



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:02 PM UTC

PDB ID : 8G5D / pdb_00008g5d
EMDB ID : EMD-29740
Title : Structure of ACLY-D1026A-products, local refinement of ASH domain
Authors : Wei, X.; Marmorstein, R.
Deposited on : 2023-02-13
Resolution : 2.50 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

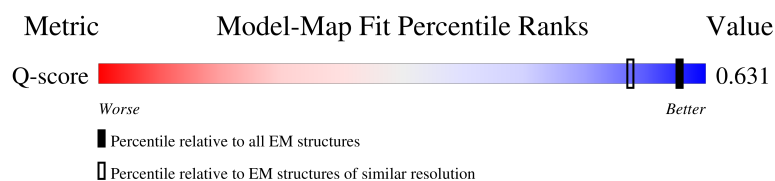
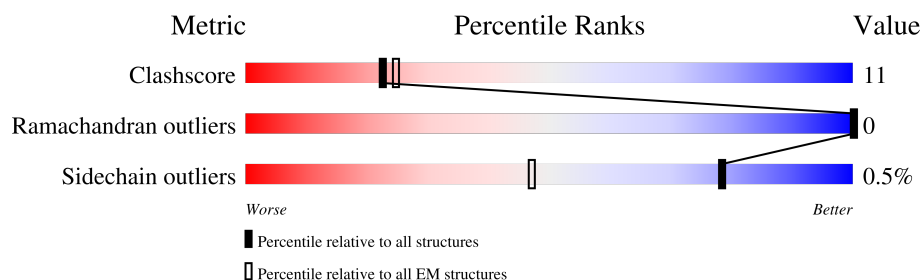
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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	7115 (2.00 - 3.00)

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	 18% 8% 75%
1	B	1101	 19% 7% 75%
1	C	1101	 18% 7% 75%
1	D	1101	 72% 22% 6%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 14852 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.

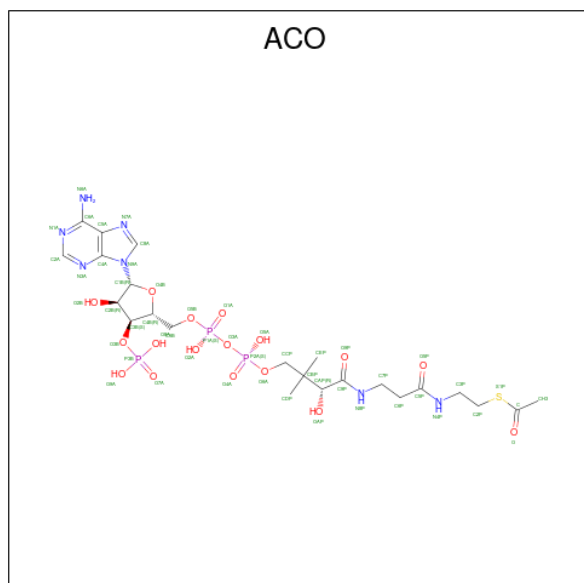
- Molecule 1 is a protein called ATP-citrate synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	279	Total	C	N	O	S	0	0
			2157	1386	369	385	17		
1	B	279	Total	C	N	O	S	0	0
			2157	1386	369	385	17		
1	C	279	Total	C	N	O	S	0	0
			2157	1386	369	385	17		
1	D	1037	Total	C	N	O	S	1	0
			8012	5130	1360	1476	46		

There are 4 discrepancies between the modelled and reference sequences:

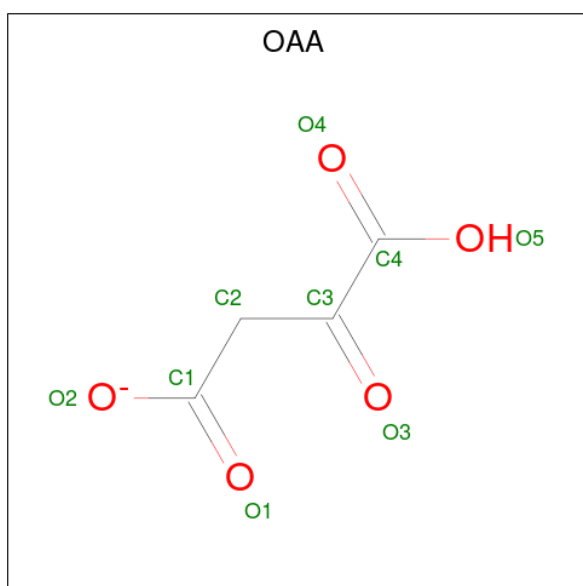
Chain	Residue	Modelled	Actual	Comment	Reference
A	1026	ALA	ASP	engineered mutation	UNP P53396
B	1026	ALA	ASP	engineered mutation	UNP P53396
C	1026	ALA	ASP	engineered mutation	UNP P53396
D	1026	ALA	ASP	engineered mutation	UNP P53396

- Molecule 2 is ACETYL COENZYME *A (CCD ID: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



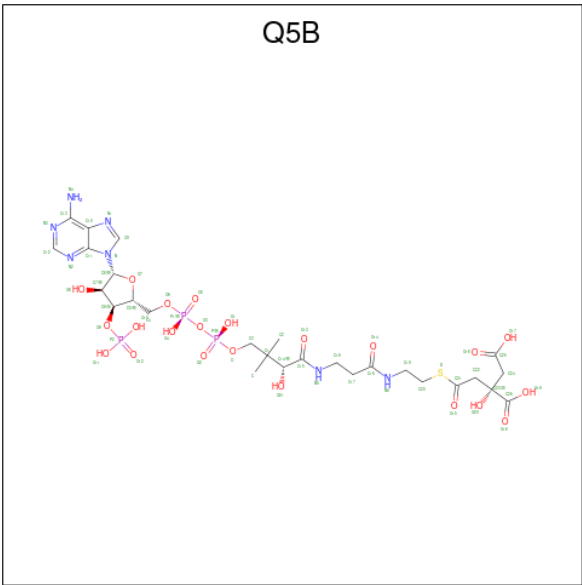
Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	
2	B	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	
2	C	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	
2	D	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	

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



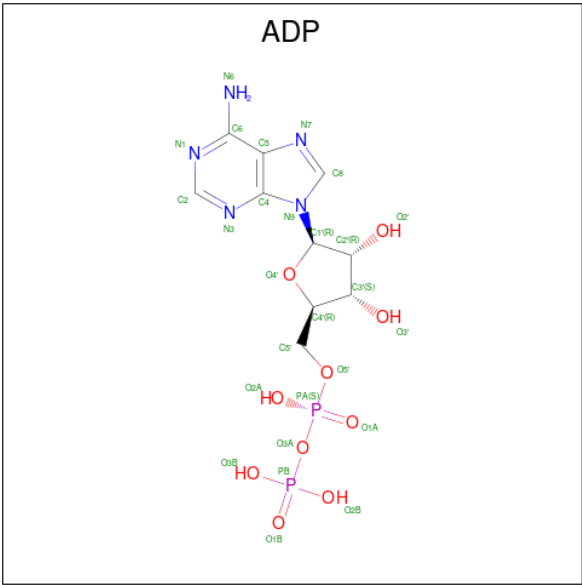
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			9	4	5	
3	B	1	Total	C	O	0
			9	4	5	
3	C	1	Total	C	O	0
			9	4	5	
3	D	1	Total	C	O	0
			9	4	5	

- Molecule 4 is (3S)-citryl-Coenzyme A (CCD ID: Q5B) (formula: $C_{27}H_{42}N_7O_{22}P_3S$) (labeled as "Ligand of Interest" by depositor).



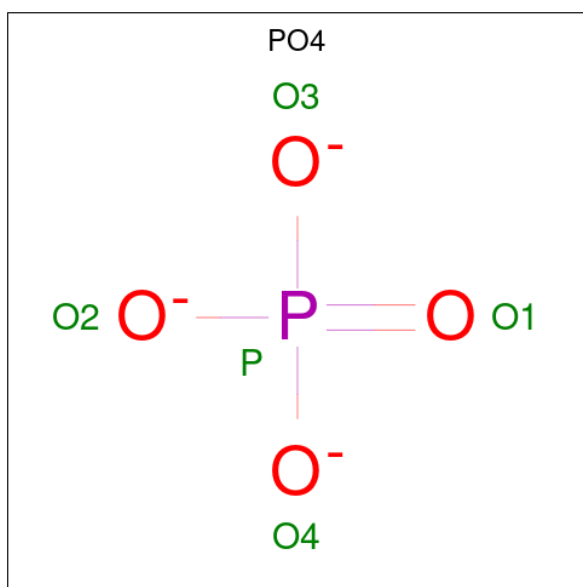
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
4	D	1	60	27	7	22	3	1	0

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



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

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

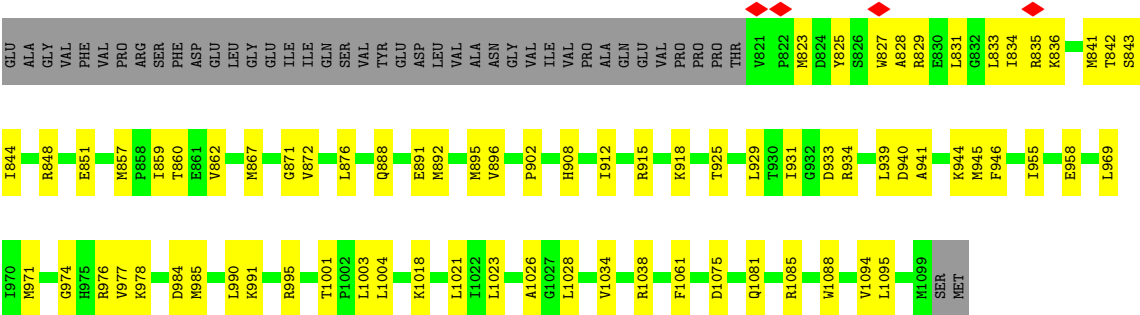


Mol	Chain	Residues	Atoms			AltConf
6	D	1	Total	O	P	0
			5	4	1	

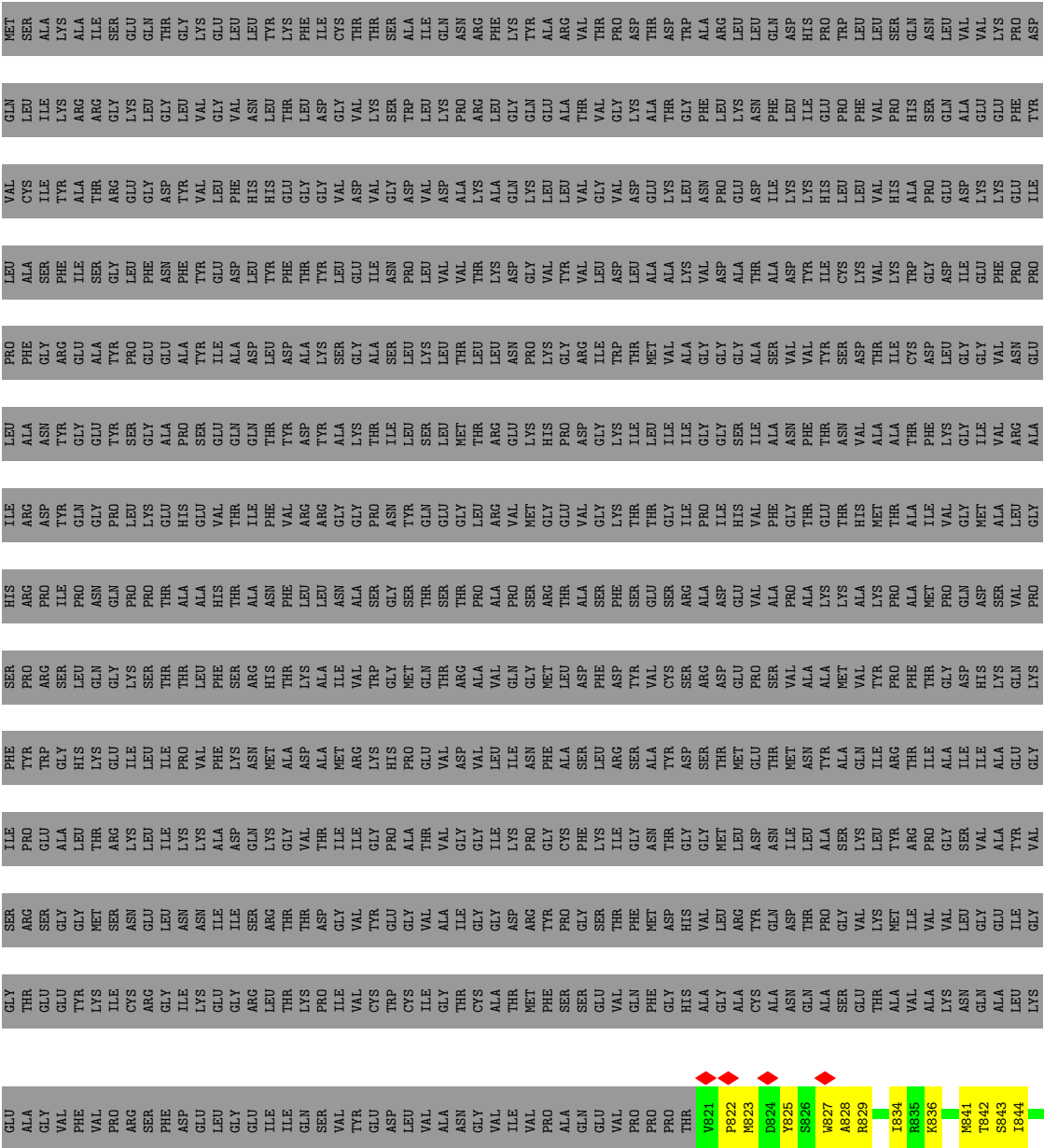
- Molecule 7 is water.

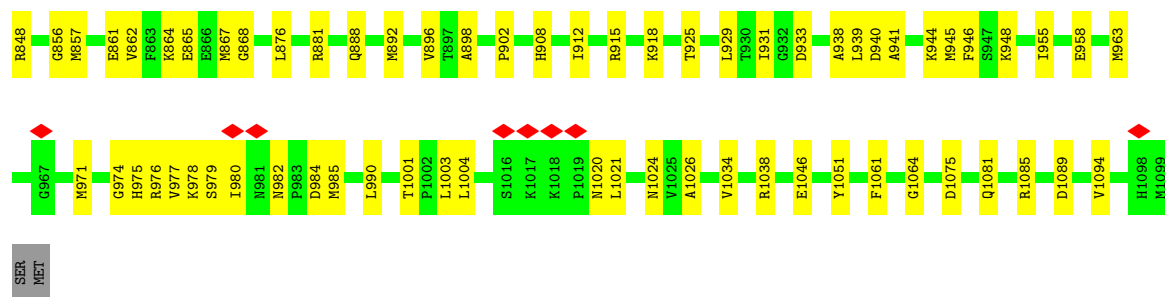
Mol	Chain	Residues	Atoms		AltConf
7	A	9	Total	O	0
			9	9	
7	B	11	Total	O	0
			11	11	
7	C	8	Total	O	0
			8	8	
7	D	9	Total	O	0
			9	9	

[illegible]

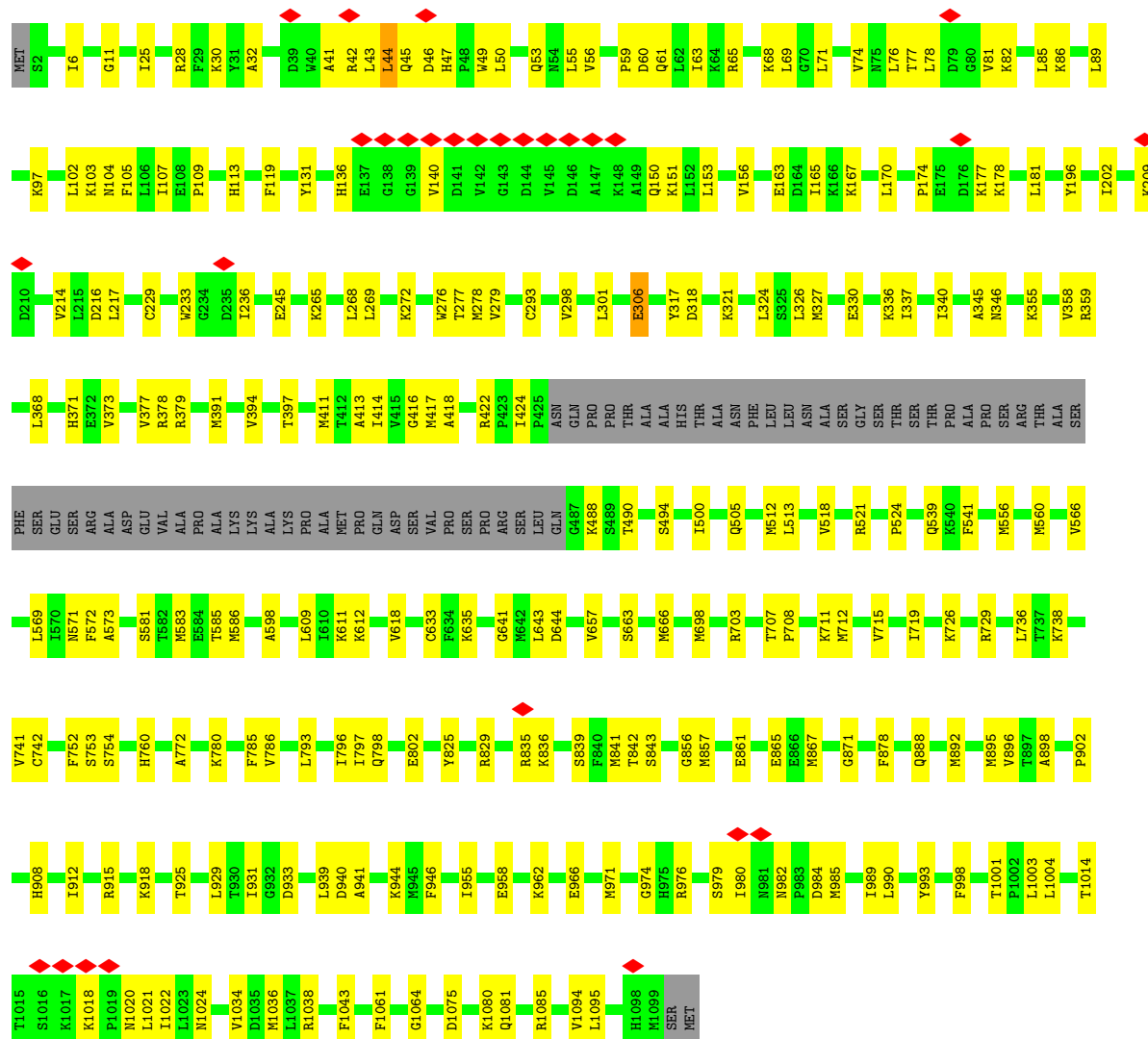


● Molecule 1: ATP-citrate synthase





• 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	613268	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	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	3.959	Depositor
Minimum map value	-1.957	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.170	Depositor
Recommended contour level	0.35	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: ACO, PO4, OAA, Q5B, 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	0.24	0/2203	0.41	0/2972
1	B	0.30	0/2203	0.41	0/2972
1	C	0.23	0/2203	0.39	0/2972
1	D	0.23	0/8190	0.39	0/11087
All	All	0.24	0/14799	0.40	0/20003

There are no bond length outliers.

There are no bond angle outliers.

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	2157	0	2174	75	0
1	B	2157	0	2174	60	0
1	C	2157	0	2174	68	0
1	D	8012	0	8053	172	0
2	A	51	0	34	7	0
2	B	51	0	34	5	0
2	C	51	0	34	7	0
2	D	51	0	34	5	0
3	A	9	0	2	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	9	0	2	1	0
3	C	9	0	2	1	0
3	D	9	0	2	1	0
4	D	60	0	0	1	0
5	D	27	0	12	0	0
6	D	5	0	0	1	0
7	A	9	0	0	0	0
7	B	11	0	0	0	0
7	C	8	0	0	0	0
7	D	9	0	0	0	0
All	All	14852	0	14731	335	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (335) 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	1.59	0.84
1:C:1085:ARG:HH11	2:D:3301:ACO:H62A	1.22	0.83
1:D:50:LEU:HB3	1:D:78:LEU:HD11	1.63	0.79
2:C:3301:ACO:H62A	1:D:1085:ARG:HH11	1.29	0.78
2:A:3301:ACO:H62A	1:B:1085:ARG:HH11	1.35	0.74
1:D:985:MET:HE3	1:D:985:MET:HA	1.70	0.73
1:A:847:GLU:OE1	1:D:1085:ARG:NH2	2.21	0.73
1:A:1024:ASN:HD22	2:A:3301:ACO:H31	1.53	0.73
1:A:1018:LYS:HE2	1:A:1020:ASN:HD21	1.53	0.73
1:D:663:SER:HB2	1:D:666:MET:HB2	1.71	0.72
1:A:1001:THR:HB	1:A:1004:LEU:HB3	1.72	0.71
1:D:896:VAL:HG21	1:D:990:LEU:HD11	1.72	0.71
1:C:823:MET:HE2	1:C:827:TRP:CD1	2.25	0.71
1:C:985:MET:HE3	1:C:985:MET:HA	1.73	0.69
1:A:1085:ARG:HH11	2:B:3301:ACO:H62A	1.41	0.68
1:D:44:LEU:HD11	1:D:78:LEU:HD21	1.73	0.68
1:D:60:ASP:HB3	1:D:104:ASN:HD22	1.59	0.68
1:D:170:LEU:O	1:D:178:LYS:NZ	2.26	0.68
1:D:265:LYS:HB2	1:D:306:GLU:HG3	1.76	0.68
1:A:843:SER:HB3	1:D:1094:VAL:HG23	1.75	0.67
1:D:394:VAL:HA	1:D:397:THR:HG22	1.74	0.67
1:C:825:TYR:OH	1:C:829:ARG:NH1	2.29	0.66
1:D:417:MET:HB2	1:D:424:ILE:HG12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:888:GLN:O	1:B:892:MET:HG3	1.96	0.65
1:B:1094:VAL:HG23	1:C:843:SER:HB3	1.77	0.65
1:C:896:VAL:HG21	1:C:990:LEU:HD11	1.79	0.65
1:D:793:LEU:O	1:D:797:ILE:HG13	1.97	0.65
1:D:85:LEU:O	1:D:89:LEU:N	2.23	0.64
1:D:513:LEU:HD22	1:D:524:PRO:HB3	1.80	0.64
1:A:939:LEU:HD22	1:A:1061:PHE:HB2	1.79	0.63
1:B:857:MET:HG2	1:B:862:VAL:HG23	1.78	0.63
1:C:975:HIS:HD2	1:C:978:LYS:HB2	1.64	0.63
1:D:330:GLU:O	1:D:371:HIS:NE2	2.30	0.63
1:B:825:TYR:OH	1:B:829:ARG:NH1	2.31	0.62
1:B:843:SER:HB3	1:C:1094:VAL:HG23	1.81	0.62
1:A:1083:LEU:HD13	1:B:934:ARG:HB3	1.81	0.61
1:B:976:ARG:HD2	2:B:3301:ACO:H2B	1.81	0.61
1:A:939:LEU:HD12	1:A:1026:ALA:HA	1.82	0.61
1:B:896:VAL:HG21	1:B:990:LEU:HD11	1.83	0.61
1:D:61:GLN:HB2	1:D:63:ILE:HD11	1.82	0.61
1:A:925:THR:HG23	1:C:925:THR:HG23	1.83	0.60
1:D:488:LYS:NZ	1:D:618:VAL:O	2.30	0.60
1:C:1001:THR:HB	1:C:1004:LEU:HB3	1.82	0.60
1:B:1001:THR:HB	1:B:1004:LEU:HB3	1.83	0.60
1:D:77:THR:OG1	1:D:78:LEU:N	2.35	0.59
1:C:836:LYS:HE3	1:D:836:LYS:HE3	1.84	0.59
1:D:825:TYR:OH	1:D:829:ARG:NH1	2.35	0.59
1:D:888:GLN:O	1:D:892:MET:HG3	2.02	0.59
1:D:276:TRP:CD1	1:D:327:MET:HG3	2.38	0.59
1:A:976:ARG:HG3	1:A:977:VAL:HG13	1.84	0.59
1:D:86:LYS:H	1:D:86:LYS:HD3	1.67	0.59
1:D:177:LYS:O	1:D:181:LEU:HB2	2.02	0.58
1:D:41:ALA:O	1:D:45:GLN:HG2	2.02	0.58
1:D:974:GLY:C	1:D:1024:ASN:HD21	2.12	0.58
2:D:3301:ACO:HH33	3:D:3302:OAA:H21	1.85	0.58
1:B:867:MET:HB2	1:B:871:GLY:HA3	1.85	0.58
1:D:378:ARG:HB2	1:D:414:ILE:HG21	1.86	0.57
1:A:836:LYS:HE3	1:B:836:LYS:HE3	1.84	0.57
1:B:891:GLU:O	1:B:895:MET:HG3	2.04	0.57
1:C:974:GLY:HA2	1:C:1021:LEU:HA	1.86	0.57
1:A:896:VAL:HG21	1:A:990:LEU:HD11	1.85	0.57
1:D:65:ARG:HD3	1:D:68:LYS:HE2	1.87	0.57
1:A:1094:VAL:HG21	1:D:841:MET:HE3	1.87	0.57
1:D:644:ASP:N	1:D:644:ASP:OD1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:991:LYS:O	1:B:995:ARG:HG2	2.04	0.57
1:D:337:ILE:HG21	1:D:418:ALA:HB1	1.85	0.57
1:C:976:ARG:HD2	2:C:3301:ACO:H2B	1.88	0.56
1:D:378:ARG:CZ	1:D:411:MET:HB2	2.34	0.56
1:B:925:THR:HG23	1:D:925:THR:HG23	1.86	0.56
1:A:976:ARG:HD2	2:A:3301:ACO:H2B	1.87	0.56
1:A:888:GLN:O	1:A:892:MET:HG3	2.04	0.56
1:A:908:HIS:O	1:A:912:ILE:HG12	2.06	0.56
1:B:908:HIS:O	1:B:912:ILE:HG12	2.06	0.56
1:D:867:MET:HB2	1:D:871:GLY:HA3	1.88	0.56
1:C:979:SER:HB3	1:C:1020:ASN:HA	1.88	0.55
1:D:102:LEU:HB3	1:D:105:PHE:HE1	1.71	0.55
1:C:823:MET:HE2	1:C:827:TRP:HD1	1.72	0.55
1:D:69:LEU:HB2	1:D:71:LEU:HD23	1.89	0.55
1:B:842:THR:HG21	1:D:902:PRO:HG3	1.88	0.55
1:B:843:SER:OG	1:D:1075:ASP:OD1	2.24	0.55
1:C:939:LEU:HD12	1:C:1026:ALA:HA	1.89	0.55
1:C:888:GLN:O	1:C:892:MET:HG3	2.08	0.54
1:C:975:HIS:CD2	1:C:978:LYS:HB2	2.41	0.54
1:D:55:LEU:HD11	1:D:78:LEU:HD12	1.89	0.54
1:D:980:ILE:C	1:D:982:ASN:H	2.15	0.54
1:D:25:ILE:HG23	1:D:28:ARG:HD2	1.89	0.54
1:D:340:ILE:HB	1:D:377:VAL:HG22	1.89	0.54
1:D:86:LYS:HD3	1:D:86:LYS:N	2.22	0.54
1:D:780:LYS:HG3	1:D:786:VAL:HB	1.89	0.54
1:A:1024:ASN:ND2	2:A:3301:ACO:H31	2.22	0.54
1:D:940:ASP:OD2	1:D:944:LYS:NZ	2.34	0.54
1:D:539:GLN:HG2	1:D:541:PHE:CE2	2.42	0.54
1:D:68:LYS:HZ2	1:D:140:VAL:HG13	1.73	0.54
1:D:908:HIS:O	1:D:912:ILE:HG12	2.08	0.54
1:A:842:THR:HG21	1:C:902:PRO:HG3	1.89	0.53
1:D:719:ILE:HD12	1:D:772:ALA:H	1.72	0.53
1:D:974:GLY:HA2	1:D:1021:LEU:HA	1.90	0.53
1:D:1001:THR:HB	1:D:1004:LEU:HB3	1.89	0.53
1:A:946:PHE:HB3	1:A:1003:LEU:HD11	1.89	0.53
1:A:962:LYS:NZ	1:A:966:GLU:OE2	2.42	0.53
1:C:939:LEU:HD22	1:C:1061:PHE:HB2	1.90	0.53
1:D:931:ILE:HD12	1:D:1061:PHE:HE2	1.74	0.53
1:B:931:ILE:HD12	1:B:1061:PHE:HE2	1.74	0.53
1:A:1078:ARG:HD2	1:C:1051:TYR:CE1	2.43	0.52
1:B:941:ALA:HB1	1:B:971:MET:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:ASP:OD1	1:D:217:LEU:N	2.42	0.52
1:D:174:PRO:O	1:D:178:LYS:HG3	2.08	0.52
1:A:1034:VAL:O	1:A:1038:ARG:HG2	2.09	0.52
1:D:413:ALA:O	1:D:417:MET:HG2	2.10	0.52
1:C:908:HIS:O	1:C:912:ILE:HG12	2.09	0.52
1:D:163:GLU:H	1:D:163:GLU:CD	2.17	0.52
1:D:416:GLY:HA3	1:D:422:ARG:HE	1.74	0.52
1:A:931:ILE:HD12	1:A:1061:PHE:HE2	1.76	0.51
1:D:119:PHE:HE1	1:D:136:HIS:ND1	2.08	0.51
1:B:872:VAL:HG21	1:D:895:MET:HG2	1.92	0.51
1:C:1085:ARG:NH1	2:D:3301:ACO:H62A	1.99	0.51
1:B:969:LEU:HD22	4:D:3303:Q5B:C10	2.40	0.51
1:C:822:PRO:HB2	1:D:835:ARG:HG3	1.93	0.51
1:A:980:ILE:C	1:A:982:ASN:H	2.17	0.51
1:B:1095:LEU:HD23	1:C:856:GLY:H	1.76	0.51
1:B:1088:TRP:NE1	1:C:847:GLU:OE1	2.39	0.51
1:A:976:ARG:HG3	1:A:977:VAL:N	2.27	0.51
1:C:948:LYS:NZ	1:C:948:LYS:HB3	2.25	0.50
1:A:974:GLY:HA2	1:A:1021:LEU:HA	1.92	0.50
2:C:3301:ACO:HH33	3:C:3302:OAA:H21	1.94	0.50
1:D:698:MET:HE1	1:D:736:LEU:HD11	1.92	0.50
1:A:823:MET:HE3	1:A:827:TRP:CD1	2.46	0.50
1:A:1018:LYS:HE2	1:A:1020:ASN:ND2	2.24	0.50
2:A:3301:ACO:HH33	3:A:3302:OAA:H21	1.93	0.50
1:D:82:LYS:O	1:D:86:LYS:HE2	2.11	0.50
1:D:760:HIS:HE2	6:D:3305:PO4:P	2.34	0.50
1:A:861:GLU:O	1:A:865:GLU:HG2	2.11	0.50
1:B:976:ARG:HG3	2:B:3301:ACO:H3B	1.93	0.50
1:C:857:MET:HE2	1:C:862:VAL:HA	1.94	0.50
1:D:391:MET:O	1:D:394:VAL:HG12	2.11	0.50
1:D:962:LYS:O	1:D:966:GLU:HG3	2.12	0.49
1:D:6:ILE:HG21	1:D:236:ILE:HD11	1.93	0.49
1:A:902:PRO:HG3	1:C:842:THR:HG21	1.95	0.49
2:B:3301:ACO:HH33	3:B:3302:OAA:H21	1.92	0.49
1:D:65:ARG:HA	1:D:65:ARG:CZ	2.42	0.49
1:C:933:ASP:OD1	1:C:933:ASP:N	2.44	0.49
1:D:32:ALA:HB1	1:D:43:LEU:HD11	1.94	0.49
1:C:844:ILE:HD12	1:C:876:LEU:HD22	1.94	0.49
1:D:941:ALA:HB1	1:D:971:MET:HG3	1.95	0.49
1:C:861:GLU:O	1:C:865:GLU:HG2	2.13	0.48
1:C:980:ILE:C	1:C:982:ASN:H	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:GLU:C	1:D:165:ILE:H	2.22	0.48
1:D:1018:LYS:HE2	1:D:1020:ASN:OD1	2.13	0.48
1:D:785:PHE:HB3	1:D:796:ILE:HD11	1.95	0.48
1:A:1085:ARG:NH1	2:B:3301:ACO:H62A	2.09	0.48
1:D:865:GLU:HB2	1:D:867:MET:HE3	1.96	0.48
1:A:1075:ASP:OD1	1:C:843:SER:OG	2.31	0.48
1:D:156:VAL:O	1:D:611:LYS:NZ	2.33	0.48
1:A:856:GLY:H	1:D:1095:LEU:HD23	1.78	0.48
1:D:102:LEU:HB3	1:D:105:PHE:CE1	2.48	0.48
1:D:707:THR:O	1:D:738:LYS:NZ	2.47	0.48
1:B:946:PHE:HB3	1:B:1003:LEU:HD11	1.95	0.48
1:D:293:CYS:HB3	1:D:298:VAL:HB	1.96	0.48
1:A:933:ASP:OD1	1:A:933:ASP:N	2.47	0.47
1:A:948:LYS:O	1:A:952:SER:OG	2.29	0.47
1:D:46:ASP:OD1	1:D:47:HIS:ND1	2.47	0.47
1:D:30:LYS:HE3	1:D:30:LYS:HB2	1.59	0.47
1:C:865:GLU:HB2	1:C:867:MET:HE3	1.97	0.47
1:D:318:ASP:HA	1:D:321:LYS:HE3	1.96	0.47
1:D:68:LYS:NZ	1:D:140:VAL:HG13	2.29	0.47
1:C:945:MET:HE2	1:C:963:MET:SD	2.54	0.47
1:D:933:ASP:N	1:D:933:ASP:OD1	2.47	0.47
1:D:512:MET:HE3	1:D:635:LYS:O	2.14	0.47
1:A:925:THR:CG2	1:C:925:THR:HG23	2.45	0.47
1:A:985:MET:HE3	1:A:985:MET:HA	1.95	0.47
1:B:1075:ASP:OD1	1:D:843:SER:OG	2.33	0.47
1:D:163:GLU:OE1	1:D:163:GLU:N	2.46	0.47
1:D:301:LEU:HD23	1:D:752:PHE:HZ	1.80	0.47
1:A:843:SER:OG	1:C:1075:ASP:OD1	2.33	0.46
1:A:844:ILE:HD12	1:A:876:LEU:HD22	1.98	0.46
1:C:931:ILE:HD12	1:C:1061:PHE:HE2	1.81	0.46
1:D:269:LEU:HD13	1:D:752:PHE:CE1	2.51	0.46
1:B:902:PRO:HG3	1:D:842:THR:HG21	1.98	0.46
1:D:30:LYS:HG2	1:D:109:PRO:HG2	1.98	0.46
1:D:518:VAL:HG11	1:D:643:LEU:HD11	1.97	0.46
1:C:976:ARG:HG3	1:C:977:VAL:N	2.30	0.46
1:D:245:GLU:H	1:D:245:GLU:CD	2.23	0.46
1:D:798:GLN:HG2	1:D:802:GLU:OE2	2.14	0.46
1:D:898:ALA:HA	1:D:1064:GLY:O	2.15	0.46
1:A:857:MET:HE2	1:A:862:VAL:HA	1.97	0.46
1:A:827:TRP:O	1:A:831:LEU:HG	2.15	0.46
1:A:1003:LEU:HB3	1:A:1035:ASP:OD1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:857:MET:HG3	1:C:861:GLU:OE1	2.15	0.46
1:D:1034:VAL:O	1:D:1038:ARG:HG2	2.15	0.46
1:C:1024:ASN:HD22	2:C:3301:ACO:H31	1.81	0.46
1:D:1018:LYS:CG	1:D:1021:LEU:HG	2.46	0.46
1:B:974:GLY:HA2	1:B:1021:LEU:HA	1.98	0.46
1:D:391:MET:HE2	1:D:391:MET:HB2	1.89	0.46
1:D:984:ASP:O	1:D:985:MET:HB2	2.15	0.46
1:D:317:TYR:CD1	1:D:359:ARG:HG2	2.51	0.46
1:C:938:ALA:HB1	2:C:3301:ACO:H32	1.97	0.45
1:D:55:LEU:HB2	1:D:76:LEU:O	2.16	0.45
1:D:974:GLY:O	1:D:1024:ASN:ND2	2.46	0.45
1:B:985:MET:HE3	1:B:985:MET:HA	1.97	0.45
1:C:955:ILE:HG13	1:C:958:GLU:H	1.80	0.45
1:A:925:THR:HG23	1:C:925:THR:CG2	2.46	0.45
1:A:1011:GLU:HG3	1:A:1023:LEU:H	1.81	0.45
1:D:61:GLN:HE22	1:D:103:LYS:NZ	2.14	0.45
1:A:1095:LEU:HD23	1:D:856:GLY:H	1.81	0.45
1:C:823:MET:HG2	1:C:828:ALA:HB2	1.99	0.45
1:A:929:LEU:O	1:B:918:LYS:NZ	2.40	0.45
1:A:945:MET:SD	1:A:963:MET:HE2	2.57	0.45
1:D:857:MET:HG3	1:D:861:GLU:HG2	1.98	0.45
1:B:925:THR:HG23	1:D:925:THR:CG2	2.46	0.45
1:D:11:GLY:HA3	1:D:217:LEU:HD11	1.97	0.45
1:D:505:GLN:HG3	1:D:572:PHE:CG	2.51	0.45
1:C:984:ASP:O	1:C:985:MET:HB2	2.15	0.45
1:B:933:ASP:OD1	1:B:933:ASP:N	2.48	0.45
1:D:741:VAL:HG22	1:D:785:PHE:HB2	1.99	0.45
1:A:901:GLY:HA3	1:C:847:GLU:HG2	1.99	0.44
1:B:925:THR:CG2	1:D:925:THR:HG23	2.48	0.44
1:B:984:ASP:O	1:B:985:MET:HB2	2.17	0.44
1:D:272:LYS:HA	1:D:272:LYS:HD3	1.78	0.44
1:D:346:ASN:O	1:D:641:GLY:HA2	2.18	0.44
1:D:955:ILE:HG13	1:D:958:GLU:H	1.81	0.44
1:A:823:MET:HB3	1:B:833:LEU:O	2.17	0.44
1:C:929:LEU:HD13	1:D:925:THR:HG22	2.00	0.44
1:D:657:VAL:HG13	1:D:712:MET:HG3	1.99	0.44
1:D:586:MET:HB2	1:D:612:LYS:HE2	1.99	0.44
1:B:823:MET:SD	1:B:827:TRP:CD1	3.11	0.44
1:B:860:THR:HA	1:D:989:ILE:HD11	1.99	0.44
1:A:929:LEU:HD13	1:B:925:THR:HG22	1.99	0.44
1:D:324:LEU:HD22	1:D:368:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:715:VAL:O	1:D:742:CYS:HA	2.17	0.44
1:B:859:ILE:O	1:B:862:VAL:HB	2.18	0.44
1:D:946:PHE:HB3	1:D:1003:LEU:HD11	2.00	0.44
1:B:844:ILE:HD12	1:B:876:LEU:HD22	2.00	0.43
1:D:209:LYS:CE	1:D:209:LYS:H	2.31	0.43
1:D:976:ARG:HG3	2:D:3301:ACO:O3A	2.17	0.43
1:A:1011:GLU:HG3	1:A:1023:LEU:N	2.33	0.43
1:C:971:MET:HA	2:C:3301:ACO:H61	1.99	0.43
1:A:984:ASP:HB3	1:A:987:VAL:H	1.83	0.43
1:D:888:GLN:HB3	1:D:993:TYR:OH	2.18	0.43
1:D:1080:LYS:HE2	1:D:1080:LYS:HB2	1.73	0.43
1:C:829:ARG:HD2	1:C:834:ILE:HG13	2.01	0.43
1:C:898:ALA:HA	1:C:1064:GLY:O	2.18	0.43
1:A:994:VAL:HG13	1:A:998:PHE:CD2	2.54	0.43
1:B:851:GLU:OE2	1:B:860:THR:HG23	2.18	0.43
1:D:278:MET:HB2	1:D:340:ILE:HG12	2.00	0.43
1:C:918:LYS:NZ	1:D:929:LEU:O	2.45	0.43
1:D:209:LYS:H	1:D:209:LYS:HE2	1.84	0.43
1:A:831:LEU:HD12	1:A:833:LEU:HD11	2.01	0.43
1:B:827:TRP:O	1:B:831:LEU:HG	2.19	0.43
1:A:940:ASP:OD2	1:A:944:LYS:NZ	2.41	0.43
1:C:867:MET:HE1	1:C:881:ARG:HD3	2.00	0.43
1:C:925:THR:HG22	1:D:929:LEU:HD13	2.01	0.43
1:D:56:VAL:HG23	1:D:74:VAL:HA	2.01	0.42
1:D:202:ILE:HG23	1:D:214:VAL:HG23	2.01	0.42
1:A:835:ARG:N	1:B:823:MET:O	2.52	0.42
1:C:1046:GLU:CD	1:C:1046:GLU:H	2.27	0.42
1:D:229:CYS:HB2	1:D:233:TRP:CE2	2.54	0.42
1:D:49:TRP:HB2	1:D:53:GLN:HE22	1.85	0.42
1:D:150:GLN:H	1:D:150:GLN:HG2	1.58	0.42
1:D:209:LYS:HE2	1:D:209:LYS:HB2	1.90	0.42
1:D:939:LEU:HD22	1:D:1061:PHE:HB2	2.01	0.42
1:C:941:ALA:HB1	1:C:971:MET:HG3	2.02	0.42
1:D:569:LEU:HD22	1:D:585:THR:HG21	2.01	0.42
1:A:979:SER:HB3	1:A:1020:ASN:HA	2.02	0.42
1:B:1023:LEU:HD23	1:B:1028:LEU:HD23	2.00	0.42
1:B:1034:VAL:O	1:B:1038:ARG:HG2	2.20	0.42
1:D:268:LEU:HD21	1:D:326:LEU:HD22	2.00	0.42
1:D:571:ASN:HD21	1:D:581:SER:HB2	1.83	0.42
1:D:915:ARG:HG2	1:D:1081:GLN:HB2	2.01	0.42
1:D:1014:THR:HB	1:D:1021:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:979:SER:O	1:A:1022:ILE:HG21	2.20	0.42
1:C:940:ASP:OD2	1:C:944:LYS:NZ	2.40	0.42
1:D:131:TYR:CE2	1:D:153:LEU:HD13	2.55	0.42
1:D:521:ARG:HD2	1:D:633:CYS:O	2.20	0.42
1:A:823:MET:O	1:B:834:ILE:HA	2.20	0.42
1:B:1018:LYS:CG	1:B:1021:LEU:HG	2.50	0.42
1:D:490:THR:HA	1:D:703:ARG:HG2	2.02	0.42
1:A:857:MET:HG3	1:A:861:GLU:OE1	2.20	0.41
1:A:925:THR:HG22	1:B:929:LEU:HD13	2.02	0.41
1:D:998:PHE:CE2	1:D:1036:MET:HB2	2.54	0.41
1:A:898:ALA:HA	1:A:1064:GLY:O	2.20	0.41
1:B:940:ASP:OD1	1:B:944:LYS:NZ	2.49	0.41
1:C:915:ARG:HG2	1:C:1081:GLN:HB2	2.01	0.41
1:D:494:SER:C	1:D:633:CYS:HB3	2.45	0.41
1:A:915:ARG:HG2	1:A:1081:GLN:HB2	2.02	0.41
1:C:841:MET:HE2	1:C:841:MET:HB3	1.93	0.41
1:C:946:PHE:HB3	1:C:1003:LEU:HD11	2.01	0.41
2:C:3301:ACO:H21	2:C:3301:ACO:HH32	1.76	0.41
1:D:53:GLN:HE21	1:D:109:PRO:HG3	1.85	0.41
1:D:59:PRO:HA	1:D:105:PHE:HA	2.02	0.41
1:D:97:LYS:HD2	1:D:753:SER:HA	2.02	0.41
1:A:823:MET:O	1:B:835:ARG:N	2.51	0.41
1:A:984:ASP:O	1:A:985:MET:HB2	2.21	0.41
1:B:915:ARG:HG2	1:B:1081:GLN:HB2	2.02	0.41
1:B:939:LEU:HD12	1:B:1026:ALA:HA	2.03	0.41
1:C:1034:VAL:O	1:C:1038:ARG:HG2	2.20	0.41
1:A:971:MET:HA	2:A:3301:ACO:H61	2.03	0.41
1:B:823:MET:HG3	1:B:828:ALA:HB2	2.02	0.41
1:C:848:ARG:H	1:C:848:ARG:HG2	1.73	0.41
1:D:979:SER:O	1:D:1022:ILE:HG21	2.20	0.41
1:A:844:ILE:HG22	1:A:879:GLN:OE1	2.21	0.41
1:D:726:LYS:HG2	1:D:729:ARG:HH12	1.86	0.41
1:D:857:MET:HE1	1:D:867:MET:HE1	2.03	0.41
1:B:977:VAL:HG23	1:B:978:LYS:HG2	2.03	0.41
1:A:867:MET:H	1:A:867:MET:HG2	1.65	0.41
1:A:1078:ARG:HD2	1:C:1051:TYR:CZ	2.55	0.41
1:C:929:LEU:O	1:D:918:LYS:HG2	2.21	0.41
1:D:196:TYR:HD1	1:D:229:CYS:SG	2.43	0.41
1:D:573:ALA:O	1:D:598:ALA:HB2	2.20	0.41
1:A:1090:ASP:OD2	1:D:839:SER:HB2	2.20	0.41
2:A:3301:ACO:HH32	2:A:3301:ACO:H21	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:985:MET:HA	1:C:985:MET:CE	2.47	0.41
1:D:556:MET:O	1:D:560:MET:HG2	2.21	0.41
1:D:583:MET:SD	1:D:609:LEU:HD23	2.61	0.41
1:D:708:PRO:O	1:D:711:LYS:NZ	2.54	0.41
1:A:895:MET:SD	1:C:868:GLY:HA2	2.61	0.41
1:B:848:ARG:H	1:B:848:ARG:HG3	1.66	0.41
1:B:945:MET:HE3	1:B:971:MET:HG2	2.03	0.41
1:B:955:ILE:HG13	1:B:958:GLU:H	1.86	0.41
1:D:42:ARG:HA	1:D:42:ARG:NE	2.35	0.41
1:D:277:THR:HB	1:D:279:VAL:HG23	2.03	0.41
1:A:929:LEU:O	1:B:918:LYS:HG2	2.21	0.40
1:C:864:LYS:HE3	1:C:864:LYS:HB2	1.80	0.40
1:D:113:HIS:ND1	1:D:113:HIS:C	2.79	0.40
1:D:151:LYS:HE2	1:D:151:LYS:HB2	1.81	0.40
1:D:726:LYS:HG2	1:D:729:ARG:NH1	2.36	0.40
1:A:910:THR:OG1	1:A:927:GLY:HA3	2.21	0.40
1:D:32:ALA:HB3	1:D:107:ILE:HB	2.03	0.40
1:D:78:LEU:O	1:D:81:VAL:HG12	2.21	0.40
1:A:941:ALA:HB3	1:A:971:MET:HG2	2.02	0.40
1:D:336:LYS:HB2	1:D:373:VAL:HG22	2.03	0.40
1:D:878:PHE:HB3	1:D:1043:PHE:HE2	1.86	0.40
1:D:500:ILE:HG13	1:D:566:VAL:HG11	2.03	0.40
1:B:1023:LEU:HD12	1:B:1023:LEU:HA	1.97	0.40
1:D:345:ALA:HB2	1:D:379:ARG:NH2	2.37	0.40
1:D:355:LYS:HA	1:D:358:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	277/1101 (25%)	266 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	277/1101 (25%)	267 (96%)	10 (4%)	0	100	100
1	C	277/1101 (25%)	265 (96%)	12 (4%)	0	100	100
1	D	1034/1101 (94%)	999 (97%)	35 (3%)	0	100	100
All	All	1865/4404 (42%)	1797 (96%)	68 (4%)	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	227/908 (25%)	225 (99%)	2 (1%)	70	87
1	B	227/908 (25%)	226 (100%)	1 (0%)	84	93
1	C	227/908 (25%)	226 (100%)	1 (0%)	84	93
1	D	851/908 (94%)	847 (100%)	4 (0%)	81	92
All	All	1532/3632 (42%)	1524 (100%)	8 (0%)	78	92

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

Mol	Chain	Res	Type
1	A	955	ILE
1	A	965	LYS
1	B	841	MET
1	C	1089	ASP
1	D	44	LEU
1	D	167	LYS
1	D	306	GLU
1	D	754	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	888	GLN
1	A	961	ASN
1	A	996	GLN
1	A	1020	ASN
1	A	1058	ASN
1	B	909	ASN
1	B	982	ASN
1	C	961	ASN
1	C	988	GLN
1	C	1058	ASN
1	C	1081	GLN
1	D	27	ASN
1	D	45	GLN
1	D	53	GLN
1	D	61	GLN
1	D	75	ASN
1	D	299	ASN
1	D	332	HIS
1	D	365	GLN
1	D	403	HIS
1	D	545	HIS
1	D	563	HIS
1	D	638	ASN
1	D	757	GLN
1	D	766	ASN
1	D	767	GLN
1	D	888	GLN
1	D	1024	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

11 ligands 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$
3	OAA	A	3302	-	8,8,8	1.34	1 (12%)	8,10,10	1.39	1 (12%)
5	ADP	D	3304	-	28,29,29	1.38	4 (14%)	43,45,45	1.89	10 (23%)
2	ACO	B	3301	-	51,53,53	1.16	6 (11%)	73,79,79	1.61	16 (21%)
2	ACO	D	3301	-	51,53,53	1.12	5 (9%)	73,79,79	1.57	12 (16%)
2	ACO	A	3301	-	51,53,53	1.18	6 (11%)	73,79,79	1.55	11 (15%)
2	ACO	C	3301	-	51,53,53	1.16	6 (11%)	73,79,79	1.65	11 (15%)
3	OAA	B	3302	-	8,8,8	1.38	1 (12%)	8,10,10	1.40	1 (12%)
6	PO4	D	3305	-	4,4,4	0.94	0	6,6,6	0.75	0
3	OAA	C	3302	-	8,8,8	1.38	1 (12%)	8,10,10	1.33	1 (12%)
3	OAA	D	3302	-	8,8,8	1.33	1 (12%)	8,10,10	1.37	1 (12%)
4	Q5B	D	3303	-	60,62,62	2.76	18 (30%)	87,93,93	2.17	24 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OAA	A	3302	-	-	6/8/8/8	-
5	ADP	D	3304	-	-	3/16/32/32	0/3/3/3
2	ACO	B	3301	-	-	16/51/67/67	0/3/3/3
2	ACO	D	3301	-	-	17/51/67/67	0/3/3/3
2	ACO	A	3301	-	-	17/51/67/67	0/3/3/3
2	ACO	C	3301	-	-	12/51/67/67	0/3/3/3
3	OAA	B	3302	-	-	6/8/8/8	-
3	OAA	C	3302	-	-	4/8/8/8	-
3	OAA	D	3302	-	-	6/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	Q5B	D	3303	-	-	18/66/83/83	0/3/3/3

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3303	Q5B	C6-C5	-8.01	1.32	1.52
4	D	3303	Q5B	P-O3	7.71	1.67	1.59
4	D	3303	Q5B	P1-O3	7.05	1.67	1.59
4	D	3303	Q5B	C18-N6	6.83	1.49	1.33
4	D	3303	Q5B	O7-C5	5.92	1.58	1.45
4	D	3303	Q5B	C15-N5	5.28	1.46	1.33
5	D	3304	ADP	C5-C4	4.46	1.47	1.39
4	D	3303	Q5B	C21-S	4.45	1.86	1.76
2	A	3301	ACO	C5A-C4A	4.39	1.46	1.39
2	C	3301	ACO	C5A-C4A	4.27	1.46	1.39
4	D	3303	Q5B	O7-C8	4.12	1.51	1.42
2	D	3301	ACO	C5A-C4A	4.09	1.46	1.39
2	B	3301	ACO	C5A-C4A	4.06	1.46	1.39
4	D	3303	Q5B	C7-C6	3.91	1.61	1.53
4	D	3303	Q5B	C10-C11	-3.90	1.32	1.39
4	D	3303	Q5B	C13-N4	3.73	1.43	1.34
4	D	3303	Q5B	P2-O9	3.18	1.65	1.59
4	D	3303	Q5B	O21-C14	-2.93	1.37	1.42
2	A	3301	ACO	C5A-C6A	2.74	1.48	1.41
2	C	3301	ACO	C5A-C6A	2.70	1.48	1.41
5	D	3304	ADP	C5-C6	2.68	1.48	1.41
2	B	3301	ACO	C4A-N9A	-2.57	1.32	1.37
2	D	3301	ACO	C5A-C6A	2.55	1.48	1.41
4	D	3303	Q5B	C17-C18	2.52	1.56	1.51
2	B	3301	ACO	C5A-C6A	2.45	1.47	1.41
2	A	3301	ACO	C5A-N7A	-2.38	1.34	1.39
2	D	3301	ACO	C5A-N7A	-2.32	1.34	1.39
2	D	3301	ACO	C4A-N9A	-2.32	1.32	1.37
5	D	3304	ADP	C8-N7	2.30	1.36	1.31
5	D	3304	ADP	C5-N7	-2.30	1.34	1.39
2	B	3301	ACO	C8A-N7A	2.29	1.36	1.31
2	B	3301	ACO	C5A-N7A	-2.29	1.34	1.39
4	D	3303	Q5B	O13-C15	-2.28	1.19	1.23
2	A	3301	ACO	P2A-O3A	2.27	1.61	1.59
2	C	3301	ACO	C5A-N7A	-2.25	1.35	1.39
4	D	3303	Q5B	C9-N	-2.21	1.33	1.37
2	A	3301	ACO	C8A-N7A	2.19	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3303	Q5B	C22-C23	-2.17	1.51	1.54
2	A	3301	ACO	P1A-O3A	2.16	1.61	1.59
2	B	3301	ACO	P1A-O3A	2.15	1.61	1.59
2	C	3301	ACO	C8A-N7A	2.13	1.35	1.31
3	B	3302	OAA	O3-C3	-2.13	1.18	1.23
3	C	3302	OAA	O3-C3	-2.10	1.18	1.23
3	A	3302	OAA	O3-C3	-2.09	1.18	1.23
2	C	3301	ACO	C4A-N9A	-2.08	1.33	1.37
2	D	3301	ACO	C8A-N7A	2.07	1.35	1.31
4	D	3303	Q5B	C23-C26	-2.06	1.51	1.53
3	D	3302	OAA	O3-C3	-2.06	1.18	1.23
2	C	3301	ACO	P1A-O3A	2.02	1.61	1.59

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3303	Q5B	C11-N-C8	-6.41	111.64	126.63
4	D	3303	Q5B	N3-C12-N2	-6.07	119.39	128.58
2	A	3301	ACO	C5A-C4A-N3A	-5.92	118.57	126.72
5	D	3304	ADP	C5-C4-N3	-5.77	118.77	126.72
2	C	3301	ACO	C5A-C4A-N3A	-5.68	118.90	126.72
4	D	3303	Q5B	C14-C15-N5	5.48	126.89	116.48
2	D	3301	ACO	C5A-C4A-N3A	-5.35	119.36	126.72
4	D	3303	Q5B	C8-N-C9	5.22	138.68	127.09
4	D	3303	Q5B	N-C9-N1	-5.11	106.69	113.94
2	B	3301	ACO	C5A-C4A-N3A	-4.81	120.10	126.72
5	D	3304	ADP	N3-C4-N9	4.66	135.10	127.17
2	C	3301	ACO	N3A-C4A-N9A	4.39	134.63	127.17
2	A	3301	ACO	N3A-C4A-N9A	4.37	134.61	127.17
2	C	3301	ACO	C3P-N4P-C5P	-4.34	114.74	122.82
2	D	3301	ACO	N3A-C4A-N9A	4.23	134.36	127.17
2	B	3301	ACO	N3A-C2A-N1A	-4.14	122.32	128.58
2	D	3301	ACO	N3A-C2A-N1A	-4.03	122.48	128.58
4	D	3303	Q5B	N4-C13-N3	-4.03	109.41	118.38
2	C	3301	ACO	C2A-N3A-C4A	3.91	121.39	111.83
2	A	3301	ACO	C4A-C5A-N7A	-3.87	106.16	110.58
2	D	3301	ACO	C2A-N3A-C4A	3.87	121.27	111.83
4	D	3303	Q5B	C10-C11-N2	-3.86	121.40	126.72
2	A	3301	ACO	C2A-N3A-C4A	3.84	121.20	111.83
2	C	3301	ACO	C4A-C5A-N7A	-3.79	106.25	110.58
4	D	3303	Q5B	O13-C15-N5	-3.78	114.97	122.98
2	B	3301	ACO	C2A-N3A-C4A	3.75	120.99	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	3304	ADP	C2-N3-C4	3.74	120.97	111.83
4	D	3303	Q5B	C11-N-C9	3.73	109.66	105.74
2	C	3301	ACO	N3A-C2A-N1A	-3.68	123.01	128.58
4	D	3303	Q5B	C16-N5-C15	3.66	129.13	122.55
2	B	3301	ACO	N3A-C4A-N9A	3.66	133.39	127.17
2	D	3301	ACO	C4A-C5A-N7A	-3.53	106.54	110.58
4	D	3303	Q5B	C22-C21-S	3.53	118.02	113.56
5	D	3304	ADP	C4-C5-N7	-3.52	106.56	110.58
2	B	3301	ACO	C7P-C6P-C5P	-3.48	106.60	112.39
4	D	3303	Q5B	C12-N2-C11	3.42	120.17	111.83
4	D	3303	Q5B	C2-C1-C14	3.39	114.55	108.77
4	D	3303	Q5B	C17-C16-N5	-3.34	104.88	112.00
2	A	3301	ACO	N3A-C2A-N1A	-3.32	123.55	128.58
5	D	3304	ADP	N3-C2-N1	-3.27	123.63	128.58
2	B	3301	ACO	C4A-C5A-N7A	-3.22	106.90	110.58
4	D	3303	Q5B	C19-N6-C18	-3.22	116.83	122.82
2	D	3301	ACO	C4A-N9A-C8A	3.19	109.09	105.74
5	D	3304	ADP	C4-N9-C8	3.13	109.03	105.74
2	B	3301	ACO	CEP-CBP-CAP	3.12	114.08	108.77
2	C	3301	ACO	O6A-CCP-CBP	-3.06	105.62	110.55
2	C	3301	ACO	C4A-N9A-C8A	2.99	108.88	105.74
2	B	3301	ACO	C4A-N9A-C8A	2.94	108.83	105.74
2	C	3301	ACO	C5A-N7A-C8A	2.88	107.97	103.45
2	B	3301	ACO	C6A-C5A-N7A	2.83	137.55	132.09
4	D	3303	Q5B	O19-C26-C23	2.83	118.56	113.14
2	A	3301	ACO	C5A-N7A-C8A	2.82	107.88	103.45
4	D	3303	Q5B	C10-N1-C9	2.80	107.85	103.45
2	A	3301	ACO	C3B-C2B-C1B	2.79	106.02	99.89
4	D	3303	Q5B	C7-C6-C5	2.78	108.10	103.24
2	D	3301	ACO	C6A-C5A-N7A	2.70	137.29	132.09
2	D	3301	ACO	C5A-N7A-C8A	2.69	107.67	103.45
5	D	3304	ADP	C5-N7-C8	2.68	107.67	103.45
2	A	3301	ACO	C3P-N4P-C5P	-2.66	117.87	122.82
2	C	3301	ACO	C6A-C5A-N7A	2.63	137.17	132.09
2	B	3301	ACO	C3B-C2B-C1B	2.60	105.61	99.89
4	D	3303	Q5B	C22-C23-C26	-2.58	104.34	110.03
2	D	3301	ACO	N9A-C8A-N7A	-2.49	110.41	113.94
2	C	3301	ACO	N9A-C8A-N7A	-2.47	110.43	113.94
2	A	3301	ACO	C6A-C5A-N7A	2.46	136.83	132.09
2	B	3301	ACO	C2A-N1A-C6A	2.37	122.62	118.73
2	D	3301	ACO	C2A-N1A-C6A	2.37	122.62	118.73
5	D	3304	ADP	C3'-C2'-C1'	2.37	105.94	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3303	Q5B	N2-C11-N	2.35	131.17	127.17
2	A	3301	ACO	C4A-N9A-C8A	2.34	108.20	105.74
5	D	3304	ADP	N9-C8-N7	-2.33	110.62	113.94
3	B	3302	OAA	O5-C4-C3	2.33	120.04	113.59
2	B	3301	ACO	C5A-N7A-C8A	2.32	107.09	103.45
2	B	3301	ACO	N9A-C8A-N7A	-2.31	110.66	113.94
2	D	3301	ACO	C7P-C6P-C5P	-2.29	108.58	112.39
3	A	3302	OAA	O5-C4-C3	2.27	119.88	113.59
3	D	3302	OAA	O5-C4-C3	2.26	119.85	113.59
4	D	3303	Q5B	C10-C13-N3	2.24	123.20	117.51
5	D	3304	ADP	C6-C5-N7	2.23	136.39	132.09
4	D	3303	Q5B	O15-C21-S	-2.19	119.89	122.68
4	D	3303	Q5B	C17-C18-N6	2.19	120.33	116.34
2	B	3301	ACO	C4A-N9A-C1B	-2.16	121.58	126.63
4	D	3303	Q5B	O3-P-O2	-2.15	104.25	110.70
3	C	3302	OAA	O5-C4-C3	2.12	119.46	113.59
2	B	3301	ACO	O5P-C5P-C6P	-2.11	118.19	122.02
2	A	3301	ACO	N9A-C8A-N7A	-2.11	110.94	113.94
2	D	3301	ACO	O6A-CCP-CBP	-2.07	107.21	110.55
2	B	3301	ACO	O9A-P3B-O8A	2.00	115.30	107.80

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3301	ACO	C5B-O5B-P1A-O2A
2	A	3301	ACO	CCP-O6A-P2A-O3A
2	A	3301	ACO	S1P-C2P-C3P-N4P
2	A	3301	ACO	O-C-S1P-C2P
2	A	3301	ACO	CH3-C-S1P-C2P
2	B	3301	ACO	C5B-O5B-P1A-O2A
2	B	3301	ACO	CCP-O6A-P2A-O3A
2	B	3301	ACO	CCP-O6A-P2A-O4A
2	B	3301	ACO	CDP-CBP-CCP-O6A
2	B	3301	ACO	CEP-CBP-CCP-O6A
2	B	3301	ACO	CAP-CBP-CCP-O6A
2	B	3301	ACO	C6P-C5P-N4P-C3P
2	B	3301	ACO	O5P-C5P-N4P-C3P
2	B	3301	ACO	O-C-S1P-C2P
2	B	3301	ACO	CH3-C-S1P-C2P
2	C	3301	ACO	CDP-CBP-CCP-O6A
2	C	3301	ACO	CEP-CBP-CCP-O6A

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Mol	Chain	Res	Type	Atoms
2	C	3301	ACO	CAP-CBP-CCP-O6A
2	C	3301	ACO	C5P-C6P-C7P-N8P
2	C	3301	ACO	S1P-C2P-C3P-N4P
2	C	3301	ACO	O-C-S1P-C2P
2	C	3301	ACO	CH3-C-S1P-C2P
2	D	3301	ACO	O4B-C4B-C5B-O5B
2	D	3301	ACO	C5B-O5B-P1A-O1A
2	D	3301	ACO	C5B-O5B-P1A-O2A
2	D	3301	ACO	CDP-CBP-CCP-O6A
2	D	3301	ACO	CEP-CBP-CCP-O6A
2	D	3301	ACO	O-C-S1P-C2P
2	D	3301	ACO	CH3-C-S1P-C2P
3	A	3302	OAA	O3-C3-C4-O4
3	A	3302	OAA	O3-C3-C4-O5
3	A	3302	OAA	C2-C3-C4-O4
3	A	3302	OAA	C2-C3-C4-O5
3	B	3302	OAA	O2-C1-C2-C3
3	B	3302	OAA	O3-C3-C4-O4
3	B	3302	OAA	C2-C3-C4-O4
3	B	3302	OAA	C2-C3-C4-O5
3	C	3302	OAA	O3-C3-C4-O4
3	C	3302	OAA	C2-C3-C4-O4
3	C	3302	OAA	C2-C3-C4-O5
3	D	3302	OAA	O3-C3-C4-O4
3	D	3302	OAA	O3-C3-C4-O5
3	D	3302	OAA	C2-C3-C4-O4
3	D	3302	OAA	C2-C3-C4-O5
4	D	3303	Q5B	C-C1-C14-C15
4	D	3303	Q5B	C-C1-C14-O21
4	D	3303	Q5B	C2-C1-C14-C15
4	D	3303	Q5B	C3-C1-C14-C15
4	D	3303	Q5B	C14-C15-N5-C16
4	D	3303	Q5B	N5-C16-C17-C18
4	D	3303	Q5B	C22-C21-S-C20
4	D	3303	Q5B	O15-C21-S-C20
4	D	3303	Q5B	C21-C22-C23-C24
4	D	3303	Q5B	C21-C22-C23-C26
4	D	3303	Q5B	C21-C22-C23-O20
4	D	3303	Q5B	P1-O3-P-O
4	D	3303	Q5B	P-O3-P1-O6
5	D	3304	ADP	C5'-O5'-PA-O1A
5	D	3304	ADP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
4	D	3303	Q5B	O13-C15-N5-C16
2	B	3301	ACO	C3B-C4B-C5B-O5B
2	A	3301	ACO	C3B-C4B-C5B-O5B
2	B	3301	ACO	O4B-C4B-C5B-O5B
2	A	3301	ACO	C4B-C3B-O3B-P3B
2	C	3301	ACO	C4B-C3B-O3B-P3B
2	A	3301	ACO	O4B-C4B-C5B-O5B
2	D	3301	ACO	C3B-C4B-C5B-O5B
4	D	3303	Q5B	O6-C4-C5-O7
2	D	3301	ACO	S1P-C2P-C3P-N4P
2	C	3301	ACO	C2B-C3B-O3B-P3B
4	D	3303	Q5B	C2-C1-C14-O21
4	D	3303	Q5B	O6-C4-C5-C6
2	B	3301	ACO	P1A-O3A-P2A-O6A
2	D	3301	ACO	P1A-O3A-P2A-O6A
3	A	3302	OAA	O2-C1-C2-C3
3	D	3302	OAA	O2-C1-C2-C3
2	B	3301	ACO	O9P-C9P-CAP-OAP
2	D	3301	ACO	O5P-C5P-N4P-C3P
2	A	3301	ACO	C5B-O5B-P1A-O3A
2	A	3301	ACO	CCP-O6A-P2A-O5A
2	B	3301	ACO	C5B-O5B-P1A-O3A
2	D	3301	ACO	C5B-O5B-P1A-O3A
4	D	3303	Q5B	C3-C1-C14-O21
5	D	3304	ADP	C5'-O5'-PA-O2A
2	A	3301	ACO	C2B-C3B-O3B-P3B
2	A	3301	ACO	C3B-O3B-P3B-O9A
3	C	3302	OAA	O1-C1-C2-C3
2	D	3301	ACO	C6P-C5P-N4P-C3P
2	B	3301	ACO	N8P-C9P-CAP-OAP
2	A	3301	ACO	P2A-O3A-P1A-O2A
2	A	3301	ACO	C5P-C6P-C7P-N8P
3	B	3302	OAA	C1-C2-C3-O3
3	A	3302	OAA	O1-C1-C2-C3
3	D	3302	OAA	O1-C1-C2-C3
2	C	3301	ACO	CAP-C9P-N8P-C7P
2	C	3301	ACO	P2A-O3A-P1A-O1A
2	C	3301	ACO	P2A-O3A-P1A-O2A
2	D	3301	ACO	C3B-O3B-P3B-O9A
2	A	3301	ACO	C2B-C1B-N9A-C8A
2	A	3301	ACO	C3P-C2P-S1P-C
2	D	3301	ACO	CAP-CBP-CCP-O6A

Continued on next page...

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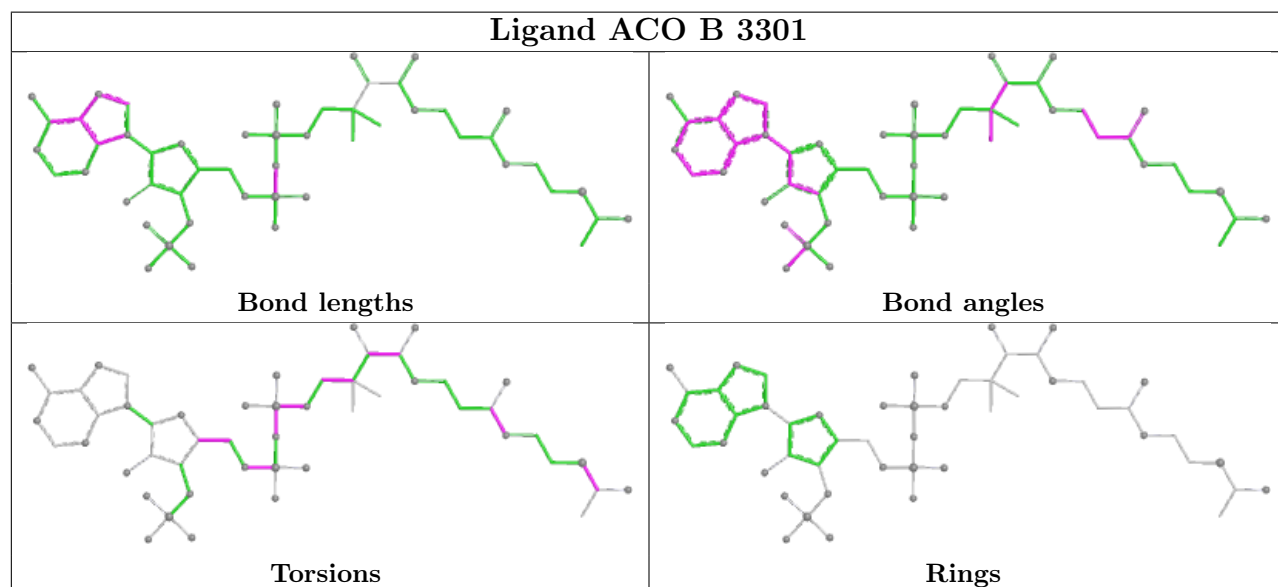
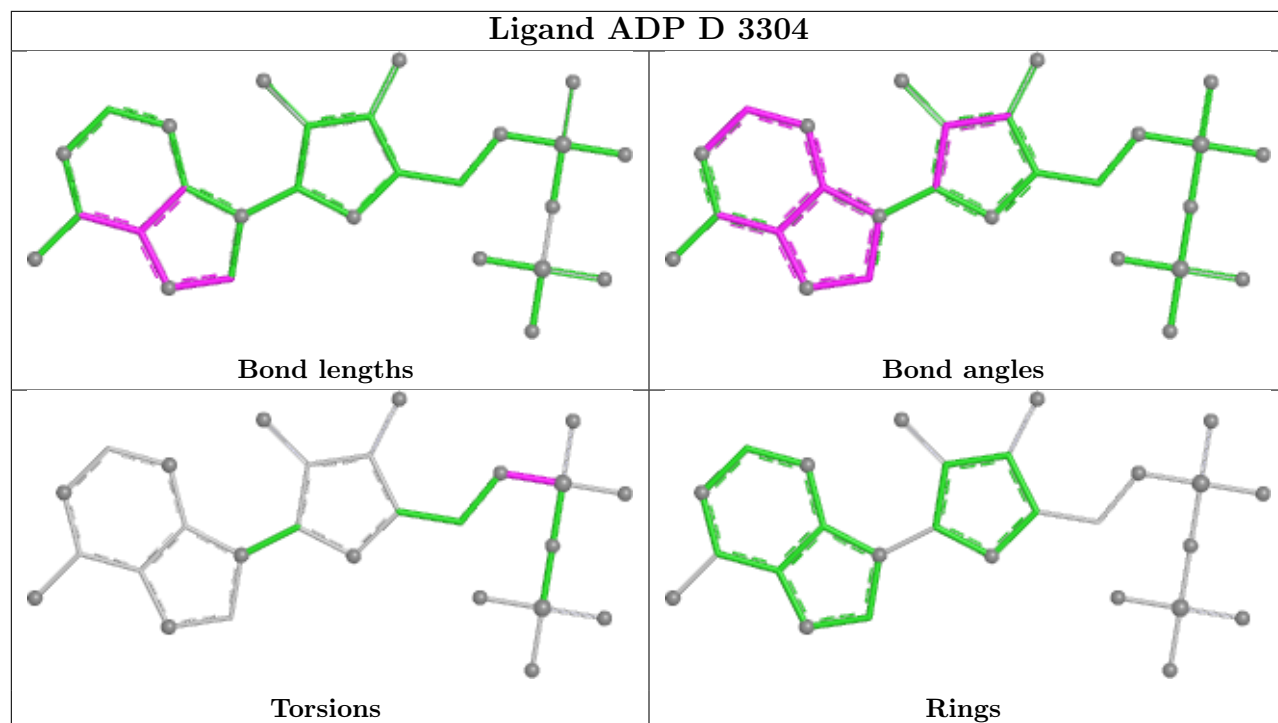
Mol	Chain	Res	Type	Atoms
3	B	3302	OAA	C1-C2-C3-C4
2	A	3301	ACO	P1A-O3A-P2A-O5A
2	D	3301	ACO	P2A-O3A-P1A-O1A
2	D	3301	ACO	P2A-O3A-P1A-O2A

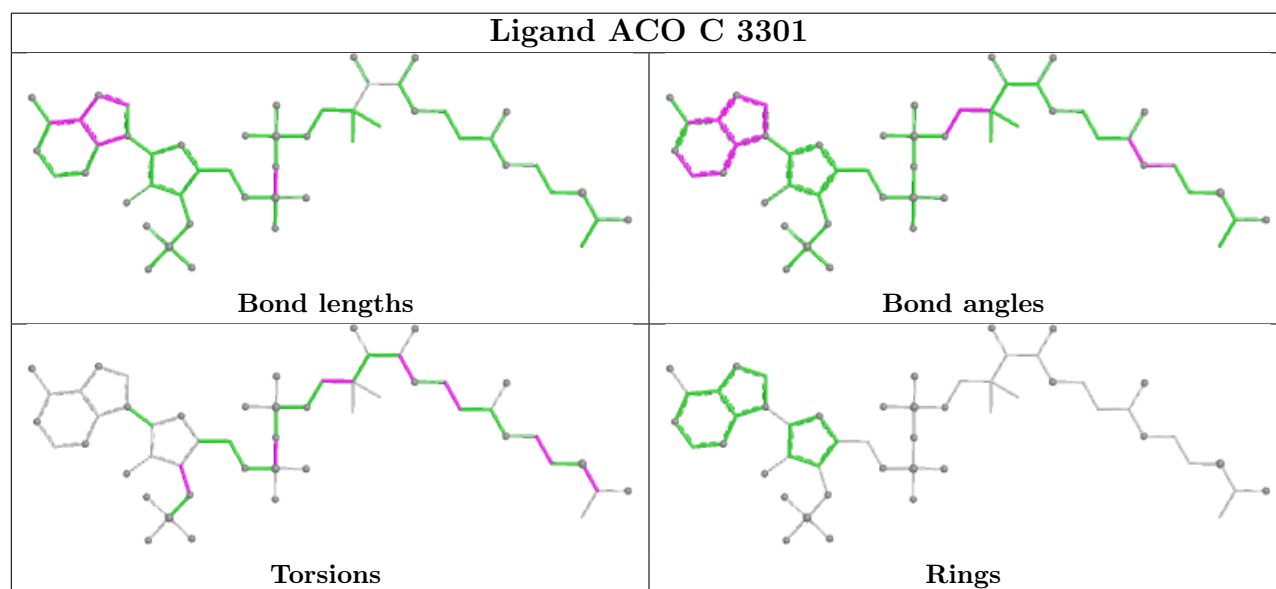
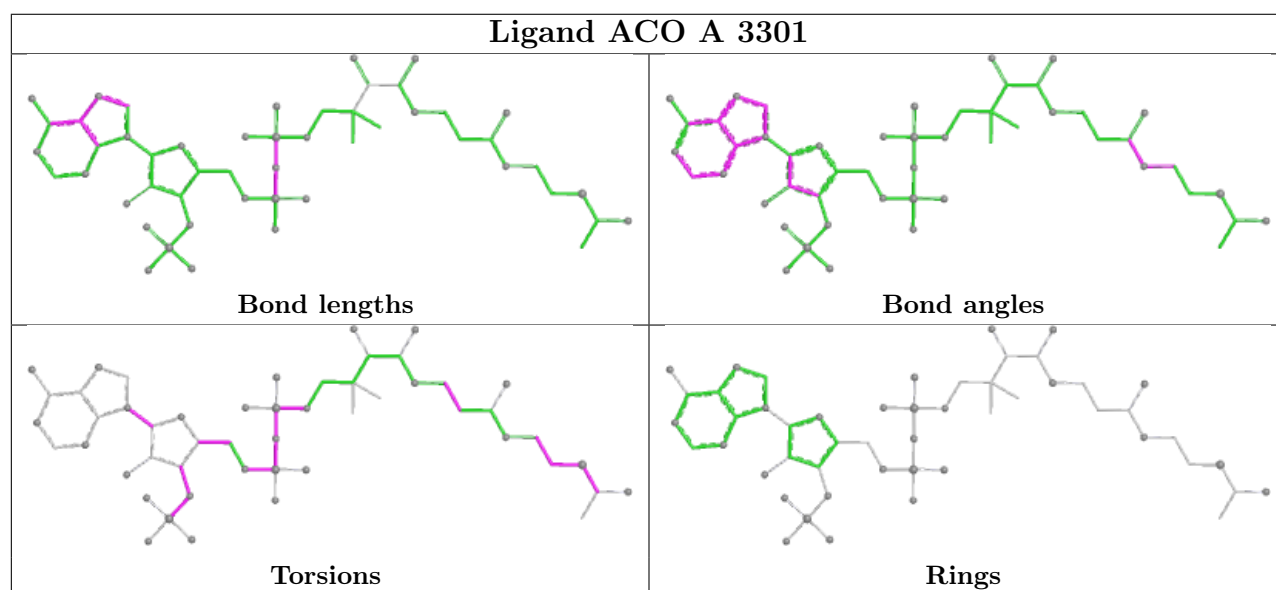
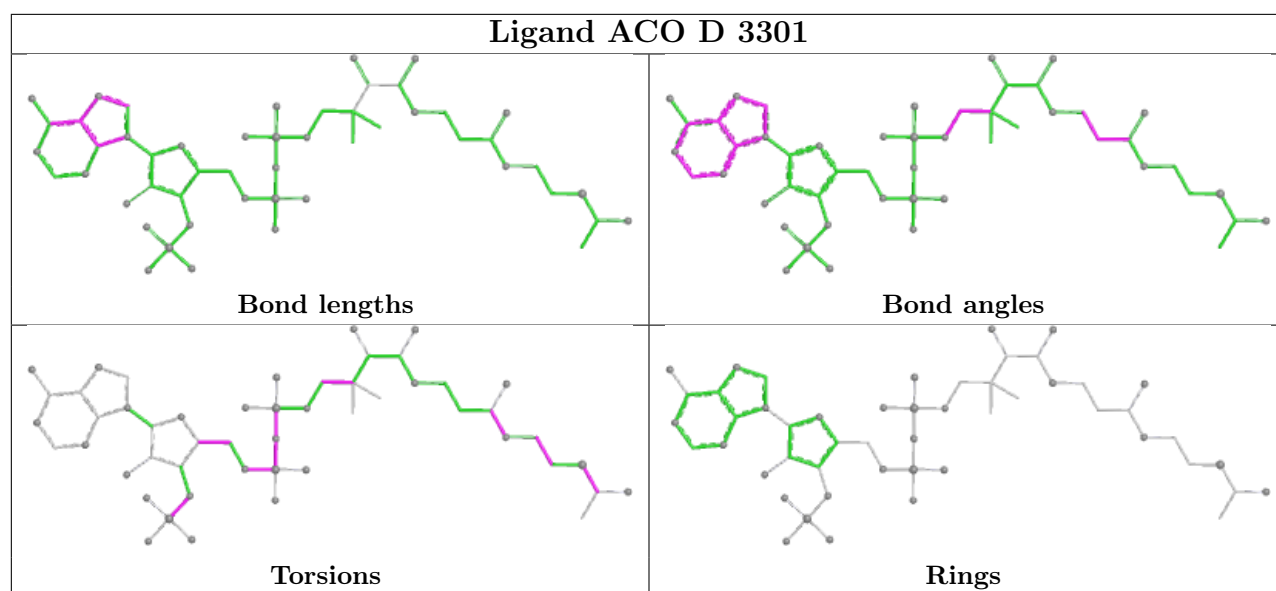
There are no ring outliers.

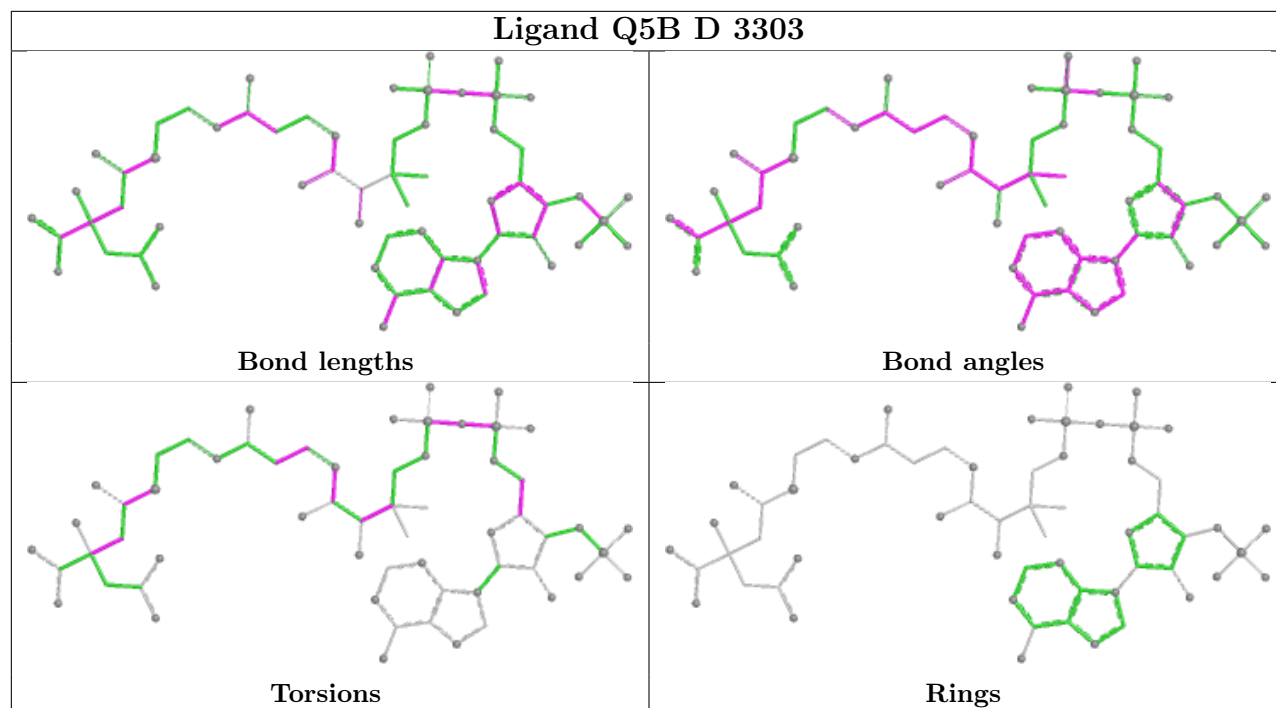
10 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3302	OAA	1	0
2	B	3301	ACO	5	0
2	D	3301	ACO	5	0
2	A	3301	ACO	7	0
2	C	3301	ACO	7	0
3	B	3302	OAA	1	0
6	D	3305	PO4	1	0
3	C	3302	OAA	1	0
3	D	3302	OAA	1	0
4	D	3303	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.

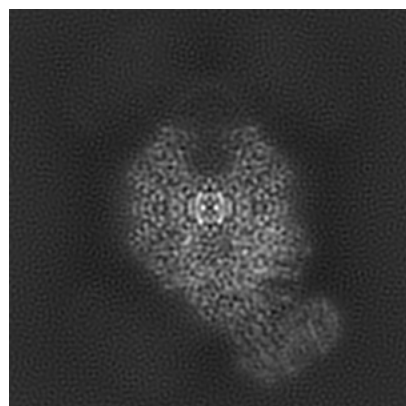
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29740. These allow visual inspection of the internal detail of the map and identification of artifacts.

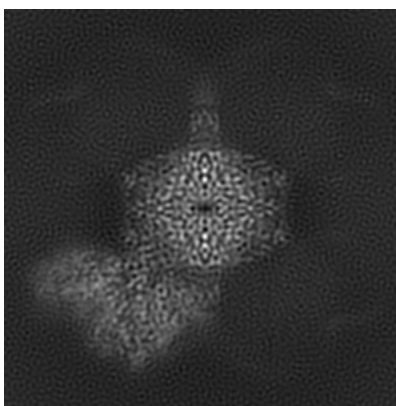
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

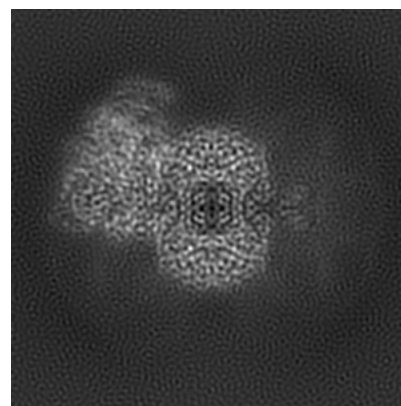
6.1.1 Primary map



X

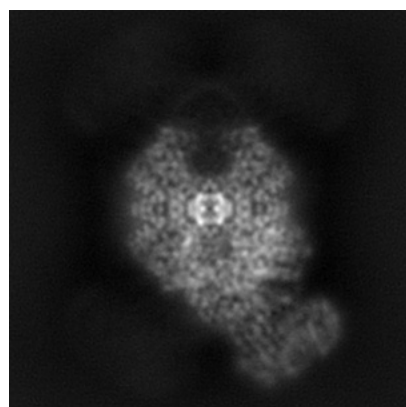


Y

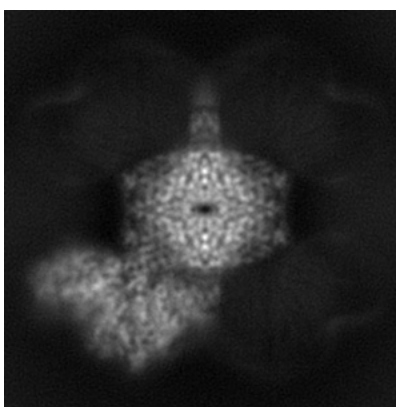


Z

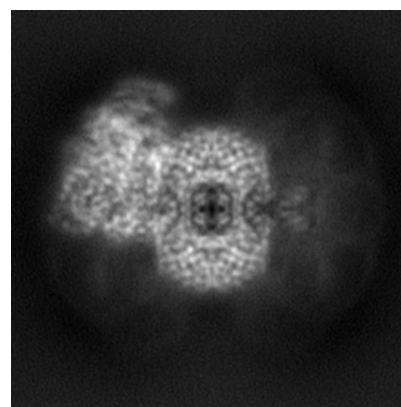
6.1.2 Raw map



X



Y

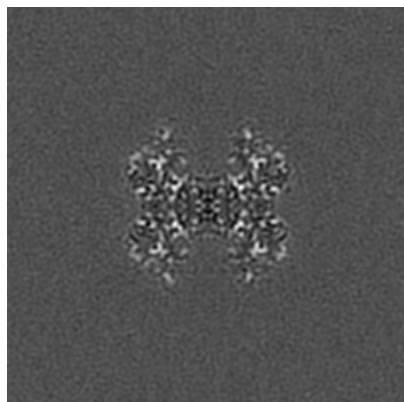


Z

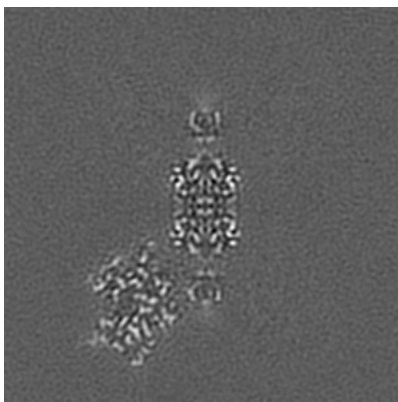
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

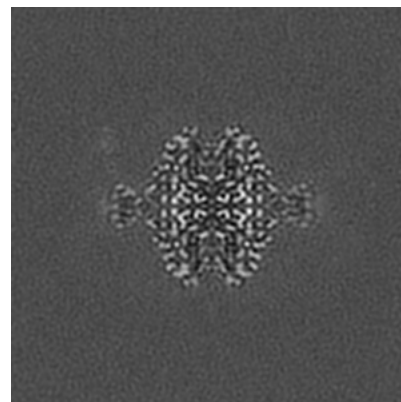
6.2.1 Primary map



X Index: 110

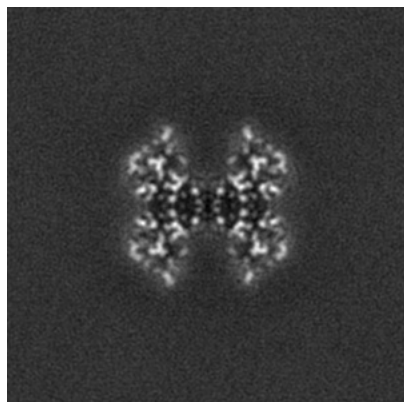


Y Index: 110

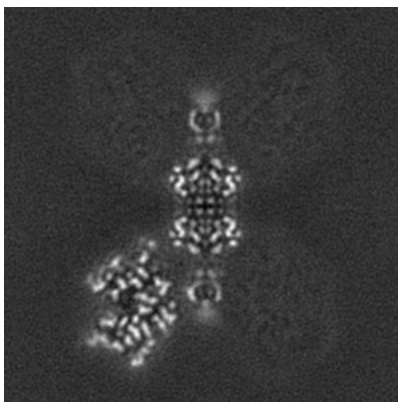


Z Index: 110

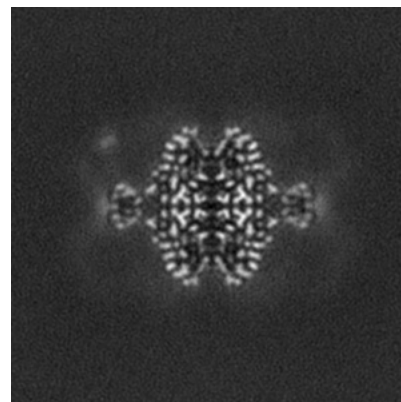
6.2.2 Raw map



X Index: 110



Y Index: 110

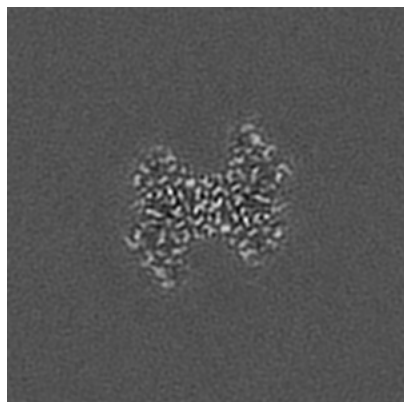


Z Index: 110

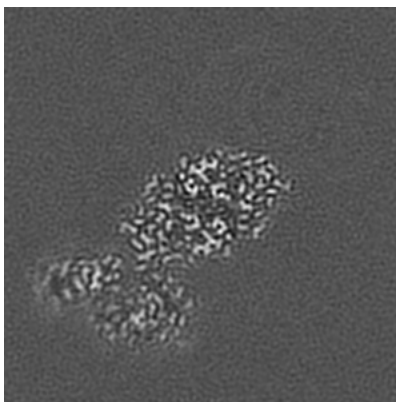
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

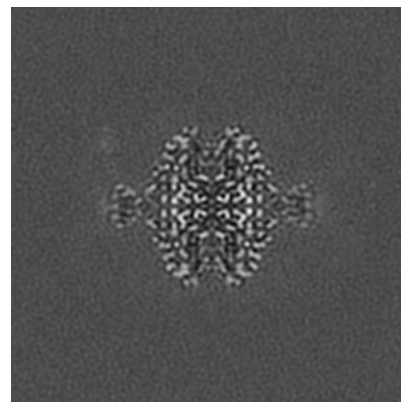
6.3.1 Primary map



X Index: 118

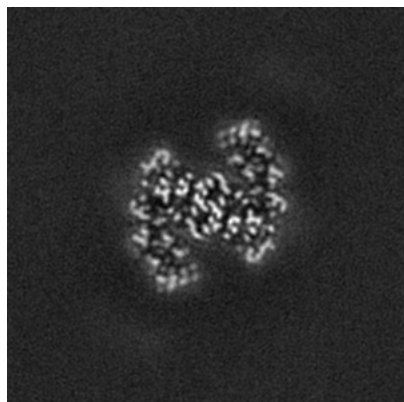


Y Index: 137

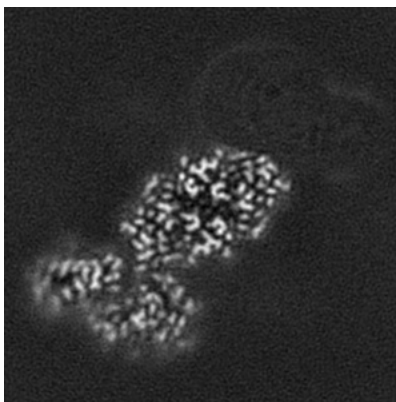


Z Index: 110

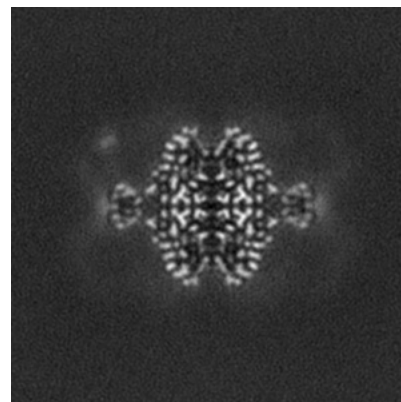
6.3.2 Raw map



X Index: 123



Y Index: 137

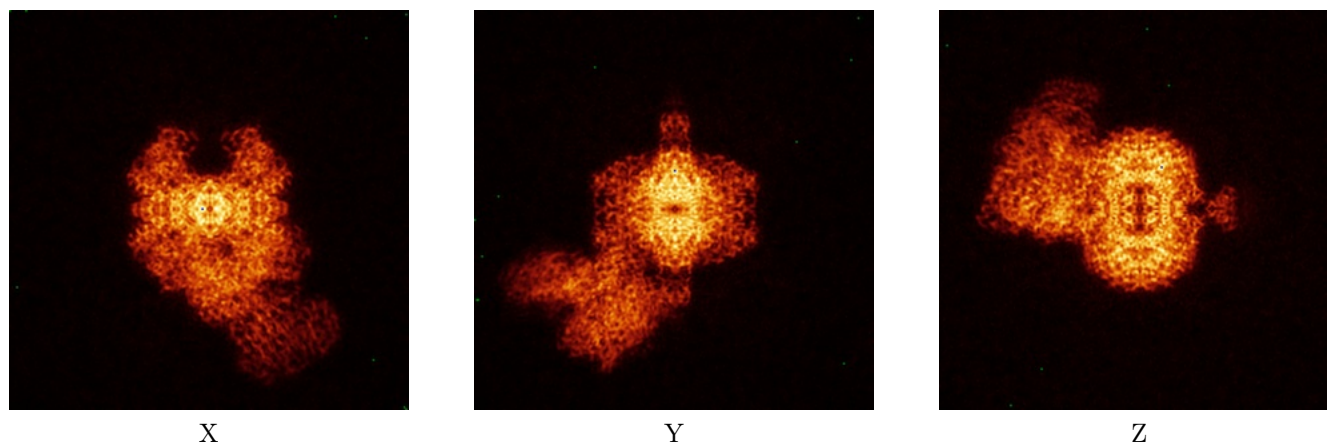


Z Index: 110

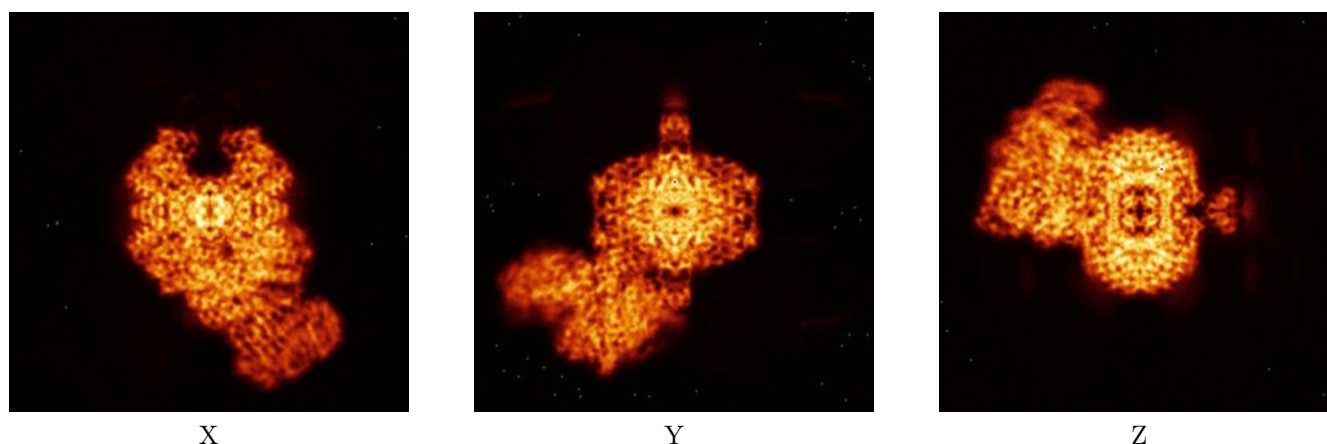
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

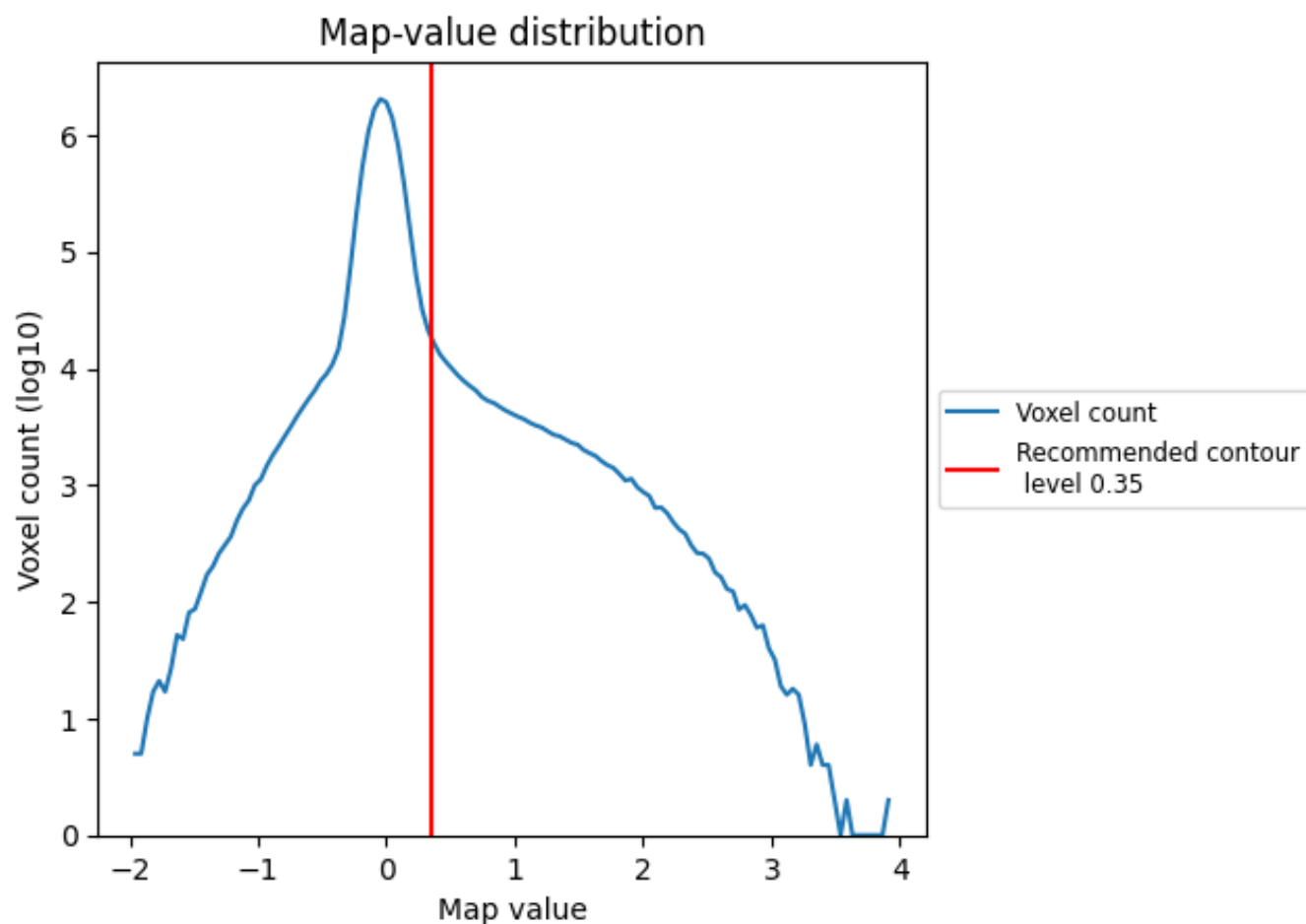
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

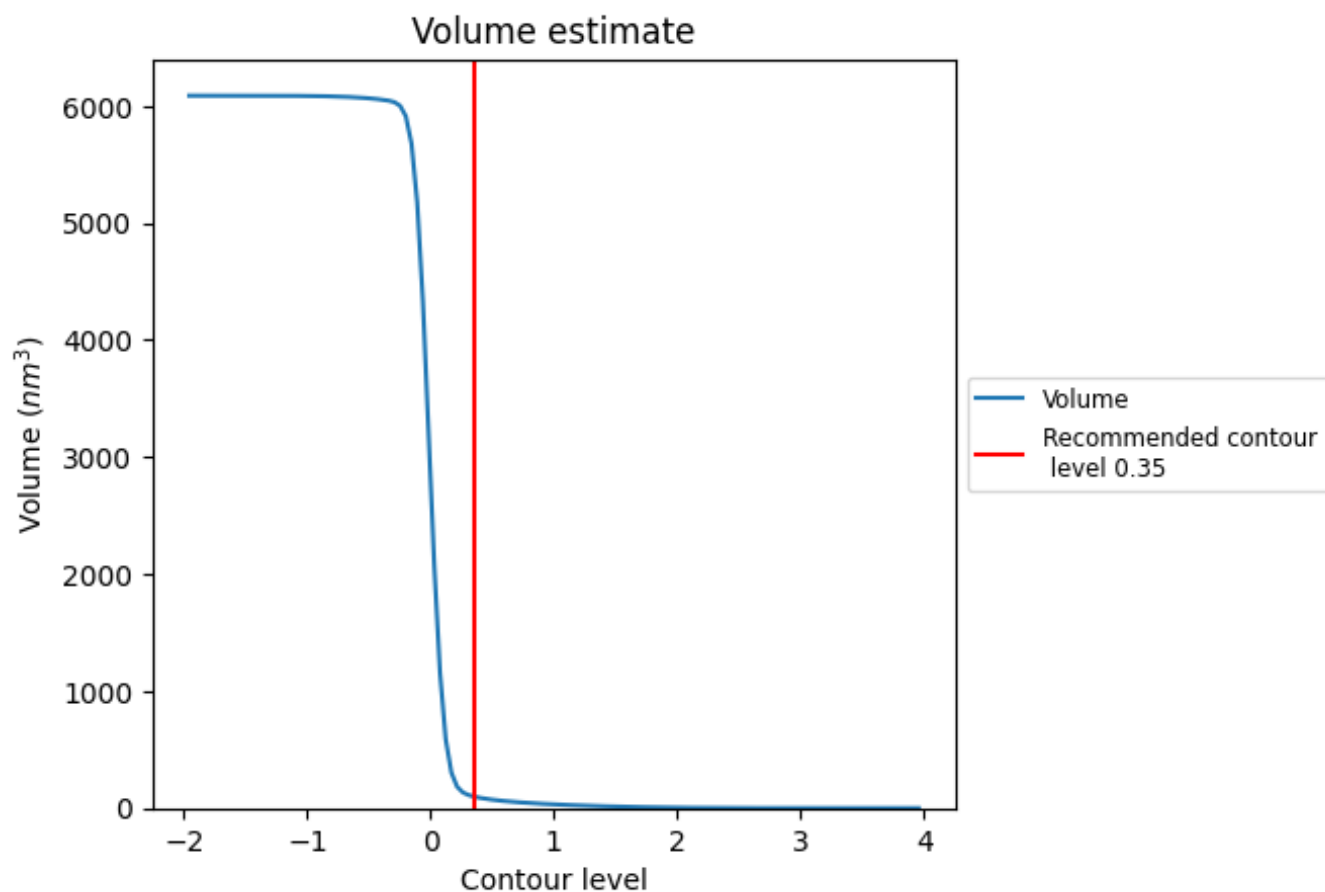
This section contains the results of statistical analysis of the map.

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.

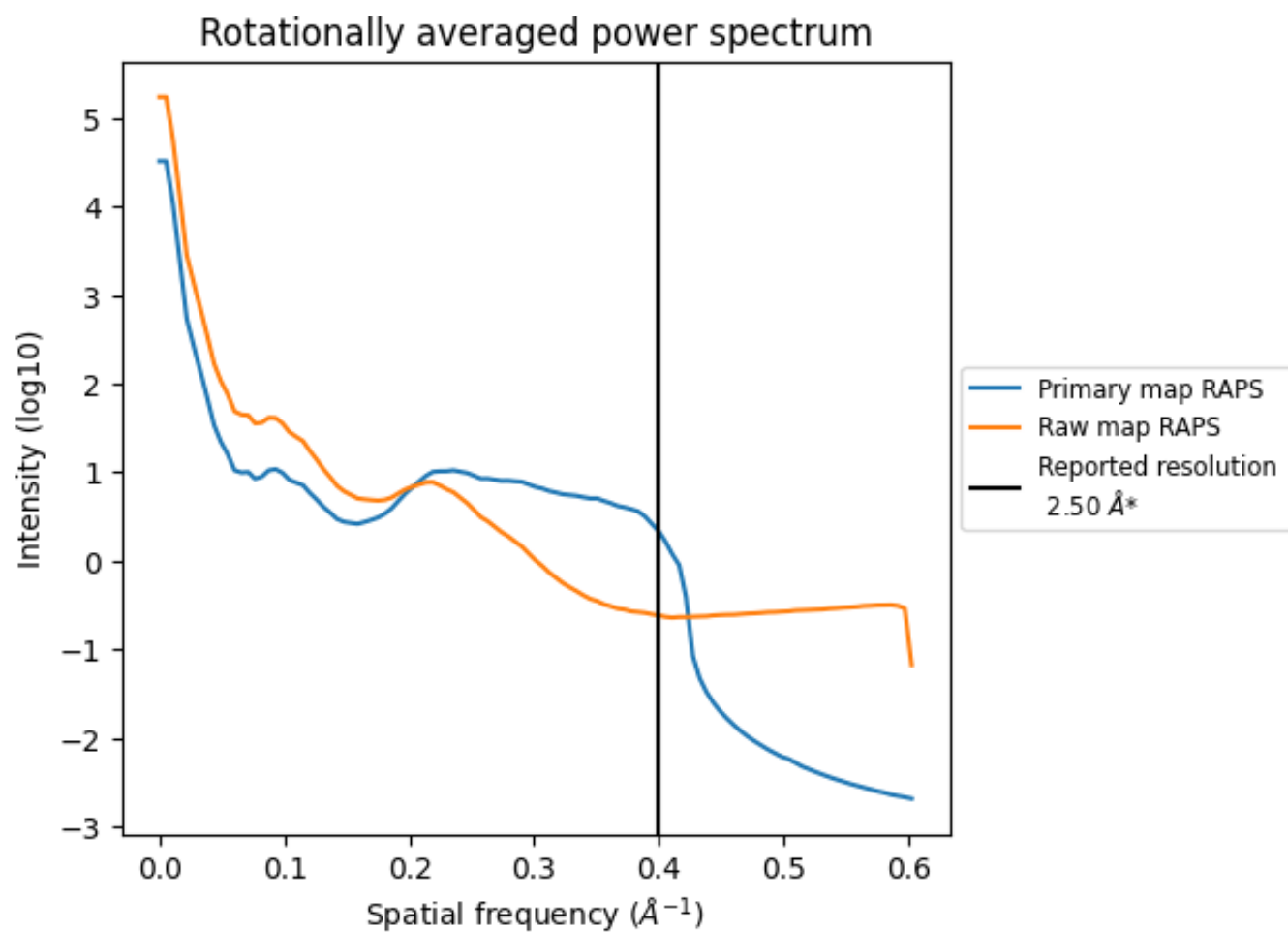
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 99 nm^3 ; this corresponds to an approximate mass of 90 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 ⓘ

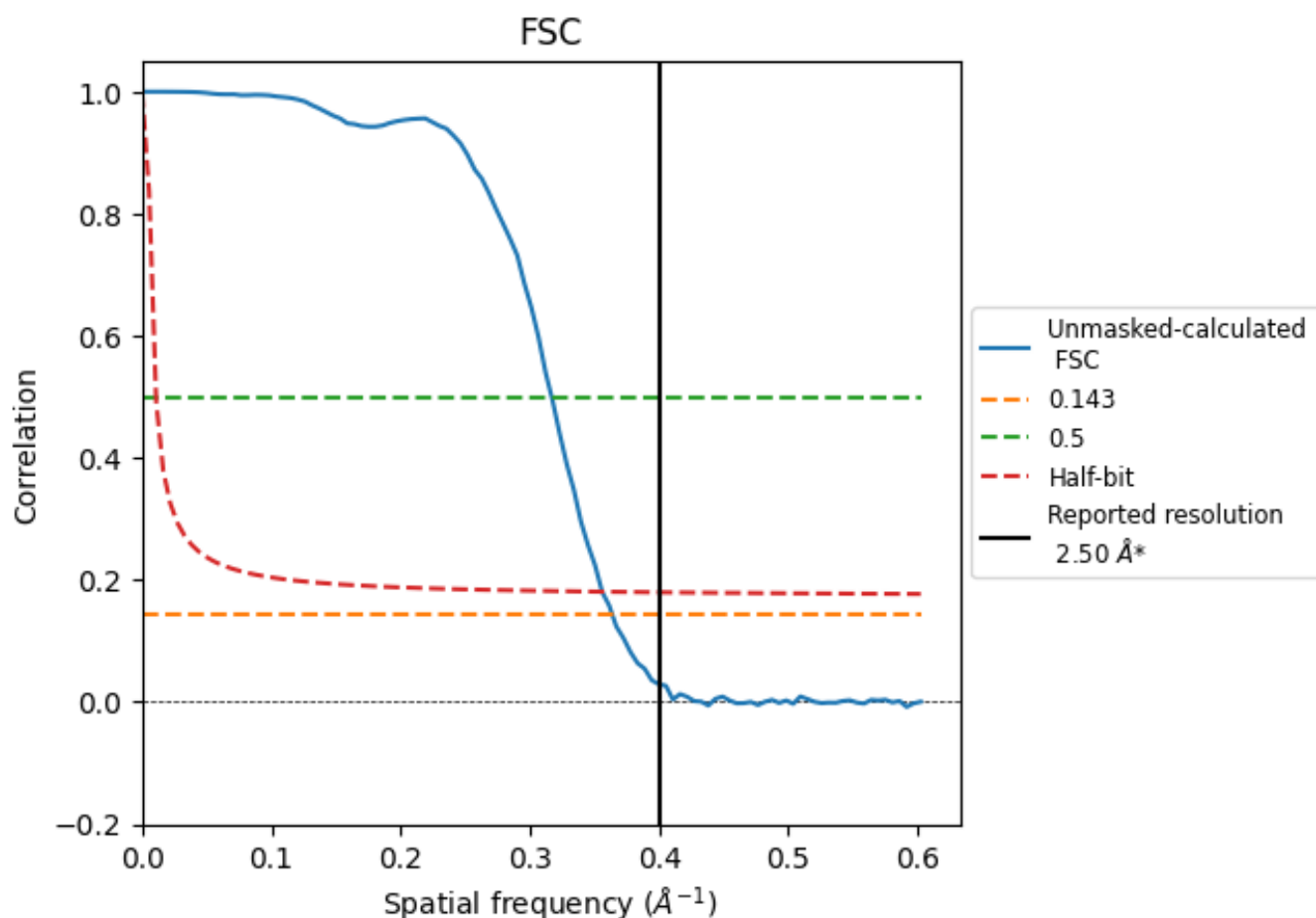


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

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 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.75	3.16	2.81

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

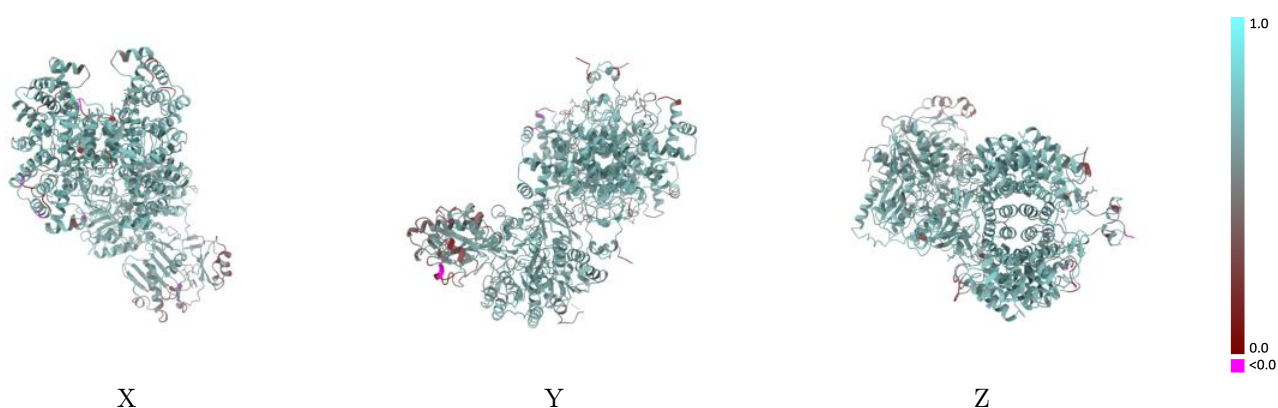
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-29740 and PDB model 8G5D. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

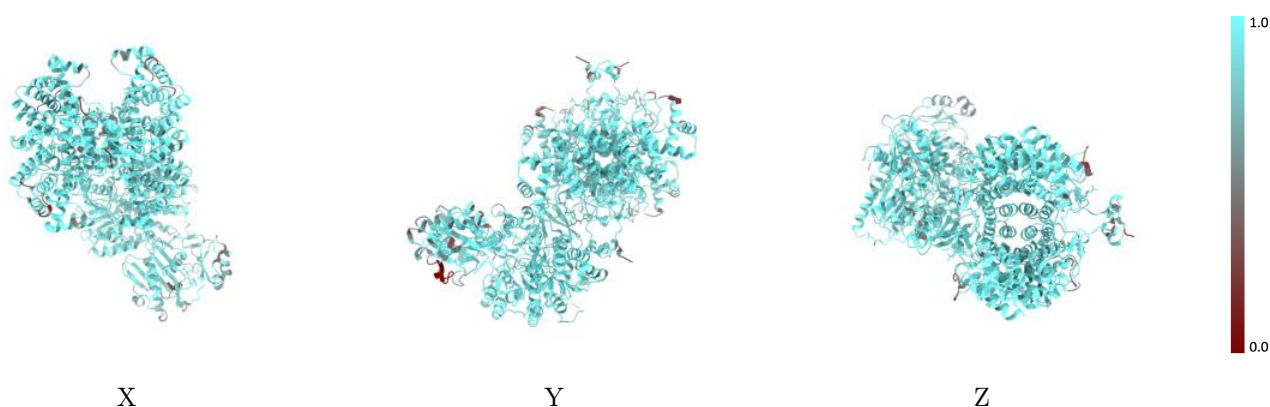
This section was not generated.

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



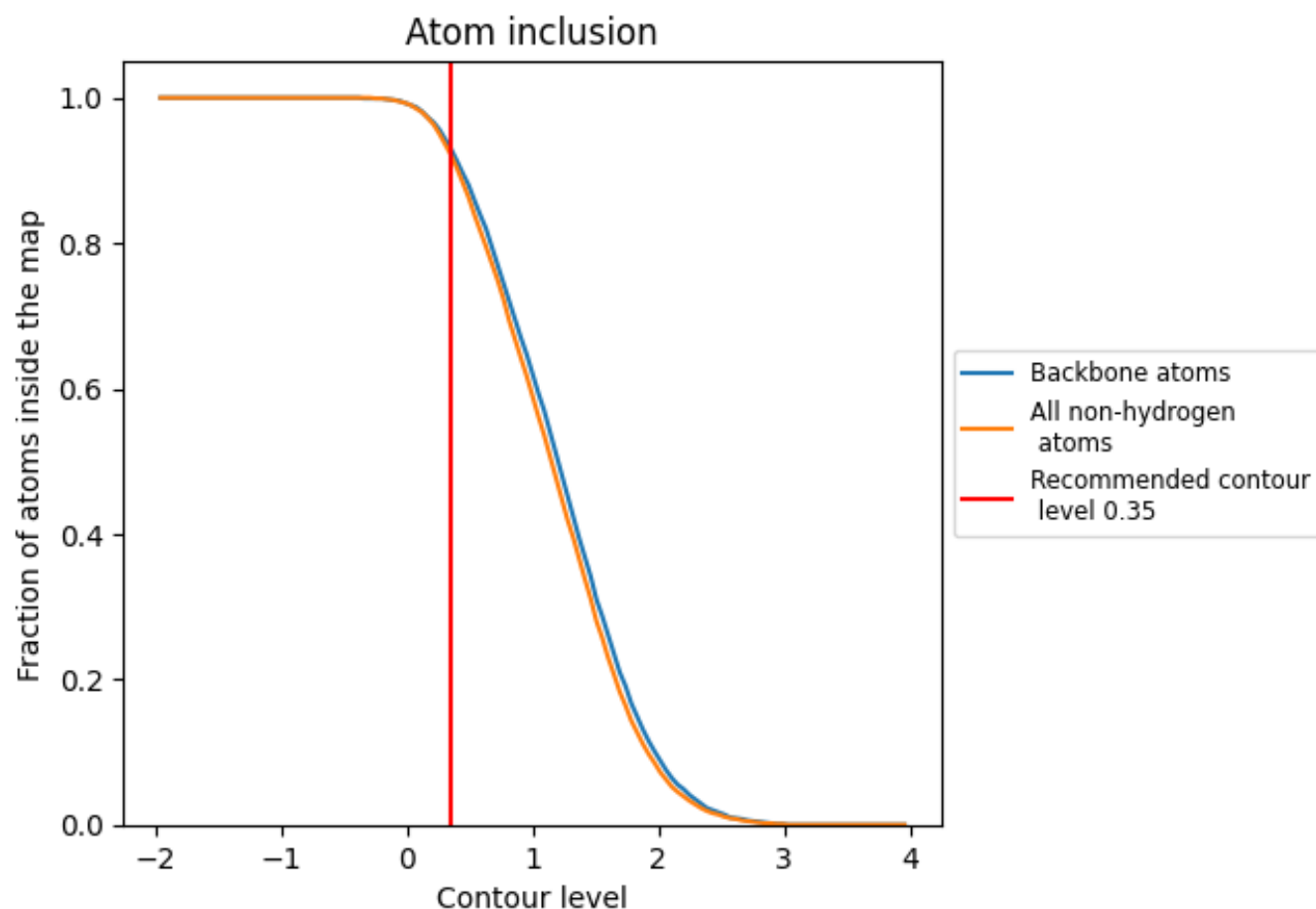
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 92% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9220	0.6310
A	0.9240	0.6390
B	0.9500	0.6590
C	0.9260	0.6400
D	0.9150	0.6190

