



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:18 PM UTC

PDB ID : 6SB0 / pdb_00006sb0
EMDB ID : EMD-10132
Title : cryo-EM structure of mTORC1 bound to PRAS40-fused active RagA/C GT-Pases
Authors : Anandapadamanaban, M.; Berndt, A.; Masson, G.R.; Perisic, O.; Williams, R.L.
Deposited on : 2019-07-18
Resolution : 5.50 Å (reported)
Based on initial models : 6BCX, 6S6A

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

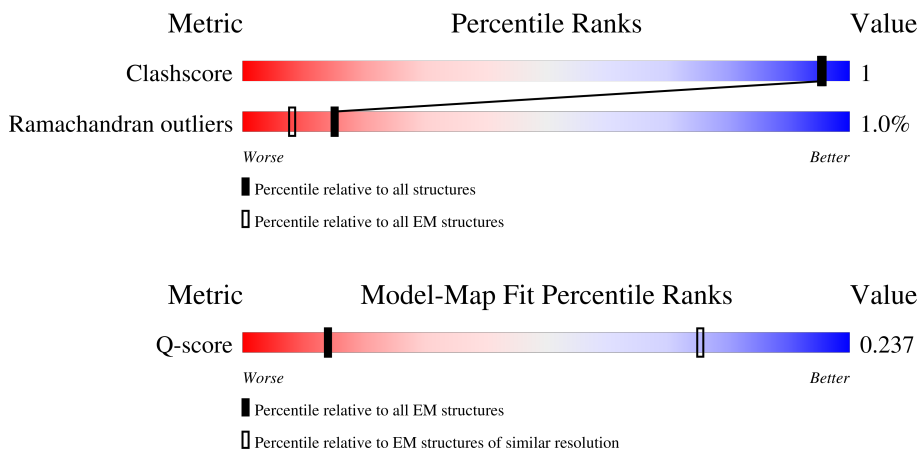
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 5.50 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	-
Q-score	-	25397	520 (5.00 - 6.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2549	 7% 81% 5% 15%
1	B	2549	 6% 80% 6% 15%
2	E	326	 93% . .
2	H	326	 93% . .

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Mol	Chain	Length	Quality of chain
3	C	313	88%7%5%
3	I	313	88%7%5%
4	D	399	63%5%32%
4	J	399	64%.32%
5	N	1335	75%.21%
5	Y	1335	74%.21%
6	O	256	11%.86%
6	T	256	11%.86%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 41284 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 mTOR,Serine/threonine-protein kinase mTOR,mTOR,Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	2178	Total	C	N	O	0	0
			10799	6443	2178	2178		
1	B	2178	Total	C	N	O	0	0
			10799	6443	2178	2178		

- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	317	Total	C	N	O	0	0
			1562	928	317	317		
2	H	317	Total	C	N	O	0	0
			1562	928	317	317		

- Molecule 3 is a protein called Ras-related GTP-binding protein A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	298	Total	C	N	O	0	0
			1483	887	298	298		
3	I	298	Total	C	N	O	0	0
			1482	886	298	298		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	66	LEU	GLN	engineered mutation	UNP Q7L523
I	66	LEU	GLN	engineered mutation	UNP Q7L523

- Molecule 4 is a protein called Ras-related GTP-binding protein C.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	272	Total	C	N	O	0	0
			1349	805	272	272		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	273	Total	C	N	O	0	0
			1354	808	273	273		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	90	ASN	THR	engineered mutation	UNP Q9HB90
J	90	ASN	THR	engineered mutation	UNP Q9HB90

- Molecule 5 is a protein called Regulatory-associated protein of mTOR.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	Y	1052	Total	C	N	O	0	0
			5214	3110	1052	1052		
5	N	1052	Total	C	N	O	0	0
			5214	3110	1052	1052		

- Molecule 6 is a protein called Proline-rich AKT1 substrate 1.

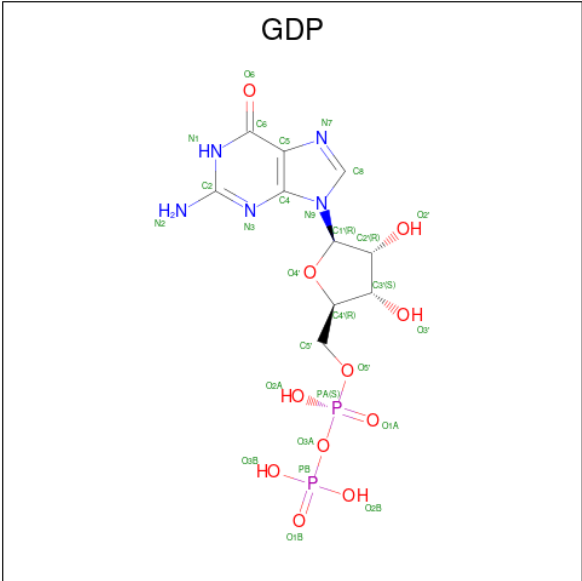
Mol	Chain	Residues	Atoms				AltConf	Trace
6	T	35	Total	C	N	O	0	0
			173	103	35	35		
6	O	35	Total	C	N	O	0	0
			173	103	35	35		

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	C	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	I	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂) (labeled as "Ligand of Interest" by depositor).

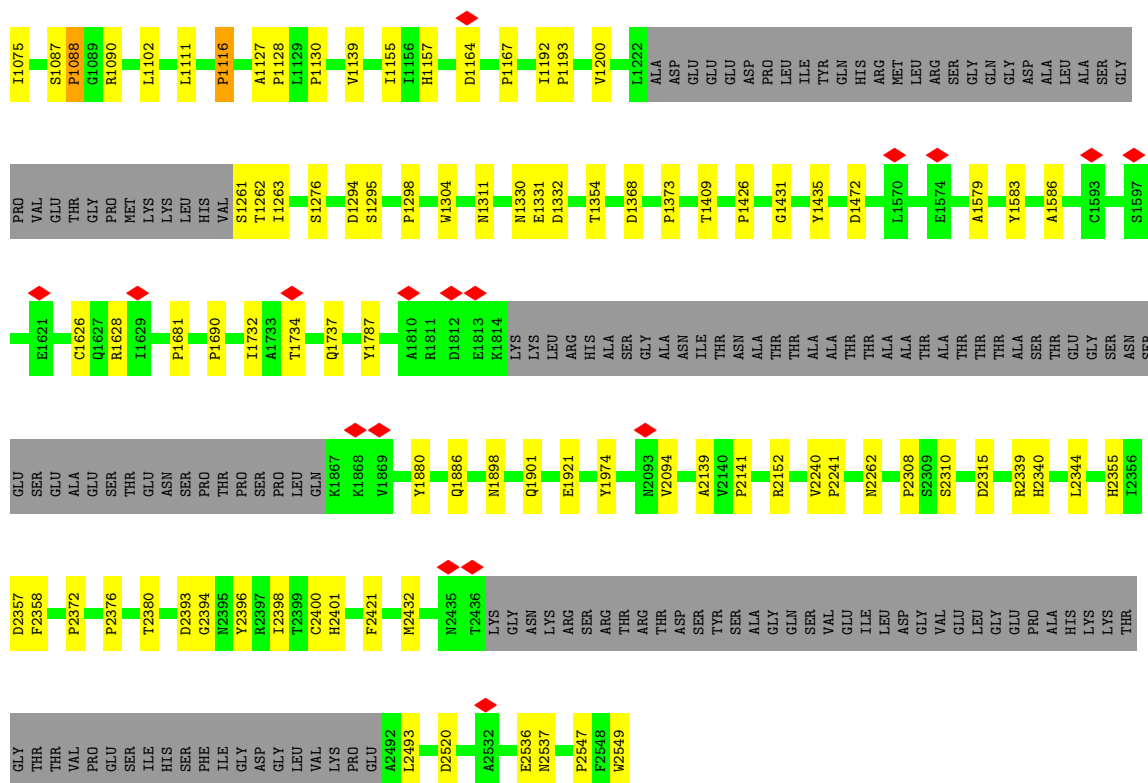


Mol	Chain	Residues	Atoms					AltConf
8	D	1	Total	C	N	O	P	0
			28	10	5	11	2	

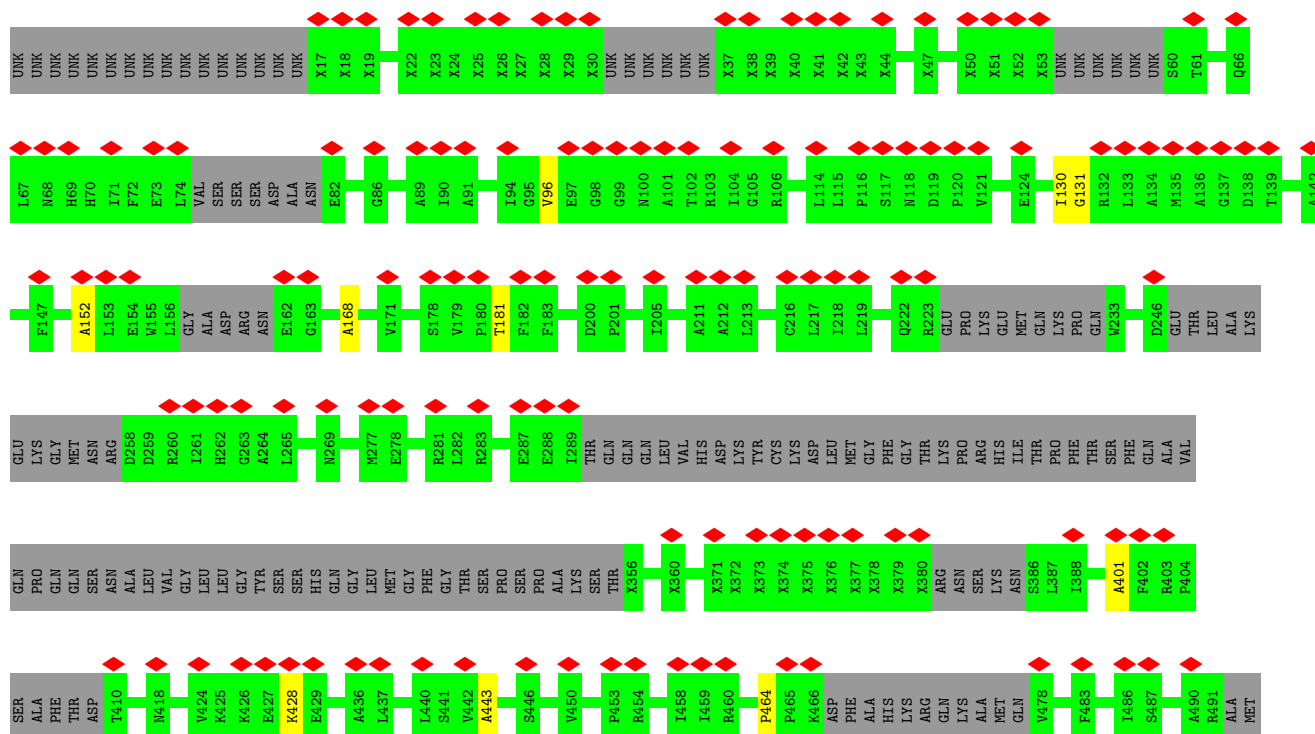
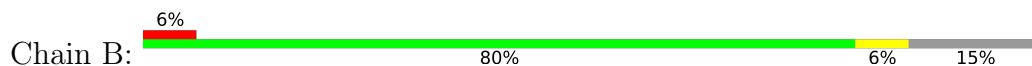
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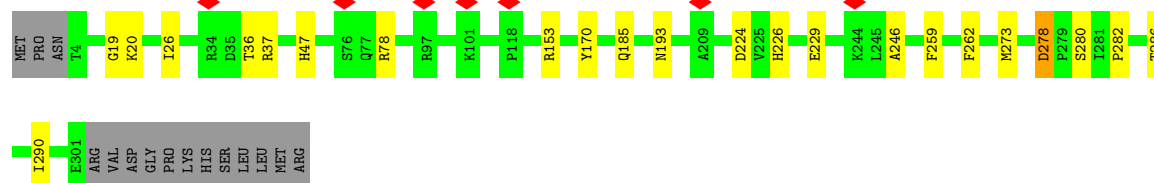
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
8	J	1	28	10	5	11	2	0



- Molecule 1: mTOR, Serine/threonine-protein kinase mTOR, mTOR, Serine/threonine-protein kinase mTOR

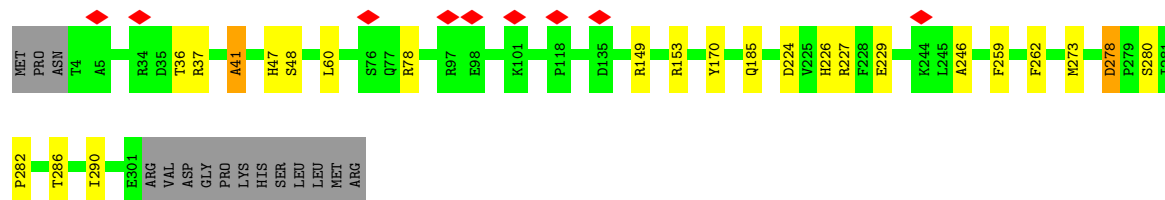


Chain C: 



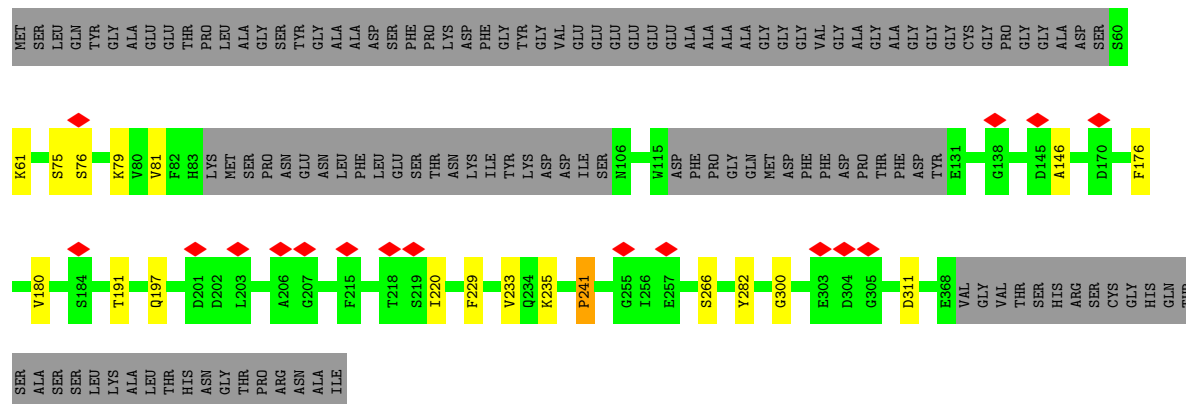
- Molecule 3: Ras-related GTP-binding protein A

Chain I: 



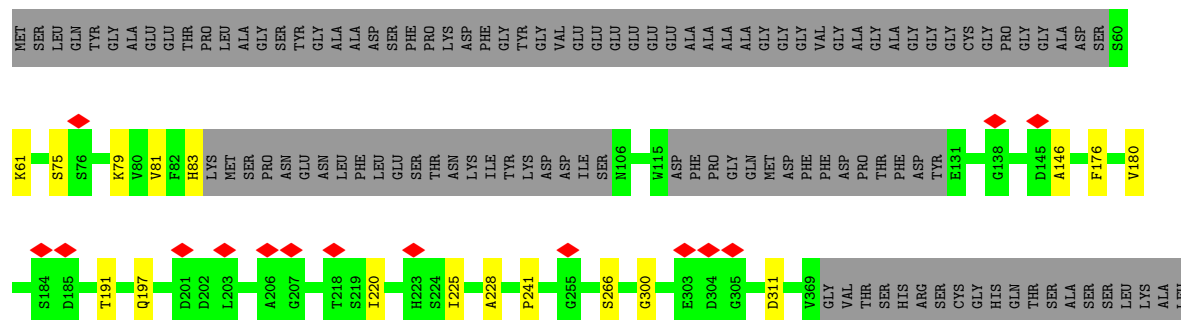
- Molecule 4: Ras-related GTP-binding protein C

Chain D: 

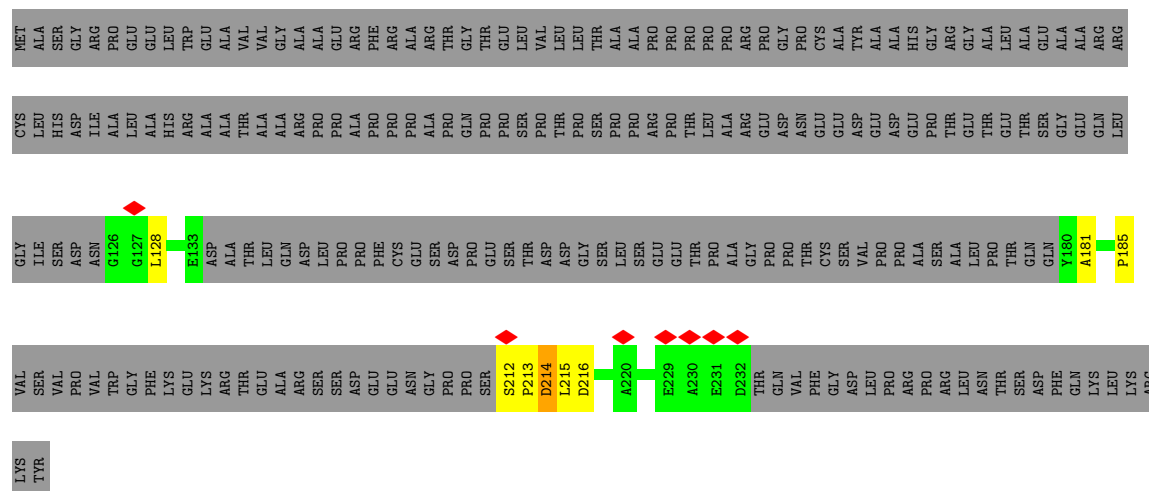


- Molecule 4: Ras-related GTP-binding protein C

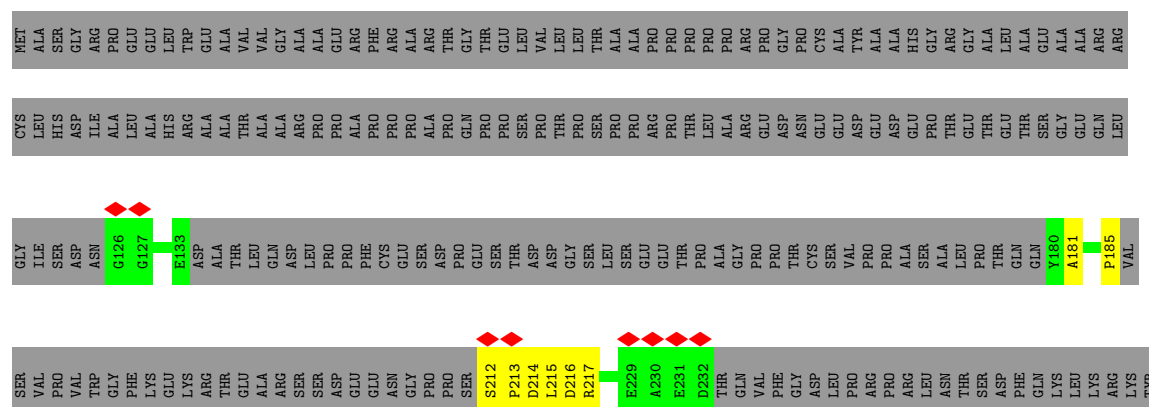
Chain J: 



- Molecule 6: Proline-rich AKT1 substrate 1



- Molecule 6: Proline-rich AKT1 substrate 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	90809	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.118	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	500.49997, 500.49997, 500.49997	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.43, 1.43, 1.43	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, GDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.88	4/10502 (0.0%)	1.63	118/14621 (0.8%)
1	B	0.92	2/10502 (0.0%)	1.72	154/14621 (1.1%)
2	E	0.86	0/1561	1.54	13/2170 (0.6%)
2	H	0.82	0/1561	1.49	11/2170 (0.5%)
3	C	0.91	0/1482	1.77	13/2069 (0.6%)
3	I	0.90	0/1481	1.76	16/2067 (0.8%)
4	D	0.98	0/1346	1.84	15/1873 (0.8%)
4	J	0.98	0/1351	1.82	9/1880 (0.5%)
5	N	0.88	1/5208 (0.0%)	1.57	57/7254 (0.8%)
5	Y	0.93	2/5208 (0.0%)	1.65	63/7254 (0.9%)
6	O	0.93	0/170	2.15	4/232 (1.7%)
6	T	0.92	0/170	2.05	3/232 (1.3%)
All	All	0.90	9/40542 (0.0%)	1.67	476/56443 (0.8%)

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	A	0	5
1	B	0	6
2	E	0	2
2	H	0	2
5	N	0	2
5	Y	0	3
All	All	0	20

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2549	TRP	C-O	7.30	1.38	1.23
1	A	2398	ILE	C-O	5.64	1.30	1.24
1	A	2549	TRP	C-O	5.57	1.34	1.23
5	Y	415	ALA	C-O	-5.40	1.17	1.24
1	A	951	SER	CA-CB	-5.40	1.45	1.53
1	A	1087	SER	CA-CB	-5.32	1.45	1.53
1	B	1403	GLU	C-O	-5.25	1.18	1.24
5	N	415	ALA	C-O	-5.21	1.18	1.24
5	Y	381	ALA	C-O	-5.12	1.18	1.24

All (476) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	434	PRO	N-CA-CB	-14.99	87.19	103.39
1	B	1681	PRO	N-CA-CB	13.83	116.78	103.51
1	B	1426	PRO	N-CA-CB	-13.34	89.24	103.25
1	A	1681	PRO	N-CA-CB	13.12	116.11	103.51
5	N	434	PRO	N-CA-CB	-11.40	91.44	103.52
1	A	2241	PRO	CB-CA-C	-11.13	96.40	110.98
5	Y	429	PRO	CB-CA-C	-11.12	97.35	110.92
1	B	2241	PRO	CB-CA-C	-11.01	96.53	110.95
6	O	217	ARG	N-CA-C	-10.95	102.14	114.62
1	B	1072	PRO	N-CA-CB	-10.68	92.03	103.25
1	B	2372	PRO	N-CA-CB	10.13	111.40	103.30
5	N	429	PRO	CB-CA-C	-10.03	98.68	110.92
1	B	2376	PRO	N-CA-CB	10.02	113.78	103.25
1	A	2372	PRO	N-CA-CB	9.92	111.24	103.30
5	Y	426	ASN	CB-CA-C	9.32	126.78	111.41
5	N	426	ASN	CB-CA-C	9.29	126.75	111.41
5	Y	407	PRO	N-CA-CB	-9.29	93.50	103.25
1	A	2376	PRO	N-CA-CB	9.28	113.00	103.25
1	A	1426	PRO	N-CA-CB	-9.17	93.62	103.25
5	Y	368	PRO	N-CA-CB	-8.98	93.82	103.25
1	B	1041	PHE	CB-CA-C	8.97	125.06	110.09
5	Y	430	PRO	CB-CA-C	8.96	123.13	111.21
1	A	2358	PHE	CB-CA-C	8.82	125.40	111.73
1	B	2358	PHE	CB-CA-C	8.77	125.32	111.73
1	A	1041	PHE	CB-CA-C	8.60	124.45	110.09
1	B	1130	PRO	N-CA-CB	-8.48	94.35	103.25
1	B	2310	SER	N-CA-CB	-8.47	99.32	110.59
1	A	464	PRO	N-CA-C	8.39	120.94	110.70
5	N	430	PRO	CB-CA-C	8.38	120.92	111.11
1	B	464	PRO	N-CA-C	8.27	120.78	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	1036	PRO	N-CA-CB	8.26	108.27	102.65
6	O	185	PRO	N-CA-CB	8.19	112.01	103.00
1	B	1128	PRO	CB-CA-C	-8.15	100.80	111.23
5	Y	363	THR	CB-CA-C	8.14	119.20	110.17
1	B	960	ARG	CB-CA-C	8.12	123.02	111.82
6	T	185	PRO	N-CA-CB	8.10	111.91	103.00
1	A	2547	PRO	N-CA-CB	8.08	111.00	103.41
1	B	2520	ASP	CA-C-O	-7.97	112.90	121.99
1	B	2380	THR	CA-C-O	-7.89	112.04	121.66
5	N	1036	PRO	N-CA-CB	7.88	108.01	102.65
5	Y	372	PRO	CB-CA-C	-7.85	98.61	111.56
5	N	1113	GLN	CA-C-N	7.83	128.51	120.60
5	N	1113	GLN	C-N-CA	7.83	128.51	120.60
1	A	1373	PRO	N-CA-CB	-7.79	96.80	102.25
5	Y	466	LEU	CA-C-N	7.76	131.01	120.54
5	Y	466	LEU	C-N-CA	7.76	131.01	120.54
5	Y	1113	GLN	CA-C-N	7.74	128.41	120.60
5	Y	1113	GLN	C-N-CA	7.74	128.41	120.60
1	B	1193	PRO	N-CA-CB	-7.70	94.76	103.15
5	Y	408	PHE	CB-CA-C	-7.70	98.69	110.92
5	Y	253	PRO	CB-CA-C	-7.68	100.99	111.21
1	B	2355	HIS	CB-CA-C	7.64	122.45	109.53
1	A	2520	ASP	CA-C-O	-7.59	113.33	121.99
1	B	2547	PRO	N-CA-CB	7.58	110.53	103.41
5	Y	464	VAL	O-C-N	7.54	129.18	121.87
1	B	1040	GLU	CB-CA-C	-7.42	99.18	110.90
1	A	1128	PRO	CB-CA-C	-7.41	101.74	111.23
5	N	368	PRO	N-CA-CB	-7.41	95.47	103.25
5	N	466	LEU	CA-C-N	7.41	130.53	120.38
5	N	466	LEU	C-N-CA	7.41	130.53	120.38
2	H	9	GLY	CA-C-N	7.39	131.90	120.82
2	H	9	GLY	C-N-CA	7.39	131.90	120.82
1	B	2396	TYR	N-CA-CB	7.37	120.67	109.91
5	Y	467	ALA	O-C-N	7.37	129.75	122.09
1	A	960	ARG	CB-CA-C	7.30	121.27	111.70
1	A	2380	THR	CA-C-O	-7.30	112.75	121.66
1	A	2393	ASP	CB-CA-C	7.29	123.34	110.37
1	A	1072	PRO	N-CA-CB	-7.27	95.61	103.25
1	B	1088	PRO	CB-CA-C	-7.26	99.58	111.56
2	E	195	TYR	CB-CA-C	7.25	121.70	110.67
5	Y	461	PRO	CB-CA-C	-7.24	100.92	112.21
5	N	372	PRO	CB-CA-C	-7.23	99.62	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2402	THR	CB-CA-C	-7.19	98.80	110.74
5	N	464	VAL	O-C-N	7.18	128.84	121.87
2	H	52	PRO	CA-C-N	7.17	130.60	120.28
2	H	52	PRO	C-N-CA	7.17	130.60	120.28
1	A	1088	PRO	CB-CA-C	-7.16	99.75	111.56
5	Y	428	ASN	CA-C-N	7.14	127.74	120.38
5	Y	428	ASN	C-N-CA	7.14	127.74	120.38
1	B	1787	TYR	N-CA-CB	7.13	120.41	110.07
5	Y	1022	ASN	CA-C-N	7.11	126.94	119.05
5	Y	1022	ASN	C-N-CA	7.11	126.94	119.05
2	E	52	PRO	CA-C-N	7.10	130.51	120.28
2	E	52	PRO	C-N-CA	7.10	130.51	120.28
1	B	2390	THR	CB-CA-C	-7.09	98.80	110.85
1	B	1192	ILE	CA-C-N	7.06	126.58	119.24
1	B	1192	ILE	C-N-CA	7.06	126.58	119.24
1	B	2339	ARG	CB-CA-C	7.05	120.59	111.50
5	Y	1026	PRO	N-CA-CB	-7.02	98.99	102.92
1	B	1127	ALA	CA-C-N	6.99	126.98	119.78
1	B	1127	ALA	C-N-CA	6.99	126.98	119.78
1	A	1127	ALA	CA-C-N	6.99	126.97	119.78
1	A	1127	ALA	C-N-CA	6.99	126.97	119.78
5	Y	464	VAL	CB-CA-C	-6.92	102.79	112.14
5	Y	1063	GLY	CA-C-N	6.92	130.01	120.39
5	Y	1063	GLY	C-N-CA	6.92	130.01	120.39
1	B	1075	ILE	N-CA-CB	-6.91	106.15	110.50
2	H	195	TYR	CB-CA-C	6.87	121.11	110.67
1	B	1409	THR	CB-CA-C	-6.85	98.79	109.55
5	N	329	PRO	N-CA-CB	-6.82	97.24	103.31
5	N	428	ASN	CA-C-N	6.82	127.40	120.38
5	N	428	ASN	C-N-CA	6.82	127.40	120.38
1	B	1192	ILE	CB-CA-C	-6.82	107.23	113.70
5	Y	407	PRO	CB-CA-C	6.81	122.80	111.56
5	Y	329	PRO	N-CA-CB	-6.81	97.25	103.31
1	B	960	ARG	CA-C-N	6.78	134.49	121.54
1	B	960	ARG	C-N-CA	6.78	134.49	121.54
5	N	1022	ASN	CA-C-N	6.76	126.55	119.05
5	N	1022	ASN	C-N-CA	6.76	126.55	119.05
5	N	1314	PRO	CB-CA-C	6.72	119.66	110.52
1	B	2358	PHE	CA-C-N	6.72	127.27	119.94
1	B	2358	PHE	C-N-CA	6.72	127.27	119.94
1	B	934	MET	CA-C-O	6.70	128.03	121.00
1	B	1373	PRO	N-CA-CB	-6.68	97.57	102.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	253	PRO	CB-CA-C	-6.67	102.33	111.21
1	B	1787	TYR	CB-CA-C	-6.65	100.39	110.90
5	N	1063	GLY	CA-C-N	6.63	129.60	120.39
5	N	1063	GLY	C-N-CA	6.63	129.60	120.39
1	B	2536	GLU	CA-C-O	6.61	127.98	120.90
1	A	2396	TYR	N-CA-CB	6.56	119.49	109.91
1	B	1901	GLN	CA-C-O	6.55	129.88	120.51
3	I	41	ALA	CA-C-N	6.54	131.22	120.94
3	I	41	ALA	C-N-CA	6.54	131.22	120.94
1	B	1354	THR	CB-CA-C	-6.54	100.82	110.95
5	N	363	THR	CB-CA-C	6.52	117.41	110.17
1	A	2355	HIS	CB-CA-C	6.52	120.46	109.84
1	B	2401	HIS	CB-CA-C	6.51	120.98	110.96
3	C	224	ASP	CB-CA-C	6.50	120.54	110.67
1	B	2393	ASP	CB-CA-C	6.47	122.01	110.81
1	A	2262	ASN	CB-CA-C	6.46	120.59	111.74
1	B	1793	TRP	N-CA-C	-6.45	104.17	111.07
5	N	569	PRO	N-CA-CB	-6.45	98.53	102.79
1	A	1193	PRO	N-CA-CB	-6.39	96.53	103.25
1	B	1200	VAL	CA-C-N	6.39	129.71	120.38
1	B	1200	VAL	C-N-CA	6.39	129.71	120.38
1	A	131	GLY	CA-C-N	6.38	128.84	120.28
1	A	131	GLY	C-N-CA	6.38	128.84	120.28
1	B	1116	PRO	N-CA-CB	-6.38	96.89	103.08
1	A	1040	GLU	CB-CA-C	-6.36	100.85	110.90
5	N	407	PRO	N-CA-CB	-6.36	96.57	103.25
1	A	2310	SER	N-CA-CB	-6.36	102.14	110.59
1	A	2358	PHE	CA-C-N	6.34	126.86	119.94
1	A	2358	PHE	C-N-CA	6.34	126.86	119.94
5	N	461	PRO	CB-CA-C	-6.31	102.36	112.21
3	I	224	ASP	CB-CA-C	6.29	120.23	110.67
1	B	131	GLY	CA-C-N	6.28	128.70	120.28
1	B	131	GLY	C-N-CA	6.28	128.70	120.28
5	Y	1314	PRO	CB-CA-C	6.22	121.85	111.21
5	Y	171	TYR	CB-CA-C	6.22	120.19	111.86
1	A	1116	PRO	N-CA-C	6.21	118.28	110.70
5	N	462	TRP	CA-C-O	6.21	128.29	121.02
1	B	2141	PRO	CB-CA-C	6.21	119.47	111.21
1	A	1130	PRO	N-CA-CB	-6.20	96.74	103.25
1	A	2398	ILE	O-C-N	6.18	128.33	121.90
5	N	464	VAL	CB-CA-C	-6.17	103.81	112.14
1	A	2339	ARG	CB-CA-C	6.17	119.46	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	263	PHE	CB-CA-C	-6.17	101.46	110.96
2	E	76	ASN	CB-CA-C	6.17	119.21	109.96
1	B	2400	CYS	CA-C-O	-6.16	113.89	120.42
1	B	1311	ASN	CA-C-N	6.16	126.34	119.32
1	B	1311	ASN	C-N-CA	6.16	126.34	119.32
5	Y	248	ALA	CA-C-N	6.15	128.43	120.44
5	Y	248	ALA	C-N-CA	6.15	128.43	120.44
1	B	1263	ILE	CA-C-N	6.11	128.46	120.28
1	B	1263	ILE	C-N-CA	6.11	128.46	120.28
4	D	241	PRO	N-CA-CB	6.10	109.65	103.25
1	B	941	LEU	CA-C-N	6.09	126.06	120.03
1	B	941	LEU	C-N-CA	6.09	126.06	120.03
1	B	2400	CYS	CB-CA-C	-6.08	100.51	110.85
1	A	2141	PRO	CB-CA-C	6.08	119.30	111.21
1	B	896	PRO	N-CA-CB	6.06	109.28	103.52
5	Y	462	TRP	CA-C-O	6.06	128.11	121.02
1	A	941	LEU	CA-C-N	6.06	126.40	119.92
1	A	941	LEU	C-N-CA	6.06	126.40	119.92
1	A	1311	ASN	CA-C-N	6.05	126.22	119.32
1	A	1311	ASN	C-N-CA	6.05	126.22	119.32
2	E	212	PRO	N-CA-CB	-6.04	97.80	103.17
1	B	2382	MET	CA-C-N	6.04	128.37	120.28
1	B	2382	MET	C-N-CA	6.04	128.37	120.28
1	B	1368	ASP	CB-CA-C	6.02	120.85	110.01
5	Y	371	PRO	CA-C-N	6.01	127.36	119.84
5	Y	371	PRO	C-N-CA	6.01	127.36	119.84
1	B	1111	LEU	O-C-N	6.01	129.25	122.22
5	Y	1089	ASP	CA-C-N	6.00	128.92	120.28
5	Y	1089	ASP	C-N-CA	6.00	128.92	120.28
1	A	2432	MET	CA-C-N	5.99	128.91	120.28
1	A	2432	MET	C-N-CA	5.99	128.91	120.28
5	N	467	ALA	O-C-N	5.99	128.47	122.12
1	A	2400	CYS	CA-C-O	-5.99	113.33	120.10
4	J	191	THR	CA-C-N	5.98	128.61	120.54
4	J	191	THR	C-N-CA	5.98	128.61	120.54
1	B	2240	VAL	CA-C-N	5.95	125.92	120.03
1	B	2240	VAL	C-N-CA	5.95	125.92	120.03
1	A	1200	VAL	CA-C-N	5.95	129.06	120.38
1	A	1200	VAL	C-N-CA	5.95	129.06	120.38
1	A	1298	PRO	CA-C-N	5.93	129.72	120.82
1	A	1298	PRO	C-N-CA	5.93	129.72	120.82
1	B	1298	PRO	CA-C-N	5.93	129.72	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1298	PRO	C-N-CA	5.93	129.72	120.82
1	A	130	ILE	CA-C-N	5.93	126.69	119.99
1	A	130	ILE	C-N-CA	5.93	126.69	119.99
1	A	2240	VAL	CA-C-O	5.92	122.64	119.15
1	B	1373	PRO	CA-C-O	-5.89	114.78	121.97
1	B	2315	ASP	CB-CA-C	-5.89	98.36	110.38
5	Y	587	ASN	CB-CA-C	5.89	120.10	111.73
4	D	176	PHE	N-CA-CB	5.89	119.21	110.49
1	B	2376	PRO	CB-CA-C	-5.89	101.84	111.56
5	N	171	TYR	CB-CA-C	5.89	119.75	111.86
1	B	2357	ASP	CB-CA-C	-5.89	98.70	110.42
1	A	2315	ASP	CB-CA-C	-5.88	100.86	110.85
1	B	1052	ILE	N-CA-CB	-5.87	103.05	110.57
1	A	1155	ILE	CA-C-O	-5.87	115.09	120.73
1	A	1409	THR	CB-CA-C	-5.87	100.34	109.55
6	O	215	LEU	CA-C-N	5.86	132.72	121.54
6	O	215	LEU	C-N-CA	5.86	132.72	121.54
5	N	371	PRO	CA-C-N	5.85	127.15	119.84
5	N	371	PRO	C-N-CA	5.85	127.15	119.84
4	D	191	THR	CA-C-N	5.84	128.42	120.54
4	D	191	THR	C-N-CA	5.84	128.42	120.54
1	B	1139	VAL	CB-CA-C	-5.82	104.42	112.04
1	B	1209	TYR	CB-CA-C	-5.82	102.00	110.96
1	B	1146	LEU	N-CA-CB	-5.81	101.04	110.81
5	N	951	ILE	CA-C-N	5.80	128.85	120.38
5	N	951	ILE	C-N-CA	5.80	128.85	120.38
1	A	1901	GLN	CA-C-O	5.80	128.80	120.51
1	A	1368	ASP	CB-CA-C	5.79	120.44	110.01
1	B	1435	TYR	CB-CA-C	-5.79	101.02	110.85
4	D	61	LYS	CB-CA-C	5.78	117.18	108.86
5	N	364	PRO	N-CA-CB	-5.77	98.33	103.35
1	A	1886	GLN	O-C-N	5.76	128.08	122.09
1	A	2401	HIS	CB-CA-C	5.76	119.87	110.95
5	Y	1327	VAL	CA-C-O	-5.75	113.59	120.78
1	A	934	MET	CA-C-O	5.75	127.04	121.00
1	B	1628	ARG	CB-CA-C	5.75	119.96	111.17
3	C	282	PRO	N-CA-CB	5.75	109.73	103.23
4	D	311	ASP	CA-C-N	5.75	127.98	120.28
4	D	311	ASP	C-N-CA	5.75	127.98	120.28
1	A	1787	TYR	CA-C-N	5.74	129.43	120.82
1	A	1787	TYR	C-N-CA	5.74	129.43	120.82
5	Y	194	TYR	CB-CA-C	5.74	119.61	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1075	ILE	CA-C-O	5.74	122.53	118.69
2	H	76	ASN	CB-CA-C	5.74	118.56	109.96
1	A	806	ALA	CA-C-N	5.73	127.89	120.44
1	A	806	ALA	C-N-CA	5.73	127.89	120.44
4	J	146	ALA	N-CA-C	5.73	119.45	112.23
5	Y	152	GLY	CA-C-N	5.73	128.23	120.38
5	Y	152	GLY	C-N-CA	5.73	128.23	120.38
1	B	1886	GLN	O-C-N	5.71	128.18	122.12
1	A	1192	ILE	CA-C-N	5.71	126.98	119.84
1	A	1192	ILE	C-N-CA	5.71	126.98	119.84
5	N	1089	ASP	CA-C-N	5.71	128.50	120.28
5	N	1089	ASP	C-N-CA	5.71	128.50	120.28
5	N	248	ALA	CA-C-N	5.71	127.86	120.44
5	N	248	ALA	C-N-CA	5.71	127.86	120.44
1	A	1435	TYR	CB-CA-C	-5.70	101.16	110.85
1	A	1921	GLU	CB-CA-C	-5.65	101.94	110.92
1	B	130	ILE	CA-C-N	5.64	126.37	119.99
1	B	130	ILE	C-N-CA	5.64	126.37	119.99
1	B	1408	PRO	CB-CA-C	5.64	118.29	111.46
1	B	2388	GLU	CA-C-N	5.64	129.38	120.47
1	B	2388	GLU	C-N-CA	5.64	129.38	120.47
5	N	407	PRO	CB-CA-C	5.64	120.86	111.56
1	A	896	PRO	N-CA-CB	5.64	109.12	103.48
1	A	498	GLN	CA-C-N	5.63	128.39	120.28
1	A	498	GLN	C-N-CA	5.63	128.39	120.28
5	Y	432	GLN	CB-CA-C	5.63	120.23	110.94
4	J	61	LYS	CB-CA-C	5.62	116.95	108.86
1	B	1974	TYR	CB-CA-C	5.61	122.19	113.04
5	N	456	PHE	CB-CA-C	-5.61	102.26	110.95
5	N	489	PRO	N-CA-CB	-5.60	97.17	103.33
1	B	1532	TYR	CA-C-N	5.59	128.04	120.38
1	B	1532	TYR	C-N-CA	5.59	128.04	120.38
5	Y	364	PRO	N-CA-CB	-5.59	98.49	103.35
1	B	933	GLU	CA-C-N	5.58	128.02	120.65
1	B	933	GLU	C-N-CA	5.58	128.02	120.65
2	E	28	GLN	CA-C-N	5.57	127.69	120.44
2	E	28	GLN	C-N-CA	5.57	127.69	120.44
2	H	140	GLN	CB-CA-C	5.57	119.21	111.63
5	Y	1157	LYS	CB-CA-C	5.57	119.13	110.67
1	B	2421	PHE	CB-CA-C	5.56	119.38	110.09
1	B	1111	LEU	CA-C-N	5.56	132.16	121.54
1	B	1111	LEU	C-N-CA	5.56	132.16	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2400	CYS	CB-CA-C	-5.55	100.35	110.63
4	J	197	GLN	CA-C-N	5.55	128.03	120.54
4	J	197	GLN	C-N-CA	5.55	128.03	120.54
1	B	2380	THR	O-C-N	5.54	129.29	123.03
1	B	1076	PRO	CB-CA-C	-5.54	103.01	112.64
5	N	587	ASN	CB-CA-C	5.53	119.58	111.73
5	N	408	PHE	CB-CA-C	-5.52	102.14	110.92
1	A	997	PHE	CA-C-N	5.52	127.61	120.44
1	A	997	PHE	C-N-CA	5.52	127.61	120.44
1	B	2400	CYS	O-C-N	5.51	128.44	122.15
5	Y	381	ALA	CA-C-O	-5.50	114.59	120.42
5	Y	429	PRO	N-CA-C	5.50	117.41	110.70
6	T	215	LEU	CA-C-N	5.49	132.02	121.54
6	T	215	LEU	C-N-CA	5.49	132.02	121.54
5	N	657	PRO	CA-C-N	5.49	127.95	120.54
5	N	657	PRO	C-N-CA	5.49	127.95	120.54
1	B	1304	TRP	CA-C-N	5.48	127.94	120.54
1	B	1304	TRP	C-N-CA	5.48	127.94	120.54
5	Y	290	VAL	CB-CA-C	5.48	117.17	111.09
1	A	960	ARG	CA-C-N	5.47	132.00	121.54
1	A	960	ARG	C-N-CA	5.47	132.00	121.54
1	A	1583	TYR	CA-C-N	5.47	127.93	120.54
1	A	1583	TYR	C-N-CA	5.47	127.93	120.54
1	B	1793	TRP	O-C-N	5.47	127.71	122.07
5	Y	1131	TRP	N-CA-CB	5.47	118.60	110.29
1	B	1432	VAL	CA-C-O	-5.47	115.06	120.85
1	B	498	GLN	CA-C-N	5.46	128.14	120.28
1	B	498	GLN	C-N-CA	5.46	128.14	120.28
4	D	79	LYS	CA-C-O	-5.46	115.09	120.82
1	A	1974	TYR	CB-CA-C	5.45	121.93	113.04
5	Y	951	ILE	CA-C-N	5.45	128.34	120.38
5	Y	951	ILE	C-N-CA	5.45	128.34	120.38
4	J	311	ASP	CA-C-N	5.45	127.59	120.28
4	J	311	ASP	C-N-CA	5.45	127.59	120.28
1	B	1133	LYS	CB-CA-C	-5.45	102.09	110.81
5	Y	456	PHE	CB-CA-C	-5.45	102.51	110.95
5	Y	461	PRO	O-C-N	5.44	129.23	122.22
5	Y	463	ALA	CA-C-O	-5.43	114.21	120.24
4	D	197	GLN	CA-C-N	5.43	127.87	120.54
4	D	197	GLN	C-N-CA	5.43	127.87	120.54
1	A	1628	ARG	CB-CA-C	5.42	119.47	111.17
1	B	1921	GLU	CB-CA-C	-5.41	102.31	110.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2323	SER	O-C-N	5.41	127.86	122.12
2	E	9	GLY	CA-C-N	5.41	131.87	121.54
2	E	9	GLY	C-N-CA	5.41	131.87	121.54
3	I	78	ARG	CA-C-O	-5.41	114.79	120.63
1	A	1116	PRO	N-CA-CB	-5.40	97.84	103.08
2	E	9	GLY	O-C-N	5.40	127.43	122.19
5	Y	1013	LEU	CA-C-N	5.40	130.24	121.98
5	Y	1013	LEU	C-N-CA	5.40	130.24	121.98
3	C	26	ILE	CA-C-N	5.39	127.44	120.70
3	C	26	ILE	C-N-CA	5.39	127.44	120.70
1	A	1111	LEU	O-C-N	5.38	128.29	122.15
4	D	146	ALA	N-CA-C	5.38	119.01	112.23
1	A	1022	PHE	CA-C-N	5.38	128.12	120.53
1	A	1022	PHE	C-N-CA	5.38	128.12	120.53
5	N	263	PHE	CB-CA-C	-5.38	102.61	110.95
4	J	176	PHE	N-CA-CB	5.37	118.44	110.49
1	B	181	THR	CA-C-N	5.37	128.47	120.31
1	B	181	THR	C-N-CA	5.37	128.47	120.31
2	E	138	PRO	N-CA-C	5.37	123.53	112.47
1	B	1690	PRO	CB-CA-C	-5.37	104.07	111.21
1	B	1880	TYR	CB-CA-C	-5.37	101.10	110.17
3	C	290	ILE	CA-C-N	5.36	127.47	120.28
3	C	290	ILE	C-N-CA	5.36	127.47	120.28
1	A	1354	THR	CB-CA-C	-5.36	102.64	110.95
1	A	1373	PRO	CA-C-O	-5.36	115.43	121.97
3	C	286	THR	CB-CA-C	5.36	119.96	110.85
3	I	290	ILE	CA-C-N	5.36	127.46	120.28
3	I	290	ILE	C-N-CA	5.36	127.46	120.28
1	A	1263	ILE	CA-C-N	5.36	127.46	120.28
1	A	1263	ILE	C-N-CA	5.36	127.46	120.28
1	B	1158	PRO	CB-CA-C	-5.36	103.78	112.62
2	H	138	PRO	N-CA-C	5.36	123.50	112.47
1	B	1787	TYR	CA-C-N	5.35	128.85	120.82
1	B	1787	TYR	C-N-CA	5.35	128.85	120.82
1	B	2493	LEU	CA-C-N	5.34	127.70	120.38
1	B	2493	LEU	C-N-CA	5.34	127.70	120.38
1	A	1880	TYR	CB-CA-C	-5.34	101.15	110.17
5	Y	657	PRO	CA-C-N	5.34	127.75	120.54
5	Y	657	PRO	C-N-CA	5.34	127.75	120.54
3	I	282	PRO	N-CA-CB	5.34	109.26	103.23
3	C	78	ARG	CA-C-O	-5.34	114.87	120.63
5	N	411	GLU	CB-CA-C	-5.33	100.44	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2397	ARG	N-CA-CB	5.33	118.54	110.28
1	A	1192	ILE	CB-CA-C	-5.33	108.64	113.70
2	H	28	GLN	CA-C-N	5.32	127.36	120.44
2	H	28	GLN	C-N-CA	5.32	127.36	120.44
1	B	1071	LEU	CB-CA-C	-5.32	102.86	112.76
1	A	1102	LEU	CA-C-N	5.32	127.67	120.38
1	A	1102	LEU	C-N-CA	5.32	127.67	120.38
4	D	229	PHE	CA-C-N	5.32	127.36	120.44
4	D	229	PHE	C-N-CA	5.32	127.36	120.44
3	I	286	THR	CB-CA-C	5.32	119.89	110.85
1	A	1090	ARG	CA-C-O	-5.31	115.44	121.65
1	B	1318	PHE	CA-C-N	5.31	127.71	120.54
1	B	1318	PHE	C-N-CA	5.31	127.71	120.54
1	B	1167	PRO	CA-C-N	5.30	127.69	120.54
1	B	1167	PRO	C-N-CA	5.30	127.69	120.54
1	B	2432	MET	CA-C-N	5.30	129.08	120.60
1	B	2432	MET	C-N-CA	5.30	129.08	120.60
1	B	2094	VAL	CA-C-N	5.30	127.91	120.28
1	B	2094	VAL	C-N-CA	5.30	127.91	120.28
1	A	2421	PHE	CB-CA-C	5.28	118.91	110.09
1	A	2094	VAL	CA-C-N	5.28	127.88	120.28
1	A	2094	VAL	C-N-CA	5.28	127.88	120.28
5	Y	119	TYR	CB-CA-C	5.28	118.24	109.53
1	B	1071	LEU	O-C-N	5.27	125.17	120.48
1	A	2493	LEU	CA-C-N	5.27	127.60	120.38
1	A	2493	LEU	C-N-CA	5.27	127.60	120.38
1	A	1139	VAL	CB-CA-C	-5.26	105.14	112.04
1	B	1583	TYR	CA-C-N	5.26	127.64	120.54
1	B	1583	TYR	C-N-CA	5.26	127.64	120.54
1	B	1183	GLN	CB-CA-C	-5.23	101.13	110.70
1	B	1734	THR	CB-CA-C	5.23	120.91	109.99
1	A	1167	PRO	CA-C-N	5.22	127.22	120.44
1	A	1167	PRO	C-N-CA	5.22	127.22	120.44
3	C	193	ASN	CB-CA-C	5.22	119.14	110.90
1	A	1111	LEU	CA-C-N	5.21	131.50	121.54
1	A	1111	LEU	C-N-CA	5.21	131.50	121.54
1	B	1784	ARG	CB-CA-C	5.21	119.06	110.88
1	B	1116	PRO	N-CA-C	5.21	117.06	110.70
1	B	2362	PHE	CB-CA-C	5.21	119.12	111.73
1	B	1304	TRP	O-C-N	5.19	127.43	122.03
5	N	1013	LEU	CA-C-N	5.19	130.09	121.99
5	N	1013	LEU	C-N-CA	5.19	130.09	121.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	1157	LYS	CB-CA-C	5.19	118.56	110.67
5	N	155	VAL	N-CA-CB	5.19	116.08	111.67
4	D	282	TYR	CA-C-N	5.19	127.18	120.44
4	D	282	TYR	C-N-CA	5.19	127.18	120.44
1	B	2352	LYS	CB-CA-C	5.18	118.98	109.46
1	A	2536	GLU	CA-C-O	5.16	126.69	120.92
1	B	1316	ASP	CB-CA-C	5.16	120.57	110.67
1	B	2158	PRO	N-CA-C	5.16	120.31	113.40
1	B	1737	GLN	CA-C-N	5.15	127.14	120.44
1	B	1737	GLN	C-N-CA	5.15	127.14	120.44
3	C	185	GLN	CA-C-N	5.15	127.13	120.44
3	C	185	GLN	C-N-CA	5.15	127.13	120.44
1	A	1157	HIS	CB-CA-C	-5.14	104.66	113.04
1	A	2380	THR	O-C-N	5.13	128.83	123.03
5	Y	489	PRO	N-CA-CB	-5.13	97.68	103.33
1	B	1203	ARG	CB-CA-C	5.13	120.11	112.06
1	B	1930	ILE	CA-C-N	5.12	128.15	120.87
1	B	1930	ILE	C-N-CA	5.12	128.15	120.87
1	A	1737	GLN	CA-C-N	5.11	127.09	120.44
1	A	1737	GLN	C-N-CA	5.11	127.09	120.44
1	B	2275	TYR	CA-C-N	5.11	127.38	120.38
1	B	2275	TYR	C-N-CA	5.11	127.38	120.38
5	N	194	TYR	CB-CA-C	5.11	118.57	110.19
5	N	152	GLY	CA-C-N	5.11	127.12	120.28
5	N	152	GLY	C-N-CA	5.11	127.12	120.28
1	A	2401	HIS	N-CA-C	-5.10	105.37	111.03
1	B	1262	THR	N-CA-CB	5.09	119.09	110.49
5	Y	472	ILE	CA-C-O	-5.09	113.12	119.43
3	C	226	HIS	CA-C-N	5.08	127.09	120.28
3	C	226	HIS	C-N-CA	5.08	127.09	120.28
1	B	1406	LYS	CB-CA-C	-5.08	102.21	110.85
5	Y	1162	PRO	N-CA-CB	5.08	108.06	103.34
1	A	1304	TRP	CA-C-N	5.08	127.39	120.54
1	A	1304	TRP	C-N-CA	5.08	127.39	120.54
1	B	1268	ALA	CA-C-N	5.08	127.53	120.63
1	B	1268	ALA	C-N-CA	5.08	127.53	120.63
2	E	156	ASP	CB-CA-C	5.08	118.33	109.65
3	I	149	ARG	CA-C-N	5.08	127.53	120.63
3	I	149	ARG	C-N-CA	5.08	127.53	120.63
1	A	933	GLU	CA-C-N	5.07	127.35	120.65
1	A	933	GLU	C-N-CA	5.07	127.35	120.65
1	A	2240	VAL	CA-C-N	5.07	124.97	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2240	VAL	C-N-CA	5.07	124.97	119.85
1	A	1690	PRO	CB-CA-C	-5.07	104.47	111.21
3	I	227	ARG	CA-C-N	5.07	128.42	120.82
3	I	227	ARG	C-N-CA	5.07	128.42	120.82
1	B	2548	PHE	CB-CA-C	5.06	118.51	109.29
5	N	290	VAL	CB-CA-C	5.06	116.70	111.09
1	A	1262	THR	N-CA-CB	5.06	119.03	110.49
1	B	2535	HIS	CB-CA-C	5.05	120.55	109.99
5	N	484	ALA	CA-C-N	5.05	127.75	120.38
5	N	484	ALA	C-N-CA	5.05	127.75	120.38
2	E	30	HIS	N-CA-CB	5.04	118.30	110.44
1	B	1604	GLN	CA-C-N	5.03	127.53	120.28
1	B	1604	GLN	C-N-CA	5.03	127.53	120.28
1	A	2344	LEU	CA-C-O	-5.03	114.93	120.36
1	A	1734	THR	CB-CA-C	5.03	120.49	109.99
1	A	2537	ASN	CA-C-N	5.02	127.01	120.28
1	A	2537	ASN	C-N-CA	5.02	127.01	120.28
1	B	1155	ILE	CA-C-O	-5.02	115.91	120.73
2	H	161	HIS	CA-C-O	-5.02	116.34	122.41
3	I	185	GLN	CA-C-N	5.01	126.96	120.44
3	I	185	GLN	C-N-CA	5.01	126.96	120.44
3	I	226	HIS	CA-C-N	5.01	127.00	120.28
3	I	226	HIS	C-N-CA	5.01	127.00	120.28
1	B	1356	THR	CB-CA-C	-5.01	102.33	110.85
1	B	1925	GLU	CB-CA-C	-5.01	102.47	110.79
1	B	1935	TRP	CB-CA-C	5.00	120.37	110.17

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1164	ASP	Peptide
1	A	1261	SER	Peptide
1	A	1732	ILE	Peptide
1	A	1898	ASN	Peptide
1	A	2340	HIS	Peptide
1	B	1164	ASP	Peptide
1	B	1261	SER	Peptide
1	B	1329	LEU	Peptide
1	B	1425	GLN	Peptide
1	B	1732	ILE	Peptide
1	B	2340	HIS	Peptide

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Mol	Chain	Res	Type	Group
2	E	267	GLU	Peptide
2	E	28	GLN	Peptide
2	H	267	GLU	Peptide
2	H	28	GLN	Peptide
5	N	430	PRO	Peptide
5	N	627	VAL	Peptide
5	Y	381	ALA	Mainchain
5	Y	430	PRO	Peptide
5	Y	627	VAL	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10799	0	4791	11	0
1	B	10799	0	4791	12	0
2	E	1562	0	718	0	0
2	H	1562	0	718	0	0
3	C	1483	0	651	11	0
3	I	1482	0	647	11	0
4	D	1349	0	589	5	0
4	J	1354	0	591	5	0
5	N	5214	0	2322	2	0
5	Y	5214	0	2322	6	0
6	O	173	0	82	2	0
6	T	173	0	82	2	0
7	C	32	0	12	4	0
7	I	32	0	12	4	0
8	D	28	0	12	3	0
8	J	28	0	12	2	0
All	All	41284	0	18352	62	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 1.

All (62) 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)
5:N:176:PRO:CB	6:O:181:ALA:O	2.19	0.89
3:I:41:ALA:HB1	7:I:401:GTP:O1G	1.73	0.87
5:Y:176:PRO:CB	6:T:181:ALA:O	2.23	0.86
4:D:75:SER:CB	8:D:401:GDP:O3B	2.29	0.81
3:I:37:ARG:HA	7:I:401:GTP:O3'	1.85	0.77
3:I:47:HIS:HA	3:I:60:LEU:O	1.84	0.76
1:A:724:ALA:HB2	5:Y:411:GLU:CB	2.30	0.62
6:O:212:SER:C	6:O:214:ASP:H	2.11	0.58
6:T:212:SER:C	6:T:214:ASP:H	2.11	0.58
4:J:75:SER:CB	8:J:401:GDP:O3B	2.52	0.57
3:C:259:PHE:HA	3:C:278:ASP:H	1.70	0.56
3:I:259:PHE:HA	3:I:278:ASP:H	1.70	0.56
4:J:81:VAL:O	4:J:266:SER:CB	2.54	0.56
3:C:37:ARG:HA	7:C:401:GTP:O3'	2.06	0.55
1:A:2139:ALA:HA	1:A:2152:ARG:HA	1.89	0.55
1:B:2139:ALA:HA	1:B:2152:ARG:HA	1.88	0.54
4:D:81:VAL:O	4:D:266:SER:CB	2.55	0.53
3:I:259:PHE:C	3:I:278:ASP:CB	2.83	0.52
1:A:1431:GLY:HA3	1:A:2394:GLY:HA2	1.91	0.52
3:C:259:PHE:C	3:C:278:ASP:CB	2.83	0.52
1:B:2327:MET:HA	1:B:2330:VAL:CB	2.38	0.52
1:A:858:TYR:O	1:A:862:PRO:HA	2.10	0.52
1:B:1330:ASN:O	1:B:1332:ASP:N	2.43	0.52
3:C:259:PHE:O	3:C:278:ASP:CB	2.58	0.52
1:B:893:ALA:O	1:B:1626:CYS:HA	2.10	0.51
3:I:259:PHE:O	3:I:278:ASP:CB	2.59	0.51
5:Y:378:MET:O	5:Y:381:ALA:HB3	2.11	0.50
1:B:1579:ALA:HA	1:B:1586:ALA:HB2	1.94	0.50
1:A:1330:ASN:O	1:A:1332:ASP:N	2.46	0.49
4:D:76:SER:CB	8:D:401:GDP:O1A	2.60	0.49
1:B:858:TYR:O	1:B:862:PRO:HA	2.14	0.48
1:A:1579:ALA:HA	1:A:1586:ALA:HB2	1.97	0.47
4:D:220:ILE:CB	8:D:401:GDP:C6	2.98	0.47
4:J:220:ILE:CB	8:J:401:GDP:C6	2.98	0.46
3:I:170:TYR:CB	3:I:229:GLU:CB	2.94	0.46
3:C:47:HIS:CB	5:Y:560:ALA:CB	2.93	0.46
3:C:36:THR:C	7:C:401:GTP:O2'	2.59	0.45
1:B:1431:GLY:HA3	1:B:2394:GLY:HA2	1.98	0.45
3:I:37:ARG:N	7:I:401:GTP:O2'	2.51	0.44
3:I:36:THR:C	7:I:401:GTP:O2'	2.61	0.44
5:N:51:MET:C	5:N:53:ASP:H	2.26	0.44
1:A:1431:GLY:CA	1:A:2394:GLY:HA2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:HIS:CB	5:Y:560:ALA:HB1	2.48	0.43
5:Y:51:MET:C	5:Y:53:ASP:H	2.27	0.43
3:C:170:TYR:CB	3:C:229:GLU:CB	2.97	0.42
1:B:152:ALA:O	1:B:168:ALA:HB1	2.18	0.42
3:I:48:SER:N	3:I:60:LEU:O	2.52	0.42
1:B:1294:ASP:O	1:B:1295:SER:C	2.62	0.42
1:A:401:ALA:HA	1:A:443:ALA:HB1	2.01	0.42
4:J:225:ILE:O	4:J:228:ALA:HB3	2.20	0.42
3:C:19:GLY:HA2	7:C:401:GTP:H5'	2.02	0.42
4:J:79:LYS:O	4:J:83:HIS:N	2.50	0.41
1:B:401:ALA:HA	1:B:443:ALA:HB1	2.01	0.41
1:B:1142:LEU:O	1:B:1146:LEU:CB	2.69	0.41
3:C:262:PHE:O	3:C:273:MET:HA	2.21	0.41
1:A:1294:ASP:O	1:A:1295:SER:C	2.64	0.41
3:C:20:LYS:H	7:C:401:GTP:PB	2.43	0.41
1:A:152:ALA:O	1:A:168:ALA:HB1	2.21	0.41
3:I:262:PHE:O	3:I:273:MET:HA	2.21	0.41
1:A:893:ALA:O	1:A:1626:CYS:HA	2.21	0.40
1:B:1374:LEU:O	1:B:1379:GLY:N	2.53	0.40
4:D:233:VAL:C	4:D:235:LYS:H	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2088/2549 (82%)	1951 (93%)	121 (6%)	16 (1%)	16	54
1	B	2088/2549 (82%)	1949 (93%)	124 (6%)	15 (1%)	18	56
2	E	315/326 (97%)	274 (87%)	36 (11%)	5 (2%)	7	37
2	H	315/326 (97%)	270 (86%)	40 (13%)	5 (2%)	7	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	296/313 (95%)	277 (94%)	15 (5%)	4 (1%)	9	39
3	I	296/313 (95%)	278 (94%)	14 (5%)	4 (1%)	9	39
4	D	266/399 (67%)	242 (91%)	21 (8%)	3 (1%)	11	45
4	J	267/399 (67%)	242 (91%)	22 (8%)	3 (1%)	11	45
5	N	1040/1335 (78%)	932 (90%)	99 (10%)	9 (1%)	14	50
5	Y	1040/1335 (78%)	927 (89%)	104 (10%)	9 (1%)	14	50
6	O	29/256 (11%)	23 (79%)	4 (14%)	2 (7%)	1	11
6	T	29/256 (11%)	23 (79%)	2 (7%)	4 (14%)	0	3
All	All	8069/10356 (78%)	7388 (92%)	602 (8%)	79 (1%)	15	48

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1331	GLU
1	B	1331	GLU
3	C	153	ARG
3	C	280	SER
4	D	180	VAL
3	I	153	ARG
3	I	280	SER
4	J	180	VAL
1	A	647	THR
1	A	1006	GLY
1	A	2308	PRO
1	B	647	THR
1	B	1006	GLY
1	B	1276	SER
1	B	2308	PRO
2	E	118	ASN
2	E	241	ASP
5	Y	601	HIS
5	Y	1213	TRP
2	H	118	ASN
2	H	241	ASP
5	N	1213	TRP
6	O	216	ASP
1	A	893	ALA
1	A	1276	SER
2	E	86	LYS

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Mol	Chain	Res	Type
2	E	87	ASN
2	E	269	SER
3	C	246	ALA
3	C	278	ASP
4	D	300	GLY
5	Y	1203	ARG
6	T	216	ASP
2	H	87	ASN
2	H	269	SER
3	I	278	ASP
5	N	601	HIS
5	N	1203	ARG
1	A	428	LYS
1	A	809	SER
1	A	1088	PRO
1	A	1472	ASP
1	B	428	LYS
1	B	809	SER
1	B	1088	PRO
1	B	1472	ASP
5	Y	80	PRO
5	Y	1264	GLN
2	H	86	LYS
3	I	246	ALA
4	J	300	GLY
5	N	80	PRO
5	N	1264	GLN
1	A	96	VAL
1	A	811	LEU
1	A	1028	ARG
1	B	811	LEU
6	T	213	PRO
6	T	214	ASP
4	J	241	PRO
6	O	213	PRO
1	A	812	GLU
1	A	2357	ASP
1	B	96	VAL
1	B	893	ALA
1	B	1582	SER
4	D	241	PRO
5	Y	528	PRO

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Mol	Chain	Res	Type
5	Y	954	THR
5	Y	1263	PRO
6	T	128	LEU
5	N	954	THR
5	N	1263	PRO
5	Y	372	PRO
5	N	372	PRO
1	B	1028	ARG
1	B	1643	VAL
5	N	528	PRO
1	A	1116	PRO

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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
7	GTP	C	401	-	33,34,34	0.78	2 (6%)	50,54,54	0.90	3 (6%)
8	GDP	J	401	-	29,30,30	1.77	4 (13%)	45,47,47	2.09	19 (42%)
8	GDP	D	401	-	29,30,30	2.75	3 (10%)	45,47,47	1.90	13 (28%)
7	GTP	I	401	-	33,34,34	0.99	3 (9%)	50,54,54	0.93	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
7	GTP	C	401	-	-	2/22/38/38	0/3/3/3
8	GDP	J	401	-	-	2/16/32/32	0/3/3/3
8	GDP	D	401	-	-	2/16/32/32	0/3/3/3
7	GTP	I	401	-	-	2/22/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	401	GDP	PA-O3A	13.51	1.74	1.59
8	J	401	GDP	PA-O3A	6.68	1.66	1.59
8	D	401	GDP	C5-C4	3.61	1.48	1.38
8	J	401	GDP	C5-C4	3.60	1.48	1.38
7	I	401	GTP	PG-O1G	-3.42	1.39	1.50
7	I	401	GTP	PA-O3A	2.48	1.62	1.59
8	J	401	GDP	O2'-C2'	2.25	1.48	1.43
8	D	401	GDP	C4-N9	-2.23	1.32	1.38
7	I	401	GTP	PG-O3G	-2.12	1.46	1.54
8	J	401	GDP	C8-N7	2.11	1.38	1.32
7	C	401	GTP	PA-O3A	2.03	1.61	1.59
7	C	401	GTP	PG-O1G	2.02	1.56	1.50

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	401	GDP	C5-C4-N3	-4.98	120.46	128.39
8	D	401	GDP	C5-C4-N3	-4.57	121.12	128.39
8	J	401	GDP	C2-N3-C4	4.46	119.98	112.30
8	D	401	GDP	C2-N3-C4	4.17	119.48	112.30
8	J	401	GDP	N9-C4-N3	4.05	134.05	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	401	GDP	N9-C4-N3	4.04	134.03	125.95
8	D	401	GDP	O3B-PB-O2B	3.82	122.11	107.80
8	J	401	GDP	C6-C5-N7	3.67	136.97	130.29
8	D	401	GDP	O6-C6-C5	-3.29	117.86	126.53
8	D	401	GDP	C6-C5-N7	3.19	136.09	130.29
8	J	401	GDP	O6-C6-C5	-3.09	118.37	126.53
8	J	401	GDP	O2B-PB-O1B	2.85	121.92	110.83
7	C	401	GTP	O3B-PB-O1B	-2.79	102.30	110.70
8	J	401	GDP	N9-C8-N7	-2.68	108.43	113.40
7	I	401	GTP	O3'-C3'-C2'	-2.63	103.39	111.82
8	J	401	GDP	O4'-C4'-C5'	-2.58	101.06	109.33
8	J	401	GDP	C8-N9-C4	2.52	110.75	106.03
8	J	401	GDP	O3A-PA-O1A	-2.43	103.40	110.70
8	J	401	GDP	C4-C5-N7	-2.40	106.86	110.67
8	D	401	GDP	O4'-C4'-C3'	2.34	109.79	105.15
7	I	401	GTP	O3'-C3'-C4'	2.33	117.78	111.08
8	J	401	GDP	C8-N7-C5	2.27	108.31	104.26
8	D	401	GDP	O3'-C3'-C2'	-2.27	104.53	111.82
8	J	401	GDP	O3B-PB-O3A	2.22	112.08	104.64
8	D	401	GDP	O3A-PB-O1B	-2.19	99.49	111.04
8	J	401	GDP	O2A-PA-O3A	2.19	113.19	107.27
8	D	401	GDP	C6-C5-C4	-2.19	115.54	118.83
8	J	401	GDP	O3A-PB-O1B	-2.15	99.71	111.04
8	J	401	GDP	O2'-C2'-C3'	2.14	118.69	111.82
8	D	401	GDP	O2'-C2'-C3'	2.14	118.68	111.82
7	C	401	GTP	O3'-C3'-C4'	2.13	117.19	111.08
8	D	401	GDP	C3'-C2'-C1'	2.12	105.47	101.46
8	J	401	GDP	O3'-C3'-C2'	-2.10	105.07	111.82
7	C	401	GTP	O2B-PB-O3B	2.10	112.94	107.27
8	J	401	GDP	C1'-N9-C4	-2.06	120.39	126.49
8	D	401	GDP	C5-C6-N1	2.03	118.43	113.25
8	J	401	GDP	O4'-C4'-C3'	2.01	109.15	105.15

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	401	GDP	PA-O3A-PB-O3B
8	J	401	GDP	PA-O3A-PB-O3B
7	C	401	GTP	PA-O3A-PB-O1B
8	J	401	GDP	PA-O3A-PB-O1B
8	D	401	GDP	PA-O3A-PB-O2B

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Continued from previous page...

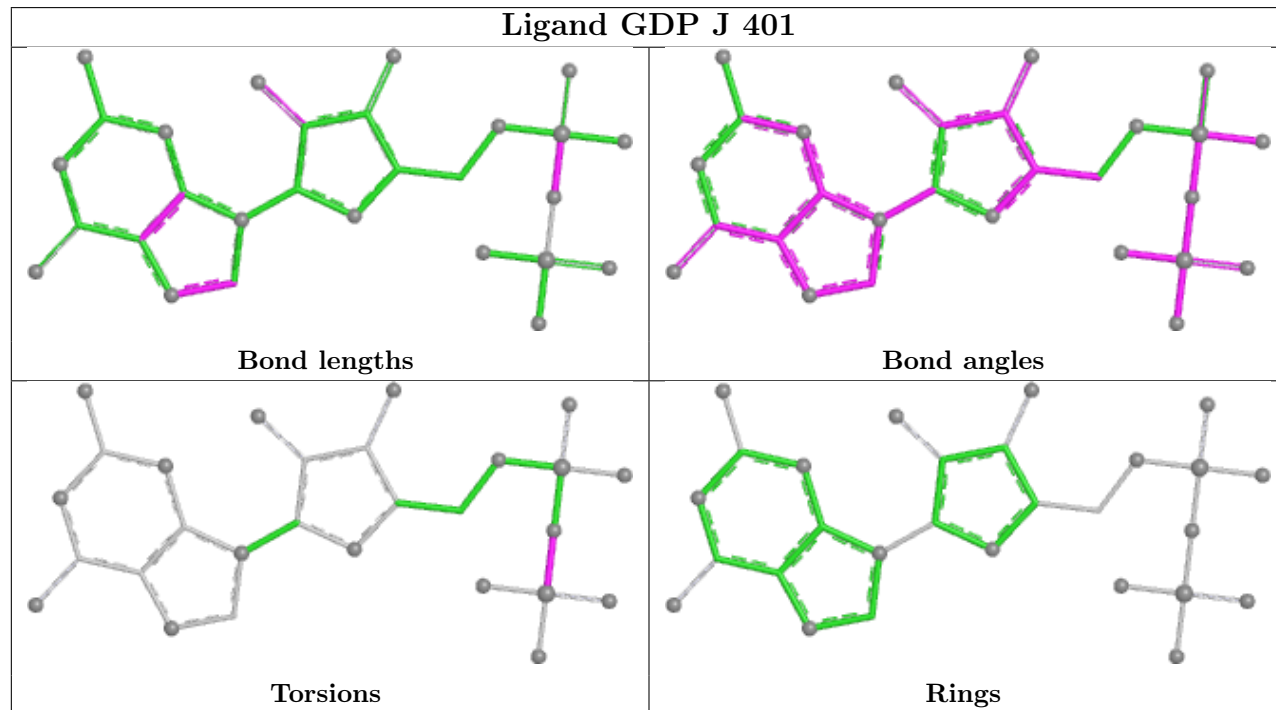
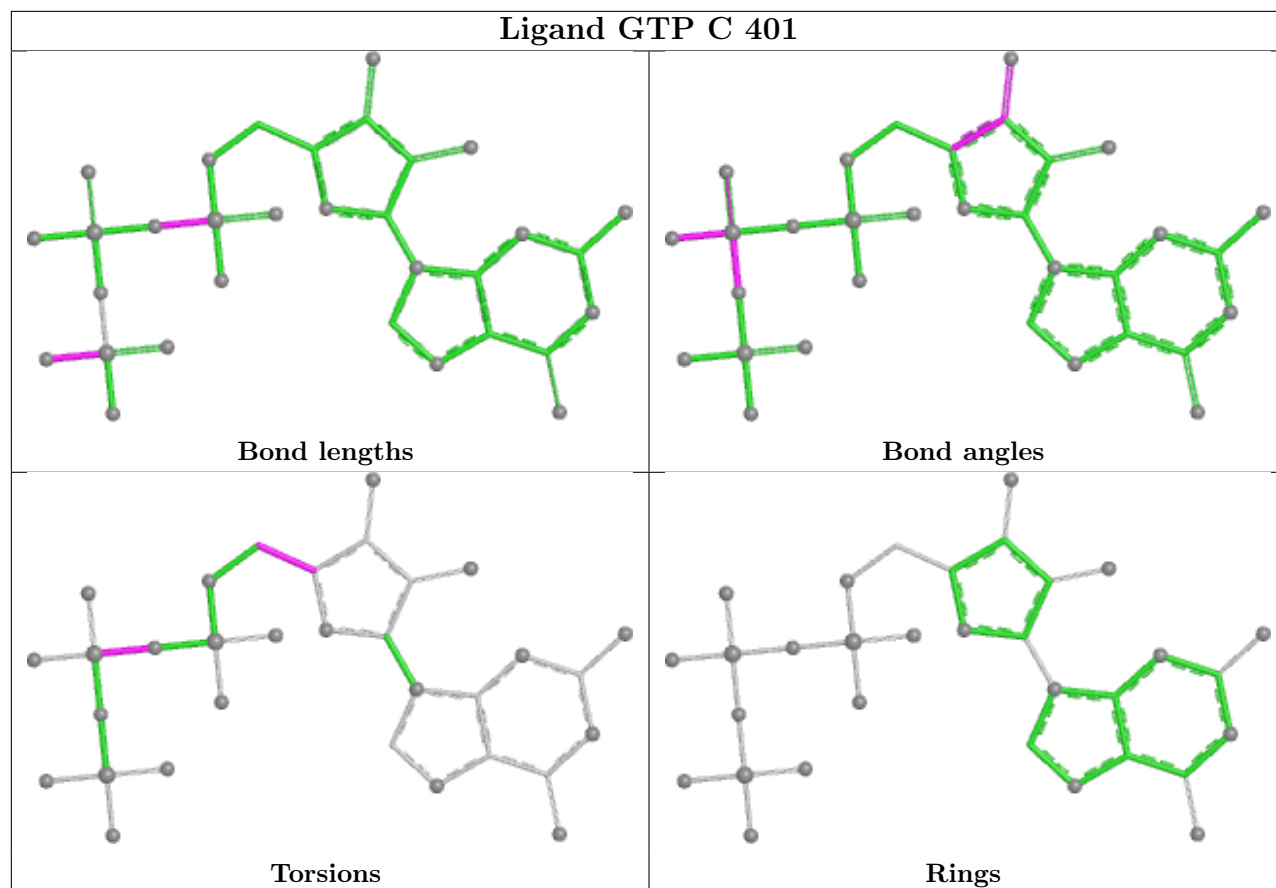
Mol	Chain	Res	Type	Atoms
7	C	401	GTP	O4'-C4'-C5'-O5'
7	I	401	GTP	PA-O3A-PB-O1B
7	I	401	GTP	PA-O3A-PB-O2B

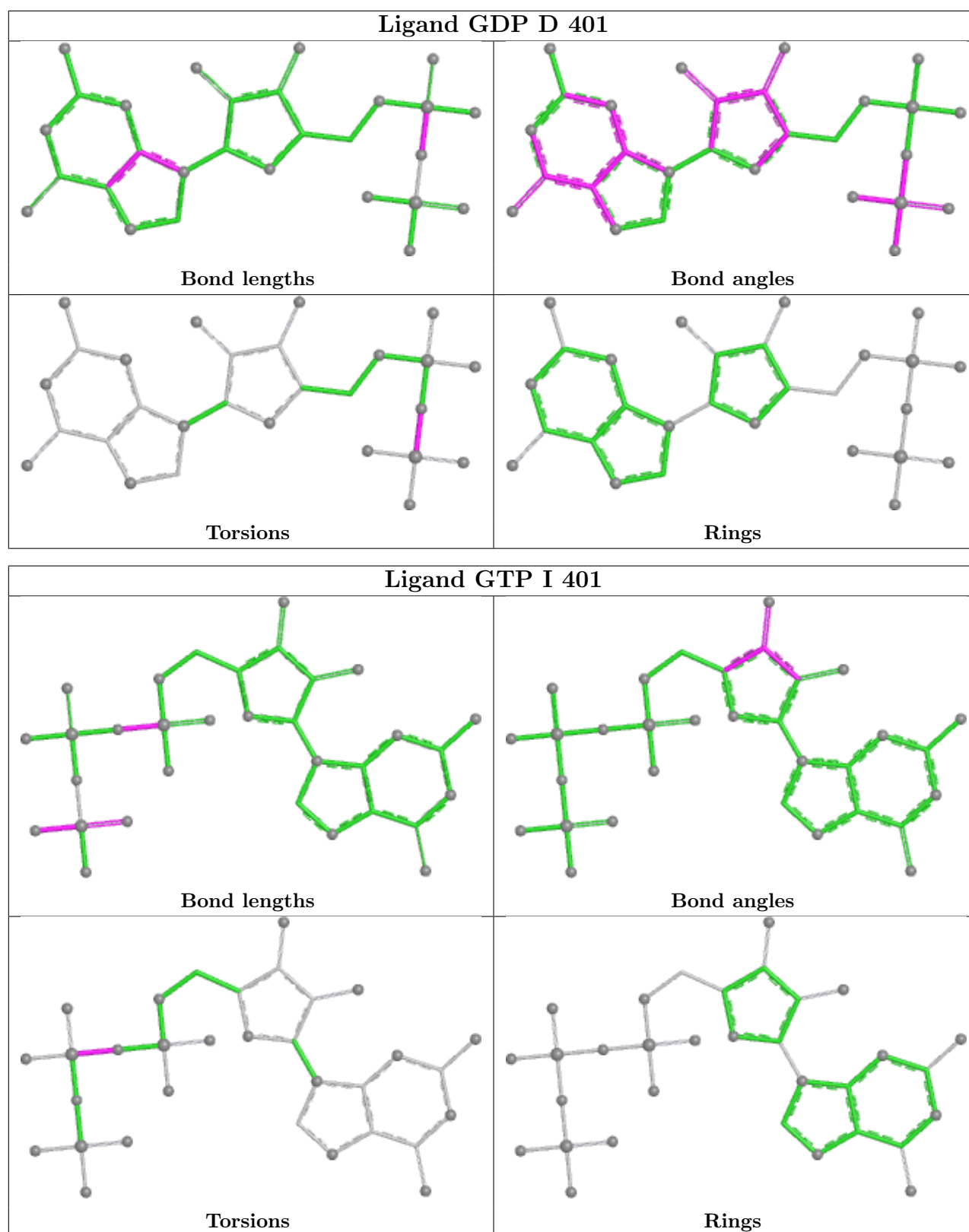
There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	401	GTP	4	0
8	J	401	GDP	2	0
8	D	401	GDP	3	0
7	I	401	GTP	4	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

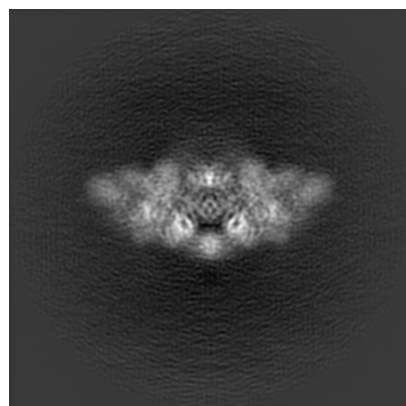
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10132. These allow visual inspection of the internal detail of the map and identification of artifacts.

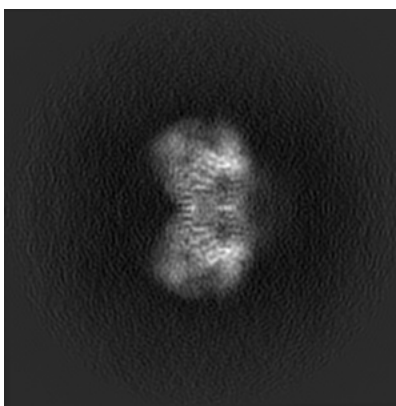
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

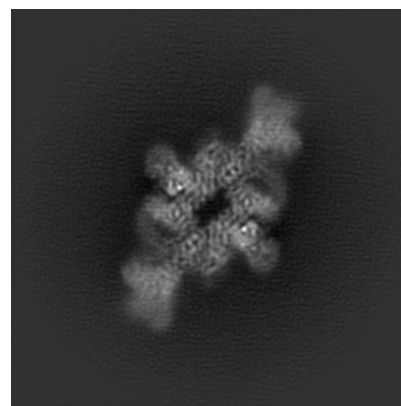
6.1.1 Primary map



X

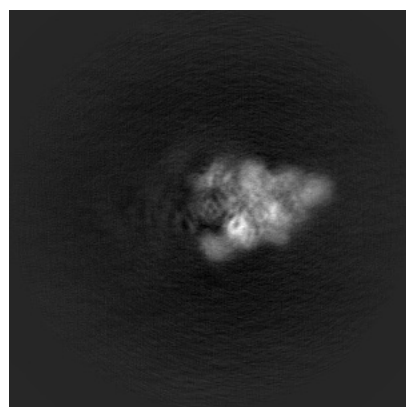


Y

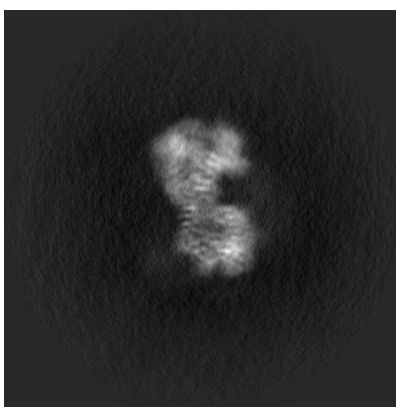


Z

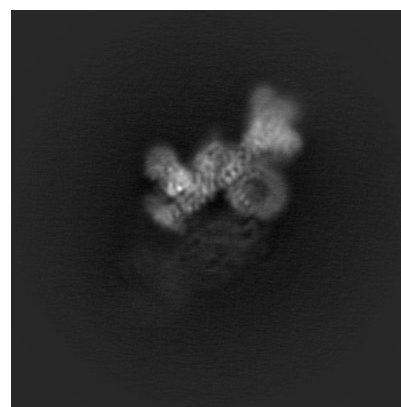
6.1.2 Raw map



X



Y

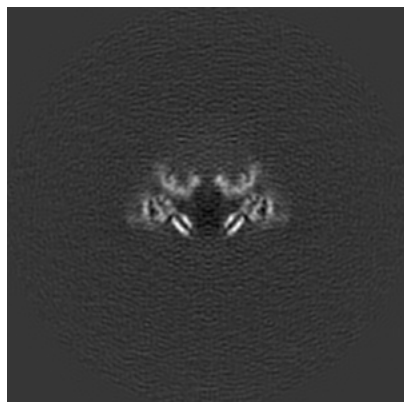


Z

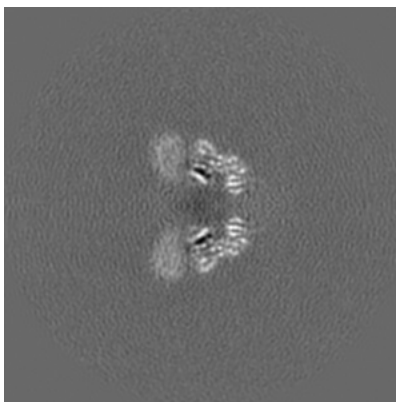
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

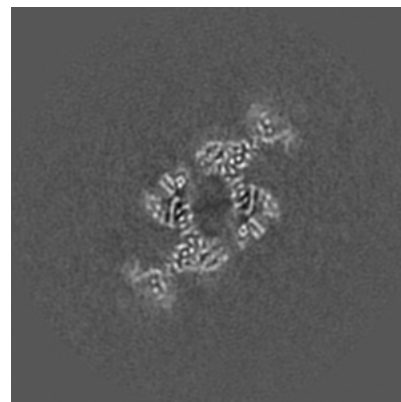
6.2.1 Primary map



X Index: 175

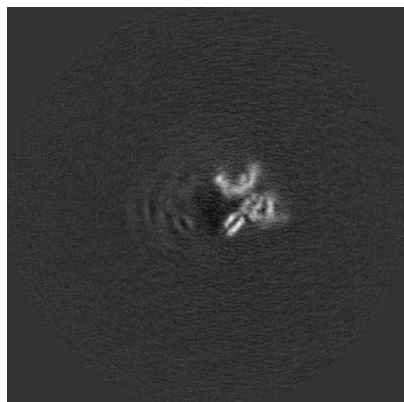


Y Index: 175

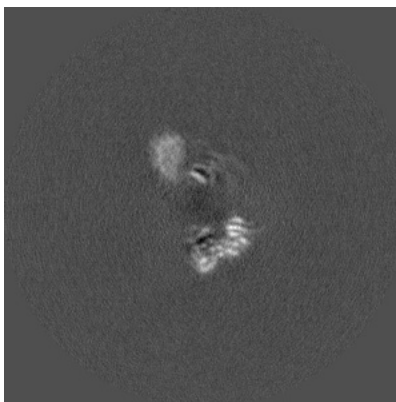


Z Index: 175

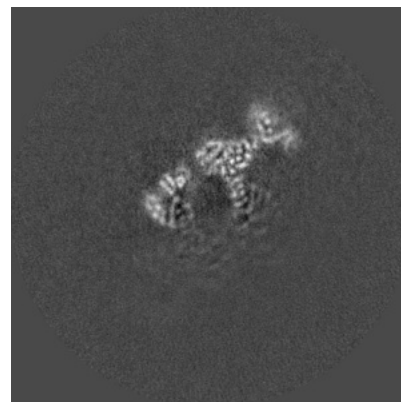
6.2.2 Raw map



X Index: 175



Y Index: 175

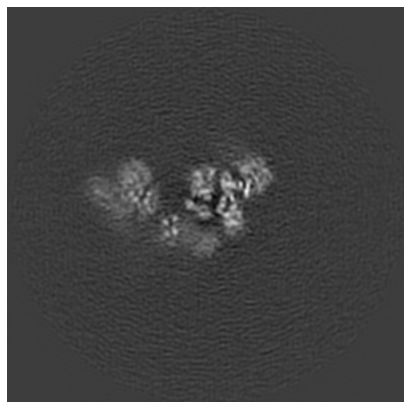


Z Index: 175

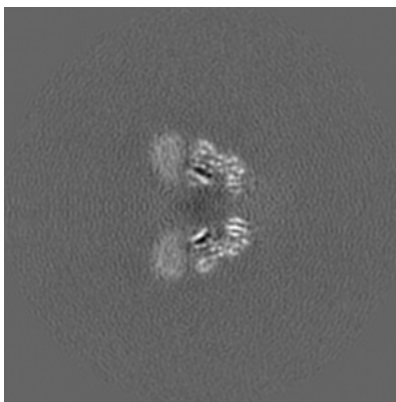
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

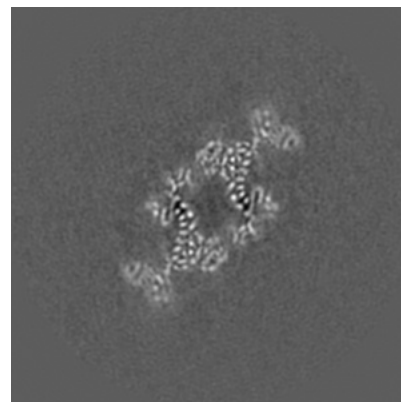
6.3.1 Primary map



X Index: 139

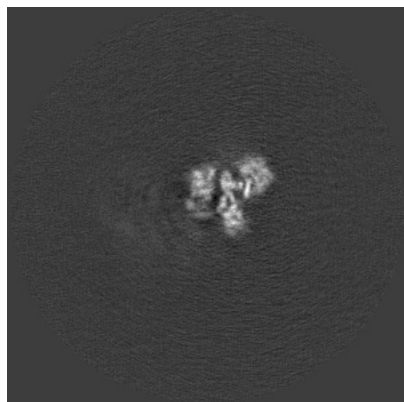


Y Index: 176

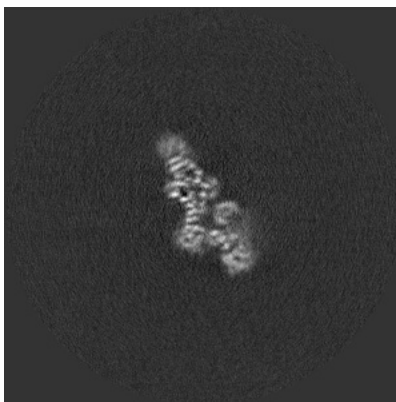


Z Index: 172

6.3.2 Raw map



X Index: 139



Y Index: 205

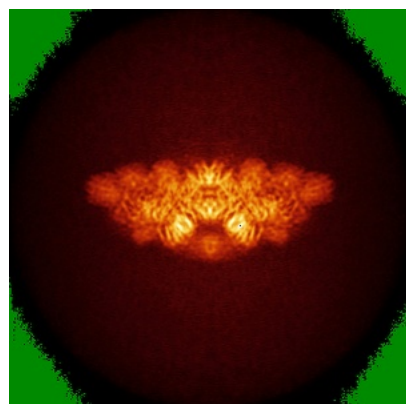


Z Index: 197

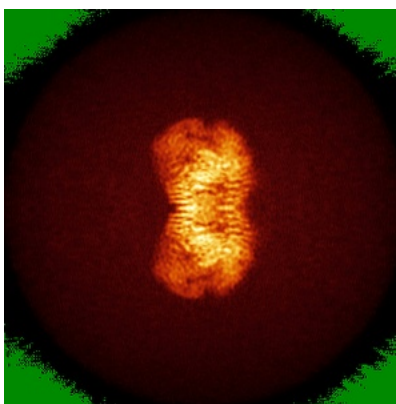
The images above show the largest variance slices of the map in three orthogonal directions.

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

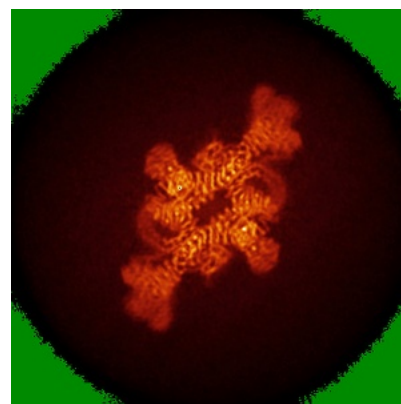
6.4.1 Primary map



X

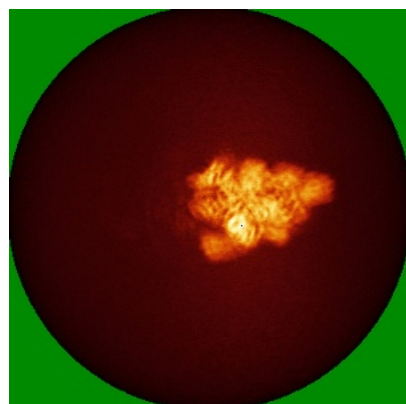


Y

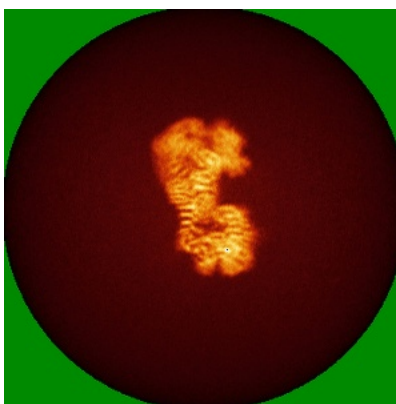


Z

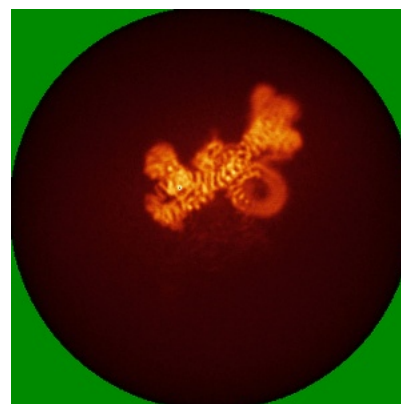
6.4.2 Raw map



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 0.018. 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.

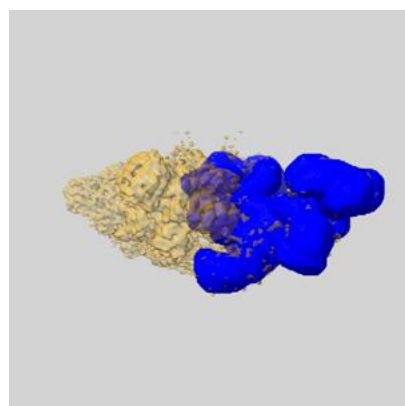
6.6 Mask visualisation [i](#)

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

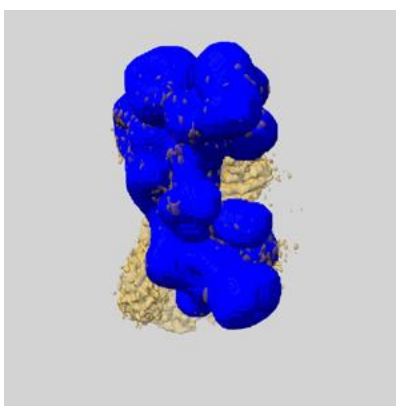
A mask typically either:

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

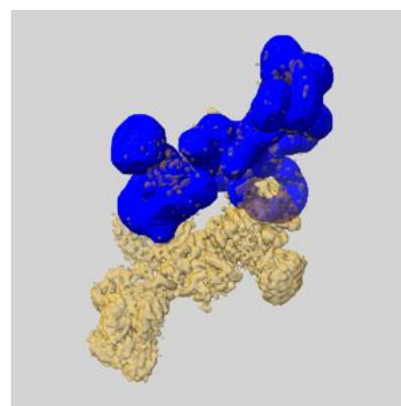
6.6.1 emd_10132_msk_1.map [i](#)



X



Y

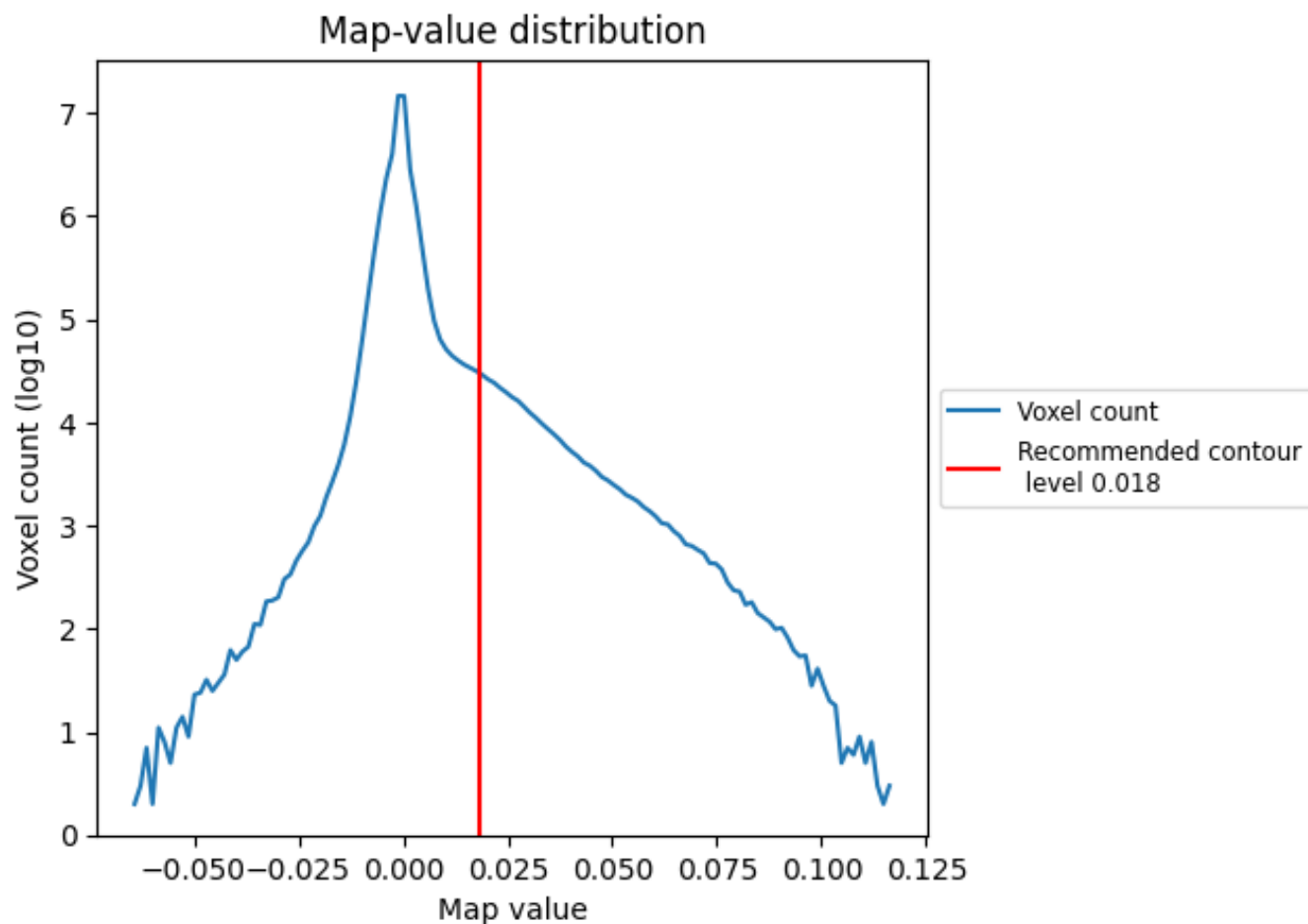


Z

7 Map analysis [i](#)

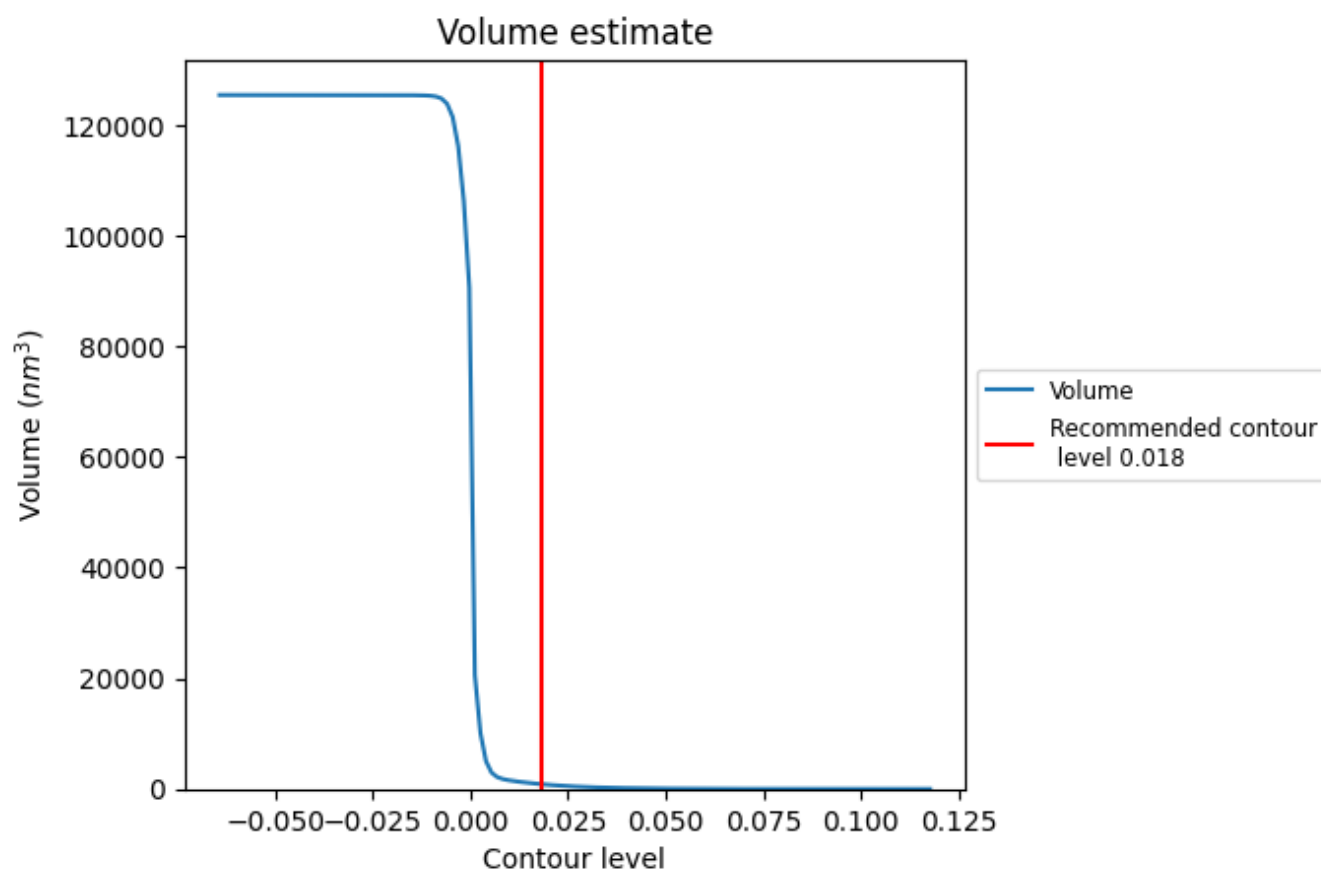
This section contains the results of statistical analysis of the map.

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.

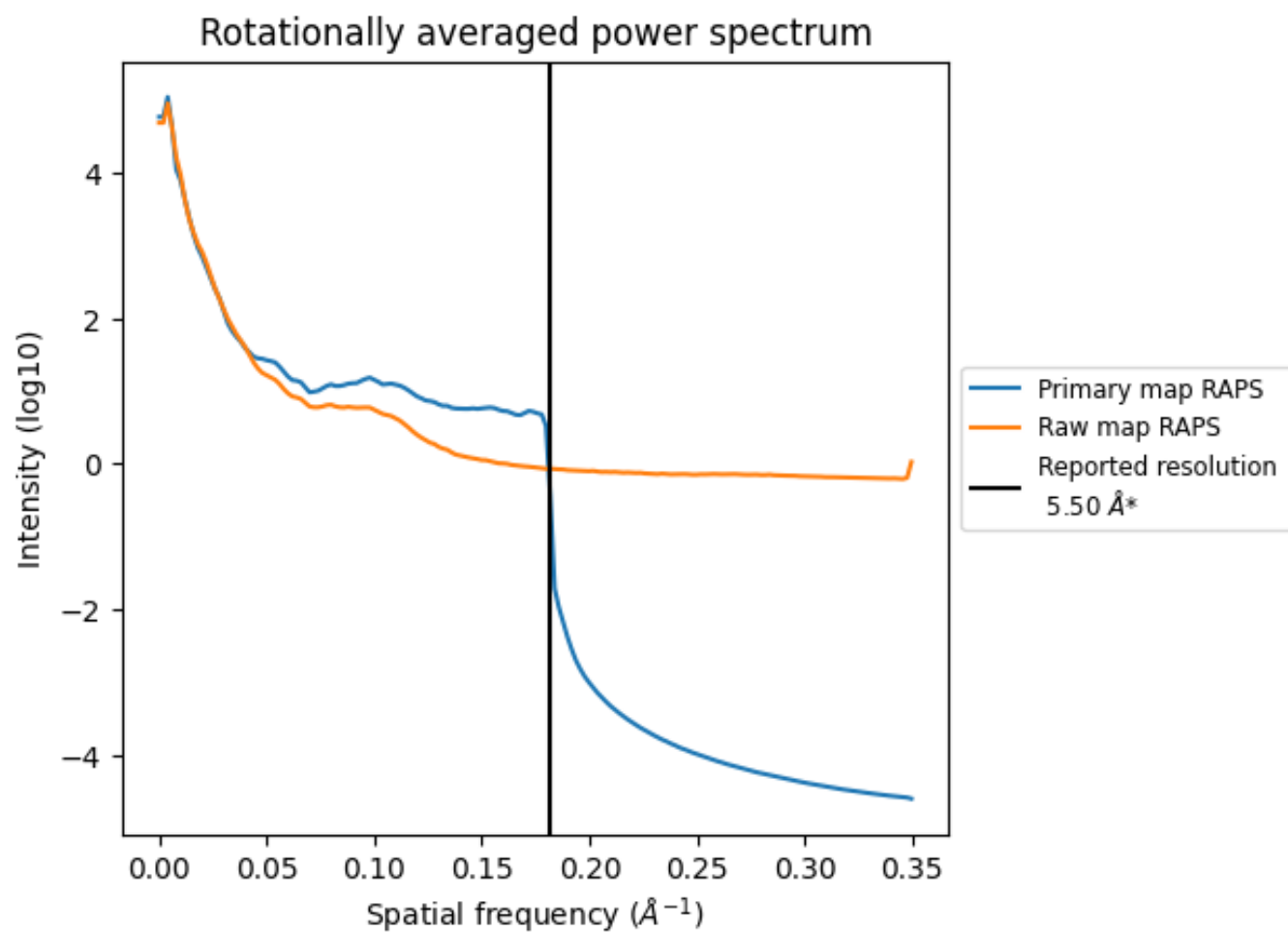
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 880 nm³; this corresponds to an approximate mass of 795 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 ⓘ

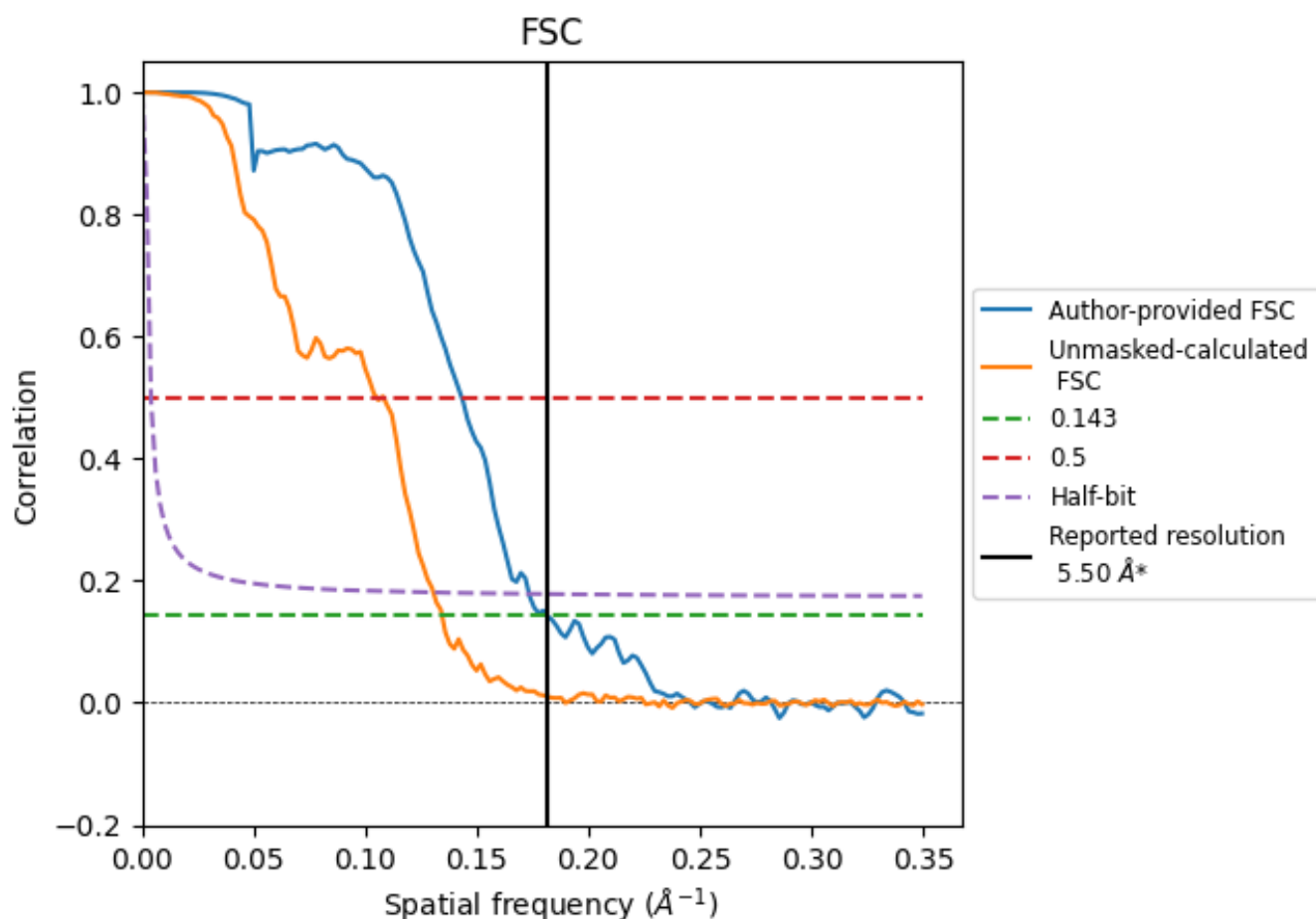


*Reported resolution corresponds to spatial frequency of 0.182 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.182 Å⁻¹

8.2 Resolution estimates [i](#)

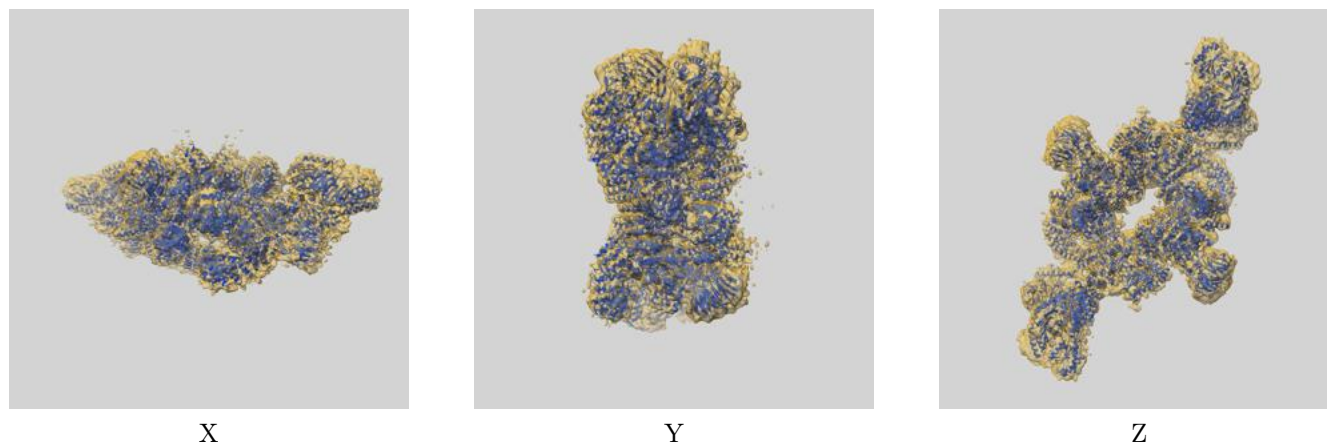
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.50	-	-
Author-provided FSC curve	5.51	6.98	5.76
Unmasked-calculated*	7.44	9.51	7.66

*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 7.44 differs from the reported value 5.5 by more than 10 %

9 Map-model fit [i](#)

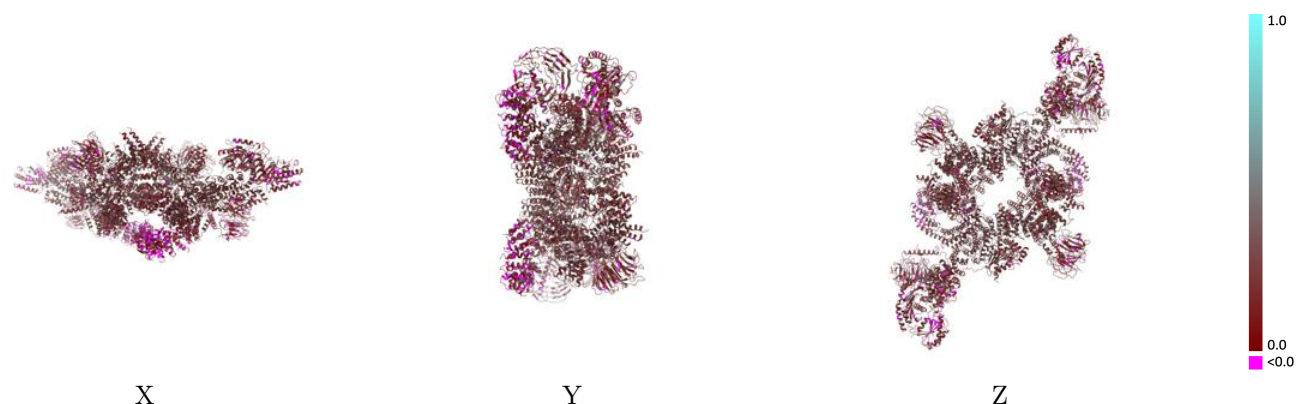
This section contains information regarding the fit between EMDB map EMD-10132 and PDB model 6SB0. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



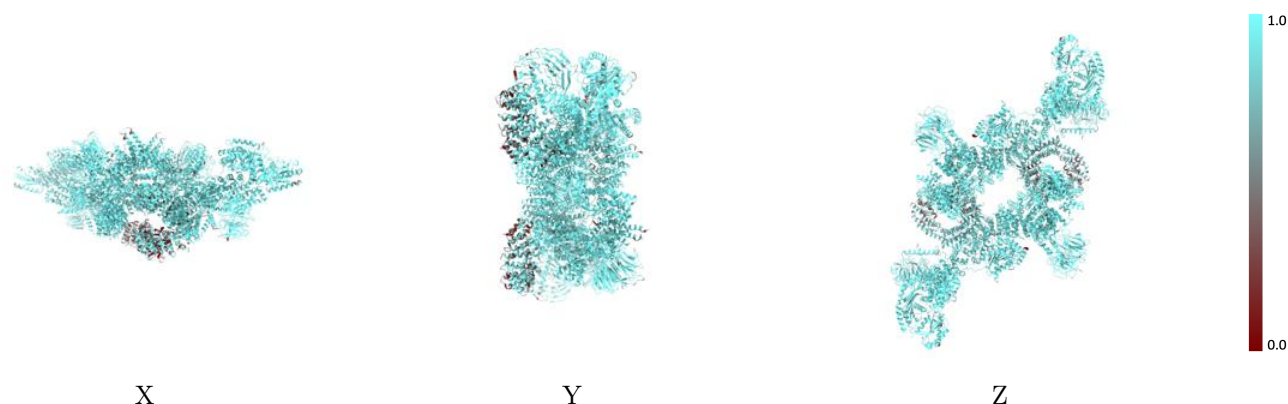
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



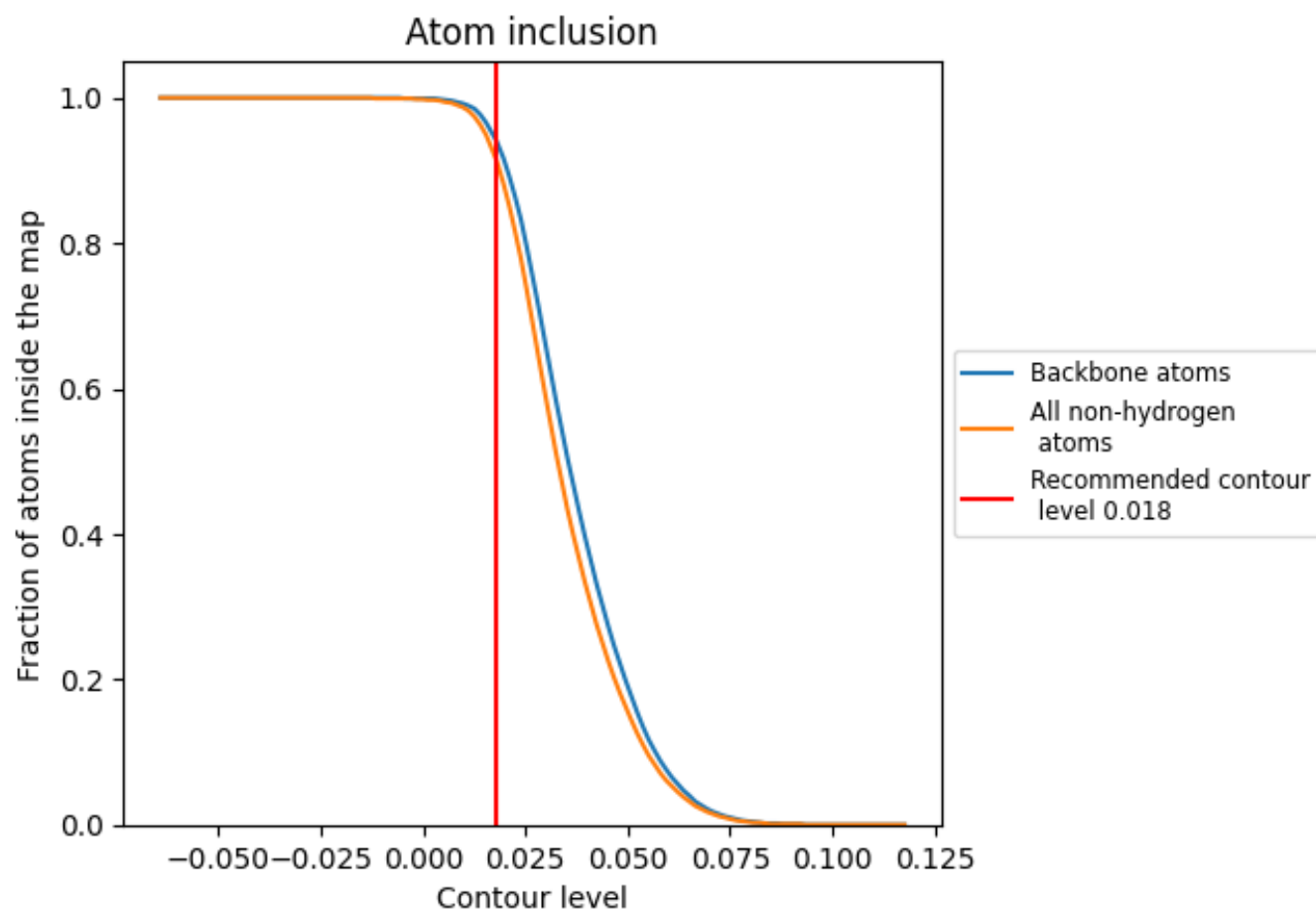
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 91% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9130	0.2370
A	0.8840	0.2290
B	0.8920	0.2350
C	0.9330	0.2270
D	0.9190	0.1820
E	0.9470	0.2320
H	0.9490	0.2240
I	0.9330	0.2250
J	0.9260	0.1860
N	0.9500	0.2630
O	0.7460	0.2690
T	0.7690	0.2640
Y	0.9500	0.2650

