



Full wwPDB EM Validation Report ⓘ

Mar 4, 2024 – 05:05 pm GMT

PDB ID : 8CQ0
EMDB ID : EMD-16792
Title : Photorhabdus luminescens TcdA1 prepore-to-pore intermediate, K567W
K2008W mutant
Authors : Nganga, P.N.; Roderer, D.; Belyy, A.; Prumbaum, D.; Raunser, S.
Deposited on : 2023-03-03
Resolution : 3.20 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.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

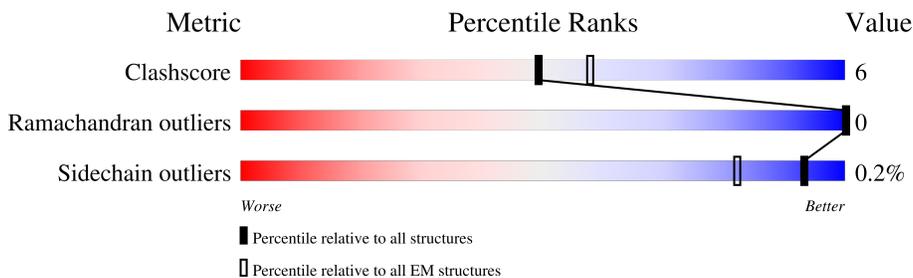
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	2535	
1	B	2535	
1	C	2535	
1	D	2535	
1	E	2535	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 84445 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 TcdA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2122	16889	10704	2868	3262	55	0	0
1	B	2122	16889	10704	2868	3262	55	0	0
1	C	2122	16889	10704	2868	3262	55	0	0
1	D	2122	16889	10704	2868	3262	55	0	0
1	E	2122	16889	10704	2868	3262	55	0	0

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP Q9RN43
A	-17	ALA	-	expression tag	UNP Q9RN43
A	-16	HIS	-	expression tag	UNP Q9RN43
A	-15	HIS	-	expression tag	UNP Q9RN43
A	-14	HIS	-	expression tag	UNP Q9RN43
A	-13	HIS	-	expression tag	UNP Q9RN43
A	-12	HIS	-	expression tag	UNP Q9RN43
A	-11	HIS	-	expression tag	UNP Q9RN43
A	-10	SER	-	expression tag	UNP Q9RN43
A	-9	SER	-	expression tag	UNP Q9RN43
A	-8	GLY	-	expression tag	UNP Q9RN43
A	-7	LEU	-	expression tag	UNP Q9RN43
A	-6	GLU	-	expression tag	UNP Q9RN43
A	-5	VAL	-	expression tag	UNP Q9RN43
A	-4	LEU	-	expression tag	UNP Q9RN43
A	-3	PHE	-	expression tag	UNP Q9RN43
A	-2	GLN	-	expression tag	UNP Q9RN43
A	-1	GLY	-	expression tag	UNP Q9RN43
A	0	PRO	-	expression tag	UNP Q9RN43
A	567	TRP	LYS	engineered mutation	UNP Q9RN43

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	2008	TRP	LYS	engineered mutation	UNP Q9RN43
B	-18	MET	-	initiating methionine	UNP Q9RN43
B	-17	ALA	-	expression tag	UNP Q9RN43
B	-16	HIS	-	expression tag	UNP Q9RN43
B	-15	HIS	-	expression tag	UNP Q9RN43
B	-14	HIS	-	expression tag	UNP Q9RN43
B	-13	HIS	-	expression tag	UNP Q9RN43
B	-12	HIS	-	expression tag	UNP Q9RN43
B	-11	HIS	-	expression tag	UNP Q9RN43
B	-10	SER	-	expression tag	UNP Q9RN43
B	-9	SER	-	expression tag	UNP Q9RN43
B	-8	GLY	-	expression tag	UNP Q9RN43
B	-7	LEU	-	expression tag	UNP Q9RN43
B	-6	GLU	-	expression tag	UNP Q9RN43
B	-5	VAL	-	expression tag	UNP Q9RN43
B	-4	LEU	-	expression tag	UNP Q9RN43
B	-3	PHE	-	expression tag	UNP Q9RN43
B	-2	GLN	-	expression tag	UNP Q9RN43
B	-1	GLY	-	expression tag	UNP Q9RN43
B	0	PRO	-	expression tag	UNP Q9RN43
B	567	TRP	LYS	engineered mutation	UNP Q9RN43
B	2008	TRP	LYS	engineered mutation	UNP Q9RN43
C	-18	MET	-	initiating methionine	UNP Q9RN43
C	-17	ALA	-	expression tag	UNP Q9RN43
C	-16	HIS	-	expression tag	UNP Q9RN43
C	-15	HIS	-	expression tag	UNP Q9RN43
C	-14	HIS	-	expression tag	UNP Q9RN43
C	-13	HIS	-	expression tag	UNP Q9RN43
C	-12	HIS	-	expression tag	UNP Q9RN43
C	-11	HIS	-	expression tag	UNP Q9RN43
C	-10	SER	-	expression tag	UNP Q9RN43
C	-9	SER	-	expression tag	UNP Q9RN43
C	-8	GLY	-	expression tag	UNP Q9RN43
C	-7	LEU	-	expression tag	UNP Q9RN43
C	-6	GLU	-	expression tag	UNP Q9RN43
C	-5	VAL	-	expression tag	UNP Q9RN43
C	-4	LEU	-	expression tag	UNP Q9RN43
C	-3	PHE	-	expression tag	UNP Q9RN43
C	-2	GLN	-	expression tag	UNP Q9RN43
C	-1	GLY	-	expression tag	UNP Q9RN43
C	0	PRO	-	expression tag	UNP Q9RN43
C	567	TRP	LYS	engineered mutation	UNP Q9RN43

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	2008	TRP	LYS	engineered mutation	UNP Q9RN43
D	-18	MET	-	initiating methionine	UNP Q9RN43
D	-17	ALA	-	expression tag	UNP Q9RN43
D	-16	HIS	-	expression tag	UNP Q9RN43
D	-15	HIS	-	expression tag	UNP Q9RN43
D	-14	HIS	-	expression tag	UNP Q9RN43
D	-13	HIS	-	expression tag	UNP Q9RN43
D	-12	HIS	-	expression tag	UNP Q9RN43
D	-11	HIS	-	expression tag	UNP Q9RN43
D	-10	SER	-	expression tag	UNP Q9RN43
D	-9	SER	-	expression tag	UNP Q9RN43
D	-8	GLY	-	expression tag	UNP Q9RN43
D	-7	LEU	-	expression tag	UNP Q9RN43
D	-6	GLU	-	expression tag	UNP Q9RN43
D	-5	VAL	-	expression tag	UNP Q9RN43
D	-4	LEU	-	expression tag	UNP Q9RN43
D	-3	PHE	-	expression tag	UNP Q9RN43
D	-2	GLN	-	expression tag	UNP Q9RN43
D	-1	GLY	-	expression tag	UNP Q9RN43
D	0	PRO	-	expression tag	UNP Q9RN43
D	567	TRP	LYS	engineered mutation	UNP Q9RN43
D	2008	TRP	LYS	engineered mutation	UNP Q9RN43
E	-18	MET	-	initiating methionine	UNP Q9RN43
E	-17	ALA	-	expression tag	UNP Q9RN43
E	-16	HIS	-	expression tag	UNP Q9RN43
E	-15	HIS	-	expression tag	UNP Q9RN43
E	-14	HIS	-	expression tag	UNP Q9RN43
E	-13	HIS	-	expression tag	UNP Q9RN43
E	-12	HIS	-	expression tag	UNP Q9RN43
E	-11	HIS	-	expression tag	UNP Q9RN43
E	-10	SER	-	expression tag	UNP Q9RN43
E	-9	SER	-	expression tag	UNP Q9RN43
E	-8	GLY	-	expression tag	UNP Q9RN43
E	-7	LEU	-	expression tag	UNP Q9RN43
E	-6	GLU	-	expression tag	UNP Q9RN43
E	-5	VAL	-	expression tag	UNP Q9RN43
E	-4	LEU	-	expression tag	UNP Q9RN43
E	-3	PHE	-	expression tag	UNP Q9RN43
E	-2	GLN	-	expression tag	UNP Q9RN43
E	-1	GLY	-	expression tag	UNP Q9RN43
E	0	PRO	-	expression tag	UNP Q9RN43
E	567	TRP	LYS	engineered mutation	UNP Q9RN43

Continued on next page...

Continued from previous page...

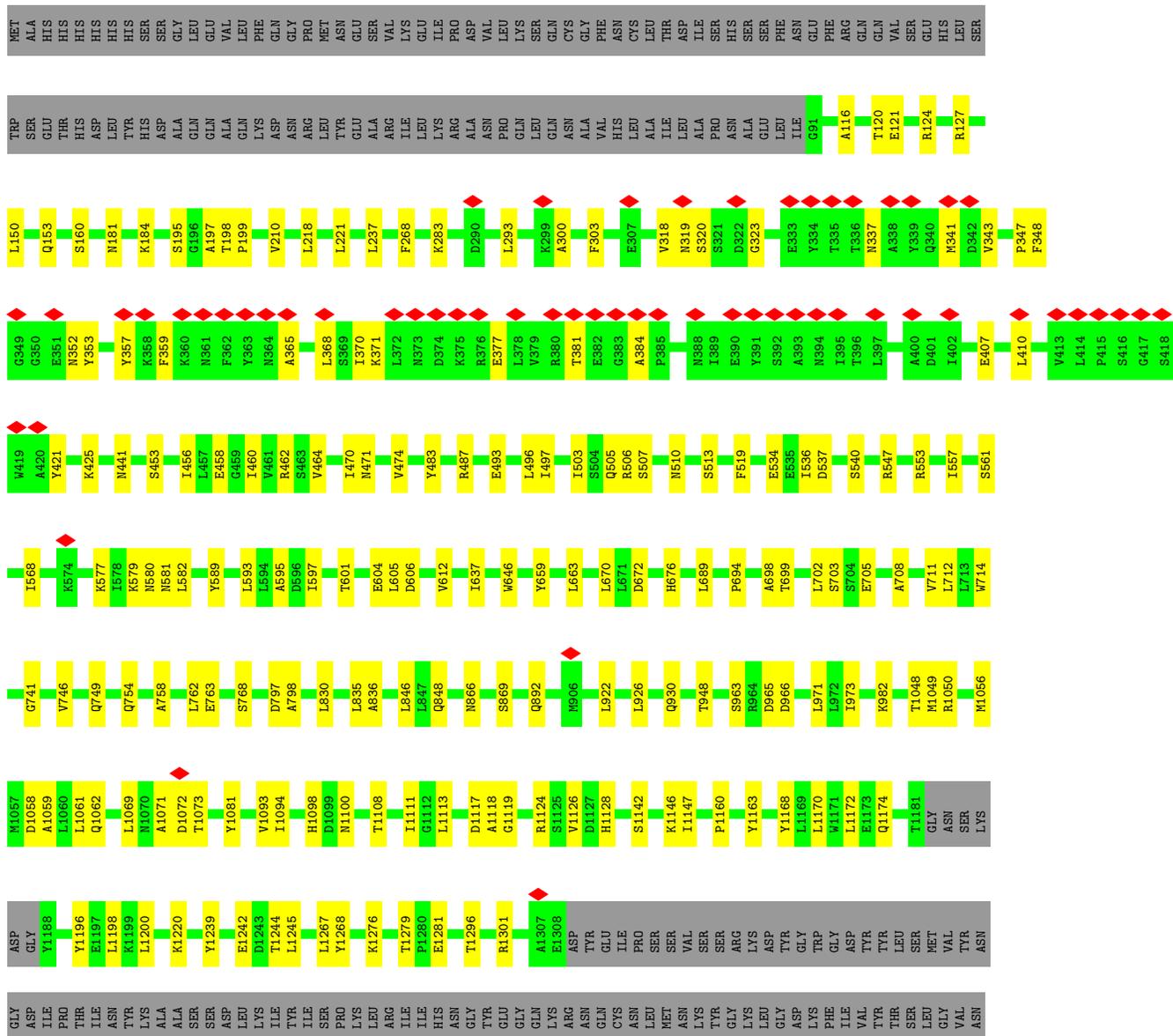
Chain	Residue	Modelled	Actual	Comment	Reference
E	2008	TRP	LYS	engineered mutation	UNP Q9RN43

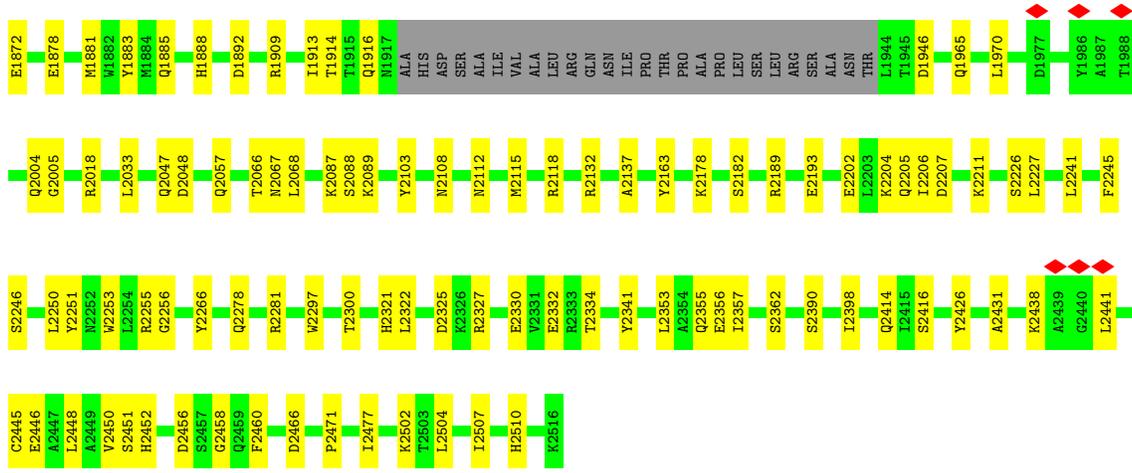
3 Residue-property plots

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.

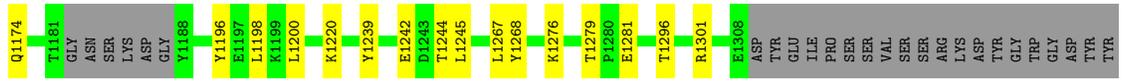
• Molecule 1: TcdA1

Chain A:





• Molecule 1: TcdA1



M441	K574	L713	TI048	Q1174	LEU	ALA	PHE	SER	HI743	I1913	Q2057	W2297	P2471
S453	K577	W714	M1049	TI1181	GLY	ILE	THR	ILE	HI766	T1914	T2066	W2300	F2472
I456	I578	A724	R1050	GLY	ASN	ASP	ALA	PRO	L1766	T1915	N2067	T2300	E2473
N580	K579	K729	ASN	ASP	PRO	ASP	ASP	VAL	F1767	Q1916	L2068	I2477	I2477
E458	I578	G741	M1056	SER	ASN	TYR	ASP	THR	H1768	N1917	K2087	H2321	K2502
I460	N581	V746	D1058	LYS	ASN	ALA	VAL	VAL	E1770	ALA	S2086	D2325	T2503
V461	E459	V746	L1060	GLY	ASN	ILE	GLN	THR	Y1774	HIS	K2089	K2326	L2504
R462	I460	Q749	L1061	Y1188	ASN	PRO	PRO	THR	Y1774	SER	S2089	R2327	L2504
S463	I460	E750	Q1062	Y1196	TYR	SER	SER	THR	L1783	ALA	Y2103	I2507	I2507
V464	L593	E750	S1067	E1197	MET	LYS	PRO	THR	E1783	ILE	N2112	H2510	H2510
I470	L594	Q754	Q1068	L1198	PHE	PRO	SER	SER	E1786	VAL	M2112	H2510	H2510
N471	A595	L762	L1069	K1199	TYR	ASP	PHE	SER	Q1787	ALA	M2115	E2332	K2516
W474	D596	E763	M1070	L1200	ASP	ASP	ASP	THR	M1606	LEU	R2118	E2332	K2516
Y483	I597	L762	A1071	L1200	VAL	LEU	GLU	THR	TI607	ARG	R2118	E2332	K2516
I497	I597	A798	M1071	L1200	TYR	ASN	MET	THR	V1644	GLN	R2132	Y2341	I2507
I503	T601	S768	D1072	K1220	GLN	TYR	TYR	THR	A1617	ASN	R2132	Y2341	I2507
S564	TI073	S768	TI073	Y1239	TYR	ILE	GLN	THR	TI618	THR	A2137	L2353	I2507
Q505	E604	D797	Y1081	E1242	ILE	ILE	PHE	ALA	I1624	PRO	Y2163	I2357	I2507
R506	I637	A798	Y1081	D1243	ASN	ASN	ASN	THR	K1797	ALA	Y2163	I2357	I2507
S507	L605	D606	ASN	T1244	THR	THR	ALA	THR	Y1798	ALA	S2362	S2362	I2507
N510	R487	D606	I1094	L1245	PRO	PRO	LEU	LEU	V1799	LEU	K2178	S2390	I2507
S513	E493	V612	I1094	L1245	LYS	LYS	GLU	GLU	M1800	SER	R2189	S2390	I2507
F519	L496	I637	H1098	L1267	LEU	LEU	ILE	ILE	S1801	LEU	R2189	S2390	I2507
E534	I497	I637	D1099	Y1268	ASN	ASN	ASP	ASP	P1802	ARG	E2193	I2398	I2507
E535	I503	W646	M1100	T1279	ILE	ILE	GLY	GLY	V1818	SER	E2193	I2398	I2507
I536	S564	Y659	TI108	P1280	ARG	THR	GLY	GLY	R1819	ASN	E2202	Q2414	I2507
D537	Q505	N660	TI108	E1281	LEU	ASP	LEU	LEU	P1820	THR	L2203	S2416	I2507
L538	Q506	K661	L1113	T1296	ASN	VAL	ASN	ASN	TI825	L1944	K2204	Y2426	I2507
N539	R506	K661	D1117	T1296	PHE	PRO	ASN	THR	Y1677	T1945	Q2205	Y2426	I2507
S540	S507	L663	A1118	R1301	ASP	VAL	ASN	SER	S1678	D1946	D2207	A2431	I2507
R547	N510	L670	R1124	E1308	GLN	GLU	ASN	SER	L1690	Q1965	K2211	K2438	I2507
R553	S513	L670	R1124	ASP	LYS	THR	THR	ALA	D1696	L1970	S2226	A2439	I2507
I557	F519	D672	V1126	TYR	ARG	THR	SER	SER	D1696	L1970	L2227	A2439	I2507
S561	E534	H676	D1127	GLU	ASN	THR	ILE	THR	L1699	D1977	K2228	L2441	I2507
L566	E534	H676	H1128	ILE	ASN	THR	THR	THR	H1704	Y1986	L2241	C2445	I2507
I567	I536	L689	TI128	ILE	LEU	THR	THR	THR	M1709	A1987	S2246	E2446	I2507
E705	D537	V691	K1135	SER	LEU	THR	THR	THR	E1872	T1988	S2246	L2448	I2507
A708	L538	V691	S1142	SER	VAL	VAL	VAL	VAL	E1872	A1998	L2250	A2449	I2507
V711	N539	P694	K1146	VAL	ASN	ALA	ALA	ALA	E1878	Q2004	Y2251	V2450	I2507
I568	S540	P694	I1147	ARG	THR	THR	THR	THR	E1878	G2005	W2253	S2451	I2507
	R547	A698	TI162	ASP	LYS	LYS	LYS	LYS	M1881	S2015	L2254	H2452	I2507
	R553	T699	Y1163	TYR	GLY	GLY	GLY	GLY	M1882	R2018	L2254	D2456	I2507
	L702	L702	Y1163	GLY	ASP	ASP	ASP	ASP	Y1883	R2018	G2256	S2457	I2507
	S703	S703	L1167	LYS	LYS	LYS	LYS	LYS	M1884	R2018	G2256	G2458	I2507
	E705	E705	Y1168	GLY	GLY	GLY	GLY	GLY	Q1885	R2018	Y2266	Q2459	I2507
	A708	A708	L1169	TYR	ILE	ILE	ILE	ILE	H1888	L2033	Y2266	F2460	I2507
	L566	L566	L1170	TYR	VAL	VAL	VAL	VAL	D1727	Q2047	Q2278	D2466	I2507
	W567	W567	W1171	LEU	THR	THR	THR	THR	D1729	D2048	R2281	L2470	I2507
	I568	I568	L1172	TYR	THR	THR	THR	THR	G1731	D2048	R2281	L2470	I2507
			E1173	SER	SER	SER	SER	SER	I1732				
									S1739				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	13356	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 ($e^-/\text{\AA}^2$)	57	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	492.8, 492.8, 492.8	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.26	0/17254	0.51	0/23440
1	B	0.26	0/17254	0.51	0/23440
1	C	0.26	0/17254	0.51	0/23440
1	D	0.26	0/17254	0.51	0/23440
1	E	0.26	0/17254	0.51	0/23440
All	All	0.26	0/86270	0.51	0/117200

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	16889	0	16504	227	0
1	B	16889	0	16504	221	0
1	C	16889	0	16504	232	0
1	D	16889	0	16504	223	0
1	E	16889	0	16504	225	0
All	All	84445	0	82520	1013	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 (1013) 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)
1:C:1108:THR:HG1	1:C:1128:HIS:HE2	1.23	0.83
1:B:1108:THR:HG1	1:B:1128:HIS:HE2	1.26	0.80
1:C:1797:LYS:HG3	1:C:1801:SER:HB2	1.64	0.80
1:E:1108:THR:HG1	1:E:1128:HIS:HE2	1.29	0.79
1:A:1797:LYS:HG3	1:A:1801:SER:HB2	1.65	0.79
1:D:1797:LYS:HG3	1:D:1801:SER:HB2	1.65	0.79
1:B:1797:LYS:HG3	1:B:1801:SER:HB2	1.65	0.78
1:E:1797:LYS:HG3	1:E:1801:SER:HB2	1.64	0.78
1:B:689:LEU:HD11	1:B:712:LEU:HB3	1.67	0.78
1:A:689:LEU:HD11	1:A:712:LEU:HB3	1.66	0.77
1:C:689:LEU:HD11	1:C:712:LEU:HB3	1.66	0.77
1:D:689:LEU:HD11	1:D:712:LEU:HB3	1.66	0.76
1:E:689:LEU:HD11	1:E:712:LEU:HB3	1.66	0.75
1:D:460:ILE:HG12	1:D:496:LEU:HD21	1.71	0.73
1:C:2089:LYS:HB2	1:C:2206:ILE:HG21	1.70	0.73
1:E:2089:LYS:HB2	1:E:2206:ILE:HG21	1.71	0.73
1:D:2089:LYS:HB2	1:D:2206:ILE:HG21	1.70	0.72
1:B:460:ILE:HG12	1:B:496:LEU:HD21	1.70	0.72
1:E:460:ILE:HG12	1:E:496:LEU:HD21	1.72	0.72
1:C:1093:VAL:HG21	1:C:1605:LEU:HD23	1.72	0.72
1:B:2089:LYS:HB2	1:B:2206:ILE:HG21	1.70	0.72
1:C:460:ILE:HG12	1:C:496:LEU:HD21	1.71	0.71
1:C:2204:LYS:O	1:D:2087:LYS:NZ	2.24	0.71
1:A:2089:LYS:HB2	1:A:2206:ILE:HG21	1.72	0.71
1:A:2204:LYS:O	1:B:2087:LYS:NZ	2.24	0.71
1:D:2204:LYS:O	1:E:2087:LYS:NZ	2.24	0.71
1:A:1059:ALA:HA	1:A:1062:GLN:HE21	1.56	0.70
1:D:1093:VAL:HG21	1:D:1605:LEU:HD23	1.73	0.70
1:A:460:ILE:HG12	1:A:496:LEU:HD21	1.71	0.70
1:E:1059:ALA:HA	1:E:1062:GLN:HE21	1.56	0.70
1:A:1093:VAL:HG21	1:A:1605:LEU:HD23	1.74	0.70
1:E:1093:VAL:HG21	1:E:1605:LEU:HD23	1.73	0.69
1:B:1093:VAL:HG21	1:B:1605:LEU:HD23	1.74	0.69
1:B:1059:ALA:HA	1:B:1062:GLN:HE21	1.57	0.69
1:A:2087:LYS:NZ	1:E:2204:LYS:O	2.24	0.69
1:D:1146:LYS:NZ	1:D:1147:ILE:O	2.26	0.69
1:D:1059:ALA:HA	1:D:1062:GLN:HE21	1.57	0.69
1:A:1146:LYS:NZ	1:A:1147:ILE:O	2.26	0.68
1:E:1916:GLN:NE2	1:E:1946:ASP:OD2	2.26	0.68
1:C:612:VAL:HG22	1:C:637:ILE:HD12	1.76	0.68
1:C:1059:ALA:HA	1:C:1062:GLN:HE21	1.57	0.68
1:E:237:LEU:HD11	1:E:483:TYR:HB2	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:LEU:HD11	1:B:483:TYR:HB2	1.75	0.68
1:A:237:LEU:HD11	1:A:483:TYR:HB2	1.76	0.67
1:C:237:LEU:HD11	1:C:483:TYR:HB2	1.76	0.67
1:E:1146:LYS:NZ	1:E:1147:ILE:O	2.25	0.67
1:D:237:LEU:HD11	1:D:483:TYR:HB2	1.77	0.67
1:C:1916:GLN:NE2	1:C:1946:ASP:OD2	2.28	0.67
1:A:2047:GLN:HB3	1:A:2251:TYR:HB3	1.77	0.67
1:A:2087:LYS:HD3	1:E:2204:LYS:HG2	1.77	0.67
1:A:2426:TYR:HB3	1:B:2334:THR:HG21	1.75	0.67
1:D:2426:TYR:HB3	1:E:2334:THR:HG21	1.77	0.67
1:A:300:ALA:HA	1:A:303:PHE:CD2	2.30	0.67
1:B:2047:GLN:HB3	1:B:2251:TYR:HB3	1.77	0.67
1:C:1146:LYS:NZ	1:C:1147:ILE:O	2.26	0.67
1:B:1916:GLN:NE2	1:B:1946:ASP:OD2	2.27	0.67
1:C:300:ALA:HA	1:C:303:PHE:CD2	2.30	0.67
1:A:612:VAL:HG22	1:A:637:ILE:HD12	1.76	0.66
1:D:300:ALA:HA	1:D:303:PHE:CD2	2.30	0.66
1:C:2204:LYS:HG2	1:D:2087:LYS:HD3	1.78	0.66
1:E:612:VAL:HG22	1:E:637:ILE:HD12	1.76	0.66
1:B:1146:LYS:NZ	1:B:1147:ILE:O	2.26	0.66
1:D:2204:LYS:HG2	1:E:2087:LYS:HD3	1.77	0.66
1:A:2205:GLN:OE1	1:B:2088:SER:OG	2.13	0.66
1:D:2205:GLN:OE1	1:E:2088:SER:OG	2.13	0.66
1:B:612:VAL:HG22	1:B:637:ILE:HD12	1.77	0.66
1:E:300:ALA:HA	1:E:303:PHE:CD2	2.31	0.66
1:E:2047:GLN:HB3	1:E:2251:TYR:HB3	1.77	0.66
1:A:2204:LYS:HG2	1:B:2087:LYS:HD3	1.77	0.66
1:B:121:GLU:HG2	1:B:124:ARG:HH21	1.60	0.66
1:D:1916:GLN:NE2	1:D:1946:ASP:OD2	2.28	0.66
1:C:830:LEU:HD21	1:C:835:LEU:HD12	1.78	0.65
1:C:963:SER:OG	1:C:965:ASP:OD1	2.14	0.65
1:B:300:ALA:HA	1:B:303:PHE:CD2	2.31	0.65
1:E:2438:LYS:HG3	1:E:2446:GLU:HG3	1.78	0.65
1:D:612:VAL:HG22	1:D:637:ILE:HD12	1.77	0.65
1:A:1916:GLN:NE2	1:A:1946:ASP:OD2	2.28	0.65
1:B:2204:LYS:O	1:C:2087:LYS:NZ	2.23	0.65
1:C:2047:GLN:HB3	1:C:2251:TYR:HB3	1.77	0.65
1:A:2334:THR:HG21	1:E:2426:TYR:HB3	1.79	0.65
1:D:963:SER:OG	1:D:965:ASP:OD1	2.15	0.65
1:D:2047:GLN:HB3	1:D:2251:TYR:HB3	1.77	0.65
1:A:121:GLU:HG2	1:A:124:ARG:HH21	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:830:LEU:HD21	1:B:835:LEU:HD12	1.79	0.64
1:E:963:SER:OG	1:E:965:ASP:OD1	2.14	0.64
1:C:1069:LEU:HD23	1:C:1786:GLU:HG3	1.80	0.64
1:A:963:SER:OG	1:A:965:ASP:OD1	2.14	0.64
1:B:2204:LYS:HG2	1:C:2087:LYS:HD3	1.77	0.64
1:A:368:LEU:N	1:A:381:THR:O	2.28	0.64
1:C:2205:GLN:OE1	1:D:2088:SER:OG	2.12	0.64
1:B:1069:LEU:HD23	1:B:1786:GLU:HG3	1.80	0.64
1:C:2182:SER:OG	1:E:1067:SER:OG	2.12	0.64
1:C:2451:SER:HB3	1:D:2332:GLU:HG2	1.80	0.64
1:D:830:LEU:HD21	1:D:835:LEU:HD12	1.79	0.64
1:B:963:SER:OG	1:B:965:ASP:OD1	2.15	0.64
1:D:121:GLU:HG2	1:D:124:ARG:HH21	1.63	0.64
1:A:210:VAL:HG11	1:A:922:LEU:HB3	1.81	0.63
1:A:2438:LYS:HG3	1:A:2446:GLU:HG3	1.78	0.63
1:D:1069:LEU:HD23	1:D:1786:GLU:HG3	1.80	0.63
1:C:121:GLU:HG2	1:C:124:ARG:HH21	1.61	0.63
1:E:121:GLU:HG2	1:E:124:ARG:HH21	1.63	0.63
1:E:1069:LEU:HD23	1:E:1786:GLU:HG3	1.80	0.63
1:A:1069:LEU:HD23	1:A:1786:GLU:HG3	1.80	0.63
1:B:2438:LYS:HG3	1:B:2446:GLU:HG3	1.81	0.63
1:D:210:VAL:HG11	1:D:922:LEU:HB3	1.79	0.63
1:E:830:LEU:HD21	1:E:835:LEU:HD12	1.79	0.63
1:C:210:VAL:HG11	1:C:922:LEU:HB3	1.81	0.63
1:D:2438:LYS:HG3	1:D:2446:GLU:HG3	1.79	0.63
1:A:2255:ARG:NH2	1:E:703:SER:O	2.25	0.62
1:E:210:VAL:HG11	1:E:922:LEU:HB3	1.80	0.62
1:A:830:LEU:HD21	1:A:835:LEU:HD12	1.80	0.62
1:B:2451:SER:HB3	1:C:2332:GLU:HG2	1.79	0.62
1:B:2205:GLN:OE1	1:C:2088:SER:OG	2.12	0.62
1:B:337:ASN:ND2	1:B:421:TYR:O	2.25	0.62
1:D:2451:SER:HB3	1:E:2332:GLU:HG2	1.81	0.62
1:B:659:TYR:HB2	1:B:754:GLN:HG2	1.82	0.62
1:E:368:LEU:N	1:E:381:THR:O	2.28	0.62
1:C:659:TYR:HB2	1:C:754:GLN:HG2	1.83	0.61
1:C:1239:TYR:CD2	1:C:1242:GLU:HB3	2.36	0.61
1:B:2460:PHE:CE1	1:C:2330:GLU:HB3	2.36	0.61
1:C:2438:LYS:HG3	1:C:2446:GLU:HG3	1.82	0.61
1:A:2332:GLU:HG2	1:E:2451:SER:HB3	1.81	0.61
1:A:2451:SER:HB3	1:B:2332:GLU:HG2	1.81	0.61
1:B:210:VAL:HG11	1:B:922:LEU:HB3	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:LEU:N	1:C:381:THR:O	2.28	0.61
1:B:1239:TYR:CD2	1:B:1242:GLU:HB3	2.36	0.61
1:C:2460:PHE:CE1	1:D:2330:GLU:HB3	2.35	0.61
1:D:659:TYR:HB2	1:D:754:GLN:HG2	1.83	0.61
1:D:1239:TYR:CD2	1:D:1242:GLU:HB3	2.36	0.61
1:A:2088:SER:OG	1:E:2205:GLN:OE1	2.13	0.61
1:D:2460:PHE:CE1	1:E:2330:GLU:HB3	2.36	0.61
1:E:1220:LYS:HE2	1:E:1267:LEU:HB3	1.83	0.60
1:D:1220:LYS:HE2	1:D:1267:LEU:HB3	1.84	0.60
1:A:337:ASN:ND2	1:A:421:TYR:O	2.25	0.60
1:A:540:SER:HB2	1:B:848:GLN:HE22	1.67	0.60
1:A:703:SER:O	1:B:2255:ARG:NH2	2.25	0.60
1:A:2460:PHE:CE1	1:B:2330:GLU:HB3	2.36	0.60
1:A:848:GLN:HE22	1:E:540:SER:HB2	1.67	0.60
1:D:124:ARG:HD3	1:D:1914:THR:HB	1.84	0.60
1:E:1239:TYR:CD2	1:E:1242:GLU:HB3	2.36	0.60
1:B:540:SER:HB2	1:C:848:GLN:HE22	1.67	0.60
1:A:659:TYR:HB2	1:A:754:GLN:HG2	1.83	0.60
1:A:2137:ALA:HB2	1:C:1118:ALA:HB2	1.82	0.59
1:A:2330:GLU:HB3	1:E:2460:PHE:CE1	2.36	0.59
1:C:337:ASN:ND2	1:C:421:TYR:O	2.25	0.59
1:A:1239:TYR:CD2	1:A:1242:GLU:HB3	2.36	0.59
1:B:2426:TYR:HB3	1:C:2334:THR:HG21	1.84	0.59
1:D:368:LEU:N	1:D:381:THR:O	2.29	0.59
1:D:540:SER:HB2	1:E:848:GLN:HE22	1.67	0.59
1:E:337:ASN:ND2	1:E:421:TYR:O	2.25	0.59
1:D:746:VAL:HB	1:D:749:GLN:HB2	1.85	0.59
1:A:1220:LYS:HE2	1:A:1267:LEU:HB3	1.85	0.59
1:B:1296:THR:HG23	1:B:1301:ARG:HH12	1.68	0.59
1:C:2137:ALA:HB2	1:E:1118:ALA:HB2	1.83	0.59
1:E:659:TYR:HB2	1:E:754:GLN:HG2	1.84	0.59
1:B:1220:LYS:HE2	1:B:1267:LEU:HB3	1.84	0.59
1:D:703:SER:O	1:E:2255:ARG:NH2	2.24	0.59
1:D:2103:TYR:CE1	1:D:2189:ARG:HG2	2.38	0.59
1:A:797:ASP:OD1	1:A:798:ALA:N	2.36	0.58
1:B:746:VAL:HB	1:B:749:GLN:HB2	1.85	0.58
1:C:746:VAL:HB	1:C:749:GLN:HB2	1.84	0.58
1:B:124:ARG:HD3	1:B:1914:THR:HB	1.85	0.58
1:D:2504:LEU:HD21	1:D:2507:ILE:HD11	1.86	0.58
1:E:124:ARG:HD3	1:E:1914:THR:HB	1.85	0.58
1:C:1774:TYR:OH	1:C:1848:TYR:OH	2.21	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1296:THR:HG23	1:D:1301:ARG:HH12	1.68	0.58
1:E:1296:THR:HG23	1:E:1301:ARG:HH12	1.67	0.58
1:A:124:ARG:HD3	1:A:1914:THR:HB	1.85	0.58
1:A:1296:THR:HG23	1:A:1301:ARG:HH12	1.68	0.58
1:D:2103:TYR:CE1	1:D:2193:GLU:HG2	2.38	0.58
1:A:2327:ARG:NH1	1:E:2445:CYS:SG	2.76	0.58
1:B:458:GLU:OE2	1:B:506:ARG:NH1	2.33	0.58
1:B:2103:TYR:CE1	1:B:2193:GLU:HG2	2.39	0.58
1:B:797:ASP:OD1	1:B:798:ALA:N	2.37	0.58
1:B:2137:ALA:HB2	1:D:1118:ALA:HB2	1.84	0.58
1:C:1296:THR:HG23	1:C:1301:ARG:HH12	1.69	0.58
1:E:2103:TYR:CE1	1:E:2189:ARG:HG2	2.39	0.58
1:D:337:ASN:ND2	1:D:421:TYR:O	2.25	0.58
1:E:2103:TYR:CE1	1:E:2193:GLU:HG2	2.38	0.58
1:A:2103:TYR:CE1	1:A:2193:GLU:HG2	2.39	0.58
1:C:1220:LYS:HE2	1:C:1267:LEU:HB3	1.86	0.58
1:D:797:ASP:OD1	1:D:798:ALA:N	2.37	0.58
1:B:703:SER:O	1:C:2255:ARG:NH2	2.25	0.57
1:C:124:ARG:HD3	1:C:1914:THR:HB	1.86	0.57
1:C:2103:TYR:CE1	1:C:2189:ARG:HG2	2.40	0.57
1:D:510:ASN:OD1	1:E:153:GLN:NE2	2.37	0.57
1:D:1865:ASP:OD1	1:D:1883:TYR:OH	2.21	0.57
1:E:746:VAL:HB	1:E:749:GLN:HB2	1.84	0.57
1:A:153:GLN:NE2	1:E:510:ASN:OD1	2.38	0.57
1:A:1865:ASP:OD1	1:A:1883:TYR:OH	2.20	0.57
1:B:519:PHE:O	1:B:553:ARG:NH2	2.38	0.57
1:A:519:PHE:O	1:A:553:ARG:NH2	2.38	0.57
1:A:1783:LEU:HD12	1:A:1788:ASN:HB3	1.87	0.57
1:B:2103:TYR:CE1	1:B:2189:ARG:HG2	2.39	0.57
1:C:2504:LEU:HD21	1:C:2507:ILE:HD11	1.86	0.57
1:E:797:ASP:OD1	1:E:798:ALA:N	2.37	0.57
1:A:746:VAL:HB	1:A:749:GLN:HB2	1.85	0.57
1:C:703:SER:O	1:D:2255:ARG:NH2	2.24	0.57
1:C:1774:TYR:HH	1:C:1848:TYR:HH	1.49	0.57
1:C:540:SER:HB2	1:D:848:GLN:HE22	1.68	0.57
1:C:2103:TYR:CE1	1:C:2193:GLU:HG2	2.39	0.57
1:C:2426:TYR:HB3	1:D:2334:THR:HG21	1.86	0.57
1:E:519:PHE:O	1:E:553:ARG:NH2	2.38	0.57
1:A:2445:CYS:SG	1:B:2327:ARG:NH1	2.78	0.57
1:B:2057:GLN:HG3	1:B:2241:LEU:HD12	1.85	0.57
1:E:2504:LEU:HD21	1:E:2507:ILE:HD11	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1072:ASP:OD1	1:E:1073:THR:N	2.38	0.57
1:B:1072:ASP:OD1	1:B:1073:THR:N	2.38	0.56
1:C:1783:LEU:HD12	1:C:1788:ASN:HB3	1.87	0.56
1:B:1655:HIS:NE2	1:B:1659:ARG:HA	2.20	0.56
1:C:797:ASP:OD1	1:C:798:ALA:N	2.37	0.56
1:A:1072:ASP:OD1	1:A:1073:THR:N	2.38	0.56
1:A:1655:HIS:NE2	1:A:1659:ARG:HA	2.20	0.56
1:B:510:ASN:OD1	1:C:153:GLN:NE2	2.38	0.56
1:C:510:ASN:OD1	1:D:153:GLN:NE2	2.38	0.56
1:E:1865:ASP:OD1	1:E:1883:TYR:OH	2.20	0.56
1:C:519:PHE:O	1:C:553:ARG:NH2	2.37	0.56
1:A:1722:GLY:O	1:A:1739:SER:HB2	2.06	0.56
1:A:2103:TYR:CE1	1:A:2189:ARG:HG2	2.40	0.56
1:C:458:GLU:OE2	1:C:506:ARG:NH1	2.35	0.56
1:C:1655:HIS:NE2	1:C:1659:ARG:HA	2.20	0.56
1:C:2057:GLN:HG3	1:C:2241:LEU:HD12	1.87	0.56
1:D:1655:HIS:NE2	1:D:1659:ARG:HA	2.20	0.56
1:E:1655:HIS:NE2	1:E:1659:ARG:HA	2.20	0.56
1:B:1783:LEU:HD12	1:B:1788:ASN:HB3	1.88	0.56
1:C:1072:ASP:OD1	1:C:1073:THR:N	2.38	0.56
1:A:2504:LEU:HD21	1:A:2507:ILE:HD11	1.87	0.56
1:D:519:PHE:O	1:D:553:ARG:NH2	2.38	0.56
1:D:1072:ASP:OD1	1:D:1073:THR:N	2.38	0.55
1:E:458:GLU:OE2	1:E:506:ARG:NH1	2.34	0.55
1:B:2504:LEU:HD21	1:B:2507:ILE:HD11	1.87	0.55
1:B:1722:GLY:O	1:B:1739:SER:HB2	2.06	0.55
1:C:1722:GLY:O	1:C:1739:SER:HB2	2.07	0.55
1:D:2057:GLN:HG3	1:D:2241:LEU:HD12	1.88	0.55
1:E:1722:GLY:O	1:E:1739:SER:HB2	2.06	0.55
1:E:1783:LEU:HD12	1:E:1788:ASN:HB3	1.87	0.55
1:E:368:LEU:HG	1:E:370:ILE:HD11	1.88	0.55
1:B:1885:GLN:HA	1:B:1888:HIS:CE1	2.42	0.55
1:C:503:ILE:HB	1:C:582:LEU:HD11	1.89	0.55
1:B:368:LEU:HG	1:B:370:ILE:HD11	1.88	0.55
1:C:1728:ASP:OD2	1:C:1730:LYS:NZ	2.40	0.55
1:A:1794:ARG:NH2	1:A:1798:TYR:OH	2.40	0.54
1:A:407:GLU:HA	1:A:425:LYS:HA	1.88	0.54
1:D:407:GLU:HA	1:D:425:LYS:HA	1.89	0.54
1:A:368:LEU:HG	1:A:370:ILE:HD11	1.88	0.54
1:A:1885:GLN:HA	1:A:1888:HIS:CE1	2.42	0.54
1:B:1865:ASP:OD1	1:B:1883:TYR:OH	2.20	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2182:SER:HG	1:E:1067:SER:HG	1.49	0.54
1:D:1722:GLY:O	1:D:1739:SER:HB2	2.07	0.54
1:B:503:ILE:HB	1:B:582:LEU:HD11	1.90	0.54
1:D:1783:LEU:HD12	1:D:1788:ASN:HB3	1.87	0.54
1:E:2033:LEU:HD11	1:E:2266:TYR:HA	1.90	0.54
1:E:2448:LEU:HD23	1:E:2471:PRO:HB2	1.90	0.54
1:A:503:ILE:HB	1:A:582:LEU:HD11	1.90	0.54
1:A:2448:LEU:HD23	1:A:2471:PRO:HB2	1.89	0.54
1:E:503:ILE:HB	1:E:582:LEU:HD11	1.90	0.54
1:D:1885:GLN:HA	1:D:1888:HIS:CE1	2.43	0.54
1:D:1728:ASP:OD2	1:D:1730:LYS:NZ	2.41	0.54
1:B:1794:ARG:NH2	1:B:1798:TYR:OH	2.41	0.54
1:D:368:LEU:HG	1:D:370:ILE:HD11	1.89	0.54
1:B:341:MET:HE1	1:B:359:PHE:CE1	2.43	0.54
1:C:407:GLU:HA	1:C:425:LYS:HA	1.89	0.54
1:C:1865:ASP:OD1	1:C:1883:TYR:OH	2.19	0.54
1:D:1790:ASP:OD1	1:D:1791:GLU:N	2.42	0.54
1:E:1790:ASP:OD1	1:E:1791:GLU:N	2.41	0.54
1:E:1885:GLN:HA	1:E:1888:HIS:CE1	2.42	0.54
1:A:2057:GLN:HG3	1:A:2241:LEU:HD12	1.90	0.53
1:C:368:LEU:HG	1:C:370:ILE:HD11	1.88	0.53
1:C:1885:GLN:HA	1:C:1888:HIS:CE1	2.43	0.53
1:E:866:ASN:HA	1:E:869:SER:HB3	1.91	0.53
1:A:510:ASN:OD1	1:B:153:GLN:NE2	2.39	0.53
1:E:2057:GLN:HG3	1:E:2241:LEU:HD12	1.89	0.53
1:A:2087:LYS:HZ2	1:E:2205:GLN:HA	1.73	0.53
1:B:407:GLU:HA	1:B:425:LYS:HA	1.89	0.53
1:C:341:MET:HE1	1:C:359:PHE:CE1	2.43	0.53
1:C:1790:ASP:OD1	1:C:1791:GLU:N	2.41	0.53
1:D:503:ILE:HB	1:D:582:LEU:HD11	1.90	0.53
1:D:2353:LEU:HD23	1:D:2357:ILE:HD11	1.90	0.53
1:D:458:GLU:OE2	1:D:506:ARG:NH1	2.34	0.53
1:A:341:MET:HE2	1:A:359:PHE:CE1	2.43	0.53
1:A:2353:LEU:HD23	1:A:2357:ILE:HD11	1.90	0.53
1:B:2205:GLN:HA	1:C:2087:LYS:HZ2	1.72	0.53
1:C:866:ASN:HA	1:C:869:SER:HB3	1.90	0.53
1:D:670:LEU:HA	1:D:699:THR:HG21	1.91	0.53
1:A:1790:ASP:OD1	1:A:1791:GLU:N	2.42	0.53
1:C:2353:LEU:HD23	1:C:2357:ILE:HD11	1.90	0.53
1:D:2033:LEU:HD11	1:D:2266:TYR:HA	1.91	0.53
1:E:1794:ARG:NH2	1:E:1798:TYR:OH	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:LEU:N	1:B:381:THR:O	2.28	0.53
1:B:2266:TYR:CZ	1:B:2297:TRP:HB2	2.43	0.53
1:B:2445:CYS:SG	1:C:2327:ARG:NH1	2.81	0.53
1:D:2448:LEU:HD23	1:D:2471:PRO:HB2	1.91	0.53
1:D:341:MET:HE1	1:D:359:PHE:CE1	2.43	0.53
1:E:341:MET:HE1	1:E:359:PHE:CE1	2.43	0.53
1:E:2266:TYR:CZ	1:E:2297:TRP:HB2	2.44	0.53
1:A:866:ASN:HA	1:A:869:SER:HB3	1.90	0.53
1:A:2266:TYR:CZ	1:A:2297:TRP:HB2	2.44	0.53
1:C:2266:TYR:CZ	1:C:2297:TRP:HB2	2.44	0.53
1:D:2341:TYR:OH	1:D:2390:SER:O	2.19	0.53
1:A:2033:LEU:HD11	1:A:2266:TYR:HA	1.90	0.52
1:B:2353:LEU:HD23	1:B:2357:ILE:HD11	1.90	0.52
1:D:866:ASN:HA	1:D:869:SER:HB3	1.91	0.52
1:E:407:GLU:HA	1:E:425:LYS:HA	1.90	0.52
1:A:497:ILE:HG21	1:A:589:TYR:HD2	1.74	0.52
1:A:1117:ASP:OD1	1:A:1118:ALA:N	2.40	0.52
1:B:1709:MET:HB3	1:B:1743:HIS:CE1	2.45	0.52
1:C:497:ILE:HG21	1:C:589:TYR:HD2	1.73	0.52
1:D:1794:ARG:NH2	1:D:1798:TYR:OH	2.43	0.52
1:B:497:ILE:HG21	1:B:589:TYR:HD2	1.74	0.52
1:D:698:ALA:HB1	1:E:2253:TRP:HA	1.90	0.52
1:D:2266:TYR:CZ	1:D:2297:TRP:HB2	2.44	0.52
1:E:1728:ASP:OD2	1:E:1730:LYS:NZ	2.41	0.52
1:A:670:LEU:HA	1:A:699:THR:HG21	1.92	0.52
1:A:1709:MET:HB3	1:A:1743:HIS:CE1	2.45	0.52
1:A:2253:TRP:HA	1:E:698:ALA:HB1	1.91	0.52
1:B:1118:ALA:HB2	1:E:2137:ALA:HB2	1.92	0.52
1:A:2068:LEU:HD22	1:A:2227:LEU:HG	1.92	0.52
1:C:1709:MET:HB3	1:C:1743:HIS:CE1	2.45	0.52
1:C:2033:LEU:HD11	1:C:2266:TYR:HA	1.91	0.52
1:D:540:SER:HB2	1:E:848:GLN:NE2	2.25	0.52
1:E:1709:MET:HB3	1:E:1743:HIS:CE1	2.44	0.52
1:A:1239:TYR:HD2	1:A:1242:GLU:HB3	1.75	0.52
1:A:1728:ASP:OD2	1:A:1730:LYS:NZ	2.41	0.52
1:B:670:LEU:HA	1:B:699:THR:HG21	1.92	0.52
1:C:1794:ARG:NH2	1:C:1798:TYR:OH	2.43	0.52
1:D:1117:ASP:OD1	1:D:1118:ALA:N	2.40	0.52
1:C:698:ALA:HB1	1:D:2253:TRP:HA	1.91	0.52
1:A:698:ALA:HB1	1:B:2253:TRP:HA	1.91	0.51
1:A:2205:GLN:HA	1:B:2087:LYS:HZ2	1.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:ILE:HD11	1:B:606:ASP:HB2	1.92	0.51
1:B:1790:ASP:OD1	1:B:1791:GLU:N	2.41	0.51
1:B:2033:LEU:HD11	1:B:2266:TYR:HA	1.91	0.51
1:E:1117:ASP:OD1	1:E:1118:ALA:N	2.40	0.51
1:E:1239:TYR:HD2	1:E:1242:GLU:HB3	1.75	0.51
1:A:343:VAL:HG23	1:A:357:TYR:HB3	1.92	0.51
1:A:848:GLN:NE2	1:E:540:SER:HB2	2.26	0.51
1:C:300:ALA:HA	1:C:303:PHE:HD2	1.76	0.51
1:C:343:VAL:HG23	1:C:357:TYR:HB3	1.93	0.51
1:D:1709:MET:HB3	1:D:1743:HIS:CE1	2.45	0.51
1:E:497:ILE:HG21	1:E:589:TYR:HD2	1.74	0.51
1:E:2353:LEU:HD23	1:E:2357:ILE:HD11	1.91	0.51
1:B:698:ALA:HB1	1:C:2253:TRP:HA	1.91	0.51
1:B:866:ASN:HA	1:B:869:SER:HB3	1.91	0.51
1:E:471:ASN:H	1:E:474:VAL:HG12	1.76	0.51
1:A:540:SER:HB2	1:B:848:GLN:NE2	2.25	0.51
1:A:2087:LYS:NZ	1:E:2205:GLN:HA	2.26	0.51
1:B:2205:GLN:HA	1:C:2087:LYS:NZ	2.26	0.51
1:B:2341:TYR:OH	1:B:2390:SER:O	2.19	0.51
1:C:2068:LEU:HD22	1:C:2227:LEU:HG	1.93	0.51
1:D:2068:LEU:HD22	1:D:2227:LEU:HG	1.92	0.51
1:C:1239:TYR:HD2	1:C:1242:GLU:HB3	1.75	0.51
1:A:1118:ALA:HB2	1:D:2137:ALA:HB2	1.93	0.51
1:E:670:LEU:HA	1:E:699:THR:HG21	1.92	0.51
1:E:470:ILE:HA	1:E:474:VAL:HG11	1.93	0.51
1:B:557:ILE:HB	1:B:561:SER:OG	2.11	0.51
1:C:471:ASN:H	1:C:474:VAL:HG12	1.76	0.51
1:C:2448:LEU:HD23	1:C:2471:PRO:HB2	1.92	0.51
1:D:497:ILE:HG21	1:D:589:TYR:HD2	1.75	0.51
1:E:343:VAL:HG23	1:E:357:TYR:HB3	1.92	0.51
1:B:540:SER:HB2	1:C:848:GLN:NE2	2.26	0.51
1:B:2068:LEU:HD22	1:B:2227:LEU:HG	1.93	0.51
1:A:568:ILE:HD11	1:A:606:ASP:HB2	1.93	0.50
1:C:670:LEU:HA	1:C:699:THR:HG21	1.92	0.50
1:C:1614:VAL:O	1:C:1618:THR:HG23	2.11	0.50
1:D:1108:THR:OG1	1:D:1128:HIS:NE2	2.36	0.50
1:D:1239:TYR:HD2	1:D:1242:GLU:HB3	1.75	0.50
1:B:120:THR:O	1:B:124:ARG:HG3	2.11	0.50
1:B:343:VAL:HG23	1:B:357:TYR:HB3	1.93	0.50
1:D:343:VAL:HG23	1:D:357:TYR:HB3	1.93	0.50
1:E:2341:TYR:OH	1:E:2390:SER:O	2.19	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2205:GLN:HA	1:B:2087:LYS:NZ	2.26	0.50
1:B:1117:ASP:OD1	1:B:1118:ALA:N	2.40	0.50
1:C:540:SER:HB2	1:D:848:GLN:NE2	2.25	0.50
1:C:2047:GLN:NE2	1:C:2048:ASP:OD1	2.44	0.50
1:D:471:ASN:H	1:D:474:VAL:HG12	1.76	0.50
1:D:2205:GLN:HA	1:E:2087:LYS:NZ	2.26	0.50
1:E:2068:LEU:HD22	1:E:2227:LEU:HG	1.92	0.50
1:B:471:ASN:H	1:B:474:VAL:HG12	1.76	0.50
1:D:2205:GLN:HA	1:E:2087:LYS:HZ2	1.75	0.50
1:C:462:ARG:HH11	1:C:506:ARG:HH11	1.60	0.50
1:E:120:THR:O	1:E:124:ARG:HG3	2.12	0.50
1:A:300:ALA:HA	1:A:303:PHE:HD2	1.75	0.50
1:A:471:ASN:H	1:A:474:VAL:HG12	1.76	0.50
1:C:120:THR:O	1:C:124:ARG:HG3	2.11	0.50
1:C:2341:TYR:OH	1:C:2390:SER:O	2.19	0.50
1:D:120:THR:O	1:D:124:ARG:HG3	2.12	0.50
1:D:470:ILE:HA	1:D:474:VAL:HG11	1.94	0.50
1:B:1168:TYR:HB3	1:B:1200:LEU:HD11	1.93	0.50
1:B:2047:GLN:NE2	1:B:2048:ASP:OD1	2.45	0.50
1:C:507:SER:HB3	1:C:513:SER:HB2	1.93	0.50
1:D:1614:VAL:O	1:D:1618:THR:HG23	2.11	0.50
1:E:1614:VAL:O	1:E:1618:THR:HG23	2.11	0.50
1:A:557:ILE:HB	1:A:561:SER:OG	2.11	0.50
1:A:1883:TYR:HD2	1:A:1970:LEU:HD11	1.77	0.50
1:B:1239:TYR:HD2	1:B:1242:GLU:HB3	1.76	0.50
1:C:2204:LYS:C	1:D:2087:LYS:HZ3	2.13	0.50
1:E:1774:TYR:OH	1:E:1848:TYR:OH	2.21	0.50
1:C:836:ALA:HB2	1:C:846:LEU:HD12	1.94	0.49
1:D:300:ALA:HA	1:D:303:PHE:HD2	1.76	0.49
1:E:300:ALA:HA	1:E:303:PHE:HD2	1.76	0.49
1:A:120:THR:O	1:A:124:ARG:HG3	2.12	0.49
1:B:698:ALA:HB2	1:C:2256:GLY:HA3	1.94	0.49
1:C:1168:TYR:HB3	1:C:1200:LEU:HD11	1.93	0.49
1:E:1883:TYR:HD2	1:E:1970:LEU:HD11	1.77	0.49
1:A:1614:VAL:O	1:A:1618:THR:HG23	2.11	0.49
1:A:2005:GLY:HA2	1:D:741:GLY:HA2	1.94	0.49
1:A:2047:GLN:NE2	1:A:2048:ASP:OD1	2.45	0.49
1:B:300:ALA:HA	1:B:303:PHE:HD2	1.76	0.49
1:B:1617:ALA:HA	1:B:1624:ILE:HD11	1.93	0.49
1:B:2448:LEU:HD23	1:B:2471:PRO:HB2	1.92	0.49
1:C:568:ILE:HD11	1:C:606:ASP:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:836:ALA:HB2	1:D:846:LEU:HD12	1.94	0.49
1:B:1614:VAL:O	1:B:1618:THR:HG23	2.11	0.49
1:B:1728:ASP:OD2	1:B:1730:LYS:NZ	2.41	0.49
1:B:2246:SER:HA	1:B:2250:LEU:HD23	1.94	0.49
1:C:557:ILE:HB	1:C:561:SER:OG	2.12	0.49
1:C:2004:GLN:H	1:C:2300:THR:HG22	1.76	0.49
1:C:2205:GLN:HA	1:D:2087:LYS:NZ	2.26	0.49
1:D:1617:ALA:HA	1:D:1624:ILE:HD11	1.94	0.49
1:E:1168:TYR:HB3	1:E:1200:LEU:HD11	1.93	0.49
1:A:197:ALA:N	1:A:948:THR:HG21	2.28	0.49
1:B:197:ALA:N	1:B:948:THR:HG21	2.27	0.49
1:D:2047:GLN:NE2	1:D:2048:ASP:OD1	2.45	0.49
1:E:2047:GLN:NE2	1:E:2048:ASP:OD1	2.46	0.49
1:A:1878:GLU:HA	1:A:1881:MET:HG3	1.94	0.49
1:A:2057:GLN:HG3	1:A:2241:LEU:CD1	2.42	0.49
1:E:347:PRO:HA	1:E:353:TYR:HA	1.95	0.49
1:A:348:PHE:CE1	1:A:352:ASN:HB3	2.48	0.49
1:B:507:SER:HB3	1:B:513:SER:HB2	1.94	0.49
1:C:1878:GLU:HA	1:C:1881:MET:HG3	1.94	0.49
1:E:348:PHE:CE1	1:E:352:ASN:HB3	2.48	0.49
1:A:470:ILE:HA	1:A:474:VAL:HG11	1.94	0.49
1:A:507:SER:HB3	1:A:513:SER:HB2	1.94	0.49
1:A:836:ALA:HB2	1:A:846:LEU:HD12	1.93	0.49
1:A:1617:ALA:HA	1:A:1624:ILE:HD11	1.94	0.49
1:A:2246:SER:HA	1:A:2250:LEU:HD23	1.94	0.49
1:D:1168:TYR:HB3	1:D:1200:LEU:HD11	1.94	0.49
1:E:568:ILE:HD11	1:E:606:ASP:HB2	1.93	0.49
1:B:348:PHE:CE1	1:B:352:ASN:HB3	2.48	0.49
1:B:836:ALA:HB2	1:B:846:LEU:HD12	1.94	0.49
1:C:197:ALA:N	1:C:948:THR:HG21	2.28	0.49
1:C:1617:ALA:HA	1:C:1624:ILE:HD11	1.94	0.49
1:D:2246:SER:HA	1:D:2250:LEU:HD23	1.94	0.49
1:E:557:ILE:HB	1:E:561:SER:OG	2.11	0.49
1:E:2057:GLN:HG3	1:E:2241:LEU:CD1	2.43	0.49
1:E:2246:SER:HA	1:E:2250:LEU:HD23	1.94	0.49
1:B:470:ILE:HA	1:B:474:VAL:HG11	1.94	0.49
1:E:197:ALA:N	1:E:948:THR:HG21	2.28	0.49
1:E:672:ASP:O	1:E:676:HIS:ND1	2.46	0.49
1:C:198:THR:HB	1:C:199:PRO:HA	1.95	0.48
1:C:371:LYS:HG2	1:C:377:GLU:HA	1.95	0.48
1:D:557:ILE:HB	1:D:561:SER:OG	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2118:ARG:HG2	1:E:2178:LYS:HB2	1.94	0.48
1:B:1870:GLN:HB3	1:B:1872:GLU:OE1	2.14	0.48
1:C:348:PHE:CE1	1:C:352:ASN:HB3	2.48	0.48
1:C:1124:ARG:NE	1:C:1142:SER:O	2.47	0.48
1:A:195:SER:HB3	1:A:198:THR:OG1	2.13	0.48
1:B:2118:ARG:HG2	1:B:2178:LYS:HB2	1.95	0.48
1:C:470:ILE:HA	1:C:474:VAL:HG11	1.93	0.48
1:C:2057:GLN:HG3	1:C:2241:LEU:CD1	2.43	0.48
1:D:348:PHE:CE1	1:D:352:ASN:HB3	2.48	0.48
1:B:347:PRO:HA	1:B:353:TYR:HA	1.95	0.48
1:B:1878:GLU:HA	1:B:1881:MET:HG3	1.95	0.48
1:C:2118:ARG:HG2	1:C:2178:LYS:HB2	1.96	0.48
1:D:198:THR:HB	1:D:199:PRO:HA	1.95	0.48
1:D:1878:GLU:HA	1:D:1881:MET:HG3	1.95	0.48
1:B:195:SER:HB3	1:B:198:THR:OG1	2.14	0.48
1:D:2057:GLN:HG3	1:D:2241:LEU:CD1	2.43	0.48
1:E:507:SER:HB3	1:E:513:SER:HB2	1.95	0.48
1:E:1172:LEU:HD11	1:E:1196:TYR:HB3	1.95	0.48
1:A:458:GLU:OE2	1:A:506:ARG:NH1	2.35	0.48
1:A:462:ARG:HH11	1:A:506:ARG:HH11	1.61	0.48
1:A:1870:GLN:HB3	1:A:1872:GLU:OE1	2.13	0.48
1:D:672:ASP:O	1:D:676:HIS:ND1	2.46	0.48
1:D:1909:ARG:HH11	1:D:1913:ILE:HD12	1.79	0.48
1:D:2204:LYS:C	1:E:2087:LYS:HZ3	2.14	0.48
1:A:1058:ASP:O	1:A:1062:GLN:HG3	2.14	0.48
1:B:462:ARG:HH11	1:B:506:ARG:HH11	1.62	0.48
1:C:1870:GLN:HB3	1:C:1872:GLU:OE1	2.14	0.48
1:D:197:ALA:N	1:D:948:THR:HG21	2.28	0.48
1:D:347:PRO:HA	1:D:353:TYR:HA	1.96	0.48
1:A:318:VAL:HG23	1:A:319:ASN:H	1.79	0.48
1:A:2182:SER:HG	1:C:1067:SER:HG	1.53	0.48
1:B:2067:ASN:HB3	1:B:2227:LEU:HD21	1.95	0.48
1:D:195:SER:HB3	1:D:198:THR:OG1	2.14	0.48
1:D:568:ILE:HD11	1:D:606:ASP:HB2	1.94	0.48
1:B:741:GLY:HA2	1:D:2005:GLY:HA2	1.95	0.48
1:D:371:LYS:HG2	1:D:377:GLU:HA	1.96	0.48
1:A:347:PRO:HA	1:A:353:TYR:HA	1.96	0.48
1:C:694:PRO:HA	1:C:705:GLU:OE1	2.14	0.48
1:C:741:GLY:HA2	1:E:2005:GLY:HA2	1.96	0.48
1:C:2246:SER:HA	1:C:2250:LEU:HD23	1.94	0.48
1:D:1124:ARG:NE	1:D:1142:SER:O	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1870:GLN:HB3	1:D:1872:GLU:OE1	2.14	0.48
1:D:2445:CYS:SG	1:E:2327:ARG:NH1	2.87	0.48
1:E:283:LYS:HB2	1:E:293:LEU:HD22	1.96	0.48
1:E:1617:ALA:HA	1:E:1624:ILE:HD11	1.94	0.48
1:A:2341:TYR:OH	1:A:2390:SER:O	2.19	0.47
1:C:181:ASN:HD21	1:C:184:LYS:HG2	1.79	0.47
1:E:198:THR:HB	1:E:199:PRO:HA	1.95	0.47
1:A:198:THR:HB	1:A:199:PRO:HA	1.96	0.47
1:A:2256:GLY:HA3	1:E:698:ALA:HB2	1.96	0.47
1:B:198:THR:HB	1:B:199:PRO:HA	1.95	0.47
1:B:2004:GLN:H	1:B:2300:THR:HG22	1.78	0.47
1:C:672:ASP:O	1:C:676:HIS:ND1	2.46	0.47
1:E:836:ALA:HB2	1:E:846:LEU:HD12	1.94	0.47
1:E:1730:LYS:HZ3	1:E:1732:ILE:HD12	1.78	0.47
1:A:1108:THR:OG1	1:A:1128:HIS:NE2	2.38	0.47
1:A:1168:TYR:HB3	1:A:1200:LEU:HD11	1.95	0.47
1:C:283:LYS:HB2	1:C:293:LEU:HD22	1.96	0.47
1:C:1909:ARG:HH11	1:C:1913:ILE:HD12	1.79	0.47
1:C:2018:ARG:NH1	1:C:2466:ASP:O	2.46	0.47
1:D:2004:GLN:H	1:D:2300:THR:HG22	1.77	0.47
1:E:195:SER:HB3	1:E:198:THR:OG1	2.14	0.47
1:E:1058:ASP:O	1:E:1062:GLN:HG3	2.15	0.47
1:E:1124:ARG:NE	1:E:1142:SER:O	2.46	0.47
1:A:371:LYS:HG2	1:A:377:GLU:HA	1.95	0.47
1:A:2004:GLN:H	1:A:2300:THR:HG22	1.79	0.47
1:B:1730:LYS:HZ3	1:B:1732:ILE:HD12	1.78	0.47
1:D:181:ASN:HD21	1:D:184:LYS:HG2	1.79	0.47
1:D:507:SER:HB3	1:D:513:SER:HB2	1.95	0.47
1:E:646:TRP:CZ2	1:E:768:SER:HB3	2.50	0.47
1:E:1878:GLU:HA	1:E:1881:MET:HG3	1.95	0.47
1:A:694:PRO:HA	1:A:705:GLU:OE1	2.15	0.47
1:A:741:GLY:HA2	1:C:2005:GLY:HA2	1.95	0.47
1:A:1730:LYS:HZ3	1:A:1732:ILE:HD12	1.79	0.47
1:B:1124:ARG:NE	1:B:1142:SER:O	2.47	0.47
1:B:1909:ARG:HH11	1:B:1913:ILE:HD12	1.79	0.47
1:C:318:VAL:HG23	1:C:319:ASN:H	1.79	0.47
1:D:462:ARG:HH11	1:D:506:ARG:HH11	1.62	0.47
1:D:698:ALA:HB2	1:E:2256:GLY:HA3	1.97	0.47
1:E:2004:GLN:H	1:E:2300:THR:HG22	1.79	0.47
1:B:672:ASP:O	1:B:676:HIS:ND1	2.47	0.47
1:B:702:LEU:HD22	1:B:708:ALA:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2204:LYS:C	1:C:2087:LYS:HZ3	2.15	0.47
1:C:195:SER:HB3	1:C:198:THR:OG1	2.14	0.47
1:C:2067:ASN:HB3	1:C:2227:LEU:HD21	1.97	0.47
1:A:672:ASP:O	1:A:676:HIS:ND1	2.47	0.47
1:B:505:GLN:HE22	1:B:582:LEU:HD13	1.79	0.47
1:C:646:TRP:CZ2	1:C:768:SER:HB3	2.50	0.47
1:C:702:LEU:HD22	1:C:708:ALA:HB2	1.96	0.47
1:C:1117:ASP:OD1	1:C:1118:ALA:N	2.40	0.47
1:C:1883:TYR:HD2	1:C:1970:LEU:HD11	1.80	0.47
1:D:646:TRP:CZ2	1:D:768:SER:HB3	2.50	0.47
1:D:1058:ASP:O	1:D:1062:GLN:HG3	2.15	0.47
1:D:1883:TYR:HD2	1:D:1970:LEU:HD11	1.79	0.47
1:E:462:ARG:HH11	1:E:506:ARG:HH11	1.63	0.47
1:E:1909:ARG:HH11	1:E:1913:ILE:HD12	1.80	0.47
1:A:698:ALA:HB2	1:B:2256:GLY:HA3	1.96	0.47
1:A:1909:ARG:HH11	1:A:1913:ILE:HD12	1.79	0.47
1:A:2118:ARG:HG2	1:A:2178:LYS:HB2	1.95	0.47
1:B:2005:GLY:HA2	1:E:741:GLY:HA2	1.97	0.47
1:A:536:ILE:HD13	1:A:547:ARG:HB2	1.96	0.47
1:C:347:PRO:HA	1:C:353:TYR:HA	1.96	0.47
1:D:702:LEU:HD22	1:D:708:ALA:HB2	1.96	0.47
1:D:1168:TYR:HD2	1:D:1200:LEU:HD11	1.80	0.47
1:E:1870:GLN:HB3	1:E:1872:GLU:OE1	2.14	0.47
1:A:127:ARG:HG3	1:A:127:ARG:HH11	1.80	0.47
1:A:1098:HIS:HE1	1:A:1100:ASN:HB3	1.81	0.47
1:B:181:ASN:HD21	1:B:184:LYS:HG2	1.79	0.47
1:B:318:VAL:HG23	1:B:319:ASN:H	1.79	0.47
1:B:1883:TYR:HD2	1:B:1970:LEU:HD11	1.80	0.47
1:D:127:ARG:HG3	1:D:127:ARG:HH11	1.80	0.47
1:D:505:GLN:HE22	1:D:582:LEU:HD13	1.79	0.47
1:E:505:GLN:HE22	1:E:582:LEU:HD13	1.80	0.47
1:A:1172:LEU:HD11	1:A:1196:TYR:HB3	1.96	0.46
1:B:694:PRO:HA	1:B:705:GLU:OE1	2.15	0.46
1:B:1058:ASP:O	1:B:1062:GLN:HG3	2.15	0.46
1:C:127:ARG:HG3	1:C:127:ARG:HH11	1.80	0.46
1:C:1058:ASP:O	1:C:1062:GLN:HG3	2.15	0.46
1:E:127:ARG:HG3	1:E:127:ARG:HH11	1.80	0.46
1:A:702:LEU:HD22	1:A:708:ALA:HB2	1.96	0.46
1:B:283:LYS:HB2	1:B:293:LEU:HD22	1.96	0.46
1:B:2183:GLU:OE1	1:C:2108:ASN:ND2	2.42	0.46
1:C:505:GLN:HE22	1:C:582:LEU:HD13	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:VAL:HG23	1:D:319:ASN:H	1.79	0.46
1:E:694:PRO:HA	1:E:705:GLU:OE1	2.15	0.46
1:A:646:TRP:CZ2	1:A:768:SER:HB3	2.51	0.46
1:D:2018:ARG:NH1	1:D:2466:ASP:O	2.47	0.46
1:D:2067:ASN:HB3	1:D:2227:LEU:HD21	1.97	0.46
1:A:1124:ARG:NE	1:A:1142:SER:O	2.47	0.46
1:B:1098:HIS:HE1	1:B:1100:ASN:HB3	1.80	0.46
1:D:283:LYS:HB2	1:D:293:LEU:HD22	1.96	0.46
1:E:318:VAL:HG23	1:E:319:ASN:H	1.79	0.46
1:E:318:VAL:HG23	1:E:319:ASN:N	2.30	0.46
1:A:1892:ASP:OD1	1:A:1892:ASP:N	2.49	0.46
1:B:127:ARG:HG3	1:B:127:ARG:HH11	1.81	0.46
1:D:1892:ASP:OD1	1:D:1892:ASP:N	2.49	0.46
1:E:1892:ASP:OD1	1:E:1892:ASP:N	2.49	0.46
1:A:2067:ASN:HB3	1:A:2227:LEU:HD21	1.96	0.46
1:B:537:ASP:HA	1:B:577:LYS:HA	1.98	0.46
1:C:1172:LEU:HD11	1:C:1196:TYR:HB3	1.96	0.46
1:D:694:PRO:HA	1:D:705:GLU:OE1	2.15	0.46
1:E:702:LEU:HD22	1:E:708:ALA:HB2	1.96	0.46
1:A:318:VAL:HG23	1:A:319:ASN:N	2.31	0.46
1:A:505:GLN:HE22	1:A:582:LEU:HD13	1.80	0.46
1:B:371:LYS:HG2	1:B:377:GLU:HA	1.96	0.46
1:D:1172:LEU:HD11	1:D:1196:TYR:HB3	1.97	0.46
1:A:711:VAL:HG11	1:A:763:GLU:OE2	2.16	0.46
1:B:646:TRP:CZ2	1:B:768:SER:HB3	2.50	0.46
1:B:2362:SER:OG	1:B:2502:LYS:NZ	2.47	0.46
1:D:536:ILE:HD13	1:D:547:ARG:HB2	1.97	0.46
1:E:371:LYS:HG2	1:E:377:GLU:HA	1.96	0.46
1:B:341:MET:HE3	1:B:410:LEU:HD22	1.98	0.46
1:B:2057:GLN:HG3	1:B:2241:LEU:CD1	2.44	0.46
1:C:370:ILE:HG13	1:C:410:LEU:HG	1.98	0.46
1:C:698:ALA:HB2	1:D:2256:GLY:HA3	1.98	0.46
1:D:318:VAL:HG23	1:D:319:ASN:N	2.31	0.46
1:D:1730:LYS:HZ3	1:D:1732:ILE:HD12	1.80	0.46
1:D:341:MET:CE	1:D:410:LEU:HD22	2.46	0.46
1:A:1168:TYR:HD2	1:A:1200:LEU:HD11	1.80	0.45
1:B:536:ILE:HD13	1:B:547:ARG:HB2	1.97	0.45
1:D:1676:ILE:HD12	1:D:1690:LEU:HD13	1.98	0.45
1:E:181:ASN:HD21	1:E:184:LYS:HG2	1.80	0.45
1:B:370:ILE:HG13	1:B:410:LEU:HG	1.98	0.45
1:B:711:VAL:HG11	1:B:763:GLU:OE2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:505:GLN:NE2	1:D:582:LEU:HD13	2.32	0.45
1:D:711:VAL:HG11	1:D:763:GLU:OE2	2.16	0.45
1:D:1071:ALA:HB2	1:D:1791:GLU:OE2	2.17	0.45
1:D:2118:ARG:HG2	1:D:2178:LYS:HB2	1.97	0.45
1:E:341:MET:CE	1:E:410:LEU:HD22	2.46	0.45
1:A:197:ALA:H	1:A:948:THR:HG21	1.82	0.45
1:A:2278:GLN:OE1	1:A:2281:ARG:NH2	2.50	0.45
1:C:505:GLN:NE2	1:C:582:LEU:HD13	2.31	0.45
1:D:370:ILE:HG13	1:D:410:LEU:HG	1.98	0.45
1:E:536:ILE:HD13	1:E:547:ARG:HB2	1.97	0.45
1:E:1098:HIS:HE1	1:E:1100:ASN:HB3	1.81	0.45
1:E:2018:ARG:NH1	1:E:2466:ASP:O	2.49	0.45
1:A:181:ASN:HD21	1:A:184:LYS:HG2	1.80	0.45
1:A:2018:ARG:NH1	1:A:2466:ASP:O	2.46	0.45
1:A:2204:LYS:C	1:B:2087:LYS:HZ3	2.14	0.45
1:B:318:VAL:HG23	1:B:319:ASN:N	2.31	0.45
1:B:1168:TYR:HD2	1:B:1200:LEU:HD11	1.81	0.45
1:C:2205:GLN:HA	1:D:2087:LYS:HZ2	1.82	0.45
1:A:341:MET:CE	1:A:410:LEU:HD22	2.46	0.45
1:A:534:GLU:OE2	1:A:580:ASN:ND2	2.49	0.45
1:C:197:ALA:H	1:C:948:THR:HG21	1.82	0.45
1:C:318:VAL:HG23	1:C:319:ASN:N	2.31	0.45
1:C:1098:HIS:HE1	1:C:1100:ASN:HB3	1.81	0.45
1:A:1056:MET:HG3	1:A:1081:TYR:HE1	1.82	0.45
1:B:1056:MET:HG3	1:B:1081:TYR:HE1	1.82	0.45
1:E:370:ILE:HG13	1:E:410:LEU:HG	1.99	0.45
1:A:283:LYS:HB2	1:A:293:LEU:HD22	1.98	0.45
1:A:505:GLN:NE2	1:A:582:LEU:HD13	2.32	0.45
1:A:1676:ILE:HD12	1:A:1690:LEU:HD13	1.98	0.45
1:B:341:MET:CE	1:B:410:LEU:HD22	2.47	0.45
1:B:1172:LEU:HD11	1:B:1196:TYR:HB3	1.97	0.45
1:C:341:MET:CE	1:C:410:LEU:HD22	2.46	0.45
1:D:1098:HIS:HE1	1:D:1100:ASN:HB3	1.81	0.45
1:D:2132:ARG:HH11	1:D:2163:TYR:HB3	1.82	0.45
1:E:210:VAL:HG22	1:E:926:LEU:HD11	1.99	0.45
1:E:1163:TYR:CD1	1:E:1245:LEU:HD22	2.52	0.45
1:E:1168:TYR:HD2	1:E:1200:LEU:HD11	1.81	0.45
1:B:197:ALA:H	1:B:948:THR:HG21	1.81	0.45
1:D:2362:SER:OG	1:D:2502:LYS:NZ	2.47	0.45
1:E:464:VAL:HG21	1:E:474:VAL:HA	1.98	0.45
1:E:505:GLN:NE2	1:E:582:LEU:HD13	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:971:LEU:O	1:A:973:ILE:HG12	2.17	0.45
1:B:505:GLN:NE2	1:B:582:LEU:HD13	2.32	0.45
1:C:1163:TYR:CD1	1:C:1245:LEU:HD22	2.52	0.45
1:C:1268:TYR:N	1:C:1276:LYS:O	2.48	0.45
1:C:2132:ARG:HH11	1:C:2163:TYR:HB3	1.81	0.45
1:B:1676:ILE:HD12	1:B:1690:LEU:HD13	1.98	0.45
1:C:1168:TYR:HD2	1:C:1200:LEU:HD11	1.81	0.45
1:C:2445:CYS:SG	1:D:2327:ARG:NH1	2.90	0.45
1:D:601:THR:HG22	1:D:604:GLU:OE1	2.17	0.45
1:D:971:LEU:O	1:D:973:ILE:HG12	2.17	0.45
1:E:2067:ASN:HB3	1:E:2227:LEU:HD21	1.98	0.45
1:A:370:ILE:HG13	1:A:410:LEU:HG	1.99	0.44
1:A:1071:ALA:HB2	1:A:1791:GLU:OE2	2.17	0.44
1:B:1892:ASP:OD1	1:B:1892:ASP:N	2.49	0.44
1:C:711:VAL:HG11	1:C:763:GLU:OE2	2.16	0.44
1:D:2416:SER:HB2	1:D:2510:HIS:HB2	1.99	0.44
1:E:197:ALA:H	1:E:948:THR:HG21	1.82	0.44
1:E:534:GLU:OE2	1:E:580:ASN:ND2	2.50	0.44
1:E:1071:ALA:HB2	1:E:1791:GLU:OE2	2.16	0.44
1:E:1676:ILE:HD12	1:E:1690:LEU:HD13	1.99	0.44
1:E:2398:ILE:HB	1:E:2477:ILE:HG21	1.99	0.44
1:A:2087:LYS:HZ3	1:E:2204:LYS:C	2.15	0.44
1:C:2398:ILE:HB	1:C:2477:ILE:HG21	1.99	0.44
1:D:341:MET:HE3	1:D:410:LEU:HD22	1.98	0.44
1:D:453:SER:HB3	1:D:456:ILE:HG12	1.99	0.44
1:E:663:LEU:HD22	1:E:749:GLN:NE2	2.33	0.44
1:E:1056:MET:HG3	1:E:1081:TYR:HE1	1.82	0.44
1:A:487:ARG:O	1:A:487:ARG:NH1	2.46	0.44
1:B:971:LEU:O	1:B:973:ILE:HG12	2.17	0.44
1:B:1071:ALA:HB2	1:B:1791:GLU:OE2	2.17	0.44
1:E:711:VAL:HG11	1:E:763:GLU:OE2	2.16	0.44
1:A:1887:LEU:HD12	1:A:1887:LEU:HA	1.88	0.44
1:A:2398:ILE:HB	1:A:2477:ILE:HG21	2.00	0.44
1:C:536:ILE:HD13	1:C:547:ARG:HB2	1.98	0.44
1:D:464:VAL:HG21	1:D:474:VAL:HA	2.00	0.44
1:D:1163:TYR:CD1	1:D:1245:LEU:HD22	2.52	0.44
1:E:1094:ILE:HD11	1:E:1113:LEU:HB2	2.00	0.44
1:C:462:ARG:NH1	1:C:506:ARG:HH11	2.16	0.44
1:C:534:GLU:OE2	1:C:580:ASN:ND2	2.50	0.44
1:C:724:ALA:O	1:C:729:LYS:NZ	2.35	0.44
1:D:197:ALA:H	1:D:948:THR:HG21	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1056:MET:HG3	1:D:1081:TYR:CE1	2.53	0.44
1:E:971:LEU:O	1:E:973:ILE:HG12	2.18	0.44
1:A:1163:TYR:CD1	1:A:1245:LEU:HD22	2.52	0.44
1:B:464:VAL:HG21	1:B:474:VAL:HA	2.00	0.44
1:B:534:GLU:OE2	1:B:580:ASN:ND2	2.50	0.44
1:C:971:LEU:O	1:C:973:ILE:HG12	2.17	0.44
1:D:1056:MET:HG3	1:D:1081:TYR:HE1	1.82	0.44
1:A:1094:ILE:HD11	1:A:1113:LEU:HB2	2.00	0.44
1:B:1094:ILE:HD11	1:B:1113:LEU:HB2	2.00	0.44
1:C:1071:ALA:HB2	1:C:1791:GLU:OE2	2.17	0.44
1:C:2362:SER:OG	1:C:2502:LYS:NZ	2.50	0.44
1:D:210:VAL:HG22	1:D:926:LEU:HD11	2.00	0.44
1:D:1094:ILE:HD11	1:D:1113:LEU:HB2	2.00	0.44
1:E:2278:GLN:OE1	1:E:2281:ARG:NH2	2.50	0.44
1:A:1050:ARG:NH2	1:A:1770:GLU:OE1	2.51	0.44
1:B:1163:TYR:CD1	1:B:1245:LEU:HD22	2.52	0.44
1:E:1056:MET:HG3	1:E:1081:TYR:CE1	2.53	0.44
1:E:1675:ILE:HD11	1:E:1678:SER:HB2	2.00	0.44
1:A:210:VAL:HG22	1:A:926:LEU:HD11	1.99	0.44
1:A:464:VAL:HG21	1:A:474:VAL:HA	1.99	0.44
1:A:1048:THR:HG23	1:A:1061:LEU:HD11	2.00	0.44
1:A:663:LEU:HD22	1:A:749:GLN:NE2	2.33	0.43
1:A:2066:THR:HG21	1:E:2226:SER:HB2	1.99	0.43
1:B:453:SER:HB3	1:B:456:ILE:HG12	2.00	0.43
1:B:1048:THR:HG23	1:B:1061:LEU:HD11	2.00	0.43
1:C:595:ALA:HB2	1:C:605:LEU:HD22	1.99	0.43
1:C:1676:ILE:HD12	1:C:1690:LEU:HD13	1.99	0.43
1:D:1135:LYS:HA	1:D:1135:LYS:HD3	1.82	0.43
1:E:2132:ARG:HH11	1:E:2163:TYR:HB3	1.83	0.43
1:B:1056:MET:HG3	1:B:1081:TYR:CE1	2.53	0.43
1:C:210:VAL:HG22	1:C:926:LEU:HD11	2.00	0.43
1:C:2458:GLY:O	1:D:2330:GLU:HB2	2.19	0.43
1:A:1056:MET:HG3	1:A:1081:TYR:CE1	2.53	0.43
1:B:2458:GLY:O	1:C:2330:GLU:HB2	2.18	0.43
1:C:601:THR:HG22	1:C:604:GLU:OE1	2.18	0.43
1:D:1652:LEU:HA	1:D:1655:HIS:HB3	2.00	0.43
1:A:601:THR:HG22	1:A:604:GLU:OE1	2.18	0.43
1:A:1268:TYR:N	1:A:1276:LYS:O	2.48	0.43
1:A:1963:LEU:HD23	1:A:1963:LEU:HA	1.93	0.43
1:B:579:LYS:HG3	1:B:581:ASN:H	1.84	0.43
1:C:453:SER:HB3	1:C:456:ILE:HG12	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:VAL:HG21	1:C:474:VAL:HA	2.01	0.43
1:C:1730:LYS:HZ3	1:C:1732:ILE:HD12	1.84	0.43
1:E:601:THR:HG22	1:E:604:GLU:OE1	2.18	0.43
1:E:1048:THR:HG23	1:E:1061:LEU:HD11	2.00	0.43
1:B:1652:LEU:HA	1:B:1655:HIS:HB3	2.01	0.43
1:C:320:SER:HB2	1:C:323:GLY:HA2	2.01	0.43
1:E:462:ARG:NH1	1:E:506:ARG:HH11	2.17	0.43
1:A:1652:LEU:HA	1:A:1655:HIS:HB3	2.00	0.43
1:B:210:VAL:HG22	1:B:926:LEU:HD11	2.00	0.43
1:C:579:LYS:HG3	1:C:581:ASN:H	1.84	0.43
1:D:534:GLU:OE2	1:D:580:ASN:ND2	2.51	0.43
1:D:595:ALA:HB2	1:D:605:LEU:HD22	2.00	0.43
1:D:1050:ARG:NH2	1:D:1770:GLU:OE1	2.51	0.43
1:A:341:MET:HE1	1:A:410:LEU:HD22	2.01	0.43
1:A:2458:GLY:O	1:B:2330:GLU:HB2	2.19	0.43
1:B:320:SER:HB2	1:B:323:GLY:HA2	2.01	0.43
1:B:2112:ASN:HA	1:B:2115:MET:HG2	2.01	0.43
1:C:537:ASP:HA	1:C:577:LYS:HA	2.00	0.43
1:C:965:ASP:OD1	1:C:966:ASP:N	2.52	0.43
1:C:1056:MET:HG3	1:C:1081:TYR:CE1	2.54	0.43
1:C:1094:ILE:HD11	1:C:1113:LEU:HB2	2.01	0.43
1:D:558:ASP:OD1	1:D:558:ASP:N	2.48	0.43
1:D:2398:ILE:HB	1:D:2477:ILE:HG21	2.00	0.43
1:A:714:TRP:CZ3	1:A:762:LEU:HD22	2.54	0.43
1:B:601:THR:HG22	1:B:604:GLU:OE1	2.19	0.43
1:B:965:ASP:OD1	1:B:966:ASP:N	2.52	0.43
1:C:116:ALA:HB1	1:C:150:LEU:HD22	2.01	0.43
1:C:848:GLN:OE1	1:C:892:GLN:NE2	2.52	0.43
1:C:1048:THR:HG23	1:C:1061:LEU:HD11	2.00	0.43
1:D:320:SER:HB2	1:D:323:GLY:HA2	2.01	0.43
1:E:2416:SER:HB2	1:E:2510:HIS:HB2	2.01	0.43
1:E:2452:HIS:CE1	1:E:2456:ASP:HB2	2.54	0.43
1:A:462:ARG:NH1	1:A:506:ARG:HH11	2.16	0.43
1:B:595:ALA:HB2	1:B:605:LEU:HD22	2.00	0.43
1:B:663:LEU:HD22	1:B:749:GLN:NE2	2.34	0.43
1:B:1766:LEU:O	1:B:1770:GLU:HB2	2.19	0.43
1:C:714:TRP:CZ3	1:C:762:LEU:HD22	2.54	0.43
1:C:1607:THR:HG21	1:C:1768:PHE:HZ	1.83	0.43
1:C:1675:ILE:HD11	1:C:1678:SER:HB2	2.01	0.43
1:D:537:ASP:HA	1:D:577:LYS:HA	2.01	0.43
1:D:1048:THR:HG23	1:D:1061:LEU:HD11	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:453:SER:HB3	1:E:456:ILE:HG12	1.99	0.43
1:A:2416:SER:HB2	1:A:2510:HIS:HB2	2.00	0.43
1:B:2226:SER:HB2	1:C:2066:THR:HG21	2.01	0.43
1:C:1652:LEU:HA	1:C:1655:HIS:HB3	2.01	0.43
1:C:1892:ASP:OD1	1:C:1892:ASP:N	2.49	0.43
1:D:2226:SER:HB2	1:E:2066:THR:HG21	2.01	0.43
1:E:595:ALA:HB2	1:E:605:LEU:HD22	2.00	0.43
1:E:714:TRP:CZ3	1:E:762:LEU:HD22	2.54	0.43
1:E:1050:ARG:NH2	1:E:1770:GLU:OE1	2.52	0.43
1:A:2330:GLU:HB2	1:E:2458:GLY:O	2.18	0.42
1:B:1050:ARG:NH2	1:B:1770:GLU:OE1	2.52	0.42
1:B:1704:HIS:CE1	1:B:1727:ARG:H	2.37	0.42
1:D:462:ARG:NH1	1:D:506:ARG:HH11	2.17	0.42
1:D:663:LEU:HD22	1:D:749:GLN:NE2	2.34	0.42
1:D:1675:ILE:HD11	1:D:1678:SER:HB2	2.01	0.42
1:D:2452:HIS:CE1	1:D:2456:ASP:HB2	2.54	0.42
1:E:368:LEU:HG	1:E:370:ILE:CD1	2.50	0.42
1:A:1766:LEU:O	1:A:1770:GLU:HB2	2.20	0.42
1:B:2398:ILE:HB	1:B:2477:ILE:HG21	2.00	0.42
1:C:663:LEU:HD22	1:C:749:GLN:NE2	2.34	0.42
1:C:1056:MET:HG3	1:C:1081:TYR:HE1	1.83	0.42
1:C:1135:LYS:HA	1:C:1135:LYS:HD3	1.82	0.42
1:D:1268:TYR:N	1:D:1276:LYS:O	2.49	0.42
1:E:1652:LEU:HA	1:E:1655:HIS:HB3	2.00	0.42
1:A:368:LEU:HG	1:A:370:ILE:CD1	2.50	0.42
1:A:453:SER:HB3	1:A:456:ILE:HG12	2.00	0.42
1:A:497:ILE:HG21	1:A:589:TYR:CD2	2.54	0.42
1:A:1675:ILE:HD11	1:A:1678:SER:HB2	2.00	0.42
1:B:253:GLU:O	1:B:442:LYS:NZ	2.38	0.42
1:C:2112:ASN:HA	1:C:2115:MET:HG2	2.01	0.42
1:C:2226:SER:HB2	1:D:2066:THR:HG21	2.00	0.42
1:C:2278:GLN:OE1	1:C:2281:ARG:NH2	2.51	0.42
1:D:1170:LEU:HD22	1:D:1198:LEU:HD11	2.01	0.42
1:A:2132:ARG:HH11	1:A:2163:TYR:HB3	1.82	0.42
1:B:368:LEU:HG	1:B:370:ILE:CD1	2.49	0.42
1:B:2441:LEU:HG	1:B:2445:CYS:HB2	2.02	0.42
1:D:368:LEU:HG	1:D:370:ILE:CD1	2.50	0.42
1:D:1766:LEU:O	1:D:1770:GLU:HB2	2.19	0.42
1:A:595:ALA:HB2	1:A:605:LEU:HD22	2.01	0.42
1:A:1607:THR:HG21	1:A:1768:PHE:HZ	1.84	0.42
1:A:2226:SER:HB2	1:B:2066:THR:HG21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:848:GLN:OE1	1:B:892:GLN:NE2	2.53	0.42
1:C:341:MET:HE3	1:C:410:LEU:HD22	2.01	0.42
1:C:1050:ARG:NH2	1:C:1770:GLU:OE1	2.53	0.42
1:C:1766:LEU:O	1:C:1770:GLU:HB2	2.19	0.42
1:D:2458:GLY:O	1:E:2330:GLU:HB2	2.19	0.42
1:E:1170:LEU:HD22	1:E:1198:LEU:HD11	2.01	0.42
1:E:1704:HIS:CE1	1:E:1727:ARG:H	2.38	0.42
1:A:926:LEU:HD22	1:A:930:GLN:HB3	2.02	0.42
1:A:2431:ALA:O	1:A:2450:VAL:HG12	2.20	0.42
1:B:174:LYS:HG2	1:B:185:VAL:HG21	2.02	0.42
1:B:2202:GLU:O	1:B:2205:GLN:HG2	2.20	0.42
1:C:926:LEU:HD22	1:C:930:GLN:HB3	2.02	0.42
1:C:2416:SER:HB2	1:C:2510:HIS:HB2	2.01	0.42
1:D:593:LEU:O	1:D:597:ILE:HG12	2.20	0.42
1:D:812:ASN:HA	1:E:1998:ALA:HB2	2.02	0.42
1:D:1607:THR:HG21	1:D:1768:PHE:HZ	1.84	0.42
1:E:537:ASP:HA	1:E:577:LYS:HA	2.01	0.42
1:A:579:LYS:HG3	1:A:581:ASN:H	1.85	0.42
1:B:462:ARG:NH1	1:B:506:ARG:HH11	2.16	0.42
1:B:1607:THR:HG21	1:B:1768:PHE:HZ	1.85	0.42
1:B:2278:GLN:OE1	1:B:2281:ARG:NH2	2.51	0.42
1:B:1113:LEU:HD11	1:B:1119:GLY:HA3	2.01	0.42
1:C:218:LEU:HB3	1:C:221:LEU:HB2	2.02	0.42
1:D:2033:LEU:CD1	1:D:2266:TYR:HA	2.50	0.42
1:E:320:SER:HB2	1:E:323:GLY:HA2	2.00	0.42
1:E:860:PRO:HA	1:E:861:PRO:HD3	1.97	0.42
1:B:218:LEU:HB3	1:B:221:LEU:HB2	2.02	0.42
1:B:593:LEU:O	1:B:597:ILE:HG12	2.20	0.42
1:B:926:LEU:HD22	1:B:930:GLN:HB3	2.02	0.42
1:B:2452:HIS:CE1	1:B:2456:ASP:HB2	2.54	0.42
1:C:1036:GLN:O	1:C:1040:TYR:N	2.41	0.42
1:D:965:ASP:OD1	1:D:966:ASP:N	2.52	0.42
1:E:579:LYS:HG3	1:E:581:ASN:H	1.84	0.42
1:E:724:ALA:O	1:E:729:LYS:NZ	2.35	0.42
1:B:2033:LEU:CD1	1:B:2266:TYR:HA	2.50	0.42
1:C:2033:LEU:CD1	1:C:2266:TYR:HA	2.50	0.42
1:D:2207:ASP:O	1:D:2211:LYS:HG2	2.20	0.42
1:E:593:LEU:O	1:E:597:ILE:HG12	2.20	0.42
1:E:1818:VAL:HG12	1:E:1820:PRO:HD2	2.02	0.42
1:E:2441:LEU:HG	1:E:2445:CYS:HB2	2.02	0.42
1:A:537:ASP:HA	1:A:577:LYS:HA	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1818:VAL:HG12	1:A:1820:PRO:HD2	2.02	0.41
1:B:371:LYS:HA	1:B:377:GLU:HA	2.02	0.41
1:C:2202:GLU:O	1:C:2205:GLN:HG2	2.20	0.41
1:C:2355:GLN:HG2	1:C:2356:GLU:OE1	2.20	0.41
1:D:1818:VAL:HG12	1:D:1820:PRO:HD2	2.02	0.41
1:A:2202:GLU:O	1:A:2205:GLN:HG2	2.20	0.41
1:A:2330:GLU:HB3	1:E:2460:PHE:CZ	2.55	0.41
1:B:1279:THR:HG22	1:B:1281:GLU:H	1.86	0.41
1:B:1675:ILE:HD11	1:B:1678:SER:HB2	2.01	0.41
1:B:1887:LEU:HD12	1:B:1887:LEU:HA	1.88	0.41
1:C:593:LEU:O	1:C:597:ILE:HG12	2.20	0.41
1:C:2441:LEU:HG	1:C:2445:CYS:HB2	2.02	0.41
1:C:2452:HIS:CE1	1:C:2456:ASP:HB2	2.55	0.41
1:C:2460:PHE:CZ	1:D:2330:GLU:HB3	2.55	0.41
1:D:160:SER:HA	1:D:982:LYS:HA	2.03	0.41
1:E:926:LEU:HD22	1:E:930:GLN:HB3	2.02	0.41
1:E:965:ASP:OD1	1:E:966:ASP:N	2.52	0.41
1:E:1135:LYS:HA	1:E:1135:LYS:HD3	1.82	0.41
1:A:848:GLN:OE1	1:A:892:GLN:NE2	2.53	0.41
1:A:2452:HIS:CE1	1:A:2456:ASP:HB2	2.54	0.41
1:A:2460:PHE:CZ	1:B:2330:GLU:HB3	2.56	0.41
1:C:1800:TRP:CZ2	1:C:1802:PRO:HG3	2.55	0.41
1:C:2431:ALA:O	1:C:2450:VAL:HG12	2.21	0.41
1:D:218:LEU:HB3	1:D:221:LEU:HB2	2.02	0.41
1:E:2112:ASN:HA	1:E:2115:MET:HG2	2.03	0.41
1:E:2431:ALA:O	1:E:2450:VAL:HG12	2.20	0.41
1:A:2112:ASN:HA	1:A:2115:MET:HG2	2.02	0.41
1:A:2207:ASP:O	1:A:2211:LYS:HG2	2.21	0.41
1:A:2470:LEU:N	1:A:2473:GLU:OE1	2.52	0.41
1:C:268:PHE:HZ	1:C:441:ASN:HB2	1.85	0.41
1:D:2441:LEU:HG	1:D:2445:CYS:HB2	2.02	0.41
1:E:661:LYS:HB2	1:E:750:GLU:HB2	2.03	0.41
1:E:2341:TYR:CD2	1:E:2353:LEU:HD11	2.55	0.41
1:A:320:SER:HB2	1:A:323:GLY:HA2	2.01	0.41
1:A:1111:ILE:HG13	1:A:1160:PRO:HD3	2.03	0.41
1:B:2416:SER:HB2	1:B:2510:HIS:HB2	2.02	0.41
1:C:538:LEU:HD12	1:C:566:LEU:HD22	2.02	0.41
1:A:218:LEU:HB3	1:A:221:LEU:HB2	2.02	0.41
1:B:2182:SER:OG	1:D:1067:SER:N	2.54	0.41
1:C:1244:THR:HG21	1:C:1268:TYR:CD1	2.55	0.41
1:C:2341:TYR:CD2	1:C:2353:LEU:HD11	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:LYS:HG2	1:D:185:VAL:HG21	2.03	0.41
1:D:926:LEU:HD22	1:D:930:GLN:HB3	2.02	0.41
1:D:1279:THR:HG22	1:D:1281:GLU:H	1.85	0.41
1:E:538:LEU:HD12	1:E:566:LEU:HD22	2.03	0.41
1:A:116:ALA:HB1	1:A:150:LEU:HD22	2.02	0.41
1:A:965:ASP:OD1	1:A:966:ASP:N	2.52	0.41
1:A:2182:SER:OG	1:C:1067:SER:N	2.54	0.41
1:A:2362:SER:OG	1:A:2502:LYS:NZ	2.49	0.41
1:B:691:VAL:O	1:B:694:PRO:HD2	2.21	0.41
1:B:2355:GLN:HG2	1:B:2356:GLU:OE1	2.21	0.41
1:C:2207:ASP:O	1:C:2211:LYS:HG2	2.21	0.41
1:D:2278:GLN:OE1	1:D:2281:ARG:NH2	2.52	0.41
1:D:2321:HIS:NE2	1:D:2325:ASP:OD2	2.53	0.41
1:E:218:LEU:HB3	1:E:221:LEU:HB2	2.02	0.41
1:E:2207:ASP:O	1:E:2211:LYS:HG2	2.20	0.41
1:A:268:PHE:HZ	1:A:441:ASN:HB2	1.86	0.41
1:A:365:ALA:HB3	1:A:384:ALA:HA	2.02	0.41
1:A:593:LEU:O	1:A:597:ILE:HG12	2.20	0.41
1:A:2033:LEU:CD1	1:A:2266:TYR:HA	2.50	0.41
1:B:714:TRP:CZ3	1:B:762:LEU:HD22	2.55	0.41
1:B:1108:THR:HB	1:B:1126:VAL:HG12	2.03	0.41
1:B:1170:LEU:HD22	1:B:1198:LEU:HD11	2.02	0.41
1:B:2207:ASP:O	1:B:2211:LYS:HG2	2.20	0.41
1:B:2460:PHE:CZ	1:C:2330:GLU:HB3	2.56	0.41
1:C:2087:LYS:HE3	1:C:2087:LYS:HB3	1.87	0.41
1:D:371:LYS:HA	1:D:377:GLU:HA	2.02	0.41
1:D:579:LYS:HG3	1:D:581:ASN:H	1.85	0.41
1:E:487:ARG:O	1:E:487:ARG:NH1	2.47	0.41
1:E:1244:THR:HG21	1:E:1268:TYR:CD1	2.56	0.41
1:A:659:TYR:CE2	1:A:758:ALA:HB2	2.56	0.41
1:A:1704:HIS:CE1	1:A:1727:ARG:H	2.39	0.41
1:A:1800:TRP:CZ2	1:A:1802:PRO:HG3	2.56	0.41
1:A:2355:GLN:HG2	1:A:2356:GLU:OE1	2.21	0.41
1:B:141:ARG:HH22	1:B:1005:GLU:CD	2.24	0.41
1:B:2132:ARG:HH11	1:B:2163:TYR:HB3	1.85	0.41
1:C:368:LEU:HG	1:C:370:ILE:CD1	2.50	0.41
1:C:2245:PHE:O	1:C:2246:SER:OG	2.39	0.41
1:D:522:PRO:O	1:D:553:ARG:NH1	2.53	0.41
1:D:1244:THR:HG21	1:D:1268:TYR:CD1	2.56	0.41
1:D:2112:ASN:HA	1:D:2115:MET:HG2	2.02	0.41
1:D:2202:GLU:O	1:D:2205:GLN:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:268:PHE:HZ	1:E:441:ASN:HB2	1.86	0.41
1:E:371:LYS:HA	1:E:377:GLU:HA	2.03	0.41
1:E:691:VAL:O	1:E:694:PRO:HD2	2.21	0.41
1:E:1607:THR:HG21	1:E:1768:PHE:HZ	1.85	0.41
1:E:1766:LEU:O	1:E:1770:GLU:HB2	2.20	0.41
1:E:2228:LYS:HE3	1:E:2228:LYS:HB2	1.82	0.41
1:A:160:SER:HA	1:A:982:LYS:HA	2.03	0.41
1:A:1244:THR:HG21	1:A:1268:TYR:CD1	2.56	0.41
1:B:538:LEU:HD12	1:B:566:LEU:HD22	2.03	0.41
1:B:1818:VAL:HG12	1:B:1820:PRO:HD2	2.02	0.41
1:B:2015:SER:HB2	1:C:2322:LEU:HD21	2.03	0.41
1:B:2431:ALA:O	1:B:2450:VAL:HG12	2.21	0.41
1:C:141:ARG:HH22	1:C:1005:GLU:CD	2.24	0.41
1:C:691:VAL:O	1:C:694:PRO:HD2	2.21	0.41
1:C:1164:LYS:HE2	1:D:1611:ARG:HG2	2.03	0.41
1:C:1170:LEU:HD22	1:C:1198:LEU:HD11	2.03	0.41
1:C:1818:VAL:HG12	1:C:1820:PRO:HD2	2.02	0.41
1:C:2321:HIS:NE2	1:C:2325:ASP:OD2	2.54	0.41
1:D:1704:HIS:CE1	1:D:1727:ARG:H	2.38	0.41
1:D:2431:ALA:O	1:D:2450:VAL:HG12	2.21	0.41
1:E:365:ALA:HB3	1:E:384:ALA:HA	2.03	0.41
1:E:2033:LEU:CD1	1:E:2266:TYR:HA	2.50	0.41
1:A:1279:THR:HG22	1:A:1281:GLU:H	1.86	0.40
1:A:2322:LEU:HD21	1:E:2015:SER:HB2	2.03	0.40
1:A:2432:ILE:HD11	1:B:2402:TYR:CE1	2.56	0.40
1:B:160:SER:HA	1:B:982:LYS:HA	2.02	0.40
1:B:1130:LYS:HZ3	1:B:1139:ASN:C	2.25	0.40
1:C:1704:HIS:CE1	1:C:1727:ARG:H	2.39	0.40
1:D:538:LEU:HD12	1:D:566:LEU:HD22	2.04	0.40
1:D:2355:GLN:HG2	1:D:2356:GLU:OE1	2.21	0.40
1:E:341:MET:HE3	1:E:410:LEU:HD22	2.03	0.40
1:E:1279:THR:HG22	1:E:1281:GLU:H	1.86	0.40
1:A:689:LEU:HD12	1:A:689:LEU:HA	1.91	0.40
1:A:1108:THR:HB	1:A:1126:VAL:HG12	2.03	0.40
1:A:2321:HIS:NE2	1:A:2325:ASP:OD2	2.54	0.40
1:A:2388:GLN:HA	1:A:2485:SER:HA	2.03	0.40
1:C:493:GLU:O	1:C:497:ILE:HG12	2.21	0.40
1:C:1108:THR:HB	1:C:1126:VAL:HG12	2.02	0.40
1:C:1111:ILE:HG13	1:C:1160:PRO:HD3	2.04	0.40
1:C:1279:THR:HG22	1:C:1281:GLU:H	1.85	0.40
1:C:1609:PHE:CZ	1:C:1613:LEU:HD13	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:538:LEU:HB2	1:D:566:LEU:HD22	2.03	0.40
1:D:661:LYS:HB2	1:D:750:GLU:HB2	2.04	0.40
1:E:1162:ILE:HD13	1:E:1167:LEU:HA	2.04	0.40
1:E:1800:TRP:CZ2	1:E:1802:PRO:HG3	2.57	0.40
1:E:2362:SER:OG	1:E:2502:LYS:NZ	2.51	0.40
1:B:268:PHE:HZ	1:B:441:ASN:HB2	1.85	0.40
1:B:1800:TRP:CZ2	1:B:1802:PRO:HG3	2.56	0.40
1:D:116:ALA:HB1	1:D:150:LEU:HD22	2.02	0.40
1:D:2328:ALA:HB2	1:D:2516:LYS:HB3	2.03	0.40
1:E:1108:THR:HB	1:E:1126:VAL:HG12	2.02	0.40
1:E:2202:GLU:O	1:E:2205:GLN:HG2	2.21	0.40
1:A:1113:LEU:HD11	1:A:1119:GLY:HA3	2.04	0.40
1:A:2341:TYR:CD2	1:A:2353:LEU:HD11	2.57	0.40
1:B:497:ILE:HG21	1:B:589:TYR:CD2	2.54	0.40
1:B:1244:THR:HG21	1:B:1268:TYR:CD1	2.56	0.40
1:C:659:TYR:CE2	1:C:758:ALA:HB2	2.56	0.40
1:D:268:PHE:HZ	1:D:441:ASN:HB2	1.87	0.40
1:D:714:TRP:CZ3	1:D:762:LEU:HD22	2.56	0.40
1:E:848:GLN:OE1	1:E:892:GLN:NE2	2.53	0.40
1:E:2470:LEU:N	1:E:2473:GLU:OE1	2.53	0.40
1:A:493:GLU:O	1:A:497:ILE:HG12	2.21	0.40
1:A:1170:LEU:HD22	1:A:1198:LEU:HD11	2.01	0.40
1:D:195:SER:OG	1:D:948:THR:HG22	2.22	0.40
1:D:659:TYR:CE2	1:D:758:ALA:HB2	2.57	0.40
1:D:689:LEU:HA	1:D:689:LEU:HD12	1.92	0.40
1:D:848:GLN:OE1	1:D:892:GLN:NE2	2.54	0.40
1:E:493:GLU:O	1:E:497:ILE:HG12	2.22	0.40
1:E:2321:HIS:NE2	1:E:2325:ASP:OD2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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	2114/2535 (83%)	2069 (98%)	45 (2%)	0	100	100
1	B	2114/2535 (83%)	2071 (98%)	43 (2%)	0	100	100
1	C	2114/2535 (83%)	2072 (98%)	42 (2%)	0	100	100
1	D	2114/2535 (83%)	2070 (98%)	44 (2%)	0	100	100
1	E	2114/2535 (83%)	2071 (98%)	43 (2%)	0	100	100
All	All	10570/12675 (83%)	10353 (98%)	217 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	1816/2173 (84%)	1812 (100%)	4 (0%)	93	98
1	B	1816/2173 (84%)	1812 (100%)	4 (0%)	93	98
1	C	1816/2173 (84%)	1812 (100%)	4 (0%)	93	98
1	D	1816/2173 (84%)	1812 (100%)	4 (0%)	93	98
1	E	1816/2173 (84%)	1812 (100%)	4 (0%)	93	98
All	All	9080/10865 (84%)	9060 (100%)	20 (0%)	93	98

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1049	MET
1	A	1174	GLN
1	A	1965	GLN
1	A	2414	GLN
1	B	1049	MET
1	B	1174	GLN
1	B	1965	GLN
1	B	2414	GLN
1	C	1049	MET
1	C	1174	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1965	GLN
1	C	2414	GLN
1	D	1049	MET
1	D	1174	GLN
1	D	1965	GLN
1	D	2414	GLN
1	E	1049	MET
1	E	1174	GLN
1	E	1965	GLN
1	E	2414	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	852	GLN
1	A	892	GLN
1	A	969	GLN
1	B	852	GLN
1	B	892	GLN
1	B	969	GLN
1	C	852	GLN
1	C	892	GLN
1	C	969	GLN
1	D	852	GLN
1	D	892	GLN
1	D	969	GLN
1	E	852	GLN
1	E	892	GLN
1	E	969	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

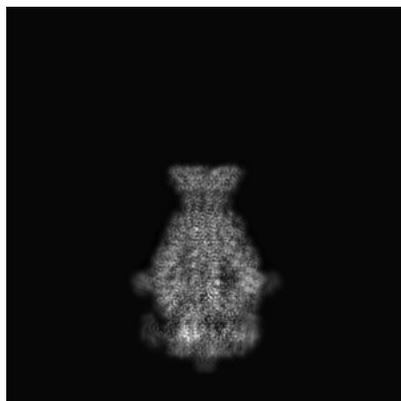
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16792. These allow visual inspection of the internal detail of the map and identification of artifacts.

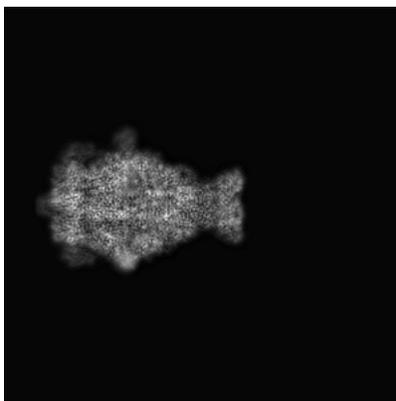
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

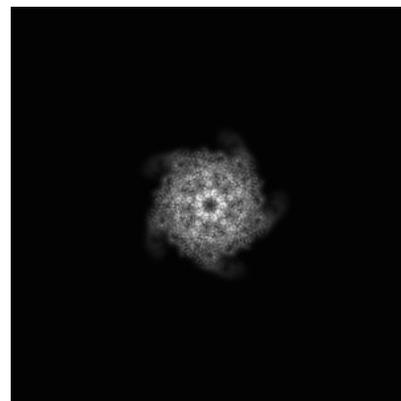
6.1.1 Primary map



X

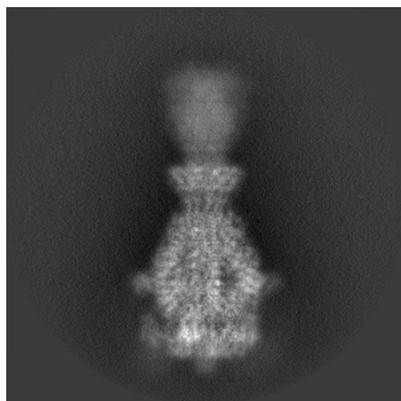


Y

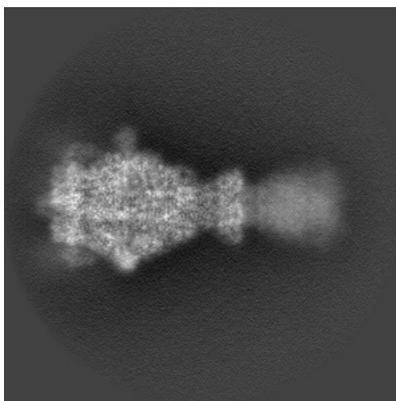


Z

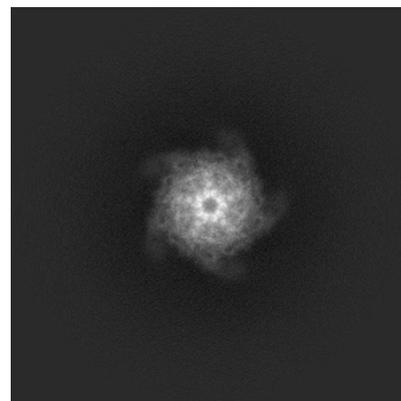
6.1.2 Raw map



X



Y

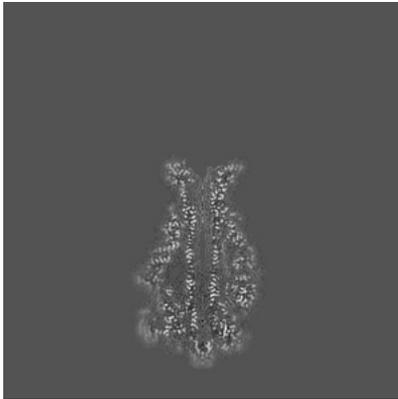


Z

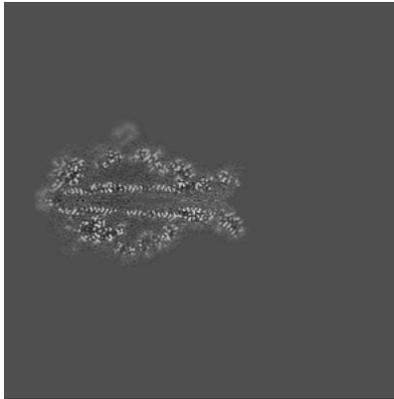
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

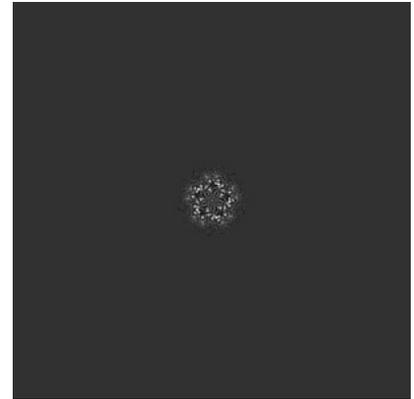
6.2.1 Primary map



X Index: 280

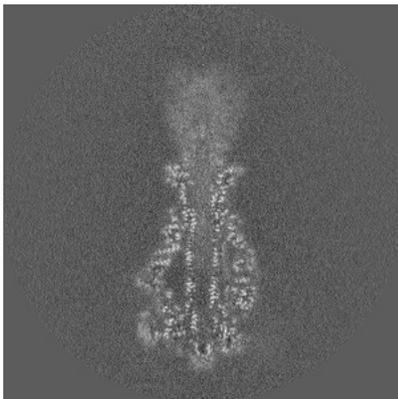


Y Index: 280

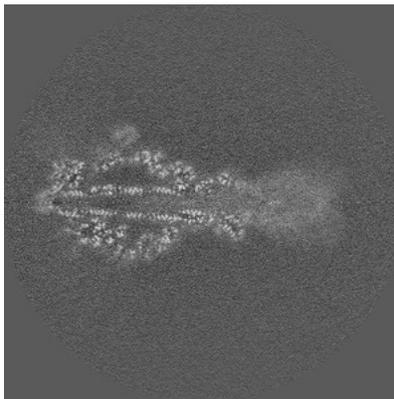


Z Index: 280

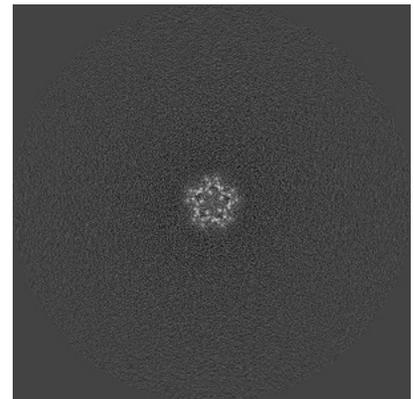
6.2.2 Raw map



X Index: 280



Y Index: 280

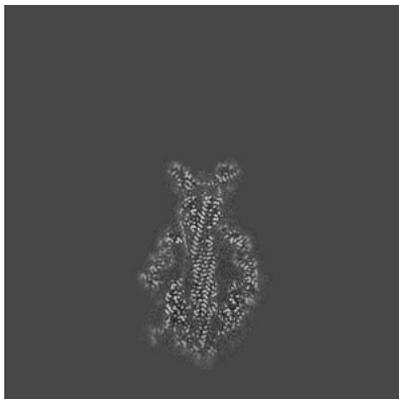


Z Index: 280

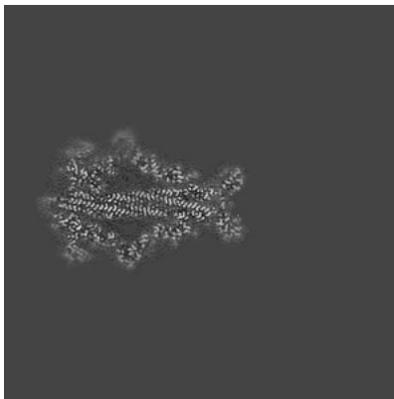
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

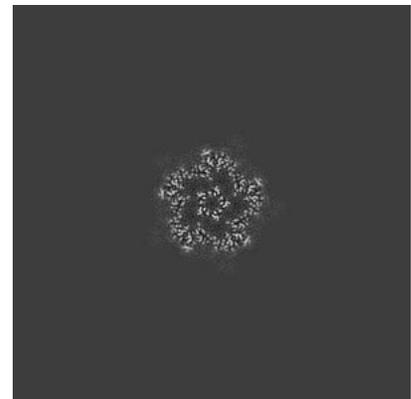
6.3.1 Primary map



X Index: 265

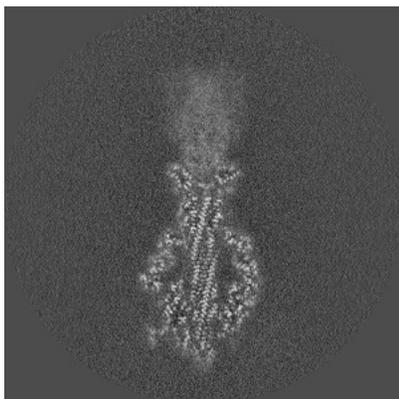


Y Index: 266

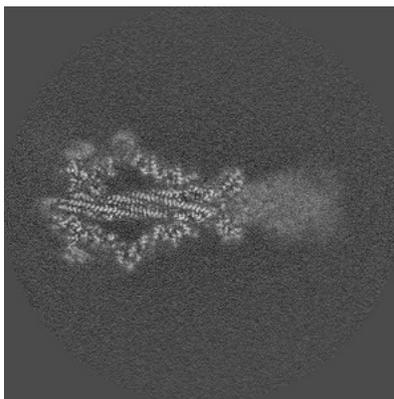


Z Index: 150

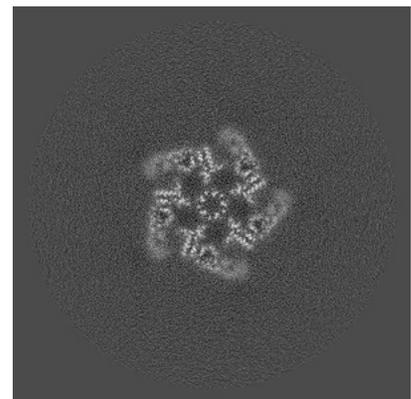
6.3.2 Raw map



X Index: 266



Y Index: 266

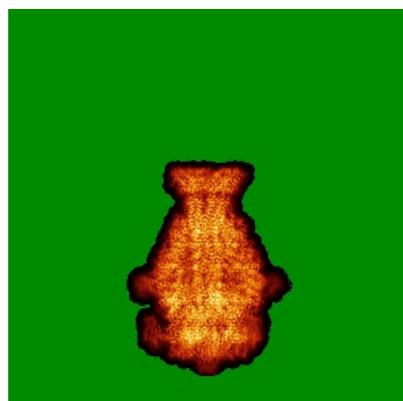


Z Index: 170

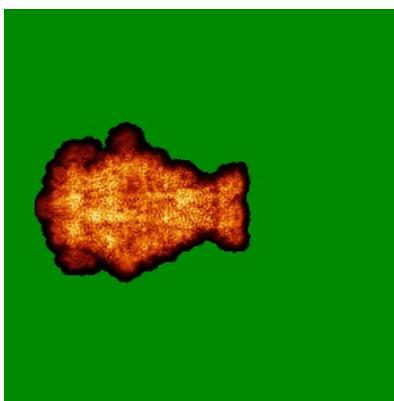
The images above show the largest variance slices of the map in three orthogonal directions.

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

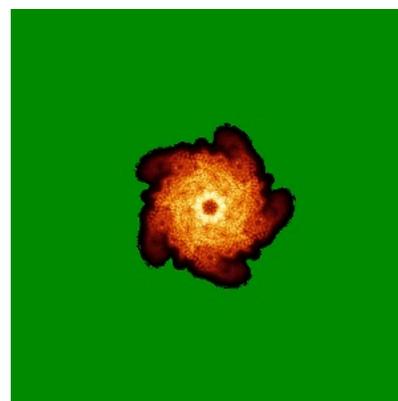
6.4.1 Primary map



X

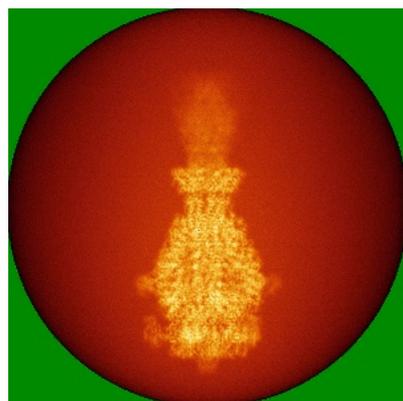


Y

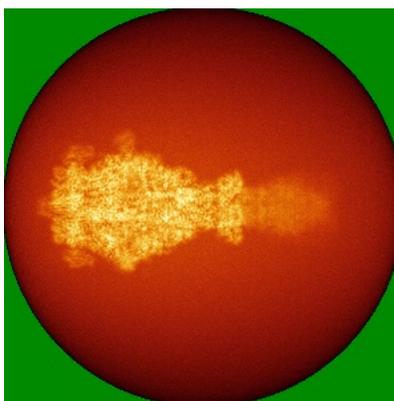


Z

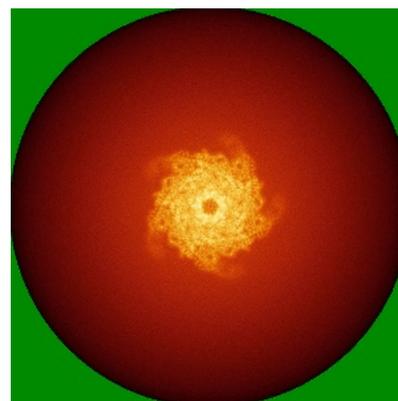
6.4.2 Raw map



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.

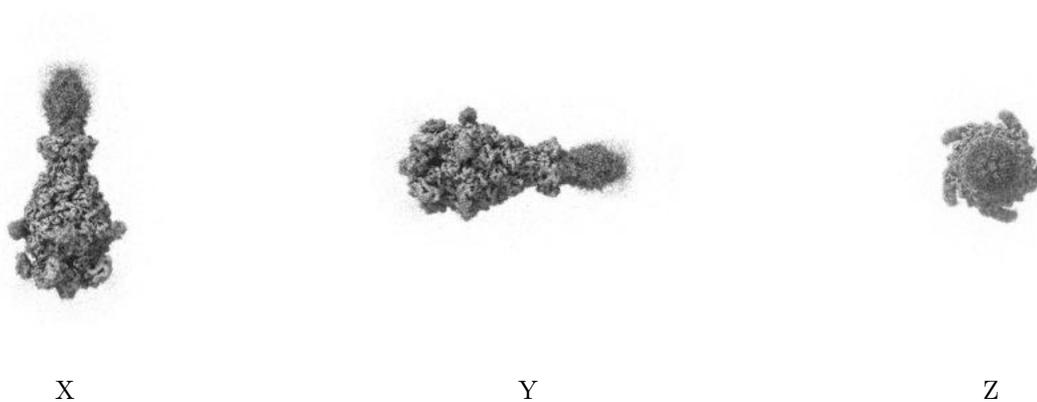
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

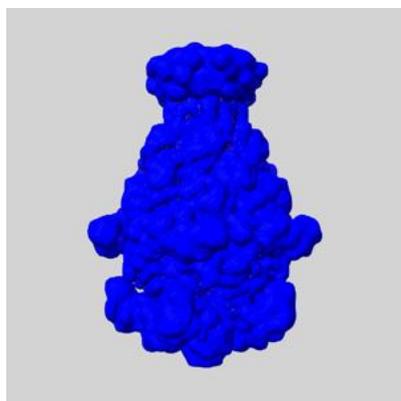
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

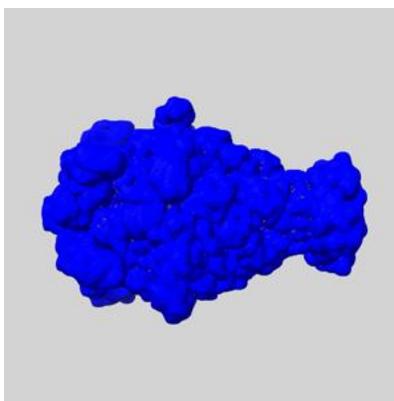
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

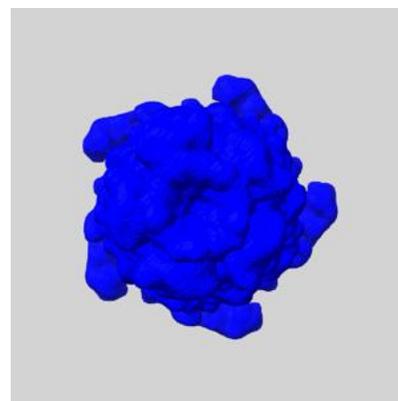
6.6.1 emd_16792_msk_1.map [i](#)



X



Y

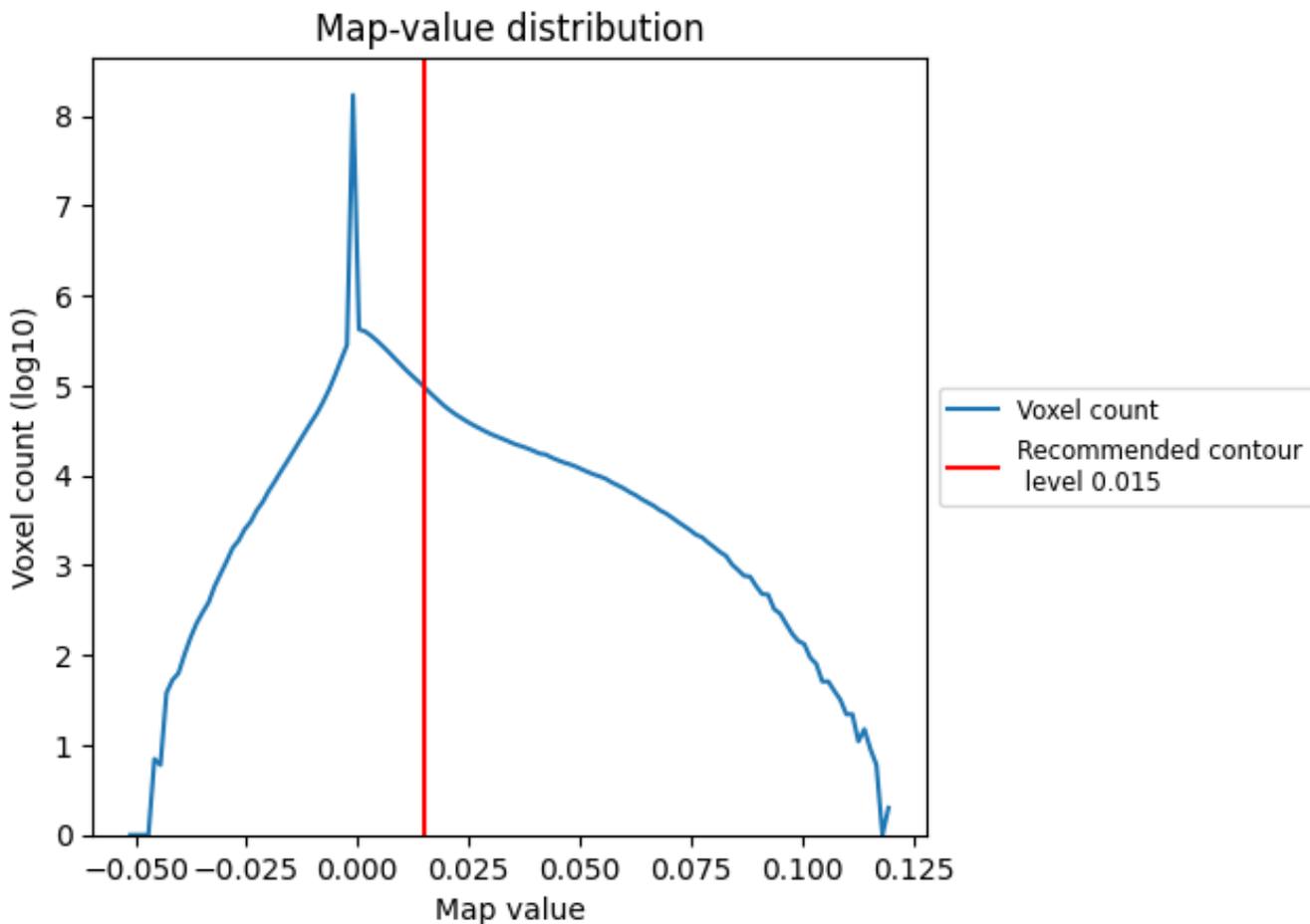


Z

7 Map analysis [i](#)

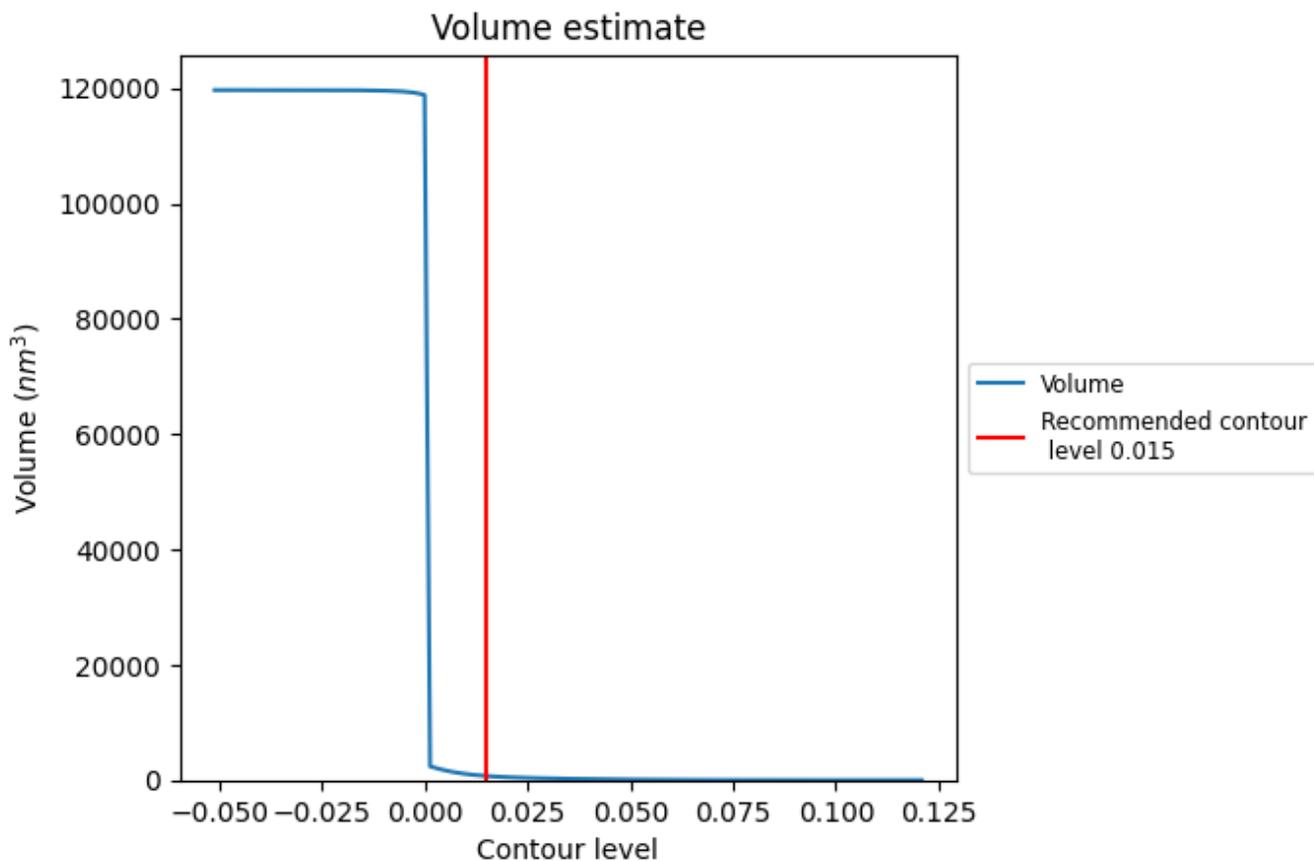
This section contains the results of statistical analysis of the map.

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.

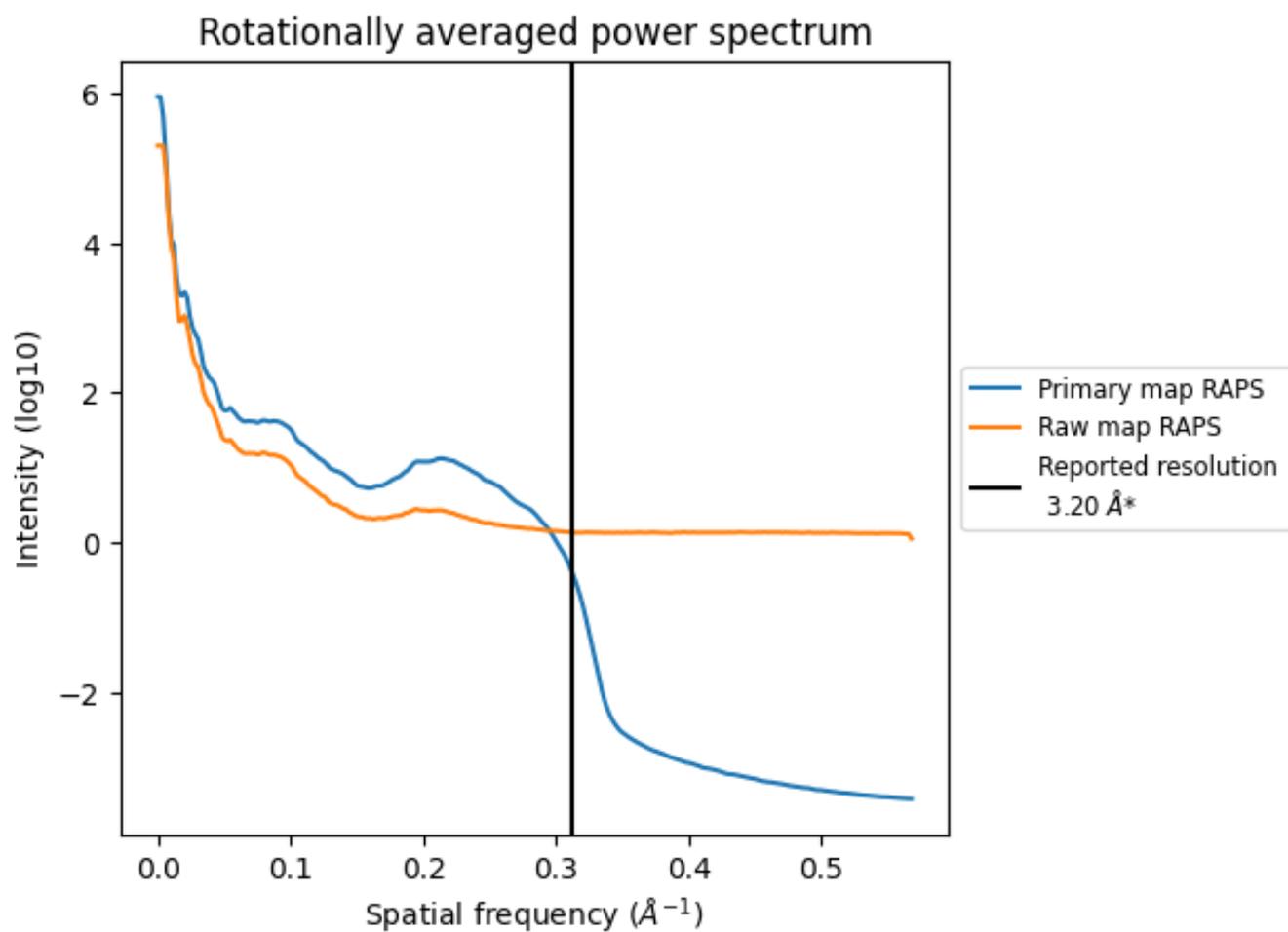
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 710 nm³; this corresponds to an approximate mass of 641 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 [i](#)

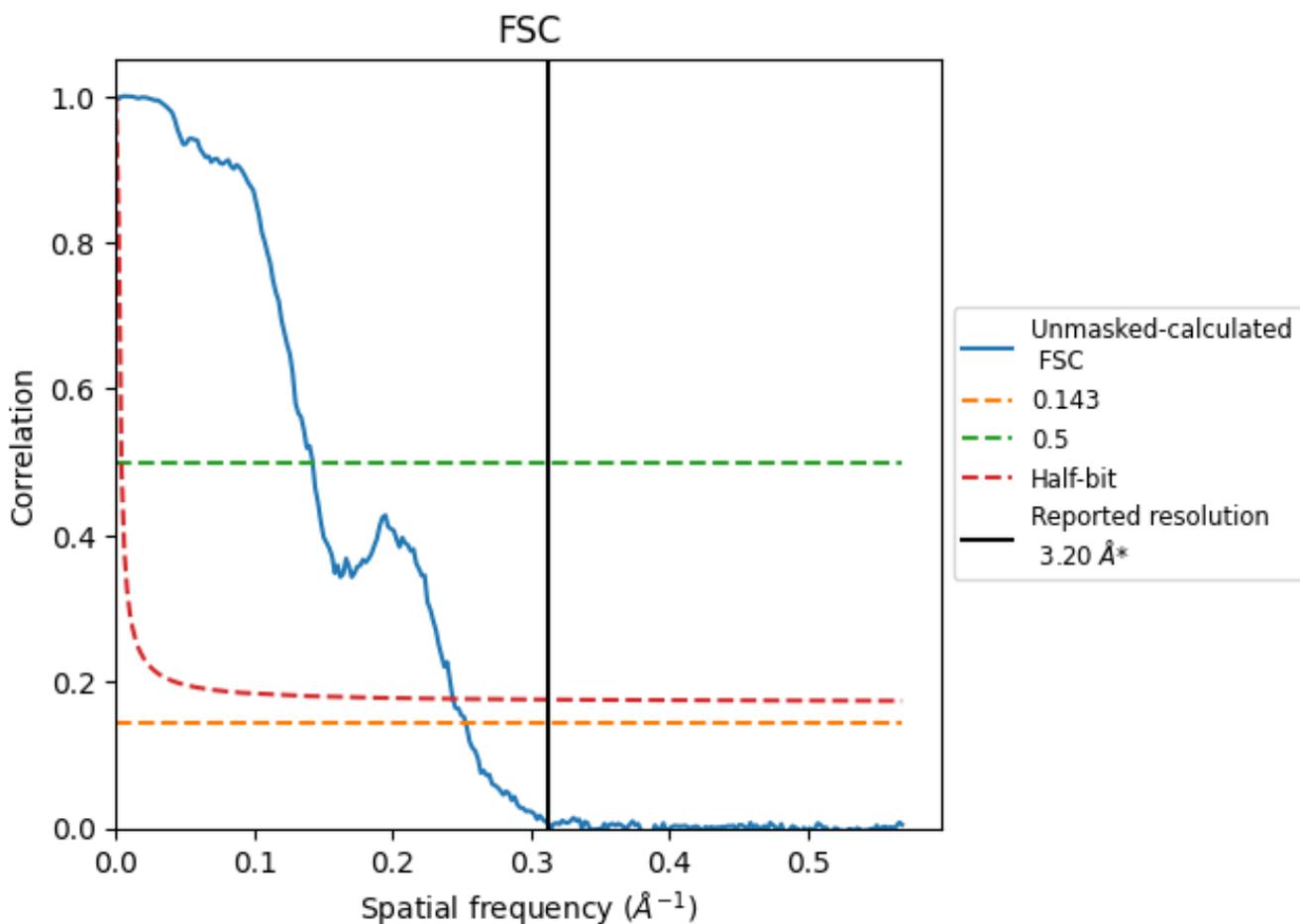


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

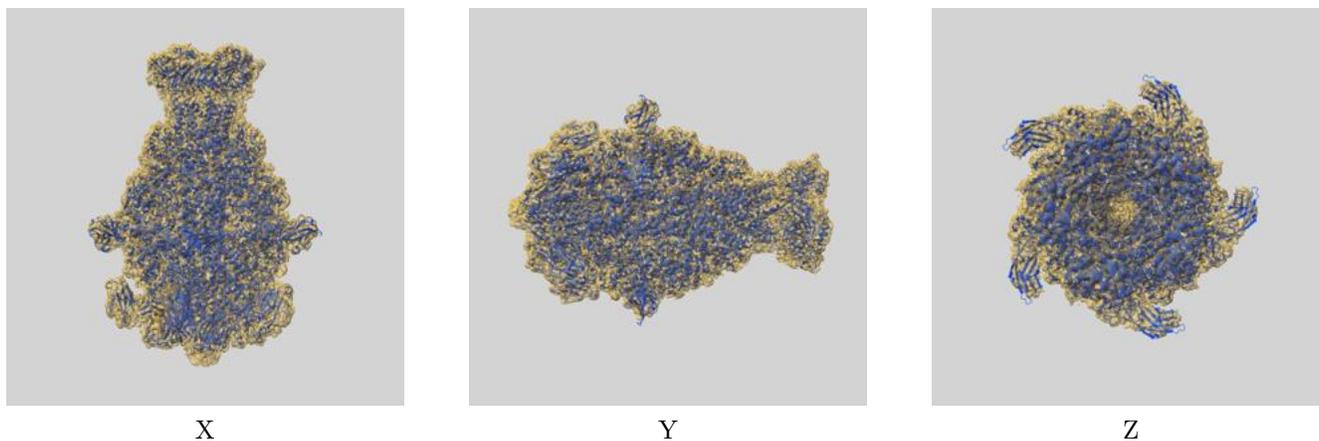
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.96	7.03	4.11

*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 3.96 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

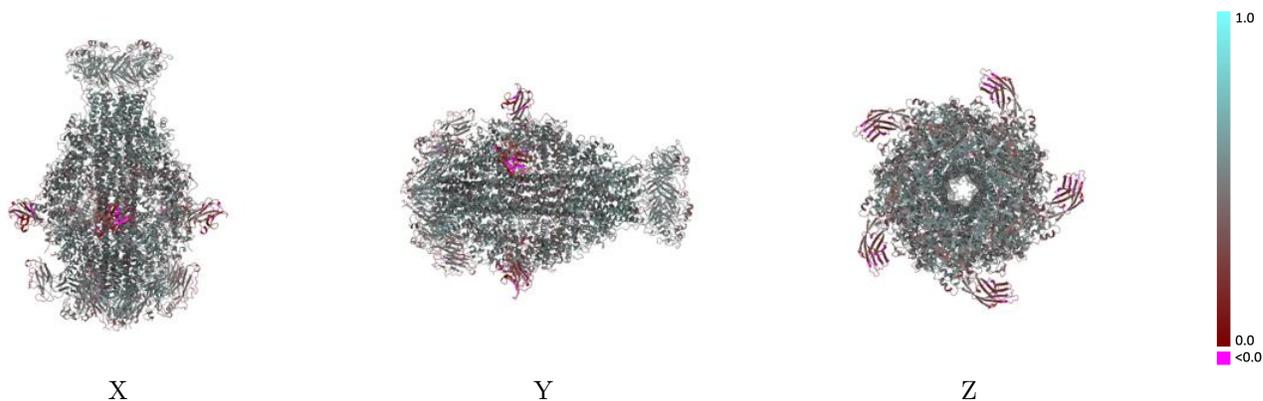
This section contains information regarding the fit between EMDB map EMD-16792 and PDB model 8CQ0. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



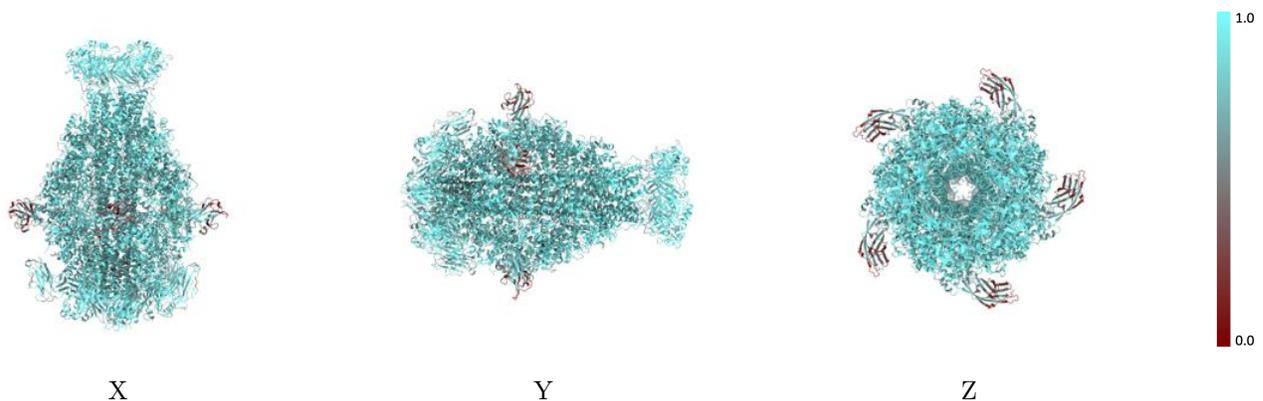
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



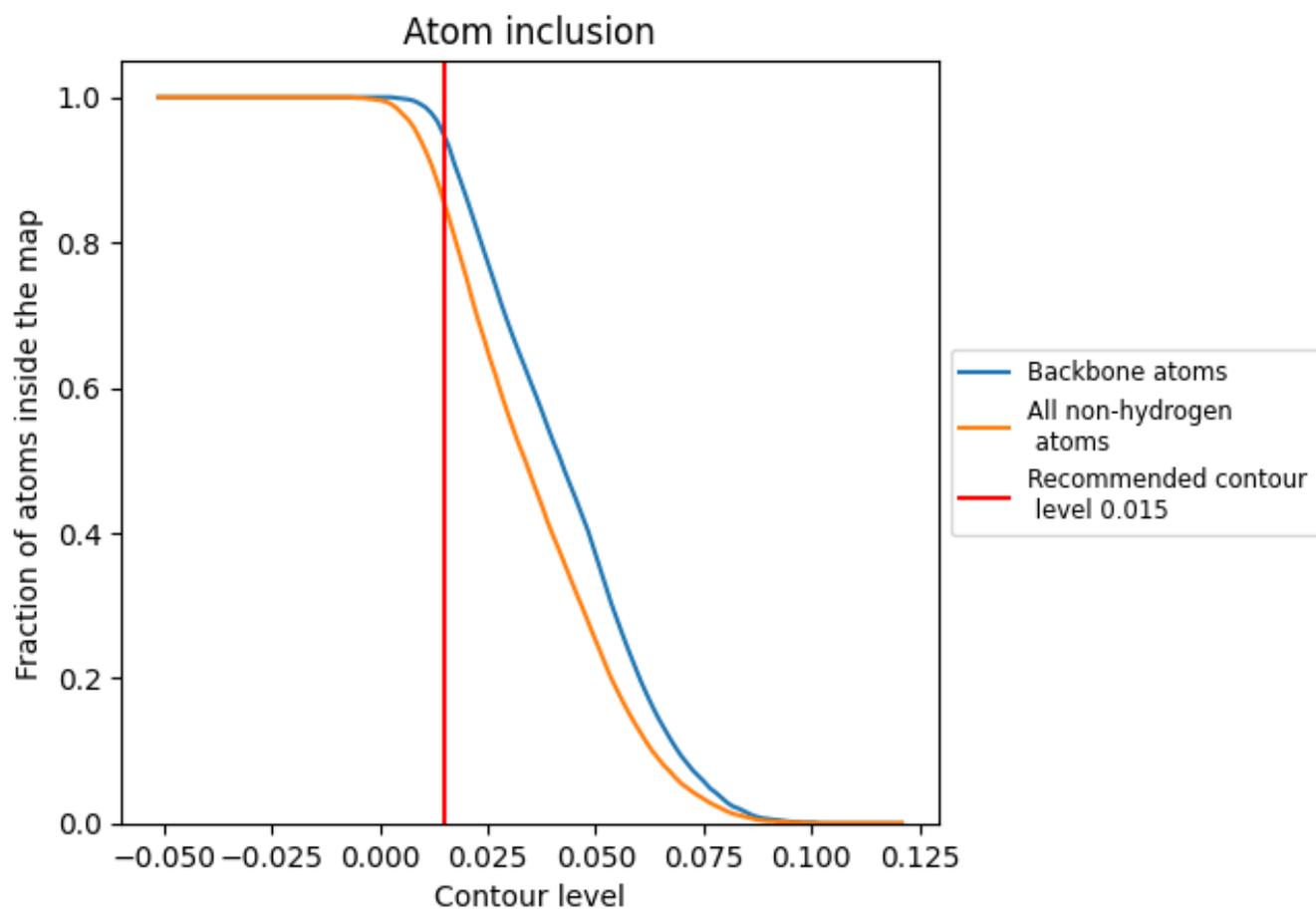
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 85% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8540	 0.4660
A	 0.8540	 0.4660
B	 0.8540	 0.4660
C	 0.8540	 0.4670
D	 0.8550	 0.4670
E	 0.8550	 0.4650

