



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 10:50 AM EDT

PDB ID : 9DB2 / pdb_00009db2
EMDB ID : EMD-46711
Title : Class Ia ribonucleotide reductase with mechanism-based inhibitor N3CDP
Authors : Westmoreland, D.E.; Drennan, C.L.
Deposited on : 2024-08-23
Resolution : 2.60 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.dev133
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) : 2.50

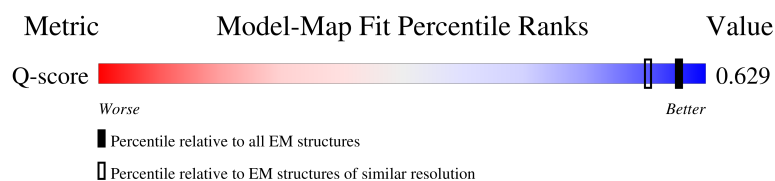
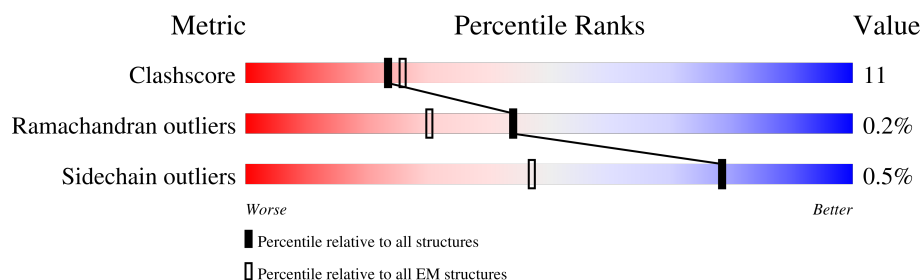
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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	8728 (2.10 - 3.10)

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	761	 75% 20% . .
1	B	761	 75% 22% .
2	C	376	 77% 22% .
2	D	376	 72% 21% . 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	UNL	A	806	-	-	X	-
8	FEO	D	401	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 18751 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.

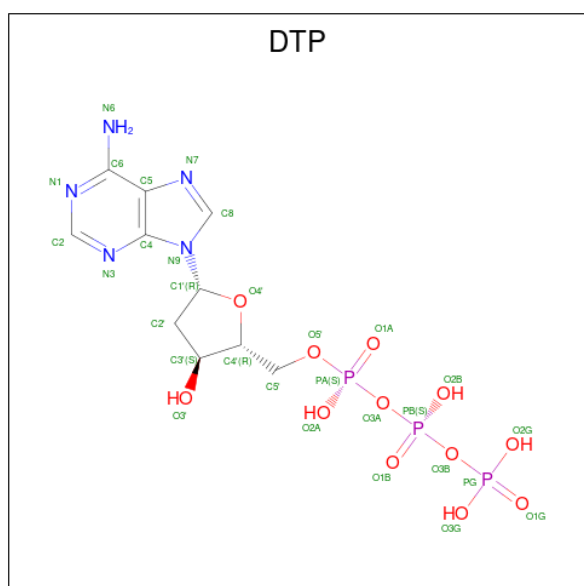
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	733	Total	C	N	O	S	14	0
			5922	3762	1018	1117	25		
1	B	744	Total	C	N	O	S	11	0
			5989	3802	1031	1132	24		

- Molecule 2 is a protein called Ribonucleoside-diphosphate reductase 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	375	Total	C	N	O	S	4	0
			3093	1971	515	594	13		
2	D	353	Total	C	N	O	S	2	0
			2903	1854	480	555	14		

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).

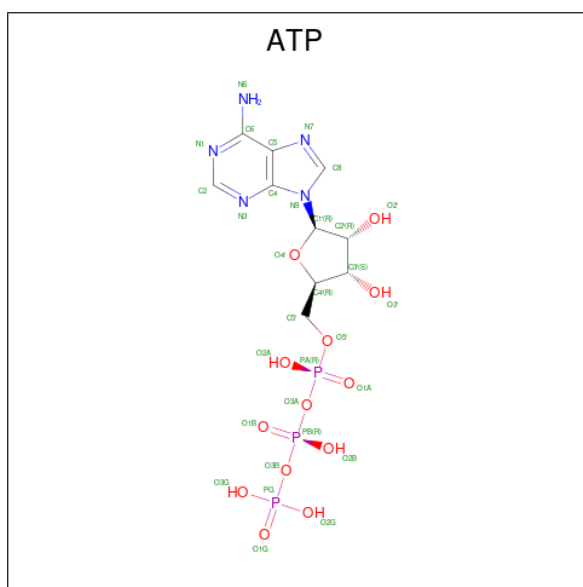


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			30	10	5	12	3	
3	B	1	Total	C	N	O	P	0
			30	10	5	12	3	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Mg	0
			2	2	
4	B	2	Total	Mg	0
			2	2	

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



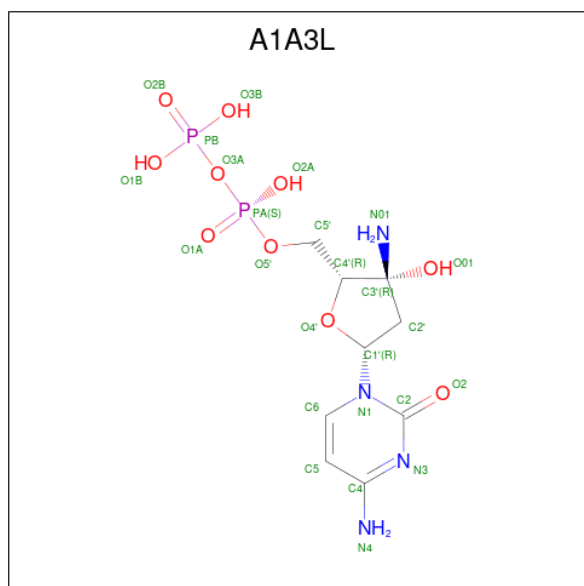
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is UNKNOWN LIGAND (CCD ID: UNL) (formula:) (labeled as "Ligand of

Interest" by depositor).

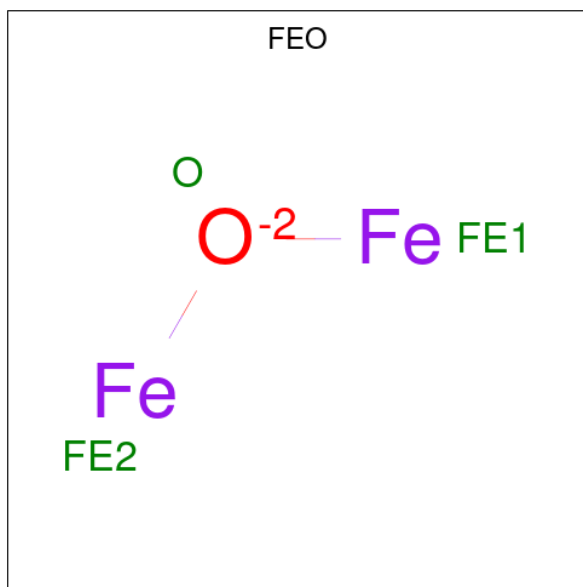
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total N 1 1	0

- Molecule 7 is 4-amino-1-[(3xi)-3-C-amino-2-deoxy-5-O-[(S)-hydroxy(phosphonooxy)phosphoryl]-beta-D-threo-pentofuranosyl]pyrimidin-2(1H)-one (CCD ID: A1A3L) (formula: $C_9H_{16}N_4O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			25	9	4	10	2	

- Molecule 8 is MU-OXO-DIIRON (CCD ID: FEO) (formula: Fe_2O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
8	C	1	Total	Fe	O	0
			3	2	1	
8	D	1	Total	Fe	O	0
			3	2	1	

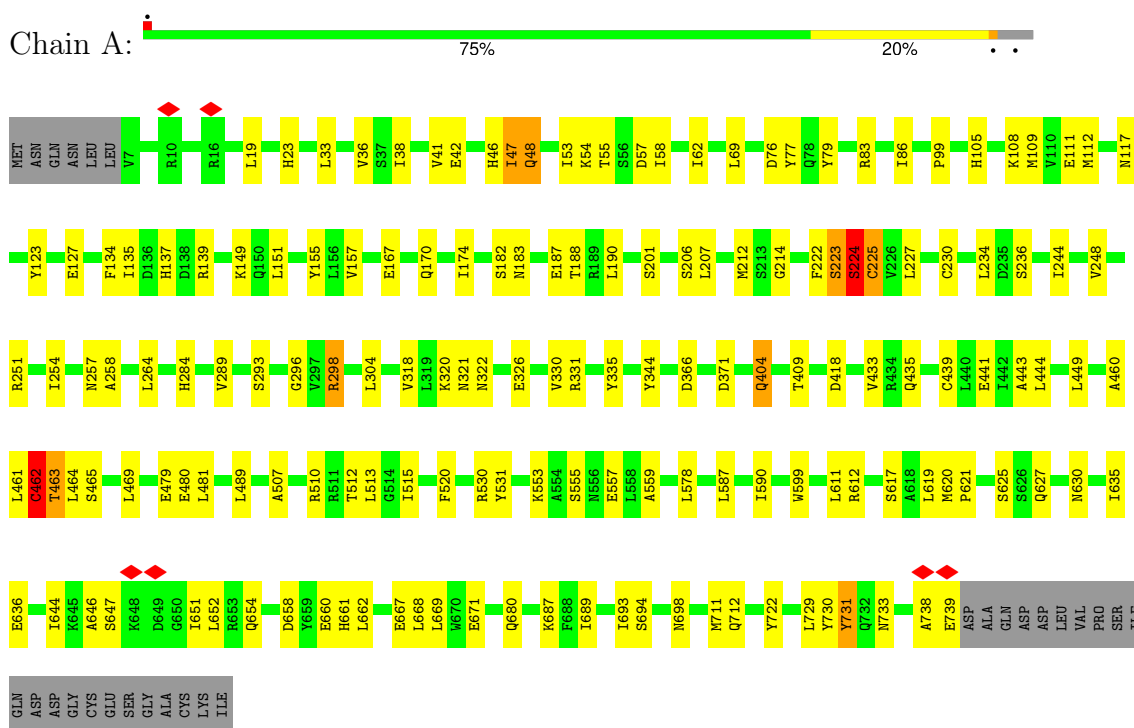
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	A	150	Total	O	0
			150	150	
9	B	296	Total	O	0
			296	296	
9	C	108	Total	O	0
			108	108	
9	D	70	Total	O	0
			70	70	

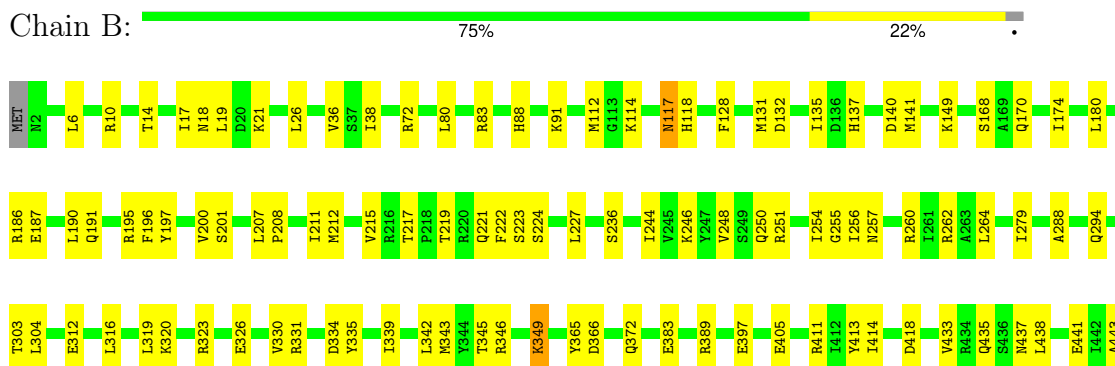
3 Residue-property plots

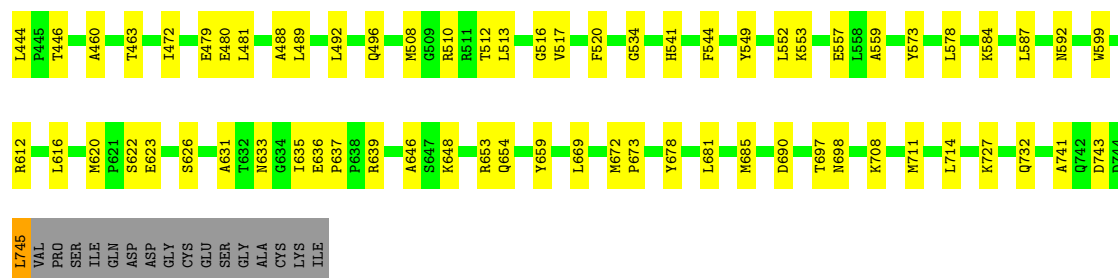
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Ribonucleoside-diphosphate reductase 1 subunit alpha



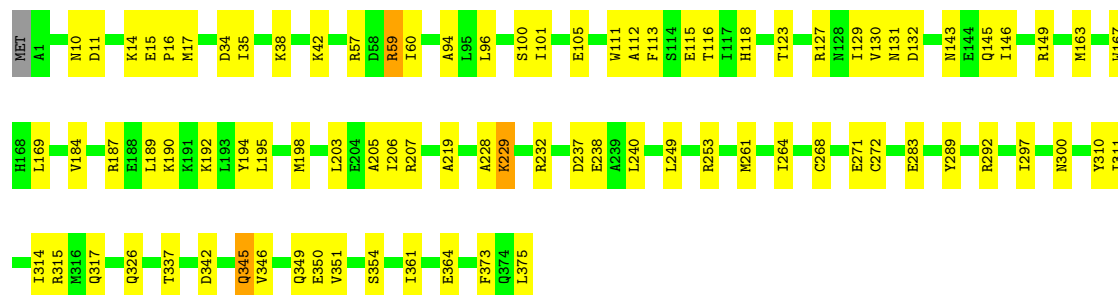
- Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha





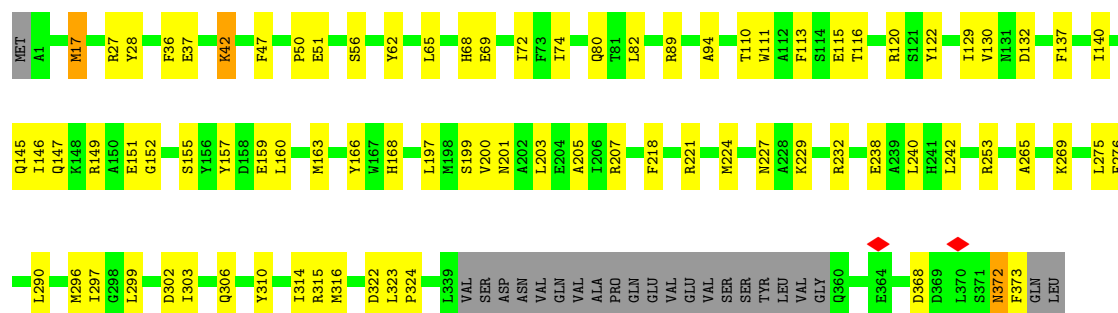
- Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta

Chain C: 77% 22%



- Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta

Chain D: 72% 21% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	440549	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTF correction using RELION's implementation of CTFFIND	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.946	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.281	Depositor
Minimum map value	-2.562	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.141	Depositor
Recommended contour level	0.235	Depositor
Map size (Å)	239.04, 239.04, 239.04	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.415, 0.415, 0.415	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: DTP, UNL, ATP, FEO, A1A3L, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	5/6090 (0.1%)	0.64	13/8245 (0.2%)
1	B	0.27	0/6150	0.47	6/8324 (0.1%)
2	C	0.38	5/3176 (0.2%)	0.47	0/4309
2	D	0.27	0/2973	0.39	2/4030 (0.0%)
All	All	0.35	10/18389 (0.1%)	0.52	21/24908 (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	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	ILE	C-N	16.57	1.59	1.33
2	C	192	LYS	N-CA	7.09	1.55	1.46
1	A	731[A]	TYR	C-O	6.22	1.31	1.24
1	A	731[B]	TYR	C-O	6.22	1.31	1.24
1	A	48	GLN	C-N	-6.03	1.26	1.33
2	C	59[A]	ARG	C-O	5.68	1.30	1.24
2	C	59[B]	ARG	C-O	5.68	1.30	1.24
2	C	59[C]	ARG	C-O	5.68	1.30	1.24
1	A	224	SER	CA-CB	-5.49	1.44	1.53
2	C	345	GLN	C-O	-5.38	1.17	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	462	CYS	N-CA-C	-16.79	81.04	108.41
1	A	48	GLN	O-C-N	-15.08	101.99	122.20
1	A	463	THR	N-CA-CB	-12.42	89.47	110.95
1	A	462	CYS	CB-CA-C	-9.26	94.78	110.16
1	A	731[A]	TYR	CA-C-O	7.80	131.66	120.51
1	A	731[B]	TYR	CA-C-O	7.80	131.66	120.51
1	B	480[A]	GLU	CA-C-O	6.89	128.05	120.82
1	B	480[B]	GLU	CA-C-O	6.89	128.05	120.82
1	A	636	GLU	CB-CA-C	-6.86	98.22	109.27
1	B	349[A]	LYS	CA-C-O	6.45	127.57	119.12
1	B	349[B]	LYS	CA-C-O	6.45	127.57	119.12
1	A	371	ASP	CA-CB-CG	6.12	118.72	112.60
1	B	117[A]	ASN	CA-C-O	5.62	126.45	120.10
1	B	117[B]	ASN	CA-C-O	5.62	126.45	120.10
2	D	42[A]	LYS	CA-C-O	5.27	126.13	120.55
2	D	42[B]	LYS	CA-C-O	5.27	126.13	120.55
1	A	404[A]	GLN	CA-C-O	5.21	125.94	120.42
1	A	404[B]	GLN	CA-C-O	5.21	125.94	120.42
1	A	731[A]	TYR	N-CA-C	5.20	121.88	110.80
1	A	731[B]	TYR	N-CA-C	5.20	121.88	110.80
1	A	298	ARG	N-CA-C	5.18	121.83	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	48	GLN	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	5922	0	5864	134	0
1	B	5989	0	5939	138	0
2	C	3093	0	3026	73	0
2	D	2903	0	2837	76	0
3	A	30	0	12	0	0
3	B	30	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	62	0	24	4	0
5	B	62	0	24	2	0
6	A	1	0	0	3	0
7	B	25	0	0	1	0
8	C	3	0	0	1	0
8	D	3	0	0	3	0
9	A	150	0	0	17	0
9	B	296	0	0	38	0
9	C	108	0	0	13	0
9	D	70	0	0	9	0
All	All	18751	0	17738	395	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 11.

All (395) 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:55:THR:HG21	5:A:804:ATP:O1B	1.48	1.11
1:A:463:THR:HG23	1:A:463:THR:O	1.62	0.97
1:A:187:GLU:HG3	1:A:188:THR:HG23	1.56	0.84
1:B:516:GLY:N	1:B:620:MET:HE1	1.93	0.84
1:B:83:ARG:HG2	1:B:141:MET:SD	2.20	0.81
1:A:19:LEU:HD13	1:A:46:HIS:CE1	2.14	0.81
1:B:516:GLY:H	1:B:620:MET:HE1	1.47	0.80
1:B:191[B]:GLN:HB3	9:B:947:HOH:O	1.81	0.79
1:A:463:THR:O	1:A:463:THR:CG2	2.31	0.78
1:B:135:ILE:HD11	1:B:174:ILE:HG21	1.65	0.78
1:A:225[B]:CYS:HB2	1:A:462:CYS:SG	2.24	0.77
1:A:331:ARG:HD2	9:A:908:HOH:O	1.84	0.75
1:B:479:GLU:HB3	9:B:972:HOH:O	1.86	0.75
1:A:298:ARG:NH1	9:A:905:HOH:O	2.19	0.75
1:A:135:ILE:HD11	1:A:174:ILE:HG21	1.69	0.74
1:A:617:SER:HB3	1:A:689:ILE:HG13	1.69	0.74
1:B:279:ILE:HG12	9:B:1082:HOH:O	1.87	0.74
1:A:53:ILE:HG13	1:A:58:ILE:HG13	1.70	0.73
1:A:23:HIS:ND1	1:A:42:GLU:OE2	2.20	0.73
2:C:373:PHE:HA	9:C:514:HOH:O	1.88	0.73
1:A:620:MET:HE1	6:A:806:UNL:N	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:VAL:O	9:B:901:HOH:O	2.06	0.73
2:D:205:ALA:HB2	2:D:242:LEU:CD1	2.19	0.72
2:C:198:MET:SD	2:C:249:LEU:HD13	2.29	0.72
2:C:123:THR:HG22	2:C:127:ARG:HD2	1.70	0.72
1:A:55:THR:CG2	5:A:804:ATP:O1B	2.34	0.71
2:D:168:HIS:ND1	9:D:501:HOH:O	2.21	0.71
2:C:163:MET:HG3	2:C:189:LEU:HD13	1.73	0.71
2:D:50:PRO:HG2	2:D:120:ARG:HG2	1.73	0.71
1:A:439:CYS:SG	1:A:620:MET:HE3	2.31	0.70
1:B:745:LEU:HD11	2:C:317:GLN:OE1	1.92	0.70
2:D:205:ALA:HB2	2:D:242:LEU:HD13	1.73	0.70
1:B:260[A]:ARG:HD3	1:B:365:TYR:CD2	2.26	0.70
1:A:99:PRO:HG2	1:A:137:HIS:CD2	2.26	0.70
1:A:331:ARG:CD	9:A:908:HOH:O	2.40	0.69
2:C:238:GLU:OE1	8:C:401:FEO:O	2.10	0.69
1:B:654:GLN:NE2	9:B:902:HOH:O	2.13	0.69
2:D:147:GLN:O	2:D:151:GLU:HG3	1.93	0.69
1:A:298:ARG:CZ	9:A:905:HOH:O	2.42	0.68
2:C:131:ASN:CB	9:C:528:HOH:O	2.42	0.68
1:B:639:ARG:HD3	9:C:537:HOH:O	1.94	0.68
1:A:33:LEU:HB3	1:A:76:ASP:OD1	1.93	0.67
1:B:227:LEU:HB2	1:B:460:ALA:HB3	1.76	0.67
1:A:55:THR:HG21	5:A:804:ATP:PB	2.33	0.67
2:C:195:LEU:HD21	2:C:271:GLU:HG2	1.75	0.67
2:D:310:TYR:O	2:D:314:ILE:HD13	1.94	0.67
1:B:587:LEU:HD11	9:B:929:HOH:O	1.94	0.66
1:B:91:LYS:HE3	5:B:801:ATP:H3'	1.78	0.66
1:B:191[A]:GLN:HB3	9:B:947:HOH:O	1.96	0.66
1:B:437:ASN:HD21	1:B:441:GLU:CD	2.03	0.66
1:B:10:ARG:HH21	1:B:88:HIS:HE1	1.41	0.65
2:C:169:LEU:HD13	2:D:166:TYR:CE1	2.32	0.65
1:A:296:GLY:CA	9:A:977:HOH:O	2.43	0.65
1:B:389:ARG:NE	9:B:916:HOH:O	2.23	0.65
2:C:57:ARG:HD3	9:C:602:HOH:O	1.96	0.65
1:A:47:ILE:HG22	1:A:47:ILE:O	1.97	0.65
1:B:446:THR:OG1	9:B:903:HOH:O	2.13	0.65
1:A:489:LEU:HB3	1:A:513:LEU:HD22	1.79	0.64
1:B:10:ARG:HH21	1:B:88:HIS:CE1	2.16	0.64
1:B:681:LEU:O	1:B:685:MET:HG3	1.97	0.64
1:B:741:ALA:O	9:B:905:HOH:O	2.15	0.64
2:D:322:ASP:HA	9:D:508:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:27:ARG:NH1	9:D:506:HOH:O	2.28	0.64
2:D:152:GLY:HA3	9:D:545:HOH:O	1.96	0.64
1:A:230:CYS:O	9:A:902:HOH:O	2.15	0.64
2:C:105:GLU:OE2	2:D:89:ARG:HB3	1.98	0.64
2:C:11:ASP:OD2	2:C:14:LYS:HG3	1.99	0.63
1:B:36:VAL:HG11	1:B:80:LEU:HD13	1.82	0.62
1:B:137:HIS:HA	1:B:170:GLN:HG3	1.81	0.62
1:B:186:ARG:NH1	9:B:945:HOH:O	2.33	0.62
1:B:195:ARG:NH1	9:B:947:HOH:O	2.33	0.62
2:D:201:ASN:HD22	2:D:276:PHE:HZ	1.46	0.62
1:A:404[B]:GLN:HG3	1:A:711:MET:HE1	1.82	0.61
1:A:722:TYR:CD2	2:D:373:PHE:HZ	2.17	0.61
2:C:143:ASN:HB3	2:C:146:ILE:HB	1.81	0.61
1:A:627:GLN:HG2	1:A:654:GLN:NE2	2.15	0.61
1:A:105:HIS:O	1:A:109:MET:HG2	2.00	0.61
1:B:257:ASN:OD1	9:B:906:HOH:O	2.16	0.61
2:D:218:PHE:CZ	2:D:296[A]:MET:CE	2.83	0.61
1:A:620:MET:CE	6:A:806:UNL:N	2.64	0.61
2:C:131:ASN:HB3	9:C:528:HOH:O	2.01	0.61
1:B:141:MET:SD	9:B:1180:HOH:O	2.56	0.60
1:B:191[A]:GLN:CB	9:B:947:HOH:O	2.48	0.60
1:B:187:GLU:OE1	1:B:187:GLU:N	2.34	0.60
1:A:510:ARG:HB3	1:A:512:THR:HG23	1.82	0.60
1:A:557:GLU:OE2	1:A:557:GLU:HA	2.01	0.60
1:A:293:SER:HB3	1:A:298:ARG:H	1.66	0.60
1:B:10:ARG:NH2	1:B:88:HIS:HE1	2.01	0.59
1:B:10:ARG:NH2	1:B:88:HIS:CE1	2.70	0.59
1:B:541:HIS:ND1	9:B:917:HOH:O	2.23	0.59
2:D:372:ASN:O	2:D:373:PHE:C	2.45	0.59
1:B:508:MET:HA	1:B:508:MET:HE2	1.85	0.59
1:B:207:LEU:HB2	1:B:212:MET:HG2	1.84	0.59
2:D:218:PHE:CE1	2:D:296[A]:MET:HE2	2.38	0.58
1:B:222:PHE:HB2	1:B:492:LEU:HD21	1.85	0.58
1:B:244:ILE:HG12	1:B:254:ILE:HG21	1.84	0.57
2:D:218:PHE:CE2	2:D:296[A]:MET:HE1	2.40	0.57
2:D:82:LEU:HD13	2:D:146:ILE:HG22	1.86	0.57
1:B:389:ARG:HA	9:B:1051:HOH:O	2.04	0.57
1:B:732:GLN:NE2	9:B:937:HOH:O	2.30	0.57
1:A:733[A]:ASN:ND2	9:A:924:HOH:O	2.38	0.56
1:B:217:THR:HG22	1:B:219:THR:H	1.70	0.56
1:A:258:ALA:HB3	1:A:304:LEU:HD21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ARG:NH2	9:B:958:HOH:O	2.39	0.56
1:A:251:ARG:HG2	1:A:251:ARG:HH11	1.71	0.56
2:C:149:ARG:HH21	2:C:283:GLU:HG2	1.70	0.56
2:D:242:LEU:HD21	2:D:315:ARG:HD2	1.87	0.56
2:C:206:ILE:HG23	2:C:311:ILE:HG23	1.87	0.56
2:D:238:GLU:OE1	8:D:401:FEO:O	2.23	0.56
1:B:326:GLU:HA	1:B:326:GLU:OE1	2.05	0.55
1:B:26:LEU:HB3	1:B:38:ILE:HD12	1.87	0.55
1:A:722:TYR:HD2	2:D:373:PHE:HZ	1.54	0.55
1:B:190:LEU:HB2	9:B:1013:HOH:O	2.05	0.55
2:C:198:MET:SD	2:C:249:LEU:HD22	2.47	0.55
2:D:205:ALA:HB2	2:D:242:LEU:HD11	1.89	0.55
1:B:669:LEU:HD11	1:B:698:ASN:ND2	2.21	0.55
1:A:627:GLN:HG2	1:A:654:GLN:HE22	1.71	0.54
2:D:323:LEU:N	9:D:508:HOH:O	2.32	0.54
1:A:439:CYS:HB2	1:A:441:GLU:OE2	2.07	0.54
2:D:145:GLN:O	2:D:149:ARG:NH1	2.40	0.54
1:A:296:GLY:HA2	9:A:977:HOH:O	2.04	0.54
1:B:334:ASP:OD2	1:B:413:TYR:OH	2.25	0.54
1:A:139:ARG:NH1	1:A:201:SER:OG	2.40	0.54
1:B:224:SER:HB2	9:B:1044:HOH:O	2.08	0.54
1:B:342:LEU:O	1:B:346:ARG:HG2	2.08	0.54
2:D:155:SER:O	2:D:159:GLU:HG3	2.07	0.53
1:B:745:LEU:HD22	2:C:314:ILE:HD13	1.91	0.53
1:B:345:THR:HG22	1:B:349[A]:LYS:HD2	1.91	0.53
2:D:302:ASP:O	2:D:306:GLN:HG3	2.08	0.53
2:C:253:ARG:HD3	9:C:588:HOH:O	2.08	0.53
1:B:244:ILE:HD11	1:B:256:ILE:HG12	1.91	0.53
1:A:137:HIS:HA	1:A:170:GLN:HG3	1.90	0.53
1:A:244:ILE:HG12	1:A:254:ILE:HG21	1.89	0.53
1:A:439:CYS:SG	1:A:620:MET:CE	2.97	0.52
2:C:42:LYS:HD3	2:C:240:LEU:HD21	1.92	0.52
2:D:80:GLN:HB3	2:D:122:TYR:CZ	2.44	0.52
2:C:253:ARG:CD	9:C:588:HOH:O	2.56	0.52
2:D:227:ASN:ND2	9:D:513:HOH:O	2.41	0.52
2:D:322:ASP:CA	9:D:508:HOH:O	2.56	0.52
2:D:218:PHE:CZ	2:D:296[A]:MET:HE1	2.44	0.52
1:A:647:SER:HA	9:A:910:HOH:O	2.10	0.52
2:C:59[B]:ARG:NH2	9:C:526:HOH:O	2.43	0.52
1:A:157:VAL:HG13	1:A:167:GLU:OE2	2.10	0.51
2:C:16:PRO:O	2:C:100:SER:OG	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:129:ILE:HG13	2:C:130:VAL:HG23	1.91	0.51
1:B:140:ASP:CG	9:B:946:HOH:O	2.54	0.51
1:B:592:ASN:OD1	1:B:592:ASN:C	2.53	0.51
2:D:137:PHE:HA	2:D:140:ILE:HD12	1.92	0.51
2:D:296[A]:MET:HG2	2:D:297:ILE:N	2.26	0.51
2:C:34:ASP:OD2	2:C:38:LYS:NZ	2.27	0.51
2:C:145[A]:GLN:HG2	2:C:289:TYR:CG	2.46	0.51
2:C:268:CYS:SG	2:C:272:CYS:N	2.82	0.51
2:C:145[B]:GLN:HG3	2:C:289:TYR:CG	2.46	0.50
1:B:516:GLY:CA	1:B:620:MET:HE1	2.41	0.50
2:C:130:VAL:HG12	2:C:132:ASP:H	1.75	0.50
1:B:646:ALA:HB3	2:C:346:VAL:HG12	1.92	0.50
1:B:187:GLU:N	1:B:187:GLU:CD	2.69	0.50
1:B:208:PRO:HD2	1:B:211:ILE:HB	1.94	0.50
1:B:584:LYS:NZ	2:C:375:LEU:O	2.42	0.50
1:A:53:ILE:CG1	1:A:58:ILE:HG13	2.41	0.50
1:B:221:GLN:HA	1:B:496:GLN:HG2	1.92	0.50
1:A:326:GLU:OE1	1:A:331:ARG:NH2	2.44	0.50
1:A:463:THR:HG21	1:A:512:THR:O	2.12	0.50
1:B:559:ALA:HB2	1:B:612:ARG:N	2.26	0.50
2:D:218:PHE:CZ	2:D:296[A]:MET:HE2	2.47	0.50
1:B:620:MET:SD	1:B:620:MET:N	2.82	0.50
2:C:35:ILE:HG22	9:C:554:HOH:O	2.11	0.50
1:B:711:MET:HE2	2:C:361:ILE:HG21	1.94	0.50
2:D:242:LEU:HD21	2:D:315:ARG:CD	2.41	0.49
1:B:196:PHE:O	1:B:200:VAL:HG22	2.12	0.49
1:B:248:VAL:O	1:B:294:GLN:HA	2.13	0.49
9:B:1114:HOH:O	2:C:342:ASP:HB2	2.10	0.49
2:D:299:LEU:HA	2:D:303:ILE:HD11	1.94	0.49
1:A:214:GLY:C	1:A:222:PHE:HE1	2.21	0.49
1:B:489:LEU:HB3	1:B:513:LEU:HD22	1.95	0.49
1:A:620:MET:HG3	1:A:621:PRO:HD2	1.93	0.49
1:B:653:ARG:HG3	9:B:1157:HOH:O	2.12	0.49
1:A:99:PRO:HG2	1:A:137:HIS:NE2	2.26	0.49
1:A:264:LEU:HD11	2:C:60:ILE:HG12	1.94	0.49
1:A:722:TYR:CD2	2:D:373:PHE:CZ	3.00	0.49
1:B:433:VAL:HG11	1:B:443:ALA:HB1	1.94	0.49
1:B:223:SER:HA	1:B:463:THR:HG22	1.95	0.49
1:A:738:ALA:O	1:A:739:GLU:C	2.55	0.49
1:B:279:ILE:HD12	1:B:319:LEU:HD21	1.93	0.49
1:A:555:SER:HB3	1:A:611:LEU:HD22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:SER:O	9:A:906:HOH:O	2.20	0.48
1:A:660:GLU:HB3	1:A:661:HIS:CD2	2.48	0.48
1:B:517:VAL:O	9:B:907:HOH:O	2.19	0.48
2:D:42[B]:LYS:HE3	2:D:240:LEU:HD11	1.95	0.48
2:C:198:MET:SD	2:C:249:LEU:CD1	3.00	0.48
2:C:118:HIS:CE1	2:C:237:ASP:HB2	2.49	0.48
2:D:62:TYR:HB2	2:D:224:MET:HE1	1.96	0.48
1:A:439:CYS:HA	1:A:730:TYR:CZ	2.49	0.48
1:A:520:PHE:HB3	1:A:635:ILE:HA	1.95	0.48
1:B:578:LEU:HD13	1:B:599:TRP:HE3	1.78	0.48
2:D:157:TYR:OH	2:D:200:VAL:HG22	2.13	0.48
2:D:203:LEU:HA	2:D:207:ARG:HD2	1.96	0.48
1:B:552:LEU:HD23	1:B:616:LEU:HD12	1.96	0.48
2:C:300:ASN:HB2	9:C:555:HOH:O	2.14	0.48
2:D:163:MET:HB2	2:D:163:MET:HE3	1.59	0.48
1:A:479:GLU:HB3	1:A:480[A]:GLU:OE1	2.14	0.48
1:A:722:TYR:HD2	2:D:373:PHE:CZ	2.31	0.48
1:B:114:LYS:HA	1:B:114:LYS:HD3	1.74	0.48
2:D:238:GLU:OE2	8:D:401:FEO:O	2.31	0.48
1:A:108:LYS:O	1:A:111:GLU:N	2.47	0.47
1:A:646:ALA:HA	1:A:651:ILE:HA	1.96	0.47
1:A:149:LYS:HG3	1:A:652:LEU:HD11	1.95	0.47
1:A:227:LEU:HB2	1:A:460:ALA:HB3	1.96	0.47
1:A:251:ARG:HG2	1:A:251:ARG:NH1	2.29	0.47
2:D:316:MET:HE2	2:D:324:PRO:HD3	1.96	0.47
1:B:256:ILE:HB	1:B:304:LEU:HD23	1.96	0.47
2:C:194:TYR:O	2:C:198:MET:HG2	2.14	0.47
1:B:573:TYR:OH	1:B:690:ASP:OD1	2.30	0.47
1:B:743:ASP:O	2:C:310:TYR:OH	2.21	0.47
2:C:232:ARG:NH2	2:C:337:THR:O	2.47	0.47
2:D:17:MET:HE2	2:D:36:PHE:CE2	2.49	0.47
1:A:590:ILE:HD13	1:A:680:GLN:HG2	1.96	0.47
1:A:712:GLN:NE2	2:D:368:ASP:OD1	2.47	0.47
2:D:238:GLU:CD	8:D:401:FEO:O	2.58	0.47
1:B:708:LYS:HE2	2:D:51:GLU:HG2	1.96	0.47
1:A:578:LEU:HD13	1:A:599:TRP:HE3	1.80	0.47
1:B:180:LEU:HD21	1:B:492:LEU:HD12	1.96	0.47
2:D:62:TYR:HA	2:D:65:LEU:HD12	1.97	0.47
1:A:668:LEU:HB2	1:A:671:GLU:HG3	1.97	0.46
1:B:128:PHE:HA	1:B:131:MET:HE3	1.97	0.46
1:B:323:ARG:HG2	2:D:47:PHE:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:THR:OG1	1:B:438:LEU:HD12	2.16	0.46
2:C:190:LYS:HB3	2:C:261:MET:HE2	1.97	0.46
1:A:155:TYR:CE2	1:A:212:MET:HG3	2.50	0.46
1:A:344:TYR:OH	9:A:904:HOH:O	2.19	0.46
1:A:465:SER:HB3	1:A:515:ILE:HG12	1.97	0.46
1:B:637:PRO:HG3	1:B:672:MET:HE2	1.97	0.46
2:D:132:ASP:OD1	2:D:132:ASP:O	2.34	0.46
1:A:33:LEU:HD12	1:A:33:LEU:N	2.30	0.46
2:C:205:ALA:HB1	2:C:315:ARG:HD2	1.97	0.46
1:B:366:ASP:OD1	9:B:909:HOH:O	2.21	0.46
2:C:203:LEU:HA	2:C:207:ARG:HD2	1.97	0.46
2:C:219:ALA:HB2	2:C:228:ALA:HB2	1.98	0.46
2:D:276:PHE:HB3	2:D:316:MET:SD	2.55	0.46
1:A:658:ASP:HB3	1:A:662:LEU:HD12	1.97	0.46
1:B:18:ASN:HA	9:B:944:HOH:O	2.16	0.46
1:B:636:GLU:OE2	1:B:678:TYR:OH	2.33	0.46
1:B:745:LEU:HD13	2:C:314:ILE:CD1	2.45	0.46
2:C:169:LEU:HD23	2:C:169:LEU:HA	1.68	0.46
1:A:553:LYS:O	1:A:557:GLU:HG2	2.16	0.46
1:B:444:LEU:HD22	1:B:512:THR:HG21	1.98	0.46
2:D:68:HIS:O	2:D:72:ILE:HG13	2.16	0.46
1:B:18:ASN:HD22	1:B:21:LYS:HE3	1.80	0.46
2:C:169:LEU:HD13	2:D:166:TYR:CD1	2.51	0.46
1:A:38:ILE:O	1:A:42:GLU:HG3	2.16	0.45
1:A:55:THR:HB	5:A:804:ATP:H5'1	1.97	0.45
1:A:439:CYS:O	1:A:694:SER:OG	2.32	0.45
2:C:112:ALA:O	2:C:116:THR:HG23	2.15	0.45
2:C:187:ARG:HG3	2:C:264:ILE:HD11	1.98	0.45
2:D:113:PHE:O	2:D:116:THR:OG1	2.29	0.45
1:A:559:ALA:HB2	1:A:612:ARG:N	2.31	0.45
2:D:72:ILE:HG23	2:D:290:LEU:HD22	1.98	0.45
2:D:269:LYS:HD3	2:D:269:LYS:HA	1.73	0.45
1:A:223:SER:O	1:A:224:SER:HB3	2.15	0.45
1:B:389:ARG:NH2	9:B:916:HOH:O	2.48	0.45
2:D:253:ARG:HG3	2:D:265:ALA:HB1	1.98	0.45
1:B:330:VAL:HB	1:B:335:TYR:OH	2.16	0.45
1:A:108:LYS:HE2	1:A:112:MET:CE	2.46	0.45
1:B:520:PHE:HB3	1:B:635:ILE:HA	1.99	0.45
1:B:672:MET:O	1:B:673:PRO:C	2.59	0.45
5:B:801:ATP:O2B	5:B:802:ATP:H2'	2.17	0.45
2:C:10:ASN:HD22	2:C:15:GLU:HG3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:LEU:HD22	2:C:59[C]:ARG:HH12	1.81	0.45
1:A:630:ASN:O	9:A:907:HOH:O	2.21	0.45
1:A:47:ILE:O	1:A:47:ILE:CG2	2.64	0.45
1:A:320:LYS:HB3	1:A:409:THR:HG21	1.99	0.45
1:B:339:ILE:HD12	1:B:414:ILE:HG23	1.98	0.45
2:C:350:GLU:OE1	9:C:502:HOH:O	2.21	0.44
1:B:255:GLY:O	1:B:435:GLN:NE2	2.43	0.44
1:B:342:LEU:HD22	1:B:343:MET:CE	2.48	0.44
1:B:727:LYS:HE2	9:B:1050:HOH:O	2.17	0.44
2:C:232:ARG:HD3	2:C:354:SER:OG	2.18	0.44
1:A:58:ILE:O	1:A:62:ILE:HG23	2.17	0.44
1:B:320:LYS:NZ	1:B:331:ARG:O	2.50	0.44
1:B:397:GLU:OE2	2:D:229:LYS:NZ	2.48	0.44
2:C:96:LEU:HD12	2:C:96:LEU:HA	1.86	0.44
1:A:322:ASN:OD1	9:A:908:HOH:O	2.21	0.44
2:D:111:TRP:O	2:D:115:GLU:HG2	2.18	0.44
1:A:461:LEU:HD23	1:A:507:ALA:HB2	1.98	0.44
1:B:622:SER:O	1:B:626:SER:OG	2.28	0.44
2:C:145[B]:GLN:HG3	2:C:289:TYR:CD1	2.52	0.44
1:A:510:ARG:HG2	9:A:960:HOH:O	2.17	0.44
1:B:372:GLN:OE1	1:B:418:ASP:HB3	2.17	0.44
1:A:36:VAL:HG13	1:A:77:TYR:CE1	2.53	0.44
2:D:129:ILE:HG13	2:D:130:VAL:HG23	1.98	0.44
1:A:157:VAL:HG22	1:A:167:GLU:HG2	2.00	0.44
1:A:330:VAL:HB	1:A:335:TYR:OH	2.18	0.44
1:A:464:LEU:N	1:A:464:LEU:HD22	2.33	0.44
1:B:219:THR:O	1:B:251:ARG:NH2	2.48	0.43
1:B:312:GLU:O	1:B:316:LEU:HG	2.18	0.43
7:B:806:A1A3L:PB	9:B:918:HOH:O	2.76	0.43
2:C:94:ALA:HA	9:C:512:HOH:O	2.17	0.43
1:A:151:LEU:HA	1:A:155:TYR:HB2	2.00	0.43
1:B:534:GLY:HA2	9:B:935:HOH:O	2.17	0.43
1:A:135:ILE:HG21	1:A:137:HIS:CE1	2.53	0.43
1:A:248:VAL:HG11	1:A:289:VAL:HA	2.00	0.43
1:B:221:GLN:OE1	1:B:496:GLN:NE2	2.47	0.43
1:B:697:THR:O	1:B:732:GLN:HA	2.18	0.43
1:A:134:PHE:CE2	1:A:190:LEU:HD12	2.54	0.43
1:B:72:ARG:HB3	1:B:659:TYR:OH	2.18	0.43
1:B:72:ARG:HG3	9:B:1111:HOH:O	2.18	0.43
2:D:17:MET:HE2	2:D:36:PHE:CZ	2.53	0.43
1:A:55:THR:HA	1:A:58:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:ARG:NH2	1:B:383:GLU:OE2	2.51	0.43
2:D:28:TYR:N	9:D:505:HOH:O	2.28	0.43
1:B:405:GLU:OE2	1:B:405:GLU:HA	2.18	0.42
1:B:510:ARG:NH1	9:B:960:HOH:O	2.39	0.42
1:B:132:ASP:OD1	9:B:911:HOH:O	2.21	0.42
1:A:234:LEU:HD23	1:A:234:LEU:HA	1.81	0.42
1:B:112:MET:HG3	1:B:114:LYS:HG2	2.00	0.42
1:B:257:ASN:HB2	1:B:435:GLN:HB3	2.01	0.42
1:B:320:LYS:HE3	1:B:411:ARG:HD3	2.00	0.42
2:C:123:THR:HG21	2:D:28:TYR:HB2	2.00	0.42
1:A:366:ASP:HA	9:A:920:HOH:O	2.19	0.42
1:A:444:LEU:HD22	1:A:512:THR:HG21	2.00	0.42
1:B:633:ASN:ND2	2:C:345:GLN:HE22	2.17	0.42
2:D:197:LEU:HD23	2:D:197:LEU:HA	1.89	0.42
1:A:79:TYR:O	1:A:83:ARG:NH1	2.52	0.42
1:A:729:LEU:HD23	1:A:729:LEU:HA	1.92	0.42
1:B:262:ARG:CZ	3:B:803:DTP:H5'1	2.49	0.42
9:B:1139:HOH:O	2:C:297:ILE:HG12	2.18	0.42
2:D:94:ALA:HB1	2:D:160:LEU:HD23	2.02	0.42
1:A:69:LEU:HD13	1:A:77:TYR:CZ	2.54	0.42
1:A:587:LEU:HD23	1:A:590:ILE:HD11	2.01	0.42
1:A:669:LEU:HD11	1:A:698:ASN:CG	2.45	0.42
1:B:544:PHE:CZ	1:B:685:MET:HE2	2.54	0.42
1:B:714:LEU:HD11	2:C:361:ILE:HD12	2.00	0.42
2:C:229:LYS:HE3	2:C:229:LYS:HB2	1.79	0.42
2:D:232:ARG:NE	9:D:522:HOH:O	2.52	0.42
2:C:326:GLN:OE1	2:C:326:GLN:HA	2.18	0.42
1:A:54:LYS:H	1:A:57:ASP:HB2	1.83	0.42
1:A:619:LEU:HB2	1:A:693:ILE:HG23	2.02	0.42
1:A:644:ILE:HD12	1:A:644:ILE:C	2.44	0.42
2:D:69:GLU:HA	2:D:72:ILE:HD12	2.01	0.42
2:D:199:SER:HA	2:D:275:LEU:HD21	2.01	0.42
1:A:225[B]:CYS:SG	6:A:806:UNL:N	2.93	0.42
2:C:289:TYR:O	2:C:292:ARG:HG2	2.20	0.42
1:B:197:TYR:O	1:B:201:SER:OG	2.30	0.41
1:B:246:LYS:O	1:B:250:GLN:HG3	2.19	0.41
2:C:111:TRP:O	2:C:115:GLU:HG2	2.20	0.41
1:A:236:SER:HA	1:A:449:LEU:O	2.20	0.41
1:B:19:LEU:N	9:B:944:HOH:O	2.32	0.41
1:B:648:LYS:HE2	2:C:351:VAL:HG12	2.02	0.41
2:C:105:GLU:OE2	2:D:89:ARG:NE	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:TYR:OH	1:A:635:ILE:O	2.31	0.41
1:B:623:GLU:OE1	2:C:345:GLN:NE2	2.54	0.41
1:A:123:TYR:HA	1:A:127:GLU:OE1	2.20	0.41
1:A:257:ASN:HB2	1:A:435:GLN:HB3	2.01	0.41
1:A:418:ASP:OD1	1:A:418:ASP:N	2.54	0.41
1:A:469:LEU:HD23	1:A:469:LEU:HA	1.92	0.41
2:C:17:MET:HG2	2:C:101:ILE:HD11	2.03	0.41
2:C:349:GLN:OE1	9:C:503:HOH:O	2.21	0.41
2:D:82:LEU:C	2:D:82:LEU:HD23	2.45	0.41
1:A:182:SER:OG	1:A:183:ASN:OD1	2.38	0.41
1:A:207:LEU:HD13	1:A:212:MET:CE	2.51	0.41
1:B:472:ILE:O	1:B:472:ILE:HG13	2.20	0.41
1:B:6:LEU:HD23	1:B:14:THR:CG2	2.51	0.41
1:B:17:ILE:HD12	1:B:17:ILE:HA	1.90	0.41
1:B:149[A]:LYS:HD2	1:B:149[A]:LYS:HA	1.73	0.41
1:B:631:ALA:O	9:B:913:HOH:O	2.22	0.41
2:D:37:GLU:OE1	2:D:37:GLU:HA	2.21	0.41
2:D:221:ARG:HD3	2:D:297:ILE:HB	2.03	0.41
1:A:646:ALA:O	9:A:910:HOH:O	2.22	0.41
1:B:149[B]:LYS:HD3	1:B:149[B]:LYS:HA	1.87	0.41
1:B:168:SER:CB	9:B:922:HOH:O	2.68	0.41
1:B:254:ILE:HG22	1:B:256:ILE:HG13	2.02	0.41
1:B:180:LEU:HD13	1:B:488:ALA:HB1	2.02	0.40
1:A:433:VAL:HG11	1:A:443:ALA:HB1	2.03	0.40
1:A:587:LEU:HD13	1:A:687:LYS:HB2	2.03	0.40
2:C:113:PHE:HE1	2:D:110:THR:HG23	1.85	0.40
1:A:318:VAL:HB	1:A:321:ASN:HD21	1.87	0.40
1:B:549:TYR:CE2	1:B:553:LYS:HD3	2.57	0.40
2:C:364:GLU:HG3	2:D:56:SER:OG	2.21	0.40
1:A:54:LYS:O	1:A:57:ASP:N	2.54	0.40
1:A:284:HIS:CE1	1:B:288:ALA:HB2	2.56	0.40
1:A:530:ARG:HB3	1:A:667:GLU:OE1	2.21	0.40
1:A:41:VAL:HG22	1:A:69:LEU:HD12	2.03	0.40
1:A:206:SER:OG	1:A:625:SER:HB3	2.21	0.40
1:B:553:LYS:O	1:B:557:GLU:HG2	2.22	0.40
2:C:167:TRP:HA	2:C:184:VAL:HG11	2.04	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	745/761 (98%)	714 (96%)	27 (4%)	4 (0%)	24	46
1	B	752/761 (99%)	730 (97%)	22 (3%)	0	100	100
2	C	378/376 (100%)	369 (98%)	9 (2%)	0	100	100
2	D	351/376 (93%)	346 (99%)	4 (1%)	1 (0%)	36	58
All	All	2226/2274 (98%)	2159 (97%)	62 (3%)	5 (0%)	44	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	SER
1	A	731[A]	TYR
1	A	731[B]	TYR
2	D	372	ASN
1	A	223	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	641/651 (98%)	637 (99%)	4 (1%)	78	91
1	B	648/651 (100%)	643 (99%)	5 (1%)	73	88
2	C	345/341 (101%)	344 (100%)	1 (0%)	86	94
2	D	322/341 (94%)	320 (99%)	2 (1%)	78	91
All	All	1956/1984 (99%)	1944 (99%)	12 (1%)	78	91

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ILE
1	A	225[A]	CYS
1	A	225[B]	CYS
1	A	462	CYS
1	B	117[A]	ASN
1	B	117[B]	ASN
1	B	236	SER
1	B	264	LEU
1	B	745	LEU
2	C	229	LYS
2	D	17	MET
2	D	74	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	88	HIS
1	A	96	GLN
1	A	137	HIS
1	A	159	ASN
1	A	284	HIS
1	A	613	ASN
1	A	654	GLN
1	A	661	HIS
1	A	680	GLN
1	B	158	GLN
1	B	183	ASN
1	B	250	GLN
1	B	257	ASN
1	B	332	HIS
1	B	453	ASN
1	B	538	ASN
1	B	691	GLN
2	C	80	GLN
2	C	92	ASN
2	C	345	GLN
2	D	71	HIS
2	D	124	HIS
2	D	227	ASN
2	D	281	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 4 are monoatomic and 1 is unknown - leaving 9 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	DTP	A	801	4	31,32,32	1.11	3 (9%)	46,50,50	2.14	12 (26%)
5	ATP	B	802	4	32,33,33	3.07	13 (40%)	48,52,52	1.82	10 (20%)
5	ATP	A	803	4	32,33,33	0.50	1 (3%)	48,52,52	0.49	0
5	ATP	A	804	4	32,33,33	0.50	1 (3%)	48,52,52	0.53	0
3	DTP	B	803	4	31,32,32	1.05	3 (9%)	46,50,50	1.77	9 (19%)
8	FEO	D	401	2,9	0,2,2	-	-	-	-	-
5	ATP	B	801	4	32,33,33	3.13	13 (40%)	48,52,52	1.73	7 (14%)
7	A1A3L	B	806	1	23,26,26	3.71	14 (60%)	28,41,41	1.47	4 (14%)
8	FEO	C	401	2,9	0,2,2	-	-	-	-	-

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	DTP	A	801	4	-	4/22/34/34	0/3/3/3
5	ATP	B	802	4	-	6/22/38/38	0/3/3/3
5	ATP	A	803	4	-	6/22/38/38	0/3/3/3
5	ATP	A	804	4	-	4/22/38/38	0/3/3/3
3	DTP	B	803	4	-	3/22/34/34	0/3/3/3
5	ATP	B	801	4	-	2/22/38/38	0/3/3/3
7	A1A3L	B	806	1	-	5/16/31/31	0/2/2/2

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	801	ATP	C2'-C3'	-9.87	1.26	1.53
5	B	802	ATP	C2'-C3'	-9.61	1.27	1.53
7	B	806	A1A3L	C6-C5	8.98	1.55	1.35
7	B	806	A1A3L	C2-N3	7.81	1.51	1.36
7	B	806	A1A3L	C4-N3	7.57	1.49	1.34
5	B	802	ATP	O4'-C1'	-5.66	1.28	1.42
5	B	801	ATP	O4'-C1'	-5.66	1.28	1.42
7	B	806	A1A3L	PA-O3A	5.32	1.65	1.59
5	B	801	ATP	PB-O3A	4.75	1.64	1.59
5	B	801	ATP	PA-O3A	4.72	1.64	1.59
5	B	802	ATP	C5'-C4'	-4.52	1.38	1.51
5	B	802	ATP	PA-O3A	4.43	1.64	1.59
5	B	801	ATP	O4'-C4'	4.42	1.54	1.45
5	B	801	ATP	C5'-C4'	-4.34	1.38	1.51
5	B	802	ATP	PB-O3A	4.33	1.64	1.59
5	B	802	ATP	O4'-C4'	4.32	1.54	1.45
5	B	802	ATP	C2'-C1'	4.30	1.67	1.53
5	B	801	ATP	C2'-C1'	4.24	1.66	1.53
7	B	806	A1A3L	C6-N1	4.23	1.48	1.38
5	B	801	ATP	C6-N6	4.18	1.44	1.34
5	B	802	ATP	C6-N6	4.14	1.44	1.34
7	B	806	A1A3L	O2-C2	-3.79	1.16	1.23
5	B	802	ATP	PB-O3B	3.69	1.63	1.59
5	B	801	ATP	PB-O3B	3.63	1.63	1.59
5	B	801	ATP	C8-N9	-3.15	1.32	1.37
5	B	802	ATP	C8-N9	-3.13	1.32	1.37
7	B	806	A1A3L	C2-N1	2.82	1.46	1.40
5	B	802	ATP	O3'-C3'	2.80	1.49	1.43
5	B	801	ATP	C5-N7	-2.76	1.34	1.39
5	B	801	ATP	O3'-C3'	2.72	1.49	1.43
3	A	801	DTP	PB-O3A	2.63	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	802	ATP	C5-N7	-2.60	1.34	1.39
5	B	802	ATP	C3'-C4'	2.42	1.59	1.53
3	A	801	DTP	PA-O3A	2.41	1.62	1.59
7	B	806	A1A3L	C4-N4	2.37	1.39	1.33
5	B	801	ATP	C3'-C4'	2.36	1.59	1.53
7	B	806	A1A3L	PB-O3B	-2.34	1.46	1.54
7	B	806	A1A3L	C5-C4	2.34	1.48	1.42
7	B	806	A1A3L	PB-O1B	-2.25	1.46	1.54
7	B	806	A1A3L	O01-C3'	2.24	1.43	1.39
3	A	801	DTP	C5-N7	-2.22	1.35	1.39
7	B	806	A1A3L	O4'-C1'	2.19	1.47	1.42
3	B	803	DTP	C5-N7	-2.16	1.35	1.39
5	A	804	ATP	PG-O2G	-2.13	1.46	1.54
7	B	806	A1A3L	PA-O2A	-2.09	1.45	1.55
3	B	803	DTP	PB-O3A	2.04	1.61	1.59
3	B	803	DTP	C8-N7	2.01	1.35	1.31
5	A	803	ATP	PG-O2G	-2.01	1.47	1.54

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	DTP	O2B-PB-O3A	5.95	123.36	107.27
5	B	801	ATP	C5-C4-N3	-5.37	119.33	126.72
3	B	803	DTP	C5-C4-N3	-5.35	119.34	126.72
5	B	802	ATP	C5-C4-N3	-5.35	119.35	126.72
3	A	801	DTP	C5-C4-N3	-5.25	119.49	126.72
5	B	802	ATP	N3-C2-N1	-4.96	121.07	128.58
3	A	801	DTP	O2A-PA-O3A	4.91	120.55	107.27
5	B	801	ATP	N3-C2-N1	-4.87	121.21	128.58
3	A	801	DTP	N3-C2-N1	-4.86	121.23	128.58
3	B	803	DTP	N3-C2-N1	-4.80	121.31	128.58
5	B	801	ATP	N3-C4-N9	4.60	134.99	127.17
5	B	802	ATP	N3-C4-N9	4.11	134.15	127.17
5	B	802	ATP	C2-N3-C4	3.79	121.09	111.83
5	B	801	ATP	C2-N3-C4	3.60	120.63	111.83
7	B	806	A1A3L	O4'-C4'-C3'	3.57	109.33	104.31
3	B	803	DTP	C2-N3-C4	3.56	120.51	111.83
3	A	801	DTP	C2-N3-C4	3.53	120.46	111.83
3	B	803	DTP	N3-C4-N9	3.49	133.10	127.17
3	B	803	DTP	N9-C8-N7	-3.47	109.02	113.94
3	A	801	DTP	N9-C8-N7	-3.46	109.03	113.94
5	B	802	ATP	N9-C8-N7	-3.44	109.05	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	DTP	N3-C4-N9	3.43	133.00	127.17
5	B	801	ATP	C4-N9-C8	3.10	109.00	105.74
3	A	801	DTP	O5'-PA-O1A	-3.09	96.67	108.94
5	B	801	ATP	N9-C8-N7	-3.07	109.58	113.94
5	B	802	ATP	C5-N7-C8	3.05	108.24	103.45
5	B	802	ATP	C4-N9-C8	3.03	108.92	105.74
5	B	802	ATP	C4-C5-N7	-2.88	107.29	110.58
7	B	806	A1A3L	O1B-PB-O3A	2.86	114.22	104.64
5	B	802	ATP	C3'-C2'-C1'	2.79	106.75	101.46
3	B	803	DTP	C4-C5-N7	-2.69	107.51	110.58
7	B	806	A1A3L	O3B-PB-O3A	2.68	113.63	104.64
3	A	801	DTP	C4-C5-N7	-2.63	107.57	110.58
3	B	803	DTP	C5-N7-C8	2.57	107.49	103.45
3	B	803	DTP	C4-N9-C8	2.56	108.43	105.74
3	A	801	DTP	C5-N7-C8	2.56	107.47	103.45
3	A	801	DTP	C4-N9-C8	2.54	108.41	105.74
5	B	801	ATP	C5-N7-C8	2.52	107.40	103.45
3	A	801	DTP	O2A-PA-O1A	-2.49	100.87	112.44
7	B	806	A1A3L	O2A-PA-O1A	-2.38	101.40	112.44
5	B	802	ATP	C2'-C3'-C4'	2.06	106.58	102.61
3	B	803	DTP	C2'-C1'-N9	-2.04	109.84	114.63

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	803	DTP	C5'-O5'-PA-O2A
3	B	803	DTP	C5'-O5'-PA-O3A
5	A	803	ATP	C5'-O5'-PA-O1A
7	B	806	A1A3L	C3'-C4'-C5'-O5'
7	B	806	A1A3L	C5'-O5'-PA-O1A
7	B	806	A1A3L	C5'-O5'-PA-O2A
7	B	806	A1A3L	C5'-O5'-PA-O3A
5	A	804	ATP	PG-O3B-PB-O1B
5	A	804	ATP	PB-O3A-PA-O1A
5	A	803	ATP	PB-O3B-PG-O1G
3	A	801	DTP	PA-O3A-PB-O1B
3	B	803	DTP	PG-O3B-PB-O1B
7	B	806	A1A3L	O4'-C4'-C5'-O5'
5	B	801	ATP	O4'-C4'-C5'-O5'
3	A	801	DTP	C5'-O5'-PA-O3A
5	A	803	ATP	C5'-O5'-PA-O3A

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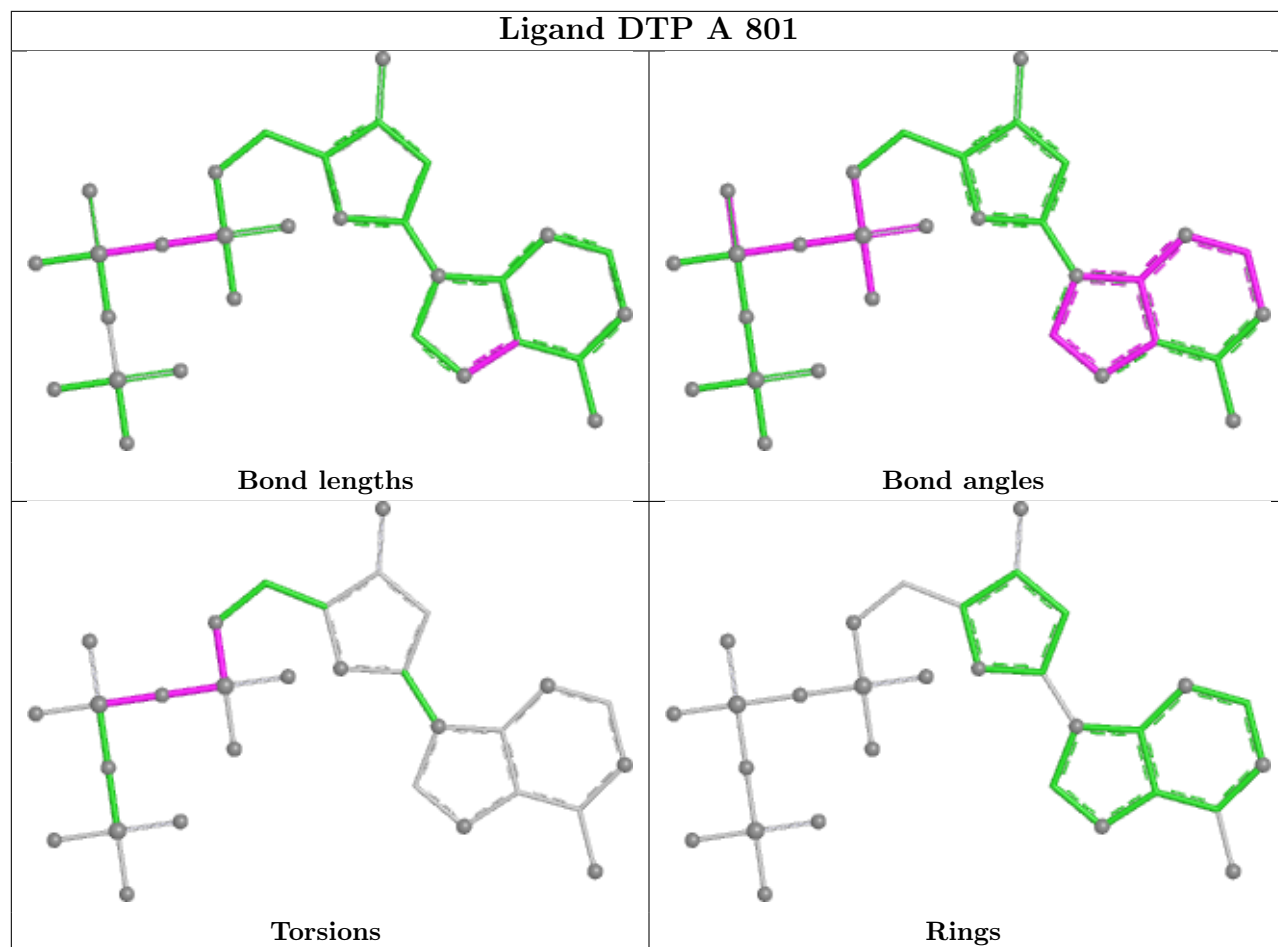
Mol	Chain	Res	Type	Atoms
5	B	802	ATP	C5'-O5'-PA-O1A
5	B	802	ATP	C5'-O5'-PA-O3A
5	B	802	ATP	PB-O3B-PG-O1G
3	A	801	DTP	PB-O3A-PA-O2A
5	A	804	ATP	PA-O3A-PB-O1B
5	A	803	ATP	PB-O3B-PG-O2G
5	A	803	ATP	PB-O3B-PG-O3G
5	B	802	ATP	PB-O3B-PG-O2G
5	B	802	ATP	PB-O3B-PG-O3G
3	A	801	DTP	PB-O3A-PA-O1A
5	A	803	ATP	PB-O3A-PA-O2A
5	A	804	ATP	PG-O3B-PB-O2B
5	B	801	ATP	PA-O3A-PB-O2B
5	B	802	ATP	PA-O3A-PB-O2B

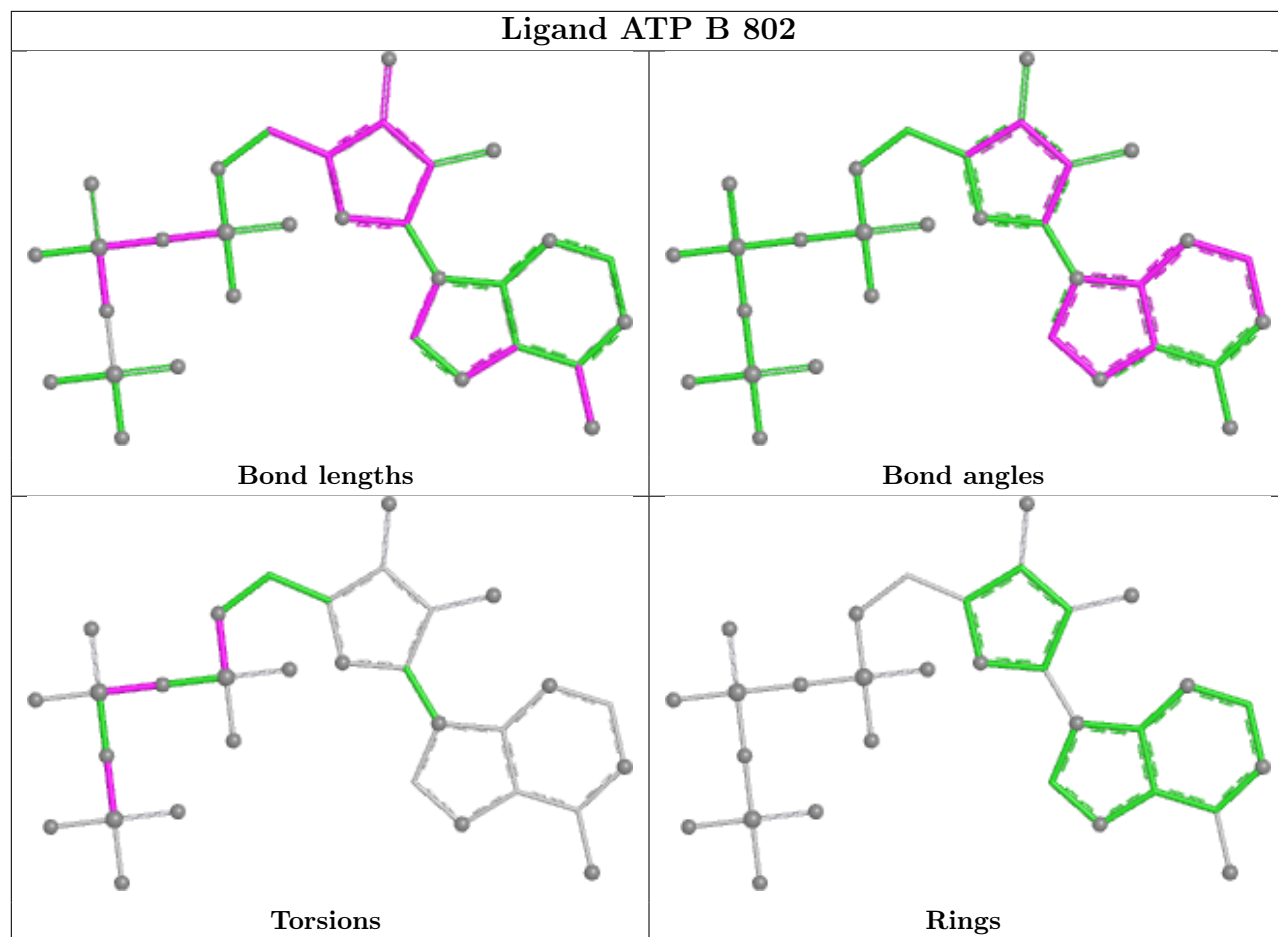
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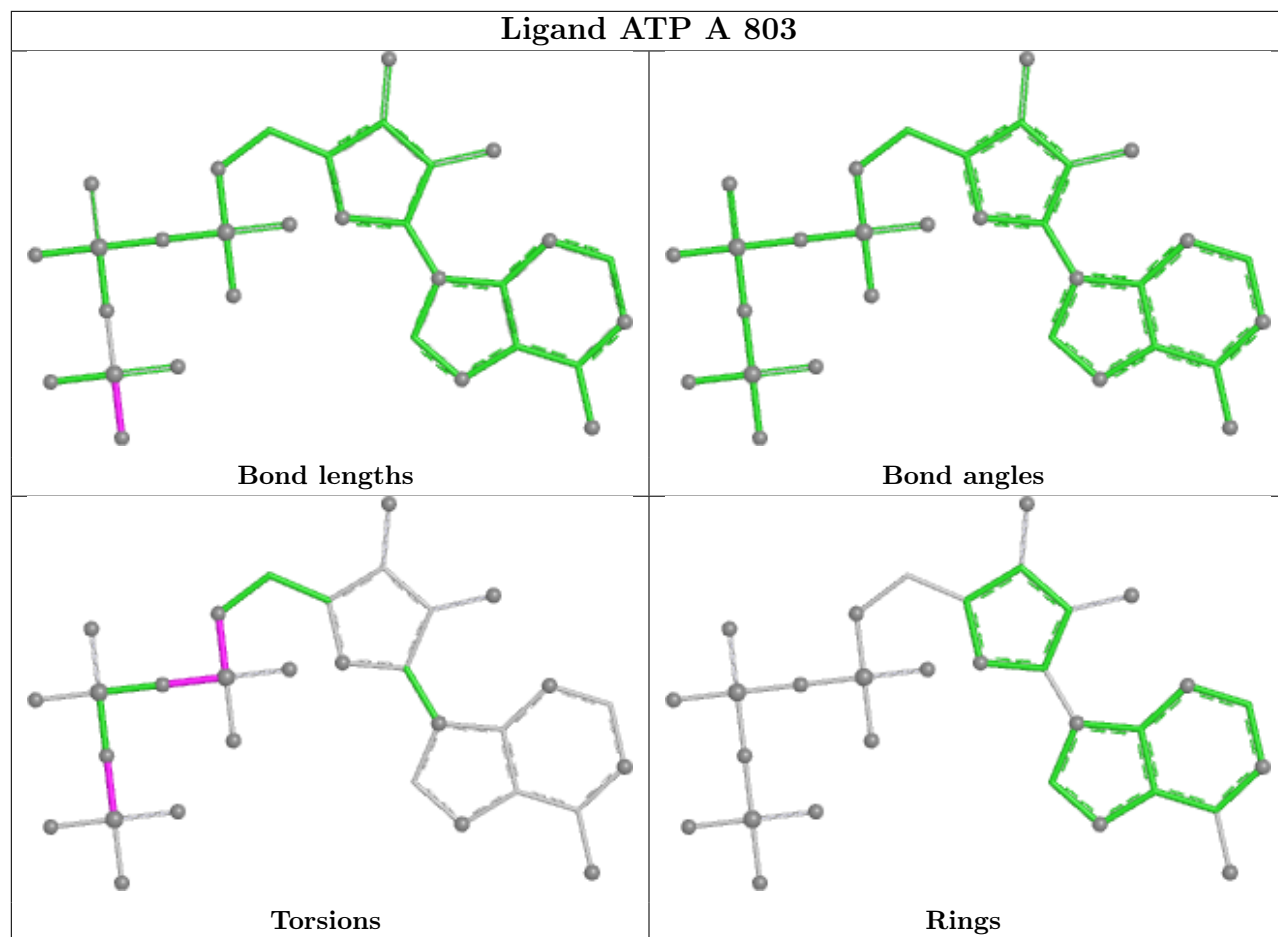
7 monomers are involved in 12 short contacts:

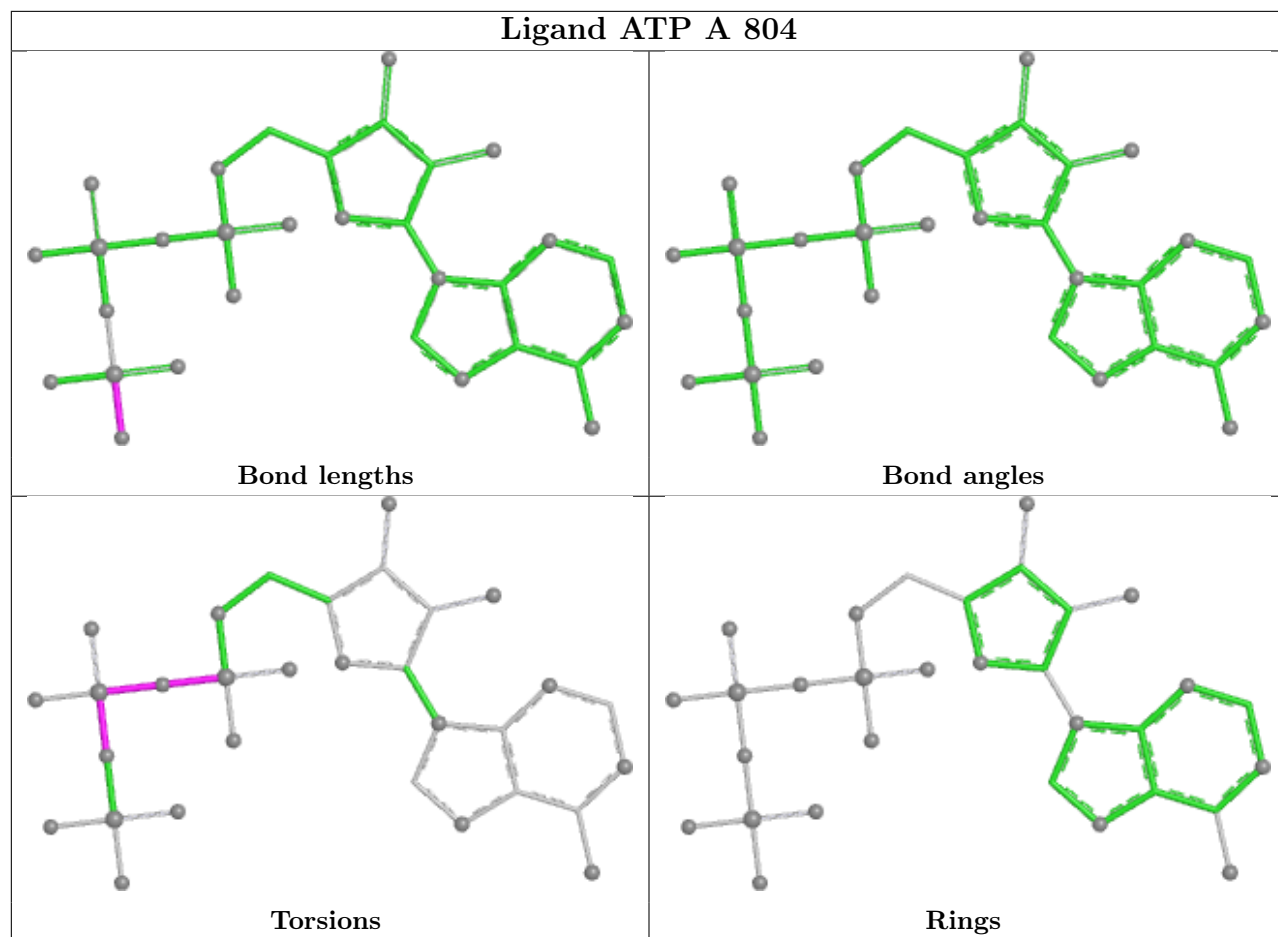
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	802	ATP	1	0
5	A	804	ATP	4	0
3	B	803	DTP	1	0
8	D	401	FEO	3	0
5	B	801	ATP	2	0
7	B	806	A1A3L	1	0
8	C	401	FEO	1	0

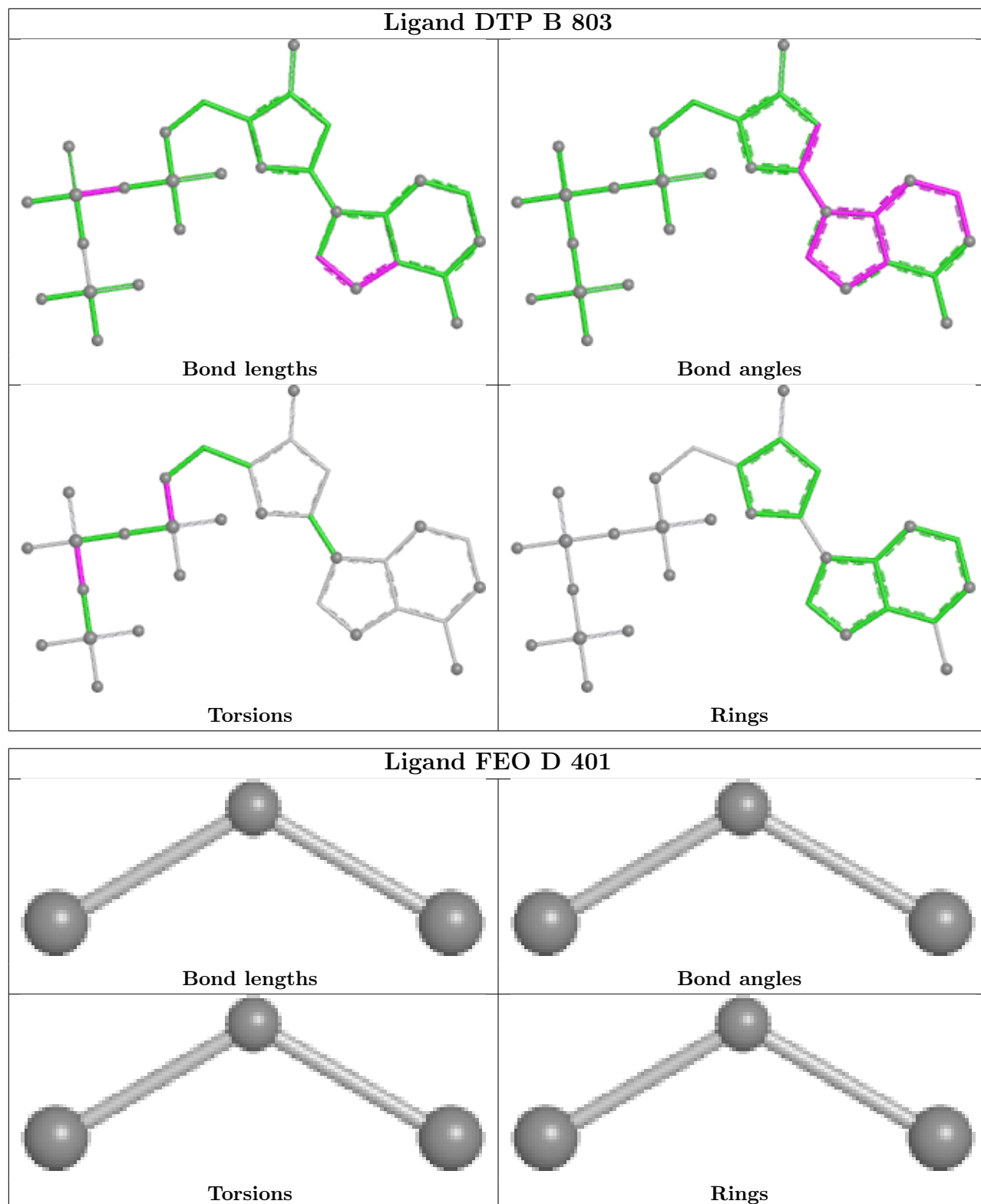
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

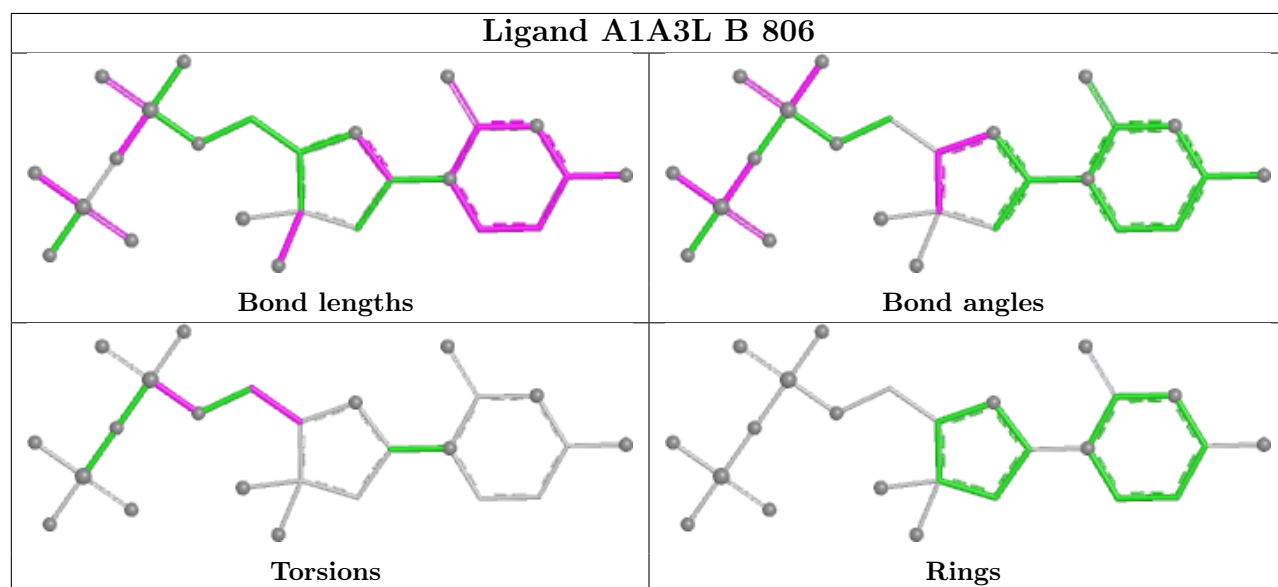
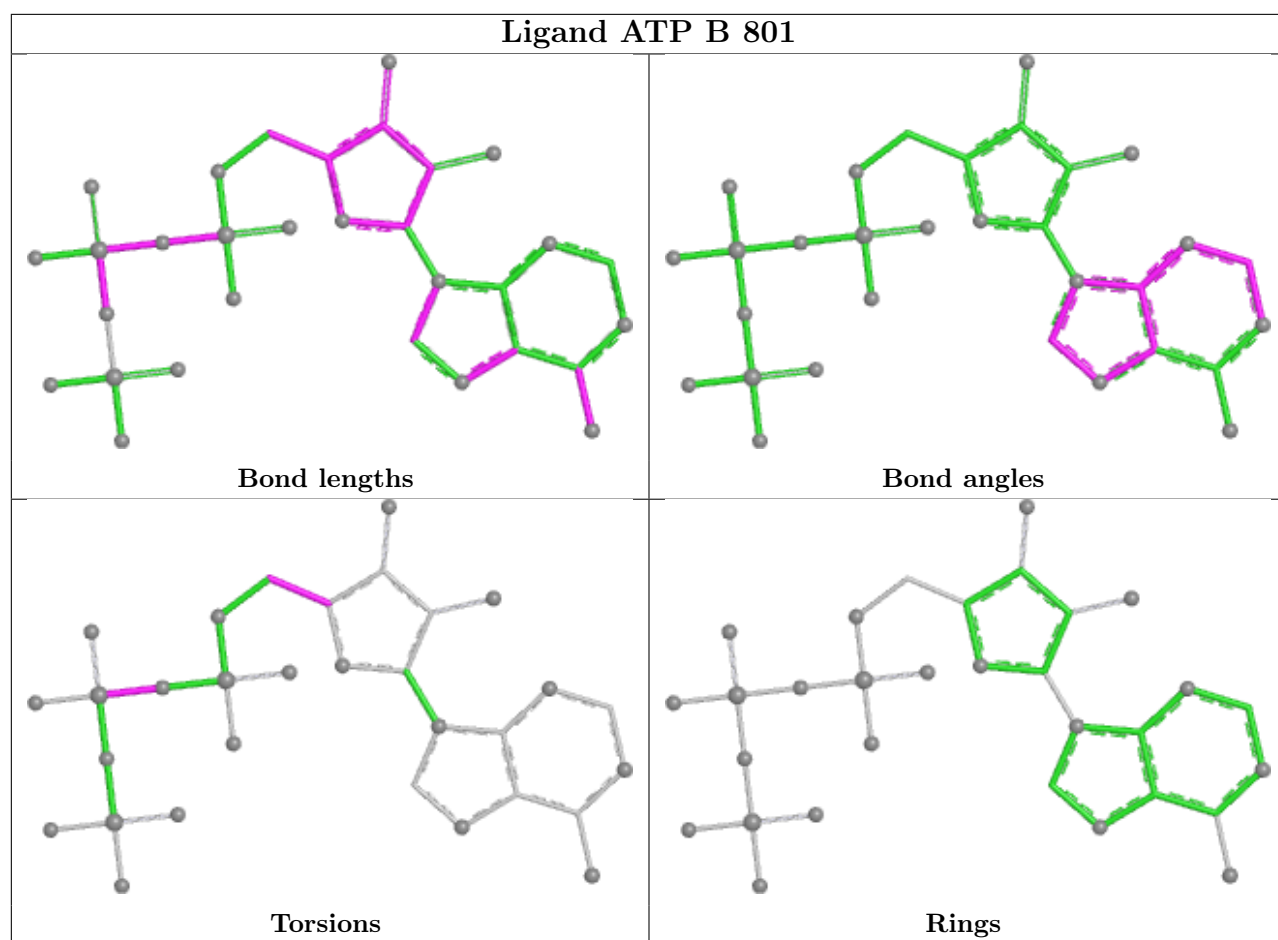


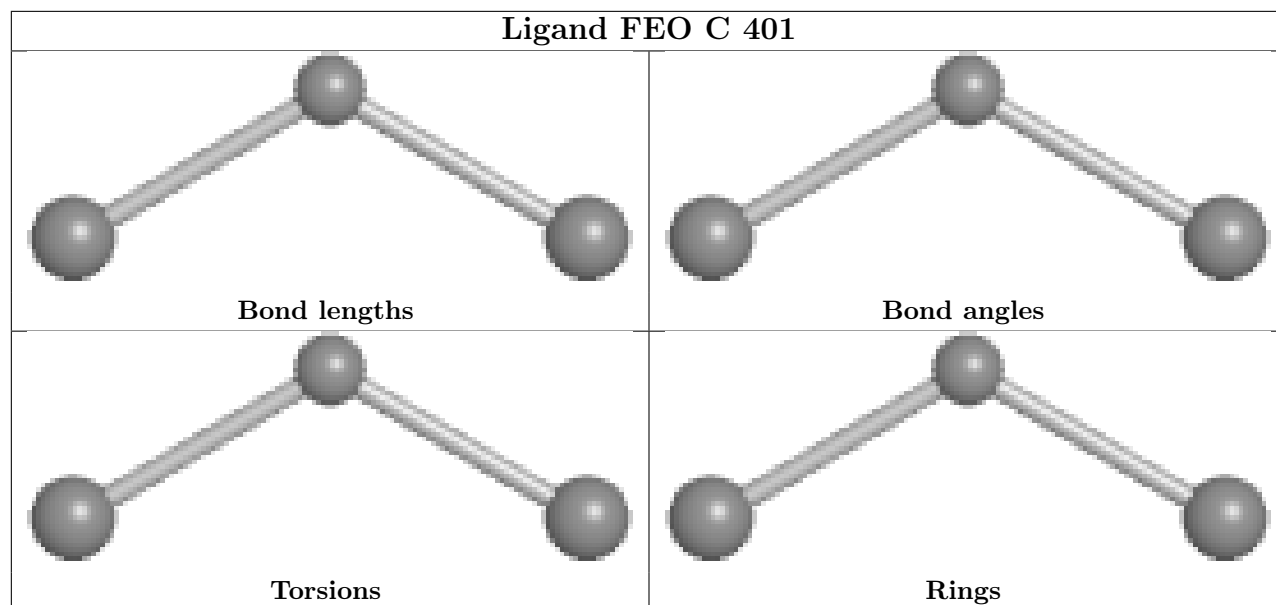












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

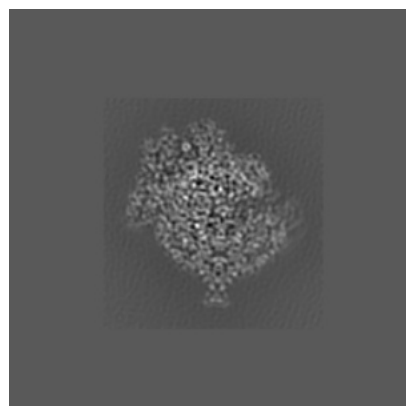
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46711. These allow visual inspection of the internal detail of the map and identification of artifacts.

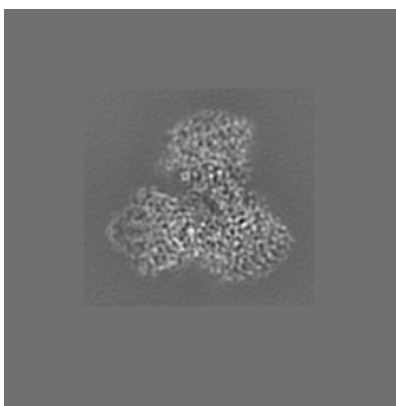
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

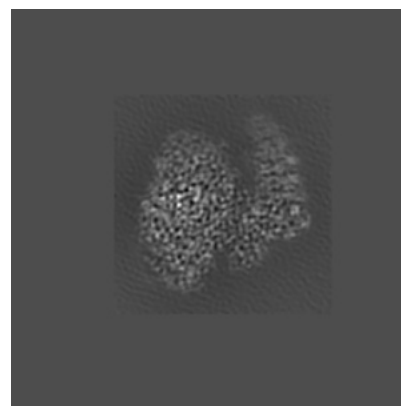
6.1.1 Primary map



X

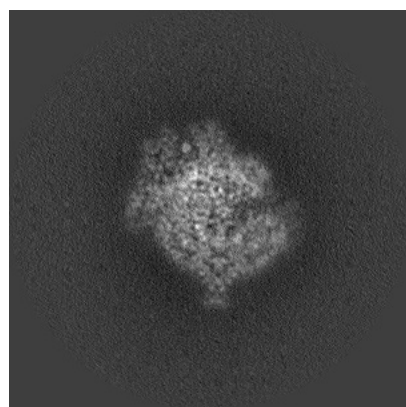


Y

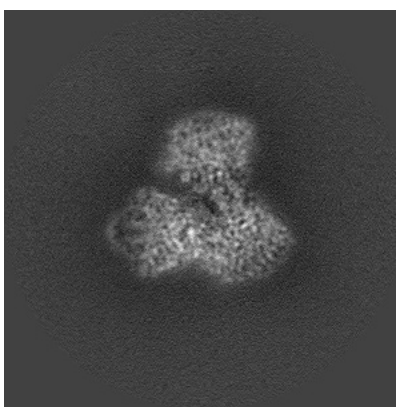


Z

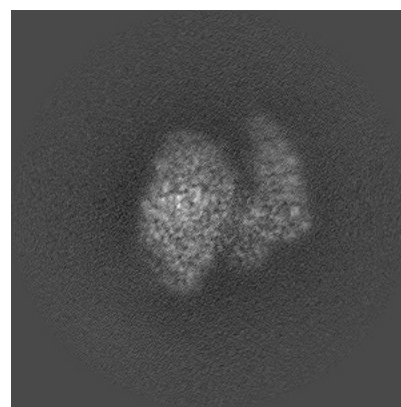
6.1.2 Raw map



X



Y

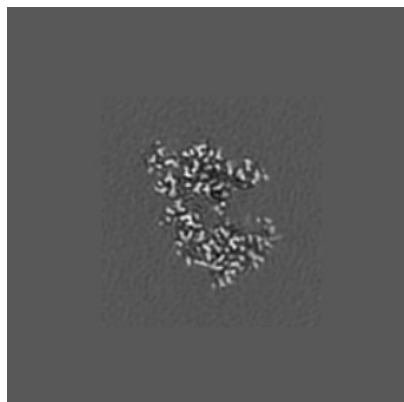


Z

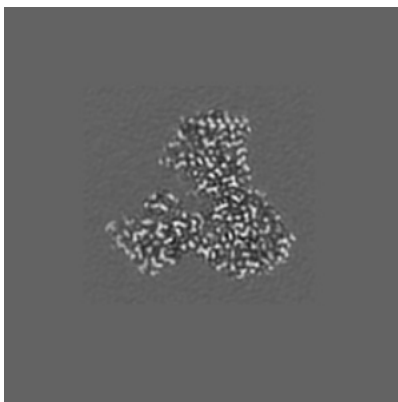
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

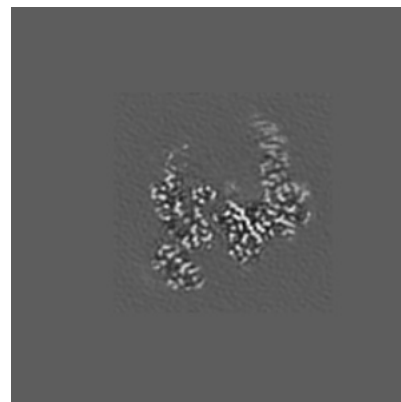
6.2.1 Primary map



X Index: 288

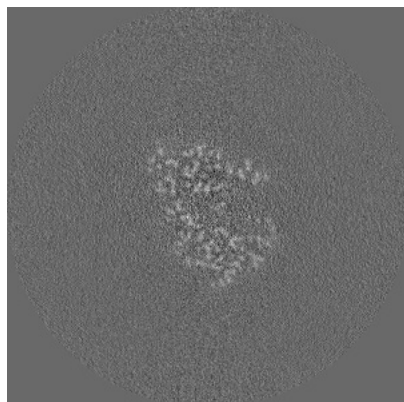


Y Index: 288

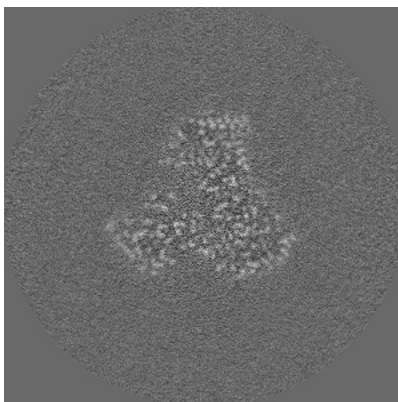


Z Index: 288

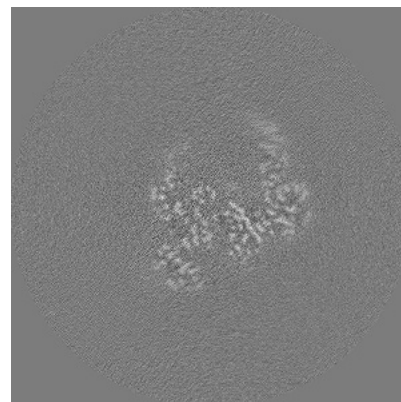
6.2.2 Raw map



X Index: 288



Y Index: 288

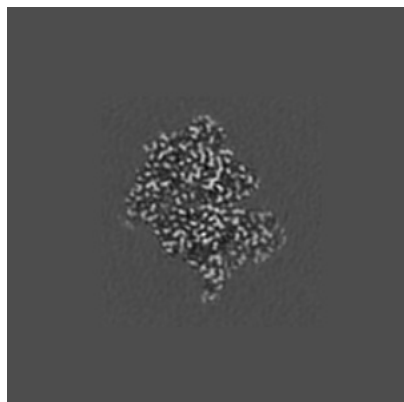


Z Index: 288

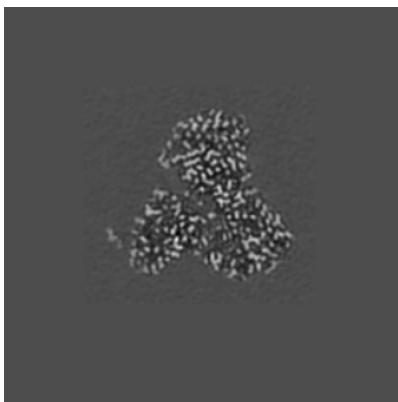
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

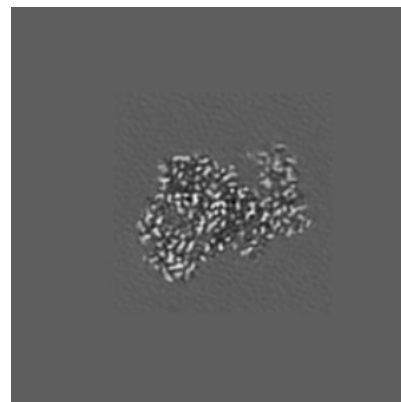
6.3.1 Primary map



X Index: 241

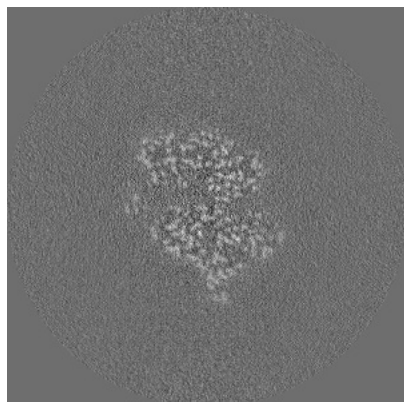


Y Index: 282

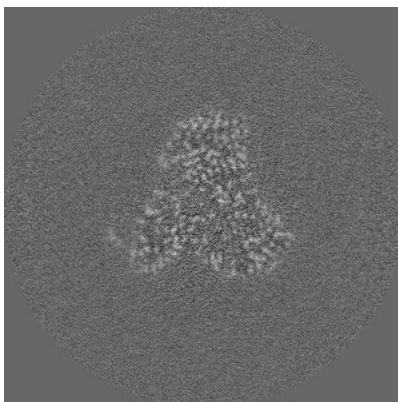


Z Index: 318

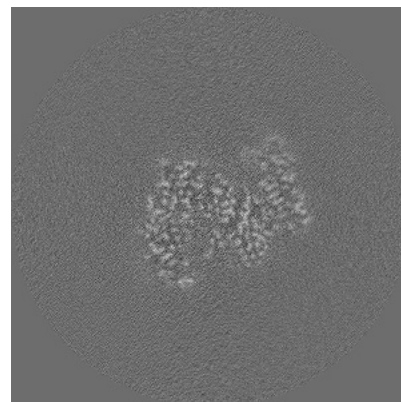
6.3.2 Raw map



X Index: 268



Y Index: 282

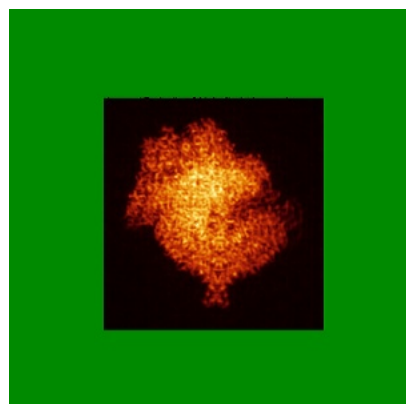


Z Index: 309

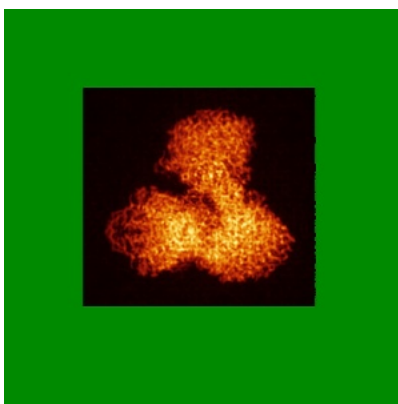
The images above show the largest variance slices of the map in three orthogonal directions.

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

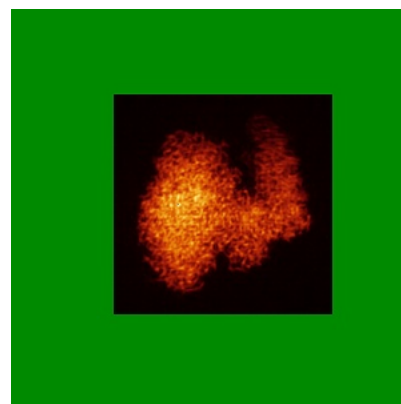
6.4.1 Primary map



X

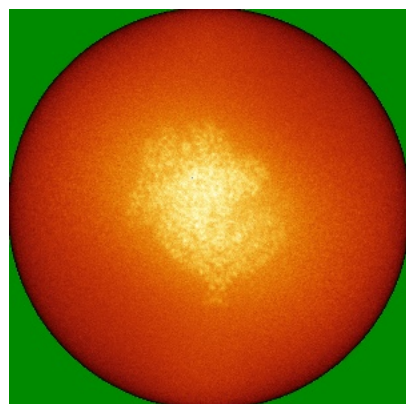


Y

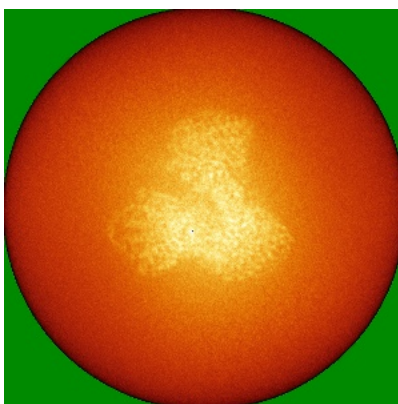


Z

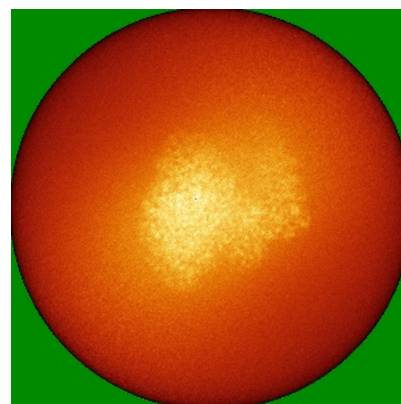
6.4.2 Raw map



X



Y

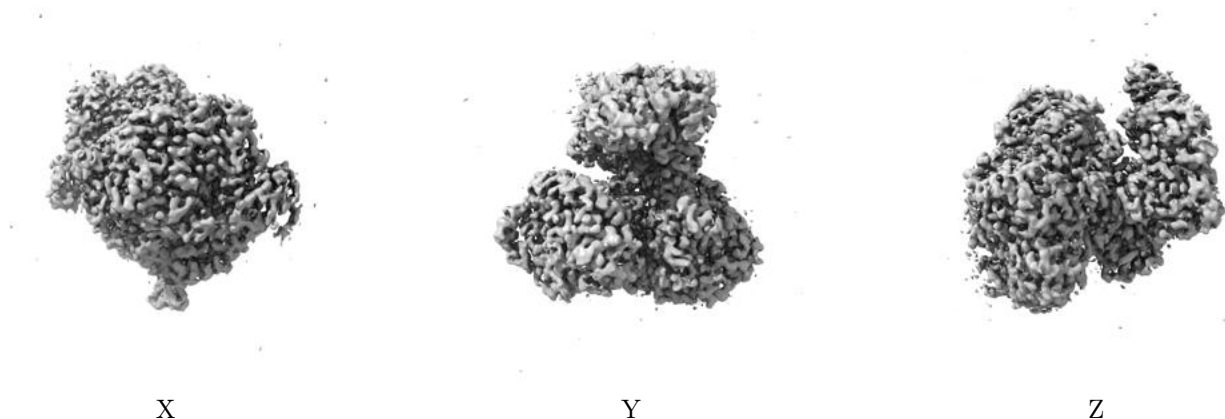


Z

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.

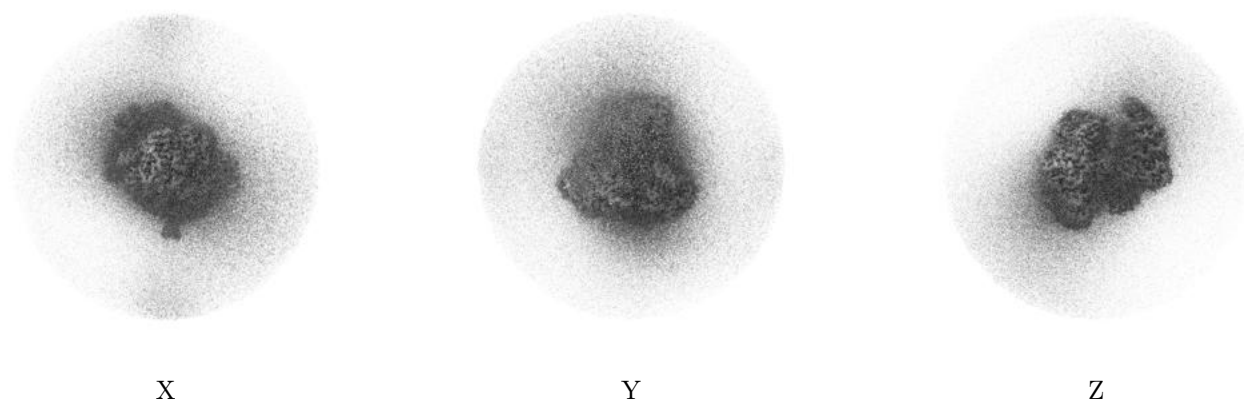
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.235. 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.

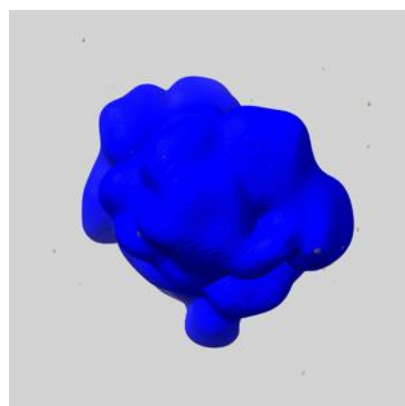
6.6 Mask visualisation [i](#)

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

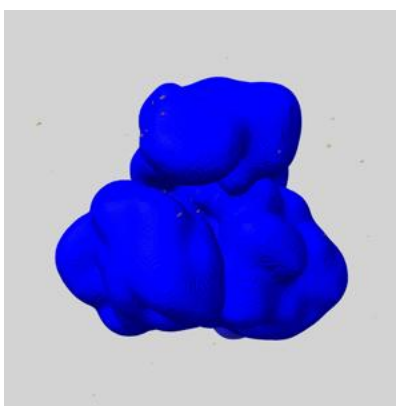
A mask typically either:

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

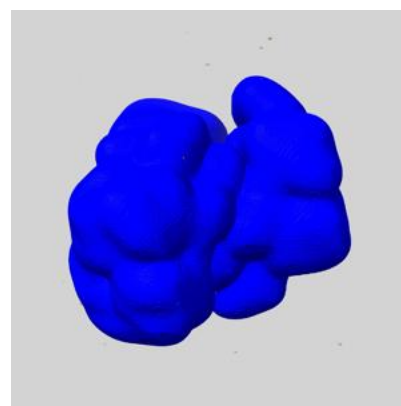
6.6.1 emd_46711_msk_1.map [i](#)



X



Y

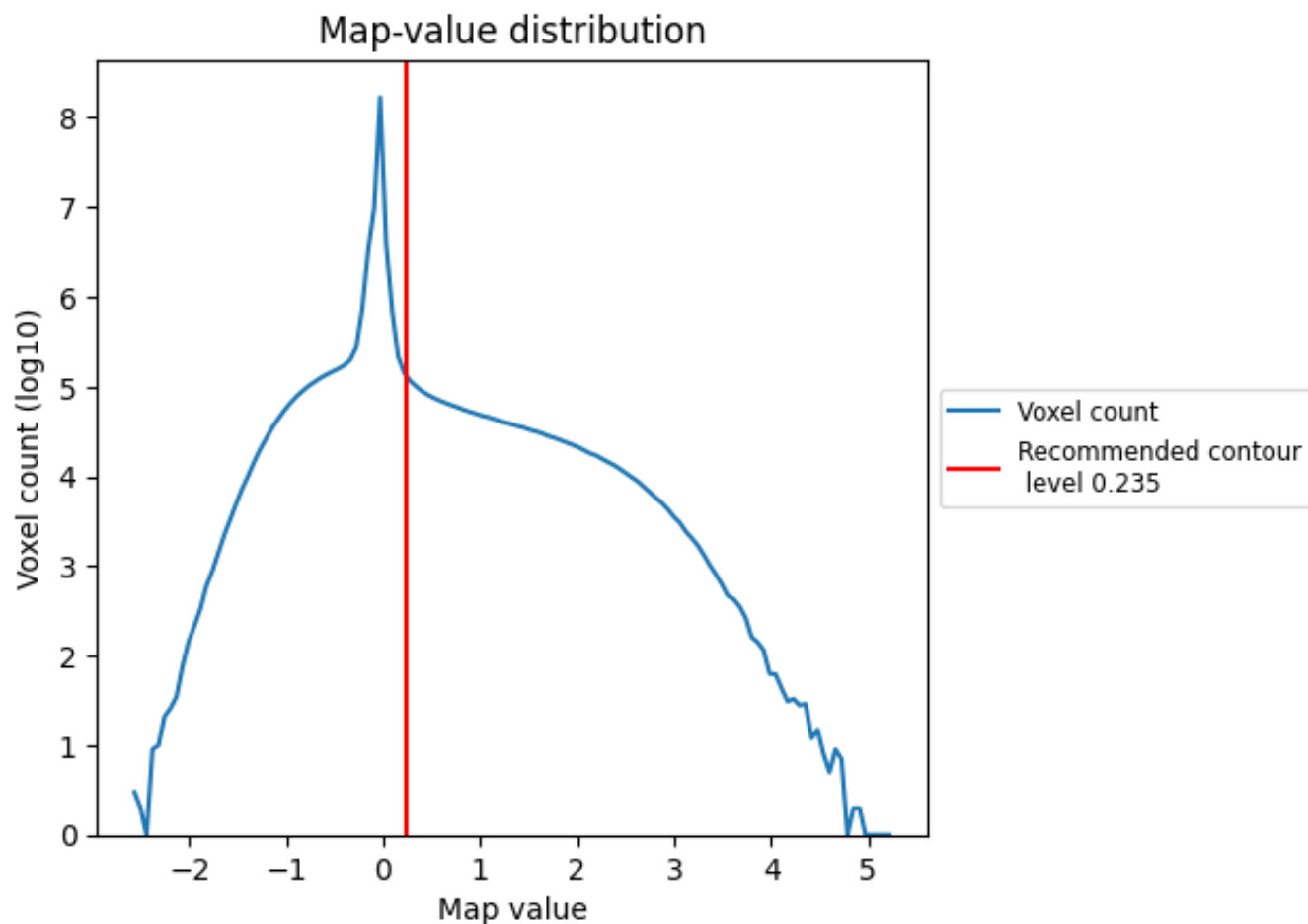


Z

7 Map analysis [i](#)

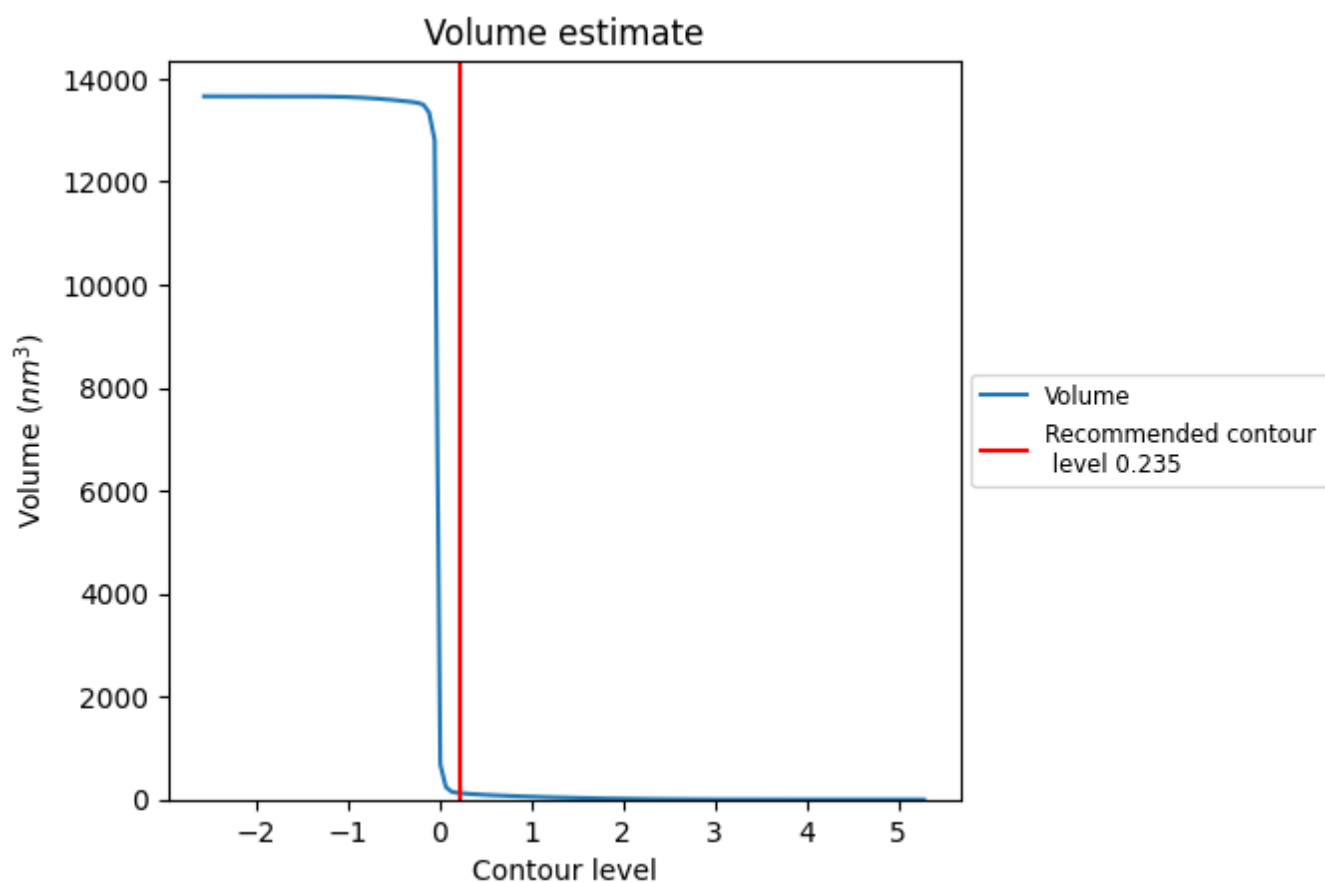
This section contains the results of statistical analysis of the map.

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.

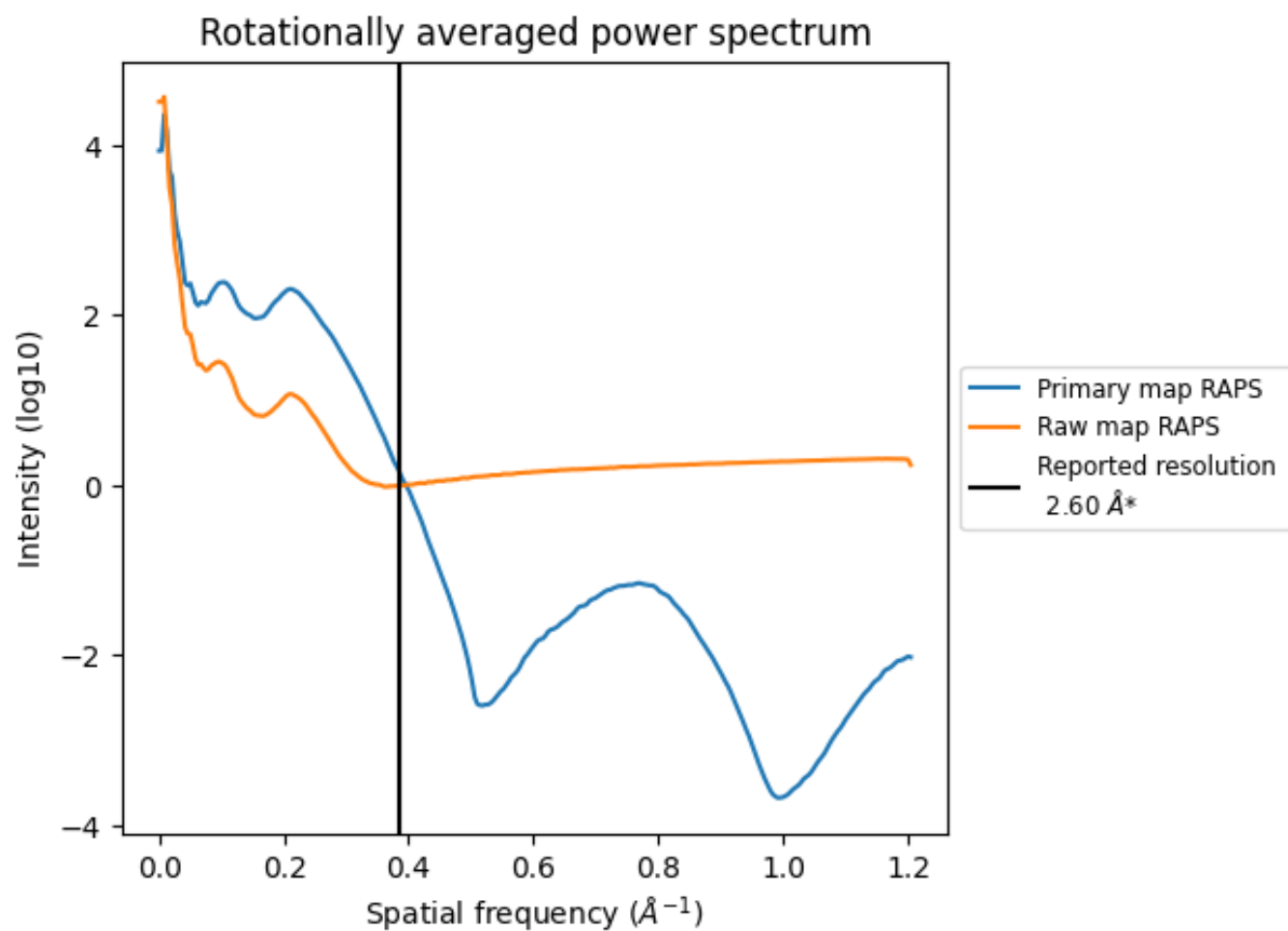
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 124 nm³; this corresponds to an approximate mass of 112 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 ⓘ

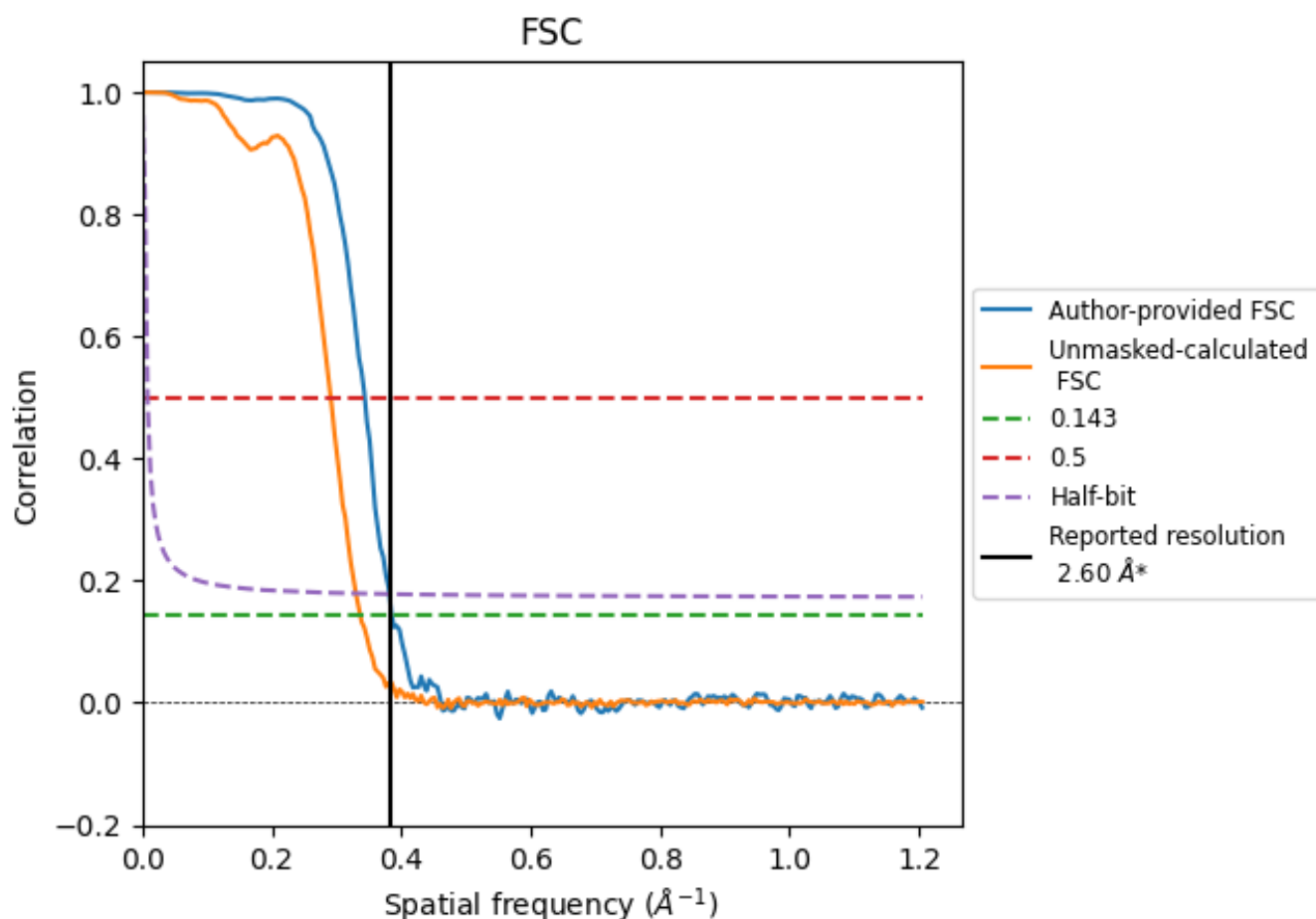


*Reported resolution corresponds to spatial frequency of 0.385 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

8.2 Resolution estimates

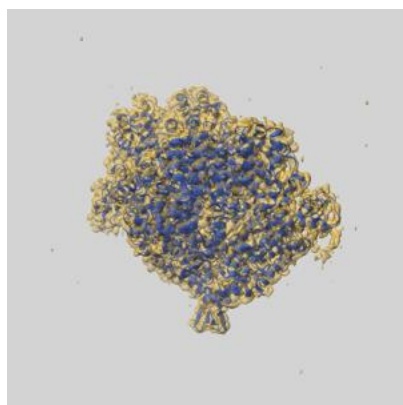
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.59	2.91	2.62
Unmasked-calculated*	2.97	3.43	3.03

*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 2.97 differs from the reported value 2.6 by more than 10 %

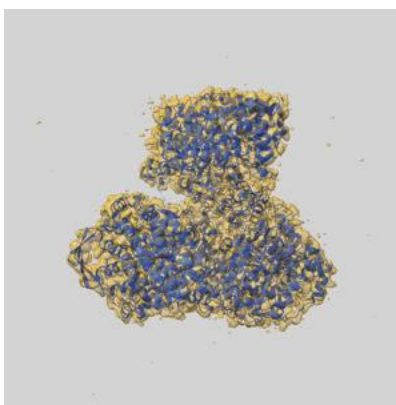
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46711 and PDB model 9DB2. Per-residue inclusion information can be found in section [3](#) on page [8](#).

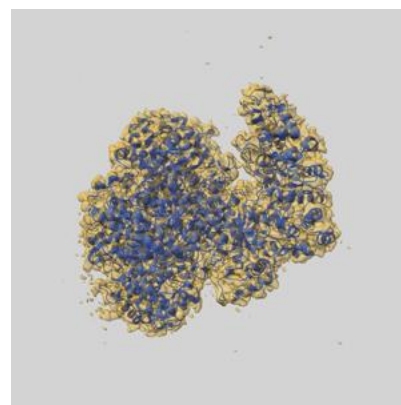
9.1 Map-model overlay [i](#)



X



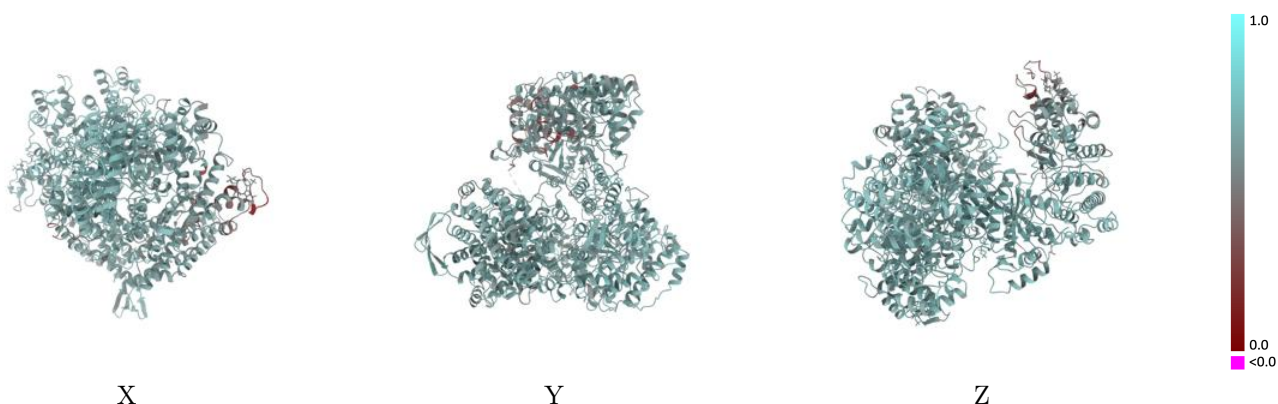
Y



Z

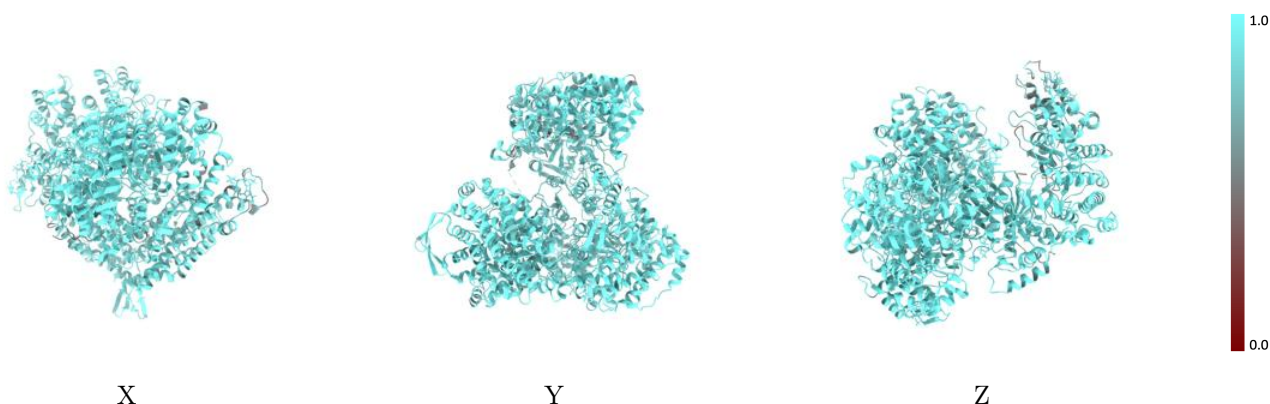
The images above show the 3D surface view of the map at the recommended contour level 0.235 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



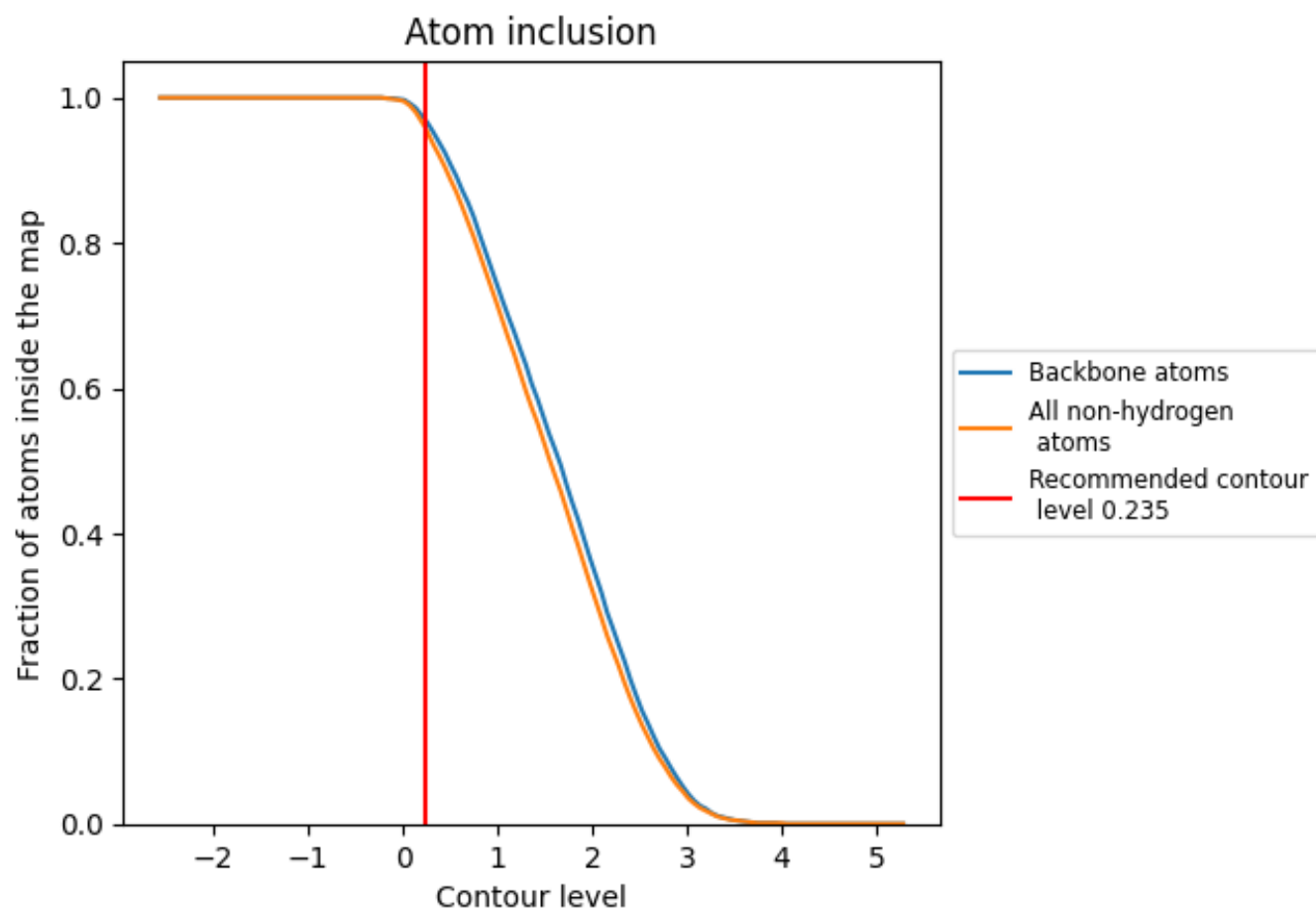
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.235).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 96% 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 (0.235) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9590	0.6290
A	0.9410	0.6090
B	0.9790	0.6500
C	0.9700	0.6390
D	0.9470	0.6140

