



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 07:12 PM UTC

PDB ID : 7SGL / pdb_00007sgl
EMDB ID : EMD-25113
Title : DNA-PK complex of DNA end processing
Authors : Liu, L.; Li, J.; Chen, X.; Yang, W.; Gellert, M.
Deposited on : 2021-10-06
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

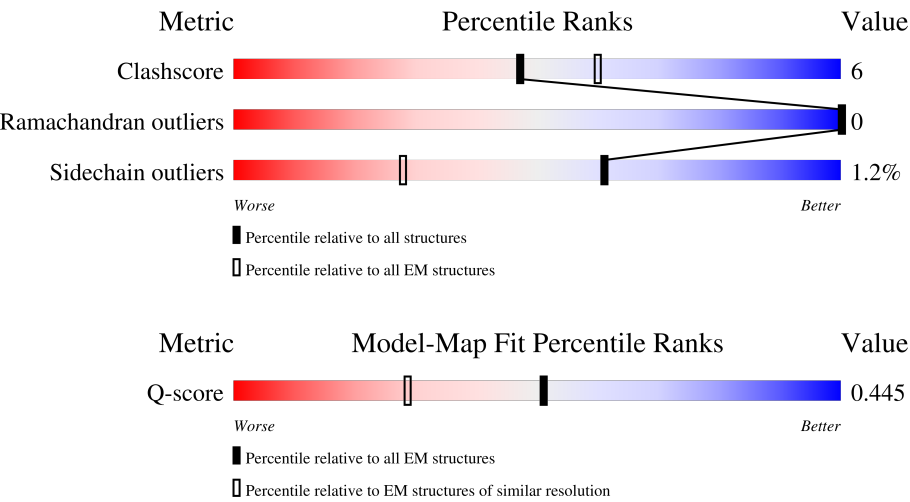
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	4128	80%13%7%
2	B	612	70%13%17%
3	C	732	8% 69%17%14%
4	D	701	49%9%42%

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Mol	Chain	Length	Quality of chain
5	E	54	 46% 54%
5	F	54	 15% 85%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 44704 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3852	Total	C	N	O	P	S	
			30853	19740	5219	5691	4	199	
								5	0

- Molecule 2 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	507	Total	C	N	O	S		
			4102	2625	694	765	18	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P12956
B	-1	PRO	-	expression tag	UNP P12956
B	0	VAL	-	expression tag	UNP P12956

- Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	631	Total	C	N	O	S		
			5099	3267	856	950	26	0	0

- Molecule 4 is a protein called Protein artemis.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	406	Total	C	N	O	S		
			3311	2111	578	601	21	1	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	693	ALA	-	expression tag	UNP Q96SD1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	694	ALA	-	expression tag	UNP Q96SD1
D	695	ALA	-	expression tag	UNP Q96SD1
D	696	LEU	-	expression tag	UNP Q96SD1
D	697	GLU	-	expression tag	UNP Q96SD1
D	698	VAL	-	expression tag	UNP Q96SD1
D	699	LEU	-	expression tag	UNP Q96SD1
D	700	PHE	-	expression tag	UNP Q96SD1
D	701	GLN	-	expression tag	UNP Q96SD1

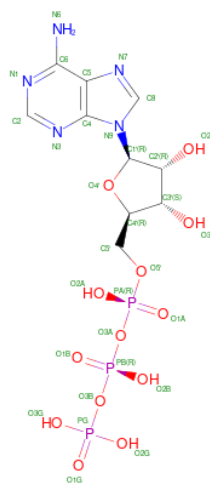
- Molecule 5 is a DNA chain called Hairpin_1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	54	Total	C	N	O	P	0	0
			1104	528	201	322	53		
5	F	8	Total	C	N	O	P	0	0
			164	78	30	48	8		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

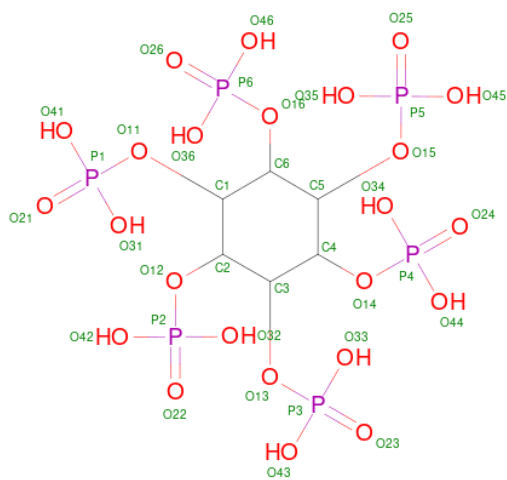
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Mg	0
			1	1	
6	D	2	Total	Mg	0
			2	2	

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 8 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $\text{C}_6\text{H}_{18}\text{O}_{24}\text{P}_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
8	B	1	Total	C	O	P	0
			36	6	24	6	

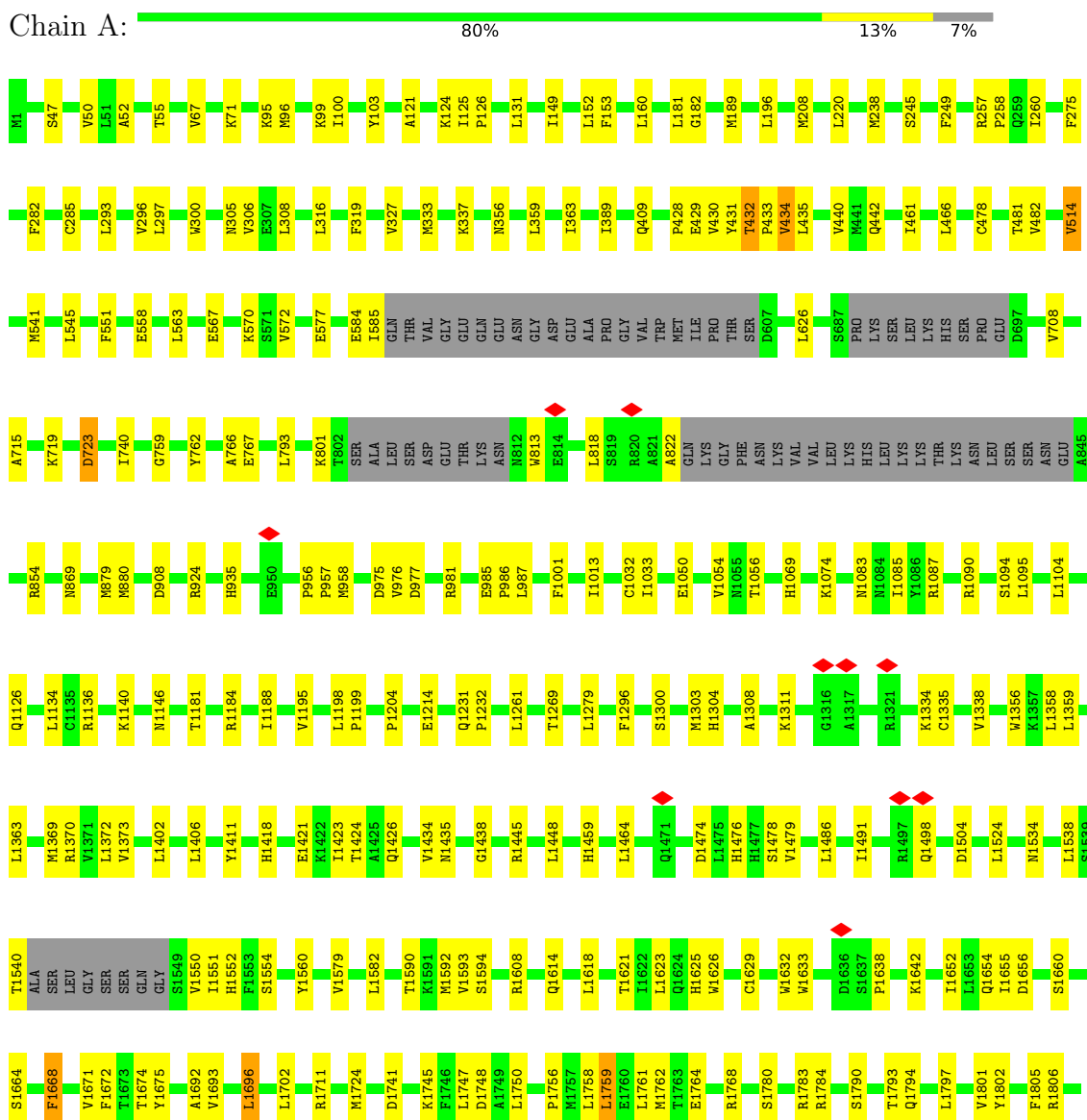
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

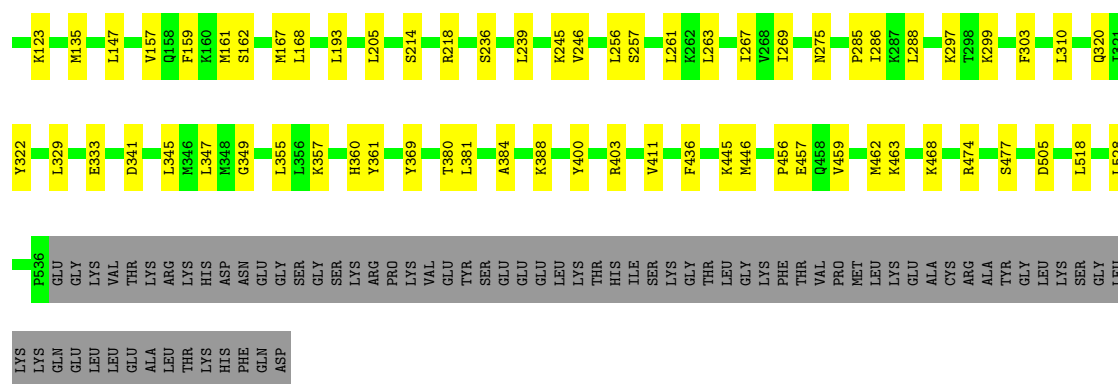
Mol	Chain	Residues	Atoms		AltConf
9	D	1	Total	Zn	0
			1	1	

3 Residue-property plots

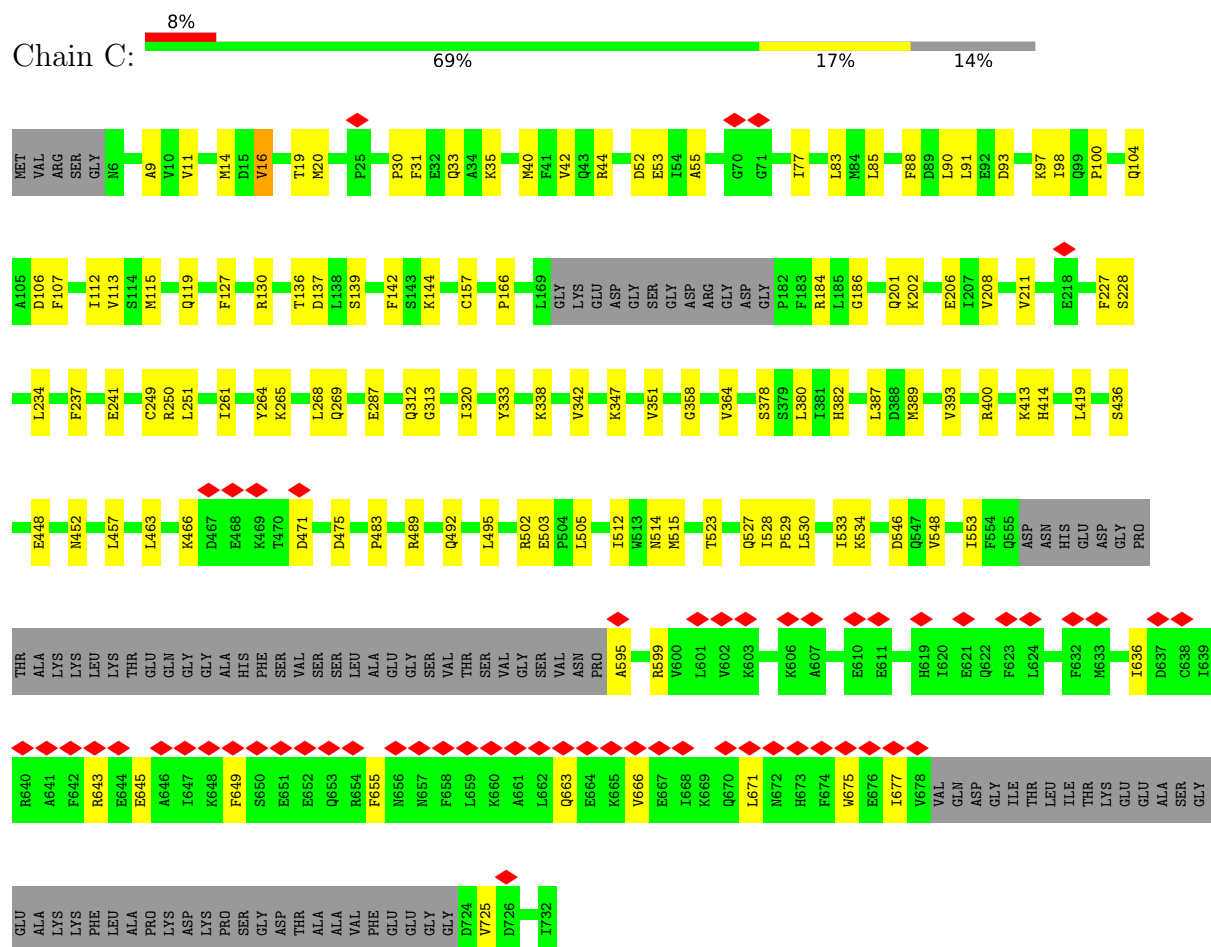
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: DNA-dependent protein kinase catalytic subunit

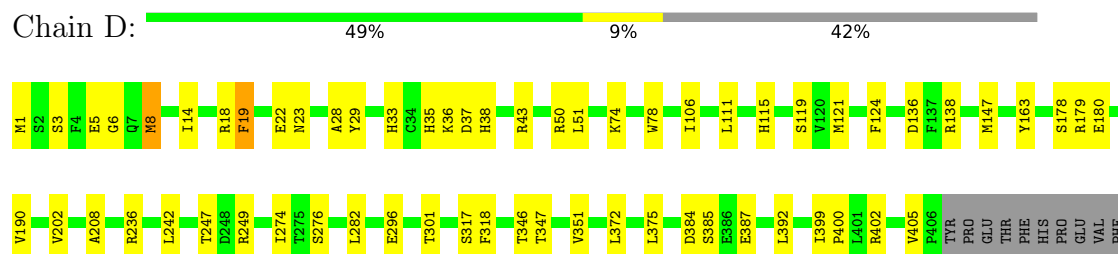




• Molecule 3: X-ray repair cross-complementing protein 5



• Molecule 4: Protein artemis



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	161380	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 ($e^-/\text{\AA}^2$)	55.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.024	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0056	Depositor
Map size (Å)	399.84, 399.84, 399.84	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.833, 0.833, 0.833	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: IHP, ATP, ZN, MG, TPO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.13	0/31449	0.33	4/42499 (0.0%)
2	B	0.11	0/4184	0.29	0/5638
3	C	0.10	0/5200	0.31	0/7007
4	D	0.18	0/3397	0.34	0/4600
5	E	1.59	0/1238	0.79	0/1909
5	F	0.67	0/183	0.67	0/280
All	All	0.29	0/45651	0.35	4/61933 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	LEU	N-CA-C	9.16	120.87	111.07
1	A	1823	SER	N-CA-C	7.87	121.39	111.24
1	A	434	VAL	CB-CA-C	6.39	121.77	111.29
1	A	1822	ARG	CB-CA-C	5.08	119.86	110.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	30853	0	31141	323	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4102	0	4174	50	0
3	C	5099	0	5128	79	0
4	D	3311	0	3298	43	0
5	E	1104	0	607	49	0
5	F	164	0	91	22	0
6	A	1	0	0	0	0
6	D	2	0	0	0	0
7	A	31	0	12	0	0
8	B	36	0	6	3	0
9	D	1	0	0	0	0
All	All	44704	0	44457	531	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 (531) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1924:THR:CG2	1:A:1975:LEU:CD1	2.26	1.13
1:A:1924:THR:HG22	1:A:1975:LEU:CD1	1.80	1.11
1:A:1924:THR:CG2	1:A:1975:LEU:HD11	1.85	1.03
1:A:1924:THR:HG22	1:A:1975:LEU:HD12	1.37	1.02
1:A:1924:THR:HG21	1:A:1975:LEU:HD11	1.47	0.93
5:E:26:DT:H2'	5:E:27:DG:C2	2.11	0.85
1:A:1984:LEU:HD23	1:A:1984:LEU:O	1.79	0.81
1:A:1924:THR:CG2	1:A:1975:LEU:HD12	2.03	0.80
5:E:53:DC:O2	5:F:48:DG:N2	2.16	0.78
5:E:25:DA:H2''	5:E:26:DT:H5''	1.72	0.71
1:A:1924:THR:HG21	1:A:1975:LEU:CD1	2.10	0.70
1:A:1664:SER:H	1:A:1668:PHE:HD2	1.40	0.69
4:D:6:GLY:HA3	4:D:18:ARG:HB3	1.75	0.67
1:A:95:LYS:O	1:A:96:MET:HE2	1.94	0.67
1:A:3578:LEU:HD11	1:A:3687:MET:HE1	1.77	0.66
4:D:38:HIS:NE2	4:D:136:ASP:OD2	2.29	0.66
1:A:1304:HIS:HB2	1:A:1308:ALA:HB2	1.78	0.66
2:B:157:VAL:HG12	2:B:159:PHE:H	1.62	0.65
3:C:186:GLY:H	3:C:228:SER:HB2	1.62	0.64
1:A:3622:ALA:HB3	1:A:3625:LEU:HB2	1.79	0.64
5:E:1:DT:H5''	5:F:54:DG:H1'	1.77	0.64
1:A:2091:HIS:HB3	1:A:2094:MET:HB2	1.80	0.64
5:E:6:DA:H2''	5:E:7:DG:H8	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3924:HIS:CE1	1:A:3927:ASN:ND2	2.66	0.64
3:C:88:PHE:HA	3:C:91:LEU:HD12	1.81	0.63
5:E:26:DT:H2'	5:E:27:DG:N3	2.13	0.63
1:A:3646:LYS:O	1:A:3646:LYS:HG2	1.99	0.63
1:A:1845:VAL:HG23	1:A:1846:ASP:H	1.63	0.62
1:A:2152:ASN:OD1	1:A:2152:ASN:O	2.17	0.62
1:A:149:ILE:HG23	1:A:181:LEU:HD22	1.81	0.62
1:A:3922:ASP:O	1:A:3927:ASN:ND2	2.32	0.62
1:A:1845:VAL:HG23	1:A:1846:ASP:N	2.15	0.62
1:A:1900:PHE:CG	1:A:1901:HIS:N	2.66	0.62
5:E:45:DG:H2''	5:E:46:DA:C8	2.35	0.61
1:A:1900:PHE:CD2	1:A:1901:HIS:N	2.69	0.61
1:A:1652:ILE:HA	1:A:1655:ILE:HG22	1.82	0.61
1:A:3789:ARG:CG	1:A:3789:ARG:HH21	2.13	0.61
2:B:95:ASN:HD21	2:B:102:ILE:HB	1.65	0.61
3:C:457:LEU:HD22	3:C:533:ILE:HG13	1.81	0.61
1:A:1780:SER:O	1:A:1783:ARG:HG2	2.01	0.61
1:A:3763:ARG:NH2	1:A:4008:GLU:OE1	2.34	0.61
4:D:29:TYR:OH	4:D:50:ARG:NH1	2.34	0.60
2:B:297:LYS:HD2	2:B:299:LYS:HE3	1.83	0.60
1:A:2216:LEU:HD22	1:A:2249:LEU:HD13	1.81	0.60
1:A:3894:PRO:HG2	1:A:3895:GLU:OE2	2.01	0.60
2:B:463:LYS:HG3	3:C:387:LEU:HD11	1.82	0.60
4:D:35:HIS:HE1	4:D:115:HIS:NE2	2.00	0.60
1:A:3169:PRO:HG3	1:A:3182:ILE:HD12	1.84	0.60
1:A:2169:LEU:HD22	1:A:2193:ILE:HD13	1.83	0.60
1:A:327:VAL:HG23	1:A:333:MET:HB3	1.84	0.59
1:A:3645:GLY:HA3	1:A:3650:LYS:H	1.67	0.59
3:C:364:VAL:HB	3:C:419:LEU:HB2	1.83	0.59
1:A:1359:LEU:HB2	1:A:1363:LEU:HD22	1.83	0.59
3:C:144:LYS:O	3:C:144:LYS:HG2	2.02	0.59
1:A:3447:VAL:HG22	1:A:3468:LEU:HD22	1.85	0.59
1:A:1623:LEU:HA	1:A:1626:TRP:HD1	1.67	0.59
1:A:1924:THR:HG22	1:A:1924:THR:O	2.00	0.59
3:C:11:VAL:HG22	3:C:55:ALA:HB3	1.85	0.58
3:C:595:ALA:O	3:C:599:ARG:HB2	2.03	0.58
2:B:361:TYR:OH	3:C:358:GLY:N	2.34	0.58
5:E:52:DT:H2''	5:E:53:DC:OP2	2.03	0.58
5:E:25:DA:N3	5:E:25:DA:H2'	2.17	0.58
4:D:296:GLU:O	4:D:296:GLU:HG3	2.03	0.58
4:D:346:THR:HG22	4:D:347:THR:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:25:DA:H2''	5:E:26:DT:C5'	2.33	0.57
2:B:462:MET:HG2	3:C:380:LEU:HA	1.87	0.57
1:A:1621:THR:O	1:A:1625:HIS:ND1	2.37	0.57
5:E:6:DA:H2''	5:E:7:DG:C8	2.39	0.57
1:A:429:GLU:HB2	1:A:1498:GLN:HB3	1.87	0.57
2:B:297:LYS:CD	2:B:299:LYS:HE3	2.34	0.57
1:A:1311:LYS:O	1:A:1311:LYS:HG2	2.04	0.57
1:A:2923:TRP:CE2	1:A:2946:GLU:HG2	2.40	0.57
3:C:42:VAL:HG21	3:C:90:LEU:HD22	1.86	0.57
1:A:584:GLU:HG2	1:A:585:ILE:N	2.20	0.56
1:A:1815:THR:HG22	1:A:1819:PHE:CE2	2.39	0.56
1:A:1741:ASP:O	1:A:1745:LYS:HG2	2.06	0.56
1:A:1759:LEU:HD13	1:A:1797:LEU:HD22	1.88	0.56
1:A:3447:VAL:HA	1:A:3468:LEU:HD22	1.86	0.56
2:B:261:LEU:HD23	2:B:269:ILE:HD11	1.86	0.56
3:C:666:VAL:HG13	3:C:671:LEU:HB2	1.86	0.56
1:A:2368:THR:HG21	1:A:2375:ALA:HB2	1.88	0.56
5:E:17:DA:H2''	5:E:18:DT:H71	1.88	0.56
3:C:249:CYS:SG	3:C:250:ARG:N	2.78	0.56
1:A:1924:THR:HG22	1:A:1975:LEU:HD11	1.57	0.56
2:B:320:GLN:NE2	2:B:322:TYR:OH	2.38	0.56
2:B:456:PRO:HA	2:B:459:VAL:HG12	1.88	0.56
3:C:251:LEU:HB2	3:C:261:ILE:HD13	1.87	0.56
1:A:2958:LEU:HD11	1:A:4101:GLU:HG2	1.87	0.55
1:A:333:MET:HG3	1:A:337:LYS:HE3	1.88	0.55
1:A:3992:ARG:NH1	1:A:4103:GLN:OE1	2.40	0.55
8:B:701:IHP:O31	3:C:414:HIS:NE2	2.39	0.55
4:D:8:MET:HG3	4:D:163:TYR:CE1	2.40	0.55
1:A:1146:ASN:HB3	1:A:1199:PRO:HG3	1.88	0.55
3:C:489:ARG:HD2	3:C:492:GLN:HE21	1.71	0.55
1:A:767:GLU:OE1	1:A:854:ARG:NH1	2.40	0.55
3:C:19:THR:OG1	3:C:137:ASP:OD2	2.25	0.55
5:F:48:DG:O5'	5:F:48:DG:H8	1.88	0.55
1:A:297:LEU:HD13	1:A:316:LEU:HA	1.87	0.54
5:E:23:DA:C8	5:E:23:DA:H5''	2.42	0.54
5:F:51:DA:H2''	5:F:52:DT:H5''	1.89	0.54
1:A:1656:ASP:OD1	1:A:1660:SER:OG	2.26	0.54
3:C:14:MET:HE1	3:C:35:LYS:HG3	1.90	0.54
4:D:35:HIS:CE1	4:D:115:HIS:NE2	2.74	0.54
5:F:47:DC:H2''	5:F:48:DG:H8	1.71	0.54
5:F:48:DG:H2''	5:F:49:DA:H2'	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1435:ASN:HD21	1:A:1486:LEU:HD11	1.73	0.54
4:D:8:MET:CG	4:D:163:TYR:CE1	2.90	0.54
1:A:1961:PHE:HZ	3:C:725:VAL:HG22	1.73	0.54
1:A:2304:VAL:HA	1:A:2323:LEU:HD11	1.90	0.54
3:C:119:GLN:NE2	3:C:157:CYS:SG	2.81	0.54
1:A:1474:ASP:O	1:A:1478:SER:N	2.41	0.54
1:A:3553:GLU:OE1	1:A:3557:ARG:NH2	2.41	0.54
1:A:282:PHE:HB3	1:A:285:CYS:HB2	1.89	0.53
5:E:17:DA:C2'	5:E:18:DT:H71	2.38	0.53
3:C:93:ASP:O	3:C:98:ILE:HG12	2.08	0.53
1:A:1356:TRP:HB2	1:A:1411:TYR:HE2	1.73	0.53
1:A:3328:ILE:HD11	1:A:3412:ALA:HB2	1.91	0.53
4:D:384:ASP:OD1	4:D:385:SER:N	2.41	0.53
1:A:305:ASN:OD1	1:A:306:VAL:N	2.42	0.53
1:A:3332:THR:HG23	1:A:3335:ARG:HH11	1.73	0.53
3:C:107:PHE:HB3	3:C:136:THR:HG21	1.90	0.53
1:A:1876:ILE:HG22	1:A:1880:MET:HE3	1.91	0.53
1:A:2161:ALA:HB3	1:A:2199:LEU:HD11	1.91	0.53
1:A:1981:LEU:HD12	1:A:1982:ILE:HG12	1.90	0.53
1:A:3323:PHE:CE2	1:A:3327:ASN:ND2	2.76	0.53
2:B:236:SER:HB3	2:B:239:LEU:HD13	1.90	0.53
4:D:178:SER:OG	4:D:180:GLU:OE2	2.27	0.53
1:A:3447:VAL:HA	1:A:3468:LEU:CD2	2.38	0.53
3:C:466:LYS:HB3	3:C:471:ASP:HA	1.90	0.53
1:A:1296:PHE:O	1:A:1300:SER:OG	2.24	0.52
3:C:184:ARG:HB3	3:C:514:ASN:HD22	1.74	0.52
5:F:50:DT:H5'	5:F:50:DT:C6	2.44	0.52
1:A:1756:PRO:HA	1:A:1759:LEU:HD22	1.92	0.52
1:A:584:GLU:HG2	1:A:585:ILE:H	1.74	0.52
1:A:3636:PHE:HE1	1:A:3669:LYS:HG3	1.74	0.52
1:A:305:ASN:HB3	1:A:308:LEU:HB3	1.92	0.52
8:B:701:IHP:O25	3:C:413:LYS:NZ	2.42	0.52
1:A:975:ASP:OD1	1:A:976:VAL:N	2.42	0.52
1:A:1372:LEU:HD13	1:A:1402:LEU:HD23	1.92	0.52
1:A:1369:MET:HE1	1:A:1406:LEU:HD13	1.92	0.52
2:B:214:SER:HA	2:B:218:ARG:HB2	1.91	0.52
4:D:36:LYS:HE3	5:E:27:DG:H2'	1.92	0.52
1:A:182:GLY:HA2	1:A:189:MET:HG3	1.91	0.52
1:A:2425:ARG:HH21	1:A:2457:PRO:HB3	1.75	0.52
4:D:399:ILE:HD12	4:D:400:PRO:HD2	1.92	0.52
1:A:1668:PHE:HD1	1:A:1672:PHE:HB2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:468:LYS:HG2	2:B:518:LEU:HA	1.91	0.51
1:A:708:VAL:HG22	1:A:740:ILE:HG23	1.91	0.51
2:B:109:ASP:OD1	2:B:110:ASN:N	2.39	0.51
1:A:3093:GLN:HE22	4:D:375:LEU:HA	1.75	0.51
3:C:448:GLU:OE1	3:C:452:ASN:ND2	2.43	0.51
1:A:67:VAL:HG22	1:A:71:LYS:HE2	1.93	0.51
1:A:1871:MET:O	1:A:1875:LYS:HG2	2.10	0.51
2:B:333:GLU:OE1	3:C:505:LEU:HD12	2.11	0.51
4:D:190:VAL:HG22	4:D:202:VAL:HG11	1.91	0.51
1:A:1303:MET:HE3	1:A:1370:ARG:HG2	1.91	0.51
2:B:69:SER:HA	2:B:245:LYS:HE2	1.93	0.51
5:E:23:DA:C2	5:E:25:DA:N6	2.78	0.51
1:A:2464:HIS:O	1:A:2470:ARG:NH1	2.39	0.51
1:A:2519:LEU:HA	1:A:2522:ARG:HG2	1.92	0.51
1:A:3885:ARG:HA	1:A:3888:VAL:HG22	1.93	0.51
3:C:83:LEU:HD21	3:C:127:PHE:HE2	1.76	0.51
5:F:47:DC:H2''	5:F:48:DG:C8	2.45	0.51
1:A:1438:GLY:O	1:A:1445:ARG:NH1	2.39	0.51
1:A:1724:MET:HA	1:A:1768:ARG:HH22	1.74	0.50
3:C:636:ILE:HG13	3:C:677:ILE:HG13	1.93	0.50
1:A:2310:VAL:HG11	1:A:2356:MET:HE1	1.94	0.50
1:A:2604:PRO:HG2	1:A:3725:ARG:HE	1.76	0.50
3:C:338:LYS:NZ	5:E:49:DA:OP1	2.44	0.50
1:A:3031:TRP:HZ3	1:A:3077:ILE:HD11	1.77	0.50
1:A:3789:ARG:CG	1:A:3789:ARG:NH2	2.73	0.50
2:B:288:LEU:HD21	3:C:320:ILE:HG21	1.93	0.50
3:C:466:LYS:HE3	3:C:471:ASP:HB3	1.94	0.50
1:A:1083:ASN:ND2	1:A:1126:GLN:OE1	2.44	0.50
1:A:2183:HIS:CE1	1:A:2186:VAL:HG23	2.46	0.50
1:A:2594:ASP:OD2	1:A:3818:ASN:ND2	2.44	0.50
3:C:106:ASP:HB2	3:C:142:PHE:HB3	1.93	0.50
3:C:636:ILE:HG21	3:C:677:ILE:HG21	1.93	0.50
1:A:1821:ASP:HA	1:A:1825:LEU:HD23	1.94	0.50
5:E:21:DA:N1	5:E:25:DA:N6	2.52	0.50
5:F:51:DA:C2'	5:F:52:DT:H5''	2.41	0.50
1:A:1952:ILE:HG21	1:A:1966:LEU:HD11	1.93	0.50
1:A:3280:TYR:OH	4:D:392:LEU:O	2.26	0.50
1:A:1459:HIS:HB2	1:A:1464:LEU:HD22	1.93	0.49
3:C:512:ILE:HG23	3:C:515:MET:HE2	1.94	0.49
1:A:3450:MET:HB3	1:A:3468:LEU:HD11	1.93	0.49
1:A:249:PHE:HZ	1:A:293:LEU:HD11	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1750:LEU:HB2	1:A:1758:LEU:HD11	1.93	0.49
1:A:2121:ASP:OD1	1:A:2122:LEU:N	2.44	0.49
1:A:956:PRO:HG2	1:A:958:MET:HE2	1.94	0.49
1:A:1424:THR:OG1	1:A:1426:GLN:NE2	2.44	0.49
1:A:1802:TYR:CZ	1:A:1806:ARG:HD2	2.46	0.49
5:E:54:DG:N2	5:F:48:DG:C4	2.80	0.49
1:A:723:ASP:OD1	1:A:723:ASP:N	2.45	0.49
1:A:1304:HIS:O	1:A:1334:LYS:NZ	2.45	0.49
1:A:1840:PHE:CD2	1:A:1844:VAL:HG11	2.48	0.49
1:A:4064:LEU:HD13	1:A:4077:TYR:HB3	1.94	0.49
4:D:138:ARG:HG2	4:D:179:ARG:NH2	2.27	0.49
1:A:131:LEU:HD21	1:A:152:LEU:HD21	1.94	0.49
2:B:355:LEU:O	2:B:355:LEU:HG	2.12	0.49
1:A:1764:GLU:HA	1:A:1819:PHE:HE1	1.77	0.49
1:A:1877:LEU:HA	1:A:1880:MET:HG2	1.94	0.49
1:A:3278:GLN:HE21	1:A:3326:GLN:HG2	1.78	0.49
1:A:3895:GLU:CD	1:A:3895:GLU:H	2.21	0.49
3:C:16:VAL:HG12	3:C:100:PRO:HA	1.94	0.49
5:E:51:DA:C2	5:F:51:DA:C2	3.01	0.49
1:A:1356:TRP:O	1:A:1411:TYR:OH	2.29	0.49
1:A:514:VAL:HG13	4:D:301:THR:HG23	1.95	0.49
1:A:1056:THR:HG21	1:A:1095:LEU:HG	1.94	0.49
1:A:1534:ASN:O	1:A:1554:SER:OG	2.29	0.49
3:C:52:ASP:OD1	3:C:53:GLU:N	2.46	0.48
5:F:51:DA:H1'	5:F:52:DT:H5''	1.94	0.48
1:A:3416:LEU:HD21	1:A:3445:LEU:HD21	1.96	0.48
1:A:3085:GLU:N	1:A:3085:GLU:OE2	2.47	0.48
5:E:26:DT:H2'	5:E:27:DG:C4	2.48	0.48
1:A:1001:PHE:HA	1:A:1054:VAL:HG13	1.94	0.48
1:A:1925:GLU:O	1:A:1980:ASN:ND2	2.47	0.48
5:F:51:DA:C2	5:F:52:DT:C2	3.01	0.48
1:A:3809:THR:HG22	1:A:3931:ALA:HA	1.95	0.48
2:B:345:LEU:HD21	2:B:400:TYR:HD1	1.78	0.48
1:A:2432:GLN:OE1	1:A:2464:HIS:NE2	2.47	0.48
2:B:380:THR:HG23	2:B:381:LEU:N	2.29	0.48
1:A:1358:LEU:HD23	1:A:1358:LEU:H	1.79	0.48
1:A:1579:VAL:HA	1:A:1582:LEU:HG	1.95	0.48
1:A:1013:ILE:HD13	1:A:1032:CYS:HB3	1.96	0.48
1:A:1279:LEU:HD23	1:A:1279:LEU:H	1.79	0.48
1:A:2890:ILE:HG23	1:A:2926:LEU:HD11	1.96	0.48
1:A:3167:ARG:O	1:A:3186:ARG:NH2	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:27:DG:C2	5:E:28:DC:C2	3.02	0.48
1:A:985:GLU:HB3	1:A:986:PRO:HD3	1.96	0.47
1:A:1524:LEU:HD23	1:A:1524:LEU:H	1.78	0.47
1:A:2087:GLU:HA	1:A:2090:ARG:HE	1.79	0.47
1:A:3723:ASP:OD1	1:A:3724:GLU:N	2.47	0.47
1:A:3924:HIS:CE1	1:A:3927:ASN:HD21	2.32	0.47
2:B:357:LYS:NZ	8:B:701:IHP:O45	2.42	0.47
1:A:715:ALA:O	1:A:719:LYS:NZ	2.47	0.47
1:A:1069:HIS:CG	1:A:1074:LYS:HD2	2.49	0.47
2:B:286:ILE:N	3:C:313:GLY:O	2.44	0.47
3:C:347:LYS:HA	3:C:389:MET:HG2	1.95	0.47
1:A:3673:ASP:N	1:A:3673:ASP:OD1	2.48	0.47
1:A:1188:ILE:HG21	1:A:1269:THR:HG21	1.96	0.47
2:B:411:VAL:HG12	2:B:436:PHE:HA	1.96	0.47
1:A:1851:LEU:HD23	1:A:1870:LYS:HD3	1.96	0.47
2:B:43:ASP:OD1	2:B:44:ALA:N	2.46	0.47
5:E:23:DA:C2	5:E:25:DA:C6	3.01	0.47
1:A:429:GLU:O	1:A:432:THR:OG1	2.33	0.47
1:A:1911:LEU:HD23	1:A:1911:LEU:H	1.79	0.47
2:B:333:GLU:OE1	3:C:505:LEU:CD1	2.63	0.47
5:E:16:DC:H2''	5:E:17:DA:C8	2.50	0.47
1:A:563:LEU:O	1:A:567:GLU:HG2	2.15	0.47
1:A:1594:SER:HB3	1:A:1632:TRP:HZ3	1.80	0.47
1:A:1711:ARG:NE	1:A:1761:LEU:HD11	2.30	0.47
3:C:268:LEU:HD23	3:C:269:GLN:O	2.15	0.47
1:A:52:ALA:HA	1:A:55:THR:HG22	1.97	0.47
4:D:19:PHE:HA	4:D:23:ASN:HB2	1.97	0.47
5:E:22:DT:H3'	5:E:22:DT:O2	2.15	0.47
5:E:53:DC:H2''	5:E:54:DG:OP2	2.14	0.47
1:A:96:MET:HB3	1:A:99:LYS:HB3	1.96	0.47
1:A:801:LYS:NZ	1:A:879:MET:SD	2.80	0.47
1:A:3049:LEU:HD22	1:A:3085:GLU:HG3	1.97	0.47
1:A:3842:TRP:HA	1:A:3845:LYS:HG2	1.97	0.47
4:D:111:LEU:HB2	4:D:121:MET:HB2	1.97	0.47
3:C:112:ILE:HA	3:C:115:MET:HE2	1.96	0.46
3:C:546:ASP:OD1	3:C:546:ASP:N	2.48	0.46
1:A:1504:ASP:OD1	1:A:1504:ASP:N	2.46	0.46
1:A:1675:TYR:OH	1:A:1692:ALA:O	2.23	0.46
1:A:1629:CYS:HB2	1:A:1632:TRP:CD1	2.51	0.46
1:A:3118:ASP:OD1	1:A:3119:VAL:N	2.49	0.46
1:A:4042:GLN:HG2	1:A:4066:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:32:DC:H2'	5:E:33:DT:C7	2.45	0.46
1:A:275:PHE:HE2	1:A:319:PHE:HB2	1.81	0.46
1:A:1824:LEU:HD22	1:A:1876:ILE:HG12	1.97	0.46
1:A:2310:VAL:HB	1:A:2359:LYS:HG3	1.98	0.46
1:A:3576:ASP:O	1:A:3629:ARG:NH2	2.49	0.46
2:B:267:ILE:HD11	3:C:534:LYS:HB2	1.97	0.46
2:B:446:MET:HE1	3:C:264:TYR:HB2	1.97	0.46
3:C:93:ASP:HA	3:C:97:LYS:HG2	1.97	0.46
3:C:234:LEU:HB2	3:C:483:PRO:HG3	1.97	0.46
1:A:577:GLU:HG2	1:A:577:GLU:O	2.16	0.46
1:A:1850:VAL:O	1:A:1870:LYS:NZ	2.32	0.46
1:A:1087:ARG:NH2	1:A:2647:TPO:O1P	2.48	0.46
1:A:3138:ILE:HG12	1:A:3189:PHE:HZ	1.80	0.46
3:C:104:GLN:O	3:C:104:GLN:HG2	2.16	0.46
3:C:265:LYS:HD3	3:C:268:LEU:HD12	1.96	0.46
4:D:138:ARG:NH2	4:D:317:SER:O	2.47	0.46
1:A:153:PHE:HE2	1:A:196:LEU:HD22	1.81	0.46
1:A:2540:LEU:HD21	1:A:2832:ILE:HG23	1.97	0.46
1:A:3147:LYS:HB2	1:A:3150:ASN:ND2	2.30	0.46
1:A:1090:ARG:NH1	1:A:2647:TPO:O2P	2.48	0.46
1:A:2548:PRO:HB2	1:A:2848:PHE:CE2	2.51	0.46
1:A:3789:ARG:NH2	1:A:3789:ARG:HG3	2.31	0.46
5:E:54:DG:N1	5:F:48:DG:C6	2.84	0.46
1:A:440:VAL:HG23	1:A:482:VAL:HG23	1.99	0.45
1:A:1924:THR:CG2	1:A:1975:LEU:CG	2.92	0.45
2:B:83:LEU:HD12	2:B:111:PRO:HB3	1.98	0.45
1:A:249:PHE:CD2	1:A:285:CYS:HB3	2.51	0.45
1:A:1794:GLN:NE2	1:A:1832:SER:OG	2.49	0.45
1:A:1970:LYS:O	1:A:1975:LEU:HB3	2.16	0.45
1:A:3049:LEU:HD21	1:A:3088:LEU:HD12	1.98	0.45
1:A:3439:LEU:HG	1:A:3442:TYR:CD2	2.52	0.45
1:A:3535:ILE:HG21	1:A:3759:ARG:HD3	1.98	0.45
2:B:505:ASP:OD2	3:C:333:TYR:OH	2.25	0.45
3:C:91:LEU:HD13	3:C:495:LEU:HD13	1.99	0.45
5:E:18:DT:H1'	5:E:19:DG:C8	2.52	0.45
5:F:50:DT:H6	5:F:50:DT:H2'	1.57	0.45
3:C:663:GLN:HB3	3:C:675:TRP:HZ3	1.82	0.45
1:A:1560:TYR:HB2	1:A:1592:MET:HE1	1.98	0.45
4:D:36:LYS:HE3	5:E:27:DG:H5"	1.99	0.45
1:A:1924:THR:CG2	1:A:1924:THR:O	2.64	0.45
2:B:35:ARG:O	2:B:162:SER:N	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:SER:OG	2:B:161:MET:HG2	2.16	0.45
3:C:208:VAL:HA	3:C:211:VAL:HG12	1.99	0.45
1:A:100:ILE:HG23	1:A:103:TYR:HD2	1.82	0.45
1:A:478:CYS:HA	1:A:481:THR:HG22	1.98	0.45
1:A:1608:ARG:NH1	1:A:1654:GLN:O	2.39	0.45
2:B:256:LEU:HD11	2:B:275:ASN:HB3	1.97	0.45
4:D:106:ILE:HD11	4:D:124:PHE:HB3	1.98	0.45
4:D:346:THR:CG2	4:D:347:THR:N	2.80	0.45
1:A:356:ASN:ND2	1:A:409:GLN:OE1	2.49	0.45
1:A:433:PRO:O	1:A:434:VAL:C	2.59	0.45
1:A:1418:HIS:O	1:A:1421:GLU:HG3	2.17	0.45
1:A:3883:LEU:HD23	1:A:3970:LEU:HD22	1.99	0.45
3:C:523:THR:O	3:C:527:GLN:HG2	2.17	0.45
5:F:50:DT:H2''	5:F:51:DA:OP2	2.16	0.45
1:A:3273:LEU:HD22	1:A:3312:VAL:HG11	1.98	0.45
1:A:3455:LYS:HG3	1:A:3490:VAL:HG22	1.98	0.45
2:B:349:GLY:HA3	3:C:463:LEU:HG	1.99	0.45
1:A:1801:VAL:HG13	1:A:1824:LEU:HD12	1.99	0.45
1:A:2535:THR:HA	1:A:2565:MET:HE1	1.98	0.45
2:B:147:LEU:HB3	2:B:193:LEU:HD11	1.99	0.45
2:B:285:PRO:HB3	3:C:312:GLN:HG3	1.99	0.45
1:A:813:TRP:HB3	1:A:818:LEU:HD11	1.99	0.44
1:A:1540:THR:HG23	1:A:1551:ILE:H	1.82	0.44
1:A:3367:SER:HB2	1:A:3372:LYS:HG3	1.99	0.44
5:E:46:DA:H1'	5:E:47:DC:H5'	1.99	0.44
1:A:1633:TRP:CD1	1:A:1674:THR:HG23	2.53	0.44
1:A:1790:SER:O	1:A:1793:THR:OG1	2.35	0.44
1:A:3285:HIS:NE2	1:A:3333:THR:OG1	2.43	0.44
1:A:1231:GLN:HB2	1:A:1232:PRO:HD3	1.98	0.44
1:A:1812:LEU:HG	1:A:1814:PHE:H	1.82	0.44
1:A:1958:GLU:OE1	1:A:1961:PHE:HE2	2.00	0.44
1:A:2442:MET:HE2	1:A:2446:LEU:HD21	2.00	0.44
1:A:3701:ILE:O	1:A:3704:GLN:HG3	2.17	0.44
1:A:3842:TRP:HA	1:A:3845:LYS:HE2	1.98	0.44
5:E:1:DT:H71	5:F:54:DG:H2'	2.00	0.44
1:A:1033:ILE:HG22	1:A:1085:ILE:HG21	1.99	0.44
1:A:1181:THR:HG22	1:A:1184:ARG:HH12	1.82	0.44
1:A:2304:VAL:HG22	1:A:2348:GLN:HG3	1.98	0.44
1:A:2371:PHE:HD2	1:A:2374:LEU:HB2	1.82	0.44
2:B:303:PHE:HB3	2:B:310:LEU:HD23	2.00	0.44
4:D:236:ARG:HA	4:D:242:LEU:HD22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:53:DC:N3	5:F:48:DG:N1	2.62	0.44
1:A:1836:LEU:H	1:A:1836:LEU:HD12	1.83	0.44
1:A:2036:LEU:HD23	4:D:147:MET:HG2	2.00	0.44
1:A:2634:GLN:HG3	1:A:2772:TYR:HB3	2.00	0.44
3:C:139:SER:HB3	3:C:201:GLN:HE21	1.83	0.44
3:C:400:ARG:HH22	5:E:45:DG:H21	1.65	0.44
4:D:1:MET:N	5:E:24:DT:C2	2.78	0.44
1:A:428:PRO:HB2	1:A:431:TYR:HD2	1.82	0.44
1:A:1214:GLU:OE1	1:A:1214:GLU:N	2.51	0.44
1:A:1594:SER:HB3	1:A:1632:TRP:CZ3	2.52	0.44
1:A:3274:VAL:HG11	1:A:3322:ALA:HB1	2.00	0.44
3:C:30:PRO:HB3	3:C:166:PRO:HG3	1.99	0.44
3:C:475:ASP:N	3:C:475:ASP:OD1	2.50	0.44
1:A:908:ASP:OD1	1:A:908:ASP:N	2.51	0.44
1:A:3701:ILE:HB	1:A:3704:GLN:NE2	2.33	0.44
1:A:1104:LEU:HA	1:A:1134:LEU:HD13	2.00	0.44
1:A:2123:PRO:HD2	1:A:2126:MET:HB2	1.99	0.44
1:A:2227:LYS:HB3	1:A:2230:VAL:HG12	1.99	0.44
1:A:567:GLU:HA	1:A:570:LYS:HG2	2.00	0.43
1:A:2135:ASN:HB3	1:A:2138:VAL:HG23	2.00	0.43
4:D:249:ARG:HB3	4:D:274:ILE:HG21	1.99	0.43
1:A:1140:LYS:HB3	1:A:2644:PHE:CZ	2.54	0.43
1:A:2313:LYS:HA	1:A:2316:TYR:CE2	2.53	0.43
1:A:2580:PRO:HB3	1:A:2784:GLN:HE21	1.82	0.43
2:B:263:LEU:HG	2:B:347:LEU:HD22	2.00	0.43
2:B:445:LYS:NZ	3:C:241:GLU:O	2.33	0.43
4:D:208:ALA:HB2	5:E:25:DA:H4'	2.00	0.43
1:A:257:ARG:HD3	1:A:258:PRO:HD2	1.99	0.43
1:A:1890:HIS:HB2	1:A:1955:VAL:HG11	2.00	0.43
1:A:3503:VAL:O	1:A:3540:TYR:OH	2.27	0.43
2:B:341:ASP:OD1	2:B:341:ASP:N	2.51	0.43
2:B:384:ALA:O	2:B:388:LYS:HG2	2.18	0.43
3:C:342:VAL:HG22	3:C:393:VAL:HG12	1.99	0.43
4:D:14:ILE:HG22	4:D:28:ALA:HB3	2.00	0.43
1:A:47:SER:HB3	1:A:50:VAL:HG12	1.98	0.43
4:D:346:THR:CG2	4:D:351:VAL:HG23	2.48	0.43
4:D:385:SER:OG	4:D:387:GLU:OE1	2.30	0.43
1:A:1672:PHE:HE2	1:A:1702:LEU:HG	1.84	0.43
4:D:402:ARG:HA	4:D:402:ARG:HD3	1.91	0.43
1:A:121:ALA:HA	1:A:124:LYS:HB3	2.00	0.43
1:A:1373:VAL:HG11	1:A:1418:HIS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3759:ARG:O	1:A:3763:ARG:HG2	2.19	0.43
2:B:38:LEU:HD21	2:B:167:MET:HE2	2.00	0.43
1:A:466:LEU:HD11	1:A:541:MET:HG3	2.00	0.43
1:A:584:GLU:CG	1:A:585:ILE:N	2.82	0.43
1:A:2953:THR:HG23	1:A:2993:PHE:HE2	1.84	0.43
1:A:3786:LEU:HD21	1:A:3983:ILE:HD12	2.01	0.43
2:B:257:SER:OG	2:B:403:ARG:NH1	2.44	0.43
4:D:5:GLU:HA	4:D:5:GLU:OE1	2.19	0.43
1:A:2428:ASP:HB3	1:A:2431:ARG:HB3	2.01	0.43
1:A:260:ILE:HB	3:C:553:ILE:HG23	2.01	0.43
1:A:1638:PRO:O	1:A:1642:LYS:HG2	2.18	0.43
1:A:2260:PHE:HA	1:A:2270:ASN:HA	2.00	0.43
1:A:2866:ALA:HB2	1:A:2899:ARG:NH2	2.34	0.43
1:A:3916:TRP:CE2	1:A:4107:LEU:HD21	2.54	0.43
2:B:59:PRO:HB3	2:B:205:LEU:HD13	2.01	0.43
4:D:43:ARG:CZ	4:D:74:LYS:HD3	2.49	0.43
1:A:2467:THR:OG1	1:A:2514:ASN:ND2	2.50	0.42
1:A:3269:ARG:HG2	1:A:3270:ASP:H	1.84	0.42
1:A:3467:ARG:HB2	1:A:4000:ASN:HD21	1.83	0.42
1:A:3604:LYS:O	1:A:3607:GLU:HG3	2.19	0.42
4:D:3:SER:O	4:D:3:SER:OG	2.37	0.42
4:D:276:SER:HA	4:D:282:LEU:HG	2.00	0.42
5:F:53:DC:H6	5:F:53:DC:H2'	1.63	0.42
1:A:160:LEU:HD23	1:A:160:LEU:HA	1.90	0.42
5:E:23:DA:H2	5:E:24:DT:C2	2.37	0.42
5:E:46:DA:H8	5:E:46:DA:OP2	2.02	0.42
5:E:51:DA:C5	5:E:52:DT:C4	3.07	0.42
1:A:1538:LEU:O	1:A:1552:HIS:ND1	2.52	0.42
1:A:1935:GLU:CD	1:A:1935:GLU:H	2.27	0.42
1:A:924:ARG:NH2	1:A:977:ASP:OD1	2.53	0.42
1:A:1852:LYS:HA	1:A:1918:LEU:HD11	2.00	0.42
1:A:2563:LEU:HD11	1:A:2808:LEU:HD21	2.02	0.42
1:A:2836:LEU:HD23	1:A:2836:LEU:HA	1.82	0.42
1:A:3091:LEU:HD21	1:A:3142:ILE:HG12	2.01	0.42
1:A:3281:CYS:HB2	1:A:3329:LEU:HD13	2.00	0.42
3:C:31:PHE:HZ	3:C:98:ILE:HG22	1.84	0.42
5:F:47:DC:H2''	5:F:48:DG:O5'	2.18	0.42
1:A:584:GLU:CG	1:A:585:ILE:H	2.32	0.42
1:A:818:LEU:HD22	1:A:3077:ILE:HG22	2.01	0.42
1:A:880:MET:HE1	1:A:3903[A]:HIS:CE1	2.55	0.42
1:A:1335:CYS:HA	1:A:1338:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2085:MET:O	1:A:2184:TYR:OH	2.28	0.42
1:A:2184:TYR:HA	1:A:2187:VAL:HG22	2.02	0.42
4:D:51:LEU:HD11	4:D:78:TRP:CZ2	2.54	0.42
5:F:48:DG:O5'	5:F:48:DG:C8	2.72	0.42
1:A:296:VAL:HG22	1:A:300:TRP:CD1	2.55	0.42
1:A:2421:VAL:O	1:A:2425:ARG:HG2	2.19	0.42
1:A:2426:HIS:O	1:A:2432:GLN:NE2	2.53	0.42
1:A:2455:LEU:HD12	1:A:2458:VAL:HB	2.02	0.42
1:A:2876:VAL:HG11	1:A:2892:LEU:HD23	2.02	0.42
1:A:3531:TYR:HB2	1:A:3532:PRO:HD3	2.01	0.42
1:A:3847:SER:HB2	1:A:3857:LEU:HB2	2.02	0.42
3:C:548:VAL:HG23	3:C:553:ILE:HD11	2.01	0.42
1:A:359:LEU:O	1:A:363:ILE:HG12	2.20	0.42
1:A:956:PRO:HA	1:A:957:PRO:HD3	1.89	0.42
1:A:1997:PRO:HG2	1:A:2000:ARG:HB2	2.01	0.42
2:B:474:ARG:HB2	2:B:477:SER:OG	2.20	0.42
1:A:430:VAL:HB	1:A:1498:GLN:O	2.20	0.42
3:C:528:ILE:HB	3:C:529:PRO:HD3	2.01	0.42
1:A:793:LEU:HD12	1:A:869:ASN:HB2	2.02	0.42
1:A:1693:VAL:O	1:A:1696:LEU:HB2	2.20	0.42
1:A:3452:LYS:HA	1:A:3455:LYS:HE2	2.02	0.42
3:C:9:ALA:HB3	3:C:130:ARG:HG2	2.02	0.42
3:C:643:ARG:HA	3:C:655:PHE:CZ	2.55	0.42
1:A:1845:VAL:CG2	1:A:1846:ASP:N	2.82	0.41
1:A:2414:GLN:OE1	1:A:2414:GLN:N	2.48	0.41
1:A:3640:PHE:O	1:A:3644:PHE:HB2	2.20	0.41
1:A:3813:LYS:HB2	1:A:3925:LEU:HB3	2.01	0.41
3:C:44:ARG:HD3	3:C:237:PHE:CZ	2.54	0.41
3:C:502:ARG:O	3:C:503:GLU:HG3	2.20	0.41
4:D:35:HIS:ND1	5:E:25:DA:OP1	2.52	0.41
1:A:935:HIS:CD2	1:A:987:LEU:HD22	2.54	0.41
1:A:1195:VAL:HG11	1:A:1204:PRO:HA	2.02	0.41
1:A:1985:LYS:O	1:A:1985:LYS:HG2	2.19	0.41
1:A:2003:LYS:O	1:A:2006:GLU:HG2	2.20	0.41
1:A:3414:MET:HE2	1:A:3460:GLU:HG2	2.02	0.41
2:B:369:TYR:OH	3:C:436:SER:O	2.36	0.41
3:C:20:MET:HG2	3:C:30:PRO:HB2	2.02	0.41
5:E:44:DT:H2''	5:E:45:DG:C8	2.55	0.41
1:A:238:MET:SD	1:A:245:SER:OG	2.68	0.41
1:A:545:LEU:HD23	1:A:551:PHE:HB3	2.02	0.41
1:A:1758:LEU:O	1:A:1762:MET:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1828:LEU:O	1:A:1883:ARG:NH2	2.42	0.41
5:E:47:DC:H2''	5:E:48:DG:C8	2.54	0.41
1:A:125:ILE:HB	1:A:126:PRO:HD3	2.02	0.41
1:A:1050:GLU:HG2	1:A:1094:SER:HB3	2.01	0.41
1:A:3528:ALA:HB2	1:A:3705:TYR:CG	2.56	0.41
3:C:44:ARG:HD3	3:C:237:PHE:CE2	2.55	0.41
1:A:759:GLY:HA3	1:A:766:ALA:HB2	2.02	0.41
1:A:1655:ILE:HD12	1:A:1655:ILE:HA	1.95	0.41
1:A:3100:LYS:HA	1:A:3103:ILE:HG22	2.02	0.41
3:C:33:GLN:HB3	3:C:227:PHE:HB3	2.02	0.41
4:D:8:MET:HG2	4:D:163:TYR:CE1	2.54	0.41
5:E:20:DC:C4	5:E:26:DT:C4	3.08	0.41
5:E:32:DC:H2'	5:E:33:DT:H72	2.03	0.41
2:B:357:LYS:HD2	2:B:360:HIS:NE2	2.36	0.41
1:A:208:MET:HG3	1:A:220:LEU:HD21	2.02	0.41
1:A:1614:GLN:O	1:A:1618:LEU:HG	2.19	0.41
1:A:3424:LEU:HD23	1:A:3439:LEU:HD23	2.01	0.41
1:A:3466:PRO:HB2	1:A:4004:VAL:HG21	2.03	0.41
2:B:41:LEU:HD23	2:B:168:LEU:HD13	2.03	0.41
1:A:2327:LEU:HD21	1:A:2341:LEU:HB3	2.02	0.41
1:A:3095:ASP:OD1	1:A:3098:ARG:HG2	2.20	0.41
1:A:4090:ARG:NH2	1:A:4113:ASP:OD2	2.38	0.41
3:C:378:SER:O	3:C:382:HIS:ND1	2.47	0.41
3:C:645:GLU:O	3:C:649:PHE:HB3	2.20	0.41
4:D:43:ARG:HD3	4:D:74:LYS:HB3	2.03	0.41
1:A:975:ASP:O	1:A:981:ARG:NH1	2.54	0.41
1:A:1761:LEU:HD12	1:A:1761:LEU:H	1.86	0.41
1:A:1783:ARG:HG3	1:A:1784:ARG:N	2.36	0.41
1:A:1934:LEU:H	1:A:1934:LEU:HD12	1.85	0.41
1:A:2341:LEU:HD23	1:A:2341:LEU:HA	1.93	0.41
1:A:3050:LYS:NZ	1:A:3181:ASP:HA	2.35	0.41
4:D:37:ASP:OD1	4:D:37:ASP:N	2.54	0.41
5:E:27:DG:H1'	5:E:28:DC:C6	2.56	0.41
5:E:50:DT:H1'	5:E:51:DA:H5''	2.02	0.41
5:E:51:DA:H5'	5:E:51:DA:C8	2.55	0.41
5:E:54:DG:C2	5:F:48:DG:C2	3.08	0.41
2:B:457:GLU:HG3	2:B:528:LEU:HD21	2.02	0.41
1:A:541:MET:HE1	1:A:558:GLU:HA	2.03	0.40
1:A:572:VAL:HG22	1:A:626:LEU:HD11	2.03	0.40
1:A:1866:GLN:O	1:A:1870:LYS:HG2	2.21	0.40
1:A:3190:LEU:HB3	1:A:3231:ILE:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:ILE:HG21	3:C:113:VAL:HG21	2.02	0.40
5:E:53:DC:H1'	5:E:54:DG:O5'	2.21	0.40
1:A:759:GLY:HA2	1:A:762:TYR:O	2.21	0.40
1:A:1839:PHE:O	1:A:1843:ILE:HG12	2.21	0.40
1:A:3954:PRO:HD3	1:A:4028:ILE:HG13	2.04	0.40
1:A:442:GLN:HE22	1:A:461:ILE:HD11	1.85	0.40
1:A:1476:HIS:HA	1:A:1479:VAL:HG12	2.02	0.40
4:D:33:HIS:HB3	4:D:119:SER:HA	2.02	0.40
1:A:1136:ARG:NH2	1:A:2645:TPO:O	2.51	0.40
1:A:4121:TRP:CD1	1:A:4123:GLY:H	2.40	0.40
1:A:822:ALA:HB2	1:A:3073:LEU:HG	2.03	0.40
1:A:3772:ASN:HB3	1:A:3787:GLN:HE22	1.86	0.40
2:B:103:TYR:HB3	2:B:135:MET:HE3	2.04	0.40
2:B:120:ASP:OD1	2:B:123:LYS:HE3	2.21	0.40
3:C:53:GLU:HG2	3:C:85:LEU:HD12	2.03	0.40
3:C:202:LYS:O	3:C:206:GLU:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3829/4128 (93%)	3731 (97%)	98 (3%)	0	100	100
2	B	505/612 (82%)	497 (98%)	8 (2%)	0	100	100
3	C	623/732 (85%)	605 (97%)	18 (3%)	0	100	100
4	D	405/701 (58%)	394 (97%)	11 (3%)	0	100	100
All	All	5362/6173 (87%)	5227 (98%)	135 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3431/3667 (94%)	3386 (99%)	45 (1%)	61	81
2	B	461/550 (84%)	459 (100%)	2 (0%)	84	90
3	C	571/649 (88%)	566 (99%)	5 (1%)	70	85
4	D	372/639 (58%)	365 (98%)	7 (2%)	50	76
All	All	4835/5505 (88%)	4776 (99%)	59 (1%)	61	82

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	389	ILE
1	A	432	THR
1	A	514	VAL
1	A	723	ASP
1	A	1198	LEU
1	A	1261	LEU
1	A	1423	ILE
1	A	1434	VAL
1	A	1448	LEU
1	A	1491	ILE
1	A	1550	VAL
1	A	1590	THR
1	A	1593	VAL
1	A	1668	PHE
1	A	1671	VAL
1	A	1696	LEU
1	A	1747	LEU
1	A	1748	ASP
1	A	1759	LEU
1	A	1805	PHE
1	A	1933	LEU
1	A	1976	LEU
1	A	1993	GLU
1	A	2013	GLU

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Mol	Chain	Res	Type
1	A	2097	LEU
1	A	2169	LEU
1	A	2449	VAL
1	A	2631	VAL
1	A	2770	VAL
1	A	2806	LYS
1	A	2899	ARG
1	A	3073	LEU
1	A	3077	ILE
1	A	3426	LYS
1	A	3480	LEU
1	A	3553	GLU
1	A	3564	GLN
1	A	3607	GLU
1	A	3680	LEU
1	A	3694	PHE
1	A	3789	ARG
1	A	3845	LYS
1	A	3977	THR
1	A	4028	ILE
1	A	4031	ILE
2	B	246	VAL
2	B	329	LEU
3	C	16	VAL
3	C	40	MET
3	C	287	GLU
3	C	351	VAL
3	C	530	LEU
4	D	8	MET
4	D	19	PHE
4	D	22	GLU
4	D	247	THR
4	D	318	PHE
4	D	372	LEU
4	D	405	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	98	GLN
1	A	281	GLN

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Mol	Chain	Res	Type
1	A	334	HIS
1	A	356	ASN
1	A	409	GLN
1	A	415	GLN
1	A	442	GLN
1	A	485	GLN
1	A	562	HIS
1	A	857	GLN
1	A	935	HIS
1	A	982	GLN
1	A	1115	HIS
1	A	1287	GLN
1	A	1418	HIS
1	A	1426	GLN
1	A	1435	ASN
1	A	1442	GLN
1	A	1477	HIS
1	A	1552	HIS
1	A	1737	ASN
1	A	1738	ASN
1	A	1794	GLN
1	A	1931	ASN
1	A	1946	ASN
1	A	1974	ASN
1	A	2103	HIS
1	A	2105	HIS
1	A	2152	ASN
1	A	2275	GLN
1	A	2493	ASN
1	A	2508	GLN
1	A	2523	ASN
1	A	2784	GLN
1	A	2799	GLN
1	A	2807	GLN
1	A	2834	GLN
1	A	3093	GLN
1	A	3112	GLN
1	A	3139	GLN
1	A	3154	GLN
1	A	3251	ASN
1	A	3278	GLN
1	A	3319	ASN

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Mol	Chain	Res	Type
1	A	3379	GLN
1	A	3384	HIS
1	A	3515	GLN
1	A	3516	HIS
1	A	3564	GLN
1	A	3573	ASN
1	A	3787	GLN
1	A	3818	ASN
1	A	3944	HIS
1	A	3951	GLN
1	A	3966	GLN
1	A	3986	HIS
1	A	4000	ASN
1	A	4015	ASN
1	A	4018	GLN
1	A	4088	ASN
1	A	4110	GLN
2	B	110	ASN
2	B	137	HIS
2	B	174	ASN
2	B	320	GLN
2	B	405	ASN
2	B	426	GLN
3	C	119	GLN
3	C	188	HIS
3	C	200	GLN
3	C	201	GLN
3	C	423	GLN
3	C	450	GLN
3	C	509	GLN
3	C	510	GLN
3	C	514	ASN
3	C	555	GLN
4	D	23	ASN
4	D	35	HIS
4	D	336	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	A	2645	1	8,10,11	1.11	0	10,14,16	2.15	1 (10%)
1	TPO	A	2609	1	8,10,11	1.65	1 (12%)	10,14,16	2.10	1 (10%)
1	TPO	A	2647	1	8,10,11	0.78	0	10,14,16	1.03	1 (10%)
1	TPO	A	2638	1	8,10,11	1.64	1 (12%)	10,14,16	2.10	1 (10%)

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
1	TPO	A	2645	1	-	0/9/11/13	-
1	TPO	A	2609	1	-	3/9/11/13	-
1	TPO	A	2647	1	-	1/9/11/13	-
1	TPO	A	2638	1	-	2/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2609	TPO	P-O1P	3.55	1.61	1.50
1	A	2638	TPO	P-O1P	3.52	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2645	TPO	P-OG1-CB	-6.19	106.50	123.33
1	A	2609	TPO	P-OG1-CB	-6.03	106.94	123.33
1	A	2638	TPO	P-OG1-CB	-6.01	107.01	123.33
1	A	2647	TPO	O-C-CA	-2.50	118.33	124.77

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	2638	TPO	O-C-CA-CB
1	A	2638	TPO	CB-OG1-P-O1P
1	A	2609	TPO	CB-OG1-P-O2P
1	A	2609	TPO	CB-OG1-P-O3P
1	A	2647	TPO	O-C-CA-CB
1	A	2609	TPO	CB-OG1-P-O1P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	2645	TPO	1	0
1	A	2647	TPO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	IHP	B	701	-	36,36,36	1.53	6 (16%)	60,60,60	0.77	2 (3%)
7	ATP	A	4201	6	32,33,33	0.54	0	48,52,52	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	IHP	B	701	-	-	4/30/54/54	0/1/1/1
7	ATP	A	4201	6	-	4/22/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	701	IHP	P4-O14	3.35	1.65	1.59
8	B	701	IHP	P5-O15	3.32	1.65	1.59
8	B	701	IHP	P3-O13	3.30	1.65	1.59
8	B	701	IHP	P6-O16	3.30	1.65	1.59
8	B	701	IHP	P1-O11	3.30	1.65	1.59
8	B	701	IHP	P2-O12	3.27	1.65	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	701	IHP	P6-O16-C6	-2.10	117.83	123.43
8	B	701	IHP	P2-O12-C2	-2.03	118.02	123.43

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	4201	ATP	C5'-O5'-PA-O1A
7	A	4201	ATP	C5'-O5'-PA-O2A
7	A	4201	ATP	C5'-O5'-PA-O3A
7	A	4201	ATP	PG-O3B-PB-O1B
8	B	701	IHP	C2-O12-P2-O22
8	B	701	IHP	C4-O14-P4-O24
8	B	701	IHP	C1-O11-P1-O31
8	B	701	IHP	C1-O11-P1-O21

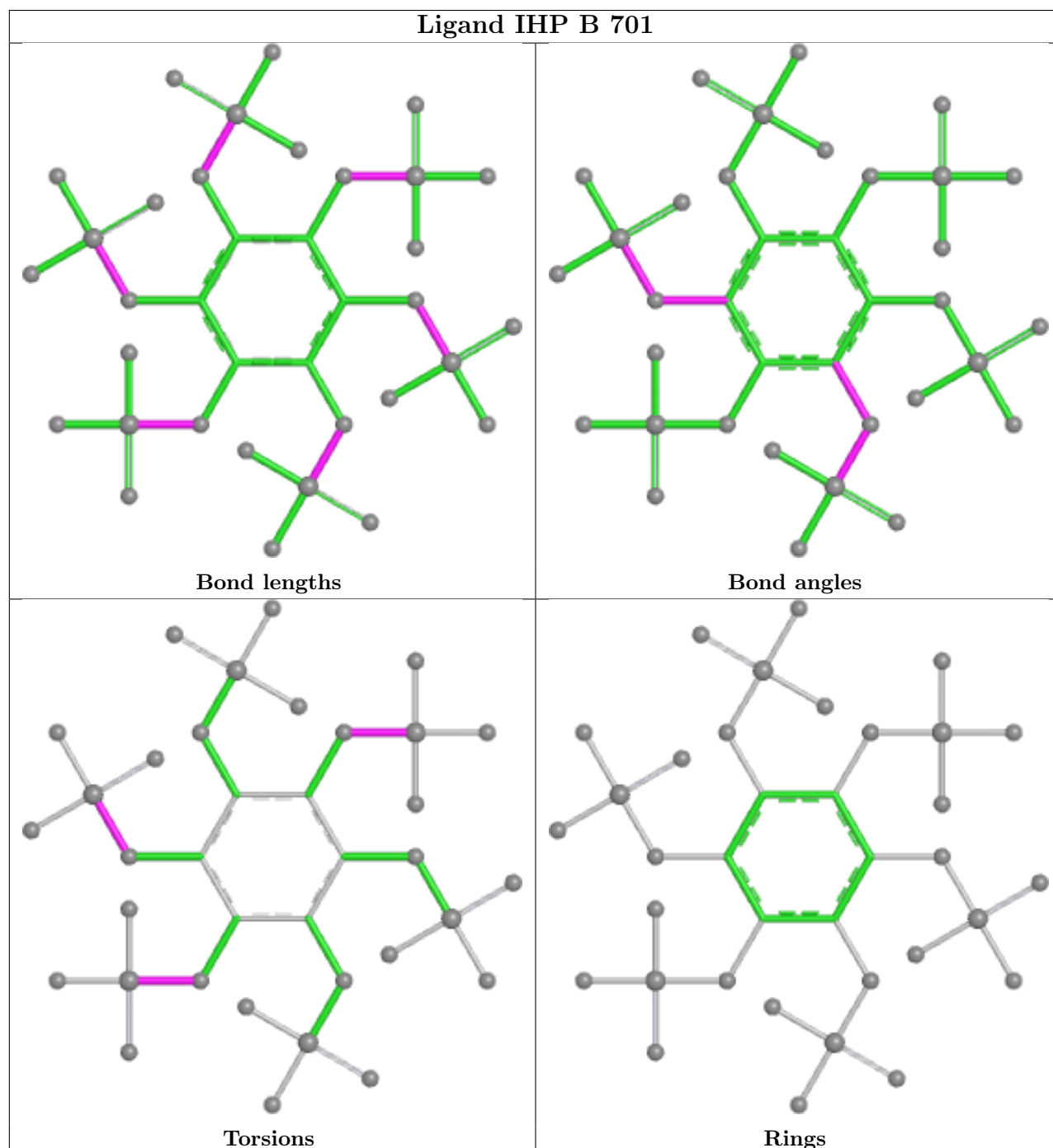
There are no ring outliers.

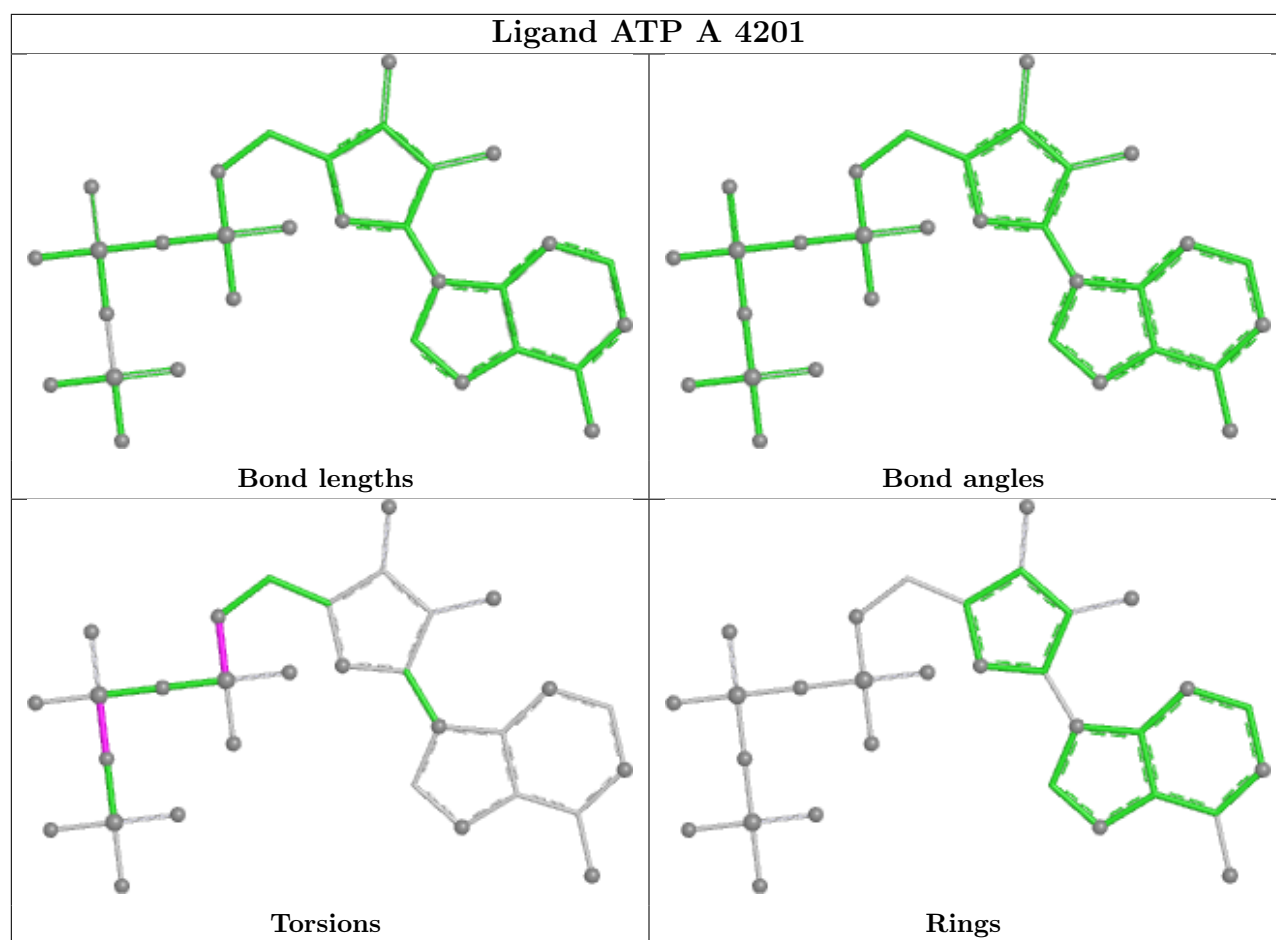
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	701	IHP	3	0

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

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





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.

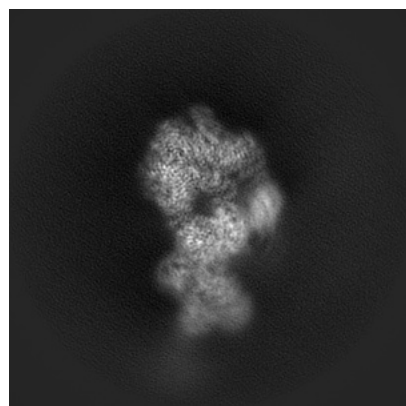
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25113. These allow visual inspection of the internal detail of the map and identification of artifacts.

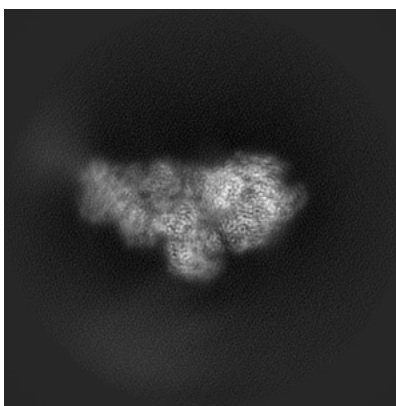
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

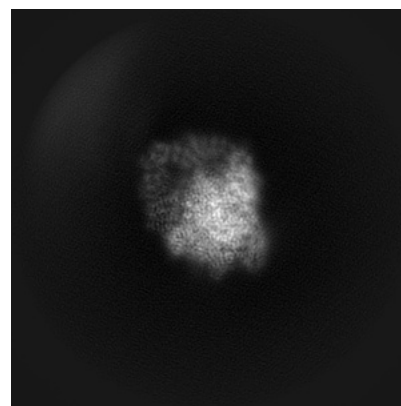
6.1.1 Primary map



X

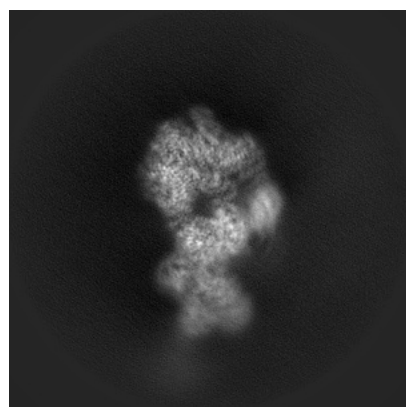


Y

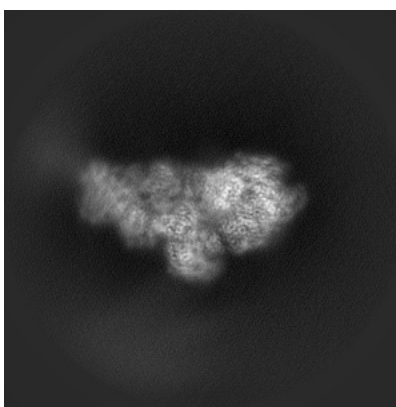


Z

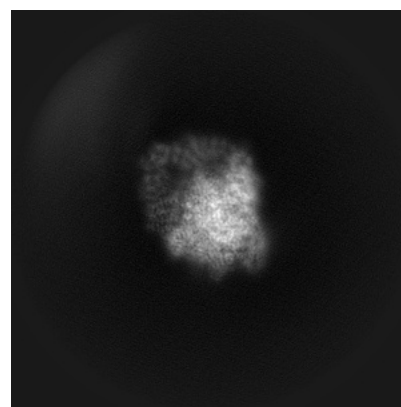
6.1.2 Raw map



X



Y

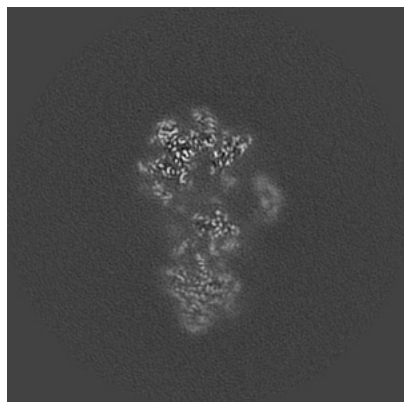


Z

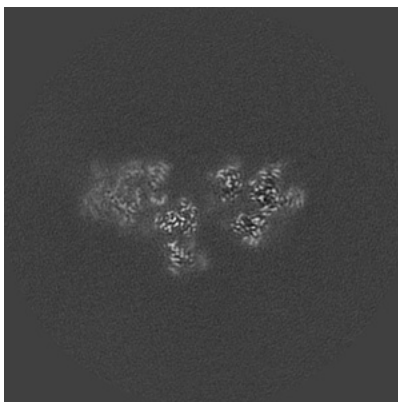
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

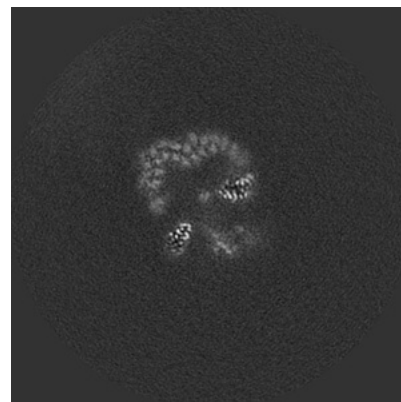
6.2.1 Primary map



X Index: 240

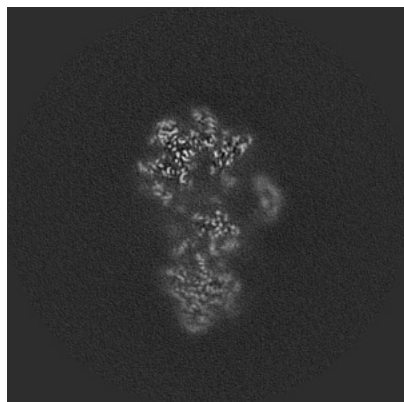


Y Index: 240

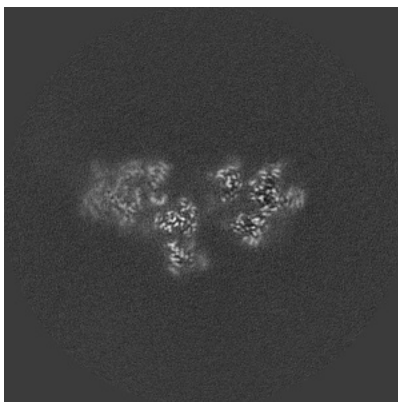


Z Index: 240

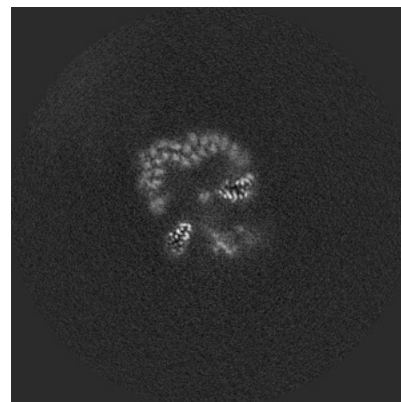
6.2.2 Raw map



X Index: 240



Y Index: 240

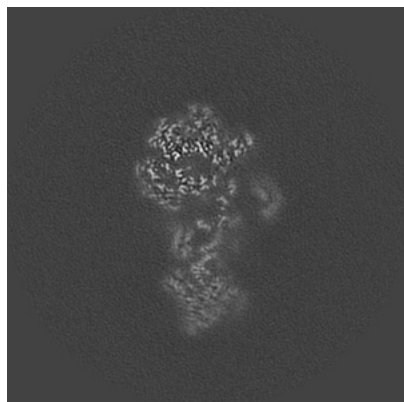


Z Index: 240

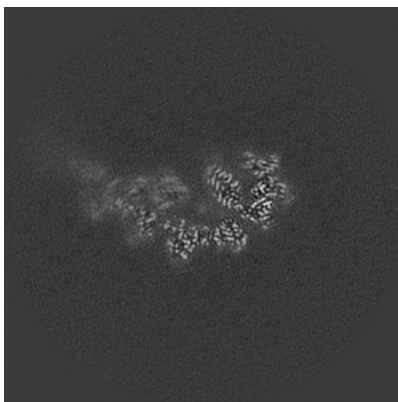
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

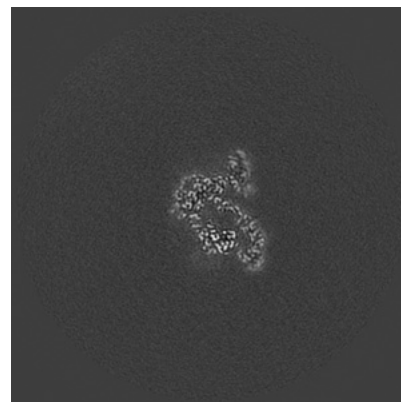
6.3.1 Primary map



X Index: 248

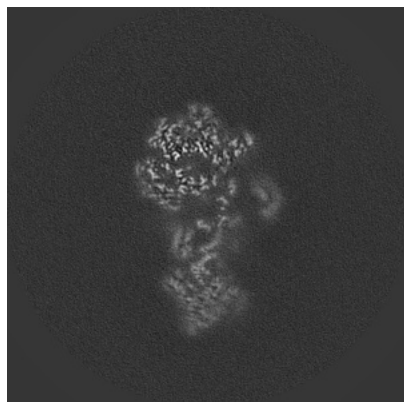


Y Index: 211

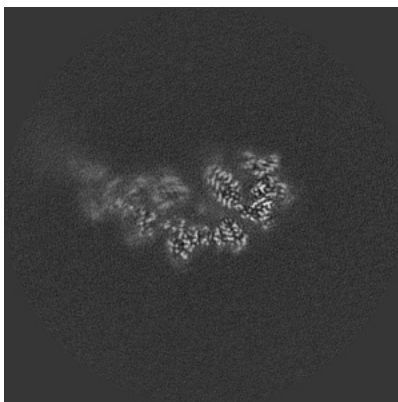


Z Index: 300

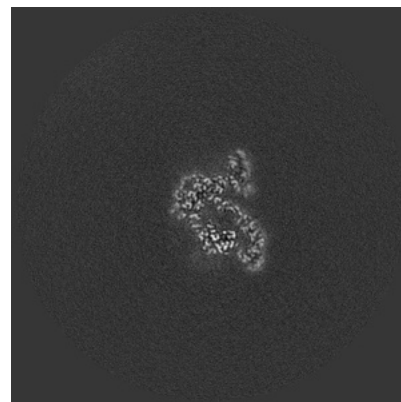
6.3.2 Raw map



X Index: 248



Y Index: 211

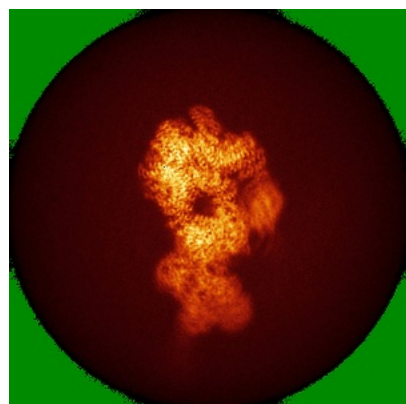


Z Index: 300

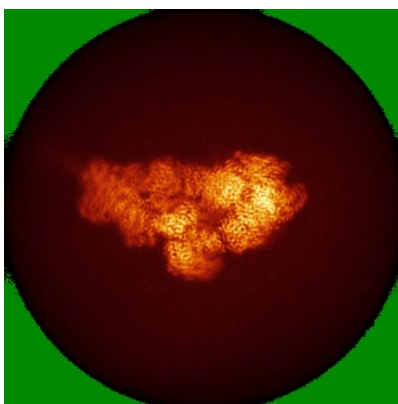
The images above show the largest variance slices of the map in three orthogonal directions.

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

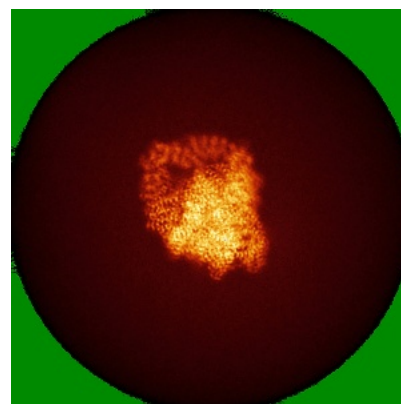
6.4.1 Primary map



X

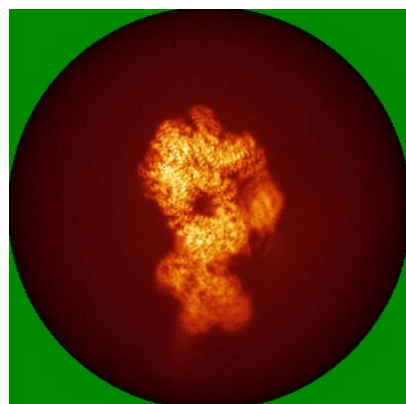


Y

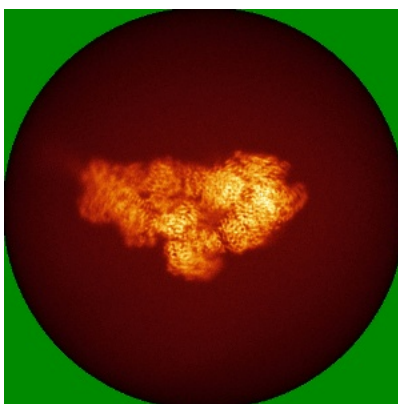


Z

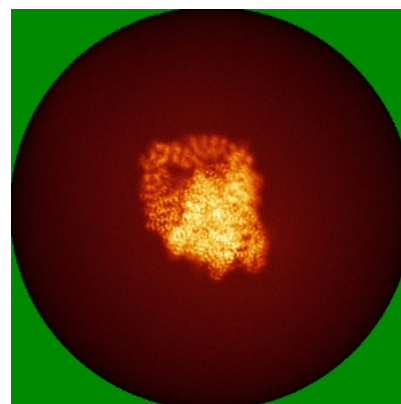
6.4.2 Raw map



X



Y

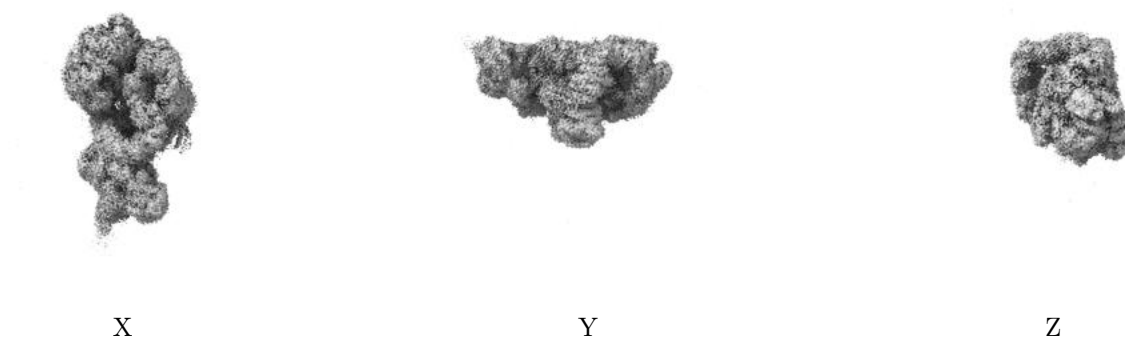


Z

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.

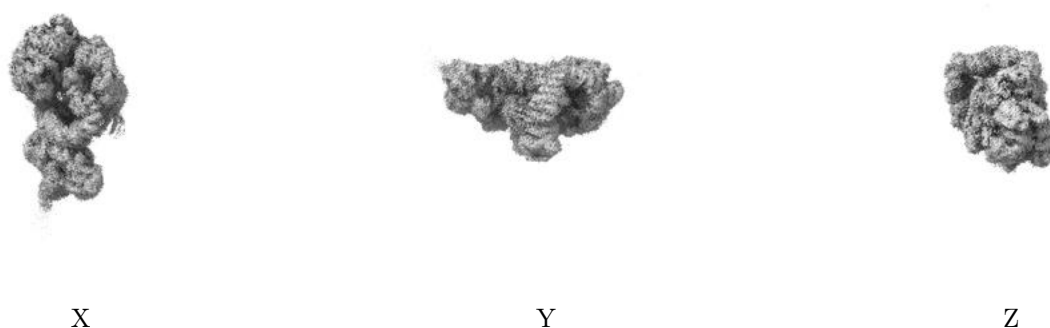
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0056. 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.

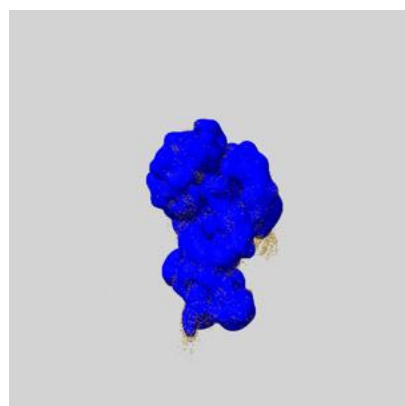
6.6 Mask visualisation [i](#)

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

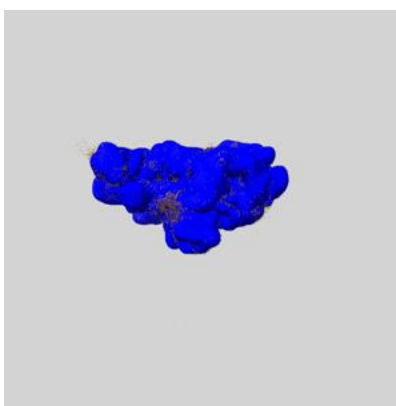
A mask typically either:

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

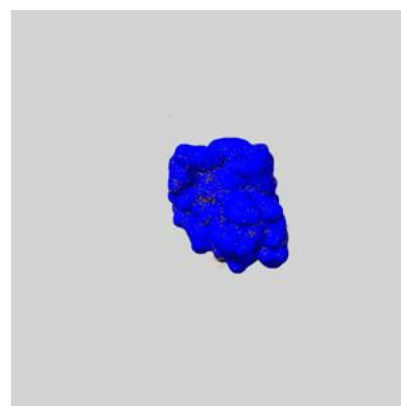
6.6.1 emd_25113_msk_1.map [i](#)



X



Y

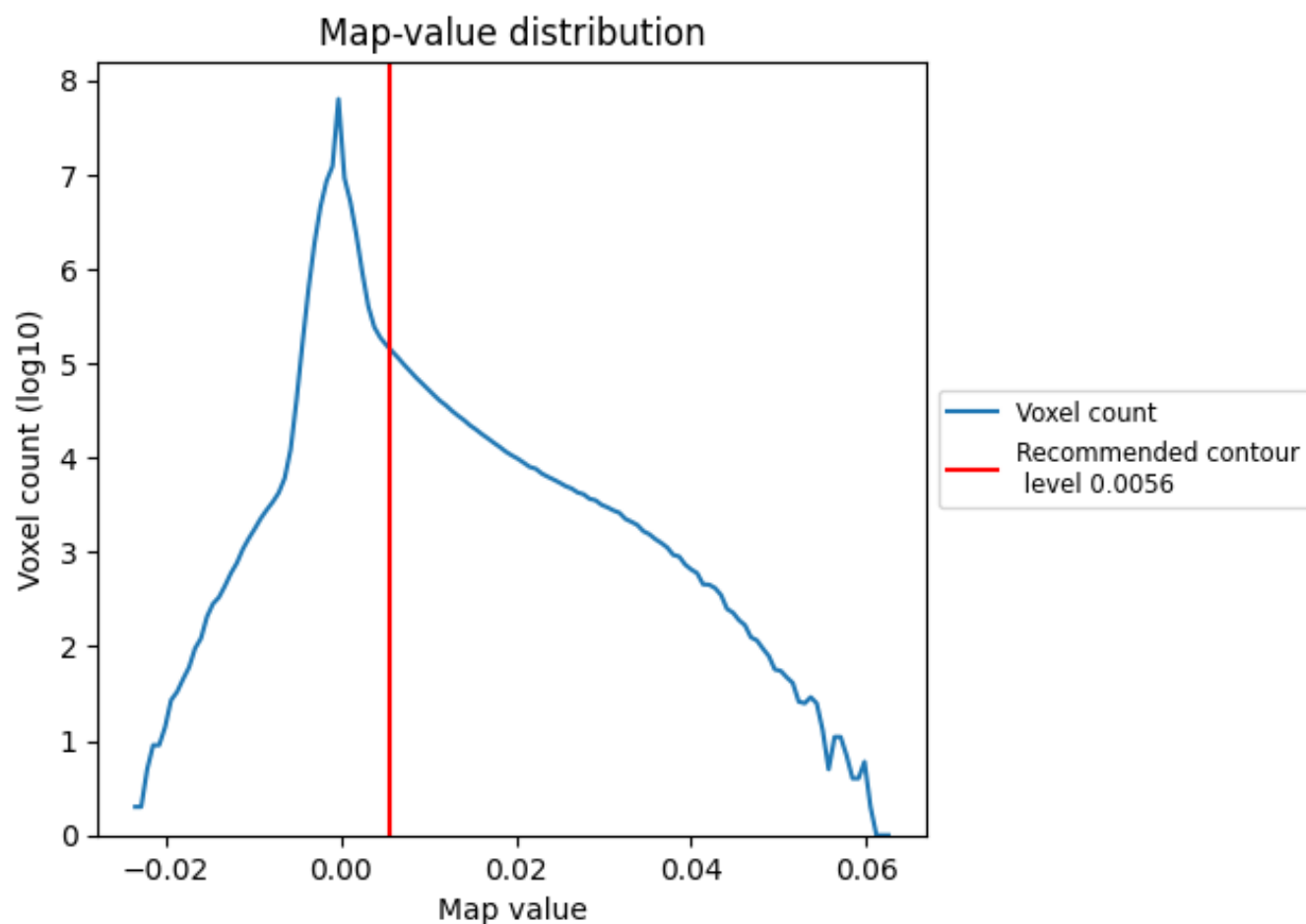


Z

7 Map analysis [i](#)

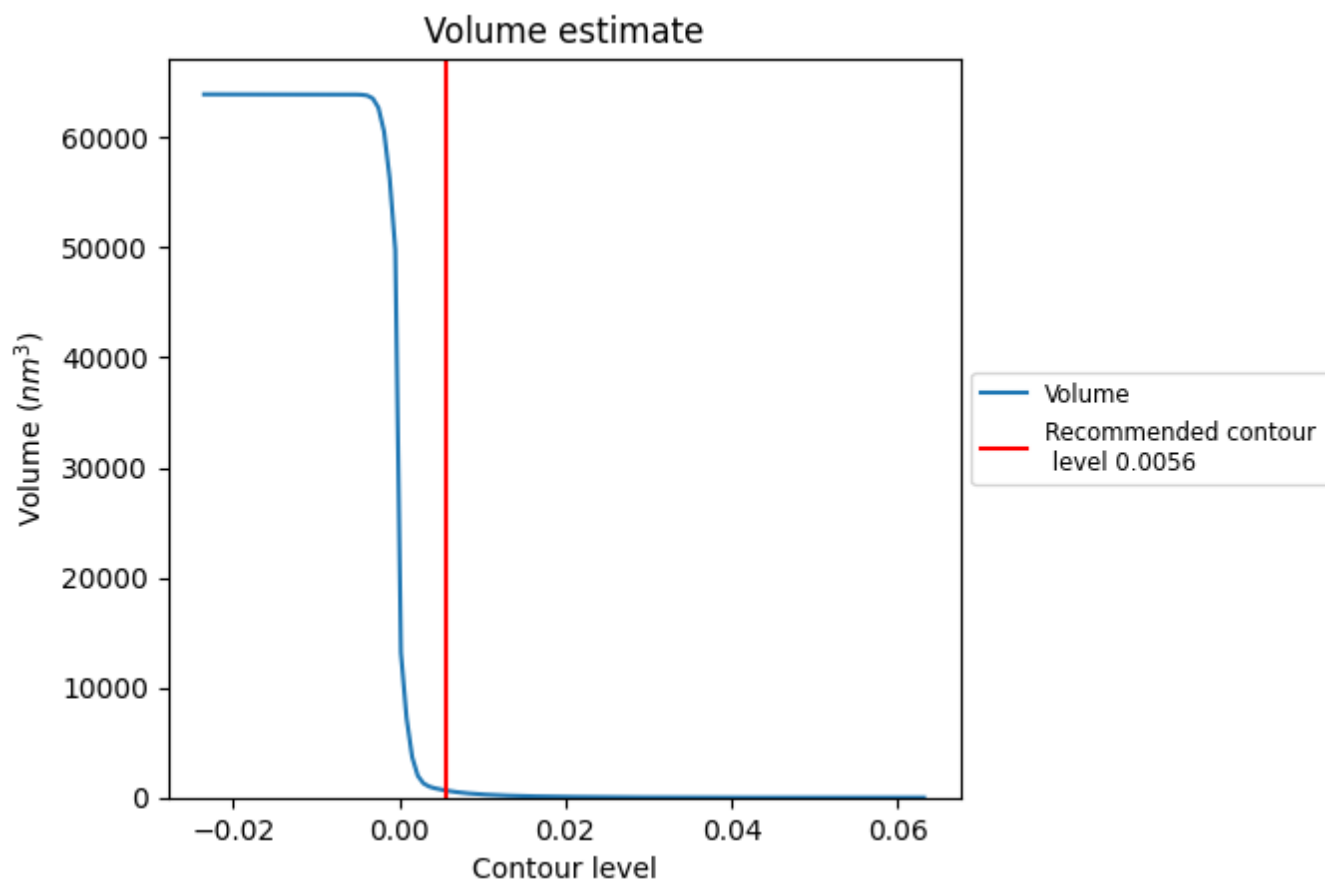
This section contains the results of statistical analysis of the map.

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.

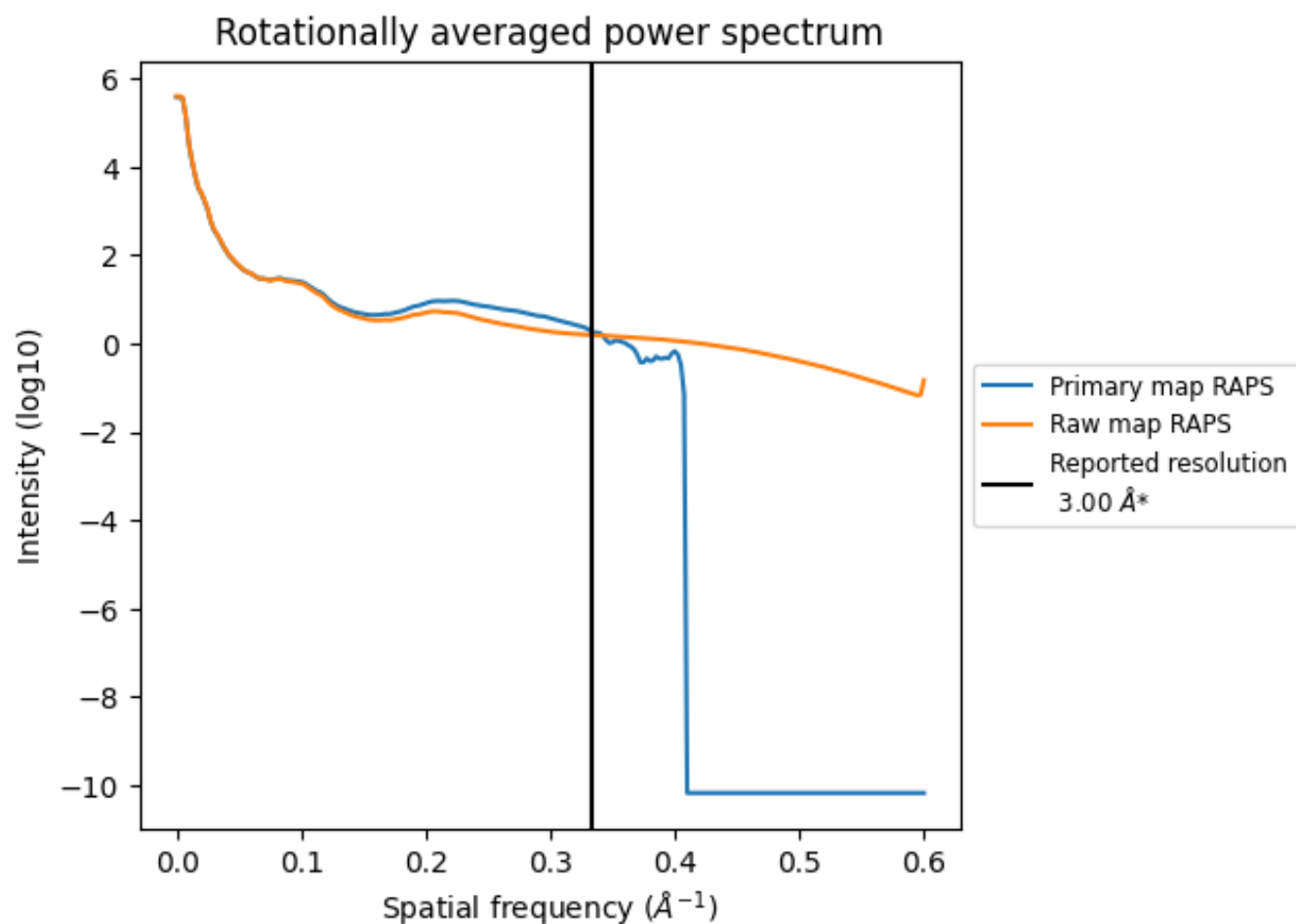
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 643 nm³; this corresponds to an approximate mass of 581 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 ⓘ

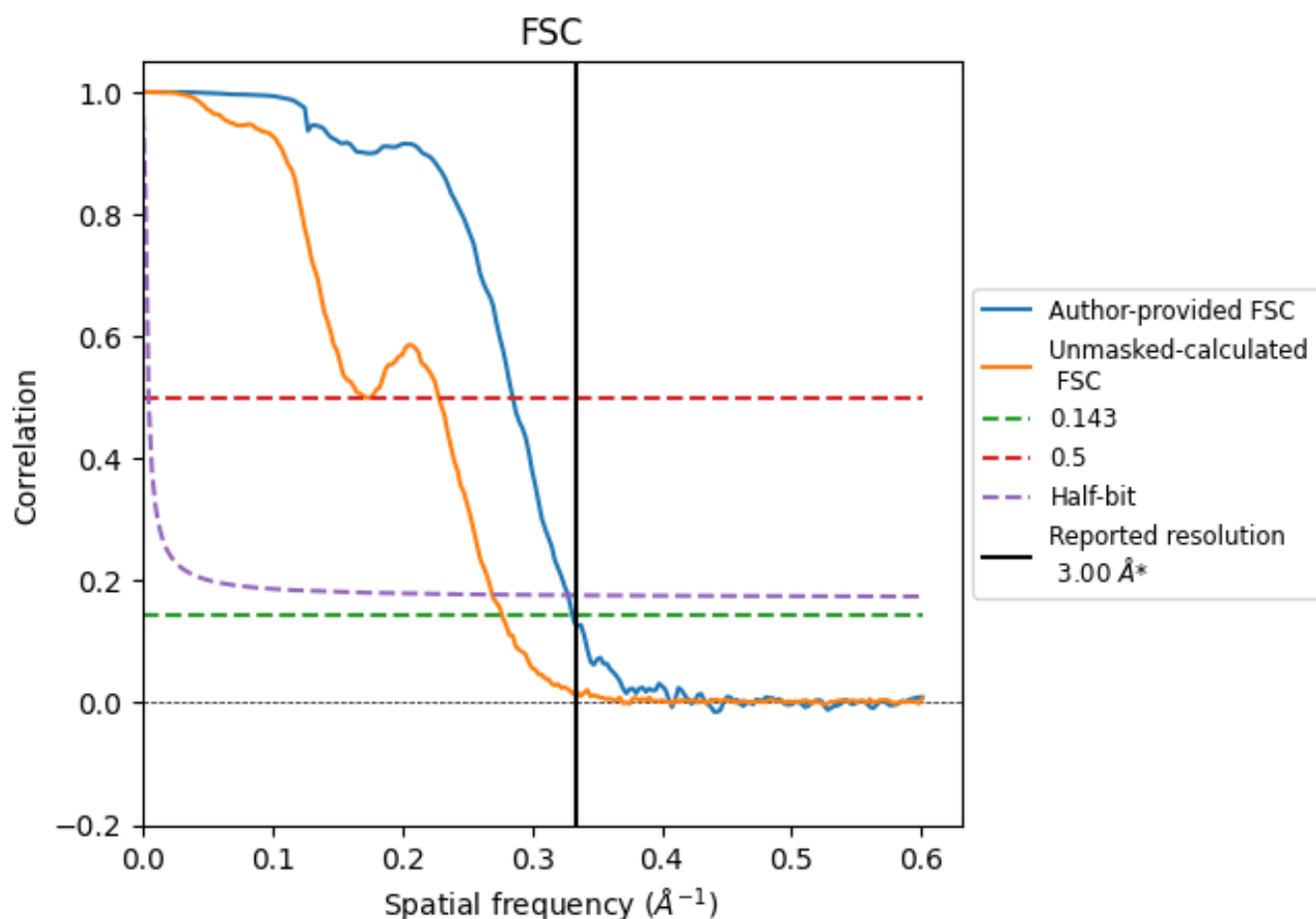


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

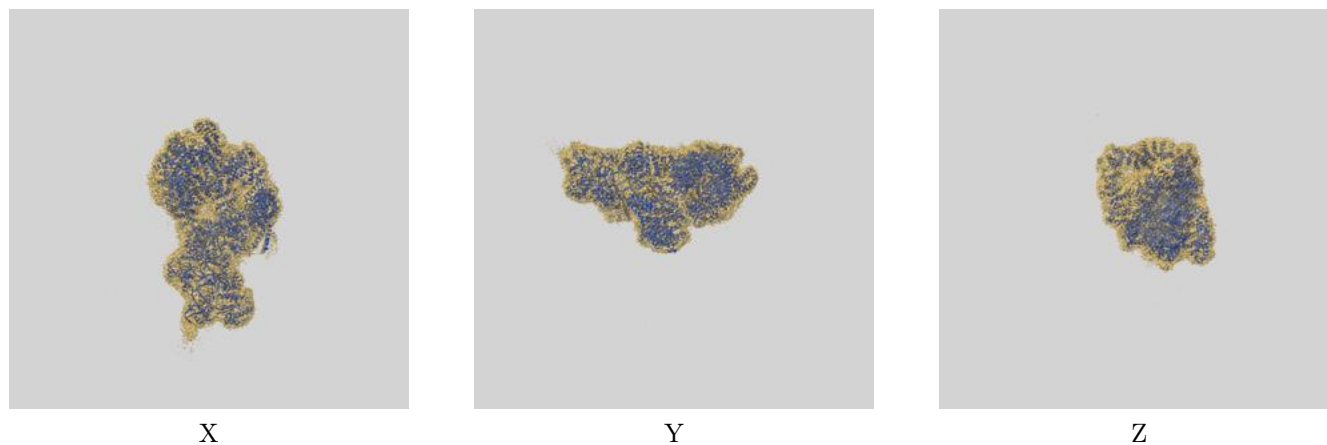
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.02	3.51	3.05
Unmasked-calculated*	3.61	5.81	3.71

*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 3.61 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

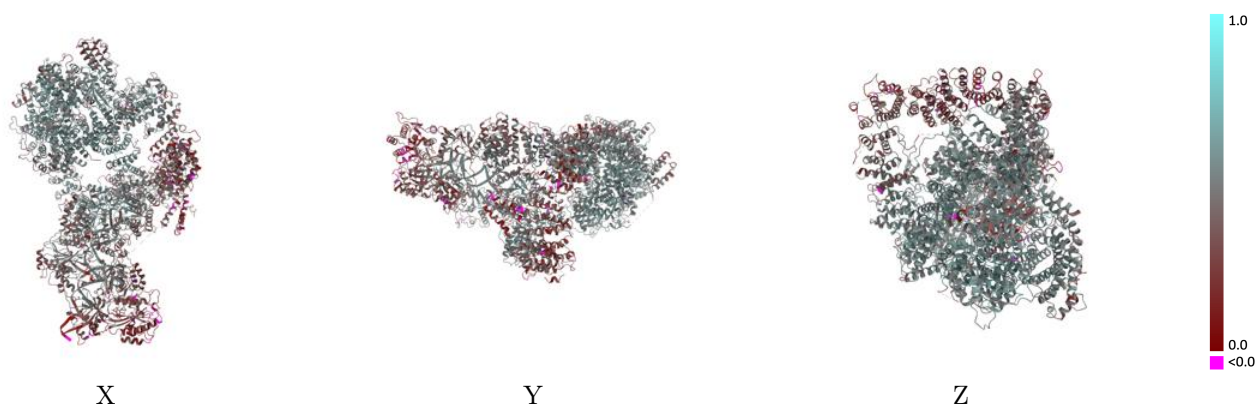
This section contains information regarding the fit between EMDB map EMD-25113 and PDB model 7SGL. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



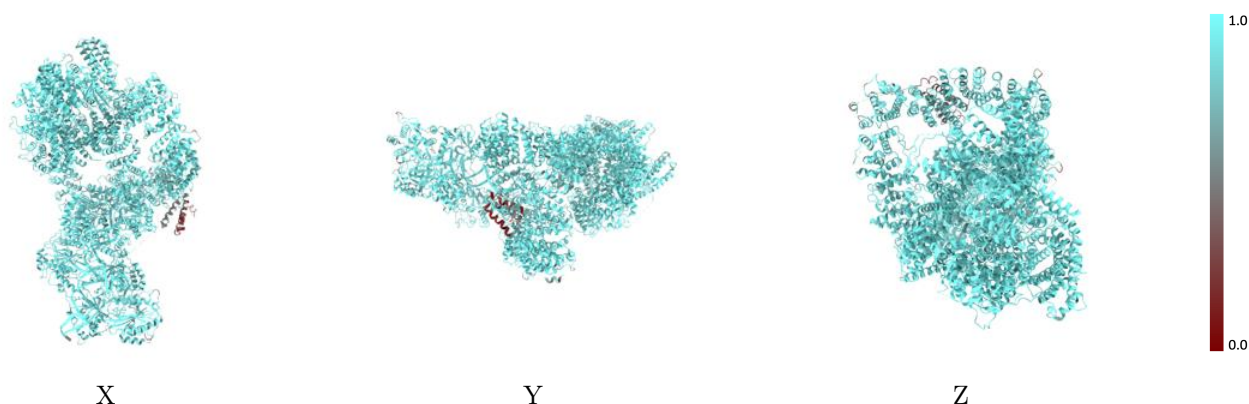
The images above show the 3D surface view of the map at the recommended contour level 0.0056 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



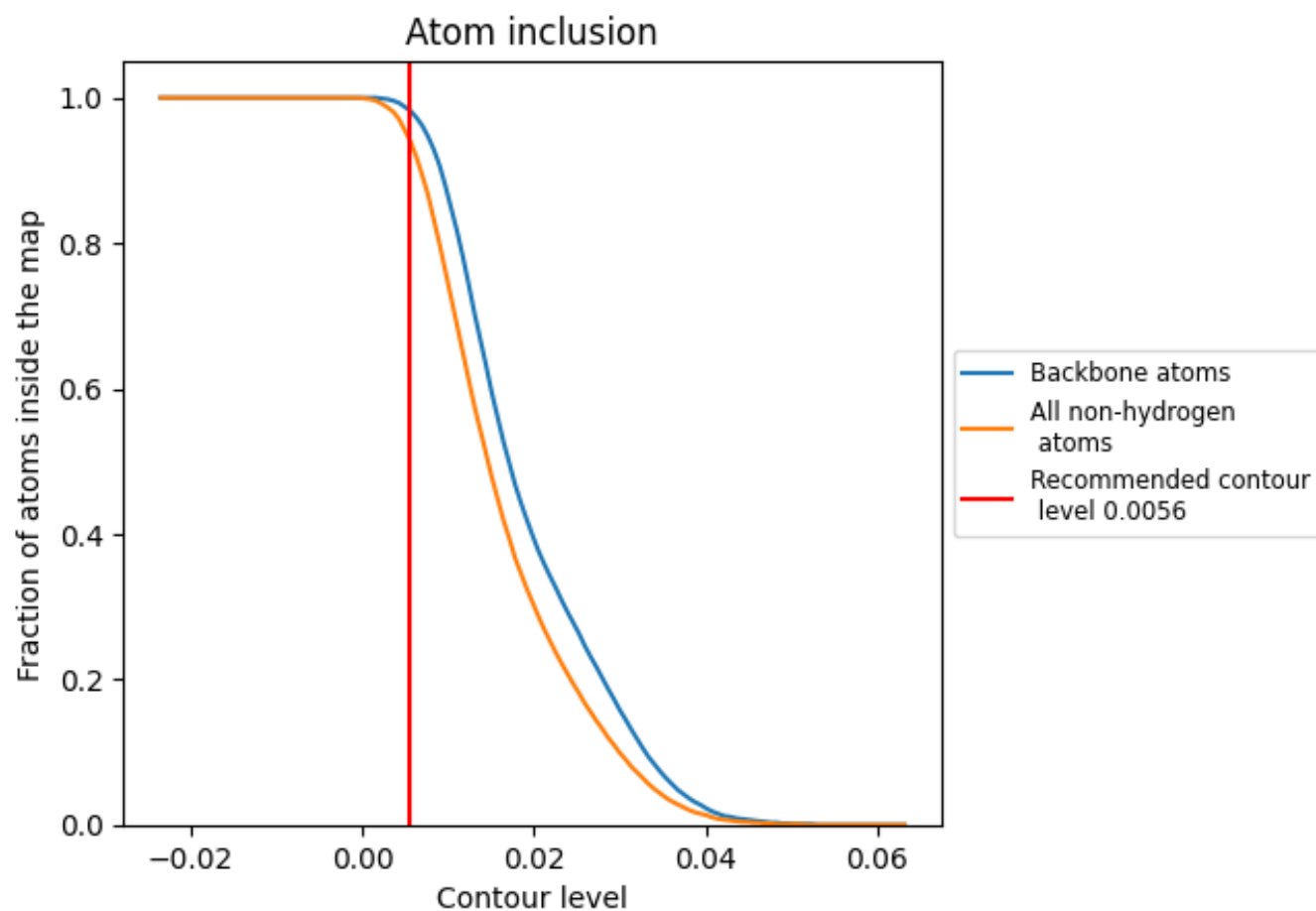
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0056).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 94% 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 (0.0056) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9400	0.4450
A	0.9540	0.4700
B	0.9410	0.3950
C	0.8290	0.2840
D	0.9680	0.5290
E	0.9910	0.4780
F	0.8480	0.1890

1.0

0.0

<0.0