



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 03:41 AM UTC

PDB ID : 8G1E / pdb_00008g1e
EMDB ID : EMD-29668
Title : Structure of ACLY-D1026A-products-asy
Authors : Wei, X.; Marmorstein, R.
Deposited on : 2023-02-02
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

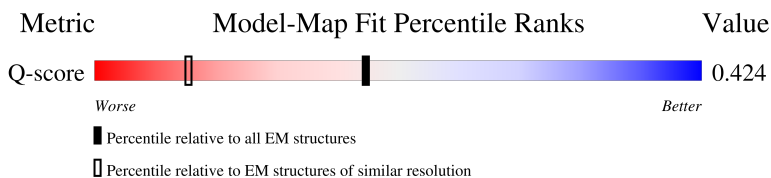
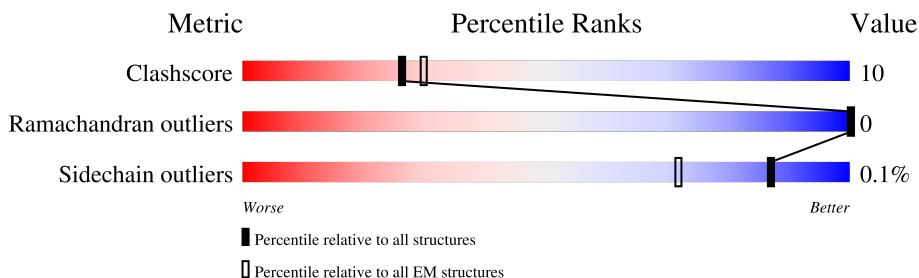
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	11806 (2.30 - 3.30)

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	1101	
1	B	1101	
1	C	1101	
1	D	1101	

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
4	UNL	B	2301	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 32649 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.

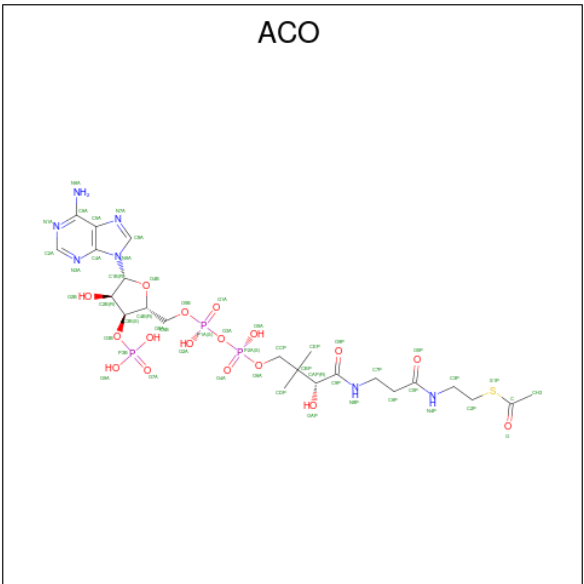
- Molecule 1 is a protein called ATP-citrate synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1037	Total	C	N	O	S	2	0
			8017	5133	1360	1478	46		
1	B	1037	Total	C	N	O	S	2	0
			8017	5133	1360	1478	46		
1	C	1037	Total	C	N	O	S	2	0
			8017	5133	1360	1478	46		
1	D	1037	Total	C	N	O	S	2	0
			8017	5133	1360	1478	46		

There are 4 discrepancies between the modelled and reference sequences:

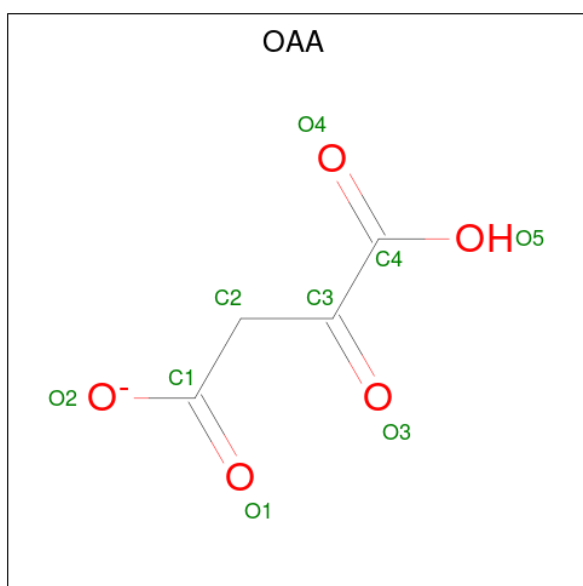
Chain	Residue	Modelled	Actual	Comment	Reference
A	1026	ALA	ASP	engineered mutation	UNP P53396
B	1026	ALA	ASP	engineered mutation	UNP P53396
C	1026	ALA	ASP	engineered mutation	UNP P53396
D	1026	ALA	ASP	engineered mutation	UNP P53396

- Molecule 2 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



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

- Molecule 3 is OXALOACETATE ION (CCD ID: OAA) (formula: $C_4H_3O_5$).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			9	4	5	
3	A	1	Total	C	O	0
			9	4	5	
3	C	1	Total	C	O	0
			9	4	5	
3	D	1	Total	C	O	0
			9	4	5	

- Molecule 4 is UNKNOWN LIGAND (CCD ID: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

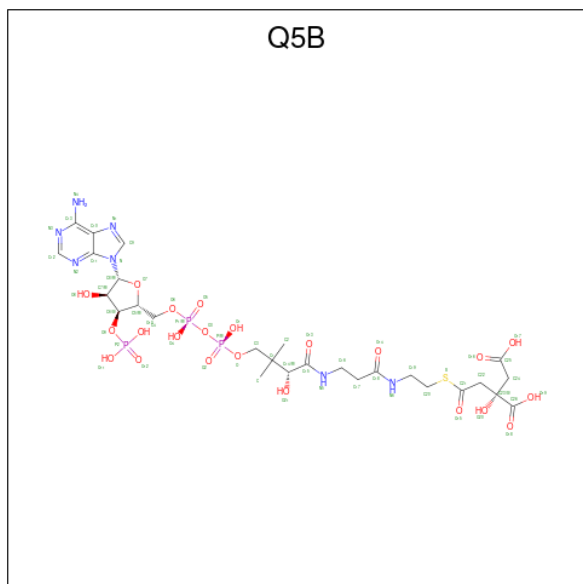
Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	C	0
			1	1	

Continued on next page...

Continued from previous page...

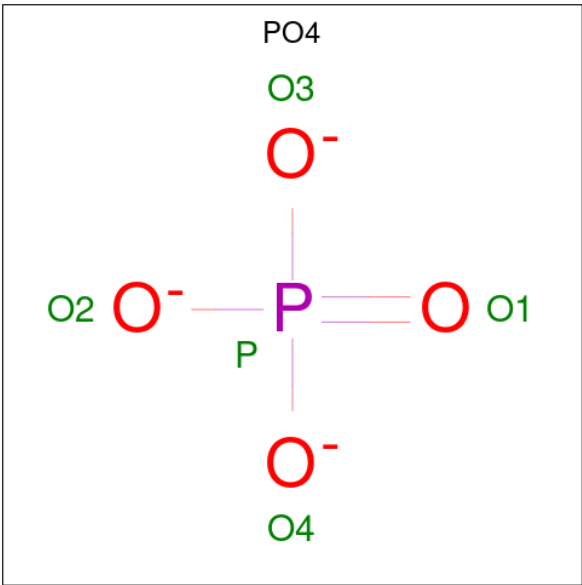
Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total	C	0
			1	1	

- Molecule 5 is (3S)-citryl-Coenzyme A (CCD ID: Q5B) (formula: $C_{27}H_{42}N_7O_{22}P_3S$).



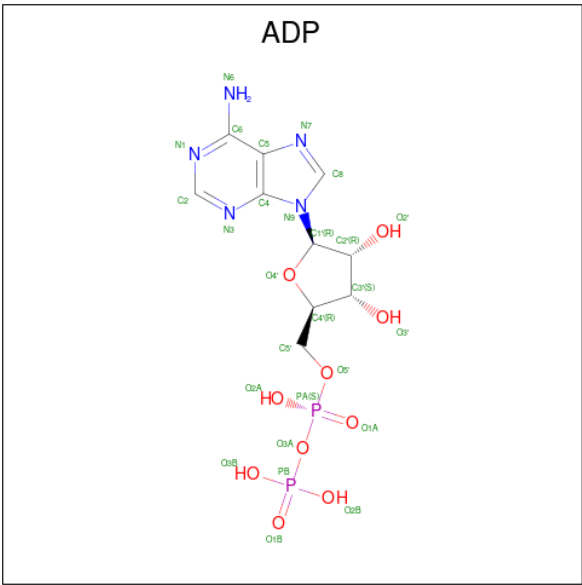
Mol	Chain	Residues	Atoms						AltConf
5	B	1	Total	C	N	O	P	S	0
			60	27	7	22	3	1	
5	C	1	Total	C	N	O	P	S	0
			60	27	7	22	3	1	
5	D	1	Total	C	N	O	P	S	0
			60	27	7	22	3	1	

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			AltConf
6	B	1	Total	O	P	0
			5	4	1	
6	C	1	Total	O	P	0
			5	4	1	
6	D	1	Total	O	P	0
			5	4	1	

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

Continued on next page...

Continued from previous page...

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

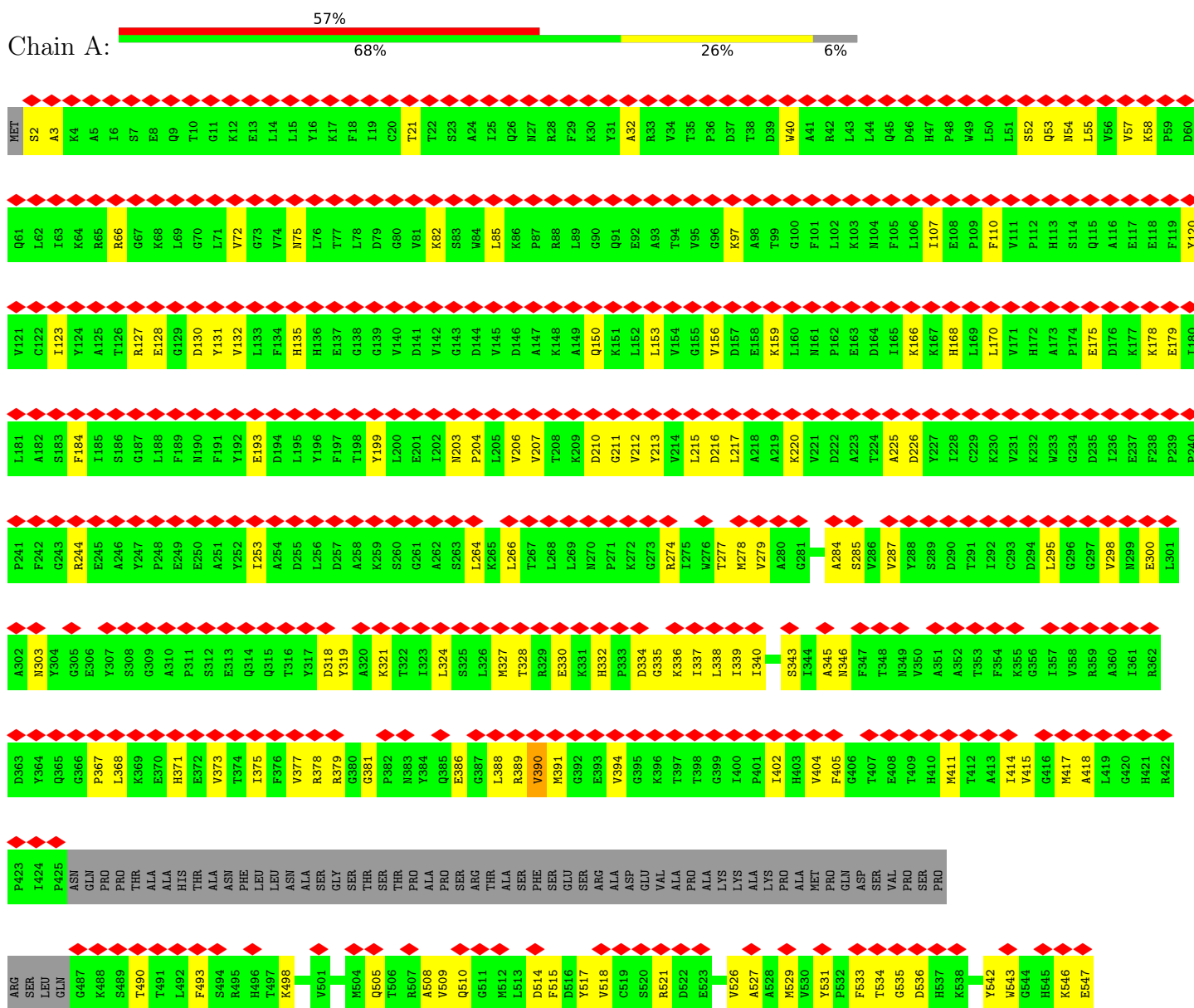
- Molecule 8 is water.

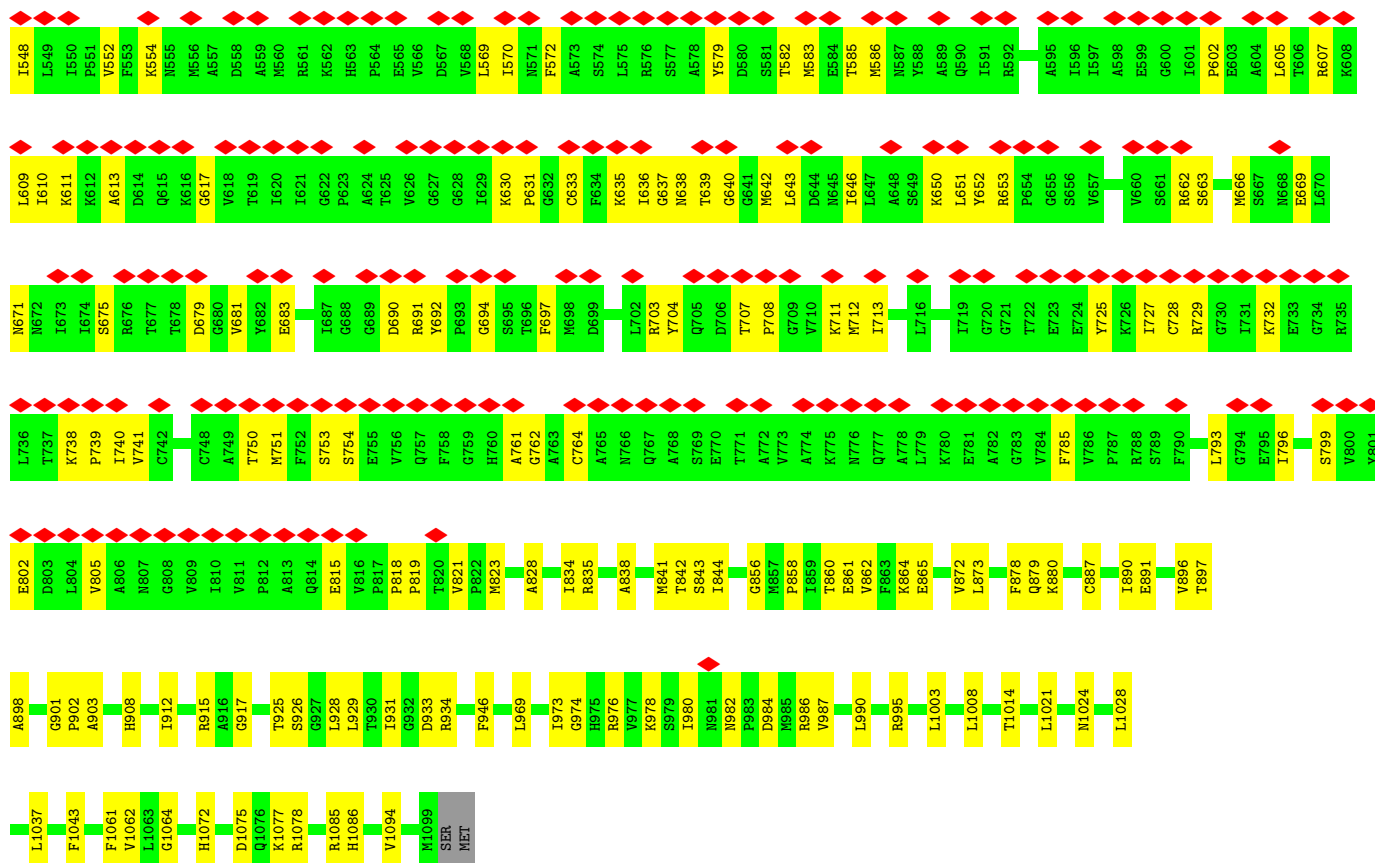
Mol	Chain	Residues	Atoms		AltConf
8	A	23	Total	O	0
			23	23	
8	B	18	Total	O	0
			18	18	
8	C	29	Total	O	0
			29	29	
8	D	20	Total	O	0
			20	20	

3 Residue-property plots

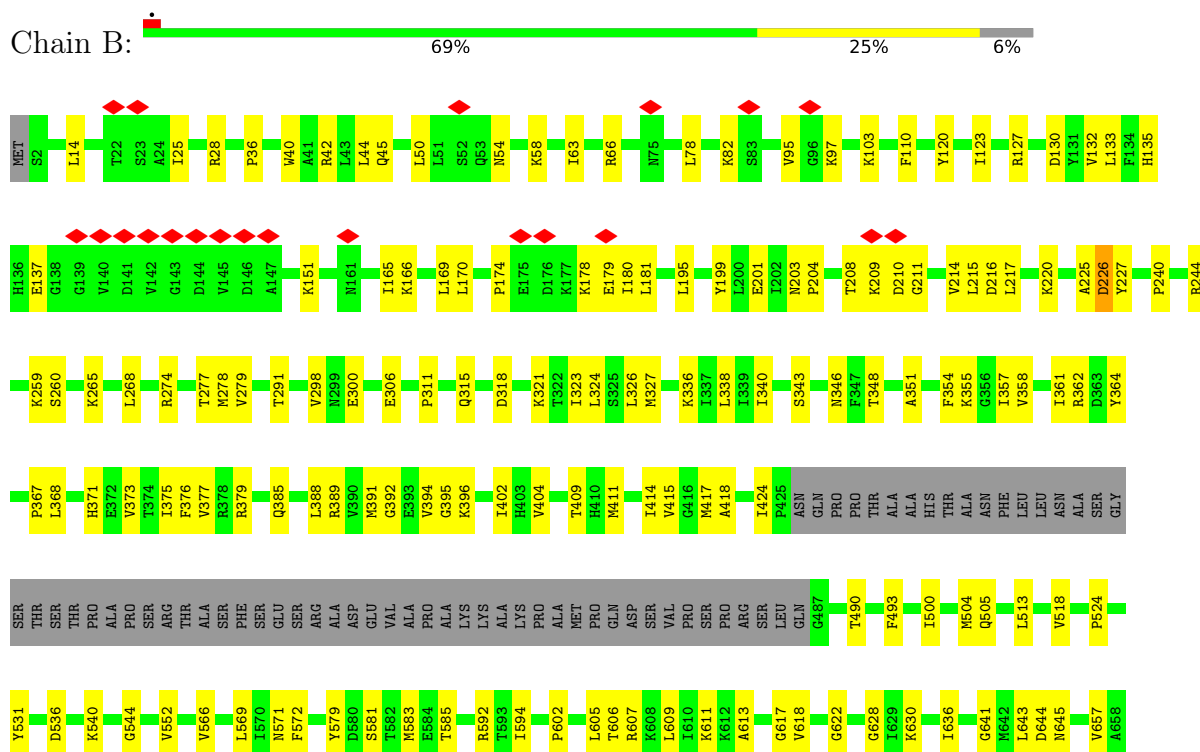
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



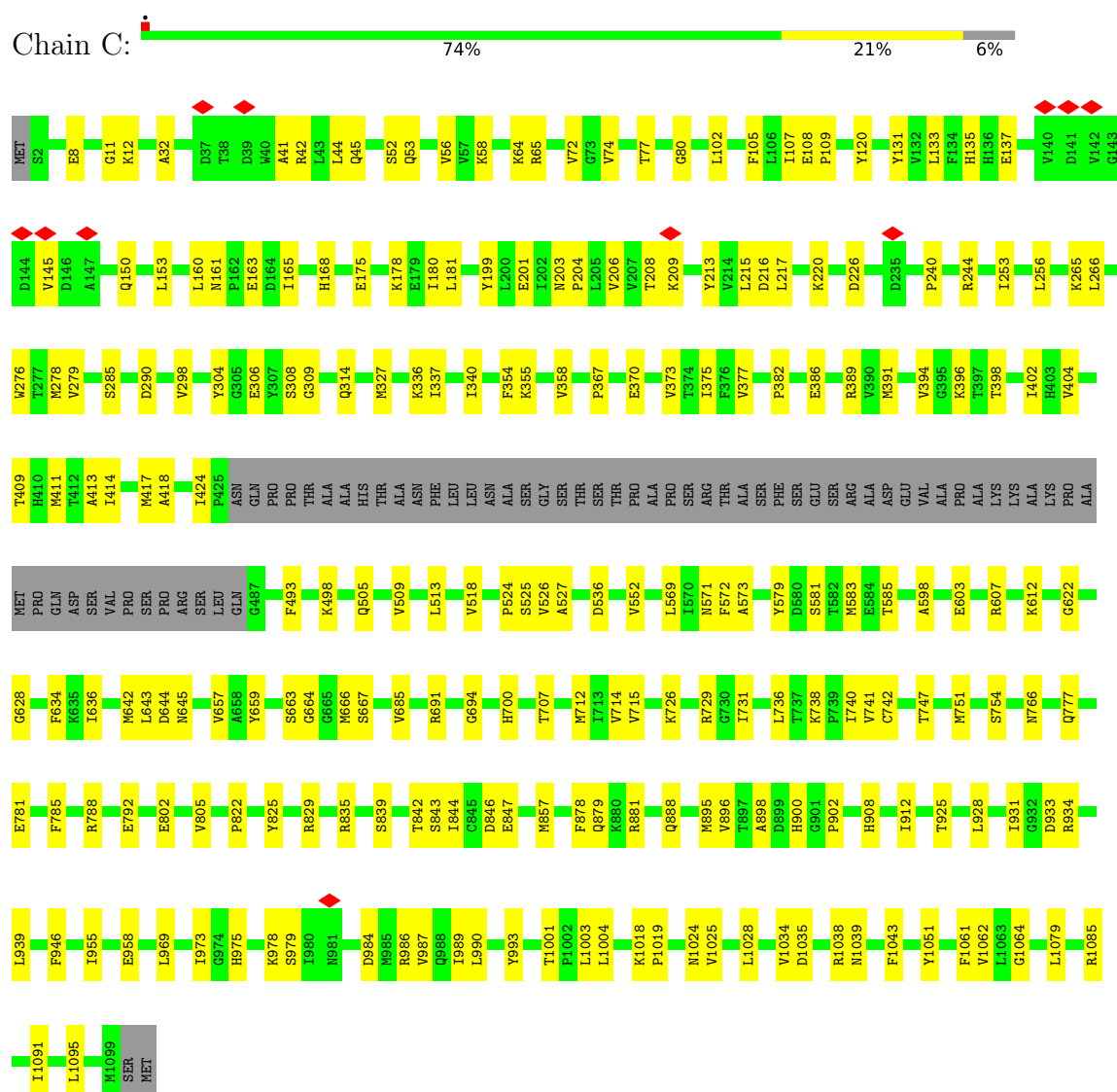


• Molecule 1: ATP-citrate synthase

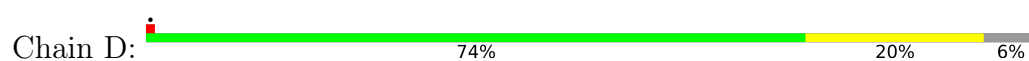




• Molecule 1: ATP-citrate synthase



• Molecule 1: ATP-citrate synthase





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	183036	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 ($e^-/\text{\AA}^2$)	40.00	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.003	Depositor
Minimum map value	-1.655	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.155	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	182.59999, 182.59999, 182.59999	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: Q5B, UNL, OAA, ACO, PO4, ADP

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	0.11	0/8198	0.30	2/11098 (0.0%)
1	B	0.14	0/8198	0.31	0/11098
1	C	0.12	0/8198	0.30	0/11098
1	D	0.10	0/8198	0.29	0/11098
All	All	0.12	0/32792	0.30	2/44392 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	VAL	CA-C-N	-5.30	111.86	120.72
1	A	390	VAL	C-N-CA	-5.30	111.86	120.72

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	8017	0	8057	202	0
1	B	8017	0	8057	188	0
1	C	8017	0	8057	150	0
1	D	8017	0	8057	153	0
2	A	51	0	34	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	51	0	34	8	0
2	C	51	0	34	5	0
2	D	51	0	34	17	0
3	A	18	0	4	2	0
3	C	9	0	2	0	0
3	D	9	0	2	1	0
4	B	1	0	0	2	0
4	C	1	0	0	0	0
5	B	60	0	0	0	0
5	C	60	0	0	1	0
5	D	60	0	0	3	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	1	0
7	C	27	0	12	0	0
7	D	27	0	12	0	0
8	A	23	0	0	2	0
8	B	18	0	0	0	0
8	C	29	0	0	0	0
8	D	20	0	0	0	0
All	All	32649	0	32396	656	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 10.

All (656) 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:D:976:ARG:HD2	2:D:3301:ACO:H2B	1.37	1.06
1:A:1085:ARG:HH11	2:B:2303:ACO:H62A	1.10	0.96
1:C:382:PRO:HA	1:C:642:MET:HE2	1.56	0.86
1:B:925:THR:HG23	1:D:925:THR:HG23	1.60	0.83
1:A:1085:ARG:NH1	2:B:2303:ACO:H62A	1.81	0.78
1:A:925:THR:HG23	1:C:925:THR:HG23	1.66	0.77
1:B:1026:ALA:HB2	2:B:2303:ACO:HH32	1.68	0.75
1:A:642:MET:HE3	1:A:643:LEU:H	1.53	0.73
1:A:97:LYS:HE3	1:A:753:SER:HA	1.71	0.73
1:D:976:ARG:HG3	2:D:3301:ACO:O1A	1.89	0.73
1:A:391:MET:HA	1:A:394:VAL:HG12	1.72	0.71
1:D:663:SER:HB2	1:D:666:MET:HB2	1.72	0.71
1:C:58:LYS:HB3	1:C:72:VAL:HG23	1.71	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ILE:HG23	1:B:169:LEU:HD23	1.72	0.70
1:A:987:VAL:HG13	1:A:1028:LEU:HD22	1.72	0.70
1:A:536:ASP:HA	1:A:552:VAL:O	1.90	0.70
1:D:167:LYS:HE3	1:D:168:HIS:CE1	2.28	0.69
1:B:974:GLY:O	1:B:1024:ASN:ND2	2.23	0.69
1:A:713:ILE:HB	1:A:740:ILE:HG12	1.74	0.68
1:D:367:PRO:O	1:D:371:HIS:ND1	2.22	0.68
1:A:327:MET:HE1	1:A:338:LEU:HD13	1.75	0.68
1:A:653:ARG:NH2	1:A:679:ASP:O	2.27	0.68
1:B:278:MET:HB2	1:B:340:ILE:HA	1.76	0.68
1:C:939:LEU:HD22	1:C:1061:PHE:HB2	1.76	0.68
1:B:123:ILE:HG13	1:B:132:VAL:HG22	1.76	0.68
1:C:1085:ARG:HG2	2:D:3301:ACO:N6A	2.09	0.68
1:A:327:MET:O	1:A:336:LYS:NZ	2.27	0.67
1:A:338:LEU:HB3	1:A:375:ILE:HG12	1.77	0.67
1:B:504:MET:HE3	1:B:531:TYR:HB2	1.75	0.67
1:D:206:VAL:HG23	1:D:213:TYR:HB2	1.76	0.67
1:B:971:MET:HA	2:B:2303:ACO:H62	1.76	0.67
1:A:277:THR:HG22	1:A:339:ILE:HB	1.77	0.67
1:B:367:PRO:O	1:B:371:HIS:ND1	2.23	0.67
1:A:842:THR:HG21	1:C:902:PRO:HG3	1.76	0.66
1:A:896:VAL:HG21	1:A:990:LEU:HD11	1.78	0.66
1:B:976:ARG:HD2	2:B:2303:ACO:H2B	1.77	0.66
1:C:120:TYR:HD1	1:C:203:ASN:HD22	1.44	0.66
1:A:902:PRO:HG3	1:C:842:THR:HG21	1.77	0.66
1:A:934:ARG:NH1	1:B:915:ARG:O	2.29	0.66
1:A:278:MET:HE1	1:A:338:LEU:HD11	1.76	0.66
1:A:156:VAL:O	1:A:611:LYS:NZ	2.25	0.65
2:A:1201:ACO:H62A	1:B:1085:ARG:NH1	1.95	0.65
1:D:27:ASN:HA	1:D:30:LYS:HD3	1.77	0.65
1:C:120:TYR:HB3	1:C:135:HIS:HB3	1.79	0.65
1:A:206:VAL:HG23	1:A:213:TYR:HB2	1.77	0.64
1:B:58:LYS:NZ	1:B:215:LEU:O	2.30	0.64
1:A:838:ALA:O	1:B:540:LYS:NZ	2.26	0.64
1:A:343:SER:O	1:A:379:ARG:NH1	2.30	0.64
1:C:336:LYS:HB2	1:C:373:VAL:HG22	1.80	0.64
1:D:156:VAL:HB	1:D:611:LYS:HD2	1.79	0.64
1:D:793:LEU:O	1:D:797:ILE:HG13	1.98	0.64
1:A:509:VAL:HG23	1:A:526:VAL:HG21	1.80	0.64
1:C:835:ARG:HG3	1:D:822:PRO:HB2	1.80	0.63
1:D:513:LEU:HD22	1:D:524:PRO:HB3	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:MET:HE3	1:B:402:ILE:HD13	1.79	0.63
1:B:583:MET:HE3	1:B:609:LEU:HD23	1.80	0.63
1:B:896:VAL:HG21	1:B:990:LEU:HD11	1.80	0.63
1:A:1037:LEU:HD22	1:A:1043:PHE:HE2	1.61	0.63
1:B:120:TYR:HB3	1:B:135:HIS:HB3	1.81	0.63
1:D:857:MET:HE1	1:D:881:ARG:HD3	1.81	0.63
1:C:896:VAL:HG21	1:C:990:LEU:HD11	1.81	0.63
1:D:512:MET:HE2	1:D:637:GLY:H	1.64	0.63
1:D:338:LEU:HB3	1:D:375:ILE:HG12	1.81	0.62
1:D:691:ARG:HH11	1:D:692:TYR:HE1	1.45	0.62
1:A:802:GLU:HA	1:A:805:VAL:HG12	1.80	0.62
1:B:741:VAL:HG22	1:B:785:PHE:HB2	1.80	0.62
1:C:513:LEU:HD22	1:C:524:PRO:HB3	1.81	0.62
1:A:510:GLN:OE1	1:B:835:ARG:NH1	2.30	0.62
1:C:150:GLN:NE2	1:C:168:HIS:O	2.32	0.62
1:C:979:SER:HB3	1:C:1019:PRO:HB2	1.81	0.62
1:D:1024:ASN:HD22	2:D:3301:ACO:H21	1.64	0.62
1:A:498:LYS:HD2	1:A:527:ALA:HB2	1.82	0.62
1:A:946:PHE:HB3	1:A:1003:LEU:HD11	1.81	0.62
1:A:976:ARG:HB2	2:A:1201:ACO:H3B	1.81	0.62
1:B:170:LEU:O	1:B:178:LYS:NZ	2.32	0.62
1:B:987:VAL:HG13	1:B:1028:LEU:HD22	1.81	0.62
1:C:265:LYS:HB2	1:C:306:GLU:HG3	1.82	0.62
1:C:340:ILE:HB	1:C:377:VAL:HG22	1.82	0.61
1:A:976:ARG:HD2	2:A:1201:ACO:H2B	1.81	0.61
1:B:513:LEU:HD22	1:B:524:PRO:HB3	1.82	0.61
1:A:378:ARG:HB2	1:A:414:ILE:HG21	1.83	0.61
1:C:337:ILE:HG21	1:C:418:ALA:HB1	1.83	0.61
1:D:278:MET:HB2	1:D:340:ILE:HA	1.83	0.61
1:D:987:VAL:HG13	1:D:1028:LEU:HD22	1.81	0.61
1:A:691:ARG:NH1	1:A:764:CYS:O	2.32	0.61
1:A:505:GLN:HB3	1:A:508:ALA:HB3	1.83	0.61
1:B:823:MET:HE1	4:B:2301:UNL:C	2.31	0.60
1:D:133:LEU:HD23	1:D:145:VAL:HG22	1.83	0.60
1:D:896:VAL:HG21	1:D:990:LEU:HD11	1.83	0.60
1:C:691:ARG:NH2	1:C:766:ASN:OD1	2.34	0.60
1:C:902:PRO:HG2	1:D:1091:ILE:HD13	1.82	0.60
1:B:662:ARG:HG3	1:B:718:GLU:HG2	1.83	0.60
1:C:628:GLY:H	1:C:636:ILE:HB	1.66	0.60
1:B:689:GLY:HA3	1:B:760:HIS:HD1	1.66	0.60
1:A:841:MET:HE3	1:C:1079:LEU:HD22	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:628:GLY:H	1:B:636:ILE:HB	1.66	0.60
1:D:120:TYR:HB3	1:D:135:HIS:HB3	1.83	0.60
1:A:662:ARG:HH22	1:A:762:GLY:HA3	1.67	0.59
1:B:842:THR:HG21	1:D:902:PRO:HG3	1.84	0.59
1:B:338:LEU:HB3	1:B:375:ILE:HG12	1.82	0.59
1:C:32:ALA:HB3	1:C:107:ILE:HB	1.85	0.59
1:B:376:PHE:HE2	1:B:418:ALA:HA	1.68	0.59
1:A:66:ARG:NH2	1:A:216:ASP:OD2	2.36	0.59
1:A:860:THR:HG22	1:C:989:ILE:HD11	1.83	0.59
1:D:295:LEU:HD12	1:D:415:VAL:HG12	1.83	0.59
1:B:518:VAL:HG11	1:B:643:LEU:HD11	1.83	0.59
1:A:707:THR:O	1:A:738:LYS:NZ	2.35	0.59
1:B:44:LEU:HD11	1:B:78:LEU:HD11	1.83	0.59
1:D:928:LEU:HD22	1:D:1062:VAL:HG13	1.84	0.59
1:A:974:GLY:HA2	1:A:1021:LEU:HA	1.85	0.58
1:D:170:LEU:O	1:D:178:LYS:NZ	2.35	0.58
1:D:277:THR:HB	1:D:279:VAL:HG23	1.84	0.58
1:A:166:LYS:HZ1	1:A:179:GLU:HG3	1.67	0.58
1:B:721:GLY:N	1:B:770:GLU:OE1	2.36	0.58
1:A:903:ALA:HB2	1:B:1091:ILE:HD11	1.86	0.58
1:B:36:PRO:HG2	1:B:103:LYS:HG3	1.85	0.58
1:B:505:GLN:HG3	1:B:572:PHE:CG	2.38	0.58
1:D:844:ILE:HG22	1:D:879:GLN:NE2	2.19	0.58
1:B:592:ARG:NH2	1:B:617:GLY:O	2.36	0.58
1:D:974:GLY:O	2:D:3301:ACO:H143	2.02	0.58
1:A:741:VAL:HG22	1:A:785:PHE:HB2	1.85	0.58
1:B:340:ILE:HB	1:B:377:VAL:HG22	1.86	0.58
1:D:166:LYS:HE3	1:D:178:LYS:HB3	1.86	0.58
1:B:602:PRO:HB2	1:B:605:LEU:HD23	1.86	0.58
1:A:569:LEU:HD22	1:A:585:THR:HG21	1.86	0.57
1:C:934:ARG:NH1	1:D:915:ARG:O	2.37	0.57
1:D:97:LYS:HE3	1:D:753:SER:HA	1.85	0.57
1:C:1085:ARG:HG2	2:D:3301:ACO:H62A	1.69	0.57
1:D:976:ARG:HH11	2:D:3301:ACO:H8A	1.68	0.57
1:A:127:ARG:HG3	1:A:692:TYR:CE1	2.40	0.57
1:C:12:LYS:NZ	1:C:108:GLU:OE1	2.38	0.57
1:D:204:PRO:HD2	1:D:215:LEU:HB2	1.87	0.57
1:D:628:GLY:H	1:D:636:ILE:HB	1.69	0.57
1:C:498:LYS:HD2	1:C:527:ALA:HB2	1.86	0.57
1:B:327:MET:O	1:B:336:LYS:NZ	2.31	0.57
1:B:933:ASP:OD1	1:B:934:ARG:N	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1078:ARG:NH2	1:D:879:GLN:OE1	2.38	0.57
1:D:167:LYS:HE3	1:D:168:HIS:HE1	1.67	0.57
1:D:194:ASP:O	1:D:232:LYS:NZ	2.34	0.57
1:D:340:ILE:HB	1:D:377:VAL:HG22	1.87	0.57
1:D:358:VAL:HG11	1:D:390:VAL:HG12	1.86	0.57
1:D:976:ARG:HD2	2:D:3301:ACO:H8A	1.86	0.57
1:A:974:GLY:O	2:A:1201:ACO:H143	2.05	0.56
1:D:788:ARG:NH2	1:D:792:GLU:OE2	2.38	0.56
1:A:253:ILE:HG13	1:A:266:LEU:HD23	1.87	0.56
1:A:872:VAL:HG21	1:C:895:MET:HG2	1.86	0.56
1:B:260:SER:HB3	1:D:1019:PRO:HD3	1.87	0.56
1:B:1088:TRP:NE1	1:C:847:GLU:OE2	2.30	0.56
1:C:42:ARG:HD2	1:C:45:GLN:HE22	1.70	0.56
1:C:685:VAL:HG11	1:C:700:HIS:CE1	2.41	0.56
1:C:825:TYR:OH	1:C:829:ARG:NH2	2.38	0.56
1:B:343:SER:HB2	1:B:669:GLU:HG2	1.87	0.56
1:A:388:LEU:HA	1:A:391:MET:SD	2.46	0.56
1:A:823:MET:HE3	1:A:828:ALA:HB2	1.88	0.56
1:B:714:VAL:HG21	1:B:797:ILE:HD12	1.85	0.56
1:B:802:GLU:HA	1:B:805:VAL:HG12	1.87	0.56
1:B:375:ILE:HB	1:B:402:ILE:HG12	1.87	0.56
1:B:750:THR:HG21	1:B:771:THR:HB	1.88	0.56
1:B:1005:ASP:O	1:B:1009:GLU:HG2	2.05	0.56
1:A:54:ASN:HD21	1:A:75:ASN:HA	1.71	0.56
1:B:66:ARG:NH2	1:B:216:ASP:OD2	2.38	0.56
1:A:799:SER:O	1:A:802:GLU:HG3	2.06	0.56
2:A:1201:ACO:HH33	3:A:1202:OAA:H22	1.88	0.56
1:C:822:PRO:HB2	1:D:835:ARG:HB2	1.88	0.56
1:C:1091:ILE:HD13	1:D:902:PRO:HG2	1.87	0.56
1:D:518:VAL:HG11	1:D:643:LEU:HD11	1.87	0.56
1:B:902:PRO:HG3	1:D:842:THR:HG21	1.88	0.55
1:A:324:LEU:HA	1:A:327:MET:HG3	1.89	0.55
1:D:509:VAL:HG21	1:D:529:MET:HE3	1.88	0.55
1:A:570:ILE:HD13	1:A:637:GLY:H	1.69	0.55
1:B:1094:VAL:HG23	1:C:843:SER:HB3	1.88	0.55
1:A:878:PHE:HB3	1:A:1043:PHE:HZ	1.71	0.55
1:B:844:ILE:HG22	1:B:879:GLN:NE2	2.22	0.55
1:C:53:GLN:HE21	1:C:109:PRO:HG3	1.71	0.55
1:A:216:ASP:OD1	1:A:217:LEU:N	2.39	0.55
1:A:414:ILE:HA	1:A:417:MET:HE2	1.88	0.55
1:D:644:ASP:OD1	1:D:645:ASN:N	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:LEU:O	1:A:609:LEU:HG	2.06	0.55
1:B:336:LYS:HB2	1:B:373:VAL:HG22	1.88	0.55
1:B:657:VAL:HG13	1:B:712:MET:HG3	1.89	0.55
1:B:707:THR:O	1:B:738:LYS:NZ	2.40	0.55
1:B:208:THR:HG22	1:B:209:LYS:H	1.71	0.55
1:C:908:HIS:O	1:C:912:ILE:HG12	2.07	0.55
1:A:336:LYS:HB2	1:A:373:VAL:HG22	1.89	0.54
1:C:42:ARG:HD2	1:C:45:GLN:NE2	2.22	0.54
1:D:975:HIS:CG	1:D:976:ARG:H	2.25	0.54
1:A:521:ARG:NH1	1:A:633:CYS:O	2.40	0.54
1:C:58:LYS:NZ	1:C:216:ASP:OD1	2.30	0.54
1:C:377:VAL:HG21	1:C:391:MET:HE2	1.88	0.54
1:C:644:ASP:OD1	1:C:645:ASN:N	2.41	0.54
2:C:3301:ACO:HN8	2:C:3301:ACO:H62A	1.56	0.54
1:A:834:ILE:HD11	1:B:825:TYR:HA	1.89	0.54
1:C:788:ARG:NH2	1:C:792:GLU:OE2	2.41	0.54
1:B:291:THR:HG23	1:B:415:VAL:HG11	1.88	0.54
1:A:340:ILE:HB	1:A:377:VAL:HG22	1.89	0.54
1:A:199:TYR:HB3	1:A:220:LYS:HB2	1.89	0.54
1:D:860:THR:O	1:D:864:LYS:HG3	2.07	0.54
1:D:963:MET:HG3	1:D:970:ILE:HG12	1.90	0.54
1:A:159:LYS:NZ	1:A:193:GLU:OE2	2.40	0.54
1:A:1037:LEU:HD22	1:A:1043:PHE:CE2	2.41	0.54
1:B:265:LYS:HB2	1:B:306:GLU:HG3	1.88	0.54
1:A:928:LEU:HD22	1:A:1062:VAL:HG13	1.90	0.53
1:B:199:TYR:OH	1:B:201:GLU:OE1	2.26	0.53
1:B:388:LEU:HD22	1:B:404:VAL:HB	1.90	0.53
1:B:644:ASP:OD1	1:B:645:ASN:N	2.40	0.53
1:D:324:LEU:HA	1:D:327:MET:HG2	1.90	0.53
1:A:543:TRP:HB2	1:A:548:ILE:HG23	1.89	0.53
1:B:343:SER:O	1:B:379:ARG:NH1	2.41	0.53
1:B:606:THR:HA	1:B:609:LEU:HD12	1.89	0.53
1:C:518:VAL:HG11	1:C:643:LEU:HD11	1.90	0.53
1:A:908:HIS:O	1:A:912:ILE:HG12	2.08	0.53
1:C:77:THR:HG23	1:C:80:GLY:H	1.74	0.53
1:A:750:THR:OG1	1:A:751:MET:SD	2.65	0.53
1:D:976:ARG:HD3	2:D:3301:ACO:O2A	2.09	0.53
1:B:216:ASP:OD1	1:B:217:LEU:N	2.42	0.53
1:B:691:ARG:NH2	1:B:766:ASN:OD1	2.42	0.53
1:B:955:ILE:HG13	1:B:958:GLU:H	1.73	0.53
1:B:989:ILE:HD11	1:D:860:THR:HG22	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:946:PHE:HB3	1:D:1003:LEU:HD11	1.91	0.53
1:A:324:LEU:HD22	1:A:368:LEU:HD21	1.89	0.52
1:A:517:TYR:OH	1:A:542:TYR:O	2.21	0.52
1:C:726:LYS:HG2	1:C:729:ARG:NH2	2.24	0.52
1:A:535:GLY:HA2	1:A:554:LYS:HE2	1.92	0.52
1:A:514:ASP:HA	1:A:517:TYR:HD2	1.73	0.52
1:C:741:VAL:HG22	1:C:785:PHE:HB2	1.91	0.52
1:C:973:ILE:O	2:C:3301:ACO:N6A	2.41	0.52
1:A:887:CYS:O	1:A:891:GLU:HG3	2.09	0.52
1:C:131:TYR:CE1	1:C:153:LEU:HD13	2.45	0.52
1:C:987:VAL:HG13	1:C:1028:LEU:HD22	1.91	0.52
1:D:44:LEU:HD11	1:D:78:LEU:HD11	1.91	0.52
1:D:657:VAL:HG13	1:D:712:MET:HG3	1.92	0.52
1:B:940:ASP:OD2	1:B:944:LYS:NZ	2.38	0.52
1:C:946:PHE:HB3	1:C:1003:LEU:HD11	1.91	0.52
1:D:54:ASN:HD21	1:D:75:ASN:HA	1.75	0.52
1:A:375:ILE:HB	1:A:402:ILE:HG12	1.90	0.52
1:A:902:PRO:HG2	1:B:1091:ILE:HD13	1.92	0.52
1:C:569:LEU:HD22	1:C:585:THR:HG21	1.91	0.52
1:D:505:GLN:HG3	1:D:572:PHE:CG	2.44	0.52
1:B:199:TYR:HB3	1:B:220:LYS:HB2	1.91	0.52
1:A:683:GLU:HB3	1:A:704:TYR:HE1	1.74	0.52
1:A:690:ASP:HA	1:A:761:ALA:HB3	1.91	0.52
1:D:569:LEU:HD22	1:D:585:THR:HG21	1.92	0.52
2:D:3301:ACO:HH33	3:D:3302:OAA:H22	1.91	0.52
1:A:897:THR:HG21	1:A:1061:PHE:HA	1.92	0.52
1:B:622:GLY:HA2	1:B:694:GLY:H	1.75	0.51
1:B:945:MET:HE1	1:B:971:MET:N	2.26	0.51
1:C:1024:ASN:HD22	2:C:3301:ACO:H21	1.74	0.51
1:A:377:VAL:HB	1:A:404:VAL:HG12	1.93	0.51
1:B:277:THR:HB	1:B:279:VAL:HG13	1.92	0.51
1:D:31:TYR:HB2	1:D:106:LEU:HD11	1.91	0.51
1:D:664:GLY:O	1:D:667:SER:OG	2.23	0.51
1:A:32:ALA:HB3	1:A:107:ILE:HB	1.92	0.51
1:A:264:LEU:HD22	1:A:319:TYR:HE2	1.76	0.51
1:A:518:VAL:HG22	1:A:652:TYR:HB3	1.92	0.51
1:D:324:LEU:HD22	1:D:368:LEU:HD21	1.90	0.51
1:D:1026:ALA:HB2	2:D:3301:ACO:HH32	1.92	0.51
1:A:835:ARG:HB2	1:B:822:PRO:HB2	1.92	0.51
1:B:351:ALA:O	1:B:355:LYS:HG2	2.11	0.51
1:D:244:ARG:HH21	1:D:754:SER:HB3	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:LEU:HD13	1:D:303:ASN:HB3	1.92	0.51
1:A:493:PHE:O	1:A:630:LYS:NZ	2.39	0.51
1:B:908:HIS:O	1:B:912:ILE:HG12	2.10	0.51
1:C:386:GLU:HA	1:C:389:ARG:HG2	1.92	0.51
1:C:657:VAL:HG13	1:C:712:MET:HG3	1.93	0.51
1:D:971:MET:HA	2:D:3301:ACO:H61	1.92	0.51
1:A:933:ASP:OD1	1:A:934:ARG:N	2.43	0.51
2:A:1201:ACO:N6A	1:B:1085:ARG:NH1	2.59	0.51
1:B:663:SER:HB2	1:B:666:MET:HB2	1.92	0.51
1:C:505:GLN:HG3	1:C:572:PHE:CG	2.45	0.51
1:D:58:LYS:HB3	1:D:72:VAL:HG12	1.91	0.51
1:D:131:TYR:CE1	1:D:153:LEU:HD13	2.46	0.51
1:D:741:VAL:HG22	1:D:785:PHE:HB2	1.93	0.51
1:C:298:VAL:HG21	1:C:751:MET:HB3	1.92	0.51
1:C:278:MET:HB2	1:C:340:ILE:HA	1.92	0.51
1:A:1094:VAL:HG23	1:D:843:SER:HB3	1.92	0.50
1:C:53:GLN:HG3	1:C:109:PRO:HB3	1.93	0.50
1:C:928:LEU:HD22	1:C:1062:VAL:HG13	1.93	0.50
1:B:1001:THR:HB	1:B:1004:LEU:HB3	1.93	0.50
1:D:53:GLN:HE21	1:D:109:PRO:HB3	1.76	0.50
1:C:201:GLU:O	1:C:217:LEU:HA	2.10	0.50
1:C:955:ILE:HG13	1:C:958:GLU:H	1.77	0.50
1:A:515:PHE:HZ	1:A:631:PRO:HA	1.76	0.50
1:A:662:ARG:NH2	1:A:690:ASP:O	2.44	0.50
1:B:274:ARG:HG2	1:B:300:GLU:HB3	1.94	0.50
1:B:357:ILE:O	1:B:361:ILE:HG12	2.11	0.50
1:B:963:MET:HE2	1:B:963:MET:HA	1.93	0.50
1:B:857:MET:HE3	1:B:861:GLU:HG2	1.94	0.50
1:C:290:ASP:OD2	1:C:747:THR:N	2.45	0.50
1:D:851:GLU:OE1	1:D:858:PRO:HB3	2.12	0.50
1:D:59:PRO:O	1:D:66:ARG:NH1	2.40	0.50
1:B:928:LEU:HD22	1:B:1062:VAL:HG13	1.94	0.50
1:C:375:ILE:HB	1:C:402:ILE:HG12	1.94	0.50
1:C:707:THR:O	1:C:738:LYS:NZ	2.44	0.50
1:D:685:VAL:HG11	1:D:700:HIS:CE1	2.46	0.50
1:A:330:GLU:O	1:A:371:HIS:NE2	2.43	0.50
1:A:607:ARG:HA	1:A:692:TYR:HE2	1.75	0.50
1:A:332:HIS:CE1	1:A:334:ASP:HB2	2.46	0.49
1:B:54:ASN:HB3	1:B:110:PHE:HB3	1.92	0.49
1:C:1018:LYS:HE3	2:C:3301:ACO:H52A	1.94	0.49
1:D:908:HIS:O	1:D:912:ILE:HG12	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASP:OD1	1:A:607:ARG:NH1	2.44	0.49
1:A:529:MET:HB3	1:A:552:VAL:HG22	1.93	0.49
1:B:278:MET:HB2	1:B:340:ILE:HG12	1.93	0.49
1:B:311:PRO:HD2	1:B:348:THR:HG23	1.94	0.49
1:B:613:ALA:HB1	1:B:618:VAL:O	2.13	0.49
1:C:1001:THR:HB	1:C:1004:LEU:HB3	1.93	0.49
1:D:278:MET:HB2	1:D:340:ILE:HG12	1.94	0.49
1:A:253:ILE:HG21	1:A:266:LEU:HB3	1.94	0.49
1:A:328:THR:HG21	1:A:367:PRO:HB2	1.93	0.49
1:C:409:THR:HG22	1:C:411:MET:H	1.77	0.49
1:B:278:MET:SD	1:B:323:ILE:HD11	2.53	0.49
1:D:728:CYS:O	1:D:732:LYS:HG2	2.13	0.49
1:B:728:CYS:O	1:B:732:LYS:HG2	2.12	0.49
1:D:54:ASN:HB3	1:D:110:PHE:HB3	1.95	0.49
1:D:760:HIS:NE2	6:D:3305:PO4:O4	2.42	0.49
1:A:697:PHE:HB3	1:A:727:ILE:HD11	1.94	0.49
1:D:199:TYR:HB3	1:D:220:LYS:HB2	1.95	0.49
1:D:974:GLY:HA2	1:D:1021:LEU:HA	1.95	0.49
1:C:64:LYS:HG3	1:C:65:ARG:HG3	1.95	0.49
1:D:567:ASP:N	1:D:567:ASP:OD1	2.44	0.49
1:D:976:ARG:NH1	2:D:3301:ACO:H8A	2.28	0.49
1:A:860:THR:O	1:A:864:LYS:HG2	2.12	0.48
1:A:128:GLU:OE2	1:A:131:TYR:OH	2.20	0.48
1:A:517:TYR:OH	1:A:543:TRP:HA	2.13	0.48
1:A:582:THR:HG21	1:A:609:LEU:HD22	1.95	0.48
1:C:175:GLU:HA	1:C:178:LYS:HG2	1.95	0.48
1:D:293:CYS:HB3	1:D:751:MET:SD	2.53	0.48
1:D:659:TYR:HA	1:D:714:VAL:O	2.13	0.48
1:A:652:TYR:OH	1:A:815:GLU:OE1	2.21	0.48
1:D:265:LYS:HB2	1:D:306:GLU:HG3	1.95	0.48
1:A:708:PRO:O	1:A:711:LYS:NZ	2.47	0.48
1:B:358:VAL:O	1:B:362:ARG:HG3	2.13	0.48
1:B:976:ARG:HG3	2:B:2303:ACO:O1A	2.14	0.48
1:C:663:SER:HB3	1:C:666:MET:HB3	1.95	0.48
1:A:123:ILE:HG23	1:A:132:VAL:HG22	1.94	0.48
1:A:490:THR:HA	1:A:703:ARG:HG2	1.96	0.48
1:A:901:GLY:HA3	1:C:847:GLU:HB3	1.94	0.48
1:A:1078:ARG:NH1	1:C:1051:TYR:OH	2.46	0.48
1:D:208:THR:HG22	1:D:209:LYS:H	1.77	0.48
1:A:691:ARG:HA	1:A:762:GLY:HA2	1.95	0.48
1:C:844:ILE:HG22	1:C:879:GLN:OE1	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1201:ACO:H141	2:A:1201:ACO:H32	1.96	0.48
1:D:888:GLN:HB3	1:D:993:TYR:OH	2.13	0.48
1:A:582:THR:O	1:A:586:MET:HG2	2.14	0.48
1:B:324:LEU:HA	1:B:327:MET:HG2	1.96	0.48
1:B:931:ILE:HD12	1:B:1061:PHE:HE2	1.78	0.48
1:C:203:ASN:O	1:C:216:ASP:HB2	2.14	0.48
1:C:253:ILE:HG13	1:C:266:LEU:HD23	1.96	0.48
1:C:571:ASN:HD21	1:C:581:SER:HB2	1.79	0.48
1:D:9:GLN:OE1	1:D:33:ARG:NH2	2.47	0.48
1:A:671:ASN:HD22	1:A:681:VAL:HG21	1.79	0.48
1:A:1085:ARG:NH2	3:A:1203:OAA:O5	2.37	0.48
1:A:1085:ARG:HD3	2:B:2303:ACO:N7A	2.29	0.48
1:B:945:MET:HE1	1:B:971:MET:H	1.79	0.48
1:A:345:ALA:HB3	1:A:381:GLY:HA3	1.95	0.48
1:B:42:ARG:HA	1:B:45:GLN:HG3	1.96	0.48
1:B:860:THR:HG22	1:D:989:ILE:HD11	1.96	0.48
1:A:844:ILE:HG22	1:A:879:GLN:NE2	2.28	0.47
1:B:569:LEU:HD22	1:B:585:THR:HG21	1.96	0.47
1:A:712:MET:SD	1:A:739:PRO:HB2	2.54	0.47
1:B:569:LEU:HD23	1:B:594:ILE:HG23	1.96	0.47
1:C:12:LYS:HG2	1:C:217:LEU:HD21	1.96	0.47
1:A:120:TYR:HB3	1:A:135:HIS:HB3	1.96	0.47
1:A:610:ILE:HD11	1:A:694:GLY:HA2	1.96	0.47
1:B:828:ALA:O	1:B:832:GLY:N	2.47	0.47
1:D:1035:ASP:O	1:D:1039:ASN:CB	2.62	0.47
1:A:266:LEU:HD11	1:A:303:ASN:HD22	1.79	0.47
1:A:995:ARG:HH21	1:A:1008:LEU:HD13	1.79	0.47
1:B:244:ARG:HH21	1:B:754:SER:HB3	1.79	0.47
1:C:715:VAL:O	1:C:742:CYS:HA	2.14	0.47
1:D:707:THR:O	1:D:738:LYS:NZ	2.48	0.47
1:A:793:LEU:O	1:A:796:ILE:HG22	2.15	0.47
1:B:240:PRO:HB2	1:B:244:ARG:HB3	1.96	0.47
1:B:860:THR:HG21	1:D:985:MET:HE3	1.95	0.47
1:C:664:GLY:O	1:C:667:SER:OG	2.20	0.47
1:A:531:TYR:CE2	1:A:533:PHE:HB2	2.49	0.47
1:A:986:ARG:NH1	8:A:2405:HOH:O	2.43	0.47
1:B:847:GLU:OE1	1:C:1085:ARG:NH2	2.48	0.47
1:C:8:GLU:HG2	1:C:12:LYS:HE3	1.96	0.47
1:A:295:LEU:HD12	1:A:415:VAL:HG12	1.96	0.47
1:B:298:VAL:HG23	1:B:752:PHE:HE1	1.80	0.47
1:B:708:PRO:O	1:B:711:LYS:NZ	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:823:MET:CE	4:B:2301:UNL:C	2.92	0.47
1:B:1035:ASP:O	1:B:1039:ASN:CB	2.63	0.47
1:C:622:GLY:HA2	1:C:694:GLY:H	1.79	0.47
1:C:986:ARG:CZ	1:C:1025:VAL:HG21	2.45	0.47
1:A:346:ASN:OD1	1:A:640:GLY:N	2.48	0.47
1:A:666:MET:HA	1:A:669:GLU:HB2	1.95	0.47
1:B:712:MET:HE1	1:B:797:ILE:HG13	1.97	0.47
1:B:1034:VAL:O	1:B:1038:ARG:HG2	2.14	0.47
1:C:898:ALA:HA	1:C:1064:GLY:O	2.15	0.47
1:B:794:GLY:O	1:B:797:ILE:HG22	2.15	0.47
1:A:835:ARG:NH1	1:B:544:GLY:O	2.40	0.46
1:A:873:LEU:HD22	1:A:890:ILE:HD13	1.97	0.46
1:C:204:PRO:HB2	1:C:215:LEU:HD22	1.97	0.46
1:A:207:VAL:HG12	1:A:212:VAL:HG12	1.96	0.46
1:A:244:ARG:HH21	1:A:754:SER:HB3	1.80	0.46
1:B:659:TYR:HA	1:B:714:VAL:O	2.15	0.46
1:C:208:THR:HG22	1:C:209:LYS:H	1.79	0.46
1:A:58:LYS:HB3	1:A:72:VAL:HG12	1.97	0.46
1:A:546:LYS:HG2	1:A:547:GLU:H	1.80	0.46
1:B:225:ALA:HB2	1:B:602:PRO:HB3	1.97	0.46
1:B:789:SER:OG	1:B:792:GLU:OE1	2.30	0.46
1:B:846:ASP:HB2	1:C:1095:LEU:HD22	1.96	0.46
1:C:278:MET:HB2	1:C:340:ILE:HG12	1.98	0.46
1:C:825:TYR:HH	1:C:829:ARG:NH2	2.13	0.46
1:D:240:PRO:HB2	1:D:244:ARG:HB3	1.97	0.46
1:D:898:ALA:HA	1:D:1064:GLY:O	2.16	0.46
1:B:493:PHE:HB2	1:B:630:LYS:HD3	1.98	0.46
1:C:244:ARG:HH21	1:C:754:SER:HB3	1.79	0.46
1:A:21:THR:HG21	1:A:184:PHE:HA	1.98	0.46
1:A:131:TYR:CE1	1:A:153:LEU:HD13	2.51	0.46
1:A:386:GLU:O	1:A:390:VAL:HG13	2.16	0.46
1:B:259:LYS:HD3	1:D:1016:SER:HA	1.97	0.46
1:B:986:ARG:CZ	1:B:1025:VAL:HG21	2.46	0.46
1:C:240:PRO:HB2	1:C:244:ARG:HB3	1.97	0.46
1:C:414:ILE:HA	1:C:417:MET:HE3	1.98	0.46
1:D:493:PHE:CZ	1:D:636:ILE:HD11	2.51	0.46
1:D:735:ARG:HG3	1:D:735:ARG:HH11	1.79	0.46
2:D:3301:ACO:O1A	2:D:3301:ACO:H3B	2.16	0.46
1:A:405:PHE:CE2	1:A:417:MET:HE1	2.51	0.46
1:B:97:LYS:HE3	1:B:753:SER:HA	1.97	0.46
1:C:931:ILE:HD12	1:C:1061:PHE:HE2	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:GLN:HB3	1:D:33:ARG:HH21	1.81	0.46
1:C:358:VAL:HG12	1:C:394:VAL:HG11	1.98	0.46
1:A:898:ALA:HA	1:A:1064:GLY:O	2.15	0.45
1:A:980:ILE:O	1:C:314:GLN:HG2	2.16	0.45
1:C:354:PHE:O	1:C:358:VAL:HG13	2.16	0.45
1:A:57:VAL:HG21	1:A:85:LEU:HD21	1.97	0.45
1:B:174:PRO:O	1:B:178:LYS:HG3	2.16	0.45
1:B:130:ASP:OD1	1:B:607:ARG:NH1	2.40	0.45
1:B:195:LEU:O	1:B:195:LEU:HD23	2.15	0.45
1:A:54:ASN:OD1	1:A:55:LEU:N	2.44	0.45
1:A:891:GLU:OE1	8:A:2401:HOH:O	2.21	0.45
1:B:324:LEU:HD22	1:B:368:LEU:HD21	1.98	0.45
1:C:536:ASP:HA	1:C:552:VAL:O	2.17	0.45
1:D:55:LEU:HD13	1:D:107:ILE:HG21	1.97	0.45
1:A:650:LYS:HE2	1:A:675:SER:HB2	1.97	0.45
1:B:794:GLY:HA2	1:B:797:ILE:HG22	1.98	0.45
1:C:731:ILE:HG12	1:C:736:LEU:HB2	1.99	0.45
1:C:888:GLN:HB3	1:C:993:TYR:OH	2.15	0.45
1:D:358:VAL:HG12	1:D:394:VAL:HG11	1.98	0.45
1:A:225:ALA:HB2	1:A:602:PRO:HB3	1.99	0.45
1:B:376:PHE:CE2	1:B:418:ALA:HA	2.50	0.45
1:B:1097:GLU:HG3	1:B:1098:HIS:N	2.32	0.45
1:C:11:GLY:HA3	1:C:217:LEU:HD11	1.98	0.45
1:D:101:PHE:HB2	1:D:103:LYS:NZ	2.32	0.45
1:A:414:ILE:HG22	1:A:417:MET:HE2	1.98	0.45
1:B:579:TYR:CG	1:B:605:LEU:HD12	2.52	0.45
1:A:2:SER:OG	1:A:3:ALA:N	2.49	0.45
1:A:346:ASN:HD21	1:A:640:GLY:H	1.65	0.45
1:B:14:LEU:HD21	1:B:195:LEU:HD21	1.99	0.45
1:C:394:VAL:O	1:C:398:THR:OG1	2.28	0.45
1:C:659:TYR:HA	1:C:714:VAL:O	2.17	0.45
1:D:976:ARG:NH1	2:D:3301:ACO:C8A	2.80	0.45
1:A:298:VAL:HG21	1:A:751:MET:HB3	1.98	0.45
1:B:25:ILE:HG23	1:B:28:ARG:HH21	1.81	0.45
1:C:279:VAL:HG21	1:C:285:SER:HA	1.99	0.45
1:C:573:ALA:O	1:C:598:ALA:HB2	2.17	0.45
1:A:203:ASN:HA	1:A:204:PRO:HA	1.72	0.45
1:A:856:GLY:HA3	1:D:1098:HIS:HA	1.99	0.45
1:B:389:ARG:O	1:B:392:GLY:N	2.50	0.45
1:B:414:ILE:HA	1:B:417:MET:HE3	1.98	0.45
1:B:843:SER:OG	1:D:1075:ASP:OD1	2.34	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:LYS:HD2	1:A:639:THR:O	2.17	0.44
1:A:978:LYS:HE2	1:A:982:ASN:O	2.16	0.44
1:C:969:LEU:HD22	2:C:3301:ACO:C4A	2.47	0.44
1:D:1026:ALA:HB2	2:D:3301:ACO:CH3	2.47	0.44
1:B:571:ASN:HD21	1:B:581:SER:HB2	1.83	0.44
1:C:1035:ASP:O	1:C:1039:ASN:CB	2.65	0.44
1:A:725:TYR:HB3	1:A:729:ARG:HH12	1.82	0.44
1:B:354:PHE:O	1:B:358:VAL:HG13	2.17	0.44
1:A:279:VAL:HB	1:A:285:SER:OG	2.18	0.44
1:A:976:ARG:NH1	2:A:1201:ACO:O2B	2.50	0.44
1:D:377:VAL:HG21	1:D:391:MET:HE2	1.99	0.44
1:D:662:ARG:HG3	1:D:718:GLU:HG2	1.99	0.44
1:D:983:PRO:O	1:D:985:MET:HG2	2.17	0.44
1:A:274:ARG:HD2	1:A:332:HIS:CE1	2.52	0.44
1:A:274:ARG:HG2	1:A:300:GLU:OE2	2.16	0.44
1:B:888:GLN:HB3	1:B:993:TYR:OH	2.17	0.44
1:A:843:SER:HB3	1:D:1094:VAL:HG23	1.99	0.44
1:A:858:PRO:O	1:A:862:VAL:HG23	2.18	0.44
1:B:602:PRO:O	1:B:606:THR:HG23	2.18	0.44
1:B:685:VAL:HG11	1:B:700:HIS:CE1	2.53	0.44
1:B:917:GLY:HA2	1:B:1077:LYS:NZ	2.32	0.44
1:C:1034:VAL:O	1:C:1038:ARG:HG2	2.17	0.44
1:A:278:MET:SD	1:A:340:ILE:HG12	2.58	0.44
1:C:52:SER:HB2	1:C:53:GLN:OE1	2.18	0.44
1:C:285:SER:HB3	1:C:304:TYR:CE1	2.52	0.44
1:A:514:ASP:CG	1:A:821:VAL:HG11	2.43	0.44
1:B:984:ASP:HB3	1:B:987:VAL:H	1.83	0.44
1:C:377:VAL:HB	1:C:404:VAL:HG12	2.00	0.44
1:D:257:ASP:OD1	1:D:264:LEU:N	2.32	0.44
1:A:613:ALA:O	1:A:617:GLY:N	2.51	0.44
1:A:728:CYS:O	1:A:732:LYS:HG2	2.18	0.44
1:A:926:SER:HA	1:A:929:LEU:HD12	2.00	0.44
1:B:536:ASP:HA	1:B:552:VAL:O	2.18	0.44
1:D:323:ILE:HA	1:D:326:LEU:HB2	1.98	0.44
1:D:1034:VAL:O	1:D:1038:ARG:HG2	2.17	0.44
1:A:878:PHE:HB3	1:A:1043:PHE:CZ	2.50	0.43
1:A:980:ILE:C	1:A:982:ASN:H	2.25	0.43
1:B:946:PHE:HB3	1:B:1003:LEU:HD11	1.99	0.43
1:C:509:VAL:HG13	1:C:526:VAL:HG21	1.99	0.43
1:D:343:SER:O	1:D:379:ARG:NH1	2.51	0.43
1:D:888:GLN:HB3	1:D:993:TYR:HH	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:973:ILE:HG21	1:A:1014:THR:HG21	2.00	0.43
1:B:135:HIS:NE2	1:B:137:GLU:OE1	2.51	0.43
1:B:500:ILE:HG13	1:B:566:VAL:HG21	1.98	0.43
1:B:664:GLY:O	1:B:667:SER:OG	2.26	0.43
1:B:974:GLY:HA2	1:B:1021:LEU:HA	1.99	0.43
1:D:389:ARG:O	1:D:392:GLY:N	2.51	0.43
1:C:135:HIS:NE2	1:C:137:GLU:OE1	2.52	0.43
1:D:586:MET:HB3	1:D:612:LYS:HE2	2.01	0.43
1:A:543:TRP:CD1	1:A:546:LYS:HE2	2.54	0.43
1:A:969:LEU:HD22	5:C:3305:Q5B:C10	2.48	0.43
1:B:409:THR:HG22	1:B:411:MET:H	1.83	0.43
1:B:991:LYS:O	1:B:995:ARG:HG2	2.19	0.43
1:C:391:MET:HA	1:C:394:VAL:HG12	2.00	0.43
1:D:13:GLU:OE1	1:D:14:LEU:HD22	2.19	0.43
1:A:52:SER:HB2	1:A:53:GLN:OE1	2.19	0.43
1:A:880:LYS:HG3	1:A:1043:PHE:HE1	1.83	0.43
1:A:1075:ASP:OD1	1:C:843:SER:OG	2.36	0.43
1:B:203:ASN:O	1:B:216:ASP:HB3	2.18	0.43
1:B:210:ASP:OD1	1:B:211:GLY:N	2.51	0.43
1:C:417:MET:HB3	1:C:424:ILE:HG12	2.00	0.43
1:D:917:GLY:HA2	1:D:1077:LYS:NZ	2.33	0.43
1:B:358:VAL:HG12	1:B:394:VAL:HG11	1.99	0.43
1:C:583:MET:HE1	1:C:612:LYS:HD3	2.00	0.43
1:D:255:ASP:O	1:D:259:LYS:HG2	2.18	0.43
1:D:354:PHE:O	1:D:358:VAL:HG13	2.18	0.43
1:B:729:ARG:HG3	1:B:729:ARG:HH11	1.83	0.43
1:C:308:SER:OG	1:C:309:GLY:N	2.52	0.43
1:C:355:LYS:HA	1:C:358:VAL:HG22	2.01	0.43
1:C:900:HIS:O	1:C:900:HIS:ND1	2.51	0.43
1:C:933:ASP:OD1	1:C:933:ASP:N	2.51	0.43
1:D:416:GLY:HA3	1:D:422:ARG:HE	1.82	0.43
1:A:318:ASP:HA	1:A:321:LYS:HE3	2.00	0.43
1:A:332:HIS:HE1	1:A:334:ASP:HB2	1.82	0.43
1:A:917:GLY:HA2	1:A:1077:LYS:NZ	2.33	0.43
1:D:203:ASN:HA	1:D:204:PRO:HA	1.73	0.42
2:A:1201:ACO:H62A	1:B:1085:ARG:HG3	1.84	0.42
1:B:490:THR:HA	1:B:703:ARG:HG2	2.01	0.42
1:C:102:LEU:HD23	1:C:105:PHE:CZ	2.54	0.42
1:C:206:VAL:HG23	1:C:213:TYR:HB2	2.02	0.42
1:D:599:GLU:HB2	5:D:3303:Q5B:C17	2.49	0.42
1:D:695:SER:OG	1:D:700:HIS:NE2	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:LYS:NZ	1:A:638:ASN:HA	2.34	0.42
1:B:1095:LEU:HD22	1:C:846:ASP:HB2	2.02	0.42
1:D:278:MET:SD	1:D:323:ILE:HD11	2.59	0.42
1:A:515:PHE:HA	1:A:518:VAL:HG12	2.00	0.42
1:B:203:ASN:HA	1:B:204:PRO:HA	1.71	0.42
1:B:226[B]:ASP:OD1	1:B:227:TYR:N	2.53	0.42
1:A:210:ASP:OD1	1:A:211:GLY:N	2.53	0.42
1:B:878:PHE:HB3	1:B:1043:PHE:CE2	2.54	0.42
1:C:367:PRO:HA	1:C:370:GLU:HG3	2.00	0.42
1:A:204:PRO:HD2	1:A:215:LEU:HB2	2.01	0.42
1:C:199:TYR:HB3	1:C:220:LYS:HB2	2.01	0.42
1:C:603:GLU:O	1:C:607:ARG:HG3	2.20	0.42
1:D:174:PRO:O	1:D:178:LYS:HG3	2.19	0.42
1:D:902:PRO:HB3	1:D:1072:HIS:CE1	2.55	0.42
1:D:975:HIS:CG	1:D:976:ARG:N	2.84	0.42
1:D:980:ILE:C	1:D:982:ASN:H	2.26	0.42
1:B:983:PRO:HG2	1:B:985:MET:CE	2.49	0.42
1:C:180:ILE:HG13	1:C:181:LEU:N	2.34	0.42
1:A:818:PRO:HA	1:A:819:PRO:HD3	1.95	0.42
1:A:915:ARG:NH1	1:C:839:SER:O	2.40	0.42
1:B:40:TRP:CE2	1:B:82:LYS:HE3	2.55	0.42
1:B:385:GLN:O	1:B:389:ARG:HG2	2.20	0.42
1:D:553:PHE:CE1	1:D:562:LYS:HD2	2.54	0.42
1:A:175:GLU:HA	1:A:178:LYS:HG3	2.02	0.42
1:A:284:ALA:O	1:A:287:VAL:HG12	2.20	0.42
1:C:133:LEU:HD13	1:C:145:VAL:HG22	2.02	0.42
1:C:493:PHE:CZ	1:C:636:ILE:HD11	2.55	0.42
1:A:386:GLU:O	1:A:389:ARG:HG2	2.19	0.42
1:A:505:GLN:HG3	1:A:572:PHE:CD2	2.55	0.42
1:B:133:LEU:HD11	1:B:151:LYS:HE2	2.02	0.42
1:B:395:GLY:HA3	1:B:402:ILE:HD12	2.02	0.42
1:B:729:ARG:HG3	1:B:729:ARG:NH1	2.35	0.42
1:B:898:ALA:HA	1:B:1064:GLY:O	2.20	0.42
1:D:226[B]:ASP:OD1	1:D:227:TYR:N	2.53	0.42
1:D:516:ASP:CG	1:D:525:SER:HG	2.21	0.42
1:A:902:PRO:HB3	1:A:1072:HIS:CE1	2.55	0.41
1:C:409:THR:HG23	1:C:413:ALA:HB3	2.02	0.41
1:C:777:GLN:O	1:C:781:GLU:OE1	2.37	0.41
1:C:975:HIS:CE1	1:C:978:LYS:HE2	2.55	0.41
1:D:25:ILE:HG23	1:D:28:ARG:HD2	2.02	0.41
1:D:34:VAL:CG2	1:D:105:PHE:HB2	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:ASN:ND2	1:D:109:PRO:HG2	2.35	0.41
1:A:274:ARG:HH21	1:A:335:GLY:C	2.28	0.41
1:A:337:ILE:HG21	1:A:418:ALA:HB1	2.01	0.41
1:A:531:TYR:HD2	1:A:534:THR:HG22	1.85	0.41
1:C:161:ASN:ND2	1:C:163:GLU:OE2	2.53	0.41
1:C:525:SER:HB2	1:C:634:PHE:CE1	2.55	0.41
1:C:878:PHE:HB3	1:C:1043:PHE:CE2	2.55	0.41
1:D:708:PRO:O	1:D:711:LYS:NZ	2.52	0.41
1:D:731:ILE:HG12	1:D:736:LEU:HB2	2.02	0.41
1:A:663:SER:HB2	1:A:666:MET:HE2	2.02	0.41
1:A:931:ILE:HD12	1:A:1061:PHE:HE2	1.85	0.41
1:B:180:ILE:HG13	1:B:181:LEU:N	2.36	0.41
1:B:214:VAL:HG11	1:B:217:LEU:HD23	2.02	0.41
1:B:895:MET:HG2	1:D:872:VAL:HG21	2.01	0.41
1:C:56:VAL:HG23	1:C:74:VAL:HA	2.01	0.41
1:C:276:TRP:CD1	1:C:327:MET:HE3	2.55	0.41
1:C:396:LYS:HB2	1:C:396:LYS:HE2	1.91	0.41
1:C:857:MET:HE1	1:C:881:ARG:HD3	2.02	0.41
1:D:977:VAL:HG23	1:D:978:LYS:HG3	2.02	0.41
1:A:54:ASN:HB3	1:A:110:PHE:HB3	2.02	0.41
1:A:493:PHE:CE2	1:A:636:ILE:HD11	2.54	0.41
1:A:579:TYR:O	1:A:583:MET:HG2	2.19	0.41
1:A:646:ILE:HG23	1:A:651:LEU:HB2	2.03	0.41
1:B:969:LEU:HD22	5:D:3303:Q5B:C10	2.50	0.41
1:B:44:LEU:HD13	1:B:50:LEU:HD12	2.03	0.41
1:B:689:GLY:HA3	1:B:760:HIS:ND1	2.34	0.41
1:C:666:MET:HE2	1:C:666:MET:HB2	1.84	0.41
1:D:323:ILE:HA	1:D:326:LEU:HD12	2.03	0.41
1:A:974:GLY:O	1:A:1024:ASN:ND2	2.52	0.41
1:B:260:SER:OG	1:B:315:GLN:OE1	2.30	0.41
1:D:89:LEU:O	1:D:91:GLN:NE2	2.39	0.41
1:D:525:SER:HB2	1:D:634:PHE:CE1	2.56	0.41
1:A:40:TRP:CE2	1:A:82:LYS:HE3	2.56	0.41
1:B:417:MET:SD	1:B:424:ILE:HA	2.60	0.41
1:C:579:TYR:O	1:C:583:MET:HG2	2.21	0.41
1:C:978:LYS:HD2	1:C:984:ASP:HA	2.03	0.41
1:D:166:LYS:HD2	1:D:170:LEU:HD12	2.03	0.41
1:D:878:PHE:HB3	1:D:1043:PHE:CE2	2.56	0.41
1:A:150:GLN:NE2	1:A:168:HIS:O	2.53	0.41
1:B:166:LYS:NZ	1:B:179:GLU:HA	2.36	0.41
1:B:204:PRO:HG2	1:B:215:LEU:HD12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:LYS:HB2	1:B:396:LYS:HE2	1.91	0.41
1:C:160:LEU:HG	1:C:165:ILE:HD11	2.02	0.41
1:C:731:ILE:HD11	1:C:740:ILE:HD12	2.03	0.41
1:C:802:GLU:HA	1:C:805:VAL:HG12	2.03	0.41
1:D:512:MET:HE2	1:D:637:GLY:N	2.32	0.41
1:D:976:ARG:HH11	2:D:3301:ACO:C8A	2.34	0.41
1:A:378:ARG:NH1	1:A:411:MET:SD	2.95	0.40
1:B:127:ARG:O	1:B:611:LYS:NZ	2.52	0.40
1:C:256:LEU:HD23	1:C:256:LEU:HA	1.86	0.40
1:C:878:PHE:HB3	1:C:1043:PHE:HE2	1.86	0.40
1:D:891:GLU:O	1:D:895:MET:HG3	2.20	0.40
1:A:346:ASN:ND2	1:A:640:GLY:H	2.19	0.40
1:A:861:GLU:O	1:A:865:GLU:HG2	2.21	0.40
1:B:63:ILE:HG21	1:B:95:VAL:HG21	2.03	0.40
1:A:984:ASP:HB3	1:A:987:VAL:H	1.86	0.40
1:C:41:ALA:O	1:C:44:LEU:N	2.44	0.40
1:D:735:ARG:HG3	1:D:735:ARG:NH1	2.36	0.40
5:D:3303:Q5B:O15	5:D:3303:Q5B:O20	2.38	0.40
1:A:1086:HIS:O	2:B:2303:ACO:N6A	2.47	0.40
1:B:318:ASP:HA	1:B:321:LYS:HG2	2.03	0.40
1:B:321:LYS:HB2	1:B:364:TYR:HE2	1.87	0.40
1:B:878:PHE:HB3	1:B:1043:PHE:HE2	1.85	0.40
1:D:165:ILE:O	1:D:169:LEU:HB2	2.20	0.40
1:A:170:LEU:O	1:A:178:LYS:NZ	2.55	0.40
1:B:268:LEU:HD21	1:B:326:LEU:HD13	2.04	0.40
1:B:346:ASN:O	1:B:641:GLY:HA2	2.22	0.40
1:B:713:ILE:O	1:B:740:ILE:HA	2.21	0.40
1:B:984:ASP:O	1:B:985:MET:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1035/1101 (94%)	992 (96%)	43 (4%)	0	100	100
1	B	1035/1101 (94%)	999 (96%)	36 (4%)	0	100	100
1	C	1035/1101 (94%)	1003 (97%)	32 (3%)	0	100	100
1	D	1035/1101 (94%)	1007 (97%)	28 (3%)	0	100	100
All	All	4140/4404 (94%)	4001 (97%)	139 (3%)	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	852/908 (94%)	850 (100%)	2 (0%)	87	96
1	B	852/908 (94%)	850 (100%)	2 (0%)	87	96
1	C	852/908 (94%)	850 (100%)	2 (0%)	87	96
1	D	852/908 (94%)	850 (100%)	2 (0%)	87	96
All	All	3408/3632 (94%)	3400 (100%)	8 (0%)	87	96

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	226[A]	ASP
1	A	226[B]	ASP
1	B	226[A]	ASP
1	B	226[B]	ASP
1	C	226[A]	ASP
1	C	226[B]	ASP
1	D	226[A]	ASP
1	D	226[B]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	315	GLN
1	A	332	HIS
1	A	545	HIS
1	A	777	GLN
1	A	1072	HIS
1	B	638	ASN
1	B	850	GLN
1	B	888	GLN
1	B	981	ASN
1	C	113	HIS
1	C	150	GLN
1	C	172	HIS
1	C	349	ASN
1	C	383	ASN
1	C	563	HIS
1	C	571	ASN
1	C	638	ASN
1	C	888	GLN
1	C	988	GLN
1	C	996	GLN
1	D	26	GLN
1	D	75	ASN
1	D	303	ASN
1	D	421	HIS
1	D	563	HIS
1	D	638	ASN
1	D	777	GLN
1	D	888	GLN
1	D	1024	ASN
1	D	1072	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are unknown - 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
5	Q5B	B	2302	-	60,62,62	2.87	20 (33%)	87,93,93	1.85	19 (21%)
3	OAA	A	1203	-	8,8,8	1.36	1 (12%)	8,10,10	1.40	1 (12%)
2	ACO	D	3301	-	51,53,53	1.12	4 (7%)	73,79,79	1.50	8 (10%)
2	ACO	C	3301	-	51,53,53	1.11	5 (9%)	73,79,79	1.51	12 (16%)
3	OAA	A	1202	-	8,8,8	1.34	1 (12%)	8,10,10	1.42	1 (12%)
2	ACO	B	2303	-	51,53,53	1.13	5 (9%)	73,79,79	1.51	11 (15%)
5	Q5B	D	3303	-	60,62,62	2.91	21 (35%)	87,93,93	1.79	19 (21%)
6	PO4	C	3306	-	4,4,4	0.97	0	6,6,6	0.35	0
3	OAA	D	3302	-	8,8,8	1.37	1 (12%)	8,10,10	1.43	1 (12%)
2	ACO	A	1201	-	51,53,53	1.16	5 (9%)	73,79,79	1.47	11 (15%)
7	ADP	C	3303	-	28,29,29	1.42	4 (14%)	43,45,45	1.85	9 (20%)
6	PO4	D	3305	-	4,4,4	0.96	0	6,6,6	0.45	0
7	ADP	D	3304	-	28,29,29	1.41	4 (14%)	43,45,45	1.85	9 (20%)
5	Q5B	C	3305	-	60,62,62	2.87	21 (35%)	87,93,93	1.76	20 (22%)
6	PO4	B	2304	-	4,4,4	0.97	0	6,6,6	0.46	0
3	OAA	C	3302	-	8,8,8	1.35	1 (12%)	8,10,10	1.41	1 (12%)

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
5	Q5B	B	2302	-	-	10/66/83/83	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OAA	A	1203	-	-	4/8/8/8	-
2	ACO	D	3301	-	-	15/51/67/67	0/3/3/3
2	ACO	C	3301	-	-	20/51/67/67	0/3/3/3
3	OAA	A	1202	-	-	5/8/8/8	-
2	ACO	B	2303	-	-	13/51/67/67	0/3/3/3
5	Q5B	D	3303	-	-	21/66/83/83	0/3/3/3
7	ADP	C	3303	-	-	4/16/32/32	0/3/3/3
3	OAA	D	3302	-	-	6/8/8/8	-
2	ACO	A	1201	-	-	12/51/67/67	0/3/3/3
7	ADP	D	3304	-	-	5/16/32/32	0/3/3/3
5	Q5B	C	3305	-	-	15/66/83/83	0/3/3/3
3	OAA	C	3302	-	-	6/8/8/8	-

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	3303	Q5B	P1-O3	8.54	1.68	1.59
5	C	3305	Q5B	P1-O3	8.26	1.68	1.59
5	D	3303	Q5B	C6-C5	-8.20	1.31	1.52
5	B	2302	Q5B	C6-C5	-8.17	1.31	1.52
5	B	2302	Q5B	P1-O3	8.12	1.68	1.59
5	C	3305	Q5B	C6-C5	-7.89	1.32	1.52
5	C	3305	Q5B	C7-C6	7.46	1.69	1.53
5	D	3303	Q5B	C18-N6	7.22	1.50	1.33
5	D	3303	Q5B	C7-C6	7.20	1.68	1.53
5	C	3305	Q5B	C18-N6	7.18	1.50	1.33
5	B	2302	Q5B	C18-N6	7.15	1.50	1.33
5	D	3303	Q5B	P-O3	7.15	1.67	1.59
5	C	3305	Q5B	P-O3	7.13	1.67	1.59
5	B	2302	Q5B	P-O3	7.05	1.67	1.59
5	B	2302	Q5B	C7-C6	7.03	1.68	1.53
5	D	3303	Q5B	C15-N5	6.63	1.49	1.33
5	C	3305	Q5B	C15-N5	6.59	1.49	1.33
5	B	2302	Q5B	C15-N5	6.45	1.48	1.33
7	C	3303	ADP	C5-C4	4.75	1.47	1.39
7	D	3304	ADP	C5-C4	4.73	1.47	1.39
2	D	3301	ACO	C5A-C4A	4.52	1.47	1.39
2	B	2303	ACO	C5A-C4A	4.41	1.46	1.39
2	A	1201	ACO	C5A-C4A	4.36	1.46	1.39
2	C	3301	ACO	C5A-C4A	4.28	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	3303	Q5B	O7-C5	3.81	1.53	1.45
5	D	3303	Q5B	C21-S	3.77	1.85	1.76
5	B	2302	Q5B	C9-N	-3.73	1.31	1.37
5	C	3305	Q5B	O7-C5	3.61	1.53	1.45
5	B	2302	Q5B	O7-C5	3.56	1.52	1.45
5	C	3305	Q5B	C21-S	3.51	1.84	1.76
5	C	3305	Q5B	O20-C23	-3.43	1.36	1.43
5	D	3303	Q5B	O20-C23	-3.39	1.36	1.43
5	B	2302	Q5B	C23-C26	-3.37	1.50	1.53
5	B	2302	Q5B	O20-C23	-3.31	1.36	1.43
5	B	2302	Q5B	C21-S	3.30	1.84	1.76
5	C	3305	Q5B	C9-N	-3.20	1.32	1.37
5	D	3303	Q5B	C22-C23	3.19	1.57	1.54
5	D	3303	Q5B	P2-O9	3.11	1.65	1.59
5	C	3305	Q5B	P2-O9	3.10	1.65	1.59
5	D	3303	Q5B	C9-N	-3.08	1.32	1.37
5	C	3305	Q5B	C23-C26	-2.94	1.50	1.53
5	D	3303	Q5B	O13-C15	-2.88	1.17	1.23
5	B	2302	Q5B	C-C1	-2.86	1.47	1.53
5	C	3305	Q5B	O14-C18	-2.83	1.17	1.23
5	B	2302	Q5B	O14-C18	-2.82	1.17	1.23
7	D	3304	ADP	C5-C6	2.75	1.48	1.41
7	C	3303	ADP	C5-C6	2.75	1.48	1.41
5	C	3305	Q5B	O13-C15	-2.75	1.18	1.23
5	D	3303	Q5B	C23-C26	-2.74	1.50	1.53
5	C	3305	Q5B	C22-C23	2.70	1.57	1.54
5	B	2302	Q5B	O13-C15	-2.68	1.18	1.23
5	D	3303	Q5B	O14-C18	-2.67	1.18	1.23
5	B	2302	Q5B	P2-O9	2.66	1.64	1.59
2	A	1201	ACO	C5A-C6A	2.63	1.48	1.41
5	D	3303	Q5B	C-C1	-2.59	1.48	1.53
2	B	2303	ACO	C5A-C6A	2.59	1.48	1.41
2	C	3301	ACO	C5A-C6A	2.55	1.48	1.41
2	D	3301	ACO	C5A-C6A	2.47	1.47	1.41
5	C	3305	Q5B	C-C1	-2.46	1.48	1.53
5	B	2302	Q5B	C2-C1	2.43	1.58	1.53
5	B	2302	Q5B	C22-C23	2.41	1.56	1.54
5	D	3303	Q5B	C22-C21	2.41	1.56	1.51
2	D	3301	ACO	C5A-N7A	-2.41	1.34	1.39
5	C	3305	Q5B	C22-C21	2.39	1.56	1.51
7	D	3304	ADP	C8-N7	2.33	1.36	1.31
7	C	3303	ADP	C8-N7	2.32	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3301	ACO	C5A-N7A	-2.32	1.34	1.39
2	A	1201	ACO	C5A-N7A	-2.30	1.34	1.39
2	B	2303	ACO	C5A-N7A	-2.30	1.34	1.39
5	D	3303	Q5B	C2-C1	2.28	1.58	1.53
7	C	3303	ADP	C5-N7	-2.26	1.35	1.39
5	B	2302	Q5B	C22-C21	2.25	1.55	1.51
5	B	2302	Q5B	C13-N3	-2.25	1.29	1.35
2	C	3301	ACO	C8A-N7A	2.24	1.36	1.31
2	C	3301	ACO	C4A-N9A	-2.24	1.33	1.37
7	D	3304	ADP	C5-N7	-2.23	1.35	1.39
2	A	1201	ACO	C8A-N7A	2.21	1.35	1.31
5	C	3305	Q5B	C2-C1	2.20	1.58	1.53
2	B	2303	ACO	C8A-N7A	2.20	1.35	1.31
5	D	3303	Q5B	O-C3	-2.18	1.36	1.43
5	D	3303	Q5B	P1-O6	2.17	1.67	1.59
2	A	1201	ACO	C4A-N9A	-2.16	1.33	1.37
3	D	3302	OAA	O3-C3	-2.13	1.18	1.23
2	B	2303	ACO	C4A-N9A	-2.12	1.33	1.37
3	A	1203	OAA	O3-C3	-2.10	1.18	1.23
5	B	2302	Q5B	P1-O6	2.09	1.67	1.59
5	D	3303	Q5B	C13-N3	-2.09	1.29	1.35
5	C	3305	Q5B	P1-O6	2.09	1.67	1.59
2	D	3301	ACO	C8A-N7A	2.09	1.35	1.31
3	A	1202	OAA	O3-C3	-2.08	1.18	1.23
3	C	3302	OAA	O3-C3	-2.08	1.18	1.23
5	C	3305	Q5B	C13-N3	-2.08	1.30	1.35
5	C	3305	Q5B	C13-N4	2.01	1.39	1.34

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	3303	ADP	C5-C4-N3	-5.98	118.48	126.72
7	D	3304	ADP	C5-C4-N3	-5.87	118.64	126.72
2	D	3301	ACO	C5A-C4A-N3A	-5.84	118.68	126.72
2	A	1201	ACO	C5A-C4A-N3A	-5.68	118.89	126.72
2	B	2303	ACO	C5A-C4A-N3A	-5.56	119.06	126.72
5	B	2302	Q5B	N3-C12-N2	-5.54	120.20	128.58
2	C	3301	ACO	C5A-C4A-N3A	-5.43	119.24	126.72
5	C	3305	Q5B	N3-C12-N2	-5.28	120.59	128.58
5	C	3305	Q5B	C10-C11-N2	-5.19	119.57	126.72
5	D	3303	Q5B	C10-C11-N2	-5.14	119.64	126.72
5	B	2302	Q5B	C10-C11-N2	-5.05	119.76	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	3305	Q5B	C22-C21-S	5.04	119.92	113.56
5	D	3303	Q5B	N3-C12-N2	-5.01	121.00	128.58
5	D	3303	Q5B	C22-C21-S	4.91	119.75	113.56
2	D	3301	ACO	N3A-C4A-N9A	4.73	135.21	127.17
7	C	3303	ADP	N3-C4-N9	4.72	135.20	127.17
5	B	2302	Q5B	C22-C21-S	4.63	119.40	113.56
7	D	3304	ADP	N3-C4-N9	4.63	135.03	127.17
2	A	1201	ACO	N3A-C4A-N9A	4.42	134.69	127.17
2	B	2303	ACO	N3A-C4A-N9A	4.37	134.59	127.17
2	C	3301	ACO	N3A-C4A-N9A	4.28	134.45	127.17
5	D	3303	Q5B	N2-C11-N	4.16	134.24	127.17
5	B	2302	Q5B	C12-N2-C11	4.16	121.98	111.83
5	C	3305	Q5B	C12-N2-C11	4.13	121.92	111.83
5	B	2302	Q5B	N-C9-N1	-4.00	108.27	113.94
5	D	3303	Q5B	C12-N2-C11	3.92	121.41	111.83
5	B	2302	Q5B	C11-N-C9	3.92	109.85	105.74
5	C	3305	Q5B	N2-C11-N	3.89	133.79	127.17
5	B	2302	Q5B	N2-C11-N	3.87	133.75	127.17
2	A	1201	ACO	C2A-N3A-C4A	3.82	121.17	111.83
7	C	3303	ADP	C2-N3-C4	3.74	120.98	111.83
2	B	2303	ACO	C4A-C5A-N7A	-3.71	106.34	110.58
7	D	3304	ADP	C2-N3-C4	3.70	120.86	111.83
2	D	3301	ACO	C2A-N3A-C4A	3.69	120.85	111.83
5	B	2302	Q5B	O7-C8-N	3.69	115.17	108.09
2	C	3301	ACO	C2A-N3A-C4A	3.68	120.83	111.83
2	B	2303	ACO	C2A-N3A-C4A	3.66	120.76	111.83
5	C	3305	Q5B	N-C9-N1	-3.60	108.83	113.94
2	A	1201	ACO	N3A-C2A-N1A	-3.53	123.23	128.58
2	A	1201	ACO	C4A-C5A-N7A	-3.52	106.56	110.58
2	C	3301	ACO	N3A-C2A-N1A	-3.49	123.30	128.58
7	C	3303	ADP	C4-C5-N7	-3.48	106.60	110.58
5	D	3303	Q5B	C14-C15-N5	3.46	123.04	116.48
7	D	3304	ADP	C4-C5-N7	-3.45	106.64	110.58
2	C	3301	ACO	C4A-C5A-N7A	-3.40	106.69	110.58
2	B	2303	ACO	N3A-C2A-N1A	-3.38	123.47	128.58
2	D	3301	ACO	N3A-C2A-N1A	-3.38	123.47	128.58
5	C	3305	Q5B	O19-C26-C23	3.35	119.58	113.14
5	C	3305	Q5B	C11-N-C9	3.33	109.23	105.74
5	B	2302	Q5B	C11-C10-N1	-3.29	106.82	110.58
2	D	3301	ACO	C4A-C5A-N7A	-3.28	106.83	110.58
5	D	3303	Q5B	O19-C26-C23	3.27	119.41	113.14
5	B	2302	Q5B	C10-N1-C9	3.26	108.58	103.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	3303	Q5B	C11-N-C9	3.25	109.15	105.74
5	D	3303	Q5B	N-C9-N1	-3.25	109.33	113.94
7	C	3303	ADP	N3-C2-N1	-3.23	123.69	128.58
7	D	3304	ADP	N3-C2-N1	-3.15	123.82	128.58
5	C	3305	Q5B	C11-C10-N1	-3.12	107.01	110.58
5	C	3305	Q5B	C10-N1-C9	3.08	108.29	103.45
2	B	2303	ACO	C4A-N9A-C8A	3.04	108.93	105.74
5	D	3303	Q5B	C16-C17-C18	3.02	117.42	112.39
5	B	2302	Q5B	C17-C18-N6	2.95	121.73	116.34
2	C	3301	ACO	C4A-N9A-C8A	2.94	108.83	105.74
5	B	2302	Q5B	C20-S-C21	2.82	110.17	101.84
5	D	3303	Q5B	O-C3-C1	-2.82	106.02	110.55
2	A	1201	ACO	C4A-N9A-C8A	2.81	108.69	105.74
5	B	2302	Q5B	O19-C26-C23	2.75	118.42	113.14
2	B	2303	ACO	C5A-N7A-C8A	2.73	107.74	103.45
5	D	3303	Q5B	C10-N1-C9	2.68	107.66	103.45
5	C	3305	Q5B	C20-S-C21	2.64	109.64	101.84
5	D	3303	Q5B	C-C1-C14	2.60	113.19	108.77
2	D	3301	ACO	C4A-N9A-C8A	2.59	108.45	105.74
2	A	1201	ACO	C3B-C2B-C1B	2.58	105.55	99.89
7	D	3304	ADP	C4-N9-C8	2.56	108.43	105.74
7	C	3303	ADP	C5-N7-C8	2.54	107.44	103.45
5	B	2302	Q5B	C13-C10-N1	2.54	136.98	132.09
7	D	3304	ADP	C5-N7-C8	2.53	107.42	103.45
2	A	1201	ACO	C5A-N7A-C8A	2.52	107.42	103.45
7	C	3303	ADP	C4-N9-C8	2.52	108.39	105.74
7	D	3304	ADP	C3'-C2'-C1'	2.51	106.21	101.46
5	D	3303	Q5B	C11-C10-N1	-2.48	107.74	110.58
5	C	3305	Q5B	C2-C1-C14	2.48	113.00	108.77
7	C	3303	ADP	C3'-C2'-C1'	2.46	106.12	101.46
2	A	1201	ACO	C6A-C5A-N7A	2.45	136.81	132.09
2	C	3301	ACO	C5A-N7A-C8A	2.42	107.26	103.45
5	D	3303	Q5B	C20-S-C21	2.42	109.00	101.84
5	D	3303	Q5B	O13-C15-N5	-2.41	117.88	122.98
2	B	2303	ACO	C6A-C5A-N7A	2.39	136.70	132.09
5	B	2302	Q5B	C11-N-C8	-2.39	121.05	126.63
3	D	3302	OAA	O5-C4-C3	2.37	120.15	113.59
3	A	1202	OAA	O5-C4-C3	2.35	120.11	113.59
2	D	3301	ACO	C5A-N7A-C8A	2.35	107.14	103.45
5	D	3303	Q5B	O15-C21-S	-2.34	119.71	122.68
5	C	3305	Q5B	C13-C10-N1	2.34	136.59	132.09
3	A	1203	OAA	O5-C4-C3	2.33	120.06	113.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	3305	Q5B	O15-C21-S	-2.33	119.72	122.68
3	C	3302	OAA	O5-C4-C3	2.33	120.05	113.59
2	B	2303	ACO	N9A-C8A-N7A	-2.32	110.64	113.94
2	C	3301	ACO	C6A-C5A-N7A	2.30	136.53	132.09
5	C	3305	Q5B	C16-N5-C15	-2.28	118.44	122.55
5	B	2302	Q5B	C19-N6-C18	-2.24	118.65	122.82
5	C	3305	Q5B	C17-C18-N6	2.20	120.34	116.34
2	C	3301	ACO	O4B-C1B-N9A	2.18	112.27	108.09
2	D	3301	ACO	C3B-C2B-C1B	2.18	104.67	99.89
5	C	3305	Q5B	O15-C21-C22	-2.16	120.35	123.66
2	C	3301	ACO	C3B-C2B-C1B	2.14	104.61	99.89
2	C	3301	ACO	N9A-C8A-N7A	-2.13	110.92	113.94
2	B	2303	ACO	C7P-C6P-C5P	-2.13	108.85	112.39
2	A	1201	ACO	N9A-C8A-N7A	-2.13	110.92	113.94
5	B	2302	Q5B	O15-C21-S	-2.11	120.00	122.68
5	B	2302	Q5B	C2-C1-C14	2.07	112.30	108.77
5	C	3305	Q5B	C11-N-C8	-2.05	121.83	126.63
5	D	3303	Q5B	O15-C21-C22	-2.04	120.53	123.66
7	D	3304	ADP	C6-C5-N7	2.04	136.02	132.09
2	C	3301	ACO	C2A-N1A-C6A	2.04	122.08	118.73
5	C	3305	Q5B	O-C3-C1	-2.04	107.27	110.55
5	C	3305	Q5B	C19-N6-C18	-2.03	119.04	122.82
7	C	3303	ADP	C6-C5-N7	2.03	135.99	132.09
2	B	2303	ACO	C3B-C2B-C1B	2.02	104.33	99.89
5	D	3303	Q5B	C17-C18-N6	2.01	120.01	116.34
2	A	1201	ACO	C7P-C6P-C5P	-2.01	109.04	112.39
5	B	2302	Q5B	O15-C21-C22	-2.00	120.59	123.66

There are no chirality outliers.

All (136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	ACO	CCP-O6A-P2A-O3A
2	A	1201	ACO	CCP-O6A-P2A-O4A
2	A	1201	ACO	CCP-O6A-P2A-O5A
2	A	1201	ACO	C6P-C5P-N4P-C3P
2	A	1201	ACO	O-C-S1P-C2P
2	A	1201	ACO	CH3-C-S1P-C2P
2	B	2303	ACO	CBP-CCP-O6A-P2A
2	B	2303	ACO	CDP-CBP-CCP-O6A
2	B	2303	ACO	CEP-CBP-CCP-O6A
2	B	2303	ACO	CAP-CBP-CCP-O6A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	2303	ACO	O-C-S1P-C2P
2	B	2303	ACO	CH3-C-S1P-C2P
2	C	3301	ACO	C5B-O5B-P1A-O1A
2	C	3301	ACO	CCP-O6A-P2A-O3A
2	C	3301	ACO	CDP-CBP-CCP-O6A
2	C	3301	ACO	CEP-CBP-CCP-O6A
2	C	3301	ACO	CAP-CBP-CCP-O6A
2	C	3301	ACO	CAP-C9P-N8P-C7P
2	C	3301	ACO	C6P-C5P-N4P-C3P
2	C	3301	ACO	O5P-C5P-N4P-C3P
2	C	3301	ACO	O-C-S1P-C2P
2	C	3301	ACO	CH3-C-S1P-C2P
2	D	3301	ACO	CBP-CCP-O6A-P2A
2	D	3301	ACO	CDP-CBP-CCP-O6A
2	D	3301	ACO	CEP-CBP-CCP-O6A
2	D	3301	ACO	CAP-CBP-CCP-O6A
2	D	3301	ACO	CAP-C9P-N8P-C7P
2	D	3301	ACO	O9P-C9P-N8P-C7P
2	D	3301	ACO	C5P-C6P-C7P-N8P
2	D	3301	ACO	C6P-C5P-N4P-C3P
2	D	3301	ACO	O-C-S1P-C2P
2	D	3301	ACO	CH3-C-S1P-C2P
3	A	1202	OAA	C2-C3-C4-O4
3	A	1202	OAA	C2-C3-C4-O5
3	A	1203	OAA	C2-C3-C4-O4
3	A	1203	OAA	C2-C3-C4-O5
3	C	3302	OAA	O3-C3-C4-O4
3	C	3302	OAA	O3-C3-C4-O5
3	C	3302	OAA	C2-C3-C4-O5
3	D	3302	OAA	O2-C1-C2-C3
3	D	3302	OAA	C2-C3-C4-O4
3	D	3302	OAA	C2-C3-C4-O5
5	B	2302	Q5B	C19-C20-S-C21
5	B	2302	Q5B	C22-C21-S-C20
5	B	2302	Q5B	O15-C21-S-C20
5	B	2302	Q5B	P-O3-P1-O6
5	C	3305	Q5B	N6-C19-C20-S
5	C	3305	Q5B	O20-C23-C24-C25
5	D	3303	Q5B	C3-O-P-O2
5	D	3303	Q5B	C-C1-C14-O21
5	D	3303	Q5B	C3-C1-C14-O21
5	D	3303	Q5B	C-C1-C3-O

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	D	3303	Q5B	C14-C1-C3-O
5	D	3303	Q5B	C2-C1-C3-O
5	D	3303	Q5B	C14-C15-N5-C16
5	D	3303	Q5B	N5-C16-C17-C18
5	D	3303	Q5B	C21-C22-C23-C24
5	D	3303	Q5B	C21-C22-C23-C26
5	D	3303	Q5B	C21-C22-C23-O20
5	D	3303	Q5B	P-O3-P1-O6
7	C	3303	ADP	C5'-O5'-PA-O2A
7	C	3303	ADP	C5'-O5'-PA-O3A
7	D	3304	ADP	C5'-O5'-PA-O1A
7	D	3304	ADP	C5'-O5'-PA-O2A
7	D	3304	ADP	C5'-O5'-PA-O3A
2	A	1201	ACO	O5P-C5P-N4P-C3P
2	D	3301	ACO	O5P-C5P-N4P-C3P
5	D	3303	Q5B	O13-C15-N5-C16
2	C	3301	ACO	O4B-C4B-C5B-O5B
7	C	3303	ADP	C3'-C4'-C5'-O5'
7	D	3304	ADP	C3'-C4'-C5'-O5'
2	B	2303	ACO	O5P-C5P-N4P-C3P
2	A	1201	ACO	C4B-C3B-O3B-P3B
2	C	3301	ACO	C4B-C3B-O3B-P3B
5	C	3305	Q5B	C21-C22-C23-C24
5	C	3305	Q5B	C21-C22-C23-O20
5	C	3305	Q5B	C21-C22-C23-C26
5	C	3305	Q5B	C26-C23-C24-C25
2	B	2303	ACO	C6P-C5P-N4P-C3P
7	C	3303	ADP	O4'-C4'-C5'-O5'
5	C	3305	Q5B	C22-C23-C24-C25
5	C	3305	Q5B	O6-C4-C5-O7
5	D	3303	Q5B	O6-C4-C5-O7
2	C	3301	ACO	O9P-C9P-N8P-C7P
2	C	3301	ACO	C3B-C4B-C5B-O5B
2	C	3301	ACO	O9P-C9P-CAP-OAP
5	D	3303	Q5B	C2-C1-C14-O21
5	B	2302	Q5B	N6-C19-C20-S
5	B	2302	Q5B	O6-C4-C5-O7
7	D	3304	ADP	O4'-C4'-C5'-O5'
2	C	3301	ACO	N8P-C9P-CAP-CBP
5	C	3305	Q5B	O15-C21-S-C20
5	D	3303	Q5B	O15-C21-S-C20
3	D	3302	OAA	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

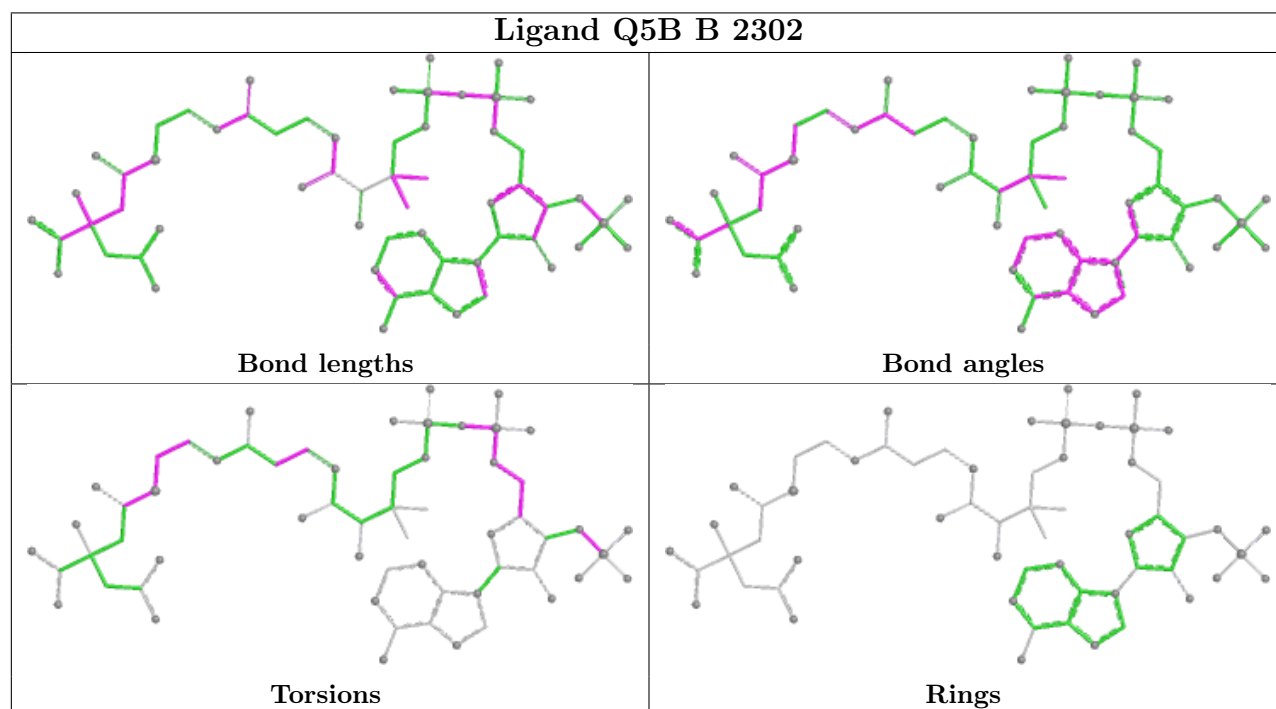
Mol	Chain	Res	Type	Atoms
5	C	3305	Q5B	O6-C4-C5-C6
2	B	2303	ACO	P1A-O3A-P2A-O6A
2	D	3301	ACO	P1A-O3A-P2A-O6A
3	C	3302	OAA	O2-C1-C2-C3
5	C	3305	Q5B	P-O3-P1-O6
5	C	3305	Q5B	C22-C21-S-C20
5	D	3303	Q5B	C22-C21-S-C20
3	A	1202	OAA	C1-C2-C3-O3
3	A	1202	OAA	O3-C3-C4-O4
3	A	1203	OAA	O3-C3-C4-O4
3	D	3302	OAA	O3-C3-C4-O4
3	C	3302	OAA	C2-C3-C4-O4
2	A	1201	ACO	O4B-C4B-C5B-O5B
3	C	3302	OAA	O1-C1-C2-C3
2	C	3301	ACO	C6P-C7P-N8P-C9P
2	B	2303	ACO	C3P-C2P-S1P-C
2	A	1201	ACO	C5B-O5B-P1A-O1A
5	B	2302	Q5B	C4-O6-P1-O5
5	D	3303	Q5B	C3-O-P-O3
2	C	3301	ACO	C2B-C3B-O3B-P3B
2	D	3301	ACO	C2B-C1B-N9A-C8A
2	B	2303	ACO	C5P-C6P-C7P-N8P
5	B	2302	Q5B	N5-C16-C17-C18
2	C	3301	ACO	O9P-C9P-CAP-CBP
2	A	1201	ACO	C2B-C1B-N9A-C8A
2	A	1201	ACO	C3B-O3B-P3B-O8A
5	B	2302	Q5B	C6-O9-P2-O10
5	C	3305	Q5B	C6-O9-P2-O10
3	A	1203	OAA	O1-C1-C2-C3
5	B	2302	Q5B	C5-C4-O6-P1
2	D	3301	ACO	C4B-C5B-O5B-P1A
5	C	3305	Q5B	C24-C23-C26-O19
3	D	3302	OAA	C1-C2-C3-O3
5	D	3303	Q5B	C7-C8-N-C9
5	D	3303	Q5B	O6-C4-C5-C6
5	C	3305	Q5B	C-C1-C14-O21
3	A	1202	OAA	O1-C1-C2-C3
5	D	3303	Q5B	C6-O9-P2-O10
2	D	3301	ACO	O4B-C1B-N9A-C8A
2	B	2303	ACO	C2B-C1B-N9A-C8A
2	C	3301	ACO	N8P-C9P-CAP-OAP
2	B	2303	ACO	C4B-C5B-O5B-P1A

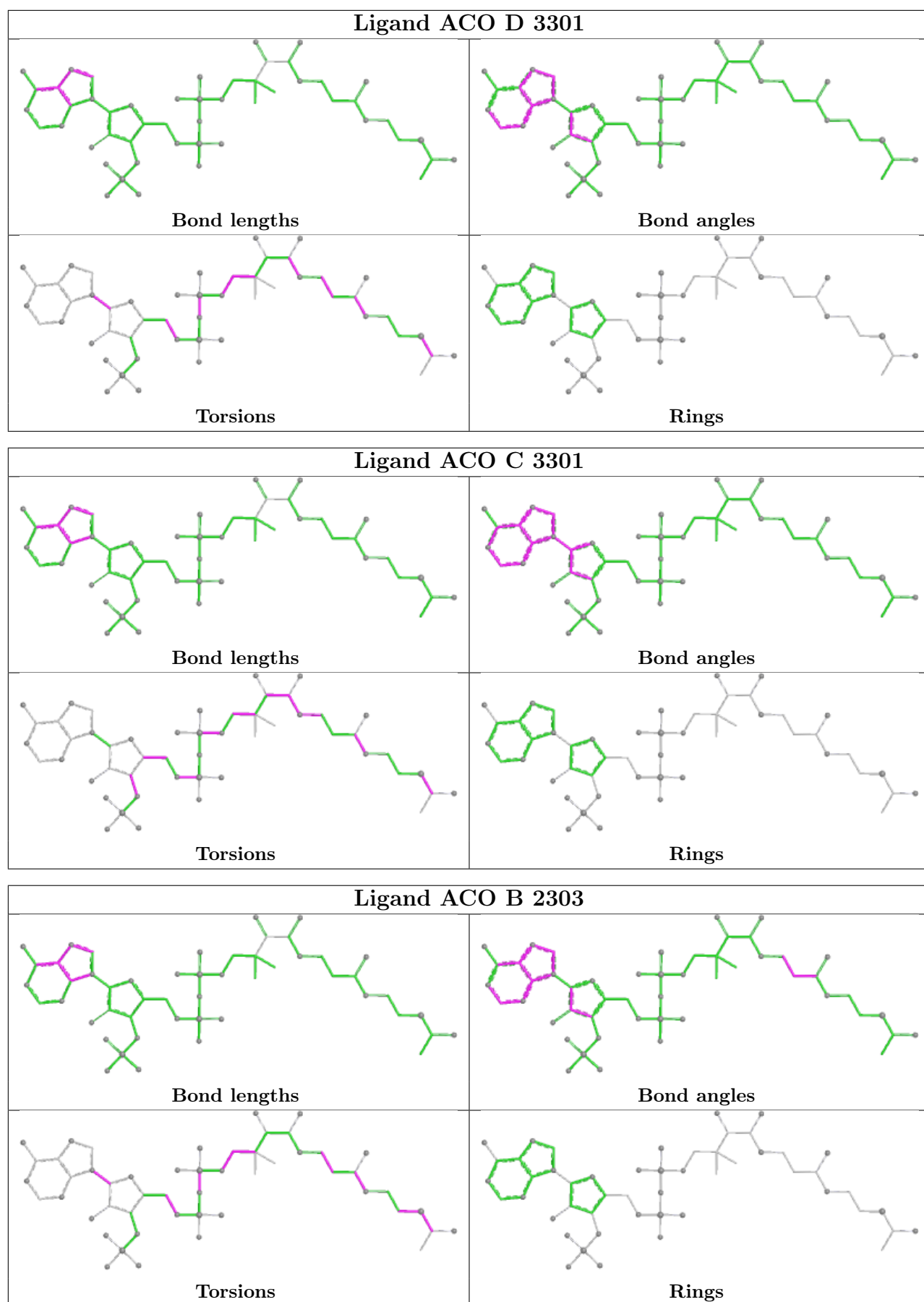
There are no ring outliers.

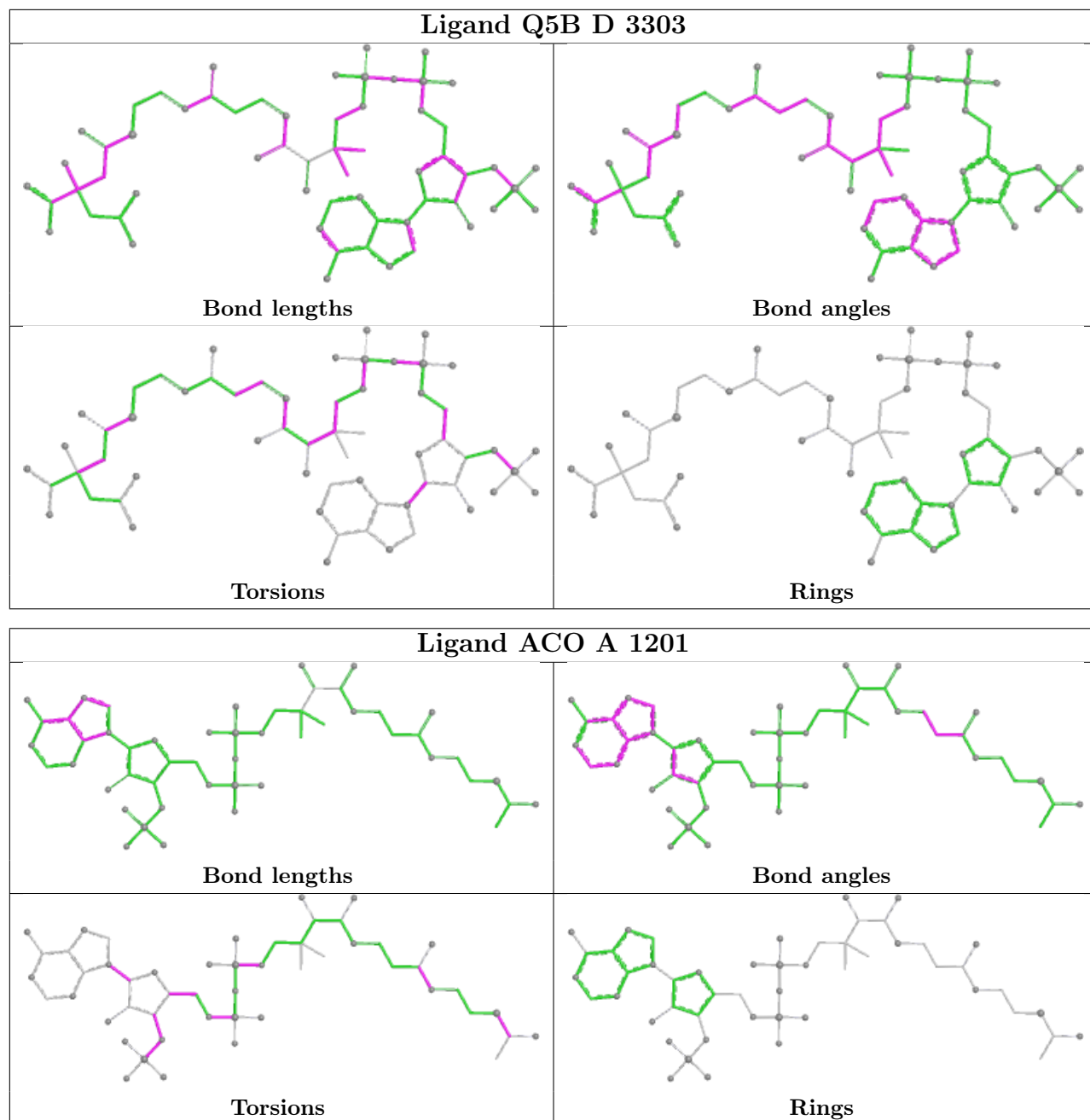
10 monomers are involved in 45 short contacts:

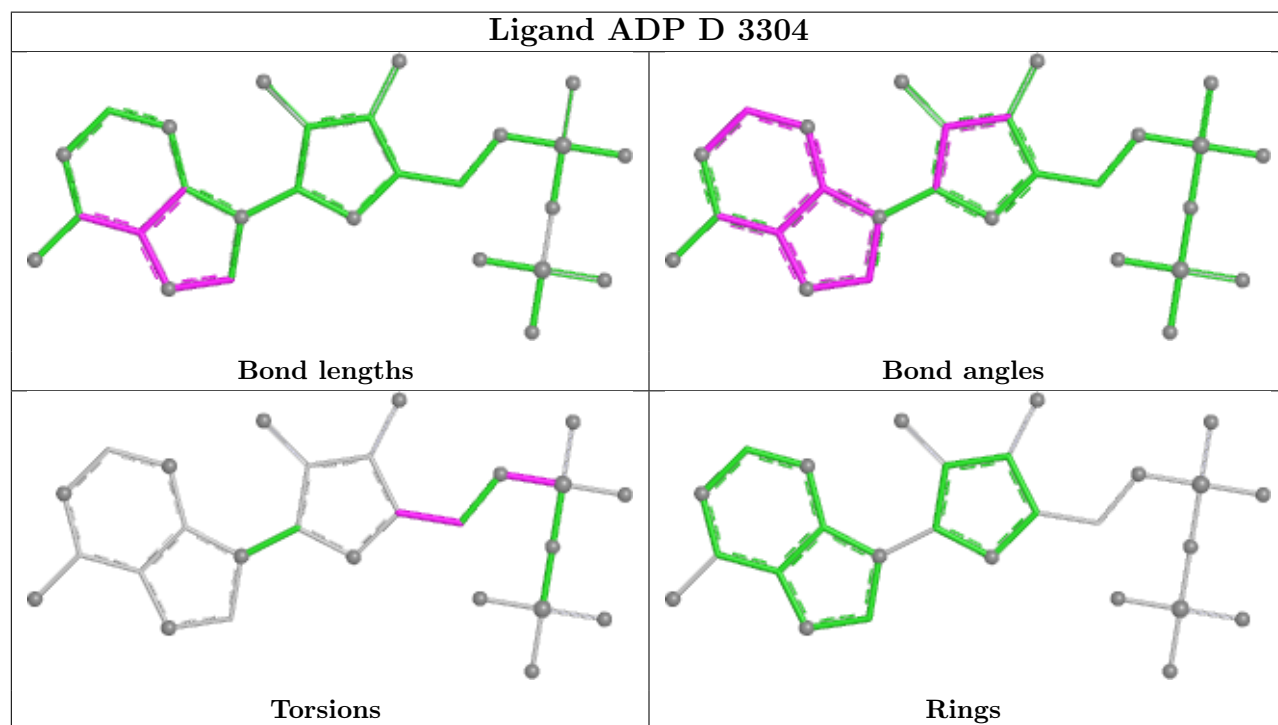
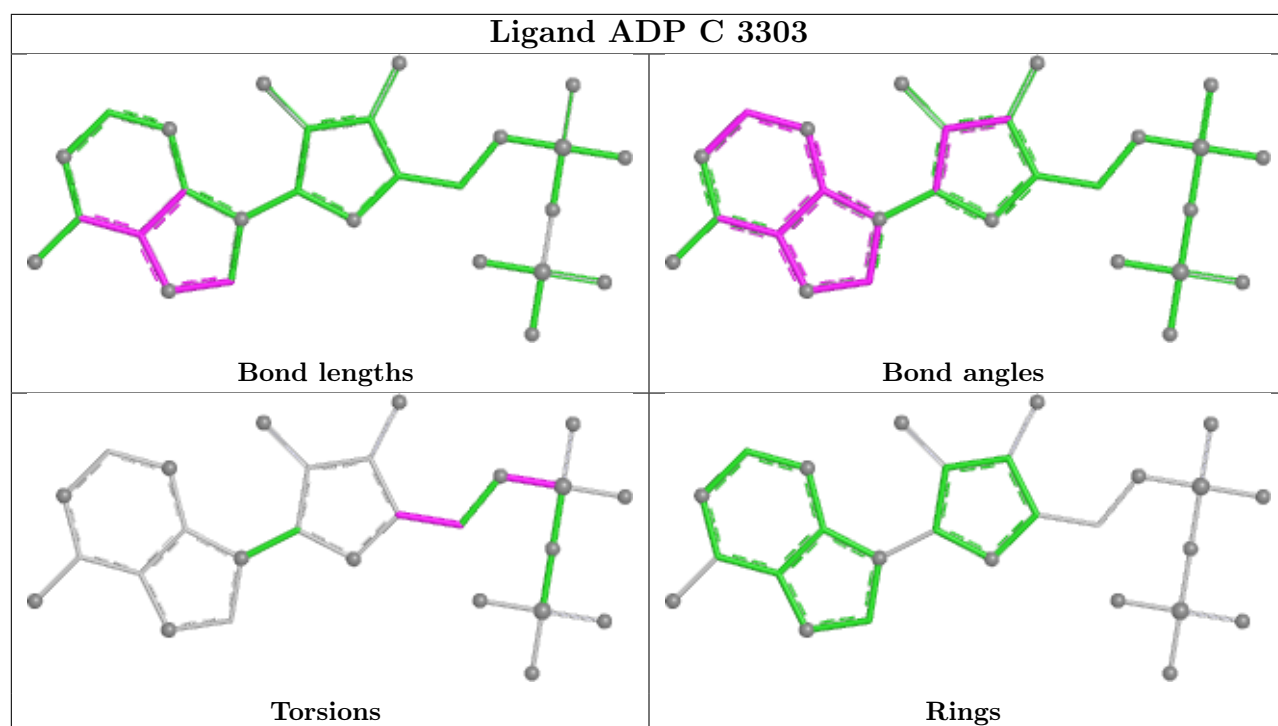
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1203	OAA	1	0
2	D	3301	ACO	17	0
2	C	3301	ACO	5	0
3	A	1202	OAA	1	0
2	B	2303	ACO	8	0
5	D	3303	Q5B	3	0
3	D	3302	OAA	1	0
2	A	1201	ACO	9	0
6	D	3305	PO4	1	0
5	C	3305	Q5B	1	0

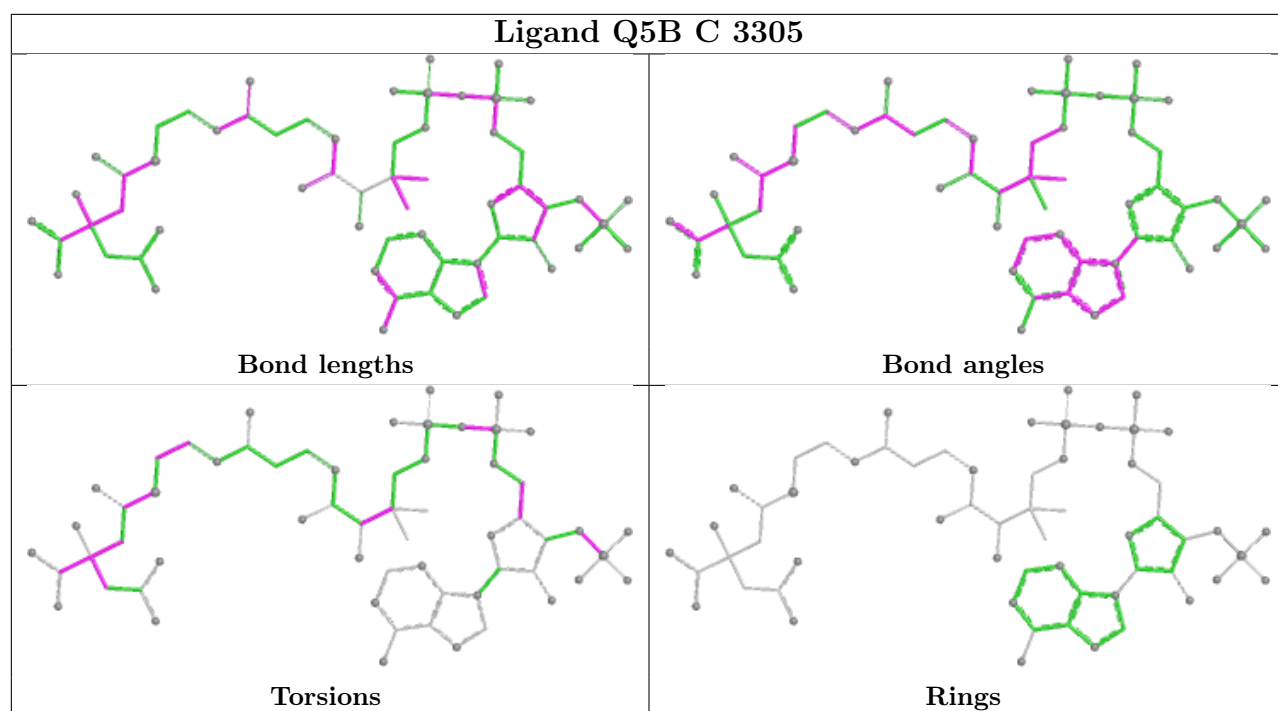
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

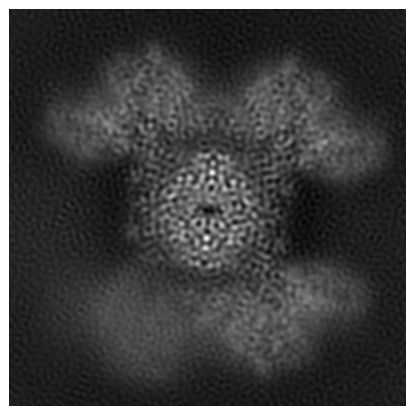
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29668. These allow visual inspection of the internal detail of the map and identification of artifacts.

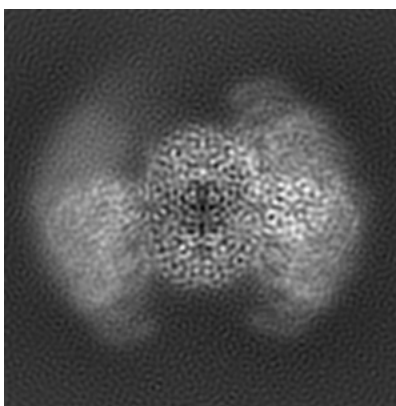
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

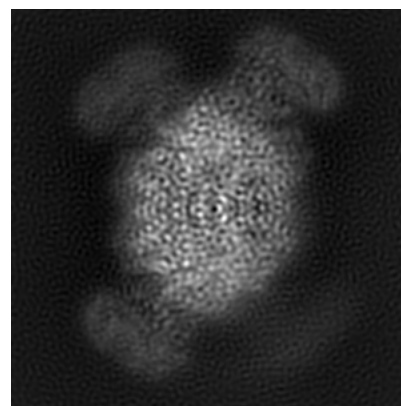
6.1.1 Primary map



X

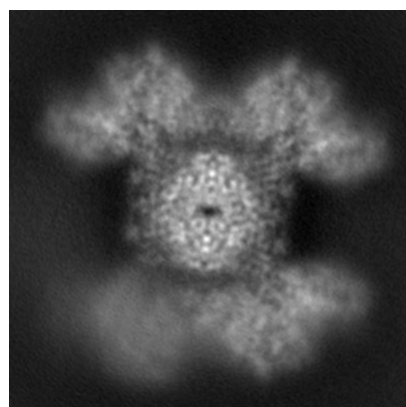


Y

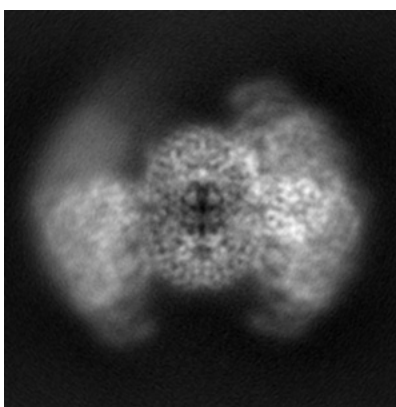


Z

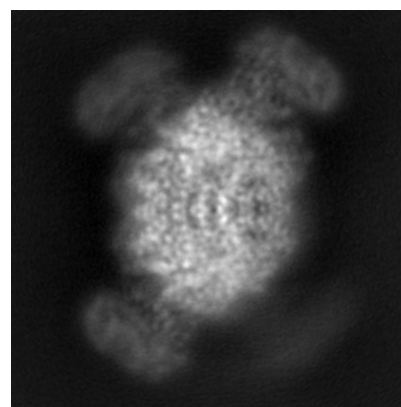
6.1.2 Raw map



X



Y

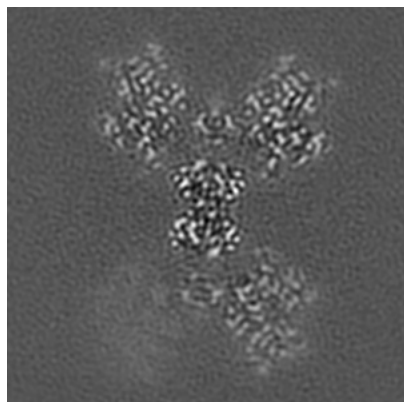


Z

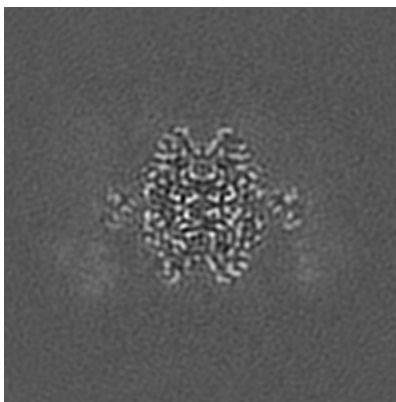
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

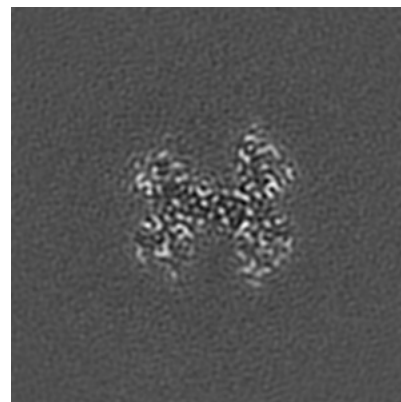
6.2.1 Primary map



X Index: 110

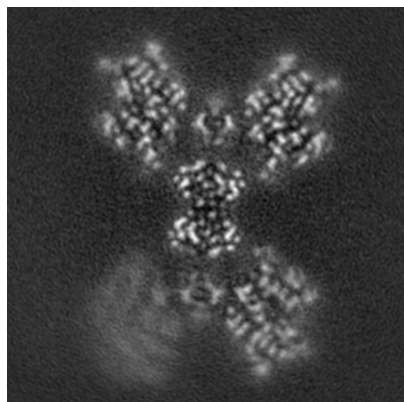


Y Index: 110

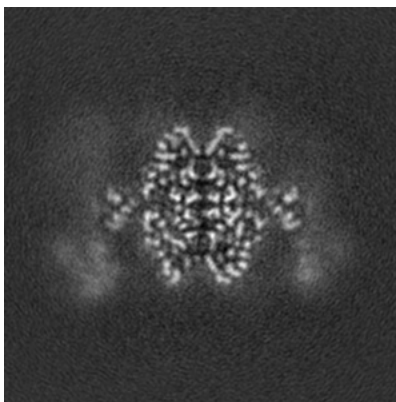


Z Index: 110

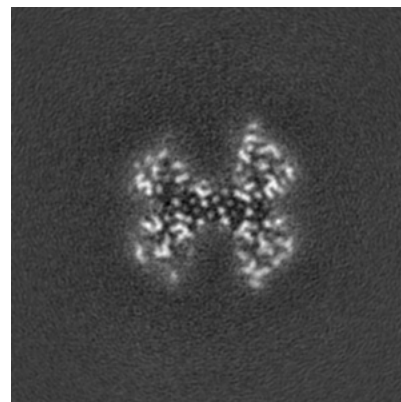
6.2.2 Raw map



X Index: 110



Y Index: 110

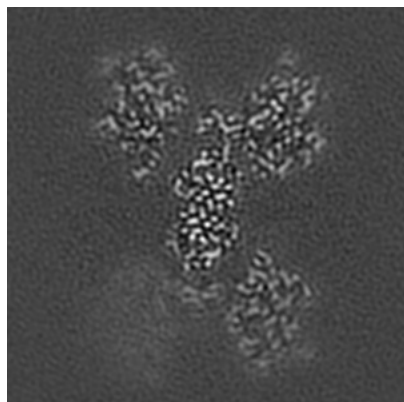


Z Index: 110

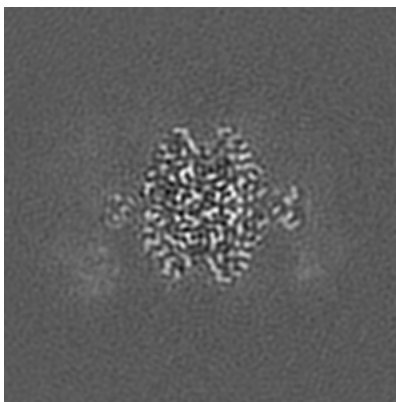
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

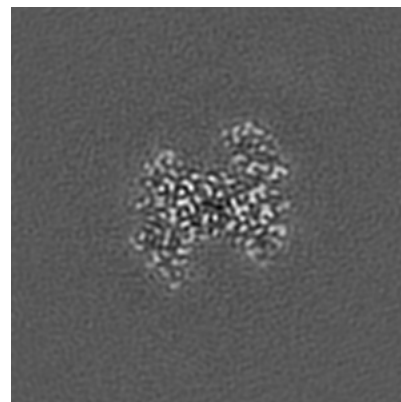
6.3.1 Primary map



X Index: 105

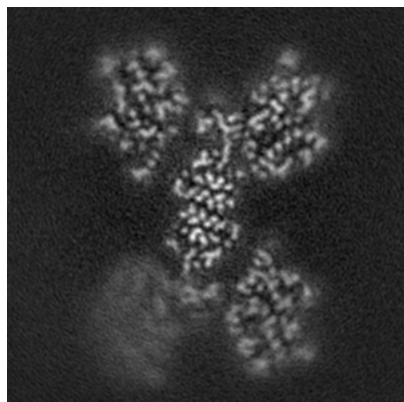


Y Index: 111

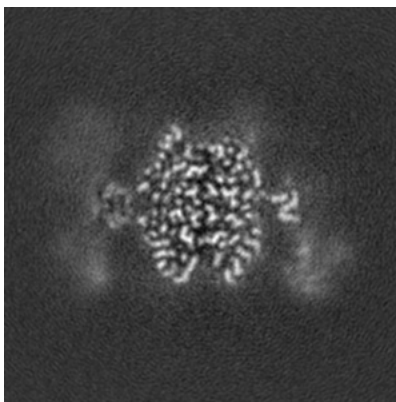


Z Index: 119

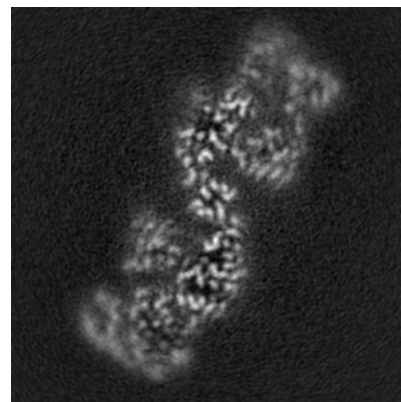
6.3.2 Raw map



X Index: 105



Y Index: 106

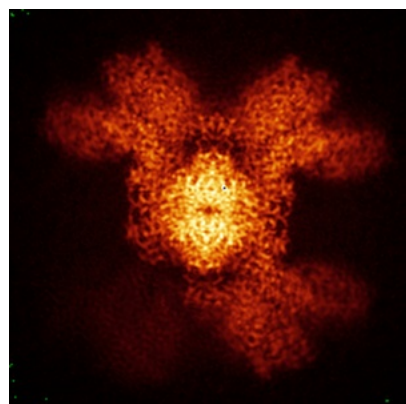


Z Index: 154

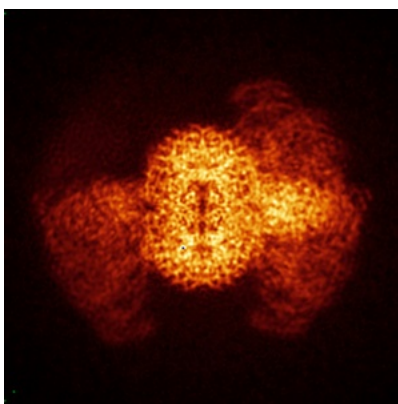
The images above show the largest variance slices of the map in three orthogonal directions.

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

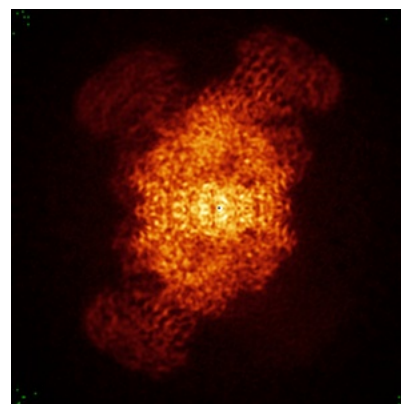
6.4.1 Primary map



X

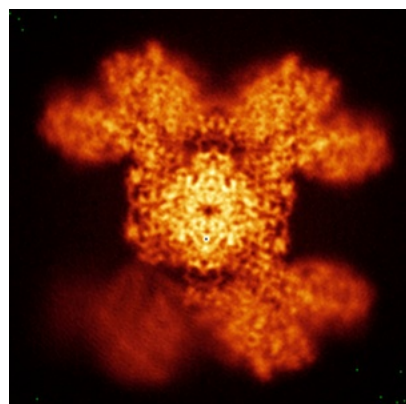


Y

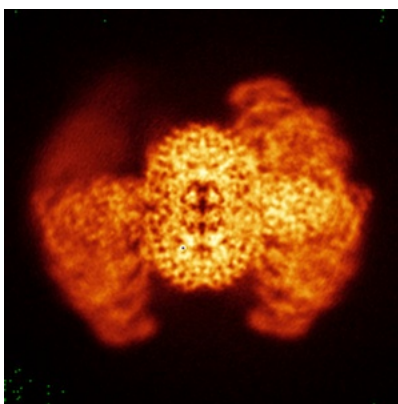


Z

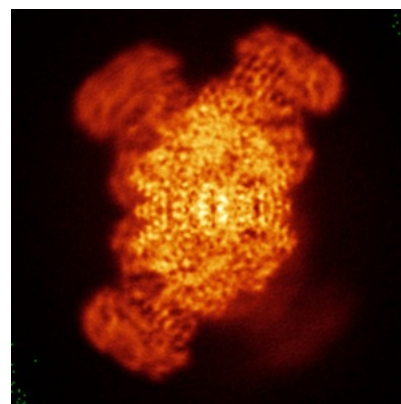
6.4.2 Raw map



X



Y

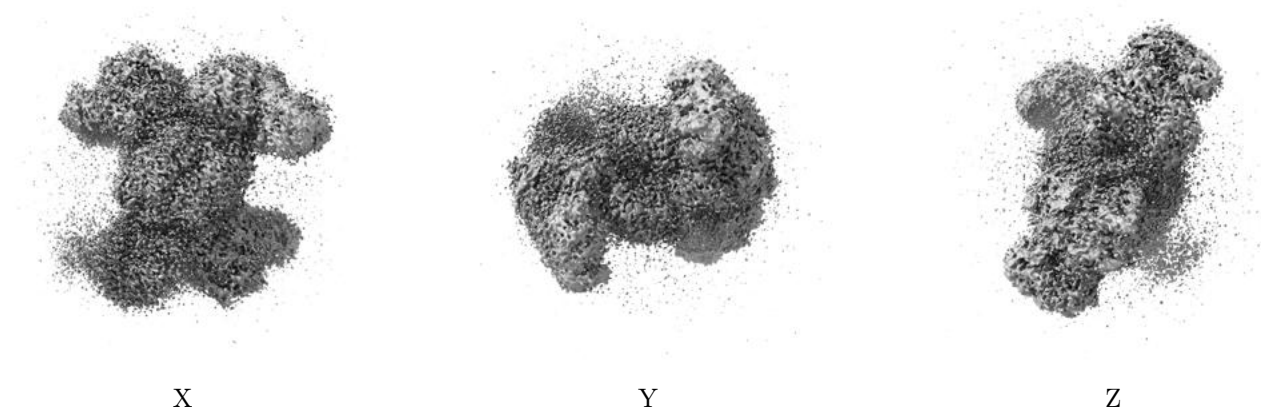


Z

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.

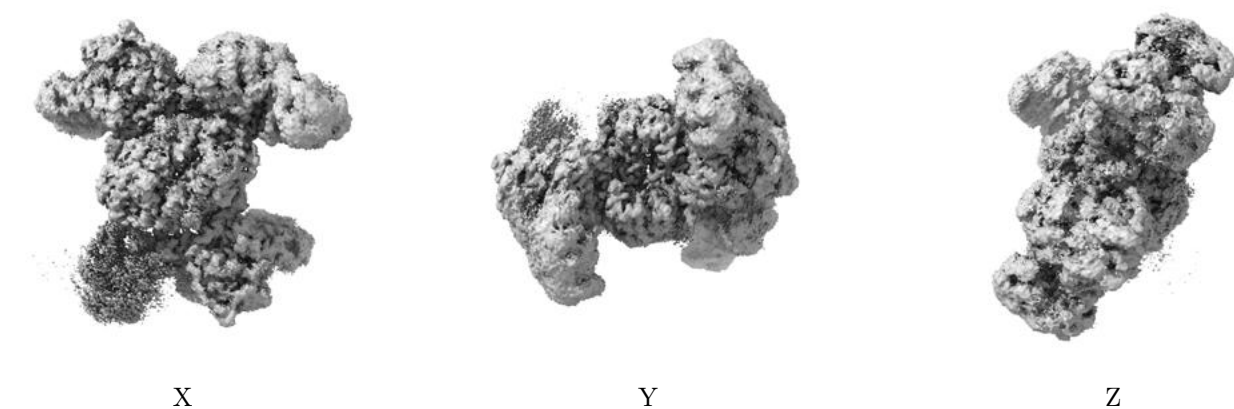
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

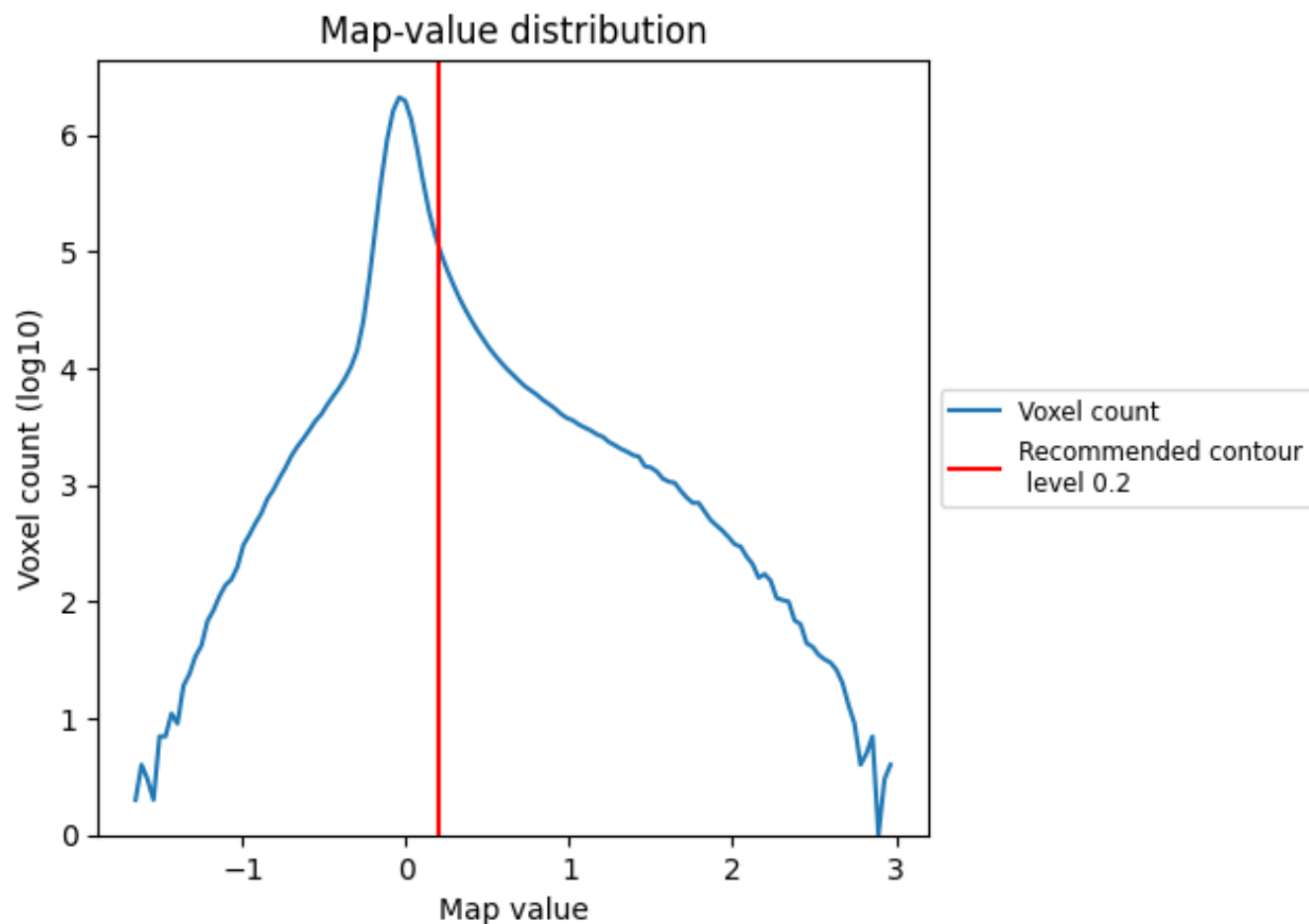
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

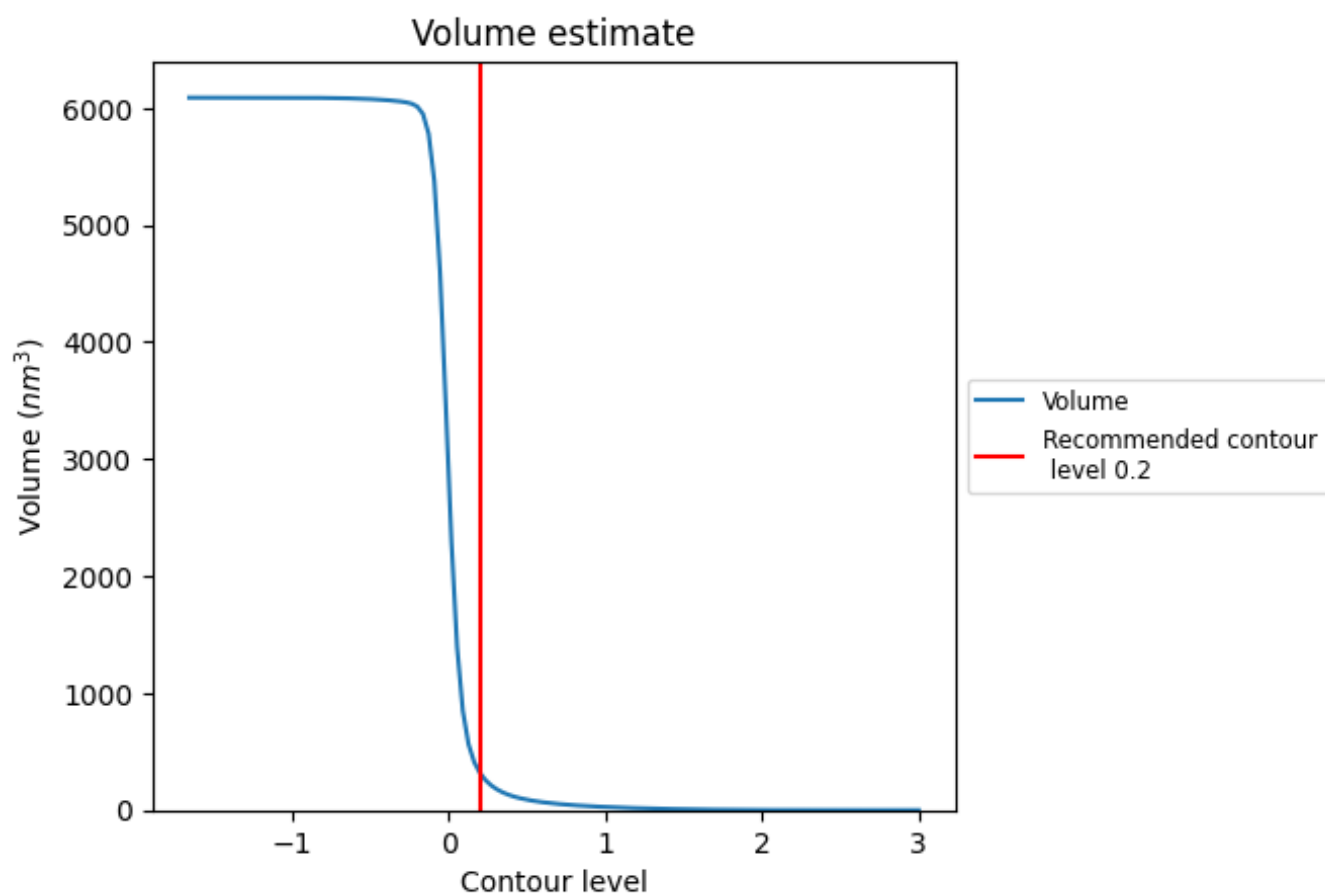
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

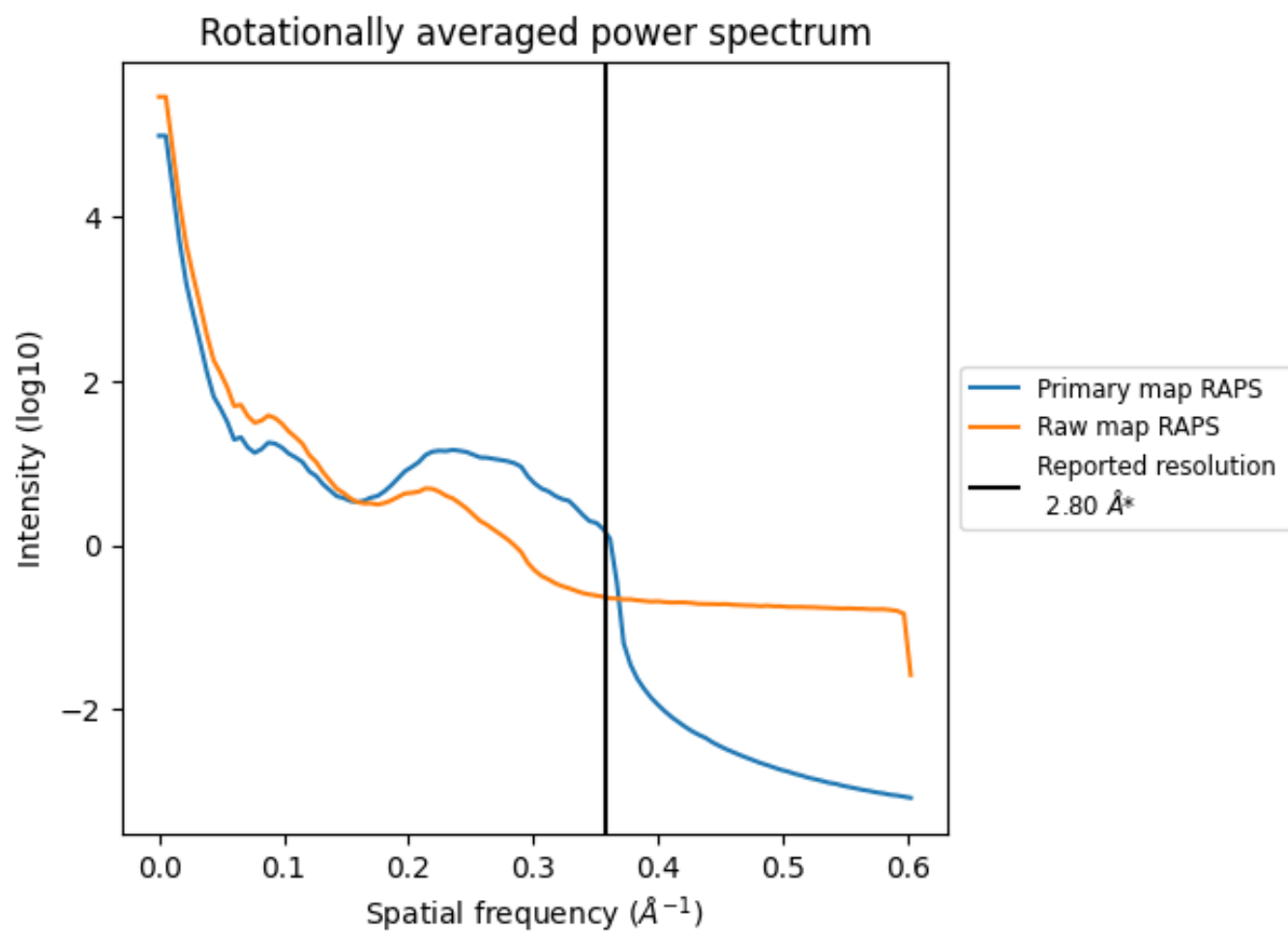
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 320 nm^3 ; this corresponds to an approximate mass of 289 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 ⓘ

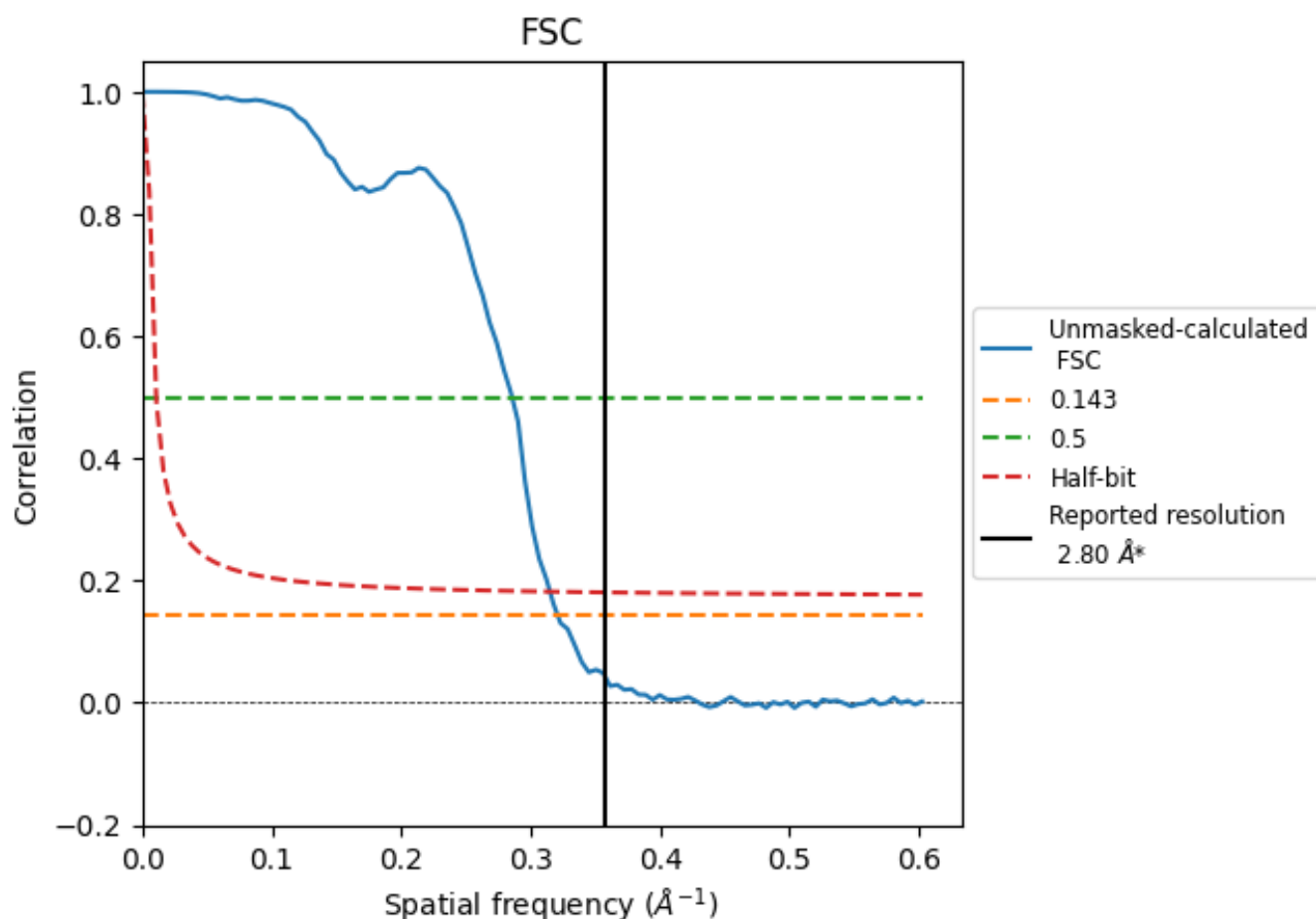


*Reported resolution corresponds to spatial frequency of $0.357 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

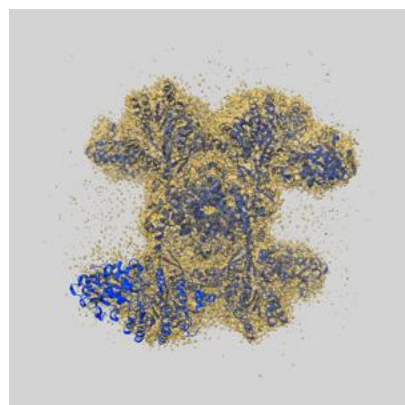
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.12	3.50	3.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.12 differs from the reported value 2.8 by more than 10 %

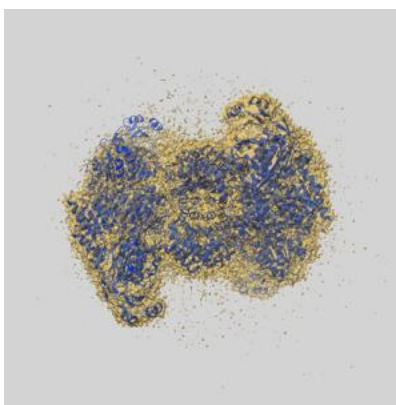
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29668 and PDB model 8G1E. Per-residue inclusion information can be found in section [3](#) on page [9](#).

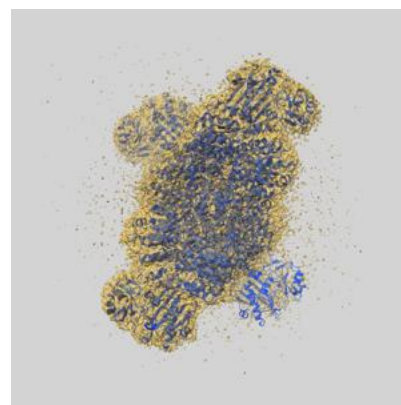
9.1 Map-model overlay [i](#)



X



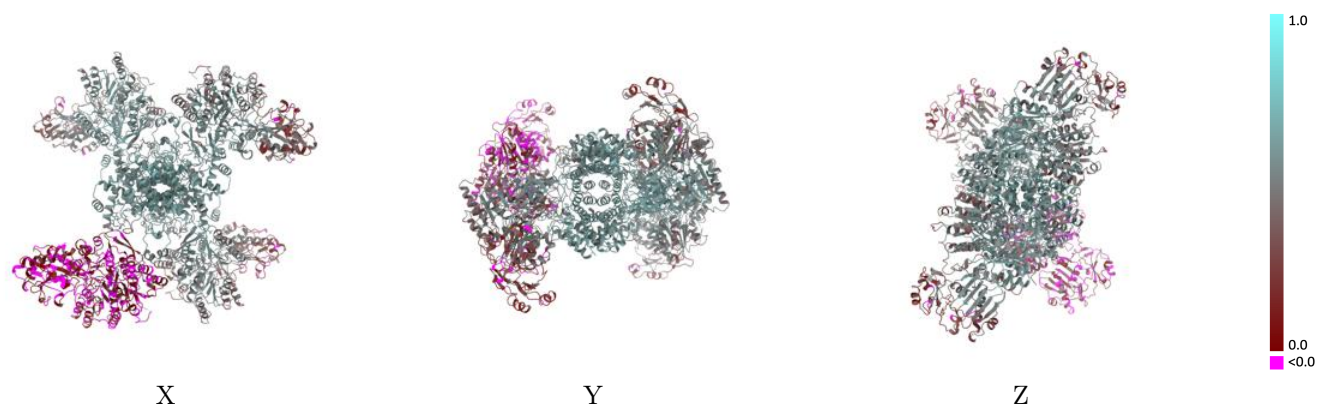
Y



Z

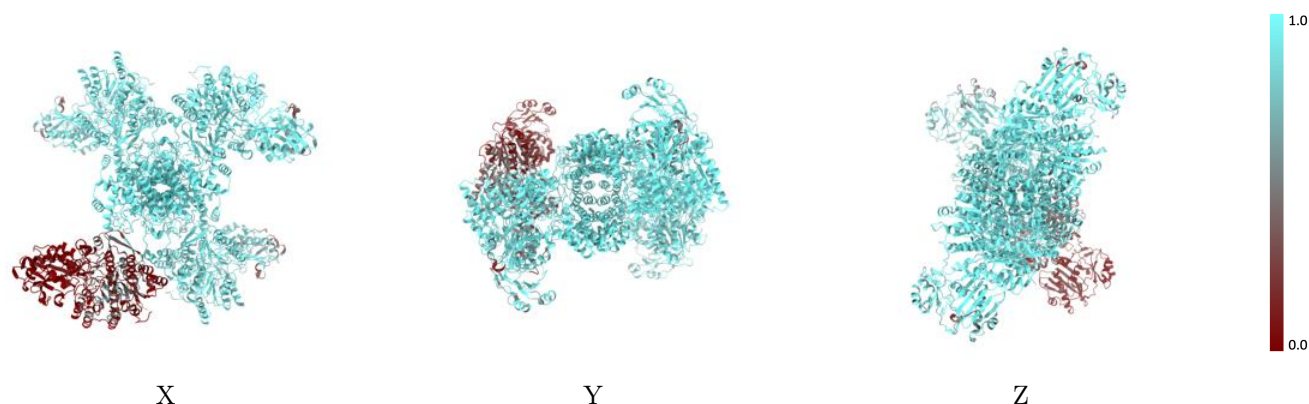
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



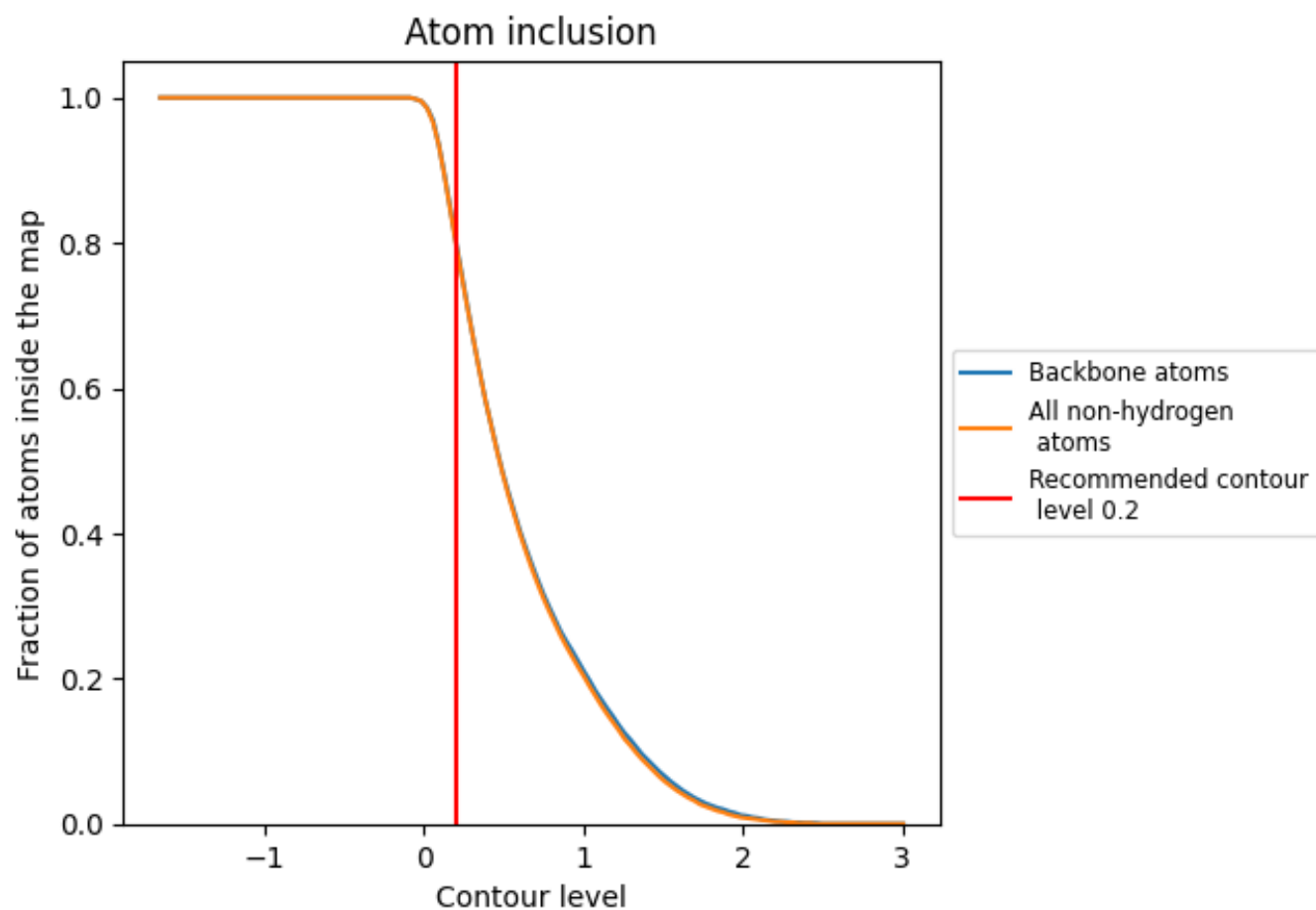
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7970	0.4240
A	0.4030	0.2090
B	0.9010	0.4570
C	0.9450	0.5150
D	0.9420	0.5120

