



Full wwPDB EM Validation Report ⓘ

Apr 20, 2026 – 01:48 PM EDT

PDB ID : 9Y07 / pdb_00009y07
EMDB ID : EMD-72387
Title : Cryo-EM structure of human VCP/p97-T122P mutant bound to ATPgammaS
Authors : Lehman, A.; Ahmed, S.; Mohajeri, A.; Yang, G.X.; Berezuk, A.M.; Mannar, D.; Cholak, S.; Tuttle, K.S.; Bennett, J.T.; Magno, J.A.; Hannibal, M.; Kovacevic, G.; Kuburovic, V.; Lewis, M.E.S.; Moldovan, O.; Nelson, Z.; Raskin, S.; Vandersteen, A.M.; Roach, J.C.; Subramaniam, S.; Patel, M.S.
Deposited on : 2025-08-28
Resolution : 2.41 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:

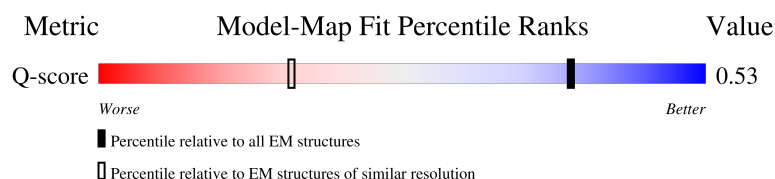
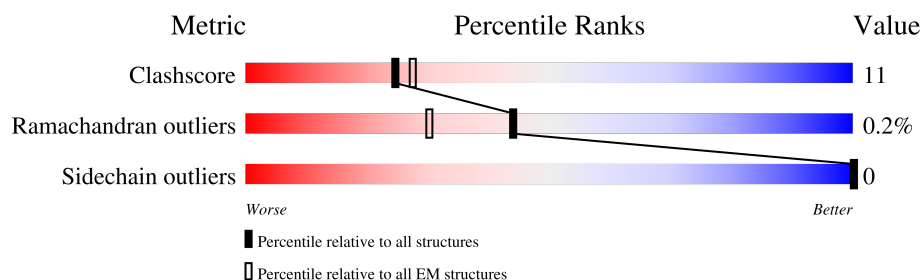
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.41 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	5662 (1.92 - 2.91)

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	822	<div> <div>6%</div> <div>50%</div> <div>17%</div> <div>33%</div> </div>
1	B	822	<div> <div>6%</div> <div>48%</div> <div>19%</div> <div>33%</div> </div>
1	C	822	<div> <div>6%</div> <div>49%</div> <div>18%</div> <div>33%</div> </div>

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Mol	Chain	Length	Quality of chain
1	D	822	<div><div></div><div>6%</div><div>50%</div><div>16%</div><div>33%</div></div>
1	E	822	<div><div></div><div>6%</div><div>50%</div><div>17%</div><div>33%</div></div>
1	F	822	<div><div></div><div>6%</div><div>48%</div><div>19%</div><div>33%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25998 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	549	Total	C	N	O	S	0	0
			4269	2689	751	807	22		
1	B	549	Total	C	N	O	S	0	0
			4269	2689	751	807	22		
1	C	549	Total	C	N	O	S	0	0
			4269	2689	751	807	22		
1	D	549	Total	C	N	O	S	0	0
			4269	2689	751	807	22		
1	E	549	Total	C	N	O	S	0	0
			4269	2689	751	807	22		
1	F	549	Total	C	N	O	S	0	0
			4269	2689	751	807	22		

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP P55072
A	-14	HIS	-	expression tag	UNP P55072
A	-13	HIS	-	expression tag	UNP P55072
A	-12	HIS	-	expression tag	UNP P55072
A	-11	HIS	-	expression tag	UNP P55072
A	-10	HIS	-	expression tag	UNP P55072
A	-9	SER	-	expression tag	UNP P55072
A	-8	SER	-	expression tag	UNP P55072
A	-7	GLY	-	expression tag	UNP P55072
A	-6	LEU	-	expression tag	UNP P55072
A	-5	VAL	-	expression tag	UNP P55072
A	-4	PRO	-	expression tag	UNP P55072
A	-3	ARG	-	expression tag	UNP P55072
A	-2	GLY	-	expression tag	UNP P55072
A	-1	SER	-	expression tag	UNP P55072
A	0	HIS	-	expression tag	UNP P55072
A	122	PRO	THR	engineered mutation	UNP P55072
B	-15	HIS	-	expression tag	UNP P55072

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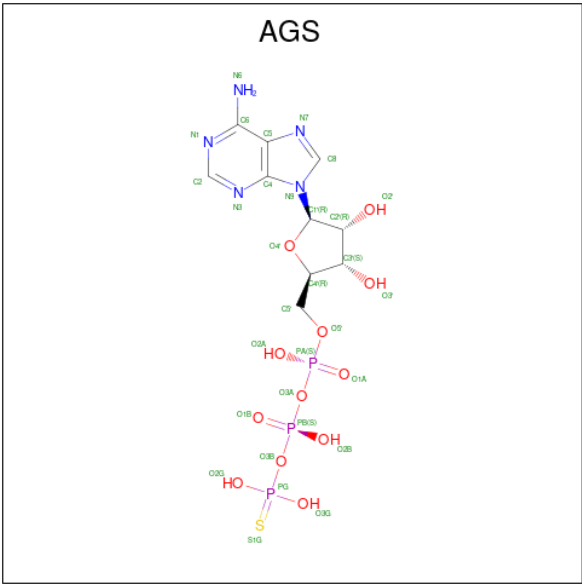
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P55072
B	-13	HIS	-	expression tag	UNP P55072
B	-12	HIS	-	expression tag	UNP P55072
B	-11	HIS	-	expression tag	UNP P55072
B	-10	HIS	-	expression tag	UNP P55072
B	-9	SER	-	expression tag	UNP P55072
B	-8	SER	-	expression tag	UNP P55072
B	-7	GLY	-	expression tag	UNP P55072
B	-6	LEU	-	expression tag	UNP P55072
B	-5	VAL	-	expression tag	UNP P55072
B	-4	PRO	-	expression tag	UNP P55072
B	-3	ARG	-	expression tag	UNP P55072
B	-2	GLY	-	expression tag	UNP P55072
B	-1	SER	-	expression tag	UNP P55072
B	0	HIS	-	expression tag	UNP P55072
B	122	PRO	THR	engineered mutation	UNP P55072
C	-15	HIS	-	expression tag	UNP P55072
C	-14	HIS	-	expression tag	UNP P55072
C	-13	HIS	-	expression tag	UNP P55072
C	-12	HIS	-	expression tag	UNP P55072
C	-11	HIS	-	expression tag	UNP P55072
C	-10	HIS	-	expression tag	UNP P55072
C	-9	SER	-	expression tag	UNP P55072
C	-8	SER	-	expression tag	UNP P55072
C	-7	GLY	-	expression tag	UNP P55072
C	-6	LEU	-	expression tag	UNP P55072
C	-5	VAL	-	expression tag	UNP P55072
C	-4	PRO	-	expression tag	UNP P55072
C	-3	ARG	-	expression tag	UNP P55072
C	-2	GLY	-	expression tag	UNP P55072
C	-1	SER	-	expression tag	UNP P55072
C	0	HIS	-	expression tag	UNP P55072
C	122	PRO	THR	engineered mutation	UNP P55072
D	-15	HIS	-	expression tag	UNP P55072
D	-14	HIS	-	expression tag	UNP P55072
D	-13	HIS	-	expression tag	UNP P55072
D	-12	HIS	-	expression tag	UNP P55072
D	-11	HIS	-	expression tag	UNP P55072
D	-10	HIS	-	expression tag	UNP P55072
D	-9	SER	-	expression tag	UNP P55072
D	-8	SER	-	expression tag	UNP P55072
D	-7	GLY	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	LEU	-	expression tag	UNP P55072
D	-5	VAL	-	expression tag	UNP P55072
D	-4	PRO	-	expression tag	UNP P55072
D	-3	ARG	-	expression tag	UNP P55072
D	-2	GLY	-	expression tag	UNP P55072
D	-1	SER	-	expression tag	UNP P55072
D	0	HIS	-	expression tag	UNP P55072
D	122	PRO	THR	engineered mutation	UNP P55072
E	-15	HIS	-	expression tag	UNP P55072
E	-14	HIS	-	expression tag	UNP P55072
E	-13	HIS	-	expression tag	UNP P55072
E	-12	HIS	-	expression tag	UNP P55072
E	-11	HIS	-	expression tag	UNP P55072
E	-10	HIS	-	expression tag	UNP P55072
E	-9	SER	-	expression tag	UNP P55072
E	-8	SER	-	expression tag	UNP P55072
E	-7	GLY	-	expression tag	UNP P55072
E	-6	LEU	-	expression tag	UNP P55072
E	-5	VAL	-	expression tag	UNP P55072
E	-4	PRO	-	expression tag	UNP P55072
E	-3	ARG	-	expression tag	UNP P55072
E	-2	GLY	-	expression tag	UNP P55072
E	-1	SER	-	expression tag	UNP P55072
E	0	HIS	-	expression tag	UNP P55072
E	122	PRO	THR	engineered mutation	UNP P55072
F	-15	HIS	-	expression tag	UNP P55072
F	-14	HIS	-	expression tag	UNP P55072
F	-13	HIS	-	expression tag	UNP P55072
F	-12	HIS	-	expression tag	UNP P55072
F	-11	HIS	-	expression tag	UNP P55072
F	-10	HIS	-	expression tag	UNP P55072
F	-9	SER	-	expression tag	UNP P55072
F	-8	SER	-	expression tag	UNP P55072
F	-7	GLY	-	expression tag	UNP P55072
F	-6	LEU	-	expression tag	UNP P55072
F	-5	VAL	-	expression tag	UNP P55072
F	-4	PRO	-	expression tag	UNP P55072
F	-3	ARG	-	expression tag	UNP P55072
F	-2	GLY	-	expression tag	UNP P55072
F	-1	SER	-	expression tag	UNP P55072
F	0	HIS	-	expression tag	UNP P55072
F	122	PRO	THR	engineered mutation	UNP P55072

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).

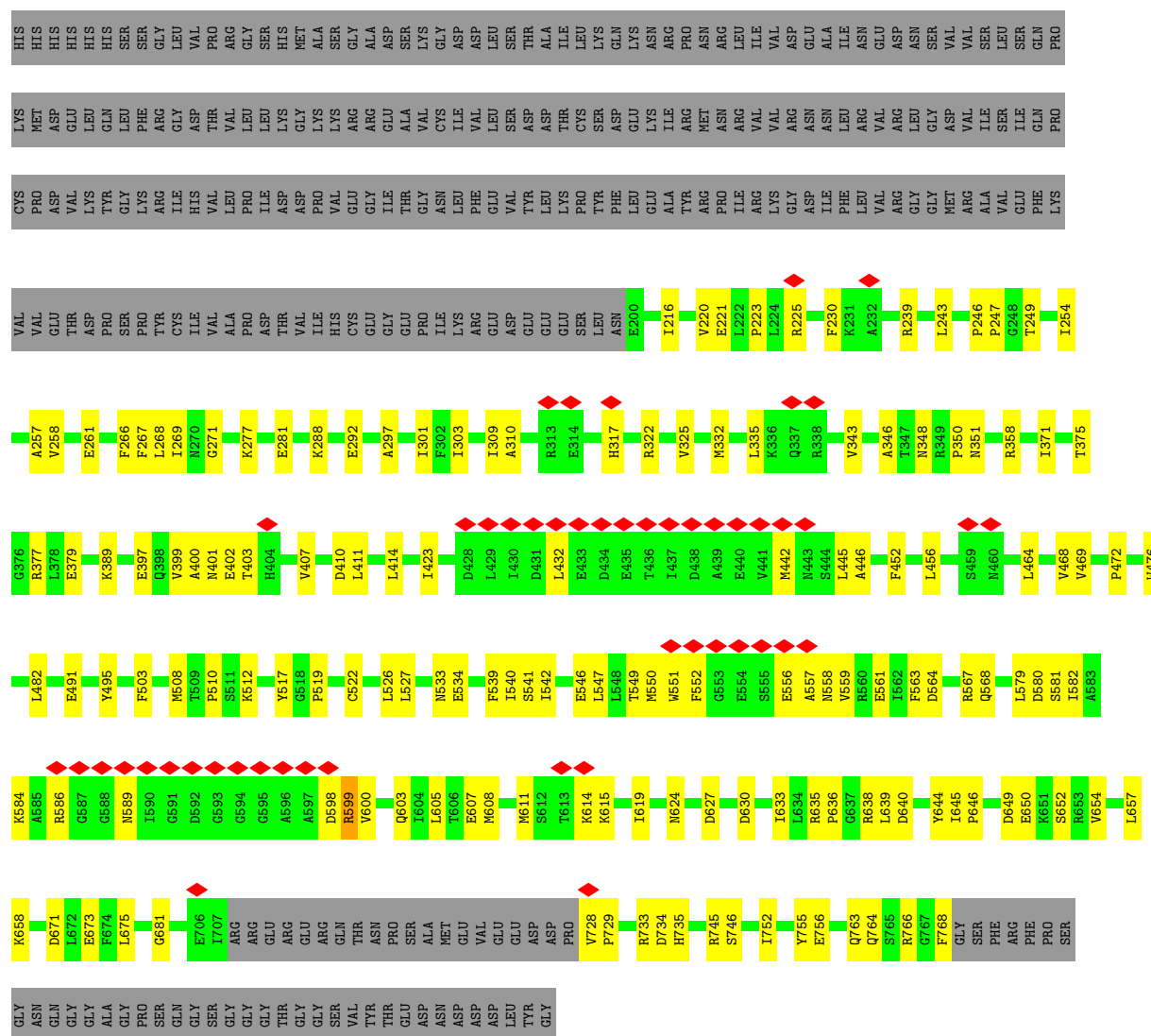


Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

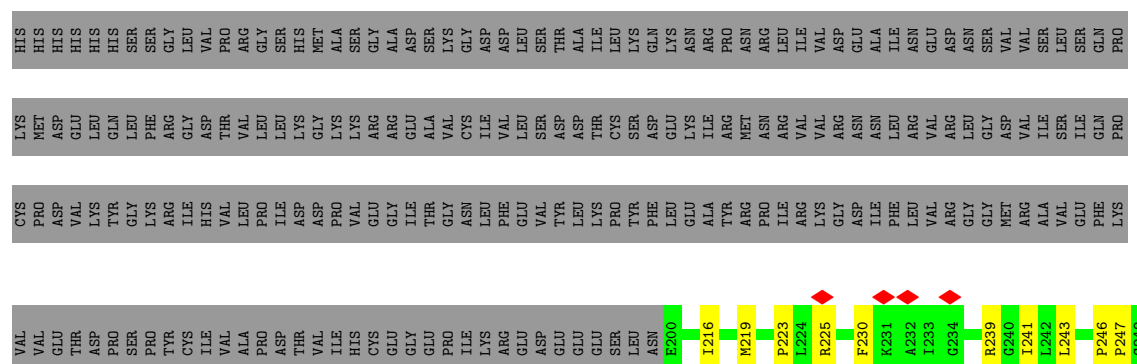
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

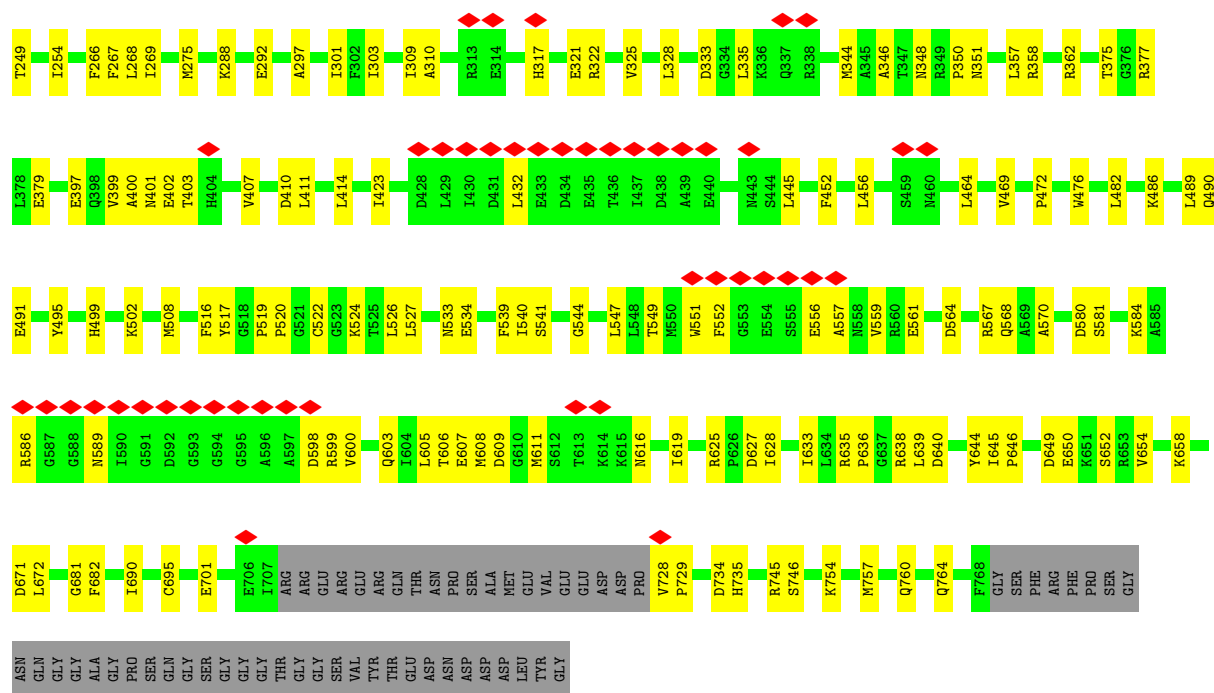
Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total 2	Mg 2	0
3	B	2	Total 2	Mg 2	0
3	C	2	Total 2	Mg 2	0
3	D	2	Total 2	Mg 2	0
3	E	2	Total 2	Mg 2	0
3	F	2	Total 2	Mg 2	0

Chain B:

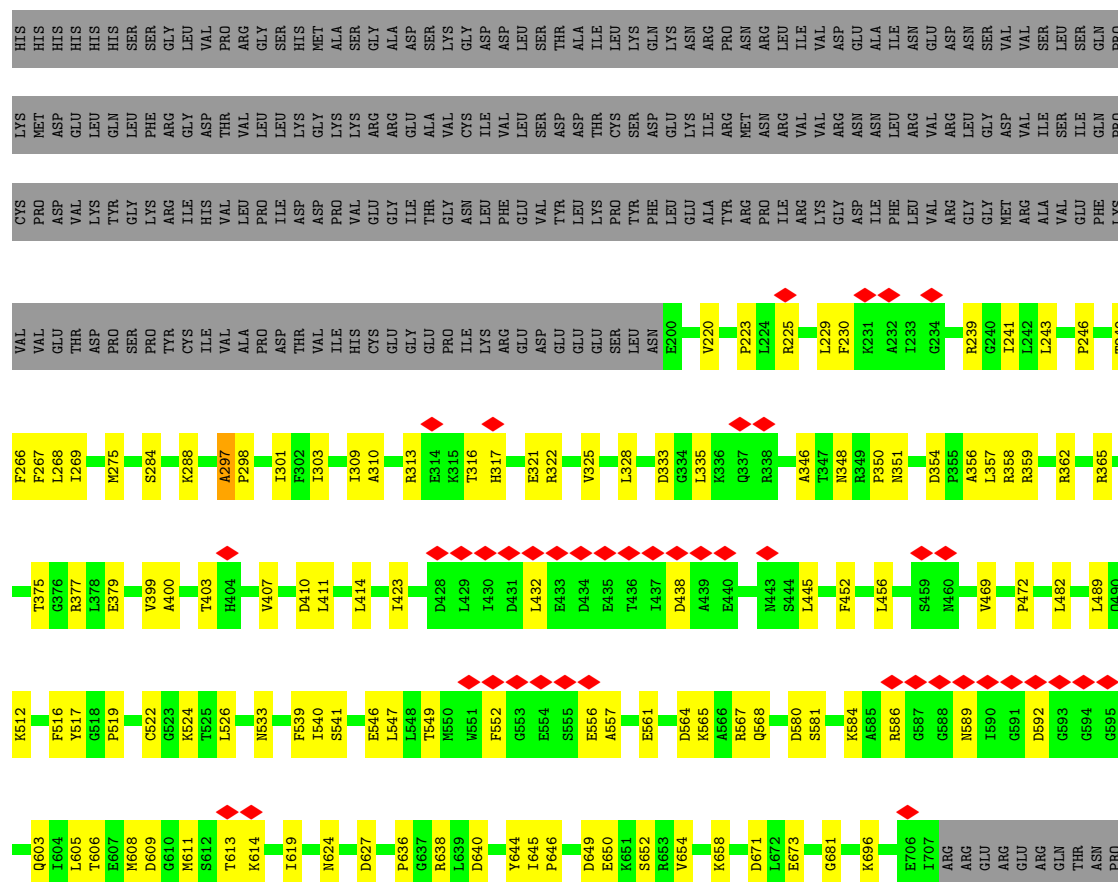


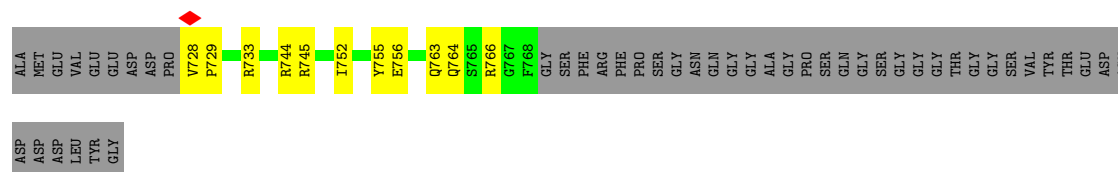
Chain C:



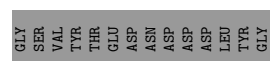
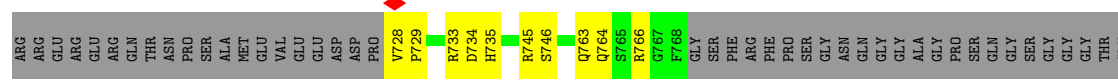
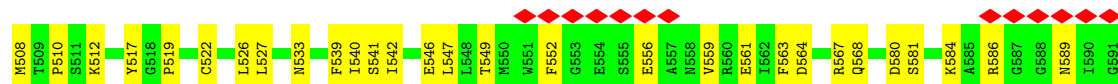
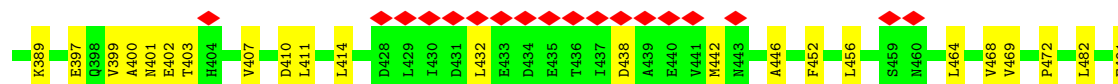
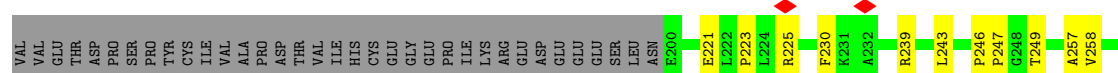
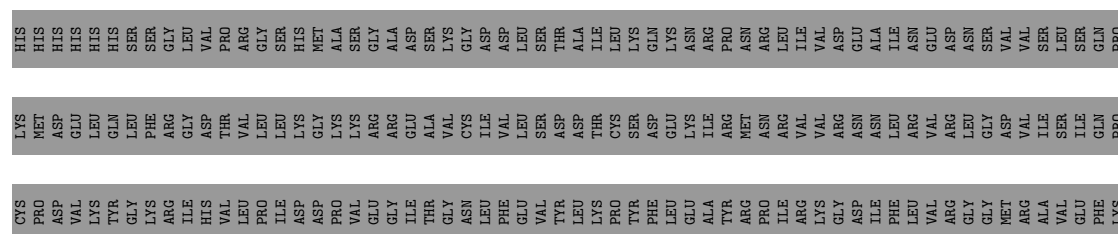


• Molecule 1: Transitional endoplasmic reticulum ATPase





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CYS	VAL	L243	R348	S459	R558	Y644	Q764
PRO	VAL		R349	R460	V559	I645	S765
ASP	GLU	P246	P350		R560	P646	S766
VAL	THR	P247	N351	L464	E561		G767
LYS	ASP	G248		V469	D564	D649	F768
TYR	PRO	T249	L357			E650	GLY
GLY	SER		R358			K651	SER
LYS	PRO	T254		P472	R567	S652	PHE
ARG	TYR	A255	R362	W476	Q568	R653	ARG
ILE	CYS	R256	R365		A569	V654	PHE
HIS	ILE			L482	A570		PRO
VAL	VAL	E261			P571	K658	SER
LEU	ALA		I371		D580	V666	GLY
PRO	PRO	F267	T375	K456	S581		ASN
ILE	ASP	L268	G376	Q490	K584	D671	GLN
ASP	THR	L269	R377	E491	A585	L672	GLY
PRO	VAL	N275	L378	Y495	R586	E673	ALA
VAL	HIS		E379			G681	GLY
GLU	CYS	K288	E397	H499	G587		PRO
GLY	GLU		Q398		G588	C695	SER
ILE	GLY	E292	V399	R502	N589		GLN
THR	PRO	A297	A400	M508	I590	E701	GLY
GLY	ASN	P298	N401		G591		GLY
ASN	ILE		E402	K512	D592	E706	GLY
LEU	LYS		T403		G593	I707	GLY
PHE	ARG	I301	H404		G594	ARG	THR
GLU	GLU	F302		Y517	G595	ARG	GLY
VAL	ASP	I303	V407	G518	A596	GLU	GLY
TYR	GLU	D304	D410	P519	P520	ARG	GLY
LEU	GLU	E305	L411	G521	A597	GLN	VAL
LYS	GLU	I309	L414	G522	D598	THR	TYR
PRO	SER	A310		G523	R599	GLU	THR
LEU	LEU			R524	V600	ASN	ASP
TYR	ASN		I423	T525		PRO	ASP
PHE	E200	R313		L526	G603	ALA	ASP
LEU		E314		L527	T604	LEU	ASP
GLU	Y203		D428		L605	GLU	ASP
ALA			I429	N533	T606	VAL	LEU
TYR		I216	E318	E534	E607	GLU	TYR
ARG		K219	V320		M608	GLU	GLY
PRO			E321	F539	D609	ASP	LYS
ILE		P223	R322	T540	G610	ASP	GLY
ARG		L224		S541	M611	PRO	ASP
LYS		R225	V325	G544	S612		ASP
GLY					T613	V728	PRO
ASP		L229		L547	K614	P729	
ILE		F230	D328	L548	K615	E730	
PHE		K231	D333	T436	N616	I731	
LEU		A232	G334	I437			
VAL		I233	R336	A439	W551	D734	
ARG		Q234	Q337	E440	F552	H735	
GLY			R338		G553		
MET			K344	N443	S444	R745	
ARG			A346	L445	E554	S746	
ALA		P237	T347	F452	E555	Q760	
VAL		P239		L456	A557		
GLU		R239					
PHE		G240					
LYS		I241					
		L242					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	279421	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.340	Depositor
Minimum map value	-0.414	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	400.0, 400.0, 400.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AGS, 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	0.12	0/4339	0.31	1/5855 (0.0%)
1	B	0.13	0/4339	0.33	1/5855 (0.0%)
1	C	0.12	0/4339	0.32	1/5855 (0.0%)
1	D	0.12	0/4339	0.31	1/5855 (0.0%)
1	E	0.12	0/4339	0.32	1/5855 (0.0%)
1	F	0.12	0/4339	0.33	1/5855 (0.0%)
All	All	0.12	0/26034	0.32	6/35130 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	599	ARG	CB-CA-C	-5.39	109.91	117.23
1	F	599	ARG	CB-CA-C	-5.38	109.91	117.23
1	E	599	ARG	CB-CA-C	-5.38	109.92	117.23
1	A	599	ARG	CB-CA-C	-5.35	109.95	117.23
1	D	599	ARG	CB-CA-C	-5.32	110.00	117.23
1	B	599	ARG	CB-CA-C	-5.22	110.12	117.23

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	4269	0	4314	103	0
1	B	4269	0	4313	105	0
1	C	4269	0	4313	105	0
1	D	4269	0	4314	97	0
1	E	4269	0	4313	94	0
1	F	4269	0	4313	114	0
2	A	62	0	24	3	0
2	B	62	0	24	3	0
2	C	62	0	24	5	0
2	D	62	0	24	3	0
2	E	62	0	24	3	0
2	F	62	0	24	4	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
All	All	25998	0	26024	549	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 11.

All (549) 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:D:547:LEU:HB3	1:D:600:VAL:HG11	1.63	0.80
1:A:547:LEU:HB3	1:A:600:VAL:HG11	1.64	0.79
1:E:547:LEU:HB3	1:E:600:VAL:HG11	1.65	0.78
1:B:547:LEU:HB3	1:B:600:VAL:HG11	1.65	0.77
1:C:760:GLN:O	1:D:744:ARG:NH2	2.20	0.75
1:D:269:ILE:HD11	1:D:303:ILE:HG12	1.70	0.74
1:F:269:ILE:HD11	1:F:303:ILE:HG12	1.68	0.73
1:E:764:GLN:NE2	1:F:745:ARG:O	2.21	0.73
1:A:744:ARG:NH2	1:F:760:GLN:O	2.20	0.73
1:D:764:GLN:NE2	1:E:745:ARG:O	2.22	0.73
1:A:269:ILE:HD11	1:A:303:ILE:HG12	1.70	0.72
1:A:764:GLN:NE2	1:B:745:ARG:O	2.22	0.72
1:B:269:ILE:HD11	1:B:303:ILE:HG12	1.72	0.71
1:E:269:ILE:HD11	1:E:303:ILE:HG12	1.72	0.70
1:C:269:ILE:HD11	1:C:303:ILE:HG12	1.72	0.69
1:F:764:GLN:O	1:F:766:ARG:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:766:ARG:NH2	2:E:902:AGS:O3G	2.28	0.67
1:C:551:TRP:HZ2	1:C:603:GLN:HE22	1.43	0.67
1:F:551:TRP:HZ2	1:F:603:GLN:HE22	1.42	0.66
1:A:766:ARG:NH2	2:B:902:AGS:O3G	2.28	0.66
1:C:423:ILE:HG12	1:C:445:LEU:HD21	1.77	0.65
1:A:317:HIS:HB3	1:F:322:ARG:HH22	1.62	0.65
1:C:764:GLN:NE2	1:D:745:ARG:O	2.30	0.64
1:C:239:ARG:NH1	1:C:335:LEU:O	2.31	0.64
1:C:603:GLN:HG2	1:D:549:THR:HG23	1.80	0.64
1:F:239:ARG:NH1	1:F:335:LEU:O	2.31	0.64
1:A:549:THR:HG23	1:F:603:GLN:HG2	1.80	0.64
1:D:350:PRO:O	1:D:358:ARG:NH2	2.31	0.63
1:A:552:PHE:HD2	1:F:556:GLU:HB3	1.64	0.63
1:B:764:GLN:NE2	1:C:745:ARG:O	2.31	0.63
1:C:322:ARG:HH22	1:D:317:HIS:HB3	1.61	0.63
1:D:556:GLU:HB3	1:E:552:PHE:HD2	1.63	0.63
1:A:442:MET:HE1	1:F:229:LEU:HA	1.81	0.63
1:B:766:ARG:NH2	2:C:902:AGS:O3G	2.28	0.62
1:B:766:ARG:HH21	1:C:520:PRO:HB3	1.65	0.62
1:E:766:ARG:NH2	2:F:902:AGS:O3G	2.28	0.62
1:A:556:GLU:HB3	1:B:552:PHE:HD2	1.64	0.61
1:B:556:GLU:HB3	1:C:552:PHE:HD2	1.65	0.61
1:A:239:ARG:NH1	1:A:335:LEU:O	2.34	0.61
1:C:219:MET:HE3	1:C:241:ILE:HD12	1.82	0.61
1:C:275:MET:HE1	1:C:321:GLU:HG2	1.83	0.61
1:F:547:LEU:HB3	1:F:600:VAL:HG11	1.83	0.61
1:C:472:PRO:O	1:C:533:ASN:ND2	2.30	0.60
1:C:476:TRP:NE1	1:C:534:GLU:OE1	2.26	0.60
1:C:556:GLU:HB3	1:D:552:PHE:HD2	1.64	0.60
1:B:239:ARG:NH1	1:B:335:LEU:O	2.34	0.60
1:B:476:TRP:NE1	1:B:534:GLU:OE1	2.32	0.60
1:C:547:LEU:HB3	1:C:600:VAL:HG11	1.82	0.60
1:C:760:GLN:HA	1:D:744:ARG:HH22	1.66	0.60
1:E:556:GLU:HB3	1:F:552:PHE:HD2	1.67	0.60
1:F:635:ARG:HH21	1:F:638:ARG:HE	1.48	0.60
1:A:350:PRO:O	1:A:358:ARG:NH2	2.35	0.59
1:F:267:PHE:HB3	1:F:301:ILE:HG22	1.84	0.59
1:C:350:PRO:O	1:C:358:ARG:NH2	2.36	0.59
1:E:350:PRO:O	1:E:358:ARG:NH2	2.35	0.59
1:F:219:MET:HE3	1:F:241:ILE:HD12	1.84	0.59
1:F:350:PRO:O	1:F:358:ARG:NH2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:744:ARG:HH22	1:F:760:GLN:HA	1.67	0.59
1:C:635:ARG:HH21	1:C:638:ARG:HE	1.48	0.59
1:D:239:ARG:NH1	1:D:335:LEU:O	2.36	0.59
1:F:288:LYS:O	1:F:292:GLU:HG2	2.03	0.59
1:F:476:TRP:NE1	1:F:534:GLU:OE1	2.26	0.58
1:B:377:ARG:HB2	1:B:411:LEU:HD11	1.86	0.58
1:F:397:GLU:OE2	1:F:401:ASN:ND2	2.37	0.58
1:B:472:PRO:O	1:B:533:ASN:ND2	2.31	0.58
1:B:267:PHE:HB3	1:B:301:ILE:HG22	1.86	0.57
1:E:239:ARG:NH1	1:E:335:LEU:O	2.38	0.57
1:E:377:ARG:HB2	1:E:411:LEU:HD11	1.86	0.57
1:B:246:PRO:HD2	1:B:249:THR:HG21	1.87	0.57
1:B:630:ASP:O	1:B:633:ILE:HG22	2.05	0.57
1:E:397:GLU:OE2	1:E:401:ASN:ND2	2.38	0.57
1:D:472:PRO:O	1:D:533:ASN:ND2	2.32	0.56
1:B:350:PRO:O	1:B:358:ARG:NH2	2.38	0.56
1:C:267:PHE:HB3	1:C:301:ILE:HG22	1.87	0.56
1:E:472:PRO:O	1:E:533:ASN:ND2	2.30	0.56
1:B:580:ASP:OD1	1:B:581:SER:N	2.39	0.56
1:E:322:ARG:HH22	1:F:317:HIS:HB3	1.70	0.56
1:F:423:ILE:HG12	1:F:445:LEU:HD21	1.85	0.56
1:B:586:ARG:NE	1:B:598:ASP:OD2	2.38	0.56
1:D:603:GLN:HG2	1:E:549:THR:HG23	1.88	0.56
1:C:288:LYS:O	1:C:292:GLU:HG2	2.05	0.56
1:E:630:ASP:O	1:E:633:ILE:HG22	2.05	0.56
1:F:472:PRO:O	1:F:533:ASN:ND2	2.28	0.56
1:D:375:THR:O	1:D:379:GLU:HG3	2.06	0.56
1:F:275:MET:HE1	1:F:321:GLU:HG2	1.88	0.56
1:E:586:ARG:NE	1:E:598:ASP:OD2	2.38	0.56
1:E:246:PRO:HD2	1:E:249:THR:HG21	1.87	0.56
1:B:288:LYS:O	1:B:292:GLU:HG2	2.06	0.55
1:C:397:GLU:OE2	1:C:401:ASN:ND2	2.37	0.55
1:D:356:ALA:HA	1:D:359:ARG:HH11	1.71	0.55
1:C:246:PRO:HD2	1:C:249:THR:HG21	1.87	0.55
1:D:229:LEU:HA	1:E:442:MET:HE1	1.87	0.55
1:E:267:PHE:HB3	1:E:301:ILE:HG22	1.87	0.55
1:B:763:GLN:HG2	1:C:746:SER:HA	1.89	0.55
1:C:377:ARG:HB2	1:C:411:LEU:HD11	1.89	0.55
1:F:580:ASP:OD1	1:F:581:SER:N	2.40	0.55
1:A:603:GLN:HG2	1:B:549:THR:HG23	1.88	0.55
1:B:348:ASN:ND2	2:B:901:AGS:S1G	2.76	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:PHE:HB3	1:A:301:ILE:HG22	1.89	0.54
1:D:586:ARG:NE	1:D:598:ASP:OD2	2.40	0.54
1:E:580:ASP:OD1	1:E:581:SER:N	2.40	0.54
1:A:375:THR:O	1:A:379:GLU:HG3	2.06	0.54
1:A:586:ARG:NE	1:A:598:ASP:OD2	2.40	0.54
1:E:288:LYS:O	1:E:292:GLU:HG2	2.07	0.54
1:A:348:ASN:ND2	2:A:901:AGS:S1G	2.78	0.54
1:D:609:ASP:OD2	1:D:638:ARG:NH2	2.40	0.54
1:F:375:THR:O	1:F:379:GLU:HG3	2.08	0.54
1:F:526:LEU:HD11	2:F:902:AGS:H2'	1.88	0.54
1:C:526:LEU:HD11	2:C:902:AGS:H2'	1.89	0.54
1:C:580:ASP:OD1	1:C:581:SER:N	2.40	0.54
1:E:414:LEU:HD11	1:E:456:LEU:HD23	1.90	0.54
1:A:229:LEU:HA	1:B:442:MET:HE1	1.88	0.54
1:A:377:ARG:HB2	1:A:411:LEU:HD11	1.90	0.54
1:C:375:THR:O	1:C:379:GLU:HG3	2.08	0.54
1:D:377:ARG:HB2	1:D:411:LEU:HD11	1.90	0.54
1:A:546:GLU:HG2	1:F:606:THR:HG23	1.90	0.54
1:D:526:LEU:HD11	2:D:902:AGS:H2'	1.88	0.54
1:D:636:PRO:HA	1:D:640:ASP:HB3	1.90	0.54
1:E:681:GLY:HA3	1:E:745:ARG:HH21	1.72	0.54
1:E:763:GLN:HG2	1:F:746:SER:HA	1.90	0.54
1:A:399:VAL:HG13	1:A:456:LEU:HD21	1.89	0.53
1:B:397:GLU:OE2	1:B:401:ASN:ND2	2.38	0.53
1:D:348:ASN:ND2	2:D:901:AGS:S1G	2.78	0.53
1:F:377:ARG:HB2	1:F:411:LEU:HD11	1.89	0.53
1:A:482:LEU:HD21	1:A:645:ILE:HG23	1.91	0.53
1:D:267:PHE:HB3	1:D:301:ILE:HG22	1.89	0.53
1:D:399:VAL:HG13	1:D:456:LEU:HD21	1.89	0.53
1:C:348:ASN:ND2	2:C:901:AGS:S1G	2.75	0.53
1:D:580:ASP:OD1	1:D:581:SER:N	2.41	0.53
1:A:580:ASP:OD1	1:A:581:SER:N	2.41	0.53
1:E:375:THR:O	1:E:379:GLU:HG3	2.09	0.53
1:A:636:PRO:HA	1:A:640:ASP:HB3	1.90	0.53
1:B:277:LYS:HB3	1:B:281:GLU:HG3	1.90	0.53
1:D:351:ASN:ND2	1:D:561:GLU:OE2	2.42	0.53
1:E:636:PRO:HA	1:E:640:ASP:HB3	1.89	0.53
1:B:414:LEU:HD11	1:B:456:LEU:HD23	1.89	0.53
1:B:322:ARG:HH22	1:C:317:HIS:HB3	1.73	0.53
1:C:351:ASN:ND2	1:C:561:GLU:OE2	2.42	0.53
1:A:414:LEU:HD11	1:A:456:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:636:PRO:HA	1:B:640:ASP:HB3	1.90	0.53
1:C:589:ASN:ND2	1:C:627:ASP:O	2.37	0.53
1:B:375:THR:O	1:B:379:GLU:HG3	2.09	0.52
1:C:482:LEU:HD21	1:C:645:ILE:HG23	1.91	0.52
1:C:606:THR:HG23	1:D:546:GLU:HG2	1.90	0.52
1:A:472:PRO:O	1:A:533:ASN:ND2	2.32	0.52
1:B:608:MET:HG2	1:B:619:ILE:HD13	1.92	0.52
1:D:482:LEU:HD21	1:D:645:ILE:HG23	1.91	0.52
1:A:526:LEU:HD11	2:A:902:AGS:H2'	1.90	0.52
1:A:681:GLY:HA3	1:A:745:ARG:HH21	1.75	0.52
1:B:603:GLN:HG2	1:C:549:THR:HG23	1.92	0.52
1:C:636:PRO:HA	1:C:640:ASP:HB3	1.92	0.52
1:B:482:LEU:HD21	1:B:645:ILE:HG23	1.92	0.52
1:D:414:LEU:HD11	1:D:456:LEU:HD23	1.91	0.52
1:F:351:ASN:ND2	1:F:561:GLU:OE2	2.42	0.52
1:F:636:PRO:HA	1:F:640:ASP:HB3	1.92	0.52
1:B:399:VAL:HG13	1:B:456:LEU:HD21	1.92	0.52
1:D:608:MET:HG2	1:D:619:ILE:HD13	1.92	0.52
1:E:277:LYS:HB3	1:E:281:GLU:HG3	1.91	0.52
1:F:414:LEU:HD11	1:F:456:LEU:HD23	1.92	0.52
1:B:223:PRO:HG3	1:B:230:PHE:HE2	1.74	0.52
1:C:247:PRO:HD2	1:C:464:LEU:HD22	1.93	0.51
1:E:603:GLN:HG2	1:F:549:THR:HG23	1.93	0.51
1:F:469:VAL:HG22	1:F:540:ILE:HG12	1.92	0.51
1:F:609:ASP:OD2	1:F:638:ARG:NH2	2.41	0.51
1:B:681:GLY:HA3	1:B:745:ARG:HH21	1.73	0.51
1:C:414:LEU:HD11	1:C:456:LEU:HD23	1.92	0.51
1:F:247:PRO:HD2	1:F:464:LEU:HD22	1.92	0.51
1:E:608:MET:HG2	1:E:619:ILE:HD13	1.93	0.51
1:A:511:SER:OG	1:A:640:ASP:OD1	2.29	0.51
1:A:322:ARG:HH22	1:B:317:HIS:HB3	1.76	0.51
1:B:540:ILE:HG22	1:B:542:ILE:HD11	1.92	0.51
1:E:351:ASN:ND2	1:E:561:GLU:OE2	2.43	0.51
1:A:608:MET:HG2	1:A:619:ILE:HD13	1.92	0.51
1:E:399:VAL:HG13	1:E:456:LEU:HD21	1.92	0.51
1:F:482:LEU:HD21	1:F:645:ILE:HG23	1.91	0.51
1:C:469:VAL:HG22	1:C:540:ILE:HG12	1.92	0.51
1:D:681:GLY:HA3	1:D:745:ARG:HH21	1.76	0.51
1:E:482:LEU:HD21	1:E:645:ILE:HG23	1.92	0.51
1:F:551:TRP:HZ2	1:F:603:GLN:NE2	2.09	0.51
1:F:650:GLU:O	1:F:654:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:ALA:HA	1:C:325:VAL:HG22	1.93	0.51
1:B:351:ASN:ND2	1:B:561:GLU:OE2	2.44	0.50
1:F:517:TYR:CZ	1:F:644:TYR:HB2	2.46	0.50
1:F:589:ASN:ND2	1:F:627:ASP:O	2.36	0.50
1:E:673:GLU:N	1:E:673:GLU:OE1	2.45	0.50
1:A:609:ASP:OD2	1:A:638:ARG:NH2	2.40	0.50
1:C:701:GLU:HG3	1:C:735:HIS:HE2	1.76	0.50
1:A:469:VAL:HG22	1:A:540:ILE:HG12	1.93	0.50
1:C:635:ARG:HH21	1:C:638:ARG:NE	2.09	0.50
1:E:671:ASP:H	1:E:733:ARG:NH1	2.09	0.50
1:D:511:SER:OG	1:D:640:ASP:OD1	2.29	0.50
1:F:671:ASP:OD1	1:F:672:LEU:N	2.44	0.50
1:B:517:TYR:CZ	1:B:644:TYR:HB2	2.47	0.50
1:E:540:ILE:HG22	1:E:542:ILE:HD11	1.93	0.50
1:B:671:ASP:H	1:B:733:ARG:NH1	2.09	0.50
1:C:605:LEU:HD22	1:C:638:ARG:HH11	1.77	0.50
1:C:671:ASP:OD1	1:C:672:LEU:N	2.45	0.50
1:E:348:ASN:ND2	2:E:901:AGS:S1G	2.79	0.50
1:C:517:TYR:CZ	1:C:644:TYR:HB2	2.47	0.50
1:C:608:MET:HG2	1:C:619:ILE:HD13	1.94	0.50
1:F:605:LEU:HD22	1:F:638:ARG:HH11	1.77	0.50
1:F:635:ARG:HH21	1:F:638:ARG:NE	2.10	0.50
1:C:564:ASP:O	1:C:568:GLN:HG2	2.12	0.49
1:F:701:GLU:HG3	1:F:735:HIS:HE2	1.77	0.49
1:C:486:LYS:O	1:C:490:GLN:HG3	2.12	0.49
1:C:650:GLU:O	1:C:654:VAL:HG23	2.11	0.49
1:E:526:LEU:HD11	2:E:902:AGS:H2'	1.94	0.49
1:E:766:ARG:HH21	1:F:520:PRO:HB3	1.78	0.49
1:F:348:ASN:ND2	2:F:901:AGS:S1G	2.73	0.49
1:F:399:VAL:HG13	1:F:456:LEU:HD21	1.94	0.49
1:F:486:LYS:O	1:F:490:GLN:HG3	2.13	0.49
1:F:681:GLY:HA3	1:F:745:ARG:HH21	1.78	0.49
1:D:322:ARG:HH22	1:E:317:HIS:HB3	1.76	0.49
1:D:469:VAL:HG22	1:D:540:ILE:HG12	1.93	0.49
1:E:517:TYR:CZ	1:E:644:TYR:HB2	2.47	0.49
1:B:673:GLU:OE1	1:B:673:GLU:N	2.44	0.49
1:C:609:ASP:OD2	1:C:638:ARG:NH2	2.41	0.49
1:E:559:VAL:HG12	1:E:607:GLU:HG3	1.95	0.49
1:C:499:HIS:HB3	1:C:502:LYS:HG2	1.95	0.49
1:C:681:GLY:HA3	1:C:745:ARG:HH21	1.76	0.49
1:F:564:ASP:O	1:F:568:GLN:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:VAL:HG22	1:B:540:ILE:HG12	1.95	0.49
1:D:310:ALA:HA	1:D:325:VAL:HG22	1.95	0.49
1:A:763:GLN:HG2	1:B:746:SER:HA	1.95	0.49
1:E:266:PHE:HE1	1:E:268:LEU:HB2	1.78	0.49
1:E:310:ALA:HA	1:E:325:VAL:HG22	1.94	0.49
1:F:275:MET:HG2	1:F:309:ILE:HG22	1.95	0.49
1:C:399:VAL:HG13	1:C:456:LEU:HD21	1.95	0.48
1:E:371:ILE:HD11	1:E:468:VAL:HG12	1.96	0.48
1:C:605:LEU:HD22	1:C:638:ARG:NH1	2.29	0.48
1:F:310:ALA:HA	1:F:325:VAL:HG22	1.94	0.48
1:A:359:ARG:HG3	1:A:359:ARG:HH11	1.78	0.48
1:A:423:ILE:HG12	1:A:445:LEU:HD21	1.96	0.48
1:B:526:LEU:HD11	2:B:902:AGS:H2'	1.94	0.48
1:C:333:ASP:OD2	1:C:362:ARG:NH2	2.43	0.48
1:C:452:PHE:O	1:C:456:LEU:HG	2.14	0.48
1:F:605:LEU:HD22	1:F:638:ARG:NH1	2.28	0.48
1:B:266:PHE:HE1	1:B:268:LEU:HB2	1.77	0.48
1:B:310:ALA:HA	1:B:325:VAL:HG22	1.94	0.48
1:B:635:ARG:HA	1:B:766:ARG:NH1	2.28	0.48
1:C:760:GLN:CA	1:D:744:ARG:HH22	2.26	0.48
1:F:203:TYR:N	1:F:261:GLU:OE2	2.42	0.48
1:F:499:HIS:HB3	1:F:502:LYS:HG2	1.95	0.48
1:F:608:MET:HG2	1:F:619:ILE:HD13	1.95	0.48
1:C:559:VAL:HG12	1:C:607:GLU:HG3	1.95	0.48
1:F:452:PHE:O	1:F:456:LEU:HG	2.14	0.48
1:F:559:VAL:HG12	1:F:607:GLU:HG3	1.95	0.48
1:C:275:MET:HG2	1:C:309:ILE:HG22	1.94	0.48
1:D:246:PRO:HG2	1:D:371:ILE:HD11	1.95	0.48
1:A:246:PRO:HG2	1:A:371:ILE:HD11	1.96	0.48
1:A:310:ALA:HA	1:A:325:VAL:HG22	1.94	0.48
1:A:564:ASP:O	1:A:568:GLN:HG2	2.14	0.48
1:A:606:THR:HG23	1:B:546:GLU:HG2	1.96	0.48
1:D:452:PHE:O	1:D:456:LEU:HG	2.14	0.48
1:F:673:GLU:OE1	1:F:673:GLU:N	2.45	0.48
1:A:491:GLU:HG2	1:A:495:TYR:CE2	2.49	0.47
1:A:658:LYS:HA	1:A:658:LYS:HE2	1.96	0.47
1:A:452:PHE:O	1:A:456:LEU:HG	2.14	0.47
1:C:482:LEU:HD13	1:C:527:LEU:HD11	1.96	0.47
1:B:564:ASP:O	1:B:568:GLN:HG2	2.14	0.47
1:C:322:ARG:HD2	1:D:321:GLU:OE2	2.14	0.47
1:A:519:PRO:HG2	1:A:522:CYS:SG	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:589:ASN:ND2	1:B:627:ASP:O	2.38	0.47
1:D:650:GLU:O	1:D:654:VAL:HG23	2.14	0.47
1:E:589:ASN:ND2	1:E:627:ASP:O	2.38	0.47
1:F:333:ASP:OD2	1:F:362:ARG:NH2	2.43	0.47
1:F:586:ARG:NE	1:F:598:ASP:OD2	2.47	0.47
1:A:744:ARG:HH22	1:F:760:GLN:CA	2.26	0.47
1:C:658:LYS:HE2	1:C:658:LYS:HA	1.96	0.47
1:D:763:GLN:HG2	1:E:746:SER:HA	1.95	0.47
1:E:539:PHE:CE2	1:E:541:SER:HB2	2.50	0.47
1:E:564:ASP:O	1:E:568:GLN:HG2	2.14	0.47
1:A:316:THR:O	1:A:322:ARG:NH2	2.47	0.47
1:E:650:GLU:O	1:E:654:VAL:HG23	2.14	0.47
1:A:246:PRO:HD2	1:A:249:THR:HG21	1.95	0.47
1:B:371:ILE:HD11	1:B:468:VAL:HG12	1.96	0.47
1:B:658:LYS:HE2	1:B:658:LYS:HA	1.96	0.47
1:D:491:GLU:HG2	1:D:495:TYR:CE2	2.49	0.47
1:D:606:THR:HG23	1:E:546:GLU:HG2	1.97	0.47
1:E:469:VAL:HG22	1:E:540:ILE:HG12	1.95	0.47
1:F:482:LEU:HD13	1:F:527:LEU:HD11	1.97	0.47
1:F:658:LYS:HA	1:F:658:LYS:HE2	1.97	0.47
1:A:650:GLU:O	1:A:654:VAL:HG23	2.15	0.47
1:C:551:TRP:HZ2	1:C:603:GLN:NE2	2.09	0.47
1:D:517:TYR:CZ	1:D:644:TYR:HB2	2.50	0.47
1:D:564:ASP:O	1:D:568:GLN:HG2	2.14	0.47
1:B:257:ALA:O	1:B:261:GLU:HG2	2.15	0.47
1:D:605:LEU:HD22	1:D:638:ARG:HH11	1.80	0.47
1:D:658:LYS:HE2	1:D:658:LYS:HA	1.96	0.47
1:C:570:ALA:HB1	1:C:616:ASN:OD1	2.14	0.46
1:D:316:THR:O	1:D:322:ARG:NH2	2.47	0.46
1:E:247:PRO:HD2	1:E:464:LEU:HD22	1.97	0.46
1:D:246:PRO:HD2	1:D:249:THR:HG21	1.96	0.46
1:F:567:ARG:HH21	1:F:611:MET:HA	1.81	0.46
1:A:223:PRO:HG3	1:A:230:PHE:HE2	1.81	0.46
1:A:605:LEU:HD22	1:A:638:ARG:HH11	1.80	0.46
1:B:247:PRO:HD2	1:B:464:LEU:HD22	1.98	0.46
1:B:559:VAL:HG12	1:B:607:GLU:HG3	1.97	0.46
1:C:586:ARG:NE	1:C:598:ASP:OD2	2.48	0.46
1:E:225:ARG:HH21	1:F:432:LEU:HD22	1.80	0.46
1:A:225:ARG:HH21	1:B:432:LEU:HD22	1.79	0.46
1:E:258:VAL:HA	1:E:261:GLU:HG2	1.98	0.46
1:F:644:TYR:CE2	1:F:646:PRO:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ARG:HH21	1:C:432:LEU:HD22	1.80	0.46
1:A:580:ASP:O	1:A:584:LYS:HG2	2.15	0.46
1:A:649:ASP:N	1:A:652:SER:OG	2.49	0.46
1:E:635:ARG:HA	1:E:766:ARG:NH1	2.31	0.46
1:A:517:TYR:CZ	1:A:644:TYR:HB2	2.51	0.46
1:A:567:ARG:HH21	1:A:611:MET:HA	1.81	0.46
1:B:452:PHE:O	1:B:456:LEU:HG	2.15	0.46
1:B:539:PHE:CE2	1:B:541:SER:HB2	2.50	0.46
1:D:567:ARG:HH21	1:D:611:MET:HA	1.81	0.46
1:D:580:ASP:O	1:D:584:LYS:HG2	2.15	0.46
1:F:407:VAL:HG22	1:F:410:ASP:OD2	2.16	0.46
1:B:650:GLU:O	1:B:654:VAL:HG23	2.15	0.46
1:E:243:LEU:O	1:E:346:ALA:HA	2.16	0.46
1:E:658:LYS:HE2	1:E:658:LYS:HA	1.97	0.45
1:A:241:ILE:HD13	1:A:365:ARG:HB2	1.99	0.45
1:A:321:GLU:OE2	1:F:322:ARG:HD2	2.16	0.45
1:C:491:GLU:HG2	1:C:495:TYR:CE2	2.51	0.45
1:C:580:ASP:O	1:C:584:LYS:HG2	2.17	0.45
1:D:243:LEU:O	1:D:346:ALA:HA	2.16	0.45
1:D:752:ILE:O	1:D:756:GLU:HG2	2.16	0.45
1:E:322:ARG:HD2	1:F:321:GLU:OE2	2.16	0.45
1:E:407:VAL:HG22	1:E:410:ASP:OD2	2.16	0.45
1:B:221:GLU:OE1	1:B:225:ARG:NH1	2.49	0.45
1:A:243:LEU:O	1:A:346:ALA:HA	2.16	0.45
1:A:407:VAL:HG22	1:A:410:ASP:OD2	2.16	0.45
1:B:258:VAL:HA	1:B:261:GLU:HG2	1.99	0.45
1:C:407:VAL:HG22	1:C:410:ASP:OD2	2.15	0.45
1:D:519:PRO:HG2	1:D:522:CYS:SG	2.55	0.45
1:E:452:PHE:O	1:E:456:LEU:HG	2.15	0.45
1:F:570:ALA:HB1	1:F:616:ASN:OD1	2.17	0.45
1:D:356:ALA:HA	1:D:359:ARG:NH1	2.30	0.45
1:D:671:ASP:H	1:D:733:ARG:NH1	2.15	0.45
1:E:257:ALA:O	1:E:261:GLU:HG2	2.16	0.45
1:F:246:PRO:HD2	1:F:249:THR:HG21	1.97	0.45
1:B:243:LEU:O	1:B:346:ALA:HA	2.16	0.45
1:C:644:TYR:CE2	1:C:646:PRO:HB3	2.51	0.45
1:A:288:LYS:O	1:A:292:GLU:HG2	2.17	0.45
1:B:491:GLU:HG2	1:B:495:TYR:CE2	2.52	0.45
1:D:223:PRO:HG3	1:D:230:PHE:HE2	1.81	0.45
1:A:752:ILE:O	1:A:756:GLU:HG2	2.17	0.45
1:B:579:LEU:HD23	1:B:582:ILE:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:PRO:HG2	1:C:522:CYS:SG	2.56	0.45
1:C:603:GLN:CG	1:D:549:THR:HG23	2.45	0.45
1:D:225:ARG:HH21	1:E:432:LEU:HD22	1.80	0.45
1:D:313:ARG:N	1:D:354:ASP:OD2	2.41	0.45
1:F:491:GLU:HG2	1:F:495:TYR:CE2	2.51	0.45
1:A:432:LEU:HD22	1:F:225:ARG:HH21	1.81	0.45
1:C:266:PHE:HE1	1:C:268:LEU:HB2	1.80	0.45
1:E:377:ARG:NH1	1:E:403:THR:O	2.50	0.45
1:F:544:GLY:HA2	1:F:547:LEU:HD12	1.99	0.45
1:A:671:ASP:H	1:A:733:ARG:NH1	2.15	0.45
1:D:328:LEU:HD23	1:D:357:LEU:HD11	1.98	0.45
1:D:407:VAL:HG22	1:D:410:ASP:OD2	2.16	0.45
1:F:649:ASP:N	1:F:652:SER:OG	2.50	0.45
1:C:649:ASP:N	1:C:652:SER:OG	2.51	0.44
1:A:284:SER:O	1:A:288:LYS:HG3	2.17	0.44
1:A:328:LEU:HD23	1:A:357:LEU:HD11	2.00	0.44
1:A:673:GLU:OE1	1:A:673:GLU:N	2.44	0.44
1:B:377:ARG:NH1	1:B:403:THR:O	2.51	0.44
1:B:614:LYS:HG2	1:C:402:GLU:OE2	2.17	0.44
1:E:221:GLU:OE1	1:E:225:ARG:NH1	2.50	0.44
1:E:580:ASP:O	1:E:584:LYS:HG2	2.16	0.44
1:F:246:PRO:HG2	1:F:371:ILE:HD11	1.99	0.44
1:A:549:THR:HG23	1:F:603:GLN:CG	2.45	0.44
1:A:603:GLN:CG	1:B:549:THR:HG23	2.47	0.44
1:C:544:GLY:HA2	1:C:547:LEU:HD12	1.99	0.44
1:C:567:ARG:HH21	1:C:611:MET:HA	1.82	0.44
1:D:649:ASP:N	1:D:652:SER:OG	2.50	0.44
1:B:508:MET:HG3	1:C:695:CYS:HB2	1.99	0.44
1:D:284:SER:O	1:D:288:LYS:HG3	2.17	0.44
1:D:673:GLU:OE1	1:D:673:GLU:N	2.44	0.44
2:C:902:AGS:O2G	2:C:902:AGS:O1A	2.35	0.44
1:E:614:LYS:HG2	1:F:402:GLU:OE2	2.18	0.44
1:B:407:VAL:HG22	1:B:410:ASP:OD2	2.17	0.44
1:A:377:ARG:HD2	1:A:400:ALA:O	2.17	0.44
1:A:625:ARG:HB3	1:A:628:ILE:HG12	2.00	0.44
1:B:581:SER:HA	1:B:584:LYS:HE2	2.00	0.44
1:B:644:TYR:CE2	1:B:646:PRO:HB3	2.53	0.44
1:C:754:LYS:HA	1:C:757:MET:HG3	1.99	0.44
1:E:649:ASP:N	1:E:652:SER:OG	2.51	0.44
1:A:754:LYS:HA	1:A:757:MET:HG3	2.00	0.44
1:B:580:ASP:O	1:B:584:LYS:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:SER:HB2	1:D:288:LYS:NZ	2.33	0.44
1:E:491:GLU:HG2	1:E:495:TYR:CE2	2.52	0.44
1:A:557:ALA:O	1:A:561:GLU:HG3	2.18	0.43
1:D:359:ARG:HE	1:E:247:PRO:HG3	1.83	0.43
1:D:377:ARG:HD2	1:D:400:ALA:O	2.17	0.43
1:E:482:LEU:HD13	1:E:527:LEU:HD11	2.00	0.43
1:A:266:PHE:HE1	1:A:268:LEU:HB2	1.83	0.43
1:F:580:ASP:O	1:F:584:LYS:HG2	2.17	0.43
1:A:539:PHE:CE2	1:A:541:SER:HB2	2.54	0.43
1:A:754:LYS:HD2	1:F:768:PHE:CG	2.52	0.43
1:B:582:ILE:HD13	1:B:600:VAL:HG21	2.00	0.43
1:D:241:ILE:HD13	1:D:365:ARG:HB2	1.99	0.43
1:D:489:LEU:HD21	1:D:516:PHE:HZ	1.83	0.43
1:D:603:GLN:CG	1:E:549:THR:HG23	2.48	0.43
1:E:728:VAL:HB	1:E:729:PRO:HD3	2.01	0.43
1:A:744:ARG:HH22	1:F:760:GLN:C	2.26	0.43
1:B:482:LEU:HD13	1:B:527:LEU:HD11	2.00	0.43
1:B:563:PHE:HD2	1:B:611:MET:HE3	1.84	0.43
1:E:644:TYR:CE2	1:E:646:PRO:HB3	2.53	0.43
1:C:407:VAL:H	1:C:410:ASP:HB2	1.84	0.43
1:E:508:MET:HG3	1:F:695:CYS:HB2	1.99	0.43
1:F:557:ALA:O	1:F:561:GLU:HG3	2.19	0.43
1:A:284:SER:HB2	1:A:288:LYS:NZ	2.33	0.43
1:D:539:PHE:CE2	1:D:541:SER:HB2	2.53	0.43
1:E:519:PRO:HG2	1:E:522:CYS:SG	2.58	0.43
1:A:275:MET:HG2	1:A:309:ILE:HG22	2.01	0.43
1:B:624:ASN:O	1:B:755:TYR:OH	2.27	0.43
1:B:649:ASP:N	1:B:652:SER:OG	2.52	0.43
1:B:734:ASP:OD1	1:B:735:HIS:N	2.52	0.43
1:D:423:ILE:HG12	1:D:445:LEU:HD21	2.01	0.43
1:C:216:ILE:HD13	1:C:254:ILE:HG21	2.01	0.43
1:D:297:ALA:HB1	1:D:298:PRO:HD2	2.01	0.43
1:D:589:ASN:ND2	1:D:627:ASP:O	2.39	0.43
1:F:328:LEU:HD23	1:F:357:LEU:HD11	2.01	0.43
1:B:681:GLY:HA3	1:B:745:ARG:HE	1.84	0.42
1:C:241:ILE:HB	1:C:344:MET:HG2	2.01	0.42
1:D:266:PHE:HE1	1:D:268:LEU:HB2	1.83	0.42
1:E:657:LEU:HD13	1:E:675:LEU:HD23	2.01	0.42
1:B:220:VAL:C	1:B:223:PRO:HD2	2.44	0.42
1:C:557:ALA:O	1:C:561:GLU:HG3	2.20	0.42
1:F:223:PRO:HG3	1:F:230:PHE:HE2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:SER:O	1:F:764:GLN:HA	2.20	0.42
1:B:503:PHE:CE2	1:B:510:PRO:HB3	2.54	0.42
1:C:734:ASP:OD1	1:C:735:HIS:N	2.52	0.42
1:F:734:ASP:OD1	1:F:735:HIS:N	2.52	0.42
1:B:423:ILE:HG12	1:B:445:LEU:HD21	2.02	0.42
1:C:328:LEU:HD23	1:C:357:LEU:HD11	2.01	0.42
1:C:508:MET:HE1	1:D:696:LYS:HG2	2.01	0.42
1:C:625:ARG:HB3	1:C:628:ILE:HG12	2.01	0.42
1:E:563:PHE:HD2	1:E:611:MET:HE3	1.84	0.42
1:E:567:ARG:HG3	1:E:611:MET:HE1	2.01	0.42
1:F:241:ILE:HB	1:F:344:MET:HG2	2.02	0.42
1:A:333:ASP:OD2	1:A:362:ARG:NH2	2.46	0.42
1:B:519:PRO:HG2	1:B:522:CYS:SG	2.59	0.42
1:B:728:VAL:HB	1:B:729:PRO:HD3	2.01	0.42
1:F:407:VAL:H	1:F:410:ASP:HB2	1.84	0.42
1:B:567:ARG:HG3	1:B:611:MET:HE1	2.01	0.42
1:B:605:LEU:HD22	1:B:638:ARG:HD3	2.02	0.42
1:B:764:GLN:N	1:B:764:GLN:OE1	2.53	0.42
1:D:524:LYS:HG2	1:D:645:ILE:HD13	2.01	0.42
1:D:557:ALA:O	1:D:561:GLU:HG3	2.19	0.42
1:D:614:LYS:HG2	1:E:402:GLU:OE2	2.20	0.42
1:F:519:PRO:HG2	1:F:522:CYS:SG	2.59	0.42
1:F:524:LYS:HG2	1:F:645:ILE:HD13	2.01	0.42
1:A:377:ARG:NH1	1:A:403:THR:O	2.53	0.42
1:A:402:GLU:OE2	1:F:614:LYS:HG2	2.20	0.42
1:A:489:LEU:HD21	1:A:516:PHE:HZ	1.83	0.42
1:B:271:GLY:HA2	1:B:309:ILE:HG23	2.01	0.42
1:C:377:ARG:HD2	1:C:400:ALA:O	2.19	0.42
1:F:728:VAL:HB	1:F:729:PRO:HD3	2.01	0.42
1:B:512:LYS:HZ1	1:B:615:LYS:HB3	1.85	0.42
1:B:768:PHE:CD2	1:C:754:LYS:HD2	2.54	0.42
1:A:297:ALA:HB1	1:A:298:PRO:HD2	2.01	0.42
1:A:611:MET:SD	1:A:619:ILE:HD11	2.60	0.42
1:E:362:ARG:HH22	1:F:305:GLU:CD	2.28	0.42
1:F:377:ARG:HD2	1:F:400:ALA:O	2.19	0.42
1:A:614:LYS:HG2	1:B:402:GLU:OE2	2.19	0.42
1:D:377:ARG:NH1	1:D:403:THR:O	2.53	0.42
1:E:605:LEU:HD22	1:E:638:ARG:HD3	2.02	0.42
1:E:605:LEU:HD22	1:E:638:ARG:HH11	1.85	0.42
1:F:243:LEU:O	1:F:346:ALA:HA	2.20	0.42
1:A:696:LYS:HG2	1:F:508:MET:HE1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:539:PHE:CE2	1:C:541:SER:HB2	2.55	0.41
1:E:503:PHE:CE2	1:E:510:PRO:HB3	2.55	0.41
1:F:539:PHE:CE2	1:F:541:SER:HB2	2.55	0.41
1:C:760:GLN:C	1:D:744:ARG:HH22	2.27	0.41
1:D:275:MET:HG2	1:D:309:ILE:HG22	2.01	0.41
1:D:333:ASP:OD2	1:D:362:ARG:NH2	2.46	0.41
1:D:438:ASP:N	1:D:438:ASP:OD1	2.53	0.41
1:A:519:PRO:HA	1:A:520:PRO:HD3	1.97	0.41
1:B:389:LYS:NZ	1:B:446:ALA:HB2	2.35	0.41
1:C:243:LEU:O	1:C:346:ALA:HA	2.19	0.41
1:C:728:VAL:HB	1:C:729:PRO:HD3	2.01	0.41
1:D:624:ASN:O	1:D:755:TYR:OH	2.22	0.41
1:F:571:PRO:HG3	1:F:616:ASN:ND2	2.35	0.41
1:A:520:PRO:HG2	1:F:766:ARG:O	2.20	0.41
1:B:657:LEU:HD13	1:B:675:LEU:HD23	2.02	0.41
1:E:438:ASP:OD1	1:E:438:ASP:N	2.53	0.41
1:E:701:GLU:HG3	1:E:735:HIS:HE2	1.86	0.41
1:A:407:VAL:H	1:A:410:ASP:HB2	1.85	0.41
1:B:768:PHE:CG	1:C:754:LYS:HD2	2.55	0.41
2:C:901:AGS:O2A	2:C:901:AGS:O2B	2.38	0.41
1:D:611:MET:SD	1:D:619:ILE:HD11	2.61	0.41
1:E:389:LYS:NZ	1:E:446:ALA:HB2	2.35	0.41
1:F:256:ARG:NH1	1:F:268:LEU:HD11	2.35	0.41
1:F:512:LYS:HZ1	1:F:615:LYS:HB3	1.86	0.41
1:A:605:LEU:HD22	1:A:638:ARG:NH1	2.35	0.41
1:B:377:ARG:HD2	1:B:400:ALA:O	2.21	0.41
1:B:752:ILE:O	1:B:756:GLU:HG2	2.21	0.41
1:C:223:PRO:HG3	1:C:230:PHE:HE2	1.85	0.41
1:C:489:LEU:HD21	1:C:516:PHE:HZ	1.86	0.41
1:A:220:VAL:C	1:A:223:PRO:HD2	2.45	0.41
1:E:271:GLY:HA2	1:E:309:ILE:HG23	2.01	0.41
1:E:734:ASP:OD1	1:E:735:HIS:N	2.53	0.41
1:F:216:ILE:HD13	1:F:254:ILE:HG21	2.02	0.41
1:A:512:LYS:HD2	1:A:613:THR:O	2.21	0.41
1:B:216:ILE:HD13	1:B:254:ILE:HG21	2.03	0.41
1:C:524:LYS:HG2	1:C:645:ILE:HD13	2.02	0.41
1:D:565:LYS:HB2	1:D:565:LYS:HE3	1.82	0.41
1:A:524:LYS:HG2	1:A:645:ILE:HD13	2.02	0.41
1:A:644:TYR:CE2	1:A:646:PRO:HB3	2.56	0.41
1:A:728:VAL:HB	1:A:729:PRO:HD3	2.02	0.41
1:A:734:ASP:OD1	1:A:735:HIS:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ARG:HD2	1:C:321:GLU:OE2	2.21	0.41
1:B:332:MET:HE1	1:B:343:VAL:HB	2.02	0.41
1:B:550:MET:SD	1:B:558:ASN:HB2	2.61	0.41
1:B:605:LEU:HD22	1:B:638:ARG:HH11	1.85	0.41
1:C:377:ARG:NH1	1:C:403:THR:O	2.54	0.41
1:C:633:ILE:HG13	1:C:639:LEU:HD12	2.03	0.41
1:D:220:VAL:C	1:D:223:PRO:HD2	2.46	0.41
1:D:512:LYS:HD2	1:D:613:THR:O	2.21	0.41
1:D:605:LEU:HD22	1:D:638:ARG:NH1	2.36	0.41
1:E:512:LYS:HZ1	1:E:615:LYS:HB3	1.86	0.41
1:F:297:ALA:HB1	1:F:298:PRO:HD2	2.03	0.41
1:F:491:GLU:HA	1:F:495:TYR:CD2	2.56	0.41
1:A:438:ASP:OD1	1:A:438:ASP:N	2.52	0.41
1:D:728:VAL:HB	1:D:729:PRO:HD3	2.02	0.41
1:F:241:ILE:HD13	1:F:365:ARG:HB2	2.03	0.41
1:B:551:TRP:CZ3	1:B:599:ARG:HB3	2.56	0.40
2:D:902:AGS:H5'1	2:D:902:AGS:S1G	2.61	0.40
1:E:377:ARG:HD2	1:E:400:ALA:O	2.21	0.40
1:F:237:PRO:HA	1:F:238:PRO:HD3	1.98	0.40
1:F:319:GLU:OE2	1:F:322:ARG:NH1	2.54	0.40
2:F:901:AGS:O2A	2:F:901:AGS:O2B	2.38	0.40
1:A:586:ARG:HB3	1:A:592:ASP:OD1	2.22	0.40
1:E:297:ALA:HB1	1:E:298:PRO:HD2	2.03	0.40
1:E:681:GLY:HA3	1:E:745:ARG:HE	1.85	0.40
1:F:438:ASP:OD1	1:F:438:ASP:N	2.53	0.40
1:A:270:ASN:HB2	1:A:273:GLU:HB3	2.04	0.40
1:A:301:ILE:HD11	1:A:343:VAL:HG22	2.02	0.40
1:A:307:ASP:OD1	1:A:347:THR:OG1	2.35	0.40
1:C:611:MET:SD	1:C:619:ILE:HD11	2.61	0.40
1:D:586:ARG:HB3	1:D:592:ASP:OD1	2.22	0.40
1:B:557:ALA:O	1:B:561:GLU:HG3	2.21	0.40
1:C:225:ARG:HH21	1:D:432:LEU:HD22	1.85	0.40
1:C:491:GLU:HA	1:C:495:TYR:CD2	2.56	0.40
1:D:644:TYR:CE2	1:D:646:PRO:HB3	2.56	0.40
1:E:223:PRO:HG3	1:E:230:PHE:HE2	1.87	0.40
2:A:902:AGS:H5'1	2:A:902:AGS:S1G	2.62	0.40
1:B:633:ILE:HG13	1:B:639:LEU:HD12	2.04	0.40
1:C:682:PHE:CE2	1:C:690:ILE:HD11	2.56	0.40
1:E:301:ILE:HD11	1:E:343:VAL:HG22	2.04	0.40
1:F:377:ARG:NH1	1:F:403:THR:O	2.55	0.40
1:F:666:VAL:HA	1:F:731:ILE:HG23	2.03	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	545/822 (66%)	528 (97%)	16 (3%)	1 (0%)	43	57
1	B	545/822 (66%)	526 (96%)	18 (3%)	1 (0%)	43	57
1	C	545/822 (66%)	528 (97%)	16 (3%)	1 (0%)	43	57
1	D	545/822 (66%)	528 (97%)	16 (3%)	1 (0%)	43	57
1	E	545/822 (66%)	528 (97%)	16 (3%)	1 (0%)	43	57
1	F	545/822 (66%)	526 (96%)	17 (3%)	2 (0%)	30	42
All	All	3270/4932 (66%)	3164 (97%)	99 (3%)	7 (0%)	44	57

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	765	SER
1	A	297	ALA
1	B	297	ALA
1	C	297	ALA
1	D	297	ALA
1	E	297	ALA
1	F	297	ALA

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	455/692 (66%)	455 (100%)	0	100	100
1	B	455/692 (66%)	455 (100%)	0	100	100
1	C	455/692 (66%)	455 (100%)	0	100	100
1	D	455/692 (66%)	455 (100%)	0	100	100
1	E	455/692 (66%)	455 (100%)	0	100	100
1	F	455/692 (66%)	455 (100%)	0	100	100
All	All	2730/4152 (66%)	2730 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN
1	A	285	ASN
1	A	296	ASN
1	A	499	HIS
1	B	285	ASN
1	B	296	ASN
1	B	499	HIS
1	C	285	ASN
1	C	296	ASN
1	C	327	GLN
1	C	458	GLN
1	C	490	GLN
1	C	603	GLN
1	D	285	ASN
1	D	296	ASN
1	D	499	HIS
1	E	285	ASN
1	E	296	ASN
1	E	499	HIS
1	E	764	GLN
1	F	285	ASN
1	F	327	GLN
1	F	458	GLN
1	F	490	GLN
1	F	603	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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$
2	AGS	B	901	3	32,33,33	0.50	1 (3%)	45,52,52	0.66	1 (2%)
2	AGS	D	901	3	32,33,33	0.50	1 (3%)	45,52,52	0.66	1 (2%)
2	AGS	E	901	3	32,33,33	0.49	1 (3%)	45,52,52	0.66	1 (2%)
2	AGS	B	902	3	32,33,33	0.48	1 (3%)	45,52,52	0.70	1 (2%)
2	AGS	C	901	3	32,33,33	0.49	1 (3%)	45,52,52	0.67	1 (2%)
2	AGS	F	901	3	32,33,33	0.49	1 (3%)	45,52,52	0.67	1 (2%)
2	AGS	C	902	3	32,33,33	0.48	1 (3%)	45,52,52	0.69	1 (2%)
2	AGS	A	902	3	32,33,33	0.46	1 (3%)	45,52,52	0.66	1 (2%)
2	AGS	E	902	3	32,33,33	0.48	1 (3%)	45,52,52	0.70	1 (2%)
2	AGS	A	901	3	32,33,33	0.50	1 (3%)	45,52,52	0.66	1 (2%)
2	AGS	F	902	3	32,33,33	0.48	1 (3%)	45,52,52	0.69	1 (2%)
2	AGS	D	902	3	32,33,33	0.46	1 (3%)	45,52,52	0.67	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
2	AGS	B	901	3	-	8/21/38/38	0/3/3/3
2	AGS	D	901	3	-	9/21/38/38	0/3/3/3
2	AGS	E	901	3	-	8/21/38/38	0/3/3/3
2	AGS	B	902	3	-	4/21/38/38	0/3/3/3
2	AGS	C	901	3	-	7/21/38/38	0/3/3/3
2	AGS	F	901	3	-	7/21/38/38	0/3/3/3
2	AGS	C	902	3	-	3/21/38/38	0/3/3/3
2	AGS	A	902	3	-	2/21/38/38	0/3/3/3
2	AGS	E	902	3	-	4/21/38/38	0/3/3/3
2	AGS	A	901	3	-	10/21/38/38	0/3/3/3
2	AGS	F	902	3	-	3/21/38/38	0/3/3/3
2	AGS	D	902	3	-	2/21/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	902	AGS	PG-S1G	2.13	1.95	1.90
2	A	901	AGS	PG-S1G	2.12	1.95	1.90
2	C	901	AGS	PG-S1G	2.11	1.95	1.90
2	F	902	AGS	PG-S1G	2.11	1.95	1.90
2	B	902	AGS	PG-S1G	2.10	1.95	1.90
2	F	901	AGS	PG-S1G	2.10	1.95	1.90
2	A	902	AGS	PG-S1G	2.09	1.95	1.90
2	B	901	AGS	PG-S1G	2.09	1.95	1.90
2	D	902	AGS	PG-S1G	2.08	1.95	1.90
2	D	901	AGS	PG-S1G	2.06	1.95	1.90
2	E	901	AGS	PG-S1G	2.05	1.95	1.90
2	E	902	AGS	PG-S1G	2.05	1.95	1.90

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	902	AGS	PB-O3B-PG	-3.85	119.10	133.17
2	B	902	AGS	PB-O3B-PG	-3.84	119.10	133.17
2	C	902	AGS	PB-O3B-PG	-3.81	119.23	133.17
2	F	902	AGS	PB-O3B-PG	-3.79	119.28	133.17
2	F	901	AGS	PB-O3B-PG	-3.68	119.71	133.17
2	E	901	AGS	PB-O3B-PG	-3.67	119.73	133.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	AGS	PB-O3B-PG	-3.67	119.75	133.17
2	C	901	AGS	PB-O3B-PG	-3.66	119.76	133.17
2	D	902	AGS	PB-O3B-PG	-3.65	119.81	133.17
2	A	901	AGS	PB-O3B-PG	-3.65	119.82	133.17
2	D	901	AGS	PB-O3B-PG	-3.64	119.86	133.17
2	A	902	AGS	PB-O3B-PG	-3.62	119.91	133.17

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	AGS	C5'-O5'-PA-O2A
2	A	901	AGS	C5'-O5'-PA-O3A
2	A	901	AGS	O4'-C4'-C5'-O5'
2	B	901	AGS	C5'-O5'-PA-O2A
2	B	901	AGS	C5'-O5'-PA-O3A
2	B	902	AGS	PB-O3B-PG-O2G
2	B	902	AGS	PB-O3B-PG-O3G
2	C	901	AGS	C5'-O5'-PA-O2A
2	C	901	AGS	C5'-O5'-PA-O3A
2	C	901	AGS	O4'-C4'-C5'-O5'
2	D	901	AGS	C5'-O5'-PA-O2A
2	D	901	AGS	C5'-O5'-PA-O3A
2	D	901	AGS	O4'-C4'-C5'-O5'
2	E	901	AGS	C5'-O5'-PA-O2A
2	E	901	AGS	C5'-O5'-PA-O3A
2	E	902	AGS	PB-O3B-PG-O2G
2	E	902	AGS	PB-O3B-PG-O3G
2	F	901	AGS	C5'-O5'-PA-O2A
2	F	901	AGS	C5'-O5'-PA-O3A
2	F	901	AGS	O4'-C4'-C5'-O5'
2	F	902	AGS	PB-O3B-PG-O2G
2	F	902	AGS	PB-O3B-PG-O3G
2	B	901	AGS	O4'-C4'-C5'-O5'
2	E	901	AGS	O4'-C4'-C5'-O5'
2	A	901	AGS	C3'-C4'-C5'-O5'
2	B	901	AGS	C3'-C4'-C5'-O5'
2	C	901	AGS	C3'-C4'-C5'-O5'
2	D	901	AGS	C3'-C4'-C5'-O5'
2	E	901	AGS	C3'-C4'-C5'-O5'
2	F	901	AGS	C3'-C4'-C5'-O5'
2	A	902	AGS	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
2	B	902	AGS	PA-O3A-PB-O1B
2	C	901	AGS	PA-O3A-PB-O2B
2	D	902	AGS	PA-O3A-PB-O1B
2	E	902	AGS	PA-O3A-PB-O1B
2	F	901	AGS	PA-O3A-PB-O2B
2	A	901	AGS	C5'-O5'-PA-O1A
2	B	901	AGS	C5'-O5'-PA-O1A
2	C	901	AGS	C5'-O5'-PA-O1A
2	D	901	AGS	C5'-O5'-PA-O1A
2	E	901	AGS	C5'-O5'-PA-O1A
2	F	901	AGS	C5'-O5'-PA-O1A
2	A	901	AGS	PA-O3A-PB-O2B
2	B	901	AGS	PA-O3A-PB-O2B
2	D	901	AGS	PA-O3A-PB-O2B
2	E	901	AGS	PA-O3A-PB-O2B
2	A	901	AGS	C4'-C5'-O5'-PA
2	C	901	AGS	C4'-C5'-O5'-PA
2	D	901	AGS	C4'-C5'-O5'-PA
2	F	902	AGS	PA-O3A-PB-O1B
2	A	901	AGS	PB-O3B-PG-O2G
2	A	901	AGS	PB-O3B-PG-O3G
2	C	902	AGS	PB-O3B-PG-O2G
2	C	902	AGS	PB-O3B-PG-O3G
2	D	901	AGS	PB-O3B-PG-O2G
2	B	901	AGS	C4'-C5'-O5'-PA
2	E	901	AGS	C4'-C5'-O5'-PA
2	F	901	AGS	C4'-C5'-O5'-PA
2	A	901	AGS	PA-O3A-PB-O1B
2	C	902	AGS	PA-O3A-PB-O1B
2	D	901	AGS	PA-O3A-PB-O1B
2	A	902	AGS	PA-O3A-PB-O2B
2	B	901	AGS	PA-O3A-PB-O1B
2	B	902	AGS	PA-O3A-PB-O2B
2	D	902	AGS	PA-O3A-PB-O2B
2	E	901	AGS	PA-O3A-PB-O1B
2	E	902	AGS	PA-O3A-PB-O2B

There are no ring outliers.

12 monomers are involved in 21 short contacts:

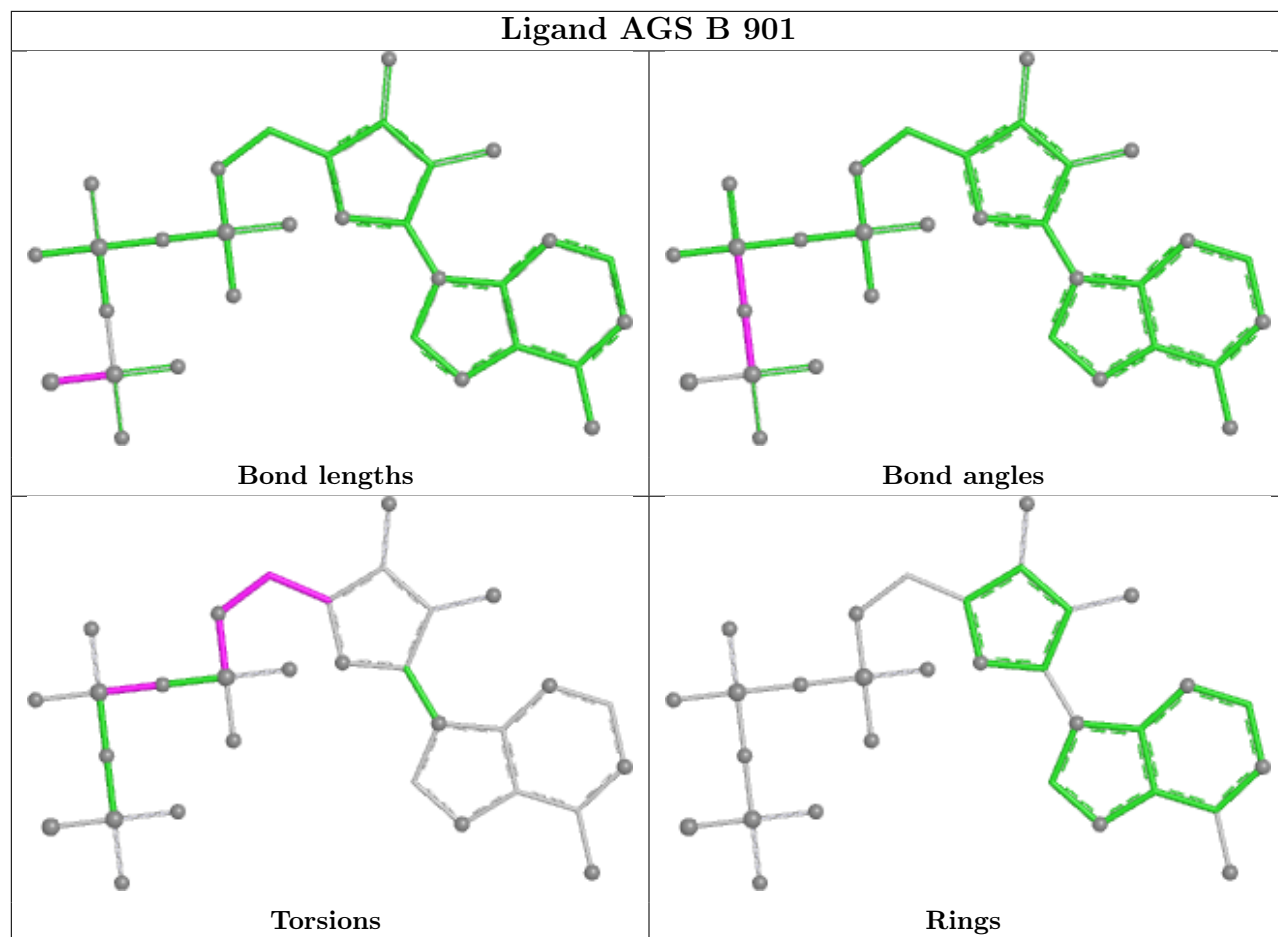
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	AGS	1	0

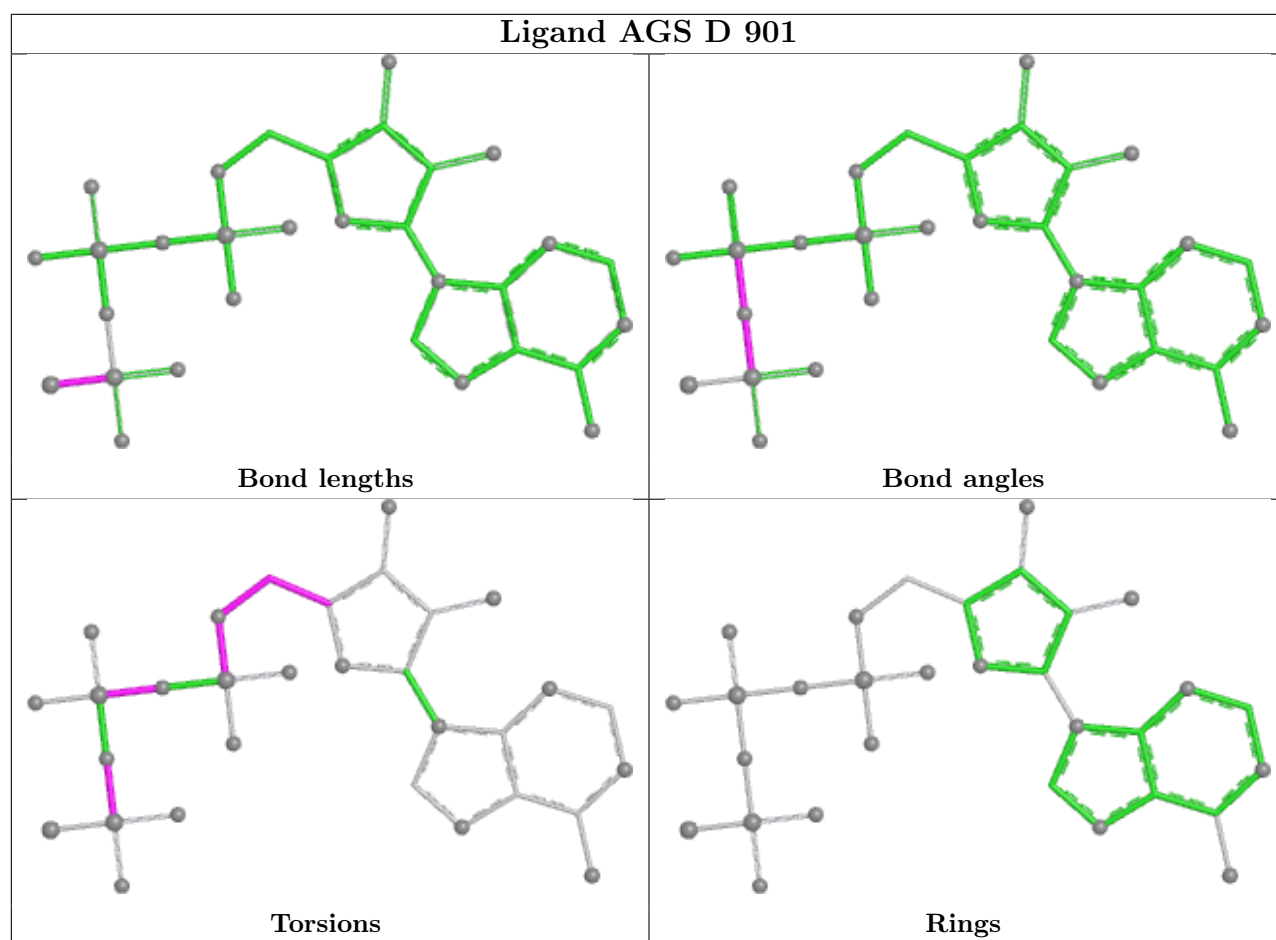
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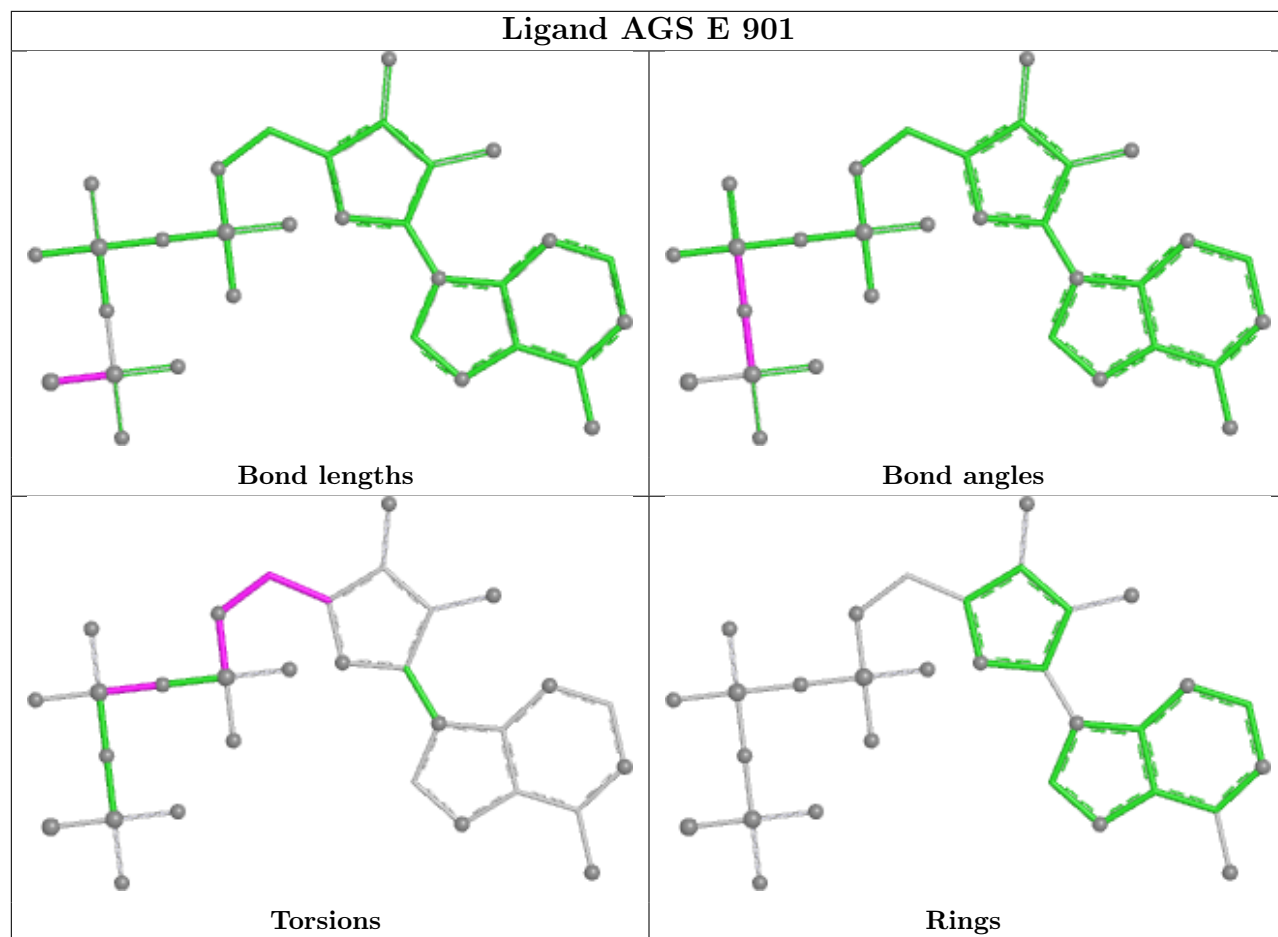
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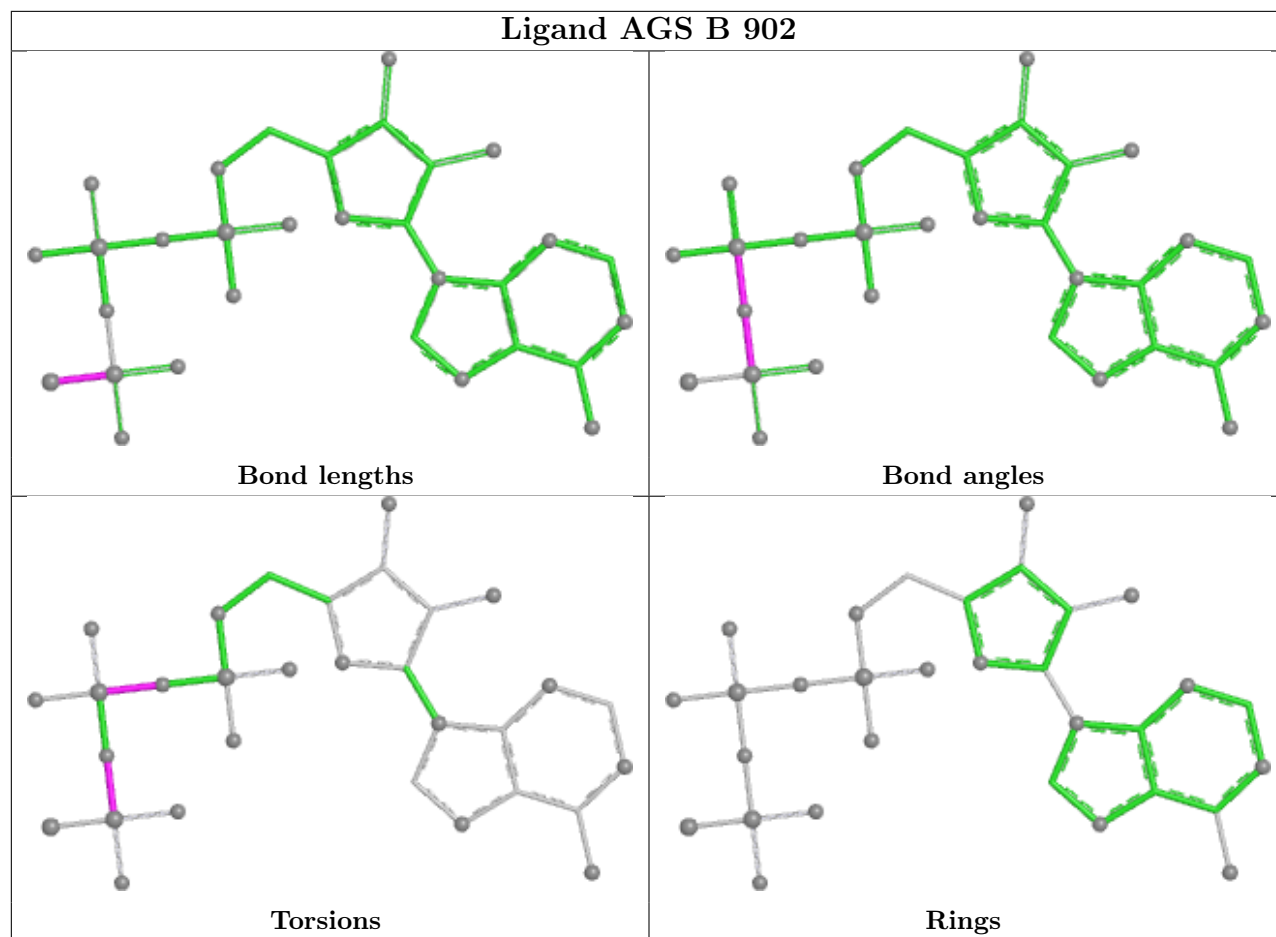
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	901	AGS	1	0
2	E	901	AGS	1	0
2	B	902	AGS	2	0
2	C	901	AGS	2	0
2	F	901	AGS	2	0
2	C	902	AGS	3	0
2	A	902	AGS	2	0
2	E	902	AGS	2	0
2	A	901	AGS	1	0
2	F	902	AGS	2	0
2	D	902	AGS	2	0

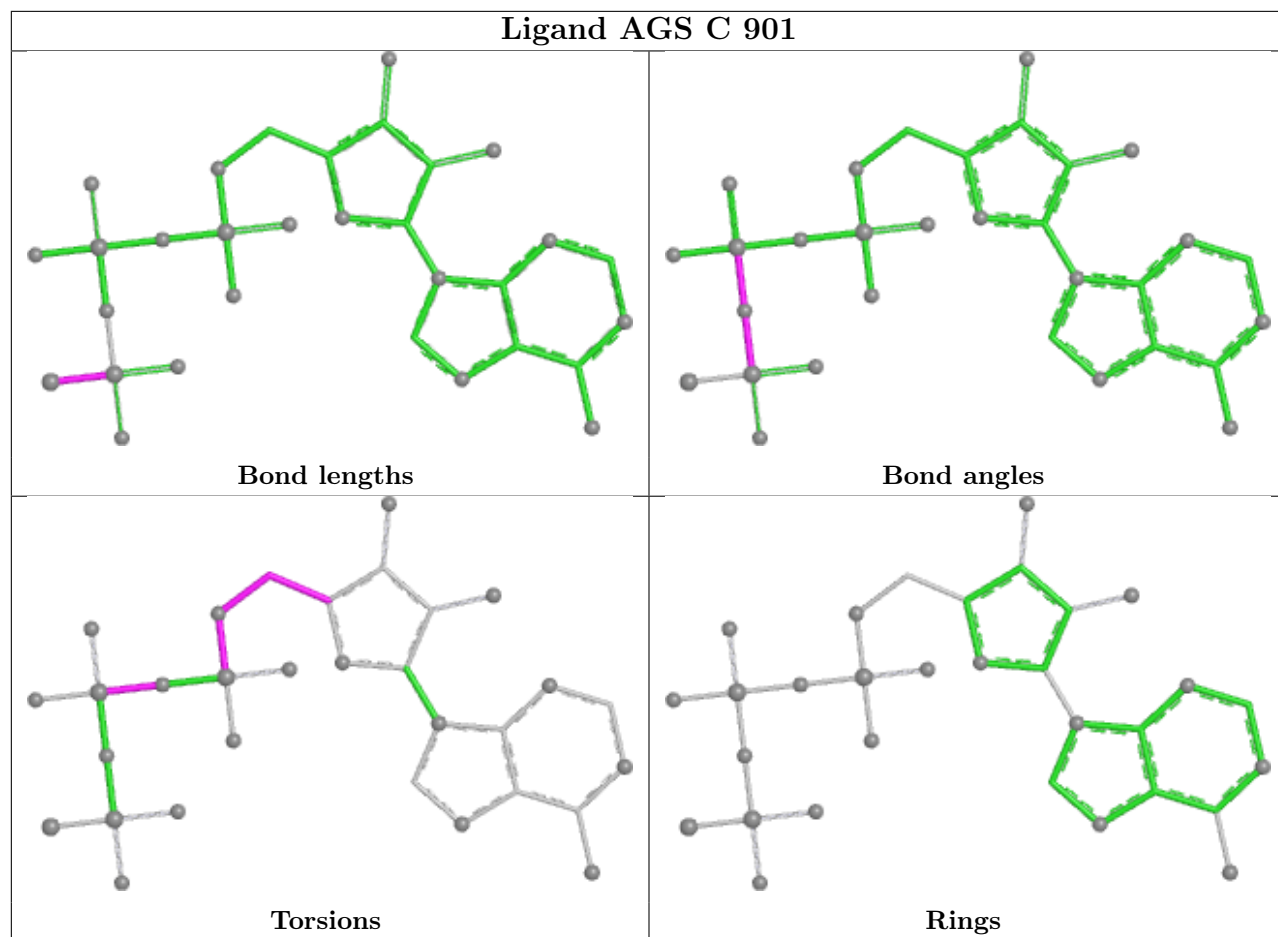
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



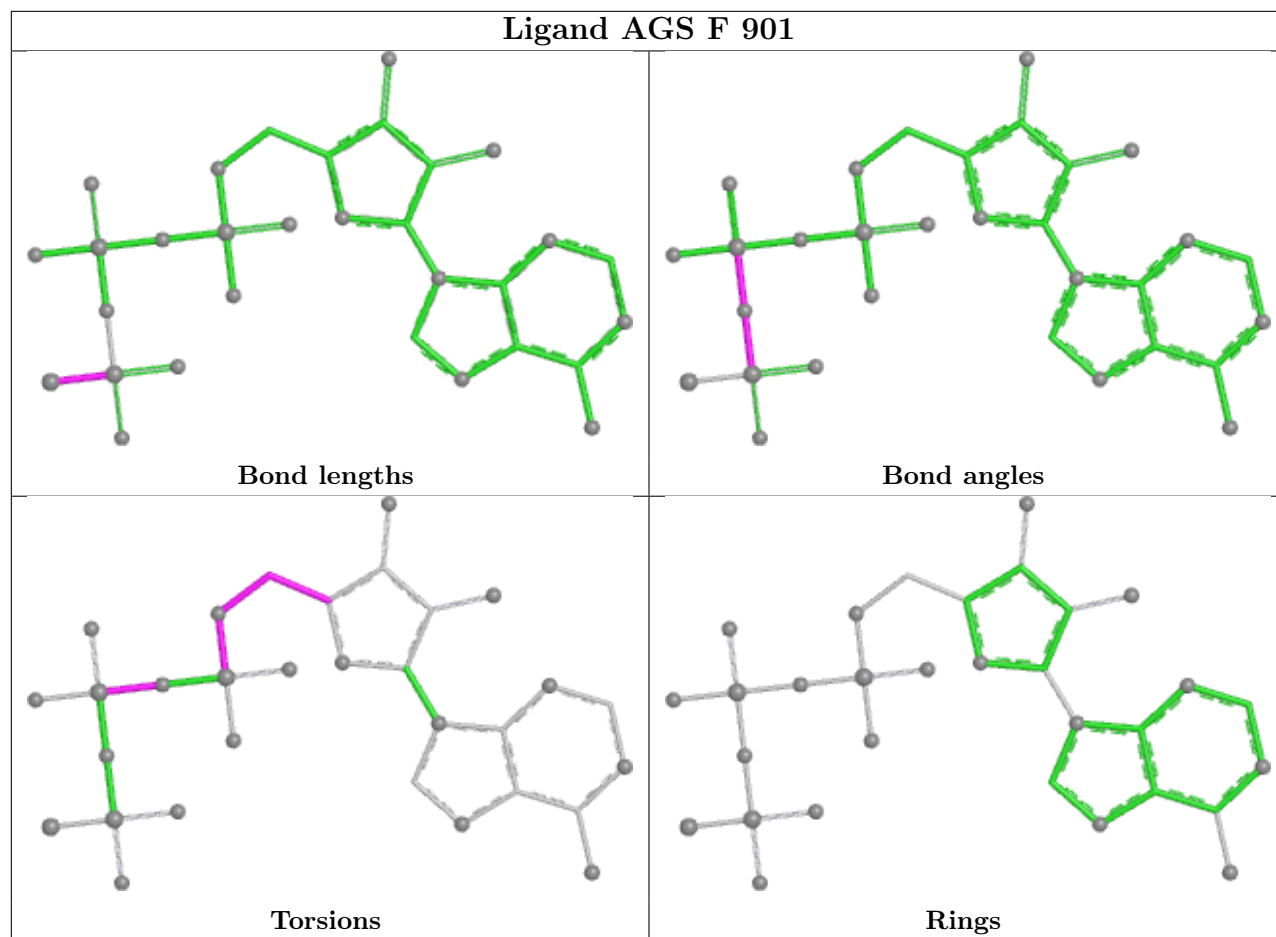


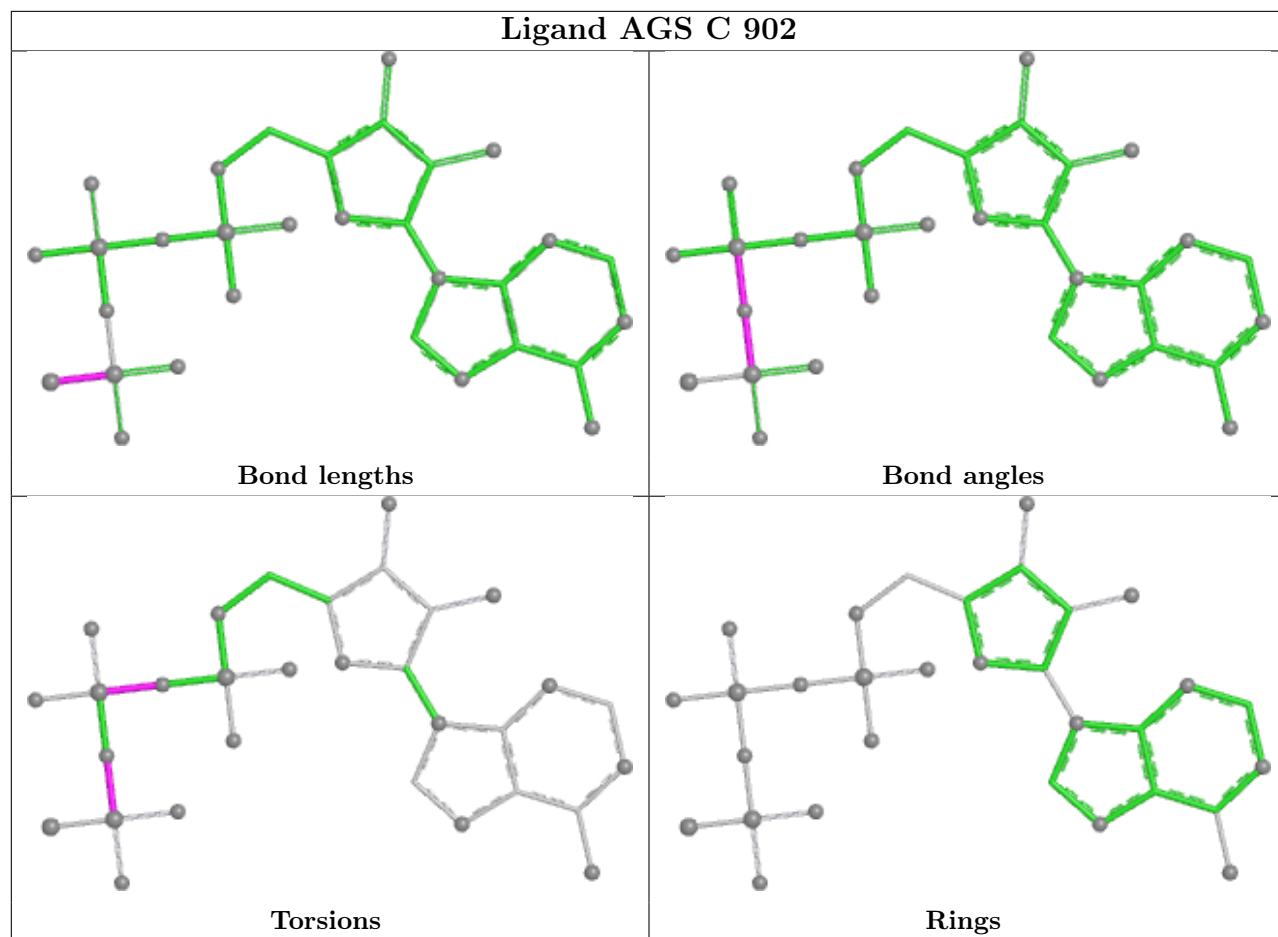


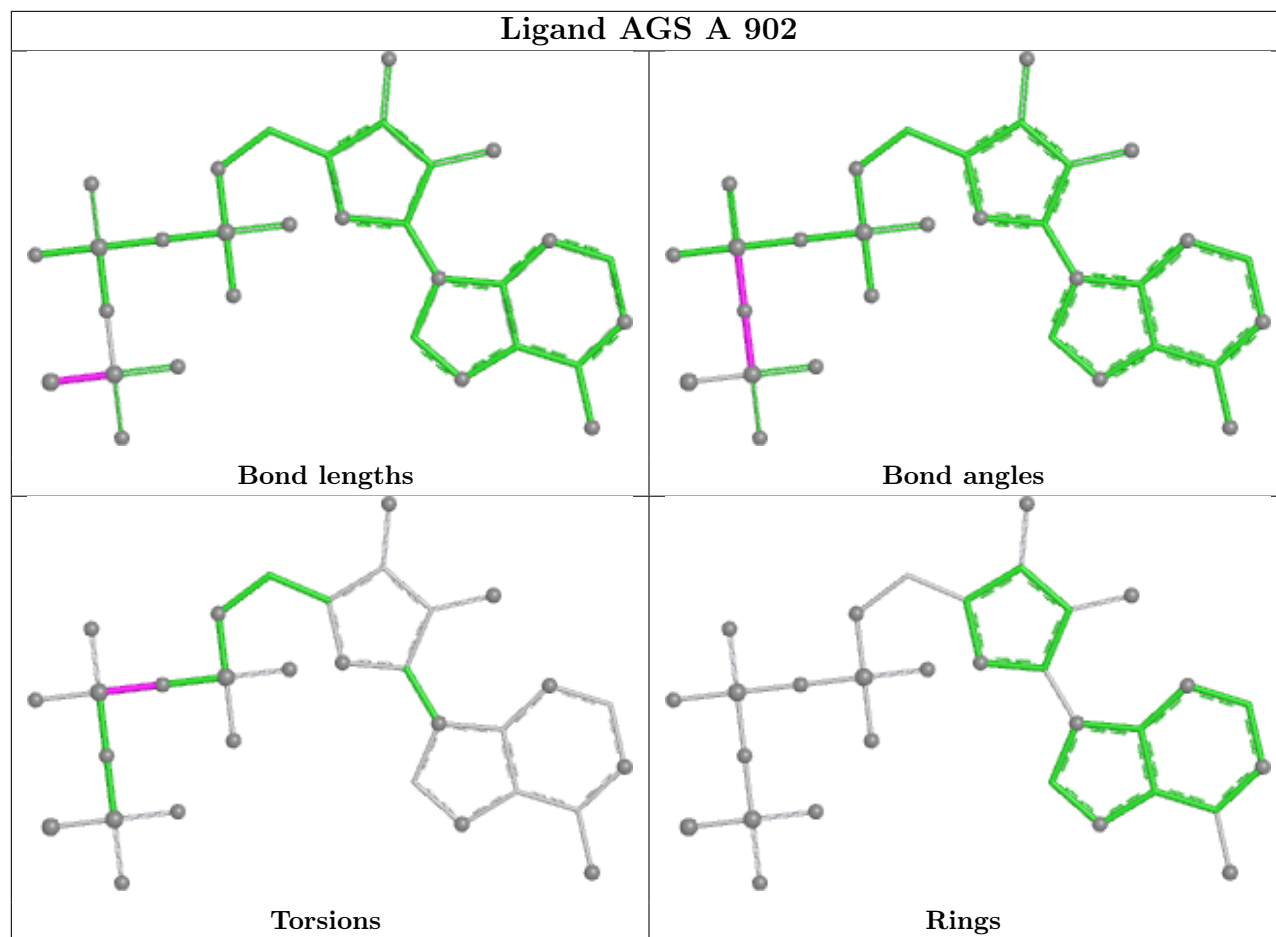


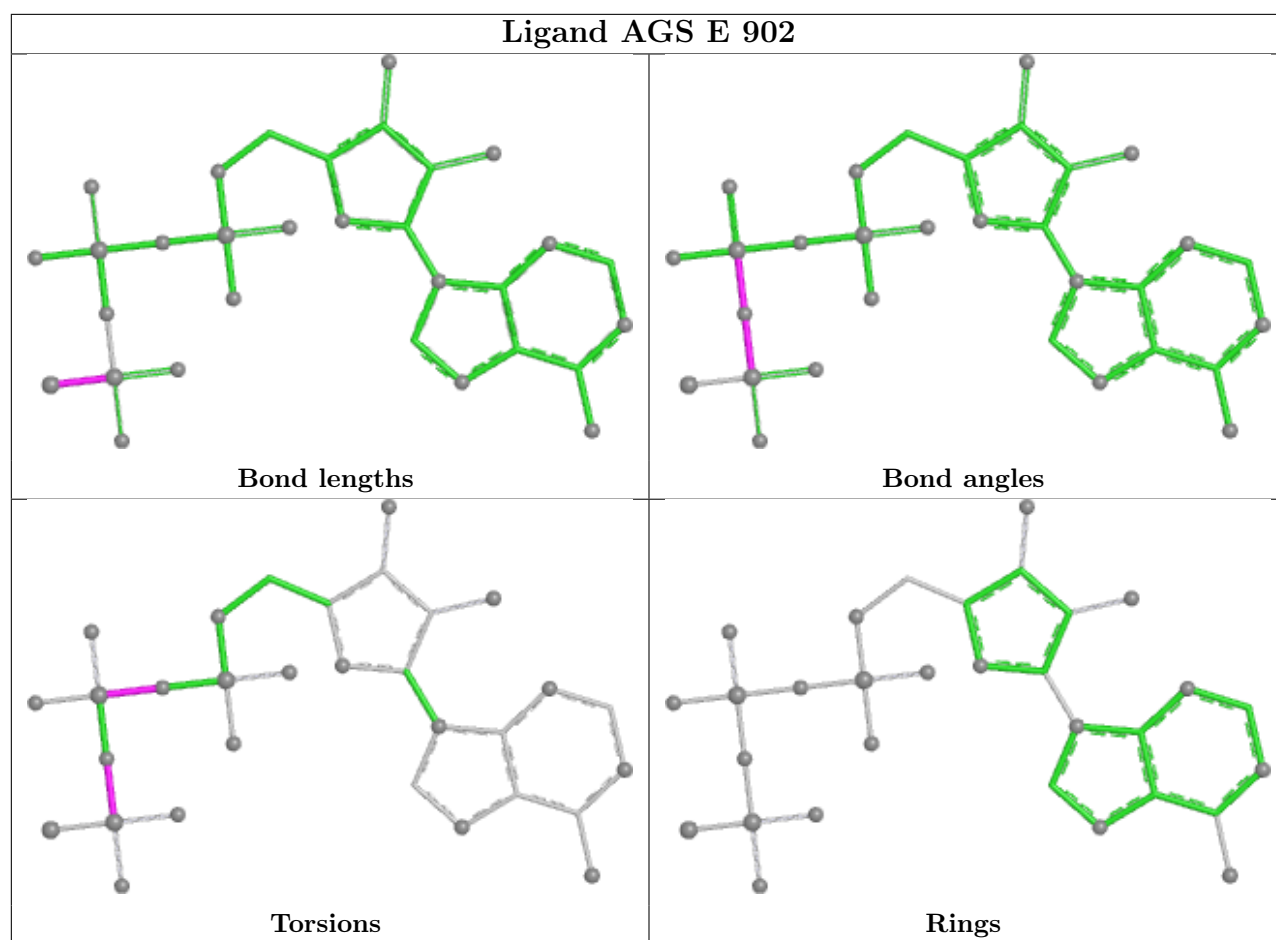


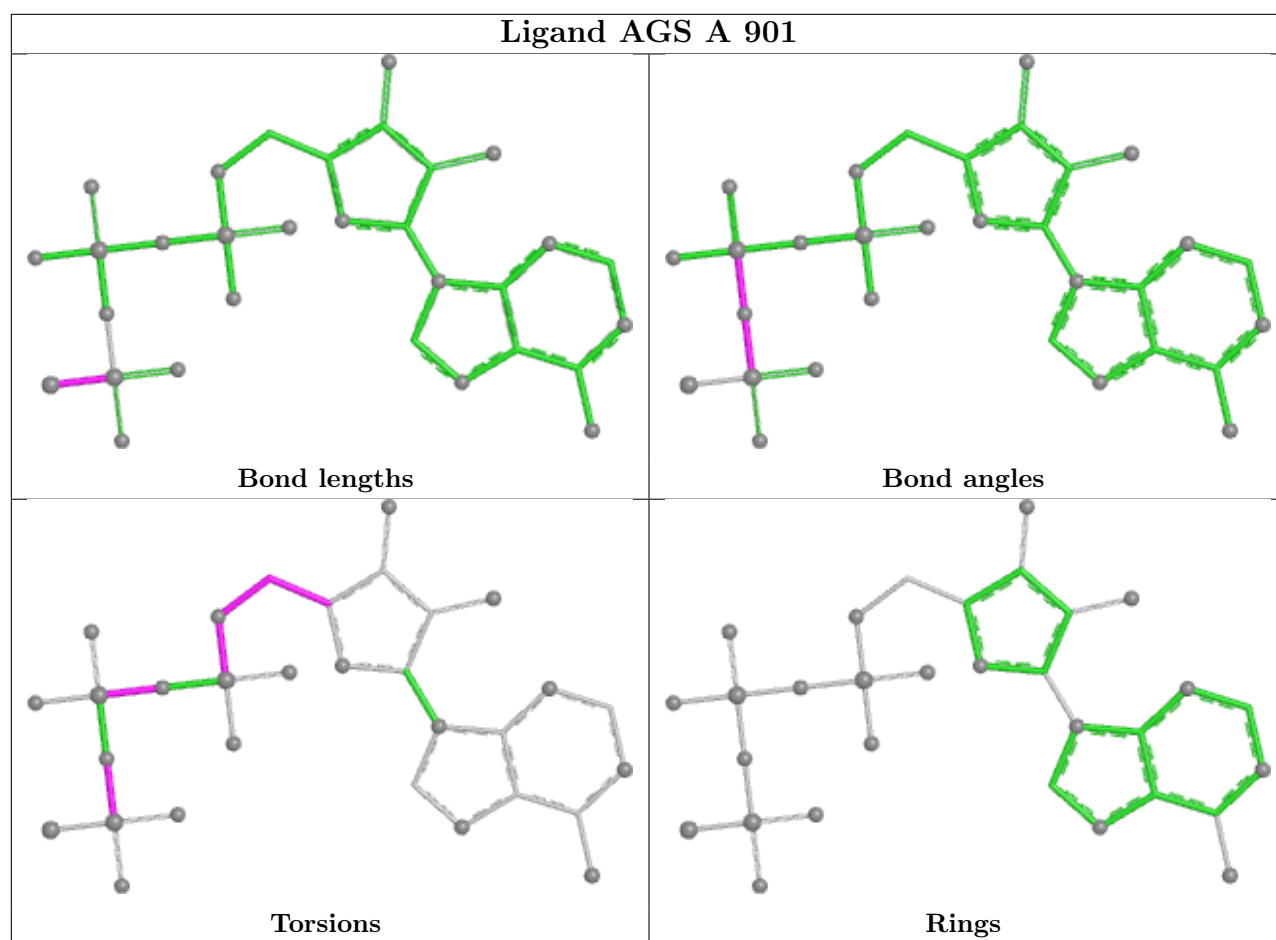
Ligand AGS F 901

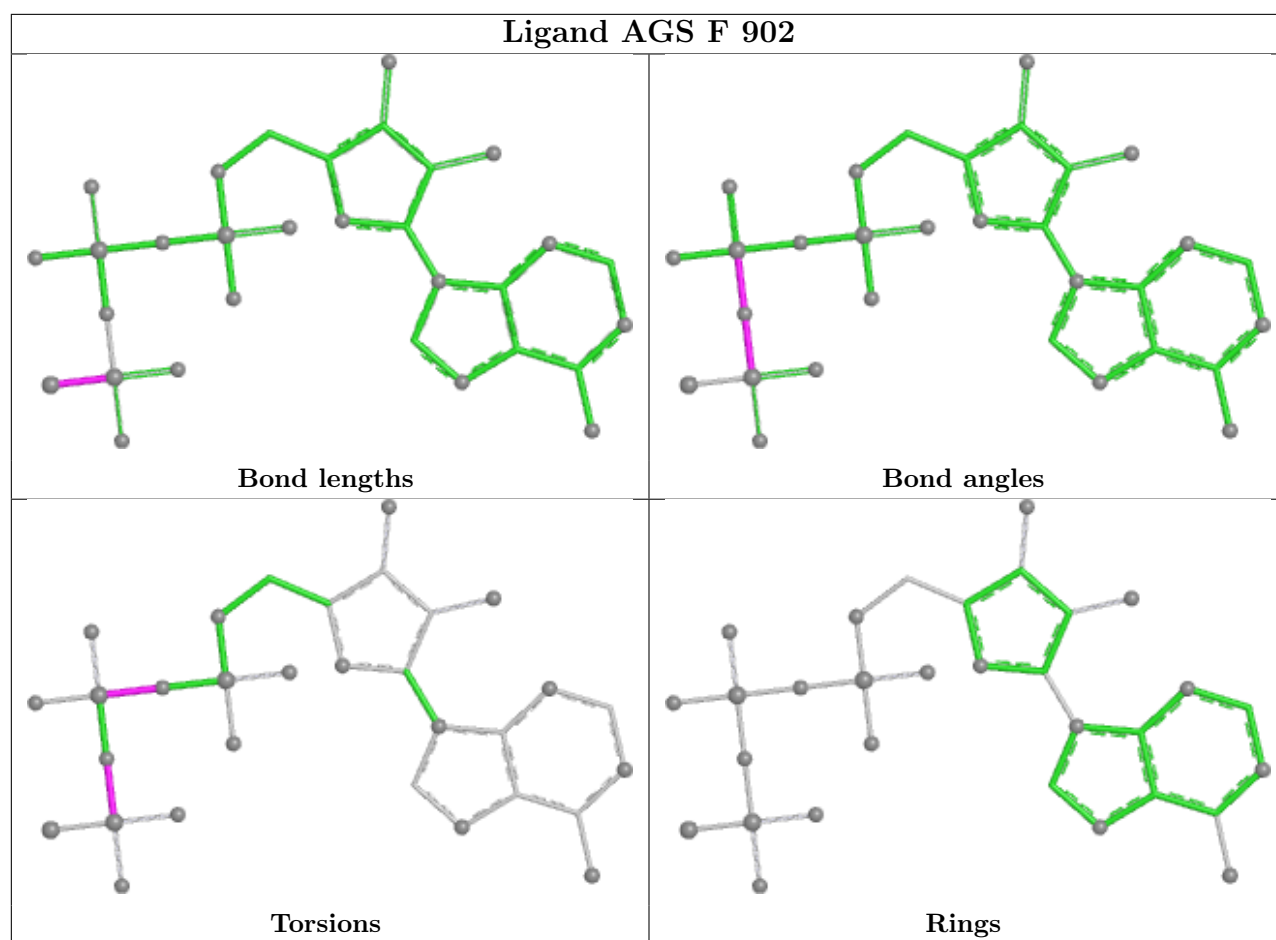


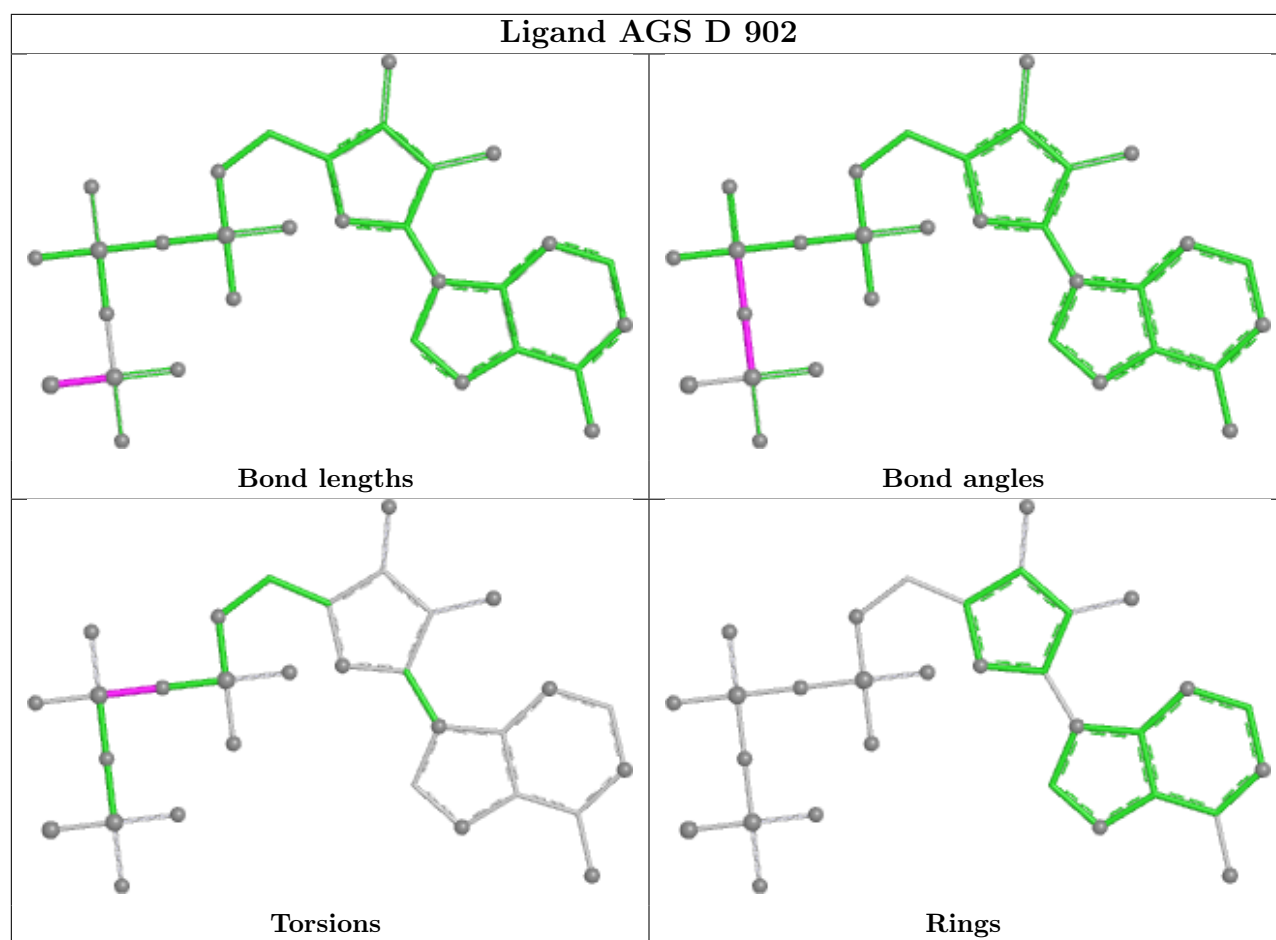












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

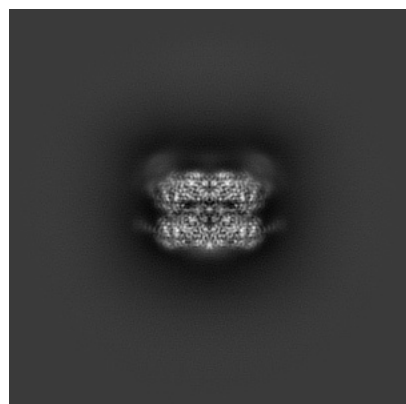
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72387. These allow visual inspection of the internal detail of the map and identification of artifacts.

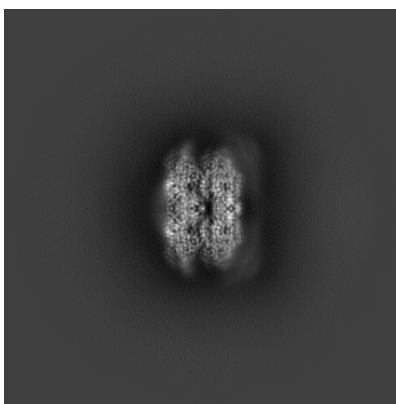
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

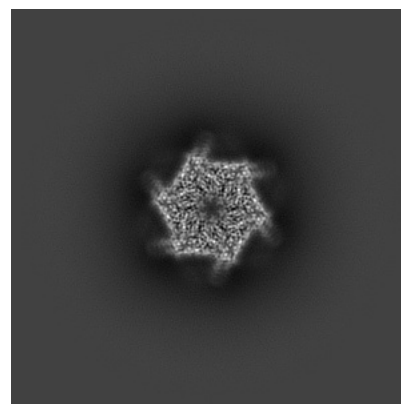
6.1.1 Primary map



X

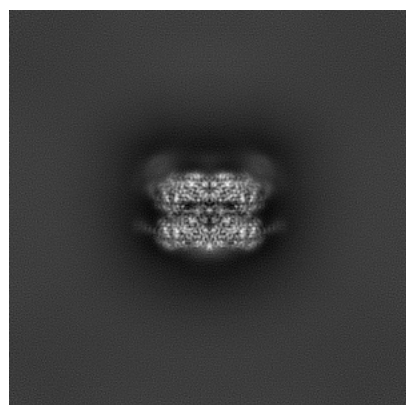


Y

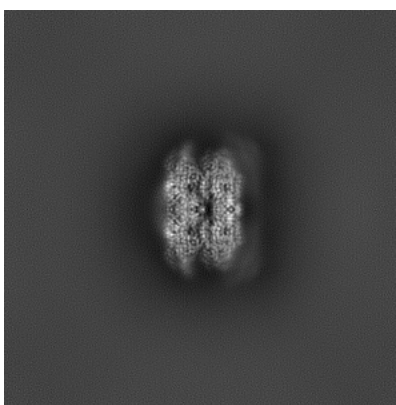


Z

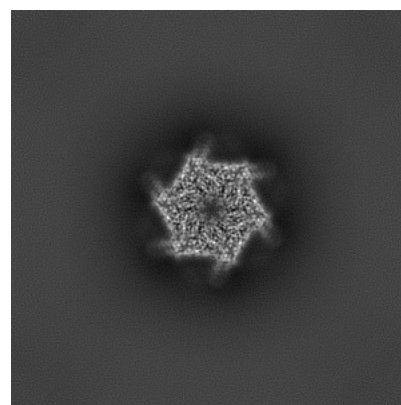
6.1.2 Raw map



X



Y

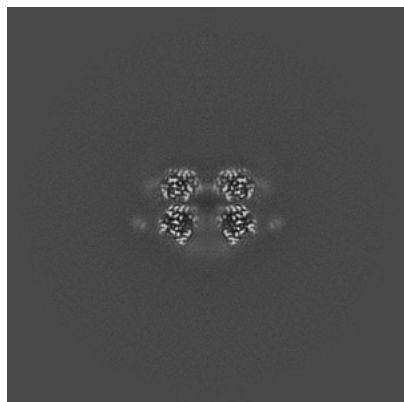


Z

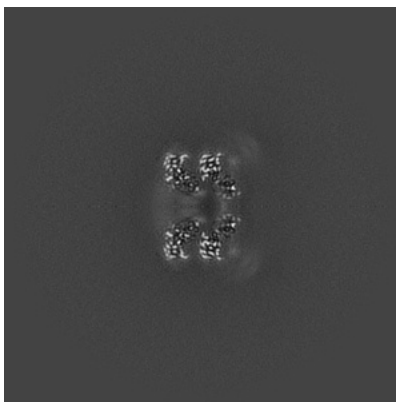
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

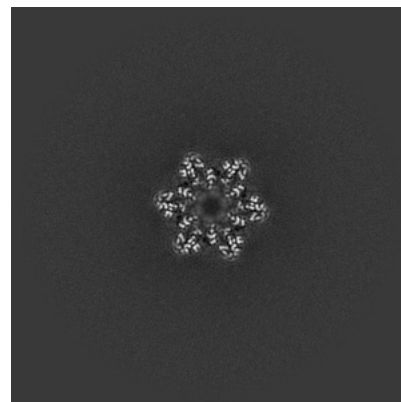
6.2.1 Primary map



X Index: 200

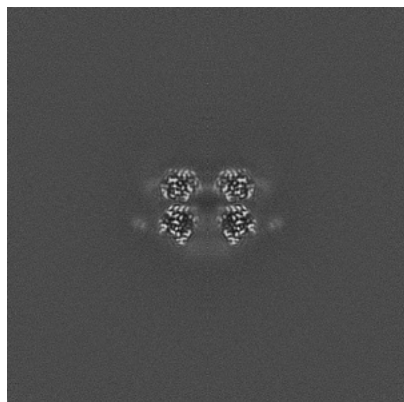


Y Index: 200

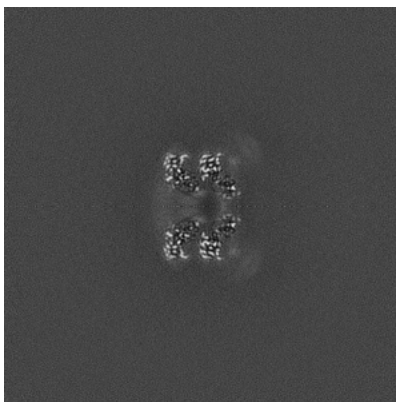


Z Index: 200

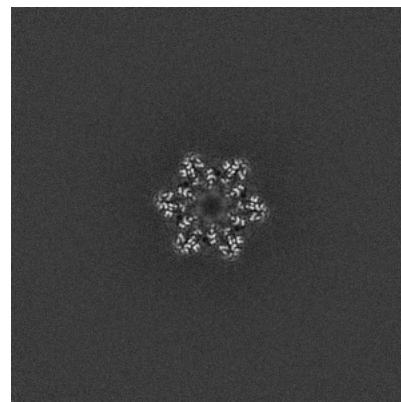
6.2.2 Raw map



X Index: 200



Y Index: 200

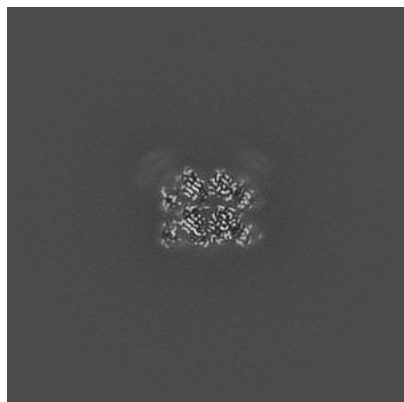


Z Index: 200

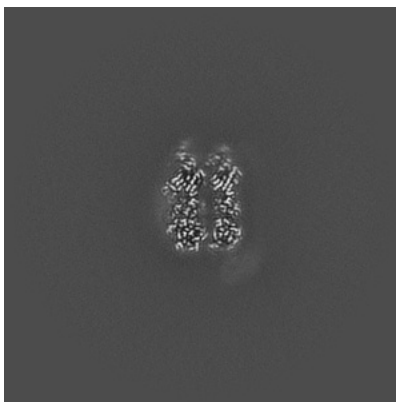
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

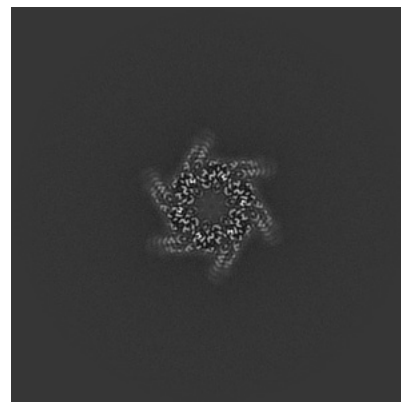
6.3.1 Primary map



X Index: 173

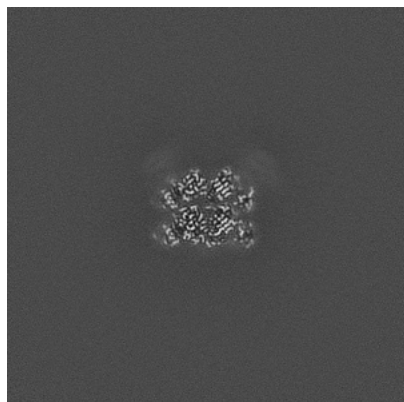


Y Index: 182

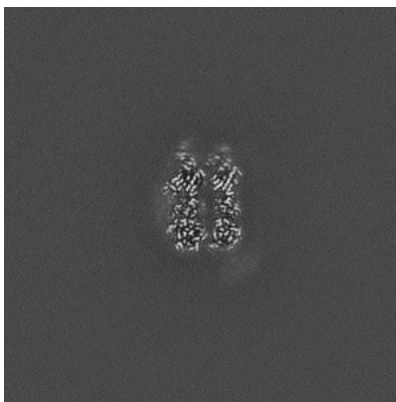


Z Index: 178

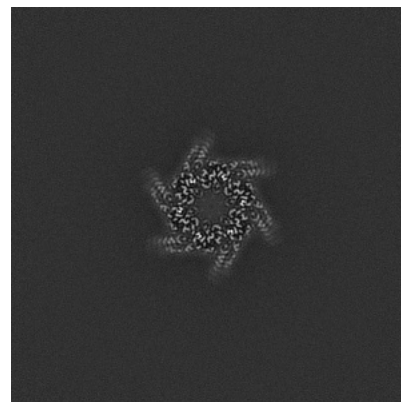
6.3.2 Raw map



X Index: 227



Y Index: 182

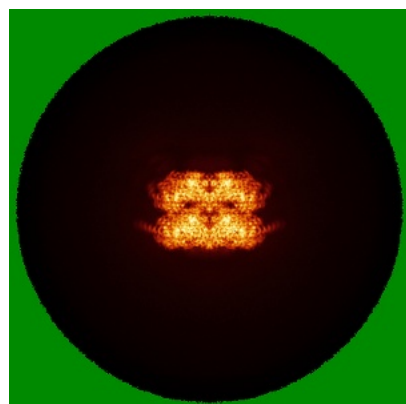


Z Index: 178

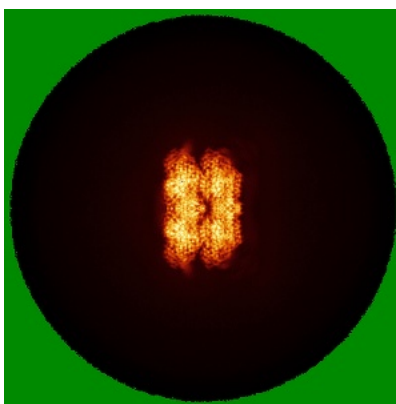
The images above show the largest variance slices of the map in three orthogonal directions.

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

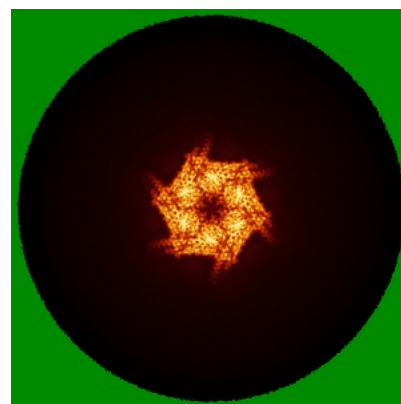
6.4.1 Primary map



X

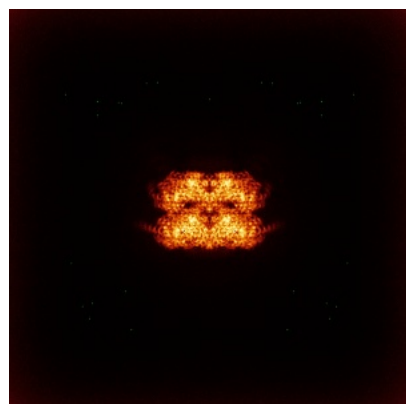


Y

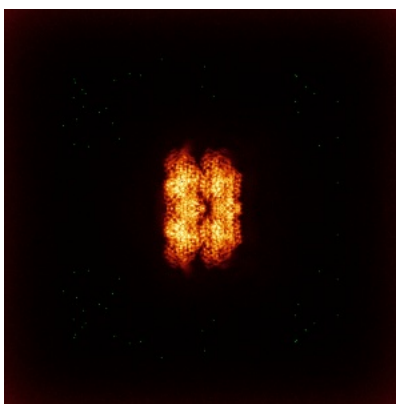


Z

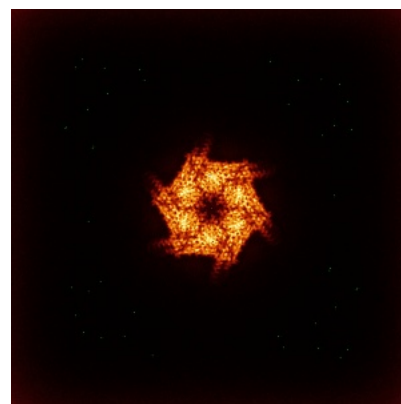
6.4.2 Raw map



X



Y

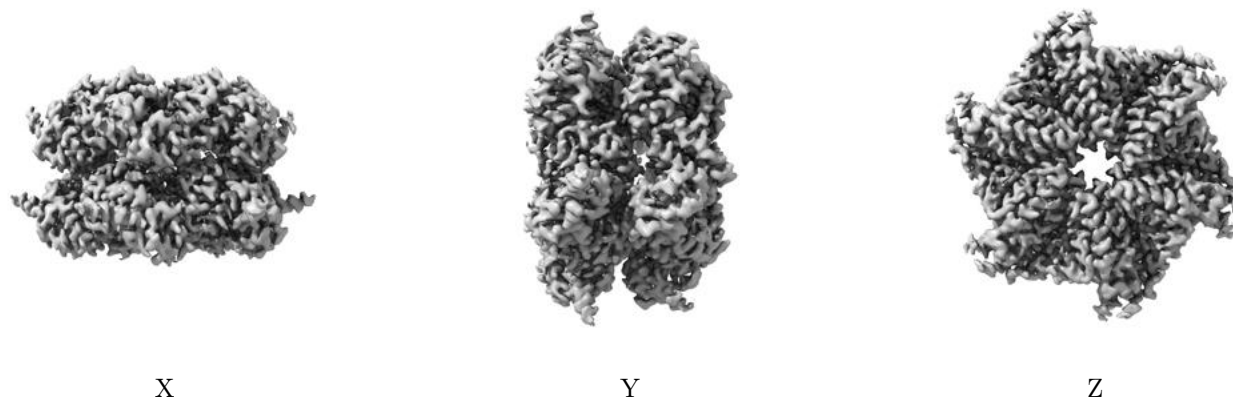


Z

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.

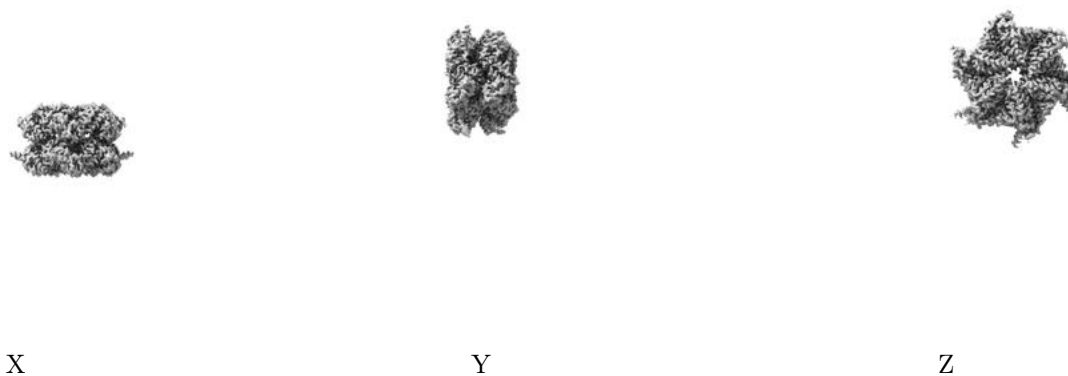
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

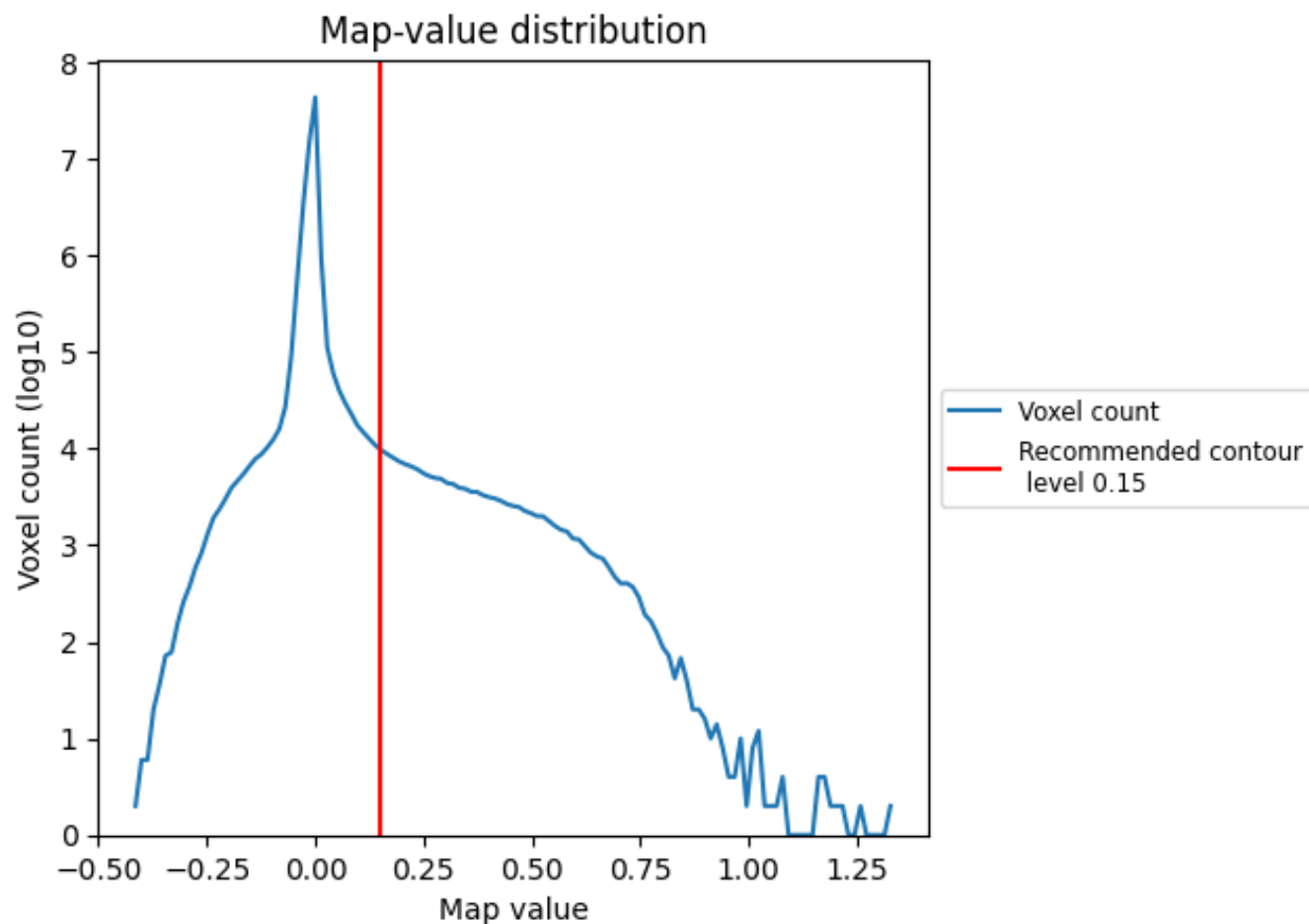
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

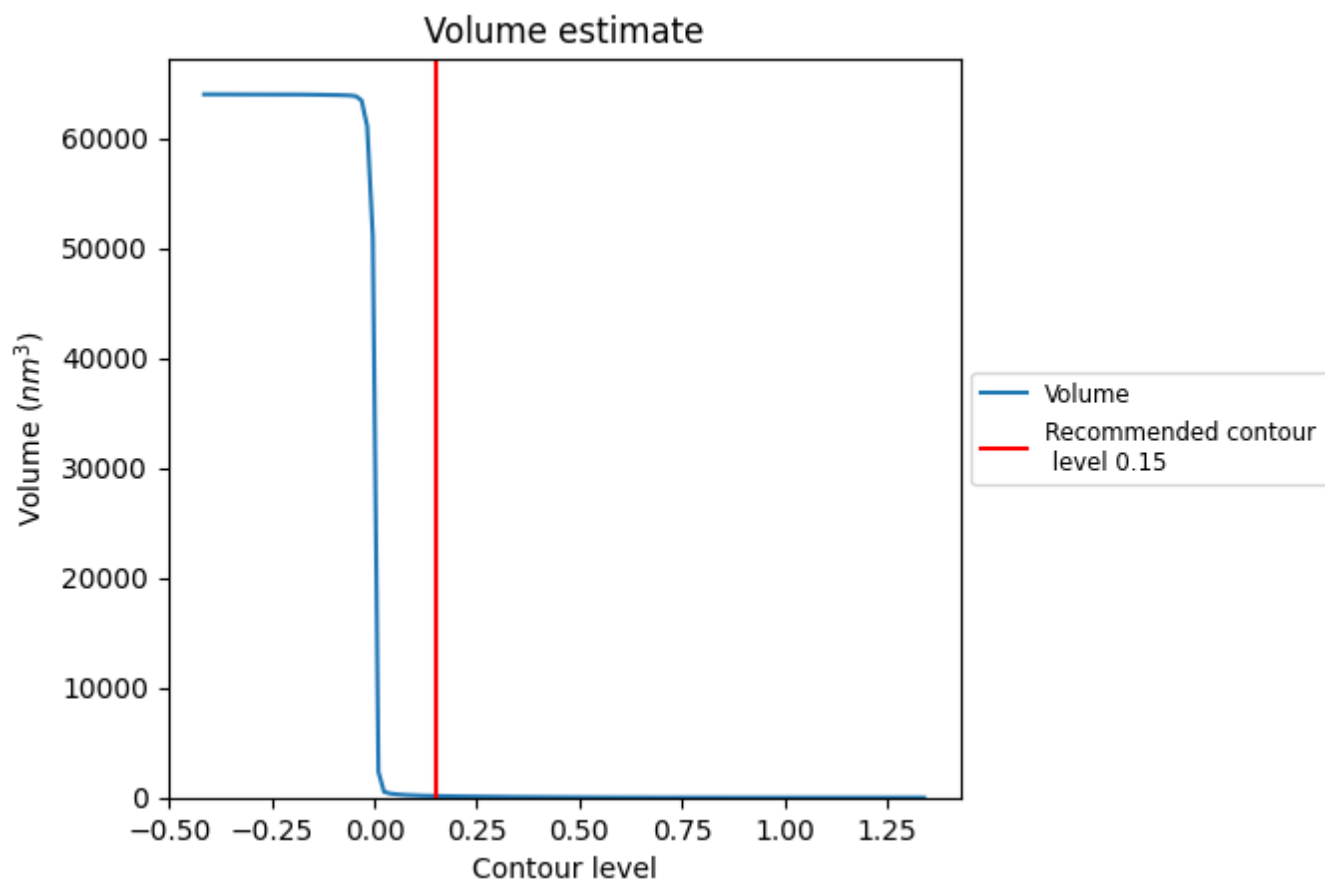
This section contains the results of statistical analysis of the map.

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.

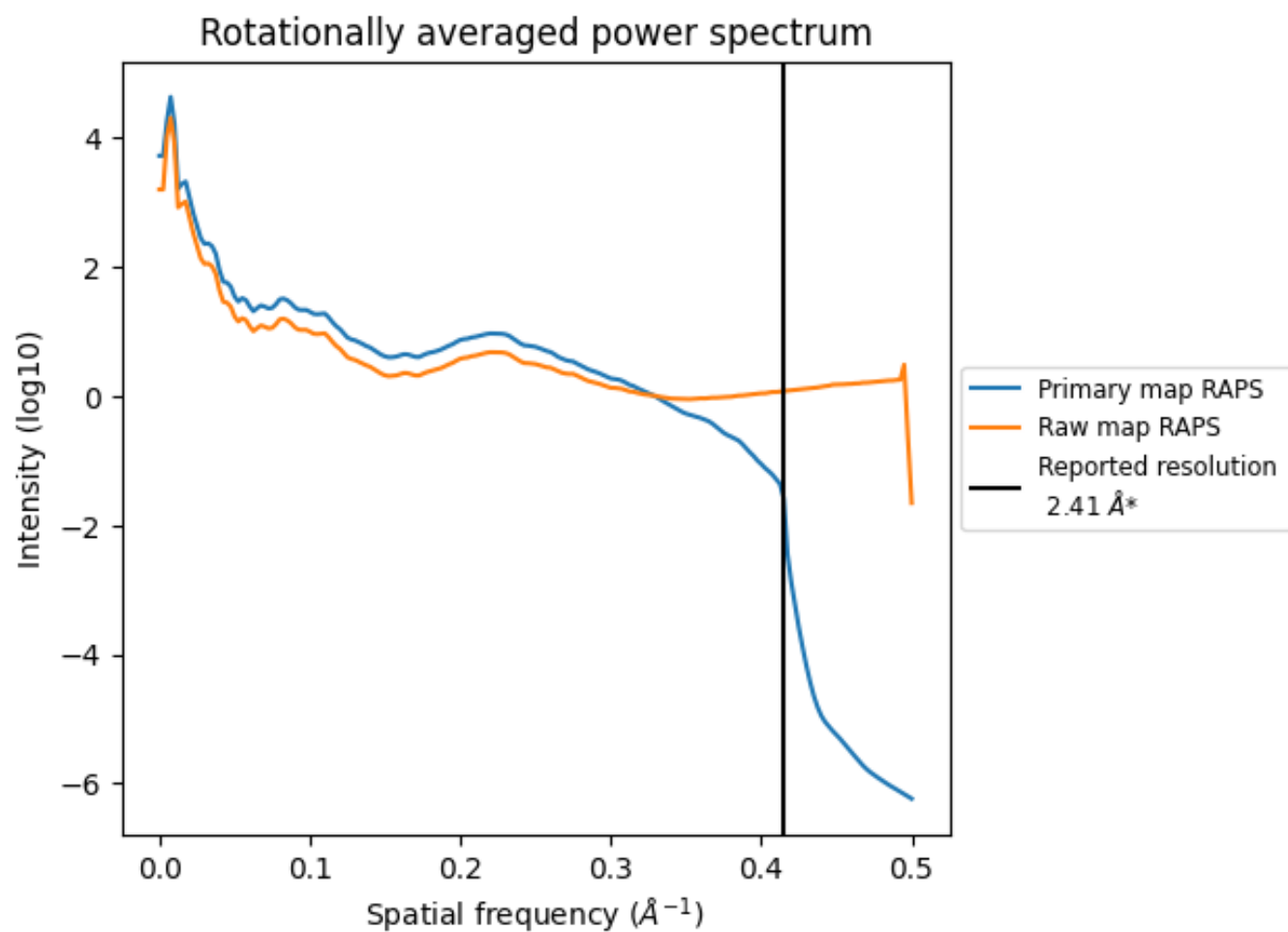
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 143 nm^3 ; this corresponds to an approximate mass of 130 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 ⓘ

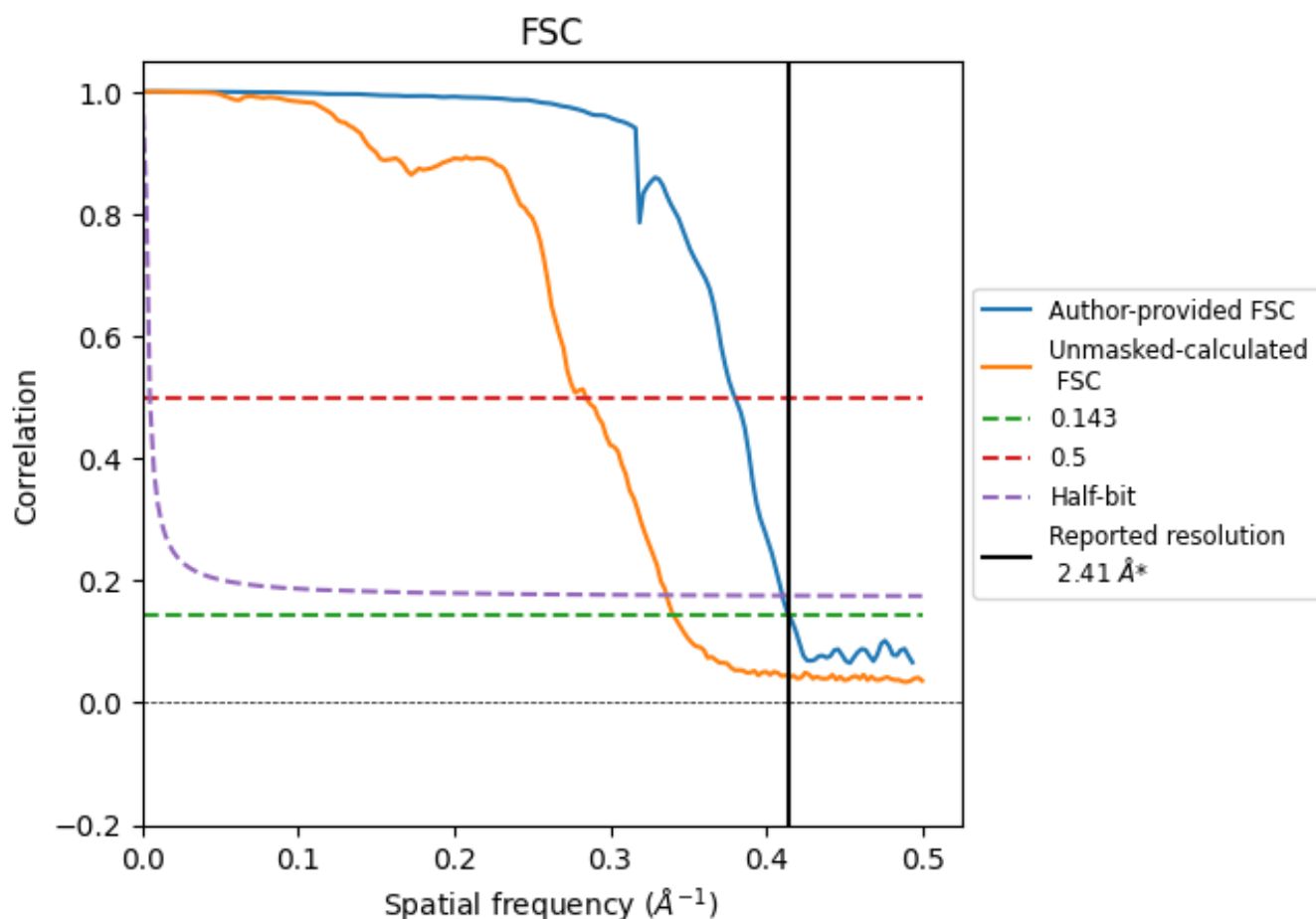


*Reported resolution corresponds to spatial frequency of 0.415 Å⁻¹

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 0.415 \AA^{-1}

8.2 Resolution estimates [i](#)

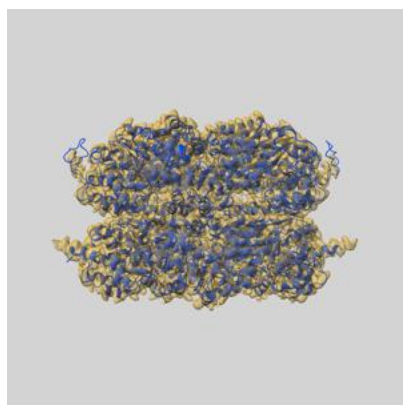
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.41	-	-
Author-provided FSC curve	2.41	2.63	2.44
Unmasked-calculated*	2.94	3.51	2.98

*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 2.94 differs from the reported value 2.41 by more than 10 %

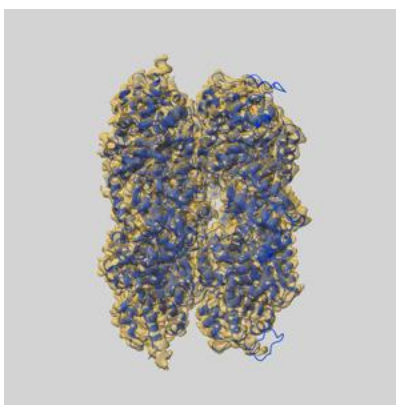
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72387 and PDB model 9Y07. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

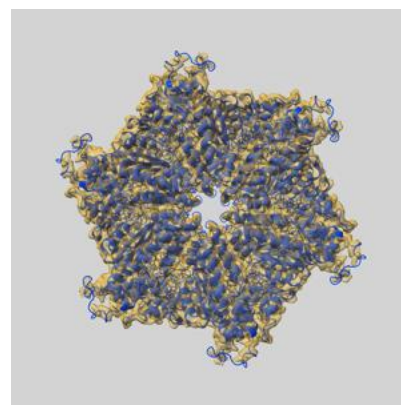
9.1 Map-model overlay [i](#)



X



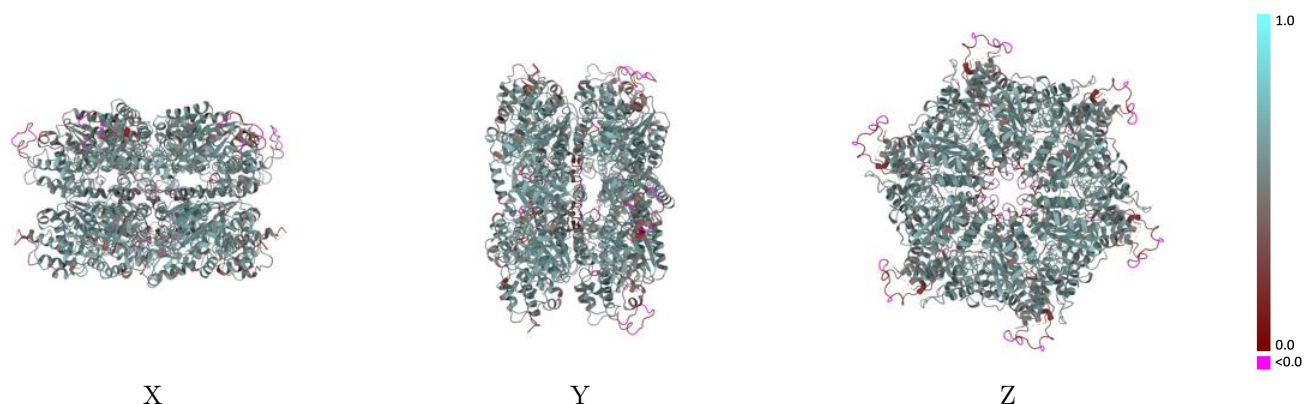
Y



Z

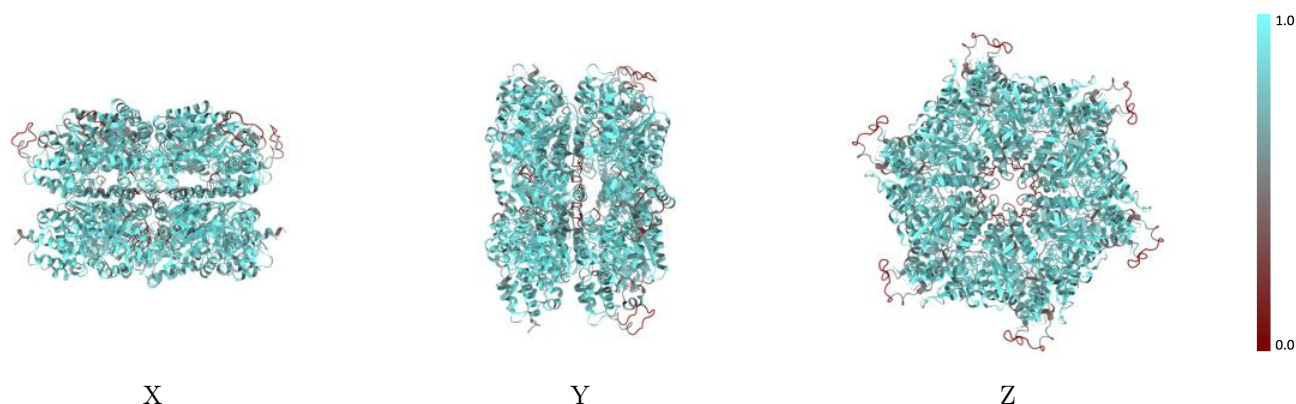
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



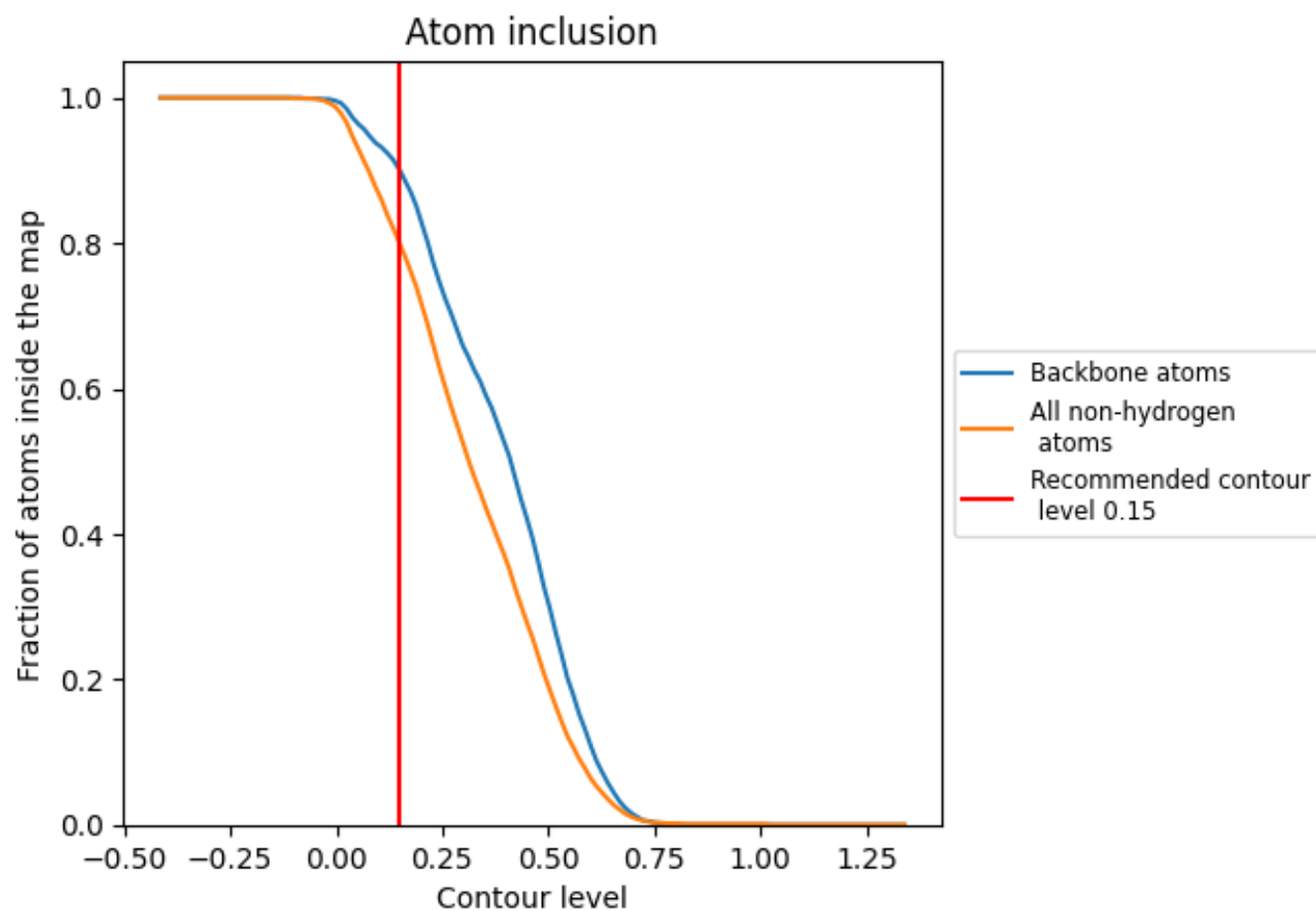
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 80% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7990	<div><div></div></div> 0.5300
A	<div><div></div></div> 0.8000	<div><div></div></div> 0.5330
B	<div><div></div></div> 0.7980	<div><div></div></div> 0.5300
C	<div><div></div></div> 0.8000	<div><div></div></div> 0.5290
D	<div><div></div></div> 0.8000	<div><div></div></div> 0.5310
E	<div><div></div></div> 0.7990	<div><div></div></div> 0.5300
F	<div><div></div></div> 0.7980	<div><div></div></div> 0.5310

1.0

0.0

<0.0