



Full wwPDB EM Validation Report ⓘ

May 11, 2026 – 06:33 PM JST

PDB ID : 9VLN / pdb_00009vln
EMDB ID : EMD-65161
Title : Structure of human MCM2-7 single hexamer without MCM3 CTE, state 1
Authors : Lam, W.H.; Fan, X.; Zhai, Y.
Deposited on : 2025-06-25
Resolution : 3.42 Å(reported)
Based on initial model : 7W1Y

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:

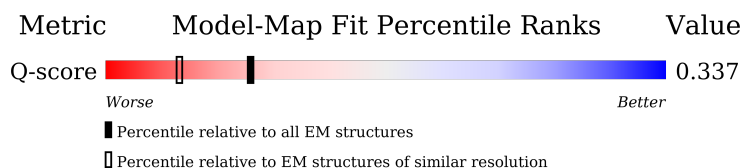
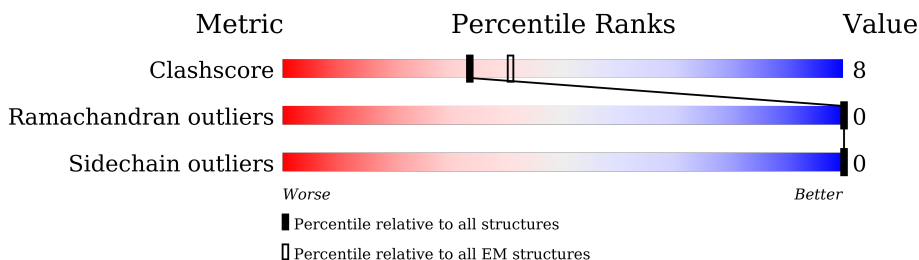
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 3.42 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	13959 (2.92 - 3.92)

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	2	904	
2	3	670	
3	4	863	
4	5	734	

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Mol	Chain	Length	Quality of chain
5	6	821	 68% 13% 19%
6	7	719	 63% 16% 22%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 28206 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 replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	697	Total	C	N	O	S	0	0
			5340	3365	936	1009	30		

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	536	Total	C	N	O	S	0	0
			4043	2533	713	776	21		

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	663	Total	C	N	O	S	0	0
			4919	3090	860	945	24		

- Molecule 4 is a protein called DNA replication licensing factor MCM5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	560	Total	C	N	O	S	0	0
			4231	2661	736	811	23		

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	666	Total	C	N	O	S	0	0
			5260	3304	926	1003	27		

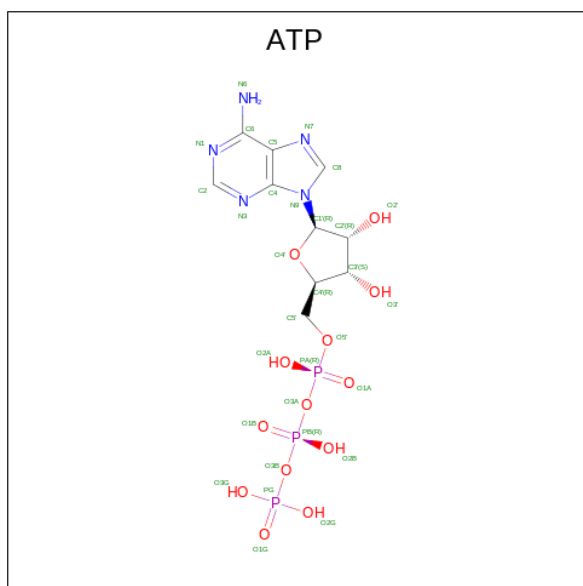
- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	564	Total	C	N	O	S	0	0
			4260	2662	743	829	26		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
7	2	1	Total	Mg	0
			1	1	
7	4	1	Total	Mg	0
			1	1	

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	2	1	Total	C	N	O	P	0
			31	10	5	13	3	
8	4	1	Total	C	N	O	P	0
			31	10	5	13	3	
8	6	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

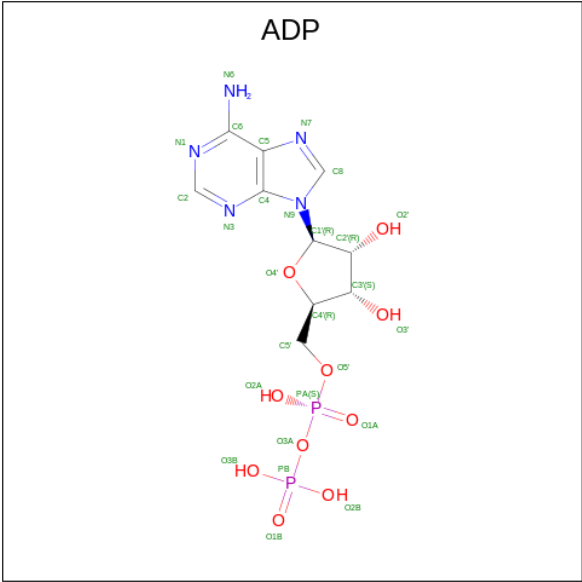
Mol	Chain	Residues	Atoms		AltConf
9	2	1	Total	Zn	0
			1	1	
9	4	1	Total	Zn	0
			1	1	
9	6	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
9	7	1	Total	Zn	0
			1	1	

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

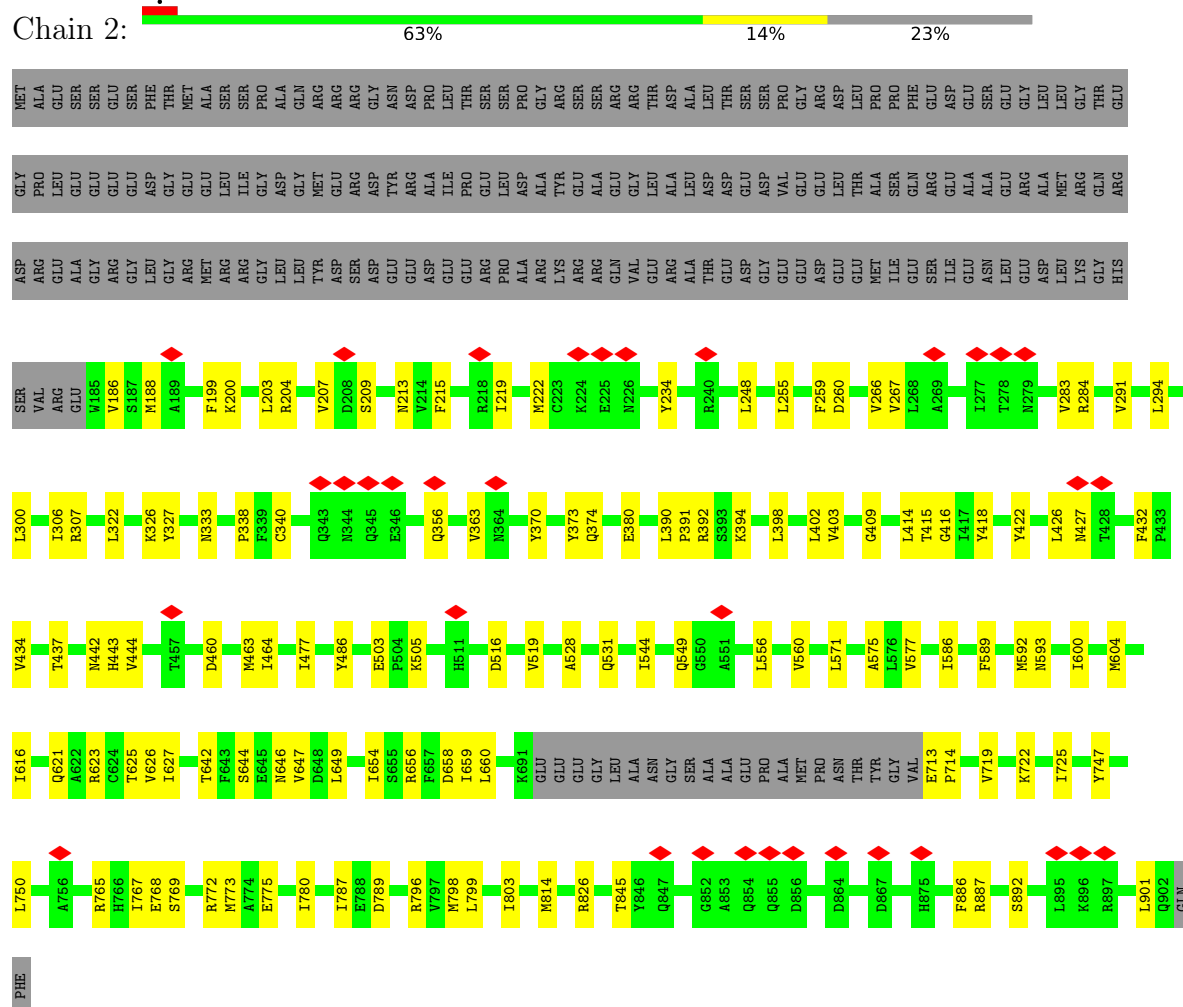


Mol	Chain	Residues	Atoms					AltConf
10	3	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	7	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots

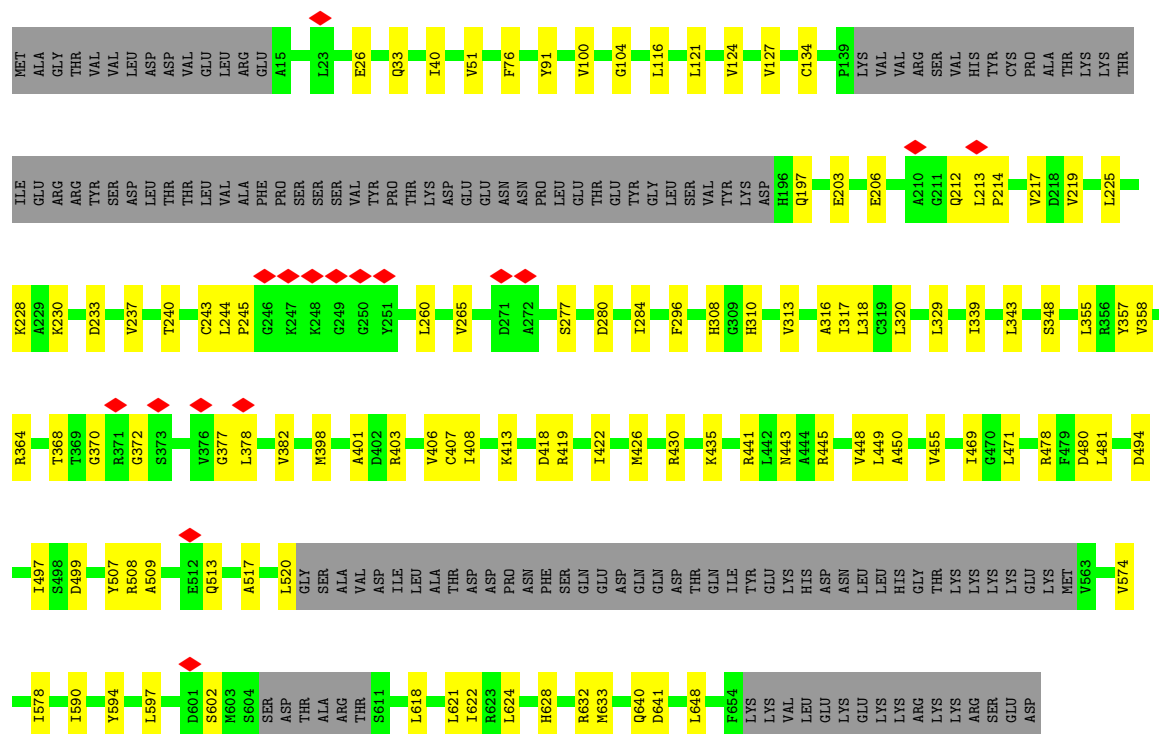
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA replication licensing factor MCM2

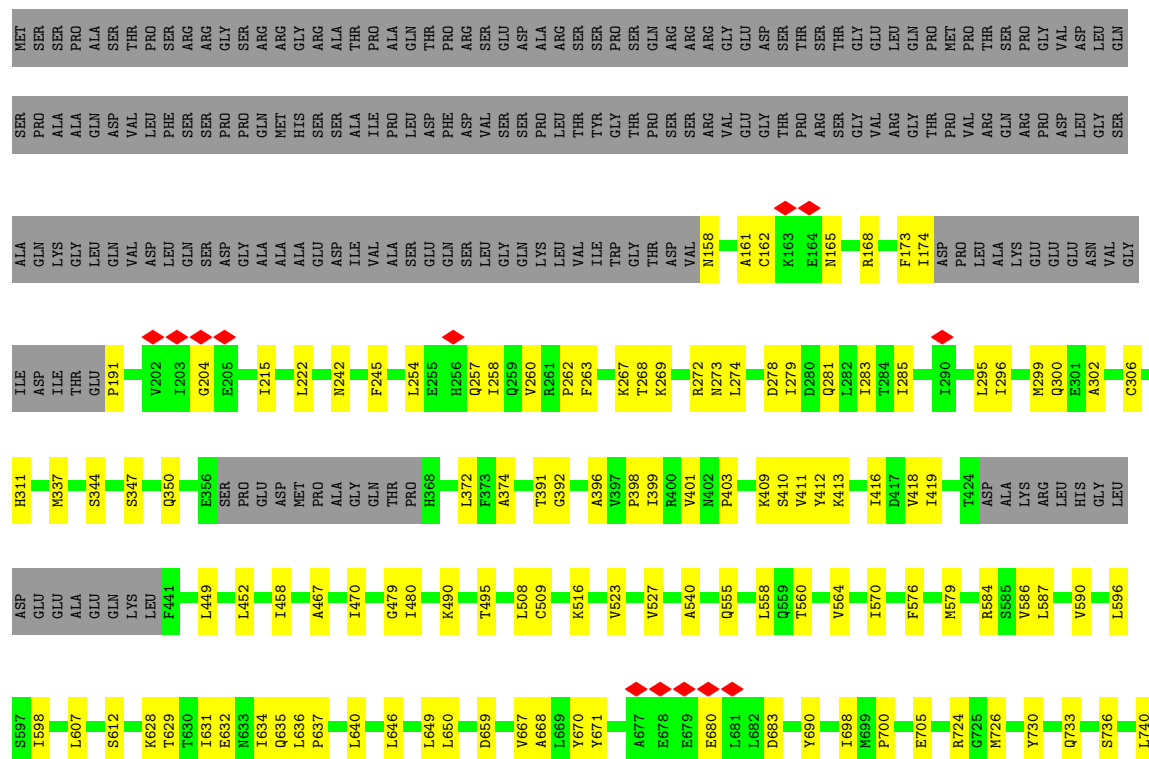


- Molecule 2: DNA replication licensing factor MCM3

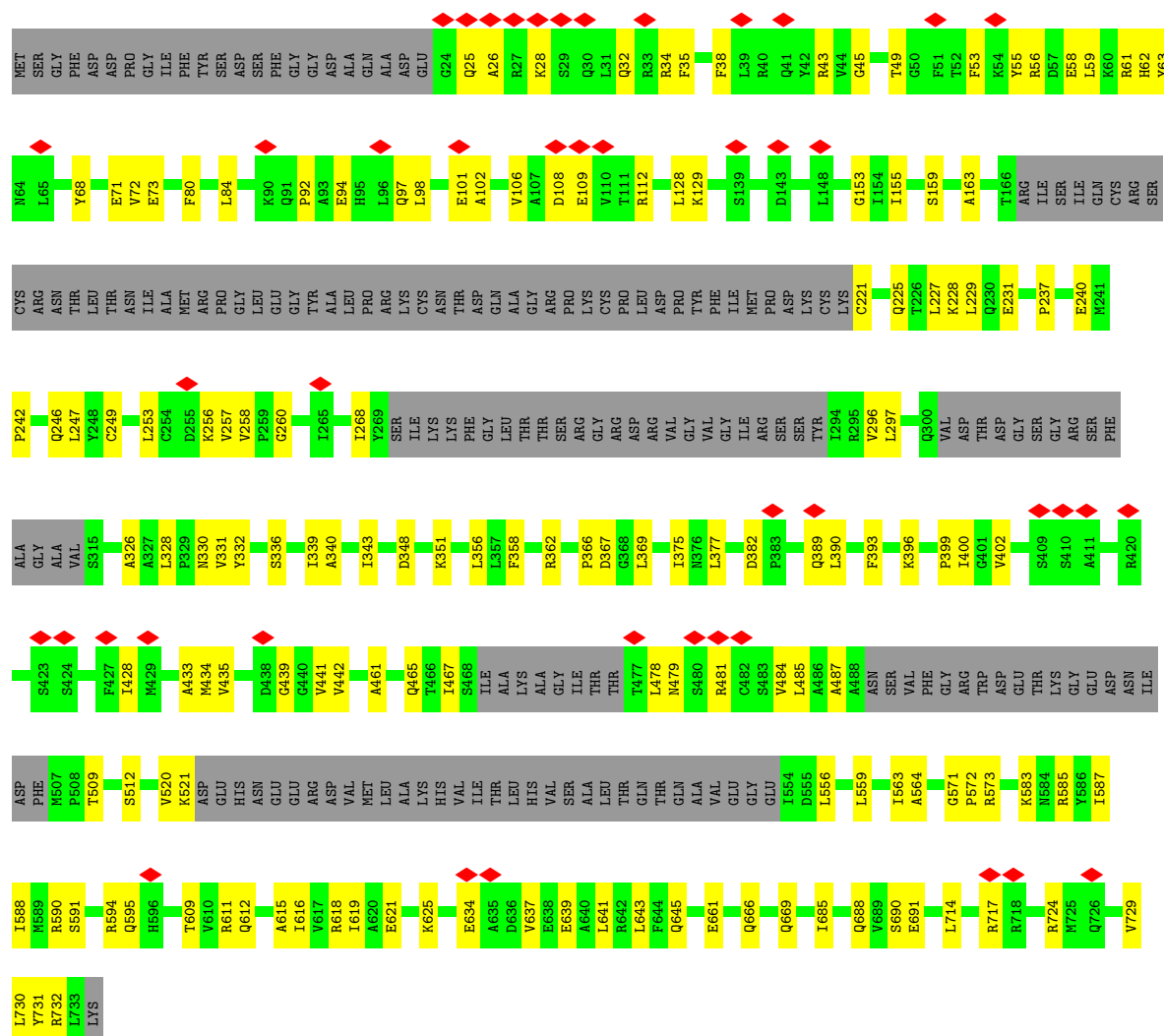




• Molecule 3: DNA replication licensing factor MCM4



- Molecule 4: DNA replication licensing factor MCM5



- Molecule 5: DNA replication licensing factor MCM6





GLY	E591	M462	V362	T262	HIS	MET
PHE	L606	T466	R367	R263	ARG	ALA
THR	L610	T467	R368	R270	LEU	LEU
PRO	R618	S468	K369	H274	MET	LYS
GLN	V622	T469	K370	T274	GLY	D5
PHE	V623	L477	K376	ILE	ARG	E9
ALA	V624	L478	K377	PHE	SER	K14
LEU	V634	L485	K378	LEU	ARG	K15
GLU	V637	L486	K383	PRO	ASP	F16
GLY	V644	L489	K384	ILE	PRO	Q17
ASN	LEU	L505	K387	LEU	GLY	Q18
VAL	GLY	L507	K391	ARG	MET	E19
ASN	GLN	L512	K394	THR	VAL	Q22
ALA	THR	L519	K395	PHE	ARG	D23
SER	ALA	D516	K396	GLY	SER	D24
ARG	ARG	L517	L397	ARG	PRO	E25
THR	THR	L518	R400	VAL	GLN	L26
ARG	GLN	L519	R401	VAL	GLN	G27
ILE	ARG	L524	T404	GLN	THR	G27
THR	ALA	H536	T405	GLY	PRO	K28
PHE	ASP	L539	G406	LEU	A128	G34
VAL	VAL	H541	S409	SER	E129	L37
ILE	ILE	V540	S410	GLU	R132	L40
PHE	ALA	H541	G411	ASP	P141	L40
THR	THR	H547	L414	ASP	R150	E44
ARG	ARG	M556	T415	GLU	G158	Q45
GLU	GLU	K557	A416	ASP	I166	L52
LEU	VAL	L558	A417	GLY	V173	A56
VAL	VAL	M559	V418	ALA	K174	V63
SER	SER	R560	V419	GLY	P175	V63
GLY	GLY	R561	R420	GLY	K176	R71
ARG	ARG	V562	D421	LEU	M177	Y11
ARG	VAL	R567	S422	THR	V178	V61
VAL	VAL	P571	V423	GLY	T199	Q87
PHE	PHE	H572	E426	THR	T213	THR
GLU	GLU	V573	L429	ARG	N214	LYS
ALA	ALA	L577	E430	GLU	R215	GLU
GLU	GLU	L584	G431	LEU	S216	GLU
GLN	GLN	V584	V434	ARG	F229	VAL
ARG	ARG	V585	L435	GLY	T236	ASN
CYS	VAL	V586	V436	ASP	K231	LYS
VAL	VAL	E587	V437	ASP	V244	VAL
SER	SER			ASP	P250	LEU
ARG	ARG			THR	V257	VAL
				ILE		THR
						ILE

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	559527	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.00	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	47170	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.275	Depositor
Minimum map value	-0.074	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.09	0/5439	0.27	0/7383
2	3	0.15	0/4099	0.30	0/5548
3	4	0.11	0/4997	0.30	0/6794
4	5	0.10	0/4289	0.29	0/5789
5	6	0.09	0/5342	0.25	0/7221
6	7	0.19	0/4323	0.35	1/5871 (0.0%)
All	All	0.12	0/28489	0.29	1/38606 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	7	178	VAL	N-CA-C	-5.17	107.79	112.96

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	2	5340	0	5176	84	0
2	3	4043	0	3999	74	0
3	4	4919	0	4658	87	0
4	5	4231	0	4150	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	6	5260	0	5203	69	0
6	7	4260	0	4119	78	0
7	2	1	0	0	0	0
7	4	1	0	0	0	0
8	2	31	0	12	1	0
8	4	31	0	12	0	0
8	6	31	0	12	3	0
9	2	1	0	0	0	0
9	4	1	0	0	0	0
9	6	1	0	0	0	0
9	7	1	0	0	0	0
10	3	27	0	12	2	0
10	7	27	0	12	0	0
All	All	28206	0	27365	461	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 (461) 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)
1:2:203:LEU:HD11	1:2:266:VAL:HG21	1.60	0.84
1:2:219:ILE:HA	1:2:222:MET:HB3	1.62	0.81
3:4:302:ALA:HA	3:4:344:SER:HB2	1.66	0.77
3:4:350:GLN:HB3	3:4:374:ALA:HB3	1.67	0.77
4:5:587:ILE:HD13	4:5:590:ARG:HH12	1.51	0.75
4:5:356:LEU:HD12	4:5:377:LEU:HB3	1.69	0.73
4:5:159:SER:H	4:5:225:GLN:HE21	1.35	0.72
4:5:641:LEU:HA	4:5:645:GLN:HB2	1.71	0.72
6:7:158:GLY:HA2	6:7:300:ALA:HB3	1.72	0.72
2:3:348:SER:HA	10:3:901:ADP:H5'1	1.71	0.71
2:3:509:ALA:HB3	2:3:513:GLN:HB2	1.71	0.71
2:3:355:LEU:HD21	2:3:449:LEU:HD22	1.73	0.71
3:4:409:LYS:HG3	3:4:411:VAL:H	1.55	0.70
4:5:231:GLU:HB3	4:5:242:PRO:HB3	1.73	0.70
3:4:794:SER:HB3	3:4:799:GLU:H	1.56	0.69
4:5:28:LYS:HA	4:5:32:GLN:HB3	1.73	0.69
6:7:173:VAL:HG13	6:7:231:LYS:HE2	1.72	0.69
3:4:162:CYS:HA	3:4:165:ASN:HB2	1.75	0.68
5:6:226:VAL:HG12	5:6:298:PHE:HB3	1.75	0.68
2:3:372:GLY:HA3	2:3:377:GLY:HA3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:631:ILE:HG13	3:4:789:GLY:HA2	1.75	0.68
5:6:520:ILE:HG22	5:6:522:LEU:H	1.60	0.66
2:3:284:ILE:HD12	2:3:574:VAL:HG21	1.76	0.66
1:2:416:GLY:HA2	1:2:442:ASN:H	1.60	0.65
5:6:126:LEU:HD11	5:6:137:ILE:HG13	1.78	0.65
6:7:622:VAL:HG22	6:7:624:VAL:H	1.62	0.65
5:6:145:HIS:HA	5:6:443:VAL:HG12	1.79	0.64
4:5:227:LEU:HB3	4:5:247:LEU:HB2	1.79	0.64
5:6:53:LEU:HD23	5:6:98:VAL:HG21	1.80	0.64
2:3:469:ILE:HG23	2:3:471:LEU:H	1.61	0.64
2:3:308:HIS:HD2	2:3:497:ILE:HG22	1.64	0.63
3:4:705:GLU:HG2	3:4:755:ALA:HB2	1.80	0.63
5:6:54:ILE:HD11	5:6:101:ARG:HH12	1.63	0.63
2:3:76:PHE:HB3	2:3:100:VAL:HG21	1.81	0.62
5:6:356:PRO:HG3	5:6:565:ARG:HE	1.64	0.62
1:2:186:VAL:HG22	1:2:188:MET:H	1.63	0.62
6:7:406:GLY:HA3	6:7:446:GLU:HB3	1.80	0.62
2:3:343:LEU:HD13	2:3:449:LEU:HD21	1.81	0.62
3:4:299:MET:HB2	3:4:347:SER:HB2	1.82	0.62
4:5:690:SER:HA	4:5:729:VAL:HA	1.82	0.61
3:4:634:ILE:O	3:4:635:GLN:HG3	2.00	0.61
4:5:59:LEU:HA	4:5:62:HIS:HD1	1.65	0.61
4:5:45:GLY:HA2	4:5:80:PHE:HB2	1.82	0.61
2:3:590:ILE:HD11	2:3:621:LEU:HB3	1.81	0.61
1:2:356:GLN:HB3	3:4:403:PRO:HG2	1.81	0.60
3:4:260:VAL:HG22	3:4:262:PRO:HD3	1.82	0.60
2:3:203:GLU:HB3	2:3:214:PRO:HG3	1.82	0.60
1:2:464:ILE:HD11	1:2:725:ILE:HG22	1.84	0.60
6:7:573:VAL:HG13	6:7:577:LEU:HD23	1.83	0.60
4:5:72:VAL:H	4:5:128:LEU:HA	1.66	0.60
3:4:586:VAL:HG13	3:4:596:LEU:HD13	1.83	0.60
6:7:512:LEU:HD12	6:7:518:LEU:HD11	1.84	0.59
4:5:58:GLU:HG2	4:5:61:ARG:HE	1.67	0.59
4:5:434:MET:HA	4:5:442:VAL:HG21	1.83	0.59
1:2:300:LEU:HD21	5:6:108:LYS:HG3	1.83	0.59
2:3:578:ILE:HG13	2:3:633:MET:HG3	1.85	0.59
3:4:306:CYS:HB3	3:4:311:HIS:H	1.67	0.59
1:2:787:ILE:HG22	1:2:789:ASP:H	1.68	0.59
4:5:71:GLU:HB2	4:5:129:LYS:HB2	1.83	0.59
6:7:244:VAL:HG21	6:7:250:PRO:HB3	1.84	0.59
4:5:328:LEU:HD23	4:5:330:ASN:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:27:GLN:HG3	5:6:93:ALA:HB2	1.85	0.58
4:5:63:TYR:HA	4:5:68:TYR:HE1	1.69	0.58
1:2:219:ILE:HD13	1:2:267:VAL:HG12	1.84	0.58
6:7:34:GLY:HA2	6:7:37:LEU:HB2	1.84	0.58
2:3:237:VAL:HG23	2:3:265:VAL:HG22	1.86	0.58
2:3:368:THR:HB	2:3:408:ILE:HG12	1.84	0.58
4:5:237:PRO:HB2	4:5:240:GLU:HB3	1.83	0.58
6:7:397:LEU:HD11	6:7:559:MET:HG2	1.84	0.58
1:2:460:ASP:HA	1:2:463:MET:HE3	1.86	0.58
5:6:370:LEU:HD21	5:6:631:MET:HG2	1.84	0.58
3:4:558:LEU:HD11	3:4:598:ILE:HD11	1.86	0.58
4:5:509:THR:HA	4:5:661:GLU:HG3	1.86	0.58
3:4:668:ALA:HA	3:4:671:TYR:HD2	1.69	0.57
3:4:272:ARG:HA	6:7:263:ARG:HH12	1.68	0.57
1:2:803:ILE:HG12	1:2:814:MET:HG3	1.85	0.57
2:3:124:VAL:HG22	2:3:240:THR:HG22	1.86	0.57
4:5:594:ARG:HH11	4:5:595:GLN:H	1.50	0.57
4:5:465:GLN:HE21	4:5:485:LEU:HD22	1.70	0.57
2:3:520:LEU:HD21	4:5:439:GLY:HA3	1.85	0.57
3:4:306:CYS:HA	3:4:337:MET:HA	1.86	0.57
5:6:395:VAL:HG22	5:6:503:ALA:HB3	1.87	0.57
1:2:374:GLN:HB3	1:2:398:LEU:HB2	1.86	0.57
2:3:403:ARG:HH11	2:3:445:ARG:HE	1.52	0.57
6:7:14:LYS:HA	6:7:18:GLN:HB3	1.87	0.57
4:5:382:ASP:HB2	4:5:520:VAL:HG11	1.87	0.57
1:2:528:ALA:HB1	1:2:531:GLN:HB2	1.87	0.57
1:2:647:VAL:HG12	1:2:649:LEU:H	1.69	0.57
4:5:666:GLN:HA	4:5:669:GLN:HB3	1.86	0.57
2:3:508:ARG:HH22	4:5:572:PRO:HA	1.70	0.56
3:4:495:THR:HA	5:6:563:ILE:HD11	1.87	0.56
4:5:393:PHE:HA	4:5:396:LYS:HG2	1.87	0.56
2:3:370:GLY:HA3	2:3:413:LYS:HB2	1.88	0.56
2:3:426:MET:HG2	2:3:478:ARG:HB3	1.87	0.56
1:2:654:ILE:HG23	1:2:660:LEU:HD21	1.86	0.56
2:3:508:ARG:O	2:3:508:ARG:HG3	2.06	0.56
3:4:274:LEU:HD21	3:4:285:ILE:HD13	1.88	0.56
2:3:355:LEU:HD22	2:3:407:CYS:HB2	1.88	0.56
5:6:396:GLY:HA3	5:6:536:LEU:HB2	1.87	0.56
2:3:213:LEU:H	4:5:479:ASN:HA	1.71	0.55
2:3:355:LEU:HA	2:3:358:VAL:HG12	1.87	0.55
6:7:150:ARG:HH21	6:7:244:VAL:HG13	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:327:TYR:HD1	1:2:363:VAL:HG22	1.72	0.55
3:4:629:THR:HG22	3:4:776:PRO:HD2	1.88	0.55
1:2:259:PHE:HB3	1:2:283:VAL:HG11	1.88	0.55
5:6:392:VAL:HG22	5:6:532:LEU:HB2	1.89	0.55
5:6:341:SER:HB3	5:6:575:TYR:HE1	1.71	0.55
4:5:106:VAL:HA	4:5:109:GLU:HG3	1.88	0.55
2:3:430:ARG:HD2	2:3:441:ARG:HD3	1.88	0.55
2:3:597:LEU:HA	2:3:602:SER:HB2	1.89	0.55
4:5:343:ILE:HG13	4:5:389:GLN:HG3	1.89	0.55
6:7:383:PRO:HG3	6:7:489:ASN:HD21	1.72	0.55
1:2:340:CYS:H	1:2:426:LEU:HD12	1.72	0.54
3:4:587:LEU:HA	3:4:590:VAL:HG12	1.90	0.54
1:2:519:VAL:HG12	1:2:659:ILE:HB	1.88	0.54
5:6:450:MET:HE3	5:6:493:LEU:HD13	1.89	0.54
1:2:207:VAL:HG23	1:2:209:SER:H	1.72	0.54
4:5:92:PRO:HG2	4:5:268:ILE:HG12	1.89	0.54
5:6:60:THR:HG22	5:6:111:TYR:HB2	1.90	0.54
1:2:390:LEU:HD12	1:2:391:PRO:HD2	1.90	0.54
6:7:394:ILE:HG21	6:7:485:LEU:HD13	1.90	0.54
2:3:622:ILE:HD13	6:7:541:HIS:HD1	1.73	0.53
3:4:540:ALA:HA	6:7:470:ALA:HB2	1.90	0.53
5:6:364:VAL:HG21	5:6:536:LEU:HD21	1.89	0.53
6:7:416:ALA:HA	6:7:431:GLY:HA2	1.89	0.53
4:5:358:PHE:HD1	4:5:563:ILE:HG22	1.73	0.53
5:6:249:ILE:HB	5:6:297:VAL:HG23	1.90	0.53
5:6:329:MET:HB2	5:6:333:GLU:HB2	1.90	0.53
3:4:158:ASN:HB3	3:4:161:ALA:HB3	1.90	0.53
4:5:73:GLU:HB3	4:5:129:LYS:HE3	1.90	0.53
3:4:508:LEU:HD23	3:4:650:LEU:HD11	1.90	0.53
2:3:624:LEU:HD21	2:3:648:LEU:HD22	1.90	0.53
4:5:62:HIS:HD2	4:5:68:TYR:HA	1.73	0.53
6:7:337:ALA:HB1	6:7:352:LYS:HG2	1.91	0.53
5:6:358:ILE:HD11	5:6:404:GLN:HB3	1.91	0.52
5:6:410:GLU:HG3	5:6:418:TYR:HB2	1.92	0.52
4:5:108:ASP:HA	4:5:112:ARG:HA	1.92	0.52
4:5:572:PRO:HD2	4:5:625:LYS:HG2	1.90	0.52
4:5:326:ALA:HA	4:5:331:VAL:HG21	1.91	0.52
6:7:414:LEU:HA	6:7:434:LEU:HD23	1.91	0.52
1:2:322:LEU:HD23	1:2:370:TYR:HD2	1.74	0.52
1:2:892:SER:H	1:2:901:LEU:HB2	1.75	0.52
4:5:227:LEU:HD21	4:5:257:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:372:LEU:HD12	3:4:418:VAL:HG13	1.92	0.52
3:4:646:LEU:HD11	3:4:740:LEU:HD21	1.91	0.52
4:5:53:PHE:CE2	4:5:55:TYR:HB2	2.44	0.52
5:6:104:ILE:HG22	5:6:106:LEU:H	1.74	0.52
4:5:25:GLN:CD	4:5:26:ALA:H	2.18	0.51
1:2:291:VAL:HG22	1:2:307:ARG:HH21	1.75	0.51
3:4:516:LYS:HG2	3:4:650:LEU:HD12	1.92	0.51
1:2:747:TYR:HD2	1:2:767:ILE:HG23	1.75	0.51
5:6:474:HIS:CD2	5:6:525:PRO:HB2	2.45	0.51
6:7:362:VAL:HG11	6:7:571:PRO:HD2	1.92	0.51
6:7:567:ARG:HA	6:7:618:ARG:HH21	1.76	0.51
2:3:508:ARG:NH1	4:5:573:ARG:HG2	2.26	0.51
3:4:607:LEU:HD21	5:6:220:ILE:HD11	1.93	0.51
6:7:556:MET:HB3	6:7:560:ARG:HH12	1.75	0.51
1:2:427:ASN:H	1:2:434:VAL:HG21	1.75	0.51
4:5:343:ILE:HG21	4:5:390:LEU:HD22	1.93	0.51
4:5:56:ARG:HA	4:5:59:LEU:HD12	1.92	0.50
5:6:371:MET:HE1	5:6:500:LEU:HD13	1.92	0.50
1:2:248:LEU:HA	1:2:255:LEU:HD22	1.93	0.50
1:2:642:THR:HG23	1:2:644:SER:H	1.75	0.50
3:4:295:LEU:HB2	3:4:555:GLN:HE22	1.76	0.50
6:7:536:HIS:CE1	6:7:547:PRO:HD2	2.46	0.50
2:3:499:ASP:HA	4:5:583:LYS:HZ2	1.76	0.50
4:5:621:GLU:O	4:5:625:LYS:HG3	2.11	0.50
6:7:404:THR:HG23	6:7:409:SER:HB2	1.93	0.50
6:7:257:VAL:HG13	6:7:262:THR:HG22	1.94	0.50
4:5:587:ILE:HA	4:5:590:ARG:NH1	2.27	0.50
5:6:601:LEU:HB2	5:6:649:PHE:HE1	1.75	0.50
6:7:584:ALA:HB1	6:7:634:ILE:HD12	1.93	0.50
2:3:212:GLN:HA	4:5:479:ASN:HA	1.94	0.50
4:5:588:ILE:HD12	4:5:591:SER:HB2	1.94	0.50
2:3:225:LEU:HD23	2:3:265:VAL:HG23	1.94	0.49
4:5:585:ARG:HG3	4:5:641:LEU:HD22	1.93	0.49
6:7:345:TYR:HB2	6:7:536:HIS:CD2	2.47	0.49
1:2:519:VAL:HG23	1:2:627:ILE:HG23	1.93	0.49
3:4:783:ILE:HG23	3:4:786:LEU:HD12	1.95	0.49
4:5:249:CYS:HA	4:5:296:VAL:HG11	1.94	0.49
1:2:370:TYR:HB3	1:2:373:TYR:HB3	1.95	0.49
1:2:646:ASN:O	1:2:646:ASN:ND2	2.45	0.49
4:5:59:LEU:HA	4:5:62:HIS:ND1	2.28	0.49
4:5:155:ILE:HG23	4:5:260:GLY:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:591:SER:HA	4:5:595:GLN:HE21	1.77	0.49
3:4:174:ILE:HD12	3:4:191:PRO:HB3	1.93	0.49
4:5:43:ARG:HA	4:5:53:PHE:CD1	2.48	0.49
6:7:466:THR:HB	6:7:477:THR:HB	1.95	0.49
3:4:279:ILE:HG13	6:7:229:PHE:CD2	2.48	0.49
4:5:163:ALA:HB1	4:5:221:CYS:HB3	1.94	0.49
4:5:615:ALA:O	4:5:618:ARG:HG2	2.13	0.49
1:2:260:ASP:HB3	1:2:283:VAL:HG12	1.94	0.49
6:7:22:GLN:HE21	6:7:23:ASP:H	1.60	0.49
2:3:121:LEU:HD22	2:3:243:CYS:HB3	1.95	0.49
3:4:636:LEU:HD22	3:4:640:LEU:HD23	1.93	0.49
1:2:773:MET:HE1	1:2:798:MET:HE2	1.94	0.48
4:5:53:PHE:CZ	4:5:56:ARG:HB2	2.48	0.48
4:5:639:GLU:HA	4:5:643:LEU:HB2	1.93	0.48
5:6:242:CYS:HA	5:6:305:PRO:HA	1.95	0.48
6:7:567:ARG:HD3	6:7:618:ARG:HH22	1.78	0.48
2:3:277:SER:HB3	2:3:280:ASP:HB2	1.95	0.48
2:3:320:LEU:HD12	2:3:339:ILE:HG23	1.96	0.48
5:6:337:VAL:HG23	5:6:575:TYR:HD1	1.76	0.48
10:3:901:ADP:H4'	4:5:611:ARG:HB2	1.96	0.48
3:4:401:VAL:HG21	6:7:199:THR:HG23	1.95	0.48
3:4:490:LYS:HD3	5:6:559:ILE:HD11	1.96	0.48
3:4:698:ILE:HG22	3:4:700:PRO:HD3	1.94	0.48
6:7:585:TYR:CG	6:7:606:LEU:HD12	2.49	0.48
3:4:784:SER:HB2	3:4:791:SER:HA	1.94	0.48
4:5:35:PHE:HA	4:5:38:PHE:HB3	1.95	0.48
4:5:590:ARG:O	4:5:594:ARG:HB3	2.14	0.48
5:6:236:ALA:HB2	5:6:303:VAL:HG11	1.96	0.48
3:4:300:GLN:CD	3:4:302:ALA:HB2	2.39	0.48
2:3:455:VAL:HG21	4:5:714:LEU:HD13	1.96	0.48
4:5:435:VAL:HA	4:5:484:VAL:HG11	1.94	0.48
5:6:576:LEU:O	5:6:580:ARG:HG2	2.14	0.48
4:5:461:ALA:HA	4:5:467:ILE:HG13	1.96	0.48
1:2:374:GLN:HB2	1:2:403:VAL:HG13	1.95	0.48
2:3:225:LEU:HA	2:3:228:LYS:HG2	1.95	0.48
3:4:283:ILE:HD11	3:4:416:ILE:HG12	1.96	0.48
3:4:372:LEU:HD13	3:4:416:ILE:HB	1.96	0.48
4:5:159:SER:H	4:5:225:GLN:NE2	2.07	0.48
1:2:418:TYR:HE1	1:2:437:THR:HB	1.78	0.48
2:3:219:VAL:HG11	2:3:237:VAL:HG21	1.96	0.48
6:7:385:VAL:HG23	6:7:387:LYS:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:589:PHE:HD2	1:2:649:LEU:HD11	1.78	0.47
6:7:357:LEU:HD23	6:7:485:LEU:HD12	1.96	0.47
1:2:294:LEU:HD12	1:2:380:GLU:HB3	1.96	0.47
4:5:53:PHE:HE2	4:5:55:TYR:HB2	1.78	0.47
5:6:353:SER:HA	5:6:565:ARG:HG2	1.95	0.47
1:2:750:LEU:HD21	1:2:799:LEU:HD21	1.94	0.47
2:3:310:HIS:HB3	2:3:313:VAL:HB	1.97	0.47
3:4:215:ILE:HD11	3:4:222:LEU:HB3	1.97	0.47
4:5:685:ILE:HA	4:5:732:ARG:HG3	1.96	0.47
5:6:165:ILE:HD13	5:6:191:PHE:HE2	1.79	0.47
1:2:432:PHE:HD1	5:6:174:TYR:HB2	1.79	0.47
3:4:785:ILE:HD11	3:4:791:SER:HB3	1.97	0.47
5:6:548:ILE:HD11	8:6:901:ATP:C2	2.50	0.47
1:2:204:ARG:HE	1:2:266:VAL:HG22	1.79	0.47
5:6:390:ILE:HD13	5:6:627:LEU:HD23	1.96	0.47
6:7:539:TYR:HB3	6:7:547:PRO:HG3	1.95	0.47
3:4:411:VAL:HG11	6:7:174:LYS:HD3	1.96	0.47
3:4:788:THR:HG22	5:6:508:GLY:HA3	1.95	0.47
4:5:340:ALA:HA	4:5:343:ILE:HD13	1.95	0.47
5:6:126:LEU:HD21	5:6:137:ILE:HD11	1.97	0.47
5:6:321:THR:HG23	5:6:323:GLU:H	1.80	0.47
1:2:284:ARG:HB3	1:2:443:HIS:HB2	1.97	0.47
1:2:516:ASP:HB3	1:2:625:THR:HG22	1.97	0.47
3:4:279:ILE:HG13	6:7:229:PHE:HD2	1.80	0.47
3:4:680:GLU:HA	3:4:683:ASP:HB2	1.95	0.47
5:6:344:LYS:HG2	5:6:345:ASN:H	1.79	0.47
2:3:26:GLU:HG2	2:3:33:GLN:HG3	1.97	0.47
3:4:242:ASN:HD22	3:4:257:GLN:HB3	1.79	0.47
5:6:462:PHE:HD2	5:6:522:LEU:HD11	1.80	0.47
2:3:116:LEU:HD22	2:3:127:VAL:HG11	1.97	0.46
3:4:452:LEU:HB3	3:4:458:ILE:HD13	1.97	0.46
1:2:215:PHE:O	1:2:219:ILE:HG13	2.15	0.46
1:2:477:ILE:HG21	1:2:780:ILE:HD12	1.96	0.46
6:7:396:ARG:HD2	6:7:556:MET:CE	2.46	0.46
1:2:604:MET:HE3	1:2:626:VAL:HG11	1.98	0.46
5:6:142:VAL:HA	5:6:446:ALA:HB2	1.97	0.46
4:5:396:LYS:HD3	4:5:556:LEU:HD21	1.97	0.46
1:2:402:LEU:HD22	1:2:444:VAL:HG12	1.97	0.46
1:2:768:GLU:HG2	1:2:772:ARG:HH12	1.81	0.46
2:3:329:LEU:HD11	6:7:540:VAL:HG13	1.98	0.46
3:4:570:ILE:HD13	3:4:612:SER:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:730:TYR:H	3:4:733:GLN:HG3	1.79	0.46
6:7:367:ARG:HD2	6:7:367:ARG:N	2.30	0.46
3:4:579:MET:HE3	3:4:584:ARG:HG2	1.98	0.46
3:4:755:ALA:O	3:4:759:GLU:HG2	2.16	0.46
4:5:332:TYR:HE2	4:5:351:LYS:HG2	1.81	0.46
6:7:558:LEU:HG	6:7:562:TYR:HE2	1.81	0.46
1:2:326:LYS:HG2	1:2:338:PRO:HA	1.98	0.46
2:3:296:PHE:CE1	2:3:318:LEU:HD22	2.51	0.46
2:3:419:ARG:HH12	4:5:717:ARG:HB3	1.80	0.46
3:4:527:VAL:HG11	3:4:570:ILE:HB	1.96	0.46
4:5:128:LEU:HD11	4:5:297:LEU:HB2	1.97	0.46
4:5:609:THR:HG23	4:5:612:GLN:H	1.81	0.46
4:5:634:GLU:HA	4:5:637:VAL:HB	1.98	0.46
3:4:480:ILE:HG21	3:4:523:VAL:HG21	1.97	0.45
1:2:549:GLN:HG2	1:2:593:ASN:HB3	1.98	0.45
1:2:719:VAL:HG13	1:2:722:LYS:H	1.82	0.45
1:2:747:TYR:HB3	1:2:767:ILE:HD12	1.98	0.45
2:3:219:VAL:HG22	2:3:260:LEU:HB2	1.97	0.45
2:3:382:VAL:HG11	2:3:435:LYS:HG2	1.98	0.45
1:2:199:PHE:CE2	1:2:259:PHE:HA	2.52	0.45
1:2:418:TYR:CE1	1:2:437:THR:HB	2.52	0.45
1:2:796:ARG:HE	1:2:826:ARG:HH21	1.64	0.45
4:5:399:PRO:HB2	4:5:400:ILE:HD12	1.98	0.45
3:4:670:TYR:CG	6:7:610:LEU:HD21	2.51	0.45
4:5:97:GLN:O	4:5:101:GLU:HG2	2.17	0.45
4:5:348:ASP:HB2	4:5:521:LYS:HE3	1.97	0.45
4:5:375:ILE:HD12	4:5:619:ILE:HD13	1.98	0.45
5:6:95:LYS:HA	5:6:110:PHE:HD2	1.81	0.45
6:7:40:LEU:HD12	6:7:45:GLN:HB3	1.99	0.45
2:3:313:VAL:O	2:3:317:ILE:HG12	2.17	0.45
3:4:726:MET:HG3	3:4:792:ALA:HB3	1.99	0.45
5:6:229:ARG:HH21	5:6:299:LEU:HD21	1.82	0.45
1:2:409:GLY:HA3	1:2:577:VAL:HG12	1.98	0.45
3:4:467:ALA:HB1	3:4:470:ILE:HD13	1.99	0.45
3:4:479:GLY:HA2	3:4:764:LEU:HD21	1.98	0.45
4:5:32:GLN:HE21	4:5:102:ALA:HB2	1.82	0.45
2:3:40:ILE:HG23	2:3:91:TYR:CG	2.52	0.45
2:3:622:ILE:HD13	6:7:541:HIS:ND1	2.32	0.45
3:4:410:SER:HB3	6:7:176:LYS:HG3	1.99	0.45
4:5:612:GLN:O	4:5:616:ILE:HG12	2.17	0.45
6:7:357:LEU:HD13	6:7:375:ILE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:503:GLU:H	1:2:775:GLU:HG2	1.82	0.45
1:2:560:VAL:HG22	1:2:571:LEU:HB3	1.99	0.45
2:3:418:ASP:O	2:3:422:ILE:HG12	2.17	0.45
4:5:253:LEU:HD12	4:5:256:LYS:HB2	1.98	0.44
5:6:598:TYR:CG	5:6:621:LEU:HD12	2.52	0.44
3:4:733:GLN:O	3:4:736:SER:HB3	2.17	0.44
4:5:688:GLN:HG2	4:5:731:TYR:HD1	1.82	0.44
6:7:435:VAL:HG21	6:7:478:LEU:HD23	1.98	0.44
3:4:245:PHE:CD1	3:4:258:ILE:HD11	2.52	0.44
4:5:691:GLU:HB3	4:5:730:LEU:HG	1.99	0.44
6:7:377:ILE:HD11	6:7:519:TRP:CD1	2.52	0.44
1:2:556:LEU:HB3	1:2:600:ILE:HD13	1.99	0.44
6:7:14:LYS:HA	6:7:19:GLU:H	1.83	0.44
6:7:270:HIS:HB2	6:7:400:ARG:NH1	2.33	0.44
6:7:468:SER:HB3	6:7:477:THR:HA	2.00	0.44
5:6:541:ASN:HB2	5:6:544:THR:HG22	2.00	0.44
6:7:505:ILE:HG13	6:7:507:LEU:H	1.83	0.44
2:3:316:ALA:HB2	2:3:648:LEU:HD21	1.99	0.44
4:5:559:LEU:O	4:5:563:ILE:HG12	2.17	0.44
5:6:358:ILE:HG23	8:6:901:ATP:N1	2.33	0.44
2:3:480:ASP:OD1	2:3:481:LEU:HG	2.18	0.44
3:4:449:LEU:HD22	3:4:690:TYR:HD2	1.83	0.44
6:7:410:SER:HA	6:7:414:LEU:HG	2.00	0.44
2:3:134:CYS:HB2	2:3:197:GLN:HE21	1.83	0.44
1:2:207:VAL:HG12	1:2:213:ASN:ND2	2.33	0.43
3:4:576:PHE:CD2	3:4:636:LEU:HD11	2.53	0.43
3:4:787:THR:HG22	3:4:788:THR:HG23	2.00	0.43
4:5:512:SER:HB2	4:5:611:ARG:NH2	2.33	0.43
6:7:378:CYS:SG	6:7:486:ALA:HB3	2.58	0.43
1:2:571:LEU:HD22	1:2:616:ILE:HG21	2.01	0.43
2:3:51:VAL:HG12	2:3:104:GLY:HA3	2.00	0.43
2:3:116:LEU:HD23	2:3:217:VAL:HG11	2.00	0.43
5:6:250:VAL:HG13	5:6:294:TYR:HB3	2.00	0.43
6:7:391:LEU:O	6:7:394:ILE:HG22	2.17	0.43
6:7:419:LEU:H	6:7:429:LEU:HD22	1.83	0.43
6:7:71:ARG:HB2	6:7:300:ALA:HB1	2.00	0.43
1:2:333:ASN:HB3	5:6:189:ARG:NE	2.34	0.43
2:3:494:ASP:HA	2:3:497:ILE:HG12	2.00	0.43
1:2:658:ASP:HB2	1:2:769:SER:OG	2.18	0.43
2:3:443:ASN:HD21	2:3:445:ARG:HH11	1.66	0.43
2:3:481:LEU:HD11	2:3:624:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:291:VAL:HG22	1:2:307:ARG:NH2	2.33	0.43
1:2:414:LEU:H	1:2:414:LEU:HD23	1.83	0.43
2:3:357:TYR:HD2	4:5:369:LEU:HD11	1.82	0.43
2:3:628:HIS:HB3	2:3:641:ASP:OD1	2.18	0.43
3:4:509:CYS:O	3:4:649:LEU:HA	2.19	0.43
6:7:637:MET:HE2	6:7:637:MET:HB2	1.91	0.43
2:3:449:LEU:HD23	2:3:450:ALA:N	2.33	0.43
3:4:267:LYS:HB3	3:4:269:LYS:HE3	2.00	0.43
3:4:296:ILE:HG13	3:4:296:ILE:O	2.19	0.43
4:5:402:VAL:HG21	4:5:433:ALA:HB1	2.00	0.43
6:7:375:ILE:HG23	6:7:516:ASP:OD2	2.18	0.43
4:5:34:ARG:HD3	4:5:84:LEU:HD11	2.00	0.43
4:5:428:ILE:HD12	4:5:478:LEU:HD21	2.00	0.43
6:7:567:ARG:HD3	6:7:618:ARG:NH2	2.34	0.43
3:4:272:ARG:HA	6:7:263:ARG:NH1	2.33	0.43
1:2:392:ARG:NE	1:2:394:LYS:HD3	2.33	0.43
1:2:486:TYR:H	8:2:1002:ATP:HN61	1.67	0.43
1:2:505:LYS:HE2	1:2:505:LYS:HB2	1.88	0.43
3:4:278:ASP:HA	3:4:281:GLN:HG3	2.00	0.43
3:4:667:VAL:HG12	3:4:671:TYR:CE2	2.54	0.43
1:2:586:ILE:HG21	1:2:589:PHE:HD1	1.84	0.42
2:3:244:LEU:HD12	2:3:245:PRO:HD2	2.01	0.42
5:6:529:ARG:CZ	5:6:619:ARG:HH12	2.32	0.42
2:3:507:TYR:CZ	4:5:366:PRO:HG3	2.54	0.42
4:5:362:ARG:HD2	4:5:485:LEU:HD11	2.01	0.42
5:6:512:ARG:HH11	5:6:537:VAL:HG21	1.84	0.42
2:3:230:LYS:HG2	2:3:233:ASP:OD2	2.19	0.42
3:4:787:THR:HG23	5:6:398:PRO:HG3	2.01	0.42
1:2:306:ILE:HD13	1:2:418:TYR:HB2	2.01	0.42
4:5:258:VAL:HG11	4:5:481:ARG:H	1.84	0.42
5:6:329:MET:HE2	5:6:329:MET:HB3	1.93	0.42
5:6:364:VAL:HG22	5:6:534:PHE:HB3	2.00	0.42
5:6:598:TYR:HB2	5:6:624:MET:HE1	2.02	0.42
6:7:524:ARG:HD3	6:7:524:ARG:H	1.84	0.42
1:2:845:THR:HG21	5:6:787:LEU:HD21	2.01	0.42
4:5:102:ALA:O	4:5:106:VAL:HG23	2.19	0.42
4:5:153:GLY:HA3	4:5:229:LEU:HD21	2.01	0.42
4:5:375:ILE:HD13	4:5:618:ARG:HG3	2.00	0.42
5:6:558:ARG:HH21	5:6:562:SER:HA	1.83	0.42
4:5:49:THR:HB	4:5:53:PHE:HA	2.02	0.42
5:6:233:VAL:HG22	5:6:234:GLU:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:296:PHE:HE1	2:3:318:LEU:HD22	1.84	0.42
4:5:399:PRO:HG3	4:5:564:ALA:HB2	2.02	0.42
5:6:55:ARG:HA	5:6:55:ARG:NE	2.34	0.42
1:2:621:GLN:HG3	1:2:623:ARG:HE	1.84	0.42
1:2:656:ARG:NH1	1:2:765:ARG:HH12	2.17	0.42
5:6:744:LYS:HD2	5:6:744:LYS:HA	1.73	0.42
6:7:166:ILE:HG22	6:7:400:ARG:HH12	1.85	0.42
2:3:357:TYR:OH	4:5:367:ASP:HB2	2.20	0.42
2:3:594:TYR:CD2	2:3:618:LEU:HD12	2.54	0.42
2:3:632:ARG:NH1	2:3:640:GLN:HE22	2.18	0.42
3:4:396:ALA:HB1	3:4:412:TYR:HB3	2.02	0.42
4:5:228:LYS:HA	4:5:246:GLN:HA	2.00	0.42
1:2:284:ARG:HD2	1:2:442:ASN:O	2.20	0.42
3:4:398:PRO:HA	3:4:412:TYR:CD1	2.55	0.42
4:5:467:ILE:HD13	4:5:484:VAL:HG13	2.02	0.42
5:6:406:LEU:HD22	5:6:458:CYS:HB3	2.01	0.42
5:6:631:MET:HE2	5:6:631:MET:HB3	1.83	0.42
6:7:37:LEU:HD21	6:7:81:VAL:HG13	2.02	0.42
1:2:556:LEU:HG	1:2:592:MET:HE1	2.02	0.41
1:2:886:PHE:HD2	1:2:887:ARG:HD3	1.85	0.41
2:3:517:ALA:HB2	4:5:571:GLY:N	2.35	0.41
6:7:56:ALA:HB2	6:7:63:VAL:HG21	2.02	0.41
1:2:307:ARG:HG3	1:2:415:THR:HG22	2.01	0.41
3:4:173:PHE:HZ	3:4:215:ILE:HA	1.85	0.41
3:4:637:PRO:HG2	3:4:640:LEU:HB3	2.01	0.41
4:5:571:GLY:HA2	4:5:625:LYS:HZ1	1.85	0.41
5:6:92:ARG:HA	5:6:95:LYS:HG2	2.02	0.41
3:4:204:GLY:HA2	3:4:254:LEU:HD21	2.03	0.41
1:2:204:ARG:HD3	1:2:266:VAL:HG13	2.01	0.41
1:2:571:LEU:HD22	1:2:616:ILE:HG13	2.02	0.41
6:7:9:GLU:HB2	6:7:16:PHE:HB2	2.03	0.41
6:7:447:PHE:CD2	6:7:507:LEU:HD11	2.55	0.41
1:2:422:TYR:OH	5:6:193:LEU:HB3	2.20	0.41
3:4:628:LYS:HD3	3:4:632:GLU:HB3	2.02	0.41
5:6:177:PRO:HB2	5:6:191:PHE:CZ	2.56	0.41
3:4:659:ASP:HB3	6:7:586:VAL:HG12	2.03	0.41
4:5:336:SER:HA	4:5:339:ILE:HG12	2.03	0.41
6:7:52:LEU:HD23	6:7:141:PRO:HB3	2.02	0.41
3:4:724:ARG:HG3	3:4:726:MET:SD	2.60	0.41
4:5:724:ARG:HA	4:5:724:ARG:NE	2.36	0.41
6:7:377:ILE:HG23	6:7:485:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:200:LYS:HE2	1:2:200:LYS:HB3	1.84	0.41
2:3:378:LEU:HA	2:3:398:MET:HG2	2.03	0.41
3:4:392:GLY:HA2	3:4:419:ILE:HG12	2.02	0.41
3:4:399:ILE:HD11	3:4:413:LYS:HG2	2.02	0.41
3:4:576:PHE:HD2	3:4:636:LEU:HD11	1.85	0.41
4:5:441:VAL:HA	4:5:487:ALA:HB3	2.02	0.41
6:7:129:GLU:HA	6:7:132:ARG:HG2	2.02	0.41
6:7:376:ASN:HD22	6:7:462:MET:HE1	1.86	0.41
6:7:443:CYS:HA	6:7:485:LEU:O	2.20	0.41
1:2:234:TYR:HE2	1:2:248:LEU:HD23	1.85	0.41
1:2:544:ILE:HD13	1:2:575:ALA:HA	2.04	0.41
2:3:426:MET:HE2	2:3:426:MET:HB2	1.83	0.41
3:4:165:ASN:O	3:4:168:ARG:HD3	2.20	0.41
3:4:773:ALA:HB1	3:4:782:ASP:H	1.86	0.41
5:6:358:ILE:HA	8:6:901:ATP:C2	2.55	0.41
2:3:401:ALA:HB3	2:3:406:VAL:HG22	2.02	0.40
5:6:98:VAL:HG12	5:6:104:ILE:HD11	2.02	0.40
1:2:713:GLU:HB3	1:2:714:PRO:HD3	2.03	0.40
3:4:268:THR:HB	3:4:273:ASN:HB3	2.02	0.40
3:4:560:THR:HB	3:4:564:VAL:HB	2.04	0.40
6:7:306:MET:HE2	6:7:306:MET:HB3	1.99	0.40
6:7:396:ARG:HD2	6:7:556:MET:HE1	2.02	0.40
6:7:348:GLU:O	6:7:352:LYS:HG3	2.22	0.40
2:3:206:GLU:OE1	2:3:364:ARG:HG3	2.22	0.40
2:3:406:VAL:HB	2:3:448:VAL:HG22	2.03	0.40
3:4:263:PHE:HA	3:4:391:THR:HG21	2.02	0.40
5:6:772:ILE:O	5:6:776:VAL:HG23	2.22	0.40
1:2:326:LYS:HD3	1:2:338:PRO:HG3	2.03	0.40
4:5:94:GLU:O	4:5:98:LEU:HG	2.20	0.40
4:5:688:GLN:HG2	4:5:731:TYR:CD1	2.56	0.40
6:7:587:GLU:O	6:7:591:GLU:HG2	2.22	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	2	693/904 (77%)	652 (94%)	41 (6%)	0	100	100
2	3	528/670 (79%)	510 (97%)	18 (3%)	0	100	100
3	4	655/863 (76%)	622 (95%)	33 (5%)	0	100	100
4	5	546/734 (74%)	513 (94%)	33 (6%)	0	100	100
5	6	658/821 (80%)	638 (97%)	20 (3%)	0	100	100
6	7	556/719 (77%)	517 (93%)	39 (7%)	0	100	100
All	All	3636/4711 (77%)	3452 (95%)	184 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	566/781 (72%)	566 (100%)	0	100	100
2	3	424/580 (73%)	424 (100%)	0	100	100
3	4	495/753 (66%)	495 (100%)	0	100	100
4	5	438/625 (70%)	438 (100%)	0	100	100
5	6	580/724 (80%)	580 (100%)	0	100	100
6	7	443/619 (72%)	443 (100%)	0	100	100
All	All	2946/4082 (72%)	2946 (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 (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	201	ASN
1	2	299	GLN

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Mol	Chain	Res	Type
1	2	421	ASN
2	3	33	GLN
2	3	308	HIS
2	3	331	ASN
2	3	573	HIS
3	4	307	GLN
3	4	341	HIS
3	4	375	HIS
3	4	518	GLN
3	4	672	GLN
3	4	751	ASN
4	5	32	GLN
4	5	41	GLN
4	5	91	GLN
4	5	246	GLN
4	5	389	GLN
4	5	584	ASN
4	5	709	HIS
5	6	72	ASN
6	7	22	GLN
6	7	243	GLN
6	7	389	GLN
6	7	459	HIS
6	7	489	ASN
6	7	522	GLN

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

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	ATP	2	1002	7	29,33,33	0.30	0	44,52,52	0.53	1 (2%)
8	ATP	4	902	7	29,33,33	0.48	0	44,52,52	0.60	0
10	ADP	7	801	-	27,29,29	1.36	4 (14%)	42,45,45	1.97	10 (23%)
10	ADP	3	901	-	27,29,29	0.43	0	42,45,45	0.58	0
8	ATP	6	901	-	29,33,33	0.49	0	44,52,52	0.59	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
8	ATP	2	1002	7	-	5/22/38/38	0/3/3/3
8	ATP	4	902	7	-	3/22/38/38	0/3/3/3
10	ADP	7	801	-	-	2/16/32/32	0/3/3/3
10	ADP	3	901	-	-	0/16/32/32	0/3/3/3
8	ATP	6	901	-	-	4/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	7	801	ADP	C5-C4	4.56	1.47	1.39
10	7	801	ADP	C5-C6	2.67	1.48	1.41
10	7	801	ADP	C8-N7	2.35	1.36	1.31
10	7	801	ADP	C5-N7	-2.20	1.34	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	7	801	ADP	C5-C4-N3	-6.32	118.50	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	7	801	ADP	N3-C4-N9	4.93	135.20	127.08
10	7	801	ADP	C2-N3-C4	3.88	120.93	111.75
10	7	801	ADP	PA-O3A-PB	-3.47	120.93	132.83
10	7	801	ADP	C4-C5-N7	-3.23	106.69	110.62
10	7	801	ADP	N3-C2-N1	-3.11	123.73	128.60
10	7	801	ADP	C5-N7-C8	2.68	107.32	103.51
10	7	801	ADP	C3'-C2'-C1'	2.60	106.36	101.43
10	7	801	ADP	C4-N9-C8	2.36	108.28	105.73
10	7	801	ADP	C6-C5-N7	2.07	135.88	132.02
8	2	1002	ATP	PB-O3B-PG	2.03	139.80	132.83

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	2	1002	ATP	PB-O3B-PG-O3G
8	2	1002	ATP	O4'-C1'-N9-C8
8	2	1002	ATP	O4'-C1'-N9-C4
8	4	902	ATP	O4'-C4'-C5'-O5'
10	7	801	ADP	O4'-C4'-C5'-O5'
8	4	902	ATP	O4'-C1'-N9-C8
8	4	902	ATP	O4'-C1'-N9-C4
10	7	801	ADP	C3'-C4'-C5'-O5'
8	2	1002	ATP	PB-O3A-PA-O2A
8	6	901	ATP	PG-O3B-PB-O1B
8	6	901	ATP	C4'-C5'-O5'-PA
8	2	1002	ATP	PG-O3B-PB-O1B
8	6	901	ATP	PG-O3B-PB-O2B
8	6	901	ATP	O4'-C4'-C5'-O5'

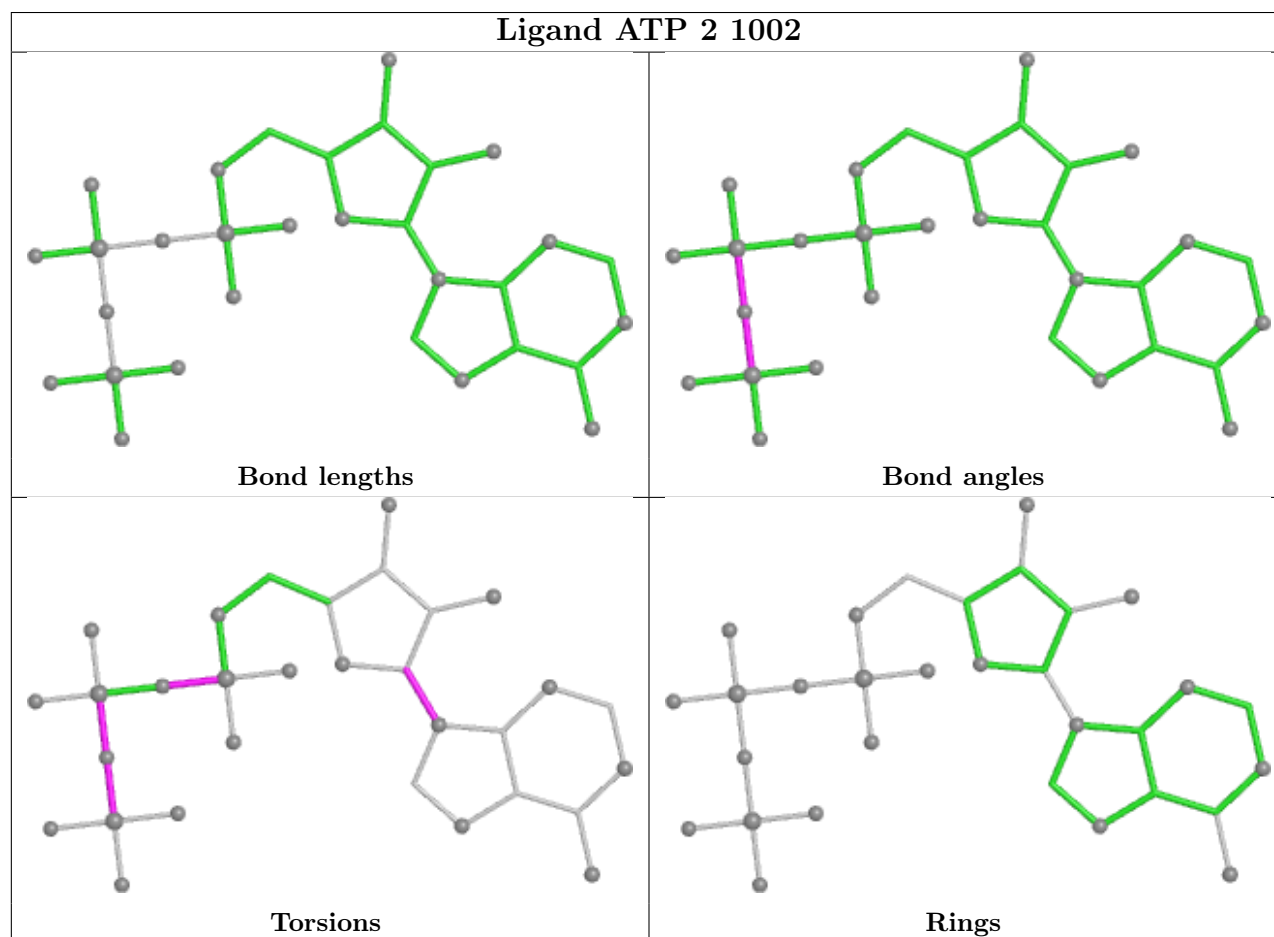
There are no ring outliers.

3 monomers are involved in 6 short contacts:

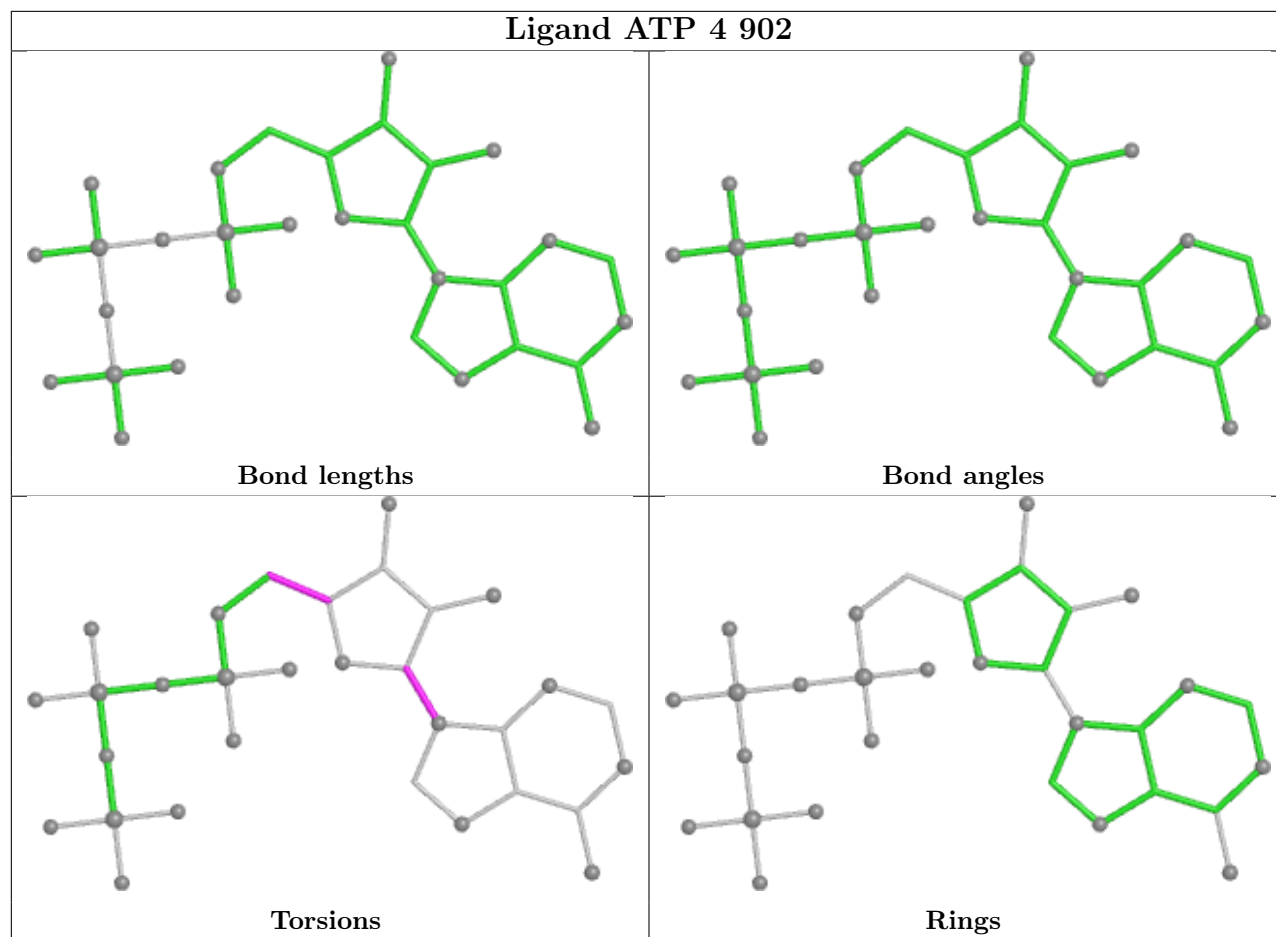
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	2	1002	ATP	1	0
10	3	901	ADP	2	0
8	6	901	ATP	3	0

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

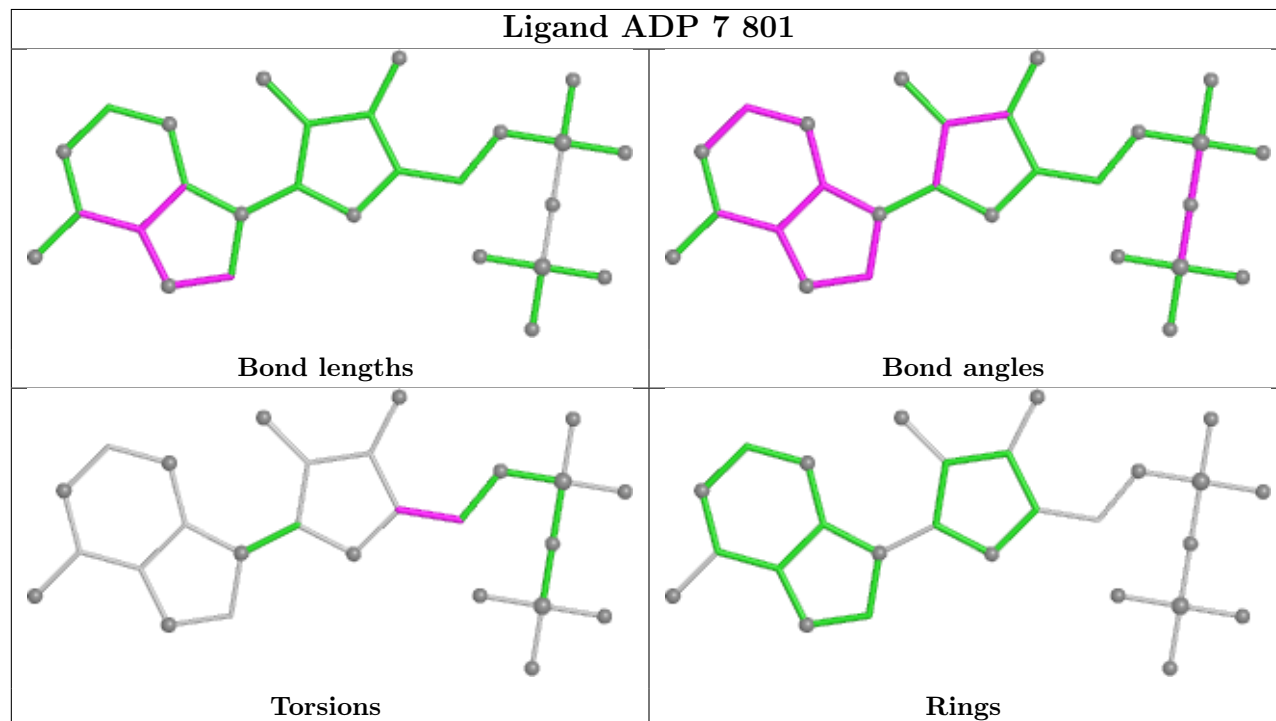
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

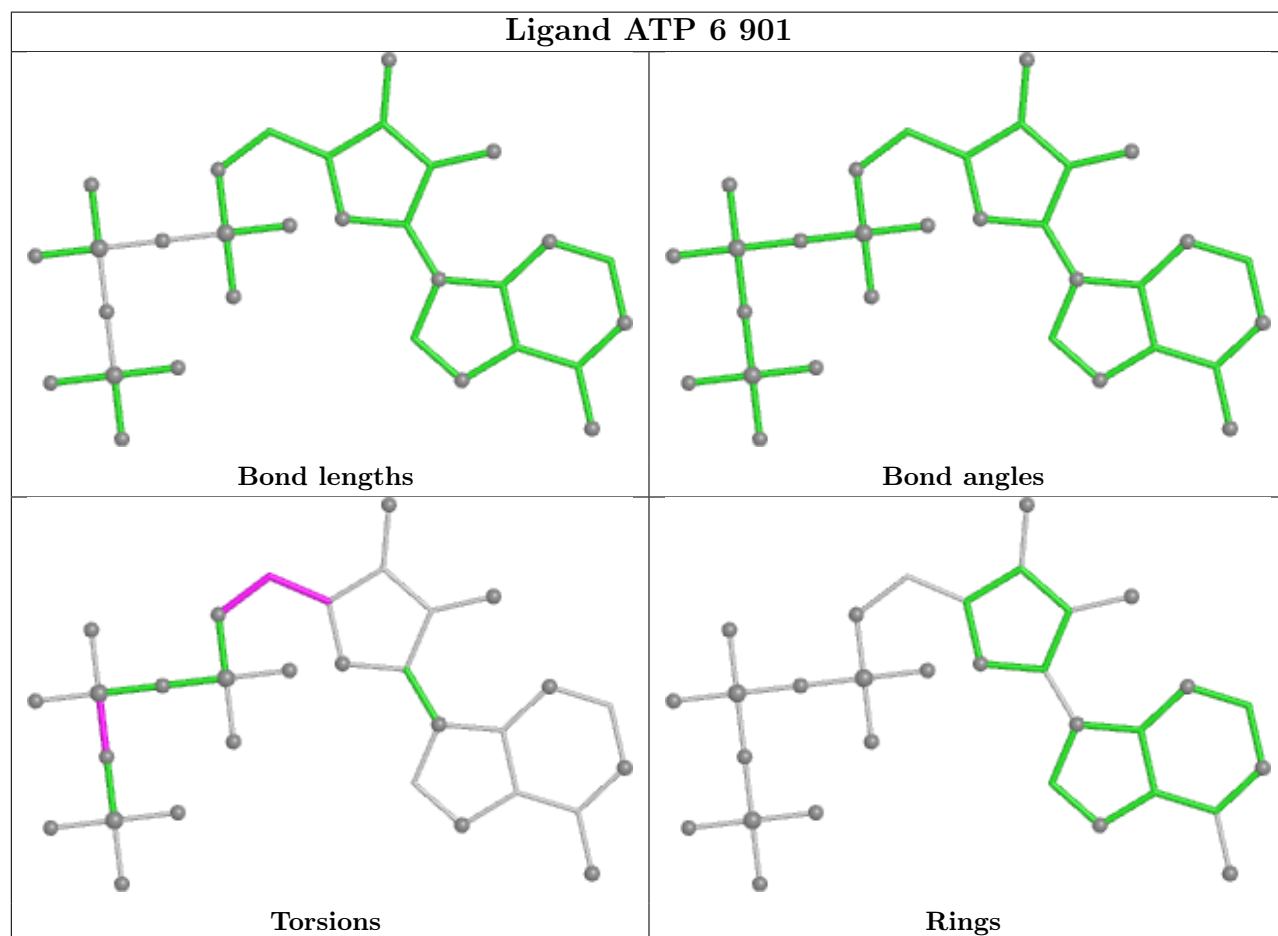
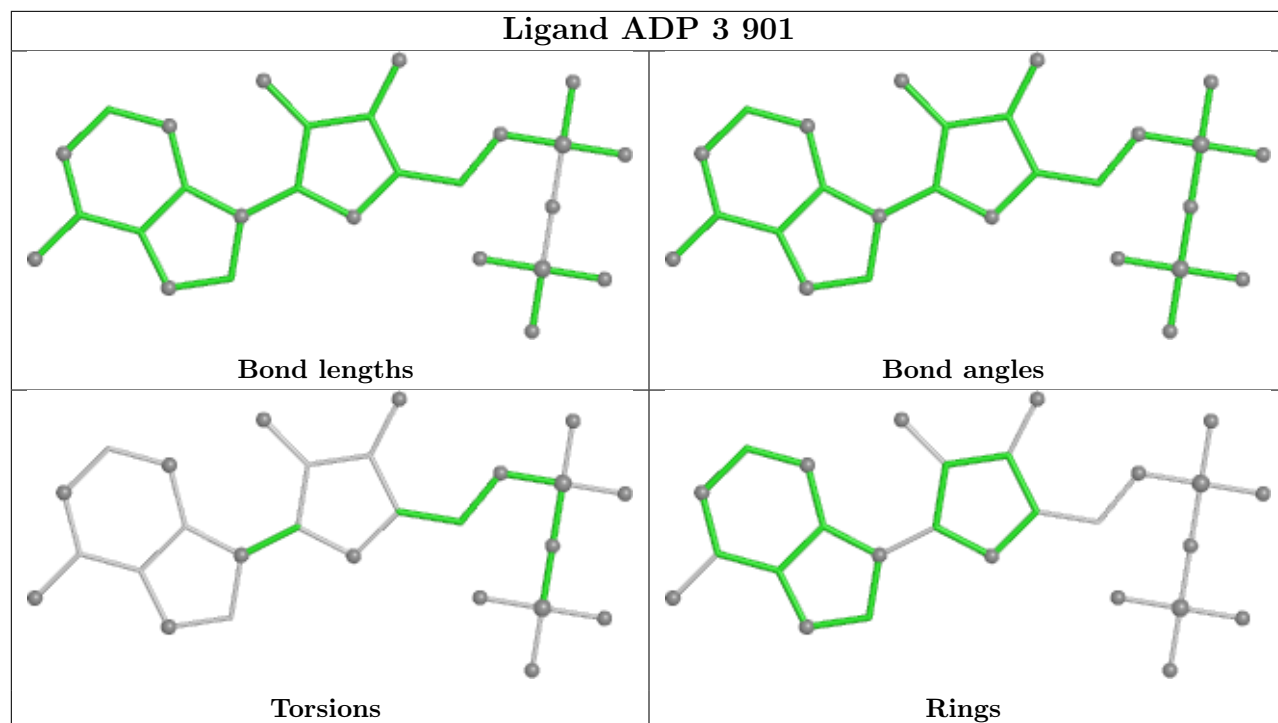


Ligand ATP 4 902



Ligand ADP 7 801





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

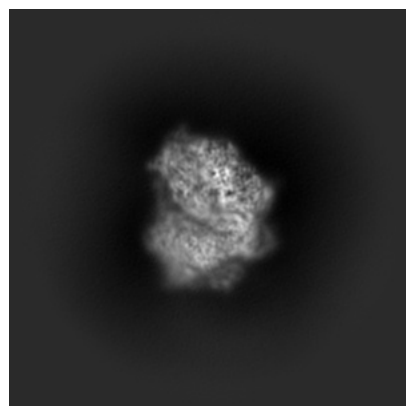
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65161. These allow visual inspection of the internal detail of the map and identification of artifacts.

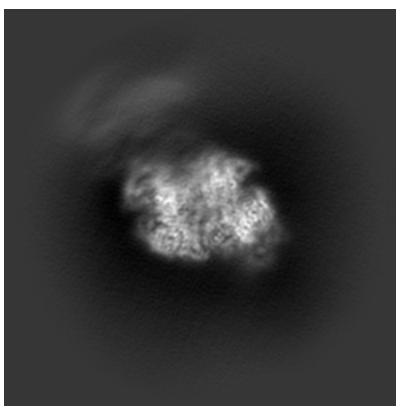
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

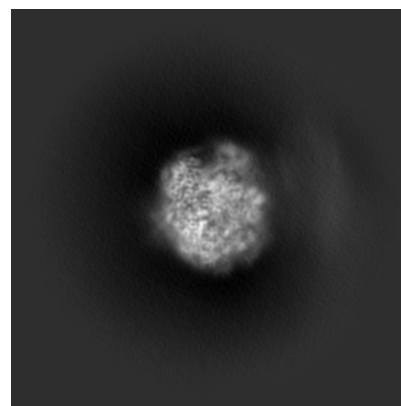
6.1.1 Primary map



X

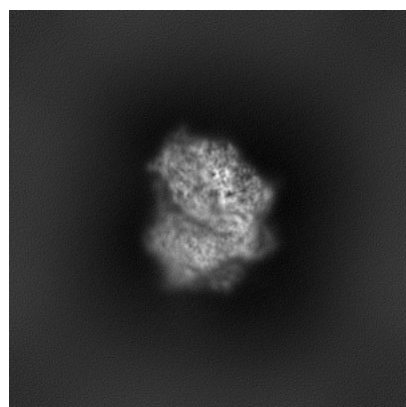


Y

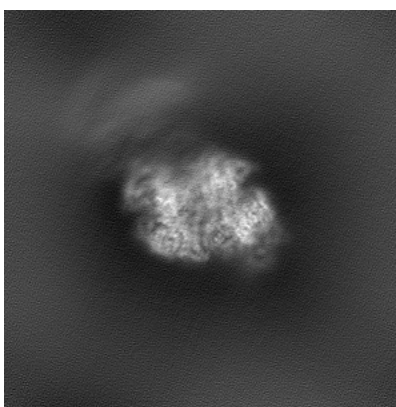


Z

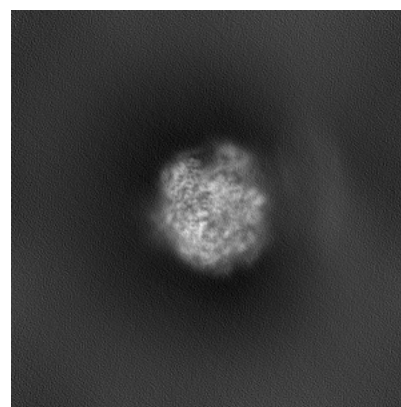
6.1.2 Raw map



X



Y

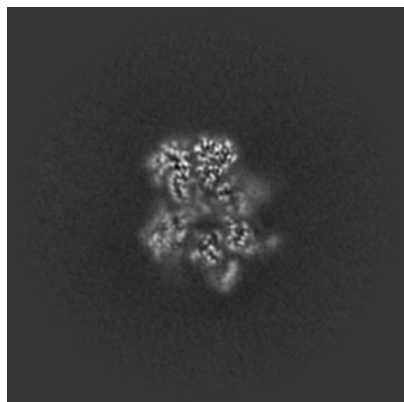


Z

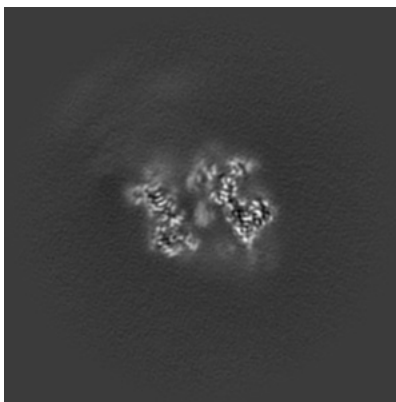
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

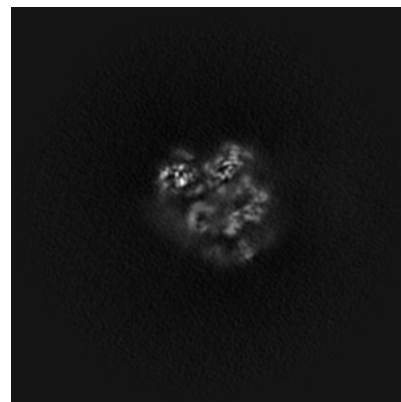
6.2.1 Primary map



X Index: 180

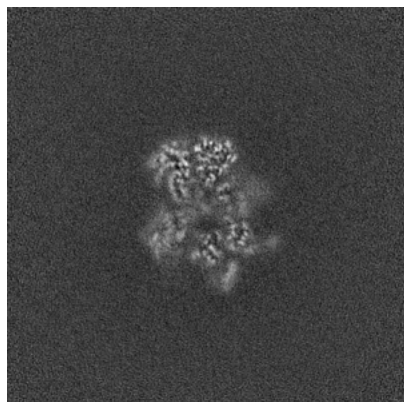


Y Index: 180

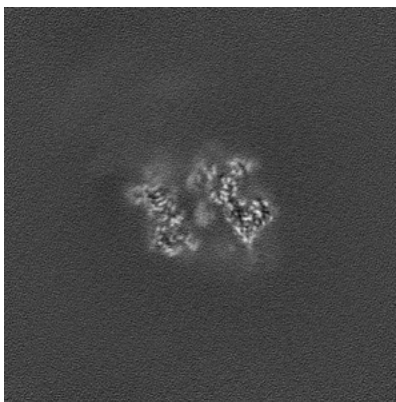


Z Index: 180

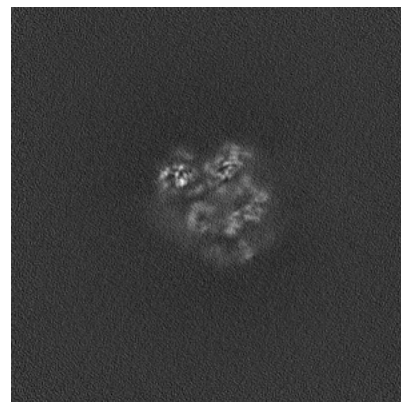
6.2.2 Raw map



X Index: 180



Y Index: 180

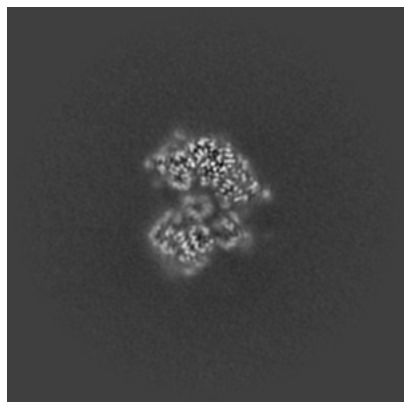


Z Index: 180

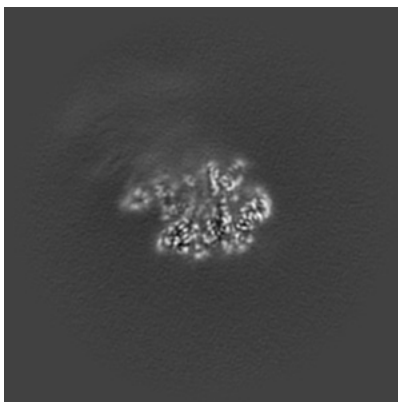
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

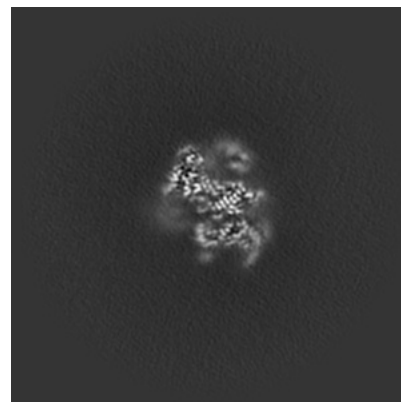
6.3.1 Primary map



X Index: 170

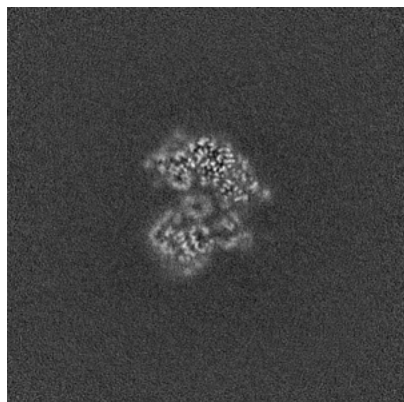


Y Index: 199

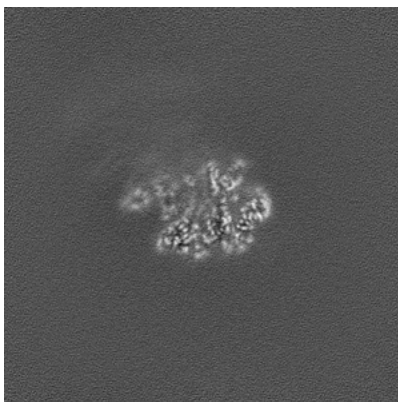


Z Index: 199

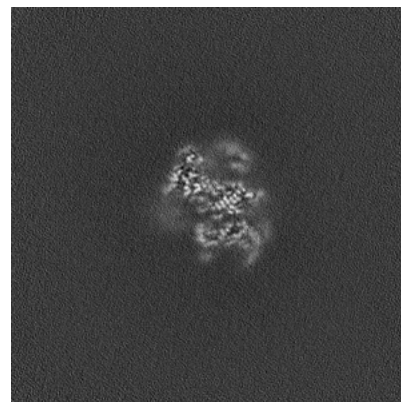
6.3.2 Raw map



X Index: 170



Y Index: 199

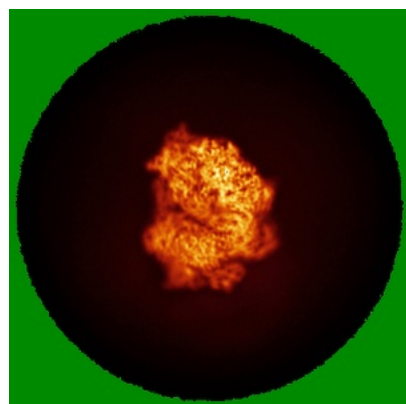


Z Index: 199

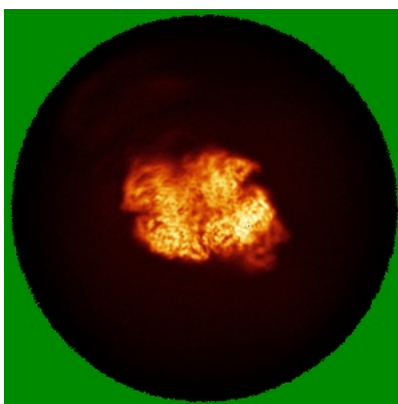
The images above show the largest variance slices of the map in three orthogonal directions.

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

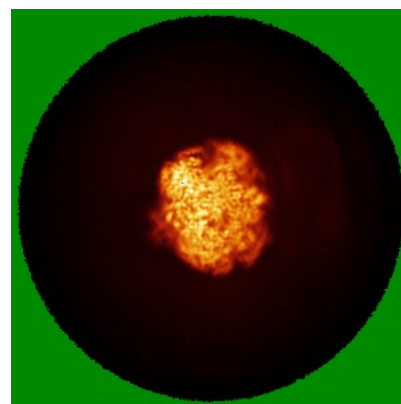
6.4.1 Primary map



X

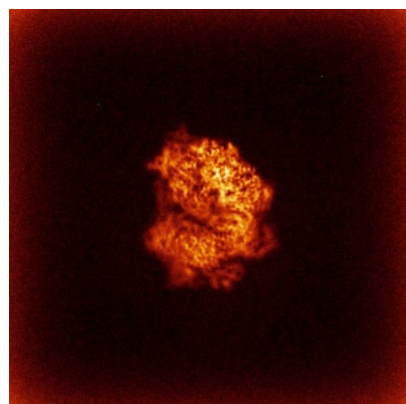


Y

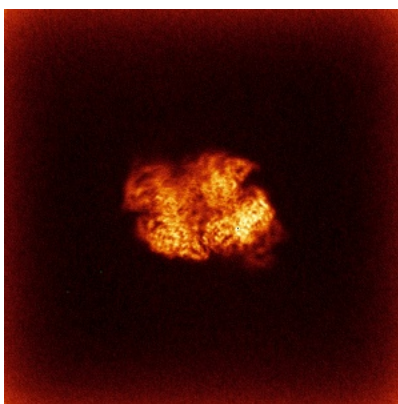


Z

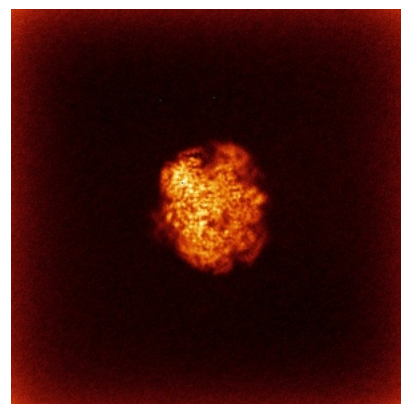
6.4.2 Raw map



X



Y

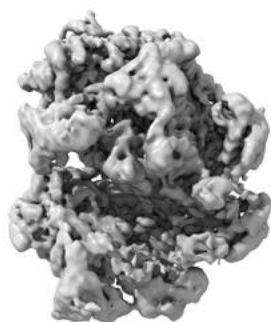


Z

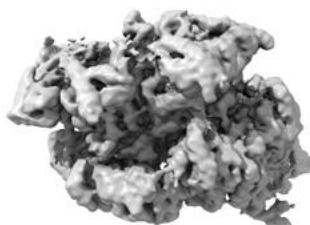
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

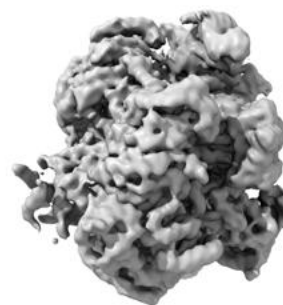
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. 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



X



Y



Z

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.

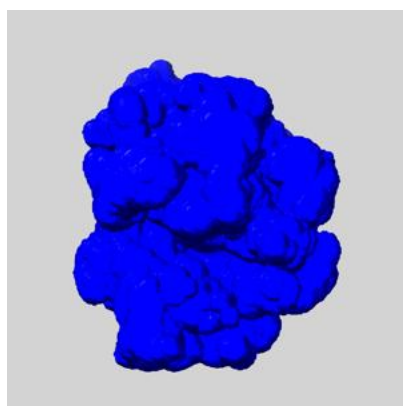
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

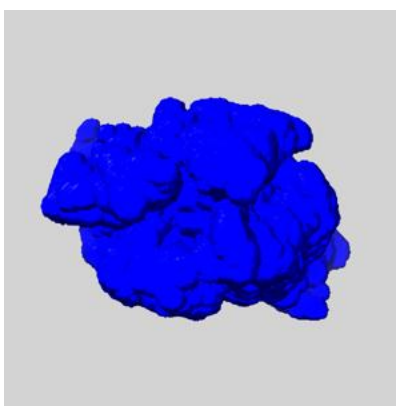
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

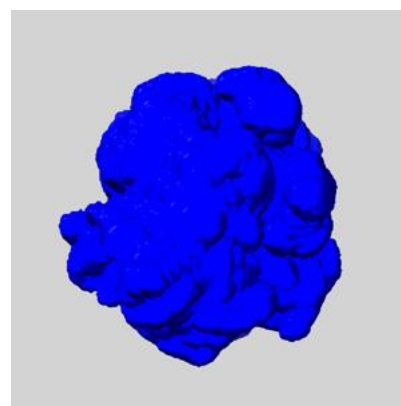
6.6.1 emd_65161_msk_1.map [i](#)



X



Y

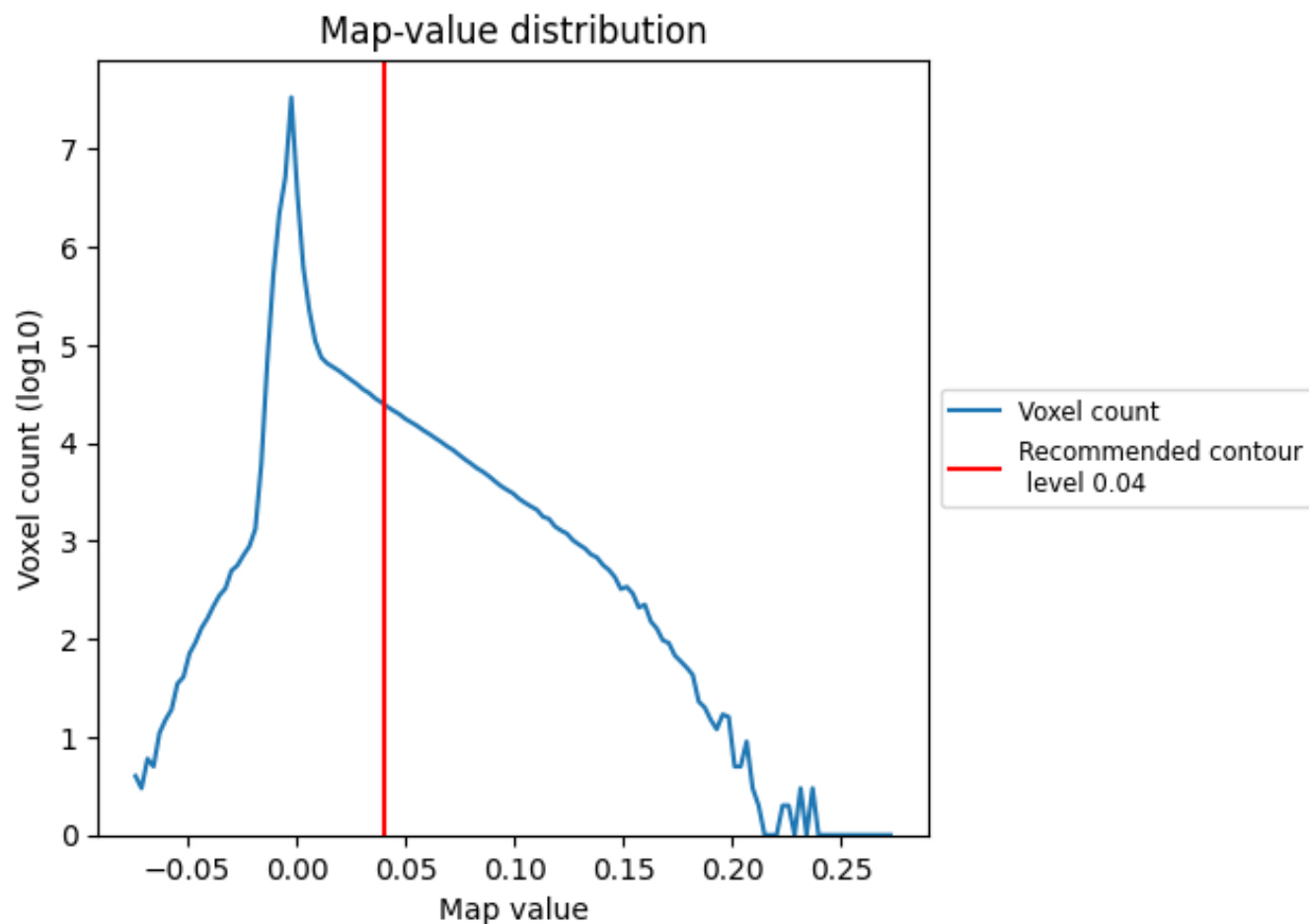


Z

7 Map analysis [i](#)

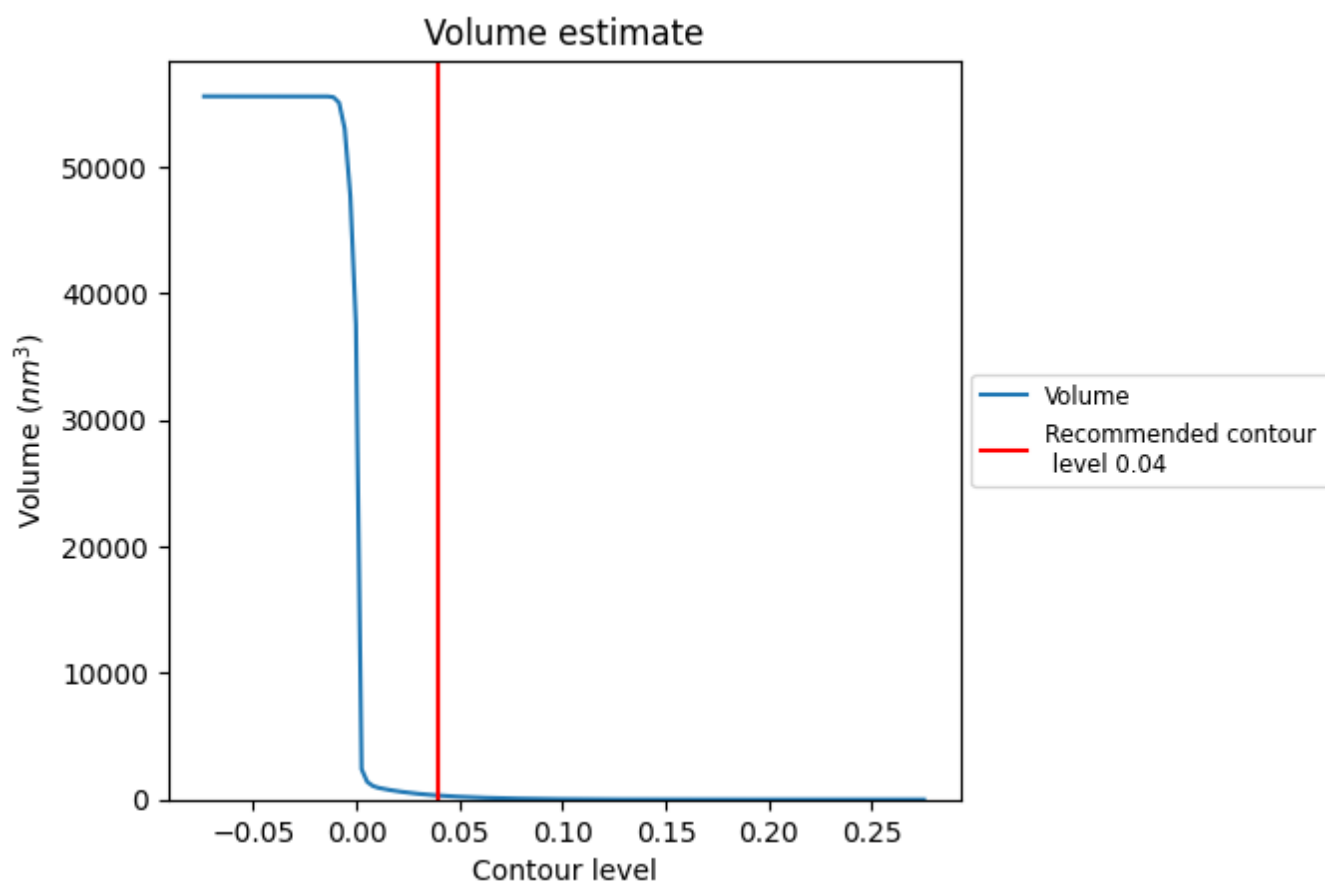
This section contains the results of statistical analysis of the map.

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.

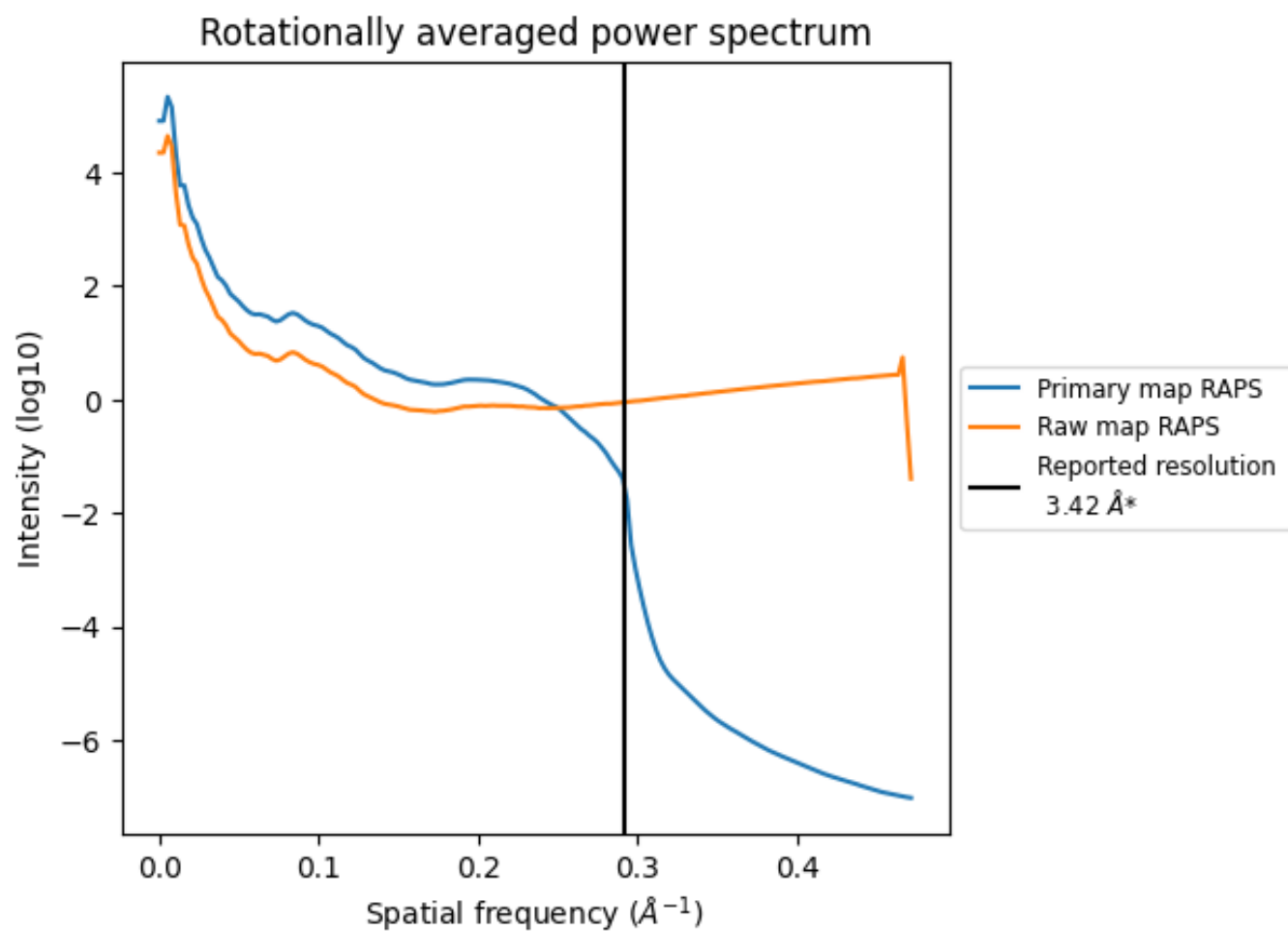
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 320 nm^3 ; this corresponds to an approximate mass of 289 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 ⓘ

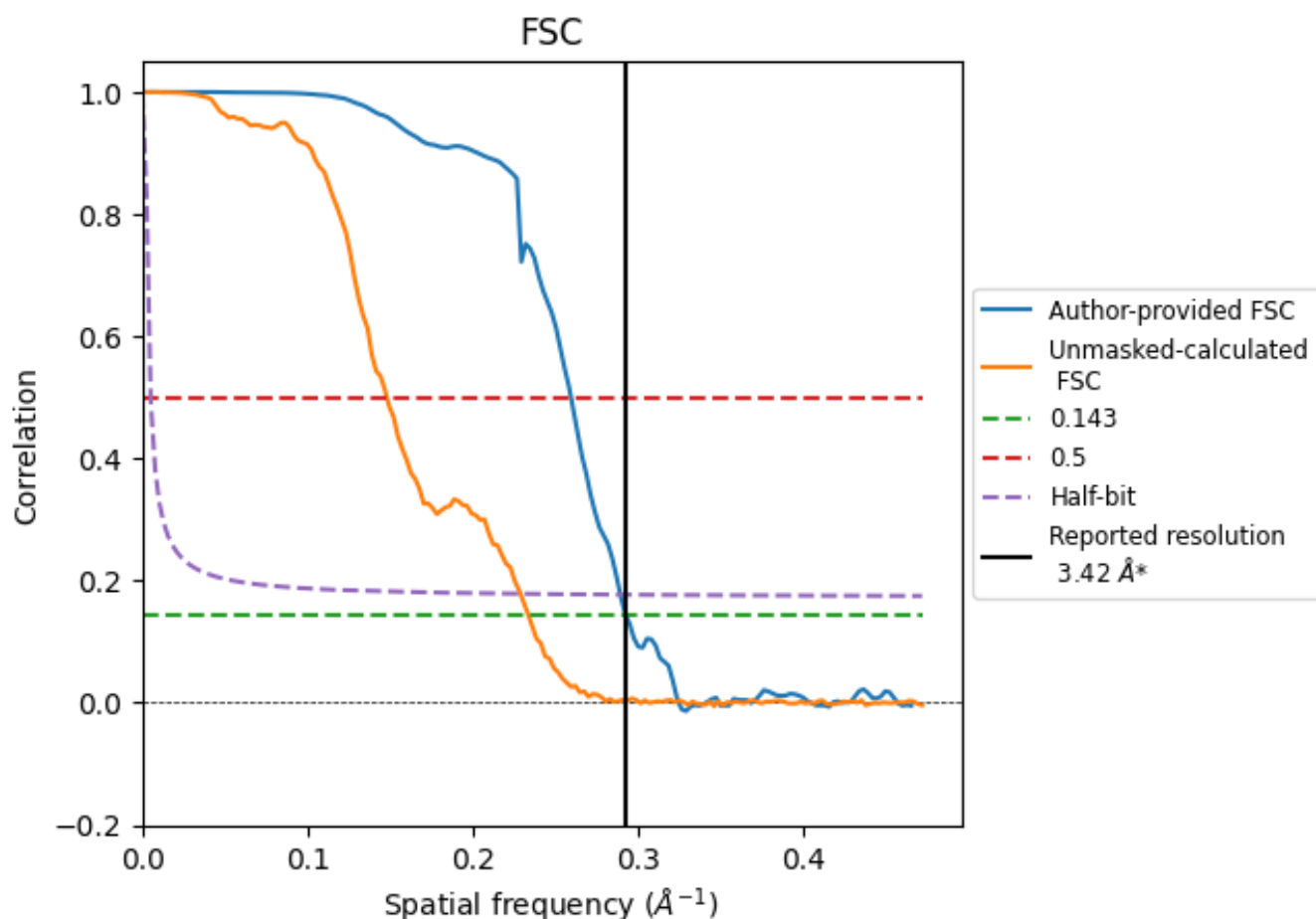


*Reported resolution corresponds to spatial frequency of 0.292 Å⁻¹

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 0.292 \AA^{-1}

8.2 Resolution estimates [i](#)

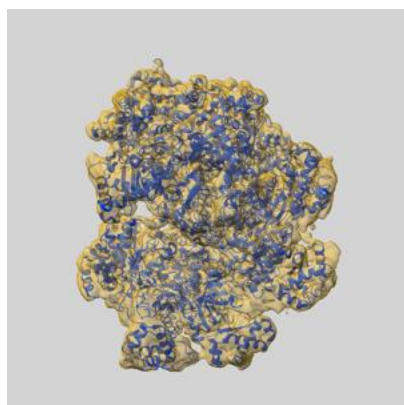
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	3.42	3.86	3.46
Unmasked-calculated*	4.28	6.76	4.37

*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 4.28 differs from the reported value 3.42 by more than 10 %

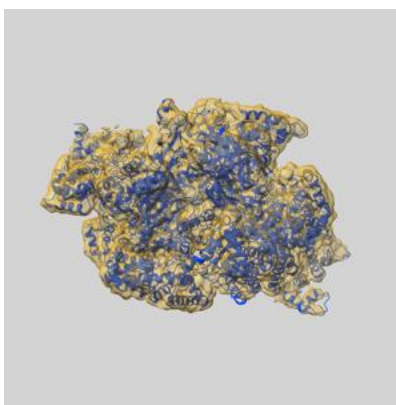
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65161 and PDB model 9VLN. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

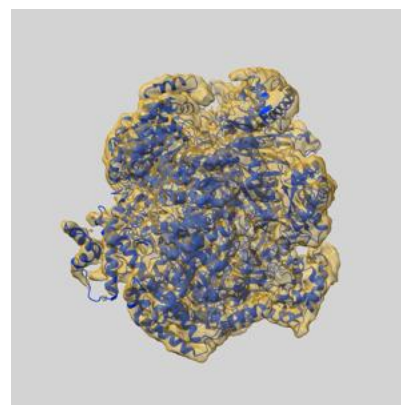
9.1 Map-model overlay [i](#)



X



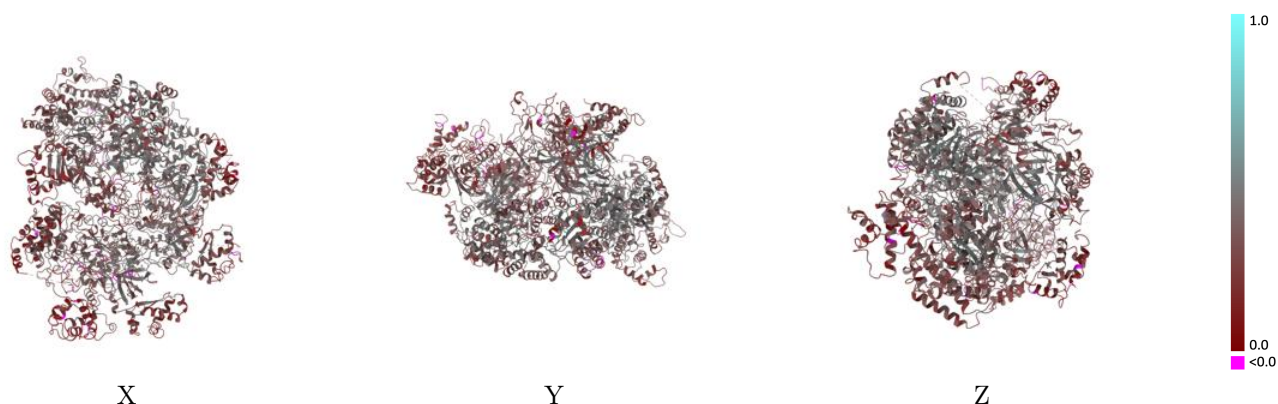
Y



Z

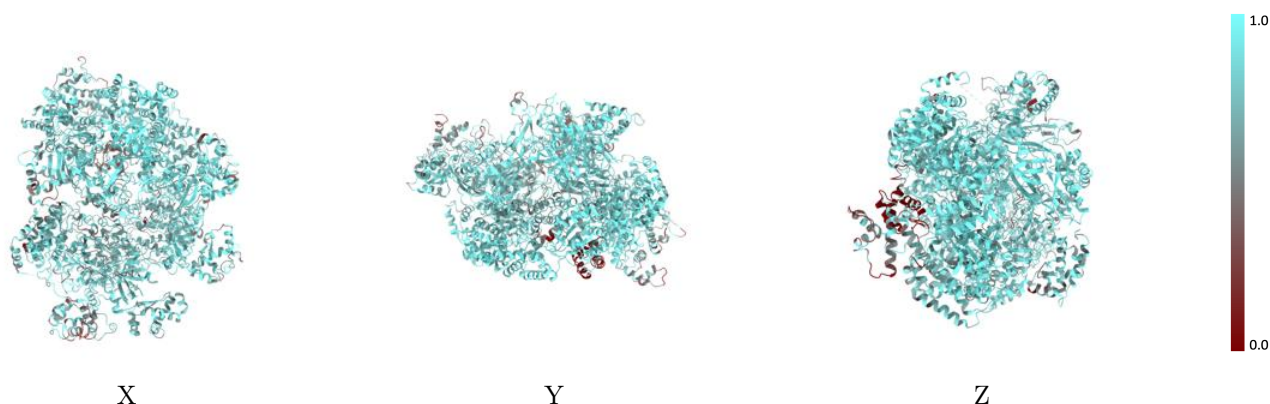
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



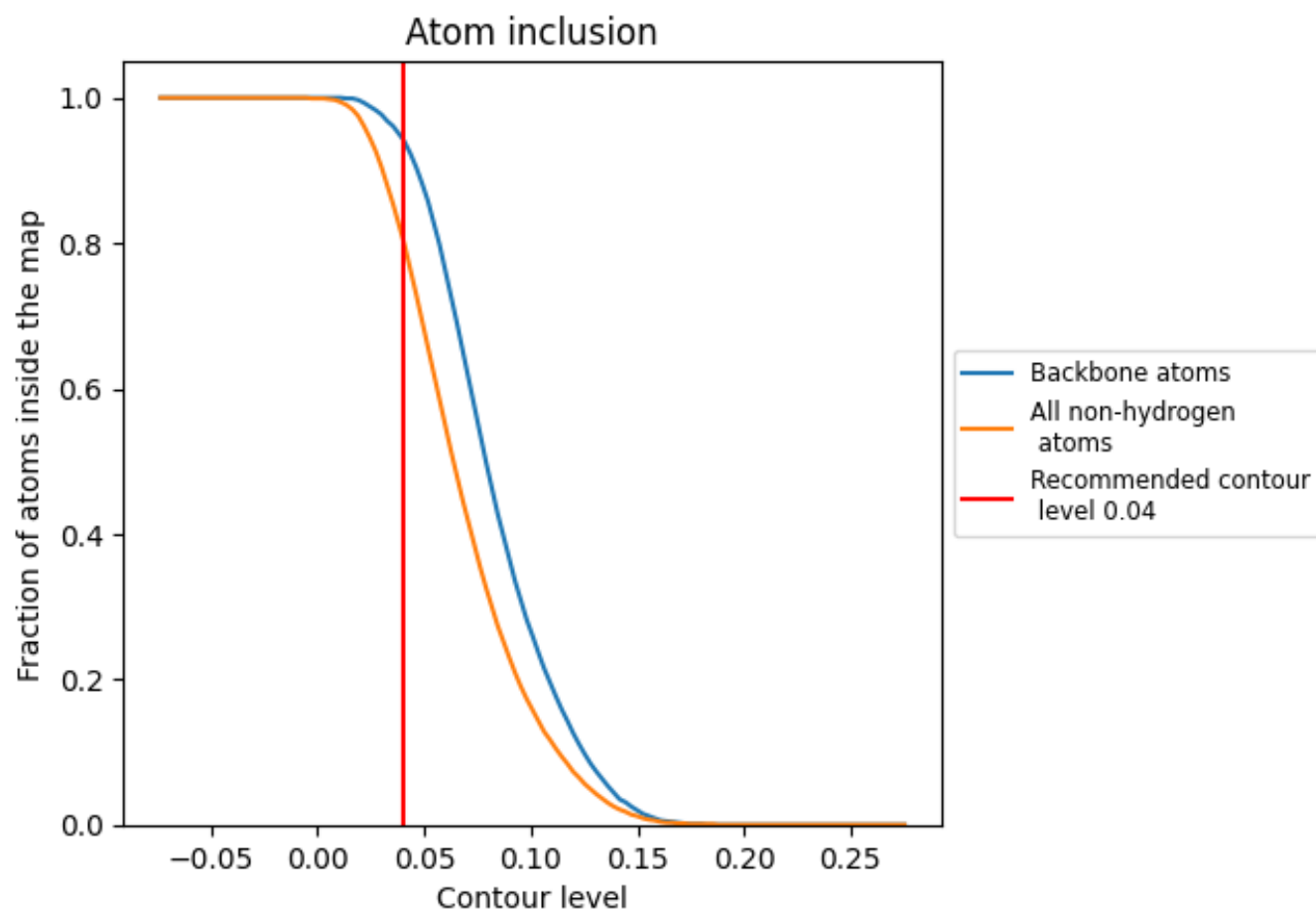
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 81% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8060</div>	<div><div></div>0.3370</div>
2	<div><div></div>0.7960</div>	<div><div></div>0.3280</div>
3	<div><div></div>0.8170</div>	<div><div></div>0.3440</div>
4	<div><div></div>0.7960</div>	<div><div></div>0.3510</div>
5	<div><div></div>0.7370</div>	<div><div></div>0.2480</div>
6	<div><div></div>0.8560</div>	<div><div></div>0.3910</div>
7	<div><div></div>0.8230</div>	<div><div></div>0.3470</div>

1.0

0.0

<0.0