



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:34 PM UTC

PDB ID : 7ZZ3 / pdb_00007zz3
EMDB ID : EMD-15033
Title : Cryo-EM structure of "BC react" conformation 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 : 2.41 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

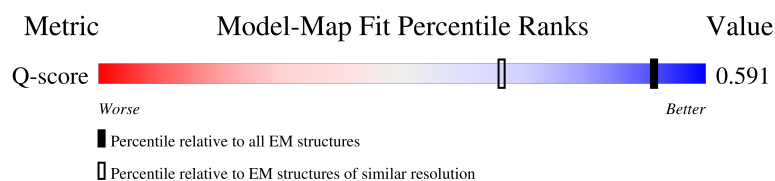
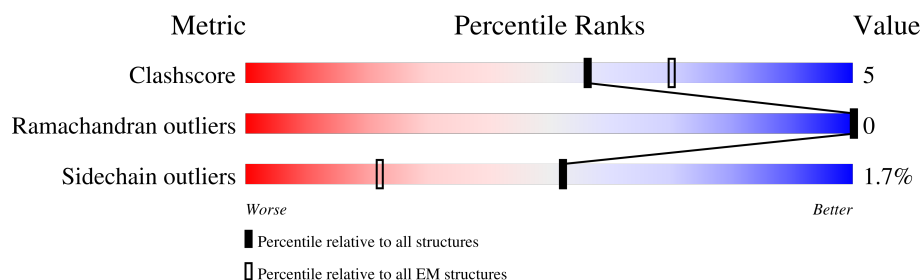
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.41 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	5662 (1.92 - 2.91)

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	86% 14%
1	B	1143	78% 14% • 8%
1	C	1143	80% 12% 7%
1	D	1143	81% 11% 7%

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
8	BCT	A	1208	-	X	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 34427 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	1138	Total	C	N	O	S	0	0
			8922	5654	1541	1692	35		
1	B	1057	Total	C	N	O	S	0	0
			8318	5275	1440	1572	31		
1	C	1058	Total	C	N	O	S	0	0
			8325	5280	1441	1573	31		
1	D	1058	Total	C	N	O	S	0	0
			8325	5280	1441	1573	31		

There are 28 discrepancies between the modelled and reference sequences:

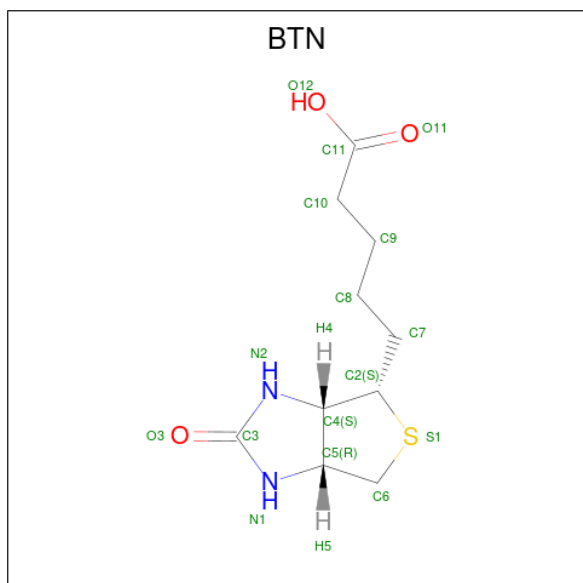
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	VAL	-	expression tag	UNP A0A2A9IR05
A	-4	PRO	-	expression tag	UNP A0A2A9IR05
A	-3	ARG	-	expression tag	UNP A0A2A9IR05
A	-2	GLY	-	expression tag	UNP A0A2A9IR05
A	-1	SER	-	expression tag	UNP A0A2A9IR05
A	0	HIS	-	expression tag	UNP A0A2A9IR05
A	1055	ALA	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 BIOTIN (CCD ID: BTN) (formula: $C_{10}H_{16}N_2O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	S	0
			15	10	2	2	1	

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

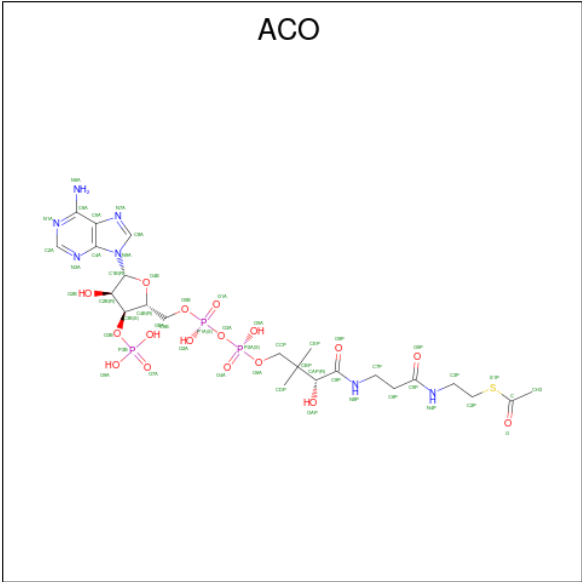
Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Mg	0
			2	2	
3	B	2	Total	Mg	0
			2	2	
3	C	2	Total	Mg	0
			2	2	
3	D	2	Total	Mg	0
			2	2	

- | Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|-----------------|---------|
| 4 | A | 1 | Total Mn
1 1 | 0 |
| 4 | B | 1 | Total Mn
1 1 | 0 |
| 4 | C | 1 | Total Mn
1 1 | 0 |
| 4 | D | 1 | Total Mn
1 1 | 0 |

- # ATP

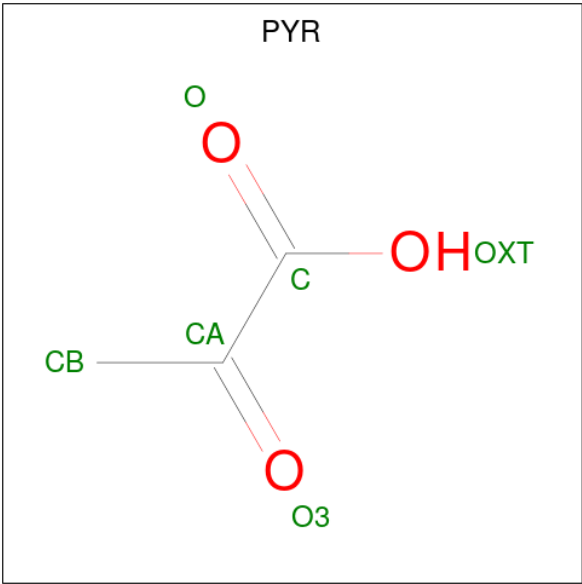
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total 31	C 10	N 5	O 13	P 3	0

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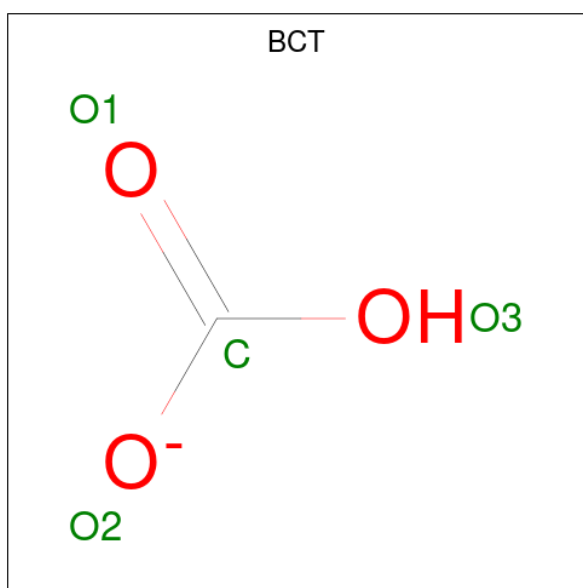
Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	
6	B	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	
6	C	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	
6	D	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	

- Molecule 7 is PYRUVIC ACID (CCD ID: PYR) (formula: C₃H₄O₃).



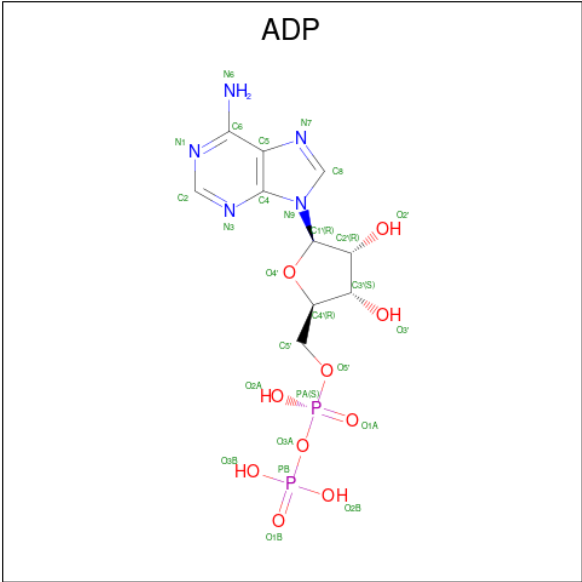
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			6	3	3	
7	B	1	Total	C	O	0
			6	3	3	
7	C	1	Total	C	O	0
			6	3	3	
7	D	1	Total	C	O	0
			6	3	3	

- Molecule 8 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			4	1	3	

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



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

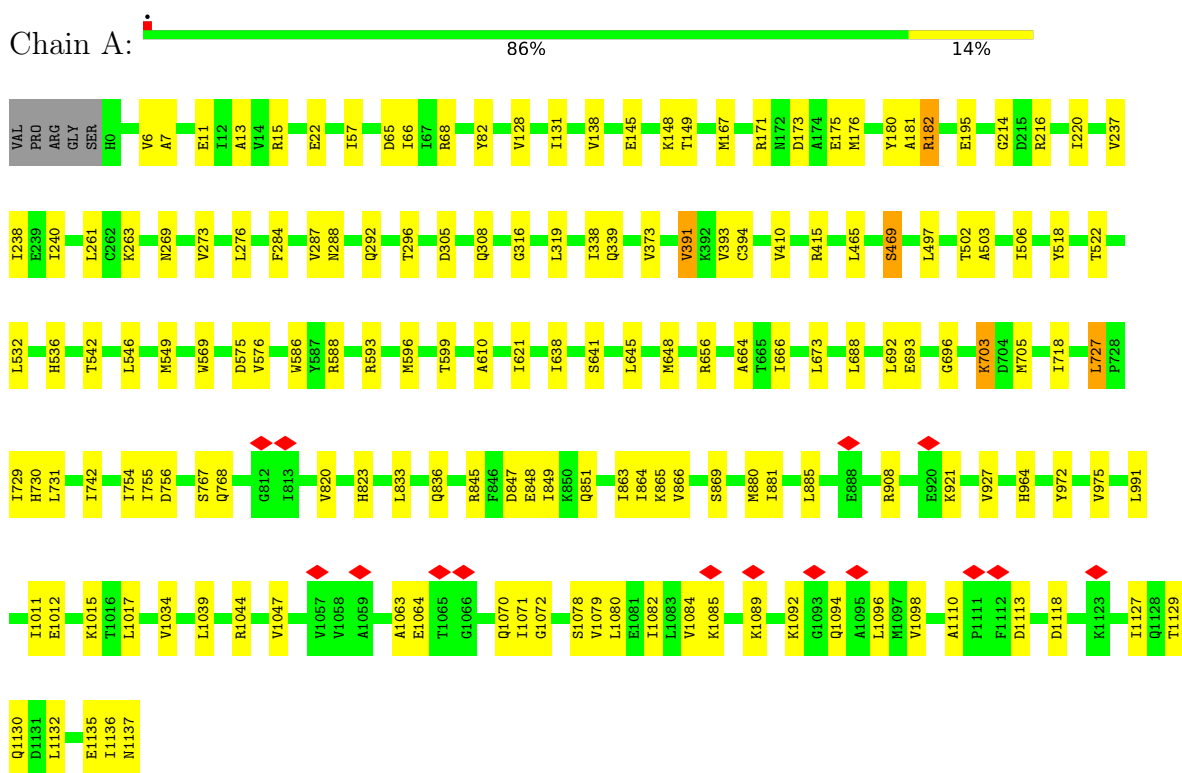
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		AltConf
10	A	58	Total	O	0
			58	58	
10	B	42	Total	O	0
			42	42	
10	C	44	Total	O	0
			44	44	
10	D	22	Total	O	0
			22	22	

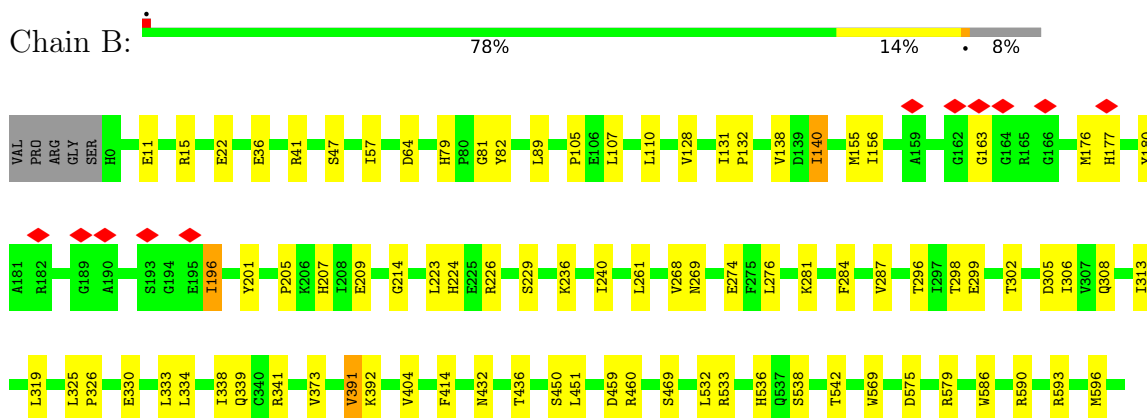
3 Residue-property plots

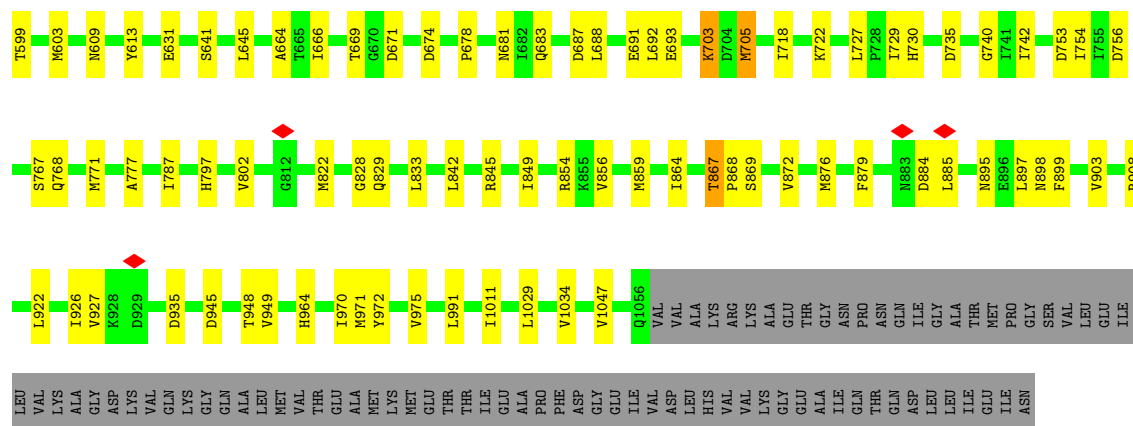
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



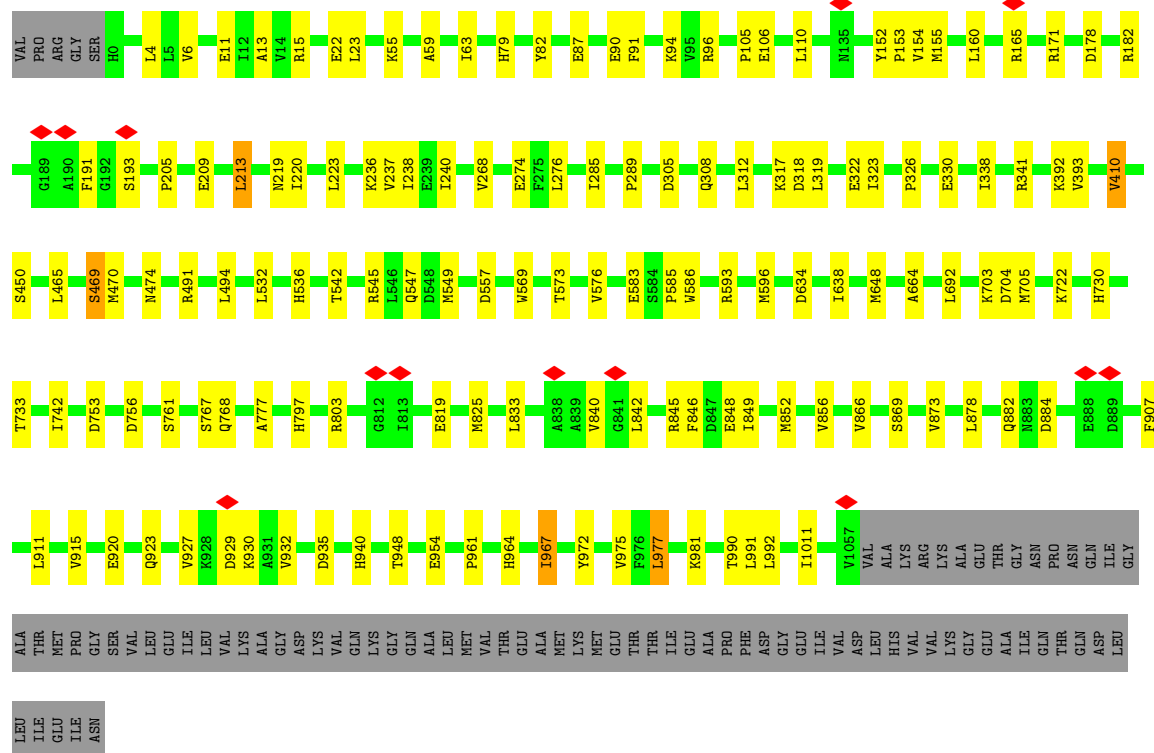
• Molecule 1: Pyruvate carboxylase





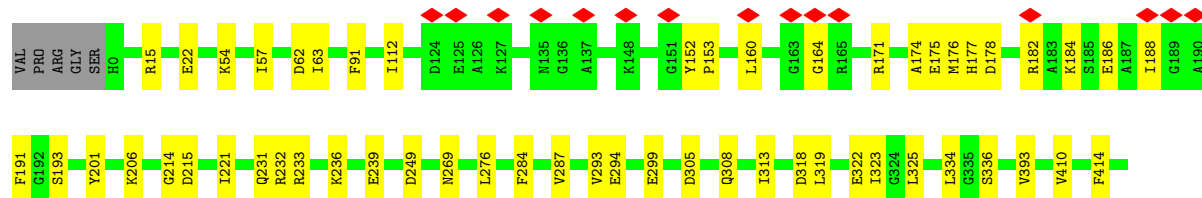
• Molecule 1: Pyruvate carboxylase

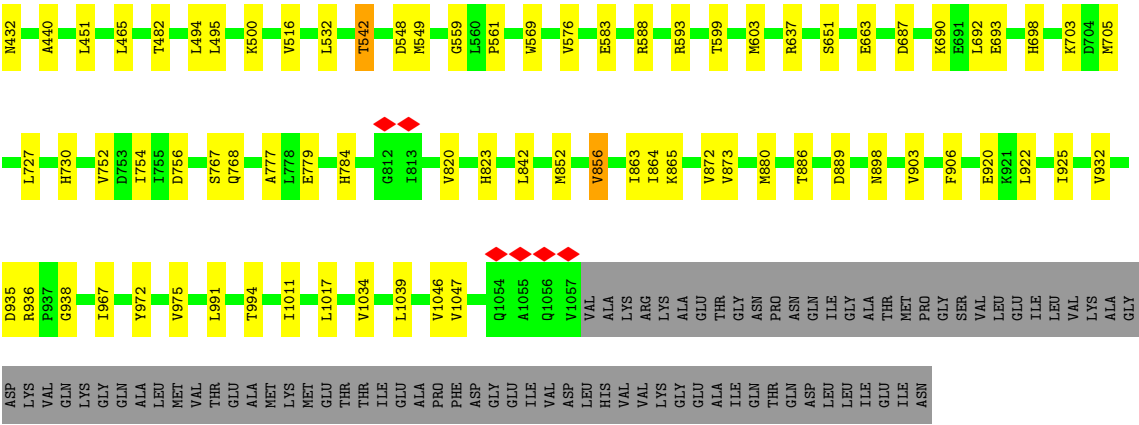
Chain C: 80% 12% 7%



• Molecule 1: Pyruvate carboxylase

Chain D: 81% 11% 7%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	128647	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	0.867	Depositor
Minimum map value	-0.244	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.143	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.15	0/9082	0.39	1/12287 (0.0%)
1	B	0.16	0/8473	0.40	0/11464
1	C	0.15	0/8480	0.38	0/11474
1	D	0.15	0/8480	0.38	0/11474
All	All	0.15	0/34515	0.39	1/46699 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	ARG	CA-CB-CG	5.54	125.18	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8922	0	8890	89	0
1	B	8318	0	8262	98	0
1	C	8325	0	8270	76	0
1	D	8325	0	8270	70	0
2	A	15	0	15	0	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	31	0	12	0	0
6	A	51	0	34	1	0
6	B	51	0	34	3	0
6	C	51	0	34	1	0
6	D	51	0	34	0	0
7	A	6	0	0	0	0
7	B	6	0	0	0	0
7	C	6	0	0	0	0
7	D	6	0	0	0	0
8	A	4	0	0	0	0
9	B	27	0	12	1	0
9	C	27	0	12	0	0
9	D	27	0	12	1	0
10	A	58	0	0	0	0
10	B	42	0	0	1	0
10	C	44	0	0	1	0
10	D	22	0	0	0	0
All	All	34427	0	33891	331	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 (331) 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:B:876:MET:HA	1:B:879:PHE:HB3	1.74	0.68
1:B:176:MET:SD	1:B:176:MET:N	2.68	0.66
1:B:842:LEU:HD12	1:B:845:ARG:HD3	1.80	0.64
1:A:1063:ALA:O	1:A:1130:GLN:NE2	2.30	0.64
1:B:822:MET:SD	1:B:854:ARG:NH1	2.70	0.64
1:D:393:VAL:HG21	1:D:410:VAL:HG11	1.80	0.63
1:B:972:TYR:HB3	1:B:975:VAL:HB	1.81	0.63
1:A:1092:LYS:HA	1:A:1110:ALA:HB3	1.81	0.63
1:C:213:LEU:HD22	1:C:223:LEU:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:HIS:HD2	1:B:81:GLY:H	1.47	0.62
1:A:1064:GLU:H	1:A:1070:GLN:HE22	1.47	0.62
1:B:156:ILE:HG23	1:B:196:ILE:HD13	1.81	0.62
1:C:840:VAL:HG12	1:C:842:LEU:H	1.65	0.60
1:B:666:ILE:O	1:B:703:KCX:N	2.34	0.60
1:A:972:TYR:HB3	1:A:975:VAL:HB	1.83	0.59
1:B:730:HIS:NE2	1:B:756:ASP:OD1	2.35	0.59
1:C:730:HIS:NE2	1:C:756:ASP:OD1	2.34	0.59
1:D:516:VAL:HG11	1:D:698:HIS:HB3	1.84	0.59
1:C:569:TRP:HE1	1:C:585:PRO:HB2	1.66	0.59
1:A:666:ILE:O	1:A:703:KCX:N	2.35	0.59
1:A:730:HIS:NE2	1:A:756:ASP:OD1	2.35	0.59
1:C:276:LEU:HG	1:C:285:ILE:HD11	1.84	0.59
1:A:1094:GLN:N	1:A:1094:GLN:OE1	2.36	0.59
1:B:223:LEU:HB3	1:B:302:THR:HG21	1.83	0.59
1:B:64:ASP:N	1:B:64:ASP:OD1	2.35	0.59
1:C:532:LEU:HD22	1:C:549:MET:HG2	1.85	0.58
1:B:22:GLU:OE1	1:B:308:GLN:NE2	2.35	0.58
1:C:825:MET:HE3	1:C:833:LEU:HD13	1.85	0.58
1:D:730:HIS:NE2	1:D:756:ASP:OD1	2.36	0.58
1:C:22:GLU:OE1	1:C:308:GLN:NE2	2.36	0.57
1:D:532:LEU:HD22	1:D:549:MET:HG2	1.86	0.57
1:B:163:GLY:N	9:B:1203:ADP:O3B	2.37	0.57
1:B:15:ARG:NH2	1:B:305:ASP:OD1	2.33	0.57
1:C:96:ARG:NH2	1:C:105:PRO:O	2.37	0.57
1:B:128:VAL:HG21	1:B:261:LEU:HB2	1.87	0.57
1:A:1012:GLU:HB3	1:A:1015:LYS:HB2	1.87	0.57
1:C:972:TYR:HB3	1:C:975:VAL:HB	1.86	0.57
1:A:532:LEU:HD22	1:A:549:MET:HG2	1.87	0.56
1:C:705:MET:HE3	1:C:866:VAL:HB	1.86	0.56
1:C:341:ARG:HG2	1:C:392:LYS:HG2	1.88	0.56
1:B:138:VAL:O	1:B:180:TYR:OH	2.22	0.56
1:C:846:PHE:HA	1:C:849:ILE:HD12	1.88	0.56
1:D:593:ARG:NH2	1:D:599:THR:O	2.37	0.56
1:D:152:TYR:OH	1:D:176:MET:SD	2.64	0.55
1:C:209:GLU:OE2	1:C:236:LYS:NZ	2.39	0.55
1:A:22:GLU:OE1	1:A:308:GLN:NE2	2.40	0.55
1:B:313:ILE:HD11	1:B:319:LEU:HD21	1.89	0.55
1:A:148:LYS:NZ	1:A:173:ASP:OD2	2.40	0.55
1:D:583:GLU:OE2	1:D:588:ARG:NH2	2.38	0.55
1:A:284:PHE:HE1	1:A:287:VAL:HG23	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:491:ARG:HE	1:C:797:HIS:HB3	1.71	0.54
1:B:645:LEU:HD22	1:B:691:GLU:HB3	1.89	0.54
1:B:829:GLN:HE21	1:B:833:LEU:HD12	1.72	0.54
1:C:15:ARG:NH2	1:C:305:ASP:OD1	2.34	0.54
1:C:593:ARG:NH2	1:C:634:ASP:OD2	2.41	0.54
1:D:319:LEU:HA	1:D:323:ILE:HD12	1.90	0.54
1:D:239:GLU:HG2	1:D:294:GLU:HG2	1.90	0.54
1:C:722:LYS:NZ	1:C:753:ASP:OD2	2.41	0.54
1:C:393:VAL:HG21	1:C:410:VAL:HG11	1.90	0.53
1:A:216:ARG:NH1	1:A:316:GLY:O	2.41	0.53
1:B:908:ARG:HG3	1:B:927:VAL:HG11	1.90	0.53
1:D:249:ASP:OD2	1:D:249:ASP:N	2.36	0.53
1:D:972:TYR:HB3	1:D:975:VAL:HB	1.91	0.53
1:D:693:GLU:HG3	1:D:727:LEU:HD22	1.91	0.53
1:A:693:GLU:HG3	1:A:727:LEU:HD13	1.88	0.53
1:B:209:GLU:OE2	1:B:236:LYS:NZ	2.39	0.53
1:B:949:VAL:HG11	1:B:970:ILE:HD11	1.90	0.53
1:A:65:ASP:OD1	1:A:68:ARG:NH2	2.41	0.53
1:D:284:PHE:HE1	1:D:287:VAL:HG23	1.74	0.52
1:B:596:MET:HE2	1:B:599:THR:HG21	1.91	0.52
1:D:206:LYS:NZ	1:D:440:ALA:O	2.41	0.52
1:B:326:PRO:HB2	1:B:330:GLU:HB2	1.92	0.52
1:A:393:VAL:HG21	1:A:410:VAL:HG11	1.92	0.52
1:A:863:ILE:O	1:A:865:LYS:NZ	2.43	0.52
1:C:845:ARG:HB2	1:C:848:GLU:HB2	1.91	0.52
1:A:1082:ILE:O	1:A:1085:LYS:NZ	2.43	0.51
1:B:140:ILE:HD11	1:B:177:HIS:HD2	1.76	0.51
1:B:533:ARG:NH2	1:B:703:KCX:OQ1	2.44	0.51
1:D:153:PRO:HB2	1:D:201:TYR:HB3	1.92	0.51
1:C:878:LEU:O	1:C:882:GLN:HB2	2.10	0.51
1:C:907:PHE:O	1:C:923:GLN:NE2	2.44	0.51
1:A:656:ARG:NH1	1:A:696:GLY:O	2.43	0.51
1:A:908:ARG:HG2	1:A:927:VAL:HG11	1.93	0.51
1:B:373:VAL:HG23	1:B:391:VAL:HB	1.92	0.51
1:A:596:MET:HE2	1:A:599:THR:HG21	1.92	0.51
1:D:852:MET:HE2	1:D:880:MET:HE2	1.93	0.51
1:B:876:MET:HB3	1:B:903:VAL:HG21	1.91	0.51
1:B:11:GLU:OE1	1:B:82:TYR:OH	2.29	0.50
1:C:106:GLU:HG2	1:C:268:VAL:HG11	1.92	0.50
1:C:991:LEU:HD13	1:C:1011:ILE:HA	1.93	0.50
1:D:886:THR:H	1:D:889:ASP:HB2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:991:LEU:HD13	1:B:1011:ILE:HA	1.94	0.50
1:B:590:ARG:NH2	1:B:631:GLU:OE2	2.45	0.50
1:B:777:ALA:HB1	1:C:742:ILE:HD13	1.93	0.50
1:B:895:ASN:OD1	1:B:895:ASN:N	2.45	0.50
1:D:863:ILE:O	1:D:865:LYS:NZ	2.44	0.50
1:D:231:GLN:HG2	1:D:236:LYS:HA	1.94	0.50
1:B:432:ASN:HD22	1:B:451:LEU:HD21	1.77	0.50
1:D:991:LEU:HD13	1:D:1011:ILE:HA	1.94	0.50
1:A:1079:VAL:HG12	1:A:1127:ILE:HD11	1.93	0.49
1:A:220:ILE:HB	1:A:263:LYS:HD3	1.93	0.49
1:D:922:LEU:HA	1:D:925:ILE:HD12	1.94	0.49
1:A:15:ARG:NH2	1:A:305:ASP:OD1	2.41	0.49
1:A:849:ILE:HG12	1:A:881:ILE:HG12	1.93	0.49
1:B:131:ILE:HD12	1:B:132:PRO:HD2	1.94	0.49
1:C:237:VAL:HG12	1:C:238:ILE:HG13	1.92	0.49
1:D:1017:LEU:HD22	1:D:1039:LEU:HD11	1.94	0.49
1:D:15:ARG:NH2	1:D:299:GLU:OE2	2.46	0.49
1:D:232:ARG:HG2	1:D:233:ARG:HG2	1.95	0.49
1:A:767:SER:OG	1:A:768:GLN:N	2.46	0.49
1:B:319:LEU:HD22	1:B:325:LEU:HD12	1.94	0.49
1:D:779:GLU:O	1:D:784:HIS:NE2	2.46	0.49
1:A:1084:VAL:HG21	1:A:1096:LEU:HD12	1.95	0.48
1:D:495:LEU:HD22	1:D:559:GLY:HA3	1.95	0.48
1:D:935:ASP:OD1	1:D:935:ASP:N	2.45	0.48
1:A:1078:SER:HA	1:A:1127:ILE:HG12	1.95	0.48
1:C:545:ARG:NH2	1:C:992:LEU:O	2.34	0.48
1:A:237:VAL:HG12	1:A:238:ILE:HG13	1.94	0.48
1:A:666:ILE:HG23	1:A:688:LEU:HD23	1.96	0.48
1:C:312:LEU:HD22	1:C:317:LYS:HD2	1.95	0.48
1:A:518:TYR:O	1:A:522:THR:OG1	2.31	0.48
1:B:1034:VAL:HG22	1:B:1047:VAL:HG22	1.95	0.48
1:C:209:GLU:HG2	1:C:274:GLU:HG2	1.96	0.48
1:C:767:SER:OG	1:C:768:GLN:N	2.47	0.48
1:B:641:SER:HB2	1:B:868:PRO:HD2	1.96	0.48
1:B:742:ILE:HD13	1:C:777:ALA:HB1	1.95	0.48
1:A:1017:LEU:HD22	1:A:1039:LEU:HD11	1.96	0.48
1:A:288:ASN:OD1	1:A:292:GLN:NE2	2.46	0.48
1:D:174:ALA:O	1:D:177:HIS:ND1	2.42	0.47
1:A:641:SER:HB3	1:A:869:SER:HB3	1.96	0.47
1:C:935:ASP:OD2	1:C:940:HIS:NE2	2.47	0.47
1:D:767:SER:OG	1:D:768:GLN:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:ASP:OD1	1:B:459:ASP:N	2.43	0.47
1:C:542:THR:HG23	1:C:576:VAL:HG11	1.97	0.47
1:C:557:ASP:HB2	1:C:596:MET:HG2	1.97	0.47
1:D:936:ARG:HG2	1:D:938:GLY:H	1.80	0.47
1:A:864:ILE:O	1:A:869:SER:OG	2.31	0.47
1:B:207:HIS:H	1:B:229:SER:HB3	1.78	0.47
1:A:296:THR:OG1	1:A:339:GLN:OE1	2.32	0.47
1:B:105:PRO:HA	1:B:268:VAL:HG23	1.97	0.47
1:B:240:ILE:HG22	1:B:338:ILE:HG12	1.96	0.47
1:B:898:ASN:OD1	1:B:898:ASN:N	2.48	0.47
1:A:845:ARG:NE	1:A:848:GLU:OE2	2.47	0.47
1:C:664:ALA:HB1	1:C:692:LEU:HD22	1.97	0.47
1:B:718:ILE:HD12	1:B:729:ILE:HG21	1.97	0.47
1:C:465:LEU:O	1:C:469:SER:OG	2.31	0.47
1:A:593:ARG:NH2	1:A:599:THR:O	2.41	0.46
1:B:460:ARG:NE	6:B:1205:ACO:O1A	2.47	0.46
1:C:638:ILE:HG22	1:C:648:MET:HG2	1.97	0.46
1:D:687:ASP:HA	1:D:690:LYS:HG2	1.97	0.46
1:A:705:MET:HE3	1:A:866:VAL:HB	1.97	0.46
1:A:991:LEU:HD13	1:A:1011:ILE:HA	1.97	0.46
1:A:273:VAL:HG22	1:A:287:VAL:HG22	1.97	0.46
1:A:1092:LYS:NZ	1:A:1113:ASP:OD2	2.48	0.46
1:A:181:ALA:HB3	1:A:182:ARG:NH1	2.31	0.46
1:B:797:HIS:NE2	1:C:819:GLU:OE2	2.40	0.46
6:B:1205:ACO:H8A	6:B:1205:ACO:O9P	2.16	0.46
1:C:927:VAL:HG23	1:C:930:LYS:HE2	1.98	0.46
1:D:318:ASP:N	1:D:322:GLU:OE1	2.49	0.46
1:C:178:ASP:O	1:C:182:ARG:HG2	2.16	0.46
1:D:214:GLY:O	1:D:269:ASN:N	2.46	0.46
1:A:240:ILE:HG22	1:A:338:ILE:HG12	1.98	0.46
1:C:866:VAL:O	1:C:869:SER:N	2.49	0.46
1:A:880:MET:O	1:A:885:LEU:N	2.48	0.45
1:B:36:GLU:O	1:B:41:ARG:NH1	2.49	0.45
1:B:334:LEU:HD22	1:D:334:LEU:HD22	1.97	0.45
1:C:920:GLU:OE2	1:C:920:GLU:N	2.47	0.45
1:B:876:MET:HE3	1:B:876:MET:HB2	1.75	0.45
1:A:145:GLU:O	1:A:149:THR:OG1	2.29	0.45
1:B:214:GLY:O	1:B:269:ASN:N	2.49	0.45
1:B:703:KCX:HD2	1:B:705:MET:HB3	1.98	0.45
1:C:55:LYS:O	1:C:59:ALA:N	2.46	0.45
1:C:704:ASP:HB3	1:C:733:THR:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:VAL:HG23	1:A:391:VAL:HB	1.98	0.45
1:C:165:ARG:HD3	1:C:191:PHE:HE2	1.80	0.45
1:D:160:LEU:HD22	1:D:191:PHE:HB3	1.98	0.45
1:A:128:VAL:HG21	1:A:261:LEU:HB2	1.99	0.45
1:A:1044:ARG:NH2	6:A:1206:ACO:O9A	2.41	0.45
1:D:898:ASN:OD1	1:D:898:ASN:N	2.46	0.45
1:D:164:GLY:N	9:D:1203:ADP:O1B	2.46	0.45
1:B:935:ASP:N	1:B:935:ASP:OD1	2.50	0.45
1:D:637:ARG:HA	1:D:663:GLU:HB3	1.98	0.45
1:C:6:VAL:HG11	1:C:13:ALA:HA	1.98	0.45
1:D:500:LYS:HD3	1:D:561:PRO:HG2	1.98	0.45
1:D:856:VAL:HG12	1:D:873:VAL:HG13	1.99	0.45
1:B:532:LEU:O	1:B:536:HIS:NE2	2.44	0.45
1:B:666:ILE:HG23	1:B:688:LEU:HD23	1.99	0.45
1:B:722:LYS:NZ	1:B:753:ASP:OD2	2.50	0.45
1:C:852:MET:HA	1:C:852:MET:HE3	1.98	0.45
1:D:184:LYS:O	1:D:188:ILE:HG13	2.16	0.45
1:A:645:LEU:HD23	1:A:692:LEU:HD23	1.98	0.44
1:B:678:PRO:O	1:B:681:ASN:ND2	2.37	0.44
1:C:326:PRO:HB2	1:C:330:GLU:HG3	1.98	0.44
1:D:160:LEU:HD13	1:D:193:SER:HB2	1.99	0.44
1:D:1034:VAL:HG22	1:D:1047:VAL:HG22	2.00	0.44
1:C:63:ILE:HG23	1:C:91:PHE:HD1	1.81	0.44
1:D:842:LEU:HD23	1:D:842:LEU:HA	1.83	0.44
1:B:41:ARG:O	1:B:47:SER:OG	2.30	0.44
1:B:281:LYS:HB3	1:B:281:LYS:HE2	1.82	0.44
1:B:341:ARG:HG2	1:B:392:LYS:HB3	1.98	0.44
1:A:833:LEU:HA	1:A:836:GLN:HG2	1.99	0.44
1:A:847:ASP:O	1:A:851:GLN:NE2	2.50	0.44
1:C:160:LEU:HD22	1:C:193:SER:HB3	1.99	0.44
1:D:54:LYS:NZ	1:D:62:ASP:OD2	2.47	0.44
1:B:671:ASP:HB3	1:B:674:ASP:HB3	2.00	0.44
1:B:693:GLU:HG3	1:B:727:LEU:HG	1.98	0.44
1:B:828:GLY:N	10:B:1317:HOH:O	2.50	0.44
1:D:432:ASN:HD22	1:D:451:LEU:HD21	1.83	0.43
1:A:465:LEU:O	1:A:469:SER:OG	2.33	0.43
1:B:79:HIS:CD2	1:B:81:GLY:H	2.31	0.43
1:D:15:ARG:NH2	1:D:305:ASP:OD1	2.36	0.43
1:D:22:GLU:OE1	1:D:308:GLN:NE2	2.49	0.43
1:D:171:ARG:O	1:D:171:ARG:NH1	2.51	0.43
1:D:175:GLU:OE2	1:D:175:GLU:N	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:PHE:HE2	1:B:287:VAL:HG23	1.82	0.43
1:B:586:TRP:CD2	1:B:964:HIS:HB2	2.54	0.43
1:B:787:ILE:HD12	1:B:787:ILE:HA	1.90	0.43
1:D:63:ILE:HG23	1:D:91:PHE:HD1	1.82	0.43
1:A:138:VAL:O	1:A:180:TYR:OH	2.30	0.43
1:A:195:GLU:OE2	1:A:195:GLU:N	2.41	0.43
1:A:638:ILE:HG22	1:A:648:MET:HG2	2.00	0.43
1:B:209:GLU:HG2	1:B:274:GLU:HG2	2.00	0.43
1:B:575:ASP:OD1	1:B:579:ARG:NH2	2.51	0.43
1:C:11:GLU:OE1	1:C:82:TYR:OH	2.36	0.43
1:C:929:ASP:OD1	1:C:929:ASP:N	2.52	0.43
1:D:313:ILE:HD11	1:D:319:LEU:HD21	1.98	0.43
1:A:1118:ASP:H	1:A:1135:GLU:HB2	1.82	0.43
1:D:692:LEU:HD23	1:D:692:LEU:HA	1.88	0.43
1:A:7:ALA:HB1	1:A:66:ILE:HD13	2.01	0.43
1:A:542:THR:HG23	1:A:576:VAL:HG11	2.00	0.43
1:B:89:LEU:HD12	1:B:110:LEU:HB3	2.01	0.43
6:C:1205:ACO:H2B	6:C:1205:ACO:H8A	1.67	0.43
1:D:276:LEU:HD23	1:D:276:LEU:HA	1.90	0.43
1:A:1034:VAL:HG22	1:A:1047:VAL:HG22	2.01	0.43
1:D:886:THR:HG23	1:D:889:ASP:H	1.83	0.43
1:B:884:ASP:OD1	1:B:885:LEU:N	2.52	0.43
1:B:645:LEU:HD13	1:B:692:LEU:HD23	2.01	0.43
6:B:1205:ACO:H8A	6:B:1205:ACO:H2B	1.65	0.43
1:B:613:TYR:HD1	1:B:868:PRO:HB3	1.83	0.42
1:B:767:SER:OG	1:B:768:GLN:N	2.50	0.42
1:B:864:ILE:O	1:B:869:SER:OG	2.27	0.42
1:B:899:PHE:CD1	1:B:926:ILE:HG12	2.54	0.42
1:C:105:PRO:HG2	1:C:110:LEU:HG	2.01	0.42
1:D:872:VAL:HG13	1:D:903:VAL:HA	2.01	0.42
1:C:155:MET:HE2	1:C:155:MET:HB2	1.86	0.42
1:C:977:LEU:O	1:C:981:LYS:HG2	2.20	0.42
1:A:546:LEU:HD13	1:A:588:ARG:HG3	2.01	0.42
1:B:205:PRO:HB2	1:B:276:LEU:HD22	2.02	0.42
1:C:219:ASN:ND2	1:C:318:ASP:OD1	2.52	0.42
1:A:586:TRP:CD2	1:A:964:HIS:HB2	2.53	0.42
1:B:226:ARG:NH1	1:B:298:THR:OG1	2.51	0.42
1:C:929:ASP:OD1	1:C:930:LYS:NZ	2.47	0.42
1:D:57:ILE:HD13	1:D:57:ILE:HA	1.92	0.42
1:D:305:ASP:HB3	1:D:308:GLN:HB2	2.00	0.42
1:D:920:GLU:OE2	1:D:920:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:586:TRP:CD2	1:C:964:HIS:HB2	2.55	0.42
1:C:884:ASP:OD1	1:C:884:ASP:N	2.53	0.42
1:A:176:MET:HE3	1:A:176:MET:HB3	1.91	0.42
1:A:1080:LEU:HD23	1:A:1098:VAL:HG13	2.00	0.42
1:B:155:MET:HE2	1:B:201:TYR:HD2	1.83	0.42
1:C:205:PRO:HB2	1:C:276:LEU:HD22	2.01	0.42
1:A:296:THR:OG1	1:A:394:CYS:SG	2.78	0.42
1:B:224:HIS:CE1	1:B:333:LEU:HD13	2.55	0.42
1:B:856:VAL:HA	1:B:859:MET:HB3	2.01	0.42
1:C:856:VAL:HG12	1:C:873:VAL:HG13	2.02	0.42
1:D:603:MET:HE3	1:D:603:MET:HB2	1.88	0.42
1:A:921:LYS:HE3	1:A:921:LYS:HB2	1.89	0.42
1:C:153:PRO:HB3	1:C:171:ARG:HD3	2.02	0.42
1:C:547:GLN:NE2	10:C:1311:HOH:O	2.53	0.42
1:C:954:GLU:HB2	1:C:961:PRO:HD3	2.02	0.42
1:A:664:ALA:HB1	1:A:692:LEU:HD22	2.02	0.42
1:B:140:ILE:HD11	1:B:177:HIS:CD2	2.55	0.42
1:C:240:ILE:HG22	1:C:338:ILE:HG12	2.02	0.42
1:C:532:LEU:O	1:C:536:HIS:NE2	2.51	0.42
1:C:583:GLU:HB3	1:C:990:THR:HB	2.02	0.42
1:D:542:THR:HB	1:D:576:VAL:HG11	2.02	0.42
1:A:319:LEU:HD12	1:A:319:LEU:HA	1.91	0.41
1:A:718:ILE:HD12	1:A:729:ILE:HG21	2.02	0.41
1:A:1089:LYS:NZ	1:A:1137:ASN:O	2.53	0.41
1:D:465:LEU:HB3	1:D:1046:VAL:HG21	2.02	0.41
1:A:214:GLY:O	1:A:269:ASN:N	2.50	0.41
1:A:415:ARG:HD3	1:A:415:ARG:HA	1.95	0.41
1:A:820:VAL:HA	1:A:823:HIS:CE1	2.55	0.41
1:A:1072:GLY:HA3	1:A:1132:LEU:HA	2.01	0.41
1:B:299:GLU:OE2	1:B:306:ILE:N	2.48	0.41
1:B:542:THR:O	1:B:542:THR:OG1	2.30	0.41
1:B:603:MET:HE3	1:B:603:MET:HB2	1.87	0.41
1:C:470:MET:SD	1:C:474:ASN:ND2	2.88	0.41
1:A:305:ASP:HB3	1:A:308:GLN:HB2	2.02	0.41
1:A:1064:GLU:OE1	1:A:1070:GLN:NE2	2.54	0.41
1:B:664:ALA:HB1	1:B:692:LEU:HD22	2.01	0.41
1:B:945:ASP:HB3	1:B:948:THR:HB	2.02	0.41
1:D:820:VAL:HA	1:D:823:HIS:CE1	2.55	0.41
1:B:333:LEU:HD12	1:B:333:LEU:HA	1.87	0.41
1:D:215:ASP:HB3	1:D:319:LEU:HG	2.01	0.41
1:B:57:ILE:HD13	1:B:57:ILE:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:593:ARG:NH2	1:B:596:MET:O	2.46	0.41
1:B:683:GLN:NE2	1:B:687:ASP:OD1	2.51	0.41
1:B:971:MET:H	1:B:971:MET:HG2	1.59	0.41
1:C:4:LEU:HD21	1:C:79:HIS:HB2	2.02	0.41
1:D:872:VAL:HG21	1:D:906:PHE:HB2	2.02	0.41
1:B:296:THR:OG1	1:B:339:GLN:OE1	2.36	0.41
1:A:167:MET:HE2	1:A:167:MET:HB3	1.93	0.41
1:A:610:ALA:HB2	1:A:621:ILE:HD12	2.03	0.41
1:B:107:LEU:H	1:B:107:LEU:HD12	1.86	0.41
1:B:404:VAL:HG11	1:B:436:THR:HG22	2.01	0.41
1:D:319:LEU:HD22	1:D:325:LEU:HD12	2.03	0.41
1:D:548:ASP:OD2	1:D:994:THR:OG1	2.36	0.41
1:A:11:GLU:OE1	1:A:82:TYR:OH	2.38	0.41
1:A:284:PHE:CE1	1:A:287:VAL:HG23	2.54	0.41
1:A:731:LEU:HB3	1:A:755:ILE:HG22	2.02	0.41
1:A:742:ILE:HD13	1:D:777:ALA:HB1	2.02	0.41
1:C:319:LEU:HA	1:C:323:ILE:HD12	2.03	0.41
1:A:171:ARG:N	1:A:175:GLU:OE1	2.45	0.41
1:A:503:ALA:HA	1:A:506:ILE:HD12	2.03	0.41
1:A:1096:LEU:HD21	1:A:1110:ALA:HB2	2.03	0.41
1:B:735:ASP:HB3	1:B:740:GLY:HA3	2.03	0.41
1:A:6:VAL:HG11	1:A:13:ALA:HA	2.02	0.40
1:A:131:ILE:HD11	1:A:276:LEU:HD12	2.04	0.40
1:B:155:MET:HE2	1:B:155:MET:HB2	1.99	0.40
1:C:317:LYS:HB3	1:C:322:GLU:HB2	2.03	0.40
1:A:1071:ILE:HD12	1:A:1136:ILE:HG21	2.02	0.40
1:C:87:GLU:HG2	1:C:289:PRO:HD2	2.03	0.40
1:C:152:TYR:HB3	1:C:171:ARG:HD2	2.04	0.40
1:B:867:THR:HA	1:B:868:PRO:HA	1.93	0.40
1:C:761:SER:O	1:C:803:ARG:NH1	2.48	0.40
1:D:178:ASP:HB2	1:D:182:ARG:NH1	2.36	0.40
1:A:532:LEU:O	1:A:536:HIS:NE2	2.50	0.40
1:C:90:GLU:OE2	1:C:94:LYS:NZ	2.49	0.40
1:C:967:ILE:HD13	1:C:967:ILE:HA	1.97	0.40
1:D:112:ILE:HD13	1:D:112:ILE:HA	1.95	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	1134/1143 (99%)	1107 (98%)	27 (2%)	0	100	100
1	B	1053/1143 (92%)	1022 (97%)	31 (3%)	0	100	100
1	C	1055/1143 (92%)	1029 (98%)	26 (2%)	0	100	100
1	D	1055/1143 (92%)	1030 (98%)	25 (2%)	0	100	100
All	All	4297/4572 (94%)	4188 (98%)	109 (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	950/954 (100%)	939 (99%)	11 (1%)	63	79
1	B	884/954 (93%)	864 (98%)	20 (2%)	44	64
1	C	885/954 (93%)	870 (98%)	15 (2%)	53	73
1	D	885/954 (93%)	868 (98%)	17 (2%)	50	70
All	All	3604/3816 (94%)	3541 (98%)	63 (2%)	52	73

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ILE
1	A	391	VAL

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Mol	Chain	Res	Type
1	A	469	SER
1	A	497	LEU
1	A	502	THR
1	A	569	TRP
1	A	575	ASP
1	A	673	LEU
1	A	727	LEU
1	A	754	ILE
1	A	1129	THR
1	B	140	ILE
1	B	196	ILE
1	B	391	VAL
1	B	414	PHE
1	B	450	SER
1	B	469	SER
1	B	538	SER
1	B	569	TRP
1	B	609	ASN
1	B	669	THR
1	B	705	MET
1	B	754	ILE
1	B	771	MET
1	B	802	VAL
1	B	849	ILE
1	B	867	THR
1	B	872	VAL
1	B	897	LEU
1	B	922	LEU
1	B	1029	LEU
1	C	23	LEU
1	C	154	VAL
1	C	213	LEU
1	C	220	ILE
1	C	410	VAL
1	C	450	SER
1	C	469	SER
1	C	494	LEU
1	C	573	THR
1	C	911	LEU
1	C	915	VAL
1	C	932	VAL
1	C	948	THR

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Mol	Chain	Res	Type
1	C	967	ILE
1	C	977	LEU
1	D	186	GLU
1	D	221	ILE
1	D	293	VAL
1	D	336	SER
1	D	414	PHE
1	D	482	THR
1	D	494	LEU
1	D	542	THR
1	D	569	TRP
1	D	651	SER
1	D	705	MET
1	D	752	VAL
1	D	754	ILE
1	D	856	VAL
1	D	864	ILE
1	D	932	VAL
1	D	967	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	GLN
1	A	492	GLN
1	A	505	ASN
1	A	598	ASN
1	A	647	GLN
1	A	817	GLN
1	A	829	GLN
1	A	851	GLN
1	A	883	ASN
1	A	913	GLN
1	A	955	GLN
1	A	1049	ASN
1	A	1070	GLN
1	B	235	GLN
1	B	492	GLN
1	B	647	GLN
1	B	658	ASN
1	B	817	GLN
1	B	829	GLN

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Mol	Chain	Res	Type
1	B	836	GLN
1	B	857	ASN
1	B	980	GLN
1	B	983	GLN
1	B	1054	GLN
1	C	21	ASN
1	C	177	HIS
1	C	234	ASN
1	C	288	ASN
1	C	375	ASN
1	C	447	ASN
1	C	609	ASN
1	C	615	ASN
1	C	653	GLN
1	C	913	GLN
1	C	983	GLN
1	C	1051	GLN
1	D	231	GLN
1	D	439	GLN
1	D	496	ASN
1	D	647	GLN
1	D	749	GLN
1	D	780	HIS
1	D	817	GLN
1	D	829	GLN
1	D	836	GLN
1	D	895	ASN
1	D	974	GLN
1	D	1038	ASN
1	D	1049	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KCX	B	703	4,1	10,11,12	0.91	0	6,12,14	1.54	1 (16%)
1	KCX	C	703	1	10,11,12	0.91	0	6,12,14	1.03	1 (16%)
1	KCX	D	703	4,1	10,11,12	0.88	0	6,12,14	1.45	1 (16%)
1	KCX	A	703	4,1	10,11,12	0.86	0	6,12,14	1.46	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	B	703	4,1	-	0/9/10/12	-
1	KCX	C	703	1	-	0/9/10/12	-
1	KCX	D	703	4,1	-	1/9/10/12	-
1	KCX	A	703	4,1	-	0/9/10/12	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	703	KCX	OQ1-CX-NZ	-3.59	119.46	124.92
1	D	703	KCX	OQ1-CX-NZ	-3.23	120.02	124.92
1	A	703	KCX	OQ1-CX-NZ	-3.19	120.08	124.92
1	C	703	KCX	OQ1-CX-NZ	-2.36	121.34	124.92

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	703	KCX	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	703	KCX	3	0
1	A	703	KCX	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 12 are monoatomic - leaving 14 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
9	ADP	D	1203	3	28,29,29	1.42	4 (14%)	43,45,45	1.84	10 (23%)
7	PYR	D	1206	-	5,5,5	3.03	3 (60%)	3,6,6	1.60	1 (33%)
6	ACO	B	1205	-	51,53,53	2.68	18 (35%)	73,79,79	2.77	20 (27%)
5	ATP	A	1204	3	32,33,33	0.29	0	48,52,52	0.28	0
7	PYR	B	1206	-	5,5,5	3.02	3 (60%)	3,6,6	1.61	1 (33%)
9	ADP	C	1203	3	28,29,29	1.41	4 (14%)	43,45,45	1.86	10 (23%)
2	BTN	A	1201	1	15,16,17	3.34	2 (13%)	20,21,23	1.76	3 (15%)
6	ACO	C	1205	-	51,53,53	2.67	18 (35%)	73,79,79	2.79	20 (27%)
7	PYR	C	1206	-	5,5,5	3.04	3 (60%)	3,6,6	1.66	1 (33%)
7	PYR	A	1207	-	5,5,5	3.03	3 (60%)	3,6,6	1.68	1 (33%)
6	ACO	A	1206	-	51,53,53	2.66	18 (35%)	73,79,79	2.78	20 (27%)
8	BCT	A	1208	-	3,3,3	3.22	1 (33%)	2,3,3	2.73	2 (100%)
6	ACO	D	1205	-	51,53,53	2.67	18 (35%)	73,79,79	2.77	19 (26%)
9	ADP	B	1203	3	28,29,29	1.40	4 (14%)	43,45,45	1.85	10 (23%)

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
9	ADP	D	1203	3	-	3/16/32/32	0/3/3/3
7	PYR	D	1206	-	-	0/4/4/4	-
6	ACO	B	1205	-	-	24/51/67/67	0/3/3/3
5	ATP	A	1204	3	-	5/22/38/38	0/3/3/3
7	PYR	B	1206	-	-	0/4/4/4	-
9	ADP	C	1203	3	-	5/16/32/32	0/3/3/3
2	BTN	A	1201	1	-	3/6/27/28	0/2/2/2
6	ACO	C	1205	-	-	25/51/67/67	0/3/3/3
7	PYR	C	1206	-	-	0/4/4/4	-
7	PYR	A	1207	-	-	0/4/4/4	-
6	ACO	A	1206	-	-	12/51/67/67	0/3/3/3
6	ACO	D	1205	-	-	28/51/67/67	0/3/3/3
9	ADP	B	1203	3	-	3/16/32/32	0/3/3/3

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	BTN	C2-S1	-9.42	1.67	1.82
2	A	1201	BTN	O3-C3	8.51	1.41	1.23
6	C	1205	ACO	C5A-N7A	7.35	1.52	1.39
6	D	1205	ACO	C5A-N7A	7.31	1.52	1.39
6	B	1205	ACO	C5A-N7A	7.28	1.52	1.39
6	A	1206	ACO	C5A-N7A	7.22	1.52	1.39
6	B	1205	ACO	C8A-N9A	-5.95	1.27	1.37
6	A	1206	ACO	C8A-N9A	-5.93	1.27	1.37
6	D	1205	ACO	C8A-N9A	-5.91	1.27	1.37
6	C	1205	ACO	C8A-N9A	-5.84	1.27	1.37
6	B	1205	ACO	P1A-O3A	5.31	1.65	1.59
8	A	1208	BCT	O1-C	5.29	1.44	1.25
6	B	1205	ACO	C9P-N8P	5.25	1.45	1.33
6	B	1205	ACO	P2A-O3A	5.22	1.65	1.59
6	A	1206	ACO	C9P-N8P	5.20	1.45	1.33
6	C	1205	ACO	P1A-O3A	5.19	1.65	1.59
6	C	1205	ACO	C5P-N4P	5.15	1.45	1.33
6	A	1206	ACO	P2A-O3A	5.14	1.65	1.59
6	A	1206	ACO	P1A-O3A	5.13	1.65	1.59
6	D	1205	ACO	C5P-N4P	5.13	1.45	1.33
6	D	1205	ACO	P1A-O3A	5.13	1.65	1.59
6	B	1205	ACO	C5P-N4P	5.11	1.45	1.33
6	C	1205	ACO	C9P-N8P	5.08	1.45	1.33
6	C	1205	ACO	P2A-O3A	5.07	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1205	ACO	C9P-N8P	5.05	1.45	1.33
6	A	1206	ACO	C5P-N4P	5.00	1.45	1.33
6	D	1205	ACO	P2A-O3A	4.94	1.64	1.59
9	D	1203	ADP	C5-C4	4.76	1.47	1.39
9	C	1203	ADP	C5-C4	4.68	1.47	1.39
6	D	1205	ACO	O4B-C1B	4.58	1.52	1.42
9	B	1203	ADP	C5-C4	4.57	1.47	1.39
6	A	1206	ACO	O4B-C1B	4.57	1.52	1.42
6	C	1205	ACO	O4B-C1B	4.56	1.52	1.42
6	D	1205	ACO	C4A-N9A	-4.54	1.28	1.37
7	A	1207	PYR	CA-C	-4.54	1.39	1.54
6	B	1205	ACO	O4B-C1B	4.52	1.52	1.42
7	C	1206	PYR	CA-C	-4.52	1.39	1.54
6	A	1206	ACO	C4A-N9A	-4.52	1.28	1.37
6	C	1205	ACO	C4A-N9A	-4.51	1.28	1.37
7	D	1206	PYR	CA-C	-4.51	1.39	1.54
7	B	1206	PYR	CA-C	-4.50	1.39	1.54
6	B	1205	ACO	C4A-N9A	-4.46	1.28	1.37
6	B	1205	ACO	C6A-N6A	4.42	1.45	1.34
6	A	1206	ACO	C6A-N6A	4.38	1.45	1.34
6	D	1205	ACO	C6A-N6A	4.38	1.45	1.34
6	C	1205	ACO	C6A-N6A	4.38	1.45	1.34
6	D	1205	ACO	C2B-C3B	-3.83	1.44	1.53
6	B	1205	ACO	C2B-C3B	-3.76	1.44	1.53
6	A	1206	ACO	C2B-C3B	-3.74	1.44	1.53
6	C	1205	ACO	C2B-C3B	-3.74	1.44	1.53
7	C	1206	PYR	O3-CA	3.61	1.31	1.23
7	D	1206	PYR	O-C	3.59	1.31	1.22
7	A	1207	PYR	O3-CA	3.59	1.31	1.23
7	B	1206	PYR	O3-CA	3.59	1.31	1.23
7	D	1206	PYR	O3-CA	3.57	1.31	1.23
7	C	1206	PYR	O-C	3.56	1.31	1.22
7	B	1206	PYR	O-C	3.54	1.31	1.22
7	A	1207	PYR	O-C	3.50	1.31	1.22
6	A	1206	ACO	O4B-C4B	3.41	1.52	1.45
6	D	1205	ACO	O4B-C4B	3.39	1.52	1.45
6	C	1205	ACO	O4B-C4B	3.39	1.52	1.45
6	B	1205	ACO	O4B-C4B	3.32	1.52	1.45
6	D	1205	ACO	P3B-O3B	3.19	1.65	1.59
6	A	1206	ACO	P3B-O3B	3.11	1.65	1.59
6	C	1205	ACO	P3B-O3B	3.10	1.65	1.59
6	B	1205	ACO	P3B-O3B	3.04	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	1203	ADP	C5-C6	2.70	1.48	1.41
9	B	1203	ADP	C5-C6	2.69	1.48	1.41
9	C	1203	ADP	C5-C6	2.67	1.48	1.41
6	D	1205	ACO	C8A-N7A	2.46	1.36	1.31
6	C	1205	ACO	C8A-N7A	2.44	1.36	1.31
6	B	1205	ACO	C8A-N7A	2.41	1.36	1.31
6	A	1206	ACO	C8A-N7A	2.41	1.36	1.31
9	C	1203	ADP	C5-N7	-2.38	1.34	1.39
6	D	1205	ACO	O9P-C9P	-2.35	1.18	1.23
9	B	1203	ADP	C5-N7	-2.35	1.34	1.39
6	A	1206	ACO	P3B-O9A	-2.31	1.46	1.54
6	C	1205	ACO	P3B-O9A	-2.31	1.46	1.54
6	A	1206	ACO	O9P-C9P	-2.30	1.19	1.23
6	B	1205	ACO	P3B-O8A	-2.30	1.46	1.54
6	C	1205	ACO	O9P-C9P	-2.29	1.19	1.23
9	D	1203	ADP	C8-N7	2.29	1.36	1.31
6	D	1205	ACO	P3B-O9A	-2.28	1.46	1.54
6	B	1205	ACO	P3B-O9A	-2.28	1.46	1.54
6	C	1205	ACO	C5A-C4A	2.27	1.43	1.39
6	B	1205	ACO	O9P-C9P	-2.27	1.19	1.23
6	A	1206	ACO	C5A-C4A	2.27	1.43	1.39
6	D	1205	ACO	P3B-O8A	-2.26	1.46	1.54
6	D	1205	ACO	C5A-C4A	2.26	1.43	1.39
6	C	1205	ACO	P3B-O8A	-2.26	1.46	1.54
6	C	1205	ACO	O5P-C5P	-2.25	1.18	1.23
9	C	1203	ADP	C8-N7	2.25	1.36	1.31
6	A	1206	ACO	P3B-O8A	-2.25	1.46	1.54
9	B	1203	ADP	C8-N7	2.24	1.36	1.31
6	A	1206	ACO	O5P-C5P	-2.23	1.18	1.23
6	B	1205	ACO	C5A-C4A	2.23	1.43	1.39
9	D	1203	ADP	C5-N7	-2.22	1.35	1.39
6	B	1205	ACO	O5P-C5P	-2.20	1.18	1.23
6	D	1205	ACO	O5P-C5P	-2.20	1.18	1.23

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1205	ACO	C4A-N9A-C8A	15.80	122.33	105.74
6	D	1205	ACO	C4A-N9A-C8A	15.77	122.30	105.74
6	A	1206	ACO	C4A-N9A-C8A	15.73	122.25	105.74
6	B	1205	ACO	C4A-N9A-C8A	15.73	122.25	105.74
6	B	1205	ACO	N3A-C4A-N9A	6.15	137.62	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1205	ACO	N9A-C8A-N7A	-6.14	105.22	113.94
6	A	1206	ACO	N3A-C4A-N9A	6.11	137.56	127.17
6	A	1206	ACO	N9A-C8A-N7A	-6.10	105.28	113.94
6	D	1205	ACO	N9A-C8A-N7A	-6.10	105.28	113.94
6	D	1205	ACO	N3A-C4A-N9A	6.07	137.48	127.17
6	B	1205	ACO	N9A-C8A-N7A	-6.04	105.36	113.94
6	C	1205	ACO	N3A-C4A-N9A	6.03	137.43	127.17
9	C	1203	ADP	C5-C4-N3	-5.94	118.54	126.72
9	D	1203	ADP	C5-C4-N3	-5.87	118.64	126.72
9	B	1203	ADP	C5-C4-N3	-5.86	118.65	126.72
6	C	1205	ACO	C4A-C5A-N7A	-5.74	104.02	110.58
2	A	1201	BTN	C4-C2-S1	5.73	111.53	105.03
6	A	1206	ACO	C4A-C5A-N7A	-5.72	104.04	110.58
6	D	1205	ACO	C4A-C5A-N7A	-5.71	104.05	110.58
6	B	1205	ACO	C4A-C5A-N7A	-5.63	104.14	110.58
6	A	1206	ACO	C5A-C4A-N3A	-5.13	119.66	126.72
6	B	1205	ACO	C5A-C4A-N3A	-5.12	119.66	126.72
6	D	1205	ACO	C5A-C4A-N3A	-5.08	119.72	126.72
6	C	1205	ACO	C5A-C4A-N3A	-5.04	119.77	126.72
9	C	1203	ADP	N3-C4-N9	4.74	135.23	127.17
9	B	1203	ADP	N3-C4-N9	4.70	135.16	127.17
9	D	1203	ADP	N3-C4-N9	4.68	135.13	127.17
6	C	1205	ACO	N3A-C2A-N1A	-4.22	122.19	128.58
6	B	1205	ACO	N3A-C2A-N1A	-4.20	122.22	128.58
6	D	1205	ACO	N3A-C2A-N1A	-4.17	122.27	128.58
6	A	1206	ACO	N3A-C2A-N1A	-4.12	122.34	128.58
9	C	1203	ADP	C2-N3-C4	3.75	120.98	111.83
9	B	1203	ADP	C2-N3-C4	3.71	120.90	111.83
9	D	1203	ADP	C2-N3-C4	3.70	120.88	111.83
6	C	1205	ACO	C4A-N9A-C1B	-3.67	118.05	126.63
6	C	1205	ACO	C4B-O4B-C1B	-3.62	101.47	109.47
6	D	1205	ACO	C4A-N9A-C1B	-3.62	118.18	126.63
6	B	1205	ACO	C4B-O4B-C1B	-3.60	101.53	109.47
6	B	1205	ACO	C4A-N9A-C1B	-3.56	118.31	126.63
6	A	1206	ACO	C4A-N9A-C1B	-3.53	118.38	126.63
6	A	1206	ACO	C4B-O4B-C1B	-3.50	101.73	109.47
6	A	1206	ACO	C1B-N9A-C8A	-3.48	119.37	127.09
9	D	1203	ADP	C4-C5-N7	-3.46	106.63	110.58
9	B	1203	ADP	C4-C5-N7	-3.45	106.63	110.58
6	B	1205	ACO	C1B-N9A-C8A	-3.45	119.43	127.09
9	C	1203	ADP	C4-C5-N7	-3.43	106.66	110.58
6	D	1205	ACO	C1B-N9A-C8A	-3.41	119.52	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1205	ACO	C1B-N9A-C8A	-3.37	119.62	127.09
6	B	1205	ACO	C2A-N3A-C4A	3.34	119.98	111.83
6	C	1205	ACO	C2A-N3A-C4A	3.32	119.95	111.83
6	D	1205	ACO	C2A-N3A-C4A	3.31	119.92	111.83
6	A	1206	ACO	C2A-N3A-C4A	3.30	119.89	111.83
9	C	1203	ADP	N3-C2-N1	-3.24	123.67	128.58
9	B	1203	ADP	N3-C2-N1	-3.24	123.68	128.58
9	D	1203	ADP	N3-C2-N1	-3.23	123.69	128.58
8	A	1208	BCT	O2-C-O1	-3.21	111.46	119.68
6	C	1205	ACO	C6A-C5A-N7A	3.15	138.17	132.09
2	A	1201	BTN	C5-C6-S1	3.10	110.33	106.06
6	D	1205	ACO	C4B-O4B-C1B	-3.08	102.66	109.47
6	D	1205	ACO	C6A-C5A-N7A	3.07	138.00	132.09
6	A	1206	ACO	C6A-C5A-N7A	3.04	137.96	132.09
6	B	1205	ACO	C6A-C5A-N7A	3.02	137.92	132.09
6	B	1205	ACO	C5A-C4A-N9A	-2.84	102.71	105.81
6	A	1206	ACO	C5A-C4A-N9A	-2.78	102.78	105.81
6	C	1205	ACO	C5A-C4A-N9A	-2.77	102.80	105.81
6	D	1205	ACO	C5A-C4A-N9A	-2.77	102.80	105.81
9	B	1203	ADP	C4-N9-C8	2.72	108.59	105.74
9	D	1203	ADP	C4-N9-C8	2.67	108.54	105.74
6	B	1205	ACO	O2A-P1A-O1A	-2.64	100.17	112.44
9	C	1203	ADP	C4-N9-C8	2.61	108.48	105.74
9	B	1203	ADP	C5-N7-C8	2.61	107.55	103.45
9	C	1203	ADP	C5-N7-C8	2.56	107.47	103.45
9	D	1203	ADP	C5-N7-C8	2.53	107.43	103.45
6	D	1205	ACO	O2A-P1A-O1A	-2.45	101.05	112.44
6	A	1206	ACO	O2A-P1A-O1A	-2.43	101.15	112.44
9	C	1203	ADP	C3'-C2'-C1'	2.42	106.03	101.46
6	B	1205	ACO	C3B-C2B-C1B	2.41	105.20	99.89
6	C	1205	ACO	O5A-P2A-O4A	-2.41	101.22	112.44
6	D	1205	ACO	C3B-C2B-C1B	2.41	105.18	99.89
6	C	1205	ACO	O2A-P1A-O1A	-2.40	101.27	112.44
9	D	1203	ADP	C3'-C2'-C1'	2.40	106.00	101.46
6	C	1205	ACO	C3B-C2B-C1B	2.40	105.16	99.89
7	A	1207	PYR	OXT-C-CA	2.39	120.21	113.59
6	B	1205	ACO	O5A-P2A-O4A	-2.38	101.35	112.44
9	B	1203	ADP	C3'-C2'-C1'	2.38	105.97	101.46
6	D	1205	ACO	O5A-P2A-O4A	-2.38	101.37	112.44
7	C	1206	PYR	OXT-C-CA	2.37	120.17	113.59
6	A	1206	ACO	O5A-P2A-O4A	-2.37	101.41	112.44
6	A	1206	ACO	CAP-C9P-N8P	2.34	120.92	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1206	PYR	OXT-C-CA	2.27	119.89	113.59
6	A	1206	ACO	C3B-C2B-C1B	2.27	104.88	99.89
6	A	1206	ACO	C7P-C6P-C5P	-2.26	108.62	112.39
7	D	1206	PYR	OXT-C-CA	2.25	119.84	113.59
6	C	1205	ACO	C2B-C3B-C4B	2.23	107.14	103.24
6	B	1205	ACO	O8A-P3B-O3B	2.21	114.47	105.85
6	A	1206	ACO	O8A-P3B-O3B	2.19	114.37	105.85
6	C	1205	ACO	O8A-P3B-O3B	2.18	114.35	105.85
6	D	1205	ACO	O8A-P3B-O3B	2.18	114.33	105.85
9	C	1203	ADP	C2'-C1'-N9	-2.14	107.99	113.30
6	C	1205	ACO	CAP-C9P-N8P	2.14	120.54	116.48
6	B	1205	ACO	C2B-C3B-C4B	2.14	106.98	103.24
8	A	1208	BCT	O3-C-O1	-2.13	114.22	119.68
6	D	1205	ACO	O9A-P3B-O3B	2.13	114.16	105.85
6	B	1205	ACO	O9A-P3B-O3B	2.12	114.10	105.85
6	C	1205	ACO	C6P-C5P-N4P	2.10	120.17	116.34
6	D	1205	ACO	C6P-C5P-N4P	2.10	120.17	116.34
6	D	1205	ACO	CAP-C9P-N8P	2.06	120.39	116.48
9	D	1203	ADP	C6-C5-N7	2.05	136.05	132.09
9	B	1203	ADP	N9-C8-N7	-2.04	111.04	113.94
6	A	1206	ACO	C6P-C5P-N4P	2.03	120.05	116.34
9	C	1203	ADP	C6-C5-N7	2.03	136.00	132.09
9	B	1203	ADP	C6-C5-N7	2.03	136.00	132.09
6	B	1205	ACO	C2P-C3P-N4P	-2.02	108.19	112.41
6	C	1205	ACO	O9A-P3B-O3B	2.02	113.73	105.85
6	B	1205	ACO	C2P-S1P-C	2.02	111.15	101.42
6	A	1206	ACO	C3P-N4P-C5P	-2.01	119.07	122.82
9	D	1203	ADP	C2'-C1'-N9	-2.00	108.33	113.30
2	A	1201	BTN	C6-C5-N1	-2.00	110.60	113.18

There are no chirality outliers.

All (108) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	BTN	C9-C10-C11-O11
5	A	1204	ATP	C5'-O5'-PA-O1A
5	A	1204	ATP	C5'-O5'-PA-O2A
5	A	1204	ATP	C5'-O5'-PA-O3A
6	A	1206	ACO	O-C-S1P-C2P
6	A	1206	ACO	CH3-C-S1P-C2P
6	B	1205	ACO	CCP-O6A-P2A-O3A
6	B	1205	ACO	CCP-O6A-P2A-O4A

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Mol	Chain	Res	Type	Atoms
6	B	1205	ACO	CCP-O6A-P2A-O5A
6	B	1205	ACO	C9P-CAP-CBP-CCP
6	B	1205	ACO	C9P-CAP-CBP-CDP
6	B	1205	ACO	N8P-C9P-CAP-OAP
6	B	1205	ACO	C3P-C2P-S1P-C
6	C	1205	ACO	P1A-O3A-P2A-O6A
6	C	1205	ACO	CCP-O6A-P2A-O3A
6	C	1205	ACO	CCP-O6A-P2A-O4A
6	C	1205	ACO	CCP-O6A-P2A-O5A
6	C	1205	ACO	CDP-CBP-CCP-O6A
6	C	1205	ACO	CEP-CBP-CCP-O6A
6	C	1205	ACO	CAP-CBP-CCP-O6A
6	C	1205	ACO	C9P-CAP-CBP-CCP
6	C	1205	ACO	C9P-CAP-CBP-CDP
6	C	1205	ACO	C9P-CAP-CBP-CEP
6	C	1205	ACO	O9P-C9P-CAP-CBP
6	C	1205	ACO	N8P-C9P-CAP-OAP
6	C	1205	ACO	C3P-C2P-S1P-C
6	D	1205	ACO	C2B-C1B-N9A-C8A
6	D	1205	ACO	C5B-O5B-P1A-O2A
6	D	1205	ACO	C5B-O5B-P1A-O3A
6	D	1205	ACO	P1A-O3A-P2A-O6A
6	D	1205	ACO	CCP-O6A-P2A-O3A
6	D	1205	ACO	CCP-O6A-P2A-O5A
6	D	1205	ACO	CDP-CBP-CCP-O6A
6	D	1205	ACO	CEP-CBP-CCP-O6A
6	D	1205	ACO	CAP-CBP-CCP-O6A
6	D	1205	ACO	C9P-CAP-CBP-CCP
6	D	1205	ACO	C9P-CAP-CBP-CDP
6	D	1205	ACO	C9P-CAP-CBP-CEP
6	D	1205	ACO	O9P-C9P-CAP-CBP
6	D	1205	ACO	N8P-C9P-CAP-OAP
9	D	1203	ADP	C5'-O5'-PA-O1A
6	D	1205	ACO	C2B-C1B-N9A-C4A
6	A	1206	ACO	S1P-C2P-C3P-N4P
6	B	1205	ACO	S1P-C2P-C3P-N4P
6	D	1205	ACO	S1P-C2P-C3P-N4P
6	B	1205	ACO	O9P-C9P-CAP-OAP
6	C	1205	ACO	O9P-C9P-CAP-OAP
6	D	1205	ACO	O9P-C9P-CAP-OAP
6	A	1206	ACO	C2B-C1B-N9A-C8A
6	B	1205	ACO	C2B-C1B-N9A-C8A

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Mol	Chain	Res	Type	Atoms
6	B	1205	ACO	OAP-CAP-CBP-CDP
6	B	1205	ACO	OAP-CAP-CBP-CEP
6	C	1205	ACO	OAP-CAP-CBP-CDP
6	C	1205	ACO	OAP-CAP-CBP-CEP
6	D	1205	ACO	OAP-CAP-CBP-CDP
6	D	1205	ACO	OAP-CAP-CBP-CEP
6	B	1205	ACO	O9P-C9P-CAP-CBP
6	C	1205	ACO	S1P-C2P-C3P-N4P
6	C	1205	ACO	N8P-C9P-CAP-CBP
6	D	1205	ACO	N8P-C9P-CAP-CBP
2	A	1201	BTN	S1-C2-C7-C8
6	C	1205	ACO	C2B-C1B-N9A-C8A
2	A	1201	BTN	C4-C2-C7-C8
6	C	1205	ACO	O5P-C5P-C6P-C7P
6	C	1205	ACO	N4P-C5P-C6P-C7P
6	B	1205	ACO	C9P-CAP-CBP-CEP
5	A	1204	ATP	PA-O3A-PB-O1B
9	B	1203	ADP	PB-O3A-PA-O2A
9	D	1203	ADP	PB-O3A-PA-O1A
6	A	1206	ACO	CDP-CBP-CCP-O6A
6	A	1206	ACO	CEP-CBP-CCP-O6A
6	B	1205	ACO	CDP-CBP-CCP-O6A
6	A	1206	ACO	C3P-C2P-S1P-C
6	B	1205	ACO	C3B-O3B-P3B-O7A
6	D	1205	ACO	C3P-C2P-S1P-C
6	B	1205	ACO	CAP-CBP-CCP-O6A
6	B	1205	ACO	C5B-O5B-P1A-O2A
6	B	1205	ACO	OAP-CAP-CBP-CCP
6	C	1205	ACO	OAP-CAP-CBP-CCP
6	D	1205	ACO	CCP-O6A-P2A-O4A
6	D	1205	ACO	OAP-CAP-CBP-CCP
9	B	1203	ADP	C5'-O5'-PA-O3A
9	C	1203	ADP	C5'-O5'-PA-O1A
9	C	1203	ADP	C5'-O5'-PA-O2A
9	C	1203	ADP	C5'-O5'-PA-O3A
6	D	1205	ACO	O4B-C4B-C5B-O5B
6	B	1205	ACO	P2A-O3A-P1A-O2A
6	A	1206	ACO	C2B-C1B-N9A-C4A
6	B	1205	ACO	C2B-C1B-N9A-C4A
6	C	1205	ACO	C2B-C1B-N9A-C4A
6	B	1205	ACO	N8P-C9P-CAP-CBP
6	A	1206	ACO	N8P-C9P-CAP-OAP

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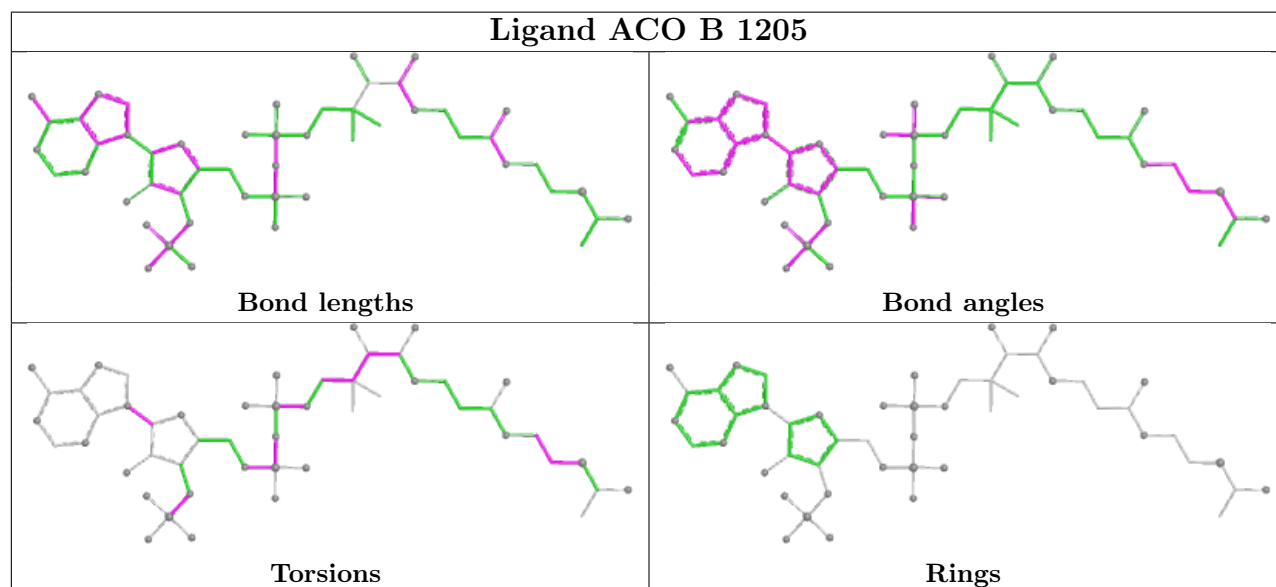
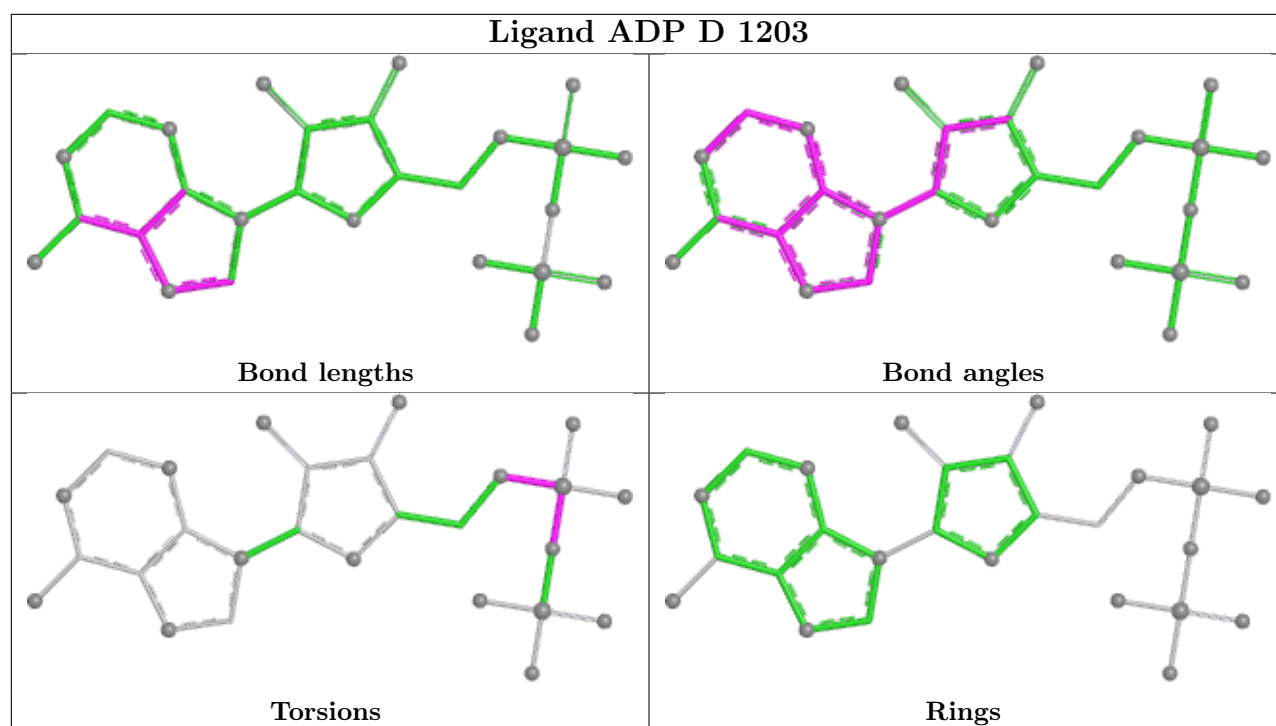
Mol	Chain	Res	Type	Atoms
6	A	1206	ACO	O9P-C9P-CAP-OAP
6	D	1205	ACO	C3B-O3B-P3B-O7A
9	B	1203	ADP	PB-O3A-PA-O1A
9	C	1203	ADP	PB-O3A-PA-O1A
6	D	1205	ACO	O5P-C5P-C6P-C7P
6	D	1205	ACO	N4P-C5P-C6P-C7P
6	A	1206	ACO	O4B-C1B-N9A-C8A
6	B	1205	ACO	O4B-C1B-N9A-C8A
6	C	1205	ACO	O4B-C1B-N9A-C8A
5	A	1204	ATP	PA-O3A-PB-O2B
9	C	1203	ADP	PB-O3A-PA-O2A
9	D	1203	ADP	PB-O3A-PA-O2A
6	C	1205	ACO	C3B-O3B-P3B-O9A
6	D	1205	ACO	C3B-O3B-P3B-O9A
6	B	1205	ACO	CEP-CBP-CCP-O6A
6	A	1206	ACO	P1A-O3A-P2A-O5A

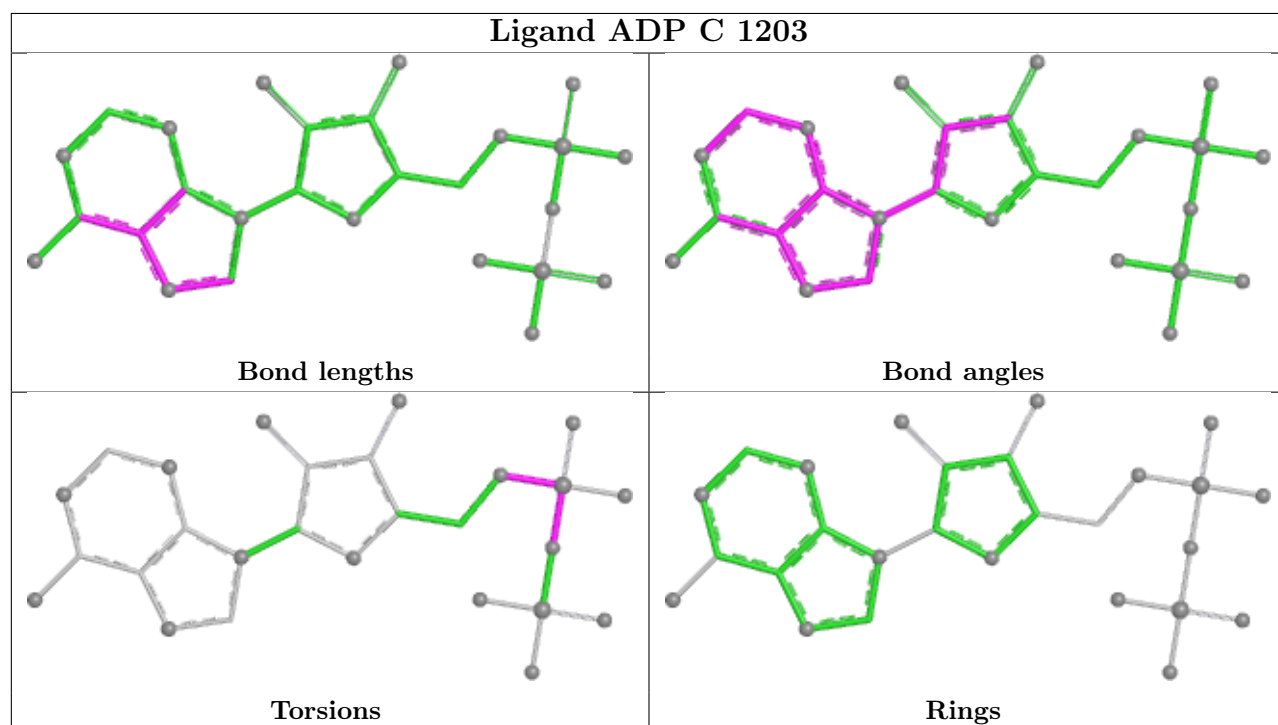
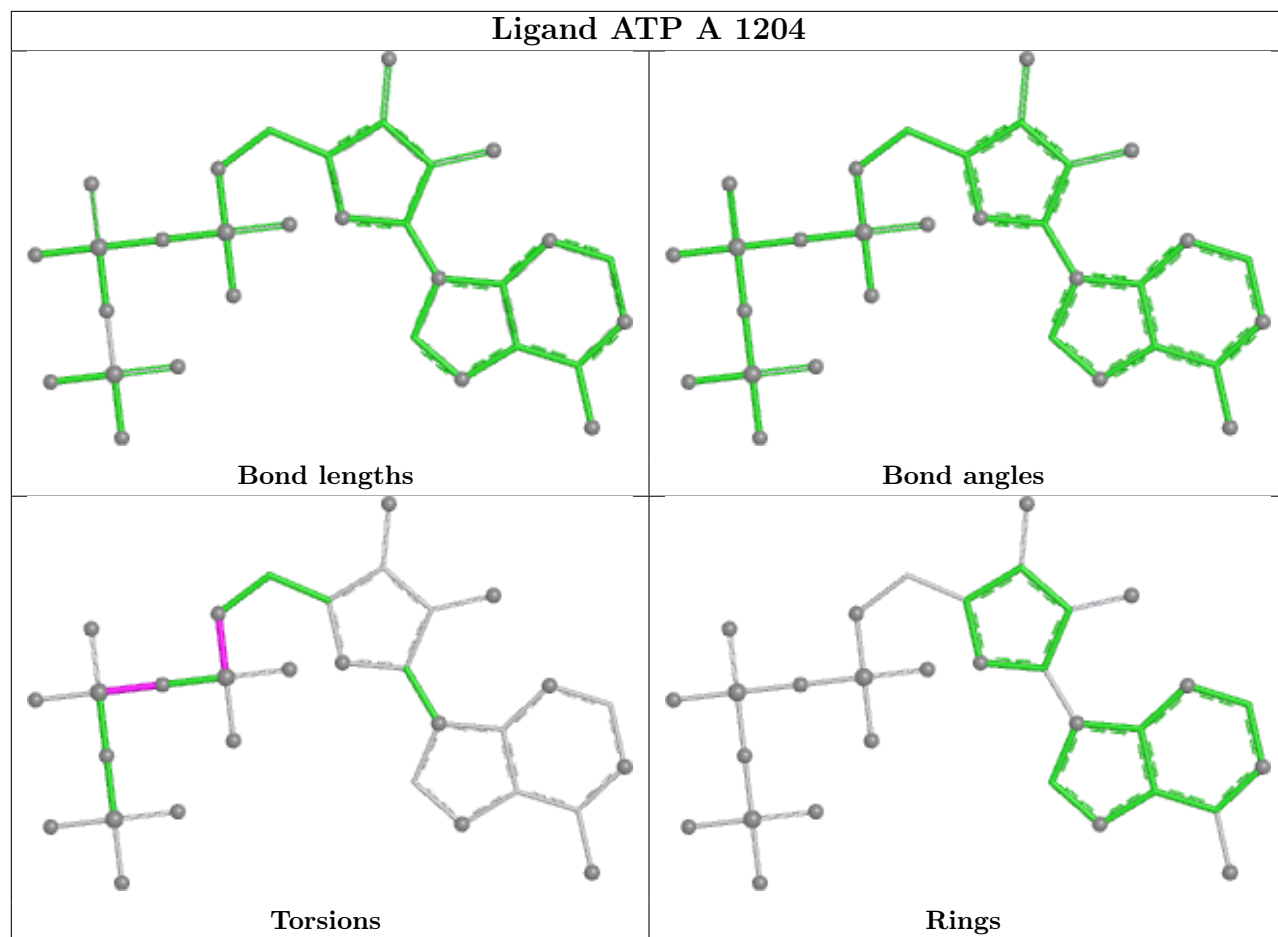
There are no ring outliers.

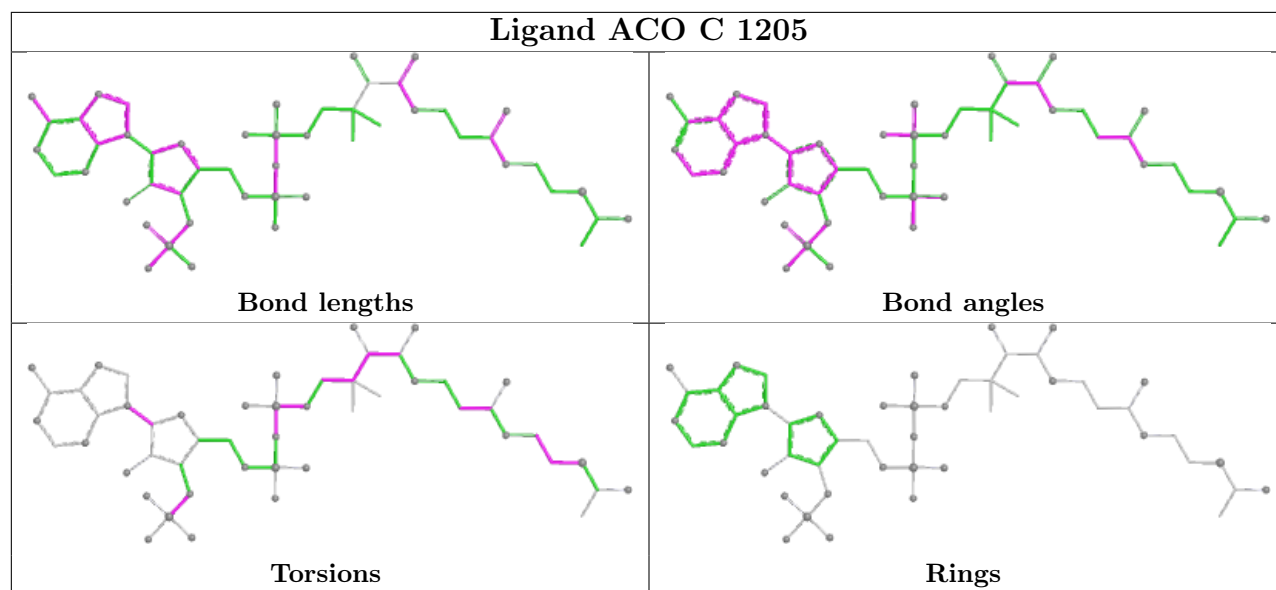
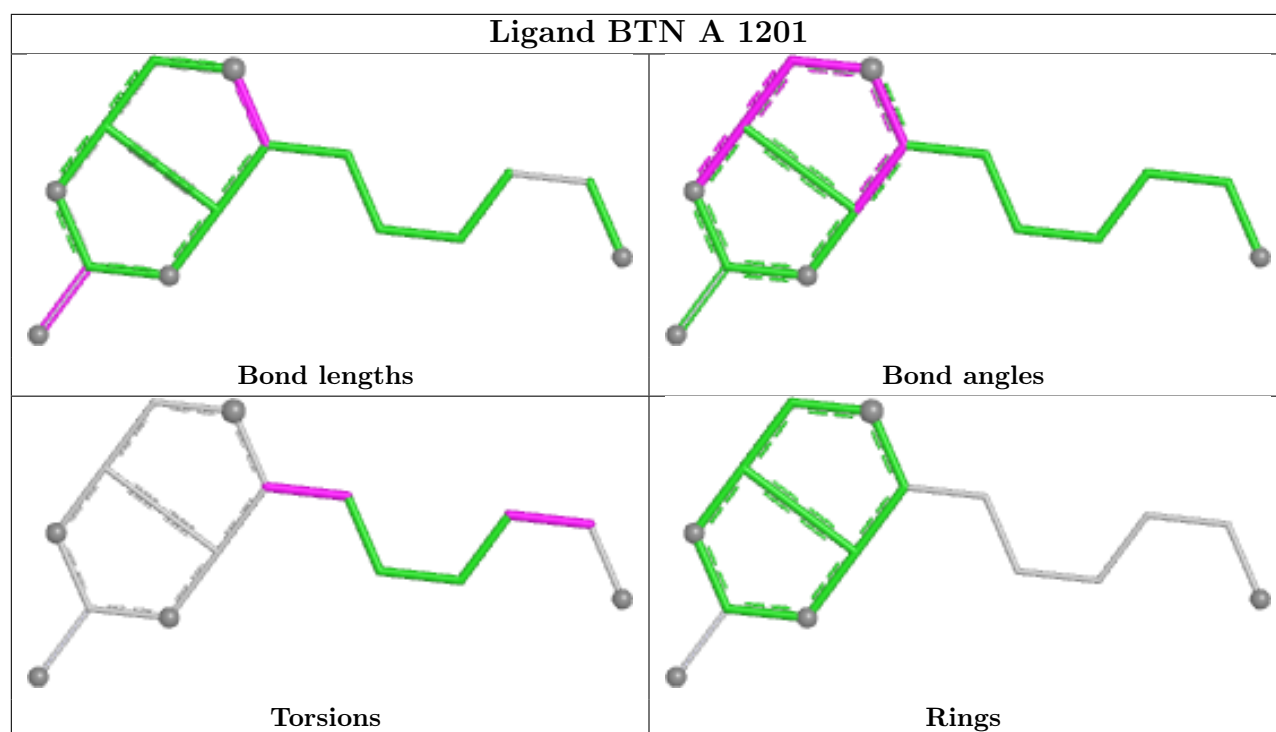
5 monomers are involved in 7 short contacts:

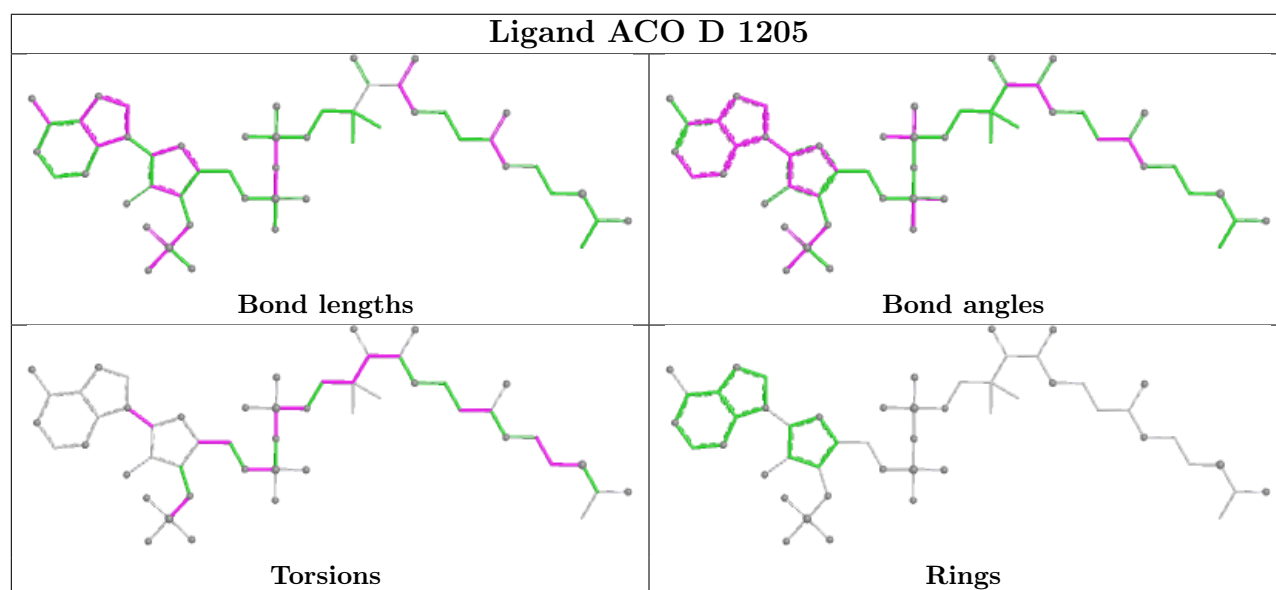
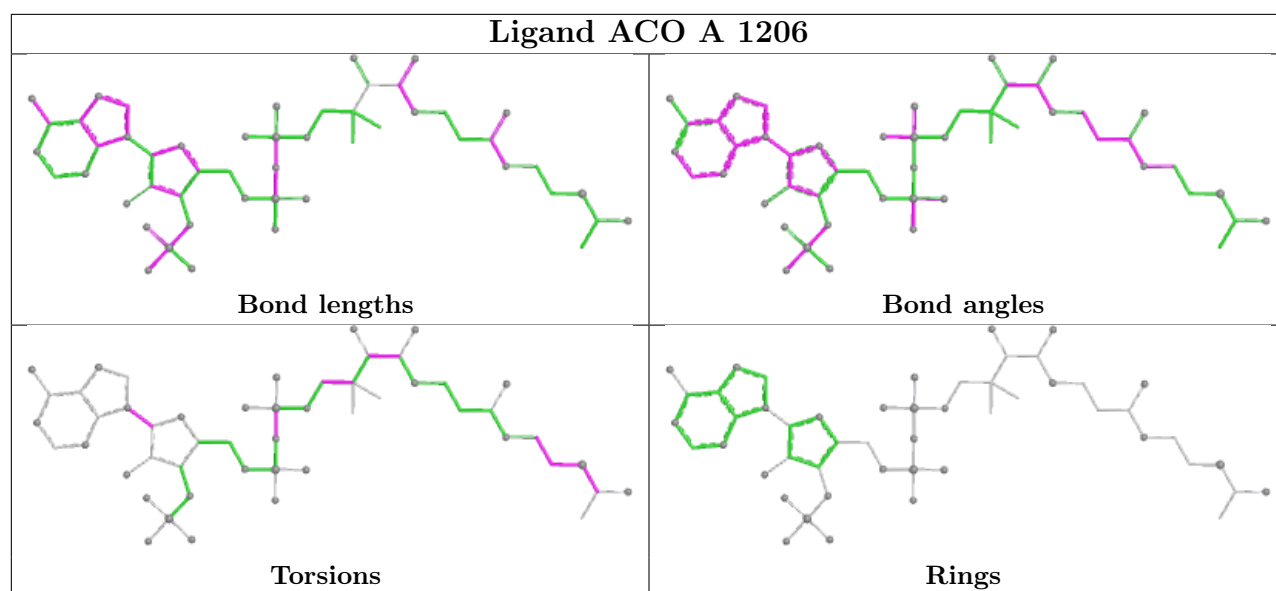
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	1203	ADP	1	0
6	B	1205	ACO	3	0
6	C	1205	ACO	1	0
6	A	1206	ACO	1	0
9	B	1203	ADP	1	0

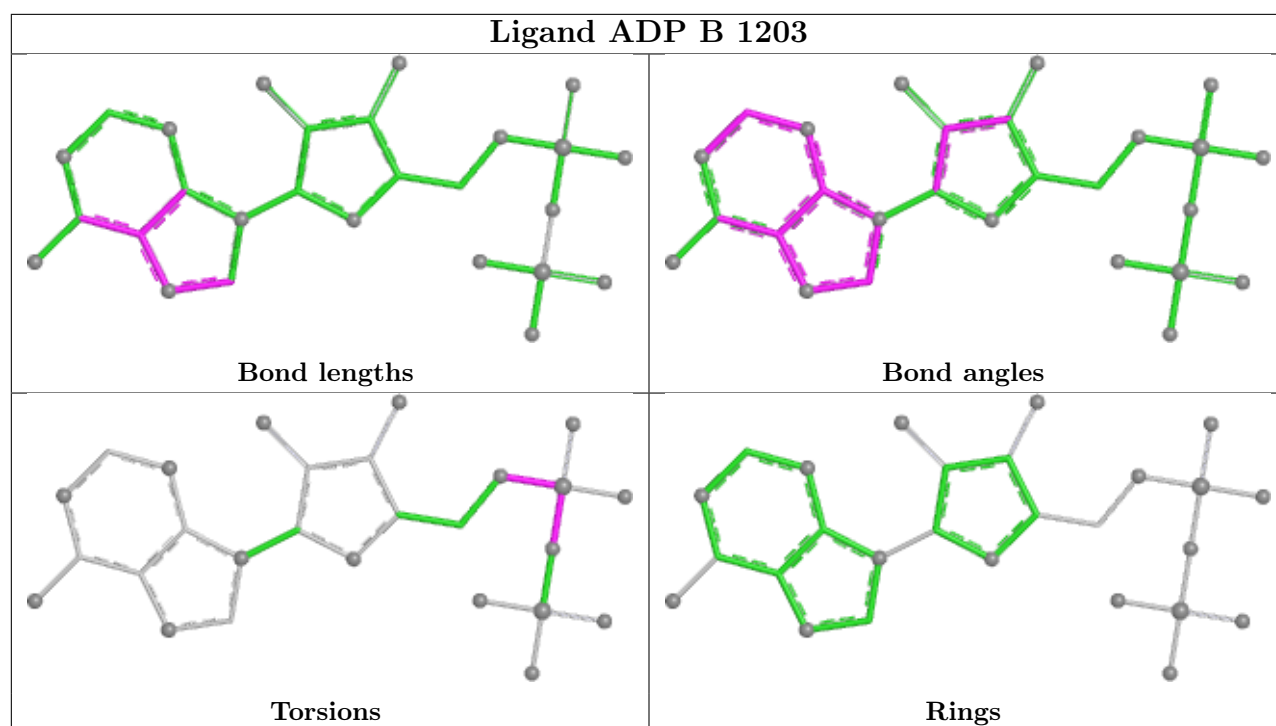
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	702:VAL	C	703:KCX	N	3.14
1	B	702:VAL	C	703:KCX	N	3.13

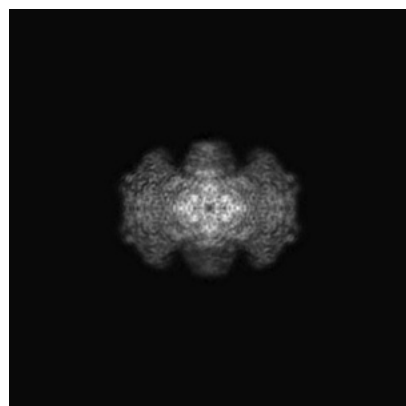
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15033. These allow visual inspection of the internal detail of the map and identification of artifacts.

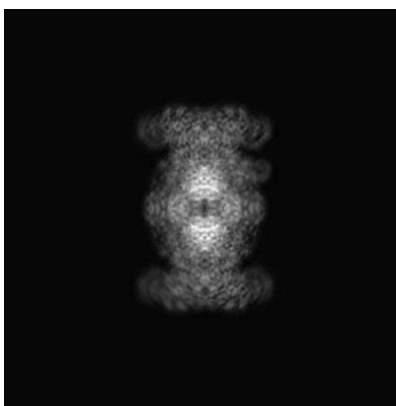
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

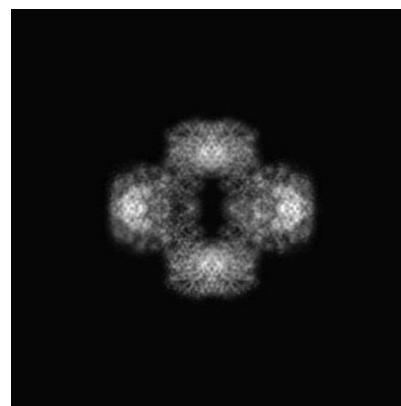
6.1.1 Primary map



X

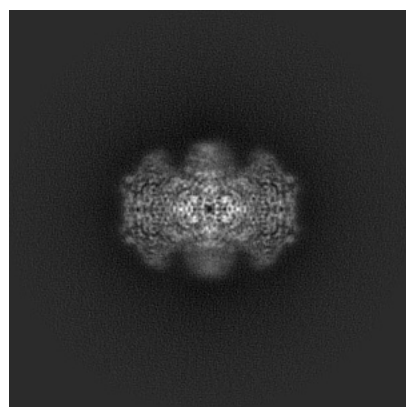


Y

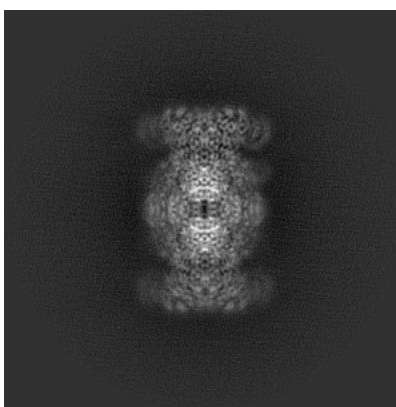


Z

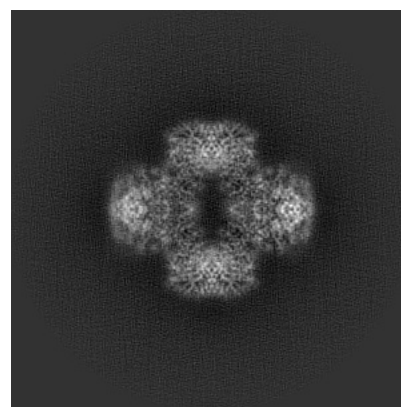
6.1.2 Raw map



X



Y

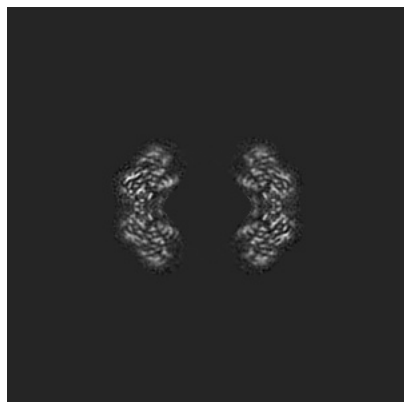


Z

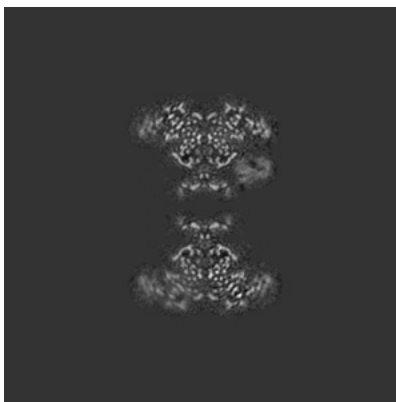
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

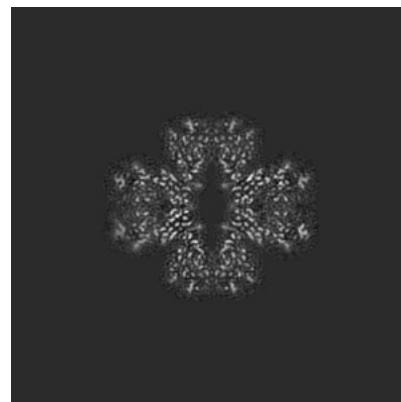
6.2.1 Primary map



X Index: 150

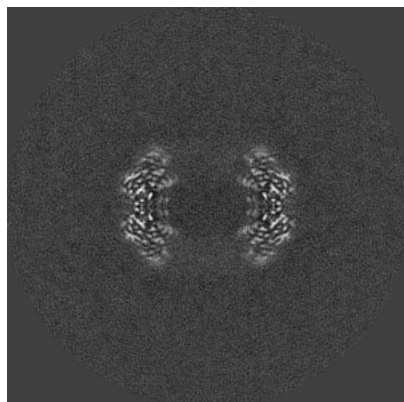


Y Index: 150

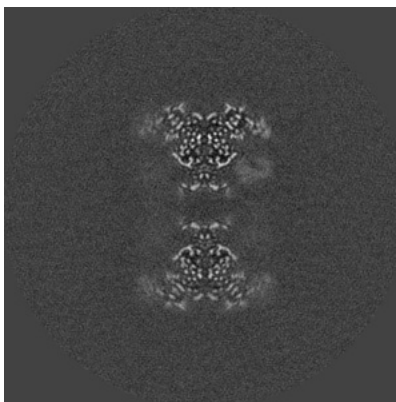


Z Index: 150

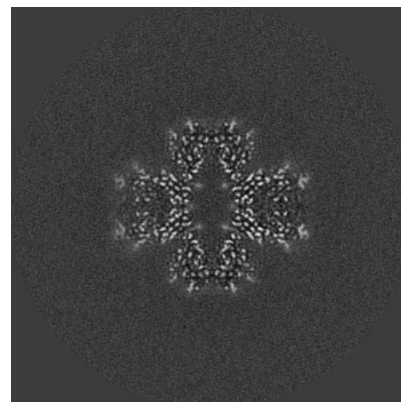
6.2.2 Raw map



X Index: 150



Y Index: 150

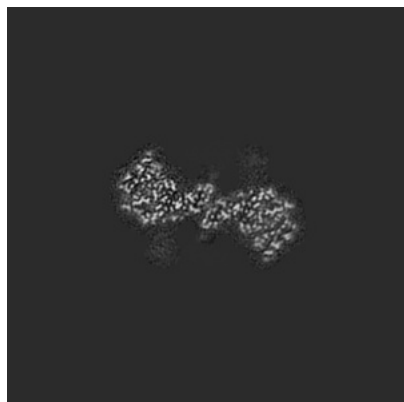


Z Index: 150

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

6.3 Largest variance slices [i](#)

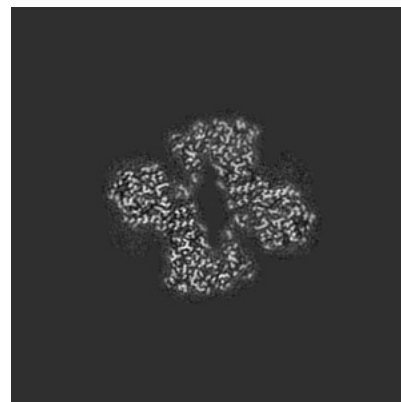
6.3.1 Primary map



X Index: 134

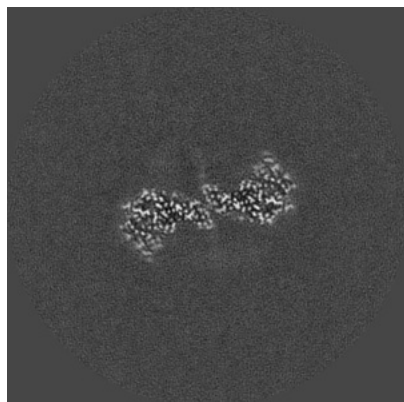


Y Index: 146

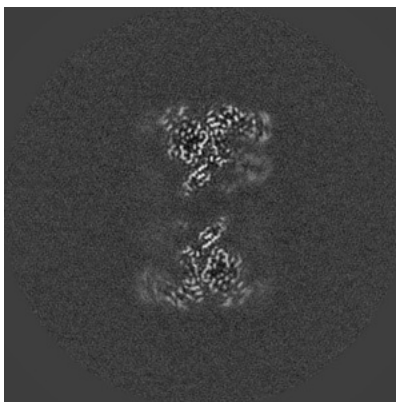


Z Index: 156

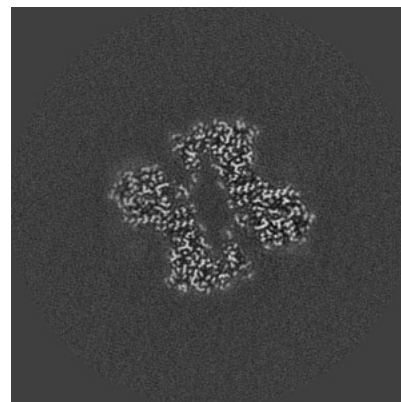
6.3.2 Raw map



X Index: 166



Y Index: 145

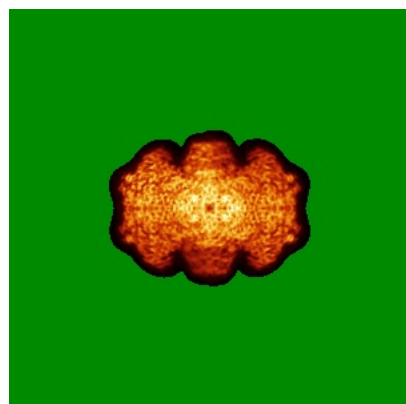


Z Index: 156

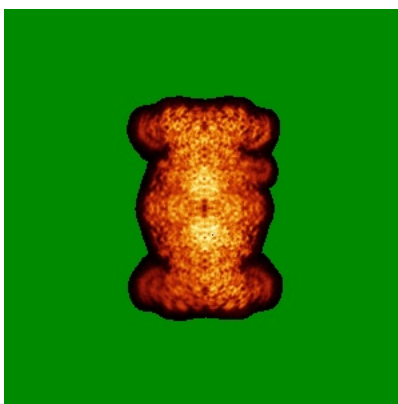
The images above show the largest variance slices of the map in three orthogonal directions.

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

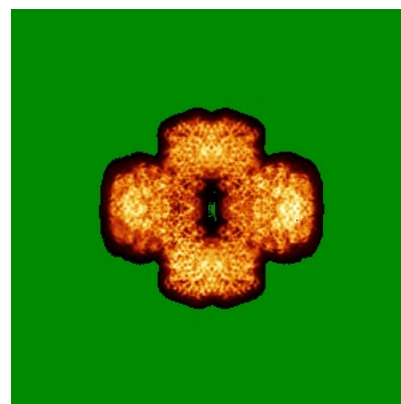
6.4.1 Primary map



X

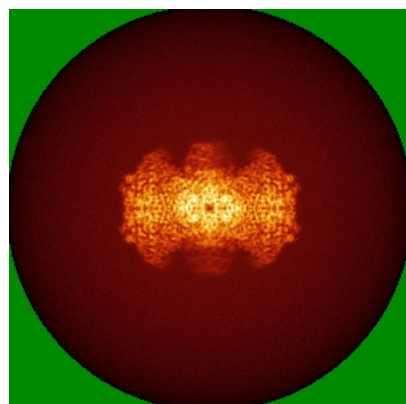


Y

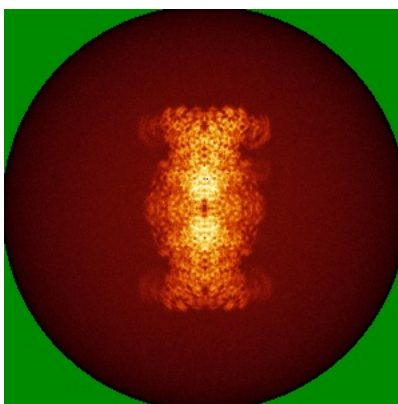


Z

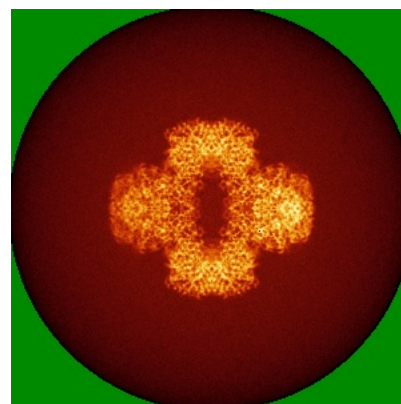
6.4.2 Raw map



X



Y

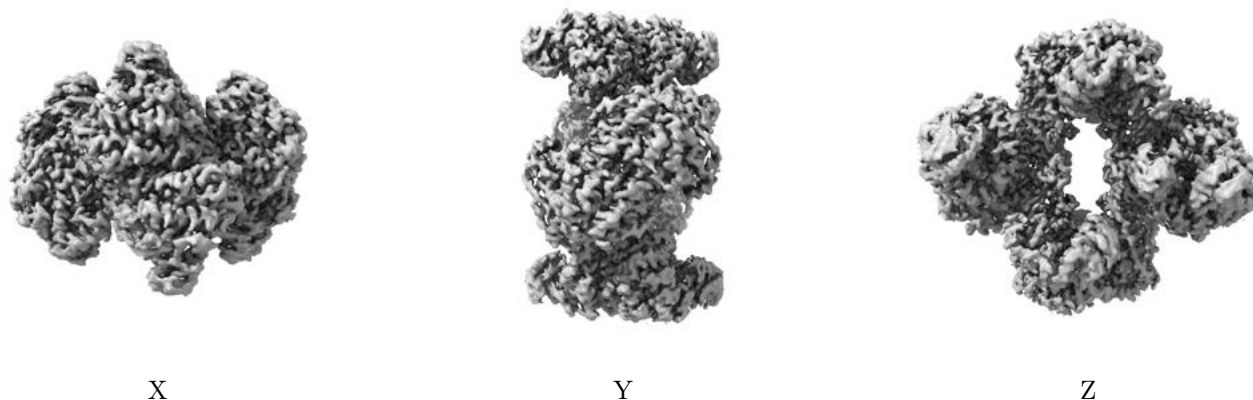


Z

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.

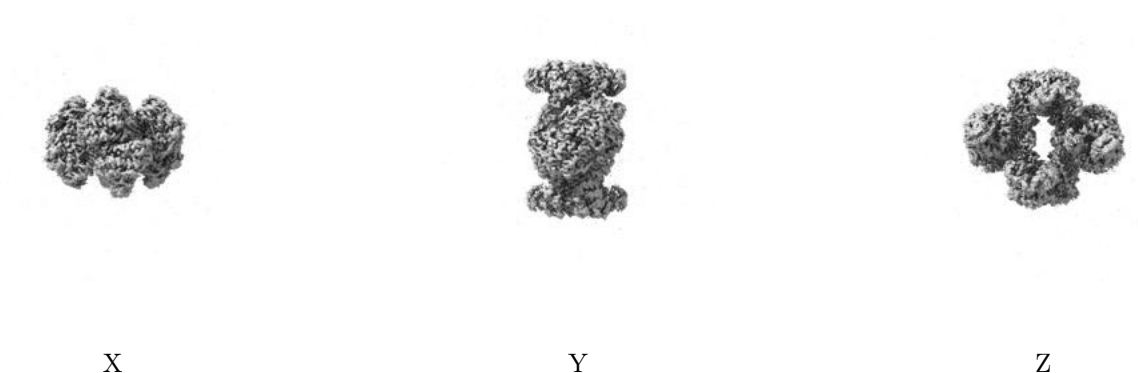
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.143. 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.

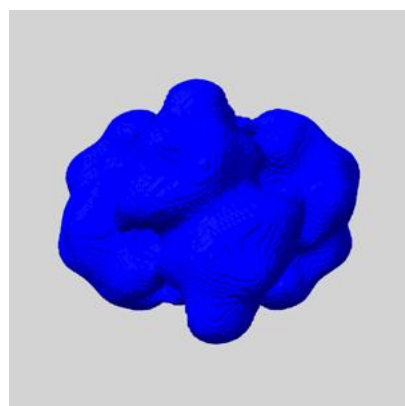
6.6 Mask visualisation [i](#)

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

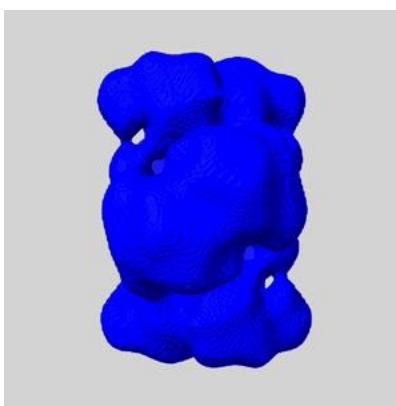
A mask typically either:

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

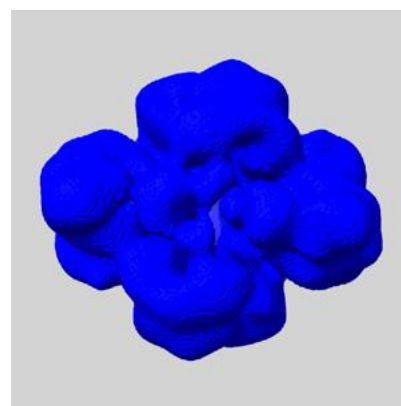
6.6.1 emd_15033_msk_1.map [i](#)



X



Y

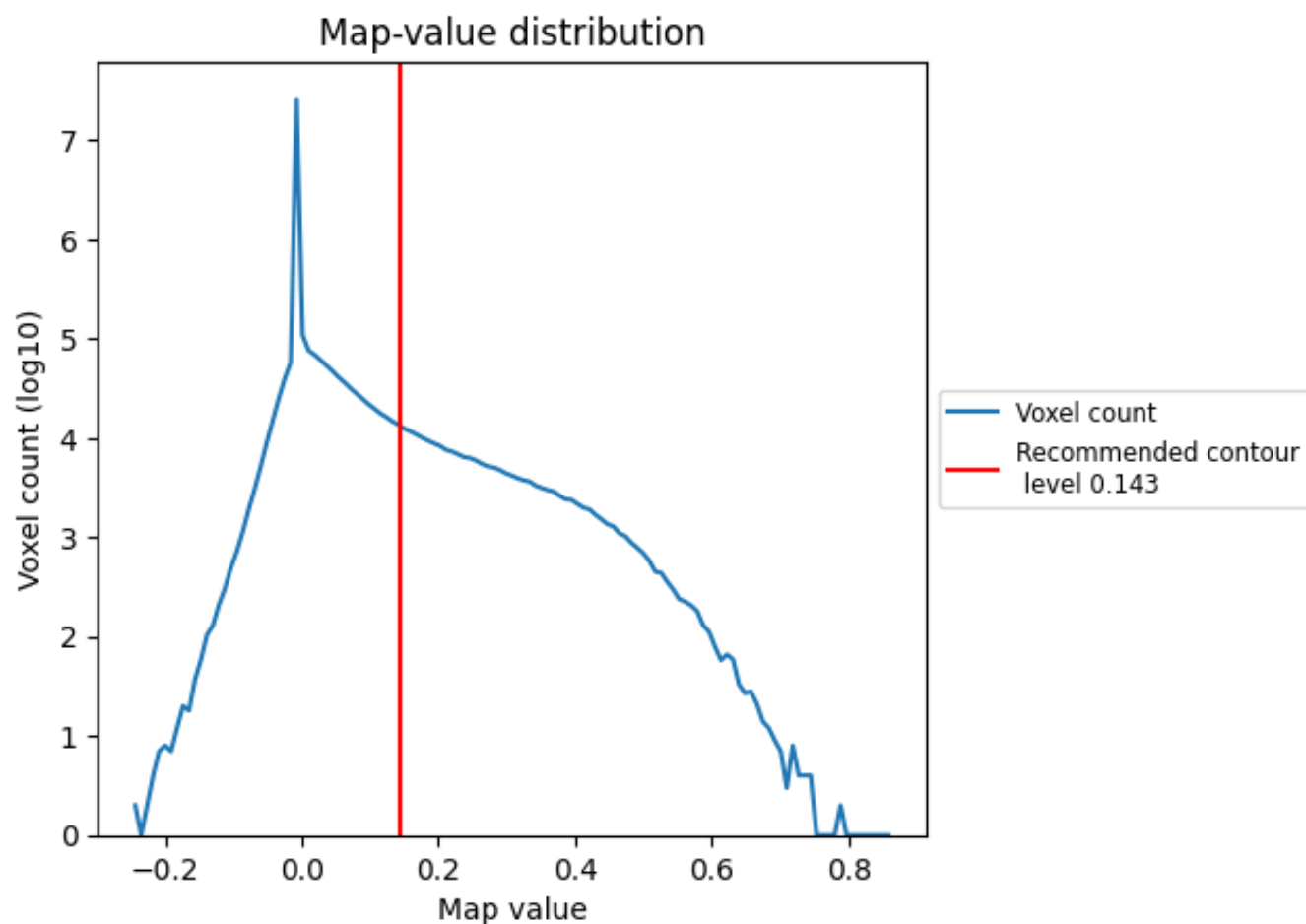


Z

7 Map analysis [i](#)

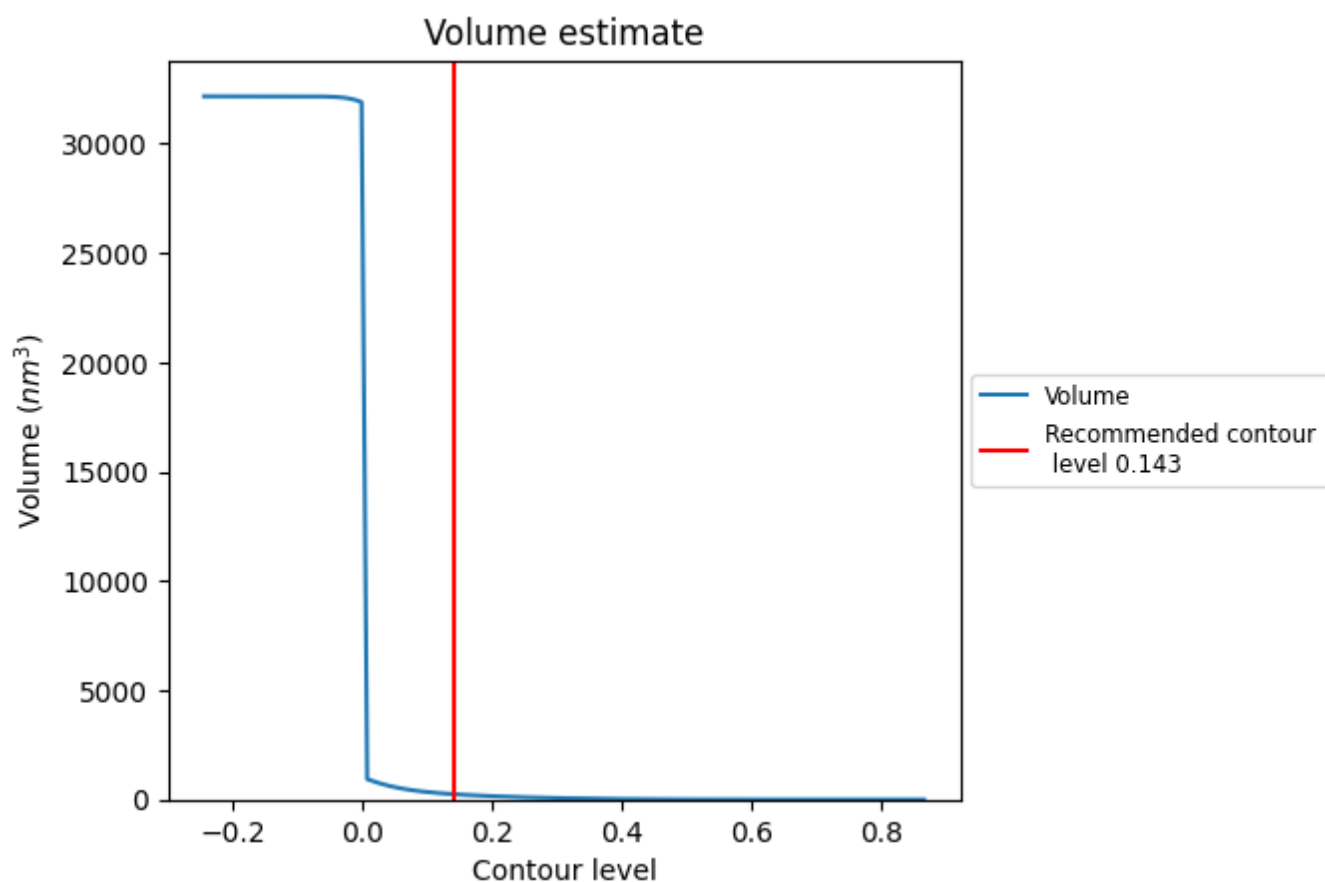
This section contains the results of statistical analysis of the map.

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.

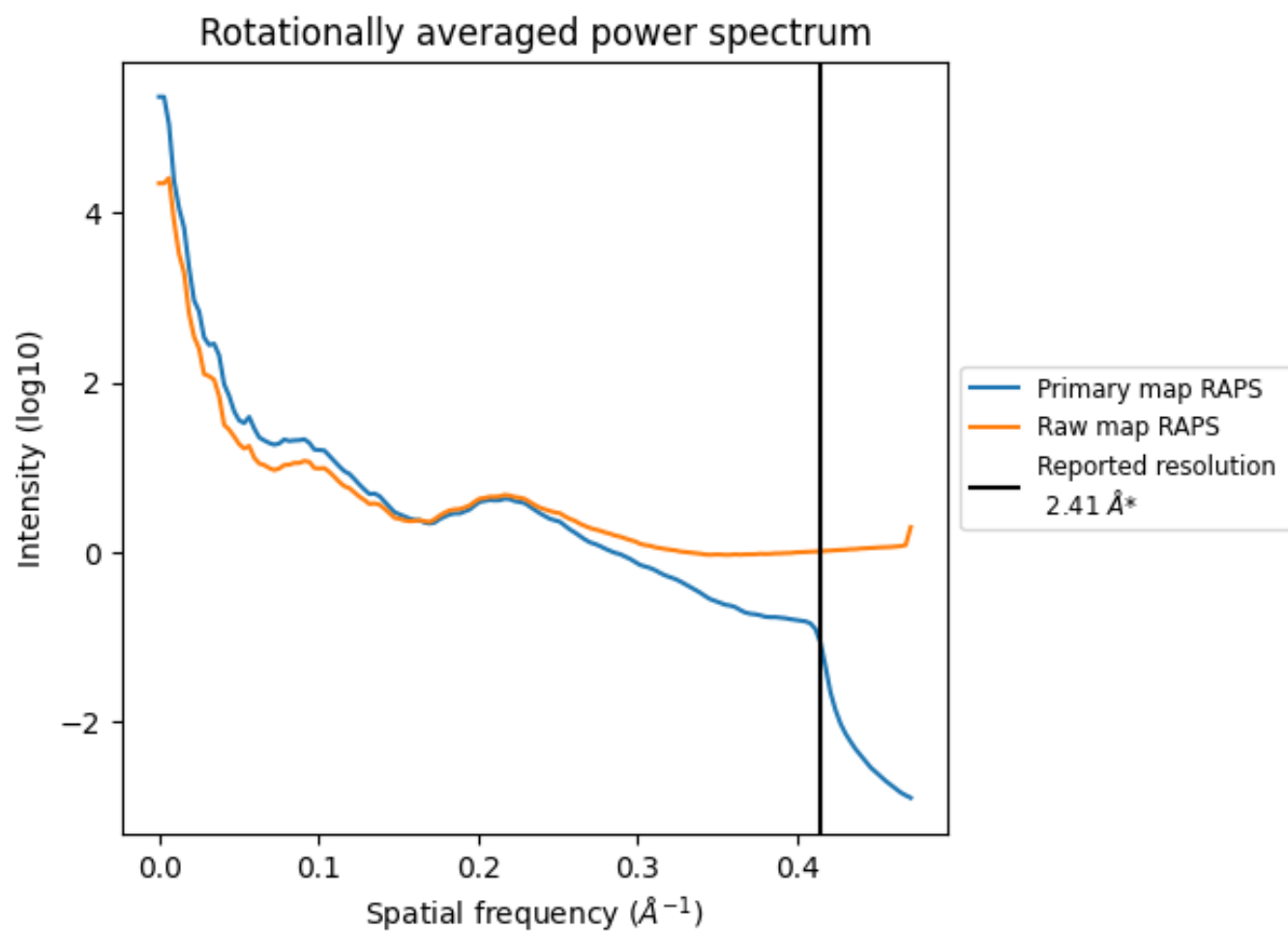
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 242 nm^3 ; this corresponds to an approximate mass of 218 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 ⓘ

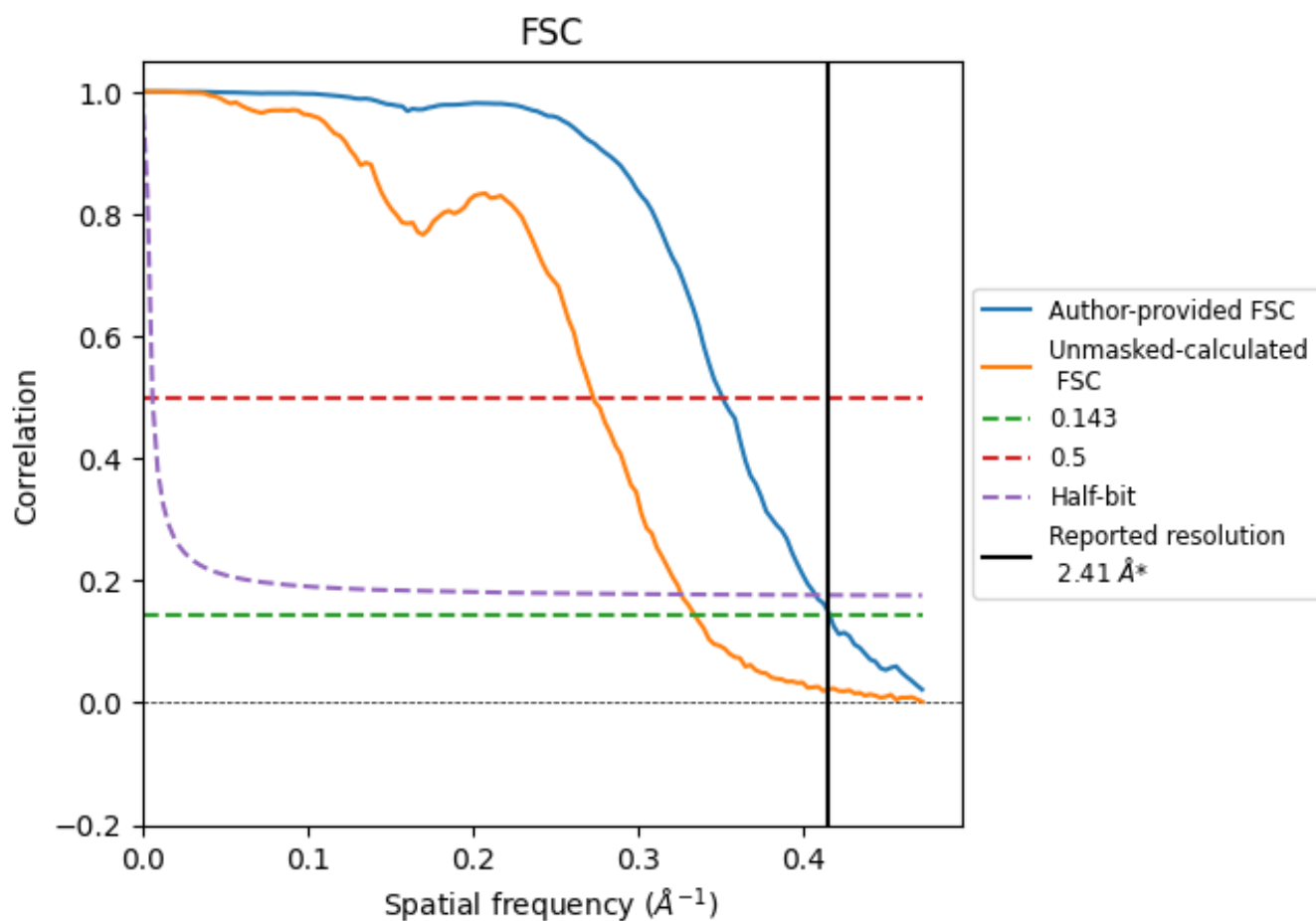


*Reported resolution corresponds to spatial frequency of 0.415 Å⁻¹

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 0.415 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

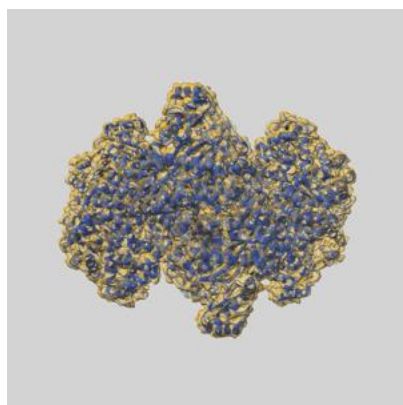
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.41	-	-
Author-provided FSC curve	2.41	2.85	2.46
Unmasked-calculated*	2.99	3.67	3.07

*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 2.99 differs from the reported value 2.41 by more than 10 %

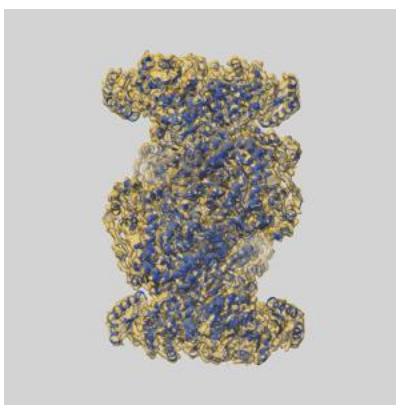
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15033 and PDB model 7ZZ3. Per-residue inclusion information can be found in section [3](#) on page [10](#).

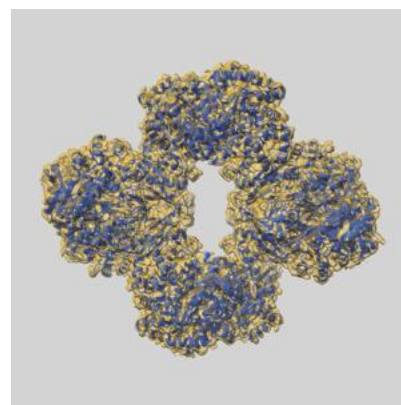
9.1 Map-model overlay [i](#)



X



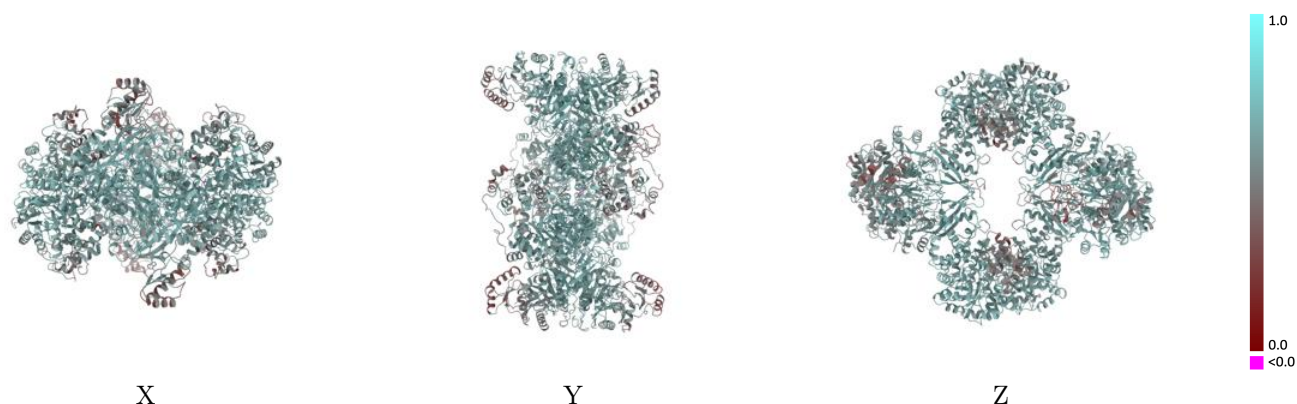
Y



Z

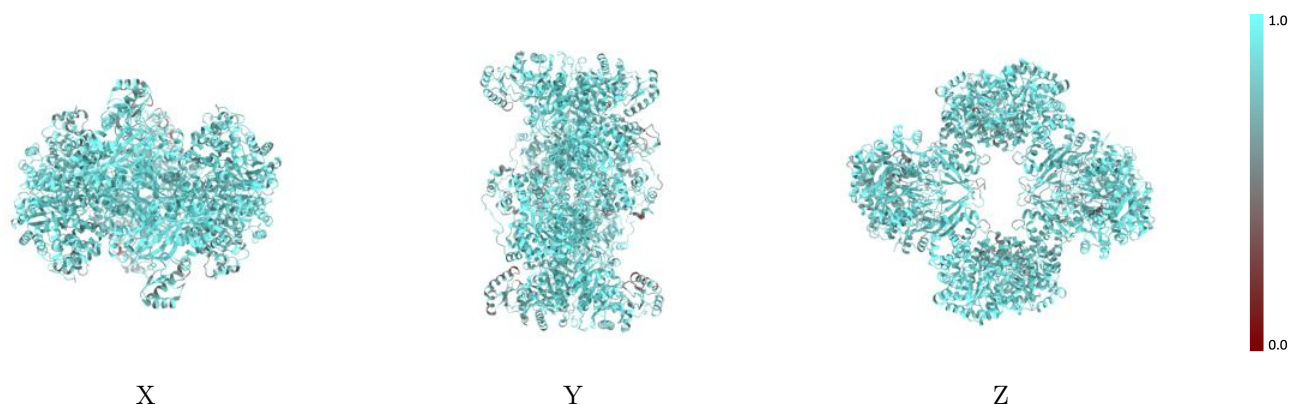
The images above show the 3D surface view of the map at the recommended contour level 0.143 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



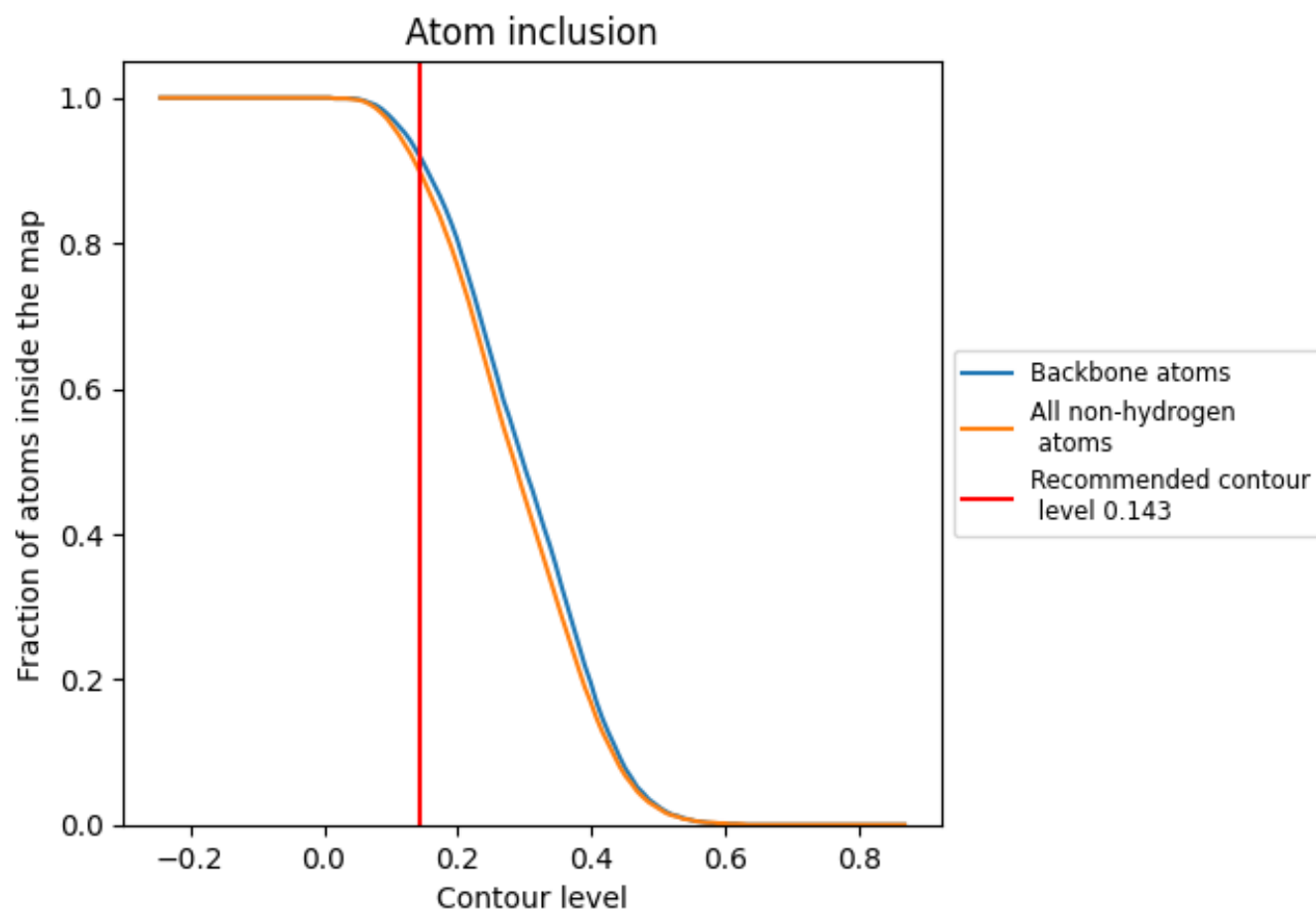
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.143).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 90% 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 (0.143) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8980	0.5910
A	0.9010	0.5900
B	0.9130	0.5970
C	0.9110	0.6020
D	0.8840	0.5760

