



Full wwPDB EM Validation Report ⓘ

May 25, 2025 – 08:46 PM EDT

PDB ID : 8S91 / pdb_00008s91
EMDB ID : EMD-40234
Title : Structure of Walker B mutated MCM8/9 heterohexamer complex with ADP
Authors : Li, C.; Gao, Y.
Deposited on : 2023-03-27
Resolution : 4.30 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

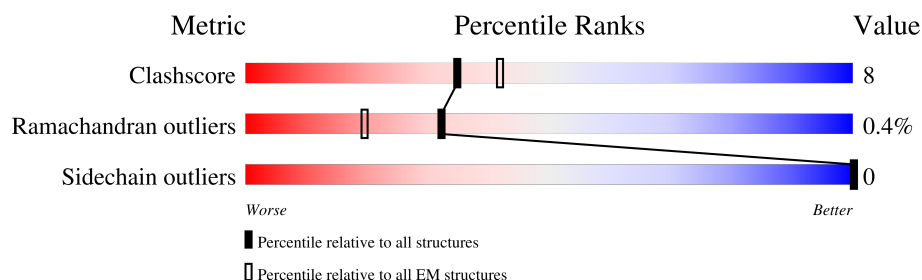
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	840	
1	B	840	
1	C	840	
2	D	1143	
2	E	1143	
2	F	1143	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29019 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 DNA helicase MCM8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	602	Total	C	N	O	S	0	0
			4703	2984	809	884	26		
1	B	602	Total	C	N	O	S	0	0
			4703	2984	809	884	26		
1	C	602	Total	C	N	O	S	0	0
			4703	2984	809	884	26		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	519	GLN	GLU	engineered mutation	UNP Q9UJA3
B	519	GLN	GLU	engineered mutation	UNP Q9UJA3
C	519	GLN	GLU	engineered mutation	UNP Q9UJA3

- Molecule 2 is a protein called DNA helicase MCM9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	621	Total	C	N	O	S	0	0
			4914	3099	841	941	33		
2	E	621	Total	C	N	O	S	0	0
			4914	3099	841	941	33		
2	F	621	Total	C	N	O	S	0	0
			4914	3099	841	941	33		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	415	GLN	GLU	engineered mutation	UNP Q9NXL9
E	415	GLN	GLU	engineered mutation	UNP Q9NXL9
F	415	GLN	GLU	engineered mutation	UNP Q9NXL9

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

- 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	B	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	D	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	

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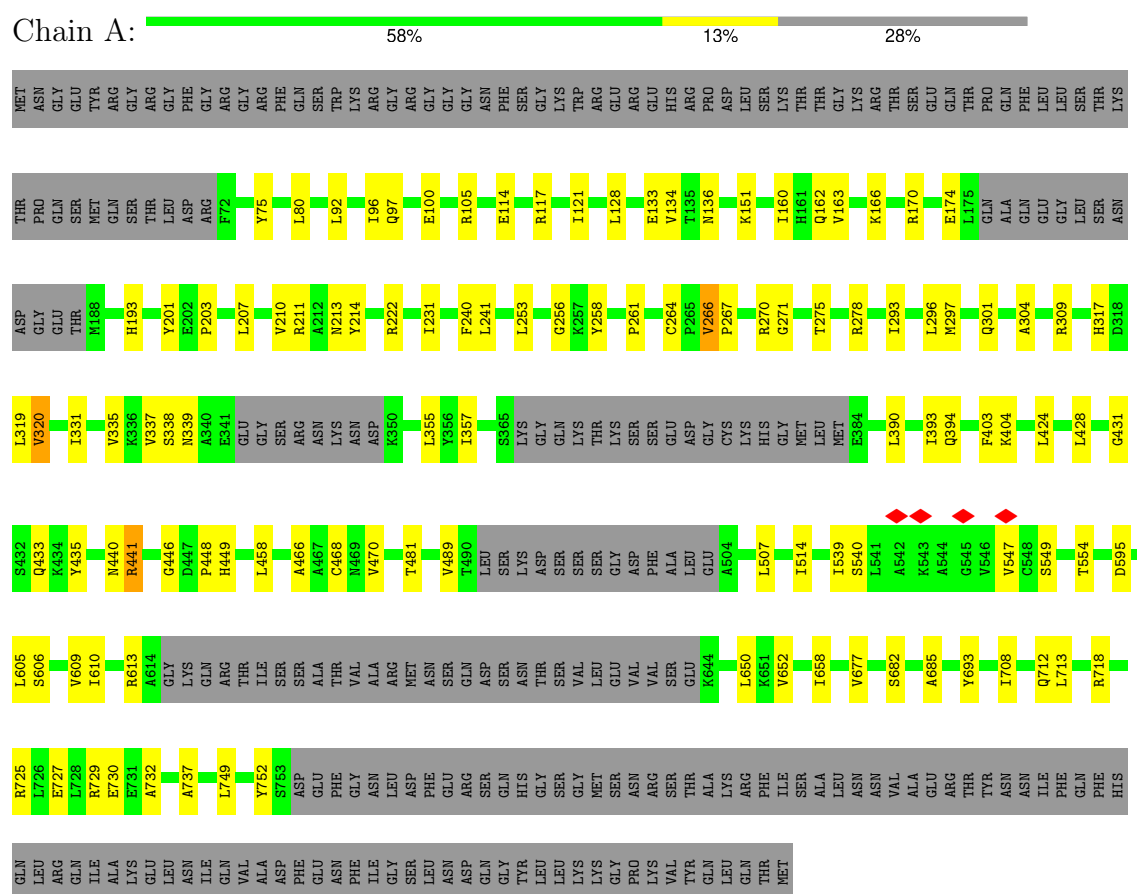
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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	F	1	1	1	0

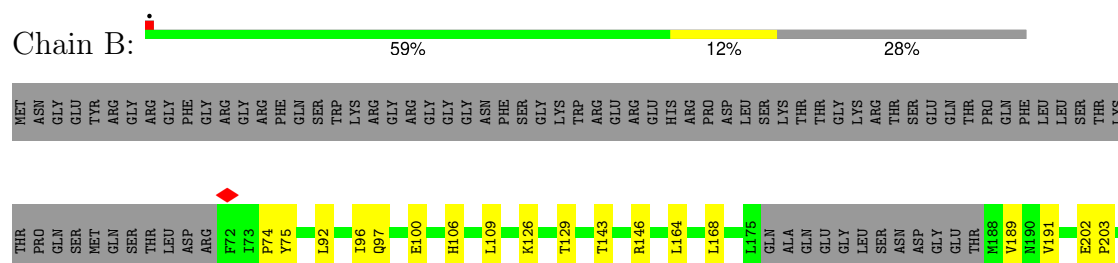
3 Residue-property plots

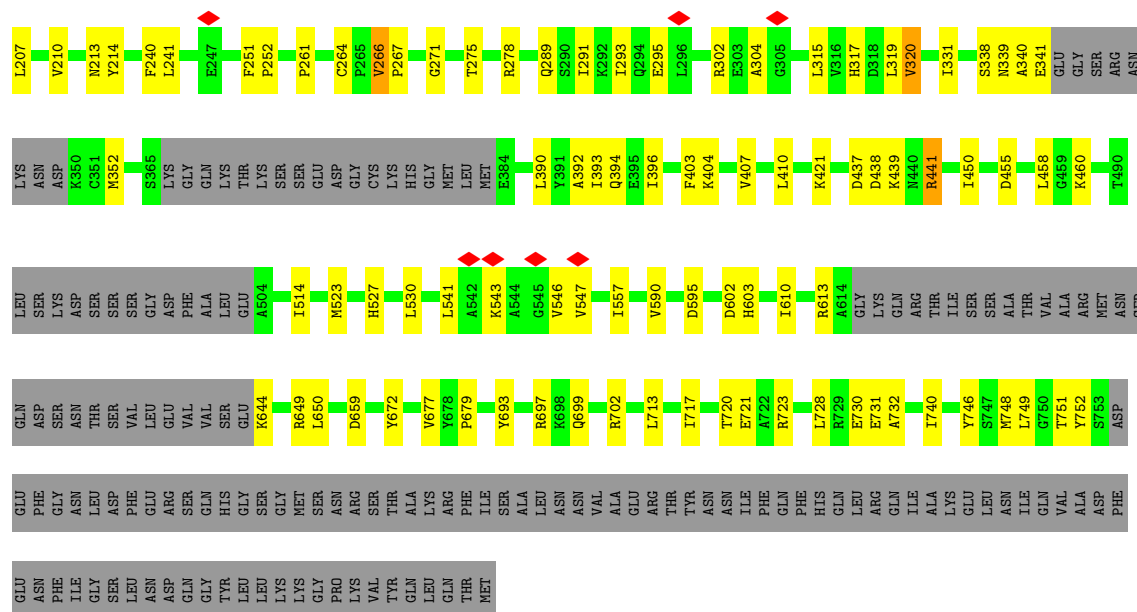
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: DNA helicase MCM8

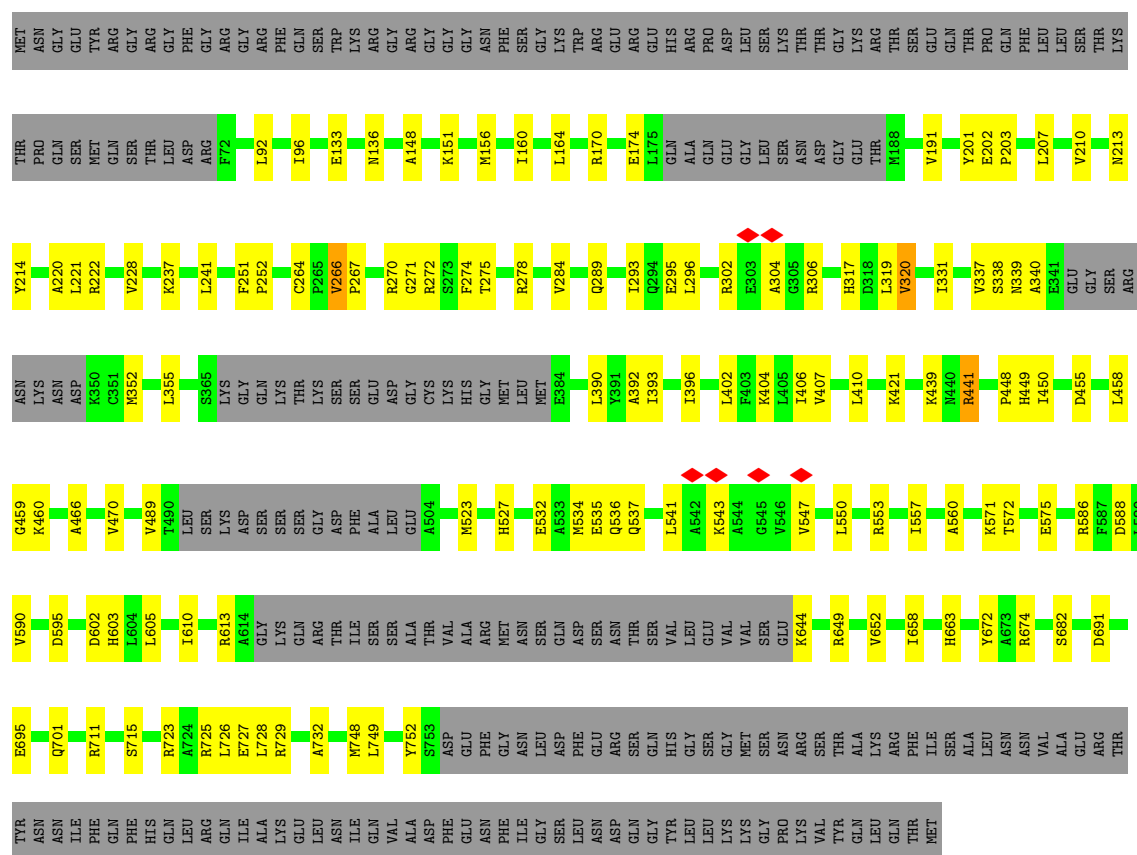


• Molecule 1: DNA helicase MCM8





• Molecule 1: DNA helicase MCM8

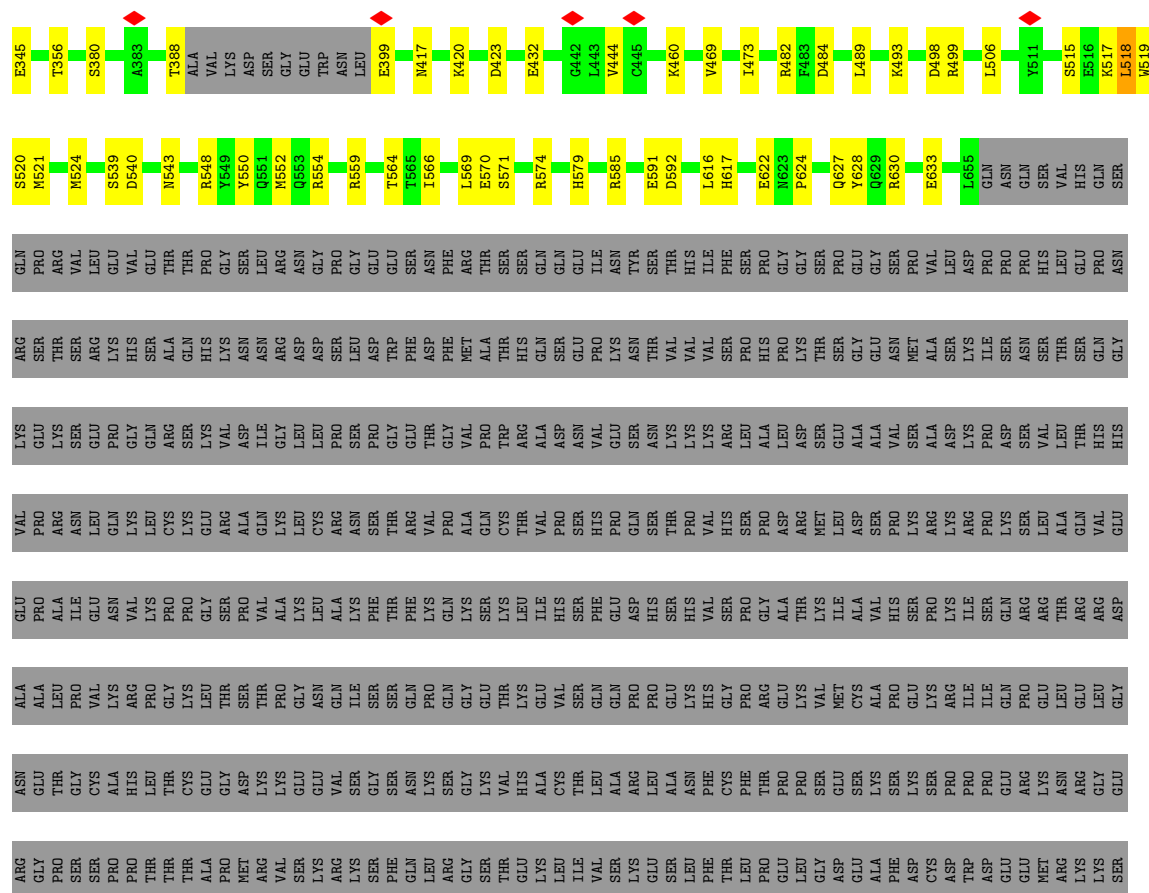


• Molecule 2: DNA helicase MCM9

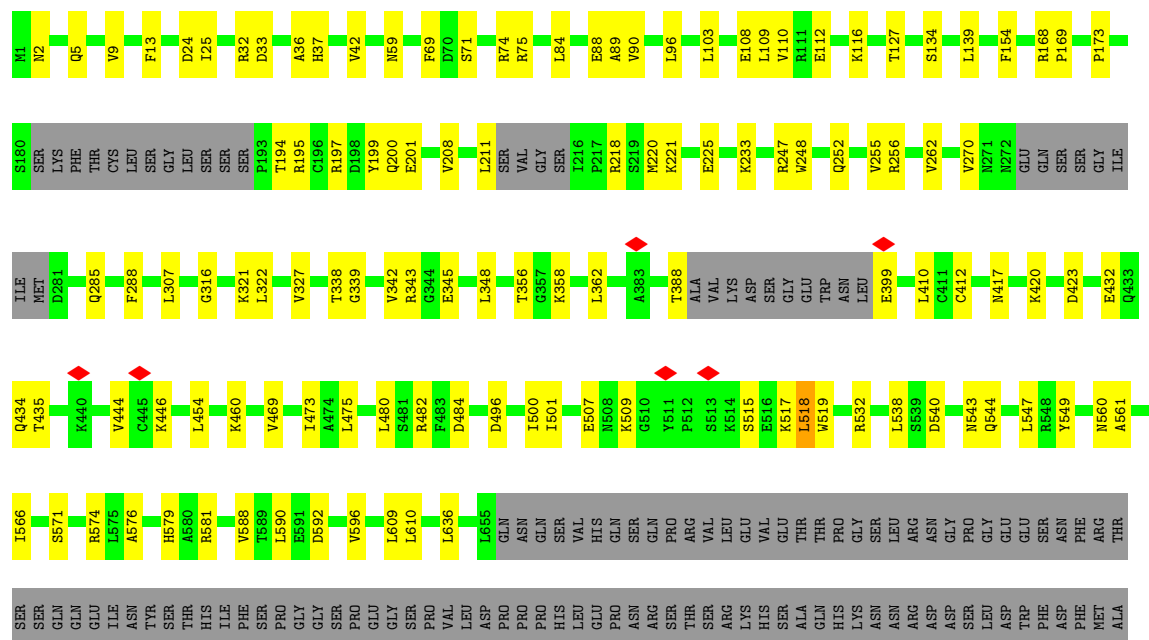




E225	V10	M1
D226	R11	M2
D227	E12	Q5
L228	H13	
C232	K18	V9
K233		G10
	L24	Q11
D236	V130	V12
		F13
		E14
L240	L139	S15
		Y16
I243	R143	R32
R247	M146	D33
W248	C147	
	M148	A36
Q252	F154	H37
		V42
V255	F166	
V262	C167	M45
L263	R168	T46
	P169	L47
L268	P173	T50
M272	S180	E56
GLJ	SER	M60
GLN	LYS	
SER	PHE	F69
SER	THR	
ILE	CYS	L73
ILE	LEU	R74
MET	SER	R75
	GLY	S76
D281	LEU	A77
	SER	L78
F300	SER	T79
A301	SER	
G302	SER	I80
	P193	
I306		
	Y199	L84
L310	E206	E88
	Q207	A89
Q313	V208	V90
M317	L211	K93
	SER	
K321	VAL	L96
L322	GLY	H97
	SER	A98
M326	I216	R99
	P217	
T338		L103
G339	W220	P104
V342	L224	L109



● Molecule 2: DNA helicase MCM9



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	227818	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 ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.189	Depositor
Minimum map value	-0.833	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.06	Depositor
Map size (\AA)	355.2, 355.2, 355.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.11, 1.11, 1.11	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, 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	0.13	0/4785	0.39	0/6474
1	B	0.13	0/4785	0.40	0/6474
1	C	0.12	0/4785	0.40	2/6474 (0.0%)
2	D	0.13	0/4992	0.38	2/6746 (0.0%)
2	E	0.14	0/4992	0.40	3/6746 (0.0%)
2	F	0.12	0/4992	0.37	2/6746 (0.0%)
All	All	0.13	0/29331	0.39	9/39660 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	560	ALA	CA-C-N	6.85	138.35	122.31
1	C	560	ALA	C-N-CA	6.85	138.35	122.31
2	F	518	LEU	CA-C-N	6.02	133.04	121.54
2	F	518	LEU	C-N-CA	6.02	133.04	121.54
2	E	518	LEU	CB-CA-C	-6.00	109.64	116.54
2	D	518	LEU	CA-C-N	5.92	132.84	121.54
2	D	518	LEU	C-N-CA	5.92	132.84	121.54
2	E	518	LEU	CA-C-N	5.11	131.30	121.54
2	E	518	LEU	C-N-CA	5.11	131.30	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4703	0	4773	74	0
1	B	4703	0	4773	73	0
1	C	4703	0	4773	79	0
2	D	4914	0	4947	85	0
2	E	4914	0	4947	97	0
2	F	4914	0	4947	80	0
3	A	27	0	12	0	0
3	B	27	0	12	1	0
3	C	27	0	12	1	0
3	D	27	0	12	0	0
3	E	27	0	12	0	0
3	F	27	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	29019	0	29232	455	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 (455) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:LEU:O	1:A:394:GLN:NE2	2.12	0.82
2:F:469:VAL:HG13	2:F:473:ILE:HD13	1.61	0.82
1:B:390:LEU:O	1:B:394:GLN:NE2	2.15	0.79
2:E:310:LEU:O	2:E:321:LYS:NZ	2.19	0.76
1:B:677:VAL:HG12	1:B:679:PRO:HD3	1.69	0.74
1:C:610:ILE:HG21	2:F:547:LEU:HD21	1.69	0.74
1:B:458:LEU:HD21	1:B:595:ASP:HB2	1.68	0.74
1:A:468:CYS:HA	1:A:514:ILE:HD11	1.71	0.73
1:A:458:LEU:HD21	1:A:595:ASP:HB2	1.69	0.72
2:F:343:ARG:HA	2:F:434:GLN:HE21	1.56	0.70
2:F:579:HIS:ND1	2:F:592:ASP:OD1	2.24	0.70
1:B:210:VAL:HG13	1:B:214:TYR:HB2	1.74	0.70
1:A:610:ILE:HD11	2:D:543:ASN:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ARG:NH2	1:A:133:GLU:OE1	2.26	0.69
1:C:458:LEU:HD21	1:C:595:ASP:HB2	1.74	0.68
2:E:559:ARG:HE	2:E:564:THR:HG21	1.59	0.68
1:C:674:ARG:O	1:C:725:ARG:NH2	2.28	0.67
1:C:210:VAL:HG13	1:C:214:TYR:HB2	1.77	0.66
2:F:362:LEU:HD12	2:F:412:CYS:HB2	1.78	0.66
1:B:679:PRO:HA	1:B:730:GLU:HG3	1.77	0.66
2:F:345:GLU:O	2:F:574:ARG:NH1	2.28	0.66
2:F:108:GLU:HG2	2:F:109:LEU:HD12	1.78	0.66
1:C:532:GLU:HG2	1:C:536:GLN:HG3	1.78	0.65
1:B:693:TYR:OH	1:B:697:ARG:NH2	2.28	0.65
2:E:36:ALA:O	2:E:37:HIS:ND1	2.29	0.65
2:D:540:ASP:OD1	2:D:544:GLN:NE2	2.29	0.65
2:D:417:ASN:HB2	2:D:460:LYS:HD3	1.78	0.64
1:A:75:TYR:HD1	1:A:162:GLN:HE21	1.45	0.64
2:D:197:ARG:NH2	2:D:225:GLU:OE2	2.30	0.64
2:E:56:GLU:HG2	2:E:60:MET:HE1	1.78	0.64
2:E:300:PHE:HD2	2:E:624:PRO:HB2	1.61	0.64
2:F:197:ARG:NH2	2:F:225:GLU:OE2	2.30	0.64
1:B:302:ARG:HD2	1:B:304:ALA:HB3	1.81	0.63
2:E:420:LYS:O	2:E:423:ASP:N	2.31	0.63
1:A:207:LEU:HB3	1:A:309:ARG:HE	1.64	0.63
2:D:345:GLU:O	2:D:574:ARG:NH1	2.30	0.63
2:E:345:GLU:O	2:E:574:ARG:NH1	2.30	0.63
1:A:210:VAL:HG13	1:A:214:TYR:HB2	1.81	0.63
1:B:390:LEU:HA	1:B:393:ILE:HG12	1.81	0.63
1:B:315:LEU:HD22	1:B:319:LEU:HD22	1.82	0.62
2:E:617:HIS:ND1	2:E:617:HIS:O	2.32	0.62
1:A:231:ILE:HG21	2:F:116:LYS:HZ1	1.65	0.62
1:C:207:LEU:HD12	1:C:295:GLU:HB2	1.81	0.62
2:E:46:THR:O	2:E:50:THR:OG1	2.08	0.61
2:D:111:ARG:NH1	2:D:119:ASP:OD2	2.33	0.61
2:D:432:GLU:OE1	2:D:482:ARG:NE	2.33	0.61
2:F:609:LEU:HD12	2:F:610:LEU:HG	1.82	0.61
2:D:343:ARG:HA	2:D:434:GLN:HE21	1.64	0.61
2:D:420:LYS:O	2:D:423:ASP:N	2.34	0.61
2:D:650:ARG:HG2	2:D:654:ARG:HH12	1.65	0.61
1:B:143:THR:HG23	1:B:146:ARG:HH21	1.64	0.61
1:C:571:LYS:HG3	1:C:572:THR:H	1.64	0.61
1:A:652:VAL:HG11	1:A:658:ILE:HD13	1.82	0.60
1:C:392:ALA:O	1:C:396:ILE:HG12	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:605:LEU:HD21	2:F:566:ILE:HD12	1.82	0.60
1:A:231:ILE:HD13	2:F:116:LYS:HZ2	1.66	0.60
1:C:572:THR:OG1	1:C:575:GLU:OE1	2.19	0.60
1:C:613:ARG:HH22	2:F:342:VAL:HG21	1.66	0.60
2:E:630:ARG:NH1	2:E:633:GLU:OE1	2.35	0.60
2:F:32:ARG:HG3	2:F:33:ASP:H	1.66	0.60
1:A:133:GLU:HA	1:A:136:ASN:HB2	1.84	0.59
2:D:521:MET:SD	2:D:525:LYS:NZ	2.74	0.59
2:E:9:VAL:HG13	2:E:13:PHE:HE2	1.67	0.59
1:B:455:ASP:O	1:B:460:LYS:NZ	2.35	0.59
2:D:222:VAL:HG12	2:D:263:LEU:HB3	1.83	0.59
1:A:211:ARG:NH2	2:D:230:ASP:OD2	2.34	0.59
2:E:322:LEU:O	2:E:326:MET:HG3	2.01	0.59
2:D:579:HIS:ND1	2:D:592:ASP:OD1	2.31	0.59
1:A:677:VAL:HG13	1:A:730:GLU:HG3	1.85	0.58
2:F:540:ASP:O	2:F:544:GLN:NE2	2.36	0.58
1:A:293:ILE:HD11	1:A:331:ILE:HD12	1.85	0.58
2:E:432:GLU:OE1	2:E:482:ARG:NE	2.37	0.58
1:B:241:LEU:HB3	1:B:275:THR:HB	1.85	0.58
1:B:613:ARG:HH22	2:E:342:VAL:HG21	1.68	0.58
1:B:717:ILE:HD11	2:D:506:LEU:HD23	1.85	0.58
2:E:45:MET:HE1	2:E:104:PRO:HG3	1.84	0.58
1:B:207:LEU:HD12	1:B:295:GLU:HB2	1.85	0.58
2:F:417:ASN:HB2	2:F:460:LYS:HD3	1.84	0.58
2:E:417:ASN:HB2	2:E:460:LYS:HD3	1.86	0.57
1:A:210:VAL:HG22	1:A:214:TYR:HD2	1.69	0.57
1:C:663:HIS:ND1	2:F:338:THR:OG1	2.36	0.57
2:D:609:LEU:HD12	2:D:610:LEU:HG	1.84	0.57
2:E:317:MET:HE1	2:E:616:LEU:HA	1.87	0.57
1:A:241:LEU:HB3	1:A:275:THR:HB	1.86	0.57
1:A:610:ILE:HG21	2:D:547:LEU:HD11	1.85	0.57
2:D:322:LEU:HG	2:D:326:MET:HE2	1.86	0.57
1:A:749:LEU:HA	1:A:752:TYR:HD1	1.70	0.57
1:B:213:ASN:HD21	2:E:36:ALA:HA	1.69	0.57
2:E:579:HIS:ND1	2:E:592:ASP:OD1	2.29	0.57
2:E:99:ARG:NH2	2:E:227:ASP:OD1	2.38	0.57
1:C:439:LYS:HE3	2:E:521:MET:HG3	1.86	0.57
1:C:749:LEU:HA	1:C:752:TYR:HD1	1.70	0.56
1:B:168:LEU:HD23	1:B:189:VAL:HG12	1.87	0.56
2:E:300:PHE:HE2	2:E:628:TYR:HB2	1.69	0.56
2:F:576:ALA:HB2	2:F:596:VAL:HG11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:MET:HE2	1:A:301:GLN:HG3	1.88	0.56
2:D:577:GLU:O	2:D:581:ARG:HG3	2.06	0.56
2:E:310:LEU:HG	2:E:524:MET:HE1	1.88	0.56
2:E:338:THR:HG23	2:E:339:GLY:H	1.71	0.56
2:F:420:LYS:O	2:F:423:ASP:N	2.38	0.56
1:A:708:ILE:HA	1:A:712:GLN:HE22	1.71	0.55
1:B:439:LYS:NZ	2:D:511:TYR:OH	2.26	0.55
2:F:59:ASN:HD21	2:F:109:LEU:HD21	1.70	0.55
1:B:403:PHE:HD2	1:B:650:LEU:HD21	1.70	0.55
1:B:613:ARG:NH2	2:E:570:GLU:OE2	2.38	0.55
1:C:241:LEU:HB3	1:C:275:THR:HB	1.89	0.55
2:F:540:ASP:OD1	2:F:544:GLN:NE2	2.39	0.55
2:F:316:GLY:O	2:F:321:LYS:NZ	2.26	0.55
2:D:140:GLU:OE2	2:D:143:ARG:NH1	2.39	0.55
1:C:534:MET:HE3	1:C:586:ARG:HD2	1.89	0.55
2:D:518:LEU:O	2:D:519:TRP:CD1	2.60	0.55
1:B:610:ILE:HD11	2:E:543:ASN:HB3	1.89	0.54
2:E:84:LEU:HD21	2:E:90:VAL:HG11	1.89	0.54
2:F:571:SER:OG	2:F:574:ARG:NH2	2.40	0.54
2:D:326:MET:HE1	2:D:599:VAL:HG11	1.88	0.54
2:E:2:ASN:HB2	2:E:5:GLN:HG3	1.89	0.54
2:E:96:LEU:O	2:E:97:HIS:ND1	2.39	0.54
2:F:220:MET:HE3	2:F:221:LYS:H	1.71	0.54
2:F:518:LEU:O	2:F:519:TRP:CD1	2.61	0.54
2:E:518:LEU:O	2:E:519:TRP:CD1	2.60	0.54
1:B:278:ARG:NH2	2:D:162:GLN:OE1	2.41	0.54
1:B:749:LEU:HA	1:B:752:TYR:CD1	2.43	0.53
1:C:202:GLU:HG2	1:C:203:PRO:HD3	1.89	0.53
2:E:36:ALA:H	2:E:93:LYS:HZ2	1.56	0.53
2:F:432:GLU:OE1	2:F:482:ARG:NE	2.41	0.53
1:B:749:LEU:HA	1:B:752:TYR:HD1	1.72	0.53
2:F:84:LEU:HD21	2:F:90:VAL:HG11	1.89	0.53
1:B:210:VAL:HG22	1:B:214:TYR:HD2	1.74	0.53
2:E:548:ARG:HH12	2:E:552:MET:HE2	1.73	0.53
2:E:9:VAL:HG13	2:E:13:PHE:CE2	2.42	0.53
2:E:42:VAL:HG21	2:E:69:PHE:HZ	1.72	0.53
2:E:103:LEU:HD21	2:E:109:LEU:HB3	1.90	0.53
2:F:484:ASP:OD1	2:F:571:SER:OG	2.22	0.53
1:A:448:PRO:O	1:A:449:HIS:ND1	2.42	0.53
1:B:202:GLU:HG2	1:B:203:PRO:HD3	1.90	0.53
2:D:540:ASP:O	2:D:544:GLN:NE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:84:LEU:HD21	2:D:90:VAL:HG11	1.90	0.53
2:D:560:ASN:OD1	2:D:561:ALA:N	2.42	0.53
2:F:532:ARG:HA	2:F:581:ARG:HH21	1.74	0.53
2:F:560:ASN:CG	2:F:561:ALA:H	2.17	0.53
1:A:605:LEU:HD21	2:D:566:ILE:HD12	1.91	0.52
2:D:24:ASP:OD1	2:D:25:ILE:N	2.42	0.52
1:C:237:LYS:HB3	1:C:284:VAL:HG22	1.91	0.52
1:A:335:VAL:HG22	1:A:357:ILE:HG12	1.91	0.52
1:C:266:VAL:HB	1:C:267:PRO:HD2	1.91	0.52
1:A:749:LEU:HG	1:A:752:TYR:HE1	1.75	0.52
2:D:88:GLU:HG2	2:D:89:ALA:H	1.74	0.52
1:A:390:LEU:HA	1:A:393:ILE:HG12	1.92	0.52
1:B:404:LYS:HA	1:B:407:VAL:HG12	1.92	0.52
2:D:550:TYR:CD2	2:D:569:LEU:HB2	2.44	0.52
2:F:338:THR:HG23	2:F:339:GLY:H	1.74	0.52
1:A:114:GLU:OE1	1:A:117:ARG:NH2	2.42	0.52
2:D:338:THR:HG23	2:D:339:GLY:H	1.74	0.52
1:B:748:MET:HE3	1:B:748:MET:HA	1.91	0.52
2:F:32:ARG:HH11	2:F:33:ASP:H	1.57	0.52
1:C:404:LYS:HA	1:C:407:VAL:HG12	1.92	0.51
1:C:602:ASP:OD1	1:C:603:HIS:N	2.43	0.51
1:B:659:ASP:OD1	1:B:659:ASP:N	2.44	0.51
2:F:110:VAL:HG12	2:F:110:VAL:O	2.10	0.51
2:D:555:GLN:O	2:D:555:GLN:HG2	2.09	0.51
1:A:231:ILE:HD13	2:F:116:LYS:NZ	2.25	0.51
2:D:539:SER:OG	2:D:540:ASP:N	2.43	0.51
1:A:121:ILE:HG13	1:A:160:ILE:HG13	1.92	0.51
2:F:112:GLU:OE1	2:F:127:THR:OG1	2.29	0.51
1:C:644:LYS:HB2	1:C:649:ARG:HD3	1.92	0.51
1:C:338:SER:OG	1:C:339:ASN:N	2.44	0.51
1:B:699:GLN:HA	1:B:702:ARG:HE	1.75	0.51
2:D:168:ARG:HE	2:D:169:PRO:HD2	1.74	0.51
1:A:727:GLU:OE1	1:A:729:ARG:NH2	2.44	0.51
1:B:240:PHE:HD2	1:B:261:PRO:HG3	1.77	0.51
1:C:272:ARG:HD2	1:C:274:PHE:H	1.76	0.50
2:D:585:ARG:NH2	2:D:591:GLU:OE2	2.43	0.50
2:E:168:ARG:HE	2:E:169:PRO:HD2	1.77	0.50
2:D:32:ARG:NH1	2:D:33:ASP:H	2.09	0.50
2:E:247:ARG:HE	2:E:262:VAL:HG11	1.76	0.50
2:E:469:VAL:O	2:E:473:ILE:HG22	2.10	0.50
1:C:278:ARG:HD2	2:E:248:TRP:CG	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:ASP:O	1:C:460:LYS:NZ	2.45	0.50
2:E:539:SER:OG	2:E:540:ASP:N	2.45	0.50
1:B:266:VAL:HB	1:B:267:PRO:HD2	1.94	0.50
2:E:300:PHE:CD2	2:E:624:PRO:HB2	2.45	0.50
1:C:133:GLU:HA	1:C:136:ASN:HB2	1.94	0.49
2:E:622:GLU:OE2	2:E:622:GLU:N	2.43	0.49
1:C:701:GLN:HB2	2:E:493:LYS:HG2	1.93	0.49
2:E:11:GLN:O	2:E:14:GLU:HG3	2.12	0.49
2:F:388:THR:HB	2:F:399:GLU:HB2	1.94	0.49
1:A:749:LEU:HA	1:A:752:TYR:CD1	2.47	0.49
2:E:571:SER:OG	2:E:574:ARG:NH2	2.45	0.49
1:C:571:LYS:HG3	1:C:572:THR:N	2.28	0.49
2:F:200:GLN:HG3	2:F:201:GLU:H	1.78	0.49
2:D:480:LEU:O	2:D:480:LEU:HD23	2.12	0.49
1:A:97:GLN:HA	1:A:100:GLU:HG2	1.95	0.49
1:A:481:THR:HG21	2:D:438:VAL:HG12	1.95	0.49
2:F:549:TYR:HE1	2:F:609:LEU:HD21	1.77	0.48
1:A:266:VAL:HB	1:A:267:PRO:HD2	1.94	0.48
1:C:170:ARG:NH1	1:C:174:GLU:OE1	2.46	0.48
2:E:88:GLU:HG2	2:E:89:ALA:H	1.78	0.48
1:C:523:MET:O	1:C:527:HIS:NE2	2.45	0.48
2:E:76:SER:O	2:E:80:ILE:HG12	2.14	0.48
2:D:110:VAL:HG12	2:D:110:VAL:O	2.13	0.48
1:B:407:VAL:HG11	1:B:650:LEU:HD22	1.95	0.48
1:B:523:MET:O	1:B:527:HIS:NE2	2.45	0.48
1:C:748:MET:HG3	1:C:749:LEU:H	1.78	0.48
2:E:146:MET:HE1	2:E:148:ASN:HB3	1.95	0.48
2:F:36:ALA:O	2:F:37:HIS:CG	2.67	0.48
2:D:356:THR:HG21	2:D:489:LEU:HD13	1.95	0.48
2:E:111:ARG:HG2	2:E:113:HIS:H	1.79	0.48
2:E:236:ASP:OD1	2:E:237:ASP:N	2.46	0.48
2:F:338:THR:HG23	2:F:339:GLY:N	2.29	0.48
1:A:80:LEU:HD21	1:A:193:HIS:HB2	1.95	0.47
2:E:154:PHE:HE1	2:E:173:PRO:HD2	1.79	0.47
1:B:338:SER:OG	1:B:339:ASN:N	2.46	0.47
2:D:388:THR:HB	2:D:399:GLU:HB2	1.96	0.47
1:B:126:LYS:HA	1:B:129:THR:HG22	1.97	0.47
2:F:2:ASN:HB2	2:F:5:GLN:HG3	1.96	0.47
2:E:13:PHE:CE1	2:E:47:LEU:HD21	2.50	0.47
2:E:220:MET:HE2	2:E:220:MET:HA	1.96	0.47
2:E:585:ARG:HH22	2:E:591:GLU:HB3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:88:GLU:HG2	2:F:89:ALA:H	1.78	0.47
2:F:220:MET:HE3	2:F:221:LYS:N	2.29	0.47
1:A:278:ARG:HD2	2:F:248:TRP:CG	2.50	0.47
1:C:264:CYS:SG	1:C:271:GLY:HA2	2.55	0.47
2:E:617:HIS:O	2:E:617:HIS:CG	2.67	0.47
2:F:71:SER:O	2:F:75:ARG:HG2	2.15	0.47
1:B:97:GLN:HA	1:B:100:GLU:HG2	1.95	0.47
1:B:450:ILE:HG22	1:B:557:ILE:HG12	1.96	0.47
1:B:679:PRO:HG2	1:B:721:GLU:OE1	2.15	0.47
1:B:713:LEU:HD11	2:D:506:LEU:HD21	1.97	0.47
2:D:38:TYR:CE2	2:D:93:LYS:HG2	2.50	0.47
2:E:338:THR:HG23	2:E:339:GLY:N	2.29	0.47
2:E:498:ASP:OD1	2:E:499:ARG:N	2.48	0.47
2:F:247:ARG:HE	2:F:262:VAL:HG11	1.79	0.47
2:E:302:GLY:O	2:E:306:ILE:HG13	2.15	0.47
2:E:380:SER:O	2:E:420:LYS:NZ	2.29	0.47
2:E:224:LEU:HD22	2:E:228:LEU:HB3	1.97	0.47
2:E:356:THR:HG21	2:E:489:LEU:HD13	1.97	0.47
2:F:154:PHE:HE1	2:F:173:PRO:HD2	1.80	0.47
1:C:652:VAL:HG21	1:C:658:ILE:HD13	1.97	0.46
2:F:473:ILE:HG22	2:F:475:LEU:HG	1.96	0.46
1:A:256:GLY:HA3	2:F:256:ARG:HE	1.81	0.46
1:A:338:SER:OG	1:A:339:ASN:N	2.46	0.46
2:D:42:VAL:HG21	2:D:69:PHE:CZ	2.51	0.46
2:F:538:LEU:HD13	2:F:588:VAL:HG21	1.98	0.46
1:C:590:VAL:HG13	1:C:590:VAL:O	2.16	0.46
2:D:36:ALA:O	2:D:37:HIS:CG	2.68	0.46
2:E:550:TYR:CD1	2:E:569:LEU:HD22	2.51	0.46
2:D:11:GLN:O	2:D:14:GLU:HG3	2.15	0.46
1:B:289:GLN:HE22	1:B:291:ILE:HG22	1.81	0.46
1:C:293:ILE:HD11	1:C:331:ILE:HD12	1.97	0.46
2:D:71:SER:O	2:D:75:ARG:HG2	2.16	0.46
2:E:226:ASP:OD1	2:E:227:ASP:N	2.49	0.46
2:F:480:LEU:O	2:F:480:LEU:HD23	2.15	0.46
2:D:329:ALA:HB3	2:D:578:ALA:HB1	1.98	0.46
2:E:232:CYS:SG	2:E:233:LYS:N	2.89	0.46
1:A:613:ARG:NH2	2:D:342:VAL:HG21	2.31	0.46
1:B:644:LYS:HB2	1:B:649:ARG:HD3	1.96	0.46
1:A:240:PHE:HD2	1:A:261:PRO:HG3	1.80	0.46
1:A:170:ARG:NH1	1:A:174:GLU:OE1	2.47	0.45
1:A:404:LYS:HG2	1:A:650:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:SER:H	1:A:732:ALA:HB3	1.82	0.45
1:C:727:GLU:OE1	1:C:729:ARG:NH2	2.45	0.45
2:D:469:VAL:O	2:D:473:ILE:HG22	2.15	0.45
2:F:24:ASP:OD1	2:F:25:ILE:N	2.49	0.45
1:B:392:ALA:O	1:B:396:ILE:HG12	2.16	0.45
2:D:179:ASP:OD1	2:D:179:ASP:N	2.47	0.45
1:C:151:LYS:HD2	1:C:151:LYS:N	2.32	0.45
1:C:749:LEU:HA	1:C:752:TYR:CD1	2.51	0.45
1:B:731:GLU:HG3	1:B:732:ALA:H	1.82	0.45
1:C:156:MET:O	1:C:160:ILE:HG12	2.16	0.45
2:D:13:PHE:CE1	2:D:47:LEU:HD21	2.51	0.45
2:D:220:MET:HE2	2:D:220:MET:HA	1.99	0.45
2:F:168:ARG:HE	2:F:169:PRO:HD2	1.80	0.45
2:F:285:GLN:O	2:F:288:PHE:N	2.49	0.45
2:F:590:LEU:HD21	2:F:636:LEU:HD21	1.97	0.45
2:D:154:PHE:HE1	2:D:173:PRO:HD2	1.82	0.45
2:E:103:LEU:HD11	2:E:109:LEU:HD13	1.98	0.45
1:B:264:CYS:SG	1:B:271:GLY:HA2	2.56	0.45
2:D:366:ALA:O	2:D:372:SER:OG	2.30	0.45
2:D:428:HIS:NE2	2:D:479:LEU:HD12	2.32	0.45
2:E:143:ARG:HE	2:E:166:PHE:HD2	1.63	0.45
1:C:571:LYS:HE3	1:C:575:GLU:CD	2.42	0.45
1:C:682:SER:H	1:C:732:ALA:HB3	1.81	0.45
2:D:152:HIS:HE1	2:D:174:SER:HB3	1.81	0.45
1:B:210:VAL:HG22	1:B:214:TYR:CD2	2.51	0.45
2:D:252:GLN:HB2	2:D:255:VAL:HG21	1.99	0.45
2:D:522:GLU:HA	2:D:525:LYS:HG2	1.99	0.45
2:D:600:MET:HE2	2:D:600:MET:HA	1.98	0.45
2:D:338:THR:HG23	2:D:339:GLY:N	2.33	0.44
1:A:222:ARG:NH2	1:A:296:LEU:HB2	2.33	0.44
1:B:438:ASP:HA	1:B:441:ARG:HG3	2.00	0.44
1:C:148:ALA:HB1	1:C:151:LYS:HG2	1.98	0.44
2:D:496:ASP:O	2:D:500:ILE:HG12	2.18	0.44
1:A:213:ASN:HD21	2:D:36:ALA:HA	1.82	0.44
1:C:489:VAL:HG21	1:C:550:LEU:HD21	1.98	0.44
1:C:588:ASP:OD1	1:C:715:SER:OG	2.24	0.44
2:E:550:TYR:OH	2:E:554:ARG:NH2	2.45	0.44
1:A:253:LEU:HD11	1:A:258:TYR:HA	1.99	0.44
1:B:319:LEU:O	1:B:320:VAL:HB	2.17	0.44
1:B:530:LEU:H	1:B:530:LEU:HD23	1.82	0.44
1:C:390:LEU:HA	1:C:393:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:ARG:O	2:E:313:GLN:NE2	2.42	0.44
1:C:672:TYR:HE2	1:C:728:LEU:HD21	1.82	0.44
2:D:74:ARG:HH12	2:D:96:LEU:H	1.64	0.44
2:D:247:ARG:HE	2:D:262:VAL:HG11	1.83	0.44
2:E:208:VAL:HG23	2:E:211:LEU:HD12	2.00	0.44
2:E:550:TYR:HD1	2:E:569:LEU:HD22	1.82	0.44
2:E:69:PHE:O	2:E:73:LEU:HD23	2.17	0.44
2:E:559:ARG:O	2:E:564:THR:OG1	2.28	0.44
1:C:448:PRO:O	1:C:449:HIS:ND1	2.51	0.44
1:C:213:ASN:HD21	2:F:36:ALA:HA	1.83	0.44
2:D:134:SER:OG	2:D:135:LEU:N	2.50	0.44
2:D:346:SER:OG	2:D:484:ASP:OD2	2.28	0.44
1:A:210:VAL:H	1:A:309:ARG:HH22	1.64	0.43
1:B:293:ILE:HD12	1:B:331:ILE:HD13	2.00	0.43
2:F:435:THR:HG21	2:F:446:LYS:HE3	1.99	0.43
1:B:514:ILE:HD11	1:B:557:ILE:HG13	1.99	0.43
1:B:679:PRO:HB3	1:B:730:GLU:HA	1.99	0.43
1:C:317:HIS:C	1:C:319:LEU:H	2.26	0.43
1:C:439:LYS:NZ	2:E:520:SER:HB2	2.34	0.43
2:F:410:LEU:HD21	2:F:454:LEU:HD12	2.00	0.43
2:F:538:LEU:HD12	2:F:543:ASN:OD1	2.18	0.43
2:D:498:ASP:OD1	2:D:499:ARG:N	2.50	0.43
2:E:16:TYR:OH	2:E:46:THR:OG1	2.34	0.43
1:A:431:GLY:O	1:A:725:ARG:NH2	2.51	0.43
1:C:402:LEU:HD23	1:C:727:GLU:HA	2.00	0.43
1:C:749:LEU:HG	1:C:752:TYR:HE1	1.84	0.43
2:F:103:LEU:HD21	2:F:109:LEU:HD23	2.00	0.43
1:B:339:ASN:OD1	1:B:340:ALA:N	2.52	0.43
1:C:459:GLY:HA2	3:C:2001:ADP:H5'2	2.01	0.43
2:D:484:ASP:O	2:D:563:ARG:NH2	2.51	0.43
2:E:506:LEU:HD23	2:E:506:LEU:HA	1.89	0.43
2:F:194:THR:C	2:F:195:ARG:HD2	2.44	0.43
1:A:92:LEU:HD11	1:A:151:LYS:HD2	2.01	0.43
2:D:601:GLU:CD	2:D:610:LEU:HB2	2.44	0.43
2:E:518:LEU:HB3	2:E:519:TRP:H	1.55	0.43
1:B:740:ILE:O	1:B:740:ILE:HG22	2.19	0.43
1:C:92:LEU:O	1:C:96:ILE:HG13	2.19	0.43
2:D:538:LEU:HD12	2:D:543:ASN:OD1	2.19	0.43
2:E:484:ASP:OD1	2:E:571:SER:OG	2.24	0.43
2:E:517:LYS:HE3	2:E:517:LYS:HB2	1.86	0.43
2:F:9:VAL:HG13	2:F:13:PHE:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:517:LYS:HE3	2:F:517:LYS:HB2	1.89	0.43
1:A:304:ALA:HB2	2:D:233:LYS:HD3	2.00	0.43
1:A:319:LEU:O	1:A:320:VAL:HB	2.19	0.43
1:B:410:LEU:HD23	1:B:421:LYS:HG2	2.01	0.43
1:C:201:TYR:CE2	1:C:203:PRO:HG2	2.53	0.43
1:C:319:LEU:O	1:C:320:VAL:HB	2.19	0.43
1:C:339:ASN:OD1	1:C:340:ALA:N	2.52	0.43
1:C:228:VAL:HG13	1:C:289:GLN:HE21	1.82	0.43
1:C:270:ARG:HD3	1:C:271:GLY:N	2.34	0.43
2:F:496:ASP:O	2:F:500:ILE:HG12	2.19	0.43
2:D:650:ARG:HG2	2:D:654:ARG:NH1	2.32	0.42
1:B:602:ASP:OD1	1:B:603:HIS:N	2.52	0.42
2:E:32:ARG:CZ	2:E:33:ASP:H	2.32	0.42
1:A:606:SER:HA	1:A:609:VAL:HG12	2.00	0.42
1:A:685:ALA:HB1	1:A:737:ALA:HB2	2.00	0.42
1:A:693:TYR:CD2	1:A:713:LEU:HD13	2.54	0.42
2:D:432:GLU:HG2	2:D:433:GLN:NE2	2.34	0.42
2:E:36:ALA:H	2:E:93:LYS:NZ	2.15	0.42
2:F:252:GLN:HB3	2:F:255:VAL:HG21	2.01	0.42
1:A:270:ARG:HD3	1:A:271:GLY:N	2.35	0.42
1:B:92:LEU:O	1:B:96:ILE:HG13	2.19	0.42
1:B:672:TYR:HE2	1:B:728:LEU:HD21	1.84	0.42
1:A:440:ASN:OD1	1:A:441:ARG:N	2.52	0.42
1:B:341:GLU:OE1	1:B:341:GLU:N	2.50	0.42
2:D:616:LEU:HD23	2:D:616:LEU:HA	1.89	0.42
2:E:111:ARG:HH12	2:E:124:LEU:HD11	1.84	0.42
2:F:507:GLU:HB3	2:F:509:LYS:HG3	2.02	0.42
1:A:92:LEU:O	1:A:96:ILE:HG13	2.18	0.42
1:B:590:VAL:O	1:B:590:VAL:HG13	2.19	0.42
1:C:302:ARG:HD2	1:C:304:ALA:HB3	2.01	0.42
2:D:42:VAL:HG21	2:D:69:PHE:HZ	1.84	0.42
1:A:240:PHE:CD2	1:A:261:PRO:HG3	2.55	0.42
1:A:317:HIS:C	1:A:319:LEU:H	2.28	0.42
2:F:2:ASN:H	2:F:5:GLN:NE2	2.18	0.42
2:F:327:VAL:HG21	2:F:348:LEU:HB2	2.01	0.42
1:C:352:MET:HE3	1:C:352:MET:HB3	1.91	0.42
2:D:518:LEU:HB3	2:D:519:TRP:H	1.68	0.42
2:E:240:ILE:HG12	2:E:268:ILE:HD13	2.01	0.42
2:F:356:THR:OG1	2:F:358:LYS:NZ	2.50	0.42
1:B:746:TYR:O	1:B:751:THR:OG1	2.34	0.42
2:D:334:ARG:HD3	2:D:334:ARG:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:550:TYR:OH	2:E:566:ILE:HA	2.20	0.42
2:E:627:GLN:HA	2:E:627:GLN:OE1	2.20	0.42
1:C:306:ARG:HB2	2:F:233:LYS:HZ2	1.84	0.42
2:F:501:ILE:HD12	2:F:501:ILE:HA	1.92	0.42
1:C:164:LEU:HD23	1:C:191:VAL:HG21	2.02	0.41
1:C:222:ARG:HH22	1:C:296:LEU:H	1.68	0.41
1:A:507:LEU:HD22	1:A:554:THR:HG21	2.02	0.41
1:C:466:ALA:O	1:C:470:VAL:HG22	2.20	0.41
1:A:337:VAL:HG22	1:A:355:LEU:HD23	2.02	0.41
1:B:720:THR:HA	1:B:740:ILE:HG13	2.02	0.41
2:D:124:LEU:HG	2:D:125:SER:H	1.85	0.41
2:D:493:LYS:HD2	2:D:493:LYS:HA	1.88	0.41
2:E:13:PHE:HB3	2:E:69:PHE:HD1	1.85	0.41
2:E:515:SER:OG	2:E:517:LYS:HE2	2.20	0.41
1:B:74:PRO:HG2	1:B:75:TYR:CD1	2.56	0.41
1:C:337:VAL:HG22	1:C:355:LEU:HD23	2.02	0.41
1:A:424:LEU:O	1:A:428:LEU:HG	2.21	0.41
1:B:546:VAL:HG23	1:B:546:VAL:O	2.20	0.41
1:A:128:LEU:HD22	1:A:134:VAL:HG11	2.02	0.41
1:A:201:TYR:CD2	1:A:203:PRO:HD2	2.55	0.41
1:A:470:VAL:HG23	1:A:470:VAL:O	2.21	0.41
2:D:296:LYS:O	2:D:296:LYS:NZ	2.48	0.41
1:A:231:ILE:HD11	2:F:218:ARG:CZ	2.50	0.41
1:A:264:CYS:SG	1:A:271:GLY:HA2	2.60	0.41
1:A:433:GLN:HG2	1:A:435:TYR:CE1	2.56	0.41
1:A:466:ALA:O	1:A:470:VAL:HG22	2.20	0.41
1:B:723:ARG:HG3	1:B:723:ARG:O	2.21	0.41
1:C:406:ILE:HG21	1:C:726:LEU:HD21	2.02	0.41
2:E:630:ARG:HD2	2:E:630:ARG:HA	1.70	0.41
1:B:403:PHE:CD2	1:B:650:LEU:HD21	2.53	0.41
1:B:437:ASP:O	1:B:441:ARG:N	2.45	0.41
1:C:410:LEU:HD23	1:C:421:LYS:HG2	2.01	0.41
2:E:139:LEU:HD23	2:E:199:TYR:HB2	2.03	0.41
2:F:134:SER:OG	2:F:201:GLU:N	2.53	0.41
1:A:540:SER:HA	1:A:549:SER:HA	2.02	0.41
1:C:220:ALA:C	1:C:221:LEU:HD12	2.45	0.41
1:C:251:PHE:HA	1:C:252:PRO:HD3	1.91	0.41
1:C:537:GLN:OE1	1:C:553:ARG:HA	2.21	0.41
2:E:75:ARG:O	2:E:78:LEU:HG	2.21	0.41
2:E:130:VAL:HG21	2:E:232:CYS:SG	2.61	0.41
2:F:307:LEU:HD11	2:F:322:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:541:LEU:HG	1:C:543:LYS:H	1.86	0.41
2:E:388:THR:HB	2:E:399:GLU:HB2	2.02	0.41
2:F:139:LEU:HD23	2:F:199:TYR:HB2	2.02	0.41
1:A:403:PHE:CD2	1:A:650:LEU:HD11	2.56	0.40
3:B:2001:ADP:C8	2:E:566:ILE:HD11	2.55	0.40
1:C:691:ASP:O	1:C:695:GLU:OE1	2.39	0.40
2:F:515:SER:OG	2:F:517:LYS:HE2	2.21	0.40
1:A:163:VAL:O	1:A:166:LYS:HG3	2.22	0.40
1:B:106:HIS:NE2	1:B:109:LEU:HD22	2.36	0.40
1:B:541:LEU:HG	1:B:543:LYS:H	1.87	0.40
1:C:228:VAL:HG13	1:C:289:GLN:NE2	2.36	0.40
2:D:302:GLY:O	2:D:306:ILE:HG13	2.21	0.40
2:E:33:ASP:OD2	2:E:36:ALA:HB2	2.21	0.40
2:E:206:GLU:HB2	2:E:217:PRO:HB2	2.03	0.40
2:E:252:GLN:HB2	2:E:255:VAL:HG21	2.03	0.40
2:F:208:VAL:HG23	2:F:211:LEU:HD12	2.03	0.40
1:A:489:VAL:HG23	1:A:539:ILE:HD13	2.03	0.40
2:F:42:VAL:HG21	2:F:69:PHE:HZ	1.86	0.40
1:A:446:GLY:HA2	1:A:718:ARG:HD3	2.04	0.40
1:B:164:LEU:HD23	1:B:191:VAL:HG21	2.03	0.40
1:C:450:ILE:HG23	1:C:557:ILE:HG23	2.03	0.40
1:C:535:GLU:CD	1:C:711:ARG:HH22	2.29	0.40
1:C:723:ARG:HG3	1:C:723:ARG:O	2.21	0.40
2:D:149:LYS:HE3	2:D:180:SER:HB3	2.03	0.40
2:E:118:LYS:O	2:E:118:LYS:NZ	2.44	0.40
2:E:243:ILE:O	2:E:263:LEU:HD12	2.22	0.40
2:F:74:ARG:HH12	2:F:96:LEU:H	1.69	0.40
1:B:251:PHE:HA	1:B:252:PRO:HD3	1.91	0.40
1:B:317:HIS:C	1:B:319:LEU:H	2.29	0.40
1:B:352:MET:HE3	1:B:352:MET:HB3	1.86	0.40
2:D:640:GLU:OE2	2:D:640:GLU:N	2.54	0.40
2:F:270:VAL:O	2:F:270:VAL:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	590/840 (70%)	527 (89%)	59 (10%)	4 (1%)	19	56
1	B	590/840 (70%)	527 (89%)	59 (10%)	4 (1%)	19	56
1	C	590/840 (70%)	525 (89%)	61 (10%)	4 (1%)	19	56
2	D	611/1143 (54%)	561 (92%)	48 (8%)	2 (0%)	37	72
2	E	611/1143 (54%)	555 (91%)	55 (9%)	1 (0%)	44	78
2	F	611/1143 (54%)	553 (90%)	57 (9%)	1 (0%)	44	78
All	All	3603/5949 (61%)	3248 (90%)	339 (9%)	16 (0%)	32	67

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	VAL
1	B	266	VAL
1	C	266	VAL
1	A	320	VAL
1	A	547	VAL
1	B	320	VAL
1	B	547	VAL
1	C	320	VAL
1	C	547	VAL
1	A	441	ARG
1	C	441	ARG
1	B	441	ARG
2	D	560	ASN
2	E	444	VAL
2	D	444	VAL
2	F	444	VAL

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	519/723 (72%)	519 (100%)	0	100	100
1	B	519/723 (72%)	519 (100%)	0	100	100
1	C	519/723 (72%)	519 (100%)	0	100	100
2	D	555/1020 (54%)	555 (100%)	0	100	100
2	E	555/1020 (54%)	555 (100%)	0	100	100
2	F	555/1020 (54%)	555 (100%)	0	100	100
All	All	3222/5229 (62%)	3222 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	A	162	GLN
1	A	209	ASN
1	A	394	GLN
1	A	401	ASN
1	A	417	HIS
1	A	462	GLN
1	A	465	GLN
1	A	608	HIS
1	B	213	ASN
1	B	289	GLN
1	B	394	GLN
1	B	465	GLN
1	B	608	HIS
1	C	566	HIS
1	C	608	HIS
2	D	5	GLN
2	D	86	GLN
2	D	152	HIS
2	D	209	GLN
2	D	434	GLN
2	D	458	ASN
2	D	551	GLN
2	D	617	HIS
2	E	5	GLN
2	E	86	GLN
2	E	95	ASN
2	E	266	ASN

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Mol	Chain	Res	Type
2	E	360	GLN
2	E	448	ASN
2	E	553	GLN
2	F	5	GLN
2	F	37	HIS
2	F	59	ASN
2	F	86	GLN
2	F	95	ASN
2	F	200	GLN
2	F	266	ASN
2	F	360	GLN
2	F	434	GLN
2	F	466	GLN
2	F	617	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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
3	ADP	A	2001	-	24,29,29	0.91	0	29,45,45	1.24	2 (6%)
3	ADP	D	2001	4	24,29,29	0.89	0	29,45,45	1.23	2 (6%)
3	ADP	C	2001	-	24,29,29	0.92	0	29,45,45	1.25	3 (10%)
3	ADP	E	2001	4	24,29,29	0.89	0	29,45,45	1.22	3 (10%)
3	ADP	F	2001	4	24,29,29	0.89	0	29,45,45	1.23	2 (6%)
3	ADP	B	2001	-	24,29,29	0.92	0	29,45,45	1.22	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	2001	-	-	3/12/32/32	0/3/3/3
3	ADP	D	2001	4	-	2/12/32/32	0/3/3/3
3	ADP	C	2001	-	-	3/12/32/32	0/3/3/3
3	ADP	E	2001	4	-	2/12/32/32	0/3/3/3
3	ADP	F	2001	4	-	4/12/32/32	0/3/3/3
3	ADP	B	2001	-	-	2/12/32/32	0/3/3/3

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2001	ADP	N3-C2-N1	-3.61	123.78	128.67
3	C	2001	ADP	N3-C2-N1	-3.60	123.78	128.67
3	D	2001	ADP	N3-C2-N1	-3.60	123.78	128.67
3	E	2001	ADP	N3-C2-N1	-3.60	123.79	128.67
3	A	2001	ADP	N3-C2-N1	-3.58	123.81	128.67
3	B	2001	ADP	N3-C2-N1	-3.51	123.90	128.67
3	B	2001	ADP	C4-C5-N7	-2.60	106.59	109.34
3	A	2001	ADP	C4-C5-N7	-2.53	106.67	109.34
3	C	2001	ADP	C4-C5-N7	-2.51	106.68	109.34
3	E	2001	ADP	C4-C5-N7	-2.47	106.73	109.34
3	D	2001	ADP	C4-C5-N7	-2.45	106.75	109.34
3	F	2001	ADP	C4-C5-N7	-2.42	106.78	109.34
3	C	2001	ADP	C4'-O4'-C1'	2.14	111.88	109.92
3	E	2001	ADP	C4'-O4'-C1'	2.06	111.81	109.92

There are no chirality outliers.

All (16) torsion outliers are listed below:

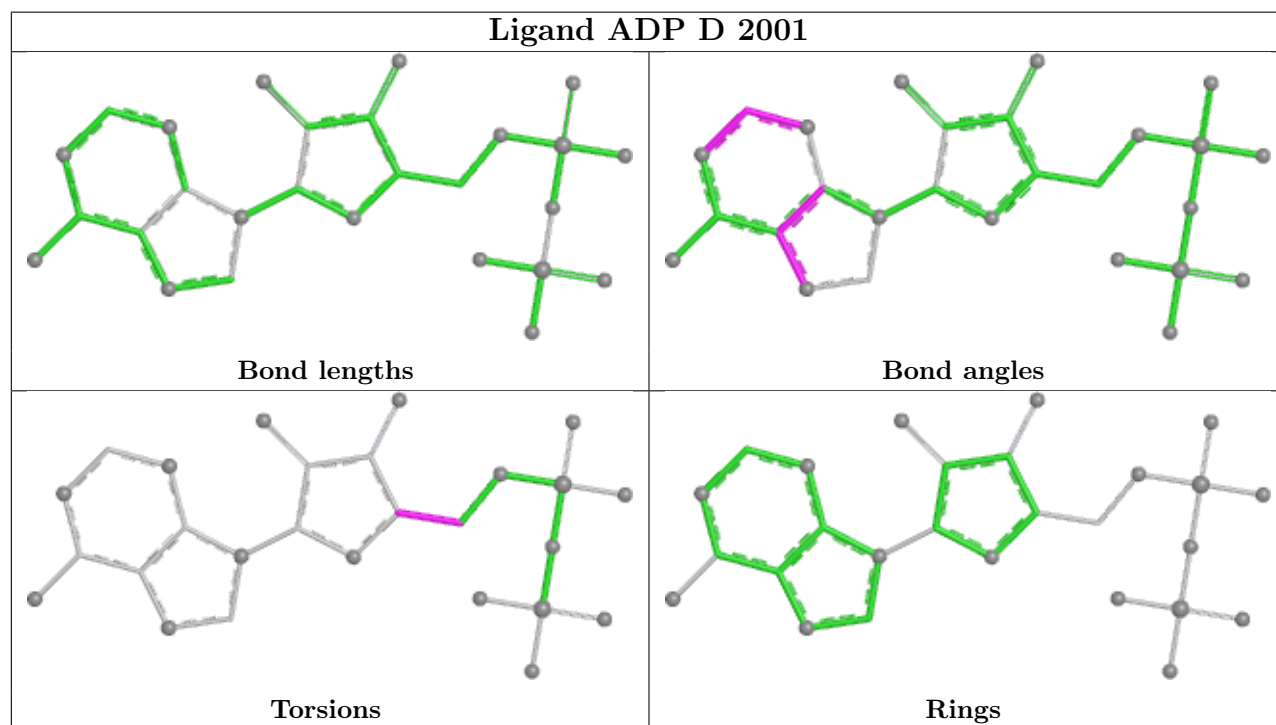
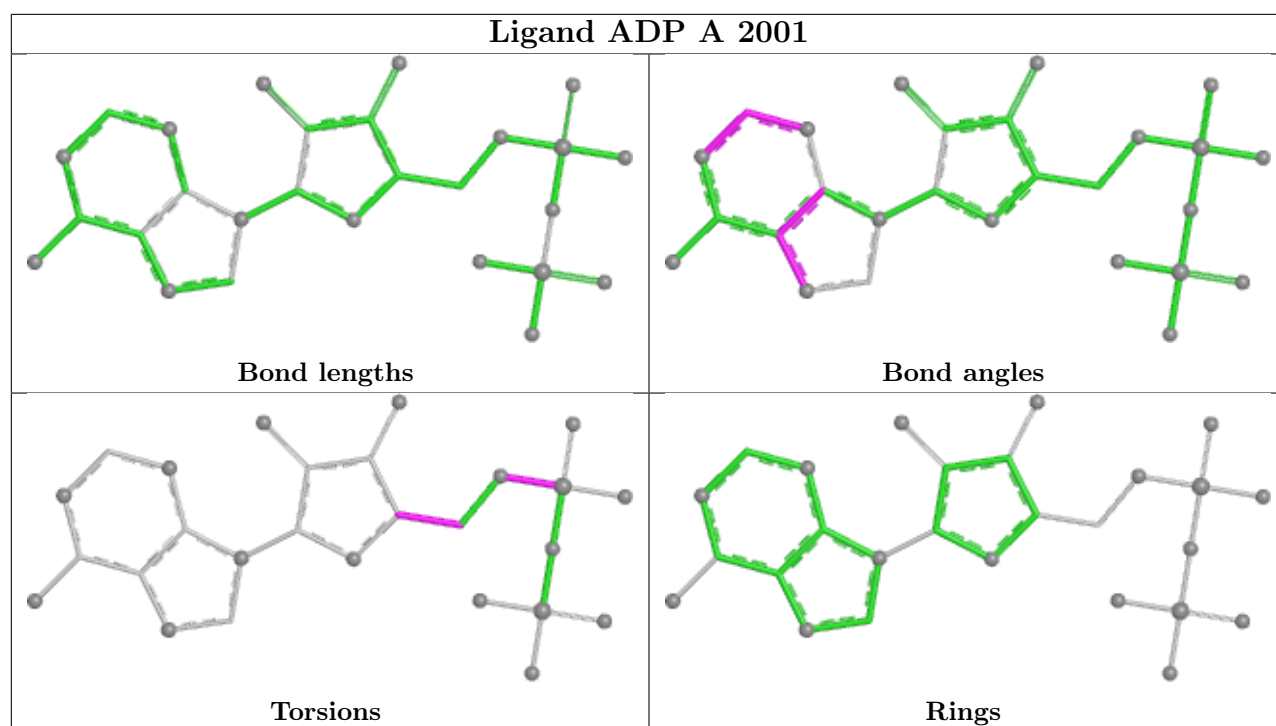
Mol	Chain	Res	Type	Atoms
3	A	2001	ADP	C5'-O5'-PA-O2A
3	A	2001	ADP	C5'-O5'-PA-O3A
3	B	2001	ADP	C5'-O5'-PA-O2A
3	B	2001	ADP	C5'-O5'-PA-O3A
3	C	2001	ADP	C5'-O5'-PA-O2A
3	C	2001	ADP	C5'-O5'-PA-O3A
3	D	2001	ADP	O4'-C4'-C5'-O5'
3	D	2001	ADP	C3'-C4'-C5'-O5'
3	E	2001	ADP	O4'-C4'-C5'-O5'
3	E	2001	ADP	C3'-C4'-C5'-O5'
3	F	2001	ADP	C3'-C4'-C5'-O5'
3	F	2001	ADP	O4'-C4'-C5'-O5'
3	F	2001	ADP	C5'-O5'-PA-O2A
3	F	2001	ADP	C5'-O5'-PA-O3A
3	C	2001	ADP	C3'-C4'-C5'-O5'
3	A	2001	ADP	C3'-C4'-C5'-O5'

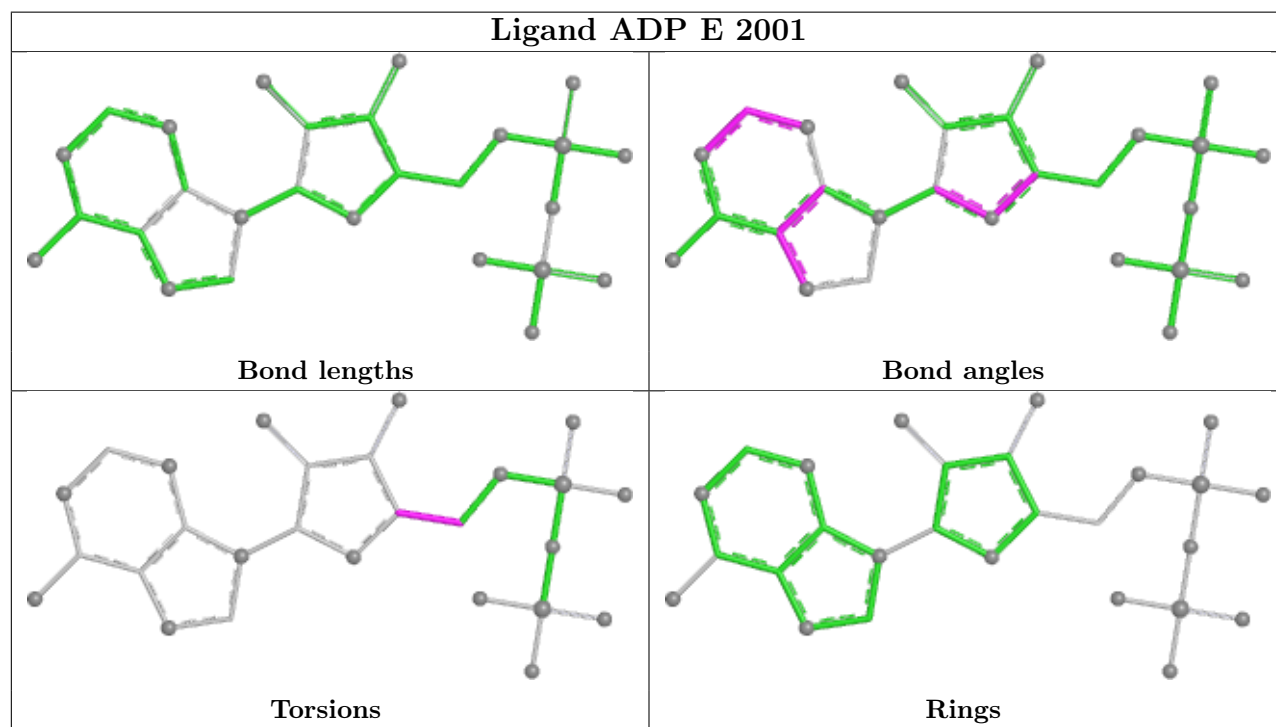
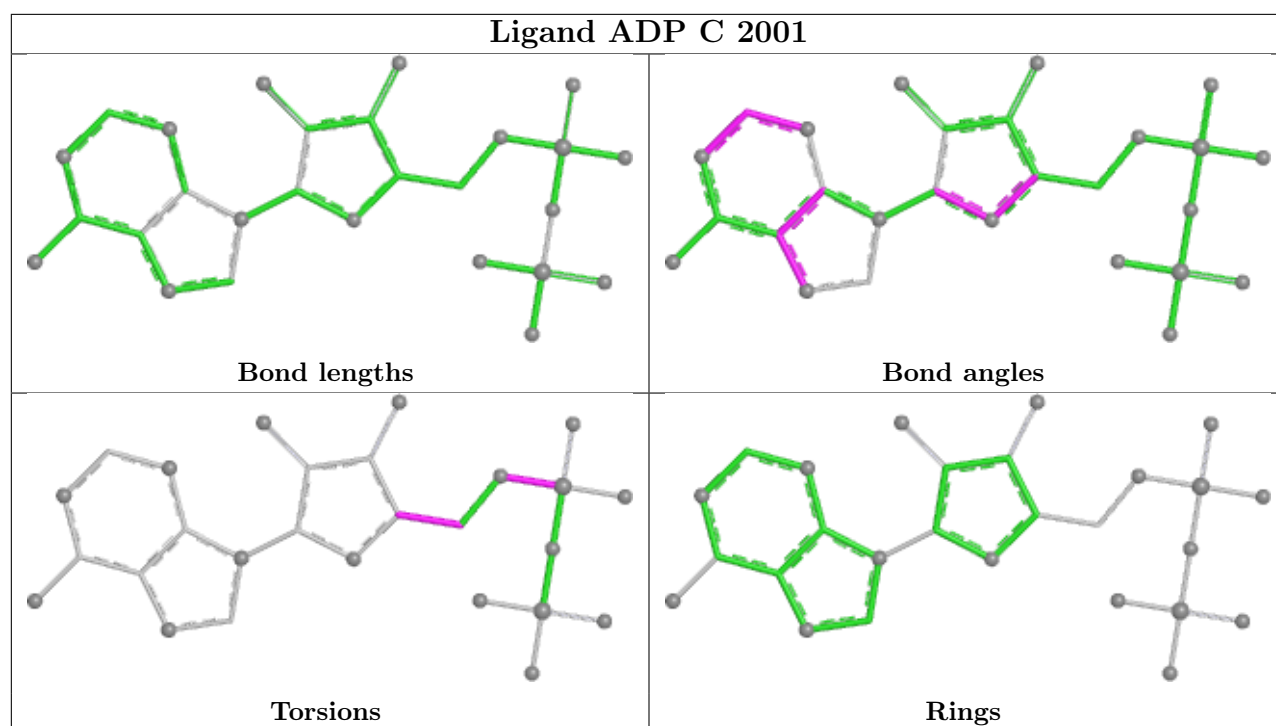
There are no ring outliers.

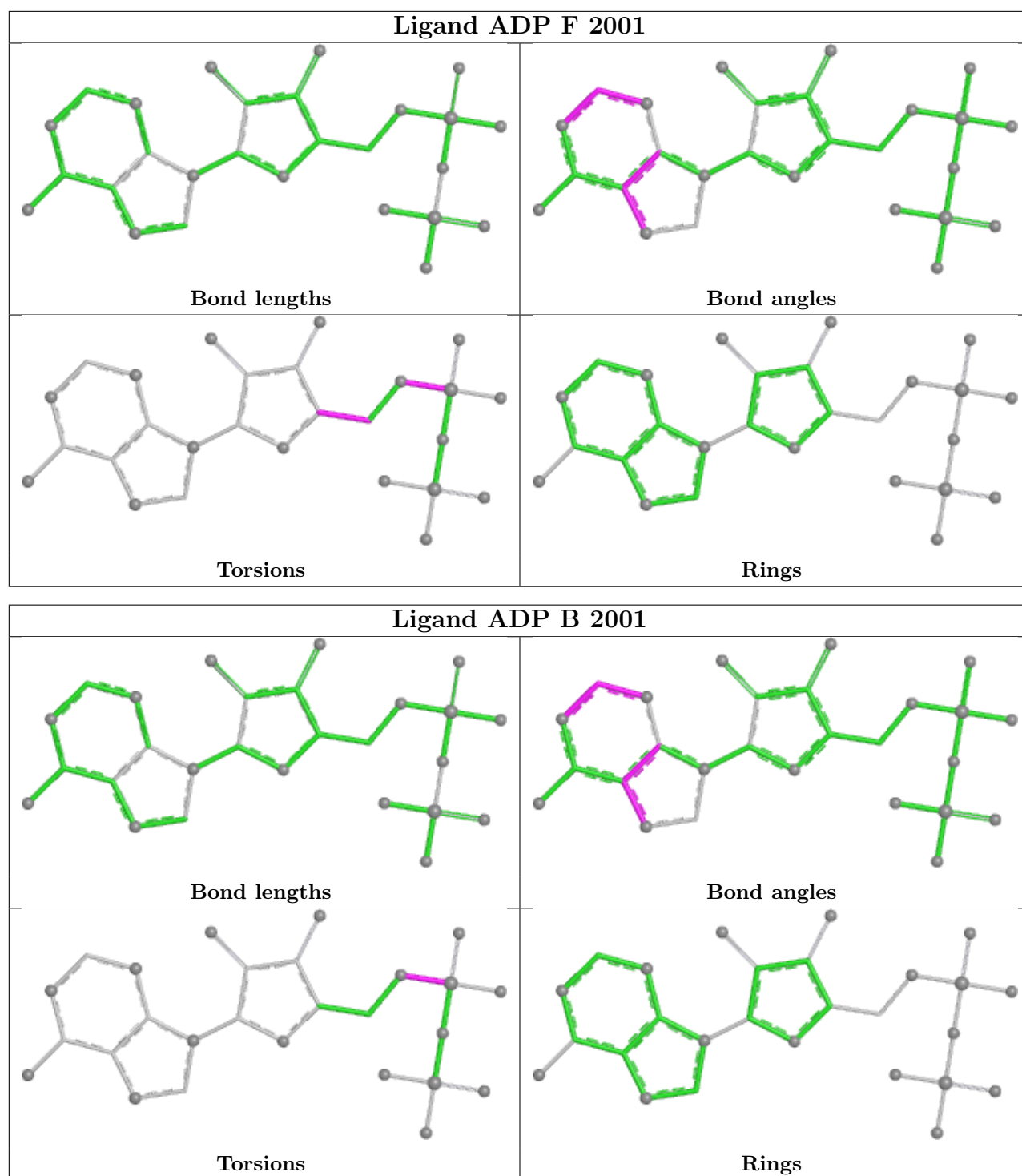
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2001	ADP	1	0
3	B	2001	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

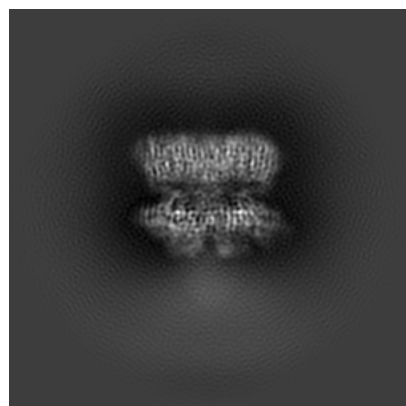
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40234. These allow visual inspection of the internal detail of the map and identification of artifacts.

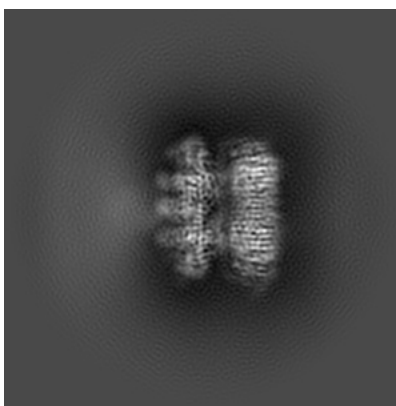
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

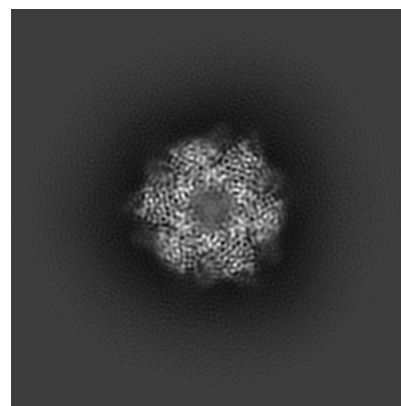
6.1.1 Primary map



X

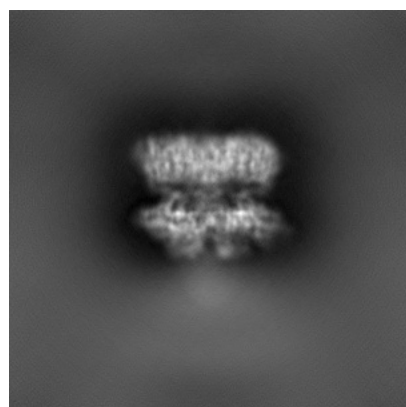


Y

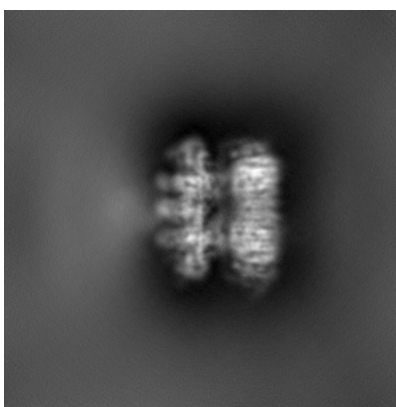


Z

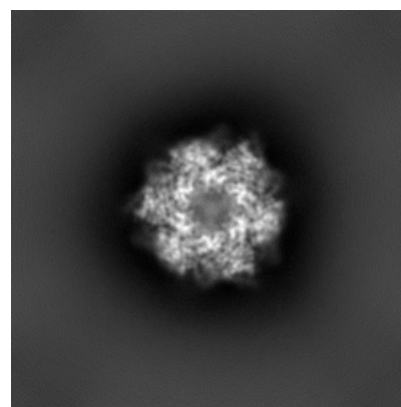
6.1.2 Raw map



X



Y

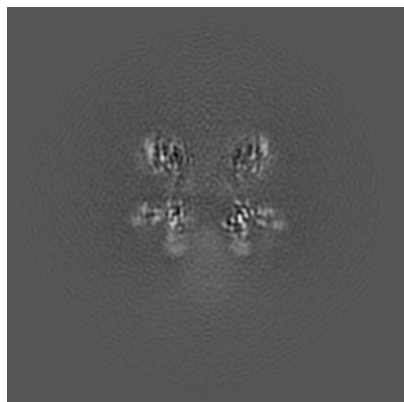


Z

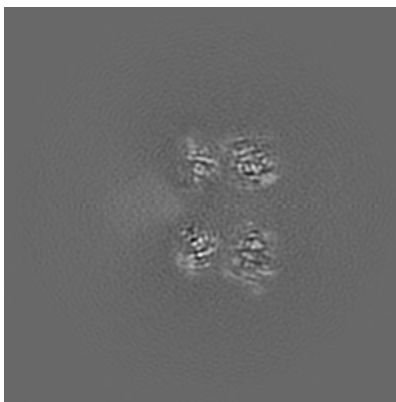
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

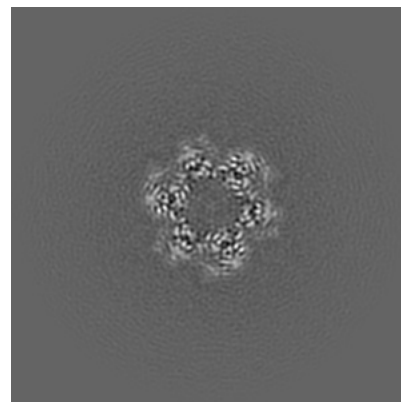
6.2.1 Primary map



X Index: 160

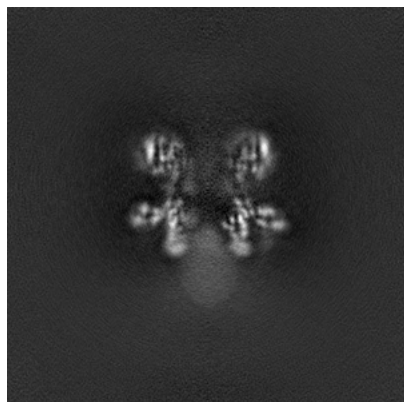


Y Index: 160

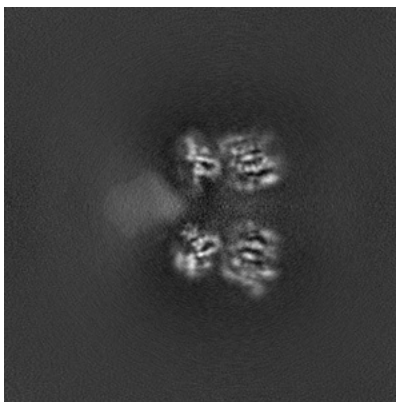


Z Index: 160

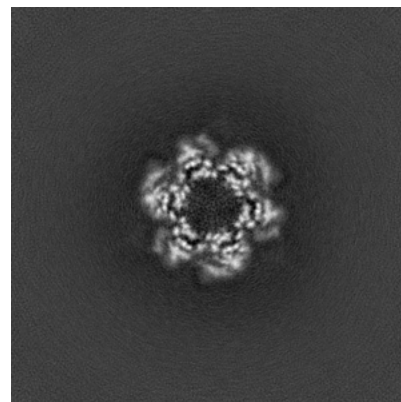
6.2.2 Raw map



X Index: 160



Y Index: 160

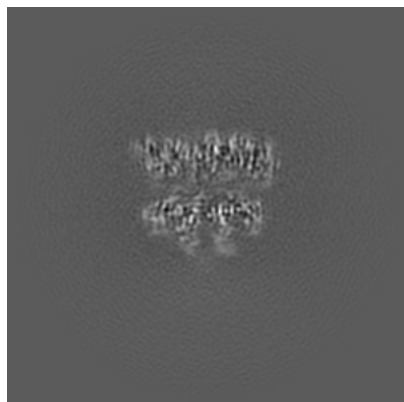


Z Index: 160

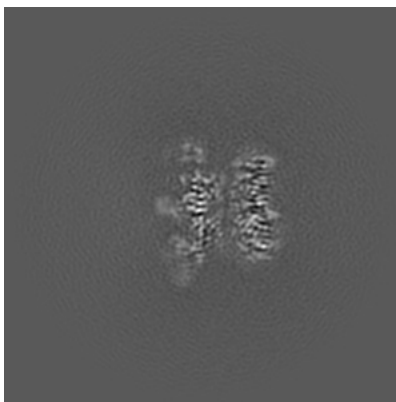
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

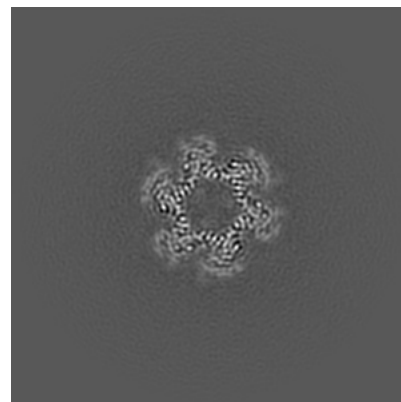
6.3.1 Primary map



X Index: 183

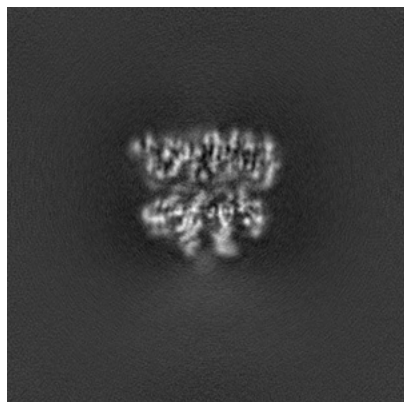


Y Index: 135

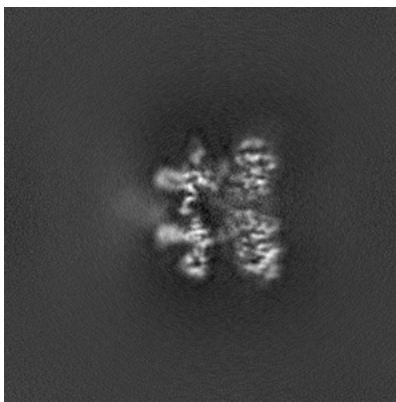


Z Index: 157

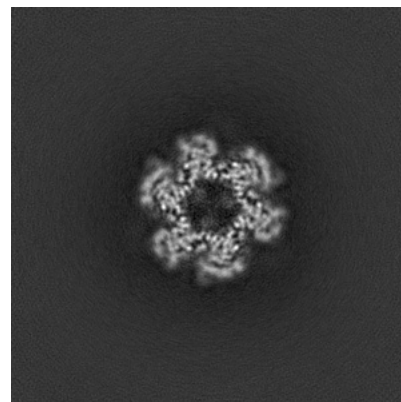
6.3.2 Raw map



X Index: 184



Y Index: 175

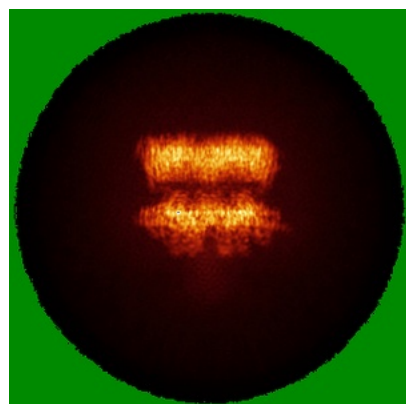


Z Index: 157

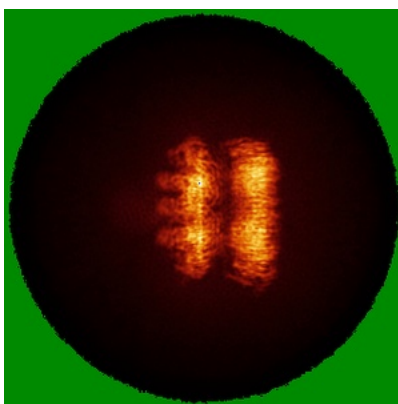
The images above show the largest variance slices of the map in three orthogonal directions.

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

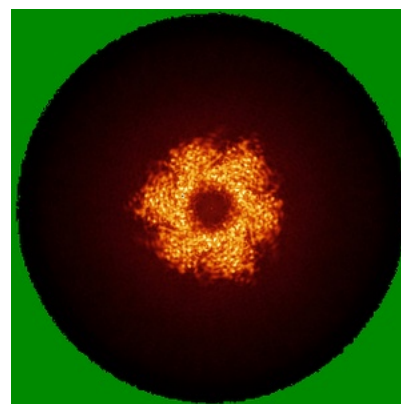
6.4.1 Primary map



X

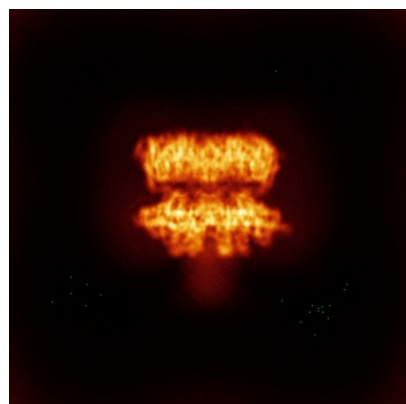


Y

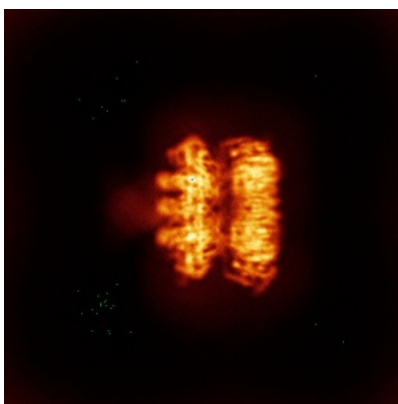


Z

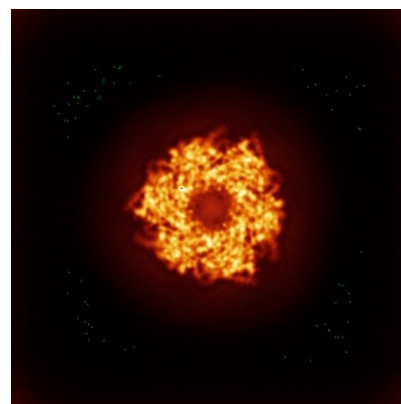
6.4.2 Raw map



X



Y

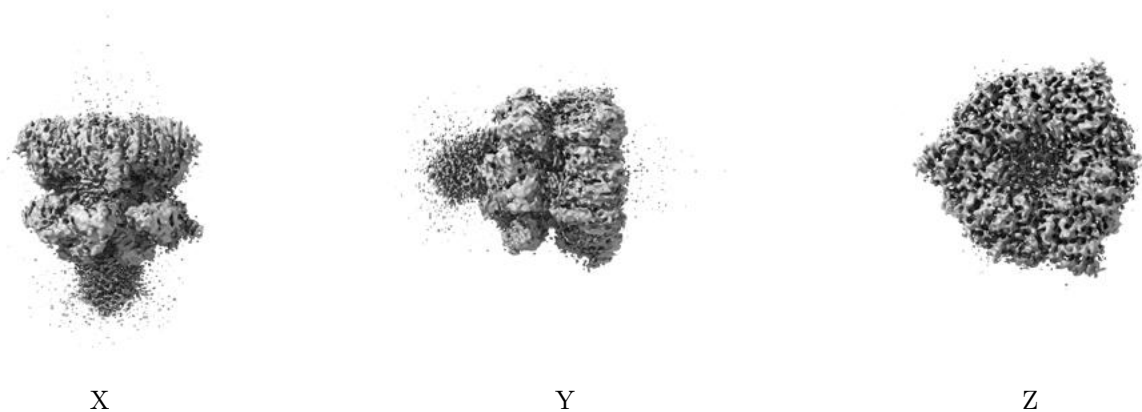


Z

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.

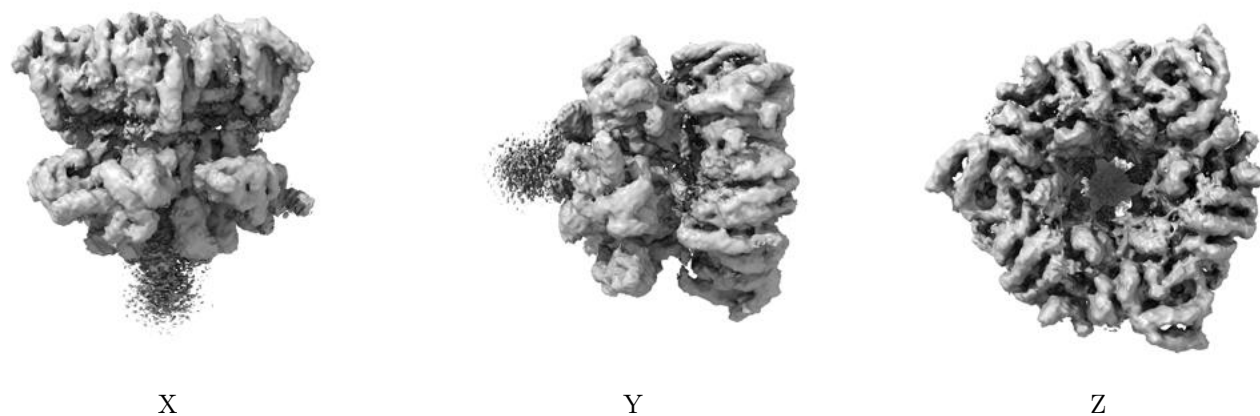
6.5 Orthogonal surface views [i](#)

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.

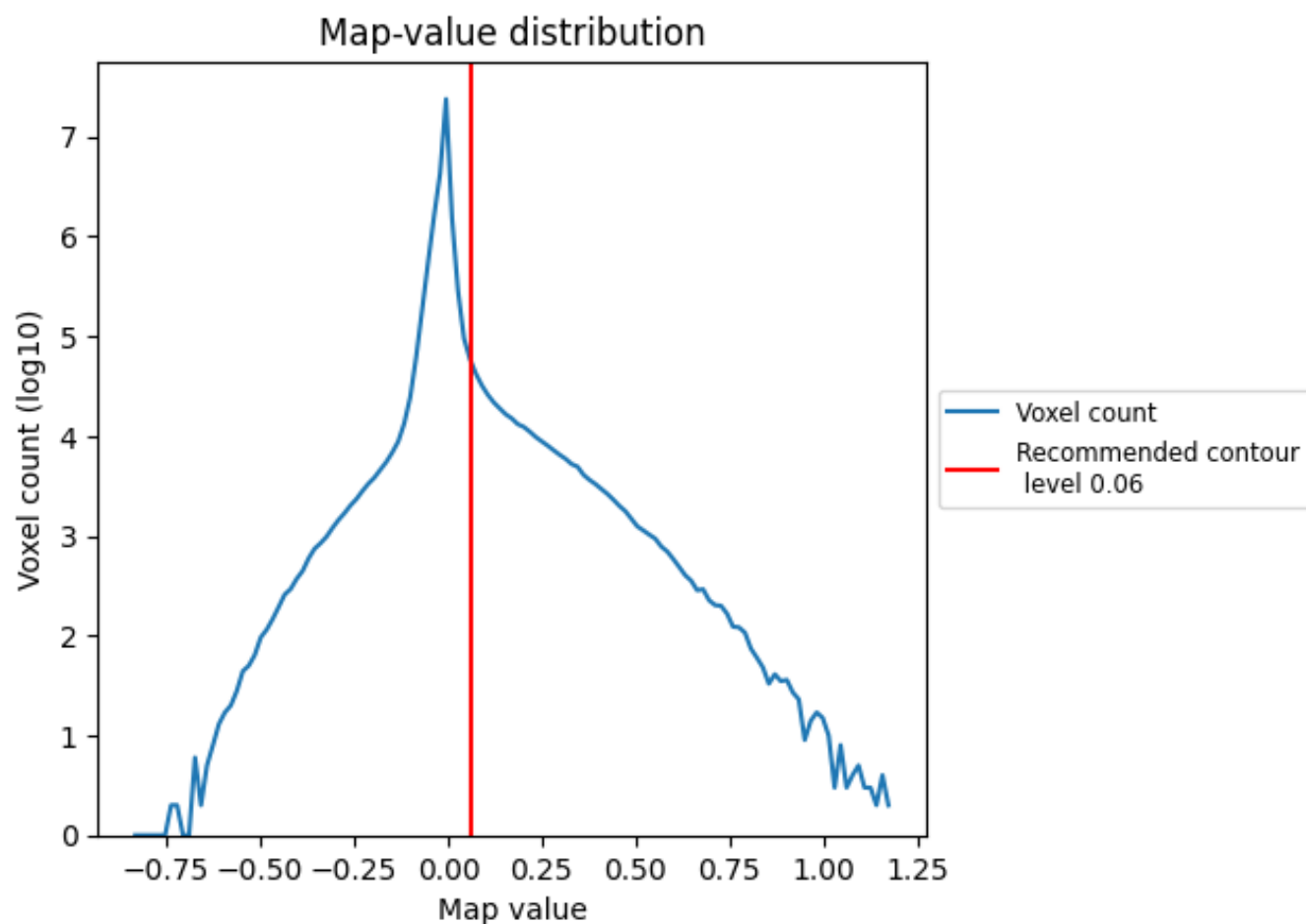
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

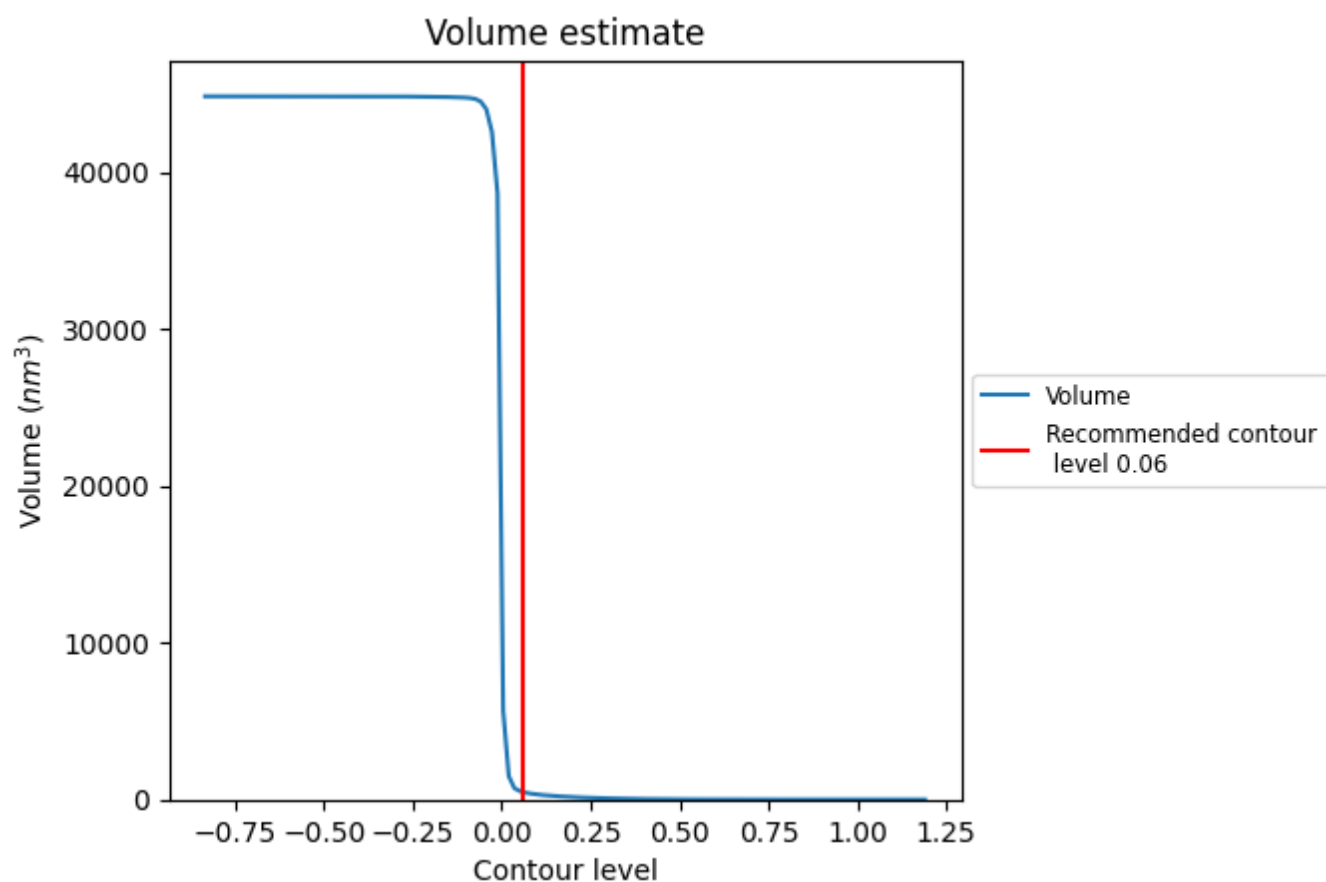
This section contains the results of statistical analysis of the map.

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.

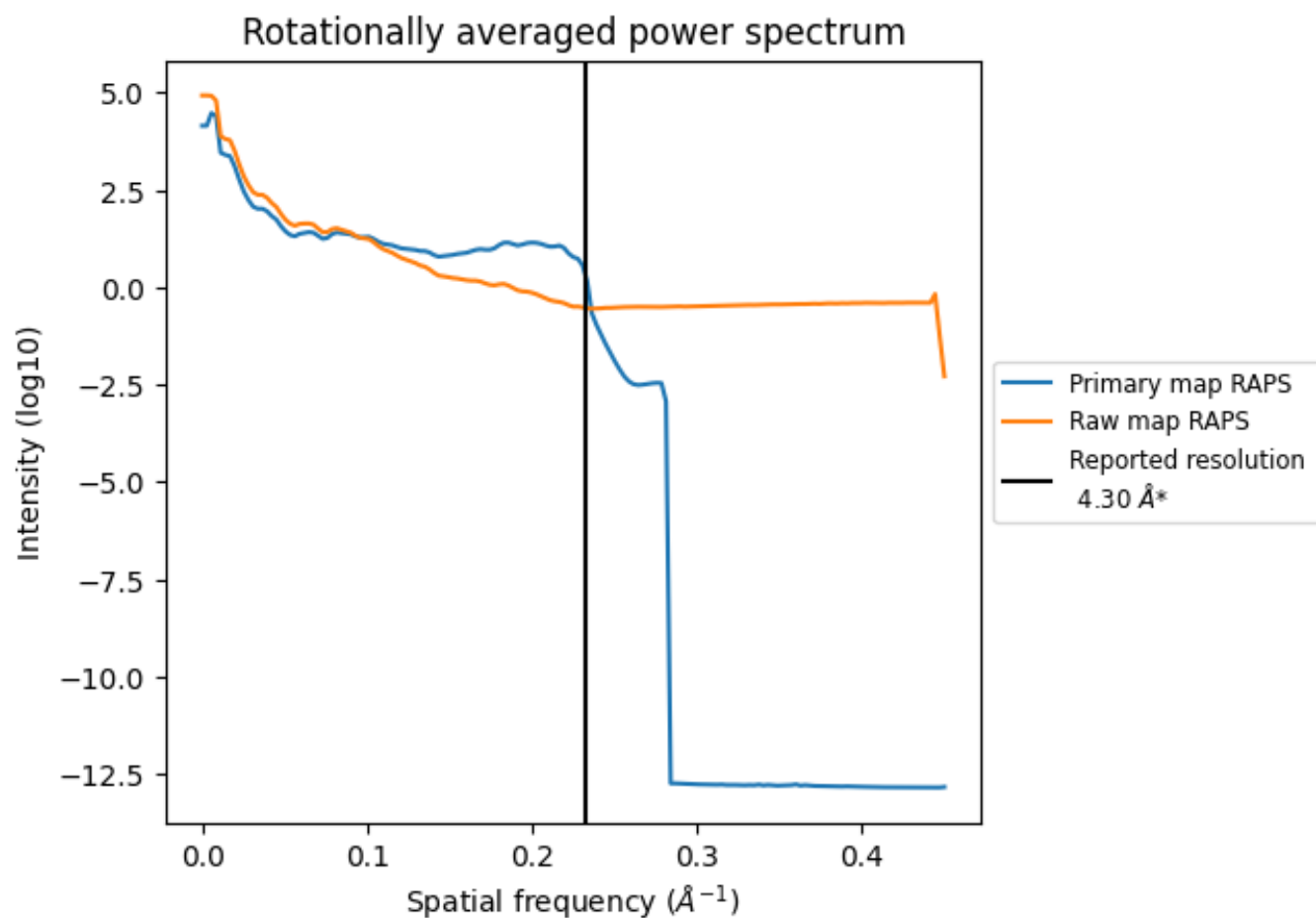
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 485 nm³; this corresponds to an approximate mass of 438 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 ⓘ

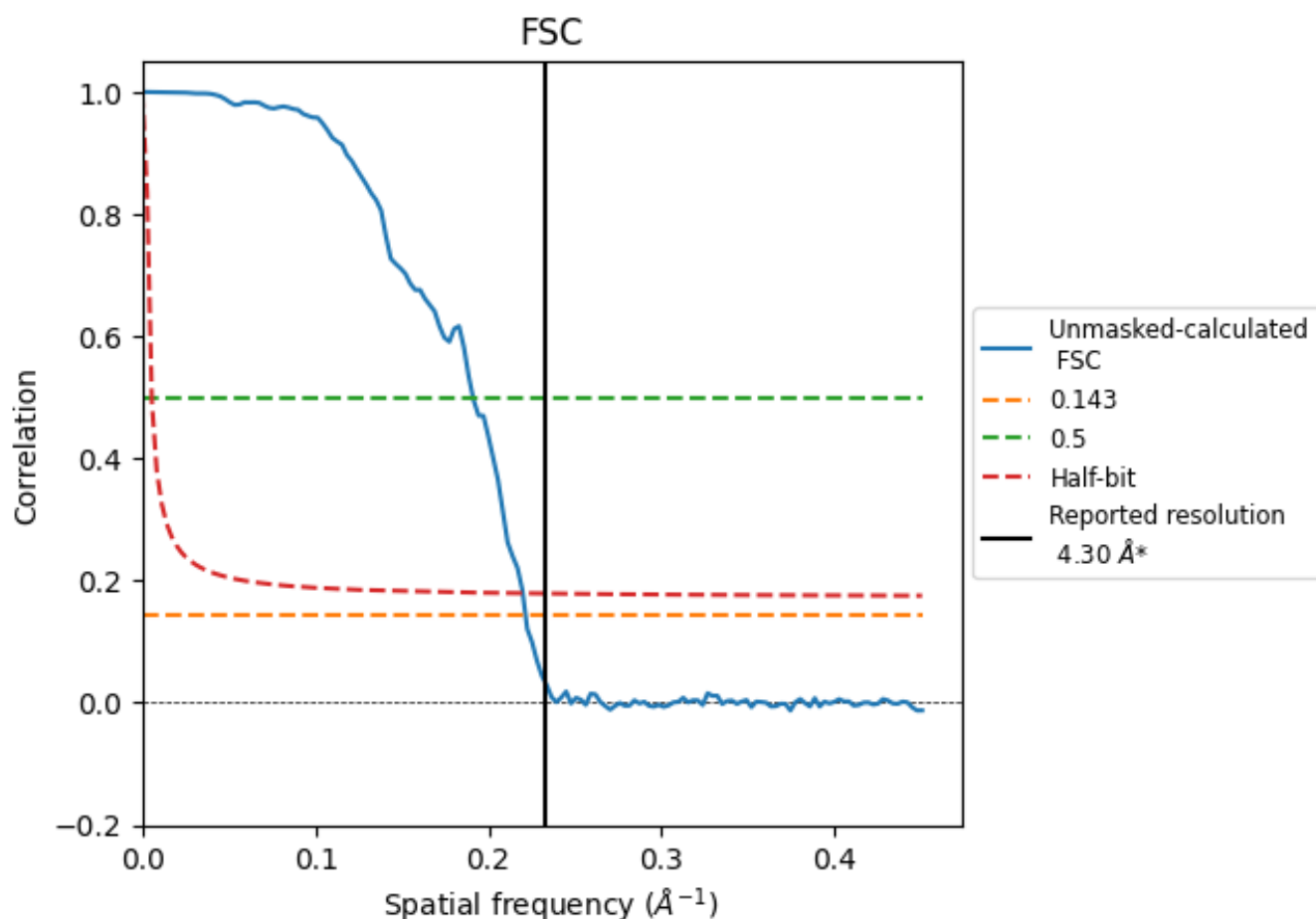


*Reported resolution corresponds to spatial frequency of 0.233 \AA^{-1}

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 0.233 \AA^{-1}

8.2 Resolution estimates [i](#)

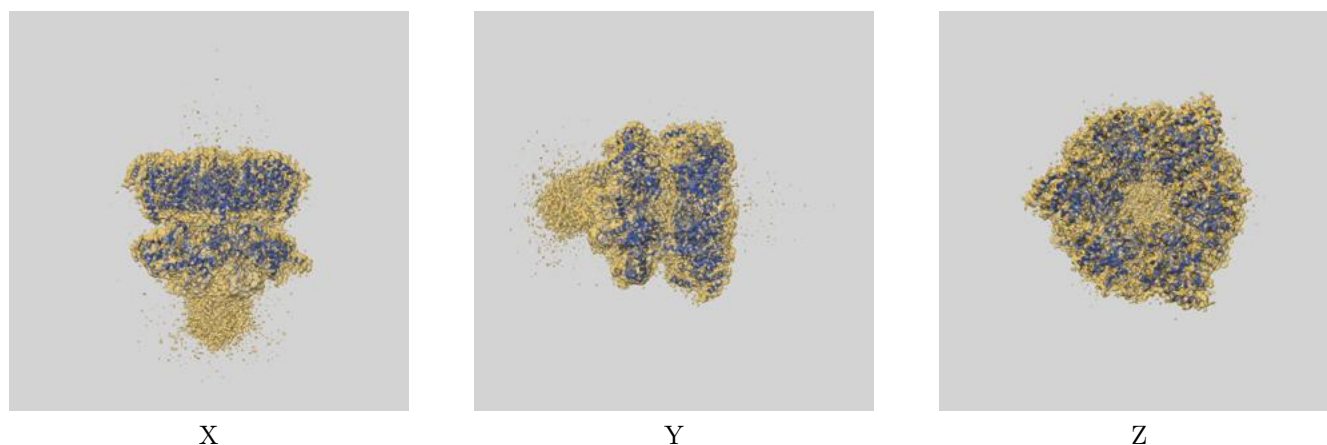
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.52	5.23	4.55

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

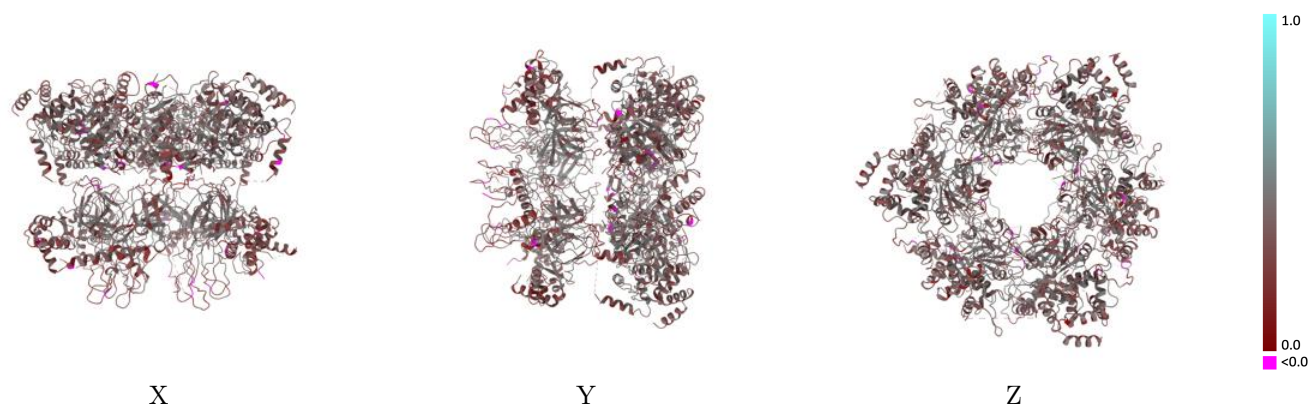
This section contains information regarding the fit between EMDB map EMD-40234 and PDB model 8S91. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



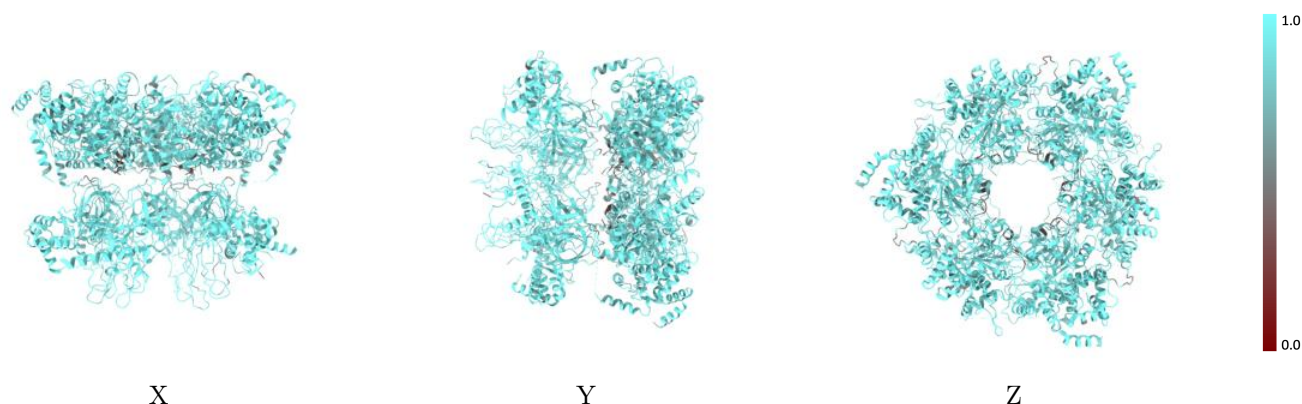
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



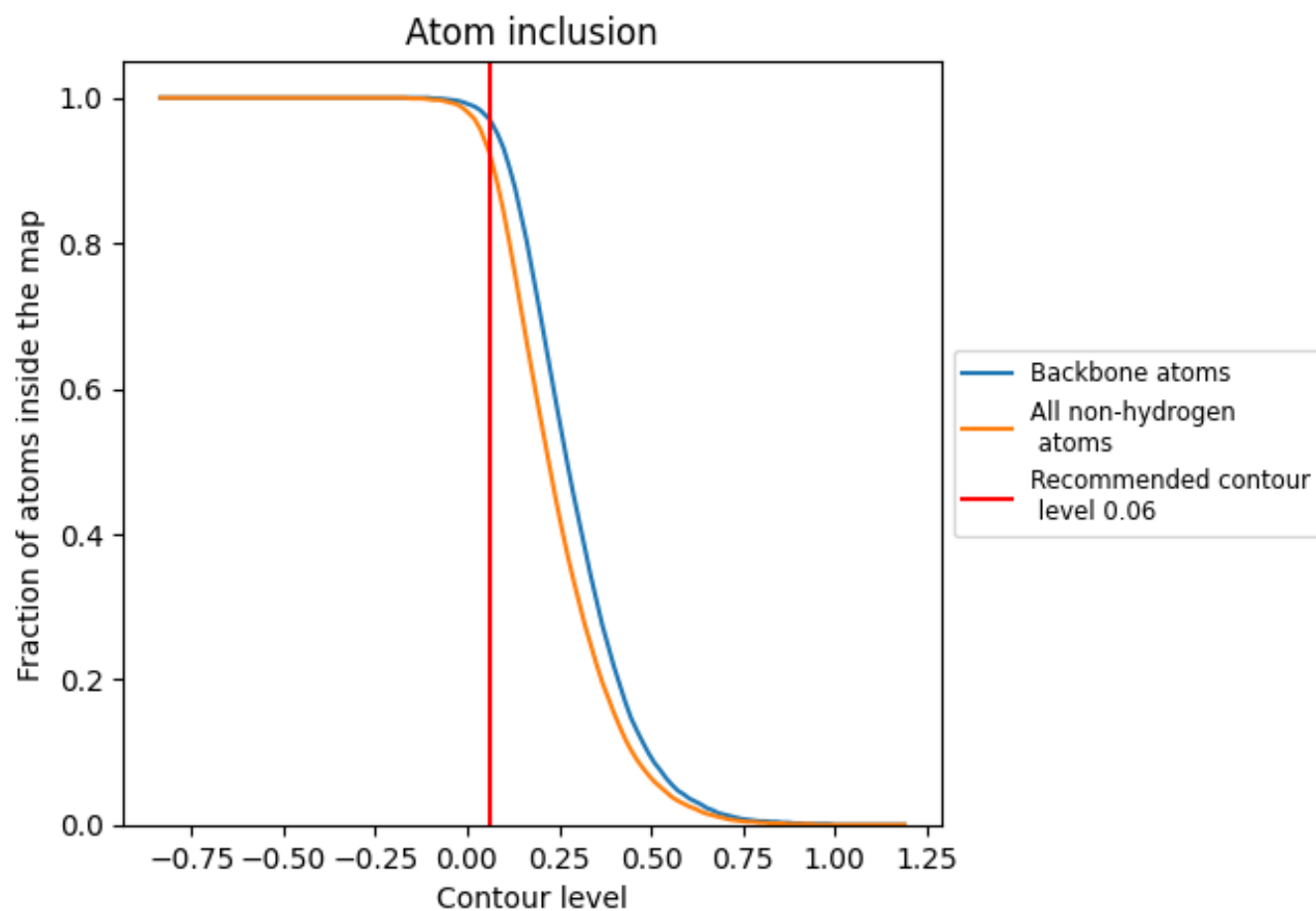
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 97% of all backbone atoms, 93% 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	<div><div></div>0.9260</div>	<div><div></div>0.3580</div>
A	<div><div></div>0.9240</div>	<div><div></div>0.3540</div>
B	<div><div></div>0.9270</div>	<div><div></div>0.3580</div>
C	<div><div></div>0.9250</div>	<div><div></div>0.3620</div>
D	<div><div></div>0.9210</div>	<div><div></div>0.3560</div>
E	<div><div></div>0.9290</div>	<div><div></div>0.3630</div>
F	<div><div></div>0.9280</div>	<div><div></div>0.3580</div>

1.0

0.0

<0.0