



Full wwPDB EM Validation Report ⓘ

Apr 20, 2026 – 10:54 PM JST

PDB ID : 9K59 / pdb_00009k59
EMDB ID : EMD-62085
Title : Structure of substrate-engaged single-cap human proteasome in state EC1
Authors : Wu, Z.; Chen, E.; Mao, Y.
Deposited on : 2024-10-21
Resolution : 4.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

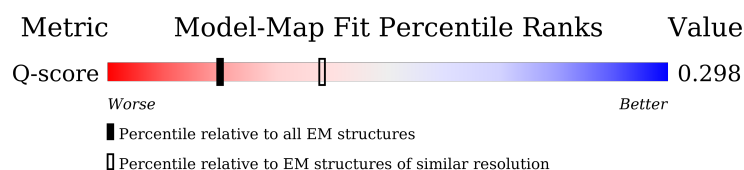
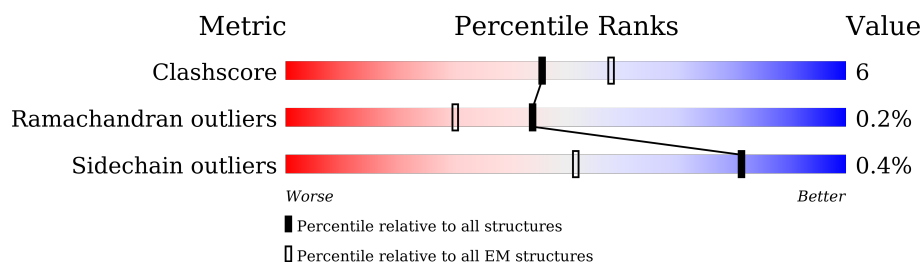
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



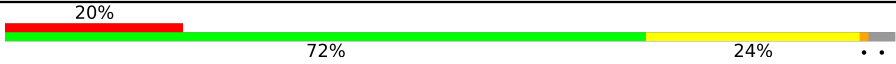

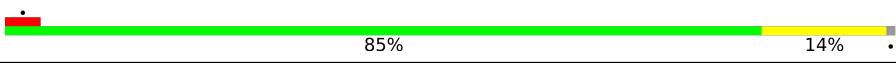

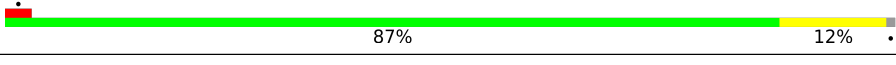
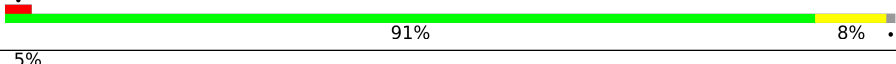
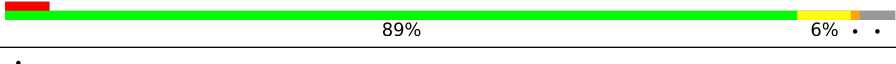

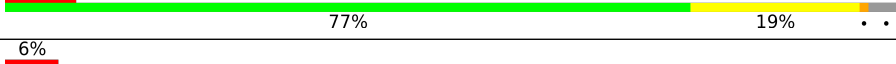


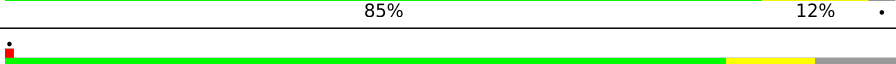
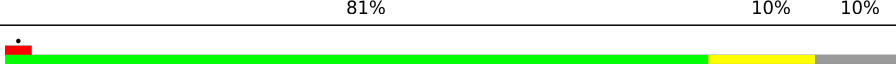
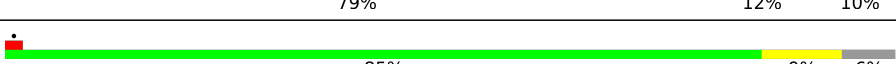

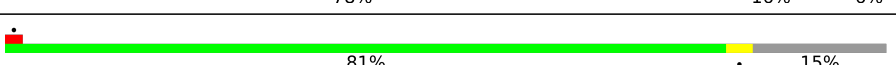
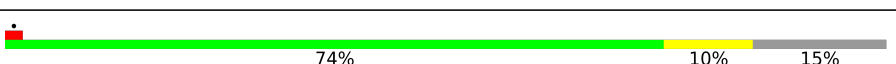
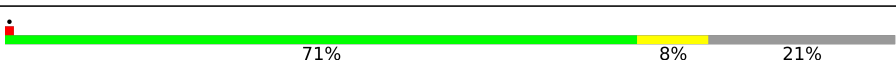
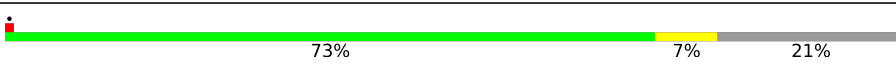
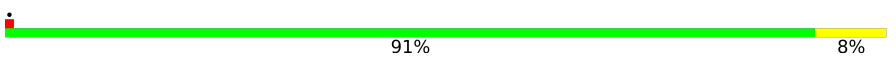

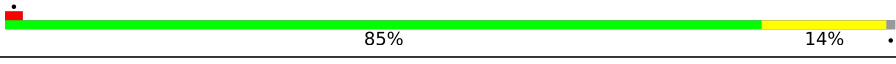
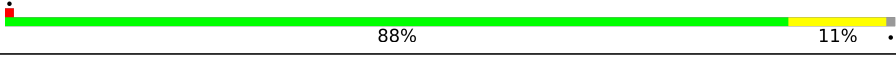


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	440	
3	C	398	
4	D	418	

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Mol	Chain	Length	Quality of chain
5	E	403	
6	F	439	
7	G	246	
7	g	246	
8	H	234	
8	h	234	
9	I	261	
9	i	261	
10	J	248	
10	j	248	
11	K	241	
11	k	241	
12	L	263	
12	l	263	
13	M	255	
13	m	255	
14	N	239	
14	n	239	
15	O	277	
15	o	277	
16	P	205	
16	p	205	
17	Q	201	
17	q	201	
18	R	263	

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Mol	Chain	Length	Quality of chain
18	r	263	
19	S	241	
19	s	241	
20	T	264	
20	t	264	
21	U	953	
22	V	534	
23	W	456	
24	X	422	
25	Y	389	
26	Z	324	
27	a	376	
28	b	377	
29	c	310	
30	d	350	
31	e	70	
32	f	908	
33	u	76	
34	v	24	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 106687 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	402	Total	C	N	O	S	0	0
			3135	1973	551	594	17		

- Molecule 2 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	399	Total	C	N	O	S	0	0
			3122	1967	529	611	15		

- Molecule 3 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	396	Total	C	N	O	S	0	0
			3105	1954	558	576	17		

- Molecule 4 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	380	Total	C	N	O	S	0	0
			3040	1923	524	580	13		

- Molecule 5 is a protein called Proteasome 26S subunit, ATPase 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	389	Total	C	N	O	S	0	0
			3097	1947	552	581	17		

- Molecule 6 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	395	Total	C	N	O	S	0	0
			3098	1951	533	596	18		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	244	Total	C	N	O	S	0	0
			1889	1198	316	362	13		
7	g	244	Total	C	N	O	S	0	0
			1880	1193	318	356	13		

- Molecule 8 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	232	Total	C	N	O	S	0	0
			1805	1152	305	342	6		
8	h	232	Total	C	N	O	S	0	0
			1805	1154	307	338	6		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	250	Total	C	N	O	S	0	0
			1955	1234	336	375	10		
9	i	250	Total	C	N	O	S	0	0
			1955	1234	336	375	10		

- Molecule 10 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	239	Total	C	N	O	S	0	0
			1880	1179	333	363	5		
10	j	239	Total	C	N	O	S	0	0
			1861	1168	332	356	5		

- Molecule 11 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	234	Total	C	N	O	S	0	0
			1777	1117	295	354	11		
11	k	234	Total	C	N	O	S	0	0
			1782	1119	295	357	11		

- Molecule 12 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	238	Total	C	N	O	S	0	0
			1866	1169	336	350	11		
12	l	238	Total	C	N	O	S	0	0
			1861	1165	335	350	11		

- Molecule 13 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	240	Total	C	N	O	S	0	0
			1876	1191	321	353	11		
13	m	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	202	Total	C	N	O	S	0	0
			1514	949	258	295	12		
14	n	202	Total	C	N	O	S	0	0
			1510	947	258	293	12		

- Molecule 15 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	220	Total	C	N	O	S	0	0
			1649	1038	279	320	12		
15	o	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		

- Molecule 16 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1587	1010	264	294	19		
16	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 17 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	199	Total	C	N	O	S	0	0
			1588	1017	270	292	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	199	Total	C	N	O	S	0	0
			1588	1017	270	292	9		

- Molecule 18 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		
18	r	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		

- Molecule 19 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1641	1041	281	309	10		
19	s	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		

- Molecule 20 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	216	Total	C	N	O	S	0	0
			1683	1062	291	318	12		
20	t	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	878	Total	C	N	O	S	0	0
			6867	4352	1163	1306	46		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	444	Total	C	N	O	S	0	0
			3612	2301	645	653	13		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	441	Total	C	N	O	S	0	0
			3596	2277	613	682	24		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	422	Total	C	N	O	S	0	0
			3335	2116	567	639	13		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	389	Total	C	N	O	S	0	0
			3202	2041	545	598	18		

- Molecule 26 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	286	Total	C	N	O	S	0	0
			2281	1457	392	427	5		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	373	Total	C	N	O	S	0	0
			2995	1911	510	559	15		

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	191	Total	C	N	O	S	0	0
			1458	910	261	279	8		

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

- Molecule 31 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	e	50	Total	C	N	O	0	0
			425	260	65	100		

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	844	Total	C	N	O	S	0	0
			6529	4126	1108	1250	45		

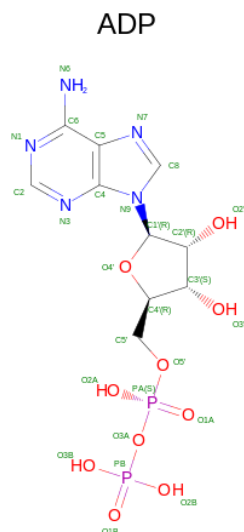
- Molecule 33 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	u	76	Total	C	N	O	S	0	0
			601	378	105	117	1		

- Molecule 34 is a protein called Substrate.

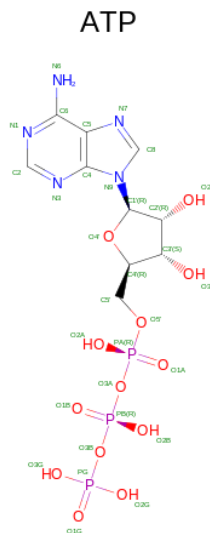
Mol	Chain	Residues	Atoms				AltConf	Trace
34	v	24	Total	C	N	O	0	0
			120	72	24	24		

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total 27	C 10	N 5	O 10	P 2	0
35	F	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
36	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

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Mol	Chain	Residues	Atoms					AltConf
36	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
37	C	1	Total	Mg	0
			1	1	
37	D	1	Total	Mg	0
			1	1	
37	E	1	Total	Mg	0
			1	1	

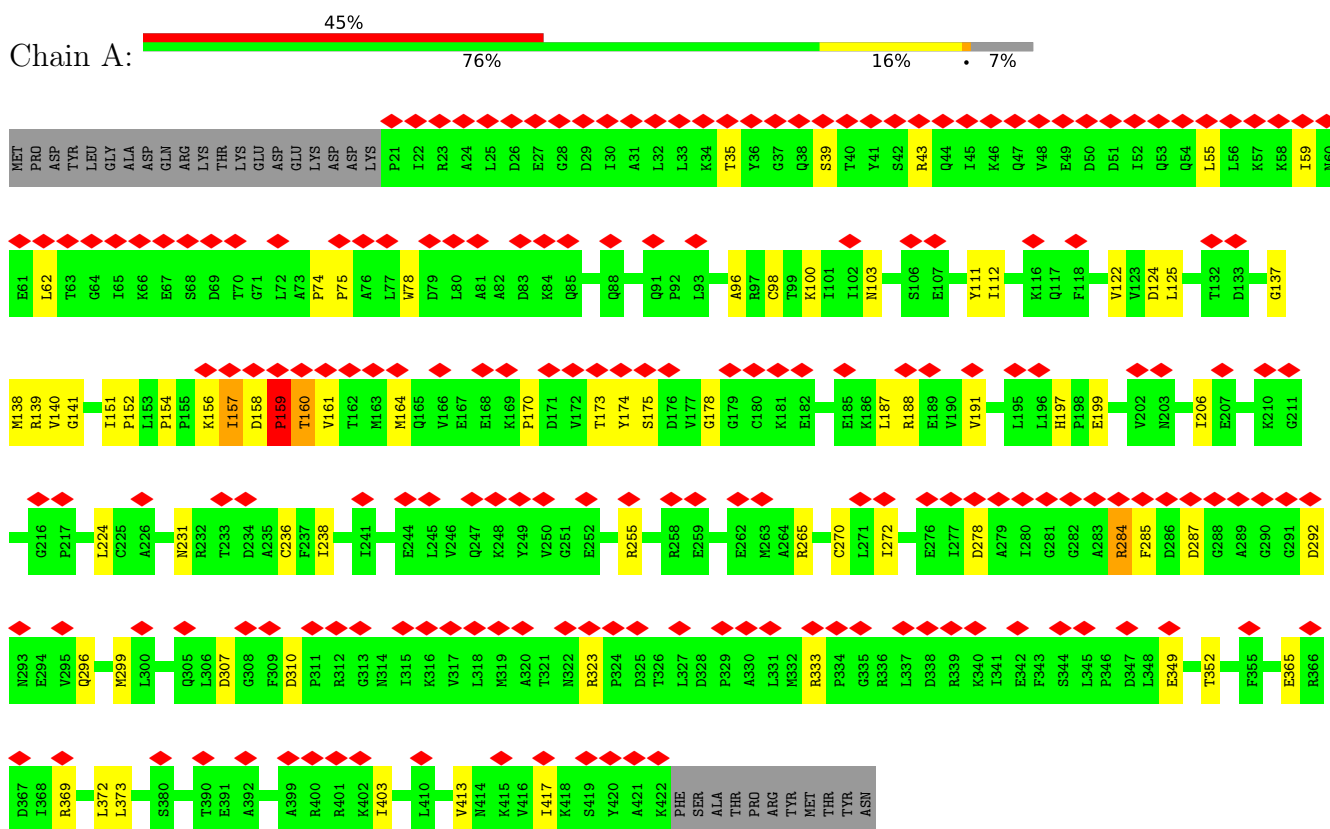
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
38	c	1	Total	Zn	0
			1	1	

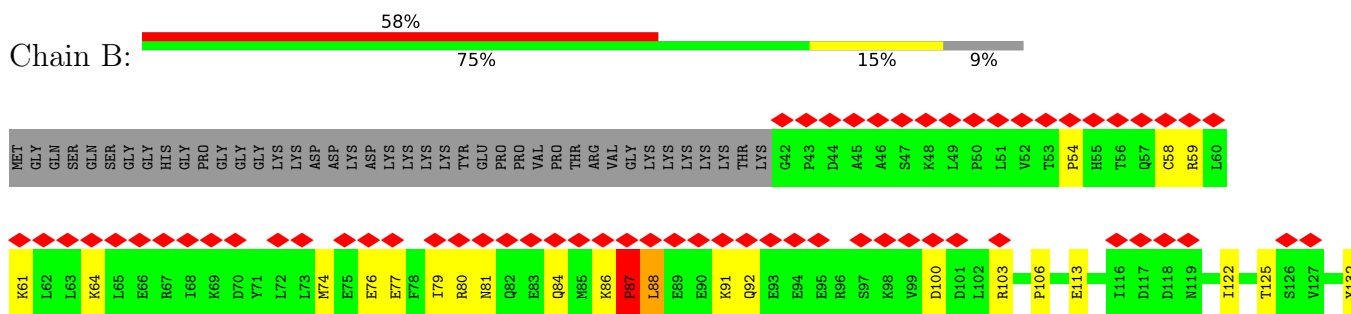
3 Residue-property plots

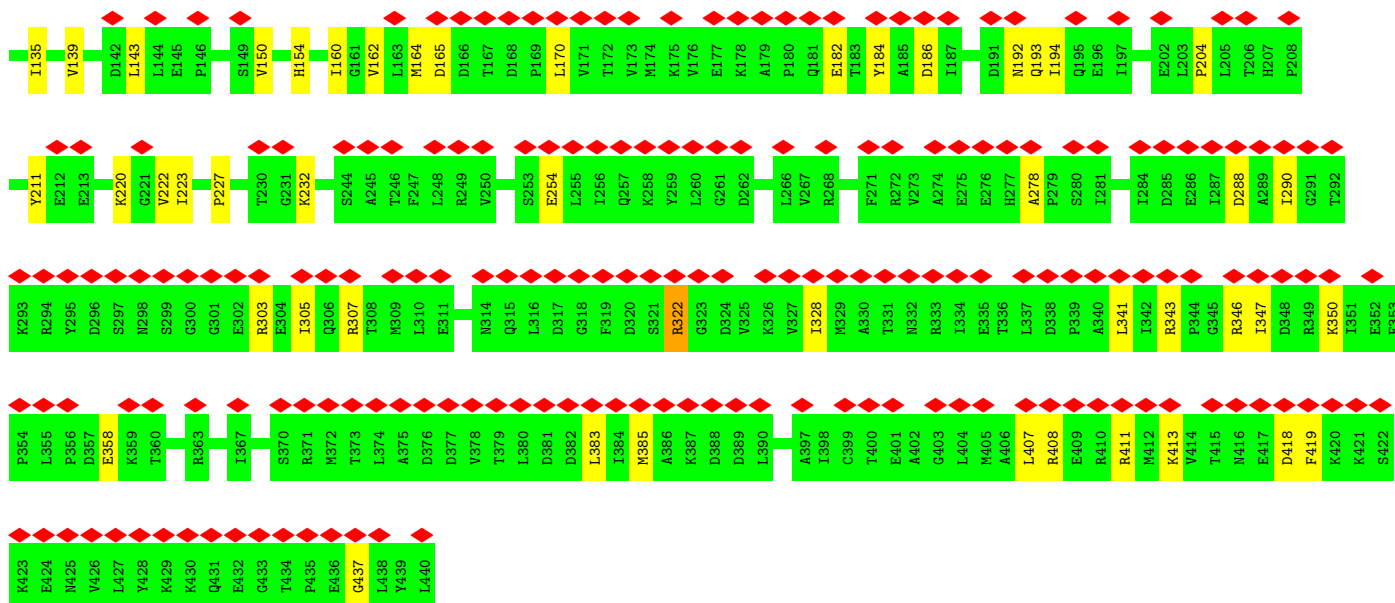
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 26S proteasome regulatory subunit 7

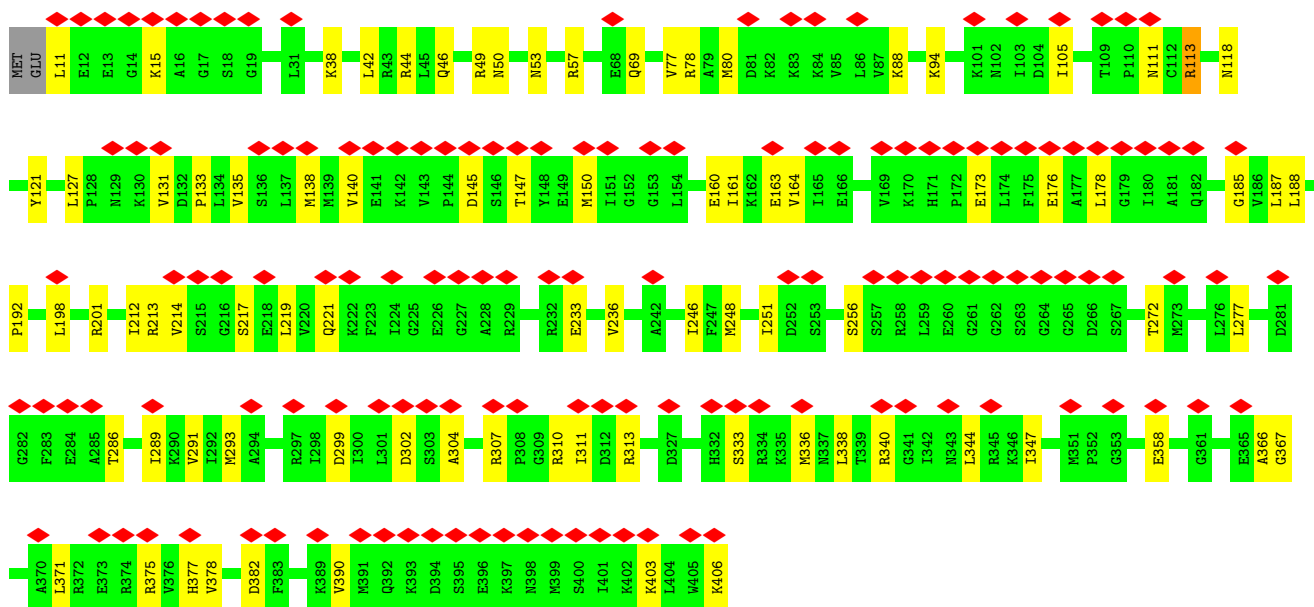
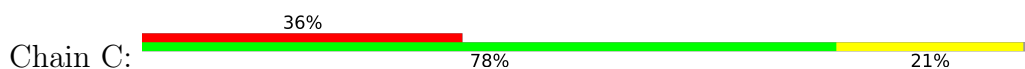


• Molecule 2: 26S proteasome regulatory subunit 4

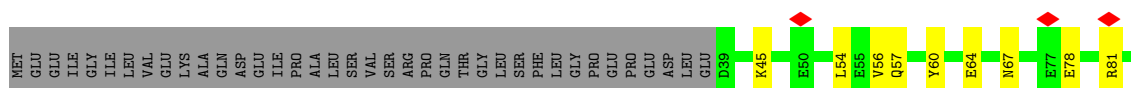


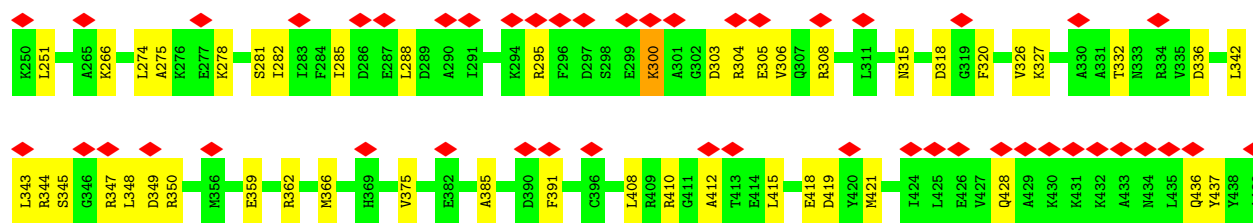


• Molecule 3: 26S proteasome regulatory subunit 8

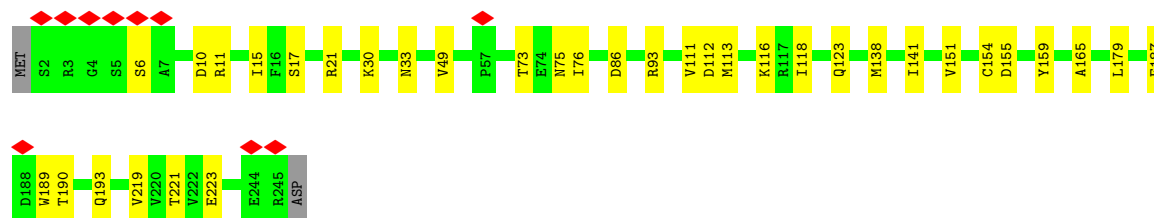
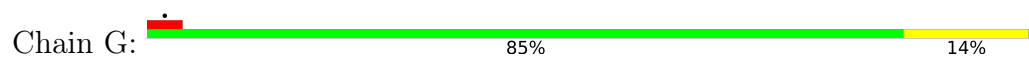


• Molecule 4: 26S proteasome regulatory subunit 6B

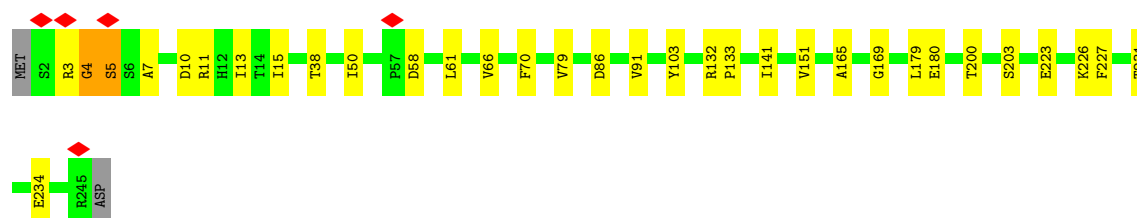
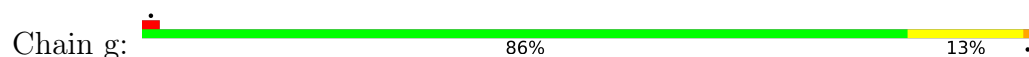




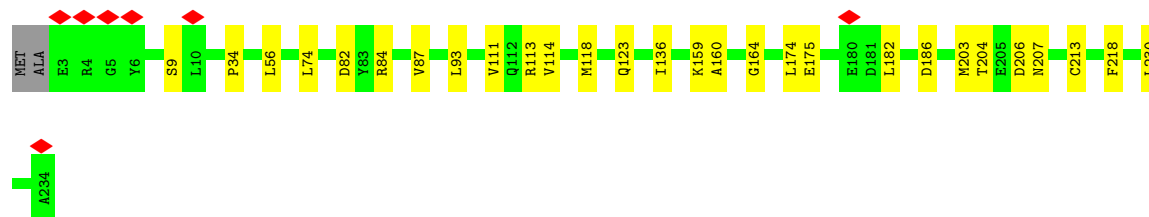
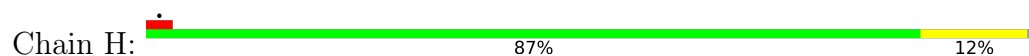
• Molecule 7: Proteasome subunit alpha type-6



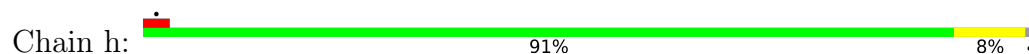
• Molecule 7: Proteasome subunit alpha type-6



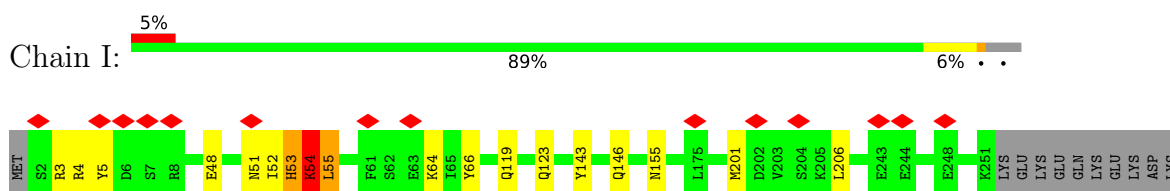
• Molecule 8: Proteasome subunit alpha type-2



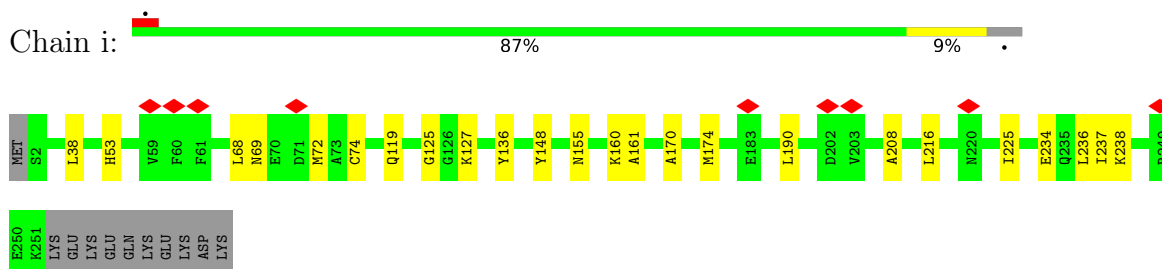
• Molecule 8: Proteasome subunit alpha type-2



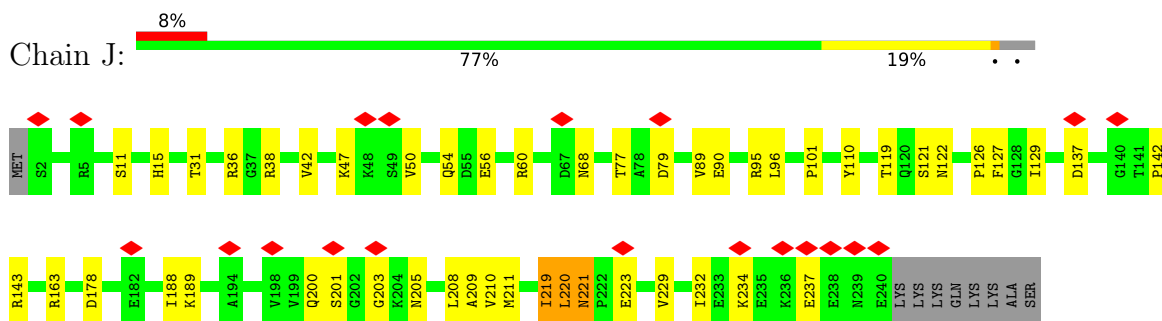
• Molecule 9: Proteasome subunit alpha type-4



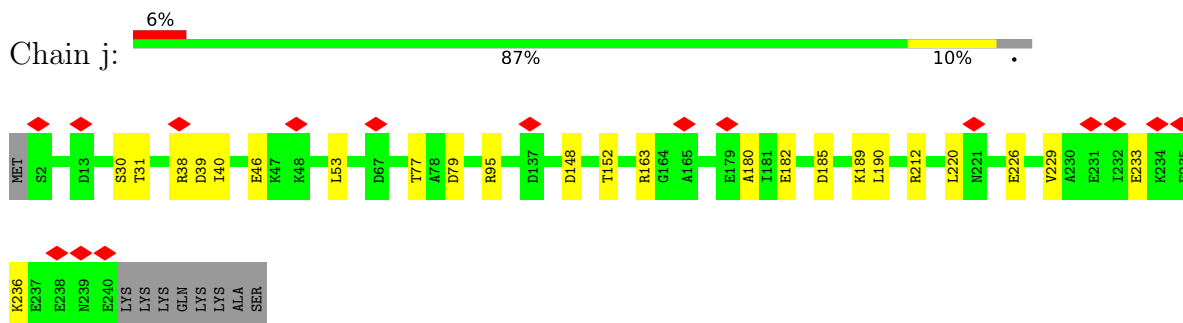
• Molecule 9: Proteasome subunit alpha type-4



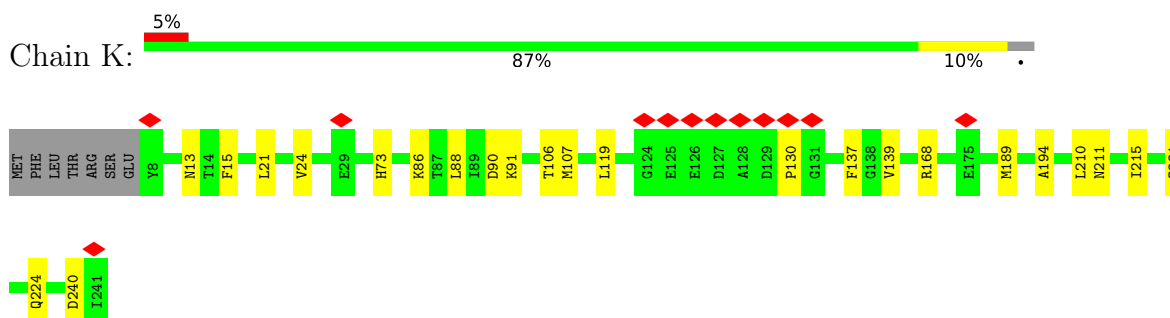
• Molecule 10: Proteasome subunit alpha type-7



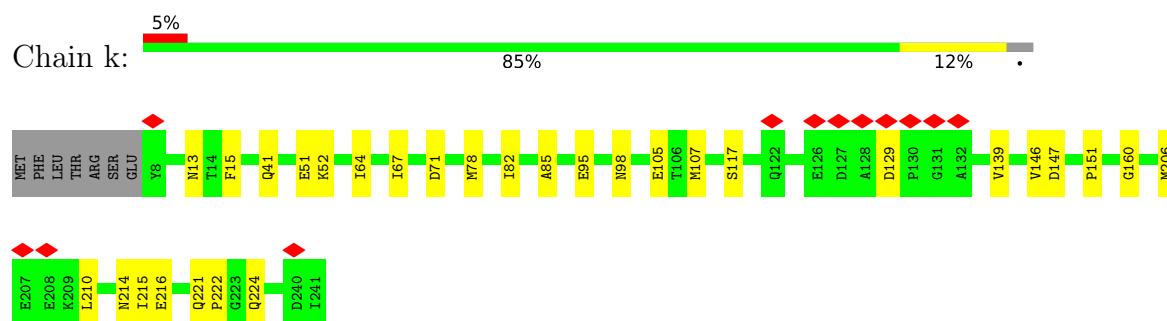
• Molecule 10: Proteasome subunit alpha type-7



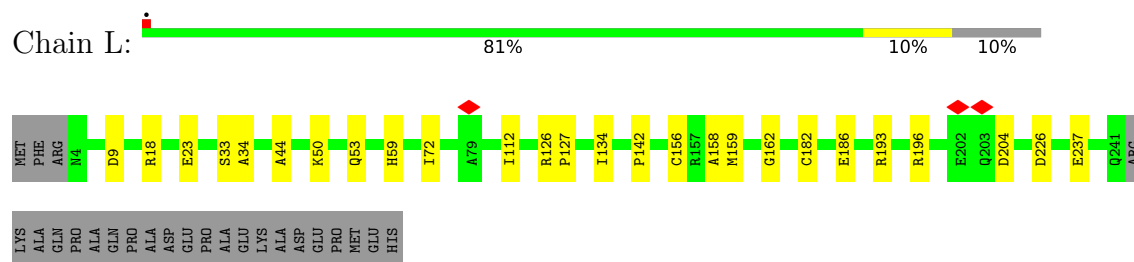
• Molecule 11: Proteasome subunit alpha type-5



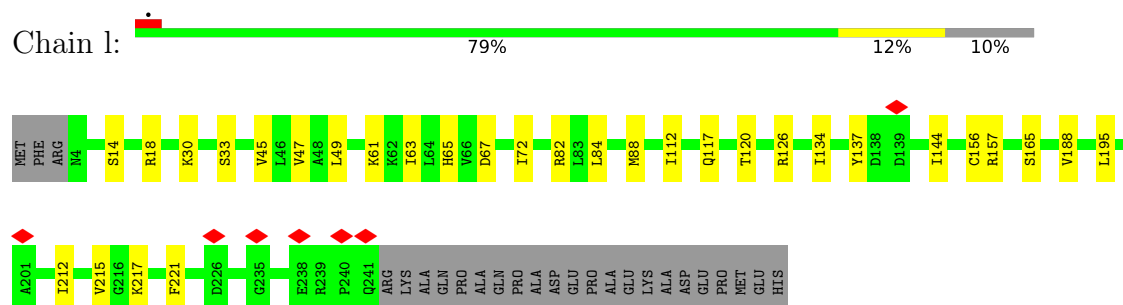
- Molecule 11: Proteasome subunit alpha type-5



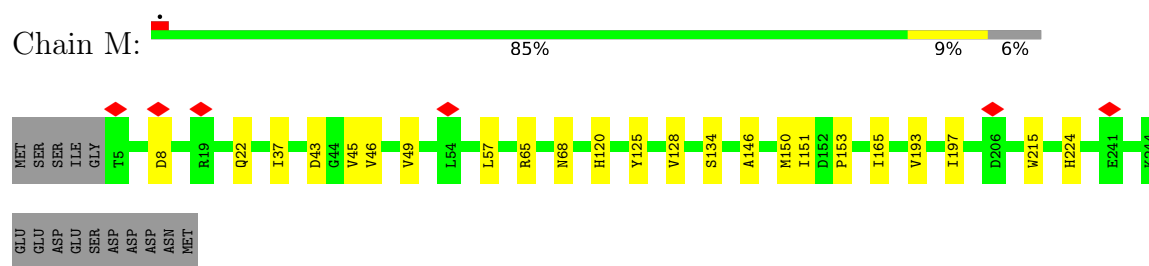
- Molecule 12: Proteasome subunit alpha type-1



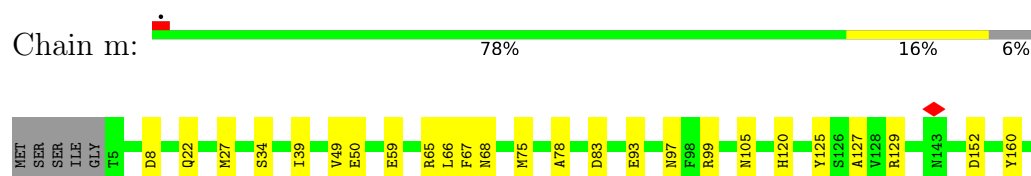
- Molecule 12: Proteasome subunit alpha type-1



- Molecule 13: Proteasome subunit alpha type-3

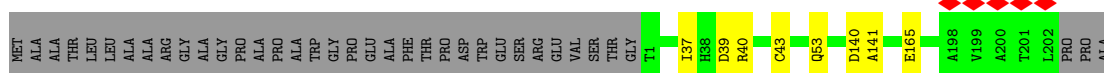
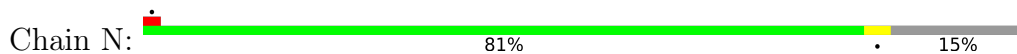


- Molecule 13: Proteasome subunit alpha type-3

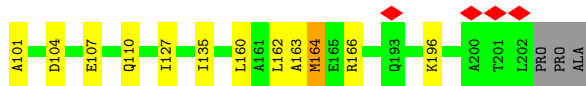
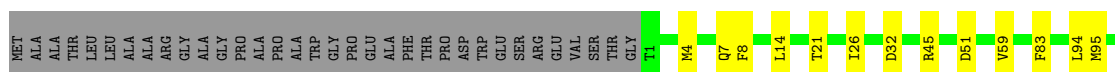




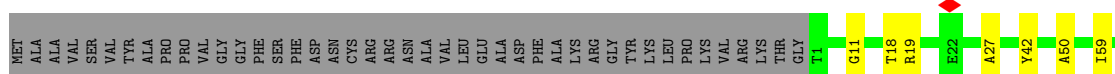
- Molecule 14: Proteasome subunit beta type-6



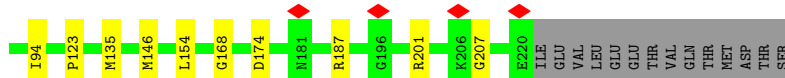
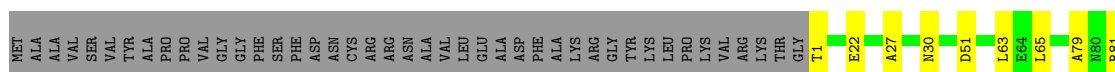
- Molecule 14: Proteasome subunit beta type-6



- Molecule 15: Proteasome subunit beta type-7

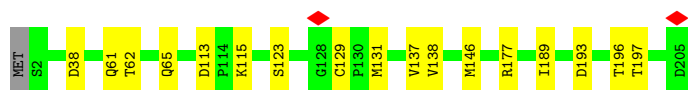


- Molecule 15: Proteasome subunit beta type-7



- Molecule 16: Proteasome subunit beta type-3





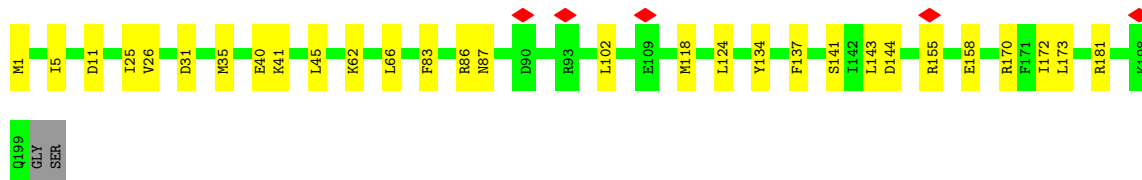
- Molecule 16: Proteasome subunit beta type-3

Chain p: 84% 16%



- Molecule 17: Proteasome subunit beta type-2

Chain Q: 85% 14%



- Molecule 17: Proteasome subunit beta type-2

Chain q: 88% 11%



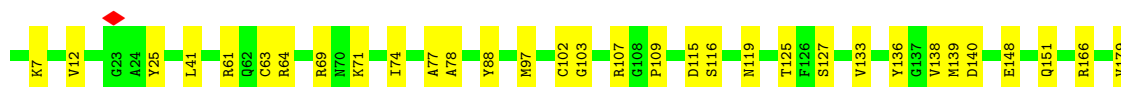
- Molecule 18: Proteasome subunit beta type-5

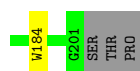
Chain R: 66% 11% 24%



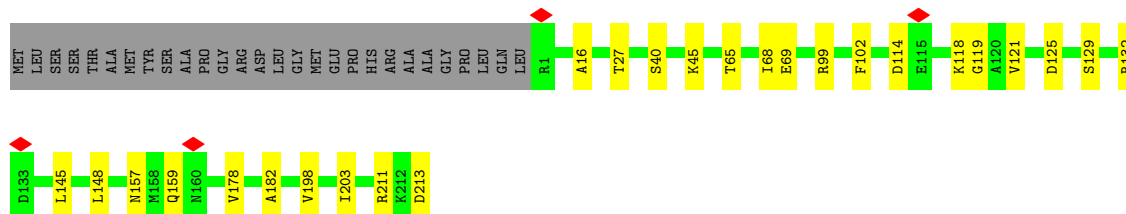
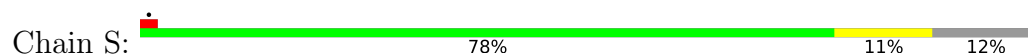
- Molecule 18: Proteasome subunit beta type-5

Chain r: 64% 13% 24%

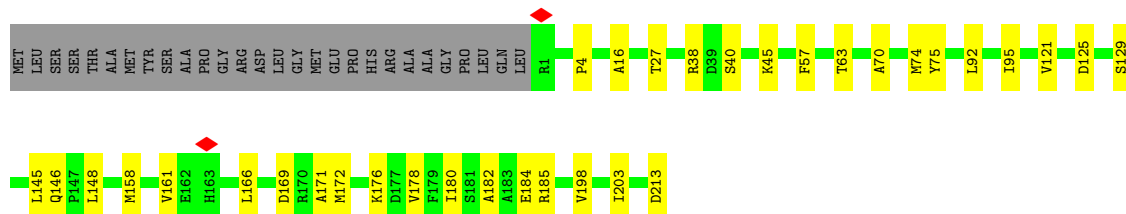




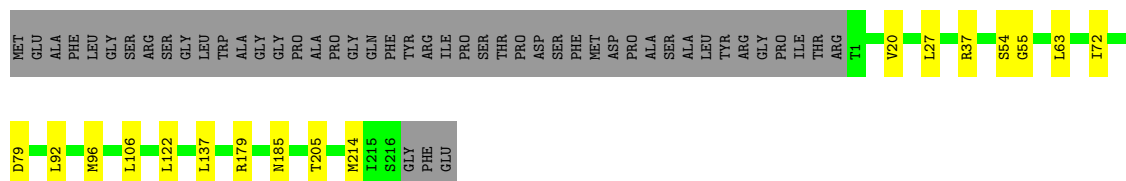
• Molecule 19: Proteasome subunit beta type-1



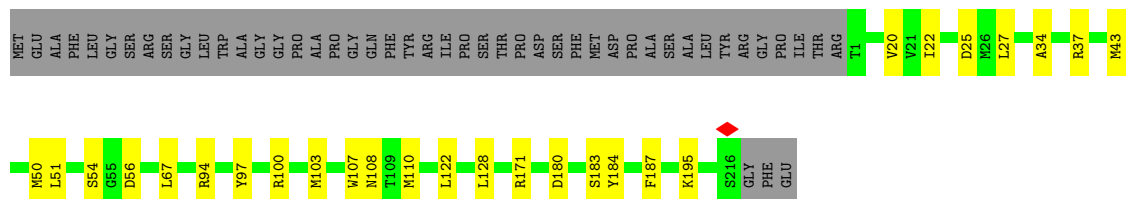
• Molecule 19: Proteasome subunit beta type-1



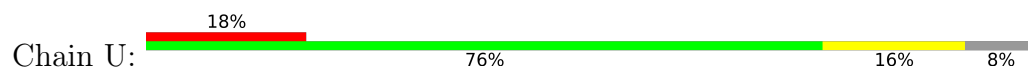
• Molecule 20: Proteasome subunit beta type-4

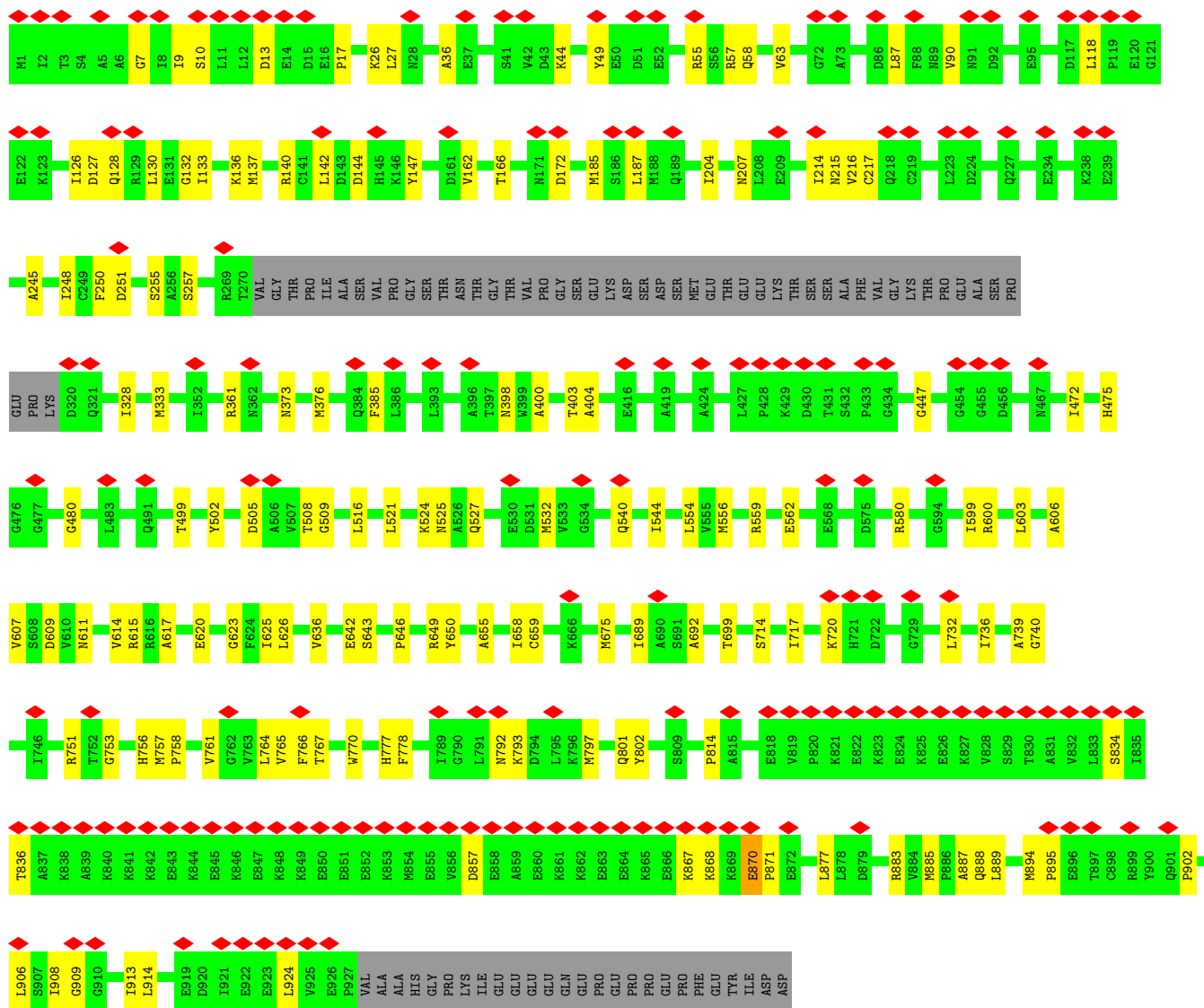


• Molecule 20: Proteasome subunit beta type-4

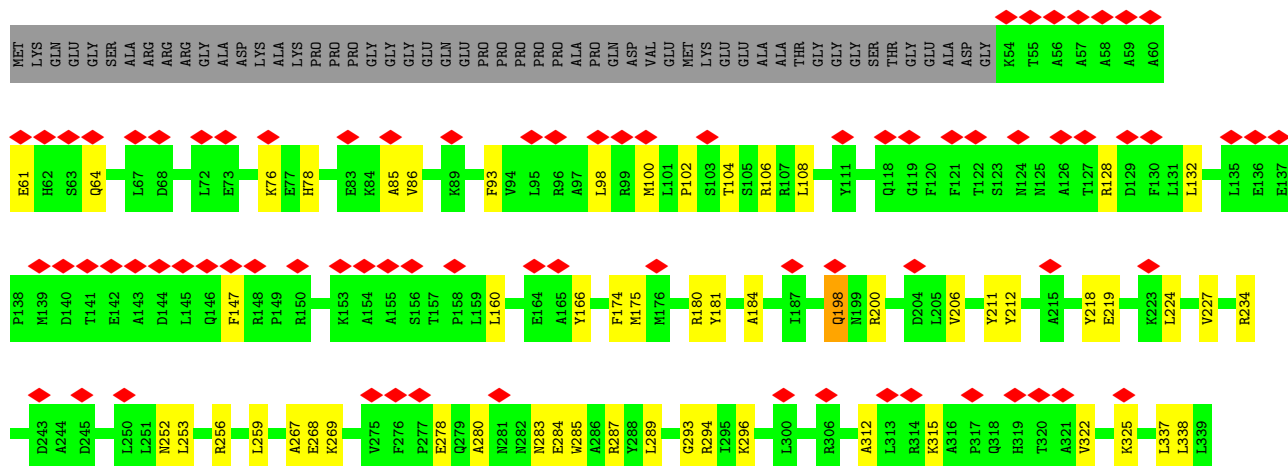


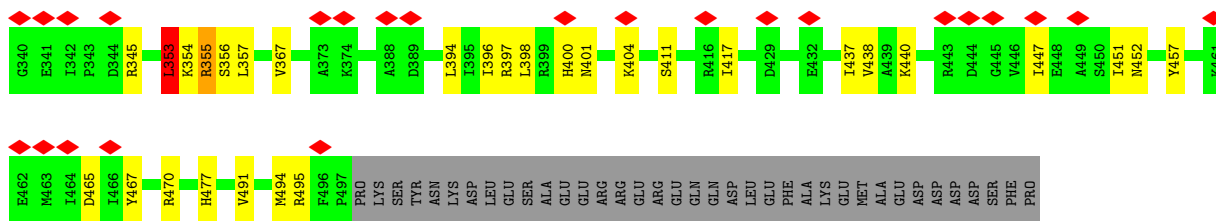
• Molecule 21: 26S proteasome non-ATPase regulatory subunit 1



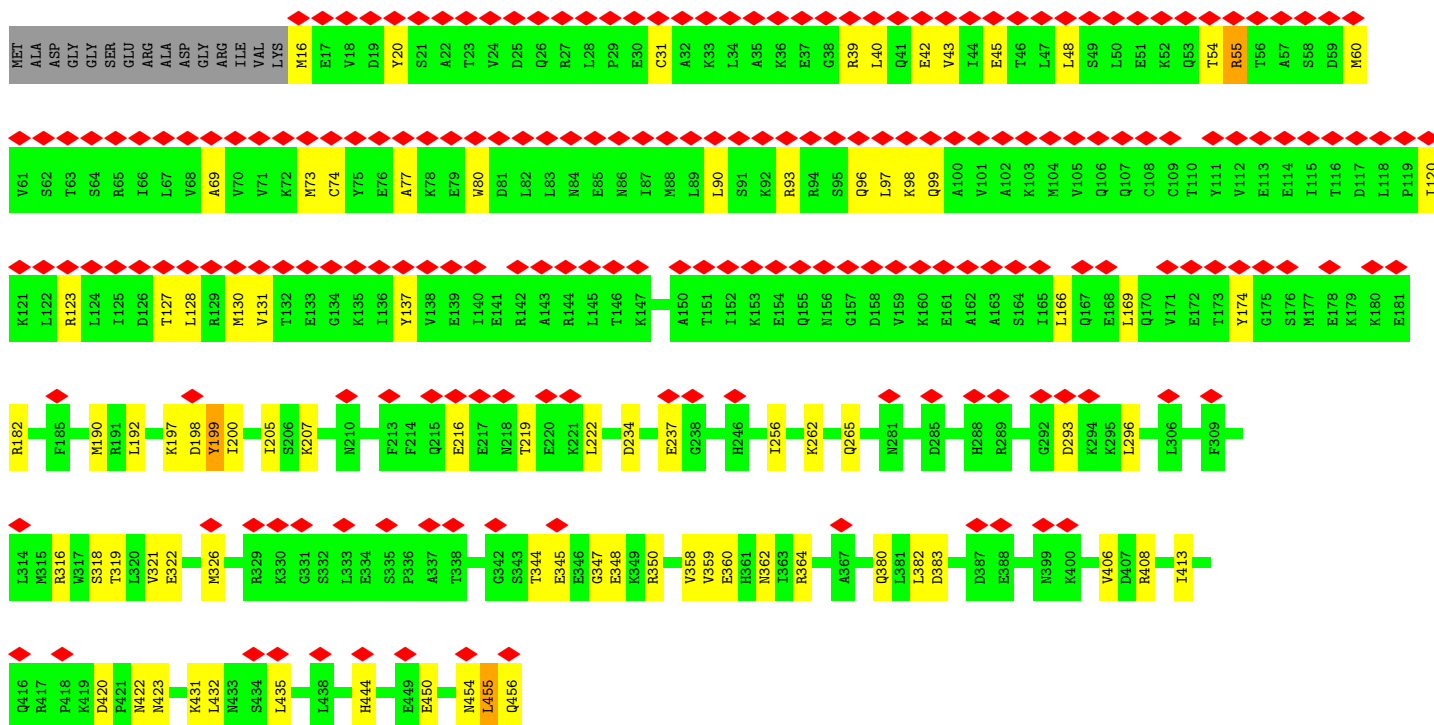
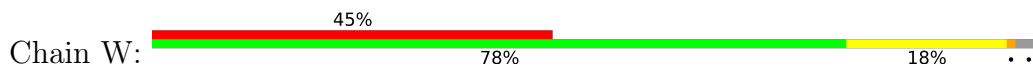


• Molecule 22: 26S proteasome non-ATPase regulatory subunit 3

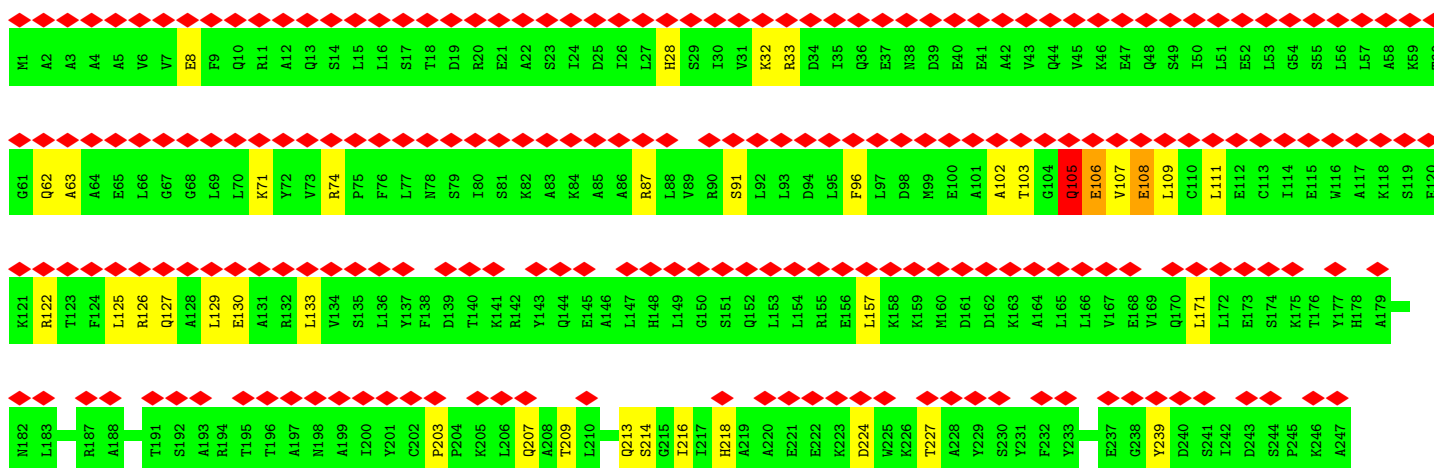
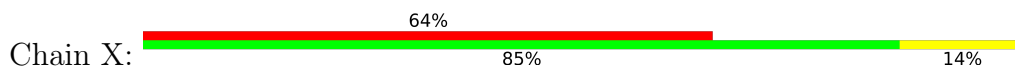


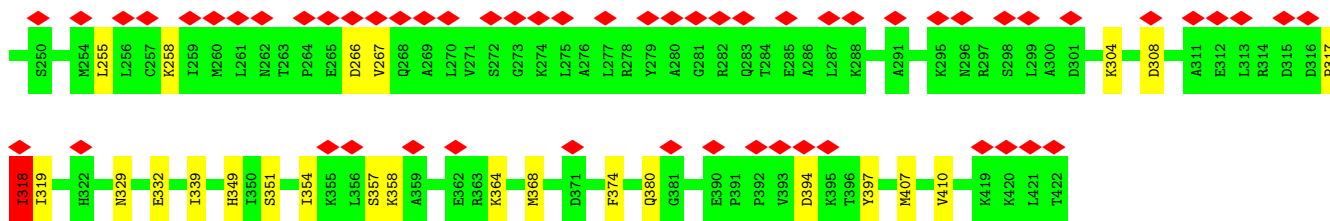


• Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

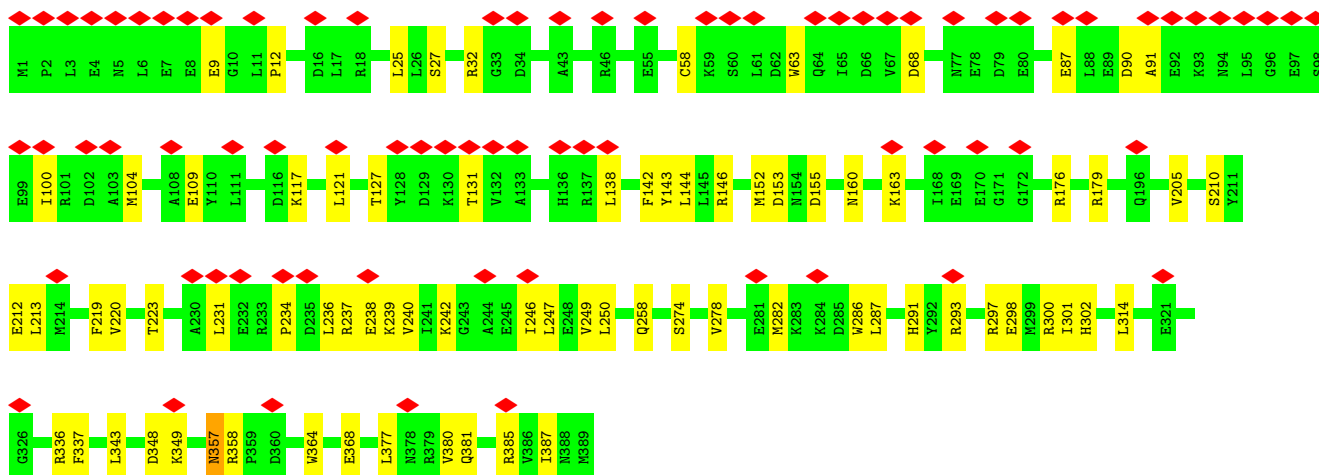
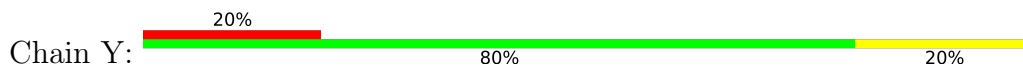


• Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

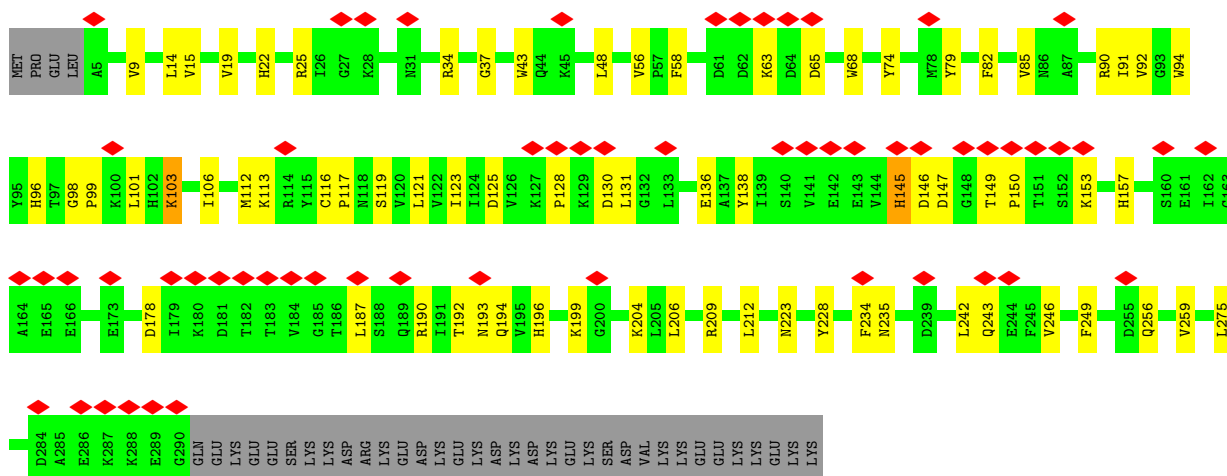




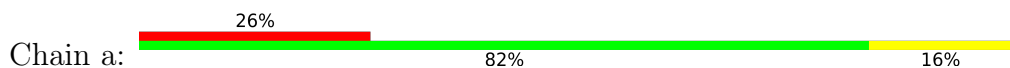
• Molecule 25: 26S proteasome non-ATPase regulatory subunit 6



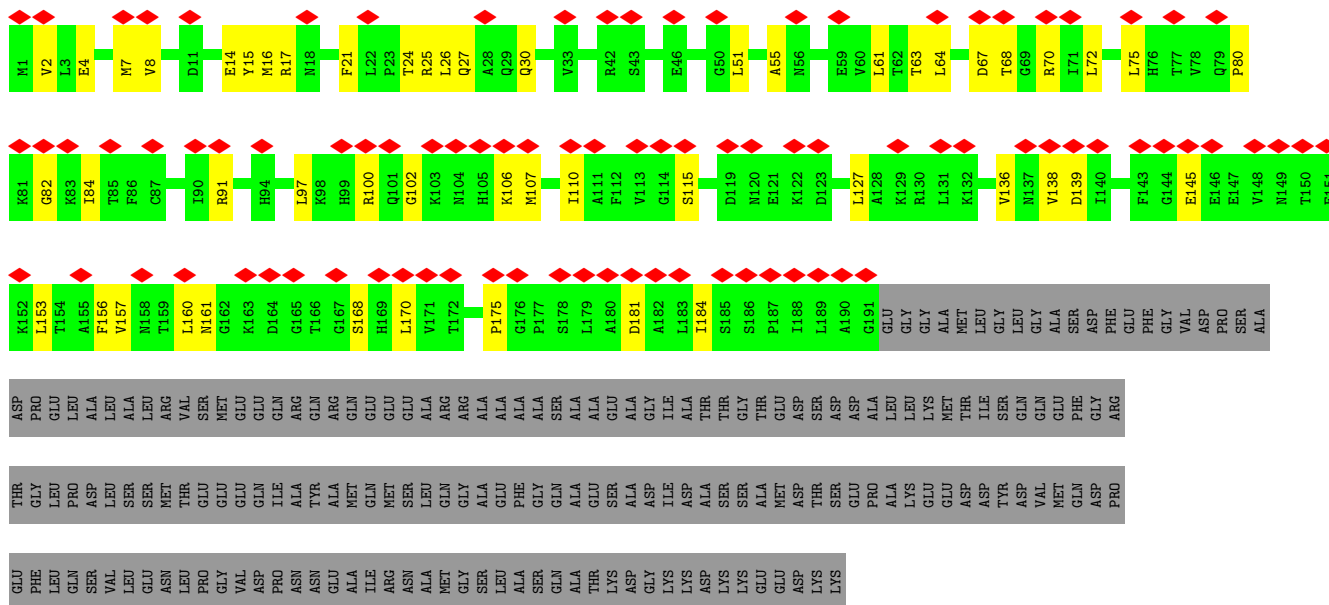
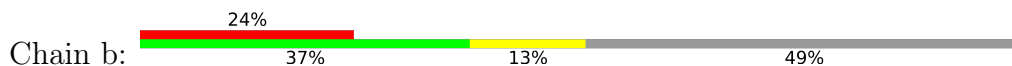
• Molecule 26: 26S proteasome non-ATPase regulatory subunit 7



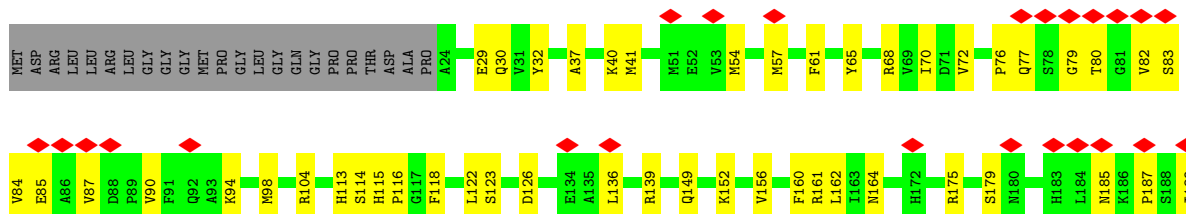
• Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

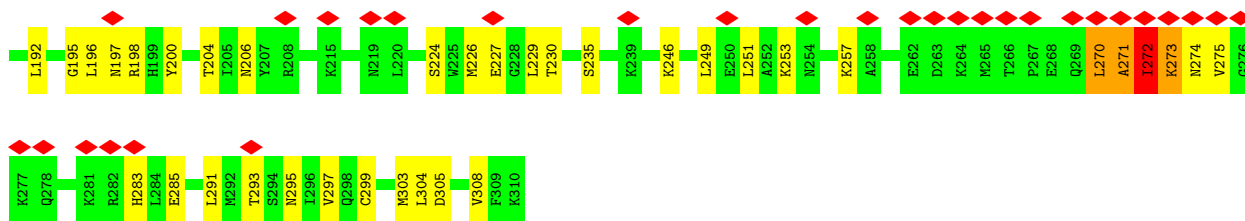


- Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

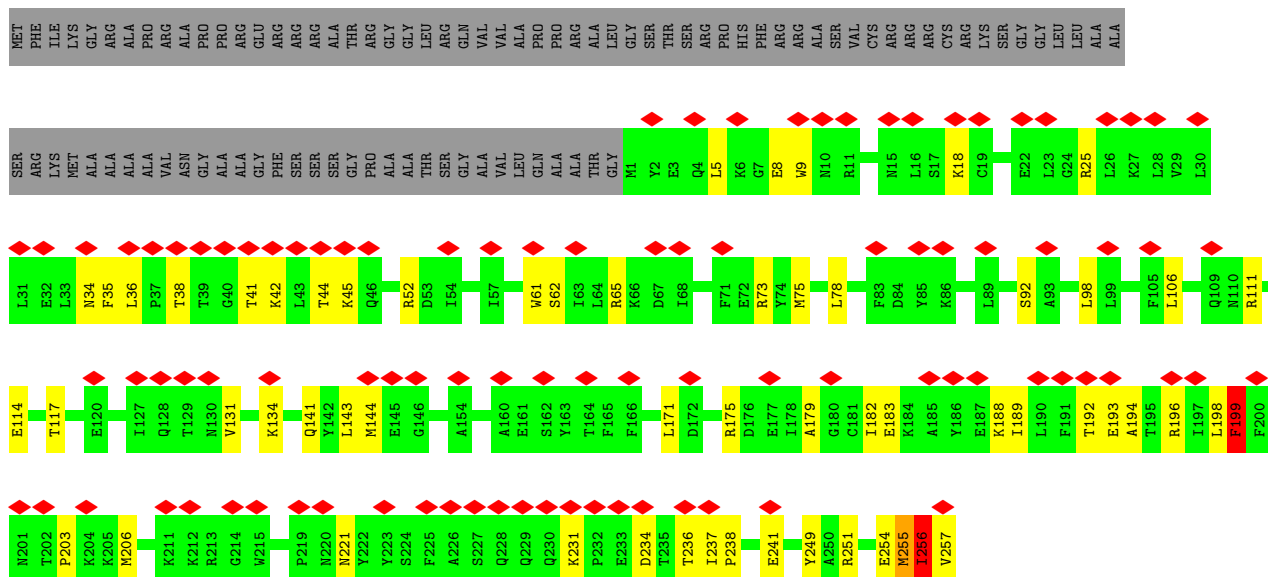


- Molecule 29: 26S proteasome non-ATPase regulatory subunit 14





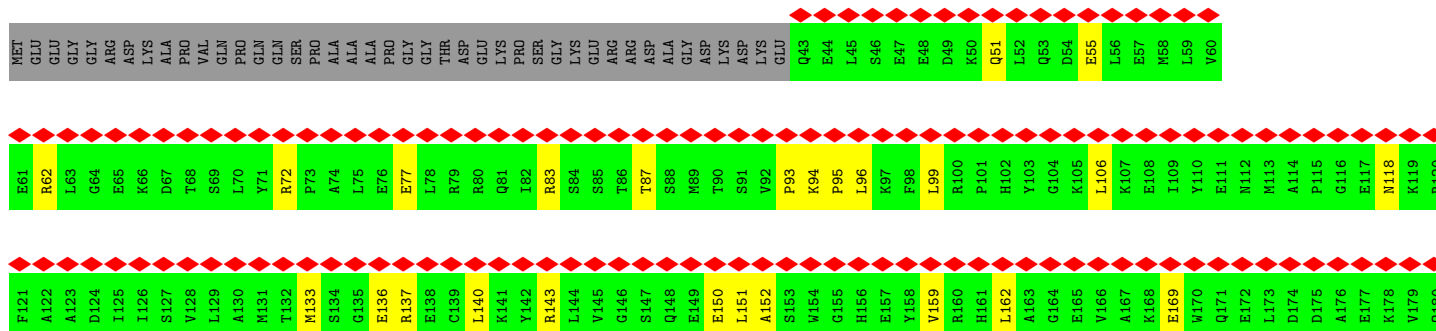
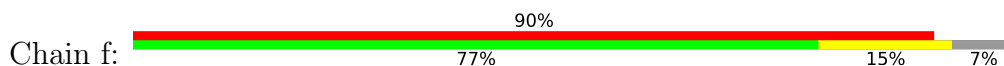
• Molecule 30: 26S proteasome non-ATPase regulatory subunit 8



• Molecule 31: 26S proteasome complex subunit SEM1

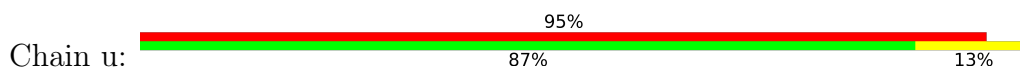


• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2



R181	P241	H301	S361	D421	S481	T541	A601	N662	S722	H782	V842
E182	E242	G302	G362	V422	I482	I542	D602	D663	V723	S783	S843
P183	P243	V303	S363	D423	F483	M543	S603	E664	M724	D784	V844
L184	E244	F304	Q364	G424	G484	E544	D604	E665	S725	R785	R845
L185	N245	L305	V365	G425	L485	K545	L607	T666	T726	Q786	V846
T186	S246	E306	D366	L426	G486	S546	V609	D667	F727	M788	Q848
L187	A247	L307	S367	T427	L487	E547	Q610	A668	A728	S789	A849
V188	L248	S308	A368	Q428	A488	T548	Q611	H670	G730	Q790	V850
K189	L249	E309	R369	I429	A489	E549	L612	A671	M731	A792	D851
E190	R250	D310	M370	D430	A490	E549	L613	L672	V732	V793	V852
I191	C251	V311	N371	K431	G491	K551	L614	T674	G733	A794	V853
V192	A252	E312	L372	Y432	S492	D552	L615	F675	S734	R795	G854
P193	L253	E313	A373	L433	M493	T553	C616	D676	M744	L804	A856
Y194	G254	Y314	S374	Y434	R494	V554	S617	H677	L745	D805	F857
N195	V255	E315	S375	S435	E495	V554	E518	L678	R746	R806	R858
M196	F256	D316	F376	S436	D496	A555	H619	L679	Q747	V807	T798
A197	R257	L317	V377	E437	V497	R556	F620	R680	L748	L808	R799
H198	K258	T318	N378	D438	L498	M557	S621	Y681	A749	L809	T800
N199	F259	E319	G379	Y439	T499	L558	LYS	G682	Q750	1810	T801
A200	S260	I320	F380	I440	L501	G561	GLU	E683	Y751	L811	R802
E201	R261	M321	V381	I441	L502	L562	LYS	D684	H752	L812	F803
H202	F262	S322	N382	S442	P503	G563	LYS	T685	A753	G812	L804
E203	P263	N323	A383	G443	V504	G564	GLU	L686	K754	R813	G864
A204	E264	V324	A384	A444	M505	L564	ASP	L687	D755	S814	D805
C205	A265	Q325	F385	L445	G506	N565	LYS	R688	P756	H815	V806
D206	L266	L326	G386	L446	D507	H566	ASP	R689	N757	Y816	R807
L207	R267	N327	Q387	A447	S508	L567	LYS	A689	N758	Y817	R808
L208	A268	S328	D388	C448	K509	G568	GLU	V690	L759	L818	R809
M209	L270	F330	K389	G449	S510	K569	LYS	P691	F760	Y819	T870
E210	L271	L331	L390	I450	S511	G570	LYS	L692	M761	L820	R871
I211	M271	A332	L391	V451	S512	A571	ASP	A693	Y762	G821	V872
E212	L272	E333	T392	M452	M513	A572	LYS	L694	V763	L822	H873
Q213	N273	L333	D393	S453	E513	I573	ASP	A695	L764	A824	L874
D214	D274	A334	D394	G454	V514	E574	LYS	L696	Q765	M825	A875
D215	M275	R335	G395	V455	A515	A575	GLU	L697	G766	Q826	H876
M216	E276	E336	N396	L456	G516	I576	ALA	S698	G767	R827	G877
L217	L277	L337	K397	M456	V517	L577	PRO	V699	L768	R828	E878
E218	V278	D338	W398	E458	T518	A578	A644	S700	T769	M829	R879
K219	E279	I339	C459	C459	A519	A579	D645	N701	Y761	G830	A880
D220	D280	M340	L399	D460	L520	L580	M646	F702	V762	L831	E881
I221	I281	E341	Y400	P461	A521	E574	G647	R703	L763	V822	L882
D222	F282	P342	K401	A462	G522	V582	A648	L704	L764	A823	T884
E223	T283	M402	K403	L463	G523	V583	H649	M705	L765	A824	R885
N224	S284	V344	D404	A464	M524	S584	D650	L706	Q766	M825	E886
A225	C285	P345	H405	L465	I525	E585	G651	L707	G767	Q826	V887
Y226	K286	D346	G406	L466	A526	P586	V652	D708	L768	R827	L888
A227	D287	D347	M407	S467	V527	F587	A653	T709	T769	M829	P889
K228	V288	I348	L408	D468	G528	R588	V654	L710	H770	L830	V890
V229	V289	Y349	S409	Y469	S529	S589	L655	S711	L771	T831	T891
C230	Q290	A410	A411	V470	C530	F590	D656	K712	L772	H832	P892
L231	Q291	T351	A412	L471	M531	A591	T657	L713	G773	F833	L893
Y232	K292	H352	A413	M473	G532	N592	L658	F714	K774	D834	L894
L233	Q293	L353	S413	S474	D533	T593	L659	S715	T775	E835	E895
T234	M294	E354	L414	M475	V534	L594	L660	H716	L776	R836	G896
S235	A295	N355	G415	T476	T535	V595	A661	D717	L777	L837	F897
C236	F296	N356	M416	T477	T537	D596		A718	L778	R838	V898
V237	M297	R357	I417	M478	L538	V597		F719	C779	L839	I899
N238	F297	F358	L418	R478	L539	A599		E720	P780	L840	L900
Y239	G299	G360	L419	L479	Q540	V600		V721	Y781	P841	R901

● Molecule 33: Ubiquitin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9319	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.023	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00636	Depositor
Map size (Å)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ATP, ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.24	0/3185	0.54	1/4299 (0.0%)
2	B	0.22	0/3168	0.55	0/4276
3	C	0.21	0/3146	0.55	1/4226 (0.0%)
4	D	0.22	0/3090	0.59	0/4168
5	E	0.24	0/3145	0.56	0/4233
6	F	0.25	0/3137	0.58	0/4223
7	G	0.19	0/1923	0.45	0/2601
7	g	0.23	0/1914	0.50	2/2590 (0.1%)
8	H	0.20	0/1844	0.46	0/2499
8	h	0.20	0/1844	0.41	0/2497
9	I	0.24	0/1985	0.50	0/2677
9	i	0.19	0/1985	0.51	0/2677
10	J	0.22	0/1906	0.47	0/2573
10	j	0.19	0/1887	0.52	2/2549 (0.1%)
11	K	0.19	0/1804	0.43	0/2436
11	k	0.18	0/1809	0.39	0/2444
12	L	0.22	0/1901	0.43	0/2570
12	l	0.20	0/1896	0.45	0/2565
13	M	0.21	0/1911	0.43	0/2573
13	m	0.19	0/1916	0.40	0/2580
14	N	0.18	0/1540	0.40	0/2085
14	n	0.20	0/1536	0.41	1/2080 (0.0%)
15	O	0.22	0/1676	0.50	0/2271
15	o	0.20	0/1686	0.41	0/2282
16	P	0.20	0/1616	0.48	0/2180
16	p	0.22	0/1620	0.49	0/2184
17	Q	0.18	0/1621	0.41	0/2194
17	q	0.19	0/1621	0.41	0/2194
18	R	0.20	0/1590	0.42	0/2147
18	r	0.20	0/1590	0.41	0/2147
19	S	0.21	0/1671	0.47	0/2252
19	s	0.21	0/1684	0.47	0/2268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.20	0/1716	0.42	0/2323
20	t	0.19	0/1720	0.41	0/2328
21	U	0.20	0/6984	0.51	0/9435
22	V	0.21	0/3681	0.50	0/4969
23	W	0.20	0/3644	0.48	0/4901
24	X	0.22	0/3381	0.50	1/4558 (0.0%)
25	Y	0.20	0/3261	0.48	0/4393
26	Z	0.23	0/2324	0.57	1/3150 (0.0%)
27	a	0.22	0/3053	0.57	1/4133 (0.0%)
28	b	0.21	0/1478	0.56	0/2001
29	c	0.29	0/2302	0.62	1/3110 (0.0%)
30	d	0.26	0/2162	0.62	1/2919 (0.0%)
31	e	0.20	0/437	0.55	0/595
32	f	0.21	0/6640	0.50	1/8988 (0.0%)
33	u	0.19	0/607	0.40	0/816
All	All	0.21	0/108237	0.50	13/146159 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	f	582	VAL	N-CA-C	-7.10	105.42	112.17
1	A	159	PRO	N-CA-CB	-6.89	96.02	103.25
10	j	220	LEU	CA-C-N	6.48	129.47	120.65
10	j	220	LEU	C-N-CA	6.48	129.47	120.65
24	X	317	PRO	N-CA-C	-6.29	104.79	113.53
27	a	189	PRO	N-CA-C	6.00	120.06	111.13
7	g	223	GLU	CA-C-N	5.88	128.73	122.26
7	g	223	GLU	C-N-CA	5.88	128.73	122.26
26	Z	92	VAL	N-CA-C	-5.75	108.25	113.71
29	c	82	VAL	N-CA-C	-5.49	108.16	113.53
3	C	105	ILE	N-CA-C	-5.20	107.76	112.96
30	d	199	PHE	N-CA-C	5.09	115.26	108.38
14	n	164	MET	CB-CG-SD	5.03	127.80	112.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3135	0	3175	46	0
2	B	3122	0	3174	51	0
3	C	3105	0	3219	58	0
4	D	3040	0	3076	66	0
5	E	3097	0	3173	77	0
6	F	3098	0	3187	67	0
7	G	1889	0	1885	23	0
7	g	1880	0	1875	22	0
8	H	1805	0	1784	17	0
8	h	1805	0	1798	16	0
9	I	1955	0	1955	16	0
9	i	1955	0	1955	15	0
10	J	1880	0	1892	30	0
10	j	1861	0	1865	15	0
11	K	1777	0	1762	16	0
11	k	1782	0	1766	20	0
12	L	1866	0	1852	17	0
12	l	1861	0	1839	22	0
13	M	1876	0	1861	15	0
13	m	1881	0	1868	27	0
14	N	1514	0	1487	6	0
14	n	1510	0	1483	15	0
15	O	1649	0	1659	15	0
15	o	1659	0	1681	13	0
16	P	1587	0	1598	13	0
16	p	1591	0	1609	23	0
17	Q	1588	0	1584	22	0
17	q	1588	0	1584	17	0
18	R	1559	0	1523	18	0
18	r	1559	0	1523	22	0
19	S	1641	0	1639	15	0
19	s	1654	0	1656	24	0
20	T	1683	0	1662	11	0
20	t	1687	0	1666	20	0
21	U	6867	0	6929	103	0
22	V	3612	0	3682	62	0
23	W	3596	0	3713	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	X	3335	0	3435	40	0
25	Y	3202	0	3204	50	0
26	Z	2281	0	2312	51	0
27	a	2995	0	3012	42	0
28	b	1458	0	1505	34	0
29	c	2260	0	2276	63	0
30	d	2116	0	2146	40	0
31	e	425	0	328	12	0
32	f	6529	0	6541	81	0
33	u	601	0	629	7	0
34	v	120	0	33	0	0
35	A	27	0	12	2	0
35	F	27	0	12	3	0
36	C	31	0	12	2	0
36	D	31	0	12	5	0
36	E	31	0	12	2	0
37	C	1	0	0	0	0
37	D	1	0	0	0	0
37	E	1	0	0	0	0
38	c	1	0	0	0	0
All	All	106687	0	107120	1324	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1324) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:LEU:HB2	2:B:92:GLN:HG2	1.47	0.95
1:A:284:ARG:HE	1:A:287:ASP:HB2	1.40	0.86
21:U:902:PRO:HG3	21:U:906:LEU:HD22	1.57	0.85
29:c:271:ALA:HA	29:c:275:VAL:HG13	1.58	0.85
6:F:163:THR:HG22	6:F:165:PRO:HD3	1.63	0.79
5:E:341:ALA:HB1	6:F:345:SER:HB2	1.64	0.79
21:U:140:ARG:O	21:U:144:ASP:HB2	1.82	0.78
23:W:55:ARG:HH22	23:W:93:ARG:HD3	1.48	0.78
6:F:189:GLY:H	35:F:501:ADP:HN62	1.32	0.77
7:g:5:SER:HB3	7:g:11:ARG:HH21	1.49	0.77
21:U:906:LEU:H	21:U:906:LEU:HD23	1.48	0.76
26:Z:145:HIS:HB2	26:Z:150:PRO:O	1.87	0.75
28:b:107:MET:HE3	28:b:136:VAL:HG22	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:192:LEU:HA	29:c:196:LEU:HB2	1.70	0.73
16:p:67:LEU:HD11	16:p:91:VAL:HG22	1.71	0.72
18:r:125:THR:HB	18:r:139:MET:HE1	1.72	0.72
4:D:67:ASN:HD22	21:U:607:VAL:HG12	1.55	0.72
30:d:254:GLU:O	30:d:255:MET:HB2	1.89	0.71
7:g:5:SER:HB3	7:g:11:ARG:NH2	2.05	0.71
32:f:570:GLY:H	32:f:599:ALA:HB1	1.56	0.70
27:a:201:GLY:HA3	27:a:233:LEU:HD21	1.73	0.70
26:Z:94:TRP:HB3	26:Z:112:MET:HE1	1.75	0.69
32:f:585:GLU:HG2	32:f:588:ARG:HH21	1.58	0.68
1:A:158:ASP:N	1:A:159:PRO:HD3	2.09	0.68
5:E:199:VAL:HG23	6:F:315:ASN:HD22	1.59	0.67
10:J:221:ASN:HD21	10:J:223:GLU:HB3	1.58	0.67
21:U:792:ASN:HB3	21:U:914:LEU:H	1.58	0.67
19:S:27:THR:HB	19:S:40:SER:H	1.60	0.67
6:F:39:GLU:HA	6:F:42:ILE:HB	1.77	0.67
16:p:45:MET:HE1	16:p:68:LYS:HA	1.76	0.66
5:E:155:ASN:HD21	23:W:207:LYS:HD3	1.60	0.66
21:U:540:GLN:HB3	29:c:68:ARG:HH22	1.61	0.66
23:W:55:ARG:HH12	23:W:93:ARG:HB3	1.61	0.65
21:U:802:TYR:HA	21:U:895:PRO:HD3	1.78	0.65
10:j:30:SER:HB3	10:j:46:GLU:HB3	1.78	0.65
25:Y:278:VAL:O	25:Y:282:MET:HB2	1.96	0.65
29:c:187:PRO:HB3	29:c:196:LEU:HD13	1.78	0.65
25:Y:238:GLU:HA	25:Y:242:LYS:HB2	1.79	0.64
28:b:138:VAL:HB	28:b:160:LEU:HD11	1.78	0.64
5:E:247:THR:O	5:E:248:SER:C	2.40	0.64
22:V:85:ALA:HB2	22:V:93:PHE:HB2	1.79	0.64
29:c:305:ASP:HA	29:c:308:VAL:HG12	1.79	0.64
22:V:128:ARG:HH21	22:V:132:LEU:HD11	1.62	0.64
1:A:140:VAL:HA	1:A:152:PRO:HA	1.79	0.64
3:C:147:THR:HG22	3:C:150:MET:HE2	1.80	0.63
21:U:699:THR:HG22	21:U:814:PRO:HD3	1.80	0.63
29:c:270:LEU:H	29:c:273:LYS:HE3	1.61	0.63
2:B:64:LYS:HD3	32:f:666:ILE:HD11	1.79	0.63
4:D:267:ILE:HB	4:D:311:THR:HG22	1.81	0.63
9:I:143:TYR:HB2	9:I:146:GLN:HE21	1.62	0.63
30:d:78:LEU:HD13	30:d:98:LEU:HD21	1.79	0.63
27:a:28:LEU:HD21	27:a:36:GLN:HG2	1.81	0.63
29:c:136:LEU:HD13	33:u:71:LEU:HD11	1.80	0.63
17:q:25:ILE:HG22	17:q:26:VAL:HG13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:394:LEU:HB2	22:V:398:LEU:HD13	1.80	0.63
21:U:204:ILE:HA	21:U:207:ASN:HB2	1.81	0.63
8:h:81:PRO:HA	8:h:84:ARG:HE	1.64	0.63
5:E:199:VAL:HG13	5:E:201:SER:H	1.64	0.63
13:M:134:SER:HB2	13:M:153:PRO:HD3	1.80	0.63
26:Z:243:GLN:H	26:Z:246:VAL:HG12	1.63	0.63
27:a:363:MET:HE2	29:c:304:LEU:HD13	1.80	0.63
19:S:198:VAL:HG22	19:S:203:ILE:HG12	1.81	0.62
30:d:75:MET:HE1	30:d:98:LEU:HG	1.81	0.62
32:f:137:ARG:HG3	32:f:140:LEU:HD22	1.81	0.62
21:U:185:MET:HE1	21:U:753:GLY:HA3	1.82	0.62
8:h:192:ILE:HD11	8:h:203:MET:HE2	1.81	0.62
32:f:267:ARG:HD3	32:f:787:LEU:HD11	1.82	0.62
3:C:138:MET:HG3	3:C:212:ILE:HG23	1.81	0.62
22:V:338:LEU:HD11	22:V:397:ARG:HB3	1.82	0.62
20:t:22:ILE:HG12	20:t:50:MET:HE1	1.81	0.62
14:N:37:ILE:HD11	14:N:43:CYS:HB3	1.80	0.61
36:C:501:ATP:O2B	4:D:323:ARG:NH2	2.32	0.61
4:D:244:PRO:HD3	4:D:288:ILE:HG12	1.81	0.61
1:A:112:ILE:HG12	1:A:122:VAL:HG22	1.81	0.61
4:D:248:ARG:HG3	4:D:295:GLN:HE22	1.64	0.61
32:f:99:LEU:HD22	32:f:106:LEU:HD11	1.81	0.61
4:D:153:MET:HE2	4:D:229:ARG:H	1.66	0.61
23:W:293:ASP:HB2	23:W:296:LEU:HD23	1.82	0.61
4:D:45:LYS:HG2	21:U:187:LEU:HB2	1.82	0.61
26:Z:259:VAL:HB	29:c:291:LEU:HD21	1.82	0.61
21:U:133:ILE:HG12	21:U:137:MET:HE1	1.82	0.61
21:U:625:ILE:HG13	21:U:626:LEU:HG	1.82	0.61
32:f:475:ASN:OD1	32:f:478:ARG:NH1	2.34	0.61
21:U:26:LYS:HE3	30:d:36:LEU:HD13	1.82	0.61
2:B:278:ALA:HB2	32:f:740:ARG:HH21	1.66	0.61
3:C:192:PRO:O	4:D:323:ARG:NH1	2.34	0.61
26:Z:74:TYR:HE1	29:c:98:MET:HB3	1.66	0.61
26:Z:34:ARG:HH22	26:Z:101:LEU:HA	1.65	0.60
2:B:437:GLY:O	9:I:155:ASN:ND2	2.34	0.60
17:Q:35:MET:HG2	17:Q:45:LEU:HG	1.84	0.60
23:W:40:LEU:HD21	23:W:74:CYS:HA	1.82	0.60
26:Z:145:HIS:HB3	26:Z:149:THR:OG1	2.01	0.60
25:Y:231:LEU:HG	25:Y:236:LEU:HD12	1.82	0.60
1:A:98:CYS:SG	1:A:139:ARG:NH1	2.75	0.60
3:C:113:ARG:HB2	3:C:127:LEU:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:303:LEU:HD23	5:E:338:PHE:HB3	1.84	0.60
5:E:198:VAL:HG12	5:E:200:SER:H	1.67	0.60
19:S:148:LEU:HD23	19:S:178:VAL:HG12	1.84	0.60
22:V:102:PRO:O	22:V:106:ARG:NH1	2.34	0.60
25:Y:258:GLN:HE22	25:Y:274:SER:HB3	1.66	0.60
29:c:123:SER:H	29:c:126:ASP:HB2	1.67	0.60
6:F:375:VAL:HG22	6:F:415:LEU:HD12	1.82	0.60
2:B:86:LYS:O	2:B:87:PRO:C	2.44	0.59
21:U:559:ARG:HB3	21:U:562:GLU:HB2	1.84	0.59
2:B:408:ARG:NH1	3:C:163:GLU:OE1	2.35	0.59
10:j:40:ILE:HG22	10:j:212:ARG:HG2	1.84	0.59
6:F:98:ASP:HA	6:F:120:LYS:HB2	1.84	0.59
7:G:30:LYS:O	7:G:33:ASN:ND2	2.35	0.59
15:o:1:THR:N	15:o:168:GLY:O	2.35	0.59
19:s:145:LEU:HD21	19:s:182:ALA:HB2	1.84	0.59
3:C:217:SER:OG	4:D:248:ARG:NH2	2.35	0.59
4:D:388:ARG:NH1	5:E:144:GLU:OE2	2.36	0.59
21:U:554:LEU:HD11	21:U:761:VAL:HG22	1.83	0.59
1:A:137:GLY:O	1:A:255:ARG:NH1	2.36	0.59
2:B:358:GLU:H	10:J:200:GLN:HE22	1.51	0.59
5:E:264:MET:HE1	5:E:294:ARG:HB2	1.85	0.59
16:P:62:THR:HG23	17:Q:86:ARG:HH12	1.68	0.59
4:D:81:ARG:HG3	29:c:152:LYS:HE2	1.84	0.59
13:M:37:ILE:HD11	13:M:193:VAL:HG13	1.85	0.59
22:V:440:LYS:NZ	30:d:143:LEU:O	2.35	0.59
18:r:63:CYS:HB2	18:r:74:ILE:HG21	1.85	0.59
3:C:135:VAL:HA	3:C:138:MET:HE2	1.85	0.59
19:s:198:VAL:HG22	19:s:203:ILE:HG12	1.85	0.58
6:F:410:ARG:NH2	6:F:419:ASP:OD2	2.36	0.58
26:Z:228:TYR:HB2	27:a:338:PRO:HB2	1.85	0.58
27:a:102:GLU:O	27:a:105:LYS:NZ	2.36	0.58
7:g:141:ILE:HG22	7:g:151:VAL:HG22	1.84	0.58
11:K:168:ARG:NH2	12:L:53:GLN:OE1	2.37	0.58
24:X:209:THR:HG1	24:X:239:TYR:HH	1.50	0.58
29:c:253:LYS:O	29:c:257:LYS:NZ	2.36	0.58
1:A:292:ASP:OD1	2:B:303:ARG:NH2	2.36	0.58
7:G:93:ARG:HH21	7:G:118:ILE:HD12	1.67	0.58
17:Q:5:ILE:HD11	17:Q:143:LEU:HD11	1.85	0.58
22:V:78:HIS:ND1	22:V:166:TYR:OH	2.36	0.58
5:E:349:GLU:OE2	6:F:350:ARG:NH1	2.37	0.58
6:F:304:ARG:HD3	6:F:308:ARG:HD3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:31:THR:OG1	10:J:163:ARG:O	2.22	0.58
32:f:486:GLY:HA3	32:f:521:ALA:HB1	1.86	0.58
3:C:221:GLN:O	4:D:245:ARG:NH2	2.36	0.58
4:D:148:ASP:HB3	5:E:61:LEU:HD13	1.85	0.58
24:X:8:GLU:OE1	24:X:33:ARG:NH2	2.37	0.58
30:d:256:ILE:O	30:d:257:VAL:HB	2.04	0.58
32:f:400:TYR:HA	32:f:407:MET:HE1	1.85	0.58
18:r:148:GLU:OE2	18:r:151:GLN:NE2	2.36	0.58
36:D:501:ATP:O1G	5:E:294:ARG:NH2	2.36	0.58
24:X:255:LEU:HD22	24:X:267:VAL:HG13	1.85	0.58
26:Z:187:LEU:HG	29:c:293:THR:HG22	1.86	0.58
2:B:222:VAL:HB	2:B:328:ILE:HG22	1.86	0.58
5:E:13:ARG:NH2	6:F:25:GLU:OE2	2.37	0.58
5:E:352:MET:HA	5:E:355:ILE:HD12	1.85	0.58
15:O:164:PHE:O	19:s:38:ARG:NH2	2.37	0.58
29:c:87:VAL:O	33:u:42:ARG:NH1	2.37	0.58
12:l:72:ILE:HG21	12:l:88:MET:HE1	1.85	0.58
10:J:56:GLU:O	10:J:60:ARG:NH1	2.35	0.58
4:D:159:LYS:HD3	4:D:160:PRO:HD2	1.85	0.57
4:D:168:GLY:O	36:D:501:ATP:N6	2.37	0.57
30:d:188:LYS:HD2	30:d:221:ASN:HD21	1.68	0.57
32:f:474:SER:HB3	32:f:477:MET:HE2	1.86	0.57
17:q:168:GLN:NE2	17:q:175:LEU:O	2.36	0.57
19:s:148:LEU:HD23	19:s:178:VAL:HG12	1.86	0.57
21:U:885:MET:HE3	21:U:887:ALA:HB3	1.84	0.57
11:K:90:ASP:OD1	18:R:69:ARG:NH2	2.37	0.57
3:C:375:ARG:NH2	3:C:382:ASP:OD2	2.37	0.57
22:V:477:HIS:HD1	30:d:249:TYR:HH	1.52	0.57
6:F:282:ILE:HG22	6:F:327:LYS:HB2	1.87	0.57
25:Y:364:TRP:NE1	25:Y:368:GLU:OE2	2.38	0.57
27:a:54:ASP:HA	27:a:57:ILE:HG22	1.87	0.57
12:l:117:GLN:NE2	13:m:83:ASP:OD1	2.37	0.57
2:B:182:GLU:HB2	2:B:186:ASP:HB2	1.86	0.57
3:C:198:LEU:HG	3:C:201:ARG:HH21	1.68	0.57
5:E:281:ARG:NH1	6:F:295:ARG:O	2.37	0.57
21:U:251:ASP:O	21:U:255:SER:CB	2.53	0.57
28:b:153:LEU:HD23	28:b:170:LEU:HD11	1.86	0.57
26:Z:196:HIS:HA	26:Z:199:LYS:HB2	1.87	0.57
22:V:76:LYS:HB2	22:V:147:PHE:HZ	1.68	0.57
8:H:175:GLU:HA	9:I:54:LYS:HZ3	1.69	0.57
19:S:159:GLN:NE2	15:o:207:GLY:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:321:LYS:HE2	27:a:336:VAL:HG21	1.87	0.57
32:f:62:ARG:NH2	32:f:77:GLU:OE1	2.37	0.57
1:A:159:PRO:HD2	1:A:160:THR:HG22	1.87	0.57
3:C:69:GLN:OE1	3:C:118:ASN:ND2	2.38	0.57
36:D:501:ATP:O1G	5:E:291:ARG:NH2	2.34	0.57
5:E:23:ASP:OD2	5:E:27:LYS:NZ	2.38	0.57
5:E:180:LYS:NZ	5:E:279:THR:O	2.37	0.57
8:h:45:VAL:HG21	8:h:188:ILE:HG12	1.85	0.57
11:k:210:LEU:HA	11:k:214:ASN:HD21	1.69	0.57
9:i:119:GLN:NE2	10:j:79:ASP:OD1	2.37	0.56
1:A:122:VAL:HB	6:F:88:TYR:HB2	1.87	0.56
5:E:75:ASN:ND2	6:F:129:ARG:O	2.38	0.56
5:E:3:ASP:HB2	6:F:36:MET:HE3	1.86	0.56
36:E:401:ATP:O2G	6:F:347:ARG:NH2	2.38	0.56
16:P:113:ASP:OD2	16:P:115:LYS:NZ	2.39	0.56
21:U:894:MET:HG2	21:U:902:PRO:HD3	1.86	0.56
23:W:128:LEU:HA	23:W:131:VAL:HG12	1.88	0.56
26:Z:190:ARG:HD3	29:c:297:VAL:HG11	1.86	0.56
29:c:79:GLY:HA3	29:c:84:VAL:HA	1.86	0.56
30:d:203:PRO:HD2	30:d:206:MET:HG2	1.86	0.56
32:f:143:ARG:NH2	32:f:169:GLU:OE2	2.38	0.56
19:s:4:PRO:HB2	20:t:100:ARG:HH21	1.71	0.56
5:E:248:SER:O	5:E:249:ALA:C	2.49	0.56
6:F:359:GLU:HB2	6:F:385:ALA:HB1	1.87	0.56
24:X:87:ARG:NH1	24:X:91:SER:OG	2.38	0.56
27:a:254:ALA:HA	27:a:261:LEU:HD23	1.86	0.56
5:E:265:ASP:OD2	5:E:294:ARG:NH2	2.39	0.56
32:f:453:SER:HA	32:f:488:ALA:HA	1.87	0.56
10:J:127:PHE:HB3	10:J:129:ILE:HG12	1.88	0.56
4:D:231:VAL:HB	4:D:234:GLU:HG2	1.87	0.56
26:Z:9:VAL:HG12	26:Z:48:LEU:HB3	1.87	0.56
16:p:11:VAL:HG11	16:p:52:GLY:HA3	1.88	0.56
16:p:35:VAL:HG12	16:p:36:THR:HG23	1.88	0.56
8:H:34:PRO:HA	8:H:164:GLY:HA3	1.87	0.56
25:Y:247:LEU:HD12	25:Y:250:LEU:HD11	1.88	0.56
32:f:466:LEU:HB3	32:f:485:LEU:HD12	1.87	0.56
17:Q:144:ASP:OD2	18:r:166:ARG:NH2	2.39	0.56
23:W:219:THR:HG22	23:W:222:LEU:HD12	1.87	0.56
24:X:102:ALA:O	24:X:106:GLU:N	2.39	0.56
28:b:161:ASN:HD21	28:b:168:SER:H	1.52	0.56
2:B:411:ARG:NH2	2:B:418:ASP:OD2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:266:GLU:OE1	5:E:262:ASN:ND2	2.39	0.56
7:G:155:ASP:OD1	7:G:159:TYR:N	2.39	0.55
17:Q:83:PHE:O	17:Q:87:ASN:ND2	2.37	0.55
24:X:103:THR:C	24:X:105:GLN:H	2.14	0.55
14:N:140:ASP:OD2	14:n:166:ARG:NH2	2.39	0.55
21:U:770:TRP:HA	29:c:179:SER:HB3	1.88	0.55
32:f:188:VAL:HG21	32:f:211:ILE:HD12	1.87	0.55
18:R:161:TYR:OH	18:R:196:HIS:ND1	2.35	0.55
25:Y:12:PRO:O	25:Y:146:ARG:NH1	2.39	0.55
1:A:206:ILE:HD13	6:F:408:LEU:HD13	1.88	0.55
3:C:164:VAL:HG21	3:C:313:ARG:HG3	1.88	0.55
21:U:649:ARG:HB3	21:U:675:MET:HE1	1.88	0.55
21:U:751:ARG:NH1	21:U:908:ILE:O	2.39	0.55
22:V:355:ARG:HH22	31:e:30:LEU:HA	1.72	0.55
33:u:5:VAL:HB	33:u:13:ILE:HB	1.87	0.55
6:F:137:ILE:HG23	6:F:160:ILE:HD12	1.86	0.55
6:F:391:PHE:HE1	6:F:428:GLN:HE21	1.53	0.55
15:O:19:ARG:NH2	19:s:213:ASP:OD2	2.40	0.55
10:J:137:ASP:OD2	10:J:143:ARG:NE	2.39	0.55
32:f:133:MET:HE3	32:f:136:GLU:H	1.70	0.55
11:k:41:GLN:NE2	11:k:151:PRO:O	2.40	0.55
11:k:95:GLU:HG3	11:k:107:MET:HE1	1.87	0.55
5:E:84:ARG:NH2	5:E:85:ARG:HG3	2.22	0.55
5:E:87:LEU:HD23	5:E:92:LEU:HD11	1.87	0.55
9:I:3:ARG:NH2	12:L:9:ASP:OD1	2.37	0.55
28:b:72:LEU:HA	28:b:75:LEU:HD12	1.88	0.55
13:m:223:ARG:NH1	13:m:224:HIS:O	2.40	0.55
16:p:62:THR:HG23	17:q:86:ARG:HH12	1.72	0.55
21:U:765:VAL:HG11	21:U:778:PHE:HD2	1.71	0.55
27:a:103:LYS:HG3	27:a:104:VAL:HG23	1.87	0.55
3:C:185:GLY:HA3	3:C:311:ILE:HA	1.89	0.55
17:Q:102:LEU:HB2	17:Q:118:MET:HB2	1.87	0.55
22:V:315:LYS:HG3	25:Y:385:ARG:HD3	1.89	0.55
1:A:35:THR:O	1:A:39:SER:OG	2.24	0.55
1:A:55:LEU:HD11	2:B:76:GLU:HG2	1.88	0.55
3:C:173:GLU:HA	3:C:176:GLU:HB2	1.88	0.55
5:E:128:GLY:HA3	5:E:185:ARG:HE	1.72	0.55
29:c:226:MET:O	29:c:230:THR:OG1	2.24	0.55
7:g:61:LEU:HD21	7:g:66:VAL:HG11	1.89	0.55
9:i:234:GLU:HA	9:i:237:ILE:HG12	1.88	0.55
4:D:200:ARG:NH1	4:D:328:ASP:OD2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:228:PRO:O	6:F:233:LYS:NZ	2.34	0.54
6:F:305:GLU:HG3	6:F:306:VAL:HG23	1.89	0.54
7:G:165:ALA:HB1	7:G:179:LEU:HD13	1.89	0.54
23:W:190:MET:HE1	23:W:205:ILE:HB	1.88	0.54
28:b:24:THR:HG22	28:b:26:LEU:H	1.72	0.54
11:k:52:LYS:NZ	11:k:64:ILE:O	2.40	0.54
16:P:65:GLN:OE1	17:Q:86:ARG:NH2	2.38	0.54
22:V:78:HIS:CD2	22:V:100:MET:HE3	2.43	0.54
25:Y:293:ARG:NH1	31:e:45:ASP:O	2.41	0.54
29:c:115:HIS:ND1	29:c:118:PHE:HE1	2.04	0.54
1:A:307:ASP:OD2	1:A:333:ARG:NH2	2.41	0.54
23:W:450:GLU:O	23:W:454:ASN:ND2	2.40	0.54
28:b:25:ARG:NH1	28:b:145:GLU:OE1	2.40	0.54
30:d:192:THR:OG1	30:d:196:ARG:NH1	2.41	0.54
1:A:170:PRO:HG2	1:A:231:ASN:HB3	1.90	0.54
3:C:88:LYS:HD3	3:C:94:LYS:HD2	1.88	0.54
3:C:338:LEU:O	3:C:340:ARG:NH1	2.41	0.54
29:c:187:PRO:HB3	29:c:196:LEU:CD1	2.37	0.54
7:g:165:ALA:HB1	7:g:179:LEU:HD13	1.89	0.54
13:M:150:MET:HE2	13:M:165:ILE:HG21	1.89	0.54
21:U:524:LYS:HA	21:U:556:MET:HE1	1.88	0.54
22:V:470:ARG:NH2	30:d:241:GLU:OE2	2.39	0.54
32:f:151:LEU:HB3	32:f:159:VAL:HG22	1.90	0.54
8:h:95:GLN:HG3	15:o:65:LEU:HG	1.89	0.54
6:F:224:LEU:HB2	6:F:348:LEU:HD21	1.89	0.54
22:V:256:ARG:NH1	31:e:21:GLU:OE1	2.41	0.54
22:V:337:LEU:HD22	22:V:367:VAL:HG11	1.88	0.54
26:Z:194:GLN:HE22	29:c:229:LEU:HB3	1.73	0.54
27:a:230:ARG:HB3	27:a:232:TRP:HD1	1.73	0.54
32:f:242:GLU:HG2	32:f:245:ASN:HD22	1.73	0.54
32:f:682:GLY:HA3	32:f:686:LEU:HD23	1.90	0.54
9:i:125:GLY:O	9:i:127:LYS:NZ	2.38	0.54
15:O:27:ALA:O	19:s:185:ARG:NH1	2.41	0.54
29:c:149:GLN:HB3	29:c:156:VAL:HG11	1.90	0.54
18:r:69:ARG:O	18:r:71:LYS:NZ	2.41	0.54
23:W:39:ARG:NH2	23:W:42:GLU:OE2	2.41	0.54
23:W:316:ARG:NH1	23:W:383:ASP:OD1	2.41	0.54
24:X:103:THR:HA	24:X:106:GLU:HB2	1.90	0.54
26:Z:178:ASP:OD1	26:Z:178:ASP:N	2.40	0.54
29:c:76:PRO:HG2	29:c:87:VAL:HG21	1.89	0.54
32:f:679:LEU:HB3	32:f:690:VAL:HG11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:103:TYR:O	15:o:81:ARG:NH2	2.40	0.54
7:g:226:LYS:NZ	7:g:227:PHE:O	2.41	0.54
11:k:160:GLY:O	12:l:82:ARG:NH2	2.41	0.54
3:C:219:LEU:HD13	3:C:272:THR:HG21	1.89	0.54
5:E:345:ASN:ND2	6:F:349:ASP:OD2	2.41	0.54
22:V:78:HIS:HD2	22:V:100:MET:HE3	1.72	0.54
28:b:100:ARG:NH1	28:b:102:GLY:O	2.41	0.54
8:H:93:LEU:HD13	8:H:113:ARG:HB3	1.89	0.54
23:W:174:TYR:O	23:W:182:ARG:NH2	2.39	0.54
28:b:7:MET:HB2	28:b:97:LEU:HD11	1.90	0.54
2:B:100:ASP:OD1	2:B:103:ARG:NH2	2.41	0.53
21:U:126:ILE:HB	21:U:130:LEU:HD11	1.89	0.53
21:U:140:ARG:O	21:U:144:ASP:CB	2.55	0.53
21:U:361:ARG:HH12	21:U:720:LYS:HG3	1.73	0.53
22:V:354:LYS:C	22:V:355:ARG:HD3	2.33	0.53
28:b:4:GLU:HG2	28:b:106:LYS:HB2	1.91	0.53
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.91	0.53
9:I:119:GLN:NE2	9:I:123:GLN:OE1	2.40	0.53
10:J:50:VAL:HB	10:J:54:GLN:HB2	1.89	0.53
13:M:49:VAL:HG11	13:M:65:ARG:HB2	1.90	0.53
24:X:122:ARG:HD2	24:X:125:LEU:HB2	1.89	0.53
29:c:90:VAL:O	29:c:94:LYS:HB2	2.07	0.53
32:f:566:HIS:HB2	32:f:573:ILE:HD11	1.90	0.53
12:l:30:LYS:NZ	12:l:165:SER:OG	2.40	0.53
1:A:238:ILE:HB	1:A:272:ILE:HG13	1.90	0.53
26:Z:82:PHE:HA	26:Z:85:VAL:HG12	1.91	0.53
7:g:165:ALA:HB3	8:h:56:LEU:HD22	1.90	0.53
17:q:102:LEU:HB2	17:q:118:MET:HB2	1.90	0.53
3:C:277:LEU:O	3:C:310:ARG:NH1	2.41	0.53
3:C:299:ASP:OD1	3:C:299:ASP:N	2.41	0.53
21:U:373:ASN:HD22	21:U:385:PHE:HD2	1.56	0.53
23:W:120:ILE:HG12	23:W:123:ARG:HH21	1.72	0.53
27:a:206:LEU:HD11	27:a:260:ASP:HB3	1.90	0.53
4:D:259:PRO:HB3	4:D:304:ASN:HB3	1.89	0.53
11:K:240:ASP:N	11:K:240:ASP:OD1	2.39	0.53
21:U:400:ALA:O	21:U:404:ALA:N	2.41	0.53
21:U:797:MET:H	21:U:924:LEU:HD11	1.72	0.53
30:d:5:LEU:HA	30:d:25:ARG:HH22	1.73	0.53
30:d:35:PHE:O	30:d:38:THR:OG1	2.26	0.53
3:C:57:ARG:NH2	21:U:643:SER:O	2.40	0.53
6:F:235:LEU:HD13	35:F:501:ADP:H2'	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:214:MET:HE3	15:o:123:PRO:HG3	1.91	0.53
1:A:161:VAL:HA	1:A:164:MET:HE2	1.90	0.53
3:C:44:ARG:HA	22:V:495:ARG:HG2	1.90	0.53
12:L:158:ALA:HB3	13:M:57:LEU:HD22	1.91	0.53
22:V:404:LYS:NZ	22:V:437:ILE:O	2.41	0.53
25:Y:27:SER:O	25:Y:32:ARG:NH2	2.39	0.53
28:b:55:ALA:HB1	28:b:82:GLY:HA3	1.89	0.53
19:s:27:THR:HB	19:s:40:SER:H	1.74	0.53
4:D:162:VAL:O	4:D:221:HIS:ND1	2.40	0.53
4:D:163:MET:HG3	4:D:165:ALA:H	1.74	0.53
10:J:188:ILE:HD12	10:J:208:LEU:HD21	1.91	0.53
12:L:226:ASP:OD1	12:L:226:ASP:N	2.40	0.53
20:T:179:ARG:NH2	15:o:135:MET:SD	2.82	0.53
32:f:490:ALA:HA	32:f:525:ILE:HA	1.89	0.53
14:n:32:ASP:O	14:n:45:ARG:NH2	2.40	0.53
16:p:70:ARG:HB3	16:p:90:MET:HE2	1.91	0.53
4:D:105:SER:OG	4:D:108:GLY:O	2.27	0.53
21:U:883:ARG:HH22	21:U:885:MET:HB2	1.74	0.53
13:m:67:PHE:HB2	13:m:75:MET:HB3	1.91	0.53
3:C:367:GLY:O	3:C:371:LEU:HB2	2.10	0.52
10:J:89:VAL:HG22	17:Q:66:LEU:HD11	1.90	0.52
32:f:470:VAL:HG11	32:f:500:LEU:HD21	1.91	0.52
4:D:272:THR:HA	4:D:317:LEU:HA	1.91	0.52
10:J:90:GLU:HG3	10:J:110:TYR:CZ	2.44	0.52
28:b:97:LEU:HD23	28:b:107:MET:HG3	1.92	0.52
32:f:698:SER:OG	32:f:701:ASN:O	2.25	0.52
7:g:86:ASP:OD1	13:m:120:HIS:NE2	2.34	0.52
2:B:411:ARG:NH1	2:B:413:LYS:O	2.43	0.52
17:Q:172:ILE:HG23	17:Q:173:LEU:HD12	1.91	0.52
23:W:359:VAL:HG23	23:W:382:LEU:HD22	1.91	0.52
29:c:57:MET:HG3	29:c:72:VAL:HG22	1.91	0.52
10:j:180:ALA:HB1	10:j:190:LEU:HD11	1.91	0.52
10:J:208:LEU:HD22	10:J:220:LEU:HG	1.92	0.52
15:O:50:ALA:HB2	16:P:129:CYS:HB2	1.90	0.52
16:P:189:ILE:HB	16:P:196:THR:HB	1.91	0.52
25:Y:152:MET:HE3	25:Y:286:TRP:HZ3	1.74	0.52
25:Y:387:ILE:HD12	26:Z:275:LEU:HD22	1.91	0.52
28:b:14:GLU:N	28:b:82:GLY:O	2.39	0.52
16:p:4:MET:HE1	16:p:106:GLU:HG2	1.91	0.52
10:J:189:LYS:HA	10:J:232:ILE:HD11	1.92	0.52
25:Y:9:GLU:OE1	25:Y:179:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:91:ARG:HD3	28:b:127:LEU:HD22	1.91	0.52
32:f:194:TYR:O	32:f:198:HIS:ND1	2.43	0.52
32:f:687:ARG:HG3	32:f:721:VAL:HG21	1.92	0.52
13:M:68:ASN:OD1	13:M:224:HIS:ND1	2.42	0.52
17:Q:11:ASP:N	17:Q:11:ASP:OD1	2.43	0.52
13:m:8:ASP:O	13:m:22:GLN:NE2	2.37	0.52
2:B:77:GLU:OE2	2:B:81:ASN:ND2	2.43	0.52
4:D:176:GLU:OE2	4:D:329:ARG:NH1	2.43	0.52
5:E:260:LEU:O	5:E:264:MET:CB	2.58	0.52
8:H:213:CYS:HB2	8:H:218:PHE:HD1	1.75	0.52
12:l:120:THR:O	13:m:129:ARG:NH1	2.37	0.52
14:n:21:THR:HG22	14:n:26:ILE:HA	1.89	0.52
4:D:64:GLU:HG3	21:U:607:VAL:HG11	1.92	0.52
7:G:165:ALA:HB3	8:H:56:LEU:HD22	1.91	0.52
8:H:111:VAL:HG22	8:H:136:ILE:HD12	1.92	0.52
19:S:114:ASP:OD1	19:S:118:LYS:N	2.41	0.52
21:U:620:GLU:HA	21:U:655:ALA:HB2	1.92	0.52
21:U:870:GLU:N	21:U:871:PRO:CD	2.73	0.52
22:V:396:ILE:HD11	30:d:141:GLN:HB2	1.91	0.52
4:D:116:LEU:HG	4:D:118:THR:H	1.75	0.52
23:W:345:GLU:HA	23:W:348:GLU:HB3	1.91	0.52
28:b:181:ASP:HA	28:b:184:ILE:HG12	1.92	0.52
9:I:155:ASN:OD1	10:J:77:THR:OG1	2.28	0.52
17:Q:31:ASP:OD1	17:Q:31:ASP:N	2.43	0.52
6:F:318:ASP:OD1	6:F:347:ARG:NH1	2.43	0.51
32:f:83:ARG:O	32:f:87:THR:OG1	2.27	0.51
19:S:211:ARG:NH2	19:S:213:ASP:OD2	2.44	0.51
28:b:157:VAL:HG21	28:b:170:LEU:HB2	1.92	0.51
2:B:383:LEU:HD11	2:B:419:PHE:HB3	1.92	0.51
22:V:278:GLU:HA	22:V:285:TRP:HZ2	1.74	0.51
22:V:477:HIS:ND1	30:d:249:TYR:OH	2.38	0.51
24:X:108:GLU:O	24:X:111:LEU:HG	2.11	0.51
27:a:54:ASP:N	27:a:54:ASP:OD1	2.43	0.51
29:c:113:HIS:CD2	29:c:115:HIS:CD2	2.99	0.51
31:e:42:ASN:OD1	31:e:43:TRP:N	2.43	0.51
1:A:296:GLN:NE2	1:A:299:MET:SD	2.84	0.51
8:h:3:GLU:N	13:m:125:TYR:HB3	2.25	0.51
2:B:290:ILE:HG13	2:B:305:ILE:HG23	1.92	0.51
21:U:499:THR:HA	21:U:502:TYR:HB2	1.92	0.51
24:X:214:SER:O	24:X:218:HIS:ND1	2.36	0.51
28:b:67:ASP:OD1	28:b:68:THR:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:54:MET:H	29:c:77:GLN:NE2	2.08	0.51
32:f:698:SER:OG	32:f:698:SER:O	2.28	0.51
8:h:39:LYS:HG3	8:h:44:VAL:HG22	1.91	0.51
13:m:215:TRP:CD1	13:m:227:VAL:HG22	2.46	0.51
19:s:16:ALA:HB2	19:s:121:VAL:HG23	1.92	0.51
21:U:36:ALA:HB1	22:V:269:LYS:HB3	1.92	0.51
24:X:126:ARG:NH1	24:X:127:GLN:OE1	2.44	0.51
8:h:148:GLN:OE1	8:h:158:TRP:NE1	2.44	0.51
33:u:5:VAL:HG22	33:u:67:LEU:HD12	1.93	0.51
4:D:147:ALA:HB1	5:E:70:ILE:HD13	1.93	0.51
13:M:125:TYR:HB2	13:M:128:VAL:HG22	1.93	0.51
28:b:63:THR:H	28:b:70:ARG:HH12	1.58	0.51
32:f:261:ARG:HG3	32:f:264:GLU:HB2	1.92	0.51
32:f:463:LEU:O	32:f:467:SER:OG	2.27	0.51
9:i:234:GLU:OE1	9:i:238:LYS:NZ	2.44	0.51
17:q:38:MET:HE3	17:q:44:LEU:HB2	1.92	0.51
3:C:188:LEU:N	3:C:293:MET:O	2.42	0.51
5:E:153:LEU:HD12	5:E:154:THR:HG23	1.92	0.51
21:U:216:VAL:HG11	21:U:248:ILE:HB	1.92	0.51
2:B:103:ARG:HD3	2:B:160:ILE:HG21	1.92	0.51
4:D:154:LEU:HD22	4:D:158:GLN:HG2	1.93	0.51
3:C:11:LEU:HD12	3:C:15:LYS:HG3	1.93	0.51
22:V:219:GLU:HA	22:V:224:LEU:HD11	1.92	0.51
22:V:491:VAL:HA	22:V:494:MET:HE1	1.92	0.51
10:j:185:ASP:OD1	10:j:185:ASP:N	2.44	0.51
20:t:43:MET:HE3	20:t:51:LEU:HD23	1.93	0.51
1:A:173:THR:HG22	1:A:175:SER:H	1.76	0.50
2:B:150:VAL:HG12	2:B:162:VAL:HA	1.93	0.50
10:J:234:LYS:HA	10:J:237:GLU:HG2	1.93	0.50
21:U:26:LYS:HD3	30:d:34:ASN:HD21	1.75	0.50
21:U:127:ASP:H	21:U:130:LEU:HD21	1.76	0.50
21:U:714:SER:HA	21:U:717:ILE:HG22	1.93	0.50
27:a:129:GLN:HG3	27:a:130:VAL:HG22	1.93	0.50
9:i:136:TYR:HB2	9:i:148:TYR:HB2	1.94	0.50
20:t:25:ASP:HA	20:t:187:PHE:HA	1.93	0.50
2:B:58:CYS:SG	2:B:59:ARG:N	2.83	0.50
2:B:164:MET:SD	2:B:164:MET:N	2.84	0.50
3:C:187:LEU:HG	3:C:293:MET:HG2	1.93	0.50
24:X:103:THR:C	24:X:105:GLN:N	2.67	0.50
25:Y:377:LEU:HA	25:Y:380:VAL:HG22	1.94	0.50
32:f:556:ARG:NH2	32:f:645:ASP:OD1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:47:VAL:HG12	12:l:195:LEU:HD22	1.94	0.50
2:B:184:TYR:HE1	2:B:194:ILE:HD12	1.75	0.50
5:E:337:GLY:O	5:E:378:LYS:NZ	2.44	0.50
24:X:216:ILE:HD12	24:X:318:ILE:HG21	1.93	0.50
26:Z:242:LEU:HG	26:Z:243:GLN:HG3	1.94	0.50
11:k:146:VAL:HG11	11:k:222:PRO:HA	1.93	0.50
13:m:49:VAL:HG11	13:m:65:ARG:HB2	1.94	0.50
4:D:147:ALA:HA	5:E:62:LYS:HD3	1.92	0.50
14:N:165:GLU:OE2	20:t:37:ARG:NH1	2.45	0.50
22:V:353:LEU:HD12	22:V:354:LYS:H	1.76	0.50
9:i:190:LEU:HB3	9:i:236:LEU:HD21	1.94	0.50
12:l:49:LEU:HG	12:l:195:LEU:HD21	1.92	0.50
5:E:260:LEU:O	5:E:264:MET:HB3	2.11	0.50
15:O:59:ILE:HD11	15:O:86:MET:HG2	1.93	0.50
18:R:58:LEU:HD23	18:R:61:ARG:HD3	1.94	0.50
22:V:198:GLN:OE1	22:V:200:ARG:HB2	2.11	0.50
25:Y:220:VAL:HG21	25:Y:249:VAL:HG21	1.93	0.50
26:Z:63:LYS:HD2	28:b:91:ARG:HH21	1.77	0.50
11:k:13:ASN:HB2	12:l:126:ARG:HG2	1.93	0.50
6:F:151:VAL:HG12	6:F:163:THR:HG23	1.93	0.50
10:J:42:VAL:HG22	10:J:210:VAL:HG12	1.93	0.50
10:J:47:LYS:HE2	10:J:205:ASN:HA	1.92	0.50
22:V:355:ARG:C	22:V:357:LEU:H	2.20	0.50
25:Y:231:LEU:HD12	25:Y:234:PRO:HD2	1.94	0.50
27:a:70:ARG:NH2	28:b:16:MET:O	2.45	0.50
2:B:192:ASN:OD1	2:B:193:GLN:NE2	2.45	0.50
3:C:375:ARG:HG2	3:C:377:HIS:H	1.76	0.50
21:U:376:MET:HA	21:U:739:ALA:HA	1.93	0.50
21:U:509:GLY:HA3	21:U:544:ILE:HG12	1.92	0.50
23:W:60:MET:HG3	23:W:97:LEU:HD21	1.94	0.50
25:Y:258:GLN:NE2	25:Y:274:SER:HB3	2.26	0.50
3:C:403:LYS:HE2	9:I:51:ASN:HD22	1.76	0.50
5:E:309:ARG:NH1	5:E:335:SER:O	2.40	0.50
6:F:288:LEU:HD21	6:F:342:LEU:HD11	1.94	0.50
12:L:193:ARG:HG2	12:L:196:ARG:HH21	1.77	0.50
17:q:44:LEU:HD11	17:q:102:LEU:HD22	1.93	0.50
2:B:288:ASP:OD1	2:B:288:ASP:N	2.44	0.50
4:D:199:PRO:HG3	4:D:329:ARG:HE	1.76	0.50
5:E:84:ARG:HH21	5:E:86:GLN:H	1.59	0.50
5:E:310:LEU:HD21	23:W:99:GLN:HE22	1.76	0.50
6:F:41:ILE:O	6:F:45:THR:OG1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:42:TYR:HE2	15:O:183:LEU:HD11	1.77	0.50
23:W:408:ARG:HH11	24:X:349:HIS:HB3	1.76	0.50
30:d:42:LYS:HD2	30:d:45:LYS:HD2	1.94	0.50
30:d:194:ALA:HA	30:d:198:LEU:HB2	1.94	0.50
32:f:688:ARG:NH1	32:f:804:LEU:O	2.45	0.50
32:f:783:SER:HB2	32:f:787:LEU:HD13	1.93	0.50
16:p:134:ASP:OD1	16:p:134:ASP:N	2.45	0.50
4:D:354:LEU:HD23	4:D:356:GLU:H	1.77	0.49
5:E:248:SER:HA	5:E:251:ARG:HH11	1.76	0.49
25:Y:87:GLU:HA	25:Y:90:ASP:HB2	1.94	0.49
7:G:190:THR:OG1	7:G:193:GLN:OE1	2.28	0.49
7:G:221:THR:HG22	7:G:223:GLU:H	1.77	0.49
14:N:39:ASP:OD2	14:N:40:ARG:NH1	2.45	0.49
21:U:792:ASN:OD1	21:U:793:LYS:N	2.45	0.49
27:a:342:ASP:OD1	27:a:342:ASP:N	2.42	0.49
30:d:234:ASP:OD1	30:d:236:THR:OG1	2.26	0.49
9:i:69:ASN:OD1	9:i:72:MET:N	2.40	0.49
3:C:344:LEU:HA	3:C:347:ILE:HD12	1.94	0.49
11:K:91:LYS:HG2	11:K:119:LEU:HD11	1.95	0.49
22:V:211:TYR:OH	22:V:234:ARG:NE	2.44	0.49
27:a:284:ARG:HD3	27:a:288:HIS:H	1.78	0.49
28:b:8:VAL:HA	28:b:110:ILE:HG13	1.94	0.49
13:m:27:MET:HE1	13:m:152:ASP:HB2	1.93	0.49
5:E:327:ASP:H	5:E:364:GLN:HG3	1.77	0.49
5:E:348:THR:HG22	5:E:352:MET:HE2	1.94	0.49
6:F:39:GLU:HB2	6:F:43:GLN:HB2	1.94	0.49
21:U:142:LEU:HD22	21:U:147:TYR:HE1	1.77	0.49
21:U:251:ASP:O	21:U:255:SER:HB3	2.13	0.49
23:W:40:LEU:HD22	23:W:77:ALA:HB3	1.93	0.49
25:Y:336:ARG:HH21	25:Y:337:PHE:HE1	1.60	0.49
17:q:35:MET:HG3	17:q:45:LEU:HG	1.93	0.49
18:r:25:TYR:OH	19:s:146:GLN:OE1	2.25	0.49
10:J:11:SER:OG	10:J:15:HIS:N	2.45	0.49
24:X:105:GLN:HA	24:X:108:GLU:HB3	1.93	0.49
32:f:887:PHE:HB3	32:f:900:LEU:HD12	1.93	0.49
3:C:248:MET:HE1	3:C:291:VAL:HB	1.93	0.49
5:E:195:PHE:HD1	5:E:229:ILE:HG23	1.78	0.49
5:E:285:LEU:HB2	5:E:290:LEU:HD11	1.94	0.49
31:e:50:ASP:OD1	31:e:55:GLN:NE2	2.35	0.49
9:i:155:ASN:OD1	10:j:77:THR:OG1	2.31	0.49
18:R:80:SER:OG	18:R:120:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:128:GLN:O	21:U:132:GLY:N	2.45	0.49
1:A:236:CYS:HB3	1:A:270:CYS:HA	1.95	0.49
5:E:116:ASP:O	5:E:118:LEU:N	2.46	0.49
13:m:68:ASN:OD1	13:m:224:HIS:ND1	2.44	0.49
14:n:7:GLN:NE2	14:n:8:PHE:O	2.46	0.49
5:E:119:VAL:HA	5:E:122:MET:HG2	1.95	0.49
10:J:38:ARG:NH2	10:J:178:ASP:O	2.46	0.49
22:V:78:HIS:HE1	22:V:104:THR:HG21	1.77	0.49
30:d:106:LEU:HD21	30:d:114:GLU:HB3	1.95	0.49
3:C:160:GLU:OE1	3:C:313:ARG:NH2	2.46	0.49
6:F:436:GLN:HG3	6:F:437:TYR:H	1.77	0.49
18:R:115:ASP:OD1	18:R:119:ASN:N	2.44	0.49
21:U:333:MET:SD	21:U:333:MET:N	2.82	0.49
26:Z:79:TYR:HE1	26:Z:90:ARG:HA	1.78	0.49
27:a:335:TRP:NE1	27:a:337:GLN:O	2.46	0.49
32:f:408:LEU:HD23	32:f:439:TYR:HD1	1.78	0.49
11:k:147:ASP:OD1	11:k:147:ASP:N	2.46	0.49
4:D:377:SER:O	5:E:297:ARG:NH2	2.45	0.48
22:V:491:VAL:HG11	30:d:256:ILE:HG12	1.94	0.48
27:a:35:HIS:NE2	28:b:17:ARG:HB2	2.28	0.48
8:h:175:GLU:OE2	9:i:53:HIS:NE2	2.47	0.48
3:C:53:ASN:ND2	21:U:642:GLU:O	2.45	0.48
3:C:366:ALA:HB1	3:C:378:VAL:HG21	1.96	0.48
6:F:31:GLU:HA	6:F:35:LYS:HZ3	1.76	0.48
7:G:86:ASP:OD1	13:M:120:HIS:NE2	2.41	0.48
21:U:214:ILE:HA	21:U:217:CYS:HB3	1.95	0.48
27:a:188:LEU:HD11	27:a:193:GLN:HG3	1.95	0.48
27:a:373:ASP:H	30:d:251:ARG:HH22	1.61	0.48
8:h:59:GLU:HG2	8:h:60:ARG:HD3	1.95	0.48
14:n:51:ASP:HB3	14:n:94:LEU:HD22	1.94	0.48
1:A:157:ILE:HG12	1:A:158:ASP:CG	2.38	0.48
1:A:224:LEU:HD11	35:A:501:ADP:H2'	1.95	0.48
21:U:376:MET:HA	21:U:740:GLY:H	1.78	0.48
23:W:197:LYS:O	23:W:199:TYR:N	2.45	0.48
26:Z:58:PHE:HE1	26:Z:68:TRP:HB2	1.78	0.48
20:t:56:ASP:HB2	20:t:107:TRP:HB3	1.94	0.48
8:H:74:LEU:HD12	8:H:87:VAL:HG22	1.95	0.48
21:U:505:ASP:HB3	21:U:508:THR:HG22	1.94	0.48
24:X:71:LYS:HA	24:X:74:ARG:HE	1.78	0.48
28:b:21:PHE:HE1	28:b:175:PRO:HA	1.79	0.48
29:c:85:GLU:HA	33:u:74:ARG:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:140:ASP:OD2	20:t:171:ARG:NH2	2.39	0.48
21:U:607:VAL:O	21:U:615:ARG:NH1	2.42	0.48
23:W:90:LEU:O	23:W:96:GLN:NE2	2.47	0.48
24:X:63:ALA:HB1	24:X:96:PHE:HE1	1.77	0.48
26:Z:125:ASP:HB3	26:Z:128:PRO:HD2	1.96	0.48
32:f:445:LEU:HD11	32:f:466:LEU:HA	1.96	0.48
10:j:148:ASP:OD1	10:j:152:THR:N	2.38	0.48
18:R:19:ARG:NH2	16:p:205:ASP:OD2	2.47	0.48
21:U:655:ALA:HA	21:U:658:ILE:HG12	1.95	0.48
23:W:326:MET:SD	23:W:326:MET:N	2.86	0.48
25:Y:117:LYS:NZ	25:Y:153:ASP:OD1	2.36	0.48
26:Z:147:ASP:OD1	26:Z:147:ASP:N	2.47	0.48
12:l:61:LYS:NZ	12:l:63:ILE:O	2.37	0.48
16:p:143:ALA:HA	16:p:146:MET:HE2	1.96	0.48
1:A:178:GLY:H	35:A:501:ADP:HN62	1.61	0.48
5:E:181:THR:OG1	36:E:401:ATP:O1B	2.31	0.48
5:E:184:ALA:HA	5:E:187:VAL:HG12	1.94	0.48
21:U:245:ALA:HA	21:U:248:ILE:HG12	1.95	0.48
25:Y:287:LEU:HD12	25:Y:291:HIS:HE1	1.79	0.48
30:d:8:GLU:HB2	30:d:18:LYS:HE3	1.96	0.48
30:d:111:ARG:HB3	30:d:114:GLU:HB2	1.95	0.48
31:e:50:ASP:OD1	31:e:50:ASP:N	2.43	0.48
32:f:325:GLN:H	32:f:325:GLN:CD	2.21	0.48
32:f:574:GLU:HA	32:f:577:LEU:HB3	1.95	0.48
32:f:779:CYS:SG	32:f:876:HIS:NE2	2.78	0.48
32:f:802:SER:HB3	32:f:809:ILE:HG21	1.95	0.48
1:A:103:ASN:ND2	6:F:167:GLU:OE2	2.47	0.48
2:B:170:LEU:HD12	2:B:254:GLU:HB3	1.96	0.48
4:D:119:ILE:O	4:D:121:ARG:NH1	2.47	0.48
4:D:296:MET:HE3	4:D:326:ARG:HD3	1.94	0.48
8:H:182:LEU:HD22	8:H:186:ASP:HB3	1.96	0.48
24:X:126:ARG:HA	24:X:129:LEU:HD12	1.96	0.48
15:O:126:THR:OG1	15:O:135:MET:HB2	2.14	0.48
25:Y:301:ILE:HD11	25:Y:343:LEU:HB2	1.96	0.48
6:F:125:LYS:HD3	6:F:131:THR:HG22	1.96	0.48
12:L:44:ALA:HB2	12:L:142:PRO:HB3	1.96	0.48
24:X:28:HIS:O	24:X:32:LYS:HB2	2.13	0.48
29:c:162:LEU:HD12	29:c:200:TYR:HB3	1.95	0.48
32:f:51:GLN:NE2	32:f:55:GLU:OE2	2.46	0.48
9:i:161:ALA:HB3	10:j:53:LEU:HD23	1.95	0.48
20:t:27:LEU:HD11	20:t:34:ALA:HB1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:PRO:HA	1:A:78:TRP:NE1	2.29	0.47
6:F:42:ILE:HG13	27:a:66:GLU:HG2	1.96	0.47
21:U:868:LYS:HD3	21:U:871:PRO:HG3	1.96	0.47
20:t:180:ASP:HB3	20:t:183:SER:HB3	1.96	0.47
19:S:119:GLY:O	19:S:132:ARG:NH2	2.47	0.47
23:W:216:GLU:O	23:W:219:THR:OG1	2.30	0.47
26:Z:121:LEU:HD11	26:Z:138:TYR:HD2	1.79	0.47
12:l:157:ARG:HD2	13:m:59:GLU:HB3	1.95	0.47
10:J:96:LEU:HB2	17:Q:62:LYS:HE3	1.96	0.47
13:M:45:VAL:HG23	13:M:146:ALA:HB1	1.96	0.47
13:M:46:VAL:HG22	13:M:215:TRP:HB3	1.96	0.47
18:R:114:VAL:HG22	18:R:120:ARG:HG3	1.96	0.47
21:U:857:ASP:OD1	21:U:857:ASP:N	2.47	0.47
22:V:218:TYR:HD2	22:V:227:VAL:HG21	1.79	0.47
25:Y:121:LEU:HD23	25:Y:144:LEU:HD22	1.97	0.47
25:Y:205:VAL:HA	25:Y:219:PHE:HE2	1.78	0.47
28:b:51:LEU:HD11	28:b:61:LEU:HD23	1.96	0.47
32:f:650:GLN:HB3	32:f:686:LEU:HD13	1.96	0.47
10:j:31:THR:OG1	10:j:163:ARG:O	2.32	0.47
3:C:46:GLN:O	3:C:50:ASN:ND2	2.48	0.47
11:k:98:ASN:OD1	18:r:61:ARG:NH2	2.48	0.47
36:D:501:ATP:O2G	5:E:291:ARG:NE	2.47	0.47
6:F:93:VAL:HG21	6:F:145:LEU:HD21	1.95	0.47
21:U:251:ASP:O	21:U:255:SER:HB2	2.15	0.47
25:Y:246:ILE:HG22	25:Y:250:LEU:HD23	1.95	0.47
2:B:227:PRO:O	2:B:232:LYS:NZ	2.47	0.47
17:Q:1:MET:HE3	17:Q:134:TYR:HB2	1.95	0.47
19:S:125:ASP:OD1	19:S:129:SER:N	2.47	0.47
23:W:166:LEU:HD12	23:W:169:LEU:HD21	1.96	0.47
1:A:39:SER:O	1:A:43:ARG:NH1	2.47	0.47
4:D:200:ARG:H	4:D:200:ARG:HD3	1.79	0.47
7:G:118:ILE:HG13	7:G:138:MET:HE1	1.96	0.47
21:U:257:SER:HB2	21:U:757:MET:HE3	1.96	0.47
23:W:450:GLU:OE2	26:Z:223:ASN:ND2	2.39	0.47
26:Z:192:THR:O	26:Z:196:HIS:ND1	2.48	0.47
32:f:150:GLU:HG3	32:f:152:ALA:H	1.80	0.47
10:j:38:ARG:NH2	10:j:182:GLU:O	2.48	0.47
11:k:78:MET:HE1	11:k:82:ILE:HA	1.95	0.47
15:o:146:MET:HE1	15:o:154:LEU:HD22	1.96	0.47
18:r:7:LYS:HD2	18:r:109:PRO:HB2	1.97	0.47
6:F:169:ASP:OD2	6:F:266:LYS:NZ	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:204:ASP:N	12:L:204:ASP:OD1	2.46	0.47
25:Y:231:LEU:HD21	25:Y:239:LYS:HZ1	1.79	0.47
26:Z:209:ARG:HH12	27:a:354:GLU:HG2	1.80	0.47
27:a:374:ILE:HG23	30:d:255:MET:HE1	1.96	0.47
14:n:104:ASP:OD1	14:n:104:ASP:N	2.47	0.47
10:J:119:THR:HG22	10:J:126:PRO:HB3	1.97	0.47
13:M:8:ASP:O	13:M:22:GLN:NE2	2.41	0.47
21:U:732:LEU:HD21	21:U:766:PHE:HZ	1.80	0.47
25:Y:91:ALA:HB1	25:Y:100:ILE:HG22	1.95	0.47
32:f:143:ARG:HD3	32:f:162:LEU:HD12	1.96	0.47
13:m:50:GLU:OE2	13:m:201:HIS:ND1	2.47	0.47
16:p:45:MET:HE3	16:p:71:LEU:HD23	1.96	0.47
4:D:410:ASP:OD1	4:D:410:ASP:N	2.48	0.47
5:E:229:ILE:HD11	5:E:276:ILE:HG13	1.96	0.47
6:F:49:ASP:O	6:F:53:LYS:NZ	2.43	0.47
23:W:358:VAL:O	23:W:362:ASN:ND2	2.48	0.47
25:Y:297:ARG:HG3	25:Y:300:ARG:HH21	1.80	0.47
16:p:123:SER:HB3	16:p:137:VAL:HB	1.96	0.47
5:E:153:LEU:HD23	5:E:274:LYS:HD3	1.96	0.46
20:T:20:VAL:HG11	20:T:122:LEU:HD13	1.97	0.46
21:U:215:ASN:OD1	21:U:216:VAL:N	2.42	0.46
22:V:252:ASN:ND2	22:V:284:GLU:OE2	2.48	0.46
24:X:364:LYS:HG3	24:X:368:MET:HE1	1.97	0.46
25:Y:212:GLU:HG2	25:Y:213:LEU:HD22	1.97	0.46
32:f:282:PHE:HZ	32:f:317:LEU:HD21	1.79	0.46
32:f:618:GLU:O	32:f:650:GLN:NE2	2.48	0.46
12:l:45:VAL:HG11	12:l:188:VAL:HG22	1.96	0.46
15:o:30:ASN:OD1	15:o:187:ARG:NH2	2.48	0.46
16:p:83:LYS:HB3	16:p:83:LYS:HE2	1.71	0.46
20:t:20:VAL:HG11	20:t:122:LEU:HD13	1.97	0.46
1:A:413:VAL:HG13	1:A:417:ILE:HD12	1.96	0.46
6:F:240:CYS:O	6:F:244:THR:OG1	2.32	0.46
13:M:150:MET:HE1	13:M:165:ILE:HD13	1.96	0.46
14:N:141:ALA:HB2	14:n:162:LEU:HD11	1.96	0.46
21:U:580:ARG:HG3	21:U:617:ALA:HB2	1.97	0.46
23:W:69:ALA:HB1	23:W:73:MET:HE2	1.96	0.46
23:W:360:GLU:HG2	23:W:364:ARG:HH21	1.79	0.46
19:s:125:ASP:OD1	19:s:129:SER:N	2.49	0.46
12:L:50:LYS:HB3	12:L:59:HIS:HB3	1.96	0.46
18:R:166:ARG:NH1	16:p:34:MET:O	2.48	0.46
20:T:79:ASP:OD1	20:T:79:ASP:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:764:LEU:O	21:U:767:THR:OG1	2.33	0.46
27:a:219:HIS:CD2	27:a:221:VAL:HG22	2.51	0.46
29:c:160:PHE:HE1	29:c:196:LEU:HD21	1.80	0.46
11:k:51:GLU:HB2	11:k:206:MET:HE3	1.97	0.46
13:m:34:SER:OG	13:m:65:ARG:NH1	2.40	0.46
2:B:347:ILE:O	2:B:350:LYS:NZ	2.48	0.46
3:C:375:ARG:NE	3:C:377:HIS:O	2.46	0.46
4:D:159:LYS:HD2	4:D:221:HIS:HA	1.98	0.46
5:E:171:LEU:HB3	5:E:298:LYS:HG2	1.96	0.46
6:F:300:LYS:HA	6:F:300:LYS:HD3	1.50	0.46
6:F:344:ARG:C	6:F:349:ASP:HB2	2.40	0.46
12:L:34:ALA:HA	12:L:162:GLY:HA3	1.96	0.46
16:P:138:VAL:HG11	16:P:146:MET:HB3	1.98	0.46
17:Q:141:SER:HB3	18:r:138:VAL:HG23	1.97	0.46
18:R:19:ARG:O	18:R:33:LYS:NZ	2.43	0.46
22:V:289:LEU:HB3	22:V:312:ALA:HB2	1.96	0.46
23:W:422:ASN:HD21	29:c:235:SER:HA	1.81	0.46
27:a:243:GLY:HA3	27:a:279:GLU:HG3	1.97	0.46
29:c:270:LEU:HB3	29:c:271:ALA:H	1.60	0.46
30:d:231:LYS:HD2	30:d:234:ASP:HB2	1.97	0.46
16:p:45:MET:HE2	16:p:67:LEU:HD23	1.98	0.46
5:E:223:ARG:O	5:E:226:GLN:NE2	2.49	0.46
19:S:16:ALA:HB2	19:S:121:VAL:HG23	1.96	0.46
22:V:337:LEU:O	22:V:401:ASN:ND2	2.44	0.46
30:d:179:ALA:HA	30:d:182:ILE:HG22	1.96	0.46
10:j:39:ASP:OD1	10:j:39:ASP:N	2.49	0.46
13:m:39:ILE:HD12	13:m:193:VAL:HG12	1.98	0.46
15:o:174:ASP:OD2	15:o:187:ARG:NH1	2.49	0.46
16:p:2:SER:OG	16:p:3:ILE:N	2.49	0.46
3:C:187:LEU:HA	3:C:293:MET:HB3	1.98	0.46
8:H:114:VAL:HG12	8:H:118:MET:HE2	1.96	0.46
23:W:127:THR:HA	23:W:130:MET:HG3	1.98	0.46
3:C:286:THR:HG21	3:C:289:ILE:HD12	1.98	0.46
5:E:385:ASP:OD1	5:E:385:ASP:N	2.44	0.46
9:I:52:ILE:O	9:I:53:HIS:C	2.59	0.46
21:U:162:VAL:O	21:U:166:THR:OG1	2.26	0.46
25:Y:138:LEU:HD13	25:Y:176:ARG:HG3	1.96	0.46
12:l:14:SER:OG	12:l:18:ARG:N	2.42	0.46
1:A:157:ILE:C	1:A:159:PRO:HD3	2.41	0.46
11:K:189:MET:HE3	11:K:194:ALA:HB2	1.98	0.46
15:O:112:SER:HB3	15:O:125:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:25:ILE:HG22	17:Q:26:VAL:HG13	1.97	0.46
18:R:39:PRO:HA	18:R:184:TRP:HE1	1.81	0.46
21:U:13:ASP:HB3	30:d:73:ARG:HH21	1.80	0.46
21:U:403:THR:HG23	21:U:777:HIS:HE2	1.81	0.46
23:W:20:TYR:HB2	23:W:54:THR:HG22	1.98	0.46
23:W:431:LYS:HA	23:W:435:LEU:HD13	1.98	0.46
24:X:380:GLN:HB2	25:Y:314:LEU:HA	1.98	0.46
29:c:270:LEU:HD13	29:c:270:LEU:HA	1.79	0.46
9:i:68:LEU:HD11	9:i:74:CYS:HB3	1.97	0.46
11:k:105:GLU:OE2	19:s:75:TYR:OH	2.33	0.46
6:F:336:ASP:OD1	6:F:336:ASP:N	2.48	0.46
11:K:13:ASN:HB3	12:L:126:ARG:HB3	1.98	0.46
11:K:21:LEU:HB2	11:K:24:VAL:HG12	1.97	0.46
13:M:43:ASP:OD1	13:M:43:ASP:N	2.48	0.46
21:U:756:HIS:HB3	21:U:758:PRO:HD2	1.96	0.46
22:V:283:ASN:ND2	31:e:17:ASP:H	2.14	0.46
23:W:55:ARG:HD2	23:W:96:GLN:HG2	1.97	0.46
25:Y:237:ARG:O	25:Y:242:LYS:N	2.41	0.46
25:Y:298:GLU:HG3	25:Y:302:HIS:CD2	2.51	0.46
12:l:72:ILE:HG22	12:l:134:ILE:HG12	1.97	0.46
17:q:53:THR:HG22	17:q:100:VAL:HG12	1.98	0.46
19:s:63:THR:OG1	20:t:94:ARG:NH1	2.43	0.46
20:t:51:LEU:HD11	20:t:110:MET:HE2	1.97	0.46
6:F:247:THR:HB	6:F:281:SER:HA	1.98	0.46
6:F:251:LEU:HB2	6:F:285:ILE:HG12	1.97	0.46
12:L:18:ARG:NH1	12:L:23:GLU:OE2	2.49	0.46
22:V:452:ASN:HB3	22:V:457:TYR:HB2	1.97	0.46
24:X:339:ILE:HG21	24:X:374:PHE:HE1	1.81	0.46
25:Y:357:ASN:O	25:Y:358:ARG:C	2.58	0.46
26:Z:91:ILE:HG22	26:Z:116:CYS:HB2	1.98	0.46
33:u:59:TYR:HB2	33:u:61:ILE:HG13	1.98	0.46
4:D:211:GLY:HA3	4:D:214:MET:HE1	1.97	0.45
4:D:230:VAL:HG12	4:D:264:ILE:HG22	1.97	0.45
7:G:6:SER:OG	7:G:11:ARG:NH1	2.49	0.45
10:J:209:ALA:HB2	10:J:219:ILE:HD12	1.98	0.45
18:R:18:SER:OG	18:R:173:ALA:N	2.49	0.45
26:Z:193:ASN:HA	26:Z:196:HIS:CE1	2.51	0.45
27:a:246:GLU:HG2	27:a:249:GLN:HB2	1.97	0.45
11:k:210:LEU:HD12	11:k:215:ILE:HD13	1.97	0.45
19:s:70:ALA:O	19:s:74:MET:HG3	2.16	0.45
3:C:256:SER:O	3:C:302:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:267:ILE:HG22	4:D:271:ALA:HB2	1.97	0.45
5:E:309:ARG:HG2	5:E:343:LEU:HD11	1.99	0.45
23:W:444:HIS:CD2	26:Z:204:LYS:HG2	2.52	0.45
24:X:407:MET:HA	24:X:410:VAL:HG22	1.96	0.45
27:a:156:TYR:HE2	27:a:196:ARG:HH12	1.65	0.45
14:n:135:ILE:HD13	14:n:163:ALA:HB2	1.98	0.45
17:q:19:ARG:HD3	17:q:177:THR:HG22	1.97	0.45
3:C:145:ASP:OD1	3:C:145:ASP:N	2.49	0.45
5:E:56:ILE:HG23	6:F:130:GLN:HE22	1.81	0.45
6:F:278:LYS:HB2	6:F:281:SER:HB3	1.99	0.45
10:J:209:ALA:HA	10:J:219:ILE:HA	1.98	0.45
18:R:122:SER:OG	18:R:123:GLY:N	2.48	0.45
20:T:122:LEU:HG	20:T:137:LEU:HD12	1.97	0.45
23:W:347:GLY:HA2	23:W:350:ARG:HD2	1.99	0.45
24:X:224:ASP:OD2	24:X:227:THR:OG1	2.30	0.45
17:q:7:ILE:HD12	17:q:14:LEU:HD23	1.97	0.45
8:H:159:LYS:HB2	9:I:55:LEU:HD22	1.98	0.45
15:O:163:ILE:HG12	15:O:170:GLY:HA2	1.97	0.45
27:a:230:ARG:HB3	27:a:232:TRP:CD1	2.51	0.45
29:c:29:GLU:O	29:c:204:THR:OG1	2.33	0.45
29:c:30:GLN:OE1	29:c:206:ASN:ND2	2.49	0.45
32:f:326:LEU:HB3	32:f:420:TRP:HE1	1.79	0.45
1:A:369:ARG:HH21	1:A:372:LEU:HD13	1.81	0.45
4:D:78:GLU:HA	4:D:81:ARG:HG2	1.98	0.45
4:D:370:ILE:HG23	4:D:374:ASP:HB2	1.99	0.45
5:E:248:SER:O	5:E:251:ARG:HD3	2.16	0.45
22:V:322:VAL:HG13	22:V:325:LYS:H	1.81	0.45
23:W:55:ARG:NH2	23:W:93:ARG:HD3	2.25	0.45
26:Z:14:LEU:HD21	29:c:40:LYS:HD3	1.99	0.45
28:b:15:TYR:HD2	28:b:115:SER:HB3	1.80	0.45
11:k:71:ASP:OD1	18:r:64:ARG:NH2	2.50	0.45
7:G:116:LYS:HE2	8:H:84:ARG:HD2	1.98	0.45
10:J:68:ASN:HA	10:J:211:MET:HE1	1.98	0.45
11:K:210:LEU:HD11	11:K:215:ILE:HD13	1.98	0.45
22:V:400:HIS:ND1	30:d:144:MET:O	2.41	0.45
28:b:181:ASP:OD2	28:b:181:ASP:N	2.49	0.45
29:c:139:ARG:HB2	29:c:161:ARG:HH12	1.82	0.45
32:f:93:PRO:HG2	32:f:96:LEU:HB2	1.99	0.45
9:i:208:ALA:HB2	9:i:234:GLU:HB3	1.97	0.45
11:k:221:GLN:HB2	11:k:224:GLN:HG2	1.98	0.45
1:A:138:MET:HE2	1:A:138:MET:HB3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:64:LEU:HG	5:E:65:THR:HG23	1.99	0.45
6:F:182:THR:HA	6:F:242:ALA:HB1	1.99	0.45
12:L:72:ILE:HG22	12:L:134:ILE:HG12	1.99	0.45
21:U:58:GLN:HB2	21:U:87:LEU:HD12	1.98	0.45
25:Y:239:LYS:HG3	25:Y:240:VAL:HG13	1.97	0.45
25:Y:287:LEU:HD12	25:Y:291:HIS:CE1	2.52	0.45
28:b:27:GLN:NE2	28:b:30:GLN:OE1	2.50	0.45
14:n:14:LEU:HD11	14:n:101:ALA:HB3	1.99	0.45
20:t:54:SER:O	20:t:108:ASN:ND2	2.37	0.45
5:E:171:LEU:HB2	5:E:295:LEU:HD12	1.99	0.45
15:O:143:ARG:NH2	15:O:150:GLU:OE1	2.50	0.45
17:Q:26:VAL:HG21	18:R:136:TYR:HE2	1.82	0.45
20:T:63:LEU:HD21	20:T:106:LEU:HD13	1.99	0.45
25:Y:210:SER:HB3	25:Y:213:LEU:HD23	1.98	0.45
32:f:416:MET:HE3	32:f:450:ILE:HD13	1.99	0.45
7:g:50:ILE:HG21	7:g:79:VAL:HB	1.99	0.45
18:r:179:VAL:HG22	18:r:184:TRP:HB3	1.98	0.45
1:A:174:TYR:OH	1:A:188:ARG:NH2	2.49	0.45
3:C:251:ILE:HD13	3:C:293:MET:HG3	1.97	0.45
19:S:45:LYS:HE3	19:S:203:ILE:HD12	1.97	0.45
21:U:447:GLY:HA3	21:U:480:GLY:HA2	1.99	0.45
24:X:203:PRO:HG2	24:X:207:GLN:HB2	1.98	0.45
29:c:299:CYS:O	29:c:303:MET:HG3	2.17	0.45
32:f:679:LEU:HD12	32:f:680:ARG:HB3	1.98	0.45
11:k:129:ASP:N	11:k:129:ASP:OD1	2.50	0.45
4:D:309:MET:HE2	4:D:327:LEU:HD11	1.97	0.45
5:E:219:PHE:HD2	5:E:263:GLN:HB3	1.82	0.45
6:F:288:LEU:HB3	6:F:332:THR:HG22	1.98	0.45
6:F:362:ARG:O	6:F:366:MET:HG2	2.17	0.45
22:V:283:ASN:HD21	31:e:17:ASP:HB2	1.82	0.45
25:Y:348:ASP:OD1	25:Y:349:LYS:N	2.49	0.45
29:c:224:SER:HB3	29:c:227:GLU:HB2	1.98	0.45
32:f:345:PRO:HA	32:f:348:ILE:HD12	1.98	0.45
7:g:200:THR:HA	7:g:203:SER:HB3	1.99	0.45
11:k:117:SER:OG	12:l:82:ARG:NH1	2.50	0.45
18:r:77:ALA:HB3	18:r:107:ARG:HH22	1.81	0.45
1:A:141:GLY:N	1:A:151:ILE:O	2.50	0.44
4:D:87:LEU:HA	4:D:134:LYS:HG3	2.00	0.44
4:D:383:GLY:HA3	5:E:164:ILE:HD13	2.00	0.44
5:E:55:GLN:O	6:F:133:PHE:N	2.38	0.44
5:E:127:PRO:HG3	6:F:320:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:54:SER:OG	20:T:55:GLY:N	2.50	0.44
22:V:465:ASP:OD1	22:V:465:ASP:N	2.50	0.44
23:W:80:TRP:CD1	23:W:123:ARG:HH22	2.34	0.44
23:W:318:SER:O	23:W:321:VAL:HG12	2.18	0.44
12:l:84:LEU:HD11	12:l:112:ILE:HD12	2.00	0.44
12:l:137:TYR:OH	12:l:217:LYS:NZ	2.50	0.44
13:m:66:LEU:HD12	13:m:212:GLU:HG2	1.98	0.44
1:A:197:HIS:ND1	1:A:199:GLU:OE1	2.50	0.44
3:C:38:LYS:HB3	4:D:54:LEU:HD22	2.00	0.44
6:F:303:ASP:O	6:F:308:ARG:NH1	2.50	0.44
9:I:4:ARG:NH2	9:I:5:TYR:OH	2.50	0.44
17:Q:137:PHE:HB3	18:r:133:VAL:HG21	1.99	0.44
21:U:521:LEU:HD13	21:U:554:LEU:HG	1.99	0.44
23:W:344:THR:O	23:W:348:GLU:N	2.42	0.44
28:b:161:ASN:ND2	28:b:168:SER:H	2.15	0.44
30:d:237:ILE:HG13	30:d:238:PRO:HD3	2.00	0.44
9:i:38:LEU:HD23	9:i:160:LYS:HG2	1.98	0.44
13:m:99:ARG:NH2	13:m:105:ASN:OD1	2.40	0.44
20:t:27:LEU:HD22	20:t:184:TYR:HB2	1.99	0.44
1:A:96:ALA:O	2:B:132:TYR:N	2.49	0.44
3:C:49:ARG:NH2	4:D:64:GLU:OE2	2.49	0.44
3:C:161:ILE:HA	3:C:164:VAL:HG12	1.99	0.44
21:U:7:GLY:O	21:U:10:SER:OG	2.30	0.44
22:V:259:LEU:HD11	22:V:294:ARG:HG2	2.00	0.44
25:Y:109:GLU:OE2	25:Y:143:TYR:OH	2.32	0.44
32:f:94:LYS:HG3	32:f:95:PRO:HD3	1.99	0.44
15:o:22:GLU:HG2	15:o:27:ALA:HB2	2.00	0.44
2:B:343:ARG:NH2	2:B:346:ARG:HE	2.15	0.44
3:C:233:GLU:HA	3:C:236:VAL:HG12	2.00	0.44
5:E:173:TYR:HB2	5:E:282:PRO:HG3	1.99	0.44
24:X:107:VAL:HG23	24:X:133:LEU:HD11	1.99	0.44
27:a:257:GLN:HB3	27:a:261:LEU:HD22	2.00	0.44
28:b:156:PHE:O	28:b:160:LEU:HB2	2.18	0.44
32:f:344:VAL:HG13	32:f:347:ASP:H	1.83	0.44
16:p:193:ASP:OD1	16:p:193:ASP:N	2.50	0.44
18:r:41:LEU:HD23	18:r:103:GLY:HA3	2.00	0.44
6:F:172:VAL:HG12	6:F:274:LEU:HD13	1.98	0.44
19:S:99:ARG:HH21	19:S:102:PHE:HD2	1.65	0.44
21:U:692:ALA:HB1	21:U:736:ILE:HB	2.00	0.44
21:U:801:GLN:HB3	21:U:877:LEU:HB3	2.00	0.44
21:U:906:LEU:HG	21:U:906:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:110:ILE:HG22	28:b:139:ASP:HB2	1.99	0.44
29:c:37:ALA:O	29:c:41:MET:HG2	2.18	0.44
8:h:3:GLU:OE2	13:m:127:ALA:HB3	2.18	0.44
12:l:215:VAL:HB	12:l:221:PHE:HD1	1.82	0.44
13:m:192:GLU:O	13:m:196:ILE:HG12	2.17	0.44
1:A:156:LYS:O	1:A:159:PRO:HG3	2.18	0.44
1:A:278:ASP:OD1	1:A:323:ARG:NH2	2.43	0.44
3:C:78:ARG:NH1	3:C:80:MET:SD	2.90	0.44
3:C:304:ALA:O	3:C:307:ARG:NH1	2.51	0.44
19:S:65:THR:O	19:S:69:GLU:HG2	2.18	0.44
24:X:258:LYS:HD3	24:X:266:ASP:HB2	1.98	0.44
24:X:304:LYS:O	24:X:308:ASP:N	2.42	0.44
27:a:174:LYS:HA	27:a:174:LYS:HD3	1.71	0.44
8:h:81:PRO:HB3	8:h:84:ARG:HH21	1.82	0.44
1:A:265:ARG:NH1	1:A:310:ASP:OD1	2.44	0.44
2:B:88:LEU:HG	2:B:91:LYS:HB2	1.98	0.44
3:C:77:VAL:HG22	3:C:111:ASN:H	1.83	0.44
6:F:188:ILE:HB	6:F:195:ILE:HD11	1.99	0.44
21:U:792:ASN:HB3	21:U:914:LEU:N	2.31	0.44
30:d:198:LEU:C	30:d:199:PHE:CG	2.95	0.44
7:g:4:GLY:O	7:g:5:SER:HB2	2.18	0.44
17:q:7:ILE:O	17:q:14:LEU:N	2.48	0.44
18:r:127:SER:HB3	18:r:136:TYR:CE1	2.53	0.44
36:C:501:ATP:O2G	4:D:323:ARG:NH1	2.51	0.44
5:E:245:GLU:HA	5:E:251:ARG:HH21	1.82	0.44
7:G:49:VAL:HG22	7:G:219:VAL:HG22	2.00	0.44
13:M:134:SER:OG	13:M:151:ILE:O	2.33	0.44
15:O:18:THR:OG1	15:O:172:ASN:HB2	2.18	0.44
22:V:98:LEU:HD21	22:V:206:VAL:HG22	1.99	0.44
26:Z:37:GLY:HA2	26:Z:56:VAL:HG12	1.99	0.44
7:g:61:LEU:HA	13:m:160:TYR:HD1	1.83	0.44
7:g:70:PHE:HD2	7:g:91:VAL:HG21	1.82	0.44
1:A:154:PRO:HB2	1:A:157:ILE:HD12	1.99	0.44
5:E:242:ARG:HG2	5:E:254:GLN:HG2	1.99	0.44
6:F:418:GLU:HA	6:F:421:MET:HG3	2.00	0.44
22:V:252:ASN:HD22	22:V:284:GLU:HG2	1.83	0.44
26:Z:136:GLU:OE2	26:Z:157:HIS:ND1	2.39	0.44
32:f:507:ASP:HB3	32:f:509:LYS:HG3	1.99	0.44
32:f:882:LEU:HD11	32:f:900:LEU:HD11	1.99	0.44
13:m:93:GLU:OE2	13:m:97:ASN:ND2	2.43	0.44
14:n:4:MET:HG3	14:n:127:ILE:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:o:63:LEU:HD11	15:o:79:ALA:HB2	1.98	0.44
19:s:45:LYS:HE3	19:s:203:ILE:HD12	2.00	0.44
19:s:169:ASP:OD2	19:s:169:ASP:N	2.48	0.44
20:t:195:LYS:HB3	20:t:195:LYS:HE3	1.75	0.44
7:G:123:GLN:NE2	8:H:82:ASP:OD1	2.50	0.43
18:R:35:ILE:N	18:R:43:GLY:O	2.51	0.43
21:U:90:VAL:HG22	21:U:136:LYS:HE2	2.00	0.43
25:Y:104:MET:HG3	25:Y:127:THR:HG23	2.00	0.43
28:b:26:LEU:HD11	28:b:80:PRO:HG3	2.00	0.43
29:c:32:TYR:HE1	29:c:206:ASN:HD21	1.66	0.43
30:d:114:GLU:HA	30:d:117:THR:HG22	2.00	0.43
3:C:42:LEU:HD22	4:D:54:LEU:HG	2.00	0.43
8:H:203:MET:HA	8:H:207:ASN:HD21	1.83	0.43
22:V:181:TYR:HA	22:V:184:ALA:HB3	1.99	0.43
22:V:354:LYS:NZ	31:e:33:ASP:OD1	2.41	0.43
32:f:442:SER:HB2	32:f:477:MET:HA	1.98	0.43
16:p:30:ILE:HG22	16:p:31:GLN:H	1.83	0.43
17:q:52:ASP:OD1	18:r:88:TYR:OH	2.32	0.43
2:B:385:MET:HE1	10:J:201:SER:HA	1.99	0.43
5:E:145:LEU:HG	5:E:149:ILE:HD12	2.00	0.43
9:I:54:LYS:HB3	9:I:54:LYS:HE3	1.45	0.43
22:V:283:ASN:HD21	31:e:17:ASP:H	1.66	0.43
26:Z:130:ASP:OD1	26:Z:131:LEU:N	2.51	0.43
11:k:67:ILE:HG22	11:k:216:GLU:HG3	1.98	0.43
18:r:115:ASP:OD1	18:r:119:ASN:N	2.51	0.43
6:F:275:ALA:HB1	6:F:326:VAL:HG21	1.99	0.43
16:P:61:GLN:HE22	17:Q:124:LEU:HB3	1.84	0.43
22:V:293:GLY:HA2	22:V:296:LYS:HZ3	1.83	0.43
23:W:45:GLU:HA	23:W:48:LEU:HG	1.99	0.43
23:W:166:LEU:HD22	23:W:192:LEU:HD12	2.00	0.43
24:X:394:ASP:N	24:X:394:ASP:OD1	2.52	0.43
28:b:2:VAL:HG22	28:b:4:GLU:HG3	2.00	0.43
30:d:189:ILE:HD12	30:d:193:GLU:HB3	2.00	0.43
32:f:414:LEU:HD12	32:f:417:ILE:HB	2.00	0.43
32:f:662:MET:O	32:f:781:TYR:OH	2.27	0.43
4:D:232:GLY:HA3	4:D:266:GLU:HG2	2.00	0.43
7:G:138:MET:HB3	7:G:154:CYS:HB2	2.01	0.43
22:V:438:VAL:HG12	22:V:451:ILE:HD11	2.00	0.43
24:X:157:LEU:HD23	24:X:157:LEU:HA	1.87	0.43
29:c:122:LEU:HB2	29:c:200:TYR:CE1	2.54	0.43
29:c:189:ILE:HA	29:c:192:LEU:HG	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:285:GLU:N	29:c:285:GLU:OE1	2.51	0.43
32:f:573:ILE:HD12	32:f:595:VAL:HG12	2.00	0.43
7:g:180:GLU:HG2	8:h:55:ILE:HG22	2.01	0.43
4:D:380:GLN:HB3	4:D:384:MET:HE1	2.00	0.43
21:U:525:ASN:ND2	21:U:527:GLN:HE21	2.16	0.43
21:U:885:MET:H	21:U:888:GLN:HE21	1.66	0.43
26:Z:103:LYS:O	26:Z:106:ILE:HG22	2.19	0.43
10:j:233:GLU:HA	10:j:236:LYS:HG2	2.00	0.43
12:l:65:HIS:NE2	12:l:67:ASP:O	2.51	0.43
19:s:180:ILE:O	19:s:184:GLU:HG2	2.19	0.43
1:A:124:ASP:OD1	1:A:125:LEU:N	2.52	0.43
4:D:56:VAL:HG22	21:U:600:ARG:HH21	1.84	0.43
5:E:249:ALA:O	5:E:250:ASP:C	2.61	0.43
25:Y:381:GLN:HB3	25:Y:385:ARG:HH12	1.84	0.43
26:Z:235:ASN:HD21	27:a:335:TRP:HB3	1.84	0.43
1:A:349:GLU:O	1:A:352:THR:OG1	2.29	0.43
5:E:44:GLU:OE2	6:F:76:ASN:ND2	2.52	0.43
5:E:310:LEU:HG	5:E:314:LYS:HE3	2.01	0.43
21:U:172:ASP:OD1	21:U:172:ASP:N	2.51	0.43
21:U:250:PHE:HE1	21:U:328:ILE:HB	1.84	0.43
21:U:398:ASN:HB3	29:c:175:ARG:HD3	2.00	0.43
21:U:792:ASN:HA	21:U:913:ILE:HG22	1.99	0.43
22:V:108:LEU:HD11	22:V:174:PHE:HB2	2.00	0.43
22:V:175:MET:SD	22:V:180:ARG:NH1	2.92	0.43
7:g:231:THR:OG1	7:g:234:GLU:OE1	2.29	0.43
2:B:223:ILE:HG13	2:B:347:ILE:HG21	2.00	0.43
3:C:214:VAL:HB	3:C:248:MET:HA	2.01	0.43
22:V:467:TYR:OH	24:X:397:TYR:OH	2.26	0.43
27:a:53:GLY:O	27:a:57:ILE:N	2.46	0.43
32:f:533:ASP:O	32:f:536:SER:OG	2.36	0.43
13:m:65:ARG:HH21	13:m:78:ALA:HA	1.83	0.43
15:O:215:LYS:HB2	16:P:197:THR:HB	2.01	0.43
18:R:133:VAL:HG21	17:q:137:PHE:HB3	2.00	0.43
32:f:478:ARG:O	32:f:482:ILE:HG12	2.19	0.43
16:p:38:ASP:OD1	16:p:38:ASP:N	2.51	0.43
5:E:245:GLU:HG3	5:E:251:ARG:NH2	2.34	0.42
7:G:17:SER:HG	7:G:21:ARG:H	1.62	0.42
18:R:33:LYS:HA	18:R:45:MET:HE3	2.01	0.42
25:Y:25:LEU:HD12	25:Y:25:LEU:HA	1.92	0.42
29:c:195:GLY:HA3	29:c:200:TYR:CE1	2.54	0.42
30:d:131:VAL:HA	30:d:134:LYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:543:MET:HE1	32:f:582:VAL:HB	2.00	0.42
32:f:679:LEU:HD22	32:f:713:PHE:HE2	1.84	0.42
2:B:204:PRO:HG3	2:B:211:TYR:HE2	1.83	0.42
6:F:94:ILE:HD11	6:F:125:LYS:HB2	2.01	0.42
11:K:137:PHE:HB3	11:K:139:VAL:HG22	1.99	0.42
21:U:49:TYR:HA	21:U:57:ARG:HG3	2.01	0.42
21:U:611:ASN:HB3	21:U:614:VAL:HG12	2.02	0.42
32:f:209:MET:HE1	32:f:244:GLU:HB3	2.01	0.42
32:f:267:ARG:O	32:f:271:MET:HG2	2.20	0.42
7:g:3:ARG:O	7:g:4:GLY:C	2.62	0.42
11:k:15:PHE:HE2	12:l:126:ARG:HB2	1.83	0.42
2:B:54:PRO:HG2	2:B:61:LYS:HB3	2.02	0.42
2:B:143:LEU:HD21	2:B:162:VAL:HG11	2.01	0.42
3:C:358:GLU:HB2	3:C:390:VAL:HG11	2.00	0.42
6:F:234:THR:N	35:F:501:ADP:O1A	2.52	0.42
6:F:275:ALA:O	6:F:281:SER:OG	2.32	0.42
7:g:132:ARG:HA	7:g:133:PRO:HD3	1.84	0.42
14:n:196:LYS:HA	14:n:196:LYS:HD3	1.77	0.42
16:p:205:ASP:OD1	16:p:205:ASP:N	2.51	0.42
33:u:45:PHE:HE1	33:u:65:SER:HB3	1.83	0.42
2:B:79:ILE:HD12	32:f:677:HIS:CD2	2.53	0.42
3:C:131:VAL:HG12	3:C:133:PRO:HD3	2.01	0.42
5:E:248:SER:O	5:E:250:ASP:N	2.52	0.42
14:N:53:GLN:NE2	15:O:117:GLY:O	2.52	0.42
19:S:157:ASN:ND2	16:p:176:ASP:OD2	2.39	0.42
23:W:199:TYR:O	23:W:200:ILE:C	2.62	0.42
23:W:319:THR:HA	23:W:322:GLU:HG2	2.01	0.42
25:Y:220:VAL:HA	25:Y:223:THR:HG22	2.01	0.42
27:a:273:GLN:HB3	27:a:310:LEU:HD11	2.02	0.42
27:a:278:MET:HA	27:a:281:THR:HG22	2.01	0.42
1:A:59:ILE:HD13	1:A:62:LEU:HD21	2.02	0.42
6:F:150:LEU:H	6:F:165:PRO:HB3	1.84	0.42
7:G:73:THR:HG23	7:G:75:ASN:H	1.84	0.42
7:G:76:ILE:HG12	7:G:111:VAL:HG22	2.00	0.42
21:U:9:ILE:O	21:U:44:LYS:NZ	2.52	0.42
25:Y:58:CYS:HA	25:Y:63:TRP:HB2	2.01	0.42
32:f:344:VAL:HB	32:f:390:LEU:HD23	2.01	0.42
7:g:10:ASP:OD1	7:g:10:ASP:N	2.51	0.42
15:o:201:ARG:H	15:o:201:ARG:HG3	1.73	0.42
17:q:19:ARG:HD2	17:q:179:SER:HB3	2.02	0.42
18:r:74:ILE:HD11	18:r:78:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:GLU:HB2	1:A:403:ILE:HD13	2.02	0.42
2:B:143:LEU:HD11	2:B:162:VAL:HG11	2.02	0.42
4:D:258:ALA:O	4:D:260:ALA:N	2.53	0.42
5:E:359:HIS:ND1	5:E:361:PHE:O	2.52	0.42
21:U:599:ILE:HD13	21:U:625:ILE:HD11	2.01	0.42
24:X:105:GLN:HA	24:X:108:GLU:CB	2.49	0.42
24:X:171:LEU:HB3	24:X:213:GLN:HE22	1.85	0.42
25:Y:240:VAL:HA	25:Y:246:ILE:HD12	2.02	0.42
30:d:41:THR:HG22	30:d:44:THR:H	1.84	0.42
9:i:216:LEU:HD12	9:i:225:ILE:HG12	2.02	0.42
16:p:74:TYR:CZ	16:p:78:GLU:HG3	2.55	0.42
2:B:76:GLU:HA	2:B:79:ILE:HG22	2.01	0.42
18:R:144:SER:OG	18:R:145:TYR:N	2.52	0.42
21:U:472:ILE:HA	21:U:475:HIS:CE1	2.55	0.42
22:V:212:TYR:HA	22:V:253:LEU:HD11	2.02	0.42
24:X:351:SER:HA	24:X:354:ILE:HG22	2.02	0.42
26:Z:249:PHE:HE2	29:c:303:MET:HE3	1.85	0.42
28:b:7:MET:HE1	28:b:64:LEU:HB2	2.01	0.42
32:f:755:ASP:OD2	32:f:758:ASN:ND2	2.46	0.42
18:r:97:MET:H	18:r:116:SER:HB3	1.85	0.42
3:C:212:ILE:HB	3:C:246:ILE:HA	2.01	0.42
4:D:153:MET:HG2	4:D:154:LEU:H	1.83	0.42
4:D:398:ASP:OD1	4:D:398:ASP:N	2.53	0.42
9:I:53:HIS:CE1	9:I:55:LEU:HB2	2.55	0.42
12:L:182:CYS:HB3	12:L:186:GLU:HB2	2.02	0.42
21:U:17:PRO:HB2	21:U:55:ARG:HH12	1.85	0.42
26:Z:113:LYS:NZ	26:Z:117:PRO:O	2.52	0.42
26:Z:206:LEU:HA	26:Z:209:ARG:HG2	2.01	0.42
20:t:97:TYR:HA	20:t:100:ARG:HG2	2.02	0.42
1:A:96:ALA:HB3	2:B:132:TYR:HD2	1.85	0.42
3:C:140:VAL:HB	3:C:213:ARG:HE	1.84	0.42
21:U:603:LEU:HD12	21:U:606:ALA:HB3	2.00	0.42
21:U:834:SER:HB2	21:U:836:THR:HG23	2.02	0.42
21:U:889:LEU:HD13	21:U:909:GLY:H	1.84	0.42
22:V:267:ALA:O	22:V:268:GLU:C	2.62	0.42
23:W:256:ILE:HG23	23:W:262:LYS:HB3	2.01	0.42
27:a:248:PHE:CE2	27:a:249:GLN:HG2	2.55	0.42
29:c:29:GLU:HG3	29:c:65:TYR:HB2	2.01	0.42
30:d:52:ARG:HH12	30:d:92:SER:HB3	1.84	0.42
7:g:13:ILE:HG13	7:g:15:ILE:HG12	2.02	0.42
12:l:137:TYR:CZ	12:l:217:LYS:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:215:TRP:CH2	13:m:219:LEU:HD11	2.54	0.42
14:n:107:GLU:HG2	14:n:110:GLN:HE21	1.84	0.42
17:q:7:ILE:HB	17:q:14:LEU:HB3	2.01	0.42
20:t:67:LEU:HD12	20:t:67:LEU:HA	1.94	0.42
2:B:303:ARG:HG3	2:B:307:ARG:HE	1.85	0.42
4:D:57:GLN:HA	4:D:60:TYR:CE1	2.54	0.42
4:D:214:MET:HE3	36:D:501:ATP:H2'	2.02	0.42
5:E:172:LEU:HD22	5:E:301:ILE:HD11	2.01	0.42
11:K:86:LYS:HA	11:K:86:LYS:HD2	1.85	0.42
13:M:37:ILE:HG12	13:M:197:ILE:HD11	2.01	0.42
15:O:11:GLY:HA2	15:O:108:PRO:HB3	2.01	0.42
16:P:193:ASP:OD1	16:P:193:ASP:N	2.53	0.42
20:T:185:ASN:OD1	20:T:205:THR:N	2.44	0.42
21:U:27:LEU:HD23	21:U:63:VAL:HG11	2.01	0.42
21:U:689:ILE:HG12	21:U:732:LEU:HD22	2.01	0.42
22:V:283:ASN:OD1	22:V:287:ARG:NH1	2.53	0.42
24:X:130:GLU:HA	24:X:133:LEU:HB3	2.01	0.42
27:a:290:GLN:HG2	27:a:330:ARG:HB3	2.02	0.42
29:c:70:ILE:HG21	29:c:104:ARG:HH11	1.85	0.42
30:d:62:SER:HA	30:d:65:ARG:HG2	2.02	0.42
30:d:179:ALA:O	30:d:183:GLU:N	2.46	0.42
32:f:535:THR:OG1	32:f:566:HIS:HE1	2.02	0.42
8:h:100:VAL:HG13	16:p:93:ASN:HD22	1.85	0.42
1:A:74:PRO:HA	1:A:75:PRO:HD3	1.87	0.41
3:C:406:LYS:NZ	9:I:66:TYR:OH	2.52	0.41
16:P:38:ASP:OD1	16:P:38:ASP:N	2.53	0.41
18:R:53:SER:O	18:R:57:ARG:HB2	2.20	0.41
20:T:92:LEU:O	20:T:96:MET:HG2	2.20	0.41
23:W:16:MET:SD	23:W:16:MET:N	2.93	0.41
24:X:71:LYS:HB2	24:X:71:LYS:HE2	1.91	0.41
25:Y:155:ASP:OD1	25:Y:155:ASP:N	2.53	0.41
26:Z:63:LYS:C	26:Z:65:ASP:H	2.28	0.41
26:Z:256:GLN:HB2	29:c:295:ASN:OD1	2.20	0.41
29:c:76:PRO:HG2	29:c:87:VAL:HG11	2.01	0.41
30:d:171:LEU:O	30:d:175:ARG:HG2	2.19	0.41
13:m:181:MET:SD	13:m:181:MET:N	2.89	0.41
14:n:160:LEU:O	14:n:164:MET:HG2	2.20	0.41
17:q:39:SER:OG	17:q:40:GLU:N	2.52	0.41
1:A:187:LEU:O	1:A:191:VAL:HG22	2.20	0.41
17:Q:170:ARG:HH21	18:r:140:ASP:CG	2.27	0.41
21:U:609:ASP:O	21:U:615:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:234:ASP:HA	23:W:237:GLU:HG2	2.01	0.41
23:W:316:ARG:NH1	23:W:380:GLN:O	2.40	0.41
24:X:105:GLN:O	24:X:109:LEU:HD23	2.20	0.41
27:a:261:LEU:HD12	27:a:261:LEU:HA	1.81	0.41
29:c:246:LYS:O	29:c:249:LEU:HB3	2.20	0.41
32:f:253:LEU:HD13	32:f:277:LEU:HD23	2.02	0.41
32:f:658:ALA:HB3	32:f:696:LEU:HD23	2.02	0.41
2:B:80:ARG:O	2:B:84:GLN:NE2	2.53	0.41
2:B:113:GLU:HB3	2:B:122:ILE:HG23	2.02	0.41
2:B:220:LYS:HD2	2:B:322:ARG:CZ	2.50	0.41
4:D:171:ASP:OD1	4:D:171:ASP:N	2.51	0.41
4:D:228:ILE:HB	4:D:262:ILE:HA	2.03	0.41
4:D:380:GLN:NE2	5:E:165:ILE:O	2.53	0.41
17:Q:40:GLU:HG3	17:Q:41:LYS:HG2	2.01	0.41
22:V:86:VAL:HG21	22:V:160:LEU:HD13	2.01	0.41
23:W:432:LEU:HD11	29:c:305:ASP:HB2	2.02	0.41
26:Z:212:LEU:HD23	27:a:350:LYS:HG2	2.02	0.41
32:f:478:ARG:HD2	32:f:514:VAL:HG21	2.01	0.41
13:m:232:ARG:NH1	13:m:236:GLU:OE2	2.54	0.41
4:D:164:TYR:HB2	4:D:222:HIS:CD2	2.55	0.41
4:D:270:ILE:HD11	4:D:288:ILE:HB	2.03	0.41
7:G:112:ASP:OD1	7:G:112:ASP:N	2.52	0.41
11:K:88:LEU:HD23	11:K:88:LEU:HA	1.92	0.41
11:K:107:MET:SD	11:K:107:MET:N	2.82	0.41
21:U:646:PRO:O	21:U:650:TYR:N	2.49	0.41
23:W:31:CYS:HB3	23:W:43:VAL:HB	2.02	0.41
23:W:406:VAL:HG12	23:W:413:ILE:HG23	2.02	0.41
25:Y:142:PHE:HE2	25:Y:176:ARG:HD2	1.85	0.41
26:Z:96:HIS:CE1	26:Z:123:ILE:HG12	2.56	0.41
27:a:250:THR:HA	27:a:253:THR:HG22	2.03	0.41
32:f:726:ILE:HG12	32:f:748:LEU:HD21	2.01	0.41
8:h:55:ILE:HD12	8:h:55:ILE:HA	1.94	0.41
10:j:185:ASP:O	10:j:189:LYS:HG2	2.20	0.41
11:k:85:ALA:HB2	11:k:139:VAL:HG11	2.03	0.41
15:o:51:ASP:HB3	15:o:94:ILE:HG23	2.01	0.41
18:r:12:VAL:HG11	18:r:102:CYS:HB3	2.02	0.41
19:s:166:LEU:HD21	19:s:171:ALA:HB2	2.01	0.41
2:B:74:MET:HE2	2:B:74:MET:HB3	1.87	0.41
6:F:96:LEU:HD12	6:F:145:LEU:HD23	2.03	0.41
16:P:123:SER:HB3	16:P:137:VAL:HB	2.02	0.41
16:P:177:ARG:HD3	16:P:177:ARG:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:72:ILE:HD12	20:T:72:ILE:HA	1.94	0.41
21:U:867:LYS:HG3	21:U:868:LYS:H	1.86	0.41
22:V:411:SER:HB2	22:V:447:ILE:HG12	2.02	0.41
25:Y:68:ASP:OD1	25:Y:68:ASP:N	2.54	0.41
27:a:182:CYS:SG	27:a:183:VAL:N	2.93	0.41
9:i:170:ALA:O	9:i:174:MET:HG3	2.21	0.41
4:D:57:GLN:HE21	21:U:636:VAL:HG12	1.85	0.41
7:G:187:PHE:HD2	7:G:189:TRP:HD1	1.68	0.41
11:K:73:HIS:CE1	11:K:106:THR:HB	2.55	0.41
21:U:516:LEU:HD23	21:U:532:MET:HE3	2.02	0.41
21:U:524:LYS:NZ	21:U:562:GLU:O	2.54	0.41
22:V:280:ALA:HB3	22:V:285:TRP:CD1	2.55	0.41
23:W:98:LYS:HD3	23:W:137:TYR:CE2	2.56	0.41
26:Z:242:LEU:HD12	26:Z:246:VAL:HG11	2.02	0.41
29:c:272:ILE:HB	29:c:273:LYS:H	1.65	0.41
7:g:38:THR:HA	7:g:169:GLY:HA3	2.02	0.41
14:n:94:LEU:C	14:n:95:MET:HE2	2.46	0.41
19:s:158:MET:HG3	19:s:161:VAL:HG21	2.02	0.41
1:A:100:LYS:HG3	1:A:137:GLY:HA2	2.03	0.41
2:B:106:PRO:HB3	3:C:121:TYR:HB2	2.02	0.41
4:D:270:ILE:O	4:D:289:LEU:HD12	2.20	0.41
8:H:9:SER:OG	8:H:123:GLN:O	2.36	0.41
8:H:160:ALA:HB1	8:H:174:LEU:HD13	2.02	0.41
9:I:201:MET:HE2	9:I:206:LEU:HD11	2.03	0.41
16:P:131:MET:HE3	16:P:131:MET:HB2	1.84	0.41
20:T:27:LEU:HD12	20:T:37:ARG:HA	2.01	0.41
29:c:114:SER:O	29:c:116:PRO:HD3	2.21	0.41
7:g:58:ASP:OD1	7:g:58:ASP:N	2.52	0.41
10:j:95:ARG:C	17:q:62:LYS:HZ3	2.29	0.41
13:m:8:ASP:OD1	13:m:8:ASP:N	2.52	0.41
19:s:57:PHE:HZ	20:t:128:LEU:HB3	1.85	0.41
2:B:135:ILE:HD11	2:B:139:VAL:HG21	2.03	0.41
2:B:341:LEU:HB3	2:B:347:ILE:HD12	2.02	0.41
3:C:147:THR:H	3:C:150:MET:HE2	1.85	0.41
4:D:149:SER:O	4:D:150:SER:C	2.62	0.41
11:K:221:GLN:HB2	11:K:224:GLN:HG2	2.02	0.41
19:S:68:ILE:HD13	19:S:68:ILE:HA	1.95	0.41
29:c:80:THR:N	29:c:83:SER:O	2.53	0.41
29:c:164:ASN:OD1	29:c:164:ASN:N	2.53	0.41
14:n:59:VAL:HG11	14:n:83:PHE:CE2	2.56	0.41
2:B:165:ASP:OD1	2:B:165:ASP:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:333:SER:HA	3:C:336:MET:HG2	2.02	0.41
7:G:187:PHE:HD2	7:G:189:TRP:CD1	2.38	0.41
9:I:119:GLN:NE2	10:J:79:ASP:OD1	2.54	0.41
10:J:36:ARG:HD2	10:J:142:PRO:HG2	2.03	0.41
10:J:203:GLY:HA2	10:J:229:VAL:HG21	2.03	0.41
11:K:15:PHE:HE2	12:L:127:PRO:HD2	1.86	0.41
12:L:112:ILE:HD13	12:L:112:ILE:HA	1.86	0.41
19:S:145:LEU:HD21	19:S:182:ALA:HB2	2.03	0.41
21:U:26:LYS:HD2	21:U:26:LYS:HA	1.88	0.41
21:U:623:GLY:HA2	21:U:659:CYS:HB2	2.02	0.41
22:V:417:ILE:HD12	22:V:417:ILE:HA	1.98	0.41
26:Z:15:VAL:O	26:Z:19:VAL:HG23	2.21	0.41
26:Z:106:ILE:HD12	26:Z:153:LYS:HB2	2.03	0.41
26:Z:206:LEU:HD13	26:Z:209:ARG:HD3	2.02	0.41
26:Z:234:PHE:HZ	27:a:353:LEU:HD12	1.86	0.41
28:b:84:ILE:HD12	28:b:115:SER:HB2	2.03	0.41
29:c:251:LEU:HD11	29:c:283:HIS:CG	2.55	0.41
29:c:273:LYS:HZ2	29:c:274:ASN:HB2	1.86	0.41
29:c:273:LYS:NZ	29:c:274:ASN:HB2	2.36	0.41
30:d:9:TRP:HD1	30:d:61:TRP:HE1	1.68	0.41
19:s:4:PRO:HB3	20:t:103:MET:HE1	2.03	0.41
19:s:172:MET:HG3	19:s:176:LYS:HE3	2.01	0.41
5:E:382:SER:HB3	6:F:336:ASP:HA	2.02	0.41
10:J:121:SER:OG	10:J:122:ASN:N	2.54	0.41
10:J:220:LEU:HD22	10:J:220:LEU:HA	1.75	0.41
12:L:156:CYS:HB3	12:L:159:MET:HE3	2.02	0.41
24:X:329:ASN:HA	24:X:332:GLU:HG2	2.02	0.41
29:c:160:PHE:CE1	29:c:196:LEU:HD21	2.56	0.41
32:f:233:LEU:HD13	32:f:252:ALA:HB2	2.02	0.41
32:f:292:LYS:HD3	32:f:296:PHE:HE2	1.86	0.41
13:m:163:CYS:SG	13:m:164:ALA:N	2.94	0.41
1:A:111:TYR:HE2	1:A:125:LEU:HD23	1.85	0.40
2:B:407:LEU:HD21	3:C:178:LEU:HB2	2.03	0.40
8:H:203:MET:HG2	8:H:230:LEU:HD11	2.03	0.40
10:J:95:ARG:HH12	10:J:101:PRO:HG3	1.85	0.40
17:Q:35:MET:HE3	17:Q:181:ARG:HH11	1.85	0.40
24:X:62:GLN:N	24:X:62:GLN:OE1	2.53	0.40
25:Y:127:THR:O	25:Y:131:THR:OG1	2.30	0.40
25:Y:160:ASN:HA	25:Y:163:LYS:HB3	2.02	0.40
32:f:594:LEU:HB2	32:f:652:VAL:HG21	2.02	0.40
32:f:701:ASN:OD1	32:f:703:ARG:NE	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:PRO:HA	32:f:854:GLY:HA3	2.02	0.40
5:E:21:GLU:OE2	5:E:25:ARG:NH2	2.55	0.40
5:E:195:PHE:CE2	5:E:197:LYS:HB2	2.56	0.40
11:K:211:ASN:OD1	11:K:211:ASN:N	2.53	0.40
12:L:196:ARG:NH1	12:L:237:GLU:O	2.54	0.40
22:V:345:ARG:HH11	31:e:43:TRP:HB2	1.86	0.40
22:V:345:ARG:NH1	31:e:43:TRP:HB2	2.36	0.40
26:Z:116:CYS:O	26:Z:119:SER:OG	2.38	0.40
27:a:255:TRP:O	27:a:258:GLN:NE2	2.45	0.40
29:c:61:PHE:CE1	29:c:139:ARG:HD2	2.57	0.40
32:f:72:ARG:HE	32:f:118:ASN:HD21	1.69	0.40
10:j:226:GLU:HA	10:j:229:VAL:HG12	2.03	0.40
19:s:172:MET:HE2	19:s:172:MET:HB2	1.89	0.40
4:D:139:LEU:HD23	4:D:139:LEU:HA	1.87	0.40
5:E:173:TYR:CZ	5:E:300:HIS:HB2	2.57	0.40
8:H:204:THR:OG1	8:H:206:ASP:OD2	2.39	0.40
23:W:420:ASP:HB3	23:W:423:ASN:HB2	2.04	0.40
24:X:357:SER:OG	24:X:358:LYS:N	2.54	0.40
26:Z:43:TRP:HB3	26:Z:90:ARG:HH22	1.86	0.40
12:l:47:VAL:HG22	12:l:212:ILE:HG23	2.03	0.40
6:F:154:ASN:HD22	6:F:157:SER:HB3	1.86	0.40
6:F:178:ASP:HB3	6:F:179:GLU:H	1.77	0.40
7:G:113:MET:HE3	7:G:113:MET:HB2	1.95	0.40
17:Q:155:ARG:HH21	17:Q:158:GLU:HG3	1.86	0.40
22:V:61:GLU:O	22:V:64:GLN:HG3	2.21	0.40
23:W:455:LEU:HB2	23:W:456:GLN:NE2	2.36	0.40
32:f:368:ALA:HA	32:f:371:ASN:OD1	2.21	0.40
8:h:163:MET:SD	8:h:163:MET:N	2.94	0.40
19:s:92:LEU:HA	19:s:95:ILE:HG22	2.03	0.40
2:B:106:PRO:HB2	2:B:154:HIS:CE1	2.57	0.40
3:C:80:MET:SD	3:C:80:MET:N	2.95	0.40
6:F:410:ARG:HG3	6:F:412:ALA:H	1.87	0.40
7:G:10:ASP:HA	7:G:15:ILE:HG13	2.04	0.40
9:I:48:GLU:O	9:I:64:LYS:NZ	2.44	0.40
21:U:137:MET:HA	21:U:140:ARG:HB2	2.03	0.40
26:Z:22:HIS:HA	26:Z:25:ARG:HB2	2.03	0.40
26:Z:98:GLY:HA2	26:Z:99:PRO:HD3	1.93	0.40
12:l:144:ILE:HG22	12:l:156:CYS:HB2	2.04	0.40
18:r:77:ALA:HB2	18:r:107:ARG:HH12	1.86	0.40
20:t:51:LEU:HD11	20:t:110:MET:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	400/433 (92%)	352 (88%)	45 (11%)	3 (1%)	16	52
2	B	397/440 (90%)	354 (89%)	42 (11%)	1 (0%)	36	71
3	C	394/398 (99%)	349 (89%)	45 (11%)	0	100	100
4	D	378/418 (90%)	334 (88%)	44 (12%)	0	100	100
5	E	387/403 (96%)	342 (88%)	41 (11%)	4 (1%)	12	47
6	F	391/439 (89%)	355 (91%)	35 (9%)	1 (0%)	36	71
7	G	242/246 (98%)	229 (95%)	13 (5%)	0	100	100
7	g	242/246 (98%)	223 (92%)	16 (7%)	3 (1%)	10	42
8	H	230/234 (98%)	216 (94%)	14 (6%)	0	100	100
8	h	230/234 (98%)	219 (95%)	11 (5%)	0	100	100
9	I	248/261 (95%)	240 (97%)	6 (2%)	2 (1%)	16	52
9	i	248/261 (95%)	242 (98%)	6 (2%)	0	100	100
10	J	237/248 (96%)	229 (97%)	8 (3%)	0	100	100
10	j	237/248 (96%)	219 (92%)	18 (8%)	0	100	100
11	K	232/241 (96%)	220 (95%)	11 (5%)	1 (0%)	30	66
11	k	232/241 (96%)	223 (96%)	9 (4%)	0	100	100
12	L	236/263 (90%)	226 (96%)	10 (4%)	0	100	100
12	l	236/263 (90%)	222 (94%)	14 (6%)	0	100	100
13	M	238/255 (93%)	230 (97%)	8 (3%)	0	100	100
13	m	238/255 (93%)	234 (98%)	4 (2%)	0	100	100
14	N	200/239 (84%)	196 (98%)	4 (2%)	0	100	100
14	n	200/239 (84%)	194 (97%)	6 (3%)	0	100	100
15	O	218/277 (79%)	209 (96%)	9 (4%)	0	100	100
15	o	218/277 (79%)	212 (97%)	6 (3%)	0	100	100
16	P	202/205 (98%)	192 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	p	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
17	Q	197/201 (98%)	189 (96%)	8 (4%)	0	100	100
17	q	197/201 (98%)	190 (96%)	7 (4%)	0	100	100
18	R	199/263 (76%)	193 (97%)	6 (3%)	0	100	100
18	r	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
19	S	211/241 (88%)	202 (96%)	9 (4%)	0	100	100
19	s	211/241 (88%)	202 (96%)	9 (4%)	0	100	100
20	T	214/264 (81%)	209 (98%)	5 (2%)	0	100	100
20	t	214/264 (81%)	202 (94%)	12 (6%)	0	100	100
21	U	874/953 (92%)	814 (93%)	59 (7%)	1 (0%)	48	83
22	V	442/534 (83%)	417 (94%)	23 (5%)	2 (0%)	24	62
23	W	439/456 (96%)	421 (96%)	17 (4%)	1 (0%)	43	77
24	X	420/422 (100%)	395 (94%)	22 (5%)	3 (1%)	18	55
25	Y	387/389 (100%)	359 (93%)	28 (7%)	0	100	100
26	Z	284/324 (88%)	249 (88%)	33 (12%)	2 (1%)	18	55
27	a	371/376 (99%)	336 (91%)	34 (9%)	1 (0%)	36	71
28	b	189/377 (50%)	173 (92%)	16 (8%)	0	100	100
29	c	285/310 (92%)	242 (85%)	40 (14%)	3 (1%)	11	45
30	d	255/350 (73%)	220 (86%)	33 (13%)	2 (1%)	16	52
31	e	48/70 (69%)	43 (90%)	5 (10%)	0	100	100
32	f	840/908 (92%)	799 (95%)	41 (5%)	0	100	100
33	u	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
All	All	13463/14952 (90%)	12571 (93%)	862 (6%)	30 (0%)	44	77

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	PRO
2	B	87	PRO
5	E	249	ALA
9	I	54	LYS
24	X	318	ILE
5	E	84	ARG
5	E	127	PRO

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Mol	Chain	Res	Type
5	E	248	SER
23	W	199	TYR
29	c	272	ILE
7	g	4	GLY
1	A	160	THR
6	F	165	PRO
9	I	53	HIS
22	V	356	SER
24	X	108	GLU
26	Z	145	HIS
26	Z	146	ASP
27	a	69	HIS
29	c	198	ARG
30	d	255	MET
1	A	285	PHE
11	K	130	PRO
22	V	353	LEU
7	g	5	SER
24	X	105	GLN
29	c	271	ALA
7	g	7	ALA
21	U	870	GLU
30	d	256	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/372 (91%)	335 (99%)	4 (1%)	63	73
2	B	349/385 (91%)	345 (99%)	4 (1%)	65	74
3	C	340/346 (98%)	339 (100%)	1 (0%)	86	84
4	D	333/366 (91%)	331 (99%)	2 (1%)	78	80
5	E	341/353 (97%)	339 (99%)	2 (1%)	78	80
6	F	340/379 (90%)	338 (99%)	2 (1%)	78	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	205/210 (98%)	205 (100%)	0	100	100
7	g	202/210 (96%)	202 (100%)	0	100	100
8	H	188/191 (98%)	188 (100%)	0	100	100
8	h	188/191 (98%)	186 (99%)	2 (1%)	65	74
9	I	206/221 (93%)	204 (99%)	2 (1%)	68	76
9	i	206/221 (93%)	206 (100%)	0	100	100
10	J	201/211 (95%)	198 (98%)	3 (2%)	57	70
10	j	196/211 (93%)	196 (100%)	0	100	100
11	K	193/203 (95%)	193 (100%)	0	100	100
11	k	195/203 (96%)	195 (100%)	0	100	100
12	L	202/224 (90%)	201 (100%)	1 (0%)	81	81
12	l	201/224 (90%)	200 (100%)	1 (0%)	81	81
13	M	196/212 (92%)	196 (100%)	0	100	100
13	m	198/212 (93%)	198 (100%)	0	100	100
14	N	157/181 (87%)	157 (100%)	0	100	100
14	n	156/181 (86%)	156 (100%)	0	100	100
15	O	179/228 (78%)	179 (100%)	0	100	100
15	o	181/228 (79%)	181 (100%)	0	100	100
16	P	172/174 (99%)	172 (100%)	0	100	100
16	p	173/174 (99%)	173 (100%)	0	100	100
17	Q	168/171 (98%)	168 (100%)	0	100	100
17	q	168/171 (98%)	168 (100%)	0	100	100
18	R	156/202 (77%)	156 (100%)	0	100	100
18	r	156/202 (77%)	156 (100%)	0	100	100
19	S	175/199 (88%)	175 (100%)	0	100	100
19	s	178/199 (89%)	178 (100%)	0	100	100
20	T	178/215 (83%)	178 (100%)	0	100	100
20	t	179/215 (83%)	179 (100%)	0	100	100
21	U	752/816 (92%)	751 (100%)	1 (0%)	88	88
22	V	390/460 (85%)	387 (99%)	3 (1%)	73	77
23	W	406/416 (98%)	402 (99%)	4 (1%)	68	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	X	362/362 (100%)	358 (99%)	4 (1%)	65	74
25	Y	344/344 (100%)	343 (100%)	1 (0%)	86	84
26	Z	257/295 (87%)	256 (100%)	1 (0%)	84	82
27	a	333/336 (99%)	332 (100%)	1 (0%)	86	84
28	b	167/312 (54%)	167 (100%)	0	100	100
29	c	252/268 (94%)	247 (98%)	5 (2%)	48	66
30	d	231/294 (79%)	229 (99%)	2 (1%)	70	76
31	e	44/63 (70%)	44 (100%)	0	100	100
32	f	711/763 (93%)	707 (99%)	4 (1%)	78	80
33	u	68/68 (100%)	68 (100%)	0	100	100
All	All	11512/12682 (91%)	11462 (100%)	50 (0%)	81	82

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	ILE
1	A	159	PRO
1	A	284	ARG
1	A	373	LEU
2	B	87	PRO
2	B	88	LEU
2	B	125	THR
2	B	322	ARG
3	C	113	ARG
4	D	149	SER
4	D	150	SER
5	E	84	ARG
5	E	364	GLN
6	F	300	LYS
6	F	343	LEU
9	I	54	LYS
9	I	55	LEU
10	J	219	ILE
10	J	220	LEU
10	J	221	ASN
12	L	33	SER
21	U	118	LEU
22	V	198	GLN

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Mol	Chain	Res	Type
22	V	353	LEU
22	V	355	ARG
23	W	55	ARG
23	W	198	ASP
23	W	265	GLN
23	W	455	LEU
24	X	105	GLN
24	X	106	GLU
24	X	318	ILE
24	X	319	ILE
25	Y	357	ASN
26	Z	103	LYS
27	a	188	LEU
29	c	185	ASN
29	c	197	ASN
29	c	270	LEU
29	c	272	ILE
29	c	273	LYS
30	d	199	PHE
30	d	256	ILE
32	f	371	ASN
32	f	502	LEU
32	f	566	HIS
32	f	754	LYS
8	h	3	GLU
8	h	4	ARG
12	l	33	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	148	GLN
1	A	203	ASN
1	A	296	GLN
2	B	82	GLN
2	B	154	HIS
2	B	181	GLN
2	B	193	GLN
3	C	205	HIS
3	C	221	GLN
4	D	57	GLN

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Mol	Chain	Res	Type
4	D	67	ASN
4	D	257	ASN
5	E	45	ASN
5	E	124	HIS
5	E	155	ASN
5	E	263	GLN
5	E	300	HIS
5	E	307	GLN
6	F	92	ASN
6	F	130	GLN
6	F	243	GLN
6	F	315	ASN
6	F	325	GLN
6	F	428	GLN
7	G	12	HIS
7	G	33	ASN
7	G	90	GLN
7	G	128	ASN
8	H	71	HIS
8	H	88	HIS
9	I	95	GLN
9	I	102	GLN
9	I	146	GLN
10	J	54	GLN
10	J	92	GLN
10	J	175	ASN
11	K	73	HIS
11	K	97	GLN
12	L	5	GLN
12	L	69	HIS
14	N	154	GLN
16	P	18	ASN
16	P	93	ASN
16	P	145	GLN
17	Q	82	ASN
17	Q	110	HIS
17	Q	168	GLN
18	R	162	GLN
19	S	58	HIS
21	U	58	GLN
21	U	267	ASN
21	U	355	ASN

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Mol	Chain	Res	Type
21	U	415	HIS
21	U	475	HIS
21	U	491	GLN
21	U	527	GLN
21	U	665	ASN
21	U	685	GLN
21	U	718	ASN
22	V	193	GLN
22	V	260	HIS
22	V	282	ASN
22	V	478	GLN
23	W	361	HIS
23	W	426	ASN
24	X	105	GLN
24	X	213	GLN
24	X	367	GLN
24	X	405	GLN
25	Y	71	ASN
25	Y	136	HIS
25	Y	363	ASN
26	Z	24	ASN
26	Z	102	HIS
26	Z	109	ASN
26	Z	145	HIS
27	a	52	GLN
27	a	62	ASN
27	a	164	GLN
27	a	194	GLN
28	b	27	GLN
28	b	76	HIS
28	b	161	ASN
29	c	77	GLN
29	c	130	GLN
29	c	197	ASN
29	c	219	ASN
29	c	237	HIS
29	c	278	GLN
29	c	283	HIS
32	f	245	ASN
32	f	325	GLN
32	f	371	ASN
32	f	493	ASN

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Mol	Chain	Res	Type
32	f	531	ASN
32	f	565	ASN
32	f	566	HIS
32	f	650	GLN
32	f	750	GLN
32	f	848	GLN
9	i	40	ASN
9	i	167	ASN
10	j	154	HIS
10	j	175	ASN
11	k	41	GLN
11	k	73	HIS
11	k	224	GLN
12	l	59	HIS
12	l	175	HIS
13	m	72	HIS
14	n	7	GLN
15	o	165	ASN
17	q	82	ASN
17	q	99	HIS
17	q	101	ASN
18	r	29	GLN
18	r	85	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	ADP	A	501	-	27,29,29	1.36	4 (14%)	42,45,45	1.98	10 (23%)
35	ADP	F	501	-	27,29,29	1.35	4 (14%)	42,45,45	2.08	9 (21%)
36	ATP	C	501	37	29,33,33	0.30	0	44,52,52	0.48	1 (2%)
36	ATP	D	501	37	29,33,33	0.32	0	44,52,52	0.54	1 (2%)
36	ATP	E	401	37	29,33,33	0.33	0	44,52,52	0.55	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ADP	A	501	-	-	5/16/32/32	0/3/3/3
35	ADP	F	501	-	-	1/16/32/32	0/3/3/3
36	ATP	C	501	37	-	4/22/38/38	0/3/3/3
36	ATP	D	501	37	-	7/22/38/38	0/3/3/3
36	ATP	E	401	37	-	9/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A	501	ADP	C5-C4	4.59	1.47	1.39
35	F	501	ADP	C5-C4	4.57	1.47	1.39
35	A	501	ADP	C5-C6	2.66	1.48	1.41
35	F	501	ADP	C5-C6	2.54	1.48	1.41
35	F	501	ADP	C5-N7	-2.50	1.34	1.39
35	A	501	ADP	C8-N7	2.31	1.36	1.31
35	F	501	ADP	C8-N7	2.22	1.35	1.31
35	A	501	ADP	C5-N7	-2.18	1.34	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	F	501	ADP	C5-C4-N3	-6.97	117.66	126.75
35	A	501	ADP	C5-C4-N3	-6.30	118.53	126.75
35	F	501	ADP	N3-C4-N9	5.59	136.29	127.08
35	A	501	ADP	N3-C4-N9	5.06	135.41	127.08
35	F	501	ADP	C2-N3-C4	4.02	121.25	111.75
35	A	501	ADP	C2-N3-C4	3.95	121.08	111.75
35	A	501	ADP	PA-O3A-PB	-3.63	120.38	132.83
35	F	501	ADP	PA-O3A-PB	-3.27	121.61	132.83
35	A	501	ADP	N3-C2-N1	-3.20	123.59	128.60
35	F	501	ADP	C4-C5-N7	-3.11	106.83	110.62
35	A	501	ADP	C4-C5-N7	-3.08	106.87	110.62
35	F	501	ADP	N3-C2-N1	-3.05	123.83	128.60
35	F	501	ADP	C3'-C2'-C1'	3.04	107.20	101.43
35	F	501	ADP	C5-N7-C8	2.88	107.61	103.51
35	A	501	ADP	C5-N7-C8	2.61	107.21	103.51
35	A	501	ADP	C4-N9-C8	2.54	108.48	105.73
35	A	501	ADP	C3'-C2'-C1'	2.25	105.71	101.43
35	F	501	ADP	C4-N9-C8	2.22	108.13	105.73
35	A	501	ADP	C6-C5-N7	2.05	135.84	132.02
36	C	501	ATP	PB-O3B-PG	2.01	139.74	132.83
36	D	501	ATP	PB-O3B-PG	2.01	139.71	132.83
36	E	401	ATP	PB-O3B-PG	2.00	139.71	132.83

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	A	501	ADP	C5'-O5'-PA-O1A
35	A	501	ADP	O4'-C4'-C5'-O5'
36	D	501	ATP	C5'-O5'-PA-O2A
36	E	401	ATP	C5'-O5'-PA-O1A
36	E	401	ATP	C5'-O5'-PA-O2A
36	E	401	ATP	O4'-C4'-C5'-O5'
36	E	401	ATP	C3'-C4'-C5'-O5'
35	A	501	ADP	C3'-C4'-C5'-O5'
36	D	501	ATP	PG-O3B-PB-O3A
36	E	401	ATP	C4'-C5'-O5'-PA
36	E	401	ATP	PB-O3B-PG-O1G
36	D	501	ATP	C5'-O5'-PA-O3A
36	C	501	ATP	PB-O3A-PA-O2A
35	A	501	ADP	C5'-O5'-PA-O2A
36	D	501	ATP	C5'-O5'-PA-O1A
36	D	501	ATP	PA-O3A-PB-O2B

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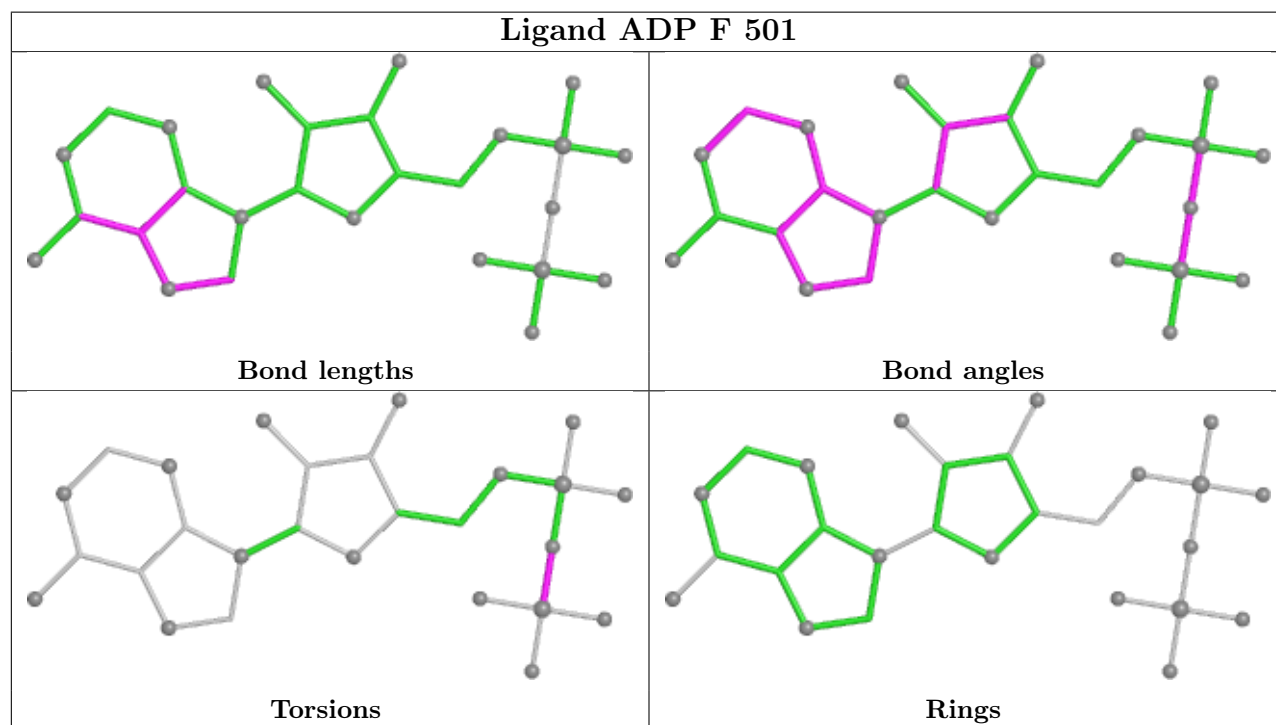
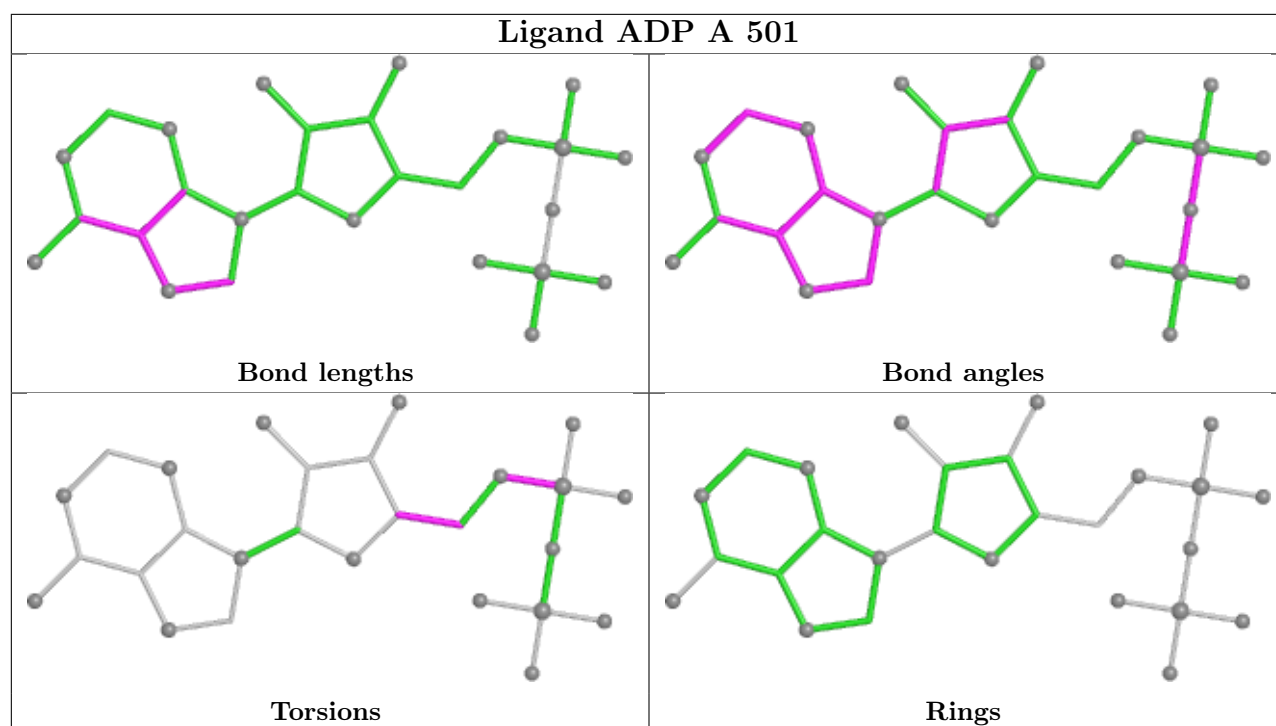
Mol	Chain	Res	Type	Atoms
36	C	501	ATP	C4'-C5'-O5'-PA
35	F	501	ADP	PA-O3A-PB-O1B
36	E	401	ATP	PB-O3B-PG-O2G
36	E	401	ATP	PB-O3B-PG-O3G
35	A	501	ADP	C5'-O5'-PA-O3A
36	E	401	ATP	C5'-O5'-PA-O3A
36	C	501	ATP	PB-O3A-PA-O1A
36	D	501	ATP	PG-O3B-PB-O1B
36	D	501	ATP	PA-O3A-PB-O1B
36	C	501	ATP	C5'-O5'-PA-O1A

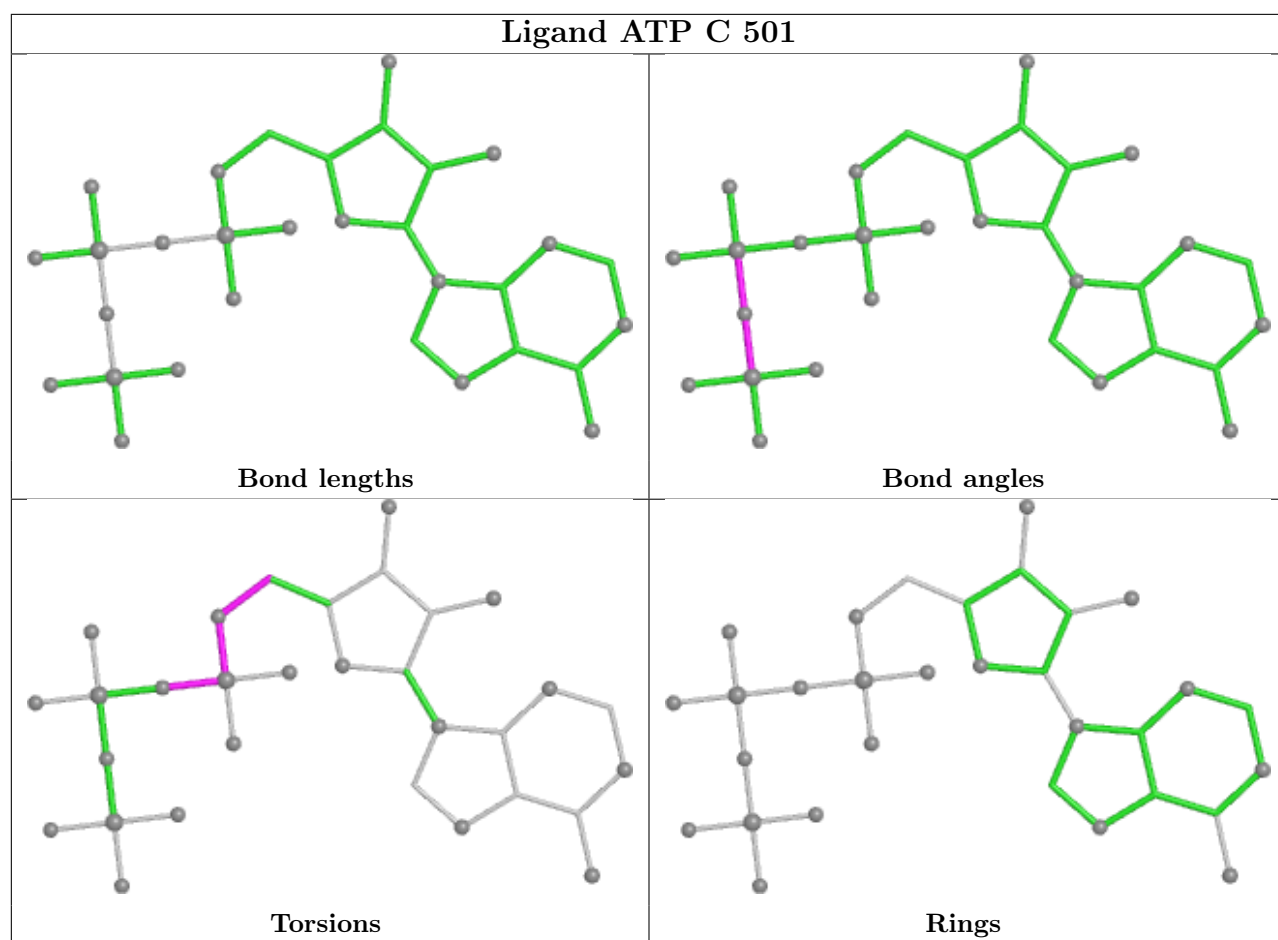
There are no ring outliers.

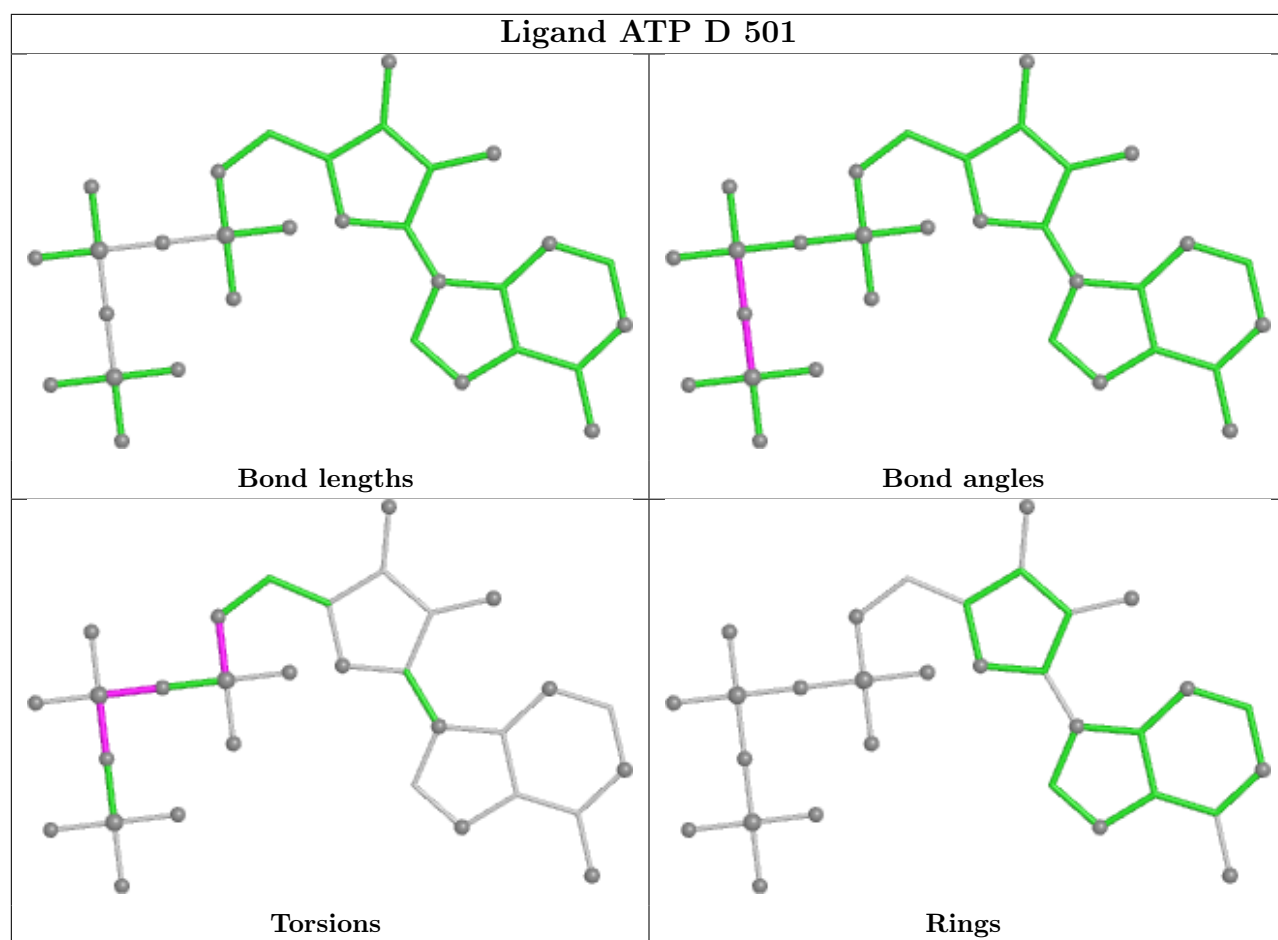
5 monomers are involved in 14 short contacts:

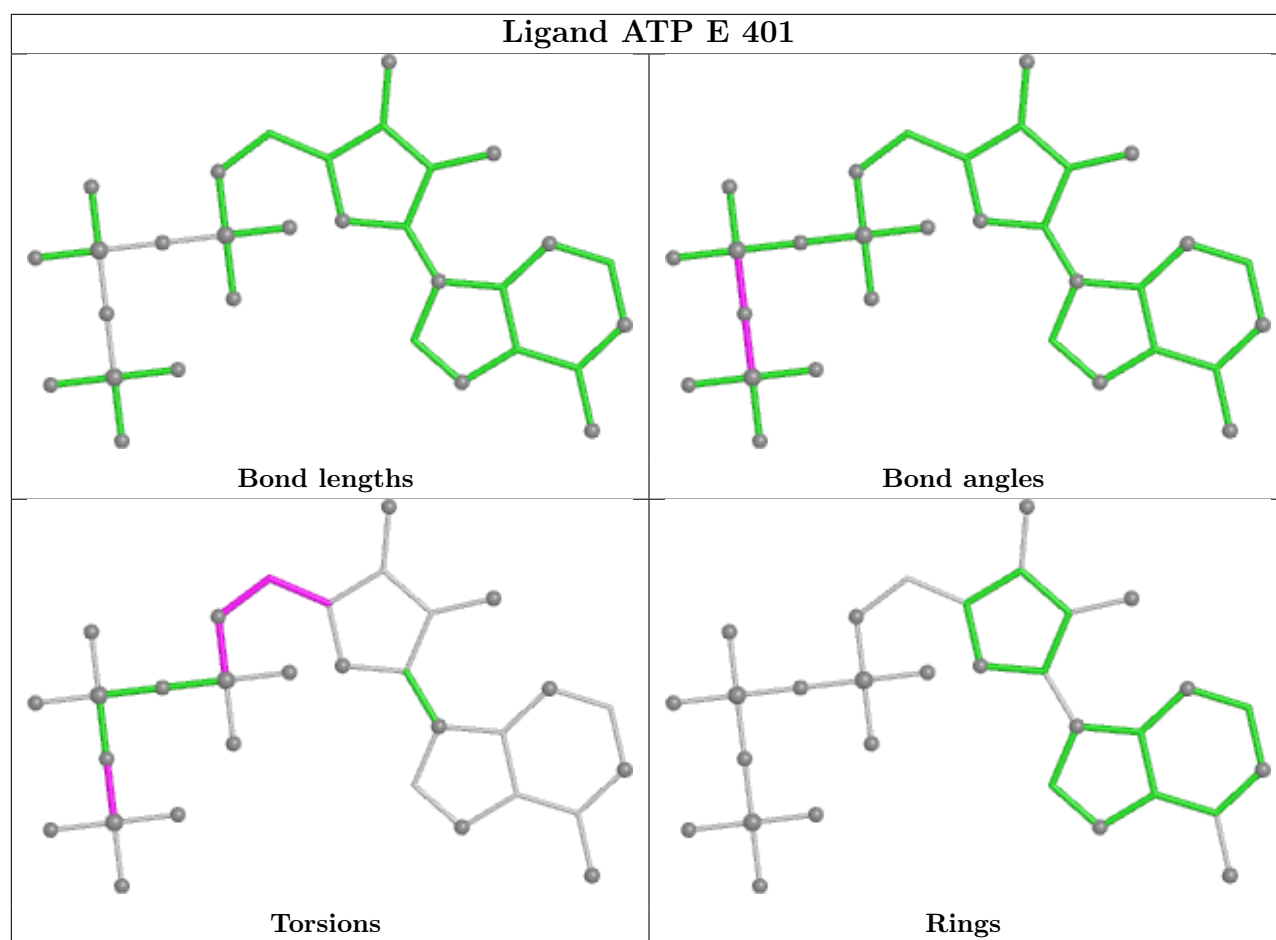
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	A	501	ADP	2	0
35	F	501	ADP	3	0
36	C	501	ATP	2	0
36	D	501	ATP	5	0
36	E	401	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

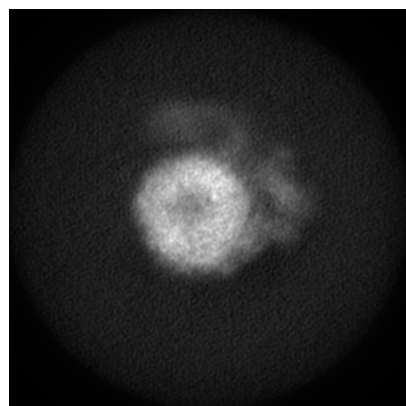
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62085. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

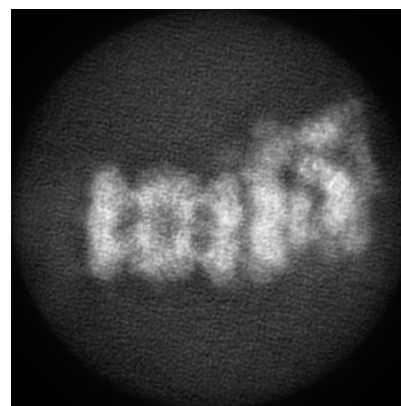
6.1.1 Primary map



X

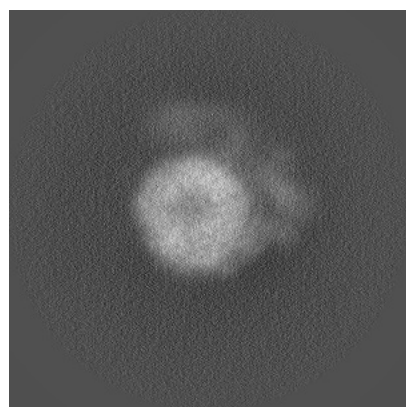


Y

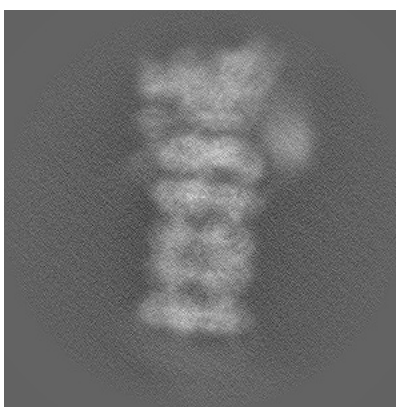


Z

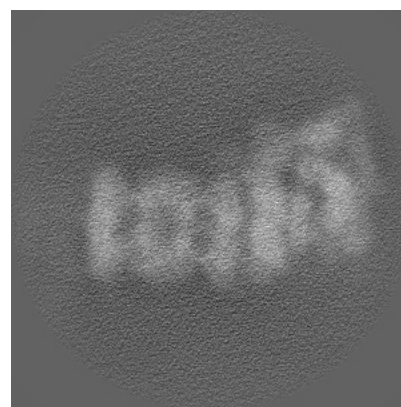
6.1.2 Raw map



X



Y

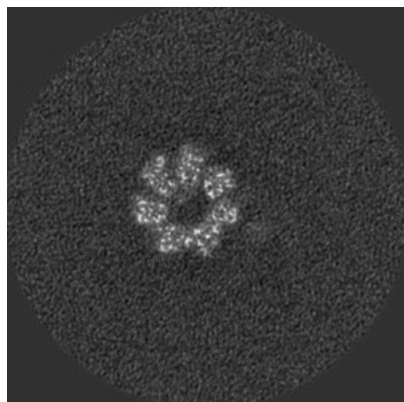


Z

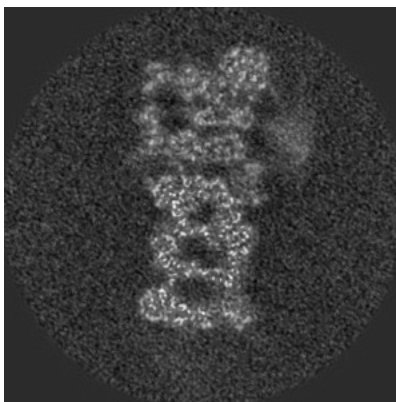
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

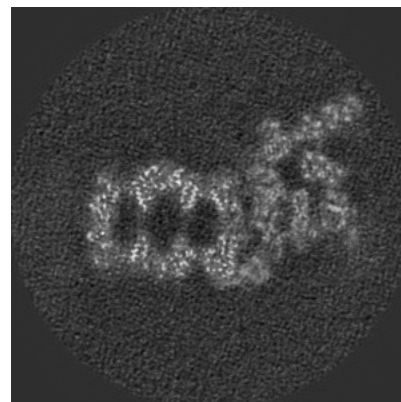
6.2.1 Primary map



X Index: 300

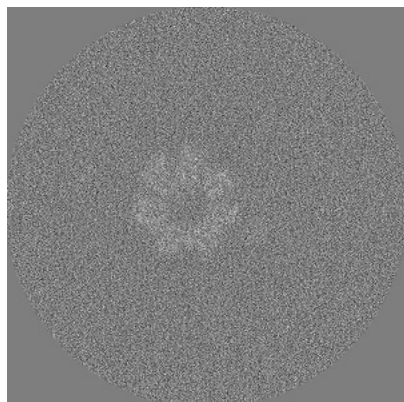


Y Index: 300

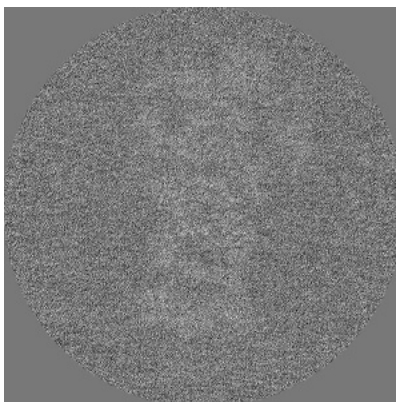


Z Index: 300

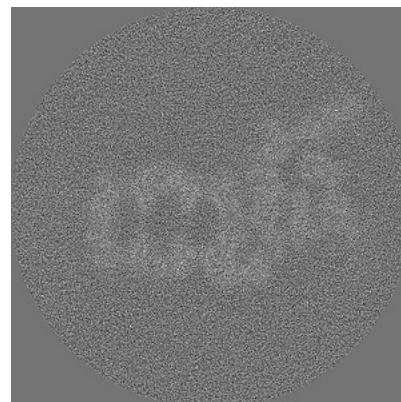
6.2.2 Raw map



X Index: 300



Y Index: 300

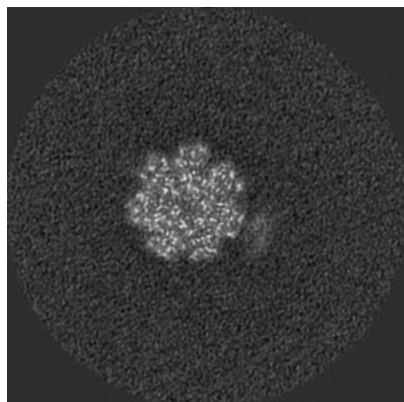


Z Index: 300

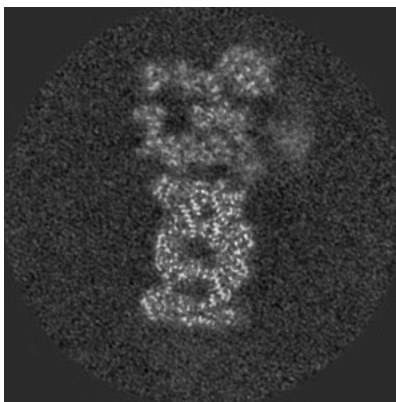
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

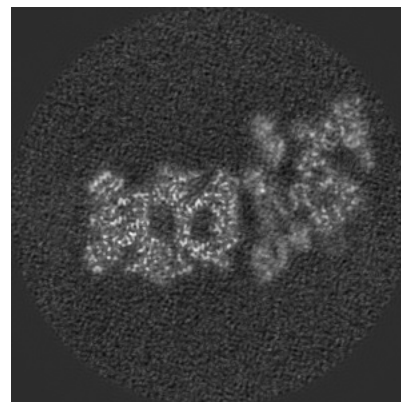
6.3.1 Primary map



X Index: 316

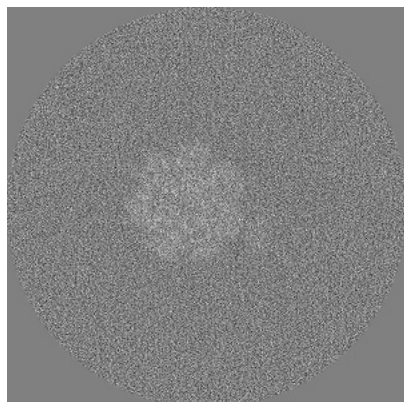


Y Index: 309

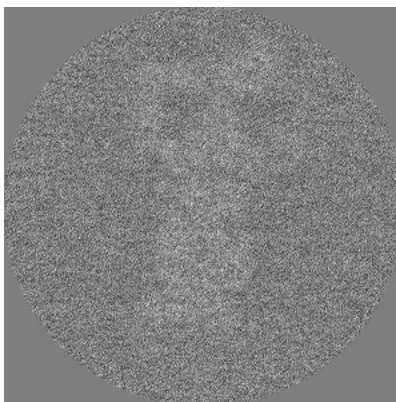


Z Index: 328

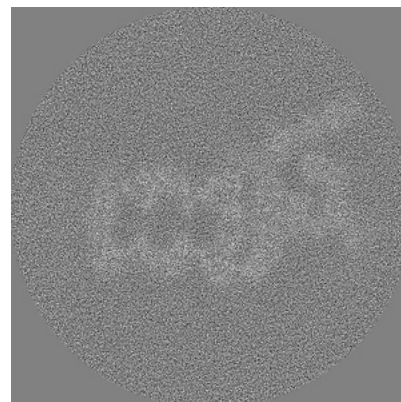
6.3.2 Raw map



X Index: 316



Y Index: 320

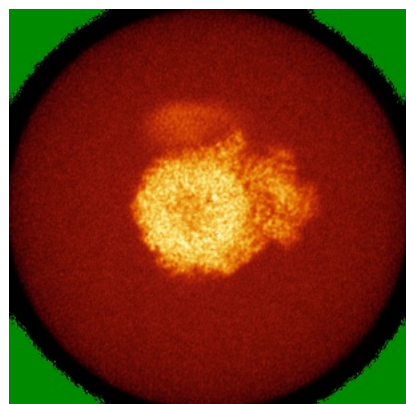


Z Index: 293

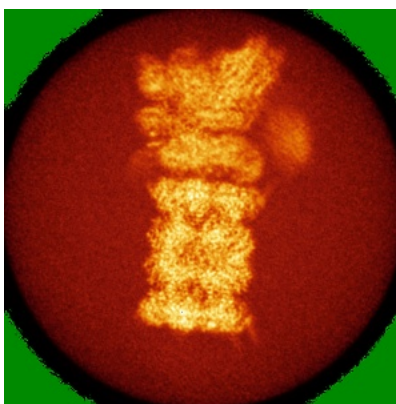
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

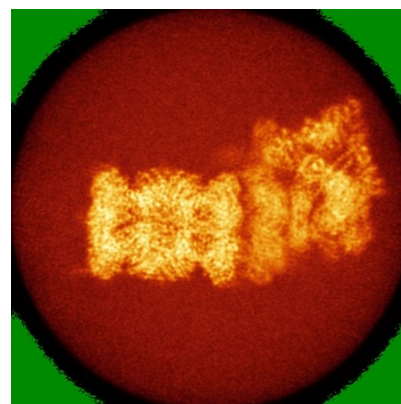
6.4.1 Primary map



X

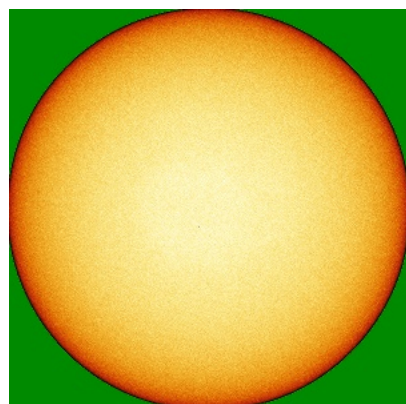


Y

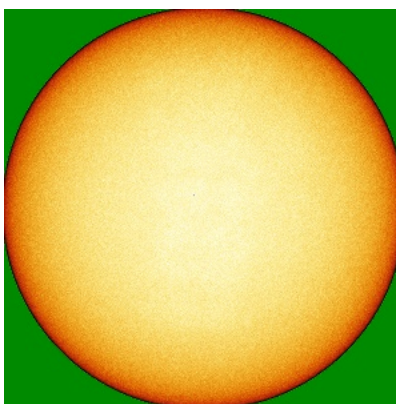


Z

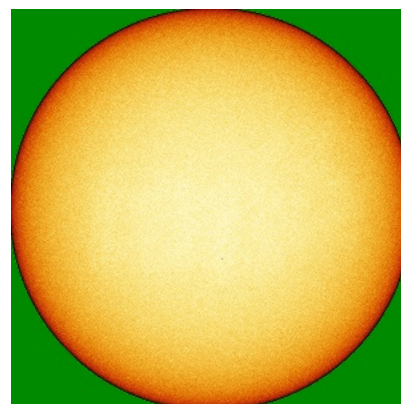
6.4.2 Raw map



X



Y

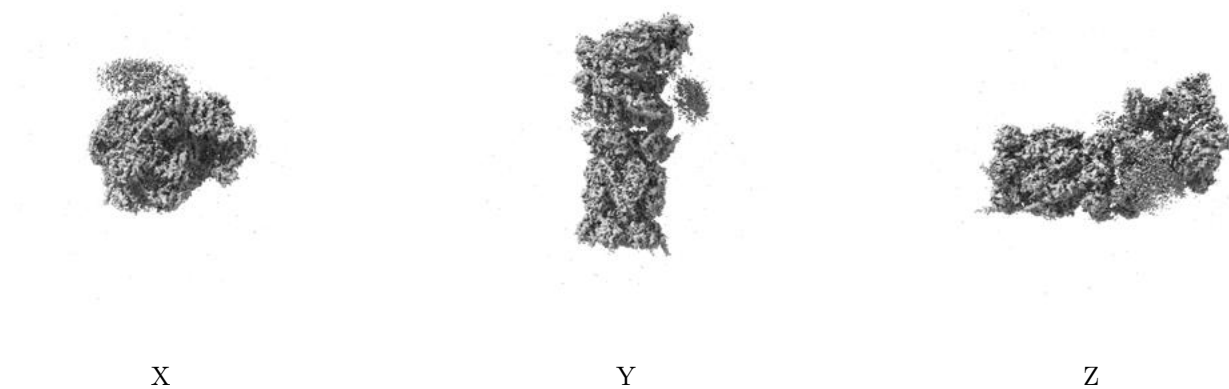


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

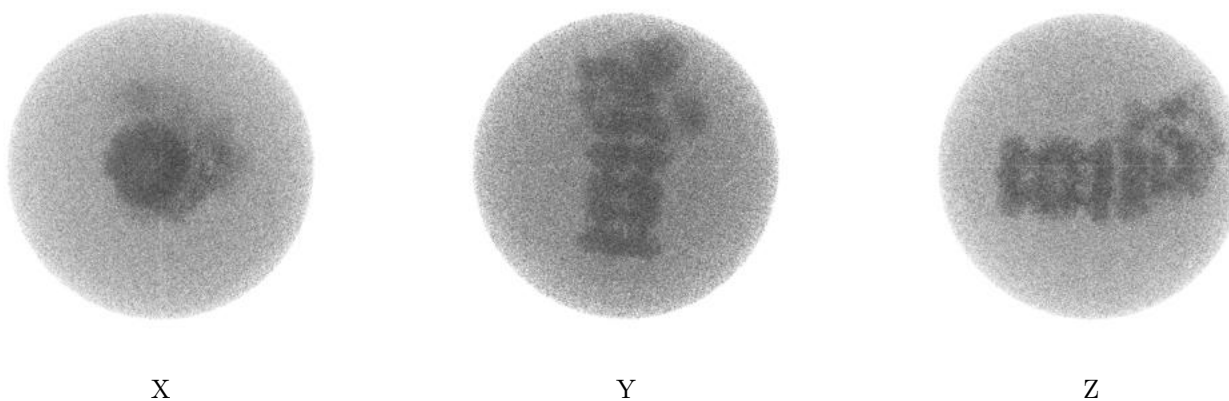
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00636. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

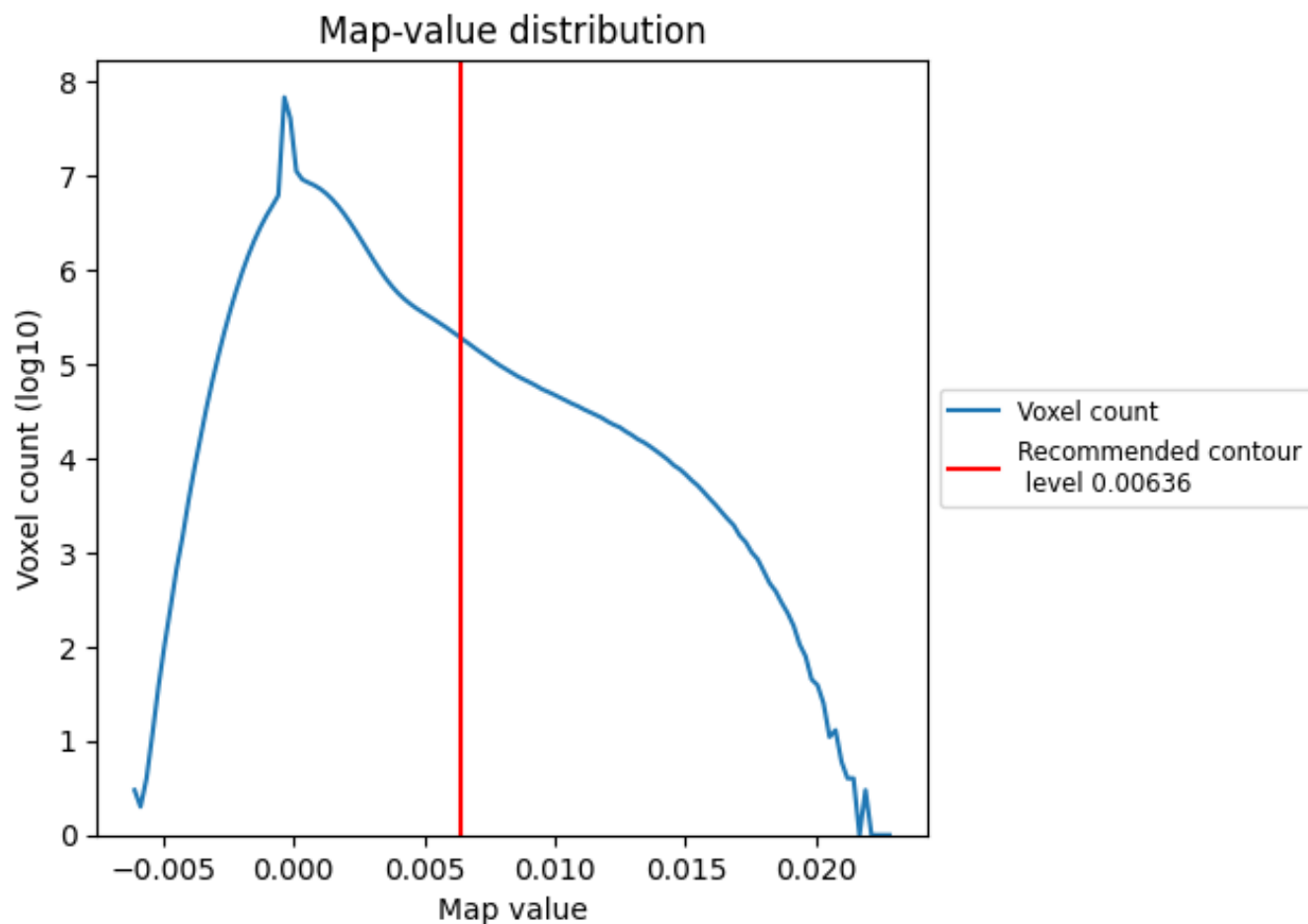
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

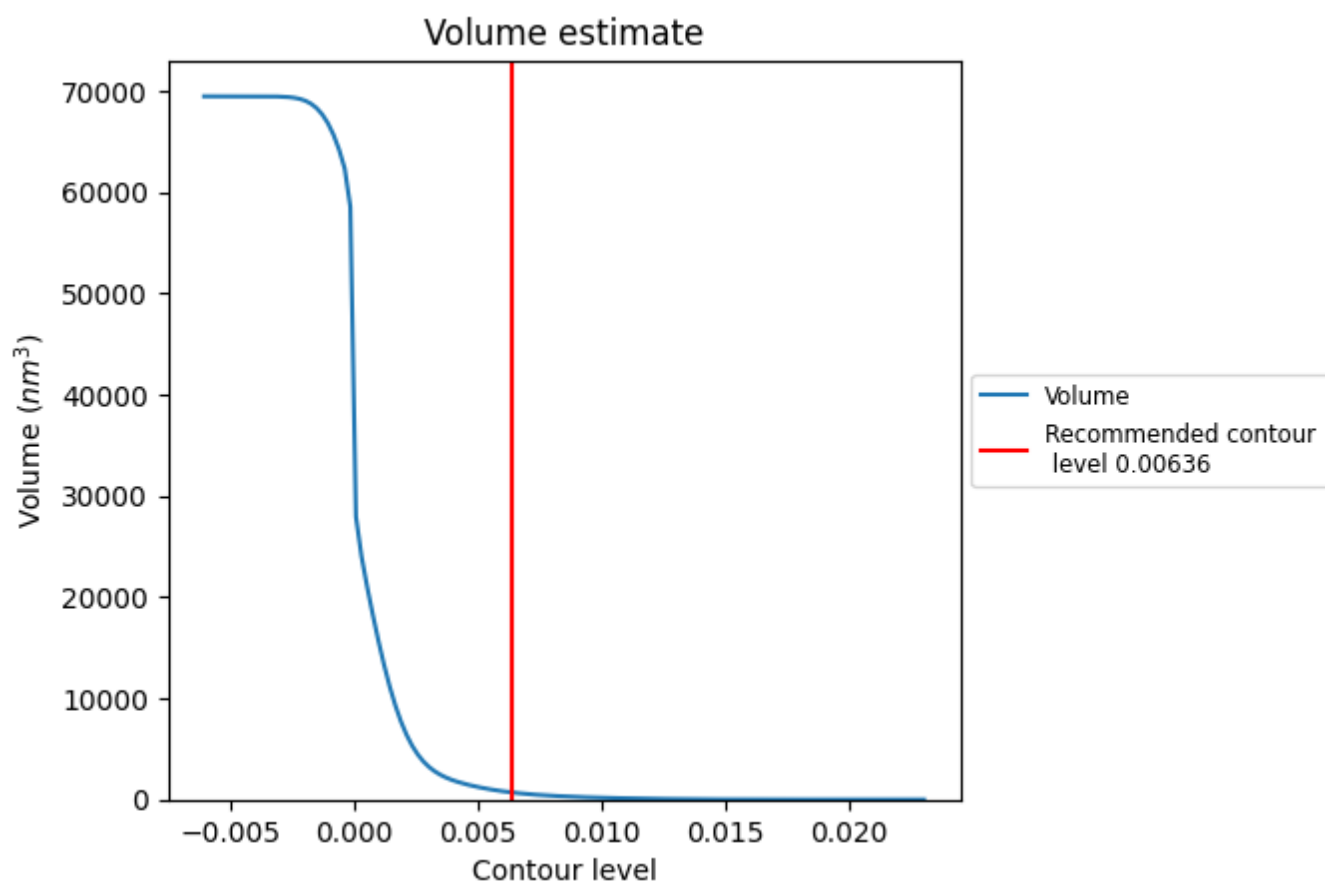
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

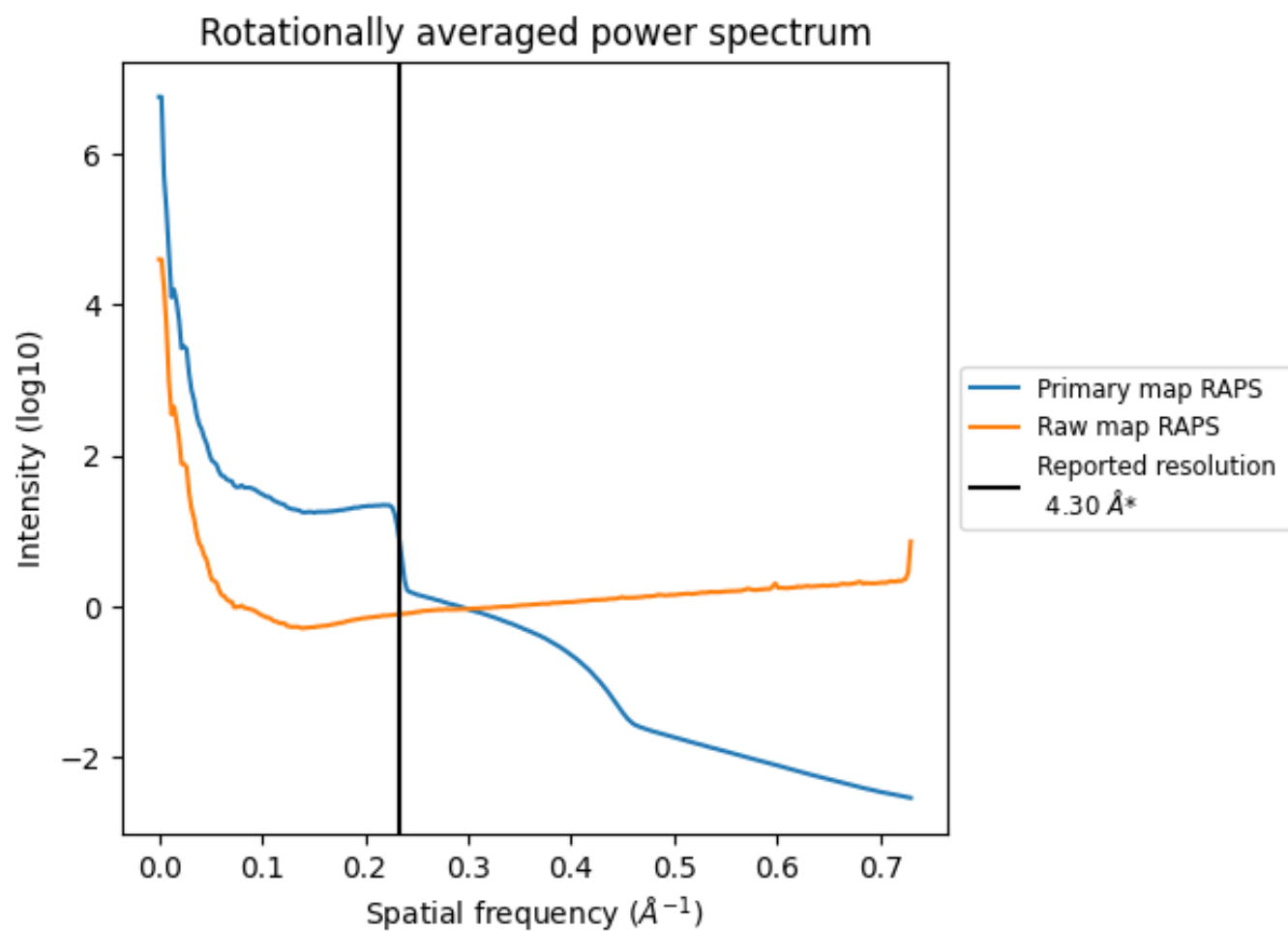
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 704 nm³; this corresponds to an approximate mass of 636 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

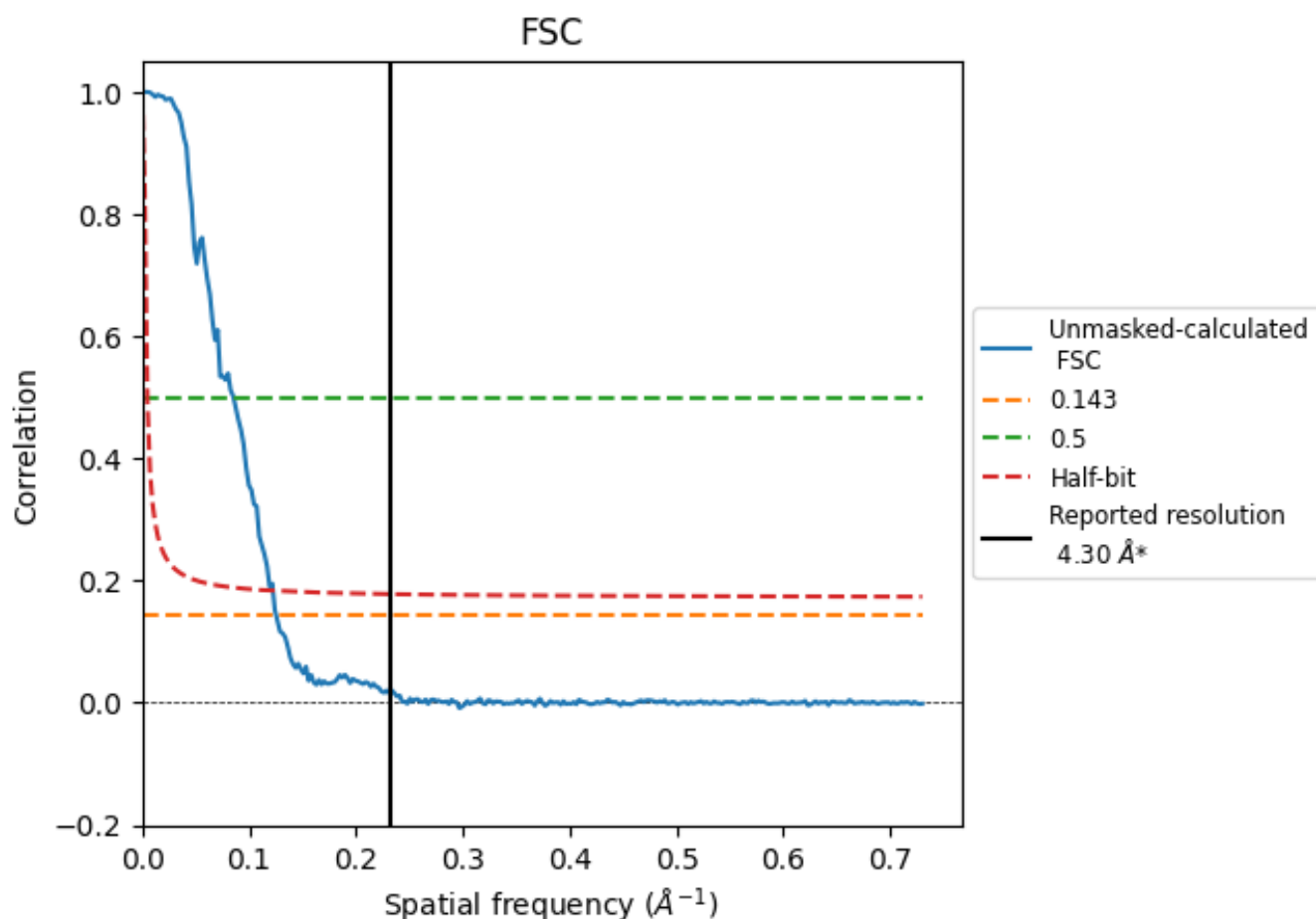


*Reported resolution corresponds to spatial frequency of 0.233 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.233 \AA^{-1}

8.2 Resolution estimates [i](#)

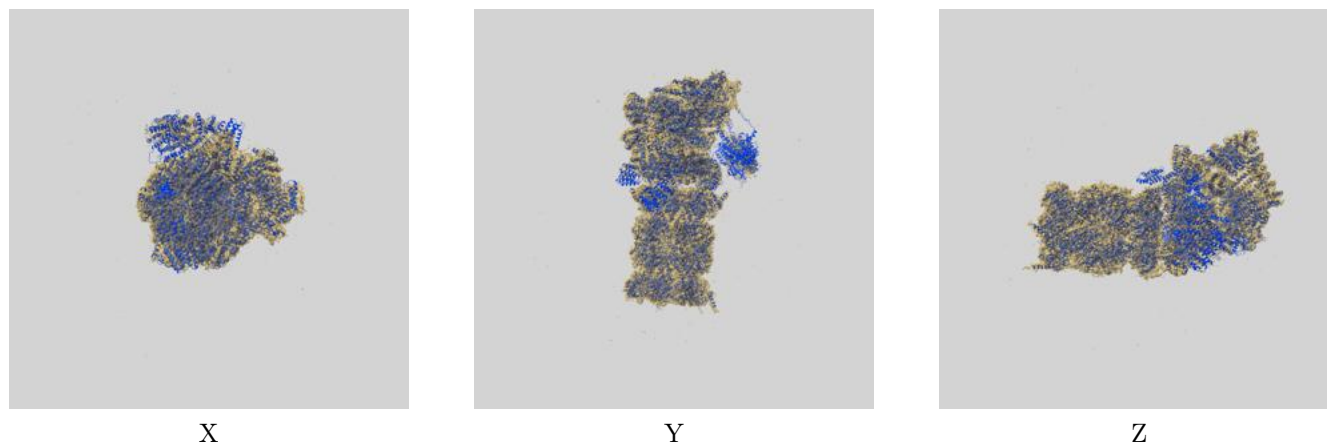
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.98	11.72	8.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.98 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

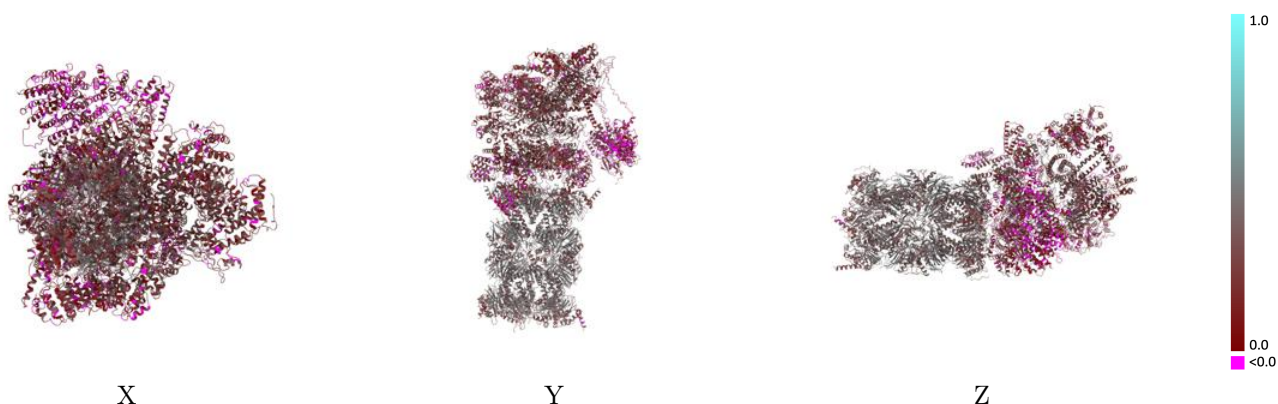
This section contains information regarding the fit between EMDB map EMD-62085 and PDB model 9K59. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



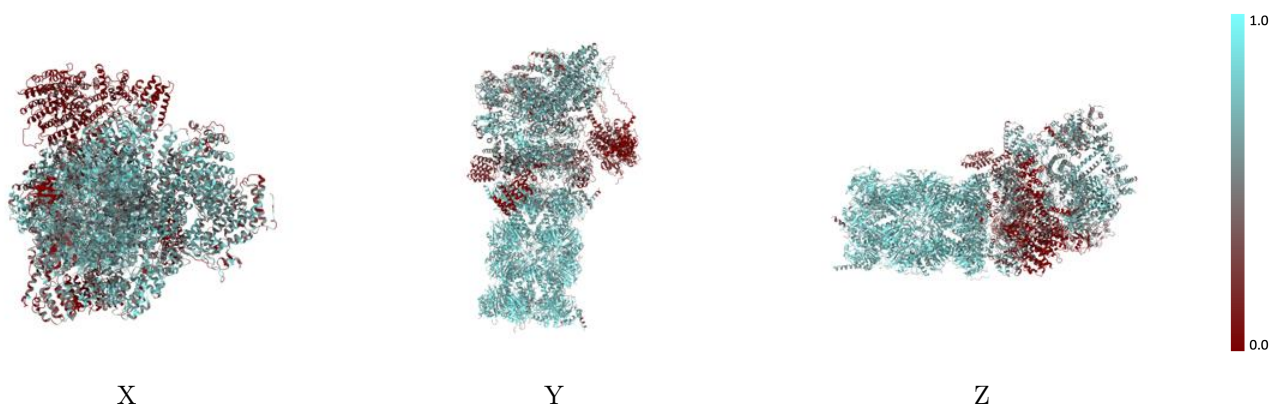
The images above show the 3D surface view of the map at the recommended contour level 0.00636 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



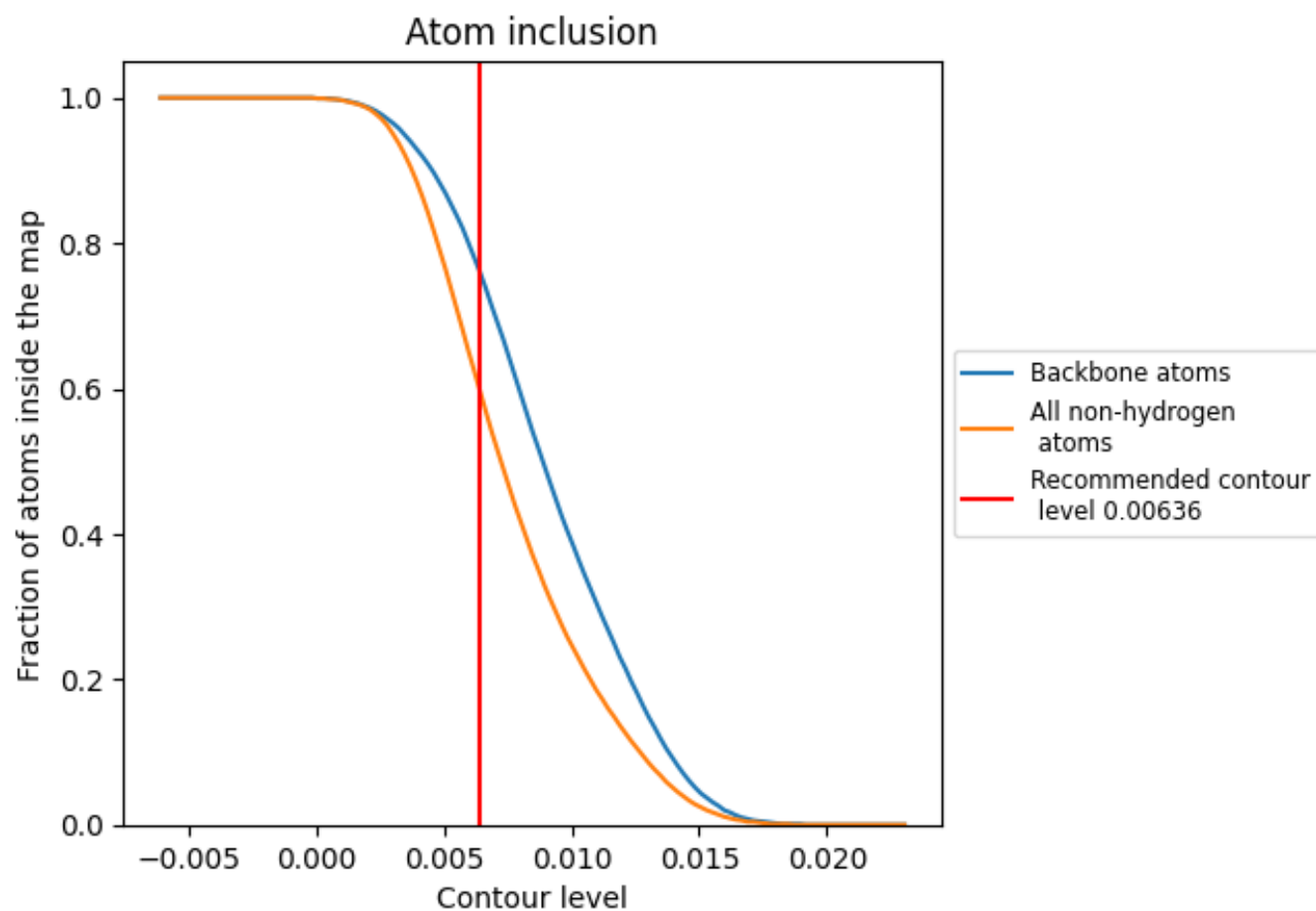
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00636).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





























The table lists the average atom inclusion at the recommended contour level (0.00636) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6030	 0.2980
A	 0.4160	 0.1870
B	 0.2890	 0.1680
C	 0.5000	 0.2570
D	 0.5930	 0.2720
E	 0.6050	 0.2810
F	 0.5400	 0.2510
G	 0.7570	 0.3880
H	 0.7790	 0.3860
I	 0.7180	 0.3640
J	 0.6930	 0.3470
K	 0.7270	 0.3700
L	 0.7940	 0.3870
M	 0.7790	 0.3760
N	 0.8040	 0.4040
O	 0.8020	 0.3930
P	 0.8140	 0.4120
Q	 0.8010	 0.3960
R	 0.8250	 0.4090
S	 0.7830	 0.4060
T	 0.8410	 0.4080
U	 0.5870	 0.2500
V	 0.5670	 0.2560
W	 0.4160	 0.2250
X	 0.2980	 0.2040
Y	 0.6050	 0.2650
Z	 0.5830	 0.2680
a	 0.5370	 0.2070
b	 0.4000	 0.2010
c	 0.5980	 0.2950
d	 0.4660	 0.2030
e	 0.4460	 0.2470
f	 0.0660	 0.0940
g	 0.7900	 0.3780
h	 0.8010	 0.3760



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Chain	Atom inclusion	Q-score
i	 0.7580	 0.3710
j	 0.7480	 0.3630
k	 0.7550	 0.3730
l	 0.7960	 0.3900
m	 0.8010	 0.3850
n	 0.8110	 0.4100
o	 0.8030	 0.4000
p	 0.8300	 0.4140
q	 0.8170	 0.3980
r	 0.8280	 0.4140
s	 0.7970	 0.4100
t	 0.8110	 0.4080
u	 0.0370	 0.1960
v	 0.1830	 0.2430