



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:27 AM UTC

PDB ID : 9GM7 / pdb_00009gm7
EMDB ID : EMD-51443
Title : MukBEF in a nucleotide-bound state with open neck gate (monomer)
Authors : Burmann, F.; Lowe, J.
Deposited on : 2024-08-28
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:

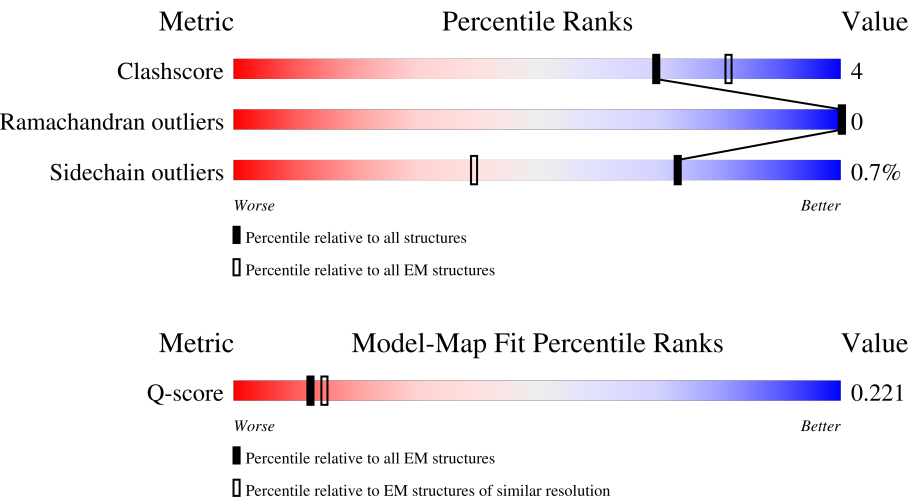
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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	C	440	13% 88% 11% .
1	D	440	9% 60% 5% 34%
2	E	240	. 69% 18% . 12%
2	F	240	. 69% 13% 18%

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Mol	Chain	Length	Quality of chain
3	G	78	
3	I	78	
4	A	1482	
4	B	1482	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	4HH	G	36	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 67711 atoms, of which 33622 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 Chromosome partition protein MukF.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	C	440	Total	C	H	N	O	S	0	0
			6982	2218	3451	614	686	13		
1	D	290	Total	C	H	N	O	S	0	0
			4567	1444	2260	402	451	10		

- Molecule 2 is a protein called Chromosome partition protein MukE.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	212	Total	C	H	N	O	S	0	0
			3441	1090	1719	301	322	9		
2	F	198	Total	C	H	N	O	S	0	0
			3246	1029	1627	284	298	8		

- Molecule 3 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	72	Total	C	H	N	O	P S	0	0
			1147	360	564	87	133	1 2		
3	I	72	Total	C	H	N	O	P S	0	0
			1147	360	564	87	133	1 2		

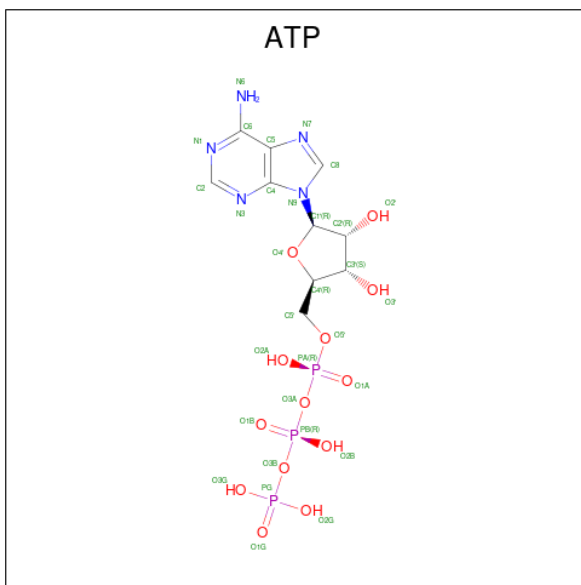
- Molecule 4 is a protein called Chromosome partition protein MukB.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	A	1467	Total	C	H	N	O	S	0	0
			23547	7298	11707	2188	2314	40		
4	B	1467	Total	C	H	N	O	S	0	0
			23546	7298	11706	2188	2314	40		

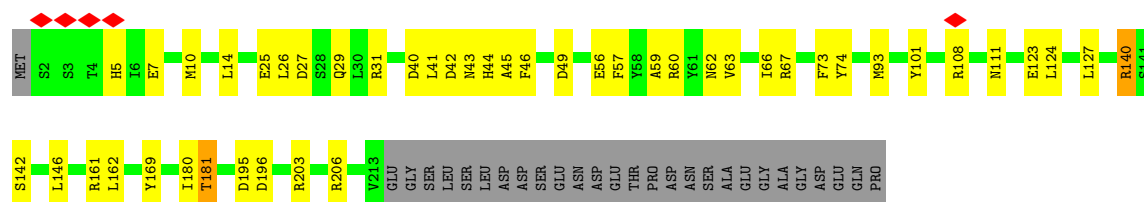
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	
5	B	1	Total	Mg	0
			1	1	

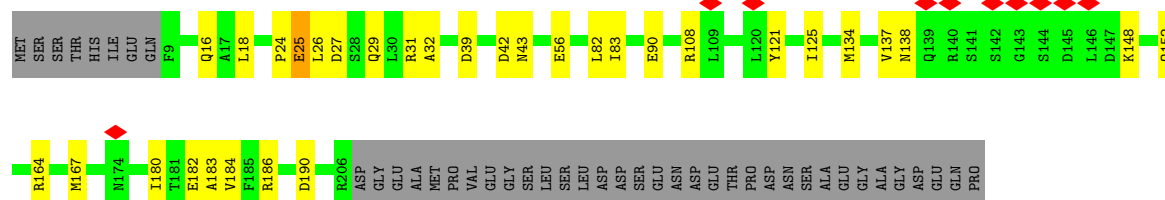
- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
6	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0



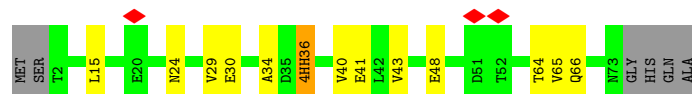
• Molecule 2: Chromosome partition protein MukE



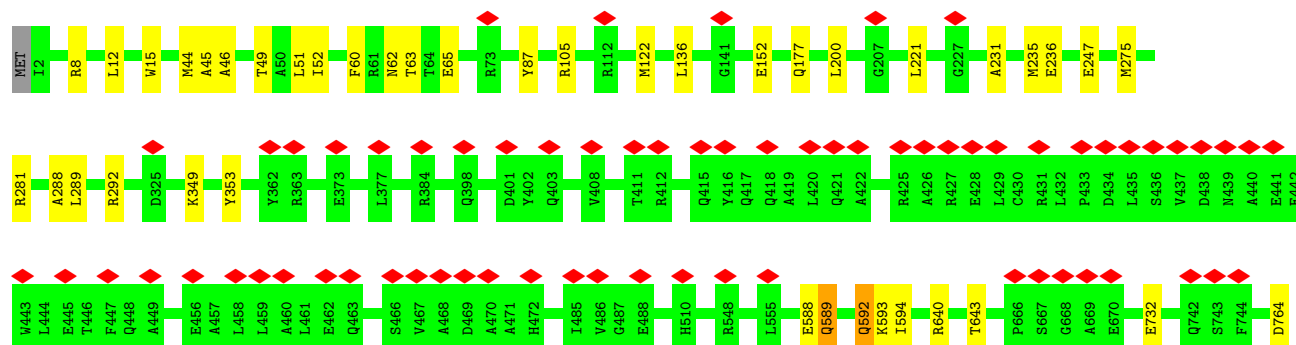
• Molecule 3: Acyl carrier protein

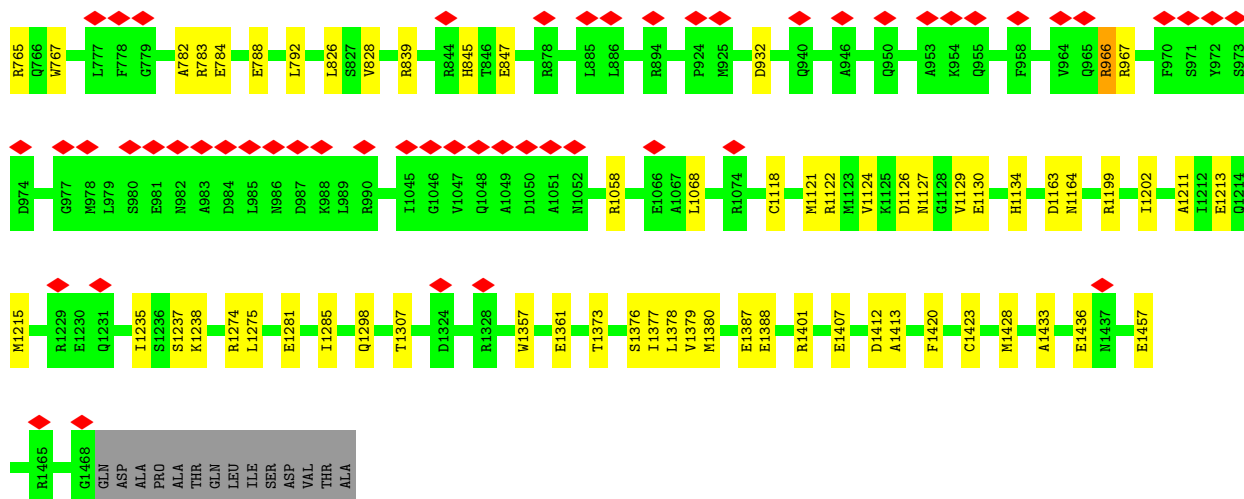


• Molecule 3: Acyl carrier protein

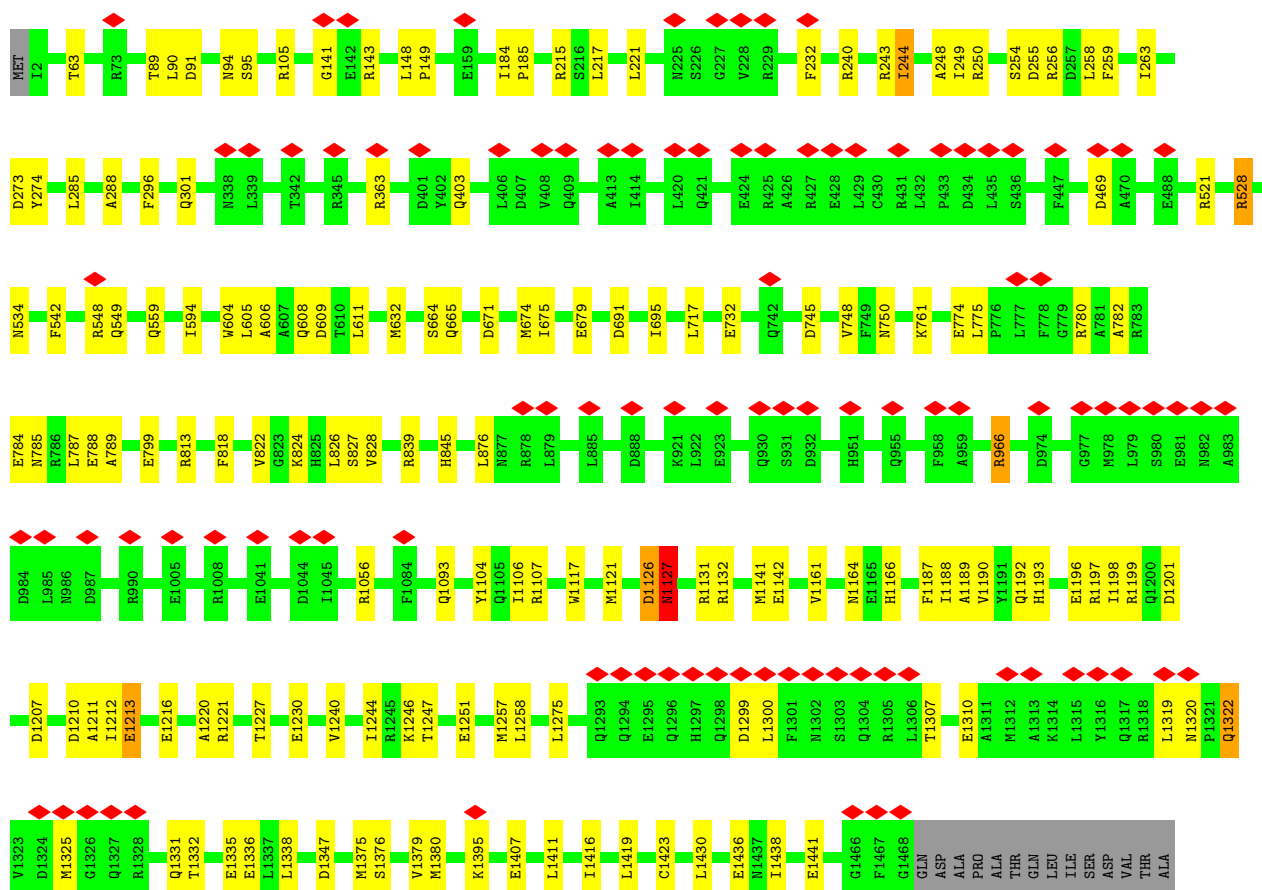
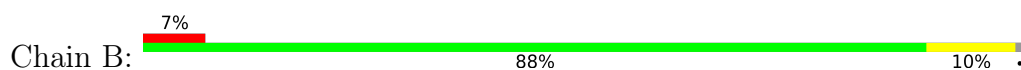


• Molecule 4: Chromosome partition protein MukB





● Molecule 4: Chromosome partition protein MukB



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34436	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.044	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	460.97998, 460.97998, 460.97998	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4775, 1.4775, 1.4775	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, 4HH, 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	C	0.77	5/3592 (0.1%)	1.24	16/4862 (0.3%)
1	D	0.69	0/2343	1.23	7/3165 (0.2%)
2	E	1.50	19/1753 (1.1%)	1.68	43/2361 (1.8%)
2	F	0.77	8/1648 (0.5%)	0.88	8/2218 (0.4%)
3	G	0.13	0/558	0.28	0/754
3	I	0.13	0/558	0.27	0/754
4	A	0.54	4/11999 (0.0%)	0.98	5/16166 (0.0%)
4	B	0.81	33/11999 (0.3%)	1.15	59/16166 (0.4%)
All	All	0.75	69/34450 (0.2%)	1.11	138/46446 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	8
1	D	0	5
2	E	0	3
4	A	0	3
4	B	0	2
All	All	0	21

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	ARG	C-N	-24.29	1.04	1.33
4	A	589	GLN	C-N	13.55	1.51	1.33
4	B	296	PHE	C-N	-8.97	1.22	1.33
4	B	1193	HIS	CE1-NE2	-8.80	1.23	1.32
4	B	1166	HIS	CE1-NE2	-8.77	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	44	HIS	CE1-NE2	-8.76	1.23	1.32
4	B	1166	HIS	CD2-NE2	-8.05	1.28	1.37
4	B	1193	HIS	CD2-NE2	-8.04	1.29	1.37
2	E	44	HIS	CD2-NE2	-8.03	1.29	1.37
2	F	31	ARG	CZ-NH2	-7.68	1.23	1.33
4	B	1132	ARG	CZ-NH2	-7.68	1.23	1.33
4	B	1131	ARG	CZ-NH2	-7.66	1.23	1.33
2	E	203	ARG	CZ-NH2	-7.63	1.23	1.33
2	E	31	ARG	CZ-NH2	-7.62	1.23	1.33
4	B	1093	GLN	C-N	7.61	1.44	1.33
4	B	1199	ARG	CZ-NH2	-7.57	1.23	1.33
2	E	206	ARG	CZ-NH2	-7.56	1.23	1.33
1	C	322	ARG	CZ-NH2	-7.54	1.23	1.33
4	B	1221	ARG	CZ-NH2	-7.52	1.23	1.33
4	B	240	ARG	CZ-NH2	-7.51	1.23	1.33
4	B	1197	ARG	CZ-NH2	-7.51	1.23	1.33
4	B	250	ARG	CZ-NH2	-7.48	1.23	1.33
2	F	164	ARG	CZ-NH2	-7.48	1.23	1.33
4	B	243	ARG	CZ-NH2	-7.41	1.23	1.33
2	E	67	ARG	CZ-NH2	-7.41	1.23	1.33
2	E	60	ARG	CZ-NH2	-7.36	1.23	1.33
4	B	301	GLN	C-N	7.10	1.43	1.34
4	B	1189	ALA	CA-CB	-6.57	1.43	1.53
4	A	847	GLU	C-N	6.47	1.42	1.33
4	B	248	ALA	CA-CB	-6.46	1.43	1.53
2	E	45	ALA	CA-CB	-6.34	1.43	1.53
1	C	320	ALA	CA-CB	-6.22	1.43	1.53
4	B	250	ARG	CZ-NH1	-6.21	1.24	1.32
2	F	31	ARG	CZ-NH1	-6.12	1.24	1.32
2	E	31	ARG	CZ-NH1	-6.10	1.24	1.32
4	B	240	ARG	CZ-NH1	-6.10	1.24	1.32
1	C	322	ARG	CZ-NH1	-6.10	1.24	1.32
4	B	243	ARG	CZ-NH1	-6.10	1.24	1.32
2	E	206	ARG	CZ-NH1	-6.09	1.24	1.32
2	E	67	ARG	CZ-NH1	-6.07	1.24	1.32
2	E	60	ARG	CZ-NH1	-6.07	1.24	1.32
4	B	1199	ARG	CZ-NH1	-6.06	1.24	1.32
2	F	164	ARG	CZ-NH1	-6.03	1.24	1.32
4	B	1221	ARG	CZ-NH1	-6.00	1.24	1.32
2	E	203	ARG	CZ-NH1	-5.96	1.24	1.32
4	B	1211	ALA	CA-CB	-5.96	1.43	1.53
4	B	1131	ARG	CZ-NH1	-5.94	1.24	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1197	ARG	CZ-NH1	-5.93	1.24	1.32
4	B	1132	ARG	CZ-NH1	-5.91	1.24	1.32
2	E	59	ALA	CA-CB	-5.81	1.43	1.53
2	F	83	ILE	N-CA	-5.68	1.42	1.46
2	F	32	ALA	CA-CB	-5.67	1.43	1.53
4	B	240	ARG	CD-NE	-5.39	1.38	1.46
4	A	592	GLN	C-N	5.37	1.40	1.33
4	B	1199	ARG	CD-NE	-5.33	1.38	1.46
1	C	322	ARG	CD-NE	-5.31	1.38	1.46
4	B	250	ARG	CD-NE	-5.30	1.38	1.46
4	B	1132	ARG	CD-NE	-5.26	1.38	1.46
2	E	60	ARG	CD-NE	-5.22	1.39	1.46
2	E	203	ARG	CD-NE	-5.21	1.39	1.46
2	E	31	ARG	CD-NE	-5.18	1.39	1.46
2	F	164	ARG	CD-NE	-5.17	1.39	1.46
2	E	67	ARG	CD-NE	-5.15	1.39	1.46
2	F	31	ARG	CD-NE	-5.10	1.39	1.46
4	B	243	ARG	CD-NE	-5.10	1.39	1.46
4	B	1221	ARG	CD-NE	-5.08	1.39	1.46
4	B	1197	ARG	CD-NE	-5.07	1.39	1.46
2	E	206	ARG	CD-NE	-5.03	1.39	1.46
4	A	839	ARG	C-N	-5.01	1.27	1.33

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	295	ARG	CA-C-N	22.16	147.91	120.88
1	C	295	ARG	C-N-CA	22.16	147.91	120.88
4	A	589	GLN	O-C-N	9.98	132.35	122.07
2	F	82	LEU	CA-C-N	9.53	129.45	122.59
2	F	82	LEU	C-N-CA	9.53	129.45	122.59
4	B	469	ASP	CA-CB-CG	8.76	121.36	112.60
1	D	176	ARG	CB-CG-CD	8.66	131.23	111.30
4	B	1127	ASN	CA-CB-CG	8.44	121.04	112.60
4	B	259	PHE	CA-CB-CG	7.87	121.67	113.80
4	A	589	GLN	CA-C-N	-7.85	109.63	120.38
4	A	589	GLN	C-N-CA	-7.85	109.63	120.38
1	C	294	ASN	N-CA-C	-6.96	103.74	111.82
1	D	251	LYS	CB-CG-CD	6.70	126.70	111.30
2	E	195	ASP	CA-CB-CG	6.68	119.28	112.60
2	E	44	HIS	CA-CB-CG	6.64	120.44	113.80
4	B	301	GLN	O-C-N	-6.63	115.09	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1187	PHE	CA-CB-CG	6.49	120.29	113.80
2	E	73	PHE	CA-CB-CG	6.48	120.28	113.80
2	E	43	ASN	CA-CB-CG	6.47	119.07	112.60
4	B	1207	ASP	CA-CB-CG	6.47	119.07	112.60
4	B	1164	ASN	CA-CB-CG	6.45	119.05	112.60
2	E	196	ASP	CA-CB-CG	6.42	119.02	112.60
4	B	1210	ASP	CA-CB-CG	6.37	118.97	112.60
4	B	966	ARG	NE-CZ-NH2	6.36	124.92	119.20
4	B	1131	ARG	CD-NE-CZ	6.33	133.26	124.40
4	B	255	ASP	CA-CB-CG	6.29	118.89	112.60
4	B	1193	HIS	CA-CB-CG	6.27	120.07	113.80
4	B	1201	ASP	N-CA-C	6.25	118.61	111.11
4	B	1221	ARG	CD-NE-CZ	6.21	133.10	124.40
2	E	57	PHE	CA-CB-CG	6.20	120.00	113.80
4	B	243	ARG	CA-CB-CG	6.17	126.44	114.10
4	B	1132	ARG	CD-NE-CZ	6.13	132.98	124.40
4	B	1056	ARG	NE-CZ-NH2	6.11	124.70	119.20
2	E	62	ASN	CA-CB-CG	6.06	118.66	112.60
4	B	243	ARG	CG-CD-NE	6.04	125.28	112.00
1	D	116	ARG	NE-CZ-NH2	6.01	124.61	119.20
2	E	66	ILE	CA-C-N	5.99	131.82	123.07
2	E	66	ILE	C-N-CA	5.99	131.82	123.07
2	F	27	ASP	CA-CB-CG	5.98	118.58	112.60
4	B	263	ILE	N-CA-CB	5.96	117.12	110.62
2	E	42	ASP	CA-C-N	5.94	128.16	120.44
2	E	42	ASP	C-N-CA	5.94	128.16	120.44
2	E	63	VAL	CA-C-N	5.90	130.27	122.30
2	E	63	VAL	C-N-CA	5.90	130.27	122.30
2	E	42	ASP	CA-CB-CG	5.89	118.49	112.60
2	E	60	ARG	CD-NE-CZ	5.86	132.60	124.40
2	F	31	ARG	CD-NE-CZ	5.82	132.55	124.40
2	E	31	ARG	CD-NE-CZ	5.82	132.55	124.40
2	E	74	TYR	CA-C-N	5.82	130.75	122.72
2	E	74	TYR	C-N-CA	5.82	130.75	122.72
4	B	1192	GLN	CA-C-N	5.81	128.38	120.54
4	B	1192	GLN	C-N-CA	5.81	128.38	120.54
4	B	548	ARG	CA-C-N	5.80	130.52	121.76
4	B	548	ARG	C-N-CA	5.80	130.52	121.76
2	E	25	GLU	CA-C-N	5.76	127.92	120.44
2	E	25	GLU	C-N-CA	5.76	127.92	120.44
1	C	294	ASN	CA-C-N	5.73	130.71	122.40
1	C	294	ASN	C-N-CA	5.73	130.71	122.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	249	ILE	N-CA-CB	5.72	117.24	110.55
4	B	1197	ARG	CA-C-N	5.71	128.15	120.50
4	B	1197	ARG	C-N-CA	5.71	128.15	120.50
4	B	244	ILE	N-CA-CB	5.71	116.61	110.62
2	E	27	ASP	CA-CB-CG	5.70	118.30	112.60
2	E	56	GLU	CA-C-N	5.67	128.14	120.65
2	E	56	GLU	C-N-CA	5.67	128.14	120.65
1	C	137	HIS	CB-CG-CD2	-5.66	123.84	131.20
2	E	67	ARG	CG-CD-NE	5.66	124.46	112.00
4	B	1126	ASP	CA-CB-CG	5.63	118.23	112.60
2	E	46	PHE	N-CA-CB	5.61	118.30	109.94
4	B	256	ARG	CD-NE-CZ	5.60	132.24	124.40
1	C	42	ARG	NE-CZ-NH1	-5.59	115.91	121.50
2	F	26	LEU	CA-C-N	5.59	127.71	120.44
2	F	26	LEU	C-N-CA	5.59	127.71	120.44
4	B	528	ARG	NE-CZ-NH2	5.59	124.23	119.20
4	B	1188	ILE	N-CA-CB	5.59	116.71	110.51
1	C	295	ARG	CB-CA-C	5.57	120.31	111.51
4	B	1197	ARG	CD-NE-CZ	5.55	132.16	124.40
4	B	1216	GLU	CA-C-N	5.53	127.53	120.56
4	B	1216	GLU	C-N-CA	5.53	127.53	120.56
1	C	287	THR	CA-CB-OG1	5.52	117.88	109.60
4	B	1212	ILE	N-CA-CB	5.48	116.37	110.62
2	F	24	PRO	CA-C-N	5.47	127.55	120.44
2	F	24	PRO	C-N-CA	5.47	127.55	120.44
2	E	44	HIS	CA-C-N	5.46	127.54	120.44
2	E	44	HIS	C-N-CA	5.46	127.54	120.44
1	D	219	GLN	OE1-CD-NE2	-5.45	117.16	122.60
4	B	403	GLN	OE1-CD-NE2	-5.43	117.17	122.60
2	E	43	ASN	CA-C-N	5.42	127.49	120.44
2	E	43	ASN	C-N-CA	5.42	127.49	120.44
4	B	363	ARG	NE-CZ-NH2	5.41	124.07	119.20
2	E	46	PHE	CA-CB-CG	5.40	119.20	113.80
4	B	1221	ARG	CA-CB-CG	5.39	124.88	114.10
1	C	299	GLN	CA-C-N	5.36	127.77	120.54
1	C	299	GLN	C-N-CA	5.36	127.77	120.54
4	B	1322	GLN	CA-CB-CG	5.34	124.78	114.10
2	E	62	ASN	CA-C-N	5.34	130.40	122.71
2	E	62	ASN	C-N-CA	5.34	130.40	122.71
2	E	67	ARG	CD-NE-CZ	5.32	131.85	124.40
2	E	67	ARG	CA-CB-CG	5.30	124.71	114.10
1	D	153	HIS	CB-CG-CD2	-5.30	124.31	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1220	ALA	CA-C-N	5.29	127.68	120.54
4	B	1220	ALA	C-N-CA	5.29	127.68	120.54
4	B	243	ARG	CD-NE-CZ	5.28	131.80	124.40
4	B	250	ARG	CA-C-N	5.28	127.16	120.72
4	B	250	ARG	C-N-CA	5.28	127.16	120.72
1	D	151	HIS	CB-CG-CD2	-5.28	124.34	131.20
1	C	290	ASP	N-CA-C	5.26	118.86	112.23
2	E	29	GLN	CA-C-N	5.23	127.24	120.44
2	E	29	GLN	C-N-CA	5.23	127.24	120.44
4	B	1188	ILE	CA-C-N	5.20	127.20	120.44
4	B	1188	ILE	C-N-CA	5.20	127.20	120.44
2	E	206	ARG	N-CA-CB	5.19	117.75	110.12
4	A	966	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	C	120	PHE	CA-CB-CG	-5.18	108.62	113.80
4	B	1164	ASN	N-CA-CB	5.17	117.62	110.17
1	C	151	HIS	CB-CG-CD2	-5.17	124.48	131.20
4	B	240	ARG	N-CA-CB	5.17	117.50	110.01
2	E	26	LEU	CA-C-N	5.16	127.15	120.44
2	E	26	LEU	C-N-CA	5.16	127.15	120.44
4	B	1187	PHE	CA-C-N	5.15	127.24	120.60
4	B	1187	PHE	C-N-CA	5.15	127.24	120.60
1	D	198	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	C	153	HIS	CB-CG-CD2	-5.11	124.56	131.20
4	B	559	GLN	OE1-CD-NE2	-5.09	117.51	122.60
4	A	932	ASP	CB-CA-C	5.08	115.56	109.31
4	B	255	ASP	CA-C-N	5.08	127.04	120.44
4	B	255	ASP	C-N-CA	5.08	127.04	120.44
1	C	116	ARG	NE-CZ-NH2	5.07	123.76	119.20
2	E	27	ASP	N-CA-CB	5.05	117.34	110.01
4	B	1198	ILE	CA-C-N	5.05	128.46	120.89
4	B	1198	ILE	C-N-CA	5.05	128.46	120.89
4	B	521	ARG	NE-CZ-NH2	5.04	123.74	119.20
4	B	1190	VAL	N-CA-CB	5.04	116.44	110.55
2	E	40	ASP	CA-C-N	5.03	127.33	120.54
2	E	40	ASP	C-N-CA	5.03	127.33	120.54
4	B	549	GLN	N-CA-C	-5.03	98.86	107.61
2	E	56	GLU	N-CA-CB	5.01	117.48	110.12
4	B	534	ASN	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1058	ARG	Sidechain
4	A	966	ARG	Sidechain
4	A	967	ARG	Sidechain
4	B	528	ARG	Sidechain
4	B	966	ARG	Sidechain
1	C	120	PHE	Sidechain
1	C	124	ARG	Sidechain
1	C	138	ARG	Sidechain
1	C	28	ARG	Sidechain
1	C	300	ARG	Sidechain
1	C	4	TYR	Sidechain
1	C	42	ARG	Sidechain
1	C	89	ARG	Sidechain
1	D	116	ARG	Sidechain
1	D	120	PHE	Sidechain
1	D	124	ARG	Sidechain
1	D	162	TYR	Sidechain
1	D	89	ARG	Sidechain
2	E	101	TYR	Sidechain
2	E	140	ARG	Sidechain
2	E	161	ARG	Sidechain

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	C	3531	3451	3450	24	0
1	D	2307	2260	2260	7	0
2	E	1722	1719	1718	15	0
2	F	1619	1627	1626	20	0
3	G	583	564	563	25	0
3	I	583	564	563	10	0
4	A	11840	11707	11705	78	0
4	B	11840	11706	11705	95	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	31	12	12	0	0
6	B	31	12	12	0	0
All	All	34089	33622	33614	244	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 4.

All (244) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:36:4HH:CL3	3:G:40:VAL:HG21	1.87	1.04
4:B:1127:ASN:O	4:B:1127:ASN:ND2	1.91	1.02
3:I:48:GLU:OE1	4:B:1107:ARG:NE	2.04	0.90
3:G:36:4HH:SU	4:A:292:ARG:HD3	2.14	0.87
4:B:665:GLN:NE2	4:B:671:ASP:OD2	2.11	0.84
4:B:1127:ASN:HD22	4:B:1127:ASN:C	1.88	0.81
3:G:36:4HH:HT3	3:G:56:ASP:OD1	1.85	0.76
3:G:23:THR:OG1	3:G:25:ASN:OD1	2.04	0.74
4:A:1412:ASP:OD1	4:A:1413:ALA:N	2.20	0.73
3:G:44:MET:HE1	4:A:288:ALA:HB1	1.73	0.71
3:G:36:4HH:CL3	3:G:40:VAL:CG2	2.68	0.68
3:G:36:4HH:HB2	3:G:36:4HH:HJ2	1.74	0.68
4:A:1298:GLN:N	4:A:1298:GLN:OE1	2.27	0.68
4:B:273:ASP:OD1	4:B:274:TYR:N	2.26	0.68
4:A:784:GLU:OE1	4:A:784:GLU:N	2.28	0.67
4:A:826:LEU:HD21	4:B:827:SER:HA	1.75	0.67
4:A:1436:GLU:O	4:A:1436:GLU:OE1	2.12	0.67
3:G:36:4HH:HJ2	3:G:36:4HH:CB	2.25	0.66
3:G:46:LEU:HD21	3:G:72:ILE:HD11	1.78	0.66
2:F:167:MET:HE2	2:F:167:MET:HA	1.79	0.65
4:B:1332:THR:O	4:B:1336:GLU:N	2.30	0.64
4:B:1141:MET:HE3	4:B:1141:MET:HA	1.80	0.64
4:A:1457:GLU:OE1	4:A:1457:GLU:N	2.28	0.62
3:G:36:4HH:ON	3:G:40:VAL:CG2	2.48	0.62
4:A:231:ALA:HB2	4:B:665:GLN:CB	2.30	0.62
4:B:1322:GLN:O	4:B:1322:GLN:CD	2.43	0.61
1:C:314:THR:HA	2:E:93:MET:HE2	1.81	0.60
4:B:254:SER:O	4:B:258:LEU:HD22	2.01	0.60
3:G:36:4HH:HS3	4:A:289:LEU:HD22	1.83	0.60
3:I:24:ASN:O	3:I:66:GLN:N	2.35	0.59
4:B:788:GLU:OE1	4:B:789:ALA:N	2.35	0.59
2:E:10:MET:SD	2:F:18:LEU:HD11	2.43	0.59
4:B:1142:GLU:OE1	4:B:1142:GLU:N	2.36	0.59
3:I:48:GLU:CD	4:B:1107:ARG:HE	2.13	0.57
2:F:148:LYS:HD3	2:F:148:LYS:N	2.20	0.57
4:B:674:MET:HE3	4:B:674:MET:HA	1.85	0.56
4:B:1441:GLU:OE1	4:B:1441:GLU:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:273:ASP:OD1	4:B:273:ASP:C	2.49	0.56
1:C:127:MET:HE2	1:D:159:PRO:HA	1.87	0.55
4:B:822:VAL:HA	4:B:826:LEU:HD23	1.88	0.55
4:A:231:ALA:HB2	4:B:665:GLN:HB2	1.89	0.55
2:F:137:VAL:HG23	2:F:138:ASN:H	1.72	0.55
3:G:36:4HH:HJ3	3:G:37:LEU:N	2.22	0.54
1:C:159:PRO:HA	1:D:127:MET:HE2	1.90	0.54
1:C:328:ASP:OD1	1:C:328:ASP:O	2.25	0.54
4:A:1420:PHE:HA	4:A:1423:CYS:SG	2.48	0.54
4:B:1240:VAL:HG12	4:B:1244:ILE:HD13	1.89	0.54
4:B:1258:LEU:HD21	4:B:1380:MET:HG2	1.90	0.54
4:B:1423:CYS:SG	4:B:1430:LEU:HD11	2.48	0.53
4:A:122:MET:HE1	4:A:177:GLN:HB3	1.90	0.53
1:D:79:ASN:CG	2:E:142:SER:HB3	2.33	0.53
4:B:799:GLU:C	4:B:799:GLU:OE1	2.51	0.53
4:B:1299:ASP:OD1	4:B:1300:LEU:N	2.42	0.53
4:A:65:GLU:O	4:A:65:GLU:HG3	2.08	0.53
4:A:1126:ASP:O	4:A:1127:ASN:OD1	2.27	0.53
4:A:1281:GLU:O	4:A:1285:ILE:HD12	2.08	0.53
2:E:7:GLU:OE1	2:E:7:GLU:N	2.38	0.52
4:A:236:GLU:OE2	4:A:1307:THR:HG21	2.08	0.52
4:A:828:VAL:HG12	4:A:828:VAL:O	2.08	0.52
2:E:124:LEU:C	2:E:124:LEU:HD23	2.34	0.52
3:G:36:4HH:CS	4:A:289:LEU:HD22	2.39	0.52
4:B:665:GLN:C	4:B:665:GLN:OE1	2.53	0.52
4:B:1161:VAL:HG12	4:B:1161:VAL:O	2.09	0.51
3:G:62:ILE:HG22	3:G:62:ILE:O	2.11	0.51
4:B:1246:LYS:HD2	4:B:1246:LYS:O	2.11	0.51
4:B:1395:LYS:O	4:B:1395:LYS:HD3	2.10	0.51
4:B:232:PHE:CZ	4:B:1240:VAL:HG11	2.46	0.51
2:E:140:ARG:HD2	2:E:140:ARG:O	2.11	0.51
4:B:217:LEU:HG	4:B:221:LEU:HD12	1.91	0.51
4:B:91:ASP:C	4:B:91:ASP:OD1	2.54	0.51
4:A:764:ASP:N	4:A:764:ASP:OD1	2.40	0.50
4:B:1257:MET:SD	4:B:1257:MET:C	2.95	0.50
4:B:1319:LEU:HD12	4:B:1320:ASN:N	2.26	0.50
2:E:10:MET:HE3	2:E:14:LEU:HD22	1.92	0.50
4:A:1361:GLU:OE1	4:A:1361:GLU:HA	2.12	0.50
1:C:158:ALA:HB3	1:C:159:PRO:HD3	1.94	0.50
1:C:370:GLN:OE1	1:C:370:GLN:O	2.29	0.50
4:A:44:MET:HE3	4:A:1433:ALA:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1163:ASP:OD1	4:A:1164:ASN:N	2.45	0.50
4:B:828:VAL:HG12	4:B:828:VAL:O	2.10	0.50
4:B:732:GLU:H	4:B:732:GLU:CD	2.18	0.50
2:F:16:GLN:C	2:F:16:GLN:OE1	2.55	0.50
4:A:1237:SER:OG	4:A:1238:LYS:N	2.45	0.50
4:B:1196:GLU:N	4:B:1196:GLU:OE1	2.45	0.50
3:I:36:4HH:O	3:I:40:VAL:HG23	2.12	0.49
4:A:1376:SER:O	4:A:1379:VAL:HG22	2.12	0.49
4:B:63:THR:HG21	4:B:1407:GLU:HG3	1.92	0.49
4:A:1211:ALA:O	4:A:1215:MET:HG2	2.13	0.49
1:C:358:LEU:HG	1:C:362:ILE:HD11	1.94	0.49
1:D:75:ASN:HD21	2:E:146:LEU:HB2	1.78	0.48
2:E:41:LEU:HD21	4:B:244:ILE:HD13	1.94	0.48
3:I:48:GLU:OE1	4:B:1107:ARG:CZ	2.59	0.48
4:A:200:LEU:HD12	4:A:1378:LEU:HD22	1.94	0.48
4:A:732:GLU:OE1	4:A:732:GLU:N	2.46	0.48
4:B:782:ALA:O	4:B:785:ASN:N	2.47	0.48
4:B:1322:GLN:O	4:B:1322:GLN:OE1	2.32	0.48
4:B:1376:SER:O	4:B:1379:VAL:HG22	2.13	0.48
2:F:56:GLU:OE1	2:F:56:GLU:HA	2.13	0.48
1:C:356:ASP:C	1:C:356:ASP:OD1	2.55	0.48
2:F:180:ILE:HG23	2:F:184:VAL:HG21	1.96	0.48
2:F:134:MET:N	2:F:134:MET:HE2	2.29	0.48
3:G:2:THR:OG1	3:G:3:ILE:N	2.45	0.48
1:C:292:ASP:CG	1:C:295:ARG:HA	2.39	0.48
4:A:235:MET:HA	4:A:235:MET:HE2	1.94	0.47
4:B:774:GLU:N	4:B:774:GLU:OE1	2.48	0.47
1:C:391:LEU:HD13	1:C:428:TYR:CD2	2.50	0.47
1:C:391:LEU:HD13	1:C:428:TYR:CE2	2.49	0.47
3:G:11:ILE:HG23	3:G:12:GLY:N	2.29	0.47
4:B:1117:TRP:O	4:B:1121:MET:HG2	2.14	0.47
1:C:375:PRO:HA	1:C:440:TYR:OH	2.15	0.47
4:A:588:GLU:O	4:A:592:GLN:HG3	2.15	0.47
4:B:1275:LEU:HD12	4:B:1347:ASP:O	2.15	0.47
4:B:664:SER:OG	4:B:665:GLN:HG3	2.15	0.47
4:B:824:LYS:HG2	4:B:824:LYS:O	2.15	0.47
4:B:1161:VAL:O	4:B:1161:VAL:CG1	2.62	0.47
3:I:41:GLU:OE2	4:B:285:LEU:HD13	2.15	0.46
4:B:94:ASN:OD1	4:B:95:SER:N	2.47	0.46
2:F:25:GLU:CD	2:F:25:GLU:H	2.23	0.46
2:F:39:ASP:OD1	2:F:39:ASP:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:57:GLU:OE1	3:G:57:GLU:N	2.45	0.46
4:A:8:ARG:HH21	4:A:8:ARG:HG3	1.80	0.46
2:E:49:ASP:OD2	4:B:1320:ASN:ND2	2.49	0.46
3:G:28:PHE:CE1	3:G:65:VAL:HG22	2.51	0.46
4:B:542:PHE:CD2	4:B:876:LEU:HD21	2.51	0.46
3:G:36:4HH:ON	3:G:40:VAL:HG23	2.14	0.46
4:A:12:LEU:HD21	4:A:46:ALA:HB2	1.97	0.46
4:A:275:MET:HE1	4:A:1134:HIS:ND1	2.31	0.46
3:G:36:4HH:OM	3:G:37:LEU:HA	2.17	0.45
4:A:62:ASN:OD1	4:A:63:THR:N	2.48	0.45
4:A:1275:LEU:HD23	4:A:1380:MET:HE2	1.98	0.45
4:B:782:ALA:O	4:B:785:ASN:CB	2.65	0.45
4:A:765:ARG:HH11	4:B:748:VAL:HG23	1.81	0.45
2:E:5:HIS:CD2	2:E:7:GLU:OE1	2.69	0.45
2:F:121:TYR:CZ	2:F:125:ILE:HD11	2.52	0.45
1:D:158:ALA:HB3	1:D:159:PRO:HD3	1.97	0.45
4:A:349:LYS:HE3	4:A:353:TYR:CZ	2.51	0.45
4:A:589:GLN:O	4:A:593:LYS:N	2.40	0.45
4:A:1121:MET:HA	4:A:1124:VAL:HG12	1.99	0.45
4:B:679:GLU:OE1	4:B:679:GLU:HA	2.17	0.45
4:A:1285:ILE:HD12	4:A:1285:ILE:H	1.81	0.45
2:F:190:ASP:C	2:F:190:ASP:OD1	2.60	0.45
4:B:784:GLU:HA	4:B:787:LEU:HG	1.98	0.45
4:A:1127:ASN:OD1	4:A:1127:ASN:C	2.60	0.45
4:A:1213:GLU:OE1	4:B:813:ARG:NE	2.50	0.45
4:B:691:ASP:OD1	4:B:780:ARG:HB3	2.17	0.45
4:B:611:LEU:C	4:B:611:LEU:HD23	2.42	0.45
2:F:137:VAL:HG23	2:F:138:ASN:N	2.31	0.44
4:A:247:GLU:HA	4:A:247:GLU:OE1	2.17	0.44
4:B:839:ARG:HG2	4:B:839:ARG:HH21	1.82	0.44
1:C:355:ASN:OD1	1:C:355:ASN:N	2.48	0.44
4:A:275:MET:HE1	4:A:1134:HIS:CE1	2.52	0.44
4:B:632:MET:HE1	4:B:818:PHE:HB3	2.00	0.44
1:C:426:ASN:OD1	1:C:430:ALA:HB3	2.16	0.44
4:B:1104:TYR:CE1	4:B:1107:ARG:NH1	2.86	0.44
1:C:326:MET:HE3	2:F:186:ARG:HG2	2.00	0.44
4:B:1375:MET:HG2	4:B:1419:LEU:HD11	1.98	0.44
1:C:399:ARG:O	1:C:403:ASP:OD2	2.36	0.44
3:I:64:THR:HG22	3:I:65:VAL:N	2.33	0.43
4:A:640:ARG:O	4:A:643:THR:HG22	2.17	0.43
4:A:1401:ARG:HB3	4:A:1428:MET:HE2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:89:THR:C	4:B:90:LEU:HD12	2.43	0.43
4:B:215:ARG:HG2	4:B:1325:MET:HE2	2.00	0.43
1:C:358:LEU:HA	1:C:361:MET:SD	2.59	0.43
4:A:1274:ARG:HG3	4:A:1357:TRP:CZ3	2.53	0.43
2:F:108:ARG:NH1	4:A:1285:ILE:HD11	2.34	0.43
4:A:152:GLU:OE1	4:A:152:GLU:N	2.51	0.43
4:A:1387:GLU:C	4:A:1387:GLU:OE1	2.61	0.43
4:B:1436:GLU:O	4:B:1438:ILE:HG23	2.19	0.43
2:E:180:ILE:HG22	2:E:181:THR:N	2.33	0.43
4:A:782:ALA:C	4:A:783:ARG:HD3	2.43	0.43
4:B:605:LEU:O	4:B:609:ASP:OD2	2.37	0.43
4:B:750:ASN:HB3	4:B:761:LYS:HB3	2.00	0.43
4:B:1213:GLU:H	4:B:1213:GLU:CD	2.26	0.43
4:A:1129:VAL:O	4:A:1130:GLU:C	2.61	0.43
1:C:120:PHE:CZ	1:C:218:LEU:HD12	2.54	0.43
2:E:127:LEU:C	2:E:127:LEU:HD23	2.44	0.43
4:A:51:LEU:O	4:A:52:ILE:HD13	2.18	0.43
4:B:594:ILE:HD12	4:B:845:HIS:CE1	2.54	0.43
4:B:184:ILE:HG23	4:B:185:PRO:HD2	2.00	0.43
4:B:745:ASP:OD1	4:B:745:ASP:N	2.51	0.43
4:B:782:ALA:O	4:B:785:ASN:HB3	2.18	0.42
2:F:25:GLU:O	2:F:29:GLN:HG3	2.19	0.42
3:G:36:4HH:CT	4:A:292:ARG:HD3	2.49	0.42
4:A:1373:THR:O	4:A:1377:ILE:HG12	2.19	0.42
4:B:105:ARG:C	4:B:105:ARG:HD2	2.44	0.42
2:F:167:MET:HE1	2:F:183:ALA:HB1	2.01	0.42
1:C:42:ARG:HH12	1:C:51:GLU:CD	2.27	0.42
4:B:775:LEU:N	4:B:775:LEU:HD22	2.34	0.42
3:I:40:VAL:O	3:I:43:VAL:HG12	2.19	0.42
4:A:105:ARG:HD2	4:A:105:ARG:C	2.44	0.42
4:B:1246:LYS:HD2	4:B:1246:LYS:C	2.45	0.42
4:B:1247:THR:O	4:B:1251:GLU:OE1	2.37	0.42
4:A:782:ALA:O	4:A:783:ARG:HD3	2.19	0.42
4:A:1068:LEU:C	4:A:1068:LEU:HD23	2.45	0.42
4:A:1202:ILE:O	4:A:1202:ILE:HG22	2.20	0.42
4:A:1387:GLU:C	4:A:1387:GLU:CD	2.87	0.42
1:C:108:ILE:CD1	1:D:176:ARG:HD2	2.50	0.42
1:C:201:ILE:HD13	1:C:289:ILE:HD11	2.02	0.42
4:A:1199:ARG:O	4:A:1199:ARG:HG2	2.19	0.42
4:A:12:LEU:HD22	4:A:15:TRP:CG	2.55	0.41
4:B:1126:ASP:O	4:B:1127:ASN:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1411:LEU:HB2	4:B:1416:ILE:HD11	2.02	0.41
3:G:64:THR:HG23	3:G:67:ALA:H	1.85	0.41
4:B:1227:THR:O	4:B:1230:GLU:HG3	2.21	0.41
4:A:594:ILE:HD12	4:A:845:HIS:CE1	2.55	0.41
4:A:1235:ILE:HG21	4:B:675:ILE:HD13	2.01	0.41
4:B:288:ALA:HB2	4:B:1106:ILE:HG22	2.03	0.41
1:C:4:TYR:CD1	1:D:115:ILE:HG22	2.56	0.41
4:A:767:TRP:CE3	4:B:717:LEU:HD13	2.55	0.41
4:B:1240:VAL:CG1	4:B:1244:ILE:HD13	2.50	0.41
4:A:12:LEU:HD21	4:A:46:ALA:CB	2.50	0.41
4:A:45:ALA:HB1	4:A:60:PHE:CE2	2.55	0.41
4:A:281:ARG:C	4:A:281:ARG:HD2	2.46	0.41
4:A:788:GLU:O	4:A:792:LEU:HD13	2.21	0.41
4:B:606:ALA:HA	4:B:609:ASP:OD2	2.20	0.41
1:C:357:GLN:O	1:C:361:MET:SD	2.78	0.41
3:I:15:LEU:HD22	3:I:34:ALA:HB2	2.03	0.41
4:A:46:ALA:O	4:A:49:THR:HG22	2.20	0.41
4:B:141:GLY:O	4:B:143:ARG:NH1	2.54	0.41
4:B:1142:GLU:H	4:B:1142:GLU:CD	2.28	0.41
4:B:695:ILE:N	4:B:695:ILE:HD12	2.35	0.41
2:E:41:LEU:HD21	4:B:244:ILE:CD1	2.51	0.41
4:A:1380:MET:HE3	4:A:1380:MET:HB3	1.96	0.41
2:E:108:ARG:NH1	2:E:111:ASN:HD21	2.19	0.41
4:A:87:TYR:CD2	4:A:136:LEU:HD23	2.56	0.41
4:A:1118:CYS:SG	4:A:1122:ARG:NH1	2.92	0.41
4:A:1407:GLU:OE1	4:A:1407:GLU:HA	2.21	0.41
4:B:1335:GLU:HA	4:B:1338:LEU:HG	2.03	0.41
2:F:90:GLU:HA	2:F:90:GLU:OE1	2.20	0.40
3:I:29:VAL:HG13	3:I:30:GLU:N	2.36	0.40
4:A:782:ALA:O	4:A:783:ARG:C	2.63	0.40
4:B:1331:GLN:OE1	4:B:1331:GLN:N	2.54	0.40
4:B:1338:LEU:N	4:B:1338:LEU:HD23	2.36	0.40
2:F:182:GLU:OE1	2:F:182:GLU:N	2.48	0.40
3:G:36:4HH:CB	3:G:36:4HH:CJ	2.90	0.40
4:A:87:TYR:CG	4:A:136:LEU:HD23	2.56	0.40
4:B:1307:THR:OG1	4:B:1310:GLU:HG3	2.22	0.40
3:G:7:VAL:O	3:G:11:ILE:HG22	2.21	0.40
1:C:440:TYR:N	1:C:440:TYR:CD1	2.90	0.40
2:F:42:ASP:OD1	2:F:43:ASN:N	2.54	0.40
3:G:54:ILE:O	4:A:292:ARG:NH1	2.55	0.40
4:A:1387:GLU:OE1	4:A:1388:GLU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:148:LEU:HA	4:B:149:PRO:HD3	1.96	0.40
4:B:604:TRP:CH2	4:B:608:GLN:HG3	2.56	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	C	438/440 (100%)	425 (97%)	13 (3%)	0	100	100
1	D	288/440 (66%)	281 (98%)	7 (2%)	0	100	100
2	E	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
2	F	196/240 (82%)	191 (97%)	5 (3%)	0	100	100
3	G	69/78 (88%)	68 (99%)	1 (1%)	0	100	100
3	I	69/78 (88%)	66 (96%)	3 (4%)	0	100	100
4	A	1465/1482 (99%)	1423 (97%)	42 (3%)	0	100	100
4	B	1465/1482 (99%)	1414 (96%)	51 (4%)	0	100	100
All	All	4200/4480 (94%)	4074 (97%)	126 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	C	376/376 (100%)	367 (98%)	9 (2%)	43	63
1	D	247/376 (66%)	240 (97%)	7 (3%)	38	59
2	E	189/212 (89%)	185 (98%)	4 (2%)	47	65
2	F	177/212 (84%)	175 (99%)	2 (1%)	65	74
3	G	62/66 (94%)	62 (100%)	0	100	100
3	I	62/66 (94%)	62 (100%)	0	100	100
4	A	1269/1281 (99%)	1268 (100%)	1 (0%)	88	88
4	B	1269/1281 (99%)	1267 (100%)	2 (0%)	87	85
All	All	3651/3870 (94%)	3626 (99%)	25 (1%)	73	79

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2	SER
1	C	11	LEU
1	C	83	ARG
1	C	92	SER
1	C	94	LEU
1	C	132	VAL
1	C	209	SER
1	C	287	THR
1	C	355	ASN
1	D	2	SER
1	D	92	SER
1	D	94	LEU
1	D	132	VAL
1	D	173	MET
1	D	209	SER
1	D	287	THR
2	E	123	GLU
2	E	162	LEU
2	E	169	TYR
2	E	181	THR
2	F	25	GLU
2	F	152	GLN
4	A	221	LEU
4	B	1127	ASN
4	B	1213	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53)

such sidechains are listed below:

Mol	Chain	Res	Type
1	C	88	ASN
1	C	128	GLN
1	C	198	GLN
1	C	435	HIS
1	D	75	ASN
1	D	128	GLN
1	D	181	GLN
1	D	269	GLN
2	E	8	GLN
2	E	111	ASN
2	E	201	GLN
4	A	306	GLN
4	A	331	GLN
4	A	378	GLN
4	A	404	GLN
4	A	409	GLN
4	A	472	HIS
4	A	473	ASN
4	A	508	GLN
4	A	510	HIS
4	A	516	GLN
4	A	534	ASN
4	A	652	GLN
4	A	865	GLN
4	A	882	GLN
4	A	930	GLN
4	A	955	GLN
4	A	1032	GLN
4	A	1077	GLN
4	A	1105	GLN
4	A	1109	GLN
4	A	1242	ASN
4	B	62	ASN
4	B	78	HIS
4	B	98	GLN
4	B	124	GLN
4	B	175	HIS
4	B	306	GLN
4	B	330	HIS
4	B	398	GLN
4	B	418	GLN
4	B	473	ASN

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Mol	Chain	Res	Type
4	B	546	GLN
4	B	559	GLN
4	B	566	GLN
4	B	766	GLN
4	B	986	ASN
4	B	1006	GLN
4	B	1013	GLN
4	B	1091	ASN
4	B	1166	HIS
4	B	1342	ASN
4	B	1437	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	4HH	I	36	3	22,26,27	0.47	0	27,35,37	1.75	3 (11%)
3	4HH	G	36	3	22,26,27	0.45	0	27,35,37	3.17	4 (14%)

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	4HH	I	36	3	-	7/33/35/37	-
3	4HH	G	36	3	-	5/33/35/37	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	36	4HH	O1P-P-OG	11.98	161.87	107.57
3	G	36	4HH	OG-P-O2P	-8.70	74.45	108.94
3	G	36	4HH	P-OG-CB	6.32	157.55	121.35
3	I	36	4HH	P-OG-CB	-5.46	90.07	121.35
3	I	36	4HH	O1P-P-OG	4.79	129.28	107.57
3	I	36	4HH	OG-CB-CA	4.47	112.49	108.14
3	G	36	4HH	OG-CB-CA	2.81	110.88	108.14

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	36	4HH	CB-OG-P-O3P
3	I	36	4HH	N-CA-CB-OG
3	I	36	4HH	CB-OG-P-O1P
3	I	36	4HH	CO-CP-CQ-NR
3	G	36	4HH	ON-CL3-CM-OM
3	I	36	4HH	ON-CL3-CM-OM
3	I	36	4HH	CO-CP-CQ-OR
3	G	36	4HH	CJ-O3P-P-OG
3	I	36	4HH	CB-OG-P-O2P
3	G	36	4HH	CT-CS-NR-CQ
3	G	36	4HH	NN-CL3-CM-OM
3	I	36	4HH	NN-CL3-CM-OM

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	36	4HH	1	0
3	G	36	4HH	14	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
6	ATP	A	1502	5	32,33,33	0.57	1 (3%)	48,52,52	0.75	2 (4%)
6	ATP	B	1502	5	32,33,33	0.57	1 (3%)	48,52,52	0.74	2 (4%)

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
6	ATP	A	1502	5	-	2/22/38/38	0/3/3/3
6	ATP	B	1502	5	-	2/22/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1502	ATP	PB-O3B	-2.34	1.57	1.59
6	B	1502	ATP	PB-O3B	-2.08	1.57	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1502	ATP	O2'-C2'-C3'	-2.33	104.33	111.82
6	B	1502	ATP	O2'-C2'-C3'	-2.21	104.72	111.82
6	B	1502	ATP	O3'-C3'-C2'	-2.17	104.86	111.82
6	A	1502	ATP	O3'-C3'-C2'	-2.07	105.19	111.82

There are no chirality outliers.

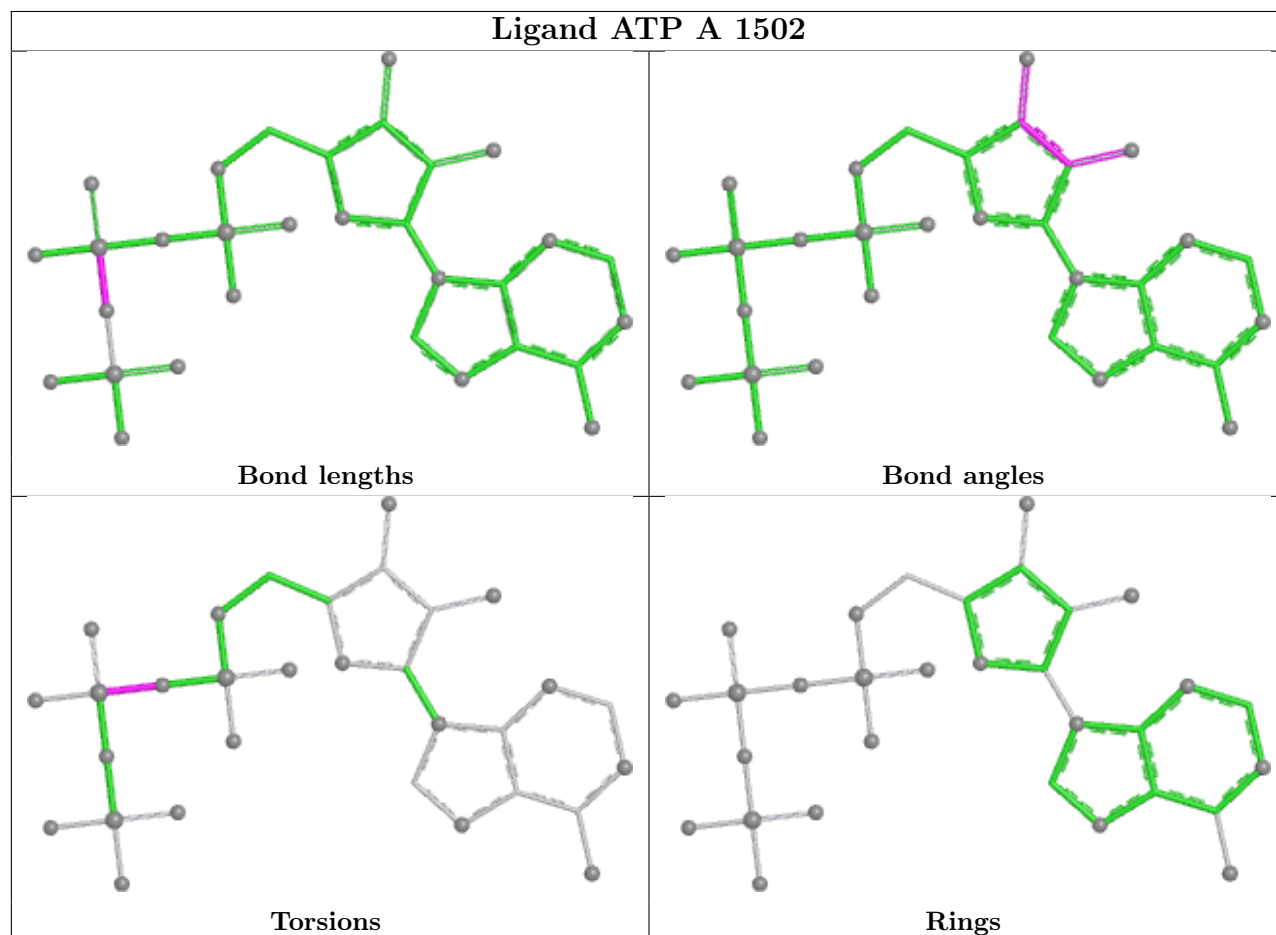
All (4) torsion outliers are listed below:

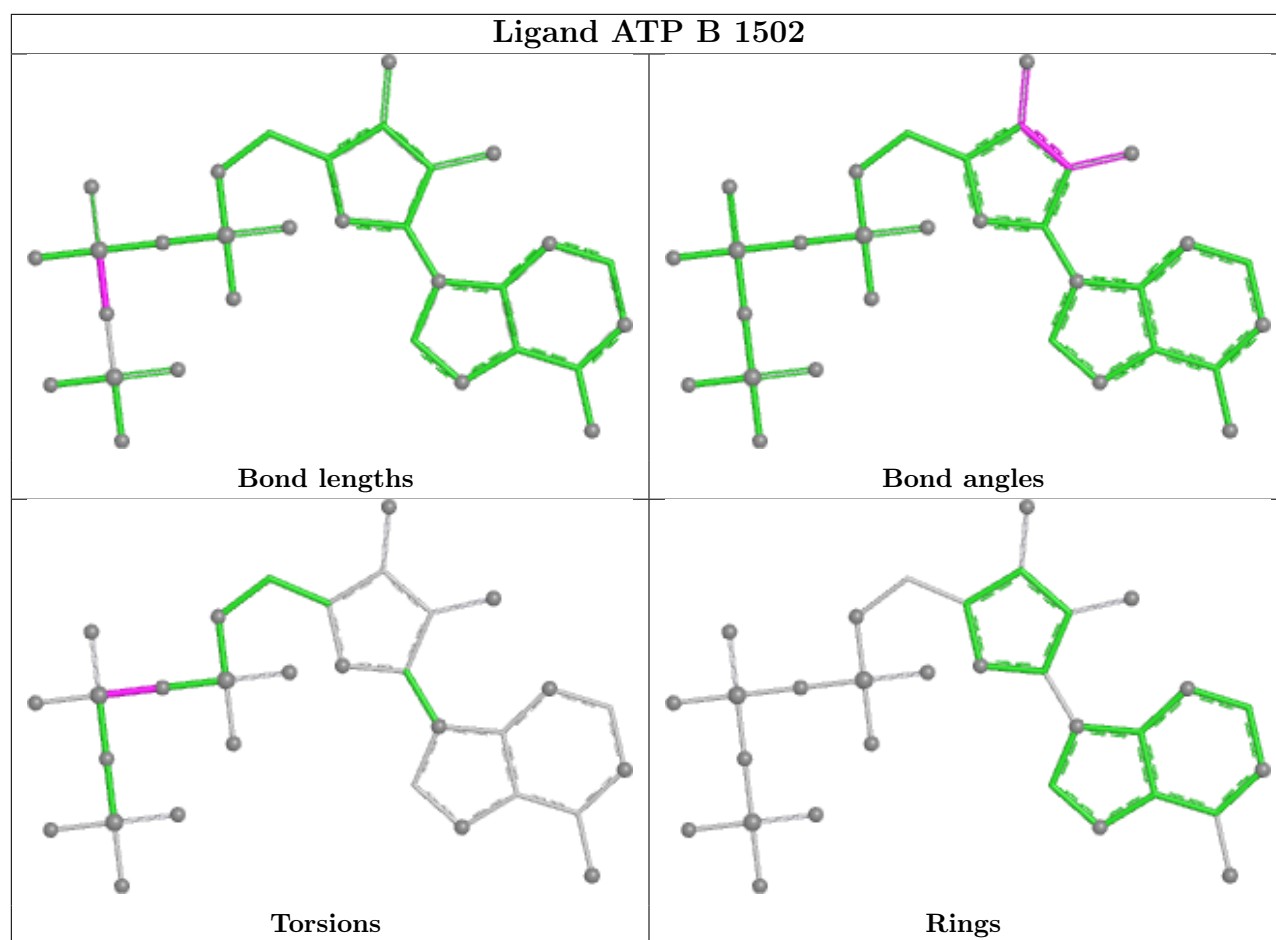
Mol	Chain	Res	Type	Atoms
6	A	1502	ATP	PA-O3A-PB-O2B
6	B	1502	ATP	PA-O3A-PB-O1B
6	B	1502	ATP	PA-O3A-PB-O2B
6	A	1502	ATP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	295:ARG	C	296:ILE	N	1.04

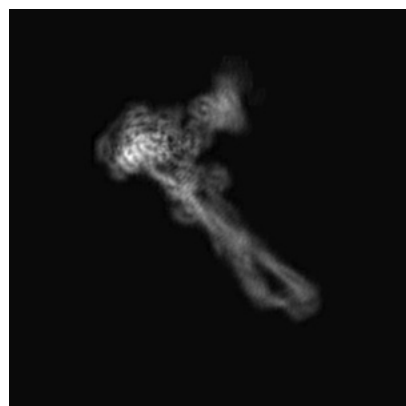
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51443. These allow visual inspection of the internal detail of the map and identification of artifacts.

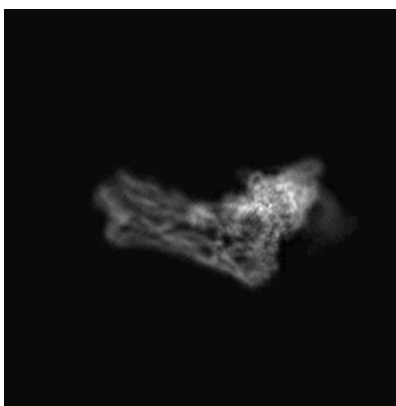
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

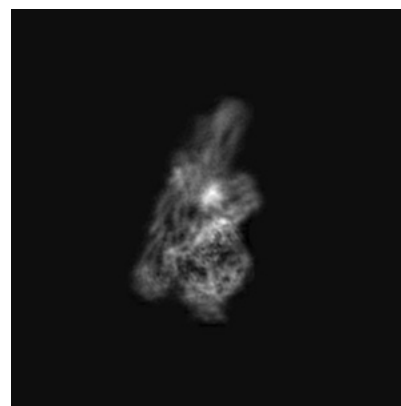
6.1.1 Primary map



X



Y

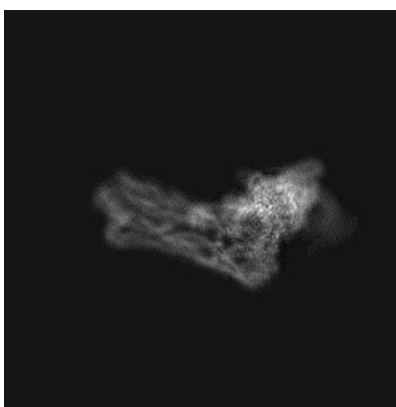


Z

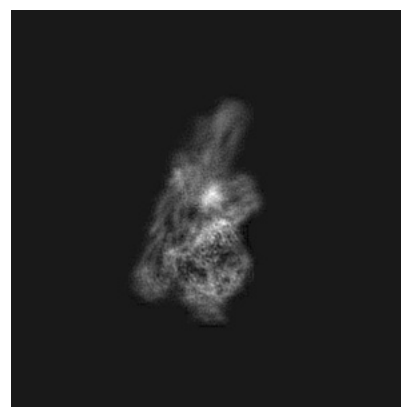
6.1.2 Raw map



X



Y

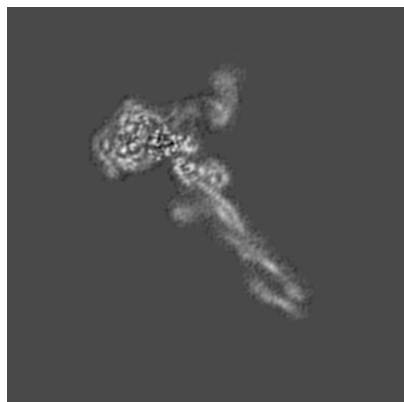


Z

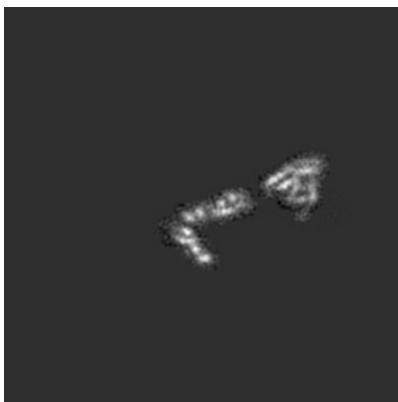
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

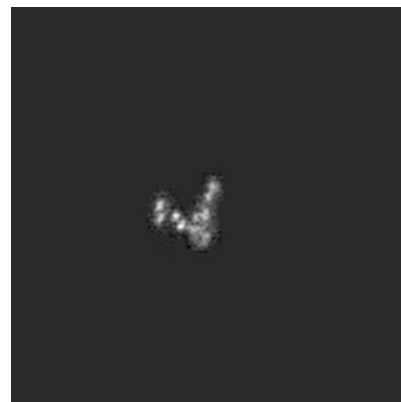
6.2.1 Primary map



X Index: 156

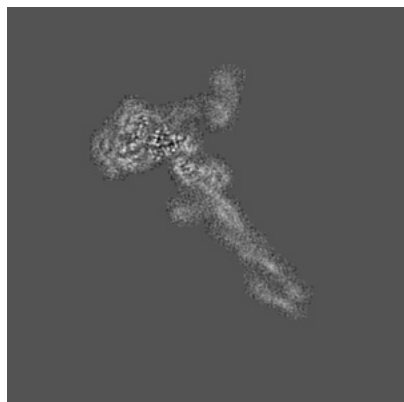


Y Index: 156

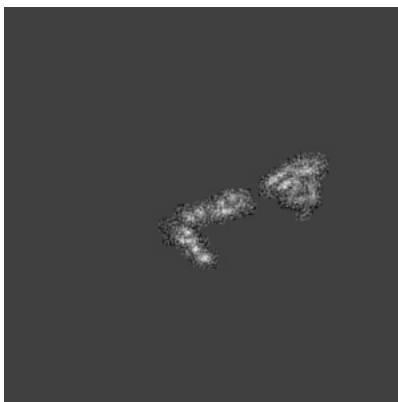


Z Index: 156

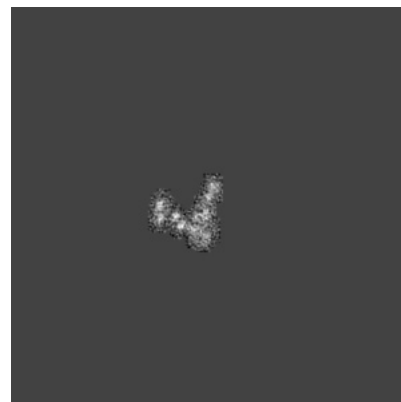
6.2.2 Raw map



X Index: 156



Y Index: 156

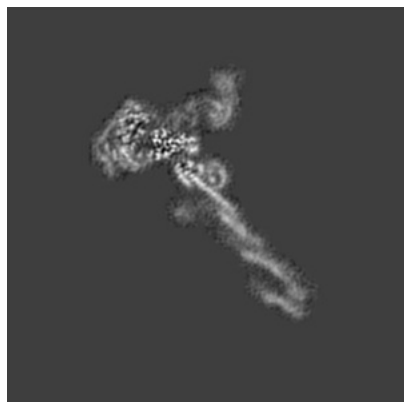


Z Index: 156

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

6.3 Largest variance slices [i](#)

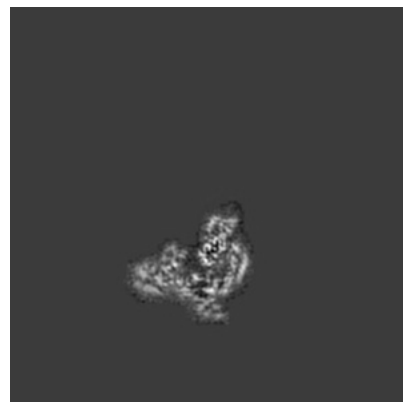
6.3.1 Primary map



X Index: 158

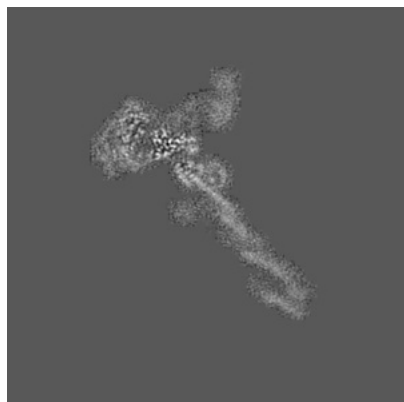


Y Index: 96



Z Index: 199

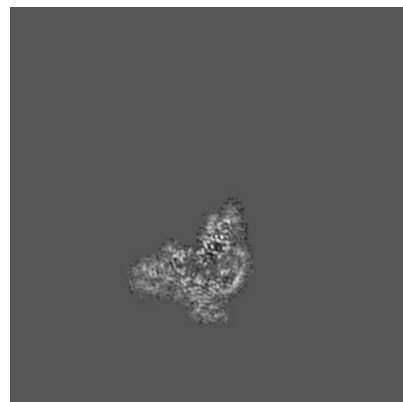
6.3.2 Raw map



X Index: 158



Y Index: 97

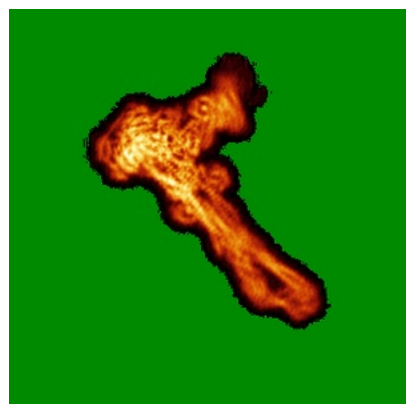


Z Index: 202

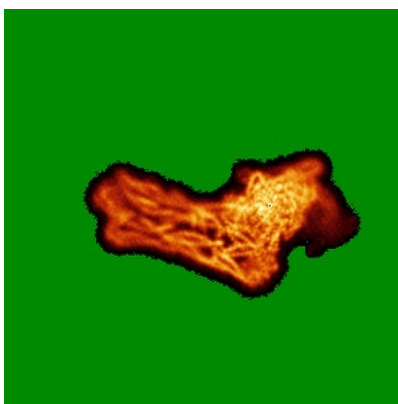
The images above show the largest variance slices of the map in three orthogonal directions.

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

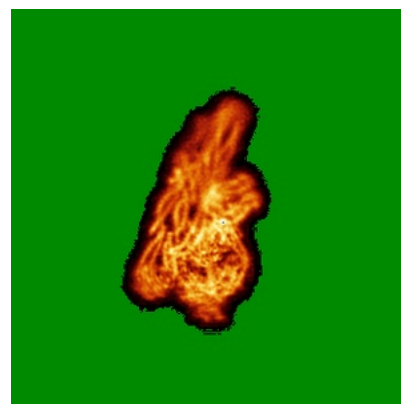
6.4.1 Primary map



X

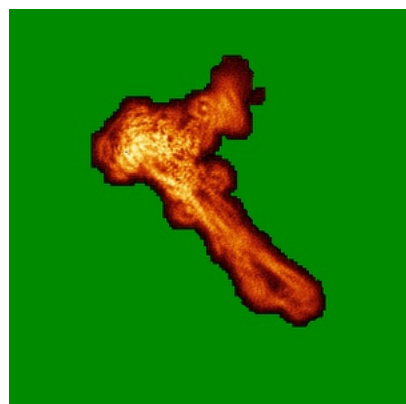


Y

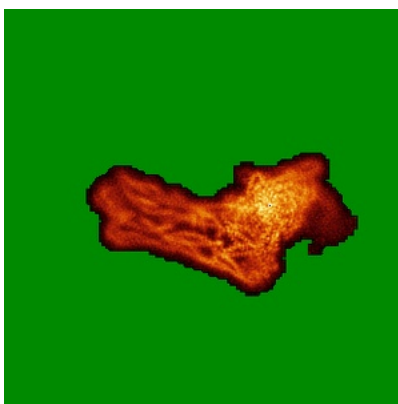


Z

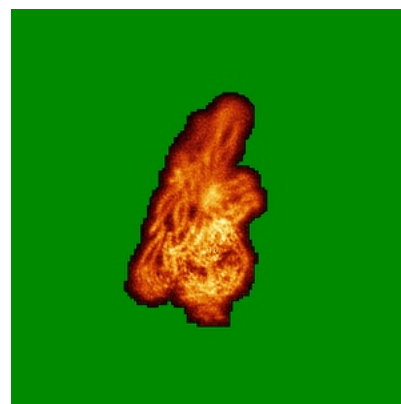
6.4.2 Raw map



X



Y

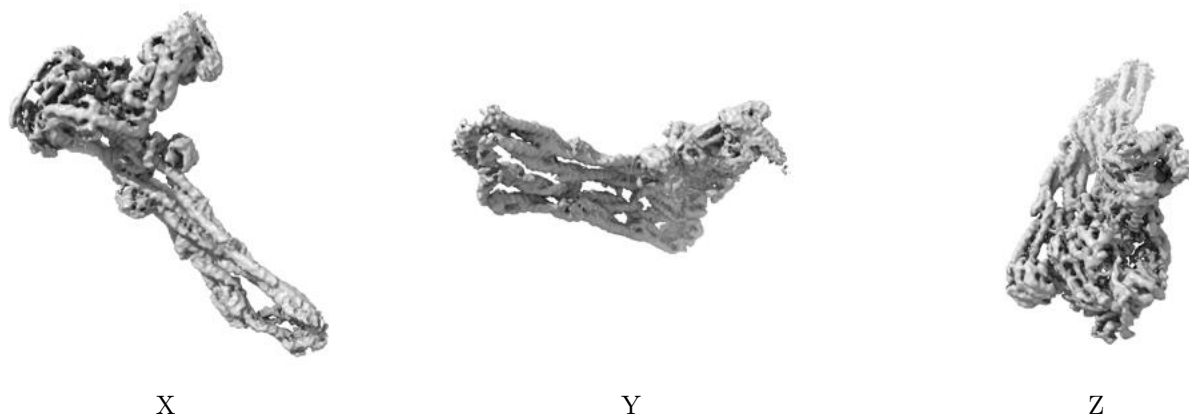


Z

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 0.012. 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.

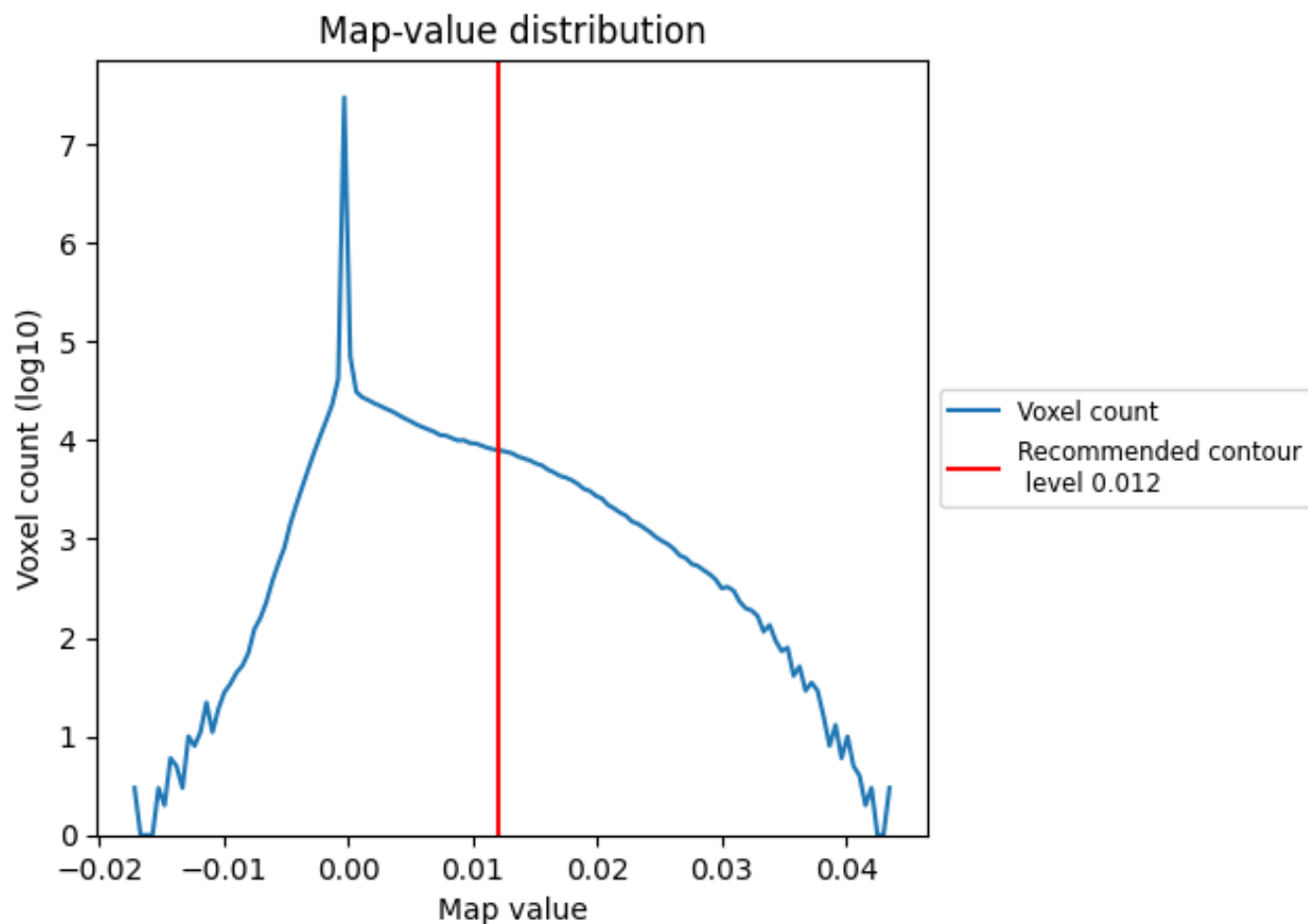
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

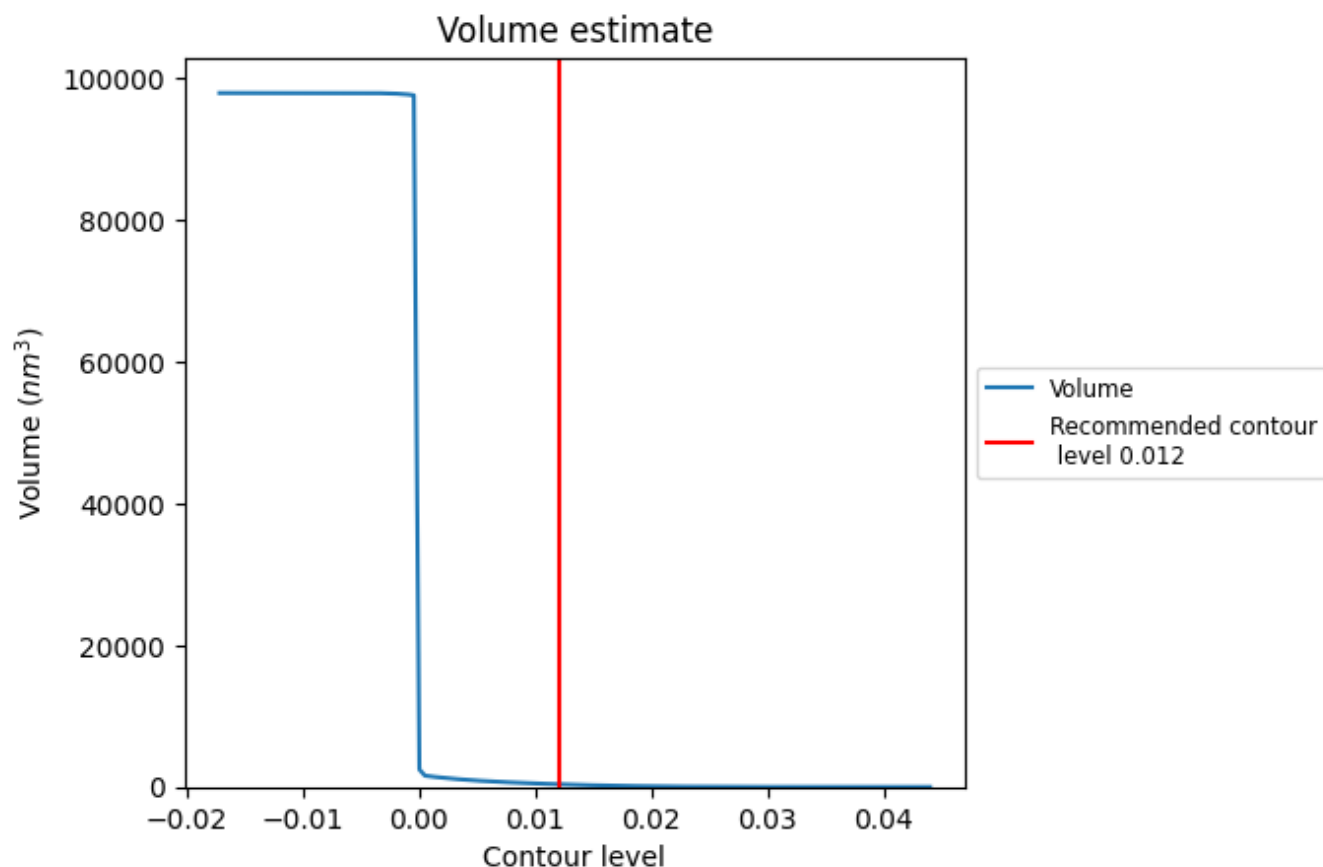
This section contains the results of statistical analysis of the map.

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.

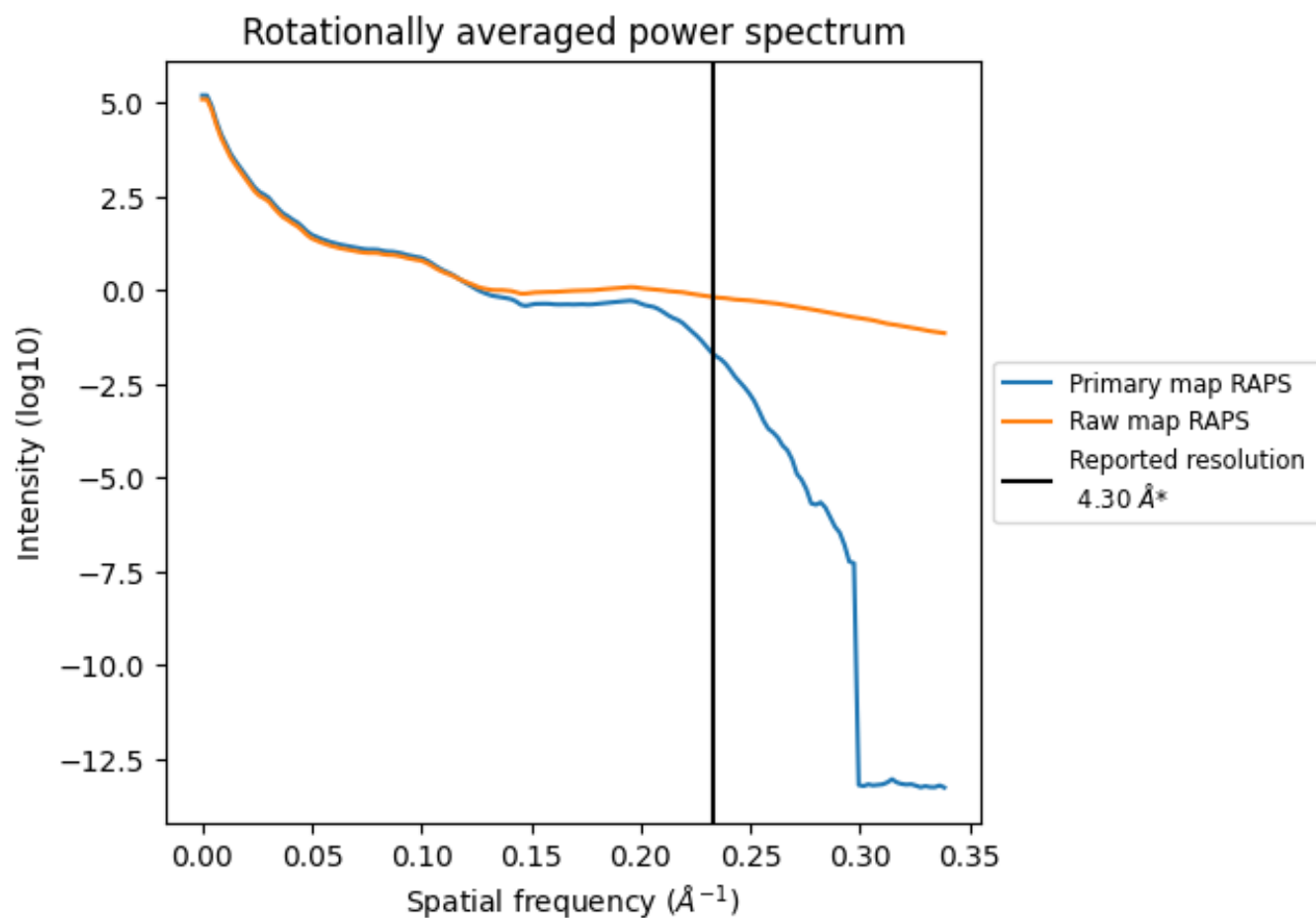
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 378 nm³; this corresponds to an approximate mass of 342 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 ⓘ

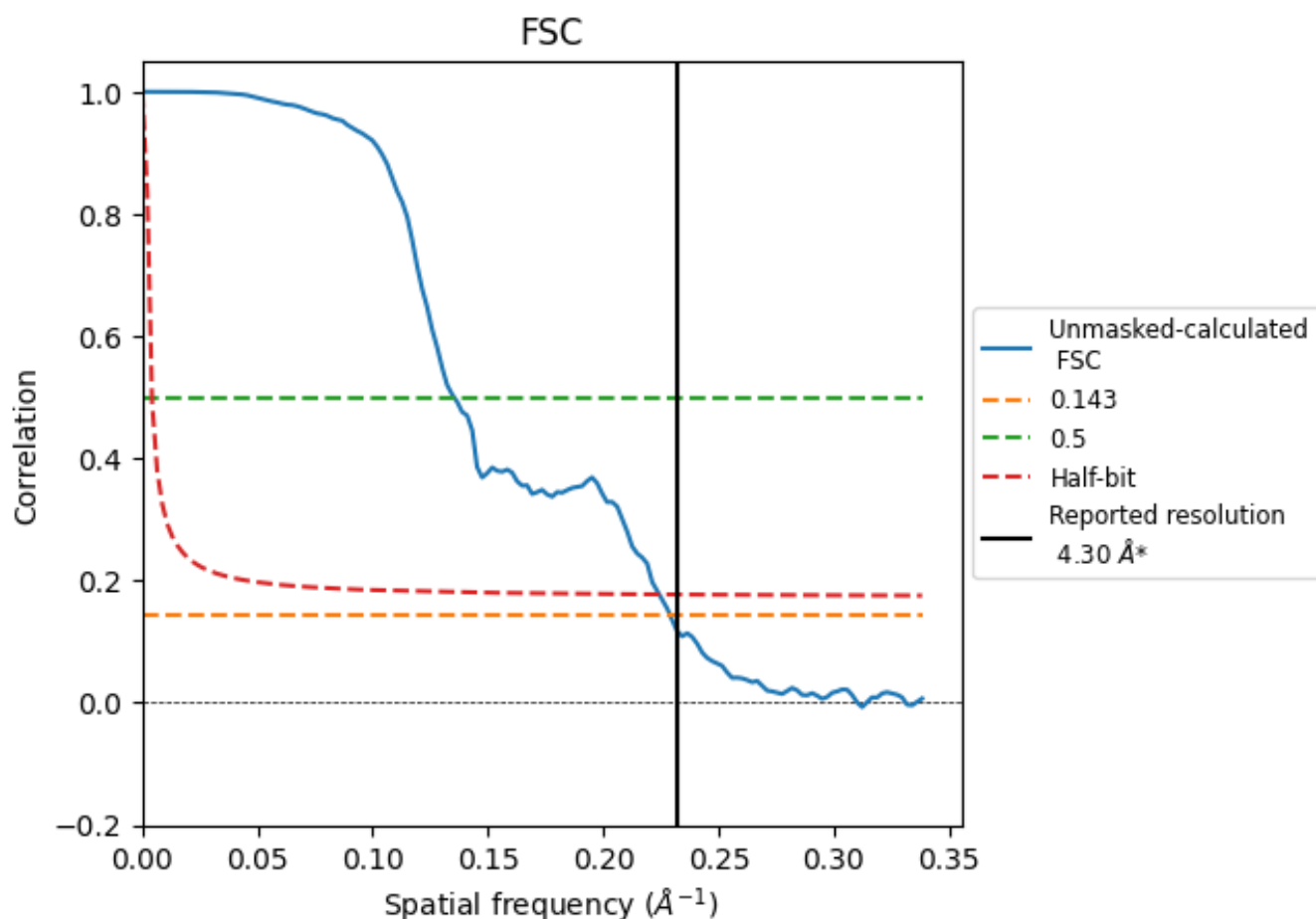


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 0.233 Å⁻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*	4.36	7.39	4.46

*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-51443 and PDB model 9GM7. Per-residue inclusion information can be found in section [3](#) on page [6](#).

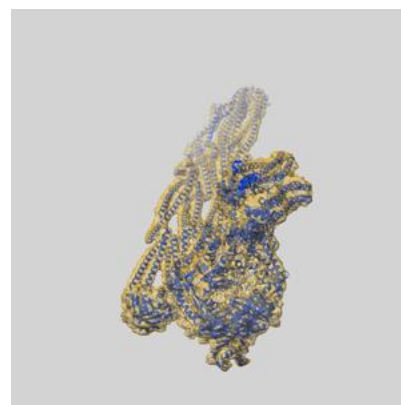
9.1 Map-model overlay [i](#)



X



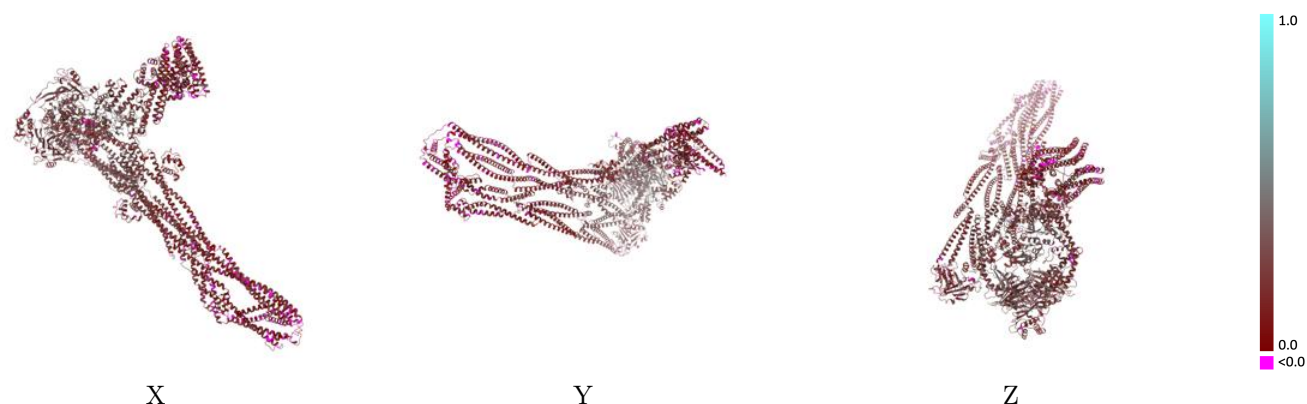
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 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](#)

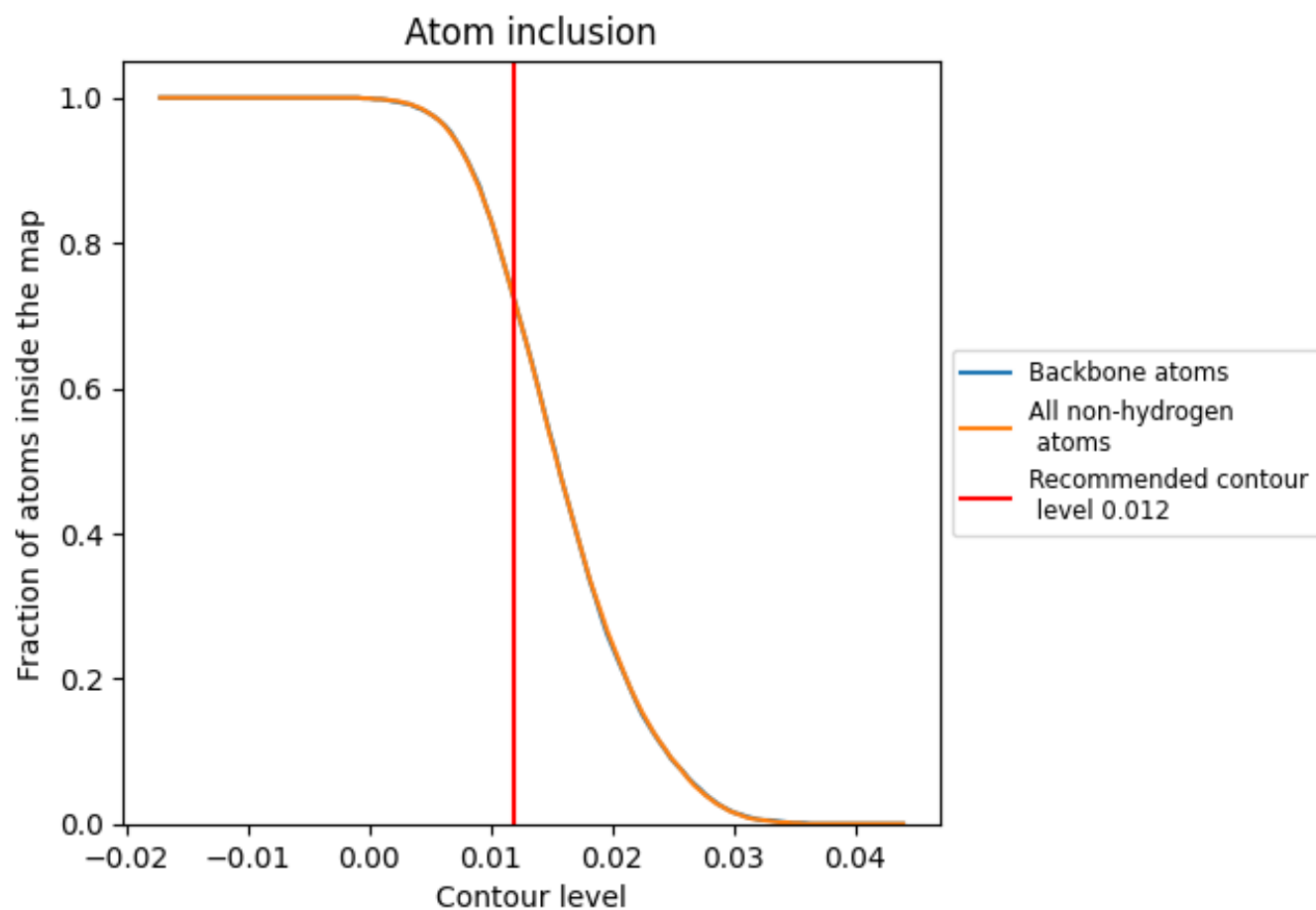


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 72% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7200	0.2210
A	0.7380	0.2220
B	0.7450	0.2190
C	0.6790	0.1900
D	0.6750	0.1470
E	0.7830	0.3280
F	0.7630	0.3060
G	0.6930	0.1900
I	0.7410	0.1730

1.0

0.0

<0.0