



Full wwPDB EM Validation Report ⓘ

Apr 21, 2026 – 01:28 PM EDT

PDB ID : 8FS3 / pdb_00008fs3
EMDB ID : EMD-29412
Title : Structure of *S. cerevisiae* Rad24-RFC loading the 9-1-1 clamp onto a 10-nt gapped DNA in step 1 (open 9-1-1 and shoulder bound DNA only)
Authors : Zheng, F.; Georgescu, R.; Yao, Y.N.; O'Donnell, M.E.; Li, H.
Deposited on : 2023-01-09
Resolution : 2.93 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

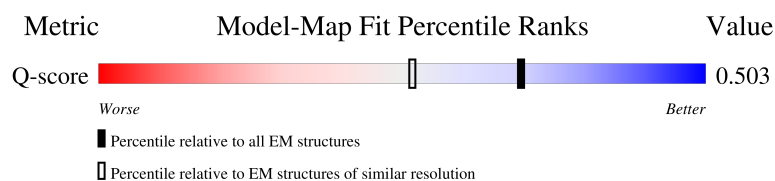
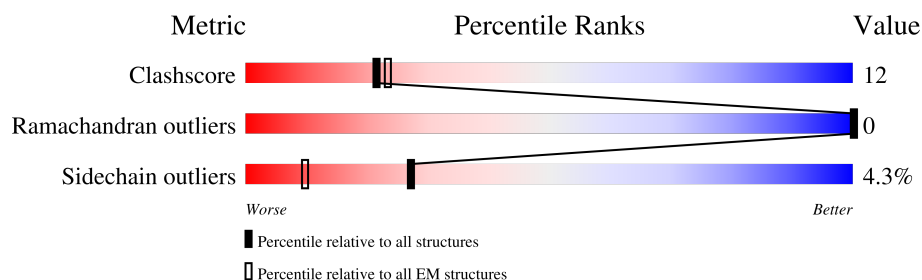
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.93 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	13037 (2.43 - 3.43)

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	545	7% 57% 22% • 20%
2	B	323	73% 25% ••
3	C	336	69% 27% ••
4	D	353	71% 21% • 7%

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Mol	Chain	Length	Quality of chain
5	E	354	68%29% ••
6	F	474	24%41%17%41% •
7	G	401	10%44%26%29% •
8	H	612	31%27%14%59%
9	I	50	20%14%66% •
10	K	20	10%20%30%50%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 21222 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	437	Total	C	N	O	S	0	0
			3564	2272	619	655	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	319	Total	C	N	O	S	0	0
			2503	1579	446	465	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	328	Total	C	N	O	S	0	0
			2593	1633	452	500	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
			2616	1653	452	501	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	346	Total	C	N	O	S	0	0
			2732	1729	475	510	18		

- Molecule 6 is a protein called DNA damage checkpoint control protein MEC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	278	Total	C	N	O	S	0	0
			2240	1439	386	396	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	285	Total	C	N	O	S	0	0
			2257	1440	366	439	12		

- Molecule 8 is a protein called DDC1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	249	Total	C	N	O	S	0	0
			2017	1299	332	374	12		

- Molecule 9 is a DNA chain called Template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	17	Total	C	N	O	P	0	0
			344	166	56	105	17		

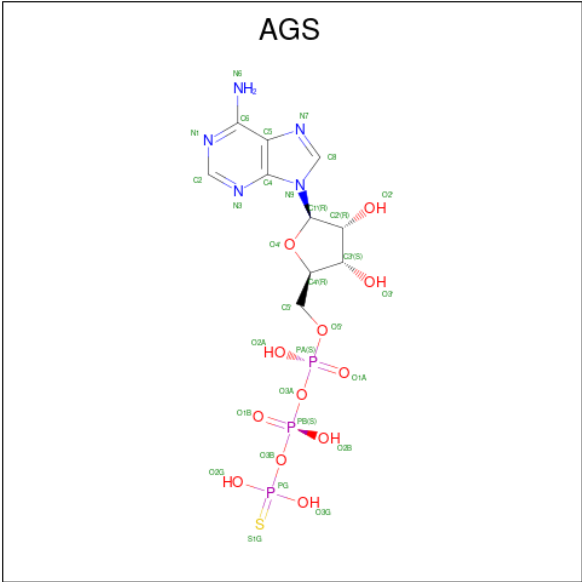
- Molecule 10 is a DNA chain called Primer strand 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	10	Total	C	N	O	P	0	0
			201	98	34	60	9		

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

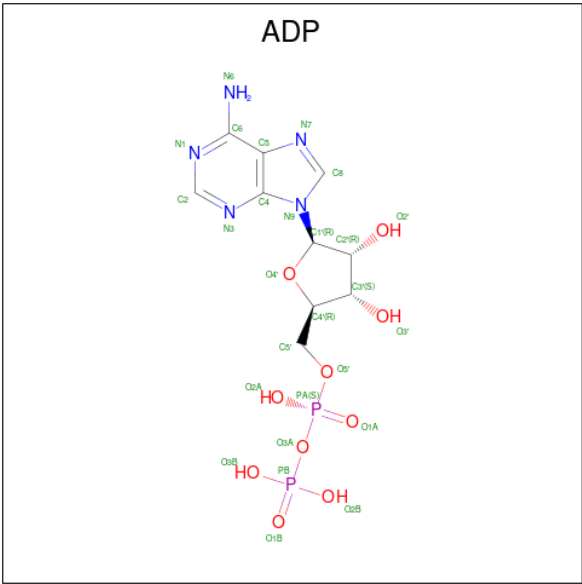
Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	Mg	0
			1	1	
11	B	1	Total	Mg	0
			1	1	
11	C	1	Total	Mg	0
			1	1	
11	D	1	Total	Mg	0
			1	1	

- Molecule 12 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



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

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

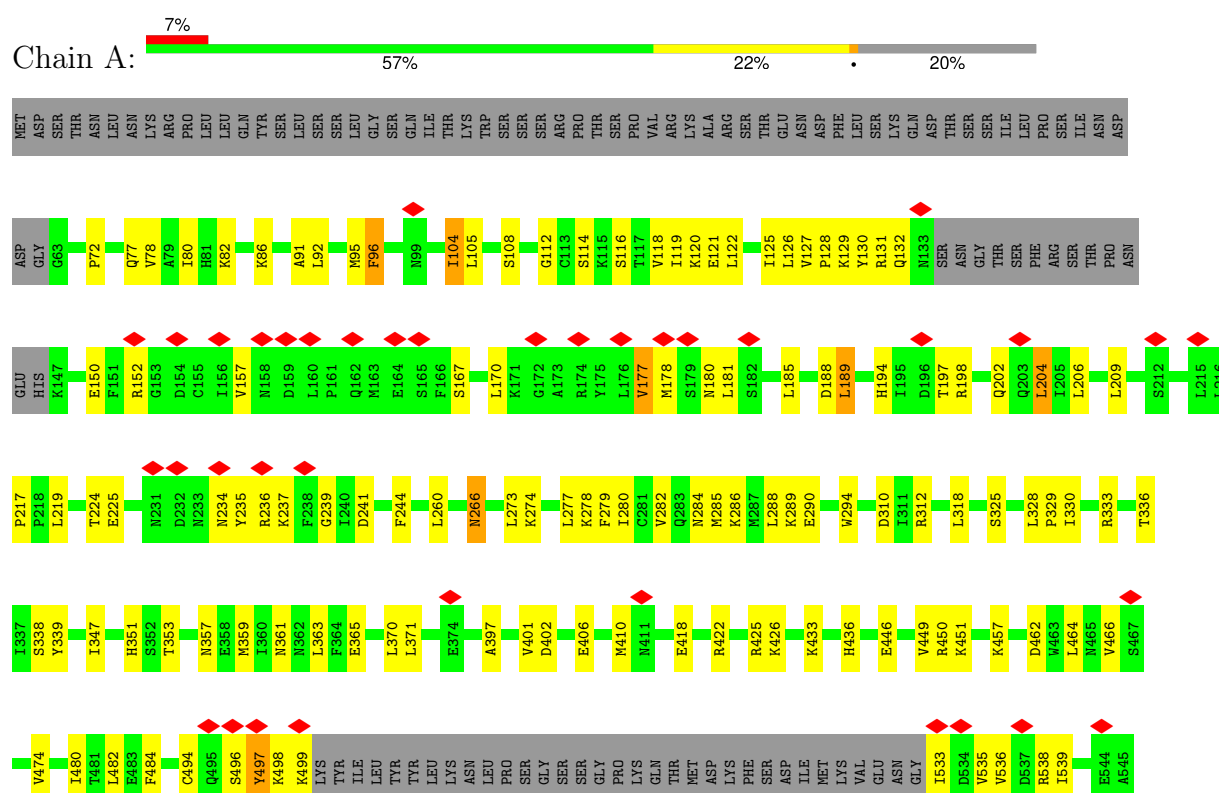


Mol	Chain	Residues	Atoms					AltConf
13	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

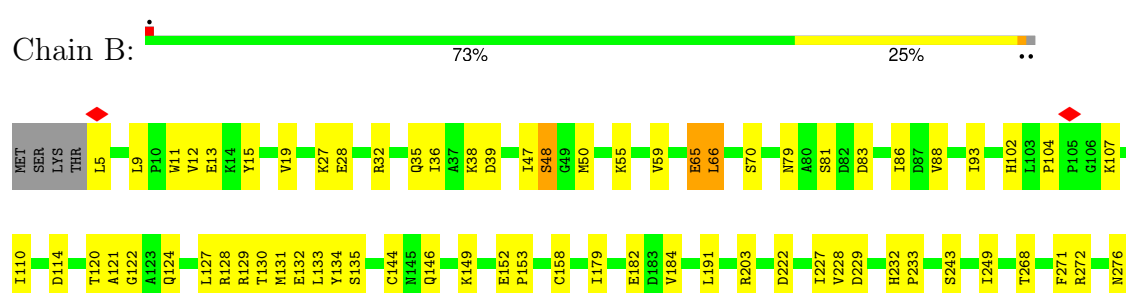
3 Residue-property plots

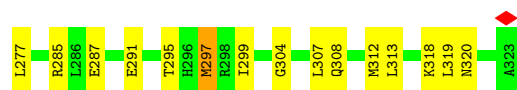
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

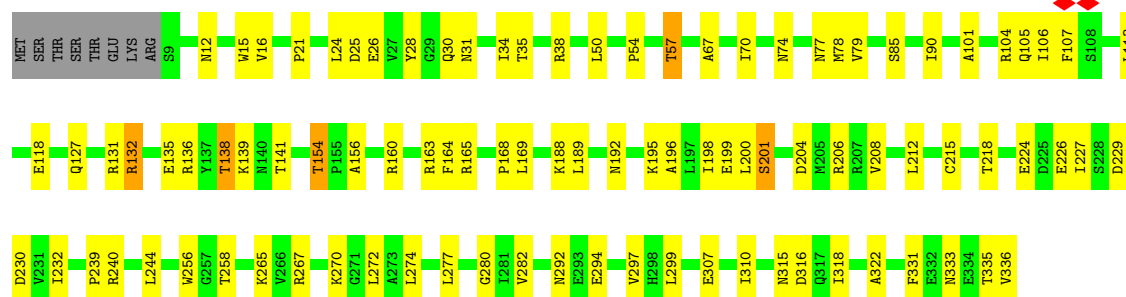


• Molecule 2: Replication factor C subunit 4

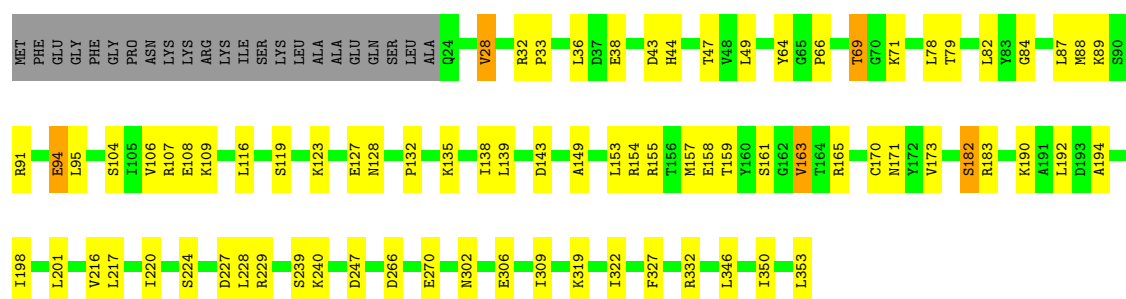




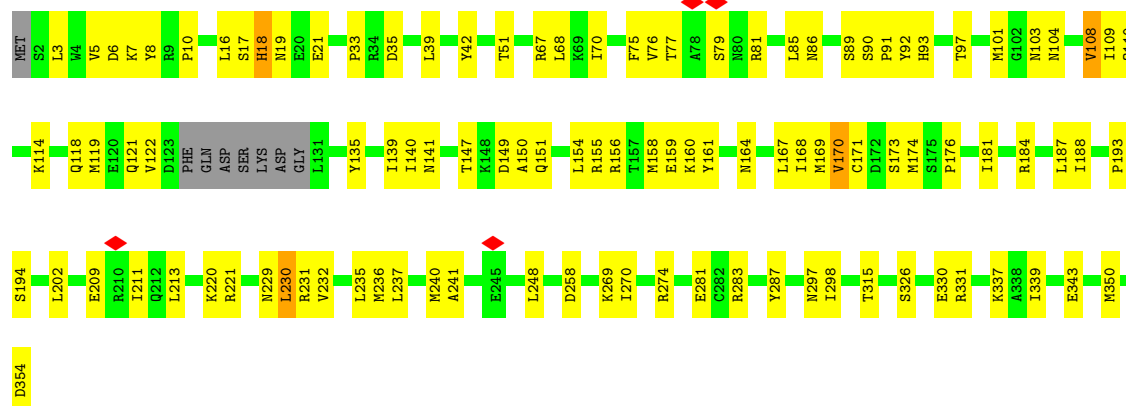
• Molecule 3: Replication factor C subunit 3



• Molecule 4: Replication factor C subunit 2



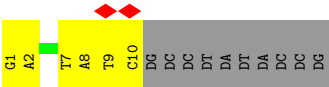
• Molecule 5: Replication factor C subunit 5



• Molecule 6: DNA damage checkpoint control protein MEC3







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	255777	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 ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.012	Depositor
Minimum map value	-1.215	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.16	Depositor
Map size ($\text{\AA}$)	347.76, 347.76, 347.76	wwPDB
Map dimensions	420, 420, 420	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: AGS, MG, 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	0.23	0/3639	0.42	0/4905
2	B	0.17	0/2538	0.35	0/3422
3	C	0.25	0/2633	0.40	0/3562
4	D	0.24	0/2661	0.39	0/3600
5	E	0.18	0/2770	0.35	0/3742
6	F	0.32	0/2278	0.51	0/3068
7	G	0.17	0/2290	0.42	0/3081
8	H	0.25	0/2053	0.41	0/2771
9	I	0.19	0/382	0.43	0/584
10	K	0.20	0/224	0.43	0/344
All	All	0.23	0/21468	0.41	0/29079

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3564	0	3569	85	0
2	B	2503	0	2598	58	0
3	C	2593	0	2623	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2616	0	2648	56	0
5	E	2732	0	2854	67	0
6	F	2240	0	2304	58	0
7	G	2257	0	2262	69	0
8	H	2017	0	2033	60	0
9	I	344	0	196	9	0
10	K	201	0	116	3	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	D	1	0	0	0	0
12	A	31	0	12	2	0
12	B	31	0	12	3	0
12	C	31	0	12	5	0
12	D	31	0	12	5	0
13	E	27	0	12	5	0
All	All	21222	0	21263	496	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 12.

All (496) 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)
8:H:9:GLU:HB2	8:H:12:LYS:HG3	1.59	0.83
7:G:24:ALA:HB1	7:G:60:LEU:HD21	1.62	0.80
8:H:353:PHE:HB3	8:H:360:ILE:HG13	1.63	0.80
6:F:39:SER:HB2	6:F:89:ASN:HB2	1.65	0.78
5:E:17:SER:H	13:E:500:ADP:HN62	1.34	0.75
4:D:116:LEU:HD21	7:G:133:SER:HB3	1.67	0.75
7:G:38:LEU:HB3	7:G:81:LYS:HE3	1.67	0.75
3:C:206:ARG:NH2	12:C:402:AGS:S1G	2.60	0.74
4:D:49:LEU:HB3	4:D:78:LEU:HD13	1.69	0.74
5:E:121:GLN:NE2	6:F:59:THR:O	2.21	0.73
4:D:171:ASN:ND2	12:D:401:AGS:S1G	2.61	0.73
2:B:203:ARG:NH2	12:B:401:AGS:S1G	2.63	0.71
6:F:164:VAL:HG23	6:F:199:LYS:HD3	1.73	0.71
6:F:213:PHE:HD1	6:F:214:ARG:H	1.35	0.71
3:C:104:ARG:NH2	7:G:312:GLU:OE2	2.24	0.71
1:A:132:GLN:OE1	1:A:132:GLN:N	2.19	0.70
1:A:538:ARG:NH1	1:A:539:ILE:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:82:LEU:HD22	4:D:132:PRO:HG2	1.73	0.69
5:E:109:ILE:HG13	5:E:150:ALA:HB1	1.74	0.69
5:E:229:ASN:HB3	5:E:232:VAL:HB	1.75	0.69
4:D:229:ARG:NH1	5:E:159:GLU:OE2	2.26	0.69
1:A:312:ARG:NH2	12:A:602:AGS:S1G	2.66	0.68
5:E:193:PRO:HG2	5:E:230:LEU:HD23	1.74	0.68
7:G:195:ILE:HG21	7:G:324:ILE:HD12	1.76	0.67
6:F:429:VAL:HB	6:F:441:HIS:HB3	1.76	0.67
3:C:21:PRO:HB3	3:C:26:GLU:HB3	1.75	0.66
2:B:13:GLU:HG3	3:C:138:THR:HG21	1.77	0.66
4:D:43:ASP:O	4:D:47:THR:HG23	1.94	0.66
2:B:299:ILE:HD13	2:B:304:GLY:HA2	1.77	0.66
3:C:230:ASP:OD1	3:C:240:ARG:NH1	2.28	0.66
8:H:241:LEU:HD13	8:H:330:LYS:HA	1.78	0.66
1:A:339:TYR:HA	1:A:370:LEU:HD21	1.78	0.66
8:H:22:VAL:HG22	8:H:331:ASN:HB3	1.77	0.66
2:B:308:GLN:NE2	3:C:307:GLU:OE1	2.29	0.66
3:C:78:MET:HE1	3:C:105:GLN:HB3	1.77	0.66
6:F:8:ASN:HB3	6:F:11:GLU:HG2	1.77	0.66
5:E:70:ILE:HD11	5:E:86:ASN:HB3	1.77	0.66
6:F:92:THR:HG23	6:F:212:LEU:HB2	1.77	0.65
4:D:161:SER:O	4:D:165:ARG:NH1	2.29	0.65
5:E:85:LEU:HB2	5:E:101:MET:HE3	1.77	0.65
8:H:19:ALA:O	8:H:23:LEU:HD12	1.96	0.65
8:H:361:LEU:HD22	8:H:362:MET:H	1.62	0.65
8:H:249:THR:HG21	8:H:326:LEU:HD13	1.78	0.65
1:A:312:ARG:NH1	2:B:132:GLU:OE2	2.29	0.65
5:E:68:LEU:HD23	5:E:90:SER:HB3	1.78	0.64
7:G:245:ILE:HG22	7:G:308:VAL:HG11	1.80	0.64
8:H:362:MET:HB2	8:H:373:LEU:HB3	1.80	0.64
4:D:36:LEU:HD11	4:D:78:LEU:HD12	1.79	0.63
4:D:155:ARG:NH1	4:D:158:GLU:OE1	2.29	0.63
6:F:228:ILE:HG13	6:F:229:GLN:HG2	1.80	0.63
7:G:190:ASN:HB2	7:G:217:LEU:HD23	1.80	0.63
2:B:79:ASN:HB2	3:C:132:ARG:HG3	1.80	0.63
7:G:221:ASP:HB2	7:G:228:ILE:HG12	1.80	0.63
1:A:418:GLU:OE1	1:A:422:ARG:NH1	2.32	0.63
3:C:299:LEU:HD11	3:C:331:PHE:HE1	1.63	0.63
4:D:28:VAL:HG11	4:D:229:ARG:HG3	1.81	0.63
7:G:50:ARG:HH21	7:G:86:ILE:HG21	1.64	0.63
6:F:84:SER:HB3	6:F:91:ILE:HD11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:171:LYS:HD3	7:G:246:ARG:HH22	1.64	0.62
1:A:328:LEU:HD23	1:A:329:PRO:HD2	1.81	0.62
1:A:114:SER:O	1:A:114:SER:OG	2.18	0.62
7:G:38:LEU:HB3	7:G:81:LYS:CE	2.30	0.61
4:D:91:ARG:NH1	4:D:119:SER:O	2.33	0.61
7:G:179:TYR:N	7:G:195:ILE:O	2.34	0.61
1:A:188:ASP:OD1	2:B:128:ARG:NH2	2.32	0.61
6:F:87:GLU:OE2	6:F:214:ARG:NH2	2.33	0.61
8:H:241:LEU:HD11	8:H:329:PHE:CD2	2.36	0.61
7:G:216:LYS:HZ3	7:G:218:GLN:HG3	1.66	0.60
1:A:235:TYR:HB2	1:A:241:ASP:OD2	2.00	0.60
6:F:30:ARG:NH2	6:F:66:GLY:O	2.34	0.60
1:A:357:ASN:OD1	1:A:422:ARG:NH2	2.35	0.60
1:A:122:LEU:O	1:A:126:LEU:HB2	2.01	0.60
1:A:494:CYS:HA	1:A:497:TYR:CD2	2.37	0.60
6:F:110:VAL:HG13	6:F:162:GLU:HG2	1.84	0.60
8:H:329:PHE:HE1	8:H:362:MET:HE1	1.67	0.59
8:H:359:PRO:HA	8:H:376:VAL:HA	1.84	0.59
1:A:361:ASN:O	1:A:365:GLU:HG3	2.02	0.59
5:E:114:LYS:O	5:E:118:GLN:HG3	2.01	0.59
2:B:86:ILE:HD11	2:B:122:GLY:HA3	1.84	0.59
1:A:170:LEU:HD12	1:A:204:LEU:HG	1.85	0.59
2:B:229:ASP:OD2	3:C:165:ARG:NH1	2.36	0.59
4:D:194:ALA:O	4:D:198:ILE:HB	2.02	0.59
2:B:32:ARG:O	2:B:36:ILE:HG13	2.03	0.58
3:C:192:ASN:OD1	3:C:195:LYS:NZ	2.36	0.58
8:H:356:PRO:HB2	8:H:379:SER:HA	1.85	0.58
1:A:116:SER:O	1:A:120:LYS:HG2	2.03	0.58
8:H:55:ARG:HB3	8:H:370:LYS:HB3	1.84	0.58
4:D:192:LEU:HD12	4:D:228:LEU:HB2	1.85	0.58
1:A:285:MET:O	1:A:289:LYS:N	2.25	0.58
4:D:201:LEU:HG	4:D:217:LEU:HD22	1.85	0.57
2:B:50:MET:O	2:B:55:LYS:NZ	2.37	0.57
6:F:38:ASN:OD1	6:F:39:SER:N	2.37	0.57
1:A:237:LYS:HG3	1:A:239:GLY:H	1.68	0.57
12:C:402:AGS:S1G	4:D:183:ARG:NH1	2.73	0.57
3:C:50:LEU:HD23	3:C:163:ARG:HG3	1.85	0.57
7:G:215:GLU:OE1	7:G:254:LYS:NZ	2.31	0.57
8:H:108:PRO:HG2	8:H:140:MET:HE3	1.84	0.57
8:H:352:TRP:CZ2	8:H:361:LEU:HG	2.39	0.57
1:A:266:ASN:N	1:A:266:ASN:OD1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:39:LEU:HD22	5:E:188:ILE:HD11	1.87	0.57
5:E:119:MET:O	5:E:164:ASN:ND2	2.37	0.57
6:F:213:PHE:CD1	6:F:214:ARG:N	2.70	0.57
7:G:49:VAL:HG22	7:G:59:GLN:HG3	1.87	0.57
5:E:236:MET:O	5:E:240:MET:HG3	2.04	0.57
1:A:533:ILE:O	1:A:535:VAL:N	2.38	0.57
6:F:19:LEU:O	6:F:23:ILE:HG12	2.05	0.57
8:H:134:LEU:HB3	8:H:150:PRO:HG2	1.87	0.56
1:A:497:TYR:CE1	1:A:498:LYS:HG3	2.39	0.56
5:E:283:ARG:NH1	5:E:343:GLU:OE1	2.37	0.56
2:B:86:ILE:HD12	9:I:32:DC:H5"	1.85	0.56
2:B:277:LEU:O	2:B:285:ARG:NH1	2.32	0.56
7:G:213:ILE:HD11	8:H:142:SER:HB2	1.88	0.56
1:A:198:ARG:O	1:A:202:GLN:HG2	2.05	0.56
5:E:154:LEU:O	5:E:158:MET:HG2	2.06	0.56
6:F:71:THR:HB	6:F:463:GLN:HG2	1.88	0.56
7:G:151:ARG:HG2	7:G:223:ASP:H	1.71	0.56
4:D:49:LEU:HB3	4:D:78:LEU:CD1	2.35	0.55
3:C:299:LEU:HD11	3:C:331:PHE:CE1	2.41	0.55
5:E:33:PRO:O	5:E:135:TYR:OH	2.24	0.55
6:F:231:MET:HE2	6:F:406:HIS:ND1	2.20	0.55
7:G:89:ILE:O	7:G:93:VAL:HG23	2.07	0.55
4:D:346:LEU:O	4:D:350:ILE:HG13	2.06	0.55
3:C:135:GLU:HG2	3:C:160:ARG:HE	1.71	0.55
4:D:107:ARG:NH2	9:I:29:DT:OP1	2.39	0.55
4:D:224:SER:OG	4:D:227:ASP:O	2.21	0.55
5:E:258:ASP:N	5:E:258:ASP:OD1	2.35	0.55
7:G:15:THR:HB	7:G:67:PHE:HD1	1.71	0.55
1:A:128:PRO:HA	1:A:131:ARG:HD3	1.89	0.55
7:G:32:GLY:O	7:G:50:ARG:NH2	2.40	0.55
1:A:333:ARG:NH1	2:B:152:GLU:OE1	2.39	0.55
6:F:39:SER:HA	6:F:82:VAL:HB	1.87	0.55
7:G:158:ILE:HD13	7:G:207:LEU:HD22	1.88	0.55
8:H:231:CYS:HB3	8:H:295:HIS:HB2	1.89	0.55
3:C:188:LYS:NZ	3:C:224:GLU:O	2.31	0.55
5:E:202:LEU:HD22	5:E:237:LEU:HD22	1.88	0.55
2:B:287:GLU:HB2	2:B:319:LEU:HD13	1.90	0.54
7:G:25:LEU:HA	7:G:28:LEU:HD12	1.89	0.54
8:H:329:PHE:CE1	8:H:362:MET:HE1	2.41	0.54
12:D:401:AGS:O3G	12:D:401:AGS:O2B	2.26	0.54
1:A:234:ASN:ND2	9:I:30:DT:O2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:VAL:O	12:B:401:AGS:O3'	2.20	0.54
4:D:332:ARG:HD3	5:E:330:GLU:HB2	1.89	0.54
8:H:140:MET:HE1	8:H:146:LYS:HE3	1.90	0.54
1:A:480:ILE:HA	1:A:484:PHE:HB2	1.89	0.54
7:G:181:TYR:CE2	7:G:328:MET:HG2	2.43	0.54
5:E:173:SER:O	5:E:176:PRO:HD2	2.08	0.54
5:E:231:ARG:HB2	13:E:500:ADP:H5'1	1.90	0.53
6:F:15:ASP:OD1	6:F:16:TYR:N	2.41	0.53
6:F:125:SER:HA	6:F:155:ALA:HB3	1.90	0.53
7:G:58:ILE:HG13	7:G:308:VAL:HG22	1.90	0.53
2:B:146:GLN:OE1	2:B:149:LYS:NZ	2.36	0.53
4:D:127:GLU:HG3	4:D:128:ASN:OD1	2.08	0.53
5:E:241:ALA:HA	5:E:248:LEU:HD21	1.90	0.53
6:F:3:LEU:HB3	6:F:123:LEU:HB2	1.90	0.53
4:D:319:LYS:HA	4:D:322:ILE:HG22	1.91	0.53
2:B:93:ILE:HG22	2:B:130:THR:HG21	1.89	0.53
4:D:104:SER:O	4:D:108:GLU:HG2	2.09	0.53
1:A:131:ARG:HG3	1:A:181:LEU:HB3	1.91	0.53
2:B:104:PRO:HB2	2:B:107:LYS:HD3	1.91	0.52
2:B:249:ILE:HD13	2:B:313:LEU:HD12	1.89	0.52
7:G:103:ILE:HG23	7:G:105:GLU:H	1.74	0.52
4:D:240:LYS:NZ	5:E:35:ASP:OD2	2.42	0.52
1:A:167:SER:HA	1:A:204:LEU:HD21	1.92	0.52
6:F:4:LYS:HG3	6:F:122:LYS:HG2	1.91	0.52
7:G:53:ASN:HB2	7:G:55:VAL:HG22	1.92	0.52
2:B:287:GLU:O	2:B:291:GLU:HG2	2.10	0.52
1:A:127:VAL:HG12	1:A:131:ARG:HD2	1.92	0.52
7:G:320:ALA:O	7:G:324:ILE:HG12	2.10	0.52
7:G:256:LEU:HB3	7:G:268:ASN:HB2	1.91	0.52
8:H:96:VAL:HG11	8:H:101:LEU:HD22	1.91	0.52
2:B:65:GLU:N	2:B:65:GLU:OE1	2.43	0.51
3:C:189:LEU:HD12	3:C:227:ILE:HB	1.92	0.51
6:F:18:LEU:HD22	6:F:444:LEU:HD23	1.93	0.51
4:D:309:ILE:O	4:D:319:LYS:NZ	2.44	0.51
6:F:156:LEU:HB2	6:F:207:VAL:HG13	1.93	0.51
6:F:23:ILE:HG13	6:F:104:PHE:CD2	2.45	0.51
4:D:32:ARG:NH1	12:D:401:AGS:O2A	2.40	0.51
8:H:7:ILE:HD11	8:H:13:GLN:HG2	1.93	0.51
2:B:227:ILE:HD11	3:C:164:PHE:HE1	1.76	0.51
7:G:260:ASP:OD1	7:G:262:HIS:N	2.43	0.51
8:H:361:LEU:HD13	8:H:362:MET:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLU:OE1	1:A:152:ARG:NH2	2.41	0.51
2:B:232:HIS:ND1	2:B:233:PRO:HD3	2.26	0.51
1:A:177:VAL:HG13	1:A:217:PRO:HD3	1.93	0.50
2:B:79:ASN:HD22	3:C:132:ARG:HB3	1.77	0.50
3:C:156:ALA:HB1	3:C:160:ARG:HH12	1.75	0.50
12:B:401:AGS:O1B	12:B:401:AGS:O2G	2.29	0.50
5:E:77:THR:HG22	5:E:81:ARG:H	1.77	0.50
3:C:90:ILE:HG21	9:I:30:DT:H3'	1.93	0.50
7:G:200:LEU:HD21	8:H:100:HIS:HB3	1.93	0.50
9:I:13:DT:H2''	9:I:14:DA:C8	2.46	0.50
6:F:48:PRO:HD2	6:F:67:GLN:HG2	1.93	0.50
7:G:170:LEU:HD11	7:G:196:SER:HB3	1.94	0.50
1:A:108:SER:OG	1:A:225:GLU:OE2	2.29	0.49
3:C:79:VAL:HG22	3:C:113:LEU:HB3	1.94	0.49
1:A:104:ILE:HD11	1:A:260:LEU:HD12	1.93	0.49
1:A:132:GLN:HE21	1:A:178:MET:HA	1.77	0.49
1:A:353:THR:O	1:A:353:THR:OG1	2.29	0.49
4:D:108:GLU:HG3	4:D:109:LYS:N	2.27	0.49
7:G:163:LEU:HD21	7:G:257:PHE:HE1	1.76	0.49
8:H:3:PHE:HB2	8:H:34:VAL:HG11	1.94	0.49
7:G:62:LEU:HB3	7:G:66:LEU:HD13	1.94	0.49
3:C:101:ALA:HB1	3:C:141:THR:HG21	1.95	0.49
4:D:153:LEU:O	4:D:157:MET:HG3	2.12	0.49
1:A:496:SER:HA	1:A:499:LYS:HG3	1.95	0.49
2:B:318:LYS:HG3	3:C:297:VAL:HG11	1.93	0.49
4:D:217:LEU:HD23	4:D:220:ILE:HD12	1.95	0.49
6:F:232:MET:N	6:F:232:MET:SD	2.86	0.49
6:F:408:VAL:HG11	6:F:432:ILE:HD12	1.94	0.49
1:A:418:GLU:HG3	2:B:271:PHE:HZ	1.77	0.49
7:G:152:ILE:H	7:G:224:SER:HB3	1.76	0.49
3:C:127:GLN:OE1	3:C:154:THR:OG1	2.30	0.49
6:F:19:LEU:HG	6:F:104:PHE:CZ	2.48	0.49
12:A:602:AGS:O1B	12:A:602:AGS:O2A	2.30	0.49
2:B:5:LEU:HB2	3:C:70:ILE:HG23	1.94	0.49
3:C:204:ASP:OD2	4:D:182:SER:OG	2.30	0.49
8:H:36:THR:O	8:H:58:LYS:NZ	2.44	0.49
8:H:5:ALA:HB1	8:H:61:PHE:CD1	2.48	0.48
8:H:44:MET:HG2	8:H:51:LEU:HD23	1.95	0.48
3:C:335:THR:O	3:C:336:VAL:C	2.56	0.48
7:G:74:ASN:ND2	7:G:77:GLU:OE1	2.37	0.48
1:A:234:ASN:OD1	1:A:236:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:156:ALA:O	3:C:160:ARG:HG2	2.13	0.48
3:C:201:SER:HB3	3:C:208:VAL:HG23	1.94	0.48
6:F:37:PHE:N	6:F:91:ILE:O	2.46	0.48
1:A:78:VAL:HG11	1:A:118:VAL:HG22	1.95	0.48
1:A:363:LEU:HG	1:A:371:LEU:HD11	1.95	0.48
1:A:121:GLU:O	1:A:125:ILE:HG12	2.12	0.48
7:G:156:ALA:HB2	7:G:217:LEU:HD13	1.96	0.48
7:G:185:GLU:OE1	7:G:186:ALA:N	2.46	0.48
4:D:89:LYS:O	4:D:89:LYS:NZ	2.41	0.48
5:E:269:LYS:NZ	5:E:281:GLU:OE1	2.46	0.48
8:H:270:VAL:HG13	8:H:278:LEU:HB2	1.95	0.48
8:H:273:LYS:HG2	8:H:274:ASN:OD1	2.14	0.48
1:A:194:HIS:HB3	1:A:197:THR:HG22	1.95	0.48
8:H:354:CYS:SG	8:H:355:HIS:HD2	2.36	0.48
6:F:154:CYS:SG	6:F:155:ALA:N	2.85	0.48
7:G:155:GLU:CD	7:G:216:LYS:HZ1	2.22	0.48
7:G:204:LYS:HE2	7:G:328:MET:SD	2.54	0.48
1:A:347:ILE:O	1:A:425:ARG:NH2	2.27	0.48
3:C:196:ALA:O	3:C:200:LEU:HG	2.13	0.48
4:D:155:ARG:O	4:D:159:THR:HG22	2.14	0.48
3:C:54:PRO:HG2	3:C:168:PRO:HG3	1.96	0.47
5:E:10:PRO:HD2	5:E:51:THR:HG21	1.96	0.47
3:C:198:ILE:O	3:C:201:SER:OG	2.31	0.47
6:F:42:LEU:HD23	6:F:72:ILE:HD11	1.95	0.47
1:A:82:LYS:HD2	1:A:86:LYS:HE3	1.97	0.47
3:C:31:ASN:O	3:C:35:THR:OG1	2.27	0.47
7:G:41:ILE:HB	7:G:80:MET:HB2	1.97	0.47
7:G:304:ILE:HD12	7:G:304:ILE:O	2.15	0.47
1:A:80:ILE:HD12	1:A:118:VAL:HG21	1.96	0.47
3:C:77:ASN:OD1	3:C:106:ILE:HG21	2.15	0.47
1:A:224:THR:HG21	2:B:153:PRO:HG3	1.96	0.47
1:A:286:LYS:O	1:A:290:GLU:N	2.45	0.47
1:A:446:GLU:O	1:A:450:ARG:HG2	2.13	0.47
4:D:84:GLY:O	4:D:88:MET:HB2	2.15	0.47
4:D:106:VAL:HG21	4:D:149:ALA:HB1	1.97	0.47
6:F:103:VAL:HG21	6:F:158:ILE:HD13	1.96	0.47
8:H:271:TYR:HA	8:H:276:ASP:O	2.14	0.47
3:C:90:ILE:N	9:I:30:DT:OP1	2.43	0.47
5:E:97:THR:HG22	5:E:141:ASN:HB2	1.96	0.47
7:G:43:ALA:O	7:G:64:ARG:NH1	2.46	0.47
1:A:484:PHE:CZ	5:E:231:ARG:HD3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:67:ARG:HA	5:E:67:ARG:NE	2.29	0.47
5:E:213:LEU:HD12	5:E:248:LEU:HD12	1.97	0.47
7:G:74:ASN:HD22	7:G:80:MET:HE2	1.79	0.47
7:G:162:ALA:HB2	7:G:213:ILE:HD13	1.96	0.47
8:H:352:TRP:CD1	8:H:352:TRP:C	2.92	0.47
3:C:118:GLU:HG2	4:D:154:ARG:CZ	2.44	0.47
3:C:229:ASP:OD1	3:C:229:ASP:N	2.45	0.47
7:G:310:MET:HE3	7:G:310:MET:HB2	1.75	0.47
3:C:25:ASP:OD1	3:C:38:ARG:NH2	2.46	0.46
3:C:244:LEU:HD23	3:C:277:LEU:HD23	1.96	0.46
4:D:143:ASP:OD1	4:D:143:ASP:N	2.47	0.46
7:G:20:HIS:ND1	7:G:66:LEU:HD21	2.30	0.46
7:G:42:ASP:O	7:G:70:TYR:OH	2.22	0.46
3:C:322:ALA:HB2	4:D:327:PHE:HB2	1.97	0.46
4:D:108:GLU:HG3	4:D:109:LYS:H	1.80	0.46
7:G:237:PHE:CE1	7:G:312:GLU:HB2	2.50	0.46
8:H:249:THR:HG21	8:H:265:ALA:HB1	1.97	0.46
4:D:155:ARG:HD2	4:D:155:ARG:HA	1.72	0.46
4:D:82:LEU:HD22	4:D:132:PRO:CG	2.45	0.46
8:H:35:THR:HG22	8:H:37:ASN:H	1.79	0.46
4:D:135:LYS:NZ	4:D:163:VAL:HG13	2.31	0.46
2:B:47:ILE:HD12	2:B:59:VAL:HG22	1.98	0.46
8:H:323:ILE:HB	8:H:378:ASP:HB3	1.97	0.46
1:A:433:LYS:H	1:A:436:HIS:CD2	2.34	0.46
4:D:87:LEU:HG	4:D:91:ARG:HG3	1.98	0.46
8:H:228:ASN:O	8:H:352:TRP:HA	2.16	0.46
8:H:351:LEU:HD12	8:H:351:LEU:N	2.30	0.46
1:A:95:MET:SD	1:A:105:LEU:HB2	2.56	0.46
4:D:95:LEU:HB2	4:D:139:LEU:HD23	1.98	0.46
7:G:247:LYS:HA	7:G:247:LYS:HD3	1.60	0.46
1:A:451:LYS:HE2	1:A:451:LYS:HA	1.98	0.46
2:B:83:ASP:O	2:B:88:VAL:HG11	2.16	0.46
3:C:106:ILE:HG23	3:C:107:PHE:HD1	1.80	0.46
3:C:315:ASN:HB3	3:C:318:ILE:HB	1.97	0.46
8:H:354:CYS:O	8:H:355:HIS:HB2	2.16	0.46
1:A:397:ALA:O	1:A:401:VAL:HG23	2.16	0.45
12:C:402:AGS:O2B	12:C:402:AGS:O1A	2.34	0.45
5:E:140:ILE:HB	5:E:169:MET:HB3	1.98	0.45
5:E:209:GLU:HB3	5:E:211:ILE:CD1	2.46	0.45
6:F:23:ILE:HG22	6:F:101:LEU:HD13	1.98	0.45
2:B:268:THR:O	2:B:272:ARG:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:34:LYS:HE3	7:G:34:LYS:HA	1.96	0.45
7:G:81:LYS:HD2	7:G:82:LEU:N	2.30	0.45
9:I:15:DC:H2"	9:I:16:DG:H8	1.82	0.45
4:D:64:TYR:HA	4:D:170:CYS:O	2.17	0.45
6:F:8:ASN:HB2	6:F:118:ASN:ND2	2.31	0.45
8:H:237:LEU:HD21	8:H:329:PHE:HZ	1.82	0.45
5:E:274:ARG:HE	5:E:354:ASP:HB3	1.81	0.45
1:A:402:ASP:OD1	5:E:331:ARG:NH1	2.49	0.45
2:B:28:GLU:CD	2:B:28:GLU:H	2.25	0.45
4:D:66:PRO:HD2	4:D:69:THR:HG21	1.98	0.45
7:G:35:ASP:O	7:G:86:ILE:HG22	2.17	0.45
1:A:178:MET:C	1:A:180:ASN:H	2.23	0.45
1:A:206:LEU:HD12	1:A:206:LEU:HA	1.87	0.45
3:C:267:ARG:NH1	3:C:316:ASP:OD1	2.49	0.45
4:D:190:LYS:H	4:D:190:LYS:HG2	1.63	0.45
7:G:119:LEU:HD12	7:G:132:TYR:HE2	1.82	0.45
2:B:121:ALA:HA	2:B:124:GLN:HG3	1.97	0.45
5:E:42:TYR:HA	5:E:171:CYS:O	2.17	0.45
8:H:361:LEU:HD22	8:H:362:MET:N	2.31	0.45
2:B:79:ASN:ND2	2:B:81:SER:OG	2.50	0.45
5:E:110:GLN:O	5:E:114:LYS:HB2	2.16	0.45
1:A:284:ASN:O	1:A:288:LEU:HB2	2.17	0.45
1:A:410:MET:HA	2:B:297:MET:SD	2.57	0.45
2:B:27:LYS:HA	2:B:27:LYS:HD3	1.63	0.45
4:D:266:ASP:O	4:D:270:GLU:HG3	2.17	0.45
7:G:154:PHE:HB2	7:G:219:VAL:HG22	1.99	0.45
2:B:179:ILE:HD11	2:B:191:LEU:HD21	1.99	0.44
3:C:28:TYR:O	12:C:402:AGS:N6	2.50	0.44
5:E:5:VAL:HG23	5:E:6:ASP:OD1	2.17	0.44
6:F:107:TYR:HD1	6:F:160:PHE:CD2	2.35	0.44
7:G:98:ARG:HG2	7:G:102:ASP:HB2	1.99	0.44
3:C:265:LYS:HE3	3:C:265:LYS:HB3	1.82	0.44
1:A:104:ILE:HB	1:A:219:LEU:HB3	1.98	0.44
1:A:112:GLY:HA3	1:A:310:ASP:OD1	2.17	0.44
6:F:65:THR:HG21	6:F:469:ALA:HB3	1.99	0.44
8:H:4:LYS:HB3	8:H:65:GLU:HG3	2.00	0.44
1:A:92:LEU:HD23	1:A:92:LEU:HA	1.76	0.44
2:B:11:TRP:CZ2	2:B:182:GLU:HG2	2.53	0.44
5:E:3:LEU:HD13	5:E:235:LEU:HD21	2.00	0.44
1:A:96:PHE:HZ	1:A:127:VAL:HG22	1.82	0.44
3:C:67:ALA:HB1	3:C:79:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:235:LEU:HD23	5:E:235:LEU:HA	1.83	0.44
6:F:154:CYS:HB2	6:F:211:LEU:HD11	2.00	0.44
10:K:9:DT:H2"	10:K:10:DC:C6	2.53	0.44
1:A:359:MET:HE3	1:A:359:MET:HB3	1.77	0.44
5:E:160:LYS:HD3	5:E:161:TYR:CE2	2.53	0.44
8:H:33:THR:HA	8:H:93:SER:HA	1.99	0.44
8:H:340:LYS:HD2	8:H:340:LYS:HA	1.75	0.44
3:C:156:ALA:HB1	3:C:160:ARG:NH1	2.32	0.44
4:D:94:GLU:HG2	4:D:138:ILE:HB	2.00	0.44
6:F:93:MET:HE1	6:F:156:LEU:HD11	1.99	0.44
1:A:189:LEU:HD23	1:A:244:PHE:HZ	1.83	0.44
1:A:402:ASP:O	1:A:406:GLU:HG3	2.18	0.44
1:A:426:LYS:HE3	1:A:426:LYS:HB3	1.81	0.44
3:C:274:LEU:HD23	3:C:310:ILE:HD11	2.00	0.44
2:B:15:TYR:OH	2:B:182:GLU:OE1	2.36	0.43
7:G:148:ASP:OD1	7:G:148:ASP:N	2.50	0.43
7:G:314:GLU:OE1	7:G:316:ILE:HG12	2.18	0.43
8:H:109:ASP:OD1	8:H:109:ASP:N	2.48	0.43
2:B:66:LEU:HD22	2:B:110:ILE:HD11	2.00	0.43
7:G:18:LEU:H	7:G:18:LEU:HD23	1.83	0.43
7:G:208:PRO:HG3	8:H:143:LEU:C	2.43	0.43
4:D:216:VAL:O	4:D:217:LEU:HB2	2.19	0.43
9:I:29:DT:H5'	9:I:29:DT:C6	2.53	0.43
10:K:1:DG:H2"	10:K:2:DA:C8	2.54	0.43
1:A:96:PHE:CZ	1:A:127:VAL:HG22	2.53	0.43
5:E:90:SER:OG	5:E:93:HIS:ND1	2.51	0.43
13:E:500:ADP:HO3'	13:E:500:ADP:HO2'	1.63	0.43
7:G:151:ARG:HD2	7:G:261:VAL:HG11	2.00	0.43
8:H:245:ASN:HB3	8:H:248:VAL:HG22	1.99	0.43
1:A:114:SER:O	1:A:118:VAL:HG23	2.18	0.43
1:A:170:LEU:HD23	1:A:170:LEU:HA	1.84	0.43
1:A:496:SER:O	1:A:499:LYS:NZ	2.41	0.43
2:B:9:LEU:HD23	2:B:9:LEU:HA	1.90	0.43
2:B:48:SER:HA	2:B:144:CYS:O	2.18	0.43
2:B:79:ASN:N	2:B:79:ASN:OD1	2.51	0.43
5:E:155:ARG:HB2	5:E:184:ARG:CZ	2.49	0.43
5:E:174:MET:HE1	5:E:187:LEU:HD13	2.01	0.43
1:A:91:ALA:O	1:A:95:MET:HE3	2.19	0.43
3:C:30:GLN:NE2	3:C:57:THR:O	2.50	0.43
4:D:44:HIS:CE1	4:D:190:LYS:HE3	2.54	0.43
4:D:302:ASN:O	4:D:306:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:141:ASN:HA	5:E:170:VAL:HG22	2.01	0.43
6:F:4:LYS:HD2	6:F:122:LYS:HE3	2.00	0.43
7:G:68:MET:H	7:G:68:MET:HG2	1.63	0.43
7:G:245:ILE:O	7:G:249:THR:HG23	2.17	0.43
7:G:260:ASP:OD1	7:G:260:ASP:C	2.61	0.43
1:A:234:ASN:HB2	9:I:29:DT:O2	2.18	0.43
1:A:279:PHE:HA	1:A:282:VAL:HG22	2.01	0.43
4:D:33:PRO:HB3	4:D:38:GLU:HB2	2.01	0.43
8:H:362:MET:HB3	8:H:362:MET:HE2	1.63	0.43
3:C:74:ASN:O	3:C:78:MET:HB2	2.19	0.43
3:C:215:CYS:SG	3:C:232:ILE:HD13	2.59	0.43
6:F:16:TYR:CE2	6:F:20:ARG:HD2	2.53	0.43
8:H:349:ILE:HD11	8:H:362:MET:CE	2.48	0.43
2:B:19:VAL:HA	2:B:65:GLU:OE2	2.19	0.43
3:C:131:ARG:HB2	3:C:160:ARG:NH1	2.34	0.43
5:E:90:SER:HG	5:E:93:HIS:CE1	2.36	0.43
5:E:147:THR:C	5:E:149:ASP:H	2.26	0.43
1:A:189:LEU:H	1:A:189:LEU:HD22	1.84	0.43
4:D:353:LEU:HD12	4:D:353:LEU:HA	1.84	0.42
6:F:255:ARG:HE	6:F:255:ARG:HB3	1.67	0.42
5:E:151:GLN:HB3	5:E:181:ILE:HG13	2.00	0.42
5:E:220:LYS:HE2	5:E:220:LYS:HB2	1.78	0.42
5:E:270:ILE:HG23	5:E:350:MET:HG3	2.01	0.42
8:H:3:PHE:HD2	8:H:120:VAL:HG12	1.84	0.42
2:B:35:GLN:HA	2:B:38:LYS:HG2	2.00	0.42
2:B:38:LYS:NZ	2:B:39:ASP:OD1	2.52	0.42
6:F:30:ARG:HH21	6:F:64:ASP:CG	2.28	0.42
6:F:107:TYR:HA	6:F:160:PHE:CE2	2.53	0.42
4:D:201:LEU:HD12	4:D:201:LEU:HA	1.82	0.42
12:D:401:AGS:O2G	5:E:184:ARG:NH2	2.53	0.42
5:E:91:PRO:HB2	5:E:92:TYR:CE2	2.54	0.42
8:H:51:LEU:N	8:H:374:VAL:O	2.53	0.42
8:H:152:PHE:CD1	8:H:152:PHE:C	2.97	0.42
2:B:295:THR:OG1	2:B:312:MET:HB2	2.20	0.42
2:B:320:ASN:OD1	2:B:320:ASN:C	2.62	0.42
5:E:7:LYS:HB3	5:E:8:TYR:CE1	2.54	0.42
1:A:338:SER:OG	1:A:339:TYR:N	2.53	0.42
5:E:75:PHE:CZ	5:E:108:VAL:HG22	2.55	0.42
5:E:118:GLN:HG2	5:E:161:TYR:CZ	2.54	0.42
5:E:156:ARG:HA	5:E:156:ARG:HD2	1.91	0.42
3:C:24:LEU:HD22	3:C:34:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:71:LYS:NZ	12:D:401:AGS:S1G	2.85	0.42
5:E:10:PRO:HB2	5:E:16:LEU:HD23	2.01	0.42
5:E:77:THR:HG23	5:E:79:SER:H	1.84	0.42
3:C:244:LEU:HD22	3:C:280:GLY:HA3	2.01	0.42
6:F:425:PHE:HE2	6:F:464:ILE:HD12	1.85	0.42
10:K:7:DT:H2''	10:K:8:DA:C8	2.54	0.42
2:B:307:LEU:HD22	3:C:282:VAL:HG21	2.01	0.42
5:E:139:ILE:HA	5:E:168:ILE:O	2.20	0.42
3:C:188:LYS:HB2	3:C:226:GLU:HA	2.02	0.41
6:F:213:PHE:O	6:F:216:GLN:HG3	2.20	0.41
1:A:132:GLN:H	1:A:132:GLN:CD	2.17	0.41
4:D:123:LYS:O	4:D:127:GLU:HG2	2.19	0.41
6:F:225:ILE:HD12	6:F:225:ILE:O	2.20	0.41
6:F:470:ARG:HD2	6:F:473:GLY:HA2	2.02	0.41
7:G:193:ALA:HA	7:G:206:LYS:HA	2.02	0.41
2:B:9:LEU:HD21	3:C:139:LYS:HA	2.01	0.41
5:E:19:ASN:O	5:E:21:GLU:N	2.51	0.41
1:A:119:ILE:HG21	1:A:185:LEU:HD22	2.01	0.41
1:A:188:ASP:HB2	2:B:129:ARG:HH11	1.84	0.41
5:E:5:VAL:O	13:E:500:ADP:O3'	2.37	0.41
5:E:18:HIS:CD2	5:E:18:HIS:C	2.97	0.41
6:F:2:LYS:HB3	6:F:2:LYS:HE3	1.72	0.41
6:F:264:LEU:HD11	6:F:415:TRP:CZ3	2.56	0.41
1:A:209:LEU:HD23	1:A:209:LEU:HA	1.84	0.41
1:A:449:VAL:HG21	5:E:287:TYR:CD1	2.55	0.41
3:C:292:ASN:C	3:C:294:GLU:H	2.27	0.41
6:F:30:ARG:NH2	6:F:64:ASP:OD1	2.52	0.41
6:F:48:PRO:HB2	6:F:58:GLY:N	2.35	0.41
1:A:241:ASP:OD1	1:A:241:ASP:C	2.63	0.41
8:H:13:GLN:HB3	8:H:107:LYS:NZ	2.35	0.41
8:H:361:LEU:HD13	8:H:361:LEU:C	2.45	0.41
1:A:72:PRO:HB3	1:A:77:GLN:HB3	2.02	0.41
7:G:147:LEU:HD21	7:G:258:ARG:NH2	2.36	0.41
7:G:170:LEU:HD23	7:G:239:PHE:CE1	2.55	0.41
1:A:129:LYS:HD2	1:A:130:TYR:CE1	2.55	0.41
2:B:55:LYS:O	2:B:59:VAL:HG23	2.21	0.41
2:B:131:MET:HE1	2:B:158:CYS:SG	2.61	0.41
6:F:263:HIS:CE1	6:F:265:MET:HG3	2.55	0.41
7:G:257:PHE:CD2	7:G:265:LEU:HD11	2.56	0.41
8:H:12:LYS:HB3	8:H:60:PHE:CZ	2.55	0.41
3:C:15:TRP:CZ3	3:C:212:LEU:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:337:LYS:HE3	5:E:337:LYS:HB3	1.67	0.41
5:E:339:ILE:HD12	5:E:339:ILE:HA	1.95	0.41
6:F:37:PHE:CE1	6:F:42:LEU:HD22	2.56	0.41
6:F:420:LYS:HE3	6:F:420:LYS:HB2	1.81	0.41
2:B:127:LEU:HD23	2:B:127:LEU:HA	1.85	0.41
2:B:133:LEU:HD22	2:B:134:TYR:CZ	2.56	0.41
6:F:253:VAL:HG22	6:F:259:VAL:HG11	2.02	0.41
8:H:45:ASN:ND2	8:H:46:GLU:H	2.19	0.41
8:H:61:PHE:HB2	8:H:64:TYR:HB2	2.03	0.41
8:H:63:GLU:O	8:H:63:GLU:HG3	2.21	0.41
8:H:320:LYS:HA	8:H:320:LYS:HD3	1.80	0.41
1:A:274:LYS:O	1:A:278:LYS:HG3	2.21	0.40
2:B:133:LEU:HD22	2:B:134:TYR:CE1	2.57	0.40
6:F:202:MET:HE2	6:F:202:MET:HB3	1.75	0.40
5:E:287:TYR:CZ	5:E:339:ILE:HG12	2.57	0.40
1:A:277:LEU:HD22	1:A:318:LEU:HD22	2.04	0.40
2:B:102:HIS:ND1	2:B:102:HIS:C	2.80	0.40
3:C:136:ARG:HH11	3:C:136:ARG:HG3	1.86	0.40
3:C:270:LYS:HE2	3:C:272:LEU:HD21	2.04	0.40
6:F:37:PHE:CD1	6:F:42:LEU:HD13	2.57	0.40
7:G:19:GLU:HG2	7:G:20:HIS:N	2.36	0.40
8:H:34:VAL:HG22	8:H:39:LEU:HD13	2.04	0.40
3:C:239:PRO:HB3	3:C:272:LEU:HD13	2.03	0.40
3:C:333:ASN:O	3:C:336:VAL:HB	2.21	0.40
5:E:91:PRO:HB2	5:E:92:TYR:CD2	2.56	0.40
5:E:231:ARG:NH2	13:E:500:ADP:O1B	2.55	0.40
12:C:402:AGS:O1B	12:C:402:AGS:O2G	2.39	0.40
7:G:252:ALA:HB2	7:G:269:ILE:HG23	2.04	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	431/545 (79%)	413 (96%)	18 (4%)	0	100	100
2	B	317/323 (98%)	302 (95%)	15 (5%)	0	100	100
3	C	326/336 (97%)	315 (97%)	11 (3%)	0	100	100
4	D	328/353 (93%)	316 (96%)	12 (4%)	0	100	100
5	E	342/354 (97%)	326 (95%)	16 (5%)	0	100	100
6	F	262/474 (55%)	251 (96%)	11 (4%)	0	100	100
7	G	277/401 (69%)	258 (93%)	19 (7%)	0	100	100
8	H	235/612 (38%)	230 (98%)	5 (2%)	0	100	100
All	All	2518/3398 (74%)	2411 (96%)	107 (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	401/504 (80%)	379 (94%)	22 (6%)	19	41
2	B	279/283 (99%)	266 (95%)	13 (5%)	23	48
3	C	285/293 (97%)	272 (95%)	13 (5%)	24	49
4	D	294/312 (94%)	285 (97%)	9 (3%)	35	60
5	E	317/324 (98%)	301 (95%)	16 (5%)	22	46
6	F	255/424 (60%)	247 (97%)	8 (3%)	35	60
7	G	259/369 (70%)	246 (95%)	13 (5%)	22	46
8	H	234/560 (42%)	228 (97%)	6 (3%)	40	65
All	All	2324/3069 (76%)	2224 (96%)	100 (4%)	27	51

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	PHE
1	A	104	ILE

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Mol	Chain	Res	Type
1	A	157	VAL
1	A	177	VAL
1	A	189	LEU
1	A	204	LEU
1	A	266	ASN
1	A	273	LEU
1	A	280	ILE
1	A	294	TRP
1	A	325	SER
1	A	330	ILE
1	A	336	THR
1	A	351	HIS
1	A	457	LYS
1	A	462	ASP
1	A	464	LEU
1	A	466	VAL
1	A	474	VAL
1	A	482	LEU
1	A	497	TYR
1	A	536	VAL
2	B	48	SER
2	B	65	GLU
2	B	66	LEU
2	B	70	SER
2	B	114	ASP
2	B	120	THR
2	B	135	SER
2	B	184	VAL
2	B	222	ASP
2	B	228	VAL
2	B	243	SER
2	B	276	ASN
2	B	297	MET
3	C	12	ASN
3	C	16	VAL
3	C	57	THR
3	C	85	SER
3	C	132	ARG
3	C	138	THR
3	C	154	THR
3	C	169	LEU
3	C	199	GLU

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Mol	Chain	Res	Type
3	C	201	SER
3	C	218	THR
3	C	256	TRP
3	C	258	THR
4	D	28	VAL
4	D	69	THR
4	D	79	THR
4	D	94	GLU
4	D	163	VAL
4	D	173	VAL
4	D	182	SER
4	D	239	SER
4	D	247	ASP
5	E	18	HIS
5	E	76	VAL
5	E	89	SER
5	E	103	ASN
5	E	104	ASN
5	E	108	VAL
5	E	122	VAL
5	E	167	LEU
5	E	170	VAL
5	E	194	SER
5	E	221	ARG
5	E	230	LEU
5	E	297	ASN
5	E	298	ILE
5	E	315	THR
5	E	326	SER
6	F	59	THR
6	F	104	PHE
6	F	207	VAL
6	F	225	ILE
6	F	286	ASN
6	F	405	THR
6	F	436	GLU
6	F	474	LEU
7	G	12	SER
7	G	21	ILE
7	G	35	ASP
7	G	37	VAL
7	G	60	LEU

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Mol	Chain	Res	Type
7	G	73	ARG
7	G	77	GLU
7	G	89	ILE
7	G	104	VAL
7	G	130	VAL
7	G	173	ILE
7	G	190	ASN
7	G	245	ILE
8	H	50	THR
8	H	144	ILE
8	H	147	GLU
8	H	252	VAL
8	H	258	VAL
8	H	352	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	ASN
1	A	298	GLN
1	A	355	ASN
1	A	438	HIS
1	A	479	ASN
2	B	35	GLN
2	B	79	ASN
2	B	276	ASN
3	C	30	GLN
3	C	291	GLN
3	C	292	ASN
4	D	317	ASN
4	D	321	GLN
4	D	338	ASN
5	E	14	ASN
5	E	277	ASN
6	F	216	GLN
7	G	79	HIS
7	G	113	HIS
7	G	268	ASN
8	H	132	ASN
8	H	355	HIS

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 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$
12	AGS	B	401	11	32,33,33	0.51	0	45,52,52	0.66	1 (2%)
12	AGS	C	402	11	32,33,33	0.52	0	45,52,52	0.73	1 (2%)
13	ADP	E	500	-	28,29,29	1.38	4 (14%)	43,45,45	1.83	8 (18%)
12	AGS	D	401	11	32,33,33	0.54	1 (3%)	45,52,52	0.69	1 (2%)
12	AGS	A	602	11	32,33,33	0.58	1 (3%)	45,52,52	0.71	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
12	AGS	B	401	11	-	6/21/38/38	0/3/3/3
12	AGS	C	402	11	-	7/21/38/38	0/3/3/3
13	ADP	E	500	-	-	4/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	AGS	D	401	11	-	5/21/38/38	0/3/3/3
12	AGS	A	602	11	-	3/21/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E	500	ADP	C5-C4	4.53	1.47	1.39
13	E	500	ADP	C5-C6	2.57	1.48	1.41
13	E	500	ADP	C5-N7	-2.32	1.34	1.39
13	E	500	ADP	C8-N7	2.25	1.36	1.31
12	A	602	AGS	PG-S1G	2.07	1.95	1.90
12	D	401	AGS	PG-S1G	2.02	1.95	1.90

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	E	500	ADP	C5-C4-N3	-5.80	118.73	126.72
13	E	500	ADP	N3-C4-N9	4.62	135.02	127.17
12	C	402	AGS	PB-O3B-PG	-4.06	118.30	133.17
12	A	602	AGS	PB-O3B-PG	-3.73	119.52	133.17
13	E	500	ADP	C2-N3-C4	3.72	120.93	111.83
12	D	401	AGS	PB-O3B-PG	-3.63	119.88	133.17
12	B	401	AGS	PB-O3B-PG	-3.55	120.18	133.17
13	E	500	ADP	C4-C5-N7	-3.41	106.68	110.58
13	E	500	ADP	N3-C2-N1	-3.31	123.57	128.58
13	E	500	ADP	C4-N9-C8	2.70	108.58	105.74
13	E	500	ADP	C5-N7-C8	2.50	107.39	103.45
13	E	500	ADP	C6-C5-N7	2.12	136.18	132.09

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	602	AGS	C5'-O5'-PA-O1A
12	A	602	AGS	C5'-O5'-PA-O3A
12	B	401	AGS	PB-O3B-PG-O2G
12	B	401	AGS	PB-O3B-PG-O3G
12	B	401	AGS	C5'-O5'-PA-O2A
12	B	401	AGS	C5'-O5'-PA-O3A
12	C	402	AGS	PB-O3B-PG-O2G
12	C	402	AGS	C5'-O5'-PA-O2A

Continued on next page...

Continued from previous page...

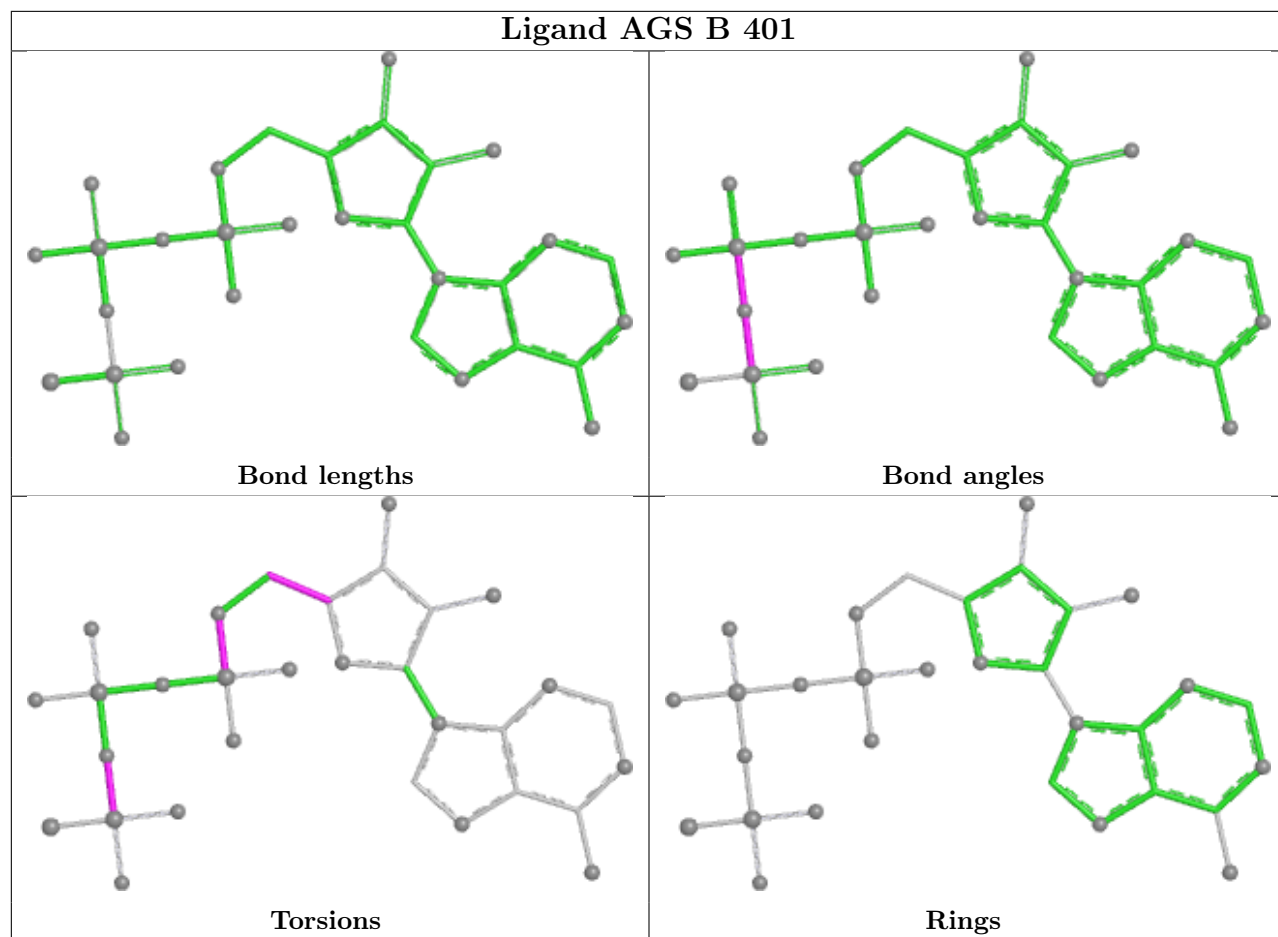
Mol	Chain	Res	Type	Atoms
13	E	500	ADP	C5'-O5'-PA-O1A
13	E	500	ADP	C5'-O5'-PA-O2A
13	E	500	ADP	C5'-O5'-PA-O3A
12	B	401	AGS	O4'-C4'-C5'-O5'
12	B	401	AGS	C3'-C4'-C5'-O5'
12	D	401	AGS	O4'-C4'-C5'-O5'
12	C	402	AGS	O4'-C4'-C5'-O5'
12	D	401	AGS	C3'-C4'-C5'-O5'
12	A	602	AGS	PB-O3A-PA-O2A
12	C	402	AGS	PB-O3A-PA-O1A
13	E	500	ADP	O4'-C4'-C5'-O5'
12	C	402	AGS	C5'-O5'-PA-O1A
12	C	402	AGS	C3'-C4'-C5'-O5'
12	D	401	AGS	PG-O3B-PB-O2B
12	D	401	AGS	PB-O3A-PA-O1A
12	C	402	AGS	PB-O3A-PA-O2A
12	D	401	AGS	PB-O3A-PA-O2A

There are no ring outliers.

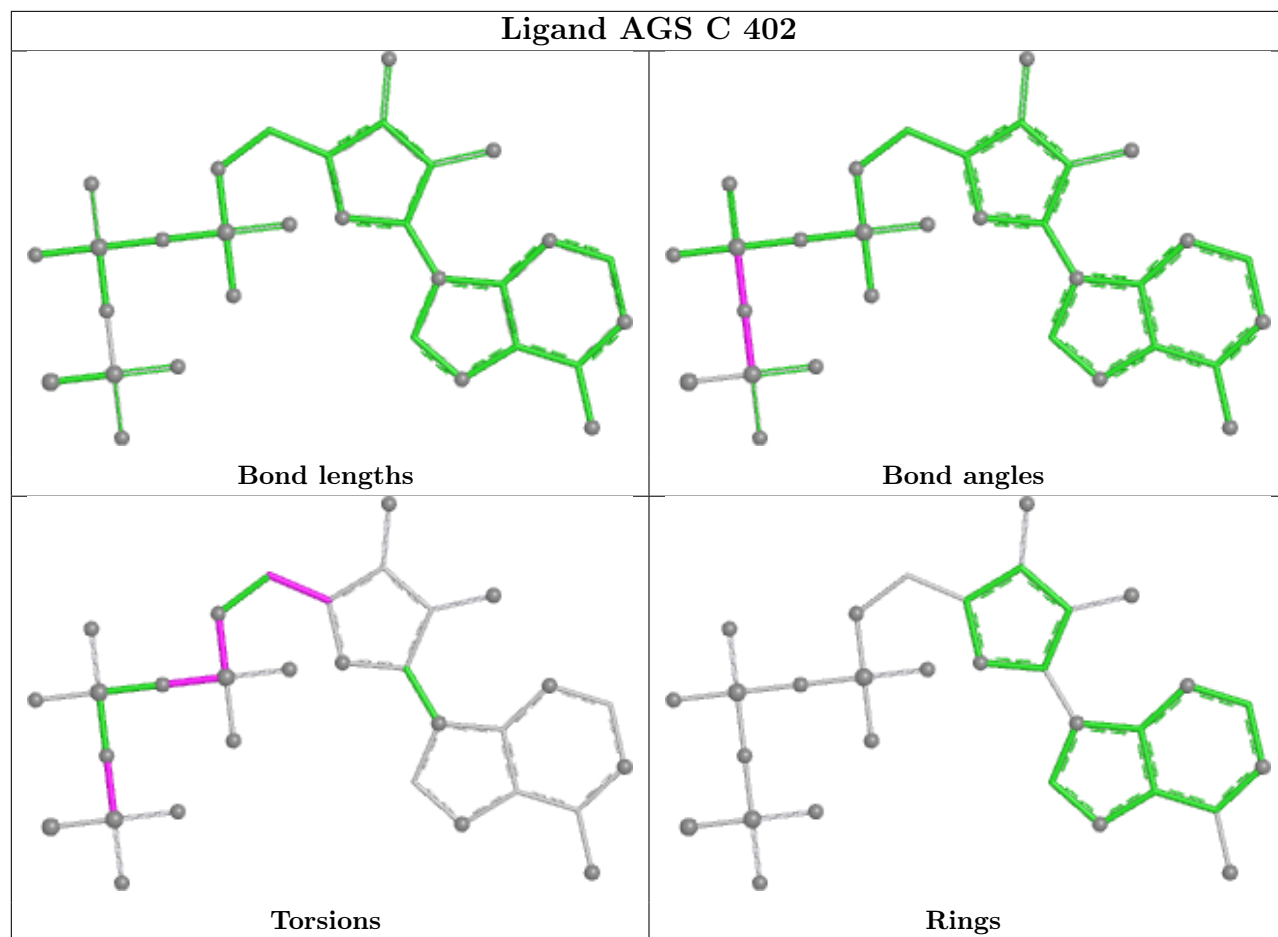
5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	401	AGS	3	0
12	C	402	AGS	5	0
13	E	500	ADP	5	0
12	D	401	AGS	5	0
12	A	602	AGS	2	0

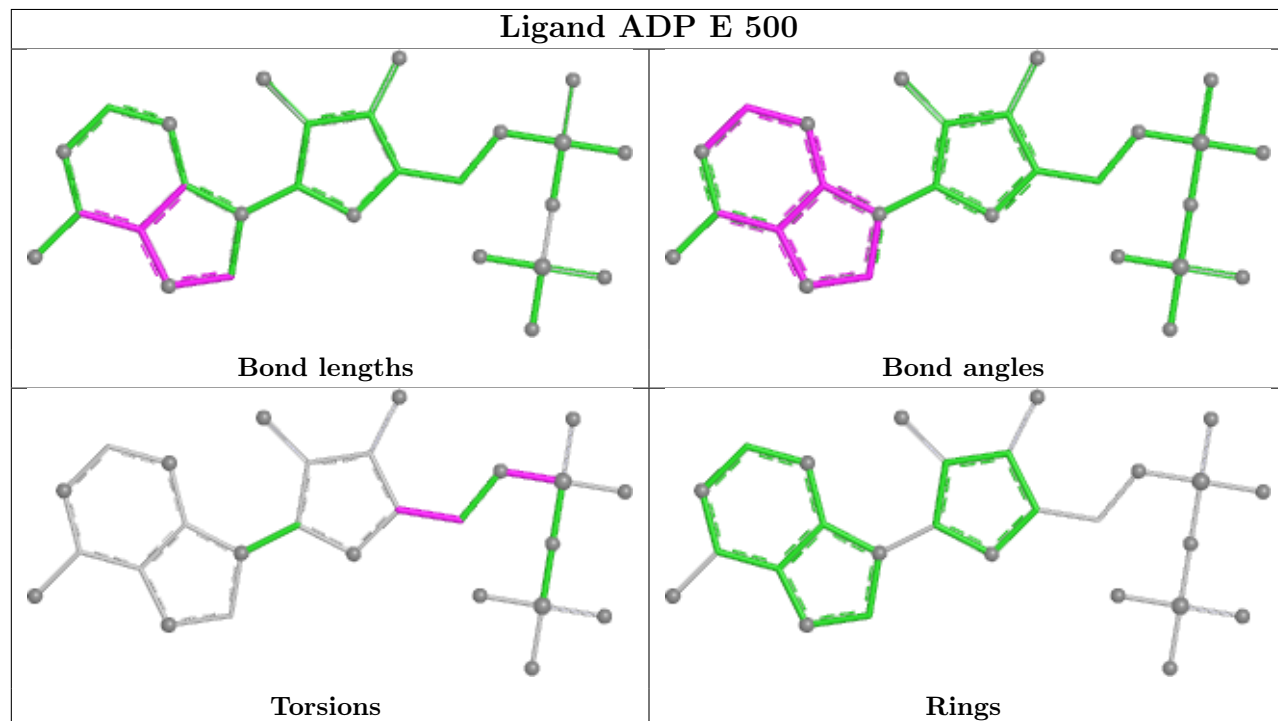
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

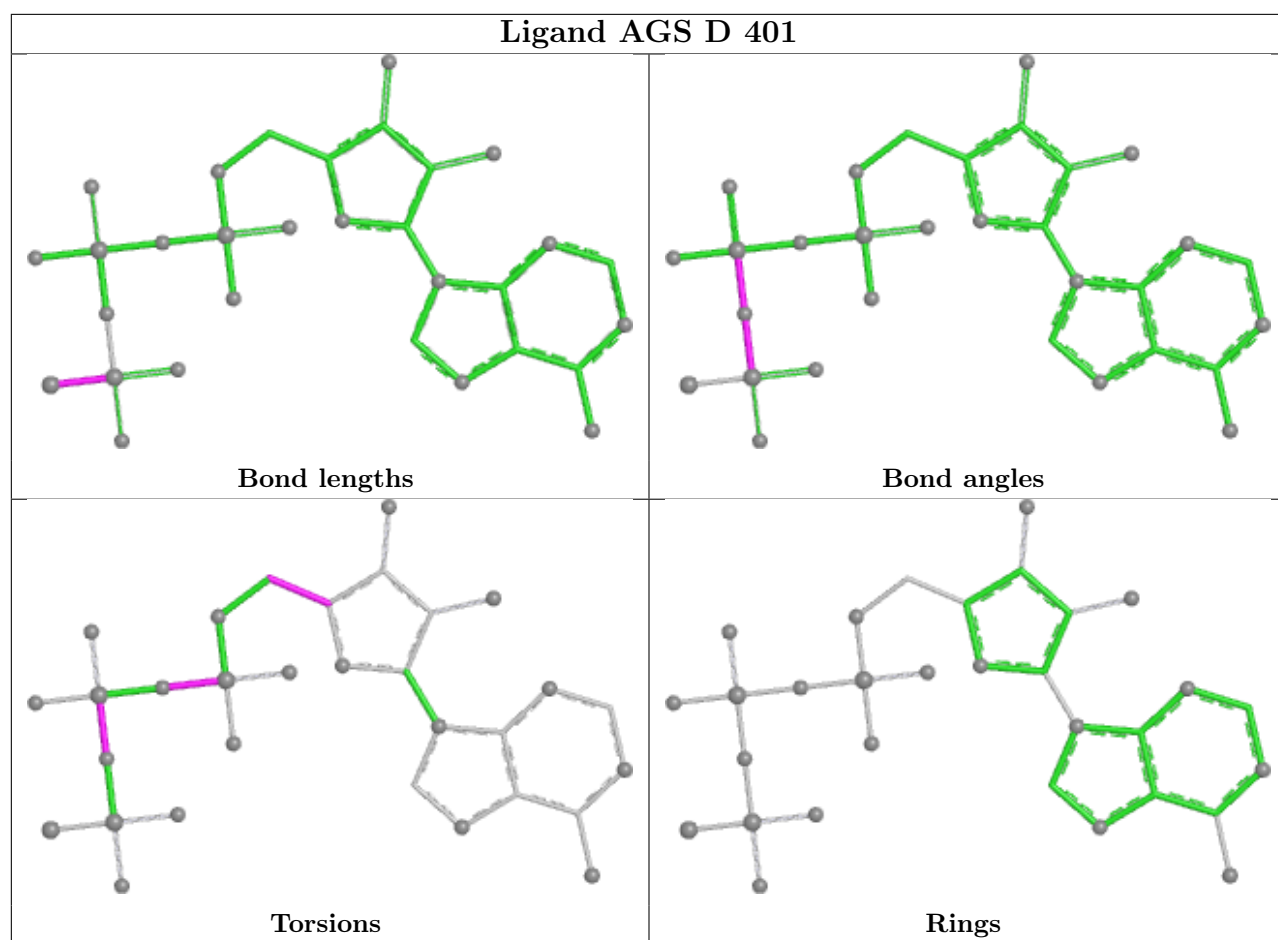


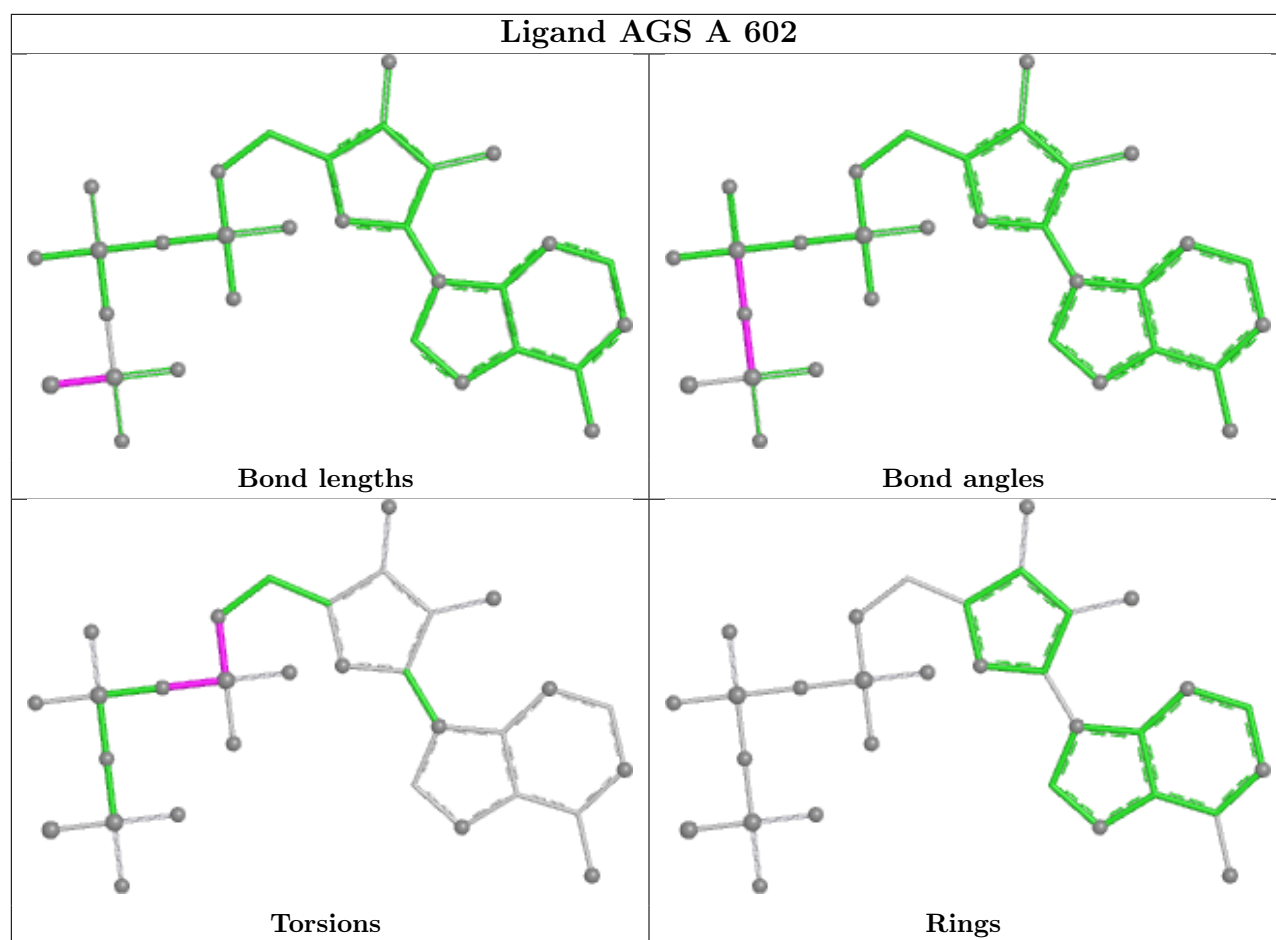
Ligand AGS C 402



Ligand ADP E 500







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.

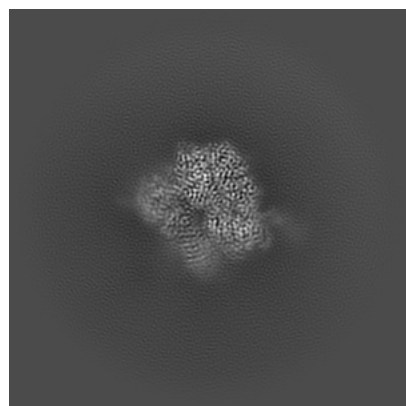
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29412. These allow visual inspection of the internal detail of the map and identification of artifacts.

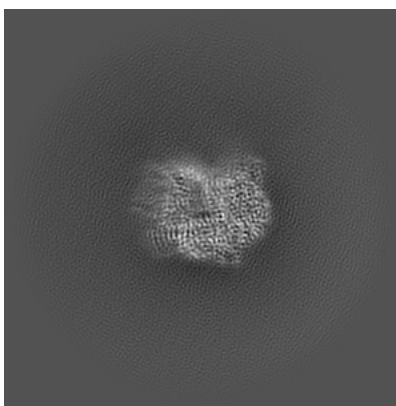
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

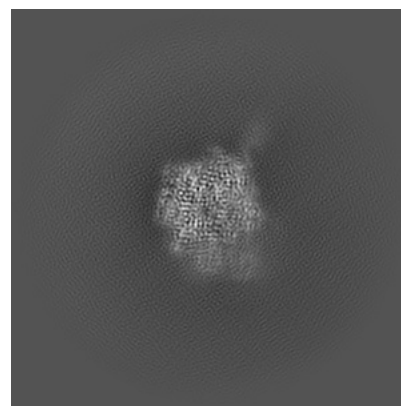
6.1.1 Primary map



X

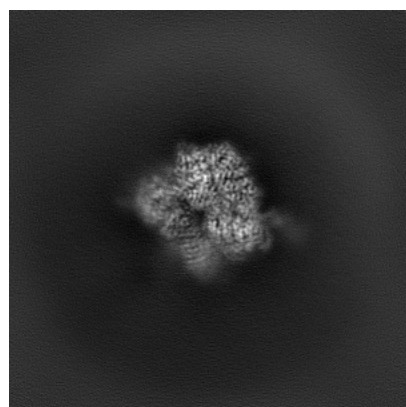


Y

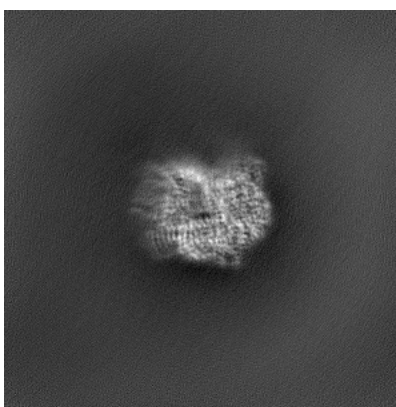


Z

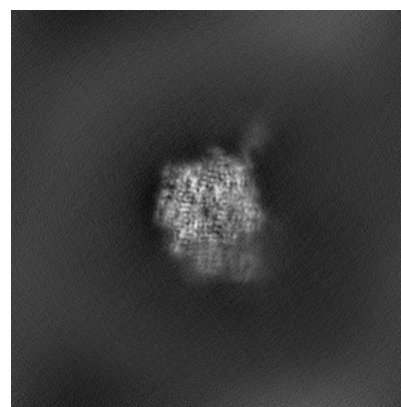
6.1.2 Raw map



X



Y

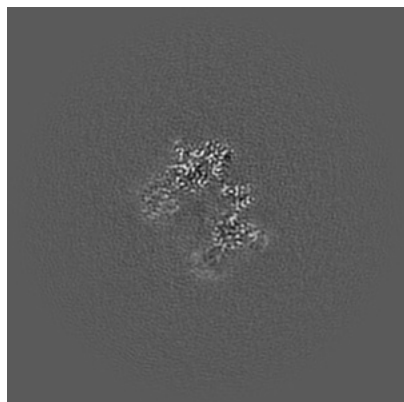


Z

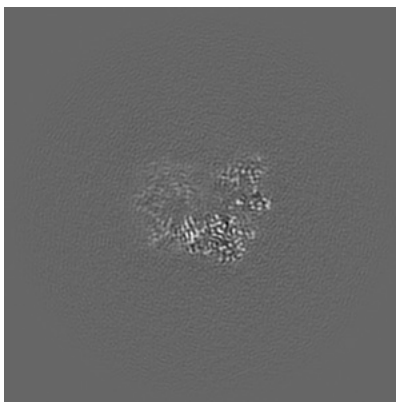
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

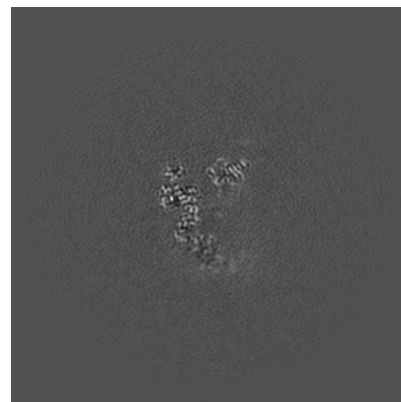
6.2.1 Primary map



X Index: 210



Y Index: 210

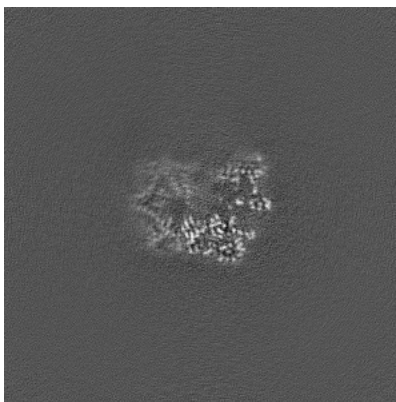


Z Index: 210

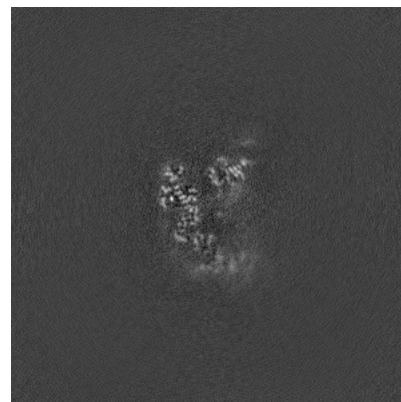
6.2.2 Raw map



X Index: 210



Y Index: 210

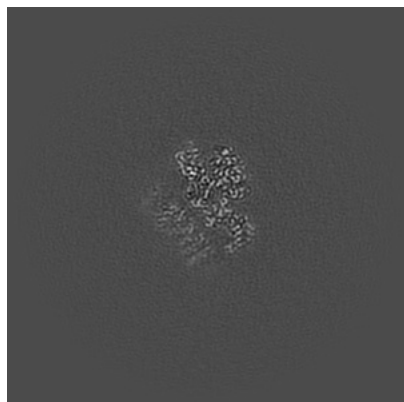


Z Index: 210

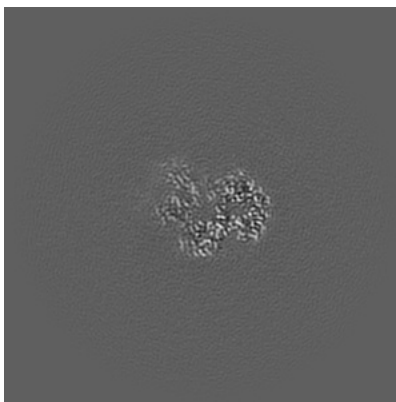
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

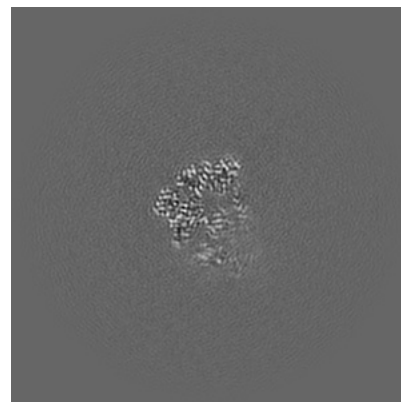
6.3.1 Primary map



X Index: 193

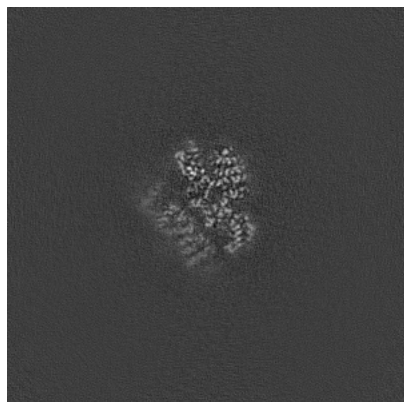


Y Index: 230

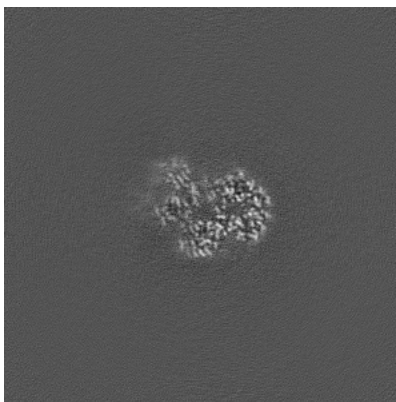


Z Index: 229

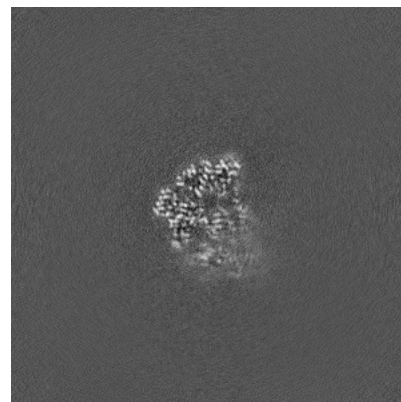
6.3.2 Raw map



X Index: 193



Y Index: 230

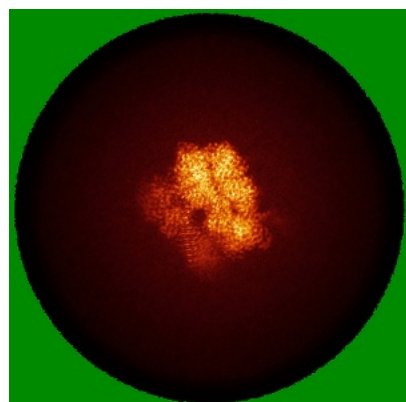


Z Index: 229

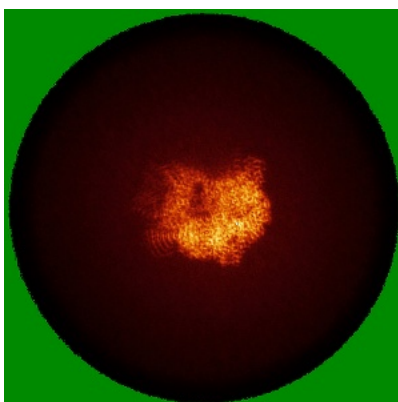
The images above show the largest variance slices of the map in three orthogonal directions.

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

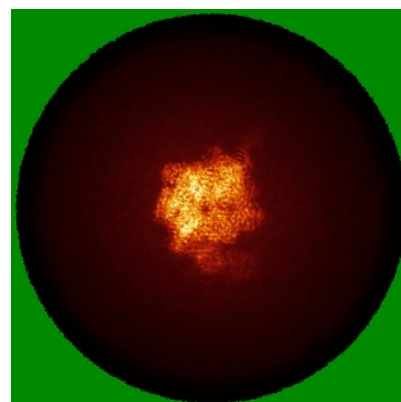
6.4.1 Primary map



X

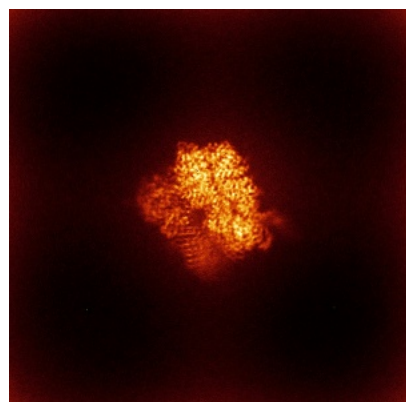


Y

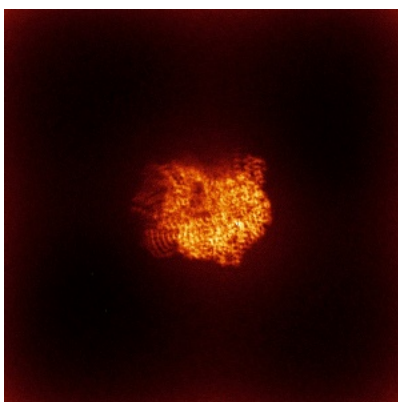


Z

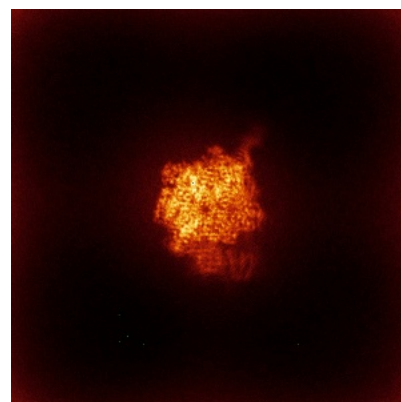
6.4.2 Raw map



X



Y

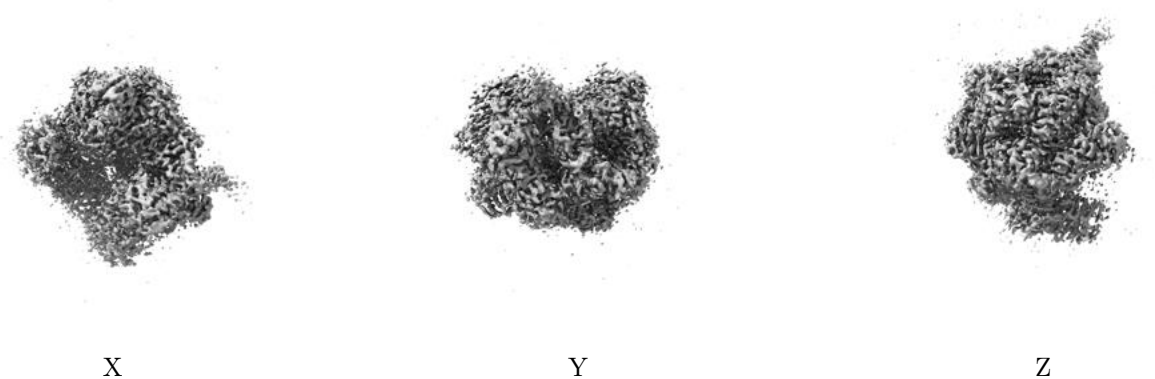


Z

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.

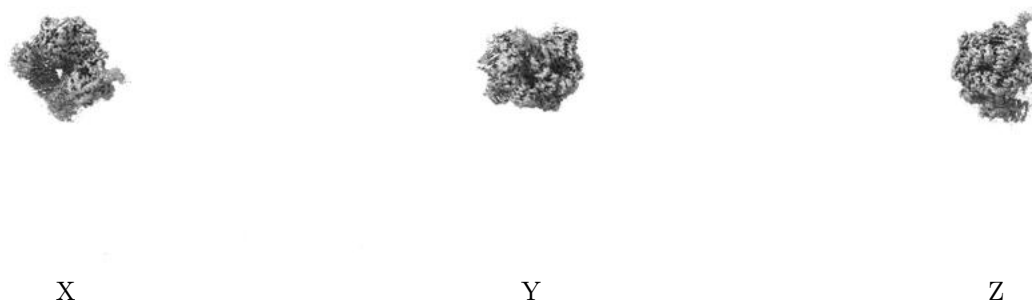
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. 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.

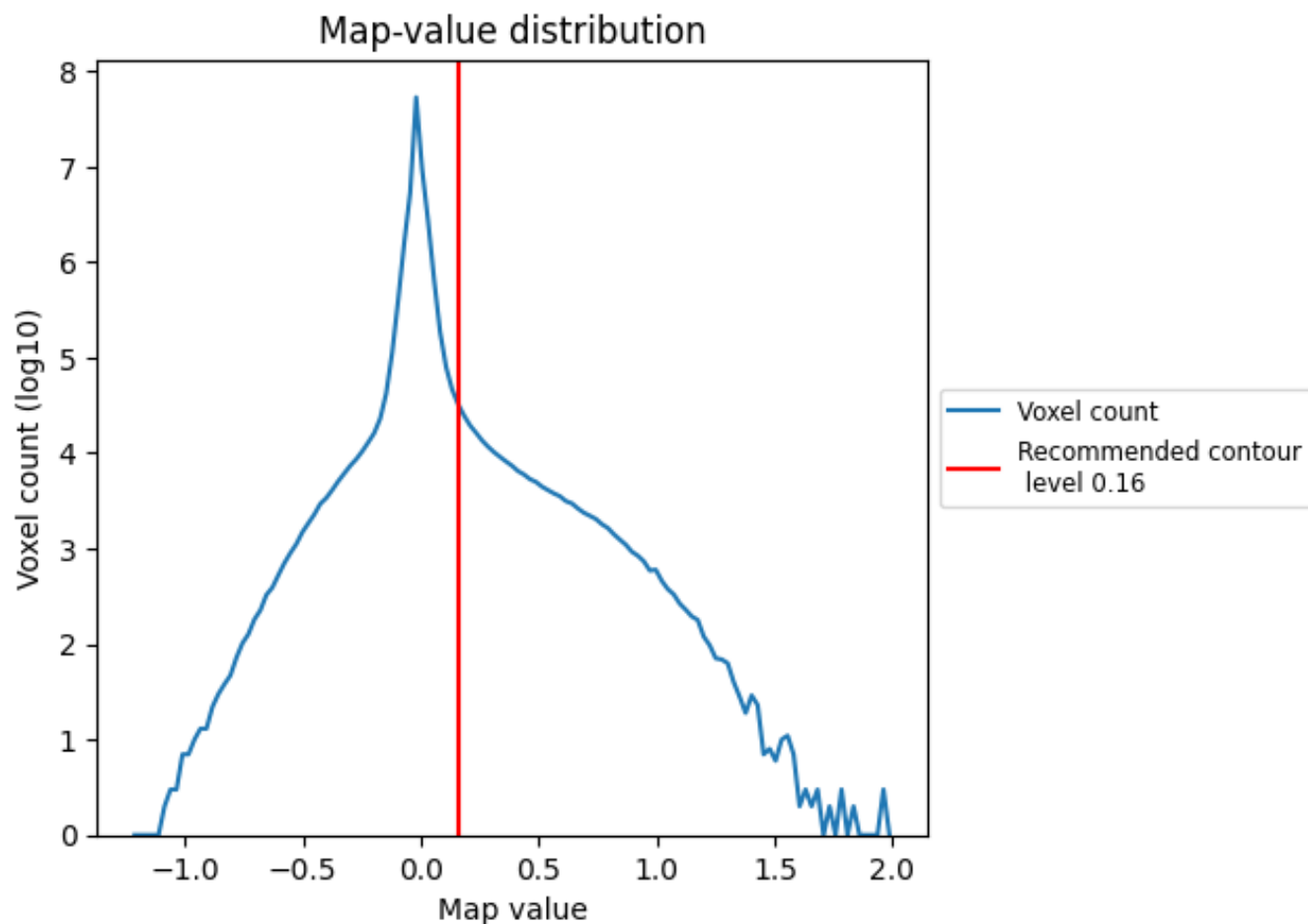
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

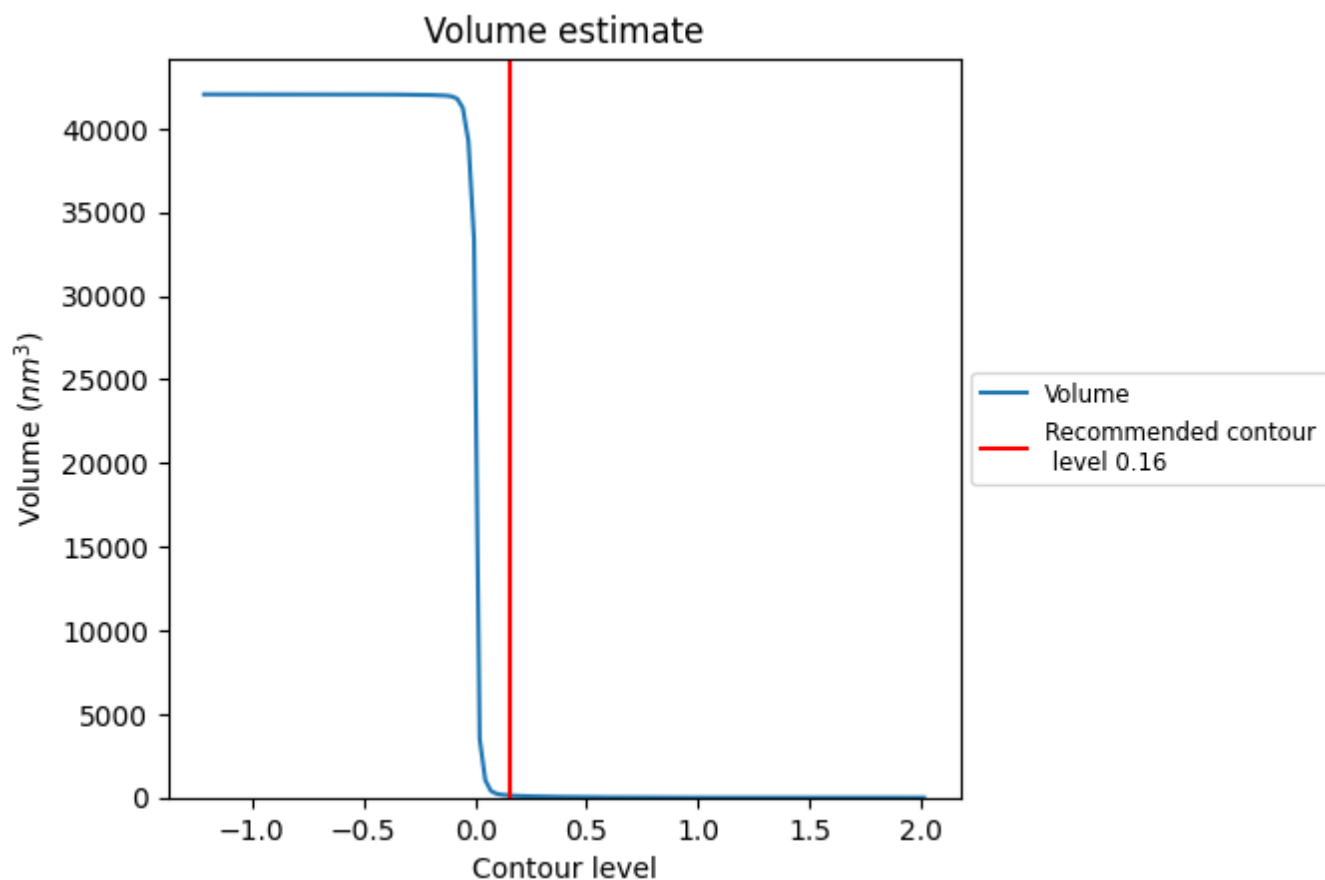
This section contains the results of statistical analysis of the map.

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.

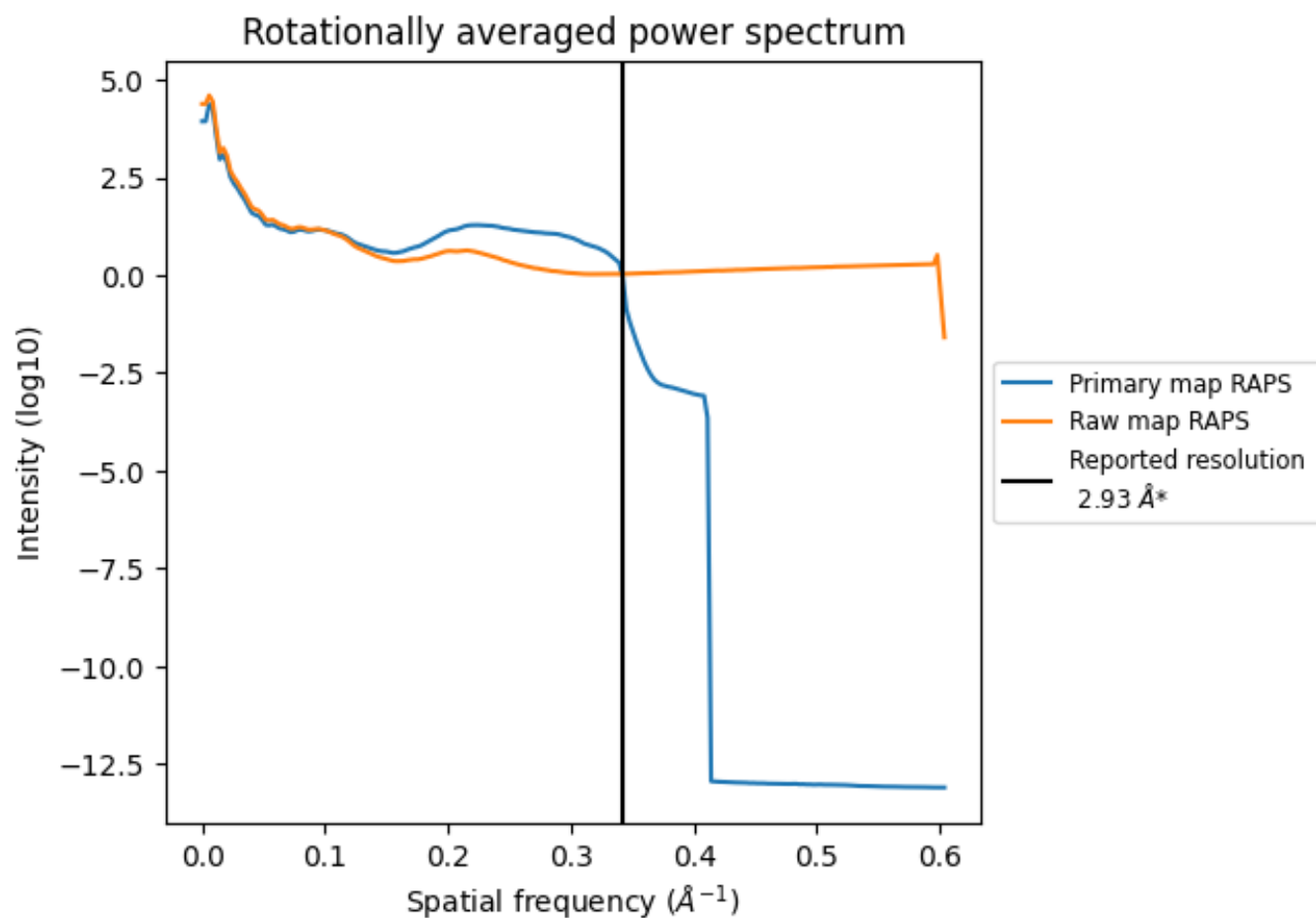
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 124 nm³; this corresponds to an approximate mass of 112 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 ⓘ

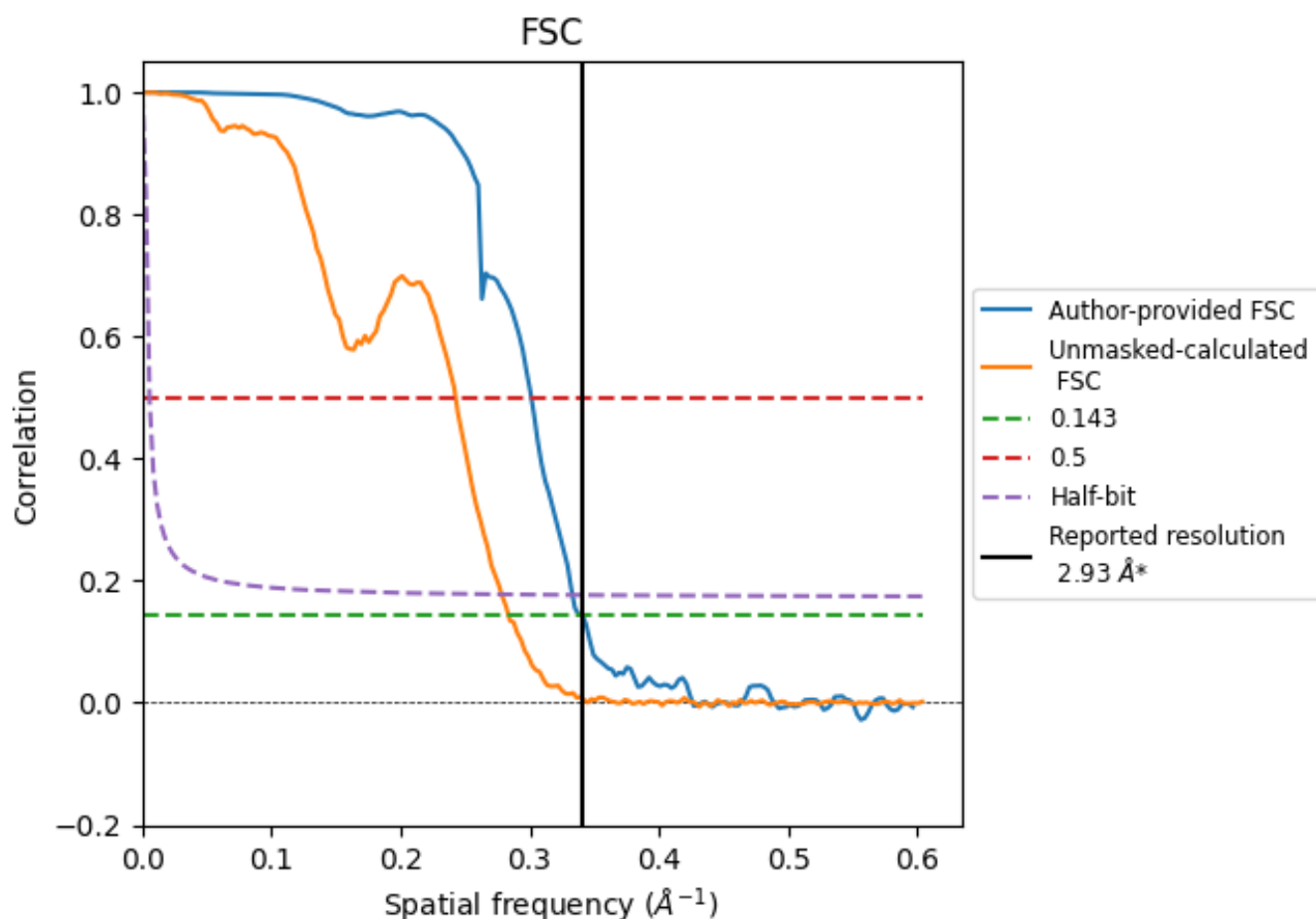


*Reported resolution corresponds to spatial frequency of 0.341 Å⁻¹

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 0.341 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.93	-	-
Author-provided FSC curve	2.93	3.32	3.00
Unmasked-calculated*	3.53	4.12	3.59

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.53 differs from the reported value 2.93 by more than 10 %

9 Map-model fit [i](#)

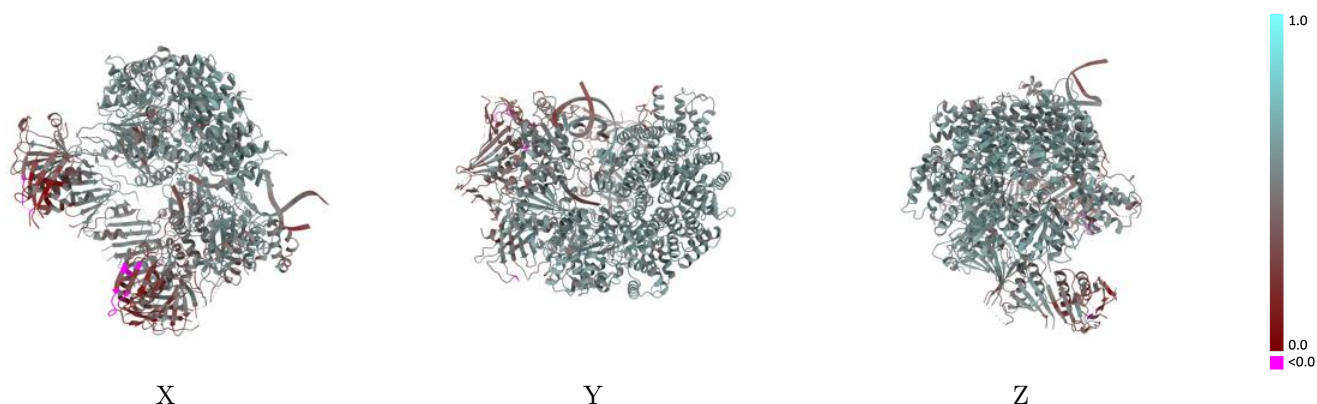
This section contains information regarding the fit between EMDB map EMD-29412 and PDB model 8FS3. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



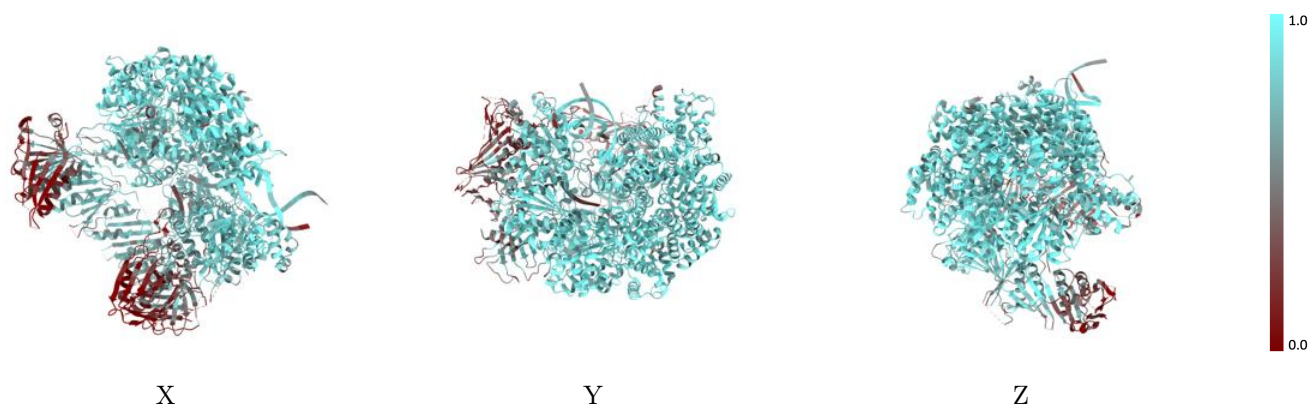
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



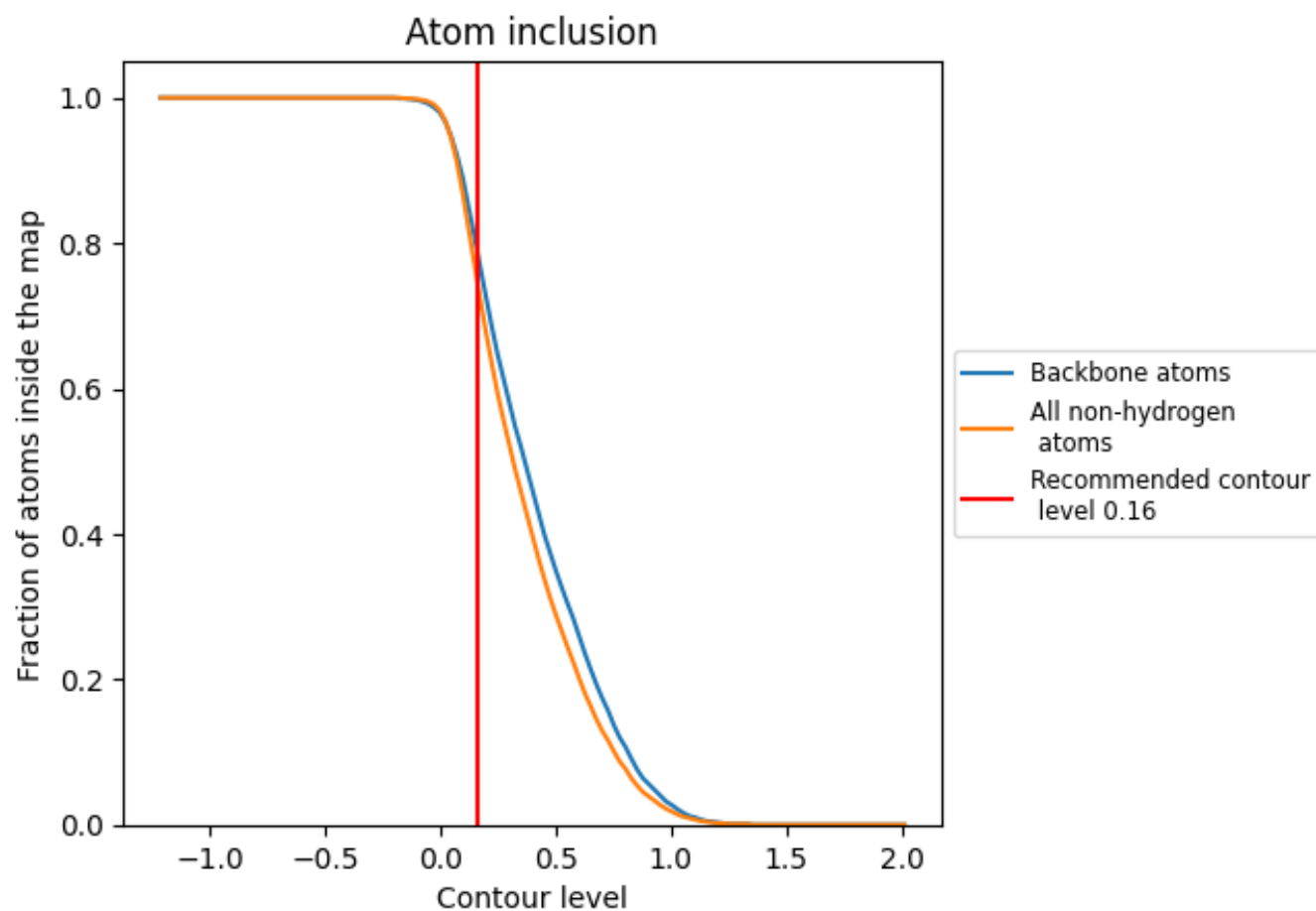
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 75% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7460	0.5030
A	0.7710	0.4930
B	0.8800	0.5600
C	0.8930	0.5690
D	0.9260	0.5810
E	0.8800	0.5590
F	0.5010	0.4060
G	0.7110	0.4870
H	0.2460	0.3270
I	0.6570	0.4320
K	0.7460	0.4370

1.0

0.0

<0.0