



## Full wwPDB EM Validation Report ⓘ

May 5, 2025 – 06:22 AM EDT

PDB ID : 7SH2 / pdb\_00007sh2  
EMDB ID : EMD-25122  
Title : Structure of the yeast Rad24-RFC loader bound to DNA and the open 9-1-1 clamp  
Authors : Zheng, F.; Georgescu, R.; Yao, Y.N.; O'Donnell, M.E.; Li, H.  
Deposited on : 2021-10-07  
Resolution : 3.23 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

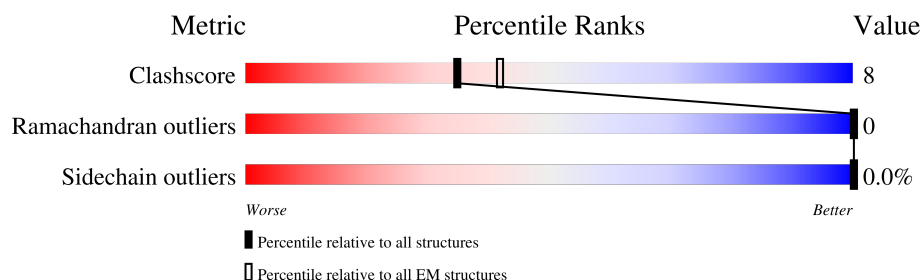
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*









The reported resolution of this entry is 3.23 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	659	
2	B	323	
3	C	340	
4	D	353	
5	E	354	
6	F	446	
7	G	401	
8	H	612	

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Mol	Chain	Length	Quality of chain
9	P	20	<div><div><div></div><div></div><div></div><div></div></div><div>5%35%15%50%</div></div>
10	T	40	<div><div><div></div><div></div><div></div><div></div></div><div>22%10%68%</div></div>

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 20933 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 Checkpoint protein RAD24.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	405	Total	C	N	O	S	0	0
			3309	2116	573	603	17		

- Molecule 2 is a protein called Replication factor C subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	317	Total	C	N	O	S	0	0
			2489	1570	444	462	13		

- Molecule 3 is a protein called Replication factor C subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	325	Total	C	N	O	S	0	0
			2569	1619	449	493	8		

- Molecule 4 is a protein called Replication factor C subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	330	Total	C	N	O	S	0	0
			2617	1653	452	502	10		

- Molecule 5 is a protein called Replication factor C subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	341	Total	C	N	O	S	0	0
			2692	1705	467	501	19		

- Molecule 6 is a protein called Mitosis Entry Checkpoint protein MEC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	269	Total	C	N	O	S	0	0
			2178	1395	374	390	19		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	MET	deletion	UNP A0A6A5PTK1
F	?	-	PRO	deletion	UNP A0A6A5PTK1
F	?	-	GLU	deletion	UNP A0A6A5PTK1
F	?	-	TRP	deletion	UNP A0A6A5PTK1
F	?	-	ASN	deletion	UNP A0A6A5PTK1
F	?	-	THR	deletion	UNP A0A6A5PTK1
F	?	-	ASN	deletion	UNP A0A6A5PTK1
F	?	-	ASN	deletion	UNP A0A6A5PTK1
F	?	-	GLY	deletion	UNP A0A6A5PTK1
F	?	-	THR	deletion	UNP A0A6A5PTK1
F	?	-	LEU	deletion	UNP A0A6A5PTK1
F	?	-	SER	deletion	UNP A0A6A5PTK1
F	?	-	GLY	deletion	UNP A0A6A5PTK1
F	?	-	GLY	deletion	UNP A0A6A5PTK1
F	?	-	THR	deletion	UNP A0A6A5PTK1
F	?	-	ALA	deletion	UNP A0A6A5PTK1
F	?	-	GLY	deletion	UNP A0A6A5PTK1
F	?	-	GLY	deletion	UNP A0A6A5PTK1
F	?	-	VAL	deletion	UNP A0A6A5PTK1
F	?	-	ASP	deletion	UNP A0A6A5PTK1
F	?	-	THR	deletion	UNP A0A6A5PTK1
F	?	-	THR	deletion	UNP A0A6A5PTK1
F	?	-	SER	deletion	UNP A0A6A5PTK1
F	?	-	LYS	deletion	UNP A0A6A5PTK1
F	?	-	PRO	deletion	UNP A0A6A5PTK1
F	?	-	ASN	deletion	UNP A0A6A5PTK1
F	?	-	PRO	deletion	UNP A0A6A5PTK1
F	?	-	ILE	deletion	UNP A0A6A5PTK1

- Molecule 7 is a protein called DNA damage checkpoint control protein RAD17.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	292	Total	C	N	O	S	0	0
			2313	1473	374	454	12		

- Molecule 8 is a protein called DNA damage checkpoint protein DDC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	266	Total	C	N	O	S	0	0
			2145	1369	358	407	11		

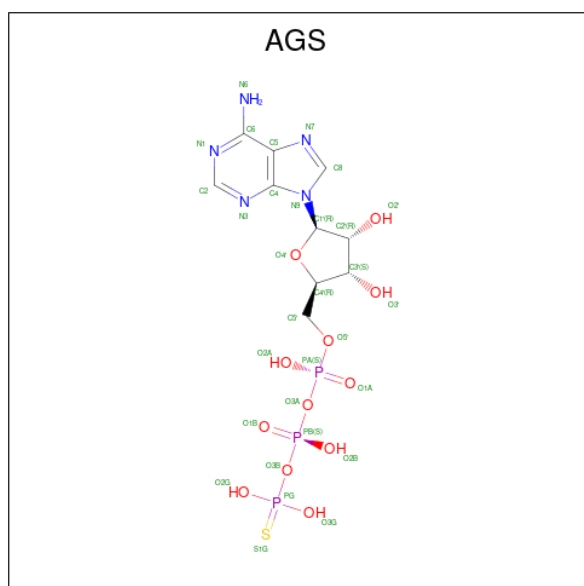
- Molecule 9 is a DNA chain called Watson strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	10	Total	C	N	O	P	0	0
			202	97	41	55	9		

- Molecule 10 is a DNA chain called Crick strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	T	13	Total	C	N	O	P	0	0
			264	127	40	84	13		

- Molecule 11 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula:  $C_{10}H_{16}N_5O_{12}P_3S$ ) (labeled as "Ligand of Interest" by depositor).

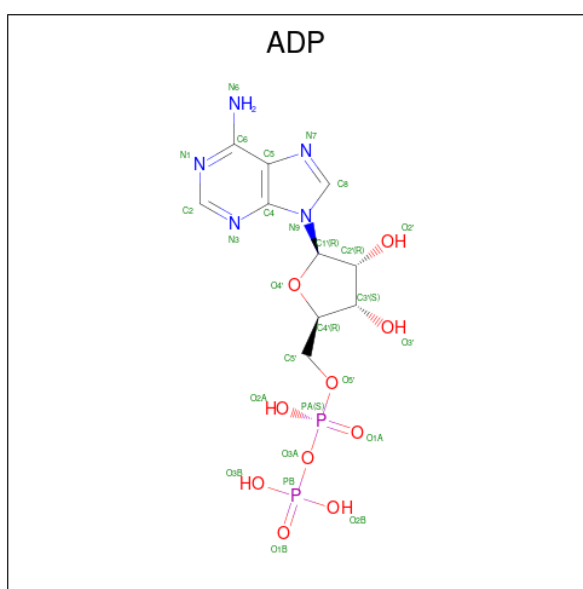


Mol	Chain	Residues	Atoms						AltConf
11	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
11	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
11	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
11	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula:  $Mg$ ) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
12	A	1	Total	Mg	0
			1	1	
12	B	1	Total	Mg	0
			1	1	
12	C	1	Total	Mg	0
			1	1	
12	D	1	Total	Mg	0
			1	1	

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).

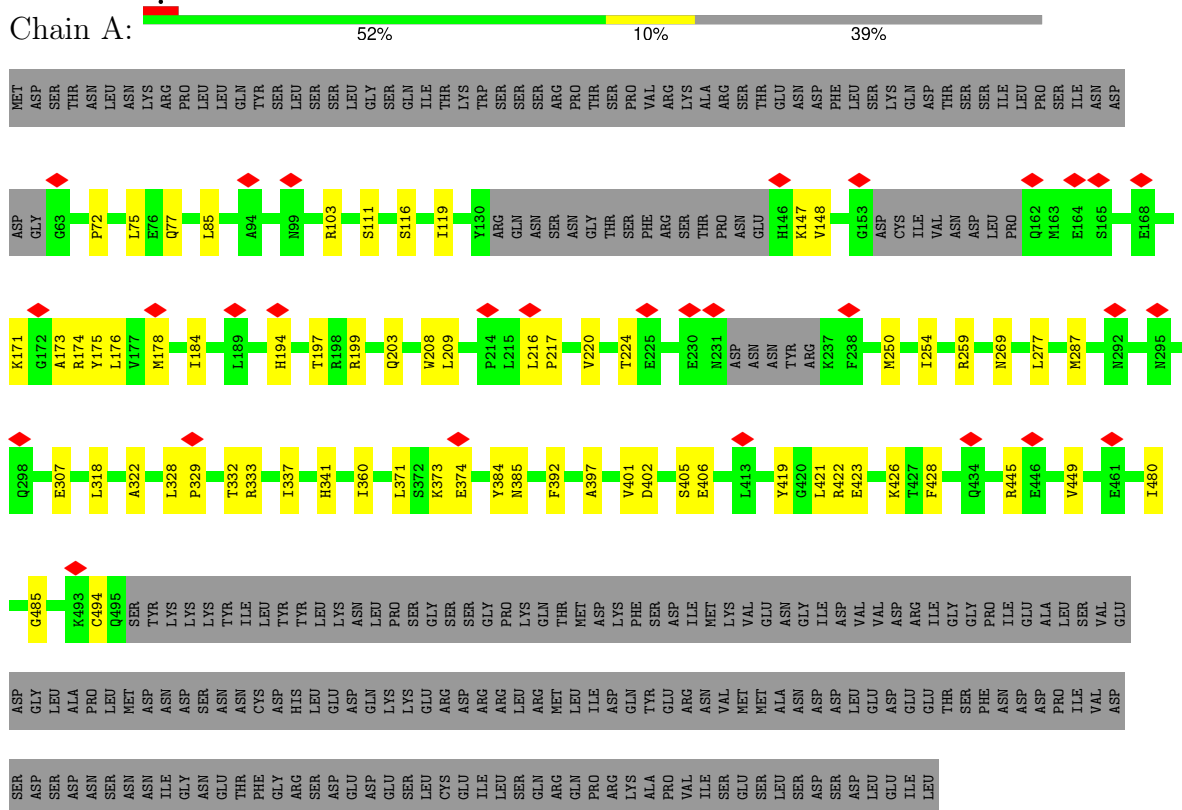


Mol	Chain	Residues	Atoms					AltConf
13	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

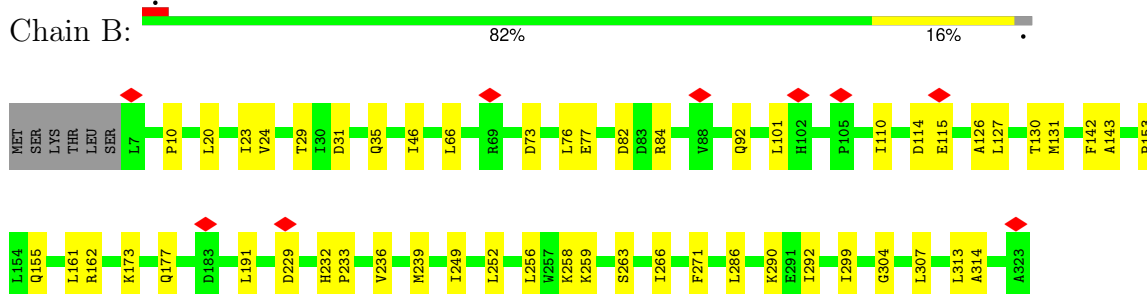
### 3 Residue-property plots

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: Checkpoint protein RAD24

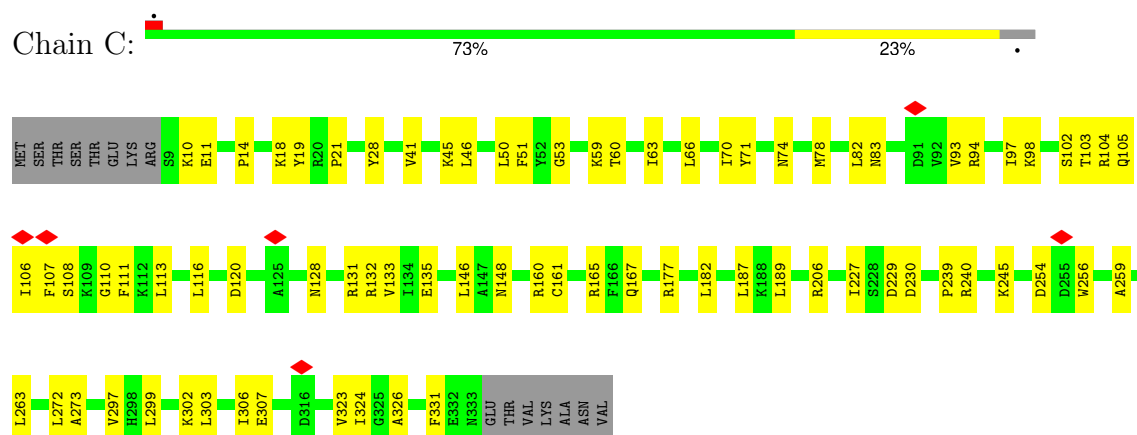


#### • Molecule 2: Replication factor C subunit 4

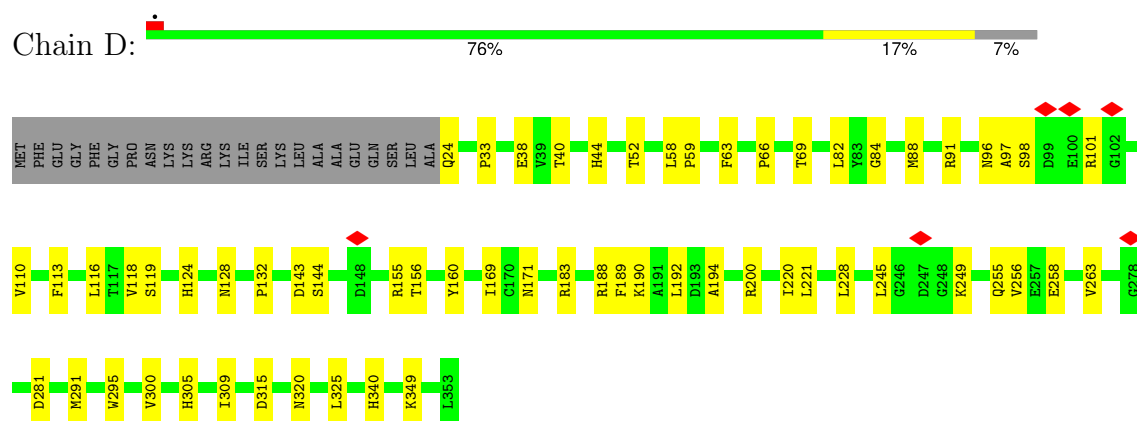




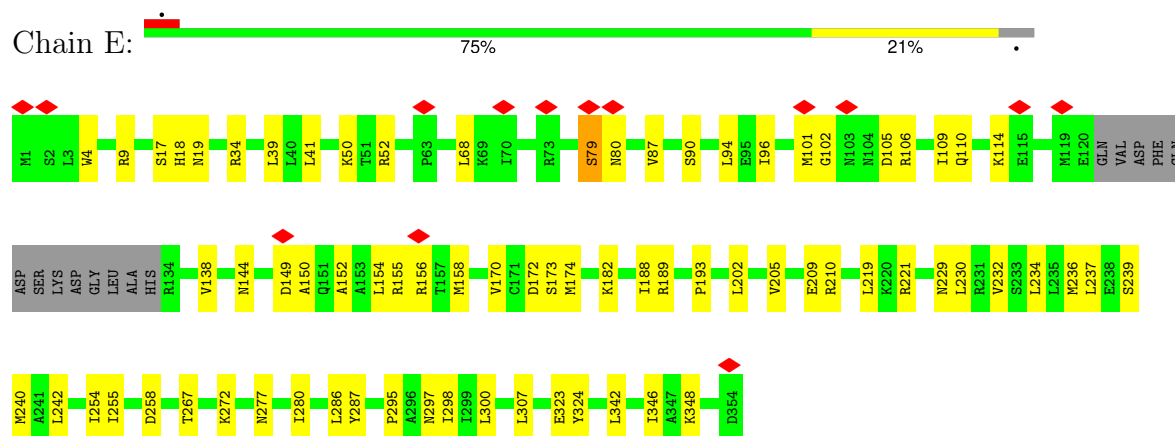
- Molecule 3: Replication factor C subunit 3



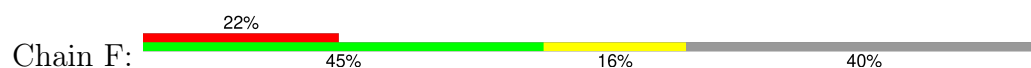
- Molecule 4: Replication factor C subunit 2



- Molecule 5: Replication factor C subunit 5



- Molecule 6: Mitosis Entry Checkpoint protein MEC3







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	302403	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	65	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.760	Depositor
Minimum map value	-0.450	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.08	Depositor
Map size ( $\text{\AA}$ )	331.2, 331.2, 331.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.828, 0.828, 0.828	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.11	0/3380	0.29	0/4552
2	B	0.09	0/2524	0.25	0/3403
3	C	0.10	0/2609	0.26	0/3529
4	D	0.10	0/2662	0.27	0/3600
5	E	0.10	0/2729	0.29	1/3686 (0.0%)
6	F	0.15	0/2216	0.38	0/2983
7	G	0.12	0/2349	0.39	0/3164
8	H	0.10	0/2182	0.29	0/2949
9	P	0.13	0/227	0.23	0/348
10	T	0.18	0/293	0.39	0/450
All	All	0.11	0/21171	0.30	1/28664 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	79	SER	CB-CA-C	-5.41	110.32	116.54

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	3309	0	3318	42	0
2	B	2489	0	2583	39	0
3	C	2569	0	2599	53	0
4	D	2617	0	2648	45	0
5	E	2692	0	2822	50	0
6	F	2178	0	2222	42	0
7	G	2313	0	2308	41	0
8	H	2145	0	2138	43	0
9	P	202	0	113	2	0
10	T	264	0	148	3	0
11	A	31	0	12	2	0
11	B	31	0	12	2	0
11	C	31	0	12	4	0
11	D	31	0	12	4	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
12	D	1	0	0	0	0
13	E	27	0	12	2	0
All	All	20933	0	20959	326	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 8.

All (326) 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)
6:F:105:LYS:HG3	6:F:106:ARG:HE	1.48	0.78
8:H:45:ASN:HB2	8:H:50:THR:HB	1.74	0.70
7:G:166:ALA:HB1	7:G:205:ILE:HD12	1.74	0.69
8:H:53:GLN:HB2	8:H:372:GLU:HB2	1.74	0.68
7:G:183:LYS:HB3	7:G:191:VAL:HB	1.74	0.68
7:G:245:ILE:HD11	7:G:308:VAL:HG11	1.76	0.67
8:H:27:GLN:HB3	8:H:43:SER:HB2	1.77	0.66
4:D:91:ARG:HH12	4:D:118:VAL:HG13	1.59	0.66
8:H:20:ILE:HG12	8:H:101:LEU:HD22	1.77	0.66
8:H:55:ARG:HB2	8:H:370:LYS:HB2	1.76	0.66
6:F:287:GLU:HB2	6:F:290:TRP:HB3	1.76	0.66
1:A:199:ARG:O	1:A:203:GLN:NE2	2.29	0.66
4:D:124:HIS:O	4:D:128:ASN:HB2	1.96	0.66
2:B:252:LEU:HG	2:B:256:LEU:HD12	1.78	0.65
1:A:360:ILE:HD13	1:A:422:ARG:HG2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:154:PHE:HE1	7:G:259:MET:HE3	1.62	0.64
4:D:40:THR:H	11:D:401:AGS:HN62	1.45	0.64
6:F:411:ARG:HE	6:F:468:ILE:HG21	1.61	0.64
7:G:190:ASN:HB3	7:G:217:LEU:HD23	1.78	0.64
8:H:238:LYS:HZ1	8:H:242:ASP:HB3	1.64	0.63
2:B:252:LEU:HD13	2:B:313:LEU:HD11	1.79	0.62
7:G:172:GLU:OE1	8:H:106:ARG:NH1	2.32	0.62
3:C:182:LEU:HD22	3:C:187:LEU:HB3	1.82	0.61
1:A:269:ASN:HD21	10:T:26:DT:H5''	1.66	0.61
8:H:241:LEU:HB3	8:H:330:LYS:HG2	1.83	0.61
6:F:84:SER:HB3	6:F:91:ILE:HG12	1.82	0.61
4:D:245:LEU:HD13	4:D:249:LYS:HE2	1.82	0.60
7:G:117:PHE:HB3	7:G:132:TYR:HB2	1.83	0.60
6:F:23:ILE:HD12	6:F:68:LEU:HD21	1.83	0.60
4:D:349:LYS:HE2	5:E:323:GLU:HG2	1.84	0.60
1:A:494:CYS:HB3	5:E:242:LEU:HD23	1.83	0.60
7:G:191:VAL:HG13	7:G:206:LYS:HE2	1.83	0.59
5:E:94:LEU:HB3	5:E:138:VAL:HG12	1.85	0.58
8:H:39:LEU:HB3	8:H:56:PHE:HB2	1.84	0.58
3:C:93:VAL:HG13	3:C:97:ILE:HD13	1.85	0.58
5:E:297:ASN:OD1	5:E:298:ILE:N	2.36	0.58
8:H:115:SER:HB3	8:H:139:GLU:HB2	1.85	0.58
7:G:320:ALA:O	7:G:323:GLU:HG3	2.04	0.58
7:G:208:PRO:HD2	7:G:213:ILE:HD11	1.85	0.58
2:B:115:GLU:OE1	3:C:131:ARG:NH2	2.37	0.58
3:C:41:VAL:HG11	3:C:66:LEU:HD11	1.86	0.58
3:C:303:LEU:O	3:C:307:GLU:HG2	2.04	0.57
2:B:10:PRO:HA	3:C:45:LYS:HE3	1.86	0.57
5:E:174:MET:HE3	5:E:182:LYS:HE3	1.87	0.57
6:F:76:VAL:O	6:F:78:ARG:NH1	2.38	0.57
7:G:58:ILE:HG13	7:G:308:VAL:HG22	1.85	0.57
2:B:229:ASP:OD1	2:B:259:LYS:NZ	2.37	0.57
5:E:52:ARG:HH12	13:E:500:ADP:HN61	1.53	0.56
8:H:272:GLY:HA3	8:H:276:ASP:HB3	1.87	0.56
6:F:443:SER:HB3	6:F:464:ILE:HB	1.87	0.56
8:H:241:LEU:HD13	8:H:330:LYS:HA	1.87	0.56
6:F:92:THR:HG21	6:F:213:PHE:HB2	1.88	0.56
3:C:94:ARG:O	3:C:98:LYS:HB2	2.07	0.55
3:C:103:THR:HG21	7:G:55:VAL:HG23	1.88	0.55
4:D:171:ASN:ND2	11:D:401:AGS:S1G	2.77	0.55
6:F:413:LYS:O	6:F:416:LYS:NZ	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:40:GLU:OE1	6:F:41:ARG:NH1	2.39	0.55
3:C:239:PRO:HB3	3:C:272:LEU:HD13	1.87	0.55
1:A:173:ALA:HA	1:A:176:LEU:HD12	1.89	0.55
2:B:173:LYS:O	2:B:177:GLN:HG3	2.06	0.55
2:B:307:LEU:HD21	3:C:303:LEU:HB3	1.88	0.55
10:T:28:DT:H2''	10:T:29:DG:H5''	1.88	0.55
1:A:72:PRO:HB3	1:A:77:GLN:HB3	1.89	0.55
3:C:10:LYS:HG3	3:C:11:GLU:H	1.71	0.55
11:C:401:AGS:S1G	4:D:183:ARG:NH2	2.80	0.55
2:B:236:VAL:HA	2:B:239:MET:HE2	1.89	0.54
2:B:256:LEU:HD13	2:B:266:ILE:HG12	1.89	0.54
1:A:250:MET:HG3	1:A:254:ILE:HD13	1.88	0.54
4:D:98:SER:HB3	5:E:114:LYS:HE3	1.88	0.54
6:F:46:SER:HB3	6:F:69:TRP:HA	1.90	0.54
6:F:410:ILE:O	6:F:470:ARG:NH1	2.41	0.54
3:C:78:MET:HE1	3:C:108:SER:HB3	1.89	0.54
4:D:91:ARG:NH2	4:D:119:SER:O	2.40	0.54
9:P:2:DC:H2'	9:P:3:DA:C8	2.43	0.54
3:C:106:ILE:HG13	3:C:107:PHE:H	1.73	0.53
6:F:17:LYS:HA	6:F:20:ARG:HG2	1.90	0.53
1:A:175:TYR:OH	8:H:251:GLU:OE1	2.27	0.53
4:D:295:TRP:CD1	5:E:189:ARG:HD2	2.44	0.53
6:F:33:ALA:HA	6:F:47:THR:HB	1.91	0.53
7:G:190:ASN:ND2	7:G:217:LEU:O	2.42	0.53
8:H:22:VAL:HG13	8:H:331:ASN:HB3	1.90	0.53
4:D:325:LEU:HD22	4:D:349:LYS:HD3	1.89	0.53
1:A:194:HIS:HB3	1:A:197:THR:HG22	1.89	0.53
2:B:76:LEU:HD21	2:B:92:GLN:HG2	1.90	0.53
3:C:105:GLN:NE2	3:C:110:GLY:O	2.41	0.53
1:A:402:ASP:O	1:A:406:GLU:HG3	2.09	0.53
1:A:277:LEU:HD22	1:A:318:LEU:HD22	1.91	0.53
6:F:22:THR:O	6:F:25:THR:OG1	2.22	0.52
7:G:153:SER:H	7:G:260:ASP:HA	1.73	0.52
8:H:324:PHE:HB2	8:H:375:GLU:HG2	1.90	0.52
8:H:51:LEU:HB3	8:H:374:VAL:HB	1.90	0.52
6:F:88:LEU:HG	6:F:90:THR:H	1.75	0.52
7:G:109:SER:HB2	7:G:118:VAL:HB	1.92	0.52
2:B:314:ALA:HB1	3:C:297:VAL:HA	1.92	0.52
3:C:10:LYS:HD2	3:C:18:LYS:HG3	1.92	0.52
5:E:286:LEU:HD11	5:E:346:ILE:HD12	1.92	0.52
5:E:295:PRO:HD2	5:E:298:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:18:LEU:O	6:F:21:THR:OG1	2.23	0.51
7:G:182:ALA:HB3	7:G:233:VAL:HB	1.93	0.51
8:H:113:ILE:HA	8:H:140:MET:HA	1.91	0.51
2:B:299:ILE:HG12	2:B:304:GLY:HA2	1.92	0.51
5:E:202:LEU:HD22	5:E:237:LEU:HD22	1.92	0.51
1:A:171:LYS:HG2	1:A:174:ARG:HH21	1.76	0.51
1:A:307:GLU:HG3	1:A:332:THR:HG21	1.92	0.51
5:E:154:LEU:O	5:E:158:MET:HG2	2.11	0.51
2:B:271:PHE:HB2	2:B:292:ILE:HG21	1.92	0.51
5:E:106:ARG:HD3	5:E:149:ASP:HB3	1.93	0.51
4:D:113:PHE:HA	4:D:116:LEU:HD23	1.94	0.50
7:G:59:GLN:HB2	7:G:307:GLU:HG2	1.92	0.50
8:H:20:ILE:HG23	8:H:102:THR:HG22	1.91	0.50
8:H:347:ASP:OD1	8:H:347:ASP:N	2.44	0.50
5:E:106:ARG:HA	5:E:150:ALA:HB2	1.93	0.50
8:H:31:LYS:HG3	8:H:95:ARG:HB3	1.93	0.50
11:D:401:AGS:O3G	11:D:401:AGS:O2B	2.29	0.50
7:G:269:ILE:HB	7:G:306:ILE:HB	1.93	0.50
8:H:140:MET:HE1	8:H:146:LYS:HG3	1.92	0.50
5:E:236:MET:O	5:E:240:MET:HG3	2.11	0.50
8:H:109:ASP:N	8:H:109:ASP:OD1	2.43	0.50
3:C:120:ASP:OD1	3:C:120:ASP:N	2.45	0.50
1:A:178:MET:HE3	1:A:178:MET:HA	1.95	0.49
6:F:98:ASP:OD1	6:F:99:SER:N	2.45	0.49
7:G:107:THR:HB	7:G:120:ILE:HB	1.94	0.49
1:A:224:THR:HG21	2:B:153:PRO:HG3	1.94	0.49
3:C:50:LEU:HB2	3:C:161:CYS:HB3	1.94	0.49
6:F:412:CYS:SG	6:F:413:LYS:N	2.84	0.49
7:G:202:PHE:CE2	7:G:204:LYS:HB2	2.48	0.49
2:B:66:LEU:HD13	2:B:110:ILE:HD11	1.95	0.49
6:F:75:ASP:OD1	6:F:76:VAL:N	2.46	0.49
8:H:140:MET:HE2	8:H:144:ILE:HG23	1.95	0.49
3:C:306:ILE:HD13	3:C:323:VAL:HG22	1.94	0.49
4:D:66:PRO:O	4:D:69:THR:OG1	2.24	0.49
7:G:35:ASP:O	7:G:50:ARG:NH1	2.46	0.49
5:E:193:PRO:HG2	5:E:230:LEU:HD21	1.94	0.49
4:D:160:TYR:HE1	7:G:138:LYS:HB2	1.78	0.48
3:C:21:PRO:HD3	11:C:401:AGS:H2'	1.94	0.48
5:E:41:LEU:HB2	5:E:170:VAL:HG12	1.94	0.48
1:A:384:TYR:HB2	1:A:428:PHE:HZ	1.76	0.48
6:F:293:GLU:HG3	7:G:129:ARG:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:55:VAL:HA	7:G:311:LEU:HD12	1.96	0.48
8:H:240:PHE:HE2	8:H:286:ASN:HB3	1.78	0.48
8:H:134:LEU:HB3	8:H:150:PRO:HG2	1.95	0.48
4:D:143:ASP:OD1	4:D:143:ASP:N	2.45	0.48
4:D:281:ASP:OD1	4:D:281:ASP:N	2.45	0.48
5:E:258:ASP:N	5:E:258:ASP:OD1	2.46	0.48
6:F:36:ARG:HH11	6:F:44:ILE:HG21	1.79	0.48
4:D:291:MET:HG3	4:D:340:HIS:CG	2.49	0.47
5:E:17:SER:H	13:E:500:ADP:HN62	1.62	0.47
7:G:202:PHE:HB3	8:H:149:CYS:HB3	1.97	0.47
5:E:9:ARG:HH22	5:E:50:LYS:HG3	1.79	0.47
4:D:96:ASN:HD22	5:E:156:ARG:HE	1.62	0.47
4:D:192:LEU:HD12	4:D:228:LEU:HB2	1.96	0.47
4:D:263:VAL:HG21	4:D:300:VAL:HG22	1.96	0.47
6:F:25:THR:HG22	6:F:101:LEU:HD11	1.96	0.47
6:F:30:ARG:NH2	6:F:64:ASP:OD1	2.45	0.47
6:F:156:LEU:HB2	6:F:207:VAL:HB	1.95	0.47
1:A:449:VAL:HG21	5:E:287:TYR:HD1	1.79	0.47
3:C:59:LYS:HB3	3:C:146:LEU:HD22	1.96	0.47
3:C:135:GLU:HG2	3:C:160:ARG:HE	1.78	0.47
6:F:301:ASP:N	6:F:301:ASP:OD1	2.47	0.47
7:G:118:VAL:HG22	7:G:131:GLU:HG2	1.97	0.47
7:G:321:GLN:HA	7:G:324:ILE:HD13	1.96	0.47
8:H:118:ILE:HD11	8:H:134:LEU:HD21	1.97	0.47
2:B:31:ASP:O	2:B:35:GLN:HG3	2.15	0.47
3:C:46:LEU:HD21	3:C:113:LEU:HD13	1.96	0.47
3:C:229:ASP:OD1	3:C:229:ASP:N	2.46	0.47
5:E:68:LEU:HD23	5:E:90:SER:HB2	1.97	0.47
5:E:239:SER:HB3	5:E:255:ILE:HD13	1.97	0.47
5:E:19:ASN:HB2	5:E:52:ARG:HH21	1.80	0.46
3:C:299:LEU:HD11	3:C:331:PHE:HE1	1.79	0.46
4:D:24:GLN:HA	5:E:34:ARG:HB3	1.97	0.46
4:D:315:ASP:OD1	4:D:315:ASP:N	2.42	0.46
8:H:241:LEU:HD21	8:H:329:PHE:HD2	1.79	0.46
2:B:236:VAL:HG22	2:B:239:MET:HE2	1.97	0.46
6:F:70:CYS:HB3	6:F:464:ILE:HG23	1.96	0.46
8:H:329:PHE:O	8:H:333:ILE:HG12	2.15	0.46
6:F:40:GLU:HG2	6:F:80:TYR:HD2	1.80	0.46
6:F:97:CYS:HA	6:F:100:LEU:HD12	1.96	0.46
1:A:385:ASN:HD22	5:E:280:ILE:HG21	1.81	0.46
3:C:256:TRP:NE1	4:D:320:ASN:OD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:ILE:O	1:A:485:GLY:N	2.48	0.46
3:C:254:ASP:HB2	3:C:259:ALA:HB2	1.97	0.46
2:B:24:VAL:H	11:B:401:AGS:HN62	1.64	0.45
3:C:104:ARG:HB2	7:G:314:GLU:HA	1.98	0.45
1:A:174:ARG:HG2	1:A:208:TRP:HE1	1.82	0.45
7:G:326:LEU:O	7:G:330:THR:OG1	2.20	0.45
2:B:77:GLU:OE2	3:C:132:ARG:NH2	2.49	0.45
2:B:82:ASP:O	3:C:94:ARG:NH1	2.49	0.45
6:F:249:PHE:HD1	6:F:294:ILE:HD12	1.82	0.45
2:B:46:ILE:HG12	2:B:142:PHE:HB2	1.98	0.45
2:B:24:VAL:O	11:B:401:AGS:N6	2.50	0.45
2:B:232:HIS:CD2	2:B:233:PRO:HD3	2.50	0.45
4:D:69:THR:HG21	4:D:189:PHE:HB3	1.99	0.45
5:E:87:VAL:HG23	5:E:96:ILE:HG22	1.99	0.45
7:G:256:LEU:HB3	7:G:268:ASN:HB2	1.98	0.45
2:B:263:SER:HA	2:B:266:ILE:HD12	1.98	0.45
2:B:20:LEU:HD23	2:B:23:ILE:HD12	1.99	0.45
4:D:84:GLY:O	4:D:88:MET:HE3	2.17	0.45
3:C:51:PHE:HB2	3:C:146:LEU:HD23	1.98	0.45
3:C:206:ARG:HD3	11:C:401:AGS:H5'1	1.98	0.45
5:E:18:HIS:CE1	5:E:193:PRO:HG3	2.52	0.45
2:B:73:ASP:HB3	2:B:101:LEU:HD21	1.99	0.45
5:E:4:TRP:HB2	5:E:234:LEU:HB3	1.99	0.45
8:H:15:ILE:HB	8:H:339:TRP:HB2	1.99	0.45
2:B:249:ILE:HD13	2:B:313:LEU:HD12	1.99	0.44
4:D:101:ARG:NH2	4:D:144:SER:OG	2.50	0.44
3:C:71:TYR:OH	3:C:111:PHE:O	2.22	0.44
4:D:249:LYS:NZ	4:D:255:GLN:OE1	2.50	0.44
4:D:295:TRP:HE1	5:E:189:ARG:NH1	2.15	0.44
3:C:97:ILE:HG22	3:C:133:VAL:HG11	2.00	0.44
4:D:305:HIS:O	4:D:309:ILE:HG12	2.17	0.44
5:E:221:ARG:HE	5:E:254:ILE:HD11	1.83	0.44
4:D:58:LEU:HD12	4:D:59:PRO:HD2	1.99	0.44
4:D:220:ILE:HD11	4:D:256:VAL:HG11	1.99	0.44
2:B:232:HIS:CG	2:B:233:PRO:HD3	2.52	0.44
6:F:433:SER:HB3	6:F:439:VAL:HG23	2.00	0.44
7:G:320:ALA:O	7:G:324:ILE:HD12	2.17	0.44
7:G:325:GLU:O	7:G:328:MET:N	2.51	0.44
8:H:262:SER:HB3	8:H:287:THR:HG23	2.00	0.44
1:A:116:SER:N	11:A:701:AGS:O1A	2.51	0.44
3:C:82:LEU:HB2	3:C:116:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:39:LEU:HD22	5:E:188:ILE:HD11	2.00	0.44
5:E:152:ALA:HA	5:E:155:ARG:HG2	1.99	0.44
1:A:371:LEU:HD23	1:A:421:LEU:HD13	2.00	0.44
3:C:83:ASN:HB2	4:D:155:ARG:HG2	2.00	0.44
9:P:10:DA:H2	10:T:21:DT:H3	1.66	0.44
6:F:14:ASP:O	6:F:17:LYS:HG2	2.18	0.44
1:A:373:LYS:HD2	1:A:374:GLU:O	2.17	0.43
2:B:114:ASP:HA	2:B:143:ALA:HB3	1.99	0.43
3:C:302:LYS:HD3	3:C:326:ALA:HB1	2.00	0.43
7:G:183:LYS:HD2	7:G:183:LYS:HA	1.76	0.43
3:C:102:SER:O	7:G:314:GLU:N	2.48	0.43
6:F:7:VAL:HG22	6:F:77:PHE:HE2	1.83	0.43
8:H:95:ARG:NH2	8:H:153:GLN:OE1	2.40	0.43
3:C:165:ARG:HH21	3:C:167:GLN:HB3	1.83	0.43
8:H:329:PHE:HE1	8:H:362:MET:HE1	1.83	0.43
3:C:28:TYR:H	11:C:401:AGS:HN62	1.66	0.43
3:C:189:LEU:HG	3:C:227:ILE:HB	1.99	0.43
4:D:63:PHE:HB2	4:D:169:ILE:HG12	1.99	0.43
5:E:267:THR:HG23	5:E:307:LEU:HG	2.00	0.43
8:H:11:GLY:O	8:H:14:ASN:ND2	2.51	0.43
1:A:119:ILE:HG12	1:A:220:VAL:HG11	2.00	0.43
1:A:147:LYS:HG2	1:A:148:VAL:HG13	2.00	0.43
1:A:173:ALA:HB1	1:A:184:ILE:HG13	2.01	0.43
1:A:333:ARG:HG2	2:B:155:GLN:HB3	2.00	0.43
3:C:71:TYR:HB3	3:C:74:ASN:HB2	2.00	0.43
4:D:44:HIS:CE1	4:D:190:LYS:HE3	2.54	0.43
8:H:141:ASP:OD1	8:H:141:ASP:N	2.51	0.43
7:G:245:ILE:HG13	7:G:310:MET:HE2	2.01	0.43
4:D:33:PRO:HB3	4:D:38:GLU:HB2	2.01	0.43
4:D:200:ARG:NE	11:D:401:AGS:H2	2.34	0.43
5:E:144:ASN:ND2	5:E:172:ASP:OD1	2.52	0.43
4:D:52:THR:HG21	4:D:58:LEU:HD13	2.01	0.43
5:E:229:ASN:HB3	5:E:232:VAL:HB	2.00	0.43
2:B:127:LEU:O	2:B:131:MET:HG3	2.19	0.42
3:C:128:ASN:HA	3:C:131:ARG:HG2	2.00	0.42
4:D:44:HIS:HE1	4:D:190:LYS:HE3	1.84	0.42
6:F:17:LYS:O	6:F:21:THR:HG23	2.19	0.42
7:G:55:VAL:HG13	7:G:56:ILE:HG22	2.01	0.42
7:G:260:ASP:OD2	7:G:262:HIS:ND1	2.52	0.42
1:A:397:ALA:O	1:A:401:VAL:HG23	2.18	0.42
8:H:4:LYS:HB3	8:H:4:LYS:HE2	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:104:ARG:HH12	7:G:312:GLU:HB3	1.84	0.42
8:H:258:VAL:HG23	8:H:259:HIS:H	1.84	0.42
3:C:273:ALA:HB2	4:D:188:ARG:HD2	2.00	0.42
2:B:84:ARG:NH1	2:B:115:GLU:O	2.49	0.42
5:E:324:TYR:CD2	5:E:348:LYS:HB3	2.54	0.42
1:A:216:LEU:HD12	1:A:217:PRO:HD2	2.00	0.42
4:D:255:GLN:O	4:D:258:GLU:HG3	2.19	0.42
7:G:264:VAL:HG12	7:G:311:LEU:HD23	2.02	0.42
8:H:237:LEU:HD21	8:H:329:PHE:CE2	2.55	0.42
6:F:163:ILE:HD11	6:F:199:LYS:HE2	2.02	0.42
3:C:230:ASP:OD1	3:C:240:ARG:NH1	2.53	0.42
4:D:110:VAL:HG12	4:D:156:THR:HG21	2.02	0.42
5:E:272:LYS:HB3	5:E:272:LYS:HE2	1.83	0.42
6:F:268:LYS:HG2	6:F:405:THR:HB	2.02	0.42
2:B:29:THR:HG23	2:B:161:LEU:HD23	2.02	0.41
4:D:82:LEU:HD22	4:D:132:PRO:HG3	2.01	0.41
4:D:194:ALA:HA	4:D:221:LEU:HD13	2.00	0.41
1:A:426:LYS:HE3	1:A:426:LYS:HB3	1.93	0.41
3:C:60:THR:HA	3:C:63:ILE:HG22	2.02	0.41
6:F:265:MET:HE2	6:F:265:MET:HB3	1.85	0.41
7:G:32:GLY:HA2	7:G:50:ARG:HE	1.84	0.41
1:A:419:TYR:CZ	2:B:290:LYS:HD3	2.54	0.41
5:E:202:LEU:HB3	5:E:219:LEU:HD22	2.01	0.41
7:G:200:LEU:HA	8:H:100:HIS:CE1	2.55	0.41
2:B:126:ALA:O	2:B:130:THR:HG23	2.20	0.41
1:A:337:ILE:HG23	1:A:341:HIS:HB3	2.03	0.41
5:E:172:ASP:OD1	5:E:173:SER:N	2.54	0.41
11:A:701:AGS:O2G	11:A:701:AGS:O2B	2.37	0.41
6:F:19:LEU:O	6:F:23:ILE:HG12	2.20	0.41
6:F:282:LYS:HB3	6:F:282:LYS:HE2	1.95	0.41
8:H:286:ASN:OD1	8:H:287:THR:N	2.53	0.41
3:C:53:GLY:O	3:C:148:ASN:ND2	2.46	0.41
5:E:300:LEU:HD12	5:E:342:LEU:HD23	2.03	0.41
1:A:111:SER:OG	1:A:333:ARG:NH1	2.47	0.41
6:F:23:ILE:HA	6:F:26:VAL:HG12	2.03	0.41
8:H:325:LYS:HA	8:H:325:LYS:HD2	1.79	0.41
1:A:75:LEU:HD11	1:A:85:LEU:HD11	2.03	0.41
1:A:103:ARG:H	1:A:259:ARG:HB3	1.85	0.41
1:A:328:LEU:HD12	1:A:329:PRO:HD2	2.03	0.41
5:E:41:LEU:HG	5:E:188:ILE:HB	2.02	0.41
5:E:202:LEU:HA	5:E:205:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:329:PHE:CE1	8:H:362:MET:HE1	2.56	0.41
1:A:103:ARG:HD3	1:A:209:LEU:HA	2.02	0.41
2:B:258:LYS:HA	2:B:258:LYS:HD3	1.87	0.41
3:C:245:LYS:HA	3:C:245:LYS:HD2	2.00	0.41
1:A:423:GLU:HA	2:B:286:LEU:HD22	2.03	0.40
2:B:162:ARG:HE	2:B:162:ARG:HB3	1.70	0.40
3:C:19:TYR:O	3:C:177:ARG:NH2	2.54	0.40
3:C:263:LEU:HD22	3:C:324:ILE:HD11	2.02	0.40
5:E:209:GLU:C	5:E:210:ARG:HD3	2.45	0.40
6:F:34:ILE:HG22	6:F:94:GLU:HB2	2.01	0.40
3:C:14:PRO:HG3	4:D:59:PRO:HA	2.03	0.40
4:D:97:ALA:O	5:E:110:GLN:NE2	2.54	0.40
5:E:79:SER:OG	5:E:80:ASN:N	2.53	0.40
5:E:101:MET:SD	5:E:102:GLY:N	2.94	0.40
8:H:18:ARG:HG3	8:H:335:ILE:HD13	2.02	0.40
1:A:445:ARG:H	1:A:445:ARG:HG2	1.70	0.40
2:B:191:LEU:HD23	2:B:191:LEU:HA	1.97	0.40
3:C:66:LEU:O	3:C:70:ILE:HG12	2.21	0.40
5:E:105:ASP:O	5:E:109:ILE:HG12	2.21	0.40
1:A:392:PHE:HE1	1:A:397:ALA:HB2	1.86	0.40
1:A:402:ASP:O	1:A:405:SER:OG	2.31	0.40
5:E:277:ASN:HA	5:E:280:ILE:HG12	2.03	0.40
6:F:9:GLY:HA3	6:F:13:PRO:HG2	2.04	0.40
1:A:287:MET:HE1	1:A:322:ALA:HB1	2.02	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	397/659 (60%)	380 (96%)	17 (4%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	315/323 (98%)	307 (98%)	8 (2%)	0	100	100
3	C	323/340 (95%)	310 (96%)	13 (4%)	0	100	100
4	D	328/353 (93%)	322 (98%)	6 (2%)	0	100	100
5	E	337/354 (95%)	328 (97%)	9 (3%)	0	100	100
6	F	255/446 (57%)	229 (90%)	26 (10%)	0	100	100
7	G	288/401 (72%)	268 (93%)	20 (7%)	0	100	100
8	H	254/612 (42%)	243 (96%)	11 (4%)	0	100	100
All	All	2497/3488 (72%)	2387 (96%)	110 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	372/612 (61%)	372 (100%)	0	100	100
2	B	277/283 (98%)	277 (100%)	0	100	100
3	C	281/296 (95%)	281 (100%)	0	100	100
4	D	294/312 (94%)	294 (100%)	0	100	100
5	E	313/324 (97%)	313 (100%)	0	100	100
6	F	248/402 (62%)	248 (100%)	0	100	100
7	G	266/369 (72%)	265 (100%)	1 (0%)	89	93
8	H	247/560 (44%)	247 (100%)	0	100	100
All	All	2298/3158 (73%)	2297 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	9	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	77	GLN
1	A	81	HIS
1	A	146	HIS
1	A	203	GLN
1	A	269	ASN
1	A	453	GLN
2	B	26	ASN
2	B	44	HIS
2	B	92	GLN
2	B	124	GLN
2	B	145	ASN
2	B	216	HIS
3	C	105	GLN
3	C	180	ASN
3	C	213	GLN
3	C	298	HIS
3	C	315	ASN
4	D	236	GLN
5	E	14	ASN
5	E	32	GLN
5	E	110	GLN
6	F	441	HIS
7	G	143	ASN
7	G	164	HIS
7	G	190	ASN
8	H	57	GLN
8	H	365	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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
13	ADP	E	500	-	24,29,29	0.91	0	29,45,45	1.21	2 (6%)
11	AGS	A	701	12	28,33,33	0.73	1 (3%)	31,52,52	0.93	2 (6%)
11	AGS	B	401	12	28,33,33	0.74	1 (3%)	31,52,52	0.93	2 (6%)
11	AGS	D	401	12	28,33,33	0.74	1 (3%)	31,52,52	0.93	2 (6%)
11	AGS	C	401	12	28,33,33	0.75	1 (3%)	31,52,52	0.92	2 (6%)

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
13	ADP	E	500	-	-	0/12/32/32	0/3/3/3
11	AGS	A	701	12	-	4/17/38/38	0/3/3/3
11	AGS	B	401	12	-	2/17/38/38	0/3/3/3
11	AGS	D	401	12	-	3/17/38/38	0/3/3/3
11	AGS	C	401	12	-	0/17/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	401	AGS	PG-S1G	2.20	1.95	1.90
11	D	401	AGS	PG-S1G	2.13	1.95	1.90
11	A	701	AGS	PG-S1G	2.13	1.95	1.90
11	B	401	AGS	PG-S1G	2.12	1.95	1.90

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	E	500	ADP	N3-C2-N1	-3.71	123.63	128.67
11	B	401	AGS	PB-O3B-PG	-3.54	120.21	133.17
11	A	701	AGS	PB-O3B-PG	-3.49	120.41	133.17
11	C	401	AGS	PB-O3B-PG	-3.43	120.63	133.17
11	D	401	AGS	PB-O3B-PG	-3.38	120.79	133.17
13	E	500	ADP	C4-C5-N7	-2.59	106.60	109.34
11	A	701	AGS	C5-C6-N6	2.31	123.83	120.31
11	C	401	AGS	C5-C6-N6	2.28	123.78	120.31
11	D	401	AGS	C5-C6-N6	2.28	123.78	120.31
11	B	401	AGS	C5-C6-N6	2.26	123.76	120.31

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	701	AGS	C5'-O5'-PA-O2A
11	A	701	AGS	C5'-O5'-PA-O3A
11	B	401	AGS	PB-O3B-PG-O2G
11	B	401	AGS	PB-O3B-PG-O3G
11	D	401	AGS	O4'-C4'-C5'-O5'
11	D	401	AGS	C3'-C4'-C5'-O5'
11	A	701	AGS	C5'-O5'-PA-O1A
11	A	701	AGS	O4'-C4'-C5'-O5'
11	D	401	AGS	PA-O3A-PB-O2B

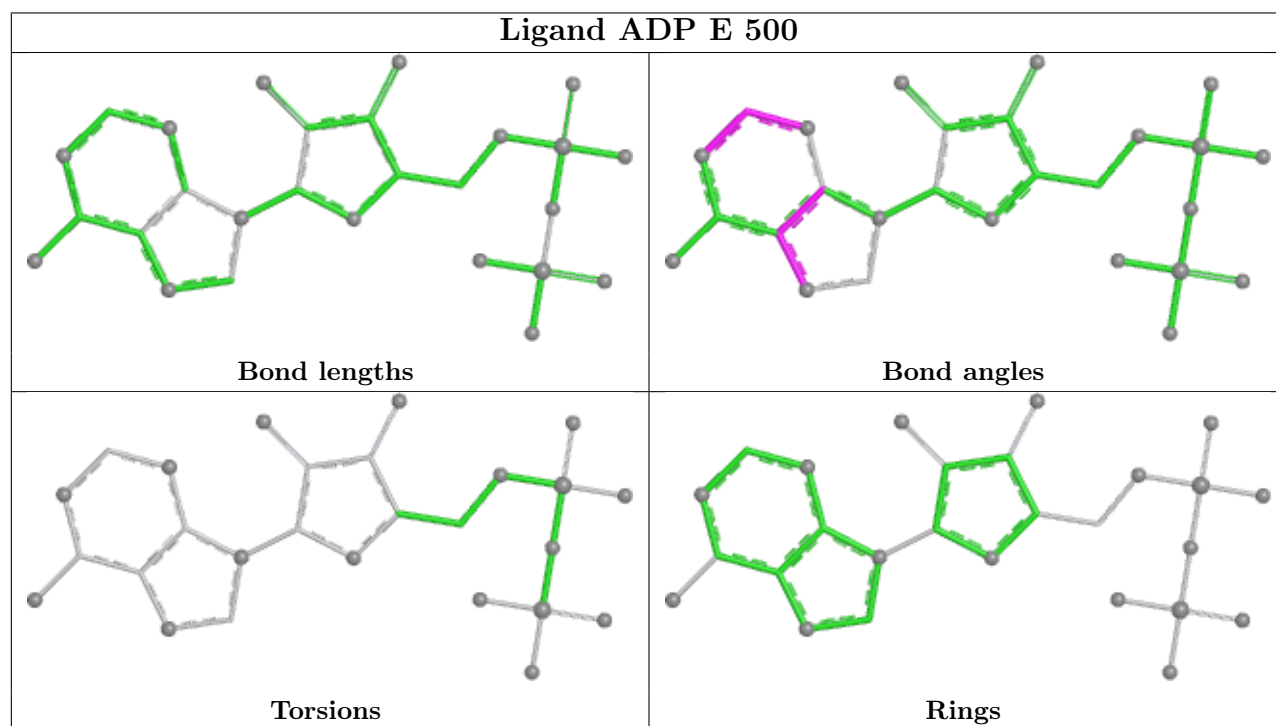
There are no ring outliers.

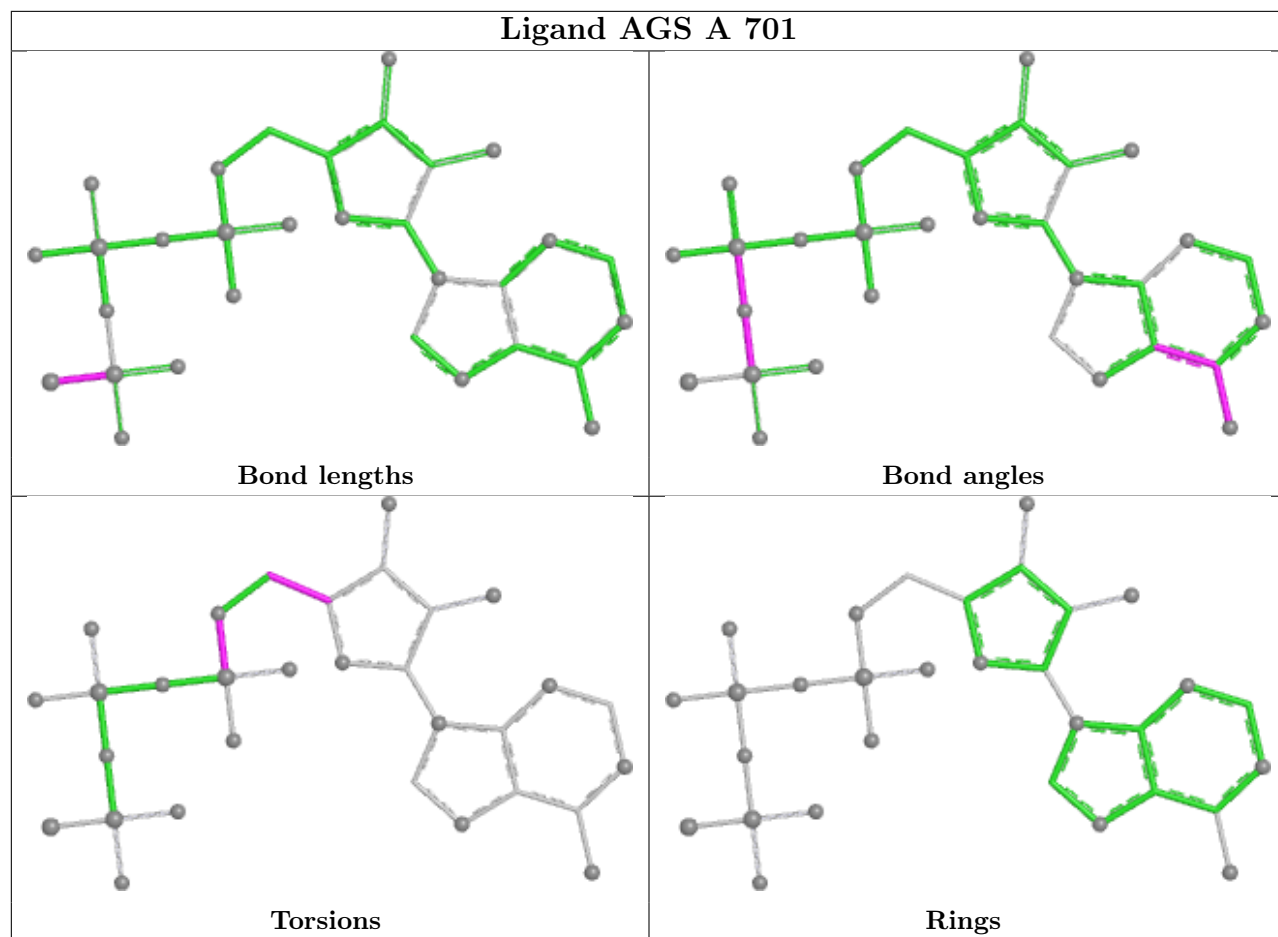
5 monomers are involved in 14 short contacts:

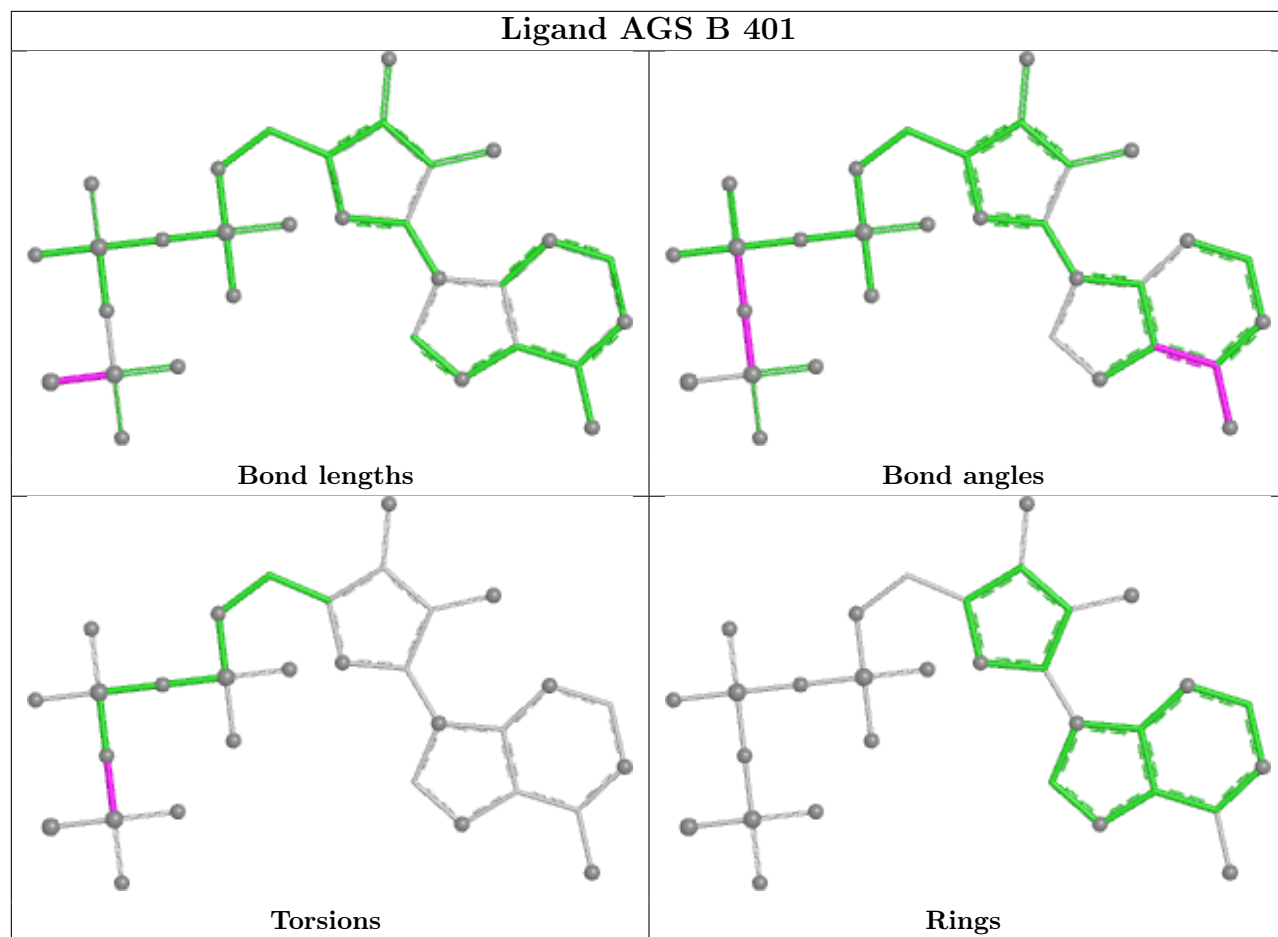
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	E	500	ADP	2	0
11	A	701	AGS	2	0
11	B	401	AGS	2	0
11	D	401	AGS	4	0
11	C	401	AGS	4	0

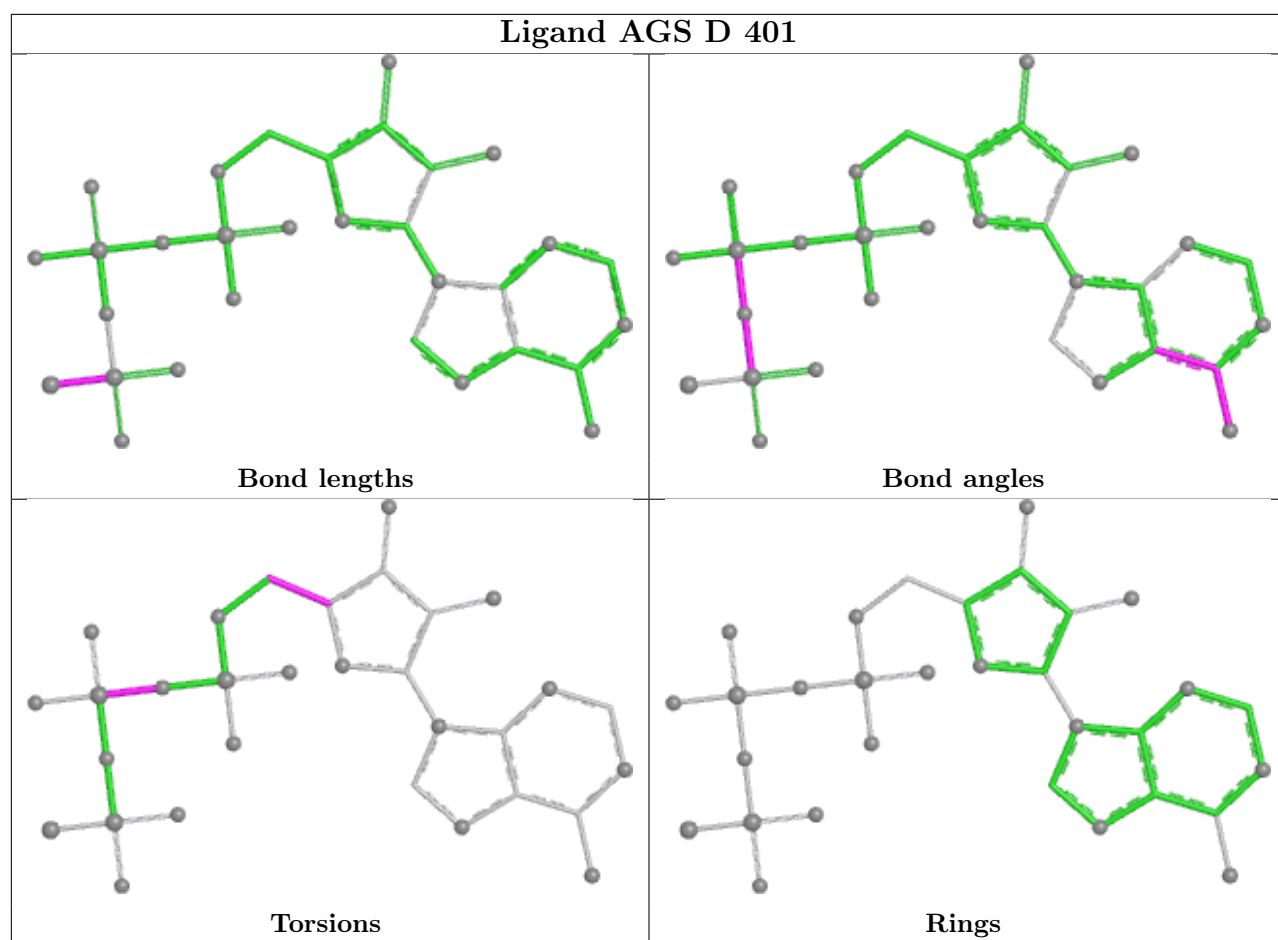
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

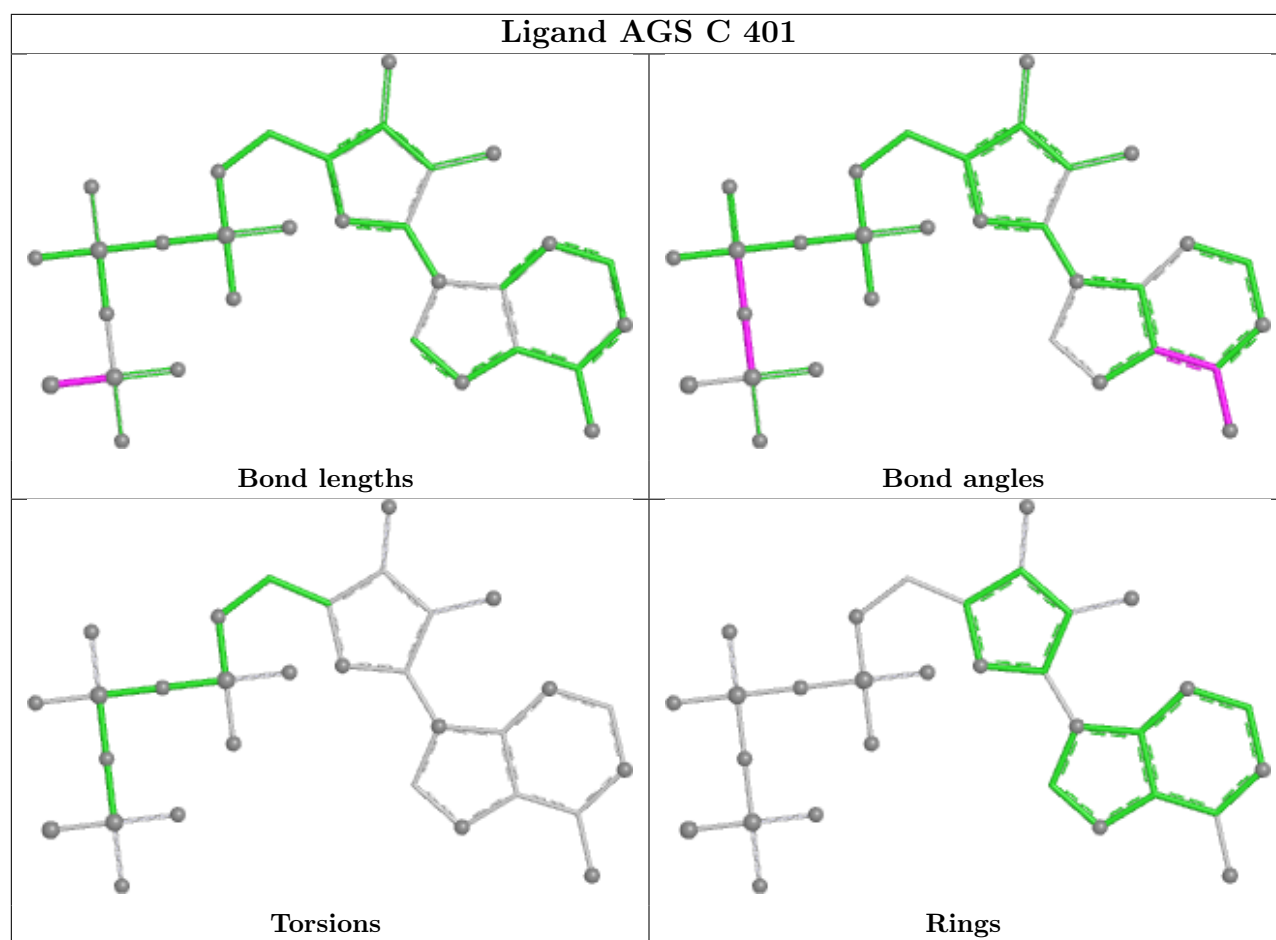
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

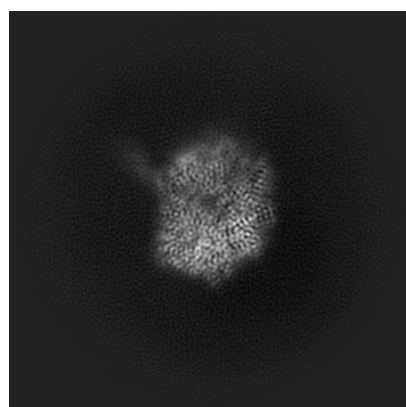
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25122. These allow visual inspection of the internal detail of the map and identification of artifacts.

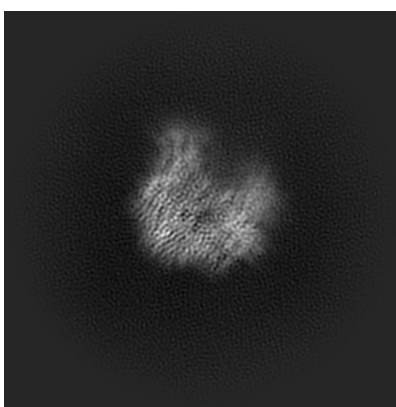
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

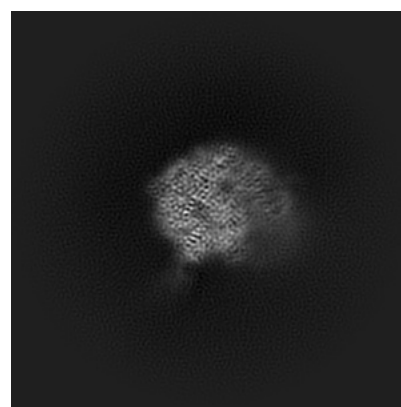
#### 6.1.1 Primary map



X



Y

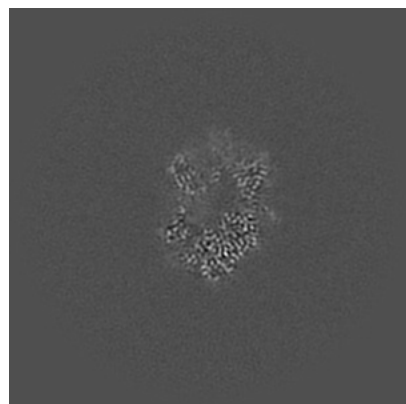


Z

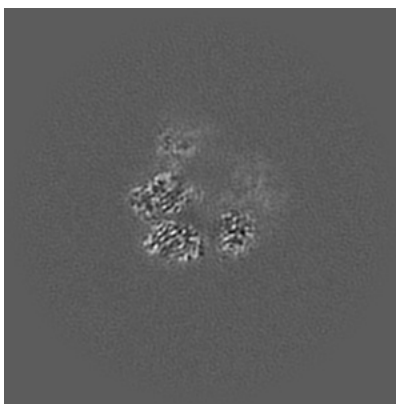
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

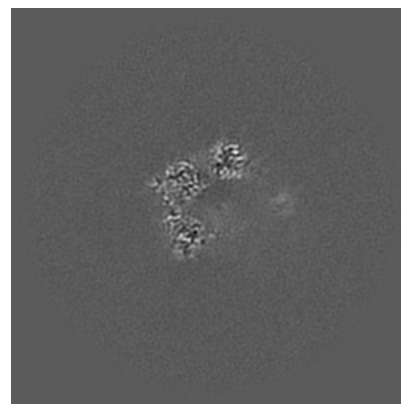
#### 6.2.1 Primary map



X Index: 200



Y Index: 200



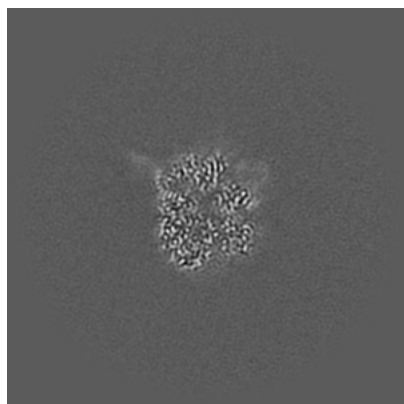
Z Index: 200



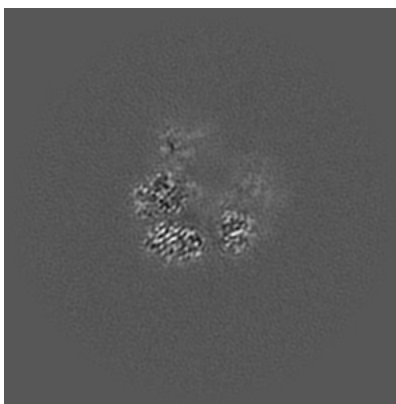
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

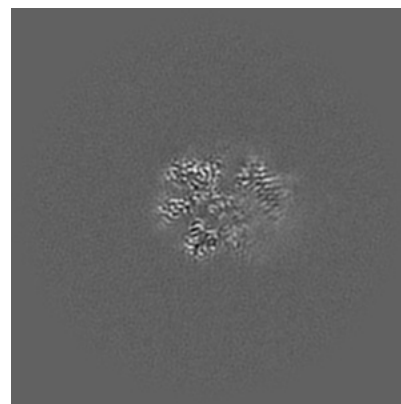
### 6.3.1 Primary map



X Index: 180



Y Index: 198

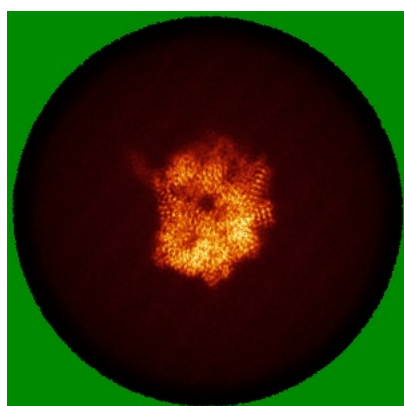


Z Index: 176

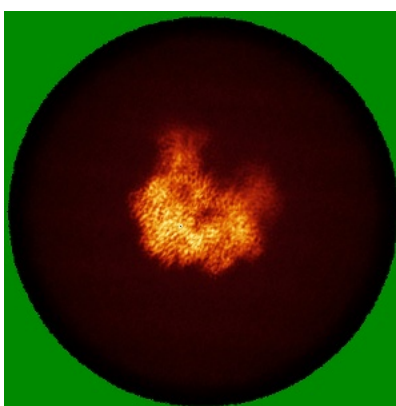
The images above show the largest variance slices of the map in three orthogonal directions.

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

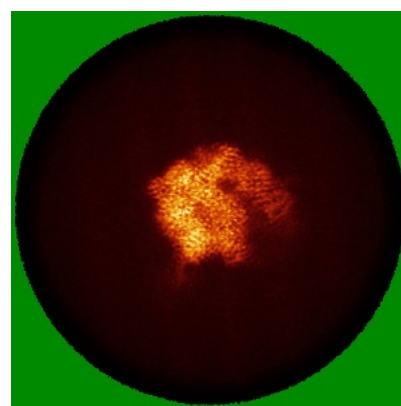
### 6.4.1 Primary map



X



Y

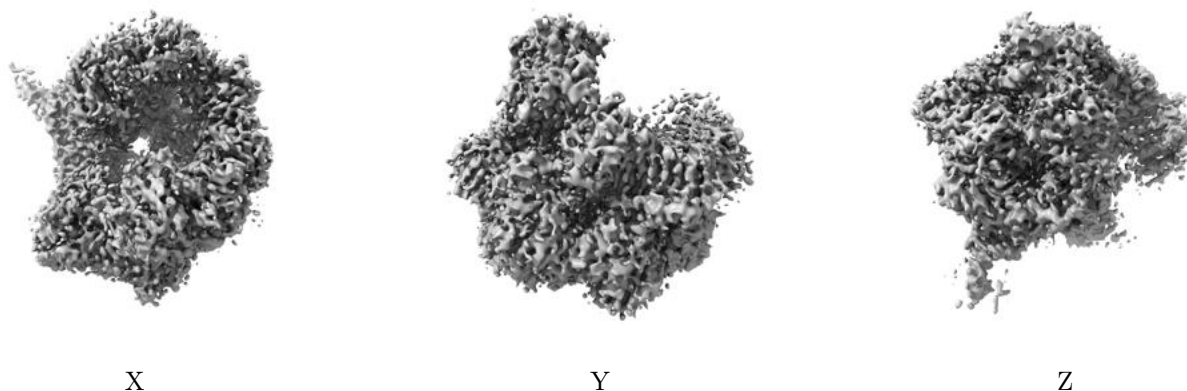


Z

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 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

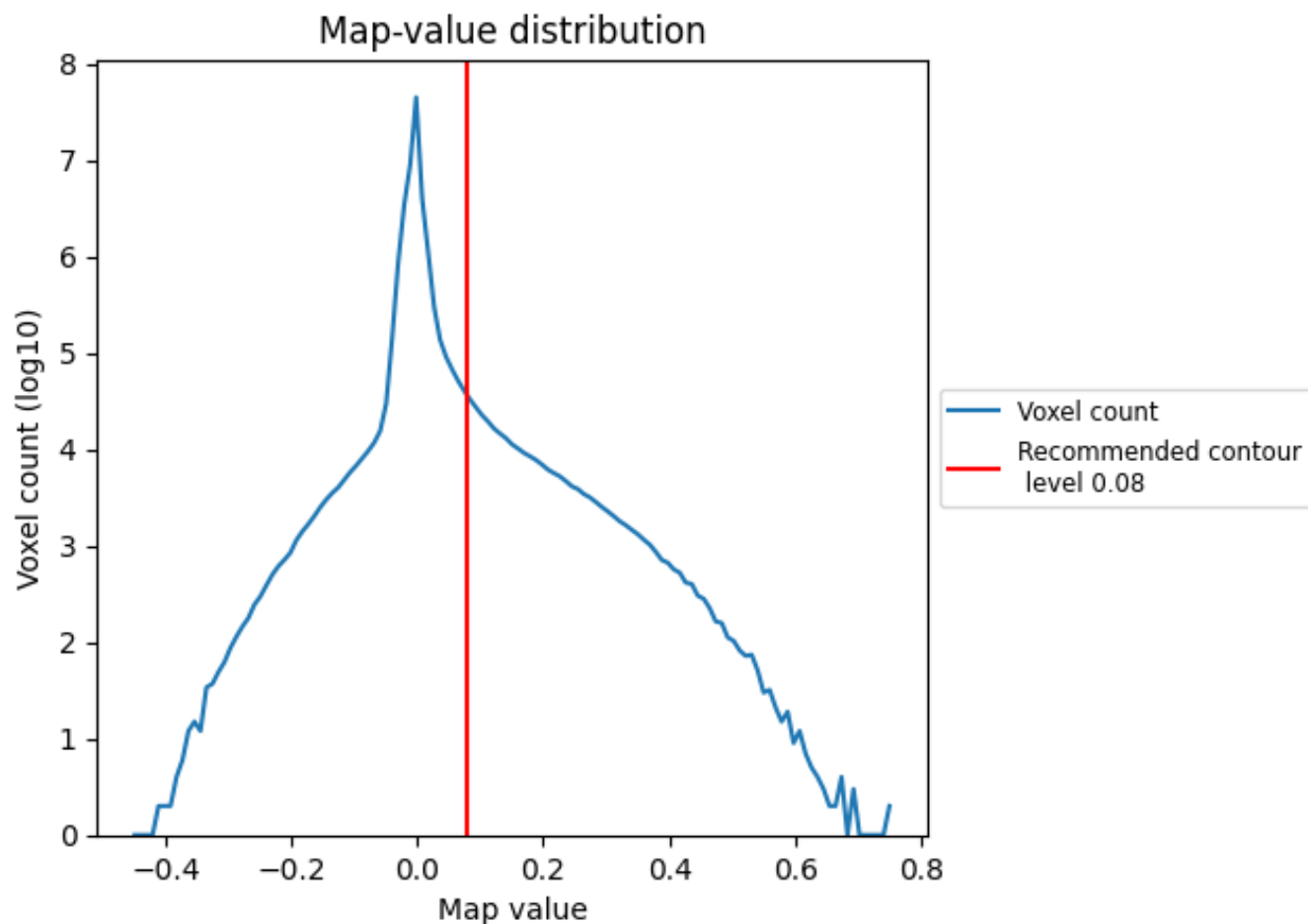
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

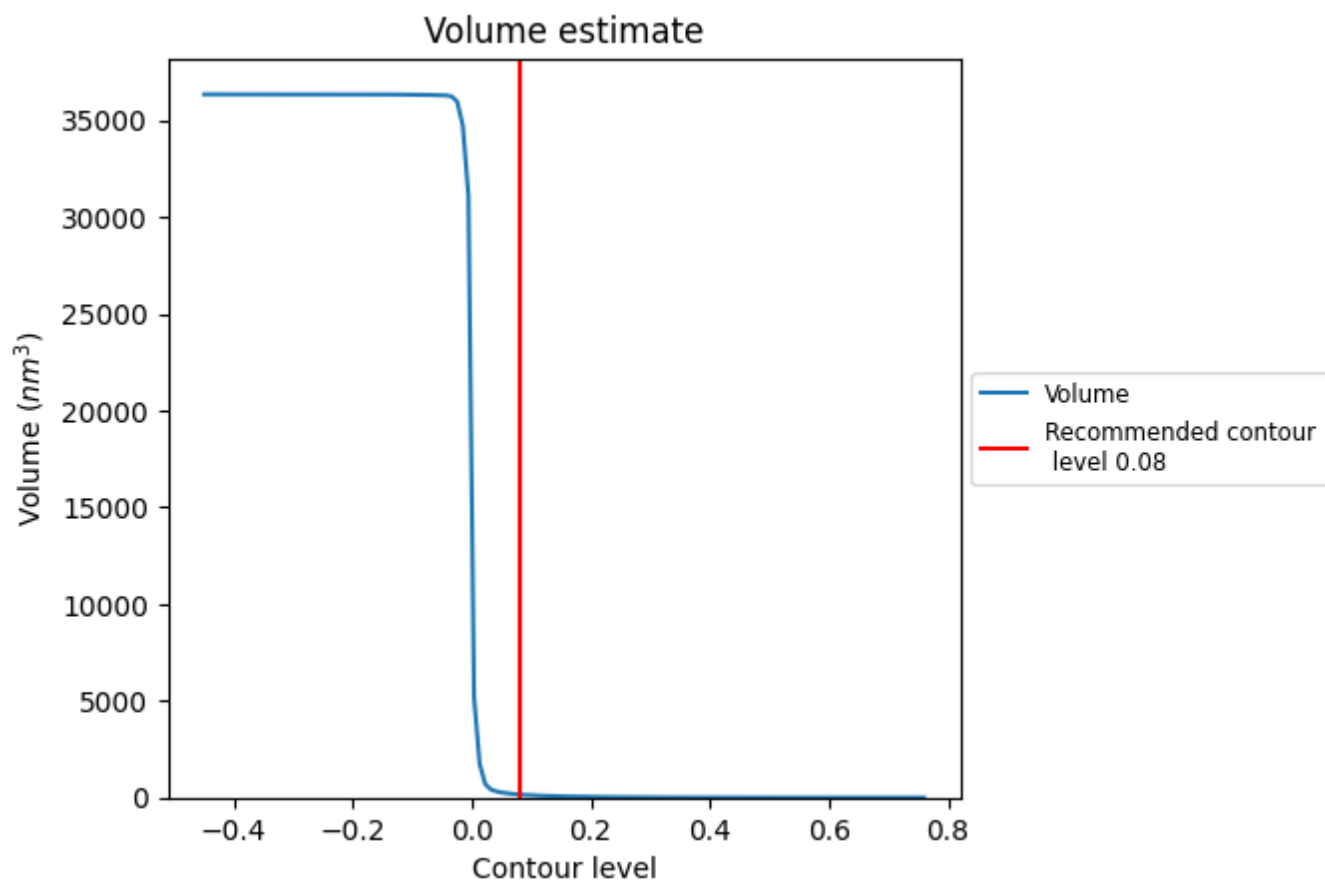
This section contains the results of statistical analysis of the map.

### 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.

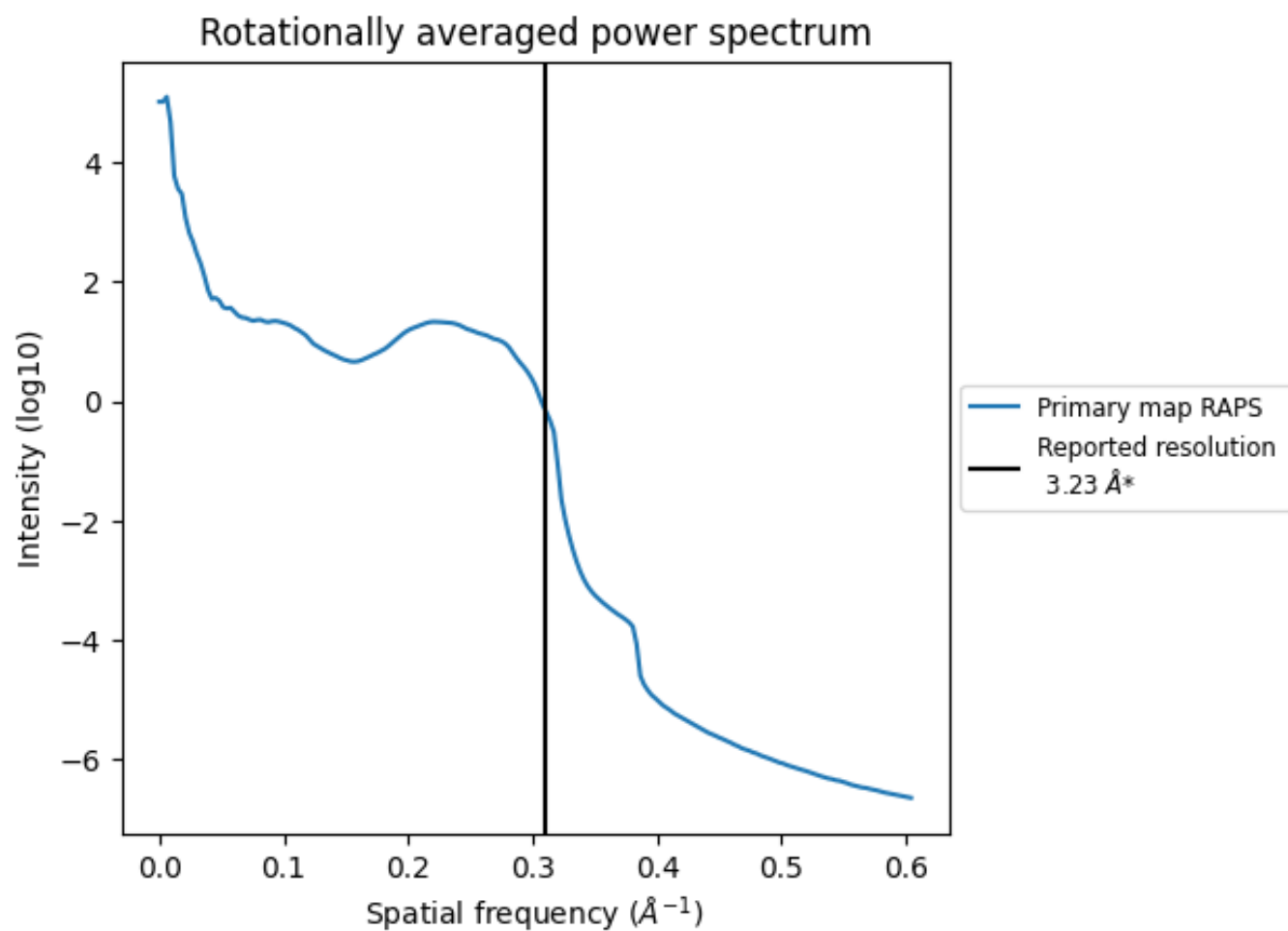
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 156 nm<sup>3</sup>; this corresponds to an approximate mass of 141 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 0.310 Å<sup>-1</sup>

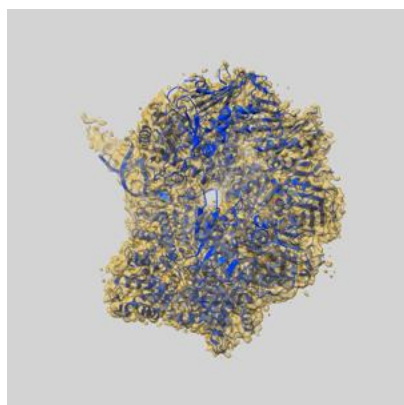
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

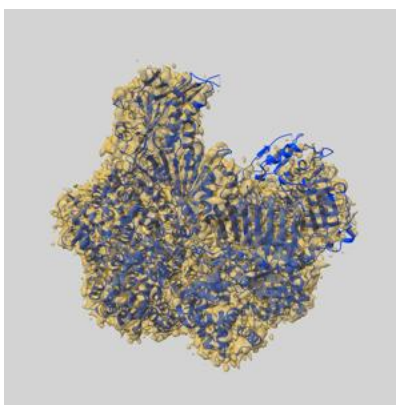
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25122 and PDB model 7SH2. Per-residue inclusion information can be found in section [3](#) on page [8](#).

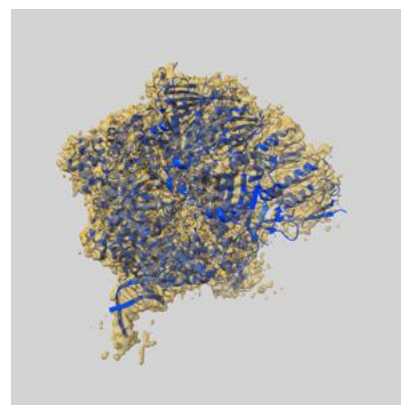
### 9.1 Map-model overlay [i](#)



X



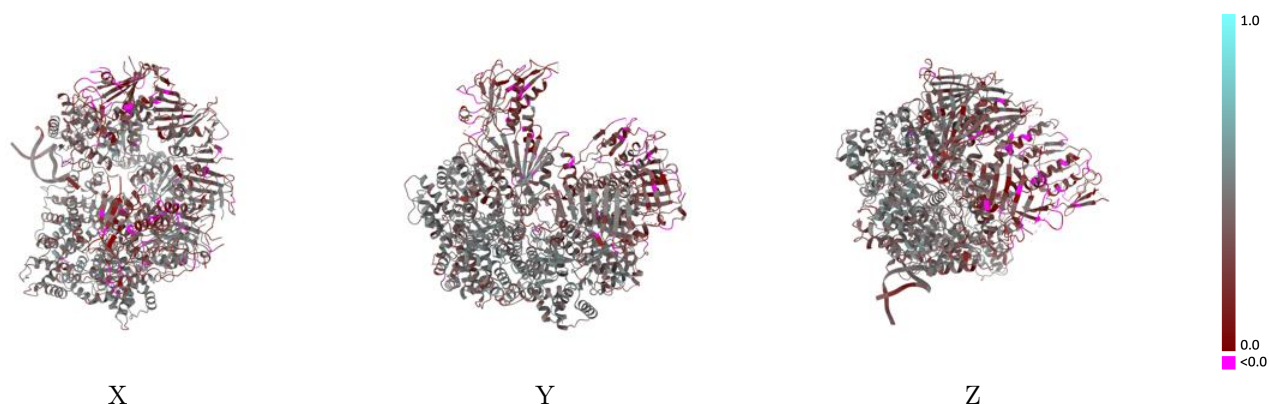
Y



Z

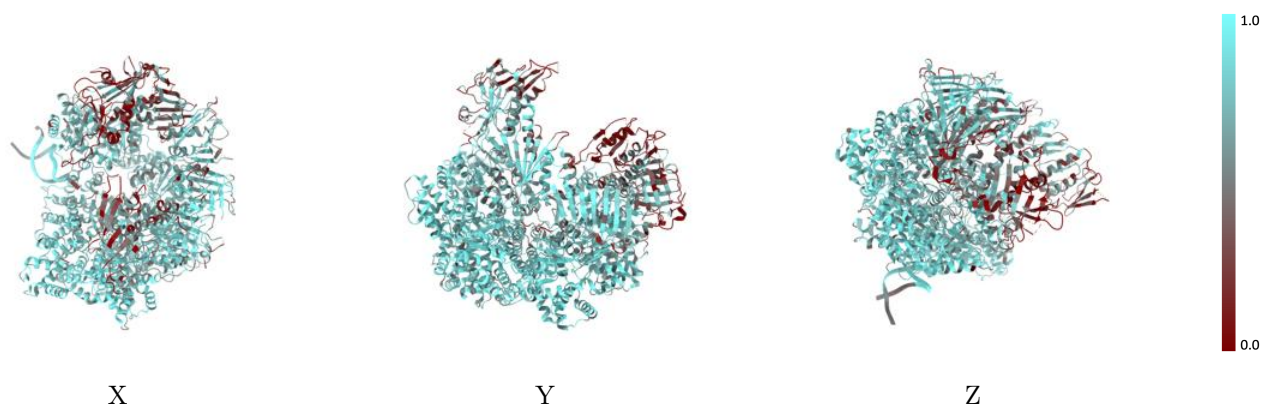
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

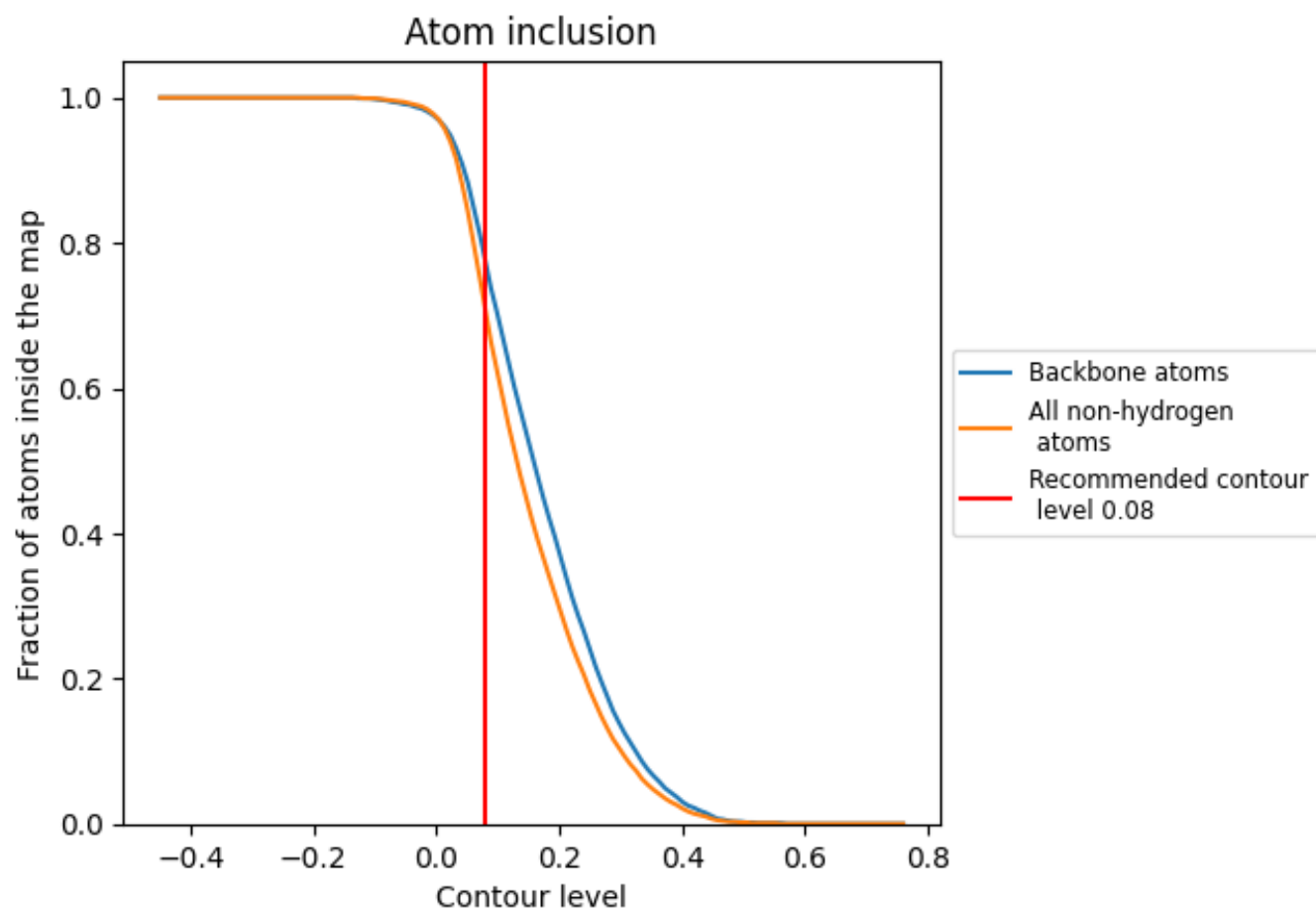
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.08).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 71% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7060	<div></div> 0.3730
A	<div></div> 0.7470	<div></div> 0.3970
B	<div></div> 0.8170	<div></div> 0.4420
C	<div></div> 0.8210	<div></div> 0.4400
D	<div></div> 0.8480	<div></div> 0.4460
E	<div></div> 0.8080	<div></div> 0.4300
F	<div></div> 0.5120	<div></div> 0.2020
G	<div></div> 0.6660	<div></div> 0.3380
H	<div></div> 0.3040	<div></div> 0.2250
P	<div></div> 0.7520	<div></div> 0.3620
T	<div></div> 0.6970	<div></div> 0.3540

1.0

0.0

<0.0