



Full wwPDB EM Validation Report ⓘ

Mar 16, 2026 – 12:25 PM UTC

PDB ID : 7ZYY / pdb_00007zyy
EMDB ID : EMD-15028
Title : Cryo-EM structure of Lactococcus lactis pyruvate carboxylase with acetyl-CoA
Authors : Lopez-Alonso, J.P.; Lazaro, M.; Gil, D.; Choi, P.H.; Tong, L.; Valle, M.
Deposited on : 2022-05-25
Resolution : 2.12 Å (reported)
Based on initial model : 5VYZ

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

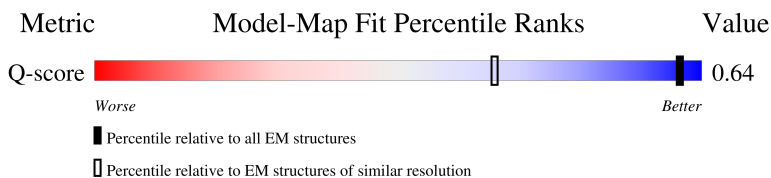
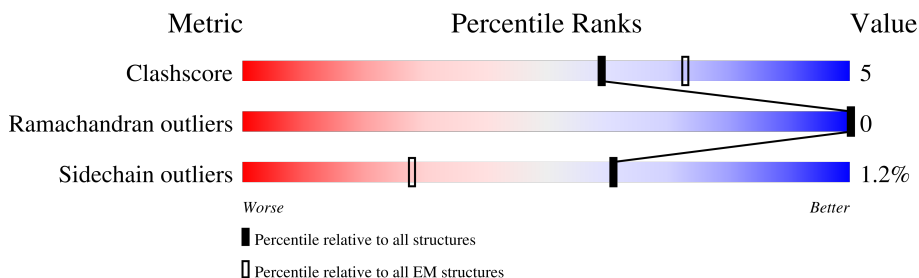
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.12 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	2398 (1.64 - 2.62)

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	1143	
1	B	1143	
1	C	1143	
1	D	1143	

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	PYR	B	1206	-	X	-	-
7	BCT	C	1207	-	X	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 33924 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 Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1056	Total	C	N	O	S	0	0
			8309	5270	1438	1570	31		
1	B	1056	Total	C	N	O	S	0	0
			8309	5270	1438	1570	31		
1	C	1056	Total	C	N	O	S	0	0
			8309	5270	1438	1570	31		
1	D	1056	Total	C	N	O	S	0	0
			8309	5270	1438	1570	31		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	VAL	-	expression tag	UNP A0A2A9IR05
A	-4	PRO	-	expression tag	UNP A0A2A9IR05
A	-3	ARG	-	expression tag	UNP A0A2A9IR05
A	-2	GLY	-	expression tag	UNP A0A2A9IR05
A	-1	SER	-	expression tag	UNP A0A2A9IR05
A	0	HIS	-	expression tag	UNP A0A2A9IR05
A	1055	ALA	THR	conflict	UNP A0A2A9IR05
B	-5	VAL	-	expression tag	UNP A0A2A9IR05
B	-4	PRO	-	expression tag	UNP A0A2A9IR05
B	-3	ARG	-	expression tag	UNP A0A2A9IR05
B	-2	GLY	-	expression tag	UNP A0A2A9IR05
B	-1	SER	-	expression tag	UNP A0A2A9IR05
B	0	HIS	-	expression tag	UNP A0A2A9IR05
B	1055	ALA	THR	conflict	UNP A0A2A9IR05
C	-5	VAL	-	expression tag	UNP A0A2A9IR05
C	-4	PRO	-	expression tag	UNP A0A2A9IR05
C	-3	ARG	-	expression tag	UNP A0A2A9IR05
C	-2	GLY	-	expression tag	UNP A0A2A9IR05
C	-1	SER	-	expression tag	UNP A0A2A9IR05
C	0	HIS	-	expression tag	UNP A0A2A9IR05
C	1055	ALA	THR	conflict	UNP A0A2A9IR05
D	-5	VAL	-	expression tag	UNP A0A2A9IR05

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	PRO	-	expression tag	UNP A0A2A9IR05
D	-3	ARG	-	expression tag	UNP A0A2A9IR05
D	-2	GLY	-	expression tag	UNP A0A2A9IR05
D	-1	SER	-	expression tag	UNP A0A2A9IR05
D	0	HIS	-	expression tag	UNP A0A2A9IR05
D	1055	ALA	THR	conflict	UNP A0A2A9IR05

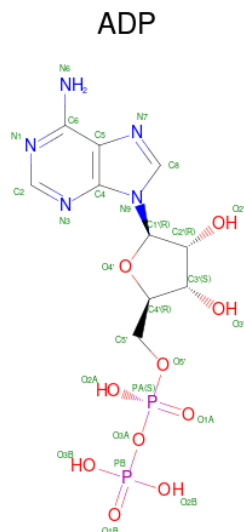
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
2	A	2	Total Mg 2 2	0
2	B	2	Total Mg 2 2	0
2	C	2	Total Mg 2 2	0
2	D	2	Total Mg 2 2	0

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

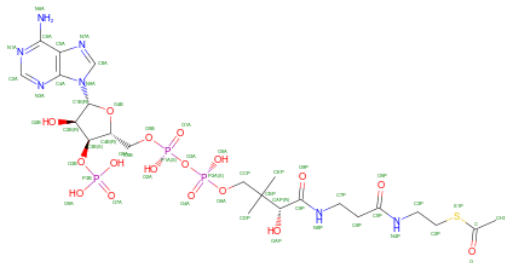
Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Mn 1 1	0
3	B	1	Total Mn 1 1	0
3	C	1	Total Mn 1 1	0
3	D	1	Total Mn 1 1	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



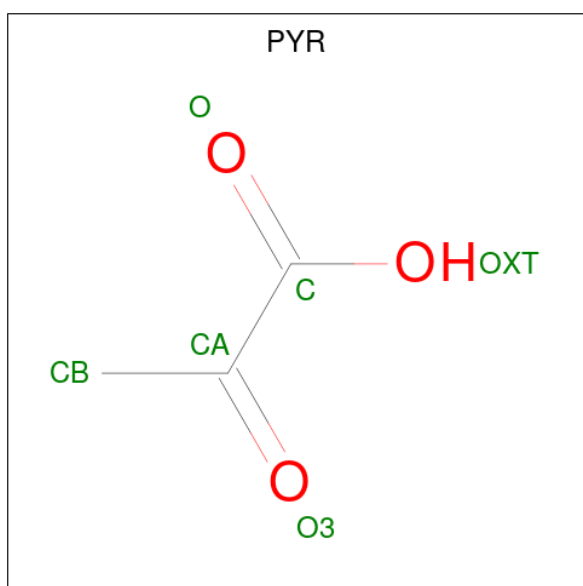
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 27	C 10	N 5	O 10	P 2	0
4	B	1	Total 27	C 10	N 5	O 10	P 2	0
4	C	1	Total 27	C 10	N 5	O 10	P 2	0
4	D	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 5 is ACETYL COENZYME *A (CCD ID: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



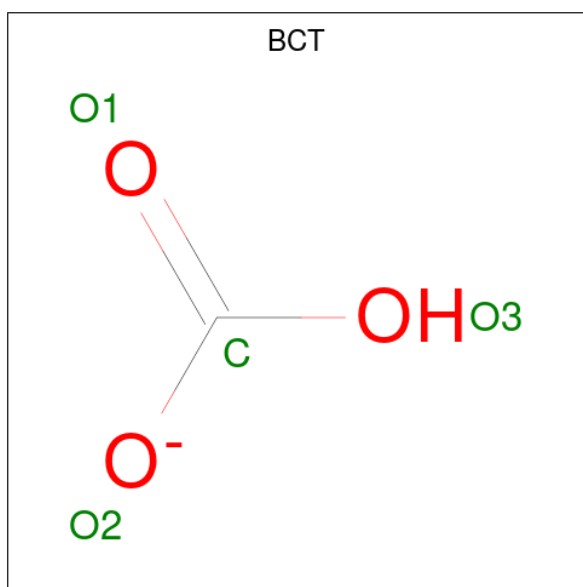
Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	
5	B	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	
5	C	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	
5	D	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	

- Molecule 6 is PYRUVIC ACID (CCD ID: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			6	3	3	
6	B	1	Total	C	O	0
			6	3	3	
6	C	1	Total	C	O	0
			6	3	3	
6	D	1	Total	C	O	0
			6	3	3	

- Molecule 7 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			4	1	3	
7	B	1	Total	C	O	0
			4	1	3	
7	C	1	Total	C	O	0
			4	1	3	
7	D	1	Total	C	O	0
			4	1	3	

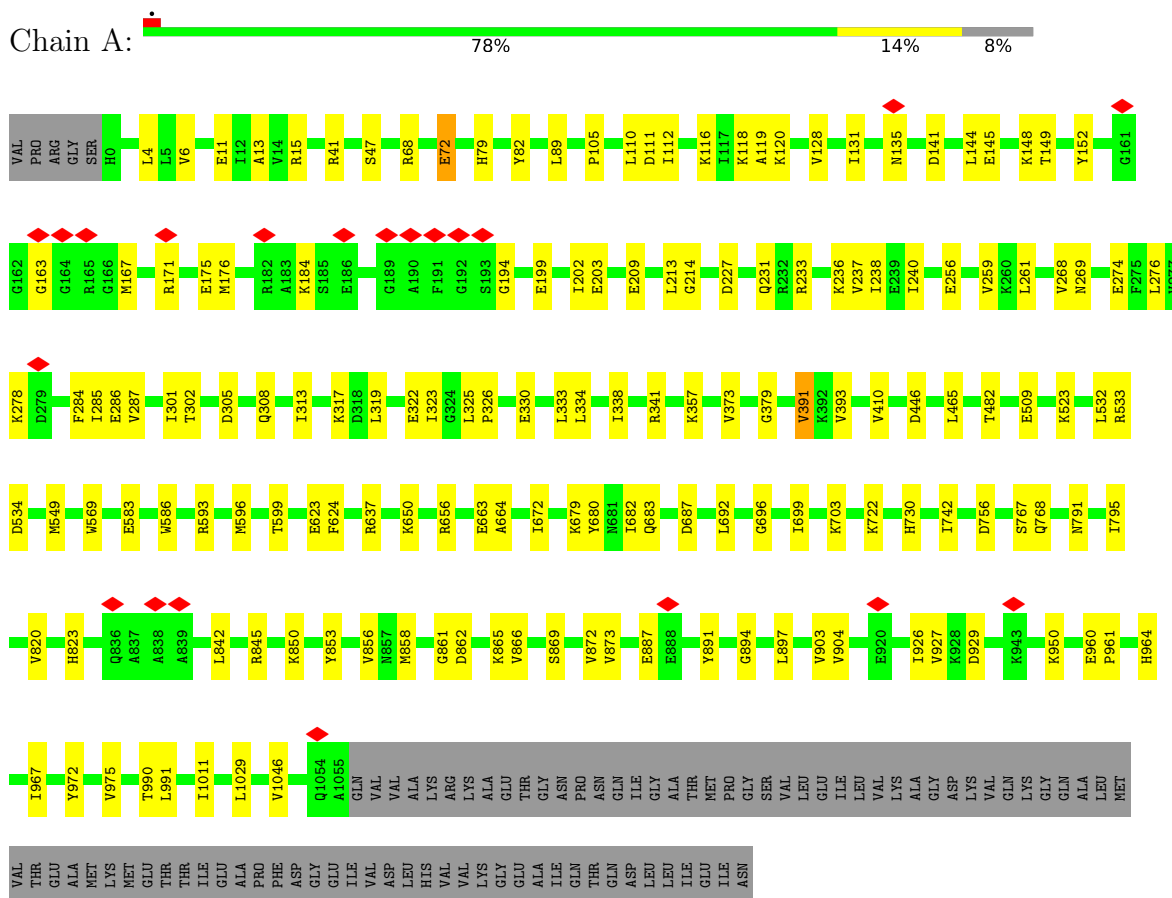
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	A	46	Total	O	0
			46	46	
8	B	155	Total	O	0
			155	155	
8	C	63	Total	O	0
			63	63	
8	D	60	Total	O	0
			60	60	

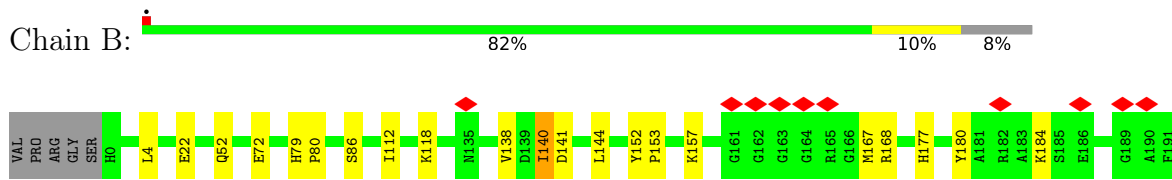
3 Residue-property plots

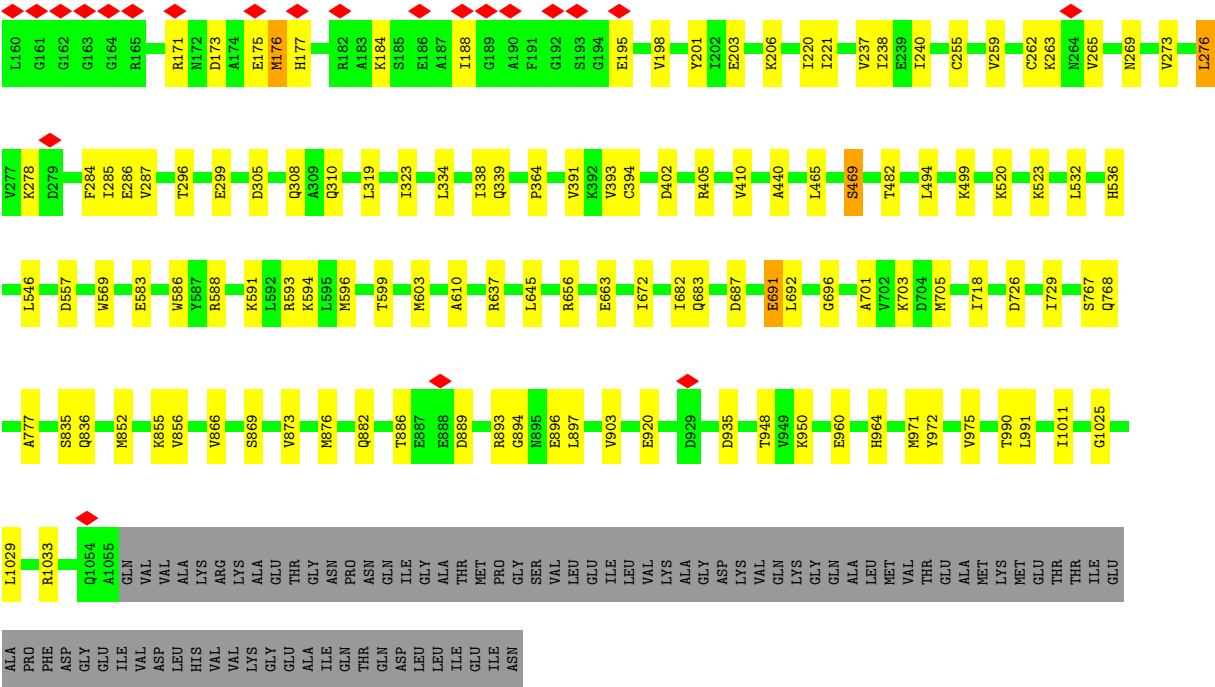
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



• Molecule 1: Pyruvate carboxylase





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1369092	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.106	Depositor
Minimum map value	-0.330	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.187	Depositor
Map size (Å)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, KCX, BCT, MG, PYR, ACO, MN

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	0.19	0/8464	0.41	2/11452 (0.0%)
1	B	0.21	0/8464	0.41	0/11452
1	C	0.19	0/8464	0.40	0/11452
1	D	0.19	0/8464	0.41	2/11452 (0.0%)
All	All	0.19	0/33856	0.41	4/45808 (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	148	LYS	CA-CB-CG	5.42	124.94	114.10
1	D	176	MET	CB-CG-SD	5.39	128.86	112.70
1	D	127	LYS	CA-CB-CG	5.33	124.76	114.10
1	A	176	MET	CB-CG-SD	5.26	128.47	112.70

There are no chirality outliers.

There are no planarity outliers.

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	8309	0	8253	91	0
1	B	8309	0	8253	67	0
1	C	8309	0	8253	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	8309	0	8252	76	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	27	0	12	3	0
4	B	27	0	12	1	0
4	C	27	0	12	1	0
4	D	27	0	12	0	0
5	A	51	0	34	0	0
5	B	51	0	34	1	0
5	C	51	0	34	1	0
5	D	51	0	34	1	0
6	A	6	0	0	0	0
6	B	6	0	0	0	0
6	C	6	0	0	1	0
6	D	6	0	0	0	0
7	A	4	0	1	0	0
7	B	4	0	1	0	0
7	C	4	0	0	0	0
7	D	4	0	1	0	0
8	A	46	0	0	0	0
8	B	155	0	0	0	0
8	C	63	0	0	0	0
8	D	60	0	0	0	0
All	All	33924	0	33198	305	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 5.

All (305) 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:C:842:LEU:HD12	1:C:845:ARG:HH22	1.58	0.69
1:C:153:PRO:HB3	1:C:171:ARG:HG2	1.77	0.66
1:D:153:PRO:HB2	1:D:201:TYR:HB3	1.79	0.65
1:A:152:TYR:HB3	1:A:171:ARG:HH12	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:ASP:HB3	1:D:118:LYS:HG3	1.79	0.64
1:B:972:TYR:HB3	1:B:975:VAL:HB	1.79	0.64
1:A:131:ILE:HD11	1:A:202:ILE:HD11	1.81	0.63
1:A:532:LEU:HD22	1:A:549:MET:HG2	1.81	0.63
1:C:972:TYR:HB3	1:C:975:VAL:HB	1.82	0.61
1:A:209:GLU:HG2	1:A:274:GLU:HG2	1.81	0.61
1:B:610:ALA:HB3	1:B:971:MET:HE1	1.82	0.61
1:D:972:TYR:HB3	1:D:975:VAL:HB	1.82	0.61
1:D:393:VAL:HG21	1:D:410:VAL:HG11	1.83	0.60
1:A:284:PHE:HE1	1:A:287:VAL:HG23	1.66	0.60
1:D:593:ARG:NH2	1:D:599:THR:O	2.34	0.60
1:C:89:LEU:HD22	1:C:111:ASP:HB3	1.82	0.60
1:A:326:PRO:HB2	1:A:330:GLU:HB3	1.84	0.59
1:B:603:MET:HG2	1:B:633:ILE:HG21	1.83	0.59
1:C:178:ASP:HA	1:C:182:ARG:HH21	1.67	0.59
1:C:115:ASP:HB3	1:C:118:LYS:HG3	1.82	0.59
1:A:972:TYR:HB3	1:A:975:VAL:HB	1.85	0.59
1:C:284:PHE:HE1	1:C:287:VAL:HG23	1.67	0.59
1:D:140:ILE:HD11	1:D:177:HIS:HD2	1.68	0.58
1:B:532:LEU:HD22	1:B:549:MET:HG2	1.86	0.58
1:B:920:GLU:OE1	1:B:920:GLU:N	2.35	0.58
1:A:276:LEU:HG	1:A:285:ILE:HD13	1.85	0.58
1:A:393:VAL:HG21	1:A:410:VAL:HG11	1.86	0.57
1:C:610:ALA:HB3	1:C:971:MET:HE1	1.85	0.57
1:A:319:LEU:HD23	1:A:323:ILE:HD12	1.87	0.57
1:A:593:ARG:NH2	1:A:599:THR:O	2.35	0.57
1:A:120:LYS:NZ	1:A:199:GLU:OE1	2.36	0.56
1:A:904:VAL:HG13	1:A:927:VAL:HG12	1.86	0.56
1:B:237:VAL:HG12	1:B:238:ILE:HG13	1.86	0.56
1:B:640:ASP:OD1	1:B:647:GLN:NE2	2.39	0.56
1:A:116:LYS:HZ2	1:A:286:GLU:HG3	1.71	0.56
1:D:894:GLY:HA2	1:D:897:LEU:HD23	1.87	0.56
1:C:276:LEU:HG	1:C:285:ILE:HD13	1.87	0.55
1:C:663:GLU:HG2	1:C:701:ALA:HB2	1.88	0.55
1:C:908:ARG:HD2	1:C:930:LYS:HB3	1.88	0.55
1:A:11:GLU:OE2	1:A:82:TYR:OH	2.23	0.55
1:C:52:GLN:OE1	1:C:52:GLN:N	2.36	0.55
1:B:683:GLN:NE2	1:B:687:ASP:OD1	2.40	0.55
1:C:593:ARG:NH2	1:C:599:THR:O	2.38	0.55
1:D:11:GLU:OE2	1:D:82:TYR:OH	2.23	0.55
1:D:284:PHE:HE1	1:D:287:VAL:HG23	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:663:GLU:HG2	1:B:701:ALA:HB2	1.89	0.54
1:B:679:LYS:NZ	1:B:861:GLY:O	2.30	0.54
1:B:319:LEU:HD23	1:B:323:ILE:HD12	1.90	0.54
1:C:236:LYS:O	1:C:341:ARG:NH2	2.40	0.54
1:C:393:VAL:HG21	1:C:410:VAL:HG11	1.90	0.54
1:B:678:PRO:O	1:B:681:ASN:ND2	2.40	0.54
1:C:319:LEU:HD23	1:C:323:ILE:HD12	1.89	0.54
1:B:593:ARG:NH2	1:B:599:THR:O	2.38	0.53
1:D:237:VAL:HG12	1:D:238:ILE:HG13	1.91	0.53
1:B:52:GLN:N	1:B:52:GLN:OE1	2.41	0.53
1:D:852:MET:SD	1:D:855:LYS:NZ	2.81	0.53
1:A:950:LYS:NZ	1:A:961:PRO:O	2.41	0.53
1:A:842:LEU:HA	1:A:845:ARG:HH12	1.74	0.52
1:A:887:GLU:O	1:A:891:TYR:HB2	2.09	0.52
1:D:663:GLU:HG2	1:D:701:ALA:HB2	1.91	0.52
1:D:1:MET:HG3	1:D:76:ASP:HB2	1.91	0.52
1:A:68:ARG:NH1	1:A:72:GLU:OE2	2.42	0.52
1:A:237:VAL:HG12	1:A:238:ILE:HG13	1.91	0.52
1:C:637:ARG:HA	1:C:663:GLU:HB3	1.92	0.52
1:A:313:ILE:HD11	1:A:319:LEU:HD21	1.90	0.52
1:C:80:PRO:HB2	1:C:86:SER:HA	1.91	0.52
1:C:852:MET:HG2	1:C:881:ILE:HG23	1.92	0.52
1:A:203:GLU:O	1:A:278:LYS:NZ	2.39	0.51
1:B:152:TYR:HD1	1:B:153:PRO:HA	1.74	0.51
1:D:637:ARG:HA	1:D:663:GLU:HB3	1.93	0.51
1:A:679:LYS:NZ	1:A:861:GLY:O	2.34	0.51
1:A:742:ILE:HD13	1:D:777:ALA:HB1	1.92	0.51
1:B:313:ILE:HD11	1:B:319:LEU:HD21	1.91	0.51
1:C:645:LEU:HD22	1:C:691:GLU:HB3	1.91	0.51
1:B:206:LYS:NZ	1:B:440:ALA:O	2.41	0.51
1:C:886:THR:OG1	1:C:887:GLU:N	2.42	0.51
1:A:357:LYS:NZ	1:A:379:GLY:O	2.44	0.51
1:A:730:HIS:NE2	1:A:756:ASP:OD1	2.43	0.51
1:B:919:PRO:HB2	1:B:922:LEU:HB3	1.93	0.51
1:D:583:GLU:HB3	1:D:990:THR:HB	1.93	0.51
1:D:950:LYS:NZ	1:D:960:GLU:OE2	2.39	0.51
1:A:233:ARG:NH2	1:A:446:ASP:OD1	2.41	0.50
1:C:373:VAL:HG23	1:C:391:VAL:HB	1.93	0.50
1:B:893:ARG:HH21	1:B:896:GLU:HB2	1.75	0.50
1:A:236:LYS:O	1:A:341:ARG:NH2	2.44	0.50
1:A:624:PHE:HA	1:A:967:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:847:ASP:HA	1:C:850:LYS:HZ3	1.75	0.50
1:D:144:LEU:HG	1:D:176:MET:HE2	1.94	0.50
1:D:546:LEU:HD13	1:D:588:ARG:HG3	1.92	0.50
1:D:203:GLU:O	1:D:278:LYS:NZ	2.40	0.50
1:C:313:ILE:HD11	1:C:319:LEU:HD21	1.93	0.50
1:C:533:ARG:NH2	1:C:534:ASP:OD2	2.45	0.50
1:D:645:LEU:HD22	1:D:691:GLU:HB3	1.94	0.50
1:D:285:ILE:HG22	1:D:286:GLU:HG3	1.94	0.49
1:B:167:MET:HE1	4:B:1203:ADP:H5'1	1.95	0.49
1:B:284:PHE:HE2	1:B:287:VAL:HG23	1.77	0.49
1:A:141:ASP:HA	1:A:144:LEU:HD12	1.95	0.49
1:A:663:GLU:HG2	1:A:699:ILE:HB	1.93	0.49
1:C:237:VAL:HG12	1:C:238:ILE:HG13	1.95	0.49
1:B:645:LEU:HD13	1:B:692:LEU:HD23	1.95	0.48
1:C:656:ARG:NH1	1:C:696:GLY:O	2.46	0.48
1:D:886:THR:H	1:D:889:ASP:HB2	1.78	0.48
1:A:89:LEU:HA	1:A:110:LEU:HD23	1.94	0.48
1:B:138:VAL:O	1:B:180:TYR:OH	2.31	0.48
1:C:22:GLU:OE1	1:C:308:GLN:NE2	2.46	0.48
1:B:590:ARG:HH12	1:B:964:HIS:CE1	2.31	0.48
1:A:586:TRP:CD2	1:A:964:HIS:HB2	2.49	0.48
1:B:637:ARG:HA	1:B:663:GLU:HB3	1.94	0.48
1:A:15:ARG:NH2	1:A:305:ASP:OD1	2.41	0.48
1:B:407:MET:HA	1:B:410:VAL:HG22	1.96	0.48
1:D:856:VAL:HG12	1:D:873:VAL:HG13	1.96	0.48
1:C:1051:GLN:O	1:C:1054:GLN:NE2	2.46	0.48
1:D:296:THR:OG1	1:D:394:CYS:SG	2.70	0.48
1:A:683:GLN:NE2	1:A:687:ASP:OD1	2.44	0.48
1:A:767:SER:OG	1:A:768:GLN:N	2.47	0.48
1:B:687:ASP:HA	1:B:690:LYS:HE3	1.96	0.48
1:C:15:ARG:NH2	1:C:305:ASP:OD1	2.38	0.47
1:D:206:LYS:NZ	1:D:440:ALA:O	2.45	0.47
1:B:586:TRP:CD2	1:B:964:HIS:HB2	2.49	0.47
1:C:908:ARG:HA	1:C:932:VAL:HG12	1.96	0.47
1:A:656:ARG:NH1	1:A:696:GLY:O	2.46	0.47
1:A:926:ILE:HG22	1:A:927:VAL:HG13	1.96	0.47
1:D:63:ILE:HG23	1:D:91:PHE:HD1	1.80	0.47
1:C:978:ASP:OD1	1:C:981:LYS:NZ	2.47	0.47
1:A:105:PRO:HA	1:A:268:VAL:HG13	1.97	0.47
1:A:373:VAL:HG23	1:A:391:VAL:HB	1.96	0.47
1:C:11:GLU:OE2	1:C:82:TYR:OH	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:603:MET:HG2	1:C:633:ILE:HG21	1.97	0.47
1:D:586:TRP:CD2	1:D:964:HIS:HB2	2.49	0.47
1:D:672:ILE:HB	1:D:682:ILE:HG13	1.96	0.47
1:A:145:GLU:O	1:A:149:THR:OG1	2.17	0.47
1:A:894:GLY:HA2	1:A:897:LEU:HD13	1.96	0.47
1:B:548:ASP:OD2	1:B:806:TYR:OH	2.27	0.47
1:C:767:SER:OG	1:C:768:GLN:N	2.48	0.46
1:A:112:ILE:HA	1:A:118:LYS:HD2	1.97	0.46
1:A:128:VAL:HG21	1:A:261:LEU:HB2	1.97	0.46
1:D:610:ALA:HB3	1:D:971:MET:HE1	1.97	0.46
1:A:135:ASN:OD1	1:A:135:ASN:N	2.49	0.46
1:A:305:ASP:HB3	1:A:308:GLN:HB2	1.97	0.46
1:B:499:LYS:HB3	1:B:499:LYS:HE3	1.65	0.46
1:C:586:TRP:CD2	1:C:964:HIS:HB2	2.50	0.46
1:D:15:ARG:NH2	1:D:299:GLU:OE2	2.41	0.46
1:D:683:GLN:NE2	1:D:687:ASP:OD1	2.48	0.46
1:D:296:THR:OG1	1:D:339:GLN:OE1	2.33	0.46
1:B:656:ARG:NH1	1:B:696:GLY:O	2.49	0.46
1:D:4:LEU:HD21	1:D:79:HIS:HB2	1.98	0.46
1:B:645:LEU:HD22	1:B:691:GLU:HB3	1.97	0.46
1:C:894:GLY:HA2	1:C:897:LEU:HD12	1.98	0.46
1:D:402:ASP:HA	1:D:405:ARG:HE	1.80	0.46
1:D:520:LYS:NZ	1:D:726:ASP:O	2.49	0.46
1:D:319:LEU:HA	1:D:323:ILE:HD12	1.98	0.46
1:C:867:THR:OG1	6:C:1206:PYR:O	2.32	0.46
1:D:645:LEU:HD13	1:D:692:LEU:HD23	1.97	0.46
1:A:680:TYR:OH	1:A:862:ASP:O	2.29	0.45
1:D:52:GLN:OE1	1:D:52:GLN:N	2.35	0.45
1:D:0:HIS:O	1:D:2:LYS:NZ	2.49	0.45
1:D:876:MET:HB2	1:D:903:VAL:HG21	1.98	0.45
1:B:140:ILE:HD11	1:B:177:HIS:HD2	1.82	0.45
1:B:767:SER:OG	1:B:768:GLN:N	2.50	0.45
1:A:4:LEU:HD21	1:A:79:HIS:HB2	1.99	0.45
1:C:4:LEU:HD21	1:C:79:HIS:HB2	1.99	0.45
1:B:276:LEU:HG	1:B:285:ILE:HD11	1.97	0.45
1:B:849:ILE:HG12	1:B:881:ILE:HG12	1.98	0.45
1:B:1034:VAL:HG22	1:B:1047:VAL:HG22	1.99	0.45
1:D:220:ILE:HG22	1:D:259:VAL:HG23	1.99	0.45
1:D:767:SER:OG	1:D:768:GLN:N	2.50	0.45
1:A:163:GLY:N	4:A:1203:ADP:O3B	2.50	0.45
1:C:319:LEU:HD22	1:C:325:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:MET:HG2	1:C:157:LYS:HG3	1.99	0.45
5:C:1205:ACO:H2B	5:C:1205:ACO:H8A	1.63	0.45
1:A:231:GLN:OE1	4:A:1203:ADP:O3'	2.34	0.45
1:A:791:ASN:O	1:A:795:ILE:HG12	2.17	0.44
1:A:991:LEU:HD13	1:A:1011:ILE:HA	1.99	0.44
1:D:148:LYS:NZ	1:D:173:ASP:OD1	2.51	0.44
1:D:276:LEU:HB2	1:D:285:ILE:HD11	1.99	0.44
5:D:1205:ACO:H8A	5:D:1205:ACO:H2B	1.66	0.44
1:B:650:LYS:NZ	1:B:650:LYS:H	2.15	0.44
1:C:791:ASN:O	1:C:795:ILE:HG12	2.17	0.44
1:D:240:ILE:HG22	1:D:338:ILE:HG12	1.98	0.44
1:B:465:LEU:O	1:B:469:SER:OG	2.35	0.44
1:D:171:ARG:N	1:D:175:GLU:OE1	2.42	0.44
1:A:856:VAL:HG12	1:A:873:VAL:HG13	1.99	0.44
1:D:156:ILE:HG13	1:D:198:VAL:HG22	1.99	0.44
1:D:935:ASP:OD1	1:D:935:ASP:N	2.51	0.44
1:A:866:VAL:O	1:A:869:SER:N	2.50	0.44
1:D:465:LEU:O	1:D:469:SER:OG	2.34	0.44
5:B:1205:ACO:H8A	5:B:1205:ACO:H2B	1.68	0.44
1:D:305:ASP:HB3	1:D:308:GLN:HB2	1.99	0.44
1:A:89:LEU:HD22	1:A:111:ASP:HB3	1.99	0.44
1:A:256:GLU:HA	1:A:259:VAL:HG12	2.00	0.44
1:D:273:VAL:HG22	1:D:287:VAL:HG22	2.00	0.44
1:D:184:LYS:O	1:D:188:ILE:HG12	2.18	0.43
1:B:184:LYS:NZ	1:B:194:GLY:O	2.39	0.43
1:B:209:GLU:HG2	1:B:274:GLU:HG2	2.00	0.43
1:A:650:LYS:HA	1:A:650:LYS:HD3	1.73	0.43
1:C:1001:MET:HE2	1:C:1001:MET:HB3	1.78	0.43
1:B:168:ARG:HH11	1:B:168:ARG:HB2	1.84	0.43
1:D:591:LYS:HD2	1:D:594:LYS:HZ3	1.83	0.43
1:D:603:MET:HE3	1:D:603:MET:HB2	1.95	0.43
1:D:718:ILE:HD12	1:D:729:ILE:HG21	2.00	0.43
1:A:184:LYS:HD3	1:A:184:LYS:HA	1.87	0.43
1:B:141:ASP:HA	1:B:144:LEU:HD12	1.99	0.43
1:C:128:VAL:HG21	1:C:261:LEU:HB2	1.99	0.43
1:D:159:ALA:HB3	1:D:195:GLU:HB2	2.01	0.43
1:A:227:ASP:HB3	1:A:240:ILE:HG13	2.00	0.43
1:A:317:LYS:HB3	1:A:322:GLU:HB2	1.99	0.43
1:B:333:LEU:HD12	1:B:333:LEU:HA	1.82	0.43
1:C:281:LYS:HB3	1:C:281:LYS:HE2	1.86	0.43
1:D:269:ASN:ND2	1:D:310:GLN:HG2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:893:ARG:NH1	1:D:896:GLU:OE1	2.52	0.43
1:D:656:ARG:NH1	1:D:696:GLY:O	2.51	0.43
1:A:523:LYS:HD3	1:A:523:LYS:HA	1.81	0.43
1:A:664:ALA:HB1	1:A:692:LEU:HD22	2.01	0.43
1:B:80:PRO:HB2	1:B:86:SER:HA	2.00	0.43
1:D:6:VAL:HG11	1:D:13:ALA:HA	2.00	0.43
1:A:334:LEU:HD22	1:C:334:LEU:HD22	2.00	0.43
1:B:326:PRO:HG2	1:B:331:ILE:HD13	2.00	0.43
1:C:155:MET:HE3	1:C:155:MET:HB2	1.79	0.43
1:D:866:VAL:O	1:D:869:SER:N	2.52	0.43
1:B:112:ILE:HA	1:B:118:LYS:HD2	2.02	0.42
1:C:170:ALA:HA	1:C:175:GLU:HG2	2.01	0.42
1:A:637:ARG:HA	1:A:663:GLU:HB2	2.00	0.42
1:C:166:GLY:HA2	1:C:186:GLU:OE1	2.19	0.42
1:C:645:LEU:HD13	1:C:692:LEU:HD23	2.01	0.42
1:D:221:ILE:HG12	1:D:319:LEU:HD21	2.00	0.42
1:B:777:ALA:HB1	1:C:742:ILE:HD13	2.02	0.42
1:A:319:LEU:HD22	1:A:325:LEU:HD12	2.02	0.42
1:B:157:LYS:HG2	1:B:167:MET:HG3	2.00	0.42
1:D:262:CYS:HA	1:D:265:VAL:HG22	2.01	0.42
1:B:305:ASP:HB3	1:B:308:GLN:HB2	2.01	0.42
1:C:167:MET:HE1	4:C:1203:ADP:O4'	2.19	0.42
1:D:255:CYS:O	1:D:259:VAL:HG12	2.18	0.42
1:D:991:LEU:HD13	1:D:1011:ILE:HA	2.01	0.42
1:B:852:MET:HE3	1:B:852:MET:HA	2.01	0.42
1:A:872:VAL:HG13	1:A:903:VAL:HA	1.99	0.42
1:B:856:VAL:HG12	1:B:873:VAL:HG13	2.01	0.42
1:A:41:ARG:O	1:A:47:SER:OG	2.31	0.42
1:B:215:ASP:HB3	1:B:319:LEU:HG	2.02	0.42
1:B:646:PRO:O	1:B:650:LYS:NZ	2.38	0.42
1:A:583:GLU:HB3	1:A:990:THR:HB	2.00	0.42
1:B:4:LEU:HD21	1:B:79:HIS:HB2	2.02	0.42
1:B:846:PHE:HA	1:B:849:ILE:HB	2.01	0.42
1:C:971:MET:HE3	1:C:971:MET:HB3	1.87	0.42
1:A:465:LEU:HB3	1:A:1046:VAL:HG21	2.02	0.42
1:A:533:ARG:NH2	1:A:534:ASP:OD2	2.53	0.42
1:A:853:TYR:HE1	1:A:865:LYS:HD2	1.84	0.42
1:C:415:ARG:HD3	1:C:415:ARG:HA	1.93	0.42
1:A:167:MET:HE1	4:A:1203:ADP:H5'1	2.02	0.41
1:A:184:LYS:NZ	1:A:194:GLY:O	2.53	0.41
1:A:623:GLU:HG3	1:A:967:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:ARG:HD3	1:B:415:ARG:HA	1.96	0.41
1:B:672:ILE:HB	1:B:682:ILE:HG13	2.02	0.41
1:C:6:VAL:HG11	1:C:13:ALA:HA	2.01	0.41
1:A:301:ILE:HG13	1:A:302:THR:HG23	2.03	0.41
1:B:825:MET:HG2	1:B:853:TYR:CE1	2.54	0.41
1:C:290:ARG:NH1	1:C:292:GLN:OE1	2.54	0.41
1:A:214:GLY:O	1:A:269:ASN:N	2.47	0.41
1:C:331:ILE:HA	1:C:332:PRO:HD3	1.94	0.41
1:C:465:LEU:HB3	1:C:1046:VAL:HG21	2.02	0.41
1:A:209:GLU:OE2	1:A:236:LYS:NZ	2.48	0.41
1:B:214:GLY:O	1:B:269:ASN:N	2.48	0.41
1:C:523:LYS:HA	1:C:523:LYS:HD3	1.80	0.41
1:D:835:SER:OG	1:D:836:GLN:NE2	2.53	0.41
1:A:213:LEU:HD23	1:A:213:LEU:HA	1.94	0.41
1:A:240:ILE:HG22	1:A:338:ILE:HG12	2.02	0.41
1:A:276:LEU:HD23	1:A:276:LEU:HA	1.90	0.41
1:A:823:HIS:CD2	1:A:850:LYS:HD2	2.55	0.41
1:B:22:GLU:OE1	1:B:308:GLN:NE2	2.49	0.41
1:B:532:LEU:O	1:B:536:HIS:NE2	2.47	0.41
1:C:583:GLU:HB3	1:C:990:THR:HB	2.01	0.41
1:D:499:LYS:HB3	1:D:499:LYS:HE3	1.76	0.41
1:D:523:LYS:HA	1:D:523:LYS:HD3	1.86	0.41
1:D:557:ASP:HB2	1:D:596:MET:HG2	2.03	0.41
1:A:116:LYS:HD3	1:A:119:ALA:HB3	2.01	0.41
1:A:333:LEU:HD12	1:A:333:LEU:HA	1.86	0.41
1:C:889:ASP:O	1:C:893:ARG:HB3	2.21	0.41
1:D:145:GLU:O	1:D:149:THR:HG22	2.21	0.41
1:D:364:PRO:HG3	1:D:410:VAL:HG13	2.01	0.41
1:D:532:LEU:O	1:D:536:HIS:NE2	2.48	0.41
1:A:171:ARG:N	1:A:175:GLU:OE1	2.54	0.41
1:A:722:LYS:HD2	1:A:722:LYS:HA	1.81	0.41
1:C:273:VAL:HG22	1:C:287:VAL:HG22	2.02	0.41
1:C:557:ASP:HB2	1:C:596:MET:HG2	2.02	0.41
1:C:615:ASN:OD1	1:C:616:TYR:N	2.54	0.41
1:D:1025:GLY:O	1:D:1033:ARG:NH1	2.54	0.41
1:A:6:VAL:HG11	1:A:13:ALA:HA	2.02	0.41
1:A:446:ASP:OD1	1:A:446:ASP:N	2.53	0.41
1:C:476:PHE:HB3	1:C:479:ILE:HG12	2.02	0.41
1:C:305:ASP:HB3	1:C:308:GLN:HB2	2.03	0.40
1:C:446:ASP:OD1	1:C:446:ASP:N	2.54	0.40
1:D:263:LYS:HB2	1:D:263:LYS:HE2	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:853:TYR:HE1	1:B:865:LYS:HD2	1.86	0.40
1:C:145:GLU:O	1:C:149:THR:HG23	2.21	0.40
1:B:118:LYS:HE3	1:B:118:LYS:HB2	1.85	0.40
1:B:967:ILE:O	1:B:971:MET:HG2	2.21	0.40
1:C:178:ASP:HA	1:C:182:ARG:NH2	2.35	0.40
1:D:173:ASP:O	1:D:177:HIS:ND1	2.55	0.40
1:A:596:MET:HB3	1:A:599:THR:HB	2.04	0.40
1:C:214:GLY:O	1:C:269:ASN:N	2.50	0.40
1:C:852:MET:HB3	1:C:877:ALA:HB1	2.03	0.40
1:A:116:LYS:HD3	1:A:116:LYS:HA	1.81	0.40
1:A:672:ILE:HB	1:A:682:ILE:HG13	2.02	0.40
1:A:820:VAL:HA	1:A:823:HIS:CE1	2.56	0.40
1:B:714:ALA:HB2	1:B:743:THR:HG23	2.04	0.40
1:B:820:VAL:HA	1:B:823:HIS:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1053/1143 (92%)	1025 (97%)	28 (3%)	0	100	100
1	B	1053/1143 (92%)	1031 (98%)	22 (2%)	0	100	100
1	C	1053/1143 (92%)	1030 (98%)	23 (2%)	0	100	100
1	D	1053/1143 (92%)	1027 (98%)	26 (2%)	0	100	100
All	All	4212/4572 (92%)	4113 (98%)	99 (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	883/954 (93%)	874 (99%)	9 (1%)	68	76
1	B	883/954 (93%)	875 (99%)	8 (1%)	70	78
1	C	883/954 (93%)	873 (99%)	10 (1%)	65	74
1	D	883/954 (93%)	869 (98%)	14 (2%)	55	63
All	All	3532/3816 (93%)	3491 (99%)	41 (1%)	61	71

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	GLU
1	A	391	VAL
1	A	482	THR
1	A	509	GLU
1	A	569	TRP
1	A	858	MET
1	A	929	ASP
1	A	960	GLU
1	A	1029	LEU
1	B	72	GLU
1	B	140	ILE
1	B	233	ARG
1	B	391	VAL
1	B	469	SER
1	B	509	GLU
1	B	569	TRP
1	B	1029	LEU
1	C	72	GLU
1	C	182	ARG
1	C	285	ILE
1	C	391	VAL
1	C	393	VAL
1	C	509	GLU
1	C	569	TRP

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Mol	Chain	Res	Type
1	C	736	THR
1	C	840	VAL
1	C	967	ILE
1	D	140	ILE
1	D	276	LEU
1	D	334	LEU
1	D	391	VAL
1	D	469	SER
1	D	482	THR
1	D	494	LEU
1	D	569	TRP
1	D	691	GLU
1	D	705	MET
1	D	882	GLN
1	D	920	GLU
1	D	948	THR
1	D	1029	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	ASN
1	A	547	GLN
1	A	609	ASN
1	A	653	GLN
1	A	882	GLN
1	A	913	GLN
1	A	983	GLN
1	A	1032	ASN
1	B	217	HIS
1	B	264	ASN
1	B	288	ASN
1	B	547	GLN
1	B	582	ASN
1	B	609	ASN
1	B	647	GLN
1	B	794	GLN
1	B	836	GLN
1	C	235	GLN
1	C	288	ASN
1	C	310	GLN
1	C	547	GLN

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Mol	Chain	Res	Type
1	C	609	ASN
1	C	614	GLN
1	C	653	GLN
1	C	683	GLN
1	C	794	GLN
1	C	817	GLN
1	C	955	GLN
1	D	108	HIS
1	D	217	HIS
1	D	447	ASN
1	D	630	HIS
1	D	653	GLN

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	KCX	D	703	3,1	10,11,12	0.86	0	6,12,14	1.41	1 (16%)
1	KCX	A	703	3,1	10,11,12	0.86	0	6,12,14	1.55	1 (16%)
1	KCX	B	703	3,1	10,11,12	0.85	0	6,12,14	1.55	1 (16%)
1	KCX	C	703	3,1	10,11,12	0.84	0	6,12,14	1.49	1 (16%)

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	KCX	D	703	3,1	-	0/9/10/12	-
1	KCX	A	703	3,1	-	5/9/10/12	-
1	KCX	B	703	3,1	-	0/9/10/12	-
1	KCX	C	703	3,1	-	2/9/10/12	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	703	KCX	OQ1-CX-NZ	-3.63	119.41	124.92
1	B	703	KCX	OQ1-CX-NZ	-3.28	119.94	124.92
1	C	703	KCX	OQ1-CX-NZ	-3.18	120.08	124.92
1	D	703	KCX	OQ1-CX-NZ	-3.12	120.19	124.92

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	703	KCX	N-CA-CB-CG
1	A	703	KCX	C-CA-CB-CG
1	C	703	KCX	O-C-CA-CB
1	A	703	KCX	CA-CB-CG-CD
1	A	703	KCX	CE-CD-CG-CB
1	C	703	KCX	CG-CD-CE-NZ
1	A	703	KCX	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 12 are monoatomic - leaving 16 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
4	ADP	C	1203	2	28,29,29	1.39	4 (14%)	43,45,45	1.89	10 (23%)
7	BCT	A	1207	-	3,3,3	1.12	0	2,3,3	4.26	2 (100%)
7	BCT	D	1207	-	3,3,3	1.10	0	2,3,3	4.13	2 (100%)
5	ACO	D	1205	-	51,53,53	2.63	20 (39%)	73,79,79	2.80	21 (28%)
4	ADP	A	1203	2	28,29,29	1.38	4 (14%)	43,45,45	1.83	11 (25%)
4	ADP	B	1203	2	28,29,29	1.42	4 (14%)	43,45,45	1.84	9 (20%)
5	ACO	A	1205	-	51,53,53	2.64	19 (37%)	73,79,79	2.79	22 (30%)
5	ACO	C	1205	-	51,53,53	2.64	19 (37%)	73,79,79	2.83	20 (27%)
6	PYR	B	1206	-	5,5,5	3.01	3 (60%)	3,6,6	1.63	1 (33%)
6	PYR	D	1206	-	5,5,5	3.04	3 (60%)	3,6,6	1.63	1 (33%)
7	BCT	C	1207	-	3,3,3	3.23	1 (33%)	2,3,3	2.73	2 (100%)
6	PYR	C	1206	-	5,5,5	3.01	3 (60%)	3,6,6	1.68	1 (33%)
4	ADP	D	1203	2	28,29,29	1.40	4 (14%)	43,45,45	1.86	9 (20%)
6	PYR	A	1206	-	5,5,5	3.03	3 (60%)	3,6,6	1.61	1 (33%)
5	ACO	B	1205	-	51,53,53	2.62	20 (39%)	73,79,79	2.81	19 (26%)
7	BCT	B	1207	-	3,3,3	1.11	0	2,3,3	4.31	2 (100%)

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
4	ADP	C	1203	2	-	6/16/32/32	0/3/3/3
5	ACO	D	1205	-	-	13/51/67/67	0/3/3/3
4	ADP	A	1203	2	-	5/16/32/32	0/3/3/3
4	ADP	B	1203	2	-	6/16/32/32	0/3/3/3
5	ACO	A	1205	-	-	14/51/67/67	0/3/3/3
5	ACO	C	1205	-	-	9/51/67/67	0/3/3/3
6	PYR	B	1206	-	-	3/4/4/4	-
6	PYR	D	1206	-	-	1/4/4/4	-
6	PYR	C	1206	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	D	1203	2	-	3/16/32/32	0/3/3/3
6	PYR	A	1206	-	-	1/4/4/4	-
5	ACO	B	1205	-	-	10/51/67/67	0/3/3/3

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1205	ACO	C5A-N7A	7.10	1.52	1.39
5	A	1205	ACO	C5A-N7A	7.09	1.52	1.39
5	D	1205	ACO	C5A-N7A	7.05	1.52	1.39
5	B	1205	ACO	C5A-N7A	6.98	1.51	1.39
5	B	1205	ACO	C8A-N9A	-6.04	1.27	1.37
5	D	1205	ACO	C8A-N9A	-6.03	1.27	1.37
5	A	1205	ACO	C8A-N9A	-6.01	1.27	1.37
5	C	1205	ACO	C8A-N9A	-5.98	1.27	1.37
7	C	1207	BCT	O1-C	5.30	1.44	1.25
5	D	1205	ACO	C9P-N8P	5.14	1.45	1.33
5	A	1205	ACO	C5P-N4P	5.13	1.45	1.33
5	A	1205	ACO	C9P-N8P	5.13	1.45	1.33
5	C	1205	ACO	P1A-O3A	5.10	1.65	1.59
5	D	1205	ACO	C5P-N4P	5.09	1.45	1.33
5	B	1205	ACO	C5P-N4P	5.07	1.45	1.33
5	C	1205	ACO	P2A-O3A	5.03	1.64	1.59
5	C	1205	ACO	C5P-N4P	5.00	1.45	1.33
5	C	1205	ACO	C9P-N8P	4.99	1.45	1.33
5	B	1205	ACO	C9P-N8P	4.97	1.45	1.33
5	A	1205	ACO	P1A-O3A	4.89	1.64	1.59
5	D	1205	ACO	P1A-O3A	4.81	1.64	1.59
5	B	1205	ACO	P2A-O3A	4.80	1.64	1.59
5	A	1205	ACO	P2A-O3A	4.73	1.64	1.59
5	D	1205	ACO	P2A-O3A	4.71	1.64	1.59
5	B	1205	ACO	P1A-O3A	4.71	1.64	1.59
4	D	1203	ADP	C5-C4	4.67	1.47	1.39
5	B	1205	ACO	C4A-N9A	-4.62	1.28	1.37
5	D	1205	ACO	C4A-N9A	-4.61	1.28	1.37
5	A	1205	ACO	C4A-N9A	-4.60	1.28	1.37
5	C	1205	ACO	C4A-N9A	-4.60	1.28	1.37
4	A	1203	ADP	C5-C4	4.55	1.47	1.39
4	B	1203	ADP	C5-C4	4.55	1.47	1.39
6	A	1206	PYR	CA-C	-4.55	1.39	1.54
4	C	1203	ADP	C5-C4	4.53	1.47	1.39
6	D	1206	PYR	CA-C	-4.52	1.39	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1206	PYR	CA-C	-4.50	1.39	1.54
6	B	1206	PYR	CA-C	-4.49	1.39	1.54
5	D	1205	ACO	O4B-C1B	4.44	1.52	1.42
5	A	1205	ACO	O4B-C1B	4.42	1.52	1.42
5	C	1205	ACO	O4B-C1B	4.40	1.52	1.42
5	B	1205	ACO	O4B-C1B	4.39	1.52	1.42
5	C	1205	ACO	C6A-N6A	4.35	1.45	1.34
5	A	1205	ACO	C6A-N6A	4.30	1.45	1.34
5	B	1205	ACO	C6A-N6A	4.27	1.45	1.34
5	D	1205	ACO	C6A-N6A	4.25	1.45	1.34
5	A	1205	ACO	C2B-C3B	-3.83	1.44	1.53
5	B	1205	ACO	C2B-C3B	-3.83	1.44	1.53
5	D	1205	ACO	C2B-C3B	-3.83	1.44	1.53
5	C	1205	ACO	C2B-C3B	-3.77	1.44	1.53
6	D	1206	PYR	O3-CA	3.59	1.31	1.23
6	B	1206	PYR	O3-CA	3.58	1.31	1.23
6	D	1206	PYR	O-C	3.57	1.31	1.22
6	A	1206	PYR	O3-CA	3.56	1.31	1.23
6	C	1206	PYR	O3-CA	3.55	1.31	1.23
6	C	1206	PYR	O-C	3.54	1.31	1.22
6	A	1206	PYR	O-C	3.51	1.31	1.22
6	B	1206	PYR	O-C	3.51	1.31	1.22
5	A	1205	ACO	O4B-C4B	3.34	1.52	1.45
5	D	1205	ACO	O4B-C4B	3.31	1.52	1.45
5	B	1205	ACO	O4B-C4B	3.29	1.52	1.45
5	C	1205	ACO	O4B-C4B	3.29	1.52	1.45
5	C	1205	ACO	P3B-O3B	2.81	1.64	1.59
5	D	1205	ACO	P3B-O3B	2.81	1.64	1.59
5	A	1205	ACO	P3B-O3B	2.80	1.64	1.59
4	B	1203	ADP	C5-C6	2.71	1.48	1.41
5	B	1205	ACO	P3B-O3B	2.70	1.64	1.59
4	D	1203	ADP	C5-C6	2.66	1.48	1.41
4	A	1203	ADP	C5-C6	2.64	1.48	1.41
4	C	1203	ADP	C5-C6	2.63	1.48	1.41
5	A	1205	ACO	O9P-C9P	-2.47	1.18	1.23
5	D	1205	ACO	O9P-C9P	-2.47	1.18	1.23
5	C	1205	ACO	O9P-C9P	-2.42	1.18	1.23
5	B	1205	ACO	P3B-O8A	-2.40	1.45	1.54
5	B	1205	ACO	O9P-C9P	-2.39	1.18	1.23
5	C	1205	ACO	P3B-O9A	-2.38	1.45	1.54
5	A	1205	ACO	P3B-O9A	-2.38	1.45	1.54
5	D	1205	ACO	P3B-O8A	-2.37	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1203	ADP	C5-N7	-2.37	1.34	1.39
5	B	1205	ACO	P3B-O9A	-2.36	1.46	1.54
4	D	1203	ADP	C5-N7	-2.36	1.34	1.39
5	A	1205	ACO	O5P-C5P	-2.36	1.18	1.23
4	C	1203	ADP	C5-N7	-2.35	1.34	1.39
5	C	1205	ACO	C8A-N7A	2.34	1.36	1.31
5	C	1205	ACO	P3B-O8A	-2.34	1.46	1.54
5	D	1205	ACO	O5P-C5P	-2.34	1.18	1.23
5	D	1205	ACO	P3B-O9A	-2.33	1.46	1.54
5	A	1205	ACO	P3B-O8A	-2.33	1.46	1.54
5	B	1205	ACO	O5P-C5P	-2.32	1.18	1.23
5	A	1205	ACO	C8A-N7A	2.32	1.36	1.31
4	A	1203	ADP	C5-N7	-2.29	1.34	1.39
4	B	1203	ADP	C8-N7	2.28	1.36	1.31
5	C	1205	ACO	O5P-C5P	-2.28	1.18	1.23
5	D	1205	ACO	C8A-N7A	2.28	1.36	1.31
5	B	1205	ACO	C8A-N7A	2.25	1.36	1.31
4	D	1203	ADP	C8-N7	2.23	1.36	1.31
5	C	1205	ACO	C5A-C4A	2.19	1.43	1.39
5	A	1205	ACO	C5A-C4A	2.19	1.43	1.39
4	A	1203	ADP	C8-N7	2.19	1.35	1.31
5	B	1205	ACO	C5A-C4A	2.18	1.43	1.39
5	D	1205	ACO	C5A-C4A	2.16	1.42	1.39
4	C	1203	ADP	C8-N7	2.14	1.35	1.31
5	C	1205	ACO	P1A-O2A	-2.09	1.45	1.55
5	B	1205	ACO	P2A-O5A	-2.04	1.45	1.55
5	D	1205	ACO	P1A-O2A	-2.02	1.46	1.55
5	B	1205	ACO	P1A-O2A	-2.02	1.46	1.55
5	A	1205	ACO	P1A-O2A	-2.01	1.46	1.55
5	D	1205	ACO	P2A-O5A	-2.00	1.46	1.55

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1205	ACO	C4A-N9A-C8A	15.91	122.44	105.74
5	B	1205	ACO	C4A-N9A-C8A	15.82	122.35	105.74
5	D	1205	ACO	C4A-N9A-C8A	15.76	122.28	105.74
5	A	1205	ACO	C4A-N9A-C8A	15.75	122.28	105.74
5	B	1205	ACO	N3A-C4A-N9A	6.25	137.79	127.17
5	C	1205	ACO	N9A-C8A-N7A	-6.23	105.10	113.94
5	D	1205	ACO	N3A-C4A-N9A	6.21	137.74	127.17
5	C	1205	ACO	N3A-C4A-N9A	6.21	137.73	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1205	ACO	N9A-C8A-N7A	-6.16	105.19	113.94
5	A	1205	ACO	N3A-C4A-N9A	6.10	137.54	127.17
5	A	1205	ACO	N9A-C8A-N7A	-6.08	105.32	113.94
5	D	1205	ACO	N9A-C8A-N7A	-6.05	105.36	113.94
4	C	1203	ADP	C5-C4-N3	-5.88	118.62	126.72
4	D	1203	ADP	C5-C4-N3	-5.87	118.64	126.72
4	B	1203	ADP	C5-C4-N3	-5.84	118.67	126.72
5	C	1205	ACO	C4A-C5A-N7A	-5.69	104.07	110.58
5	B	1205	ACO	C4A-C5A-N7A	-5.69	104.08	110.58
4	A	1203	ADP	C5-C4-N3	-5.68	118.90	126.72
7	B	1207	BCT	O2-C-O1	5.66	134.16	119.68
5	A	1205	ACO	C4A-C5A-N7A	-5.65	104.12	110.58
7	A	1207	BCT	O2-C-O1	5.62	134.05	119.68
5	D	1205	ACO	C4A-C5A-N7A	-5.57	104.21	110.58
7	D	1207	BCT	O2-C-O1	5.42	133.53	119.68
5	B	1205	ACO	C5A-C4A-N3A	-5.20	119.55	126.72
5	C	1205	ACO	C5A-C4A-N3A	-5.16	119.61	126.72
5	D	1205	ACO	C5A-C4A-N3A	-5.14	119.64	126.72
5	A	1205	ACO	C5A-C4A-N3A	-5.05	119.76	126.72
4	C	1203	ADP	N3-C4-N9	4.70	135.16	127.17
4	D	1203	ADP	N3-C4-N9	4.70	135.16	127.17
4	B	1203	ADP	N3-C4-N9	4.64	135.06	127.17
4	A	1203	ADP	N3-C4-N9	4.60	134.99	127.17
5	D	1205	ACO	N3A-C2A-N1A	-4.23	122.18	128.58
5	A	1205	ACO	N3A-C2A-N1A	-4.19	122.24	128.58
5	C	1205	ACO	N3A-C2A-N1A	-4.19	122.25	128.58
5	B	1205	ACO	N3A-C2A-N1A	-4.17	122.26	128.58
4	C	1203	ADP	C2-N3-C4	3.76	121.02	111.83
4	B	1203	ADP	C2-N3-C4	3.76	121.02	111.83
4	D	1203	ADP	C2-N3-C4	3.73	120.94	111.83
4	A	1203	ADP	C2-N3-C4	3.69	120.84	111.83
5	A	1205	ACO	C4B-O4B-C1B	-3.63	101.44	109.47
5	D	1205	ACO	C4B-O4B-C1B	-3.63	101.46	109.47
5	B	1205	ACO	C4B-O4B-C1B	-3.58	101.55	109.47
5	D	1205	ACO	C1B-N9A-C8A	-3.58	119.15	127.09
5	C	1205	ACO	C1B-N9A-C8A	-3.56	119.20	127.09
5	A	1205	ACO	C4A-N9A-C1B	-3.55	118.32	126.63
5	B	1205	ACO	C4A-N9A-C1B	-3.54	118.35	126.63
5	C	1205	ACO	C4A-N9A-C1B	-3.54	118.36	126.63
5	B	1205	ACO	C1B-N9A-C8A	-3.51	119.30	127.09
5	A	1205	ACO	C1B-N9A-C8A	-3.46	119.41	127.09
5	D	1205	ACO	C4A-N9A-C1B	-3.45	118.56	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1205	ACO	C4B-O4B-C1B	-3.37	102.02	109.47
5	D	1205	ACO	C2A-N3A-C4A	3.35	120.01	111.83
4	B	1203	ADP	C4-C5-N7	-3.35	106.75	110.58
5	B	1205	ACO	C2A-N3A-C4A	3.34	119.98	111.83
4	B	1203	ADP	N3-C2-N1	-3.31	123.58	128.58
4	A	1203	ADP	C4-C5-N7	-3.30	106.80	110.58
4	C	1203	ADP	C4-C5-N7	-3.30	106.80	110.58
5	C	1205	ACO	C2A-N3A-C4A	3.30	119.90	111.83
4	A	1203	ADP	N3-C2-N1	-3.30	123.59	128.58
5	A	1205	ACO	C2A-N3A-C4A	3.30	119.89	111.83
4	C	1203	ADP	N3-C2-N1	-3.29	123.60	128.58
4	D	1203	ADP	C4-C5-N7	-3.28	106.83	110.58
4	D	1203	ADP	N3-C2-N1	-3.27	123.63	128.58
7	C	1207	BCT	O2-C-O1	-3.13	111.66	119.68
5	A	1205	ACO	C6A-C5A-N7A	3.02	137.90	132.09
5	B	1205	ACO	C6A-C5A-N7A	2.99	137.86	132.09
5	D	1205	ACO	C6A-C5A-N7A	2.97	137.82	132.09
5	C	1205	ACO	C6A-C5A-N7A	2.96	137.80	132.09
5	D	1205	ACO	C5A-C4A-N9A	-2.93	102.62	105.81
5	B	1205	ACO	C5A-C4A-N9A	-2.90	102.65	105.81
5	C	1205	ACO	C5A-C4A-N9A	-2.89	102.66	105.81
4	B	1203	ADP	C2'-C1'-N9	-2.89	106.12	113.30
5	A	1205	ACO	C5A-C4A-N9A	-2.85	102.71	105.81
4	C	1203	ADP	C2'-C1'-N9	-2.85	106.23	113.30
4	A	1203	ADP	C4-N9-C8	2.79	108.67	105.74
5	A	1205	ACO	C6P-C5P-N4P	2.70	121.26	116.34
4	B	1203	ADP	C4-N9-C8	2.64	108.51	105.74
5	D	1205	ACO	C6P-C5P-N4P	2.55	120.99	116.34
5	C	1205	ACO	O2A-P1A-O1A	-2.54	100.64	112.44
4	D	1203	ADP	C3'-C2'-C1'	2.50	106.19	101.46
4	C	1203	ADP	C4-N9-C8	2.50	108.36	105.74
4	D	1203	ADP	C4-N9-C8	2.50	108.36	105.74
4	A	1203	ADP	C5-N7-C8	2.46	107.32	103.45
4	C	1203	ADP	C3'-C2'-C1'	2.46	106.11	101.46
5	C	1205	ACO	C3B-C2B-C1B	2.45	105.28	99.89
5	A	1205	ACO	CAP-C9P-N8P	2.44	121.11	116.48
4	B	1203	ADP	C5-N7-C8	2.43	107.26	103.45
5	C	1205	ACO	C7P-C6P-C5P	-2.42	108.35	112.39
5	B	1205	ACO	O5A-P2A-O4A	-2.42	101.19	112.44
4	D	1203	ADP	C5-N7-C8	2.42	107.25	103.45
4	C	1203	ADP	C5-N7-C8	2.41	107.24	103.45
5	C	1205	ACO	O5A-P2A-O4A	-2.41	101.25	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1203	ADP	C3'-C2'-C1'	2.39	105.98	101.46
6	C	1206	PYR	OXT-C-CA	2.37	120.16	113.59
5	A	1205	ACO	O2A-P1A-O1A	-2.37	101.43	112.44
5	D	1205	ACO	C7P-C6P-C5P	-2.35	108.47	112.39
5	D	1205	ACO	O2A-P1A-O1A	-2.35	101.52	112.44
5	A	1205	ACO	O5A-P2A-O4A	-2.35	101.53	112.44
5	D	1205	ACO	CAP-C9P-N8P	2.34	120.92	116.48
5	B	1205	ACO	O2A-P1A-O1A	-2.33	101.59	112.44
5	D	1205	ACO	O5A-P2A-O4A	-2.33	101.62	112.44
5	B	1205	ACO	O9A-P3B-O3B	2.33	114.91	105.85
5	C	1205	ACO	O8A-P3B-O3B	2.32	114.88	105.85
4	D	1203	ADP	C2'-C1'-N9	-2.31	107.56	113.30
6	D	1206	PYR	OXT-C-CA	2.30	119.97	113.59
5	D	1205	ACO	O9A-P3B-O3B	2.30	114.79	105.85
4	A	1203	ADP	C2'-C1'-N9	-2.29	107.61	113.30
6	A	1206	PYR	OXT-C-CA	2.26	119.87	113.59
7	C	1207	BCT	O3-C-O1	-2.26	113.89	119.68
7	B	1207	BCT	O3-C-O1	-2.26	113.90	119.68
6	B	1206	PYR	OXT-C-CA	2.26	119.85	113.59
5	B	1205	ACO	CAP-C9P-N8P	2.26	120.76	116.48
5	A	1205	ACO	O8A-P3B-O3B	2.24	114.58	105.85
5	B	1205	ACO	C7P-C6P-C5P	-2.23	108.67	112.39
5	D	1205	ACO	C3B-C2B-C1B	2.22	104.78	99.89
5	A	1205	ACO	O5P-C5P-N4P	-2.22	118.67	123.03
7	D	1207	BCT	O3-C-O1	-2.18	114.09	119.68
5	A	1205	ACO	C7P-C6P-C5P	-2.17	108.78	112.39
7	A	1207	BCT	O3-C-O1	-2.16	114.16	119.68
5	C	1205	ACO	C2B-C3B-C4B	2.15	107.00	103.24
5	D	1205	ACO	C2P-S1P-C	2.13	111.65	101.42
4	A	1203	ADP	C6-C5-N7	2.08	136.11	132.09
4	B	1203	ADP	C6-C5-N7	2.08	136.11	132.09
5	A	1205	ACO	C3B-C2B-C1B	2.08	104.45	99.89
5	D	1205	ACO	O5P-C5P-N4P	-2.07	118.97	123.03
5	C	1205	ACO	C6P-C5P-N4P	2.03	120.05	116.34
5	B	1205	ACO	O9P-C9P-N8P	-2.03	118.68	122.98
5	C	1205	ACO	O6A-CCP-CBP	-2.02	107.30	110.55
5	B	1205	ACO	C6P-C5P-N4P	2.01	120.01	116.34
4	C	1203	ADP	C6-C5-N7	2.01	135.96	132.09
4	A	1203	ADP	N9-C8-N7	-2.01	111.09	113.94
5	A	1205	ACO	C2P-S1P-C	2.00	111.06	101.42
5	A	1205	ACO	C2B-C3B-C4B	2.00	106.74	103.24

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1203	ADP	C5'-O5'-PA-O1A
4	A	1203	ADP	C5'-O5'-PA-O2A
4	B	1203	ADP	C5'-O5'-PA-O3A
4	C	1203	ADP	C5'-O5'-PA-O2A
4	C	1203	ADP	O4'-C4'-C5'-O5'
4	D	1203	ADP	C5'-O5'-PA-O2A
4	D	1203	ADP	C5'-O5'-PA-O3A
5	A	1205	ACO	N8P-C9P-CAP-OAP
5	A	1205	ACO	C3P-C2P-S1P-C
5	C	1205	ACO	C3P-C2P-S1P-C
5	D	1205	ACO	N8P-C9P-CAP-OAP
5	D	1205	ACO	C3P-C2P-S1P-C
6	D	1206	PYR	OXT-C-CA-CB
5	A	1205	ACO	C6P-C5P-N4P-C3P
5	D	1205	ACO	C6P-C5P-N4P-C3P
4	C	1203	ADP	C3'-C4'-C5'-O5'
5	A	1205	ACO	O5P-C5P-N4P-C3P
5	D	1205	ACO	O5P-C5P-N4P-C3P
5	A	1205	ACO	S1P-C2P-C3P-N4P
4	A	1203	ADP	O4'-C4'-C5'-O5'
5	B	1205	ACO	C2B-C1B-N9A-C8A
5	A	1205	ACO	O9P-C9P-CAP-OAP
5	D	1205	ACO	O9P-C9P-CAP-OAP
5	A	1205	ACO	C2B-C1B-N9A-C8A
5	C	1205	ACO	C2B-C1B-N9A-C8A
5	D	1205	ACO	C2B-C1B-N9A-C8A
4	A	1203	ADP	C3'-C4'-C5'-O5'
5	D	1205	ACO	S1P-C2P-C3P-N4P
5	B	1205	ACO	N8P-C9P-CAP-OAP
5	C	1205	ACO	N8P-C9P-CAP-OAP
4	B	1203	ADP	PB-O3A-PA-O2A
5	B	1205	ACO	O9P-C9P-CAP-OAP
5	C	1205	ACO	O9P-C9P-CAP-OAP
5	A	1205	ACO	CDP-CBP-CCP-O6A
5	A	1205	ACO	CEP-CBP-CCP-O6A
5	B	1205	ACO	CDP-CBP-CCP-O6A
5	B	1205	ACO	C3P-C2P-S1P-C
5	D	1205	ACO	O-C-S1P-C2P
5	B	1205	ACO	C2B-C1B-N9A-C4A
4	A	1203	ADP	C5'-O5'-PA-O3A
4	B	1203	ADP	C5'-O5'-PA-O1A
4	C	1203	ADP	C5'-O5'-PA-O1A

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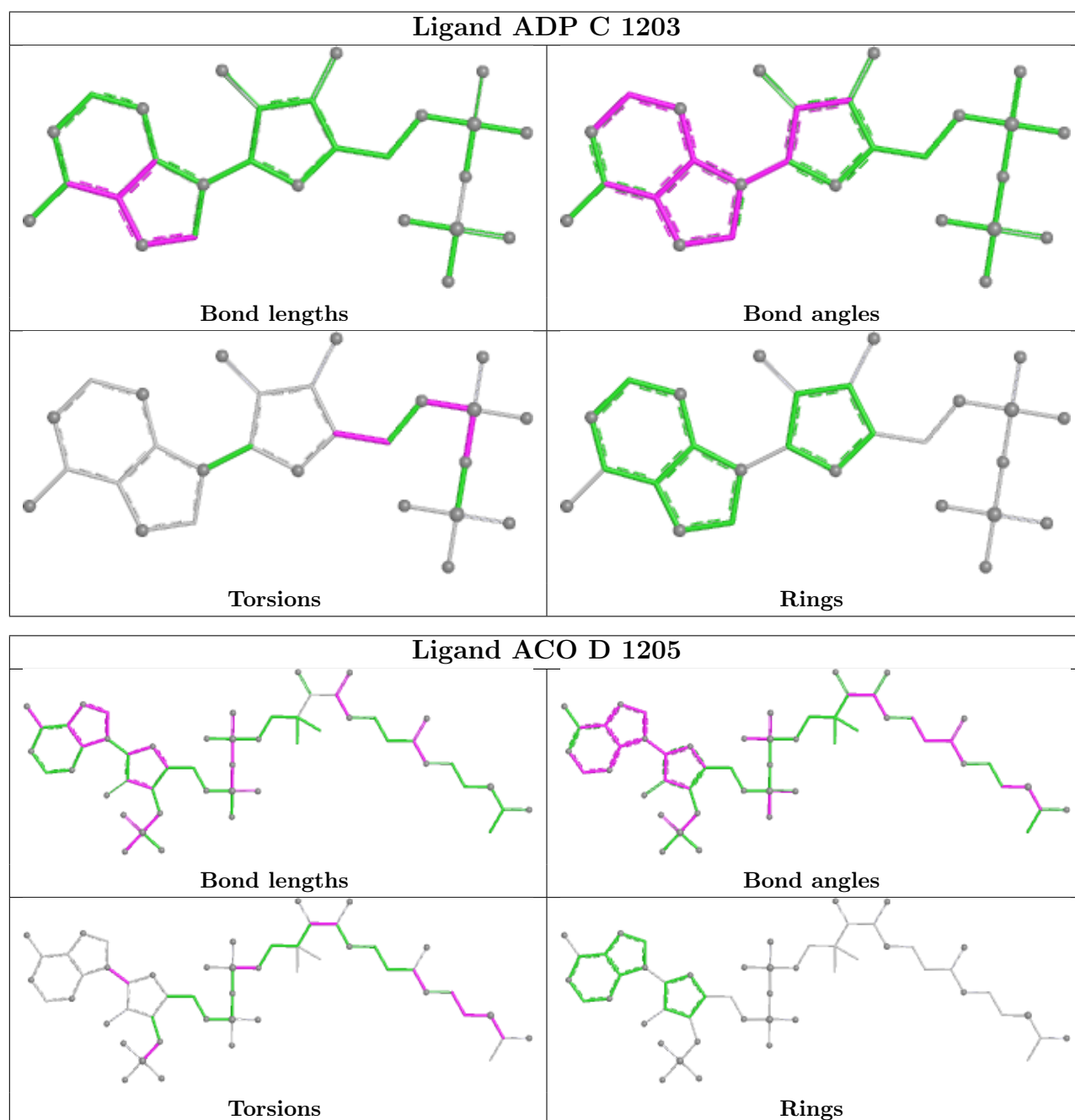
Mol	Chain	Res	Type	Atoms
4	C	1203	ADP	C5'-O5'-PA-O3A
5	C	1205	ACO	CCP-O6A-P2A-O3A
5	C	1205	ACO	CCP-O6A-P2A-O5A
5	D	1205	ACO	CCP-O6A-P2A-O5A
6	A	1206	PYR	OXT-C-CA-O3
6	B	1206	PYR	OXT-C-CA-O3
6	B	1206	PYR	OXT-C-CA-CB
6	C	1206	PYR	OXT-C-CA-CB
5	A	1205	ACO	C2B-C1B-N9A-C4A
5	C	1205	ACO	C2B-C1B-N9A-C4A
5	D	1205	ACO	C2B-C1B-N9A-C4A
5	D	1205	ACO	CH3-C-S1P-C2P
4	B	1203	ADP	PB-O3A-PA-O1A
4	D	1203	ADP	O4'-C4'-C5'-O5'
6	B	1206	PYR	O-C-CA-CB
5	A	1205	ACO	O-C-S1P-C2P
5	B	1205	ACO	O4B-C1B-N9A-C8A
5	C	1205	ACO	O4B-C1B-N9A-C8A
5	D	1205	ACO	O4B-C1B-N9A-C8A
4	C	1203	ADP	PB-O3A-PA-O1A
5	B	1205	ACO	P1A-O3A-P2A-O5A
5	A	1205	ACO	O4B-C1B-N9A-C8A
5	A	1205	ACO	C3B-O3B-P3B-O9A
5	B	1205	ACO	C3B-O3B-P3B-O8A
5	C	1205	ACO	C3B-O3B-P3B-O9A
5	D	1205	ACO	C3B-O3B-P3B-O8A
5	B	1205	ACO	CEP-CBP-CCP-O6A
4	B	1203	ADP	C3'-C4'-C5'-O5'
5	A	1205	ACO	P1A-O3A-P2A-O5A
4	B	1203	ADP	O4'-C4'-C5'-O5'

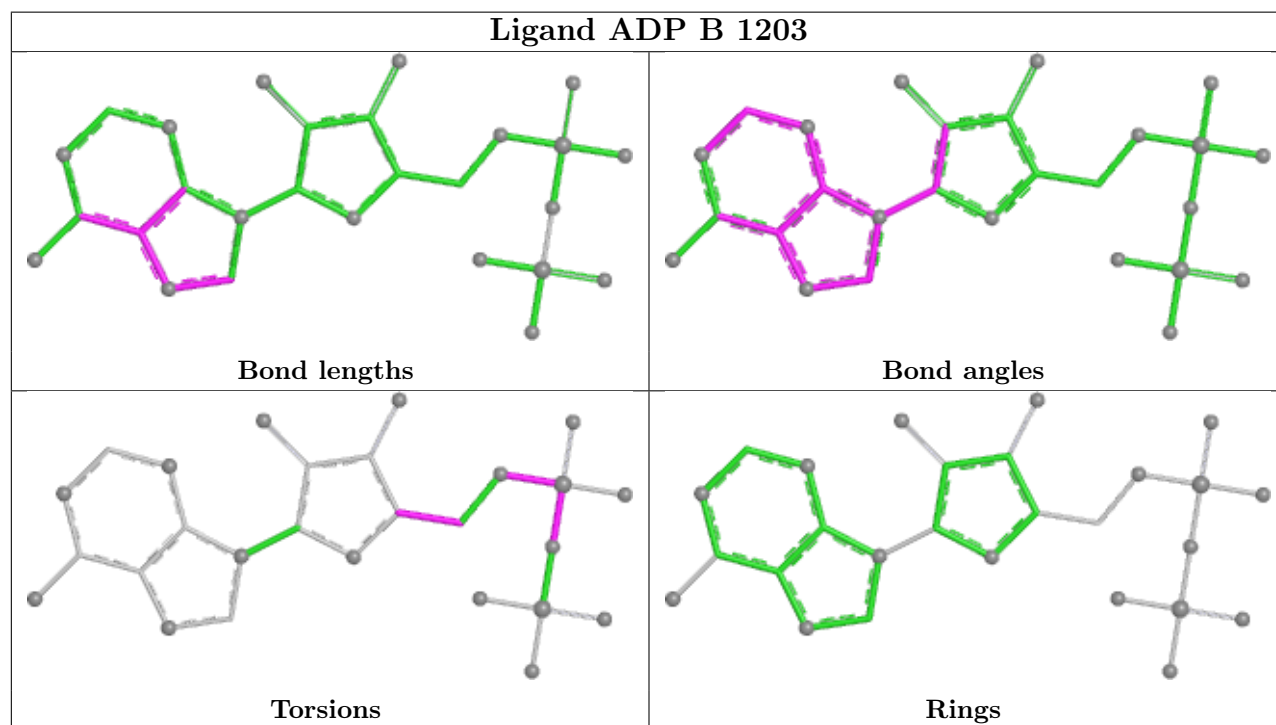
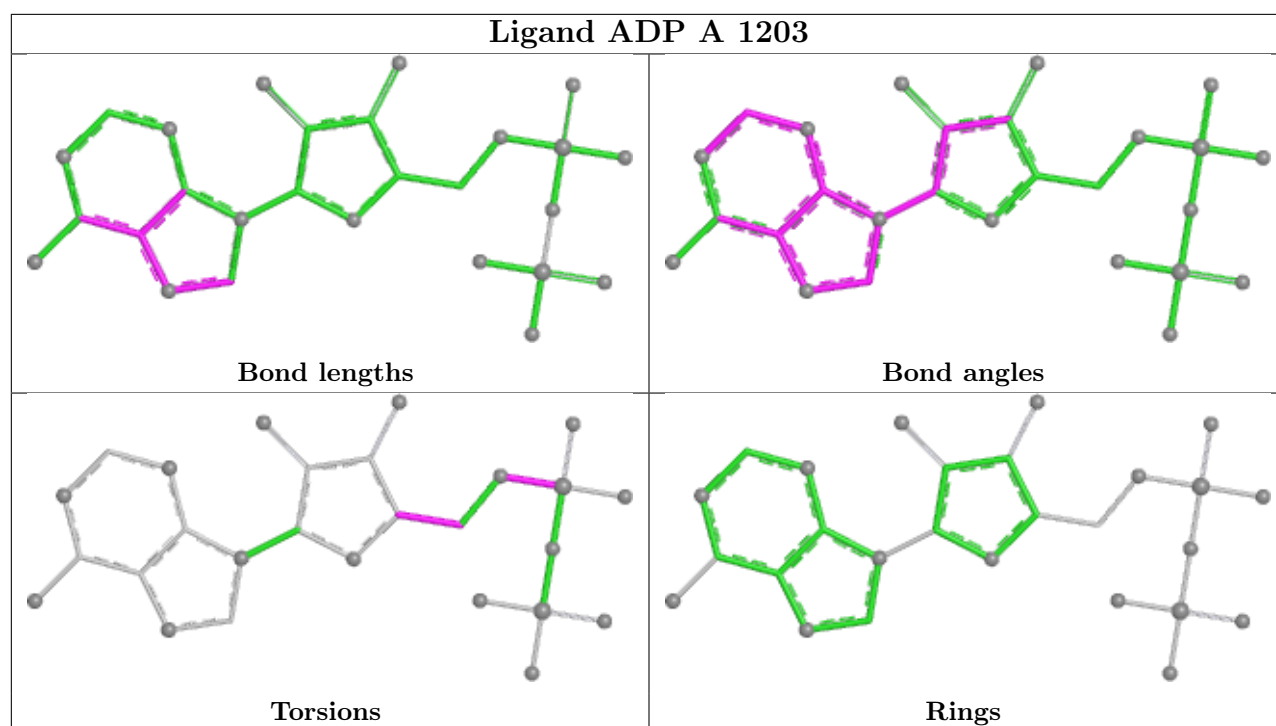
There are no ring outliers.

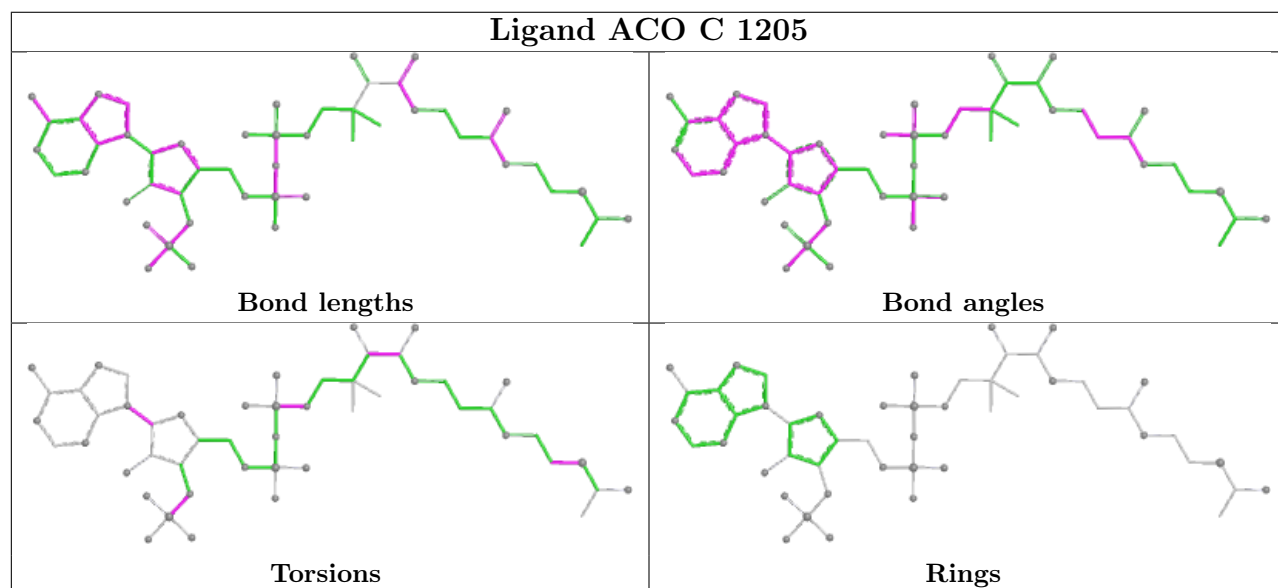
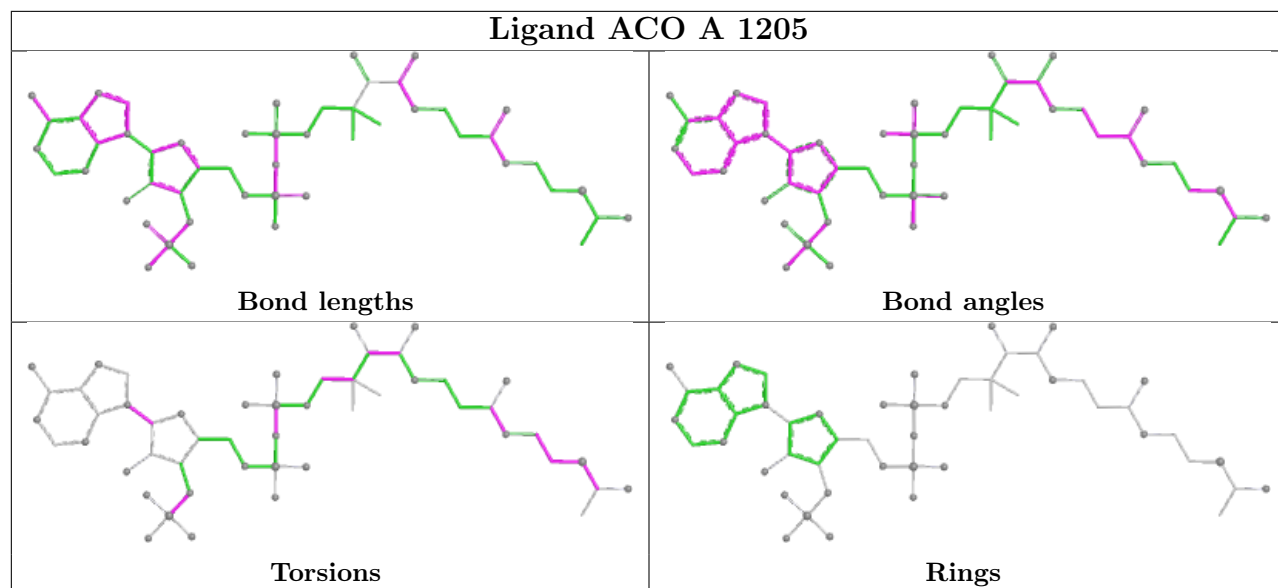
7 monomers are involved in 9 short contacts:

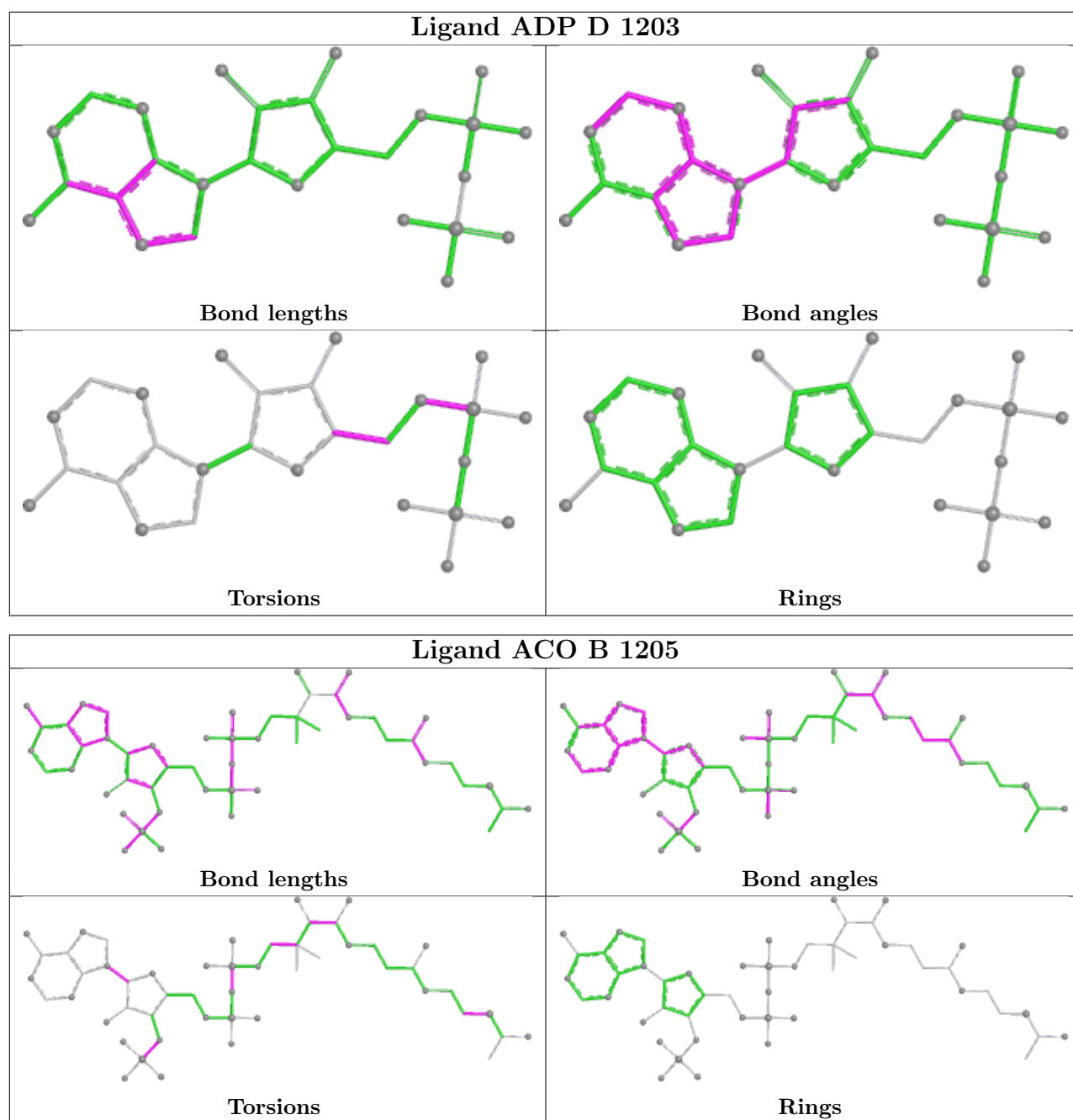
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1203	ADP	1	0
5	D	1205	ACO	1	0
4	A	1203	ADP	3	0
4	B	1203	ADP	1	0
5	C	1205	ACO	1	0
6	C	1206	PYR	1	0
5	B	1205	ACO	1	0

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.

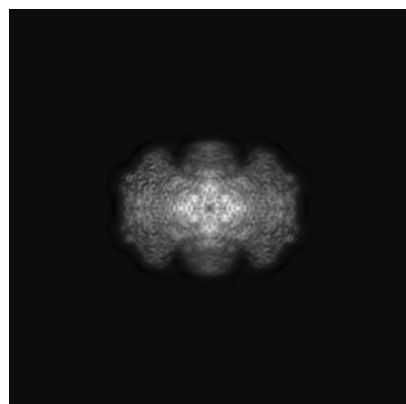
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15028. These allow visual inspection of the internal detail of the map and identification of artifacts.

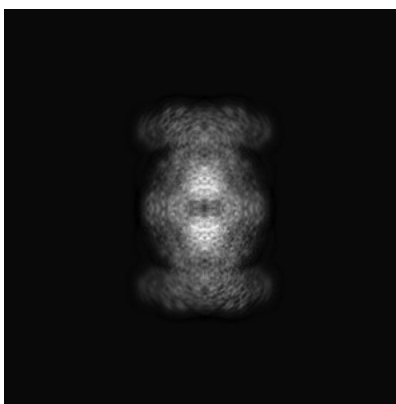
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

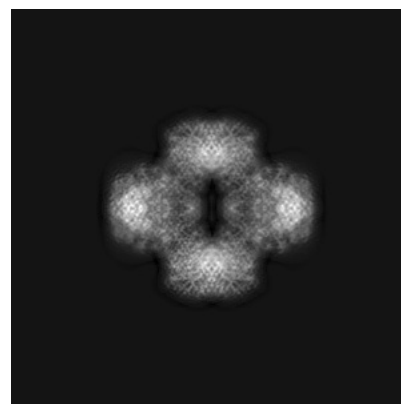
6.1.1 Primary map



X

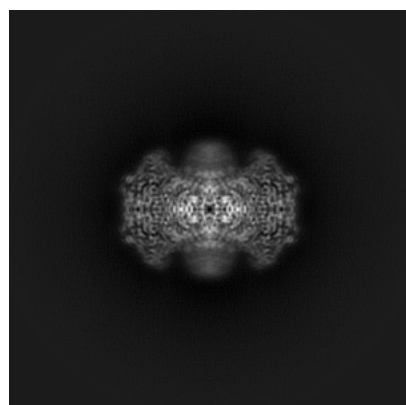


Y

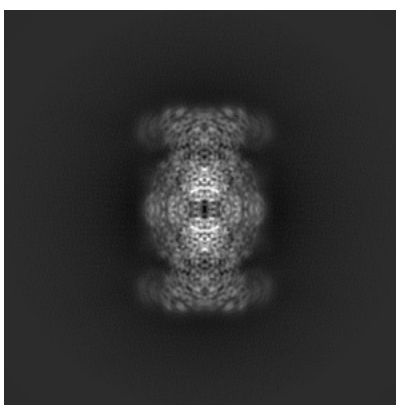


Z

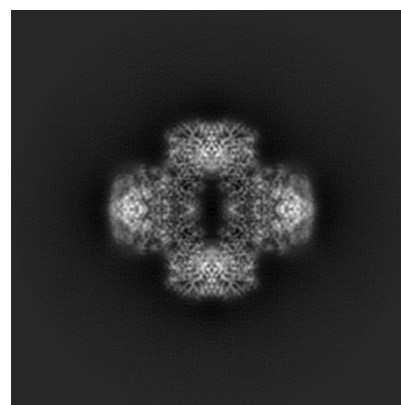
6.1.2 Raw map



X



Y

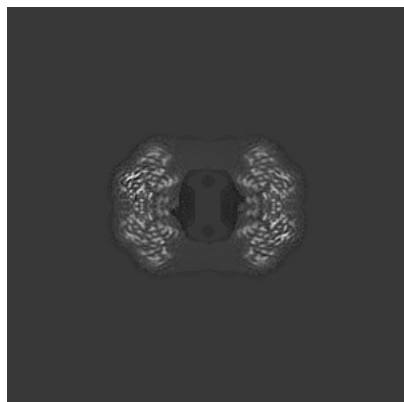


Z

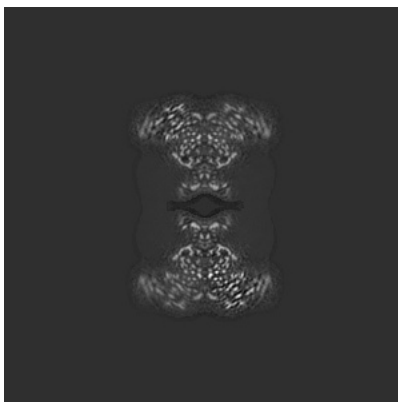
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

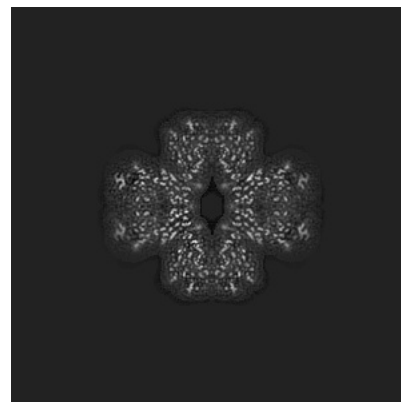
6.2.1 Primary map



X Index: 150

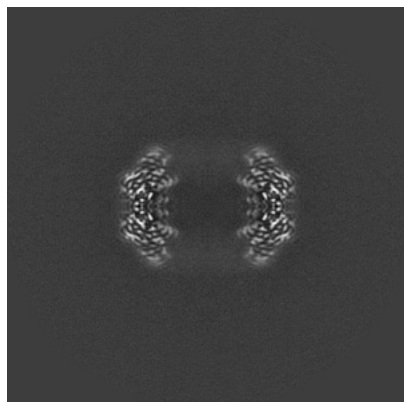


Y Index: 150

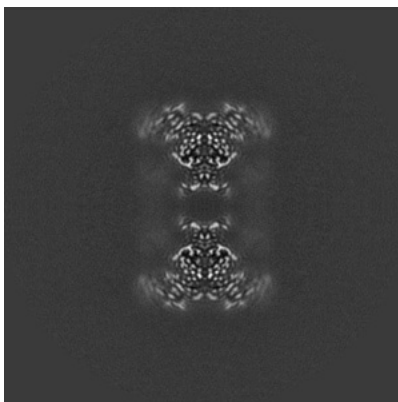


Z Index: 150

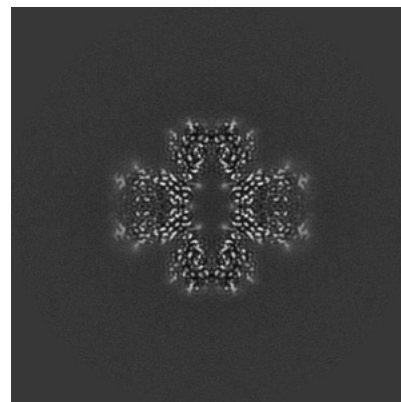
6.2.2 Raw map



X Index: 150



Y Index: 150

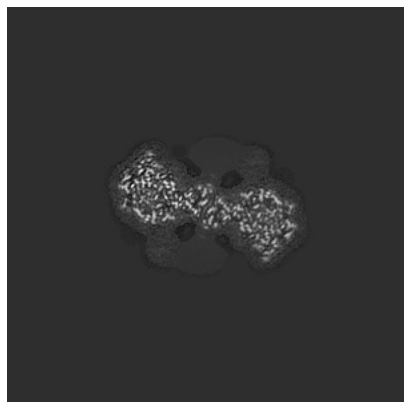


Z Index: 150

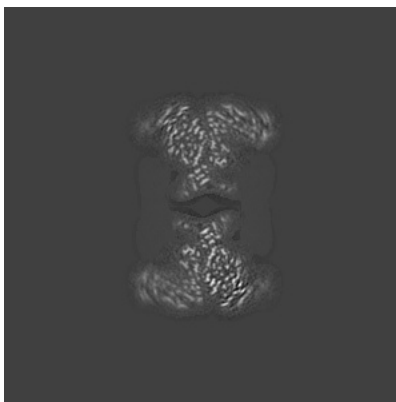
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

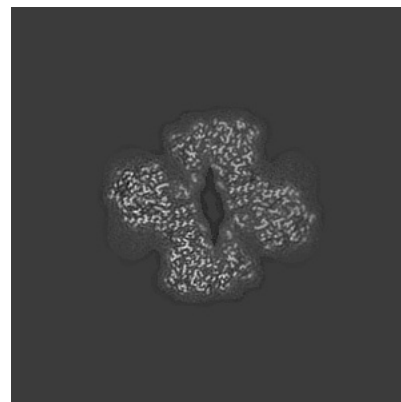
6.3.1 Primary map



X Index: 133

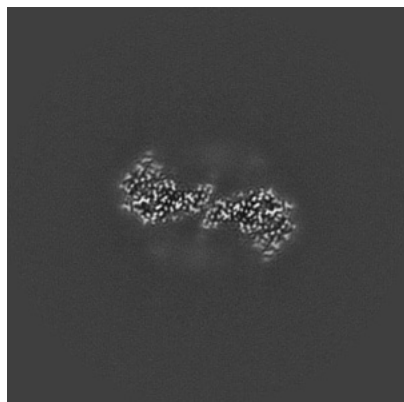


Y Index: 146

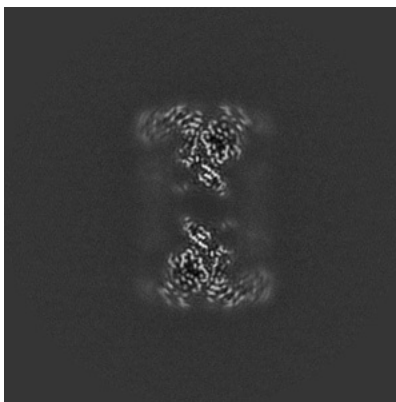


Z Index: 156

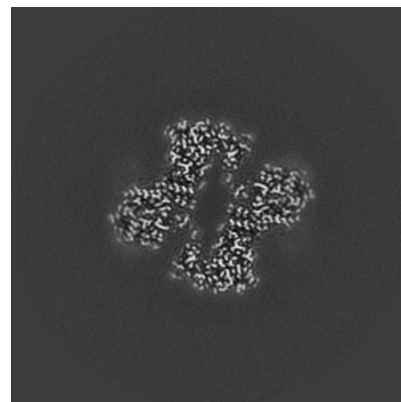
6.3.2 Raw map



X Index: 134



Y Index: 155

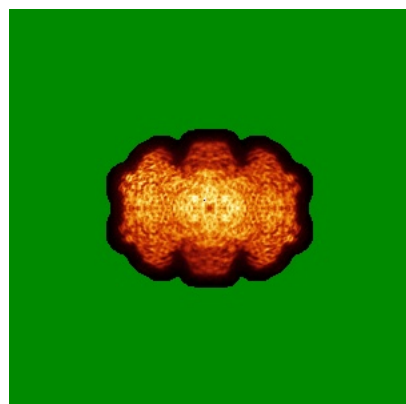


Z Index: 144

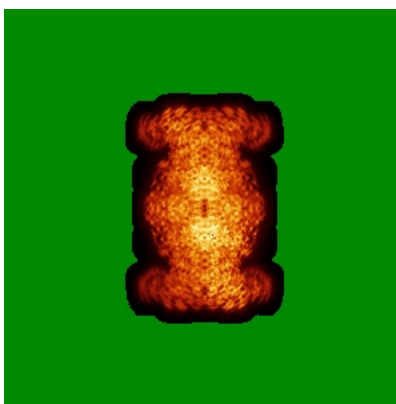
The images above show the largest variance slices of the map in three orthogonal directions.

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

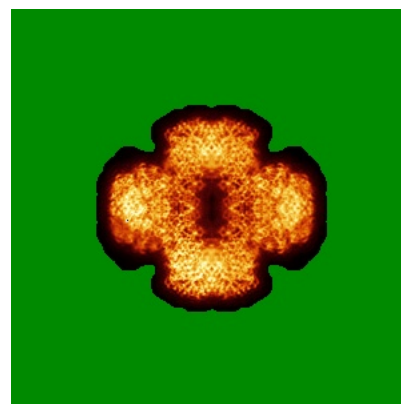
6.4.1 Primary map



X

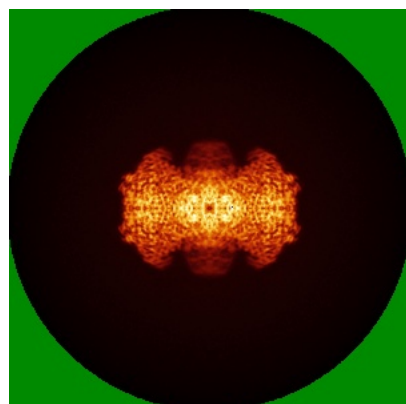


Y

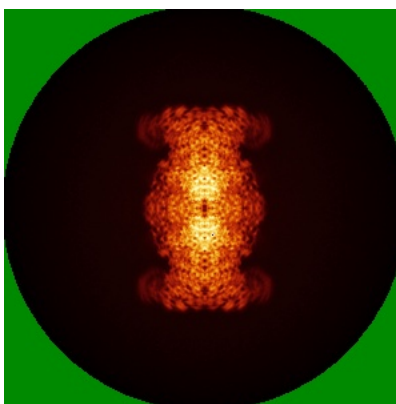


Z

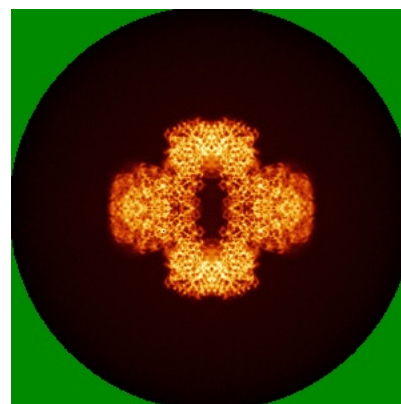
6.4.2 Raw map



X



Y

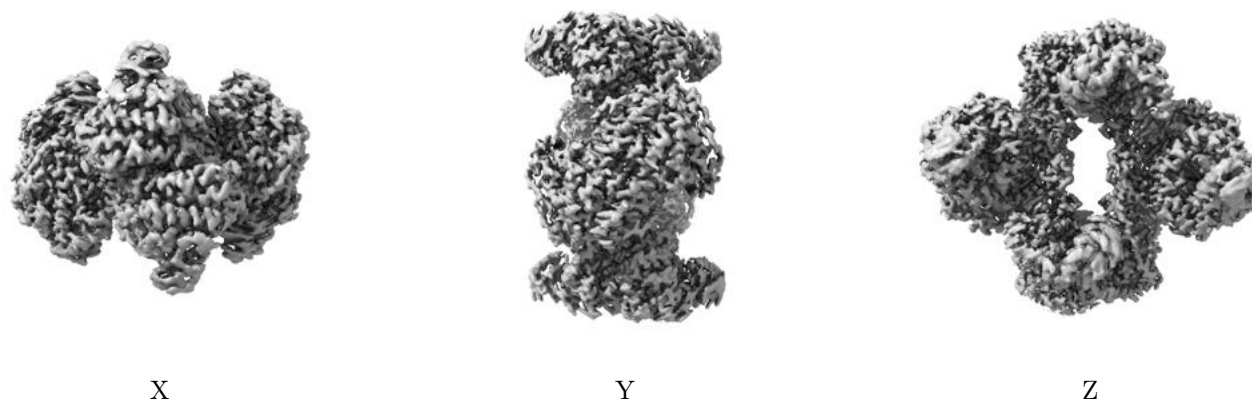


Z

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.

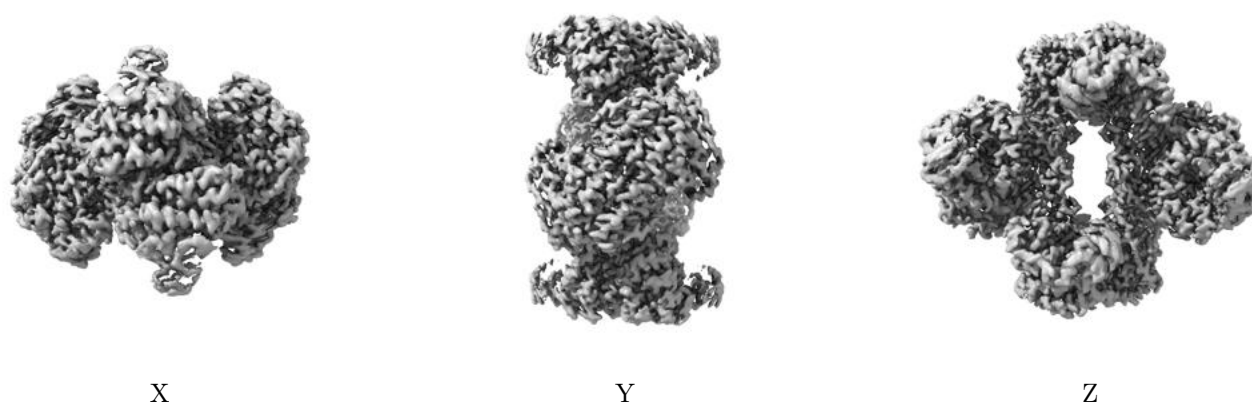
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.187. 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.

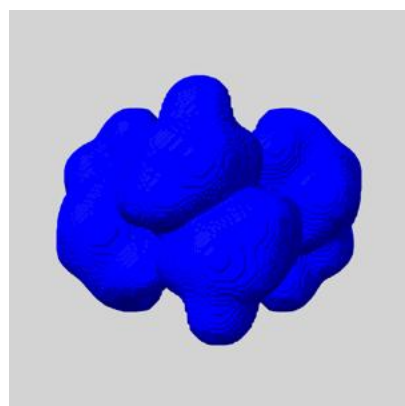
6.6 Mask visualisation [i](#)

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

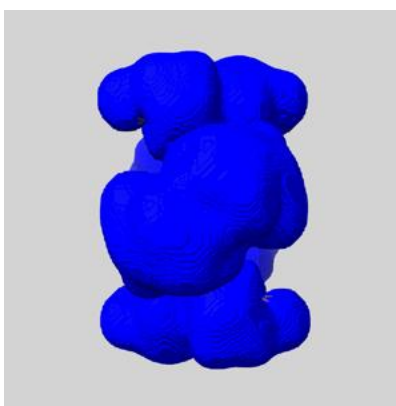
A mask typically either:

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

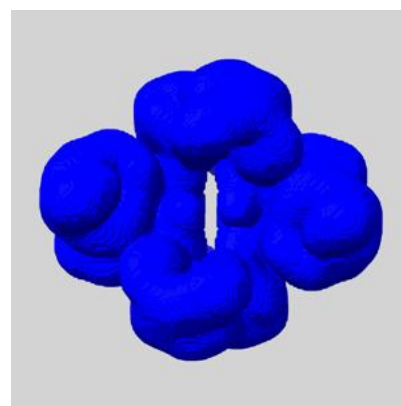
6.6.1 emd_15028_msk_1.map [i](#)



X



Y

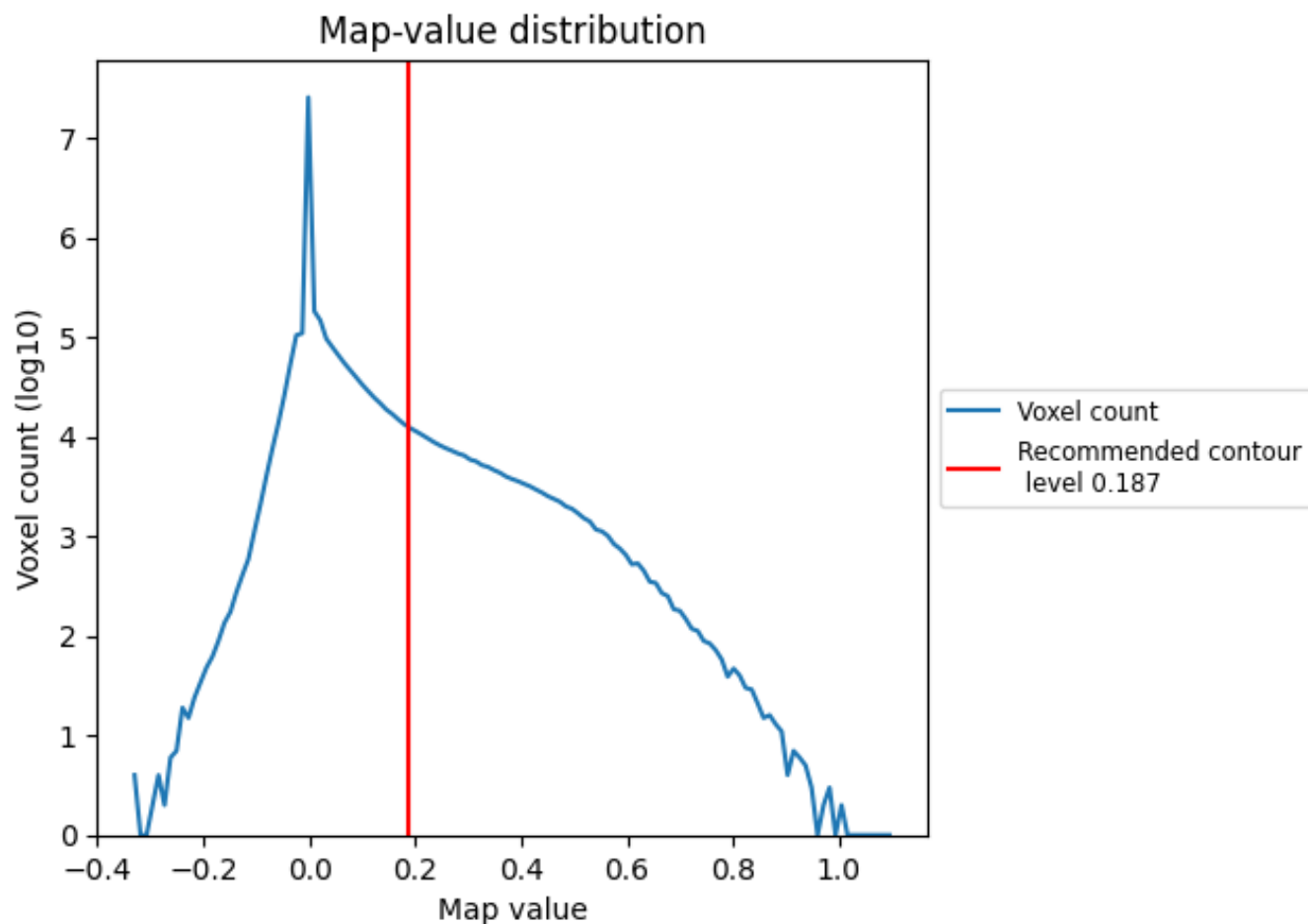


Z

7 Map analysis [i](#)

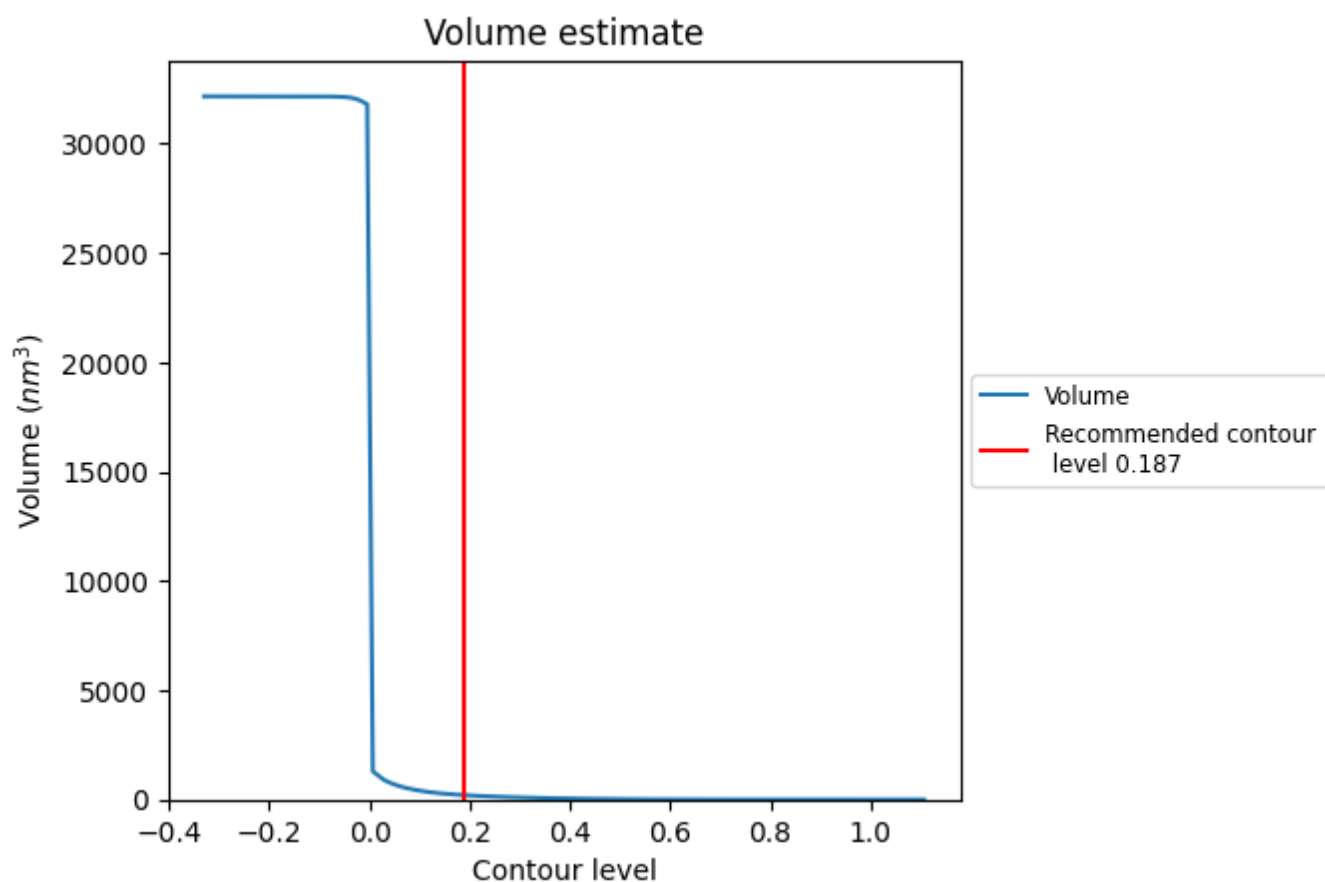
This section contains the results of statistical analysis of the map.

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.

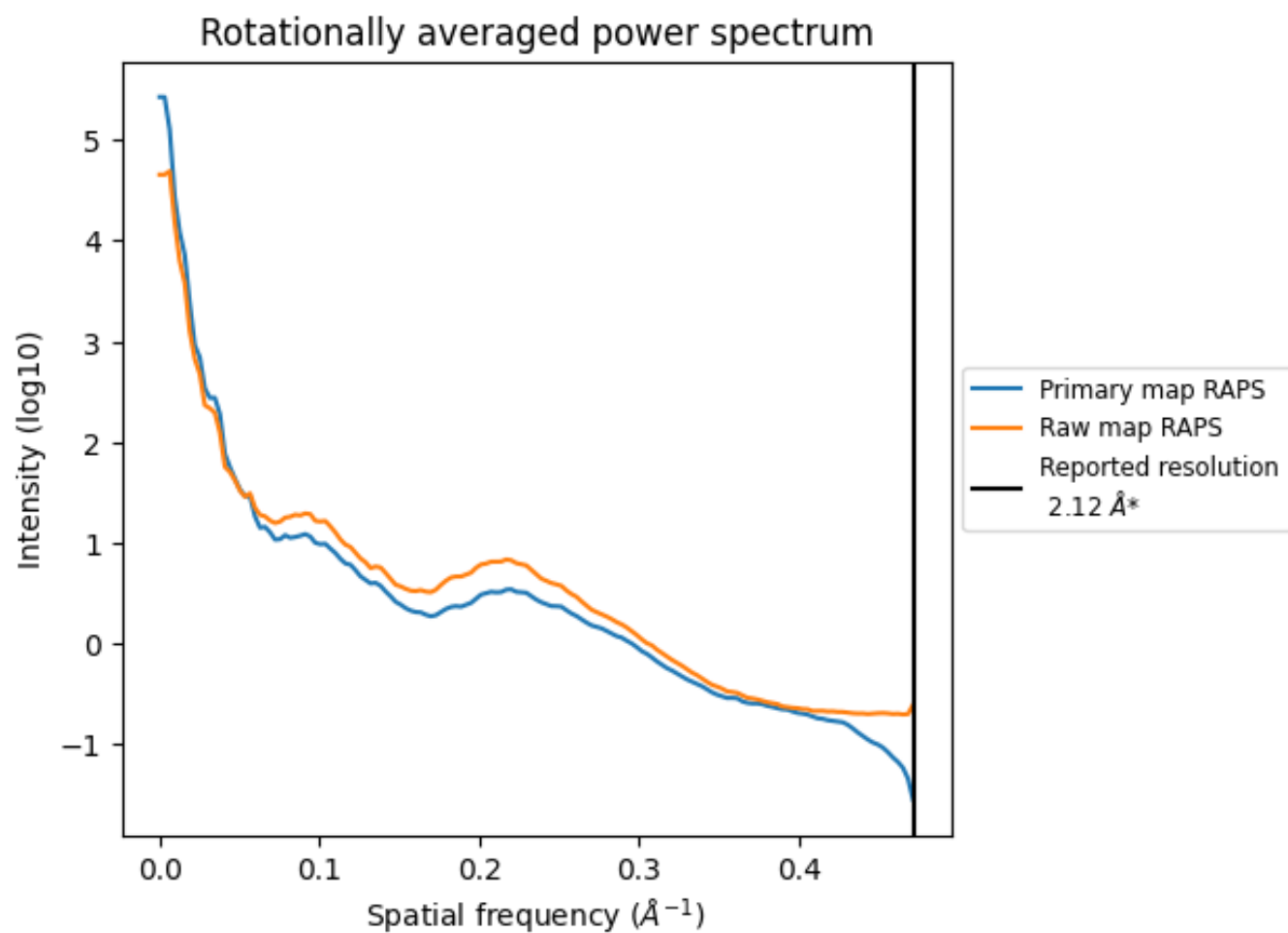
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 205 nm³; this corresponds to an approximate mass of 185 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 ⓘ

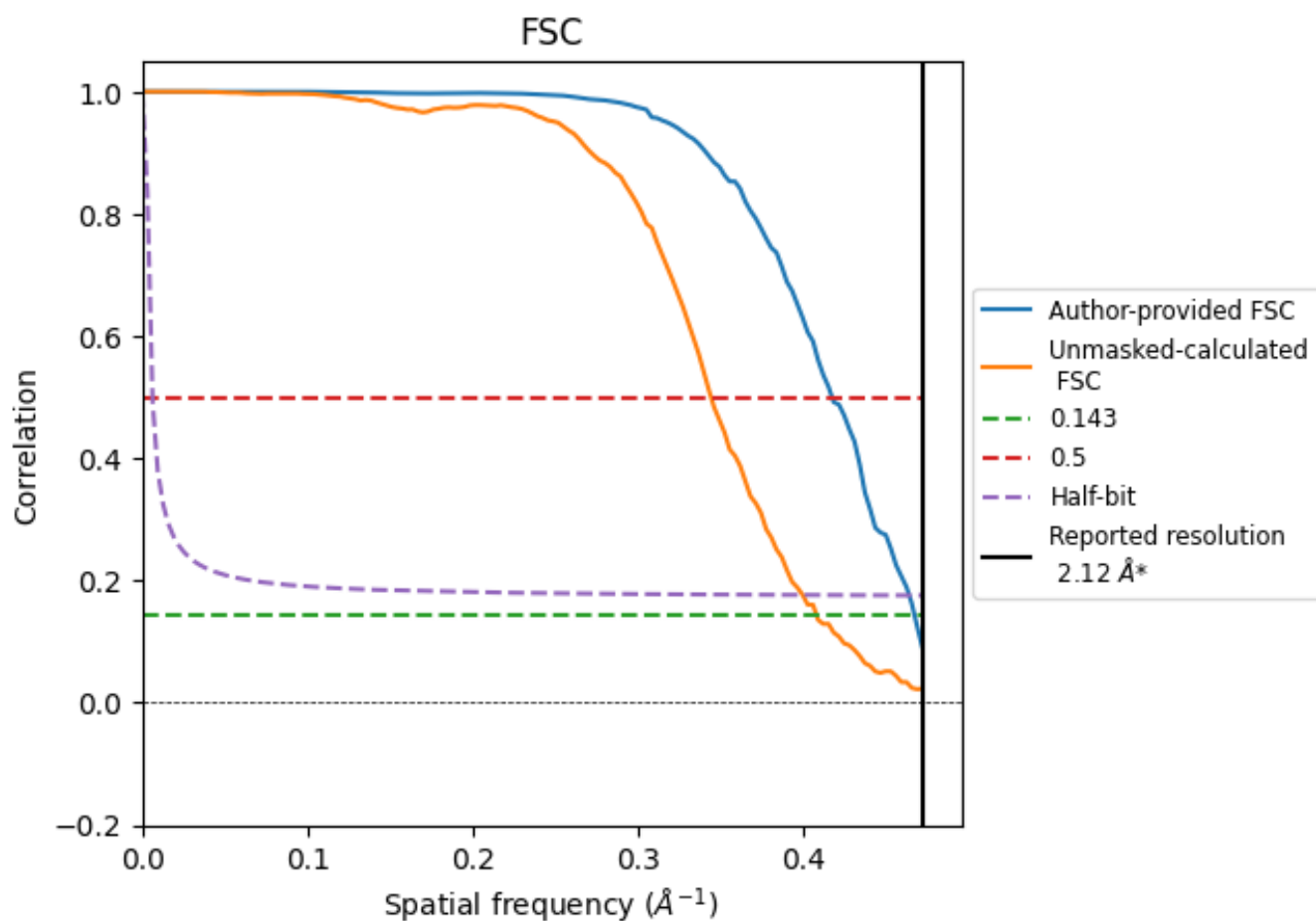


*Reported resolution corresponds to spatial frequency of 0.472 Å⁻¹

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 0.472 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

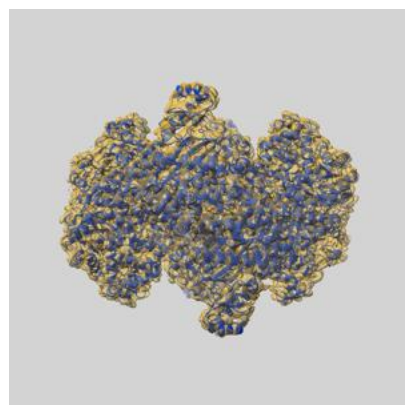
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.12	-	-
Author-provided FSC curve	2.14	2.40	2.16
Unmasked-calculated*	2.45	2.91	2.50

*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 2.45 differs from the reported value 2.12 by more than 10 %

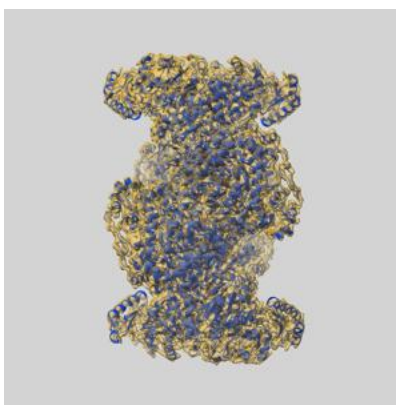
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15028 and PDB model 7ZYY. Per-residue inclusion information can be found in section [3](#) on page [9](#).

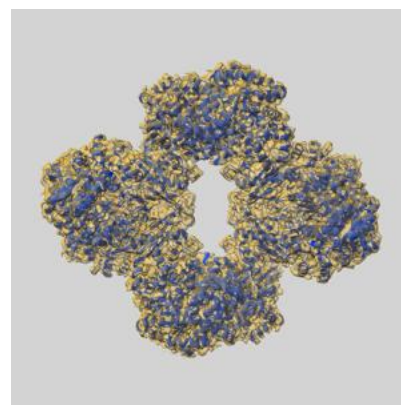
9.1 Map-model overlay [i](#)



X



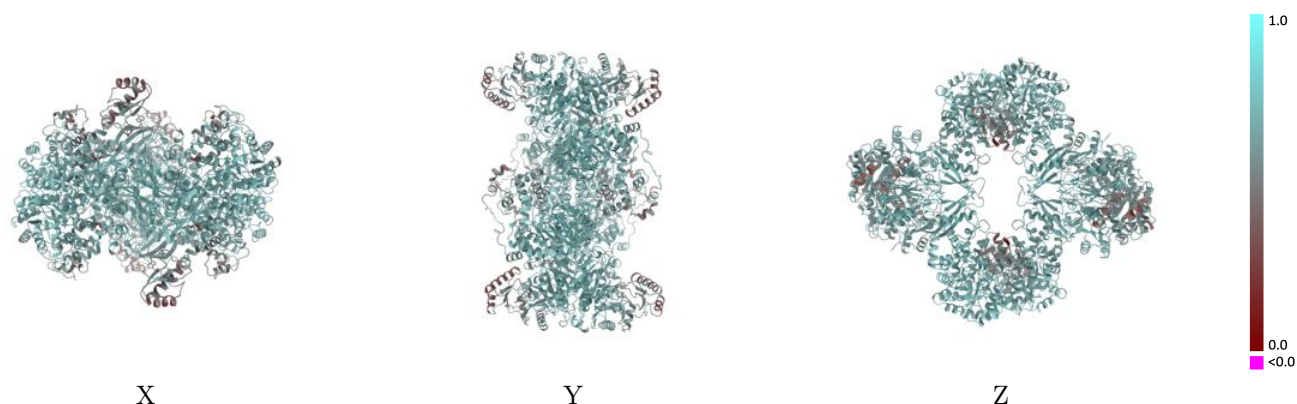
Y



Z

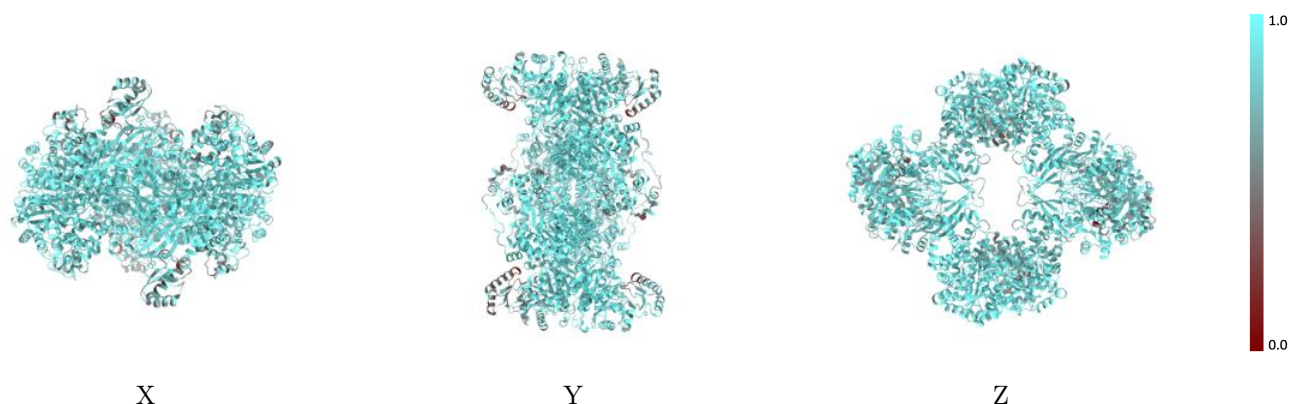
The images above show the 3D surface view of the map at the recommended contour level 0.187 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



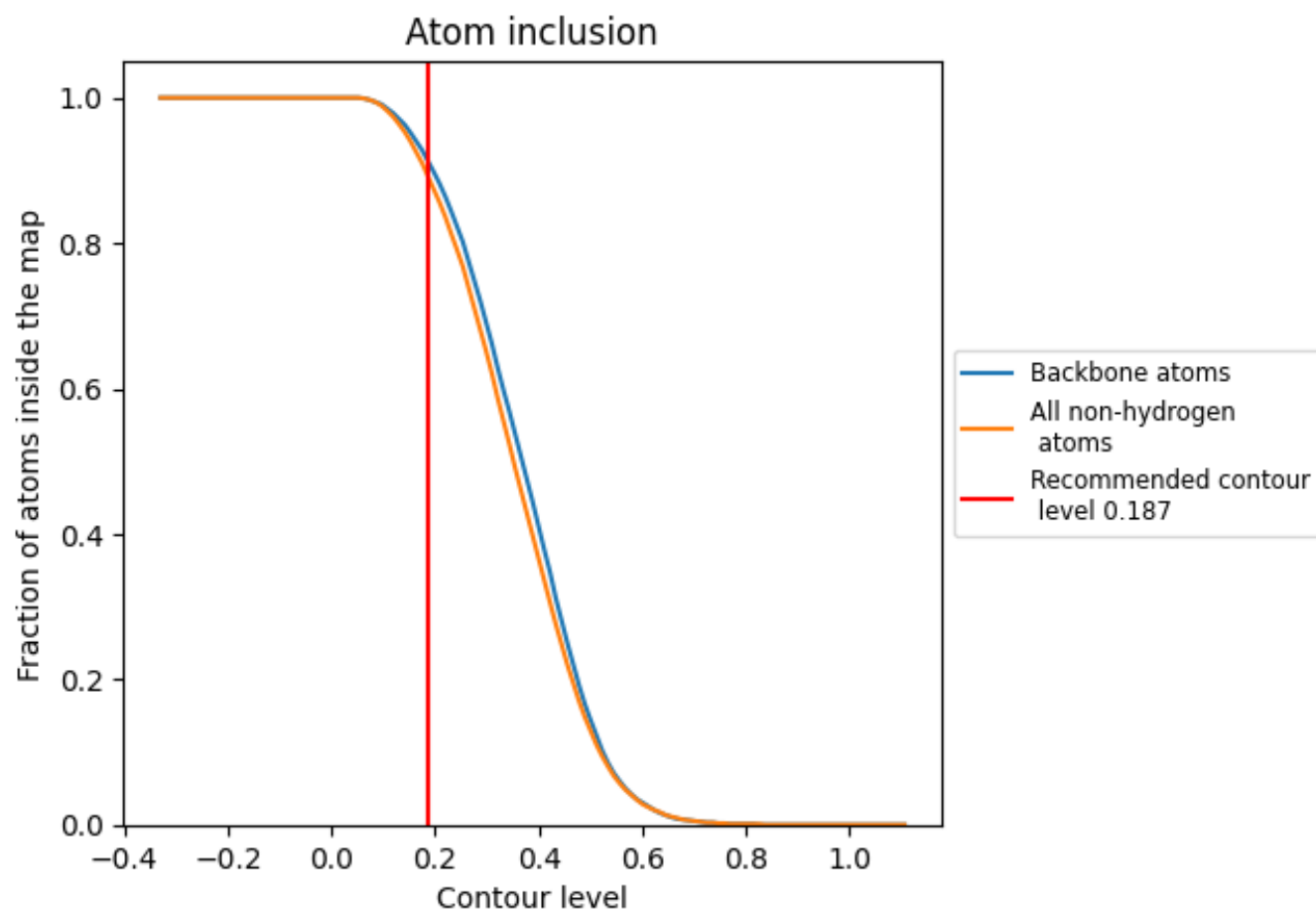
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.187).

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 89% 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 (0.187) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8910	0.6400
A	0.8820	0.6340
B	0.9190	0.6540
C	0.8990	0.6410
D	0.8740	0.6310

