



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:43 AM UTC

PDB ID : 9CI2 / pdb_00009ci2
EMDB ID : EMD-45608
Title : Anthoceros agrestis Rubisco octamer core complexed with small subunits and Arabidopsis thaliana BSD2
Authors : Ang, W.S.L.; Oh, Z.G.; Li, F.W.; Gunn, L.H.
Deposited on : 2024-07-02
Resolution : 2.90 Å (reported)
Based on initial models : 8LIM, 9CHZ, 8ILB

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

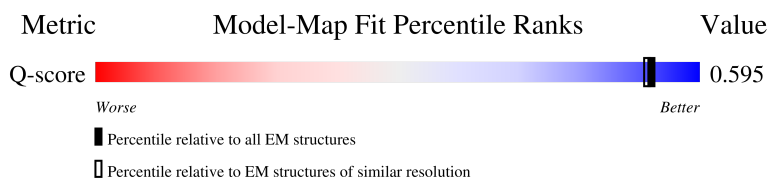
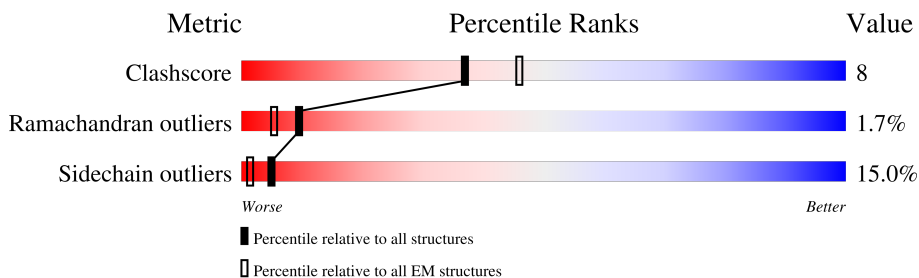
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

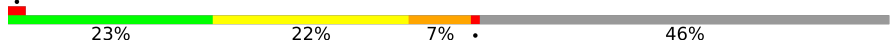
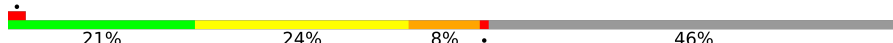
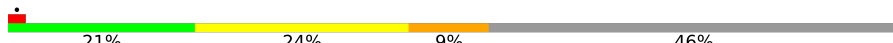
The reported resolution of this entry is 2.90 Å.

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	13054 (2.40 - 3.40)

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	1	136	
1	2	136	
1	3	136	
1	4	136	

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Mol	Chain	Length	Quality of chain
2	A	475	 72% 19% 5%
2	B	475	 76% 16% 5%
2	C	475	 72% 20% 5%
2	D	475	 77% 16% 5%
2	E	475	 72% 18% 5% 5%
2	F	475	 78% 15% 5%
2	G	475	 73% 17% 5% 5%
2	H	475	 79% 15% 5%
3	I	125	 74% 14% 6% 6%
3	J	125	 70% 19% 6% 6%
3	K	125	 71% 17% 6% 6%
3	L	125	 68% 17% 10% 6%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 34492 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 Protein BUNDLE SHEATH DEFECTIVE 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	73	Total	C	N	O	S	0	0
			519	320	91	99	9		
1	2	73	Total	C	N	O	S	0	0
			519	320	91	99	9		
1	3	73	Total	C	N	O	S	0	0
			519	320	91	99	9		
1	4	73	Total	C	N	O	S	0	0
			519	320	91	99	9		

- Molecule 2 is a protein called Rubisco large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	452	Total	C	N	O	S	0	0
			3549	2247	623	661	18		
2	B	455	Total	C	N	O	S	0	0
			3568	2257	631	662	18		
2	C	452	Total	C	N	O	S	0	0
			3549	2247	623	661	18		
2	D	455	Total	C	N	O	S	0	0
			3568	2257	631	662	18		
2	E	452	Total	C	N	O	S	0	0
			3549	2247	623	661	18		
2	F	455	Total	C	N	O	S	0	0
			3568	2257	631	662	18		
2	G	452	Total	C	N	O	S	0	0
			3549	2247	623	661	18		
2	H	455	Total	C	N	O	S	0	0
			3568	2257	631	662	18		

- Molecule 3 is a protein called Rubisco small subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	118	Total	C	N	O	S	0	0
			965	627	162	166	10		

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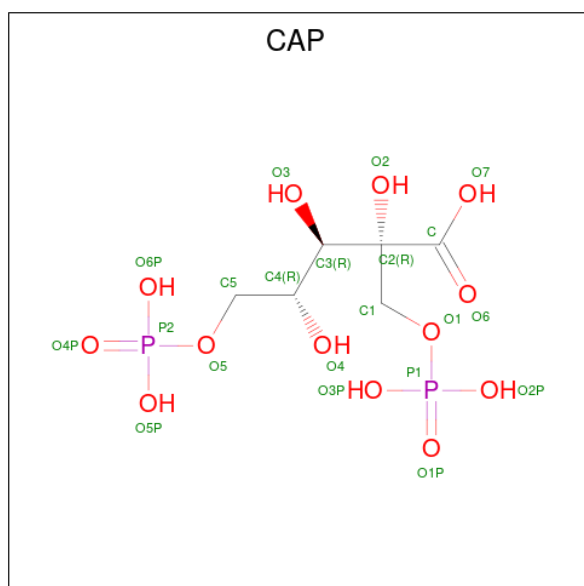
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	118	Total	C	N	O	S	0	0
			965	627	162	166	10		
3	K	118	Total	C	N	O	S	0	0
			965	627	162	166	10		
3	L	118	Total	C	N	O	S	0	0
			965	627	162	166	10		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	
4	G	1	Total	Mg	0
			1	1	

- Molecule 5 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (CCD ID: CAP) (formula: C₆H₁₄O₁₃P₂) (labeled as "Ligand of Interest" by depositor).

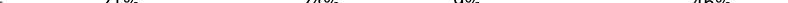


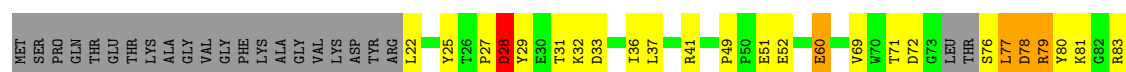
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			21	6	13	2	

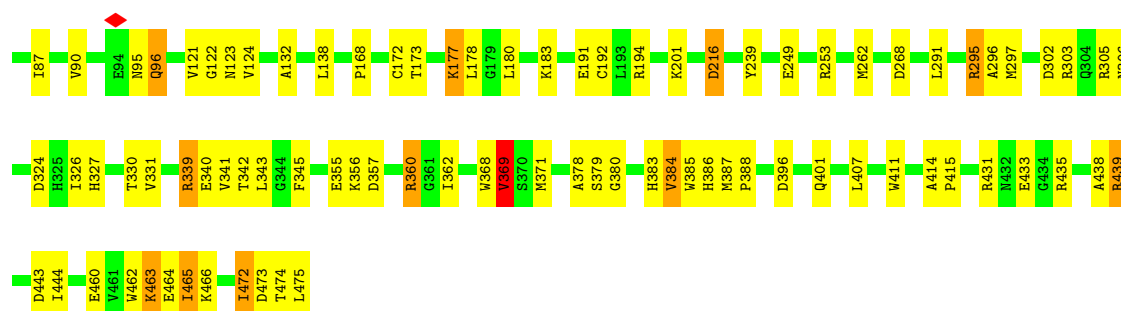
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Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	O	P	0
			21	6	13	2	
5	E	1	Total	C	O	P	0
			21	6	13	2	
5	G	1	Total	C	O	P	0
			21	6	13	2	

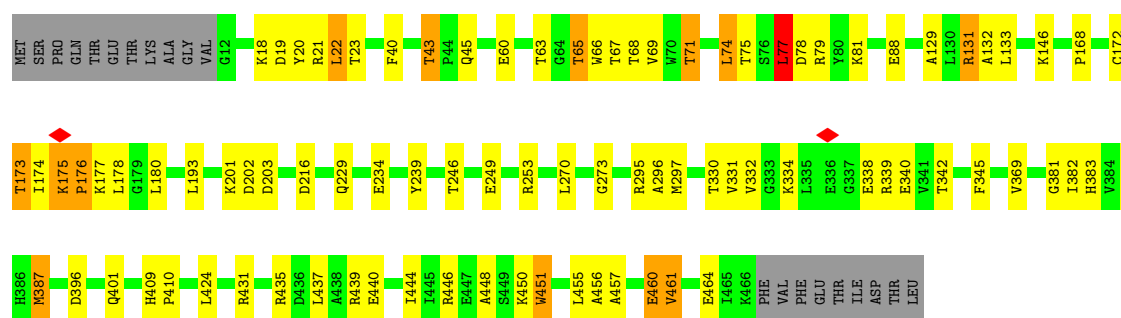
- Chain 4: 





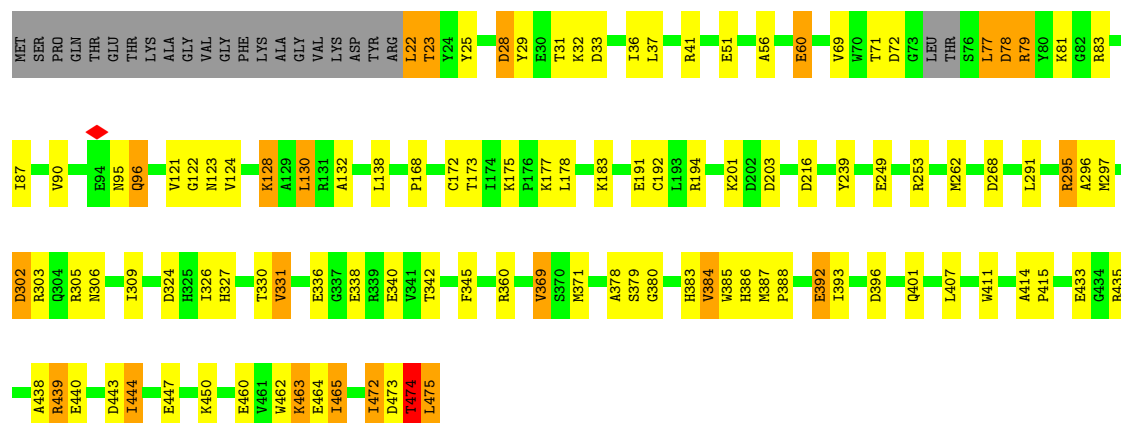
• Molecule 2: Rubisco large subunit

Chain D: 77% 16% . .



• Molecule 2: Rubisco large subunit

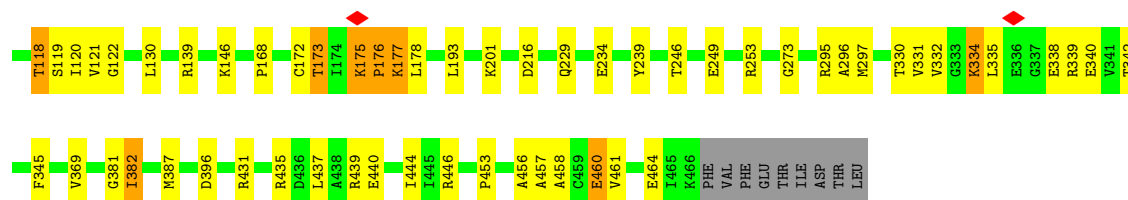
Chain E: 72% 18% 5% 5%



• Molecule 2: Rubisco large subunit

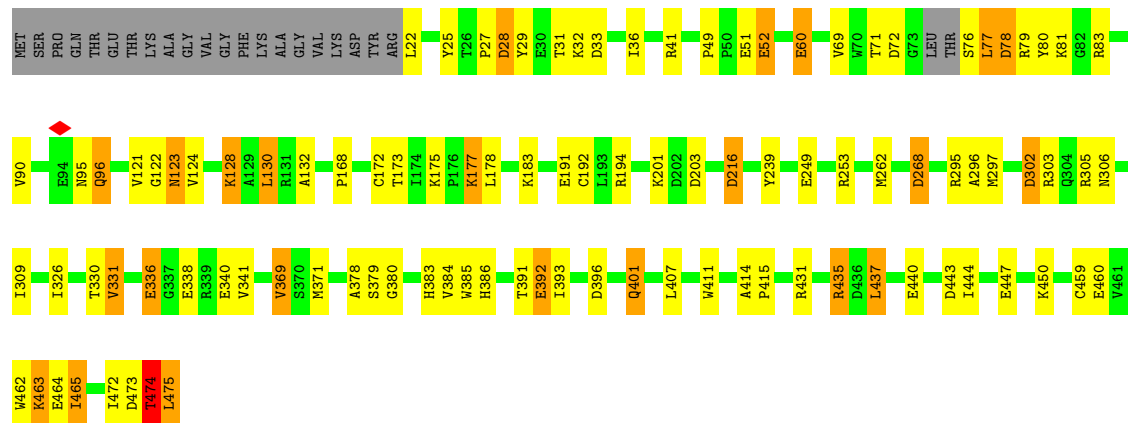
Chain F: 78% 15% . .





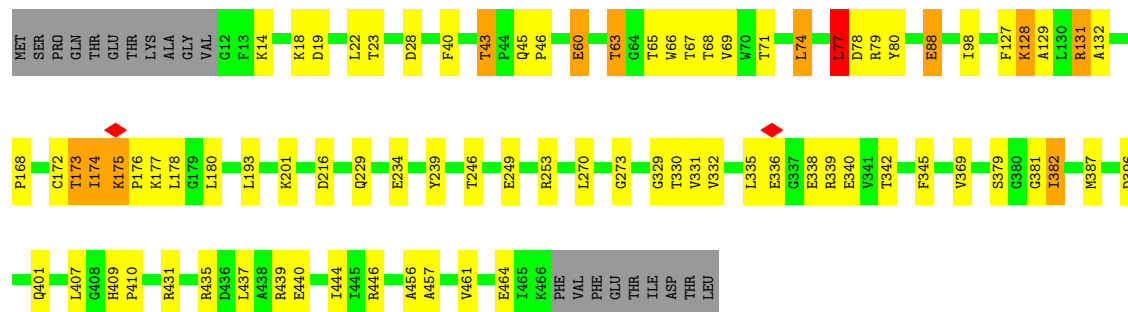
• Molecule 2: Rubisco large subunit

Chain G: 73% 17% 5% 5%



• Molecule 2: Rubisco large subunit

Chain H: 79% 15% 6%



• Molecule 3: Rubisco small subunit

Chain I: 74% 14% 6% 6%

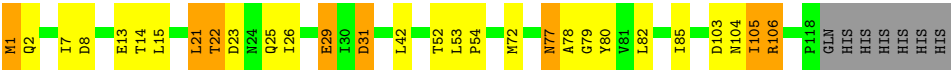


• Molecule 3: Rubisco small subunit

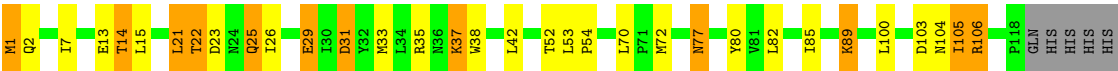
Chain J: 70% 19% 6% 6%



• Molecule 3: Rubisco small subunit



• Molecule 3: Rubisco small subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	19751	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	79000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.446	Depositor
Minimum map value	-0.230	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	281.6, 281.6, 281.6	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.55, 0.55, 0.55	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1	0.94	0/527	1.05	0/705
1	2	0.94	0/527	1.04	0/705
1	3	0.95	0/527	1.08	1/705 (0.1%)
1	4	0.91	0/527	1.05	0/705
2	A	0.72	0/3622	0.87	2/4908 (0.0%)
2	B	0.58	0/3642	0.70	1/4933 (0.0%)
2	C	0.70	0/3622	0.83	0/4908
2	D	0.57	0/3642	0.69	1/4933 (0.0%)
2	E	0.69	0/3622	0.81	1/4908 (0.0%)
2	F	0.56	0/3642	0.69	1/4933 (0.0%)
2	G	0.69	0/3622	0.81	1/4908 (0.0%)
2	H	0.54	0/3642	0.66	1/4933 (0.0%)
3	I	0.65	0/998	0.78	1/1360 (0.1%)
3	J	0.66	0/998	0.80	1/1360 (0.1%)
3	K	0.66	0/998	0.78	1/1360 (0.1%)
3	L	0.87	0/998	0.97	0/1360
All	All	0.66	0/35156	0.79	12/47624 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	129	GLY	CA-C-O	-6.41	118.06	122.22
2	A	331	VAL	N-CA-C	-5.76	107.67	113.20
2	E	331	VAL	N-CA-C	-5.72	107.71	113.20
3	I	13	GLU	CB-CA-C	-5.69	110.03	116.63
3	K	13	GLU	CB-CA-C	-5.69	110.03	116.63
2	G	331	VAL	N-CA-C	-5.68	107.75	113.20
3	J	13	GLU	CB-CA-C	-5.68	110.05	116.63
2	H	273	GLY	CA-C-O	-5.42	117.94	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	273	GLY	CA-C-O	-5.38	117.97	122.33
2	D	273	GLY	CA-C-O	-5.37	117.98	122.33
2	F	273	GLY	CA-C-O	-5.32	118.02	122.33
2	A	66	TRP	N-CA-C	-5.03	107.82	114.31

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	1	519	0	493	27	0
1	2	519	0	493	27	0
1	3	519	0	493	23	0
1	4	519	0	493	27	0
2	A	3549	0	3448	43	0
2	B	3568	0	3476	53	0
2	C	3549	0	3448	50	0
2	D	3568	0	3476	50	0
2	E	3549	0	3448	47	0
2	F	3568	0	3476	42	0
2	G	3549	0	3448	41	0
2	H	3568	0	3476	50	0
3	I	965	0	939	20	0
3	J	965	0	939	20	0
3	K	965	0	939	19	0
3	L	965	0	939	21	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	21	0	9	0	0
5	C	21	0	9	0	0
5	E	21	0	9	0	0
5	G	21	0	9	0	0
All	All	34492	0	33460	514	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 (514) 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)
3:L:77:ASN:ND2	3:L:80:TYR:CD2	1.75	1.53
3:J:77:ASN:ND2	3:J:80:TYR:CD2	1.75	1.52
3:I:77:ASN:ND2	3:I:80:TYR:CD2	1.75	1.51
3:K:77:ASN:ND2	3:K:80:TYR:CD2	1.90	1.38
3:J:77:ASN:ND2	3:J:80:TYR:HD2	1.21	1.11
3:K:77:ASN:ND2	3:K:80:TYR:HD2	1.33	1.10
3:I:77:ASN:ND2	3:I:80:TYR:HD2	1.21	1.07
3:L:77:ASN:ND2	3:L:80:TYR:CE2	2.28	1.02
3:J:77:ASN:ND2	3:J:80:TYR:CE2	2.29	1.00
3:I:77:ASN:ND2	3:I:80:TYR:CE2	2.29	1.00
3:L:77:ASN:ND2	3:L:80:TYR:HD2	1.25	0.99
2:F:175:LYS:HB3	2:F:176:PRO:HD2	1.57	0.86
2:D:175:LYS:HB3	2:D:176:PRO:HD2	1.57	0.86
3:K:77:ASN:ND2	3:K:80:TYR:CE2	2.48	0.81
2:D:383:HIS:CE1	2:D:385:TRP:HB2	2.20	0.76
2:E:433:GLU:HG2	3:J:28:ARG:HD3	1.68	0.75
1:1:134:PHE:HE2	2:B:332:VAL:HB	1.50	0.74
2:C:433:GLU:HG2	3:I:28:ARG:HD3	1.70	0.74
1:1:134:PHE:CE2	2:B:332:VAL:HB	2.24	0.72
1:2:135:ASP:HB3	2:D:330:THR:H	1.54	0.71
1:4:135:ASP:HB3	2:H:330:THR:H	1.55	0.70
1:3:134:PHE:HE2	2:F:332:VAL:HB	1.55	0.70
1:2:66:LYS:HE3	1:2:71:VAL:HB	1.72	0.70
1:4:134:PHE:HE1	2:H:382:ILE:HG23	1.57	0.70
1:4:134:PHE:HE2	2:H:332:VAL:HB	1.58	0.69
2:D:383:HIS:HE1	2:D:385:TRP:HB2	1.58	0.68
3:L:33:MET:HG3	3:L:38:TRP:HB2	1.76	0.68
1:3:81:VAL:HG23	1:3:116:VAL:HG23	1.76	0.67
2:D:45:GLN:HG2	2:D:131:ARG:HG2	1.75	0.67
2:A:438:ALA:HB3	2:A:439:ARG:HH12	1.59	0.67
2:C:460:GLU:HA	2:C:463:LYS:HE3	1.77	0.67
2:B:45:GLN:HG2	2:B:131:ARG:HG2	1.77	0.66
2:E:433:GLU:HG2	3:J:28:ARG:CD	2.24	0.66
1:1:75:CYS:HB2	1:1:79:GLY:H	1.60	0.66
2:C:433:GLU:HG2	3:I:28:ARG:CD	2.26	0.65
1:3:135:ASP:HB3	2:F:330:THR:H	1.62	0.65
1:1:135:ASP:O	1:1:136:GLU:C	2.40	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:21:LEU:HD13	3:L:25:GLN:HB2	1.79	0.65
1:1:86:CYS:HB3	1:1:107:CYS:HB2	1.77	0.64
1:2:81:VAL:HG23	1:2:116:VAL:HG23	1.79	0.64
1:1:81:VAL:HG23	1:1:116:VAL:HG23	1.78	0.64
1:4:86:CYS:HB3	1:4:107:CYS:HB2	1.79	0.64
2:E:411:TRP:HA	3:J:1:MET:HE2	1.80	0.64
1:3:134:PHE:CE2	2:F:332:VAL:HB	2.32	0.63
1:4:117:LEU:HD21	1:4:122:ASN:HA	1.79	0.63
1:4:92:ASN:HB3	1:4:96:HIS:HE1	1.63	0.63
2:G:411:TRP:HA	3:K:1:MET:HE2	1.81	0.63
3:L:22:THR:H	3:L:25:GLN:HG3	1.61	0.63
1:3:134:PHE:HE1	2:F:382:ILE:HG23	1.64	0.63
2:H:88:GLU:HG3	2:H:98:ILE:HB	1.80	0.62
2:F:88:GLU:HG3	2:F:98:ILE:HB	1.81	0.62
2:G:49:PRO:HG2	2:G:52:GLU:HB2	1.81	0.62
2:H:175:LYS:HB3	2:H:176:PRO:HD2	1.81	0.62
2:A:411:TRP:HA	3:L:1:MET:HE2	1.82	0.61
2:B:175:LYS:HB3	2:B:176:PRO:HD2	1.81	0.61
1:4:134:PHE:CE2	2:H:332:VAL:HB	2.36	0.61
2:E:438:ALA:HB3	2:E:439:ARG:HH21	1.64	0.61
2:E:22:LEU:HG	2:E:23:THR:HG22	1.83	0.61
1:3:109:LEU:HD13	2:F:457:ALA:HB1	1.83	0.61
2:F:71:THR:HA	2:F:74:LEU:HD21	1.83	0.60
1:2:136:GLU:HG3	2:D:334:LYS:HD3	1.82	0.60
2:G:460:GLU:HA	2:G:463:LYS:HD3	1.84	0.60
2:G:407:LEU:HB3	2:H:69:VAL:HG13	1.84	0.60
2:G:177:LYS:HG3	2:H:63:THR:HA	1.84	0.59
2:F:435:ARG:NH2	2:F:440:GLU:OE1	2.28	0.59
3:J:77:ASN:HD22	3:J:80:TYR:HD2	0.69	0.59
2:B:60:GLU:HG2	2:B:127:PHE:HZ	1.67	0.59
2:C:438:ALA:HB3	2:C:439:ARG:HH11	1.68	0.59
2:E:201:KCX:HG2	2:E:239:TYR:HD2	1.66	0.59
2:B:201:KCX:HG3	2:B:239:TYR:CD2	2.38	0.59
2:D:201:KCX:HG3	2:D:239:TYR:CD2	2.38	0.59
2:B:71:THR:HA	2:B:74:LEU:HD21	1.85	0.59
2:C:177:LYS:HD3	2:D:63:THR:HA	1.85	0.59
2:H:201:KCX:HG3	2:H:239:TYR:CD2	2.38	0.58
3:I:22:THR:H	3:I:25:GLN:HG3	1.68	0.58
1:3:86:CYS:HB3	1:3:107:CYS:HB2	1.84	0.58
1:3:117:LEU:HD11	1:3:122:ASN:HA	1.85	0.58
2:F:201:KCX:HG3	2:F:239:TYR:CD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:396:ASP:OD1	2:A:396:ASP:N	2.34	0.58
2:H:175:LYS:HZ3	2:H:175:LYS:HA	1.68	0.58
1:1:135:ASP:HB3	2:B:330:THR:H	1.68	0.58
1:2:86:CYS:HB3	1:2:107:CYS:HB2	1.84	0.58
3:K:77:ASN:HD21	3:K:80:TYR:H	1.52	0.58
2:A:201:KCX:HG2	2:A:239:TYR:HD2	1.69	0.58
2:E:407:LEU:HB3	2:F:69:VAL:HG13	1.86	0.58
2:F:457:ALA:HA	2:F:460:GLU:HG3	1.84	0.58
2:B:88:GLU:HG3	2:B:98:ILE:HB	1.86	0.58
1:2:135:ASP:O	1:2:136:GLU:C	2.46	0.57
2:D:71:THR:HA	2:D:74:LEU:HD21	1.86	0.57
1:2:134:PHE:HE2	2:D:332:VAL:HB	1.68	0.57
2:G:396:ASP:OD1	2:G:396:ASP:N	2.34	0.57
2:H:435:ARG:NH2	2:H:440:GLU:OE1	2.28	0.57
2:D:173:THR:HG23	2:D:175:LYS:HD3	1.85	0.57
2:A:407:LEU:HB3	2:B:69:VAL:HG13	1.86	0.57
2:G:25:TYR:O	2:G:27:PRO:HD3	2.05	0.57
1:1:92:ASN:HB3	1:1:96:HIS:HE1	1.70	0.57
3:J:22:THR:H	3:J:25:GLN:HG3	1.69	0.57
2:G:201:KCX:HG2	2:G:239:TYR:HD2	1.70	0.56
2:B:175:LYS:HA	2:B:175:LYS:HZ3	1.69	0.56
2:B:457:ALA:HA	2:B:460:GLU:HG2	1.86	0.56
2:E:379:SER:HB2	2:E:401:GLN:HB2	1.86	0.56
2:G:379:SER:HB2	2:G:401:GLN:HB2	1.87	0.56
2:H:45:GLN:HE21	2:H:129:ALA:HA	1.69	0.56
2:H:168:PRO:HG3	2:H:396:ASP:HA	1.88	0.56
2:A:90:VAL:HB	2:A:96:GLN:HB3	1.88	0.56
2:B:168:PRO:HG3	2:B:396:ASP:HA	1.88	0.56
2:C:90:VAL:HB	2:C:96:GLN:HB3	1.88	0.56
2:E:90:VAL:HB	2:E:96:GLN:HB3	1.88	0.56
2:H:71:THR:HA	2:H:74:LEU:HD21	1.87	0.56
1:3:92:ASN:HB3	1:3:96:HIS:HE1	1.71	0.56
2:G:90:VAL:HB	2:G:96:GLN:HB3	1.88	0.56
2:H:60:GLU:HG2	2:H:127:PHE:HZ	1.70	0.56
1:3:135:ASP:O	1:3:136:GLU:C	2.49	0.55
2:F:168:PRO:HG3	2:F:396:ASP:HA	1.88	0.55
2:D:168:PRO:HG3	2:D:396:ASP:HA	1.88	0.55
1:1:136:GLU:HB3	2:B:330:THR:O	2.07	0.55
2:A:379:SER:HB2	2:A:401:GLN:HB2	1.87	0.55
2:A:392:GLU:HG2	2:A:393:ILE:N	2.21	0.55
2:E:460:GLU:HA	2:E:463:LYS:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:435:ARG:NH2	2:D:440:GLU:OE1	2.28	0.55
2:E:29:TYR:CZ	2:E:31:THR:HA	2.42	0.55
1:4:75:CYS:HB2	1:4:79:GLY:H	1.72	0.55
2:B:331:VAL:HA	2:B:334:LYS:HD2	1.87	0.55
2:C:396:ASP:OD1	2:C:396:ASP:N	2.34	0.55
2:C:379:SER:HB2	2:C:401:GLN:HB2	1.87	0.54
2:C:201:KCX:HG2	2:C:239:TYR:HD2	1.71	0.54
2:G:383:HIS:CE1	2:G:385:TRP:HB2	2.43	0.54
3:L:77:ASN:HD22	3:L:80:TYR:HD2	0.67	0.54
2:B:175:LYS:O	2:B:177:LYS:HG2	2.08	0.54
2:F:173:THR:HG23	2:F:175:LYS:HD3	1.89	0.54
2:C:411:TRP:HA	3:I:1:MET:HE2	1.90	0.53
3:K:77:ASN:HD22	3:K:80:TYR:HD2	0.67	0.53
2:C:49:PRO:HG2	2:C:52:GLU:HB2	1.90	0.53
2:E:77:LEU:HD13	2:E:78:ASP:H	1.74	0.53
2:D:456:ALA:O	2:D:457:ALA:HB3	2.09	0.53
2:E:414:ALA:HB3	2:E:415:PRO:HD3	1.90	0.53
3:L:52:THR:HG22	3:L:53:LEU:H	1.74	0.53
2:C:25:TYR:O	2:C:27:PRO:HD3	2.08	0.52
2:E:462:TRP:HA	2:E:465:ILE:HD11	1.91	0.52
2:A:49:PRO:HG2	2:A:52:GLU:HB2	1.91	0.52
2:A:95:ASN:O	2:A:96:GLN:NE2	2.37	0.52
2:B:435:ARG:NH2	2:B:440:GLU:OE1	2.28	0.52
1:2:134:PHE:CE2	2:D:332:VAL:HB	2.45	0.52
2:D:448:ALA:HA	2:D:451:TRP:NE1	2.25	0.52
2:H:77:LEU:C	2:H:79:ARG:H	2.18	0.52
2:A:305:ARG:HG3	2:A:473:ASP:HA	1.92	0.52
2:G:95:ASN:O	2:G:96:GLN:NE2	2.37	0.52
2:A:387:MET:HB2	2:A:388:PRO:HD3	1.91	0.52
2:H:379:SER:HB3	2:H:401:GLN:HB2	1.92	0.52
3:I:52:THR:HG22	3:I:53:LEU:H	1.74	0.52
3:K:52:THR:HG22	3:K:53:LEU:H	1.74	0.52
3:K:82:LEU:HA	3:K:85:ILE:HD12	1.92	0.52
2:C:414:ALA:HB3	2:C:415:PRO:HD3	1.90	0.51
2:A:132:ALA:HB1	2:A:306:ASN:O	2.10	0.51
2:G:414:ALA:HB3	2:G:415:PRO:HD3	1.90	0.51
2:B:457:ALA:CA	2:B:460:GLU:HG2	2.39	0.51
2:C:342:THR:HA	2:C:345:PHE:CE2	2.45	0.51
2:G:132:ALA:HB1	2:G:306:ASN:O	2.11	0.51
2:B:456:ALA:O	2:B:457:ALA:HB3	2.10	0.51
2:D:201:KCX:HG3	2:D:239:TYR:HD2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:52:THR:HG22	3:J:53:LEU:H	1.74	0.51
2:A:414:ALA:HB3	2:A:415:PRO:HD3	1.93	0.51
2:H:446:ARG:NH1	2:H:464:GLU:OE2	2.44	0.51
2:B:60:GLU:HG2	2:B:127:PHE:CZ	2.46	0.51
2:B:335:LEU:HG	2:B:336:GLU:O	2.11	0.51
2:E:95:ASN:O	2:E:96:GLN:NE2	2.37	0.51
2:E:132:ALA:HB1	2:E:306:ASN:O	2.11	0.51
2:E:396:ASP:OD1	2:E:396:ASP:N	2.34	0.51
3:K:22:THR:H	3:K:25:GLN:HG3	1.76	0.51
2:C:132:ALA:HB1	2:C:306:ASN:O	2.11	0.50
2:F:201:KCX:HG3	2:F:239:TYR:HD2	1.76	0.50
2:B:201:KCX:HG3	2:B:239:TYR:HD2	1.76	0.50
2:D:77:LEU:C	2:D:79:ARG:H	2.19	0.50
2:D:446:ARG:NH1	2:D:464:GLU:OE2	2.44	0.50
2:F:446:ARG:NH1	2:F:464:GLU:OE2	2.44	0.50
2:B:20:TYR:HB2	2:B:52:GLU:OE1	2.11	0.50
2:E:387:MET:HB2	2:E:388:PRO:HD3	1.92	0.50
2:C:387:MET:HB2	2:C:388:PRO:HD3	1.93	0.50
2:G:383:HIS:HE1	2:G:385:TRP:HB2	1.75	0.50
1:4:86:CYS:HB2	1:4:90:GLY:H	1.77	0.49
2:A:348:LEU:HD23	2:A:354:ILE:HD13	1.94	0.49
2:D:439:ARG:HB2	2:D:439:ARG:CZ	2.42	0.49
2:H:45:GLN:HB3	2:H:131:ARG:HH11	1.77	0.49
2:F:439:ARG:HB2	2:F:439:ARG:CZ	2.42	0.49
2:G:462:TRP:HA	2:G:465:ILE:HD11	1.93	0.49
2:A:342:THR:HA	2:A:345:PHE:CE2	2.47	0.49
2:A:383:HIS:CE1	2:A:385:TRP:HB2	2.47	0.49
2:C:462:TRP:HA	2:C:465:ILE:HD11	1.95	0.49
2:F:456:ALA:C	2:F:458:ALA:H	2.19	0.49
2:D:457:ALA:HA	2:D:460:GLU:HG3	1.94	0.49
2:F:332:VAL:HG12	2:F:332:VAL:O	2.12	0.49
2:H:175:LYS:CB	2:H:176:PRO:HD2	2.43	0.49
2:A:438:ALA:HB3	2:A:439:ARG:NH1	2.27	0.49
2:G:249:GLU:O	2:G:253:ARG:HG3	2.12	0.49
2:C:168:PRO:HG3	2:C:396:ASP:HA	1.95	0.49
2:C:249:GLU:O	2:C:253:ARG:HG3	2.12	0.49
2:H:439:ARG:CZ	2:H:439:ARG:HB2	2.42	0.49
2:B:463:LYS:H	2:B:463:LYS:HZ2	1.61	0.49
2:E:249:GLU:O	2:E:253:ARG:HG3	2.12	0.49
2:A:249:GLU:O	2:A:253:ARG:HG3	2.12	0.49
2:E:168:PRO:HG3	2:E:396:ASP:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:439:ARG:HB2	2:B:439:ARG:CZ	2.42	0.48
1:2:75:CYS:HB2	1:2:79:GLY:H	1.78	0.48
1:4:117:LEU:HD22	1:4:118:CYS:N	2.27	0.48
2:H:335:LEU:HG	2:H:336:GLU:O	2.12	0.48
3:I:22:THR:O	3:I:26:ILE:HG12	2.14	0.48
2:A:463:LYS:HB3	2:A:463:LYS:HE3	1.51	0.48
2:B:175:LYS:CB	2:B:176:PRO:HD2	2.43	0.48
3:I:77:ASN:HD22	3:I:80:TYR:HD2	0.69	0.48
2:D:201:KCX:HB2	2:D:201:KCX:HE2	1.41	0.48
1:2:134:PHE:HB3	1:2:135:ASP:H	1.52	0.48
3:K:53:LEU:HD22	3:K:54:PRO:HD2	1.96	0.48
2:A:383:HIS:HE1	2:A:385:TRP:HB2	1.79	0.48
2:C:383:HIS:CE1	2:C:385:TRP:HB2	2.49	0.48
2:E:305:ARG:HH11	2:E:474:THR:HG23	1.77	0.48
3:J:22:THR:O	3:J:26:ILE:HG12	2.14	0.48
1:3:97:PHE:HE2	2:F:453:PRO:HB3	1.79	0.48
2:E:262:MET:HE2	2:E:262:MET:HA	1.95	0.48
2:G:29:TYR:CZ	2:G:31:THR:HA	2.49	0.48
3:L:53:LEU:HD22	3:L:54:PRO:HD2	1.96	0.48
1:4:130:PHE:CE1	2:G:60:GLU:HG2	2.49	0.48
2:G:262:MET:HE2	2:G:262:MET:HA	1.95	0.48
2:A:262:MET:HA	2:A:262:MET:HE2	1.95	0.47
2:H:456:ALA:O	2:H:457:ALA:HB3	2.13	0.47
3:I:53:LEU:HD22	3:I:54:PRO:HD2	1.96	0.47
3:L:89:LYS:HB2	3:L:89:LYS:HE3	1.53	0.47
2:G:168:PRO:HG3	2:G:396:ASP:HA	1.95	0.47
2:H:175:LYS:HB2	2:H:407:LEU:CD1	2.44	0.47
2:B:357:ASP:OD2	2:B:360:ARG:HD3	2.14	0.47
2:D:387:MET:HE3	2:D:424:LEU:HB2	1.96	0.47
2:E:383:HIS:CE1	2:E:385:TRP:HB2	2.48	0.47
3:J:53:LEU:HD22	3:J:54:PRO:HD2	1.96	0.47
2:B:249:GLU:O	2:B:253:ARG:HG3	2.14	0.47
2:C:262:MET:HA	2:C:262:MET:HE2	1.95	0.47
2:D:296:ALA:O	2:D:297:MET:HB3	2.13	0.47
2:H:201:KCX:HG3	2:H:239:TYR:HD2	1.76	0.47
3:J:21:LEU:HD13	3:J:25:GLN:HB2	1.96	0.47
1:2:88:GLY:HA2	1:2:114:LYS:HG2	1.97	0.47
2:D:66:TRP:CE3	2:D:67:THR:HB	2.49	0.47
2:F:396:ASP:OD1	2:F:396:ASP:N	2.45	0.47
3:K:103:ASP:OD2	3:K:106:ARG:HG3	2.14	0.47
3:L:82:LEU:HA	3:L:85:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:103:ASP:OD2	3:L:106:ARG:HG3	2.14	0.47
2:C:296:ALA:O	2:C:297:MET:HB3	2.14	0.47
2:C:472:ILE:HG13	2:C:473:ASP:N	2.29	0.47
2:E:296:ALA:O	2:E:297:MET:HB3	2.14	0.47
2:F:249:GLU:O	2:F:253:ARG:HG3	2.14	0.47
1:2:127:ILE:O	1:2:128:GLY:C	2.57	0.47
2:B:296:ALA:O	2:B:297:MET:HB3	2.14	0.47
1:4:121:CYS:O	1:4:121:CYS:SG	2.73	0.47
2:B:77:LEU:C	2:B:79:ARG:H	2.23	0.47
2:G:463:LYS:HB2	2:G:463:LYS:HE3	1.40	0.47
3:I:21:LEU:HD13	3:I:25:GLN:HB2	1.97	0.47
3:J:77:ASN:HD21	3:J:80:TYR:H	1.63	0.47
2:A:296:ALA:O	2:A:297:MET:HB3	2.14	0.46
3:I:82:LEU:HA	3:I:85:ILE:HD12	1.97	0.46
3:L:105:ILE:HD12	3:L:105:ILE:HA	1.78	0.46
1:1:121:CYS:C	1:1:123:GLY:H	2.23	0.46
3:K:22:THR:O	3:K:26:ILE:HG12	2.15	0.46
2:G:296:ALA:O	2:G:297:MET:HB3	2.14	0.46
2:H:249:GLU:O	2:H:253:ARG:HG3	2.14	0.46
2:D:249:GLU:O	2:D:253:ARG:HG3	2.14	0.46
2:G:305:ARG:HH11	2:G:474:THR:HG23	1.80	0.46
3:I:78:ALA:O	3:I:79:GLY:C	2.59	0.46
1:4:135:ASP:HB2	2:H:379:SER:O	2.16	0.46
2:C:368:TRP:O	2:C:369:VAL:C	2.59	0.46
2:E:302:ASP:HB3	2:E:309:ILE:O	2.15	0.46
3:I:26:ILE:O	3:I:29:GLU:HG2	2.16	0.46
2:F:296:ALA:O	2:F:297:MET:HB3	2.14	0.46
3:J:78:ALA:O	3:J:79:GLY:C	2.59	0.46
1:1:92:ASN:HB3	1:1:96:HIS:CE1	2.49	0.46
2:E:342:THR:HA	2:E:345:PHE:CE2	2.51	0.46
2:H:45:GLN:HB3	2:H:131:ARG:HG2	1.98	0.46
1:2:134:PHE:HD1	1:2:134:PHE:HA	1.69	0.46
1:4:133:THR:HG23	1:4:134:PHE:O	2.16	0.46
2:B:174:ILE:H	2:B:174:ILE:HG12	1.53	0.46
2:B:177:LYS:HB3	2:B:177:LYS:HE3	1.65	0.46
2:C:77:LEU:HD22	2:C:77:LEU:HA	1.76	0.46
3:L:31:ASP:OD1	3:L:31:ASP:N	2.49	0.46
1:3:66:LYS:HD3	1:3:73:ALA:HA	1.99	0.45
1:3:75:CYS:HB2	1:3:79:GLY:H	1.80	0.45
1:4:134:PHE:CE1	2:H:382:ILE:HG23	2.44	0.45
2:C:305:ARG:HG3	2:C:473:ASP:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:37:LEU:O	2:C:138:LEU:HD23	2.17	0.45
2:H:396:ASP:OD1	2:H:396:ASP:N	2.45	0.45
1:2:117:LEU:HD22	1:2:118:CYS:H	1.81	0.45
1:3:66:LYS:H	1:3:66:LYS:HG2	1.57	0.45
2:F:77:LEU:O	2:F:78:ASP:C	2.60	0.45
2:F:81:LYS:HB2	2:F:81:LYS:HE3	1.68	0.45
3:J:26:ILE:O	3:J:29:GLU:HG2	2.16	0.45
2:C:29:TYR:CZ	2:C:31:THR:HA	2.52	0.45
3:I:14:THR:HG22	3:I:15:LEU:HG	1.99	0.45
3:I:77:ASN:HD21	3:I:80:TYR:H	1.63	0.45
3:K:26:ILE:O	3:K:29:GLU:HG2	2.16	0.45
2:F:66:TRP:CE3	2:F:67:THR:HB	2.51	0.45
2:G:302:ASP:HB3	2:G:309:ILE:O	2.17	0.45
2:H:66:TRP:CE3	2:H:67:THR:HB	2.51	0.45
2:C:177:LYS:H	2:C:177:LYS:HG3	1.52	0.45
2:H:431:ARG:HB2	2:H:437:LEU:HD11	1.99	0.45
2:C:77:LEU:C	2:C:79:ARG:H	2.24	0.45
2:E:383:HIS:HE1	2:E:385:TRP:HB2	1.82	0.45
2:G:77:LEU:HD13	2:G:78:ASP:H	1.81	0.45
2:G:392:GLU:HG2	2:G:393:ILE:N	2.28	0.45
1:1:117:LEU:HA	1:1:117:LEU:HD23	1.78	0.45
1:2:106:LEU:H	1:2:106:LEU:HG	1.66	0.45
1:4:135:ASP:O	1:4:136:GLU:C	2.60	0.45
2:B:175:LYS:HB3	2:B:176:PRO:CD	2.46	0.45
2:C:78:ASP:C	2:C:80:TYR:H	2.25	0.45
2:C:339:ARG:O	2:C:343:LEU:HG	2.16	0.45
3:K:21:LEU:HD13	3:K:25:GLN:HB2	1.99	0.45
1:2:136:GLU:HB3	2:D:330:THR:O	2.17	0.45
1:3:70:LEU:H	1:3:70:LEU:HG	1.43	0.45
1:4:66:LYS:HD3	1:4:73:ALA:HA	1.99	0.45
2:C:383:HIS:HE1	2:C:385:TRP:HB2	1.82	0.45
2:F:172:CYS:SG	2:F:173:THR:N	2.90	0.45
2:G:191:GLU:HA	2:G:194:ARG:HG2	1.99	0.45
2:G:435:ARG:HE	2:G:435:ARG:HB3	1.58	0.45
2:H:174:ILE:H	2:H:174:ILE:HG12	1.53	0.45
3:I:2:GLN:HE21	3:I:2:GLN:HB2	1.58	0.45
3:J:14:THR:HG22	3:J:15:LEU:HG	1.99	0.45
3:K:78:ALA:O	3:K:79:GLY:C	2.59	0.45
3:J:82:LEU:HA	3:J:85:ILE:HD12	1.97	0.44
2:G:475:LEU:HD23	2:G:475:LEU:HA	1.73	0.44
2:H:409:HIS:CG	2:H:410:PRO:HD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:21:LEU:HD22	3:L:21:LEU:HA	1.85	0.44
2:D:342:THR:HA	2:D:345:PHE:CD2	2.53	0.44
2:G:305:ARG:HG3	2:G:473:ASP:CG	2.43	0.44
1:1:72:CYS:HB3	1:1:75:CYS:SG	2.58	0.44
2:B:20:TYR:C	2:B:22:LEU:H	2.26	0.44
2:C:191:GLU:HA	2:C:194:ARG:HG2	1.99	0.44
2:D:175:LYS:O	2:D:176:PRO:C	2.60	0.44
2:G:77:LEU:C	2:G:79:ARG:H	2.24	0.44
2:H:270:LEU:HD23	2:H:270:LEU:HA	1.86	0.44
3:K:21:LEU:HD22	3:K:21:LEU:HA	1.86	0.44
1:2:69:SER:HB2	1:2:71:VAL:HG23	1.99	0.44
2:B:342:THR:HA	2:B:345:PHE:CD2	2.53	0.44
2:B:431:ARG:HB2	2:B:437:LEU:HD11	1.99	0.44
2:C:95:ASN:O	2:C:96:GLN:NE2	2.36	0.44
2:E:128:LYS:C	2:E:130:LEU:H	2.26	0.44
2:A:128:LYS:C	2:A:130:LEU:H	2.26	0.44
2:B:66:TRP:CE3	2:B:67:THR:HB	2.52	0.44
2:D:172:CYS:SG	2:D:173:THR:N	2.90	0.44
2:E:475:LEU:HD23	2:E:475:LEU:HA	1.72	0.44
2:F:431:ARG:HB2	2:F:437:LEU:HD11	1.99	0.44
1:1:134:PHE:HE1	2:B:382:ILE:HG23	1.82	0.44
2:A:77:LEU:O	2:A:79:ARG:HG3	2.18	0.44
2:B:172:CYS:SG	2:B:173:THR:N	2.90	0.44
2:E:191:GLU:HA	2:E:194:ARG:HG2	1.99	0.44
2:H:45:GLN:HB2	2:H:46:PRO:HD2	2.00	0.44
1:2:87:LYS:HB3	1:2:87:LYS:HE2	1.52	0.44
1:2:130:PHE:CE1	2:C:60:GLU:HG2	2.53	0.44
2:A:191:GLU:HA	2:A:194:ARG:HG2	2.00	0.44
2:B:21:ARG:H	2:B:21:ARG:HG3	1.52	0.44
2:D:431:ARG:HB2	2:D:437:LEU:HD11	1.99	0.44
2:F:115:ASN:O	2:F:118:THR:HG22	2.18	0.44
2:B:116:MET:HE1	2:B:320:MET:HE1	1.99	0.44
2:B:409:HIS:CG	2:B:410:PRO:HD2	2.53	0.44
2:D:45:GLN:HG3	2:D:129:ALA:C	2.42	0.44
2:H:342:THR:HA	2:H:345:PHE:CD2	2.53	0.44
3:I:31:ASP:OD1	3:I:31:ASP:N	2.51	0.44
2:F:342:THR:HA	2:F:345:PHE:CD2	2.53	0.43
1:2:66:LYS:H	1:2:66:LYS:HG2	1.59	0.43
2:B:335:LEU:HD23	2:B:335:LEU:H	1.82	0.43
2:D:146:LYS:HB3	2:D:146:LYS:HE3	1.60	0.43
3:K:14:THR:HG22	3:K:15:LEU:HG	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:193:LEU:HD23	2:D:193:LEU:HA	1.90	0.43
2:D:457:ALA:O	2:D:461:VAL:HG12	2.18	0.43
2:E:201:KCX:HG2	2:E:239:TYR:CD2	2.50	0.43
2:H:172:CYS:SG	2:H:173:THR:N	2.90	0.43
2:H:229:GLN:HG3	2:H:234:GLU:O	2.19	0.43
3:K:105:ILE:HG22	3:K:106:ARG:HG2	1.99	0.43
2:B:457:ALA:O	2:B:461:VAL:HG12	2.19	0.43
2:D:382:ILE:HD11	2:D:401:GLN:O	2.18	0.43
2:E:342:THR:HA	2:E:345:PHE:CD2	2.54	0.43
2:F:18:LYS:HB3	2:F:18:LYS:HE2	1.67	0.43
2:F:175:LYS:O	2:F:176:PRO:C	2.61	0.43
2:F:334:LYS:HB2	2:F:335:LEU:H	1.59	0.43
1:2:97:PHE:HB3	1:2:100:GLN:CD	2.44	0.43
1:2:97:PHE:HB3	1:2:100:GLN:NE2	2.33	0.43
1:4:130:PHE:CD2	1:4:131:LEU:HG	2.53	0.43
2:D:338:GLU:C	2:D:340:GLU:H	2.27	0.43
3:L:26:ILE:O	3:L:29:GLU:HG2	2.18	0.43
1:1:134:PHE:HB3	1:1:135:ASP:H	1.60	0.43
1:4:130:PHE:HD2	1:4:131:LEU:HG	1.84	0.43
2:B:229:GLN:HG3	2:B:234:GLU:O	2.19	0.43
2:H:180:LEU:HD23	2:H:180:LEU:HA	1.90	0.43
3:L:14:THR:HG22	3:L:15:LEU:HG	2.00	0.43
1:4:72:CYS:HB3	1:4:75:CYS:SG	2.59	0.43
2:A:25:TYR:O	2:A:27:PRO:HD3	2.18	0.43
2:A:291:LEU:O	2:A:324:ASP:HB2	2.19	0.43
2:C:305:ARG:HG3	2:C:473:ASP:CG	2.44	0.43
2:C:357:ASP:OD2	2:C:360:ARG:HB2	2.19	0.43
2:D:229:GLN:HG3	2:D:234:GLU:O	2.19	0.43
1:3:134:PHE:HB3	1:3:135:ASP:H	1.69	0.43
2:B:201:KCX:HB2	2:B:201:KCX:HE2	1.40	0.43
2:A:77:LEU:HA	2:A:77:LEU:HD22	1.78	0.43
2:C:291:LEU:O	2:C:324:ASP:HB2	2.19	0.43
2:G:128:LYS:C	2:G:130:LEU:H	2.27	0.43
2:H:28:ASP:OD1	2:H:28:ASP:N	2.46	0.43
1:1:106:LEU:H	1:1:106:LEU:HG	1.64	0.42
1:1:127:ILE:O	1:1:128:GLY:C	2.62	0.42
1:4:134:PHE:HD1	1:4:134:PHE:HA	1.69	0.42
2:C:357:ASP:H	2:C:362:ILE:HB	1.83	0.42
2:D:133:LEU:HD12	2:D:133:LEU:HA	1.91	0.42
3:J:31:ASP:OD1	3:J:31:ASP:N	2.51	0.42
1:1:85:GLN:HB2	1:1:107:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:384:VAL:C	2:A:386:HIS:H	2.27	0.42
2:G:330:THR:HG22	2:G:378:ALA:HB1	2.01	0.42
1:1:66:LYS:CG	1:1:71:VAL:HB	2.49	0.42
2:B:450:LYS:HD2	2:B:450:LYS:HA	1.86	0.42
2:E:433:GLU:HG2	3:J:28:ARG:HD2	2.00	0.42
2:H:193:LEU:HD23	2:H:193:LEU:HA	1.90	0.42
2:D:409:HIS:CG	2:D:410:PRO:HD2	2.54	0.42
2:E:291:LEU:O	2:E:324:ASP:HB2	2.19	0.42
2:F:201:KCX:HB2	2:F:201:KCX:HE2	1.40	0.42
2:F:229:GLN:HG3	2:F:234:GLU:O	2.19	0.42
1:1:97:PHE:HB3	1:1:100:GLN:CD	2.45	0.42
2:A:268:ASP:OD1	2:A:268:ASP:N	2.53	0.42
2:E:28:ASP:O	2:E:29:TYR:C	2.62	0.42
2:F:338:GLU:C	2:F:340:GLU:H	2.27	0.42
1:4:92:ASN:HB3	1:4:96:HIS:CE1	2.49	0.42
2:A:475:LEU:HD23	2:A:475:LEU:HA	1.77	0.42
2:G:268:ASP:OD1	2:G:268:ASP:N	2.53	0.42
2:H:43:THR:CG2	2:H:132:ALA:HB3	2.49	0.42
3:K:31:ASP:OD1	3:K:31:ASP:N	2.52	0.42
1:2:75:CYS:O	1:2:78:GLU:HB2	2.20	0.42
2:D:331:VAL:HG12	2:D:342:THR:HG21	2.02	0.42
2:E:392:GLU:HG2	2:E:393:ILE:N	2.29	0.42
2:E:444:ILE:H	2:E:444:ILE:HG12	1.47	0.42
2:F:334:LYS:H	2:F:334:LYS:HG2	1.65	0.42
1:3:85:GLN:HB2	1:3:107:CYS:SG	2.60	0.42
2:B:338:GLU:C	2:B:340:GLU:H	2.27	0.42
2:E:77:LEU:C	2:E:79:ARG:H	2.28	0.42
1:3:92:ASN:HB3	1:3:96:HIS:CE1	2.52	0.42
2:B:133:LEU:HD12	2:B:133:LEU:HA	1.91	0.42
2:E:330:THR:HG22	2:E:378:ALA:HB1	2.02	0.42
2:G:437:LEU:HD23	2:G:437:LEU:HA	1.74	0.42
2:H:409:HIS:ND1	2:H:410:PRO:HD2	2.35	0.42
1:1:134:PHE:HD1	1:1:134:PHE:HA	1.70	0.42
1:4:95:ASP:CG	1:4:102:LYS:HA	2.45	0.42
2:A:78:ASP:C	2:A:80:TYR:H	2.28	0.42
2:A:330:THR:HG22	2:A:378:ALA:HB1	2.02	0.42
2:B:43:THR:CG2	2:B:132:ALA:HB3	2.50	0.42
2:B:201:KCX:OQ1	2:B:204:GLU:N	2.53	0.42
2:C:384:VAL:C	2:C:386:HIS:H	2.28	0.42
2:D:20:TYR:C	2:D:22:LEU:H	2.28	0.42
2:D:43:THR:CG2	2:D:132:ALA:HB3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:23:THR:C	2:E:25:TYR:H	2.28	0.42
2:E:384:VAL:C	2:E:386:HIS:H	2.28	0.42
2:F:82:GLY:C	2:F:83:ARG:HG3	2.45	0.42
2:H:338:GLU:C	2:H:340:GLU:H	2.27	0.42
2:C:407:LEU:HB3	2:D:69:VAL:HG13	2.01	0.41
1:4:107:CYS:HB3	1:4:110:CYS:SG	2.61	0.41
2:A:305:ARG:HH11	2:A:474:THR:HG23	1.84	0.41
2:G:459:CYS:O	2:G:463:LYS:HG3	2.20	0.41
1:1:66:LYS:H	1:1:66:LYS:HG2	1.49	0.41
1:1:75:CYS:CB	1:1:79:GLY:H	2.32	0.41
2:E:128:LYS:C	2:E:130:LEU:N	2.79	0.41
2:E:295:ARG:HG2	2:E:327:HIS:HB2	2.03	0.41
2:F:176:PRO:O	2:F:177:LYS:HG2	2.20	0.41
3:L:53:LEU:HD23	3:L:53:LEU:HA	1.88	0.41
1:2:66:LYS:CE	1:2:71:VAL:HB	2.44	0.41
2:A:56:ALA:O	2:A:60:GLU:HB2	2.21	0.41
2:C:330:THR:HG22	2:C:378:ALA:HB1	2.02	0.41
2:G:216:ASP:OD1	2:G:216:ASP:N	2.54	0.41
3:J:21:LEU:HD22	3:J:21:LEU:HA	1.88	0.41
1:3:121:CYS:O	1:3:121:CYS:SG	2.78	0.41
2:A:29:TYR:CE2	2:A:31:THR:HA	2.56	0.41
2:C:28:ASP:O	2:C:29:TYR:C	2.64	0.41
2:C:356:LYS:HE3	2:C:356:LYS:HB3	1.84	0.41
2:H:175:LYS:HB3	2:H:176:PRO:CD	2.46	0.41
3:L:37:LYS:HA	3:L:37:LYS:HD3	1.85	0.41
1:1:107:CYS:HB3	1:1:110:CYS:SG	2.61	0.41
1:2:121:CYS:O	1:2:121:CYS:SG	2.79	0.41
1:3:95:ASP:CG	1:3:102:LYS:HA	2.45	0.41
2:C:180:LEU:HD23	2:C:180:LEU:HA	1.82	0.41
1:2:85:GLN:HB2	1:2:107:CYS:SG	2.61	0.41
2:A:350:ARG:HD3	2:A:376:PRO:HD3	2.02	0.41
2:E:56:ALA:O	2:E:60:GLU:HB2	2.21	0.41
2:E:305:ARG:HG3	2:E:473:ASP:CG	2.45	0.41
1:1:87:LYS:HE3	1:1:87:LYS:HB3	1.48	0.41
1:3:134:PHE:HD1	1:3:134:PHE:HA	1.67	0.41
1:4:109:LEU:HD11	2:H:457:ALA:HB1	2.03	0.41
2:C:79:ARG:HE	2:C:79:ARG:HB2	1.75	0.41
2:F:20:TYR:C	2:F:22:LEU:H	2.29	0.41
2:H:45:GLN:CB	2:H:131:ARG:HH11	2.33	0.41
2:D:180:LEU:HD23	2:D:180:LEU:HA	1.90	0.41
2:D:270:LEU:HD23	2:D:270:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:135:ASP:CG	2:H:329:GLY:HA2	2.46	0.40
2:D:448:ALA:HA	2:D:451:TRP:HE1	1.87	0.40
3:I:21:LEU:HD22	3:I:21:LEU:HA	1.87	0.40
3:L:105:ILE:HG22	3:L:106:ARG:HG2	2.02	0.40
1:4:117:LEU:HD21	1:4:122:ASN:CA	2.48	0.40
2:A:334:LYS:O	2:B:128:LYS:HG2	2.20	0.40
2:A:444:ILE:H	2:A:444:ILE:HG12	1.49	0.40
2:A:462:TRP:HA	2:A:465:ILE:HD11	2.03	0.40
2:D:77:LEU:C	2:D:79:ARG:N	2.80	0.40
2:E:472:ILE:HG13	2:E:473:ASP:N	2.35	0.40
2:G:78:ASP:C	2:G:80:TYR:H	2.30	0.40
2:G:384:VAL:C	2:G:386:HIS:H	2.29	0.40
2:C:295:ARG:HG2	2:C:327:HIS:HB2	2.03	0.40
1:1:106:LEU:HD13	1:1:111:ARG:HA	2.03	0.40
1:1:130:PHE:CE2	2:A:60:GLU:HG2	2.56	0.40
1:2:70:LEU:HG	2:C:52:GLU:CD	2.47	0.40
2:A:339:ARG:O	2:A:343:LEU:HG	2.21	0.40
2:B:331:VAL:HG12	2:B:342:THR:HG21	2.02	0.40
2:C:216:ASP:OD1	2:C:216:ASP:N	2.54	0.40
2:D:65:THR:HG22	2:D:66:TRP:CD1	2.57	0.40
2:G:336:GLU:HA	2:H:128:LYS:HD3	2.02	0.40
1:3:96:HIS:HB2	1:3:101:PHE:CD2	2.57	0.40
1:3:109:LEU:CD1	2:F:457:ALA:HB1	2.50	0.40
2:D:202:ASP:HB3	2:D:203:ASP:H	1.60	0.40
2:E:37:LEU:O	2:E:138:LEU:HD23	2.22	0.40
2:F:193:LEU:HD23	2:F:193:LEU:HA	1.90	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	1	71/136 (52%)	49 (69%)	16 (22%)	6 (8%)	0	1
1	2	71/136 (52%)	44 (62%)	20 (28%)	7 (10%)	0	1
1	3	71/136 (52%)	48 (68%)	18 (25%)	5 (7%)	1	2
1	4	71/136 (52%)	48 (68%)	19 (27%)	4 (6%)	1	4
2	A	447/475 (94%)	402 (90%)	38 (8%)	7 (2%)	7	27
2	B	452/475 (95%)	405 (90%)	43 (10%)	4 (1%)	14	41
2	C	447/475 (94%)	403 (90%)	36 (8%)	8 (2%)	6	25
2	D	452/475 (95%)	401 (89%)	45 (10%)	6 (1%)	9	32
2	E	447/475 (94%)	396 (89%)	43 (10%)	8 (2%)	6	25
2	F	452/475 (95%)	402 (89%)	42 (9%)	8 (2%)	6	25
2	G	447/475 (94%)	396 (89%)	43 (10%)	8 (2%)	6	25
2	H	452/475 (95%)	405 (90%)	43 (10%)	4 (1%)	14	41
3	I	116/125 (93%)	104 (90%)	12 (10%)	0	100	100
3	J	116/125 (93%)	103 (89%)	12 (10%)	1 (1%)	14	41
3	K	116/125 (93%)	103 (89%)	13 (11%)	0	100	100
3	L	116/125 (93%)	101 (87%)	15 (13%)	0	100	100
All	All	4344/4844 (90%)	3810 (88%)	458 (10%)	76 (2%)	9	26

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	176	PRO
2	F	176	PRO
1	1	135	ASP
1	2	134	PHE
1	4	89	GLY
1	4	120	ASP
1	4	135	ASP
2	B	381	GLY
2	C	71	THR
2	D	451	TRP
2	F	122	GLY
2	G	28	ASP
1	1	89	GLY
1	2	120	ASP
1	3	89	GLY
2	A	123	ASN

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Mol	Chain	Res	Type
2	C	28	ASP
2	C	123	ASN
2	E	71	THR
2	F	77	LEU
2	F	79	ARG
2	G	71	THR
1	1	120	ASP
1	1	134	PHE
1	3	120	ASP
1	3	134	PHE
2	A	71	THR
2	B	68	THR
2	B	77	LEU
2	D	68	THR
2	D	77	LEU
2	E	28	ASP
2	E	123	ASN
2	E	474	THR
2	F	68	THR
2	H	68	THR
1	2	89	GLY
1	2	127	ILE
2	A	28	ASP
2	A	122	GLY
2	A	178	LEU
2	C	122	GLY
2	C	178	LEU
2	C	339	ARG
2	D	381	GLY
2	E	122	GLY
2	E	178	LEU
2	F	381	GLY
2	G	122	GLY
2	G	123	ASN
2	G	178	LEU
2	H	77	LEU
1	3	113	LYS
2	F	76	SER
2	G	474	THR
3	J	68	TRP
1	1	127	ILE
1	3	94	ILE

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Mol	Chain	Res	Type
2	C	369	VAL
1	2	104	GLY
1	2	128	GLY
1	4	94	ILE
2	A	380	GLY
2	B	369	VAL
2	C	380	GLY
2	D	369	VAL
2	E	380	GLY
2	F	369	VAL
2	G	380	GLY
2	H	369	VAL
1	1	94	ILE
1	2	88	GLY
2	A	369	VAL
2	E	369	VAL
2	G	369	VAL
2	H	381	GLY

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	1	54/114 (47%)	31 (57%)	23 (43%)	0	0
1	2	54/114 (47%)	29 (54%)	25 (46%)	0	0
1	3	54/114 (47%)	25 (46%)	29 (54%)	0	0
1	4	54/114 (47%)	25 (46%)	29 (54%)	0	0
2	A	366/384 (95%)	314 (86%)	52 (14%)	3	11
2	B	366/384 (95%)	326 (89%)	40 (11%)	6	20
2	C	366/384 (95%)	315 (86%)	51 (14%)	3	11
2	D	366/384 (95%)	334 (91%)	32 (9%)	9	30
2	E	366/384 (95%)	310 (85%)	56 (15%)	3	9
2	F	366/384 (95%)	326 (89%)	40 (11%)	6	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	366/384 (95%)	307 (84%)	59 (16%)	2	8
2	H	366/384 (95%)	336 (92%)	30 (8%)	10	32
3	I	105/112 (94%)	92 (88%)	13 (12%)	4	15
3	J	105/112 (94%)	88 (84%)	17 (16%)	2	8
3	K	105/112 (94%)	90 (86%)	15 (14%)	3	11
3	L	105/112 (94%)	83 (79%)	22 (21%)	1	4
All	All	3564/3976 (90%)	3031 (85%)	533 (15%)	5	10

All (533) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	65	THR
1	1	66	LYS
1	1	68	ASN
1	1	70	LEU
1	1	74	ASN
1	1	81	VAL
1	1	87	LYS
1	1	91	VAL
1	1	93	LEU
1	1	94	ILE
1	1	98	ASN
1	1	102	LYS
1	1	106	LEU
1	1	109	LEU
1	1	113	LYS
1	1	114	LYS
1	1	116	VAL
1	1	117	LEU
1	1	120	ASP
1	1	127	ILE
1	1	130	PHE
1	1	132	SER
1	1	134	PHE
1	2	65	THR
1	2	66	LYS
1	2	68	ASN
1	2	69	SER
1	2	70	LEU
1	2	71	VAL

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Mol	Chain	Res	Type
1	2	78	GLU
1	2	81	VAL
1	2	87	LYS
1	2	91	VAL
1	2	93	LEU
1	2	94	ILE
1	2	98	ASN
1	2	102	LYS
1	2	106	LEU
1	2	109	LEU
1	2	113	LYS
1	2	114	LYS
1	2	116	VAL
1	2	117	LEU
1	2	120	ASP
1	2	131	LEU
1	2	132	SER
1	2	133	THR
1	2	134	PHE
1	3	65	THR
1	3	66	LYS
1	3	68	ASN
1	3	69	SER
1	3	70	LEU
1	3	71	VAL
1	3	74	ASN
1	3	78	GLU
1	3	80	CYS
1	3	81	VAL
1	3	87	LYS
1	3	91	VAL
1	3	93	LEU
1	3	94	ILE
1	3	98	ASN
1	3	100	GLN
1	3	102	LYS
1	3	106	LEU
1	3	109	LEU
1	3	113	LYS
1	3	114	LYS
1	3	116	VAL
1	3	117	LEU

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Mol	Chain	Res	Type
1	3	120	ASP
1	3	126	PHE
1	3	130	PHE
1	3	132	SER
1	3	134	PHE
1	3	136	GLU
1	4	65	THR
1	4	66	LYS
1	4	68	ASN
1	4	69	SER
1	4	70	LEU
1	4	71	VAL
1	4	78	GLU
1	4	80	CYS
1	4	87	LYS
1	4	91	VAL
1	4	93	LEU
1	4	94	ILE
1	4	98	ASN
1	4	100	GLN
1	4	102	LYS
1	4	106	LEU
1	4	109	LEU
1	4	111	ARG
1	4	113	LYS
1	4	114	LYS
1	4	116	VAL
1	4	117	LEU
1	4	118	CYS
1	4	120	ASP
1	4	126	PHE
1	4	130	PHE
1	4	133	THR
1	4	134	PHE
1	4	136	GLU
2	A	22	LEU
2	A	28	ASP
2	A	32	LYS
2	A	33	ASP
2	A	41	ARG
2	A	51	GLU
2	A	60	GLU

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Mol	Chain	Res	Type
2	A	72	ASP
2	A	76	SER
2	A	77	LEU
2	A	78	ASP
2	A	79	ARG
2	A	81	LYS
2	A	83	ARG
2	A	87	ILE
2	A	96	GLN
2	A	121	VAL
2	A	124	VAL
2	A	128	LYS
2	A	130	LEU
2	A	172	CYS
2	A	173	THR
2	A	177	LYS
2	A	183	LYS
2	A	192	CYS
2	A	203	ASP
2	A	216	ASP
2	A	268	ASP
2	A	295	ARG
2	A	302	ASP
2	A	303	ARG
2	A	326	ILE
2	A	331	VAL
2	A	336	GLU
2	A	338	GLU
2	A	340	GLU
2	A	347	ASP
2	A	360	ARG
2	A	384	VAL
2	A	392	GLU
2	A	435	ARG
2	A	439	ARG
2	A	440	GLU
2	A	444	ILE
2	A	450	LYS
2	A	463	LYS
2	A	464	GLU
2	A	465	ILE
2	A	466	LYS

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Mol	Chain	Res	Type
2	A	472	ILE
2	A	474	THR
2	A	475	LEU
2	B	18	LYS
2	B	21	ARG
2	B	23	THR
2	B	28	ASP
2	B	30	GLU
2	B	32	LYS
2	B	40	PHE
2	B	43	THR
2	B	60	GLU
2	B	63	THR
2	B	65	THR
2	B	71	THR
2	B	74	LEU
2	B	75	THR
2	B	77	LEU
2	B	78	ASP
2	B	80	TYR
2	B	81	LYS
2	B	83	ARG
2	B	88	GLU
2	B	131	ARG
2	B	146	LYS
2	B	173	THR
2	B	174	ILE
2	B	175	LYS
2	B	177	LYS
2	B	178	LEU
2	B	180	LEU
2	B	216	ASP
2	B	246	THR
2	B	295	ARG
2	B	330	THR
2	B	334	LYS
2	B	339	ARG
2	B	382	ILE
2	B	387	MET
2	B	407	LEU
2	B	444	ILE
2	B	461	VAL

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Mol	Chain	Res	Type
2	B	463	LYS
2	C	22	LEU
2	C	28	ASP
2	C	32	LYS
2	C	33	ASP
2	C	36	ILE
2	C	41	ARG
2	C	51	GLU
2	C	60	GLU
2	C	69	VAL
2	C	72	ASP
2	C	76	SER
2	C	77	LEU
2	C	78	ASP
2	C	79	ARG
2	C	81	LYS
2	C	83	ARG
2	C	87	ILE
2	C	96	GLN
2	C	121	VAL
2	C	124	VAL
2	C	172	CYS
2	C	173	THR
2	C	177	LYS
2	C	183	LYS
2	C	192	CYS
2	C	216	ASP
2	C	268	ASP
2	C	295	ARG
2	C	302	ASP
2	C	303	ARG
2	C	326	ILE
2	C	331	VAL
2	C	340	GLU
2	C	341	VAL
2	C	355	GLU
2	C	360	ARG
2	C	369	VAL
2	C	371	MET
2	C	384	VAL
2	C	431	ARG
2	C	435	ARG

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Mol	Chain	Res	Type
2	C	439	ARG
2	C	443	ASP
2	C	444	ILE
2	C	463	LYS
2	C	464	GLU
2	C	465	ILE
2	C	466	LYS
2	C	472	ILE
2	C	474	THR
2	C	475	LEU
2	D	18	LYS
2	D	19	ASP
2	D	21	ARG
2	D	22	LEU
2	D	23	THR
2	D	40	PHE
2	D	43	THR
2	D	60	GLU
2	D	65	THR
2	D	71	THR
2	D	74	LEU
2	D	75	THR
2	D	77	LEU
2	D	78	ASP
2	D	81	LYS
2	D	88	GLU
2	D	131	ARG
2	D	173	THR
2	D	174	ILE
2	D	175	LYS
2	D	177	LYS
2	D	178	LEU
2	D	216	ASP
2	D	246	THR
2	D	295	ARG
2	D	339	ARG
2	D	387	MET
2	D	444	ILE
2	D	450	LYS
2	D	455	LEU
2	D	460	GLU
2	D	461	VAL

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Mol	Chain	Res	Type
2	E	22	LEU
2	E	23	THR
2	E	32	LYS
2	E	33	ASP
2	E	36	ILE
2	E	41	ARG
2	E	51	GLU
2	E	60	GLU
2	E	69	VAL
2	E	72	ASP
2	E	77	LEU
2	E	78	ASP
2	E	79	ARG
2	E	81	LYS
2	E	83	ARG
2	E	87	ILE
2	E	96	GLN
2	E	121	VAL
2	E	124	VAL
2	E	128	LYS
2	E	130	LEU
2	E	172	CYS
2	E	173	THR
2	E	175	LYS
2	E	177	LYS
2	E	183	LYS
2	E	192	CYS
2	E	203	ASP
2	E	216	ASP
2	E	268	ASP
2	E	295	ARG
2	E	302	ASP
2	E	303	ARG
2	E	326	ILE
2	E	331	VAL
2	E	336	GLU
2	E	338	GLU
2	E	340	GLU
2	E	360	ARG
2	E	369	VAL
2	E	371	MET
2	E	384	VAL

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Mol	Chain	Res	Type
2	E	392	GLU
2	E	435	ARG
2	E	439	ARG
2	E	440	GLU
2	E	443	ASP
2	E	444	ILE
2	E	447	GLU
2	E	450	LYS
2	E	463	LYS
2	E	464	GLU
2	E	465	ILE
2	E	472	ILE
2	E	474	THR
2	E	475	LEU
2	F	14	LYS
2	F	18	LYS
2	F	22	LEU
2	F	23	THR
2	F	30	GLU
2	F	32	LYS
2	F	40	PHE
2	F	43	THR
2	F	45	GLN
2	F	60	GLU
2	F	63	THR
2	F	65	THR
2	F	71	THR
2	F	74	LEU
2	F	77	LEU
2	F	78	ASP
2	F	81	LYS
2	F	88	GLU
2	F	118	THR
2	F	119	SER
2	F	120	ILE
2	F	121	VAL
2	F	130	LEU
2	F	139	ARG
2	F	146	LYS
2	F	173	THR
2	F	175	LYS
2	F	177	LYS

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Mol	Chain	Res	Type
2	F	178	LEU
2	F	216	ASP
2	F	246	THR
2	F	295	ARG
2	F	331	VAL
2	F	334	LYS
2	F	339	ARG
2	F	382	ILE
2	F	387	MET
2	F	444	ILE
2	F	460	GLU
2	F	461	VAL
2	G	22	LEU
2	G	28	ASP
2	G	32	LYS
2	G	33	ASP
2	G	36	ILE
2	G	41	ARG
2	G	51	GLU
2	G	52	GLU
2	G	60	GLU
2	G	69	VAL
2	G	72	ASP
2	G	76	SER
2	G	77	LEU
2	G	78	ASP
2	G	81	LYS
2	G	83	ARG
2	G	96	GLN
2	G	121	VAL
2	G	123	ASN
2	G	124	VAL
2	G	128	LYS
2	G	130	LEU
2	G	172	CYS
2	G	173	THR
2	G	175	LYS
2	G	177	LYS
2	G	183	LYS
2	G	192	CYS
2	G	203	ASP
2	G	216	ASP

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Mol	Chain	Res	Type
2	G	268	ASP
2	G	295	ARG
2	G	302	ASP
2	G	303	ARG
2	G	326	ILE
2	G	331	VAL
2	G	336	GLU
2	G	338	GLU
2	G	340	GLU
2	G	341	VAL
2	G	369	VAL
2	G	371	MET
2	G	391	THR
2	G	392	GLU
2	G	401	GLN
2	G	431	ARG
2	G	435	ARG
2	G	437	LEU
2	G	440	GLU
2	G	443	ASP
2	G	444	ILE
2	G	447	GLU
2	G	450	LYS
2	G	463	LYS
2	G	464	GLU
2	G	465	ILE
2	G	472	ILE
2	G	474	THR
2	G	475	LEU
2	H	14	LYS
2	H	18	LYS
2	H	19	ASP
2	H	22	LEU
2	H	23	THR
2	H	40	PHE
2	H	43	THR
2	H	60	GLU
2	H	63	THR
2	H	65	THR
2	H	74	LEU
2	H	77	LEU
2	H	78	ASP

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Mol	Chain	Res	Type
2	H	80	TYR
2	H	88	GLU
2	H	128	LYS
2	H	131	ARG
2	H	173	THR
2	H	174	ILE
2	H	175	LYS
2	H	177	LYS
2	H	178	LEU
2	H	216	ASP
2	H	246	THR
2	H	331	VAL
2	H	339	ARG
2	H	382	ILE
2	H	387	MET
2	H	444	ILE
2	H	461	VAL
3	I	1	MET
3	I	2	GLN
3	I	5	ASN
3	I	21	LEU
3	I	22	THR
3	I	25	GLN
3	I	29	GLU
3	I	31	ASP
3	I	42	LEU
3	I	72	MET
3	I	77	ASN
3	I	105	ILE
3	I	107	GLN
3	J	1	MET
3	J	2	GLN
3	J	8	ASP
3	J	21	LEU
3	J	22	THR
3	J	25	GLN
3	J	29	GLU
3	J	31	ASP
3	J	37	LYS
3	J	39	ILE
3	J	42	LEU
3	J	72	MET

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Mol	Chain	Res	Type
3	J	77	ASN
3	J	103	ASP
3	J	105	ILE
3	J	106	ARG
3	J	107	GLN
3	K	1	MET
3	K	2	GLN
3	K	7	ILE
3	K	8	ASP
3	K	21	LEU
3	K	22	THR
3	K	23	ASP
3	K	29	GLU
3	K	31	ASP
3	K	42	LEU
3	K	72	MET
3	K	77	ASN
3	K	104	ASN
3	K	105	ILE
3	K	106	ARG
3	L	1	MET
3	L	2	GLN
3	L	7	ILE
3	L	13	GLU
3	L	14	THR
3	L	21	LEU
3	L	22	THR
3	L	23	ASP
3	L	25	GLN
3	L	29	GLU
3	L	31	ASP
3	L	35	ARG
3	L	37	LYS
3	L	42	LEU
3	L	70	LEU
3	L	72	MET
3	L	77	ASN
3	L	89	LYS
3	L	100	LEU
3	L	104	ASN
3	L	105	ILE
3	L	106	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	92	ASN
1	1	96	HIS
1	2	98	ASN
1	3	96	HIS
1	4	96	HIS
1	4	122	ASN
2	A	115	ASN
2	A	123	ASN
2	A	207	ASN
2	A	229	GLN
2	A	292	HIS
2	A	294	HIS
2	A	298	HIS
2	A	307	HIS
2	A	325	HIS
2	A	327	HIS
2	A	383	HIS
2	B	45	GLN
2	B	298	HIS
2	B	327	HIS
2	C	115	ASN
2	C	153	HIS
2	C	229	GLN
2	C	294	HIS
2	C	298	HIS
2	C	307	HIS
2	C	327	HIS
2	C	383	HIS
2	D	96	GLN
2	D	287	ASN
2	D	298	HIS
2	D	307	HIS
2	D	327	HIS
2	D	413	ASN
2	E	115	ASN
2	E	153	HIS
2	E	156	GLN
2	E	229	GLN
2	E	294	HIS
2	E	298	HIS
2	E	307	HIS

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Mol	Chain	Res	Type
2	E	327	HIS
2	E	383	HIS
2	F	45	GLN
2	F	96	GLN
2	F	287	ASN
2	F	298	HIS
2	F	307	HIS
2	F	327	HIS
2	F	413	ASN
2	G	115	ASN
2	G	123	ASN
2	G	229	GLN
2	G	294	HIS
2	G	298	HIS
2	G	304	GLN
2	G	327	HIS
2	G	383	HIS
2	G	429	GLN
2	H	45	GLN
2	H	96	GLN
2	H	123	ASN
2	H	298	HIS
2	H	307	HIS
2	H	401	GLN
2	H	413	ASN
3	I	2	GLN
3	J	5	ASN
3	K	2	GLN
3	K	77	ASN
3	L	2	GLN
3	L	87	HIS
3	L	116	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	KCX	A	201	4,2	10,11,12	0.47	0	6,12,14	0.41	0
2	KCX	G	201	4,2	10,11,12	0.46	0	6,12,14	0.41	0
2	KCX	E	201	4,2	10,11,12	0.47	0	6,12,14	0.43	0
2	KCX	H	201	2	10,11,12	0.75	0	6,12,14	0.94	0
2	KCX	D	201	2	10,11,12	0.75	0	6,12,14	0.94	0
2	KCX	C	201	4,2	10,11,12	0.46	0	6,12,14	0.41	0
2	KCX	B	201	2	10,11,12	0.75	0	6,12,14	0.95	0
2	KCX	F	201	2	10,11,12	0.76	0	6,12,14	0.95	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KCX	A	201	4,2	-	3/9/10/12	-
2	KCX	G	201	4,2	-	3/9/10/12	-
2	KCX	E	201	4,2	-	4/9/10/12	-
2	KCX	H	201	2	-	6/9/10/12	-
2	KCX	D	201	2	-	6/9/10/12	-
2	KCX	C	201	4,2	-	3/9/10/12	-
2	KCX	B	201	2	-	6/9/10/12	-
2	KCX	F	201	2	-	6/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	KCX	OQ1-CX-NZ-CE
2	A	201	KCX	OQ2-CX-NZ-CE

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Mol	Chain	Res	Type	Atoms
2	B	201	KCX	C-CA-CB-CG
2	B	201	KCX	OQ1-CX-NZ-CE
2	B	201	KCX	OQ2-CX-NZ-CE
2	C	201	KCX	OQ1-CX-NZ-CE
2	C	201	KCX	OQ2-CX-NZ-CE
2	D	201	KCX	C-CA-CB-CG
2	D	201	KCX	OQ1-CX-NZ-CE
2	D	201	KCX	OQ2-CX-NZ-CE
2	E	201	KCX	OQ1-CX-NZ-CE
2	E	201	KCX	OQ2-CX-NZ-CE
2	F	201	KCX	C-CA-CB-CG
2	F	201	KCX	OQ1-CX-NZ-CE
2	F	201	KCX	OQ2-CX-NZ-CE
2	G	201	KCX	OQ1-CX-NZ-CE
2	G	201	KCX	OQ2-CX-NZ-CE
2	H	201	KCX	C-CA-CB-CG
2	H	201	KCX	OQ1-CX-NZ-CE
2	H	201	KCX	OQ2-CX-NZ-CE
2	B	201	KCX	CE-CD-CG-CB
2	D	201	KCX	CE-CD-CG-CB
2	F	201	KCX	CE-CD-CG-CB
2	H	201	KCX	CE-CD-CG-CB
2	A	201	KCX	CG-CD-CE-NZ
2	C	201	KCX	CG-CD-CE-NZ
2	E	201	KCX	CG-CD-CE-NZ
2	G	201	KCX	CG-CD-CE-NZ
2	B	201	KCX	CG-CD-CE-NZ
2	D	201	KCX	CG-CD-CE-NZ
2	F	201	KCX	CG-CD-CE-NZ
2	H	201	KCX	CG-CD-CE-NZ
2	D	201	KCX	CA-CB-CG-CD
2	H	201	KCX	CA-CB-CG-CD
2	B	201	KCX	CA-CB-CG-CD
2	F	201	KCX	CA-CB-CG-CD
2	E	201	KCX	CE-CD-CG-CB

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	KCX	1	0
2	G	201	KCX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	201	KCX	2	0
2	H	201	KCX	2	0
2	D	201	KCX	3	0
2	C	201	KCX	1	0
2	B	201	KCX	4	0
2	F	201	KCX	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
5	CAP	A	502	4	18,20,20	0.97	1 (5%)	23,31,31	1.18	2 (8%)
5	CAP	E	502	4	18,20,20	0.94	1 (5%)	23,31,31	1.17	2 (8%)
5	CAP	C	502	4	18,20,20	0.97	1 (5%)	23,31,31	1.12	2 (8%)
5	CAP	G	502	4	18,20,20	0.97	1 (5%)	23,31,31	1.12	2 (8%)

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
5	CAP	A	502	4	-	10/29/29/29	-
5	CAP	E	502	4	-	8/29/29/29	-
5	CAP	C	502	4	-	8/29/29/29	-
5	CAP	G	502	4	-	8/29/29/29	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	502	CAP	C2-C	-2.75	1.50	1.53
5	A	502	CAP	C2-C	-2.73	1.50	1.53
5	C	502	CAP	C2-C	-2.70	1.51	1.53
5	E	502	CAP	C2-C	-2.61	1.51	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	502	CAP	O7-C-C2	3.11	119.26	114.06
5	E	502	CAP	O7-C-C2	3.08	119.22	114.06
5	G	502	CAP	O7-C-C2	2.81	118.77	114.06
5	C	502	CAP	O7-C-C2	2.78	118.71	114.06
5	A	502	CAP	O6-C-C2	-2.51	117.65	122.32
5	E	502	CAP	O6-C-C2	-2.28	118.07	122.32
5	G	502	CAP	O6-C-C2	-2.24	118.15	122.32
5	C	502	CAP	O6-C-C2	-2.23	118.16	122.32

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	CAP	O7-C-C2-C1
5	A	502	CAP	O6-C-C2-O2
5	A	502	CAP	O7-C-C2-O2
5	A	502	CAP	C2-C3-C4-O4
5	A	502	CAP	O3-C3-C4-O4
5	A	502	CAP	O4-C4-C5-O5
5	C	502	CAP	O6-C-C2-C1
5	C	502	CAP	O7-C-C2-C1
5	C	502	CAP	O6-C-C2-O2
5	C	502	CAP	O7-C-C2-O2
5	C	502	CAP	C2-C3-C4-O4
5	C	502	CAP	O3-C3-C4-O4
5	C	502	CAP	O4-C4-C5-O5
5	E	502	CAP	O6-C-C2-C1
5	E	502	CAP	O7-C-C2-C1
5	E	502	CAP	O6-C-C2-O2
5	E	502	CAP	O7-C-C2-O2
5	E	502	CAP	C2-C3-C4-O4
5	E	502	CAP	O3-C3-C4-O4
5	E	502	CAP	O4-C4-C5-O5

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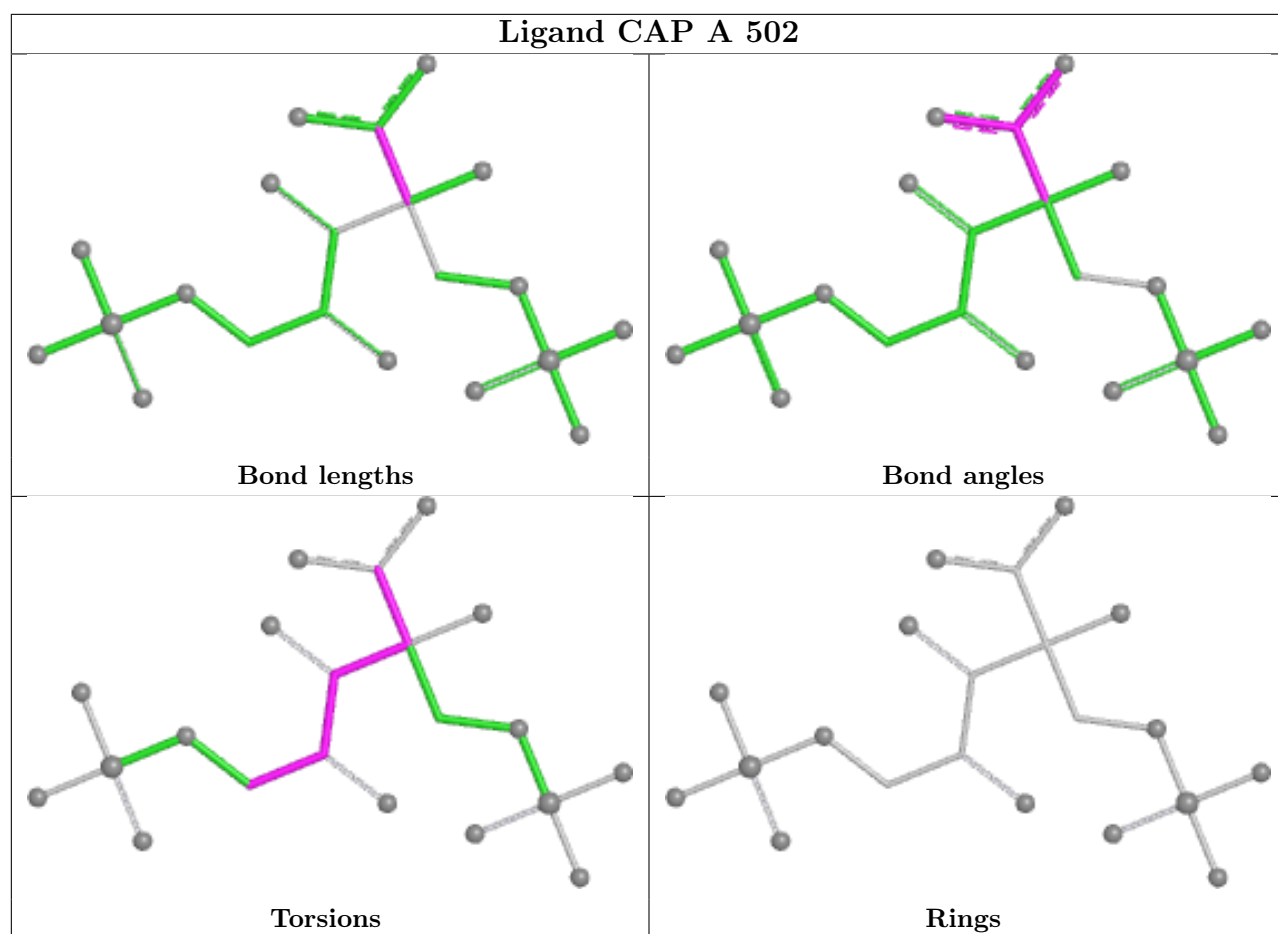
Continued from previous page...

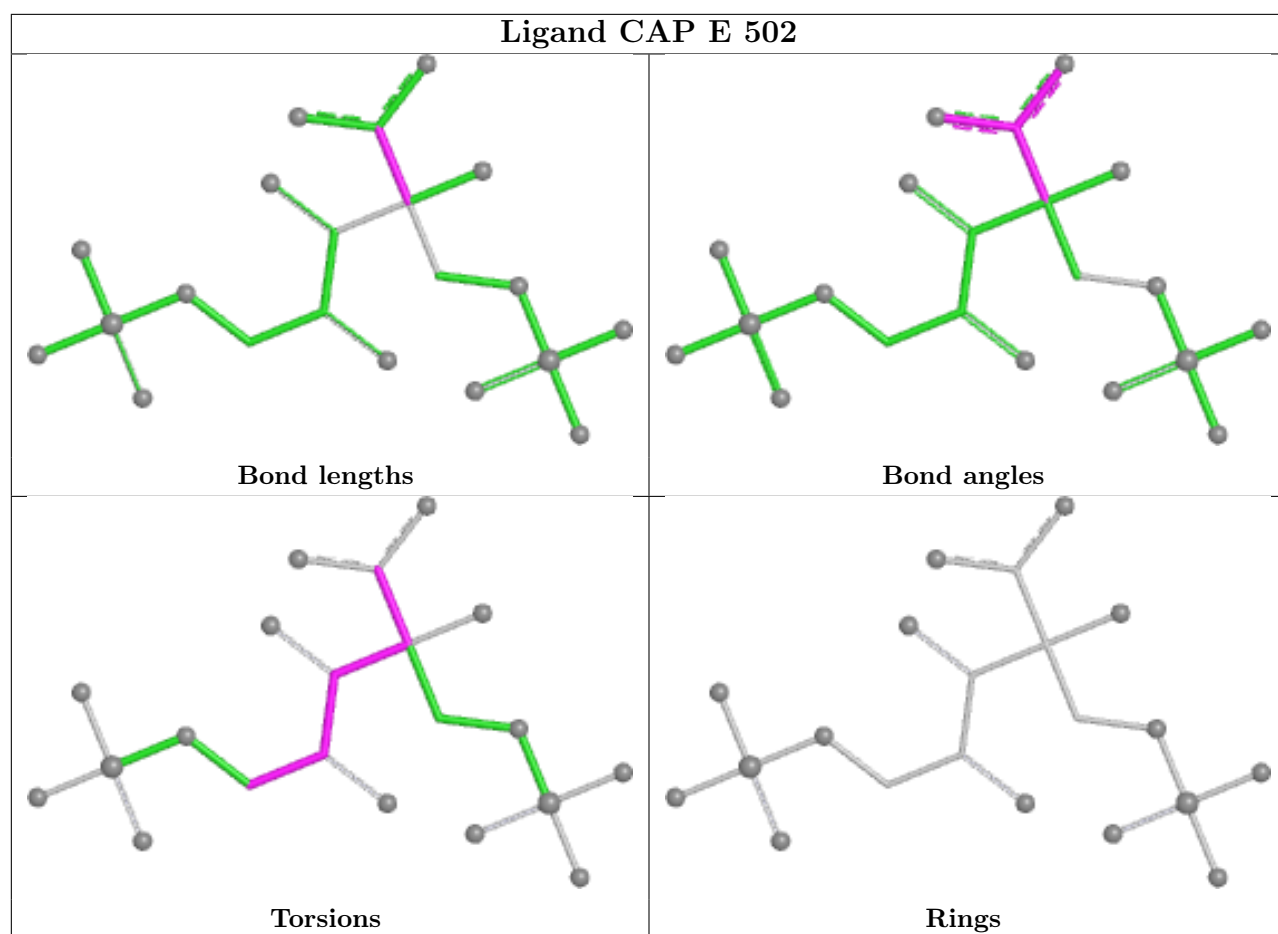
Mol	Chain	Res	Type	Atoms
5	G	502	CAP	O7-C-C2-C1
5	G	502	CAP	O6-C-C2-O2
5	G	502	CAP	O7-C-C2-O2
5	G	502	CAP	C2-C3-C4-O4
5	G	502	CAP	O3-C3-C4-O4
5	G	502	CAP	O4-C4-C5-O5
5	G	502	CAP	O6-C-C2-C1
5	A	502	CAP	O6-C-C2-C1
5	A	502	CAP	O2-C2-C3-C4
5	C	502	CAP	O2-C2-C3-C4
5	E	502	CAP	O2-C2-C3-C4
5	G	502	CAP	O2-C2-C3-C4
5	A	502	CAP	O7-C-C2-C3
5	A	502	CAP	O6-C-C2-C3

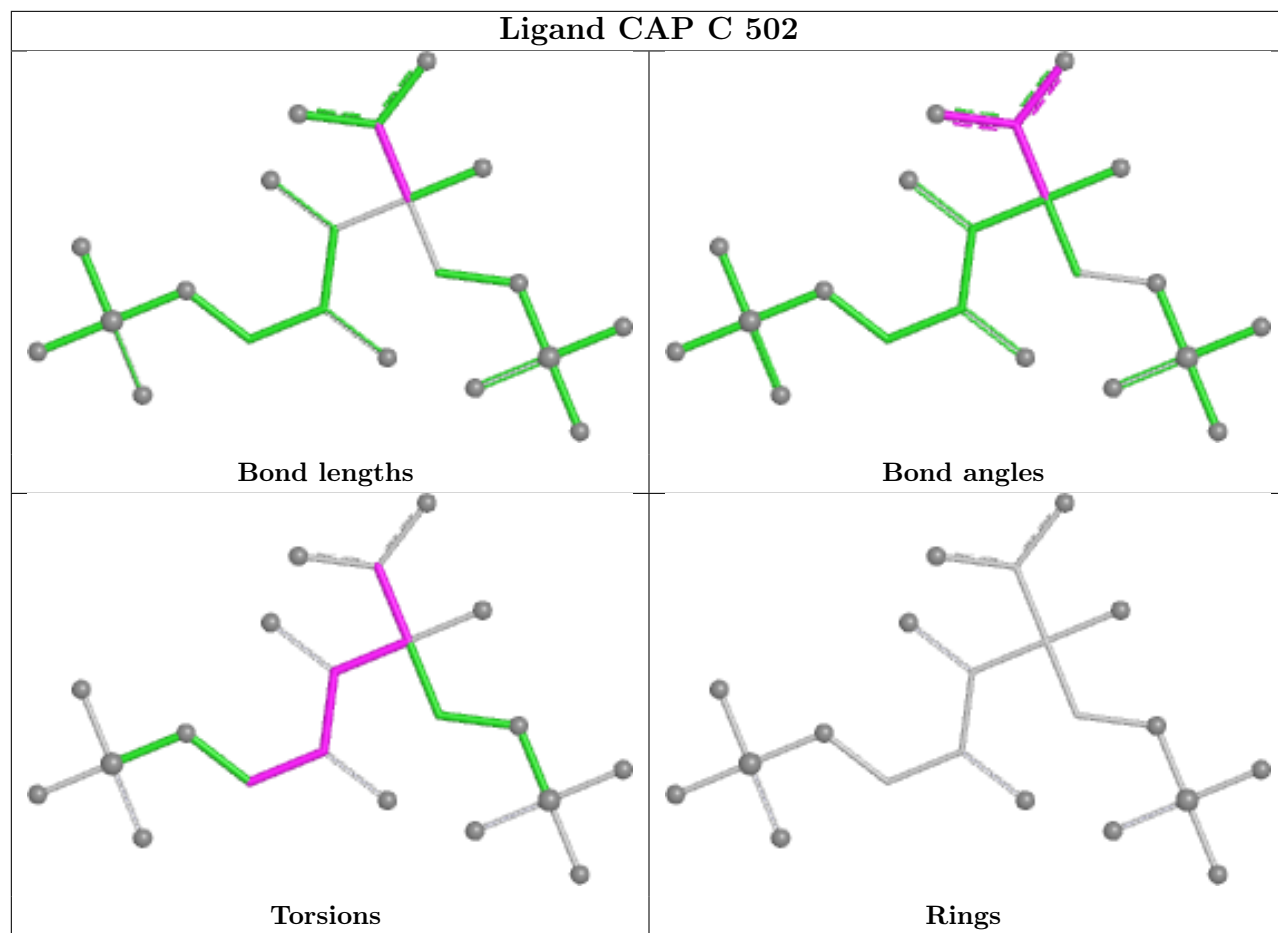
There are no ring outliers.

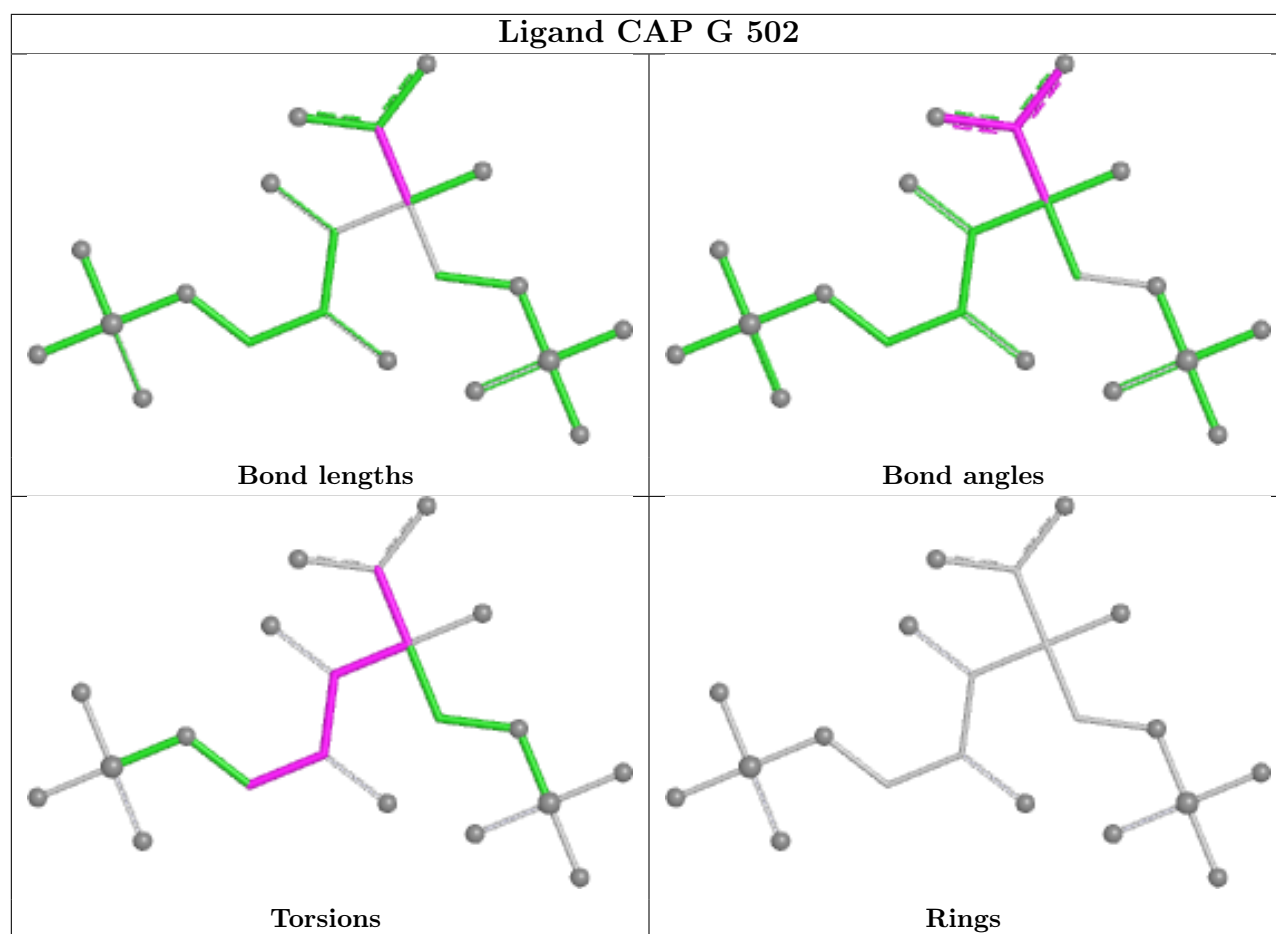
No monomer is involved in short contacts.

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.

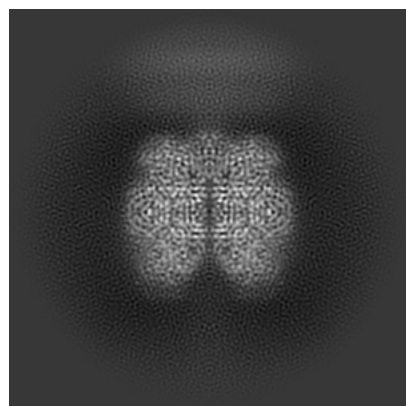
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45608. These allow visual inspection of the internal detail of the map and identification of artifacts.

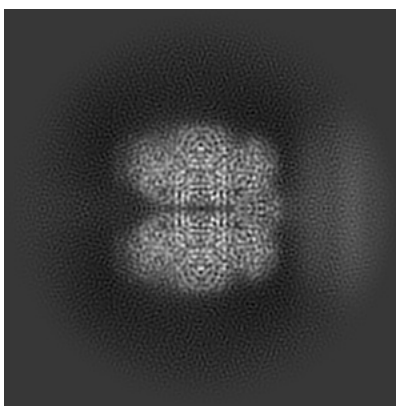
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

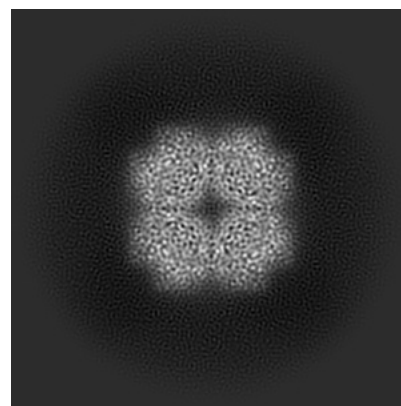
6.1.1 Primary map



X

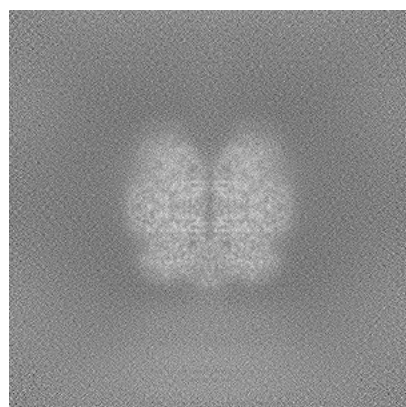


Y

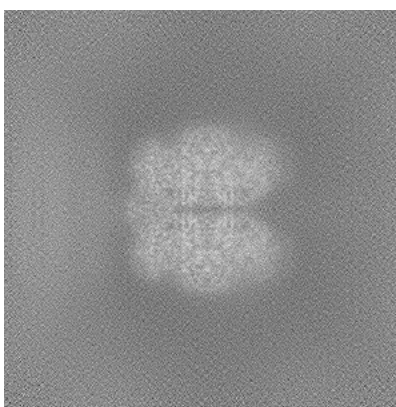


Z

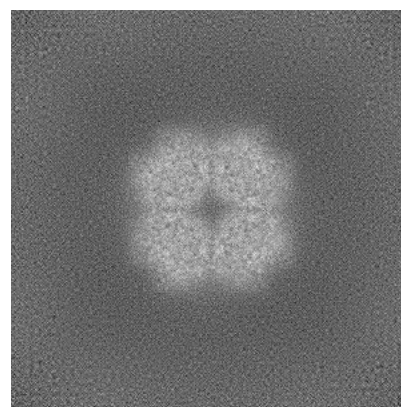
6.1.2 Raw map



X



Y

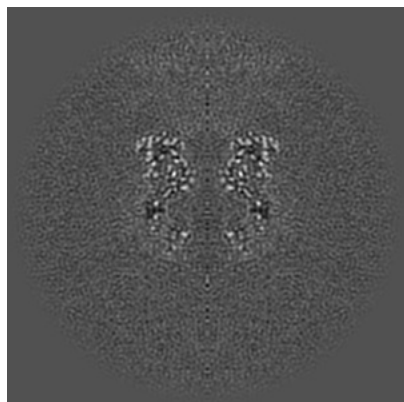


Z

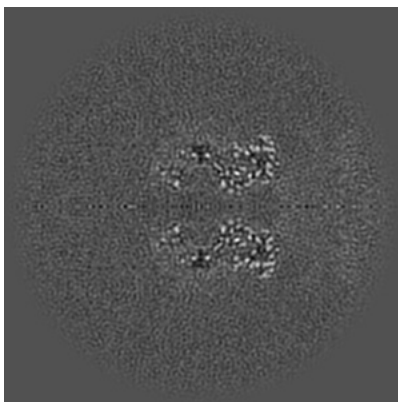
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

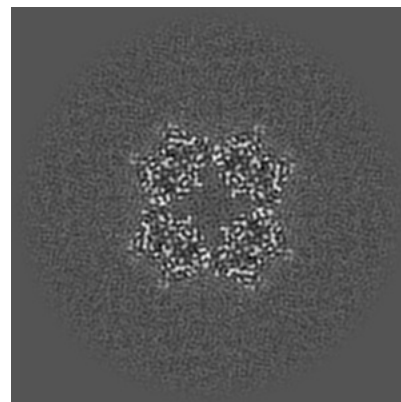
6.2.1 Primary map



X Index: 256

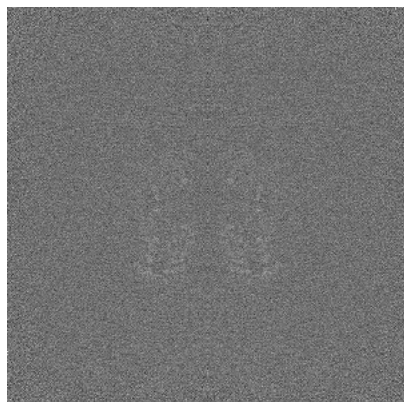


Y Index: 256

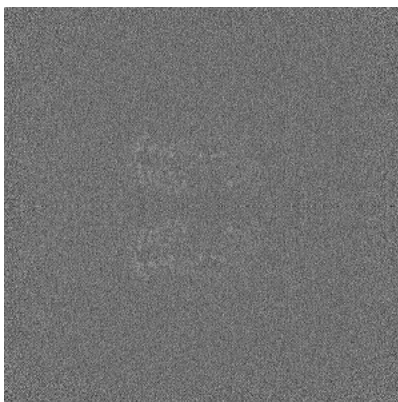


Z Index: 256

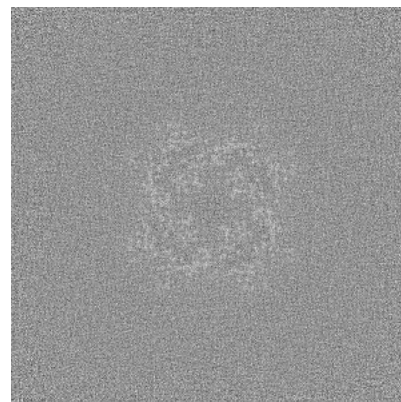
6.2.2 Raw map



X Index: 256



Y Index: 256

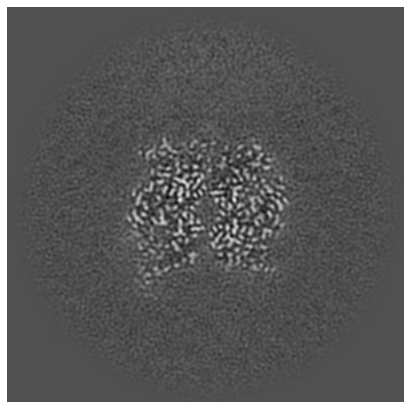


Z Index: 256

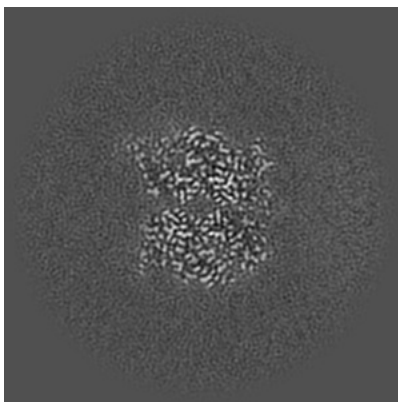
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

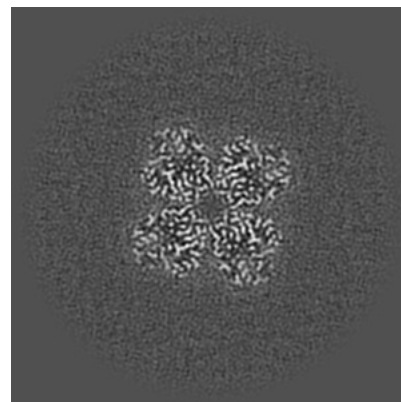
6.3.1 Primary map



X Index: 221

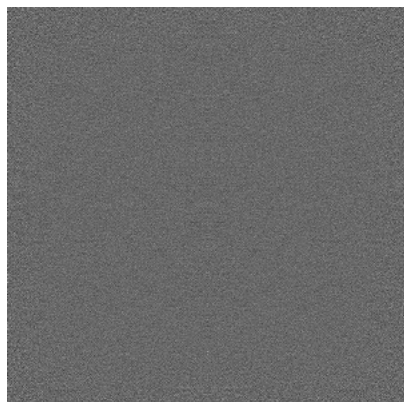


Y Index: 221

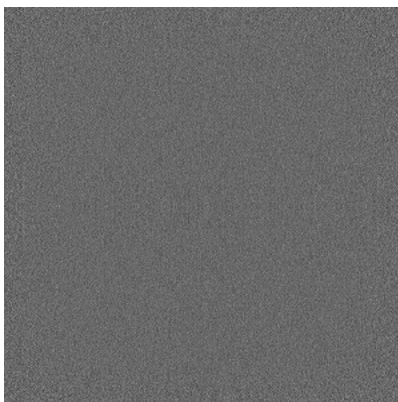


Z Index: 281

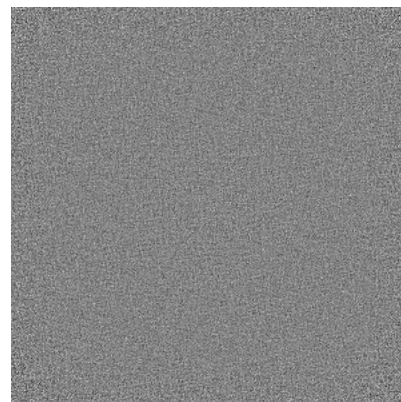
6.3.2 Raw map



X Index: 0



Y Index: 0

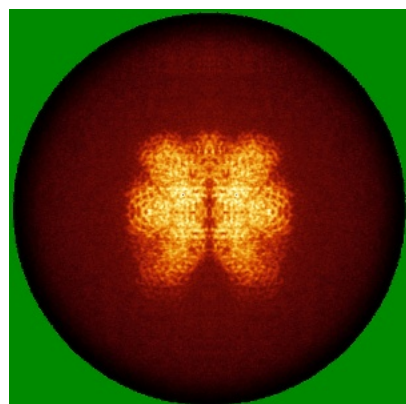


Z Index: 0

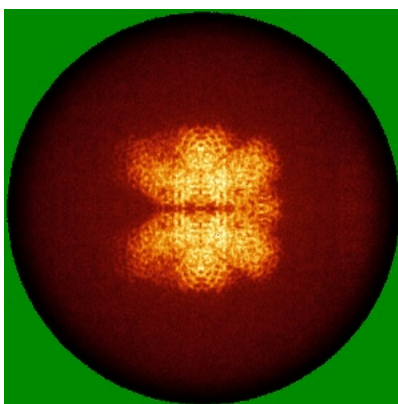
The images above show the largest variance slices of the map in three orthogonal directions.

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

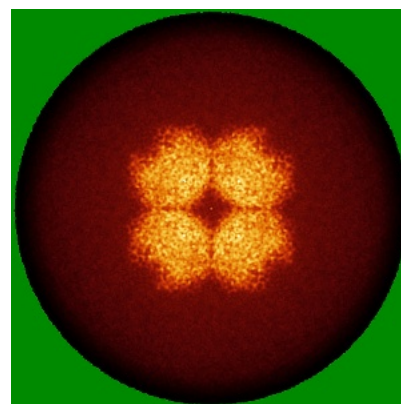
6.4.1 Primary map



X

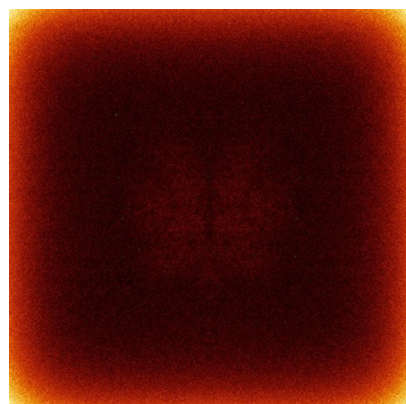


Y

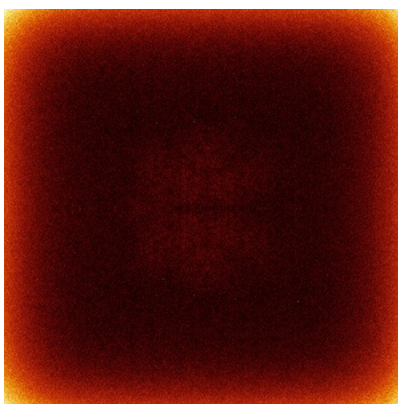


Z

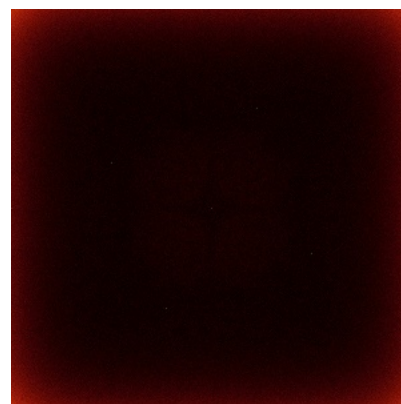
6.4.2 Raw map



X



Y

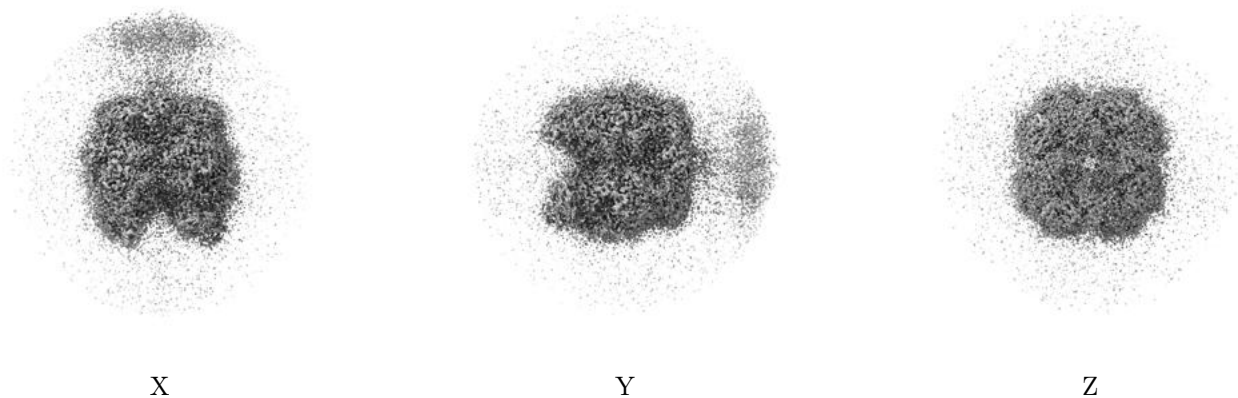


Z

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.

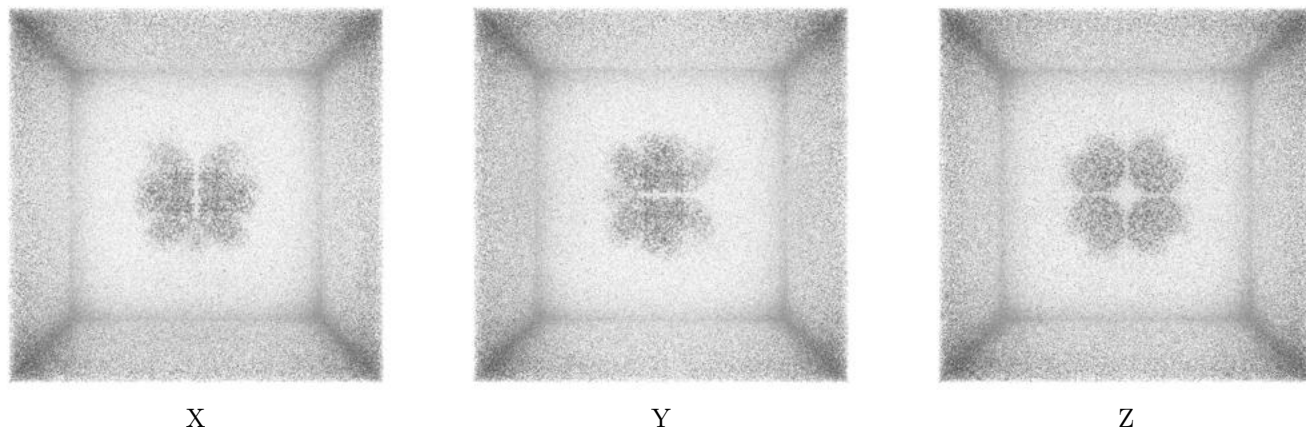
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

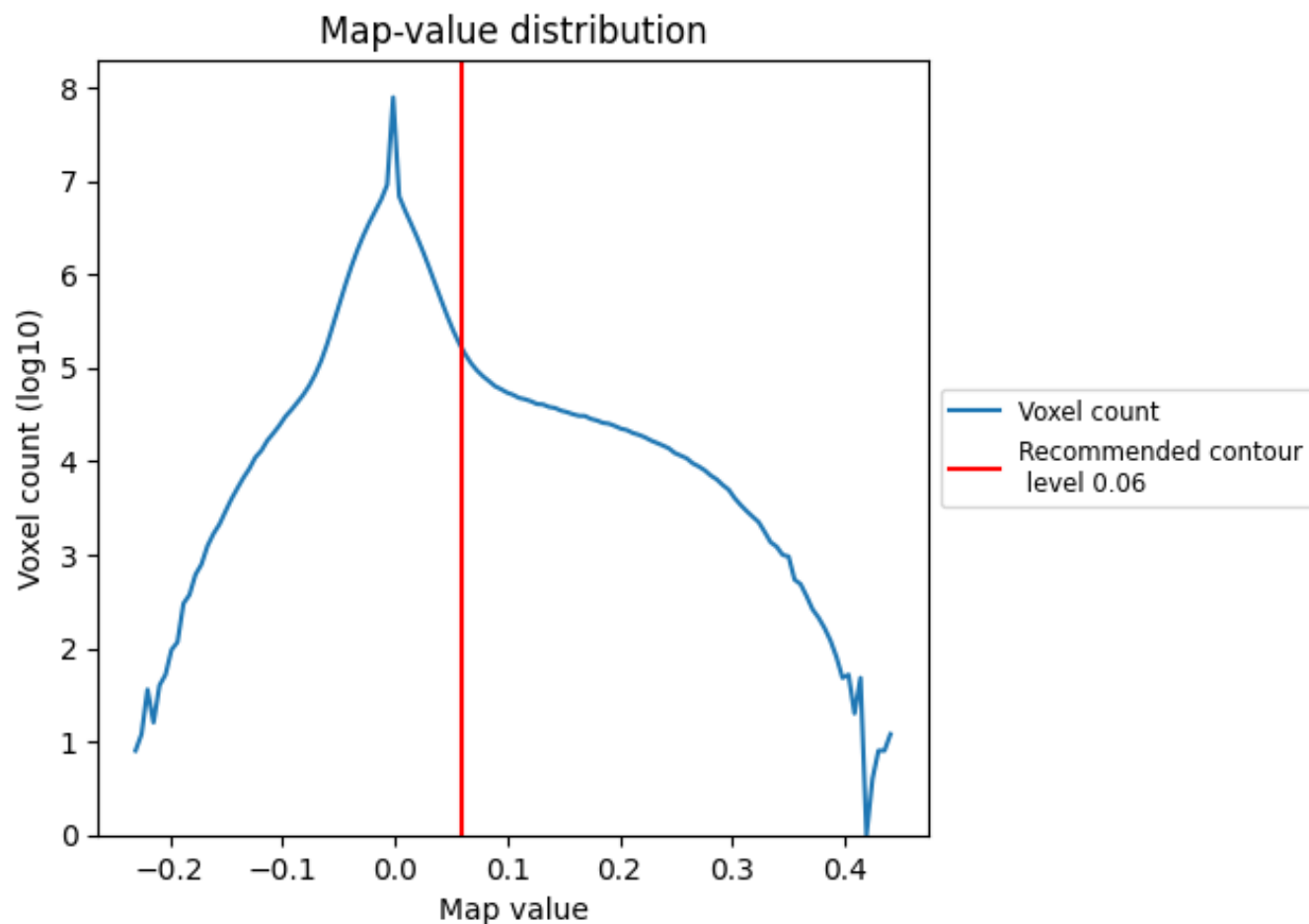
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

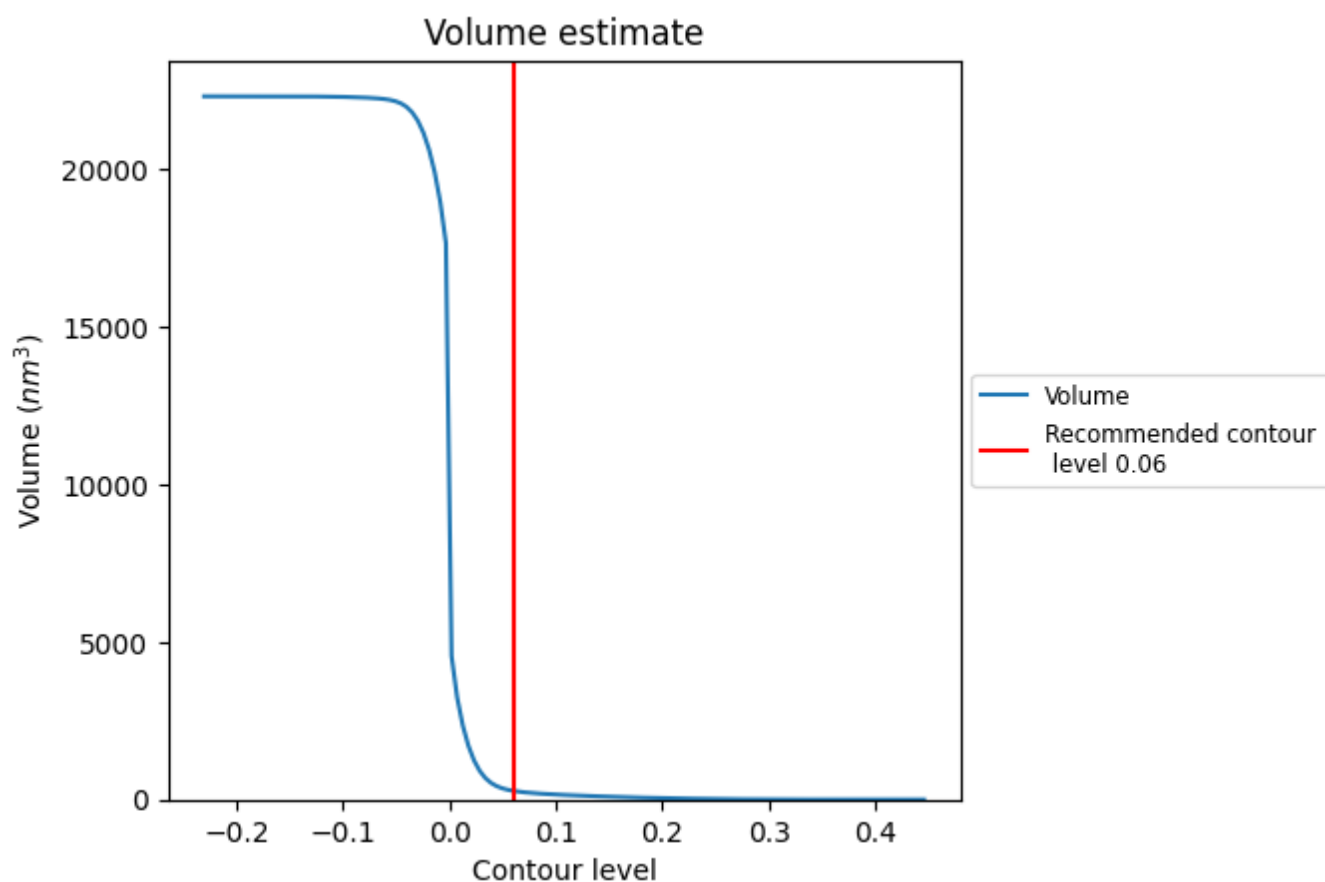
This section contains the results of statistical analysis of the map.

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.

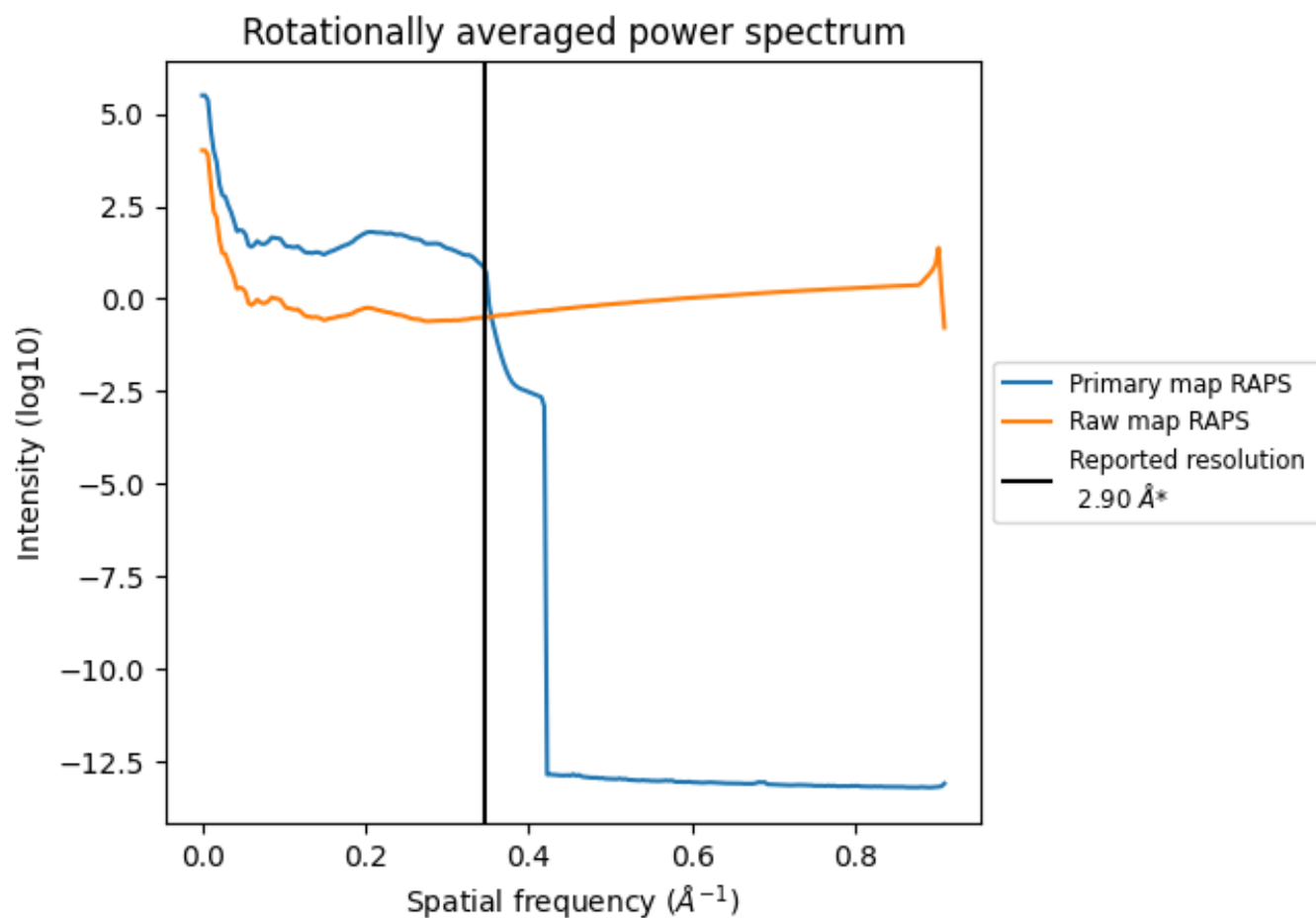
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 277 nm³; this corresponds to an approximate mass of 250 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 ⓘ

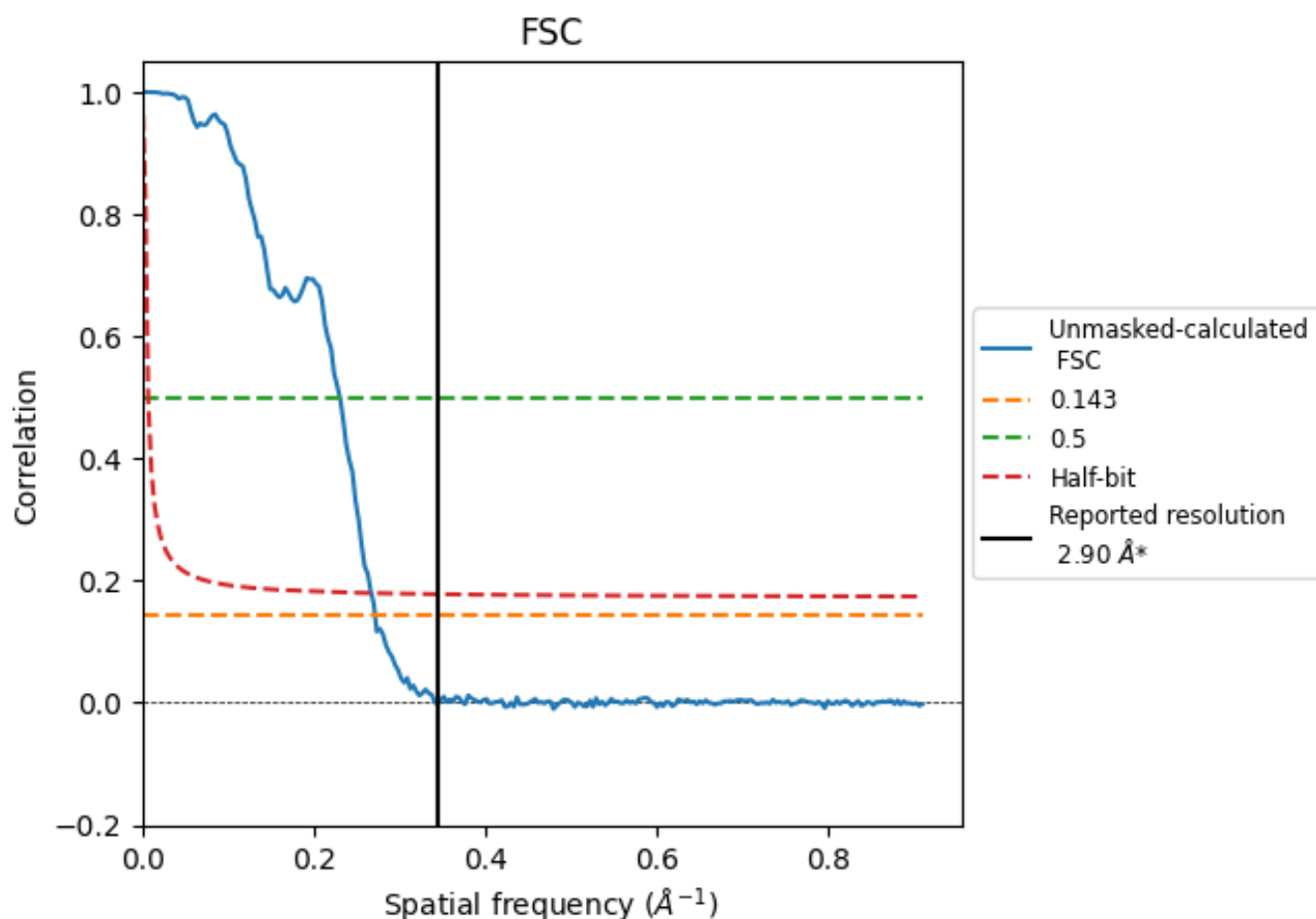


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

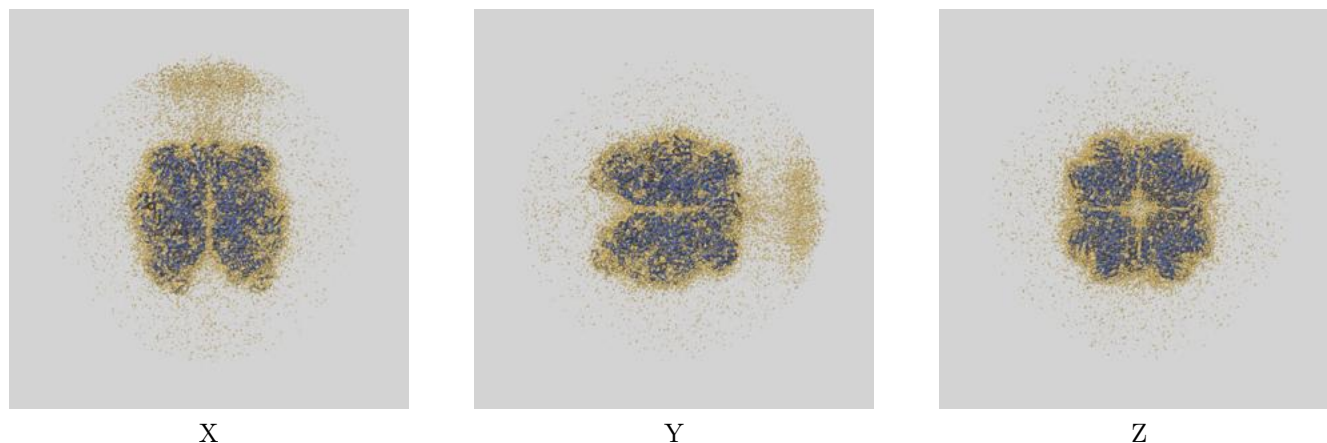
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.68	4.34	3.75

*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 3.68 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

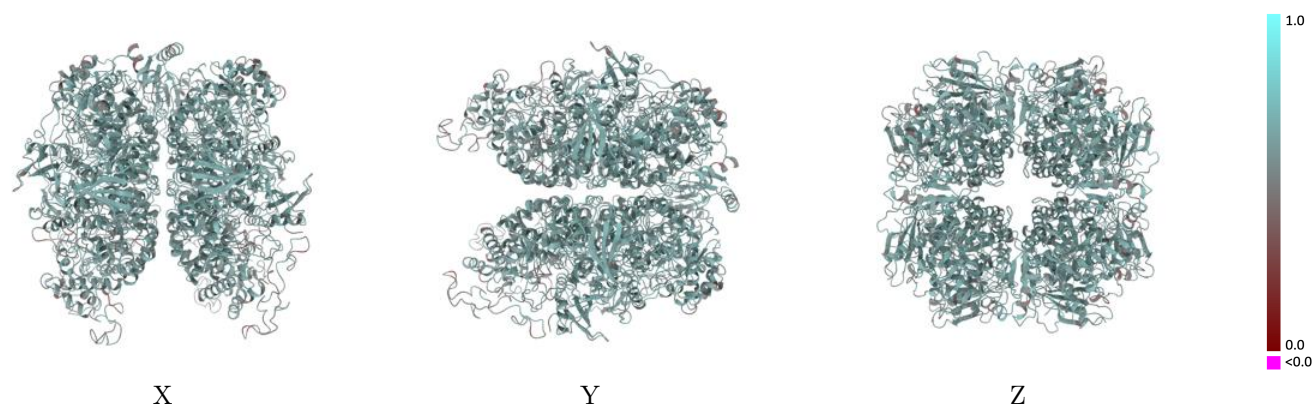
This section contains information regarding the fit between EMDB map EMD-45608 and PDB model 9CI2. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



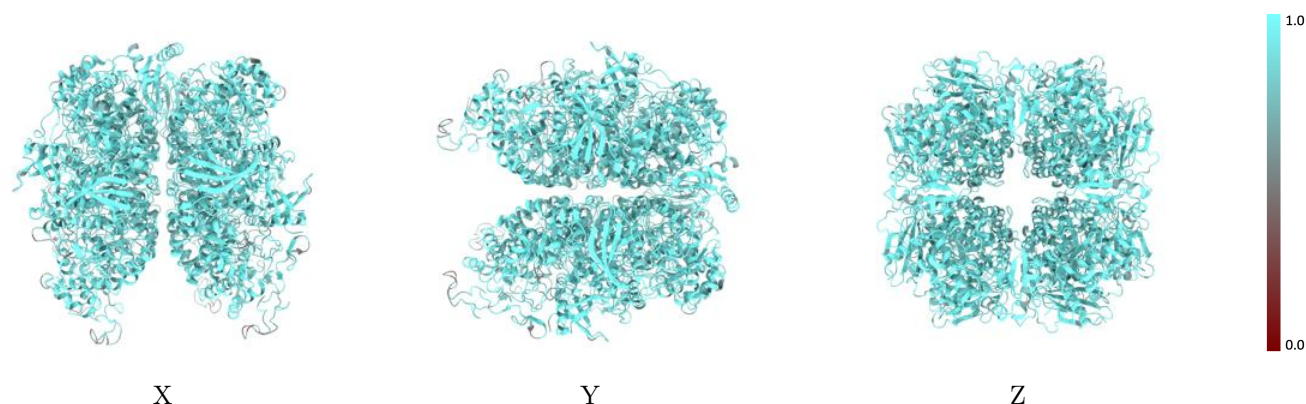
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



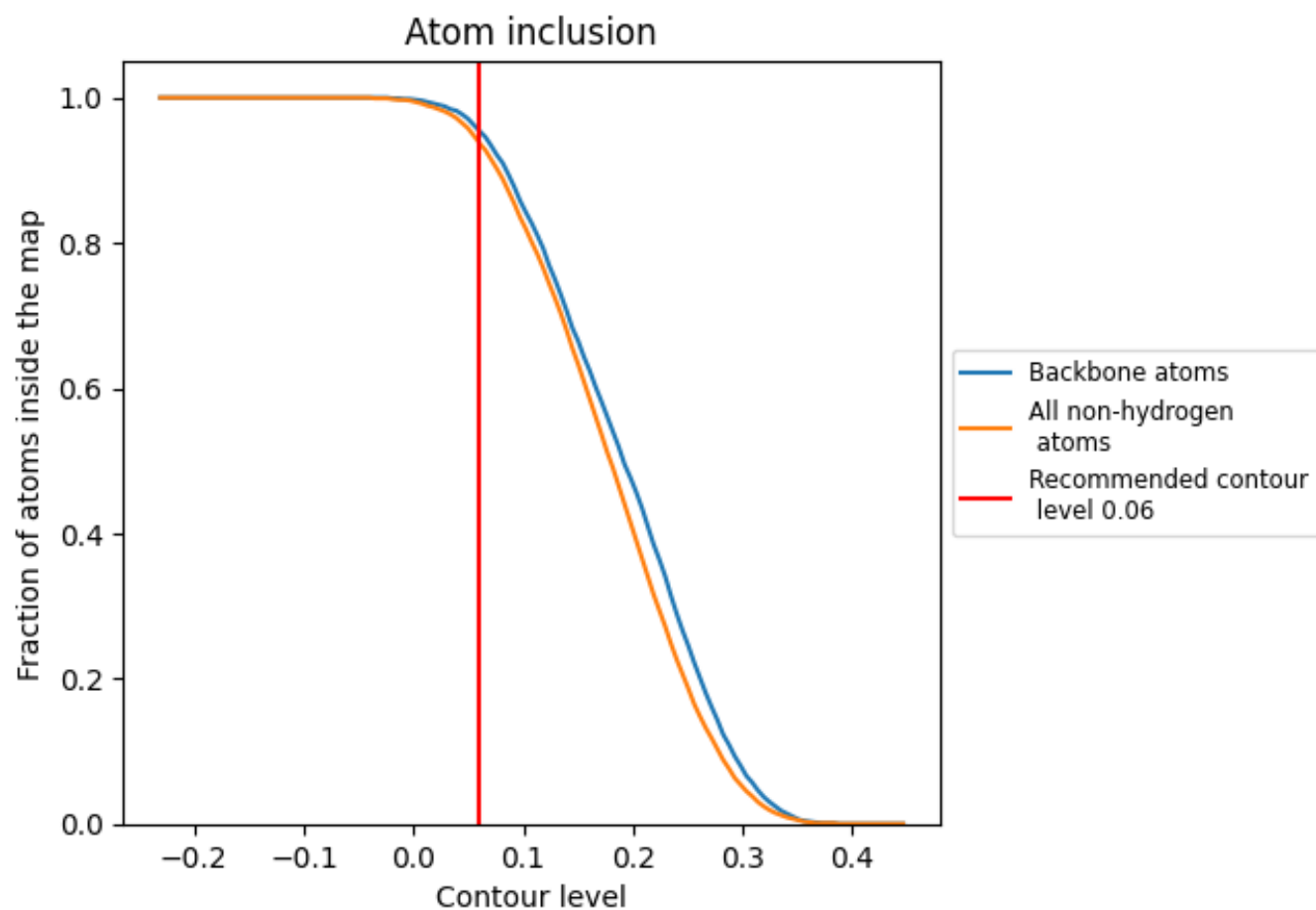
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9380	0.5950
1	0.7770	0.5050
2	0.7810	0.5010
3	0.7770	0.5030
4	0.7730	0.4940
A	0.9540	0.6080
B	0.9440	0.5960
C	0.9580	0.6090
D	0.9440	0.5950
E	0.9530	0.6090
F	0.9460	0.5970
G	0.9530	0.6090
H	0.9440	0.5970
I	0.9420	0.5960
J	0.9360	0.5930
K	0.9410	0.5930
L	0.9310	0.5870

