



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:52 AM UTC

PDB ID : 9L4D / pdb_00009l4d
EMDB ID : EMD-62811
Title : ATR-ATRIP bound with RP-3500
Authors : Wang, G.
Deposited on : 2024-12-20
Resolution : 3.79 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

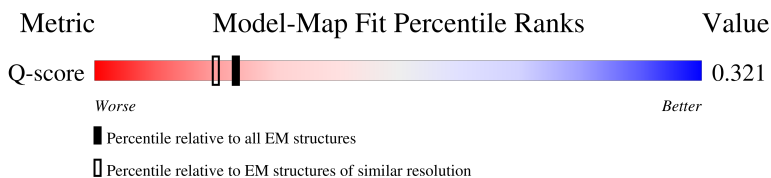
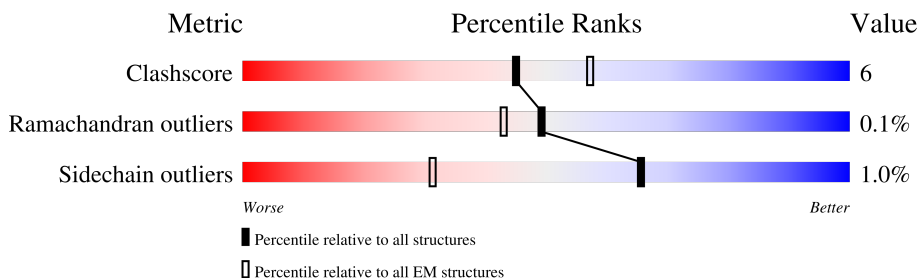
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

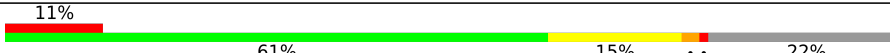
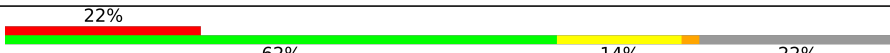
The reported resolution of this entry is 3.79 Å.

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	10018 (3.29 - 4.29)

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	2637	
1	B	2637	
2	C	491	
2	D	491	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 67221 atoms, of which 29861 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.

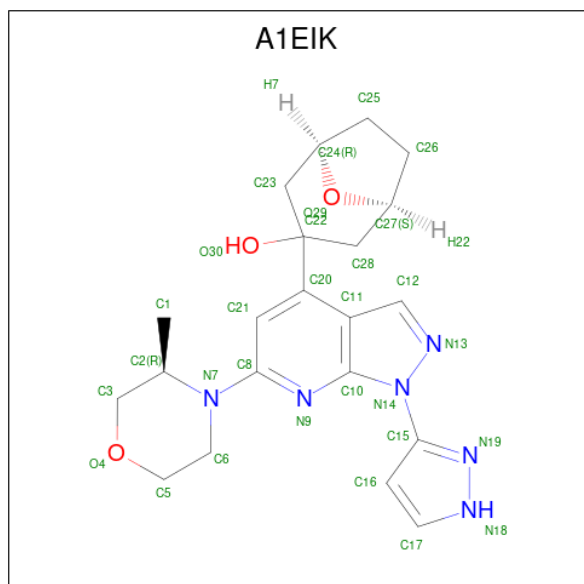
- Molecule 1 is a protein called Serine/threonine-protein kinase ATR.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2473	Total	C	H	N	O	S	0	0
			26772	9217	11475	2847	3181	52		
1	B	2497	Total	C	H	N	O	S	0	0
			31311	10642	14272	3025	3281	91		

- Molecule 2 is a protein called ATR-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	382	Total	C	H	N	O	S	0	0
			4498	1510	2026	462	485	15		
2	C	382	Total	C	H	N	O	S	0	0
			4579	1521	2088	461	485	24		

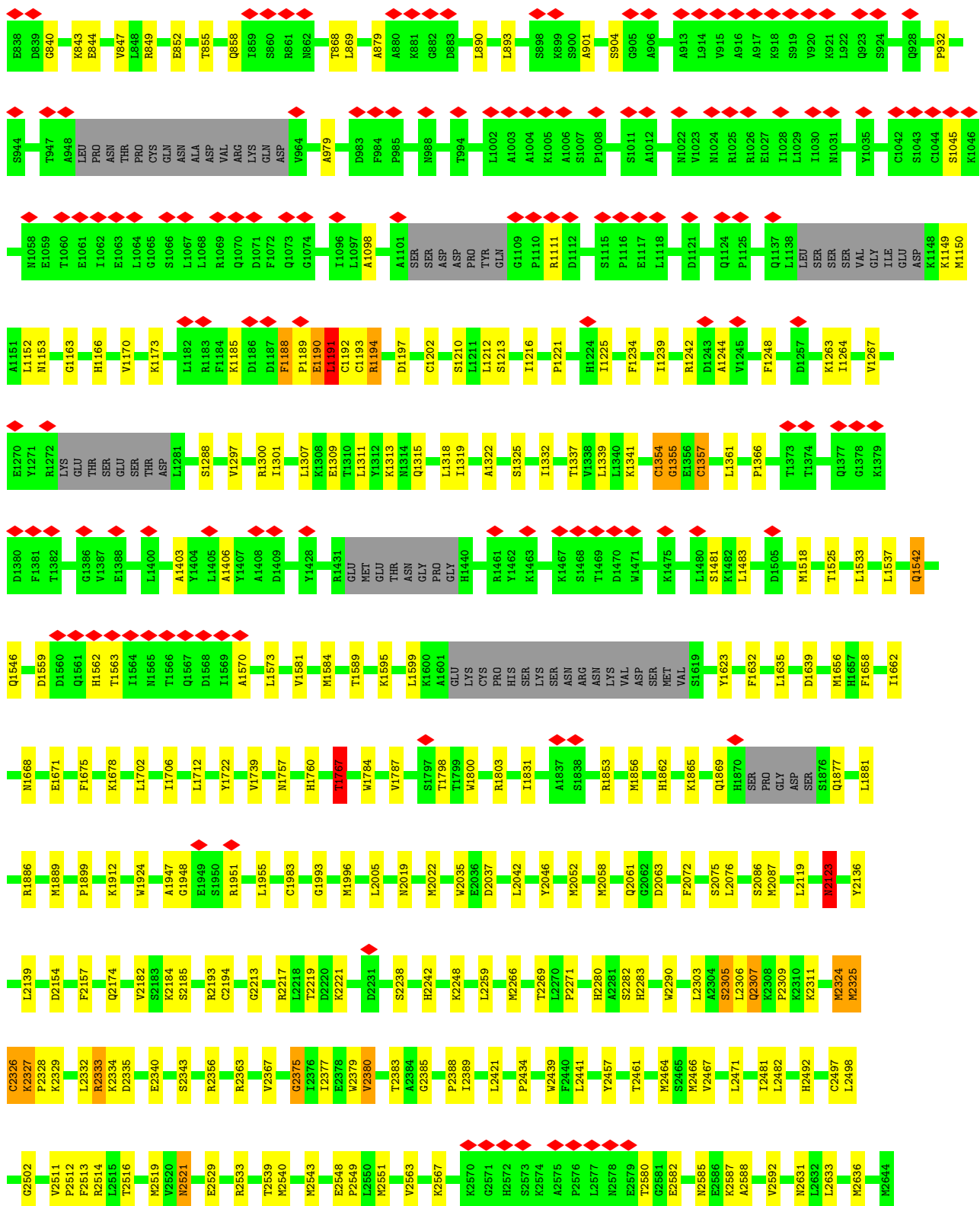
- Molecule 3 is Camonsertib (CCD ID: A1EIK) (formula: $C_{21}H_{26}N_6O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			30	21	6	3	
3	B	1	Total	C	N	O	0
			30	21	6	3	

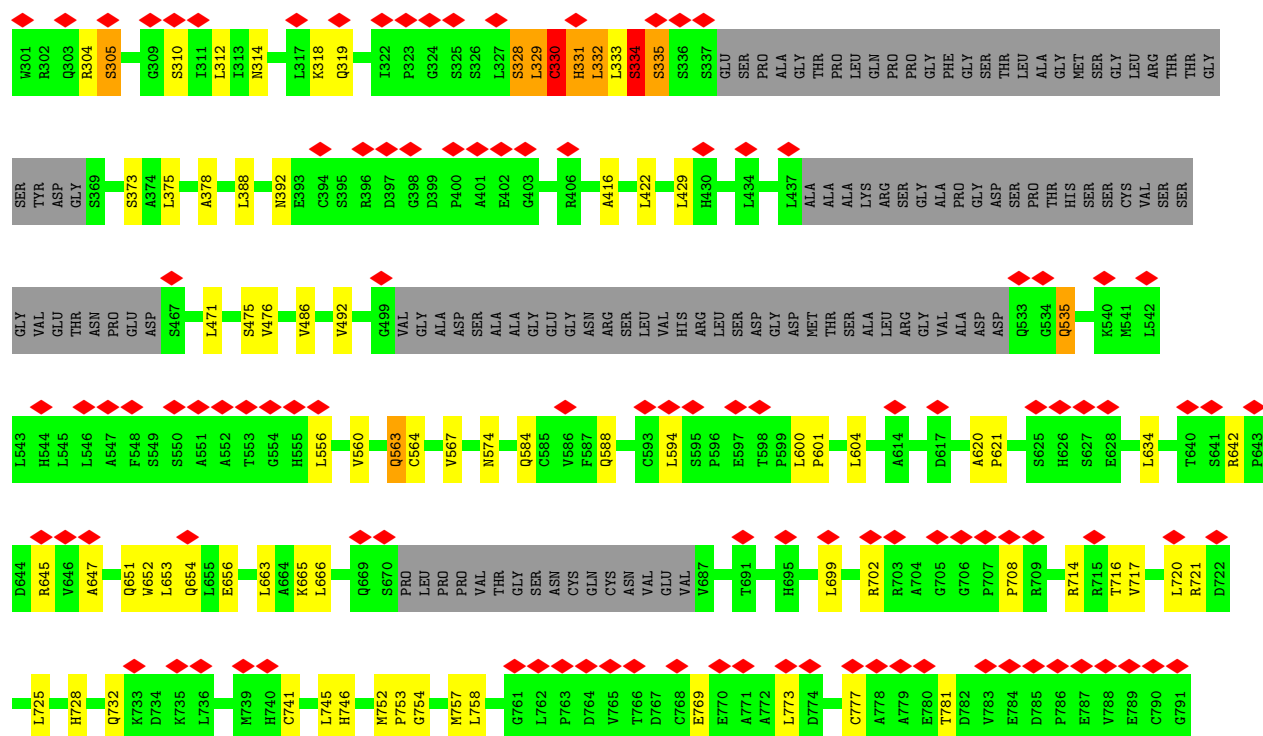
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total	Zn	0
			1	1	

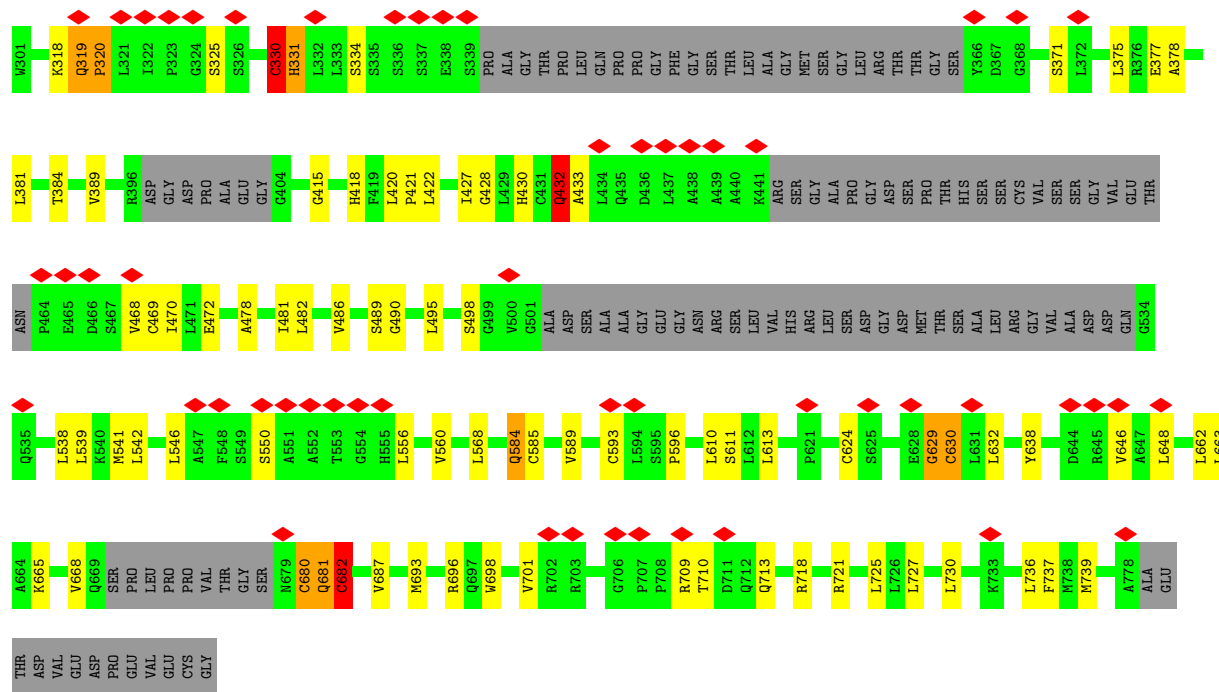


• Molecule 2: ATR-interacting protein





• Molecule 2: ATR-interacting protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77631	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.204	Depositor
Minimum map value	-0.640	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	314.88, 314.88, 314.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, A1EIK

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	0.34	10/15382 (0.1%)	0.50	16/21057 (0.1%)
1	B	0.38	6/17289 (0.0%)	0.62	38/23571 (0.2%)
2	C	0.45	2/2513 (0.1%)	0.82	12/3426 (0.4%)
2	D	0.69	6/2493 (0.2%)	0.72	7/3401 (0.2%)
All	All	0.40	24/37677 (0.1%)	0.60	73/51455 (0.1%)

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	3
1	B	0	5
2	D	0	2
All	All	0	10

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	330	CYS	C-O	-23.55	0.93	1.24
2	D	330	CYS	C-N	-5.83	1.25	1.33
1	B	751	HIS	ND1-CE1	5.61	1.38	1.32
1	B	737	HIS	ND1-CE1	5.45	1.38	1.32
1	B	830	HIS	ND1-CE1	5.42	1.38	1.32
1	A	1870	HIS	ND1-CE1	5.37	1.38	1.32
1	A	2289	HIS	ND1-CE1	5.28	1.37	1.32
1	A	2437	HIS	ND1-CE1	5.27	1.37	1.32
2	D	535	GLN	CD-OE1	5.22	1.33	1.23
1	A	661	GLN	CD-OE1	5.18	1.33	1.23
2	D	584	GLN	CD-OE1	5.16	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	GLN	CD-OE1	5.15	1.33	1.23
2	D	588	GLN	CD-OE1	5.15	1.33	1.23
1	A	2631	ASN	CG-OD1	5.14	1.33	1.23
1	B	1542	GLN	CD-OE1	5.12	1.33	1.23
2	D	563	GLN	CD-OE1	5.11	1.33	1.23
1	A	2131	ASN	CG-OD1	5.09	1.33	1.23
1	A	1022	ASN	CG-OD1	5.08	1.33	1.23
1	A	2591	HIS	ND1-CE1	5.08	1.37	1.32
1	A	2521	ASN	CG-OD1	5.08	1.33	1.23
2	C	432	GLN	CD-OE1	5.08	1.33	1.23
1	B	2521	ASN	CG-OD1	5.05	1.33	1.23
1	B	2123	ASN	CG-OD1	5.02	1.33	1.23
2	C	584	GLN	CD-OE1	5.01	1.33	1.23

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	682	CYS	N-CA-CB	14.97	132.13	110.12
2	D	330	CYS	N-CA-CB	14.64	134.69	110.39
1	B	1188	PHE	CB-CA-C	-13.90	89.17	110.02
1	B	1189	PRO	N-CA-C	-13.87	94.82	113.40
1	B	1767	THR	CA-CB-OG1	-11.30	92.64	109.60
2	C	681	GLN	N-CA-C	-10.70	88.02	110.80
1	B	1191	LEU	CA-C-N	-10.08	106.58	120.38
1	B	1191	LEU	C-N-CA	-10.08	106.58	120.38
2	C	331	HIS	N-CA-C	-10.07	100.31	111.28
1	B	1355	GLY	N-CA-C	-9.76	101.02	112.73
1	B	1767	THR	CA-C-O	-9.71	110.26	120.55
2	D	330	CYS	O-C-N	-8.83	110.59	122.43
2	C	331	HIS	CA-C-O	-8.53	111.50	120.55
1	B	2326	CYS	N-CA-CB	8.31	122.23	109.85
2	D	334	SER	N-CA-C	-8.30	102.24	111.28
1	B	2324	MET	O-C-N	-8.22	113.39	123.33
2	C	320	PRO	N-CA-CB	-7.80	96.17	103.19
2	C	330	CYS	CB-CA-C	-7.70	96.38	110.63
1	B	1185	LYS	N-CA-C	-7.21	103.11	110.97
1	A	2326	CYS	N-CA-CB	7.15	120.63	109.83
1	B	1190	GLU	CA-C-N	7.11	129.80	120.28
1	B	1190	GLU	C-N-CA	7.11	129.80	120.28
1	B	2327	LYS	CB-CA-C	6.95	117.05	110.17
1	B	830	HIS	CB-CG-CD2	-6.70	122.50	131.20
1	B	1189	PRO	N-CA-CB	6.68	110.92	103.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2307	GLN	CB-CA-C	6.68	121.28	109.72
1	A	2591	HIS	CB-CG-CD2	-6.66	122.54	131.20
1	B	751	HIS	CB-CG-CD2	-6.66	122.55	131.20
1	A	1208	LEU	CA-C-O	-6.65	110.81	120.13
1	A	2437	HIS	CB-CG-CD2	-6.59	122.64	131.20
1	A	2289	HIS	CB-CG-CD2	-6.58	122.64	131.20
2	C	682	CYS	N-CA-C	-6.57	104.12	111.28
1	B	737	HIS	CB-CG-CD2	-6.56	122.67	131.20
1	A	1870	HIS	CB-CG-CD2	-6.53	122.71	131.20
1	A	2432	HIS	CB-CG-CD2	-6.51	122.74	131.20
2	D	330	CYS	N-CA-C	-6.49	104.63	112.54
1	B	2306	LEU	N-CA-C	-6.42	104.28	111.28
1	B	1191	LEU	CA-C-O	-6.38	113.79	120.55
1	B	1191	LEU	N-CA-CB	6.33	119.43	110.12
1	B	1188	PHE	N-CA-C	6.15	120.32	108.45
2	C	680	CYS	CA-CB-SG	6.12	128.48	114.40
1	B	1357	CYS	CB-CA-C	-6.03	100.78	110.79
1	B	1173	LYS	N-CA-C	-6.00	104.81	111.36
2	C	319	GLN	N-CA-C	-5.95	100.23	109.87
1	B	2375	GLY	CA-C-O	-5.90	115.68	121.76
1	B	1589	THR	N-CA-C	-5.85	104.81	111.07
1	B	830	HIS	CB-CG-ND1	5.78	131.37	122.70
1	A	1870	HIS	CB-CG-ND1	5.78	131.37	122.70
1	B	751	HIS	CB-CG-ND1	5.70	131.25	122.70
1	A	2324	MET	O-C-N	-5.70	116.66	123.27
1	A	2591	HIS	CB-CG-ND1	5.64	131.16	122.70
1	B	737	HIS	CB-CG-ND1	5.62	131.13	122.70
1	A	2437	HIS	CB-CG-ND1	5.62	131.13	122.70
2	D	332	LEU	N-CA-CB	5.62	118.37	110.12
1	A	2289	HIS	CB-CG-ND1	5.55	131.02	122.70
1	A	2432	HIS	CB-CG-ND1	5.53	131.00	122.70
2	D	330	CYS	CB-CA-C	-5.51	98.80	110.31
1	B	1354	CYS	CB-CA-C	5.38	120.05	109.72
1	B	1045	SER	CA-C-O	-5.38	115.86	121.99
1	B	2335	ASP	CA-C-N	5.38	127.93	120.29
1	B	2335	ASP	C-N-CA	5.38	127.93	120.29
2	C	681	GLN	N-CA-CB	5.29	119.42	110.49
2	C	682	CYS	CA-CB-SG	5.22	126.41	114.40
1	B	2325	MET	N-CA-C	5.21	117.40	108.90
1	B	1197	ASP	N-CA-C	-5.20	105.04	111.33
2	C	680	CYS	CA-C-O	-5.14	114.29	120.10
1	A	1208	LEU	CA-C-N	5.14	125.68	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1208	LEU	C-N-CA	5.14	125.68	119.98
1	B	2481	ILE	CA-C-O	-5.12	115.72	121.36
1	B	979	ALA	CA-C-O	-5.12	115.12	120.55
1	A	504	THR	N-CA-C	-5.07	105.94	111.82
1	B	504	THR	N-CA-C	-5.06	105.76	111.28
2	D	331	HIS	N-CA-C	-5.04	100.06	110.80

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2333	ARG	Sidechain
1	A	2475	ASP	Mainchain
1	A	2547	ARG	Sidechain
1	B	1194	ARG	Sidechain
1	B	1767	THR	Mainchain
1	B	2324	MET	Mainchain
1	B	2333	ARG	Sidechain
1	B	2363	ARG	Sidechain
2	D	305	SER	Mainchain
2	D	328	SER	Mainchain

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	A	15297	11475	11498	103	0
1	B	17039	14272	14390	220	0
2	C	2491	2088	2096	56	0
2	D	2472	2026	2034	55	0
3	A	30	0	0	1	0
3	B	30	0	0	0	0
4	C	1	0	0	0	0
All	All	37360	29861	30018	424	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 6.

All (424) 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)
2:D:330:CYS:O	2:D:331:HIS:C	2.08	0.91
2:D:330:CYS:O	2:D:330:CYS:SG	2.35	0.84
1:B:2514:ARG:HG3	1:B:2519:MET:HE1	1.62	0.82
1:A:2366:ALA:HB1	1:A:2368:ILE:HD11	1.62	0.81
2:C:680:CYS:C	2:C:682:CYS:H	1.88	0.81
2:C:680:CYS:C	2:C:682:CYS:N	2.49	0.71
2:D:752:MET:HE2	2:D:777:CYS:H	1.57	0.70
2:D:330:CYS:HB2	2:D:333:LEU:CB	2.24	0.67
1:B:2585:ASN:HB3	1:B:2588:ALA:HB2	1.76	0.66
1:B:1191:LEU:HA	1:B:1194:ARG:HE	1.62	0.64
1:B:279:HIS:HB3	1:B:283:MET:HE3	1.79	0.64
1:B:23:PRO:HA	1:B:26:TYR:HB3	1.79	0.64
2:D:330:CYS:O	2:D:332:LEU:N	2.31	0.64
1:A:2481:ILE:HD12	1:A:2514:ARG:HD3	1.80	0.64
1:B:724:LEU:HA	1:B:747:ALA:HA	1.81	0.63
1:B:901:ALA:HB1	2:D:746:HIS:HA	1.81	0.63
1:B:1149:LYS:O	1:B:1153:ASN:ND2	2.33	0.62
1:B:2303:LEU:HD12	1:B:2325:MET:HE2	1.81	0.62
2:C:319:GLN:O	2:C:320:PRO:C	2.42	0.59
1:B:890:LEU:HD23	1:B:893:LEU:HD12	1.83	0.59
2:D:752:MET:HE1	2:D:773:LEU:HA	1.83	0.59
1:B:2303:LEU:HD21	1:B:2311:LYS:HD2	1.84	0.58
2:D:330:CYS:C	2:D:332:LEU:N	2.56	0.58
1:B:763:CYS:O	1:B:767:LEU:N	2.27	0.57
2:C:378:ALA:HB1	2:C:422:LEU:HA	1.86	0.57
1:B:2332:LEU:HD22	1:B:2375:GLY:HA3	1.87	0.57
2:D:331:HIS:HB2	2:C:334:SER:CB	2.34	0.57
2:D:330:CYS:CB	2:D:333:LEU:CB	2.83	0.56
1:B:1366:PRO:O	1:B:2356:ARG:NH2	2.36	0.56
1:B:890:LEU:HD11	1:B:932:PRO:CB	2.37	0.55
2:D:310:SER:C	2:D:312:LEU:H	2.14	0.55
2:C:550:SER:HG	2:C:593:CYS:HG	1.54	0.54
1:B:1656:MET:HE3	1:B:2441:LEU:HD22	1.89	0.54
2:D:330:CYS:SG	2:D:333:LEU:CB	2.96	0.54
1:B:2332:LEU:HD23	1:B:2367:VAL:HG12	1.90	0.53
1:B:2511:VAL:HG12	1:B:2636:MET:HE3	1.91	0.53
1:B:2072:PHE:O	1:B:2075:SER:OG	2.24	0.53
2:D:330:CYS:O	2:D:333:LEU:N	2.41	0.53
2:D:330:CYS:SG	2:D:334:SER:N	2.82	0.53
1:A:2276:THR:C	1:A:2278:ALA:H	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:330:CYS:O	2:C:331:HIS:C	2.52	0.53
1:B:890:LEU:HD23	1:B:893:LEU:CD1	2.39	0.52
1:B:2551:MET:HE2	1:B:2592:VAL:HG13	1.91	0.52
2:C:736:LEU:HA	2:C:739:MET:HE2	1.90	0.52
1:A:1344:GLN:HB3	1:A:1835:SER:HA	1.90	0.52
1:B:1518:MET:HE2	1:B:1525:THR:HA	1.92	0.52
2:C:371:SER:O	2:C:375:LEU:N	2.41	0.52
1:A:1677:GLN:OE1	1:A:1696:ARG:NH2	2.41	0.52
1:B:1886:ARG:HA	1:B:1889:MET:HE3	1.91	0.52
1:A:2189:MET:HE3	1:A:2580:THR:HA	1.90	0.51
2:D:378:ALA:HB1	2:D:422:LEU:HA	1.93	0.51
1:A:1204:ASP:OD2	1:A:1207:CYS:N	2.39	0.51
1:A:2464:MET:HE3	1:A:2492:HIS:HB2	1.93	0.51
1:B:656:TYR:O	1:B:660:LEU:N	2.43	0.51
1:A:963:ASP:N	1:A:963:ASP:OD1	2.43	0.50
2:D:717:VAL:O	2:D:721:ARG:HG3	2.11	0.50
2:C:495:LEU:O	2:C:498:SER:OG	2.25	0.50
2:C:468:VAL:O	2:C:472:GLU:HG2	2.12	0.50
1:A:1373:THR:OG1	1:A:1374:THR:N	2.45	0.50
1:B:2466:MET:HE2	1:B:2540:MET:HG2	1.92	0.50
1:A:2234:SER:O	1:A:2234:SER:OG	2.30	0.50
1:B:2307:GLN:HG2	1:B:2328:PRO:HD2	1.94	0.50
1:A:2327:LYS:HB3	1:A:2332:LEU:HD11	1.93	0.49
2:D:330:CYS:C	2:C:330:CYS:SG	2.94	0.49
1:A:1886:ARG:HA	1:A:1889:MET:HE2	1.94	0.49
1:B:2332:LEU:O	1:B:2333:ARG:C	2.55	0.49
1:B:2466:MET:HE2	1:B:2540:MET:CG	2.42	0.49
1:B:1152:LEU:HG	1:B:1191:LEU:HD22	1.94	0.49
2:D:331:HIS:CB	2:C:334:SER:CB	2.89	0.49
1:A:2575:ALA:HB3	1:A:2576:PRO:HD3	1.94	0.49
2:D:388:LEU:O	2:D:392:ASN:N	2.45	0.49
1:A:87:SER:OG	1:A:88:GLY:N	2.45	0.48
2:C:680:CYS:CB	2:C:682:CYS:H	2.24	0.48
1:B:787:HIS:HA	1:B:830:HIS:CE1	2.47	0.48
2:D:328:SER:O	2:D:329:LEU:CB	2.60	0.48
2:C:718:ARG:HE	2:C:721:ARG:HD3	1.78	0.48
1:A:2591:HIS:O	1:A:2595:ILE:HG12	2.13	0.48
1:B:276:LEU:O	1:B:280:LEU:HG	2.13	0.48
1:A:2416:ALA:HB3	1:A:2419:GLU:HG3	1.95	0.48
1:B:70:ASP:HA	1:B:73:GLN:NE2	2.29	0.48
1:A:2501:LYS:O	1:A:2504:THR:OG1	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1309:GLU:HG3	1:B:1313:LYS:HZ2	1.79	0.48
2:C:330:CYS:O	2:C:330:CYS:SG	2.61	0.48
1:B:203:GLU:O	1:B:244:ILE:HD11	2.14	0.48
1:B:726:SER:HA	1:B:745:LEU:HD11	1.95	0.48
1:A:1494:TRP:O	1:A:1498:LEU:HG	2.14	0.48
1:A:2338:LEU:HD11	1:A:2471:LEU:HD13	1.96	0.48
1:B:91:GLU:HG2	1:B:92:ALA:N	2.29	0.48
2:D:476:VAL:HB	2:D:563:GLN:NE2	2.29	0.48
2:C:718:ARG:HA	2:C:721:ARG:HD3	1.95	0.48
1:A:2352:ASP:HB3	1:A:2355:SER:HB3	1.95	0.47
1:B:1581:VAL:HA	1:B:1584:MET:HG2	1.96	0.47
2:D:318:LYS:HD3	2:D:319:GLN:O	2.13	0.47
2:D:754:GLY:O	2:D:758:LEU:HD23	2.14	0.47
1:B:720:GLY:HA3	1:B:749:SER:HA	1.97	0.47
1:B:2457:TYR:O	1:B:2461:THR:HG22	2.14	0.47
2:C:469:CYS:SG	2:C:470:ILE:N	2.87	0.47
1:B:2303:LEU:HD21	1:B:2311:LYS:CD	2.45	0.47
1:B:813:MET:HE1	1:B:868:THR:HB	1.96	0.47
1:A:2568:PRO:C	1:A:2570:LYS:H	2.22	0.47
1:B:554:VAL:C	1:B:556:LYS:H	2.22	0.47
2:C:687:VAL:HG22	2:C:730:LEU:HD13	1.96	0.47
1:B:1212:LEU:HD22	1:B:1248:PHE:HB3	1.97	0.47
1:B:1993:GLY:O	1:B:1996:MET:HG2	2.14	0.47
1:B:2305:SER:HB2	1:B:2309:PRO:HD3	1.97	0.47
1:B:2511:VAL:H	1:B:2636:MET:CE	2.27	0.47
2:C:320:PRO:CB	2:C:325:SER:O	2.62	0.47
1:A:626:ASP:N	1:A:626:ASP:OD1	2.46	0.47
1:A:1895:ARG:HH12	1:A:2357:ARG:NH2	2.13	0.47
1:B:281:VAL:HG22	1:B:333:VAL:HG12	1.96	0.47
2:D:600:LEU:HD21	2:D:651:GLN:HB3	1.97	0.47
2:C:648:LEU:HD23	2:C:648:LEU:H	1.79	0.47
1:B:1675:PHE:HA	1:B:1678:LYS:HD3	1.97	0.47
1:B:213:LEU:HB3	1:B:251:PHE:CZ	2.50	0.46
1:B:1297:VAL:HG22	1:B:1300:ARG:HH21	1.79	0.46
1:B:832:LEU:HD12	1:B:879:ALA:HB3	1.97	0.46
2:D:556:LEU:O	2:D:560:VAL:HG23	2.15	0.46
1:B:251:PHE:O	1:B:255:LEU:HG	2.15	0.46
1:B:304:PRO:HB2	1:B:306:GLU:HG3	1.98	0.46
1:B:760:ALA:O	1:B:762:VAL:HG22	2.16	0.46
1:B:813:MET:HE3	1:B:869:LEU:HD22	1.96	0.46
1:B:1856:MET:HE1	1:B:1899:PRO:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2174:GLN:HA	1:B:2266:MET:HE1	1.97	0.46
1:B:2380:VAL:HG23	1:B:2383:THR:HG21	1.97	0.46
1:B:53:VAL:HG11	1:B:115:SER:C	2.40	0.46
1:B:1212:LEU:O	1:B:1216:ILE:HG12	2.15	0.46
1:B:1163:GLY:HA3	1:B:1202:CYS:C	2.41	0.46
1:A:605:ASP:O	1:A:609:LYS:HG2	2.14	0.46
1:A:2608:ARG:HG3	1:B:2052:MET:HG3	1.98	0.46
1:B:279:HIS:O	1:B:283:MET:HG2	2.16	0.46
1:B:352:TYR:HA	1:B:356:PHE:HD2	1.80	0.46
1:B:1354:CYS:HA	1:B:1357:CYS:CB	2.45	0.46
1:B:1355:GLY:HA2	1:B:1831:ILE:HD11	1.97	0.46
1:B:1234:PHE:CE2	1:B:1264:ILE:HG21	2.50	0.46
2:C:632:LEU:CB	2:C:682:CYS:HB3	2.46	0.46
1:B:203:GLU:O	1:B:207:VAL:HG23	2.15	0.46
1:B:382:VAL:O	1:B:386:GLU:HG2	2.16	0.46
1:B:890:LEU:HA	1:B:893:LEU:HD12	1.96	0.46
1:B:2182:VAL:HG12	1:B:2194:CYS:HB2	1.98	0.46
1:B:2385:GLY:C	1:B:2388:PRO:HD2	2.41	0.46
1:B:296:SER:O	1:B:300:LYS:HD3	2.16	0.46
1:B:688:VAL:H	1:B:762:VAL:HG12	1.81	0.46
1:B:1798:THR:HG23	1:B:1803:ARG:NH2	2.30	0.46
1:B:2334:LYS:HB2	1:B:2563:VAL:HG21	1.98	0.46
1:B:217:ILE:HA	1:B:220:VAL:HG22	1.97	0.45
1:B:1924:TRP:HB3	1:B:1947:ALA:HB2	1.97	0.45
1:B:2154:ASP:N	1:B:2154:ASP:OD1	2.49	0.45
1:A:1691:GLY:HA3	1:A:2530:GLY:HA2	1.97	0.45
1:A:2225:LEU:HG	1:A:2243:PHE:CE2	2.52	0.45
1:A:2268:PRO:HA	1:A:2286:PHE:HD1	1.81	0.45
1:B:1166:HIS:O	1:B:1170:VAL:HG12	2.17	0.45
1:B:1403:ALA:C	1:B:1406:ALA:H	2.24	0.45
1:B:2332:LEU:CD2	1:B:2375:GLY:HA3	2.46	0.45
2:D:600:LEU:HD13	2:D:647:ALA:HB1	1.97	0.45
2:D:725:LEU:O	2:D:728:HIS:ND1	2.49	0.45
1:A:659:ALA:O	1:A:662:SER:OG	2.28	0.45
1:A:2279:ASN:HB3	1:A:2282:SER:OG	2.16	0.45
1:A:1702:LEU:HD22	1:A:1728:LEU:HD12	1.98	0.45
1:A:2379:TRP:HA	3:A:2701:A1EIK:C3	2.47	0.45
1:A:31:GLN:O	1:A:35:GLN:N	2.50	0.45
1:A:1559:ASP:HB3	1:A:1562:HIS:NE2	2.32	0.45
1:A:1895:ARG:HH22	1:A:2357:ARG:CZ	2.29	0.45
1:B:73:GLN:HB3	1:B:77:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ARG:HD2	1:B:223:ARG:N	2.32	0.45
1:B:2434:PRO:HB2	1:B:2521:ASN:OD1	2.16	0.45
2:C:662:LEU:HD23	2:C:663:LEU:HD22	1.99	0.45
1:A:1645:SER:OG	1:A:1650:ALA:O	2.34	0.45
1:B:2280:HIS:C	1:B:2282:SER:H	2.23	0.45
1:A:2385:GLY:N	1:A:2482:LEU:HD23	2.32	0.45
1:B:1188:PHE:CB	1:B:1192:CYS:H	2.30	0.45
1:B:1339:LEU:HD22	1:B:1354:CYS:SG	2.57	0.45
1:B:2136:TYR:O	1:B:2139:LEU:HB3	2.17	0.45
2:C:482:LEU:O	2:C:486:VAL:HG22	2.17	0.45
1:A:213:LEU:O	1:A:217:ILE:N	2.50	0.45
1:B:327:VAL:HA	1:B:330:GLU:HG2	1.99	0.45
1:B:2022:MET:HE3	1:B:2022:MET:HB3	1.76	0.45
1:B:2325:MET:HE3	1:B:2379:TRP:CZ3	2.52	0.45
2:D:304:ARG:O	2:D:305:SER:C	2.60	0.45
2:D:741:CYS:O	2:D:745:LEU:N	2.50	0.45
1:B:1309:GLU:HG3	1:B:1313:LYS:NZ	2.32	0.44
1:B:1639:ASP:OD1	1:B:1639:ASP:N	2.51	0.44
1:A:727:SER:OG	1:A:728:LEU:N	2.50	0.44
1:A:1633:LEU:HD23	1:A:1633:LEU:HA	1.89	0.44
1:B:124:CYS:O	1:B:125:GLU:C	2.60	0.44
2:C:539:LEU:HD23	2:C:542:LEU:HD21	2.00	0.44
1:A:1597:GLN:O	1:A:1600:LYS:HG3	2.17	0.44
1:A:2121:LYS:HA	1:A:2124:LYS:HE2	1.99	0.44
1:B:53:VAL:HG23	1:B:55:LEU:H	1.82	0.44
1:B:1542:GLN:HG3	1:B:1546:GLN:NE2	2.32	0.44
2:C:478:ALA:HA	2:C:481:ILE:HD12	1.99	0.44
1:B:340:ASP:N	1:B:340:ASP:OD1	2.51	0.44
1:B:2248:LYS:HE3	1:B:2248:LYS:HB3	1.85	0.44
1:B:2548:GLU:HB2	1:B:2549:PRO:HD3	2.00	0.44
1:A:1260:GLU:O	1:A:1264:ILE:HG12	2.18	0.44
1:A:1620:THR:OG1	1:A:1622:ASP:OD1	2.32	0.44
1:A:1815:ASP:CB	1:A:1818:ALA:HB3	2.48	0.44
1:B:106:ARG:HH21	1:B:109:ARG:HD3	1.82	0.44
1:B:1190:GLU:O	1:B:1193:CYS:CB	2.66	0.44
1:B:2119:LEU:O	1:B:2123:ASN:OD1	2.35	0.44
2:C:556:LEU:O	2:C:560:VAL:HG22	2.17	0.44
1:A:552:GLU:O	1:A:623:ARG:NH1	2.50	0.44
1:A:1015:ARG:O	1:A:1019:LYS:HG2	2.17	0.44
1:A:1175:MET:HE3	1:A:1211:LEU:HD12	2.00	0.44
1:B:134:PHE:HD2	1:B:141:ILE:HG21	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2585:ASN:HD21	1:B:2587:LYS:HG2	1.83	0.44
2:C:418:HIS:C	2:C:421:PRO:HD2	2.42	0.44
1:B:1191:LEU:HA	1:B:1194:ARG:NE	2.31	0.44
2:D:332:LEU:O	2:D:335:SER:O	2.36	0.44
2:D:486:VAL:O	2:D:574:ASN:ND2	2.51	0.44
1:B:171:TRP:HB2	1:B:172:PRO:HD3	1.99	0.44
1:B:1307:LEU:O	1:B:1311:LEU:HG	2.18	0.44
1:B:1337:THR:O	1:B:1341:LYS:HG2	2.18	0.44
1:B:2076:LEU:HD23	1:B:2076:LEU:HA	1.79	0.44
2:D:314:ASN:O	2:D:318:LYS:HB2	2.18	0.44
2:C:420:LEU:HD11	2:C:538:LEU:HD22	1.99	0.44
2:C:630:CYS:SG	2:C:630:CYS:O	2.75	0.44
1:B:2389:ILE:HG23	1:B:2439:TRP:CD1	2.53	0.43
1:A:1045:SER:O	1:A:1049:LEU:N	2.40	0.43
1:A:2434:PRO:HB2	1:A:2521:ASN:OD1	2.18	0.43
1:B:817:ASP:OD2	1:B:820:VAL:HG23	2.18	0.43
1:B:2035:TRP:CZ2	1:B:2037:ASP:HB2	2.53	0.43
1:B:2467:VAL:O	1:B:2471:LEU:HB2	2.18	0.43
1:A:355:LYS:HG3	1:A:356:PHE:N	2.33	0.43
1:B:760:ALA:C	1:B:762:VAL:H	2.25	0.43
1:B:1150:MET:SD	1:B:1150:MET:N	2.91	0.43
1:B:1668:ASN:O	1:B:1671:GLU:HG2	2.18	0.43
2:C:725:LEU:HD12	2:C:725:LEU:HA	1.79	0.43
2:D:331:HIS:CG	2:D:332:LEU:N	2.83	0.43
1:A:2528:THR:O	1:A:2532:PHE:HB3	2.19	0.43
1:A:2568:PRO:O	1:A:2570:LYS:HD3	2.19	0.43
1:B:373:ARG:O	1:B:377:LYS:HG2	2.18	0.43
1:B:1190:GLU:H	1:B:1194:ARG:HH21	1.67	0.43
1:B:1757:ASN:HA	1:B:1760:HIS:HB3	2.01	0.43
2:D:753:PRO:O	2:D:757:MET:HG2	2.19	0.43
1:A:2088:PRO:O	1:A:2092:THR:OG1	2.33	0.43
1:B:153:PHE:O	1:B:157:VAL:HG22	2.19	0.43
1:B:2340:GLU:O	1:B:2343:SER:OG	2.30	0.43
2:D:652:TRP:O	2:D:656:GLU:HG2	2.19	0.43
2:C:381:LEU:O	2:C:384:THR:OG1	2.35	0.43
2:C:472:GLU:OE1	2:C:560:VAL:HG11	2.17	0.43
1:A:693:ILE:O	1:A:697:LYS:HG2	2.18	0.43
1:B:2005:LEU:HD12	1:B:2005:LEU:HA	1.84	0.43
1:A:2326:CYS:HA	1:A:2376:ILE:HA	2.01	0.43
1:B:704:LYS:NZ	1:B:774:ILE:HG23	2.33	0.43
1:B:2058:MET:HA	1:B:2061:GLN:CD	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2539:THR:O	1:B:2543:MET:HG2	2.19	0.43
2:C:629:GLY:O	2:C:682:CYS:SG	2.77	0.43
1:A:453:HIS:CE1	1:A:533:THR:HG23	2.53	0.43
1:A:1431:ARG:HD2	1:A:1431:ARG:HA	1.74	0.43
1:A:1449:HIS:O	1:A:1453:ILE:HG12	2.19	0.43
1:B:285:THR:OG1	1:B:286:ASP:N	2.52	0.43
1:B:1595:LYS:O	1:B:1599:LEU:HG	2.19	0.43
2:C:418:HIS:O	2:C:421:PRO:HD2	2.19	0.43
1:A:2622:TYR:O	1:A:2626:GLU:HG2	2.19	0.43
1:B:735:HIS:CE1	1:B:738:VAL:HA	2.54	0.43
1:B:1635:LEU:HD23	1:B:1635:LEU:HA	1.88	0.43
1:B:2512:PRO:HB2	1:B:2513:PHE:CD1	2.53	0.43
1:B:12:ILE:N	1:B:13:PRO:HD2	2.34	0.42
1:B:135:LYS:HA	1:B:142:PHE:HB2	2.01	0.42
1:B:261:LEU:HD12	1:B:262:PRO:HD2	2.01	0.42
1:B:1318:LEU:O	1:B:1322:ALA:N	2.50	0.42
1:B:2498:LEU:HD23	1:B:2498:LEU:HA	1.86	0.42
1:B:2516:THR:H	1:B:2519:MET:HE3	1.84	0.42
2:C:489:SER:OG	2:C:490:GLY:N	2.52	0.42
1:B:1862:HIS:ND1	1:B:1881:LEU:HD21	2.34	0.42
2:D:601:PRO:O	2:D:604:LEU:HG	2.19	0.42
1:A:162:ARG:O	1:A:166:GLY:N	2.52	0.42
1:B:901:ALA:N	2:D:781:THR:O	2.50	0.42
1:B:1098:ALA:HB1	1:B:1111:ARG:CB	2.50	0.42
1:B:1865:LYS:HE3	1:B:1877:GLN:HE22	1.84	0.42
1:B:1869:GLN:HG2	1:B:1877:GLN:HB3	2.01	0.42
1:A:144:VAL:O	1:A:148:GLU:HG3	2.20	0.42
1:A:2374:CYS:SG	1:A:2375:GLY:N	2.90	0.42
1:B:760:ALA:O	1:B:762:VAL:N	2.52	0.42
1:B:1767:THR:O	1:B:1767:THR:HG22	2.19	0.42
1:B:2238:SER:O	1:B:2242:HIS:ND1	2.52	0.42
2:D:716:THR:O	2:D:720:LEU:HG	2.19	0.42
2:C:377:GLU:O	2:C:381:LEU:HD23	2.19	0.42
1:A:1175:MET:HE2	1:A:1175:MET:HB2	1.95	0.42
1:A:2411:LEU:HD12	1:A:2420:LYS:HG2	2.01	0.42
1:B:1239:ILE:HA	1:B:1242:ARG:NH2	2.35	0.42
1:B:1800:TRP:CE3	1:B:1853:ARG:HD3	2.54	0.42
1:B:2063:ASP:OD1	1:B:2063:ASP:N	2.52	0.42
1:B:2157:PHE:CZ	1:B:2193:ARG:HD2	2.54	0.42
1:A:1240:GLU:N	1:A:1240:GLU:OE1	2.52	0.42
1:B:1784:TRP:HA	1:B:1787:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2182:VAL:HA	1:B:2185:SER:OG	2.20	0.42
1:A:1258:HIS:O	1:A:1262:LYS:N	2.53	0.42
1:B:147:LYS:HD2	1:B:147:LYS:HA	1.73	0.42
1:B:317:TYR:O	1:B:321:LEU:HD23	2.19	0.42
1:B:2529:GLU:HG3	1:B:2533:ARG:HH21	1.84	0.42
2:C:428:GLY:O	2:C:432:GLN:HG3	2.19	0.42
1:A:1885:ALA:O	1:A:1889:MET:HG3	2.19	0.42
1:A:2554:LEU:HD23	1:A:2554:LEU:HA	1.91	0.42
1:B:554:VAL:C	1:B:556:LYS:N	2.77	0.42
1:B:1722:TYR:HB3	1:B:1739:VAL:HG23	2.01	0.42
2:D:653:LEU:HD11	2:D:716:THR:HA	2.01	0.42
1:A:1541:ASN:OD1	1:A:1542:GLN:N	2.53	0.42
1:B:101:ASN:HB3	1:B:178:PHE:O	2.19	0.42
1:B:714:LEU:HA	1:B:717:THR:HG22	2.02	0.42
1:B:1263:LYS:O	1:B:1267:VAL:HG13	2.19	0.42
1:B:1562:HIS:CE1	1:B:1563:THR:HG23	2.55	0.42
1:B:1570:ALA:HA	1:B:1573:LEU:HB3	2.01	0.42
1:B:2497:CYS:SG	1:B:2502:GLY:N	2.93	0.42
2:D:651:GLN:HA	2:D:654:GLN:CD	2.45	0.42
2:C:727:LEU:HD22	2:C:737:PHE:HZ	1.84	0.42
1:A:686:ASN:OD1	1:A:687:ARG:N	2.52	0.42
1:A:1080:LEU:O	1:A:1083:ILE:HG22	2.19	0.42
1:A:2276:THR:HB	1:A:2279:ASN:H	1.85	0.42
1:B:89:SER:O	1:B:93:LYS:N	2.42	0.42
1:B:230:TRP:O	1:B:234:CYS:HB2	2.20	0.42
1:B:703:VAL:HA	1:B:706:GLU:HG3	2.02	0.42
1:B:849:ARG:O	1:B:852:GLU:HG3	2.19	0.42
1:B:1658:PHE:O	1:B:1662:ILE:HG22	2.19	0.42
1:A:1696:ARG:HH12	1:A:1704:GLU:HB3	1.85	0.41
1:B:26:TYR:HE2	1:B:85:ASN:HB2	1.84	0.41
1:B:2529:GLU:HG3	1:B:2533:ARG:NH2	2.34	0.41
2:D:699:LEU:HA	2:D:702:ARG:HH21	1.85	0.41
2:C:389:VAL:HG13	2:C:415:GLY:HA3	2.01	0.41
1:B:2213:GLY:O	1:B:2217:ARG:HD3	2.19	0.41
1:B:2580:THR:HG22	1:B:2582:GLU:HB2	2.02	0.41
1:A:139:PRO:O	2:C:668:VAL:HA	2.20	0.41
1:B:352:TYR:HA	1:B:356:PHE:CD2	2.55	0.41
1:B:2019:ASN:HA	1:B:2022:MET:HB2	2.02	0.41
1:B:2259:LEU:HD12	1:B:2290:TRP:HB3	2.02	0.41
2:C:585:CYS:O	2:C:589:VAL:HG23	2.20	0.41
1:A:895:CYS:O	1:A:898:SER:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LYS:O	1:B:36:ILE:HG12	2.20	0.41
1:B:142:PHE:CZ	1:B:219:ILE:HG23	2.56	0.41
1:B:1288:SER:HB3	1:B:1307:LEU:HD12	2.02	0.41
1:B:1297:VAL:O	1:B:1301:ILE:HG12	2.20	0.41
1:B:1332:ILE:HG23	1:B:1361:LEU:HD21	2.03	0.41
1:B:1948:GLY:HA2	1:B:1955:LEU:HD22	2.02	0.41
1:B:2184:LYS:NZ	1:B:2219:THR:OG1	2.45	0.41
2:C:611:SER:O	2:C:665:LYS:NZ	2.54	0.41
1:A:1236:TYR:O	1:A:1240:GLU:HB2	2.20	0.41
1:B:12:ILE:O	1:B:16:ARG:HG2	2.20	0.41
1:B:256:PHE:HD1	1:B:301:THR:HG22	1.85	0.41
1:A:581:SER:OG	1:A:587:LEU:HD11	2.21	0.41
1:A:1172:VAL:O	1:A:1176:THR:HG23	2.21	0.41
1:A:2422:LYS:O	1:A:2426:GLU:HG2	2.20	0.41
1:B:1242:ARG:C	1:B:1244:ALA:H	2.28	0.41
1:B:1559:ASP:HB3	1:B:1562:HIS:ND1	2.36	0.41
1:B:1599:LEU:HD22	1:B:1623:TYR:CD1	2.55	0.41
1:B:2385:GLY:HA2	1:B:2482:LEU:HB3	2.02	0.41
1:A:1423:GLU:O	1:A:1427:ILE:HG12	2.20	0.41
1:A:1665:LYS:O	1:A:1667:GLN:HG2	2.20	0.41
1:B:1210:SER:O	1:B:1213:SER:OG	2.25	0.41
2:D:620:ALA:HB3	2:D:621:PRO:HD3	2.03	0.41
1:B:210:LEU:HD13	1:B:247:LEU:HB2	2.02	0.41
1:B:222:PHE:HB3	2:D:665:LYS:HD3	2.01	0.41
1:B:364:ALA:HB1	2:C:381:LEU:HD22	2.03	0.41
1:A:453:HIS:NE2	1:A:531:VAL:HG13	2.36	0.41
1:B:366:GLN:OE1	2:C:381:LEU:HD21	2.21	0.41
1:B:795:PHE:HD1	1:B:802:VAL:HG13	1.85	0.41
1:B:1481:SER:O	1:B:1483:LEU:N	2.54	0.41
1:B:1533:LEU:HD21	1:B:1632:PHE:HE2	1.85	0.41
1:B:1537:LEU:HD11	1:B:1632:PHE:CD2	2.56	0.41
1:B:2421:LEU:HD22	1:B:2631:ASN:OD1	2.21	0.41
2:D:373:SER:C	2:D:375:LEU:H	2.28	0.41
2:D:471:LEU:O	2:D:475:SER:N	2.53	0.41
2:D:564:CYS:HA	2:D:567:VAL:HG22	2.02	0.41
2:D:663:LEU:HD23	2:D:666:LEU:HD12	2.03	0.41
2:D:666:LEU:HD23	2:D:666:LEU:HA	1.96	0.41
2:D:721:ARG:HB3	2:D:769:GLU:OE1	2.21	0.41
2:C:427:ILE:HG22	2:C:541:MET:HG3	2.03	0.41
2:C:430:HIS:HA	2:C:433:ALA:HB3	2.02	0.41
2:C:693:MET:HA	2:C:696:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:LEU:HD22	1:A:621:SER:HB3	2.03	0.41
1:A:1714:LEU:HD23	1:A:1715:LEU:N	2.36	0.41
1:B:51:VAL:HG13	1:B:52:ALA:H	1.86	0.41
1:B:1191:LEU:CA	1:B:1194:ARG:HE	2.29	0.41
1:B:1315:GLN:O	1:B:1319:ILE:HG12	2.20	0.41
1:B:1702:LEU:O	1:B:1706:ILE:HG13	2.21	0.41
2:C:546:LEU:HD22	2:C:568:LEU:HD11	2.03	0.41
2:C:680:CYS:O	2:C:681:GLN:CB	2.69	0.41
1:A:477:LEU:HA	1:A:484:ASN:ND2	2.36	0.40
1:A:631:GLN:CD	1:A:631:GLN:H	2.29	0.40
1:A:2406:LEU:O	1:A:2410:MET:N	2.53	0.40
1:A:2421:LEU:HD11	1:A:2425:ARG:NH1	2.36	0.40
1:A:2422:LYS:HE3	1:A:2422:LYS:HB3	1.85	0.40
1:B:807:GLY:O	1:B:849:ARG:NH2	2.54	0.40
1:B:840:GLY:O	1:B:844:GLU:HG2	2.21	0.40
1:B:1559:ASP:H	1:B:1562:HIS:CE1	2.39	0.40
1:B:1912:LYS:HD2	1:B:1912:LYS:HA	1.91	0.40
2:D:728:HIS:O	2:D:732:GLN:OE1	2.39	0.40
2:C:710:THR:HG23	2:C:713:GLN:H	1.86	0.40
1:A:819:ASP:N	1:A:819:ASP:OD1	2.54	0.40
1:A:1726:ILE:HD11	1:A:1736:TYR:HA	2.04	0.40
1:A:2529:GLU:CD	1:A:2533:ARG:HE	2.29	0.40
1:B:320:MET:O	1:B:323:GLU:HG3	2.20	0.40
1:B:843:LYS:O	1:B:847:VAL:HG23	2.21	0.40
1:B:855:THR:O	1:B:858:GLN:HG3	2.20	0.40
1:B:2464:MET:HG2	1:B:2492:HIS:CD2	2.57	0.40
2:C:698:TRP:HA	2:C:701:VAL:HG12	2.03	0.40
1:A:147:LYS:O	1:A:151:GLN:OE1	2.38	0.40
1:A:2058:MET:HA	1:A:2061:GLN:CD	2.47	0.40
1:B:1212:LEU:HD13	1:B:1248:PHE:HD2	1.86	0.40
1:B:1221:PRO:O	1:B:1225:ILE:HG12	2.22	0.40
1:B:1325:SER:HA	1:B:2271:PRO:HA	2.04	0.40
1:B:1951:ARG:NH2	1:B:1983:CYS:SG	2.88	0.40
1:B:2058:MET:HA	1:B:2061:GLN:OE1	2.21	0.40
1:B:2221:LYS:HD3	1:B:2221:LYS:HA	1.89	0.40
2:C:610:LEU:HA	2:C:613:LEU:HD12	2.01	0.40
1:A:1668:ASN:HB3	1:A:1671:GLU:CD	2.46	0.40
1:A:1714:LEU:HD22	1:A:1717:ASP:HB2	2.03	0.40
1:A:2276:THR:HB	1:A:2279:ASN:HB2	2.03	0.40
1:A:2303:LEU:HD12	1:A:2309:PRO:HB2	2.02	0.40
1:A:2365:TYR:CD2	1:A:2377:ILE:HG23	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2410:MET:HE3	1:A:2410:MET:HB3	1.91	0.40
1:B:2042:LEU:HD11	1:B:2046:TYR:CZ	2.57	0.40
1:B:2269:THR:O	1:B:2283:HIS:NE2	2.51	0.40
1:B:2633:LEU:HD23	1:B:2633:LEU:HA	1.91	0.40
2:D:594:LEU:O	2:D:634:LEU:HD13	2.21	0.40
2:D:642:ARG:HB3	2:D:645:ARG:HH21	1.86	0.40
2:C:596:PRO:HA	2:C:638:TYR:CD2	2.57	0.40
2:C:709:ARG:HD3	2:C:709:ARG:H	1.86	0.40
1:A:2206:LYS:HA	1:A:2206:LYS:HD3	1.90	0.40
1:B:305:PHE:HD1	1:B:356:PHE:CE2	2.39	0.40
1:B:2086:SER:OG	1:B:2087:MET:N	2.55	0.40
2:D:416:ALA:HB3	2:D:492:VAL:HG21	2.03	0.40
2:D:429:LEU:HD12	2:D:429:LEU:HA	1.93	0.40
2:D:708:PRO:HG2	2:D:714:ARG:HG2	2.02	0.40
2:C:646:VAL:O	2:C:646:VAL:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2451/2637 (93%)	2313 (94%)	136 (6%)	2 (0%)	48	79
1	B	2471/2637 (94%)	2327 (94%)	142 (6%)	2 (0%)	48	79
2	C	370/491 (75%)	341 (92%)	27 (7%)	2 (0%)	24	57
2	D	372/491 (76%)	336 (90%)	35 (9%)	1 (0%)	36	67
All	All	5664/6256 (90%)	5317 (94%)	340 (6%)	7 (0%)	49	79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	557	LEU
2	D	329	LEU
2	C	318	LYS
1	A	2328	PRO
2	C	629	GLY
1	A	2602	VAL
1	B	904	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1021/2358 (43%)	1013 (99%)	8 (1%)	73	76
1	B	1387/2358 (59%)	1376 (99%)	11 (1%)	73	76
2	C	207/417 (50%)	201 (97%)	6 (3%)	37	58
2	D	194/417 (46%)	190 (98%)	4 (2%)	47	64
All	All	2809/5550 (51%)	2780 (99%)	29 (1%)	65	74

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	503	CYS
1	A	2325	MET
1	A	2326	CYS
1	A	2374	CYS
1	A	2383	THR
1	A	2496	ASN
1	A	2602	VAL
1	B	250	SER
1	B	1191	LEU
1	B	1712	LEU
1	B	2123	ASN
1	B	2305	SER
1	B	2326	CYS
1	B	2327	LYS

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Mol	Chain	Res	Type
1	B	2329	LYS
1	B	2377	ILE
1	B	2380	VAL
1	B	2567	LYS
2	D	330	CYS
2	D	334	SER
2	D	335	SER
2	D	535	GLN
2	C	330	CYS
2	C	432	GLN
2	C	584	GLN
2	C	624	CYS
2	C	630	CYS
2	C	682	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	GLN
1	A	457	ASN
1	A	657	ASN
1	A	1135	ASN
1	A	1153	ASN
1	A	1241	ASN
1	A	1597	GLN
1	A	1971	GLN
1	A	2199	ASN
1	A	2203	HIS
1	A	2307	GLN
1	A	2432	HIS
1	A	2480	ASN
1	A	2496	ASN
1	A	2591	HIS
1	B	73	GLN
1	B	713	GLN
1	B	787	HIS
1	B	827	ASN
1	B	1137	GLN
1	B	1414	GLN
1	B	1542	GLN
1	B	1575	GLN
1	B	1862	HIS

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Mol	Chain	Res	Type
1	B	1926	GLN
1	B	2056	ASN
1	B	2131	ASN
1	B	2382	ASN
1	B	2480	ASN
1	B	2517	HIS
2	D	303	GLN
2	D	387	ASN
2	D	424	GLN
2	D	535	GLN
2	D	574	ASN
2	D	657	GLN
2	C	306	ASN
2	C	584	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is 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
3	A1EIK	A	2701	-	33,35,35	0.62	1 (3%)	38,53,53	2.24	4 (10%)
3	A1EIK	B	2701	-	33,35,35	0.69	1 (3%)	38,53,53	2.51	5 (13%)

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	A1EIK	A	2701	-	-	3/13/44/44	0/7/6/6
3	A1EIK	B	2701	-	-	1/13/44/44	0/7/6/6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2701	A1EIK	C16-C15	-2.03	1.37	1.43
3	A	2701	A1EIK	C16-C15	-2.01	1.37	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2701	A1EIK	C15-N19-N18	12.82	110.97	103.30
3	A	2701	A1EIK	C15-N19-N18	12.56	110.81	103.30
3	B	2701	A1EIK	O4-C3-C2	-6.13	94.99	111.53
3	B	2701	A1EIK	C17-N18-N19	-3.28	105.15	111.60
3	A	2701	A1EIK	C17-N18-N19	-3.21	105.30	111.60
3	B	2701	A1EIK	C16-C17-N18	2.59	111.52	107.62
3	A	2701	A1EIK	C16-C17-N18	2.55	111.47	107.62
3	A	2701	A1EIK	O4-C3-C2	-2.37	105.13	111.53
3	B	2701	A1EIK	C5-C6-N7	-2.13	104.53	109.97

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2701	A1EIK	N9-C8-N7-C2
3	A	2701	A1EIK	N9-C8-N7-C6
3	A	2701	A1EIK	C21-C8-N7-C6
3	B	2701	A1EIK	C21-C8-N7-C2

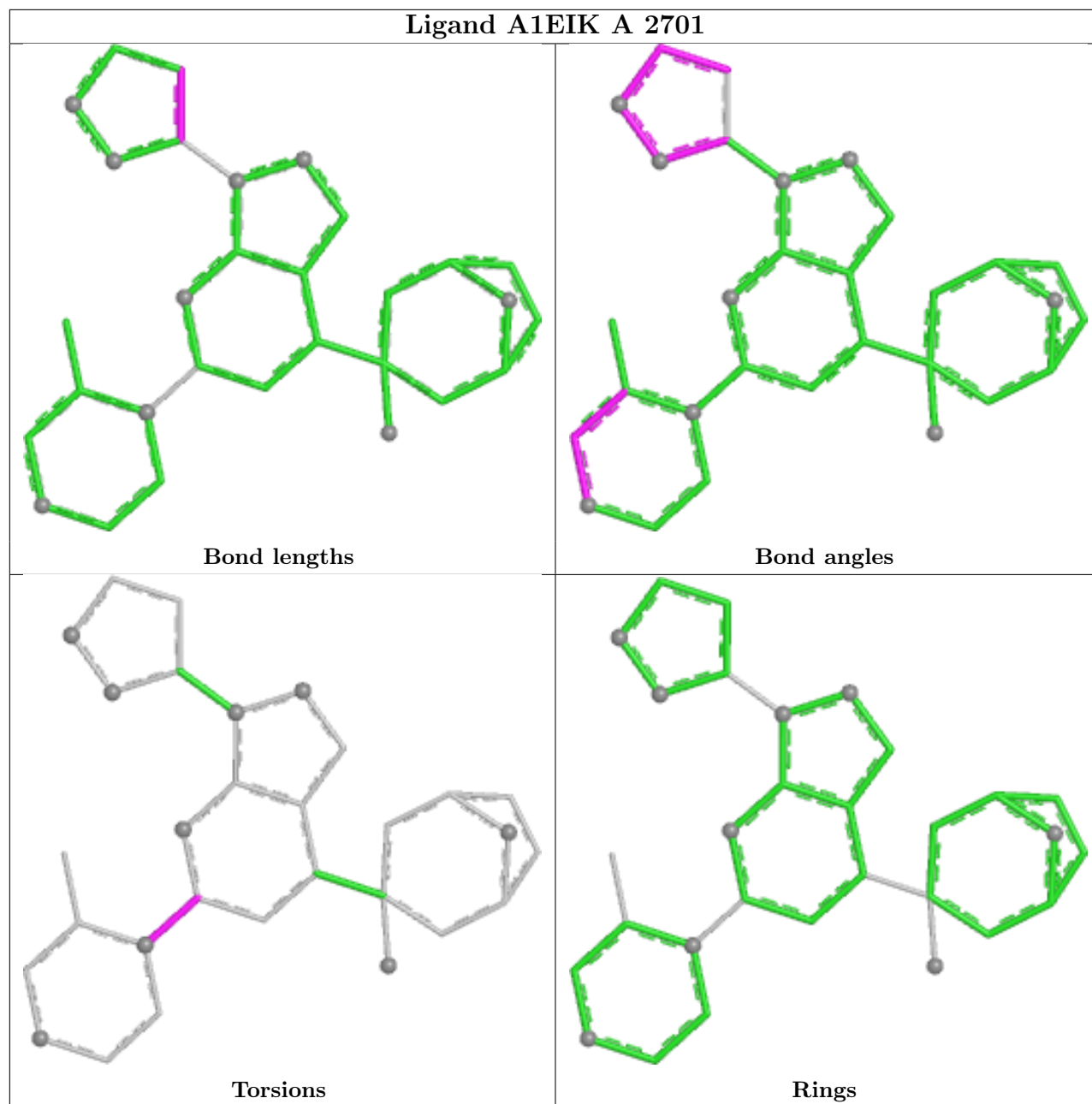
There are no ring outliers.

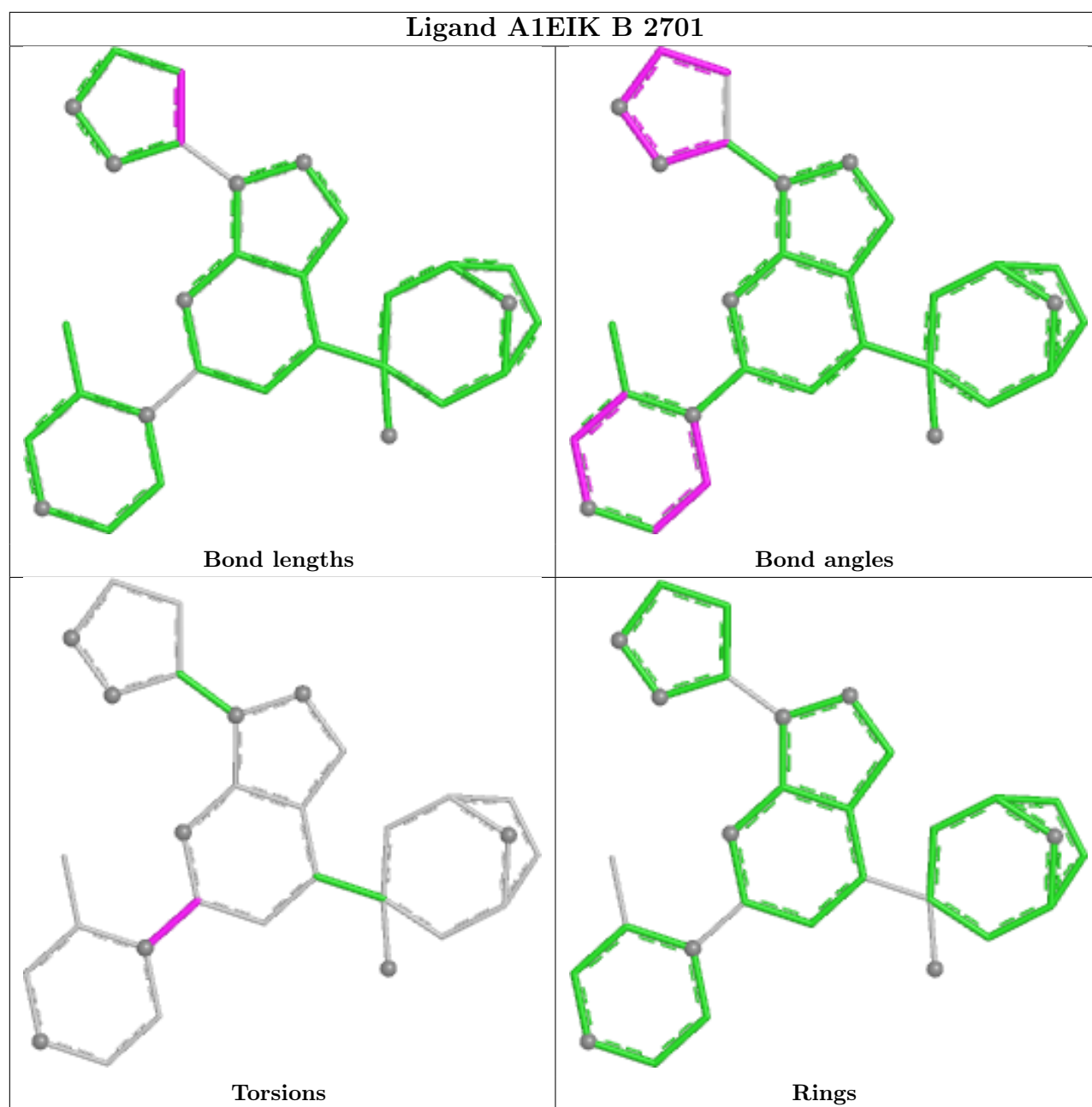
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2701	A1EIK	1	0

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

Ligand A1EIK A 2701





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

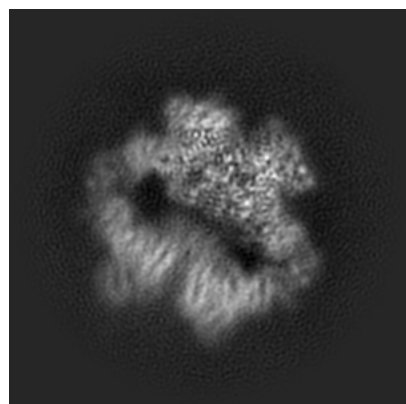
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62811. These allow visual inspection of the internal detail of the map and identification of artifacts.

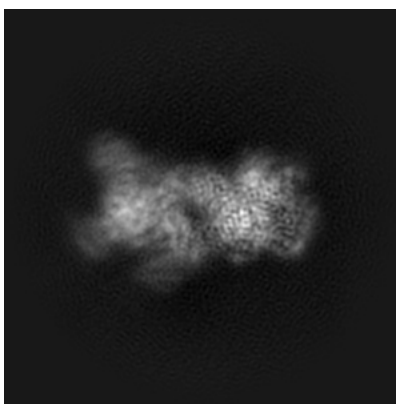
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

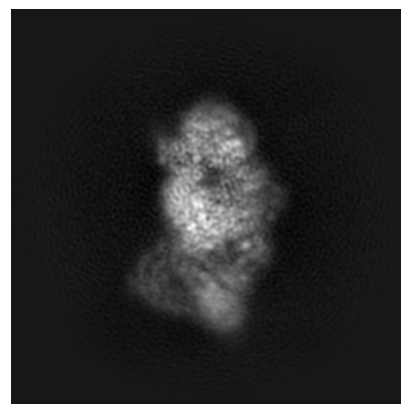
6.1.1 Primary map



X

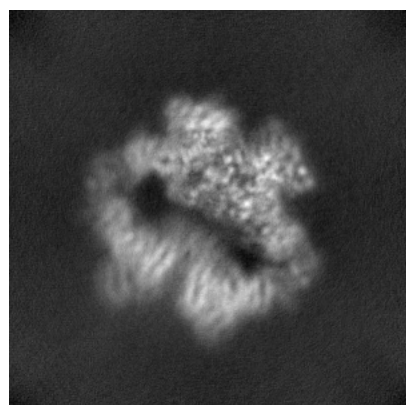


Y

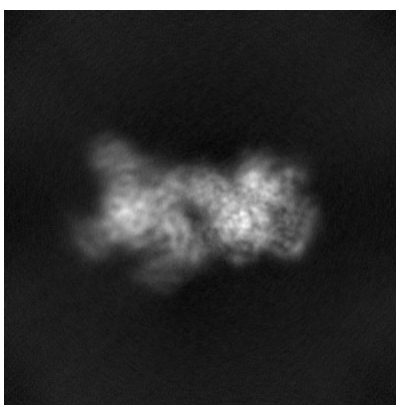


Z

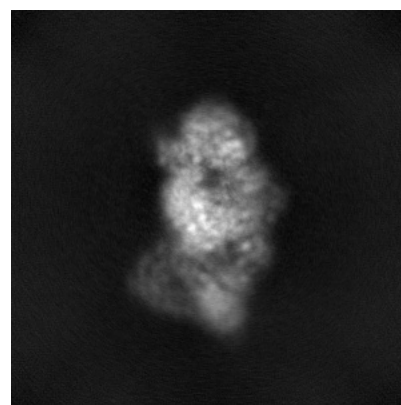
6.1.2 Raw map



X



Y

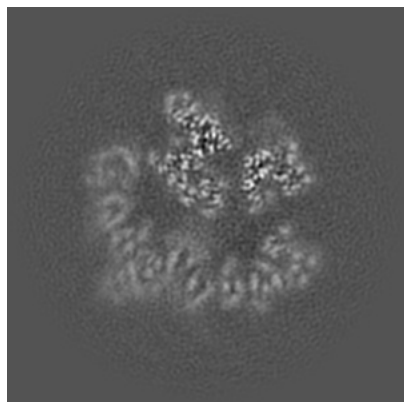


Z

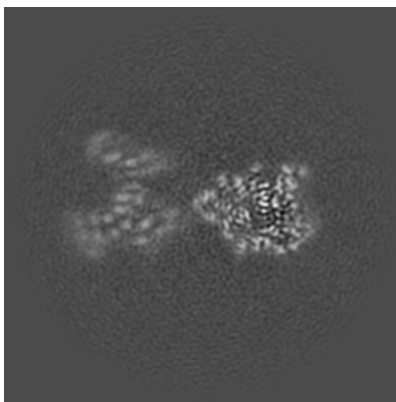
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

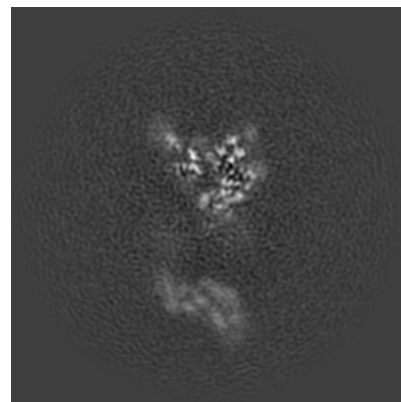
6.2.1 Primary map



X Index: 192

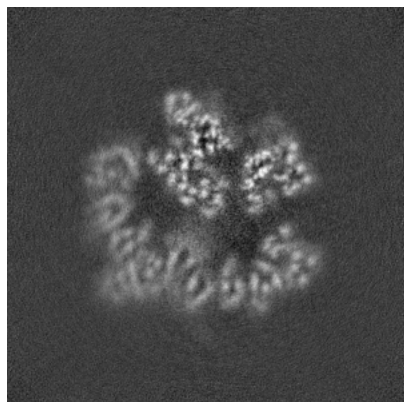


Y Index: 192

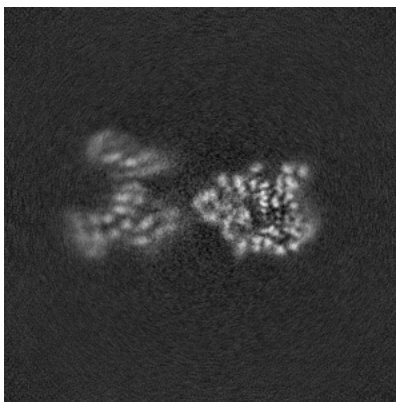


Z Index: 192

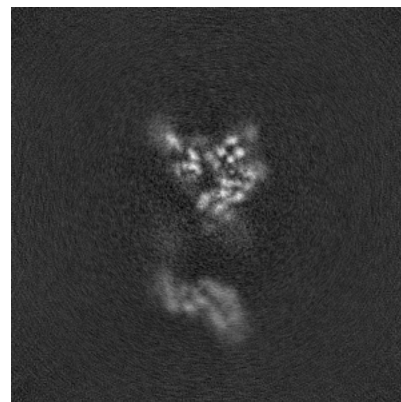
6.2.2 Raw map



X Index: 192



Y Index: 192

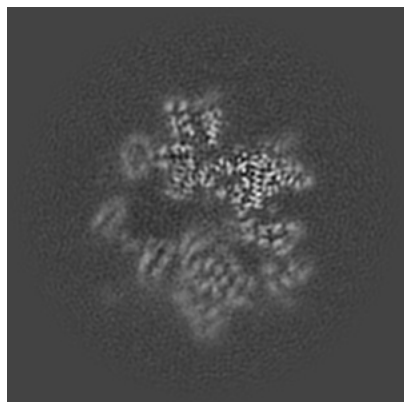


Z Index: 192

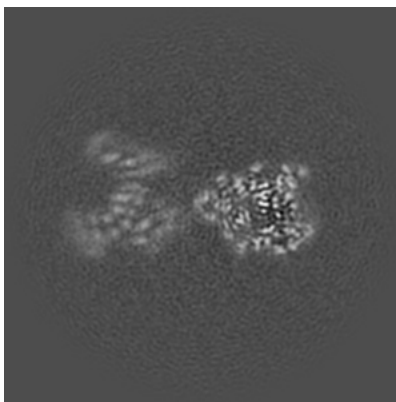
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

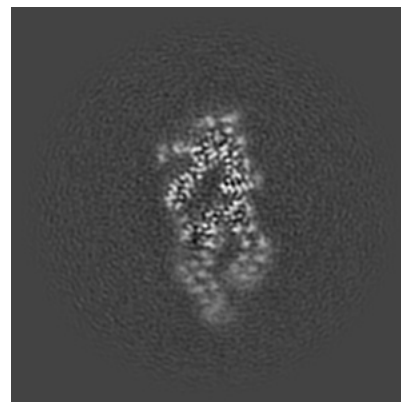
6.3.1 Primary map



X Index: 176

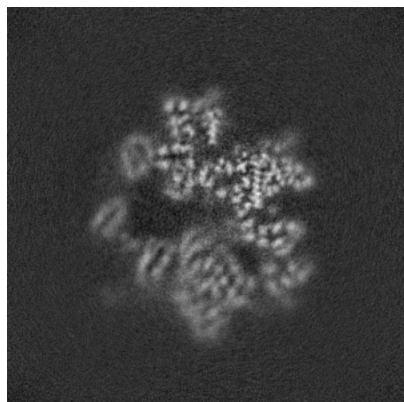


Y Index: 191

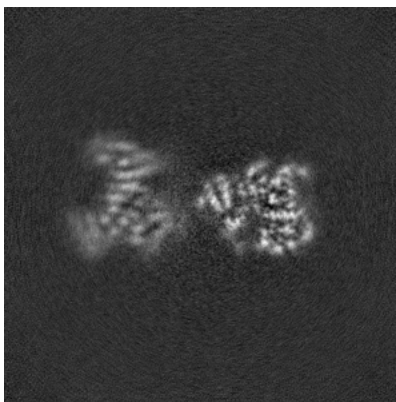


Z Index: 240

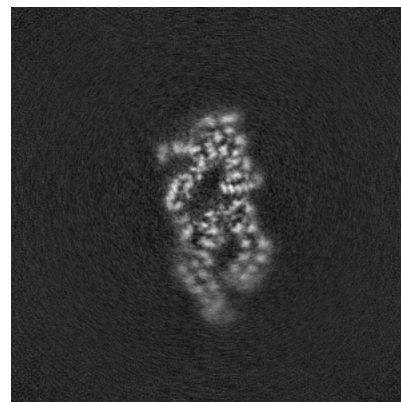
6.3.2 Raw map



X Index: 176



Y Index: 187

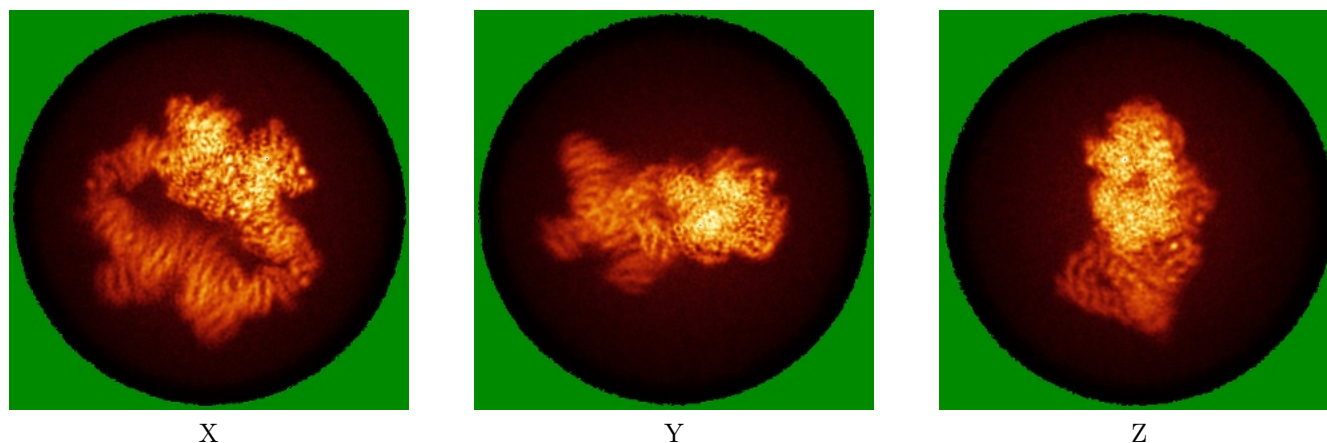


Z Index: 241

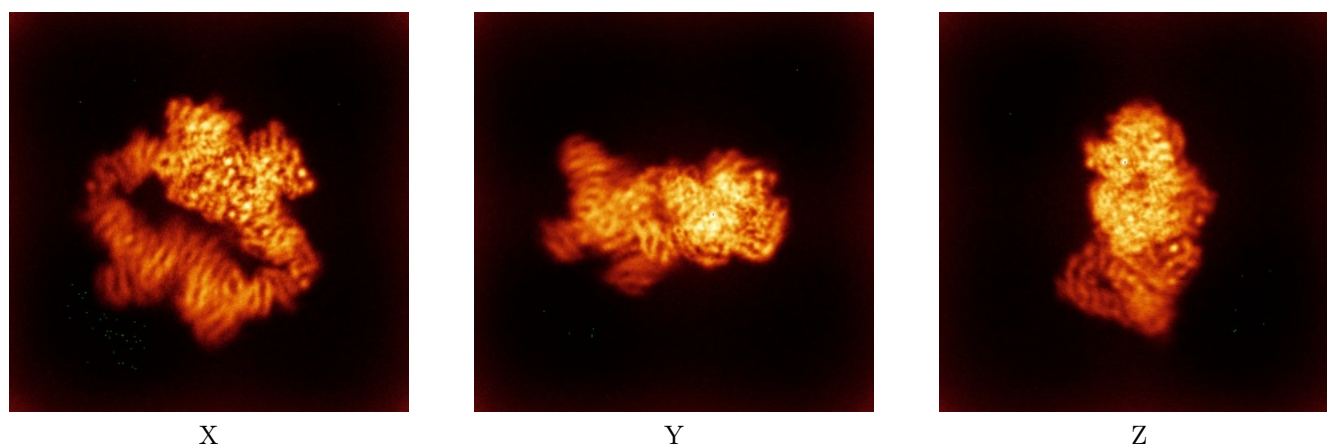
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

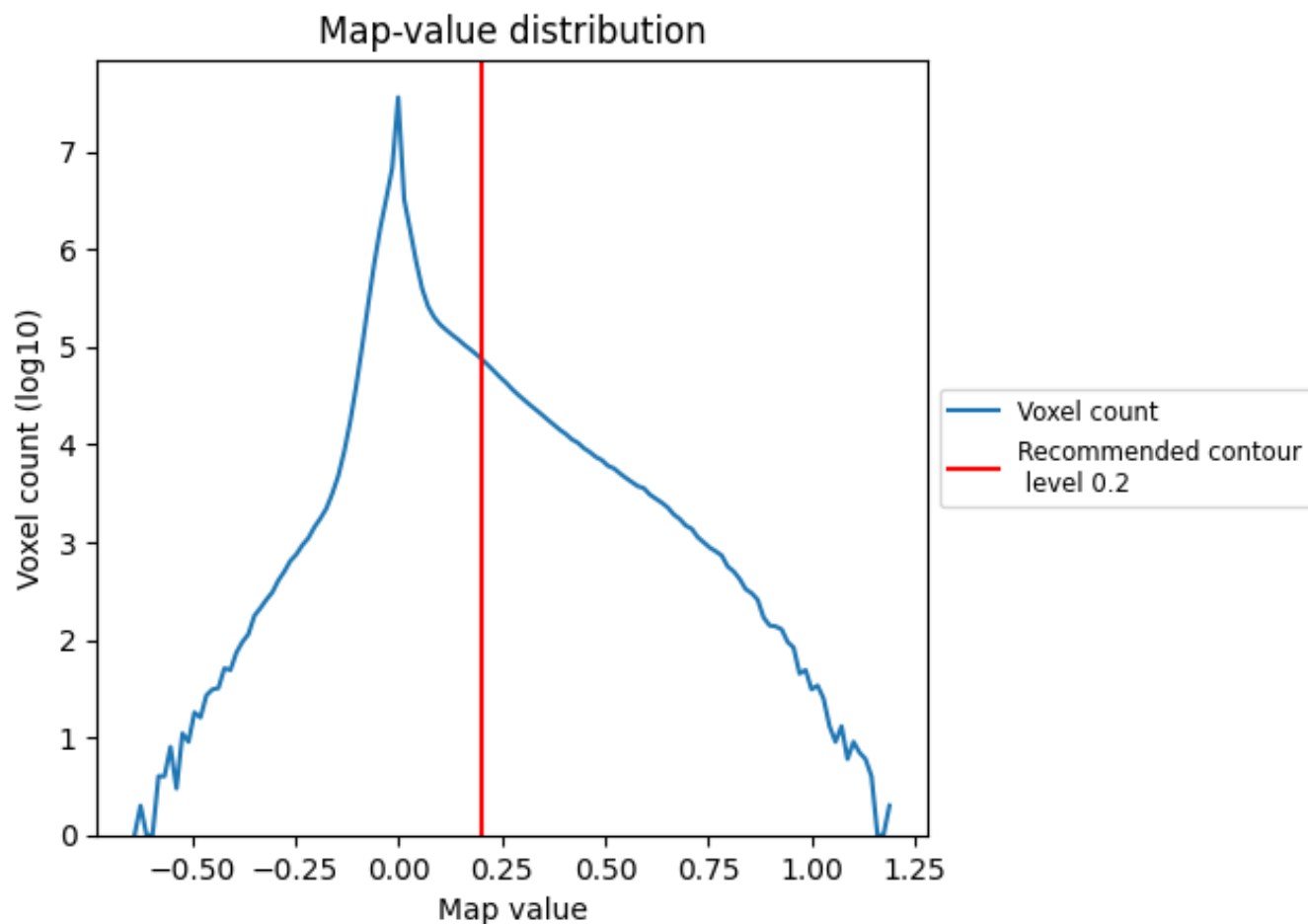
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

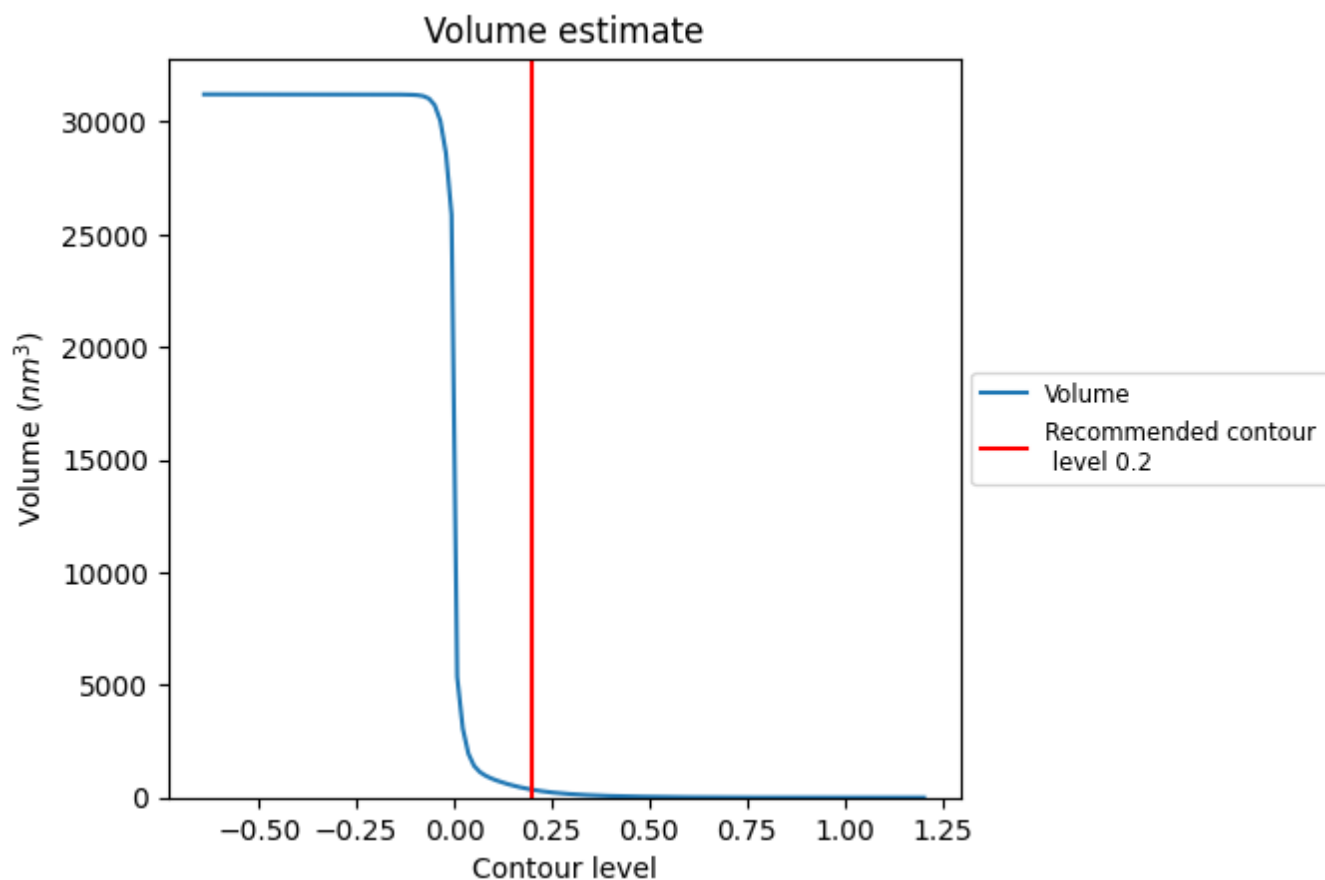
This section contains the results of statistical analysis of the map.

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.

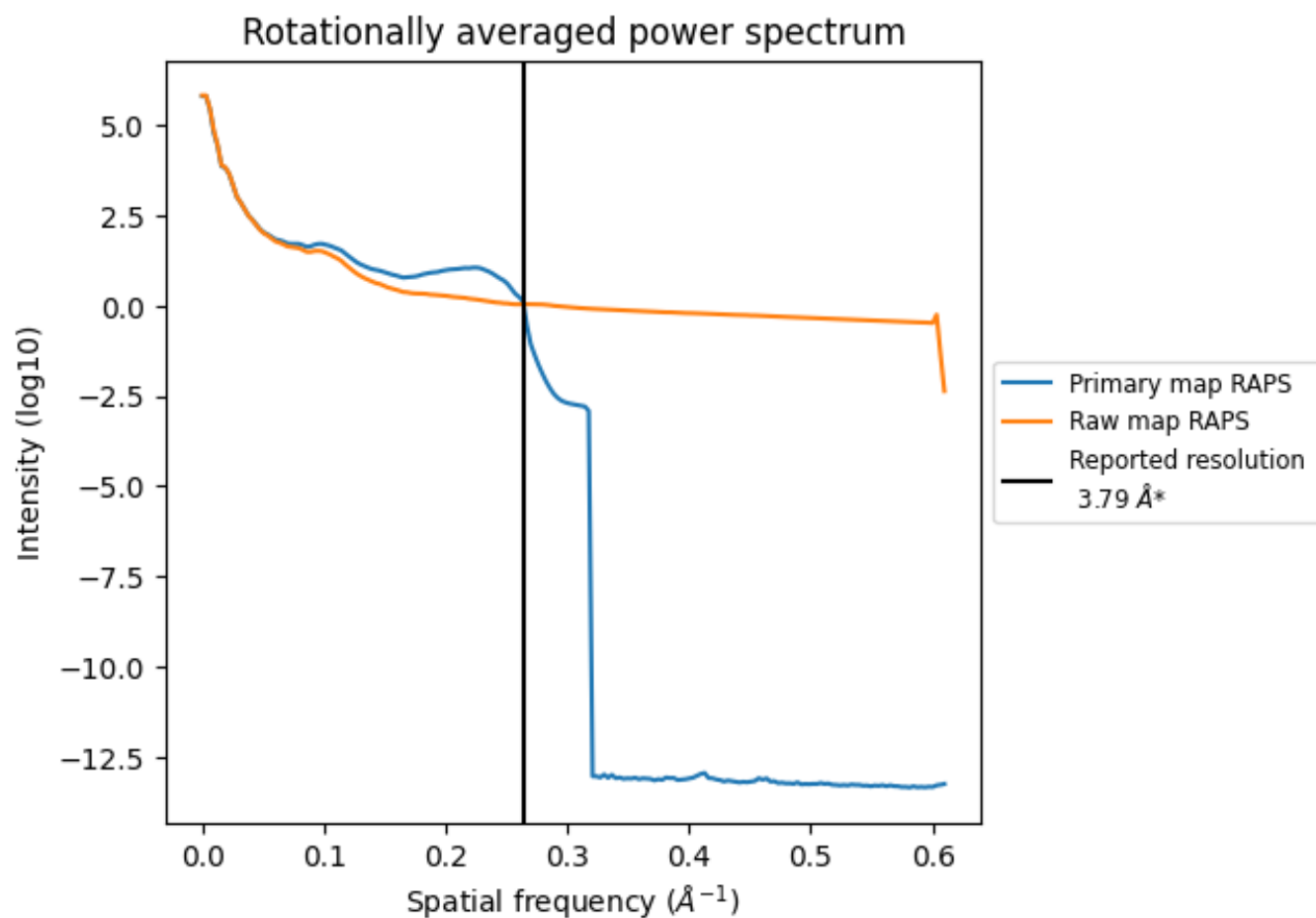
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 352 nm^3 ; this corresponds to an approximate mass of 318 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 ⓘ

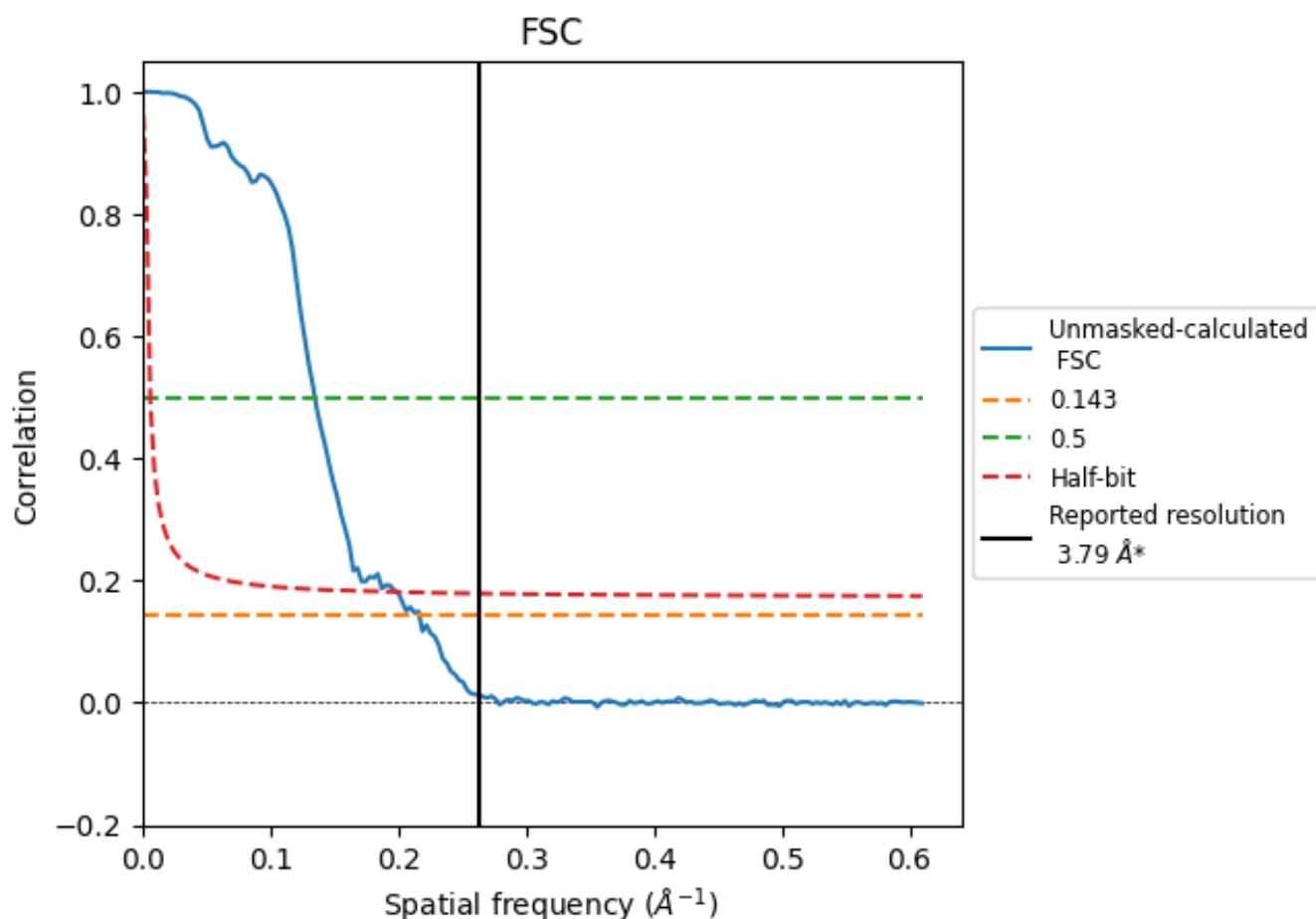


*Reported resolution corresponds to spatial frequency of 0.264 Å⁻¹

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 0.264 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.79	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.62	7.41	5.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.62 differs from the reported value 3.79 by more than 10 %

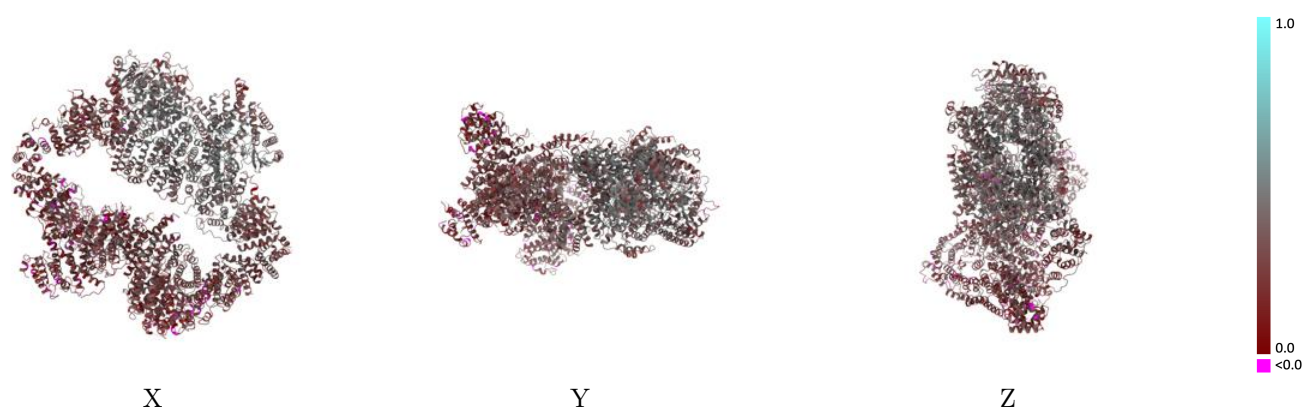
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62811 and PDB model 9L4D. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

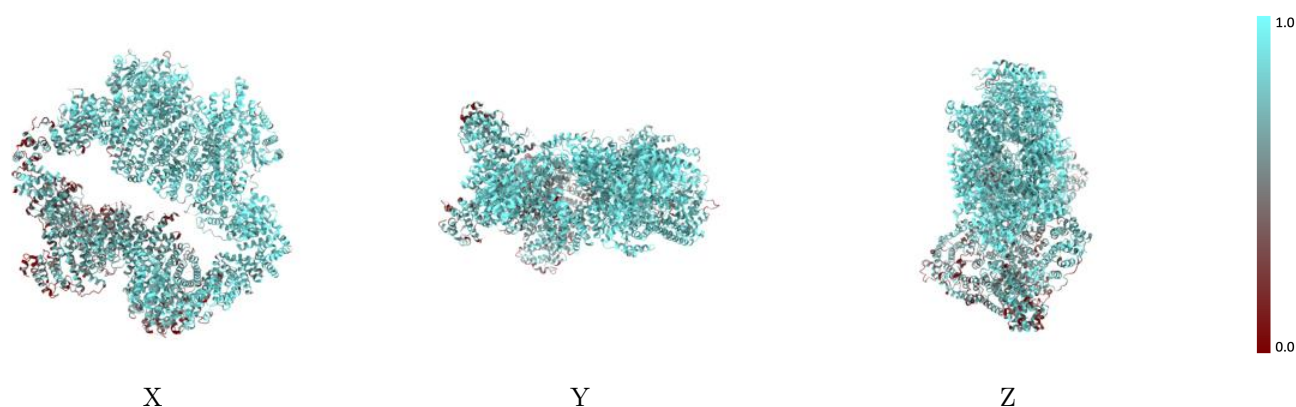
This section was not generated.

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



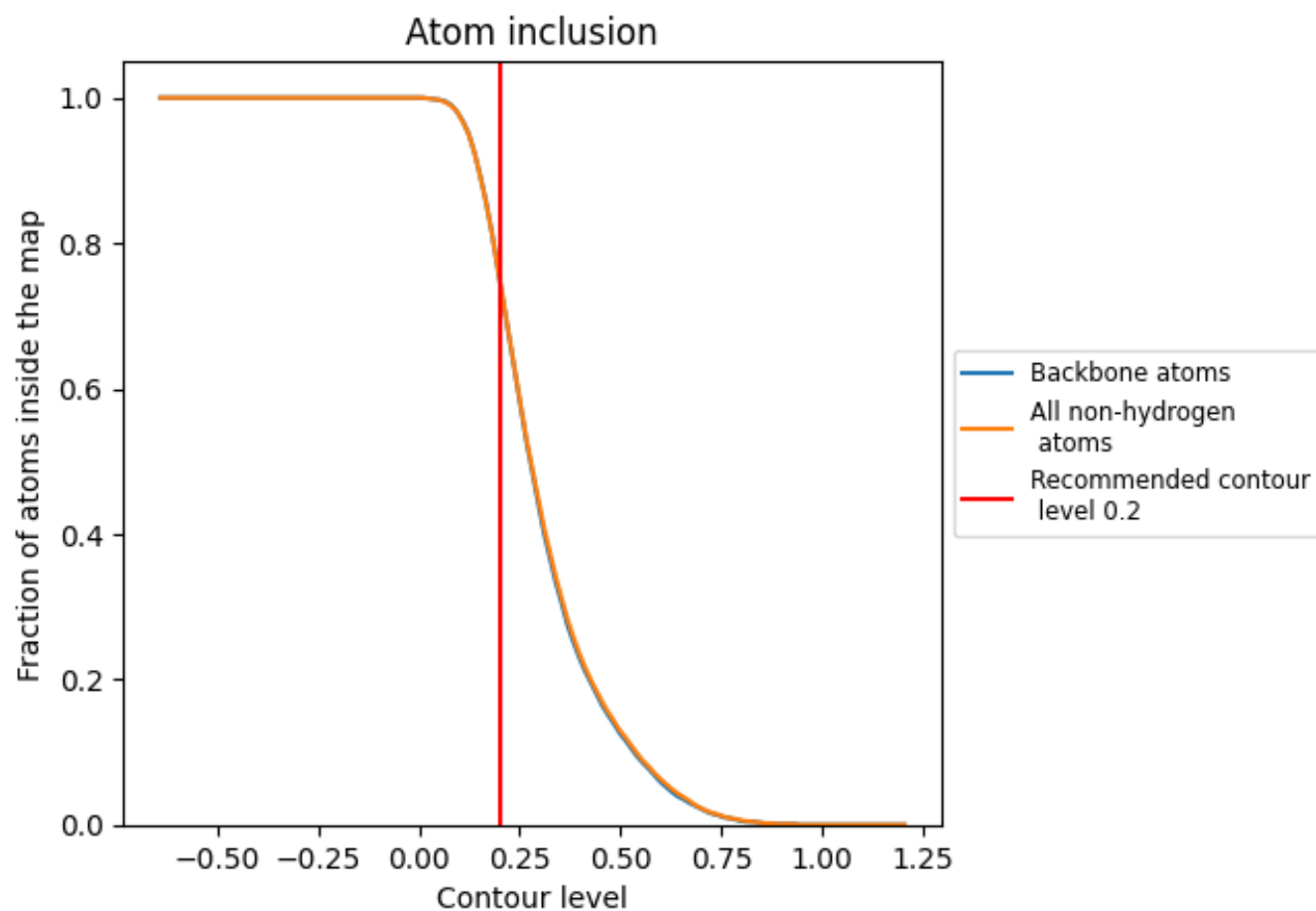
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 75% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7520	0.3210
A	0.8370	0.3490
B	0.7210	0.3180
C	0.6950	0.2660
D	0.5730	0.2270

