



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 10:46 AM UTC

PDB ID : 7WTB / pdb_00007wtb
EMDB ID : EMD-32775
Title : Cryo-EM structure of human pyruvate carboxylase with acetyl-CoA
Authors : Chai, P.; Lan, P.; Wu, J.; Lei, M.
Deposited on : 2022-02-04
Resolution : 3.70 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:

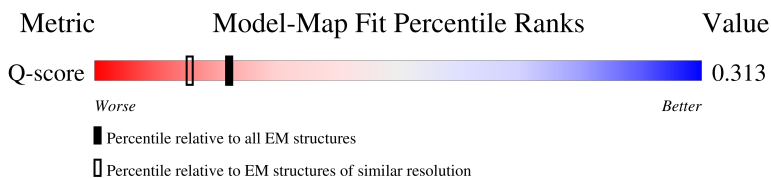
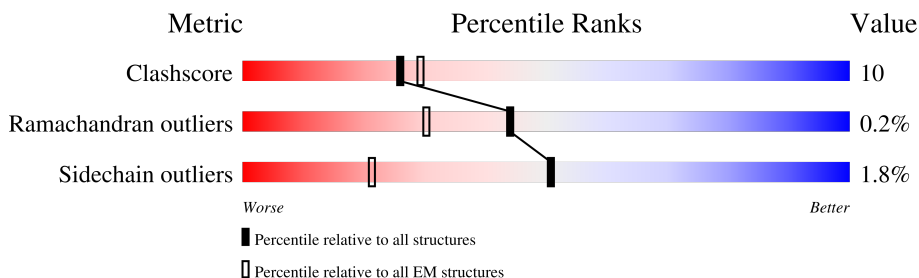
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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	1178	
1	B	1178	
1	C	1178	
1	D	1178	

2 Entry composition [i](#)

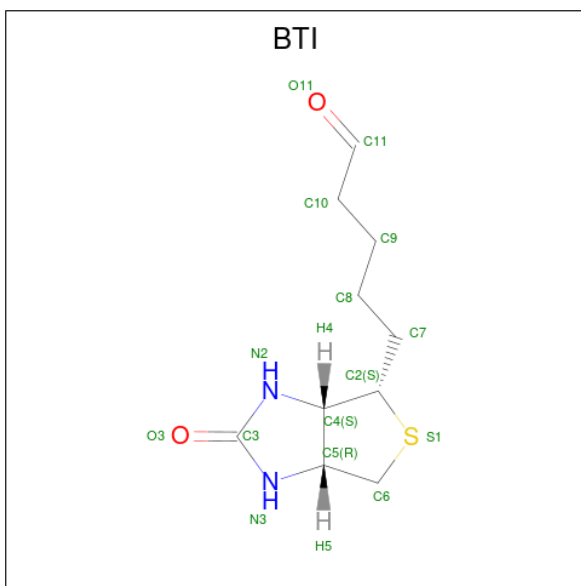
There are 4 unique types of molecules in this entry. The entry contains 28480 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pyruvate carboxylase, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1146	Total 8869	C 5612	N 1559	O 1651	S 47	0	0
1	B	1147	Total 8877	C 5618	N 1560	O 1652	S 47	0	0
1	C	684	Total 5255	C 3339	N 902	O 978	S 36	0	0
1	D	684	Total 5255	C 3339	N 902	O 978	S 36	0	0

- Molecule 2 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (CCD ID: BTI) (formula: C₁₀H₁₆N₂O₂S).



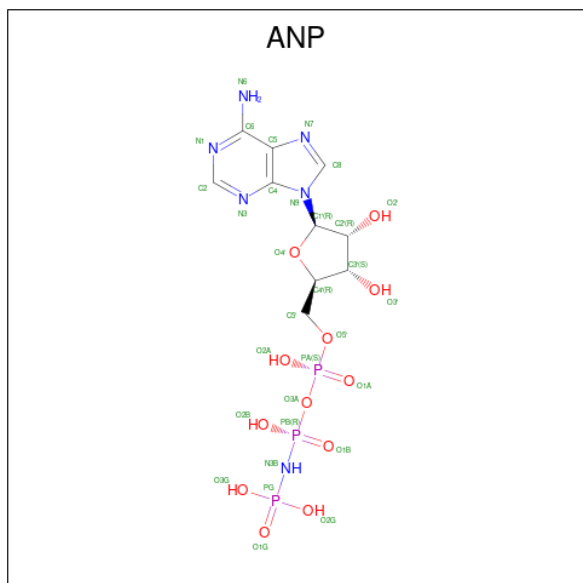
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
2	A	1	Total 15	C 10	N 2	O 2	S 1	0
2	B	1	Total 15	C 10	N 2	O 2	S 1	0

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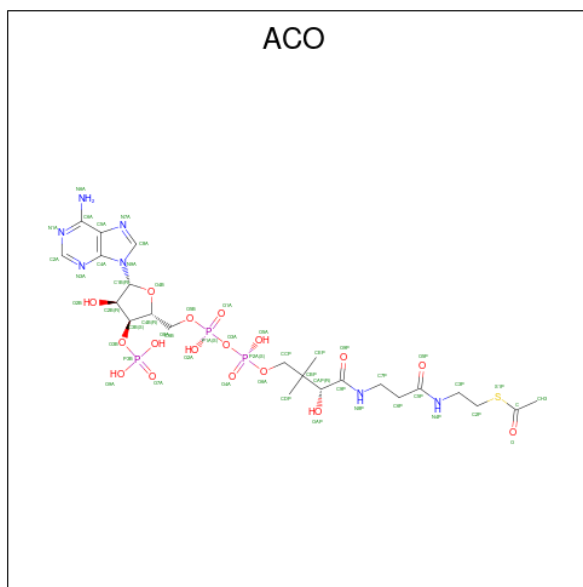
Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	S	0
			15	10	2	2	1	
2	D	1	Total	C	N	O	S	0
			15	10	2	2	1	

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	B	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 4 is ACETYL COENZYME *A (CCD ID: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).

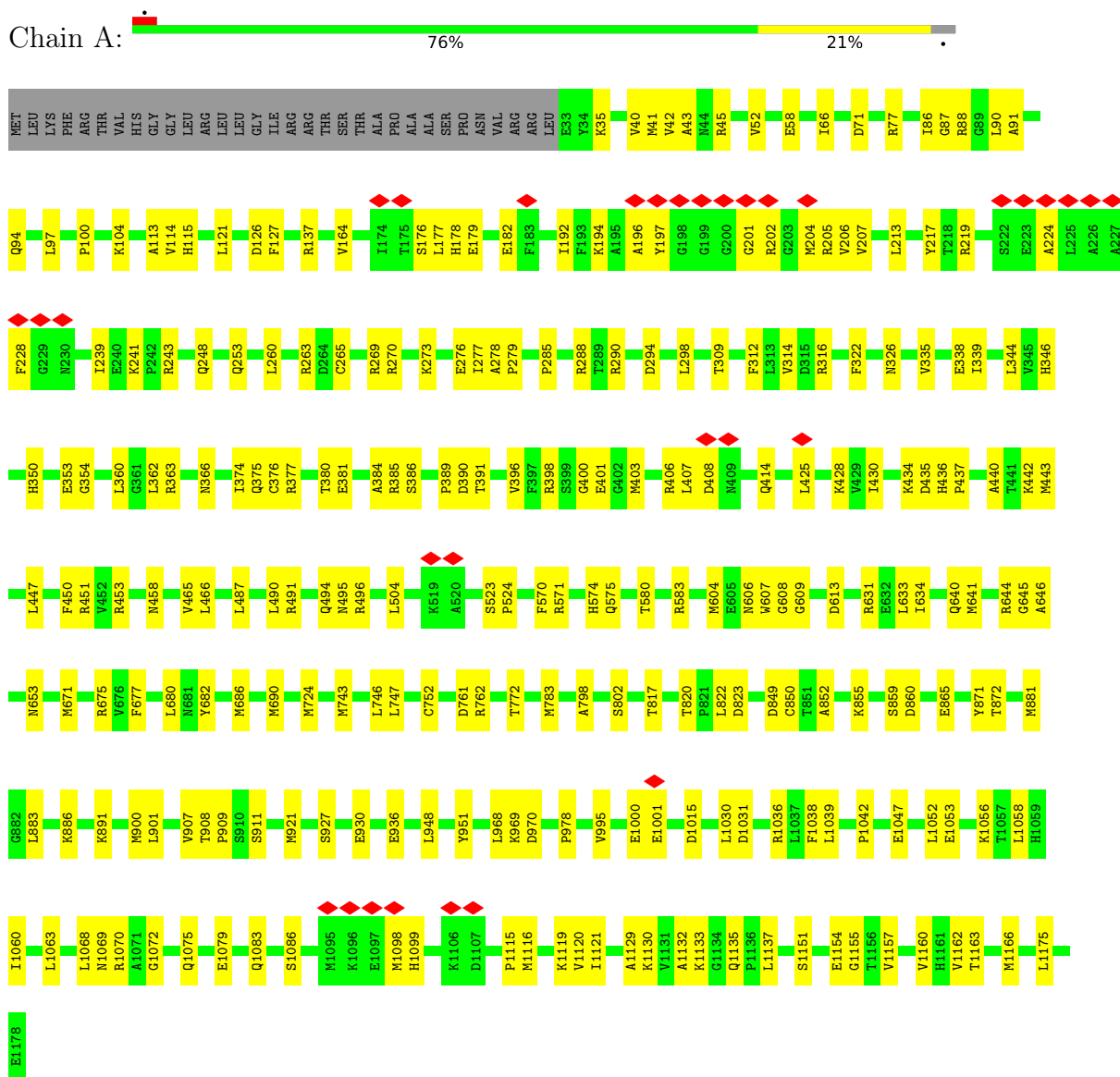


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
4	A	1	51	23	7	17	3	1	0
4	B	1	51	23	7	17	3	1	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Pyruvate carboxylase, mitochondrial



- Molecule 1: Pyruvate carboxylase, mitochondrial

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	186526	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)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.044	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size (\AA)	343.2, 343.2, 343.2	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	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: ANP, ACO, BTI

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.15	0/9060	0.37	0/12277
1	B	0.17	0/9068	0.42	1/12288 (0.0%)
1	C	0.39	1/5373 (0.0%)	0.63	8/7284 (0.1%)
1	D	0.34	0/5373	0.52	1/7284 (0.0%)
All	All	0.26	1/28874 (0.0%)	0.47	10/39133 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	507	VAL	C-N	8.03	1.44	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	507	VAL	O-C-N	8.36	130.10	121.91
1	C	1041	GLY	N-CA-C	6.65	125.90	112.34
1	C	1036	ARG	CB-CA-C	-6.55	100.59	110.88
1	C	1039	LEU	CA-C-N	-6.19	113.11	121.71
1	C	1039	LEU	C-N-CA	-6.19	113.11	121.71
1	B	590	ILE	N-CA-C	-6.08	107.93	113.71
1	C	1037	LEU	CA-C-O	-5.81	114.72	120.82
1	D	511	GLY	CA-C-O	-5.74	113.31	121.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	590	ILE	N-CA-C	-5.72	108.28	113.71
1	C	649	VAL	N-CA-C	-5.60	108.39	113.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	511	GLY	Mainchain

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	8869	0	8829	185	0
1	B	8877	0	8839	184	0
1	C	5255	0	5247	119	0
1	D	5255	0	5248	96	0
2	A	15	0	15	0	0
2	B	15	0	15	5	0
2	C	15	0	15	3	0
2	D	15	0	15	0	0
3	A	31	0	13	1	0
3	B	31	0	11	0	0
4	A	51	0	34	4	0
4	B	51	0	34	2	0
All	All	28480	0	28315	577	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 (577) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:908:THR:CG2	1:B:909:PRO:HD3	1.52	1.39
1:A:908:THR:CG2	1:A:909:PRO:HD3	1.60	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:908:THR:HG23	1:B:909:PRO:CD	1.76	1.16
1:A:908:THR:HG23	1:A:909:PRO:HD3	1.23	1.14
1:B:908:THR:HG22	1:B:909:PRO:HD3	1.19	1.12
1:B:908:THR:CG2	1:B:909:PRO:CD	2.33	1.03
1:B:908:THR:HG23	1:B:909:PRO:HD3	1.32	1.03
1:A:908:THR:HG22	1:A:909:PRO:HD3	1.39	1.02
1:A:908:THR:HG23	1:A:909:PRO:CD	1.90	1.02
1:D:908:THR:CG2	1:D:909:PRO:HD3	1.96	0.96
1:A:644:ARG:HE	1:A:908:THR:HG21	1.29	0.93
1:B:431:ALA:HB2	1:B:443:MET:HE3	1.53	0.91
1:A:908:THR:CG2	1:A:909:PRO:CD	2.48	0.91
1:A:35:LYS:HB3	1:A:137:ARG:HH22	1.40	0.87
1:C:501:LEU:HD22	1:C:1078:PHE:CG	2.10	0.87
1:A:641:MET:HB2	1:A:671:MET:HE2	1.56	0.84
1:B:570:PHE:HD1	1:B:604:MET:HE2	1.42	0.84
1:D:908:THR:HG22	1:D:909:PRO:HD3	1.57	0.84
1:D:644:ARG:HE	1:D:908:THR:HG21	1.43	0.82
1:B:190:PRO:HA	1:B:207:VAL:O	1.79	0.81
1:D:908:THR:HG23	1:D:909:PRO:HD3	1.66	0.76
1:B:1156:THR:O	1:B:1158:ARG:NH1	2.19	0.76
1:B:44:ASN:ND2	1:B:116:PRO:O	2.19	0.76
1:A:1069:ASN:OD1	1:A:1070:ARG:N	2.19	0.75
1:B:1132:ALA:HA	1:B:1154:GLU:HG2	1.67	0.75
1:B:743:MET:HE2	1:B:907:VAL:HG22	1.68	0.75
1:A:42:VAL:HG11	1:A:52:VAL:HG21	1.69	0.75
1:C:1163:THR:H	1:C:1166:MET:HE2	1.52	0.74
1:A:276:GLU:HB2	1:A:375:GLN:HB3	1.70	0.74
1:B:241:LYS:HB3	1:B:316:ARG:HD2	1.68	0.73
1:B:995:VAL:HA	1:B:999:GLY:HA3	1.67	0.73
1:B:850:CYS:HB3	1:B:854:MET:HB2	1.70	0.73
1:B:1068:LEU:HD23	1:B:1072:GLY:HA2	1.69	0.73
1:C:640:GLN:HE21	1:C:675:ARG:HD2	1.52	0.73
1:B:276:GLU:HG3	1:B:332:GLU:HG2	1.72	0.72
1:B:908:THR:HG23	1:B:909:PRO:CG	2.19	0.71
1:D:509:VAL:HB	1:D:1089:VAL:HG11	1.71	0.71
1:D:917:LEU:HG	1:D:921:MET:HE1	1.73	0.71
1:A:396:VAL:HB	1:A:453:ARG:HB2	1.71	0.71
1:D:538:PRO:O	1:D:636:ASN:ND2	2.24	0.69
1:D:502:HIS:HA	1:D:1087:ILE:HD13	1.73	0.69
1:A:772:THR:HG22	1:A:783:MET:HE2	1.74	0.69
1:B:1080:LEU:HG	1:B:1081:ASN:H	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:930:GLU:OE1	1:C:934:GLN:NE2	2.26	0.69
1:C:995:VAL:HA	1:C:999:GLY:HA3	1.74	0.69
1:B:32:LEU:N	1:B:254:TYR:HH	1.91	0.68
1:B:1101:HIS:NE2	1:B:1173:LEU:O	2.20	0.68
1:D:1090:LYS:NZ	1:D:1091:ASP:O	2.25	0.68
1:B:644:ARG:NE	1:B:908:THR:HG21	2.09	0.68
1:A:1068:LEU:HD22	1:A:1072:GLY:HA2	1.74	0.68
1:C:508:MET:HG2	1:C:1042:PRO:HA	1.75	0.68
1:C:752:CYS:SG	1:C:786:CYS:N	2.68	0.67
1:B:855:LYS:HD2	1:C:851:THR:HG21	1.75	0.67
1:C:1132:ALA:O	1:C:1151:SER:OG	2.13	0.67
1:A:948:LEU:HB3	1:A:968:LEU:HD21	1.75	0.67
1:A:414:GLN:OE1	1:A:1083:GLN:NE2	2.21	0.67
1:B:112:ASP:OD1	1:B:137:ARG:NH1	2.28	0.67
1:C:661:LYS:HD3	1:C:1008:LEU:HD21	1.75	0.67
1:B:741:LYS:HD2	1:B:771:HIS:HD2	1.60	0.67
1:D:908:THR:HG23	1:D:909:PRO:CD	2.25	0.67
1:A:1163:THR:H	1:A:1166:MET:HE1	1.60	0.67
1:C:959:PHE:HE2	1:C:964:ARG:HH11	1.43	0.67
1:B:570:PHE:CD1	1:B:604:MET:HE2	2.28	0.66
1:D:1135:GLN:HE21	1:D:1151:SER:HB2	1.59	0.66
1:C:890:VAL:HG22	1:C:922:VAL:HG11	1.77	0.66
1:A:309:THR:HB	1:A:326:ASN:HB2	1.78	0.66
1:A:398:ARG:HH21	1:A:451:ARG:HD2	1.58	0.66
1:A:269:ARG:HG3	1:A:270:ARG:HD3	1.76	0.66
1:A:260:LEU:HD11	1:A:344:LEU:HD11	1.78	0.66
1:A:743:MET:HE2	1:A:907:VAL:HG22	1.78	0.66
1:B:1158:ARG:HH21	1:B:1178:GLU:H	1.42	0.66
1:C:1143:MET:SD	1:C:1143:MET:N	2.69	0.66
1:B:1158:ARG:NH2	1:B:1178:GLU:H	1.94	0.65
1:A:1053:GLU:H	1:A:1056:LYS:HB2	1.61	0.65
1:B:445:ARG:NH1	1:B:449:GLU:OE2	2.28	0.65
1:C:1174:ILE:HG23	1:C:1175:LEU:HD23	1.78	0.65
1:D:772:THR:HG22	1:D:783:MET:HE2	1.79	0.65
1:C:771:HIS:ND1	1:C:795:ASP:OD2	2.31	0.64
1:A:907:VAL:HG12	1:A:908:THR:H	1.62	0.64
1:B:908:THR:HG23	1:B:909:PRO:N	2.12	0.63
1:A:164:VAL:HG22	1:A:322:PHE:HB2	1.81	0.63
2:B:2002:BTI:S1	1:D:651:TYR:OH	2.57	0.63
1:D:505:GLY:HA3	1:D:1087:ILE:HD11	1.81	0.63
1:A:381:GLU:OE2	1:A:458:ASN:ND2	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:752:CYS:SG	1:B:786:CYS:N	2.72	0.62
1:C:844:LEU:HD21	1:C:1036:ARG:HB3	1.81	0.62
1:B:35:LYS:HD2	1:B:137:ARG:HE	1.64	0.62
1:B:900:MET:HG3	1:B:901:LEU:HD12	1.80	0.62
1:C:1034:ASN:HB2	1:C:1037:LEU:HB3	1.79	0.62
1:B:91:ALA:HB3	1:B:94:GLN:HG2	1.81	0.62
1:C:998:HIS:CD2	1:C:1021:LYS:HG2	2.34	0.62
1:C:1121:ILE:HD13	1:C:1139:VAL:HG12	1.80	0.62
1:A:686:MET:O	1:A:690:MET:HG3	2.00	0.61
1:C:924:ASN:HB2	1:C:926:LEU:HD22	1.82	0.61
1:C:728:GLU:OE1	1:C:762:ARG:NH2	2.32	0.61
1:A:747:LEU:HD22	1:A:752:CYS:HB3	1.82	0.61
1:B:1101:HIS:HE1	1:B:1161:HIS:HB3	1.65	0.61
1:D:1133:LYS:NZ	1:D:1151:SER:O	2.31	0.61
1:C:720:LEU:HD22	1:C:754:MET:HE1	1.83	0.61
1:A:360:LEU:HB3	1:A:362:LEU:HD23	1.83	0.60
1:D:607:TRP:HE1	1:D:627:LEU:HD13	1.67	0.60
1:B:609:GLY:HA3	1:B:644:ARG:HH12	1.67	0.60
1:D:1156:THR:OG1	1:D:1158:ARG:NH2	2.35	0.60
1:A:58:GLU:OE1	1:A:346:HIS:NE2	2.34	0.60
1:A:42:VAL:HG12	1:A:115:HIS:HB3	1.84	0.60
1:A:121:LEU:HD12	1:A:127:PHE:HB2	1.84	0.60
1:A:1075:GLN:NE2	1:A:1086:SER:OG	2.24	0.60
1:B:678:ASP:H	1:B:686:MET:HE1	1.66	0.60
1:A:77:ARG:NH2	1:B:1081:ASN:OD1	2.35	0.59
1:A:606:ASN:OD1	1:A:607:TRP:N	2.35	0.59
1:C:679:SER:HB3	1:C:909:PRO:HD2	1.83	0.59
1:A:338:GLU:OE2	1:A:406:ARG:NH1	2.34	0.59
1:B:330:GLN:O	1:B:333:HIS:ND1	2.34	0.59
1:B:566:MET:HE3	1:B:795:ASP:OD1	2.02	0.59
1:B:1117:PRO:HB3	1:B:1169:GLU:HA	1.85	0.59
1:A:1120:VAL:HG21	1:A:1162:VAL:HG11	1.84	0.59
1:A:194:LYS:HA	1:A:204:MET:HE1	1.85	0.59
1:A:201:GLY:O	1:A:204:MET:HG2	2.03	0.59
1:A:241:LYS:O	1:A:316:ARG:NH1	2.36	0.59
1:C:1040:GLN:C	1:C:1042:PRO:HD3	2.27	0.59
1:B:787:ALA:HA	1:B:791:ALA:HB3	1.84	0.58
1:A:377:ARG:HG3	1:A:425:LEU:HD13	1.85	0.58
1:A:1116:MET:HE3	1:A:1116:MET:HA	1.85	0.58
1:B:334:THR:O	1:B:337:GLU:HB3	2.02	0.58
1:C:505:GLY:HA2	1:C:508:MET:HE2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:864:ASN:HB3	1:D:866:ILE:HG13	1.85	0.58
1:B:728:GLU:OE1	1:B:762:ARG:NH2	2.36	0.58
1:B:590:ILE:HG22	1:B:594:VAL:HG23	1.85	0.58
1:C:926:LEU:HB2	1:C:930:GLU:OE2	2.03	0.58
1:A:406:ARG:HB3	1:A:430:ILE:CG2	2.34	0.58
1:C:590:ILE:HG22	1:C:594:VAL:HG23	1.86	0.58
1:C:1034:ASN:HB3	1:C:1036:ARG:HG3	1.85	0.58
1:A:855:LYS:HD2	1:D:851:THR:HG21	1.86	0.58
1:B:438:THR:O	1:B:442:LYS:HG3	2.04	0.58
1:C:501:LEU:HD22	1:C:1078:PHE:CD2	2.38	0.58
1:A:1135:GLN:HE22	1:A:1137:LEU:HB3	1.69	0.58
1:D:907:VAL:HG12	1:D:908:THR:H	1.67	0.58
1:A:164:VAL:HG11	1:A:298:LEU:HD12	1.86	0.57
1:C:787:ALA:HA	1:C:791:ALA:HB3	1.86	0.57
1:A:849:ASP:OD2	1:A:852:ALA:N	2.37	0.57
1:B:382:ASP:OD2	1:B:385:ARG:NH1	2.36	0.57
1:D:761:ASP:OD1	1:D:762:ARG:N	2.38	0.57
1:C:498:GLN:HG2	1:C:1085:ARG:NH1	2.18	0.57
1:B:1133:LYS:HG3	1:B:1154:GLU:HB2	1.87	0.57
4:B:2001:ACO:OAP	4:B:2001:ACO:O1A	2.23	0.57
1:D:641:MET:HB2	1:D:671:MET:HE3	1.86	0.57
1:D:1015:ASP:O	1:D:1019:HIS:ND1	2.38	0.57
1:B:930:GLU:OE1	1:B:934:GLN:NE2	2.35	0.57
1:A:224:ALA:HA	1:A:228:PHE:HD2	1.70	0.57
1:A:380:THR:HG22	1:A:390:ASP:HB3	1.87	0.56
1:B:908:THR:HG23	1:B:909:PRO:HG3	1.87	0.56
1:A:407:LEU:N	1:B:401:GLU:OE2	2.37	0.56
1:D:501:LEU:HD11	1:D:1060:ILE:HG21	1.87	0.56
1:C:959:PHE:CE2	1:C:964:ARG:HD2	2.41	0.56
1:D:908:THR:CG2	1:D:909:PRO:CD	2.76	0.56
1:B:935:ALA:HB3	1:B:966:LYS:HE3	1.87	0.56
1:C:844:LEU:CD2	1:C:1036:ARG:HB3	2.35	0.56
1:B:783:MET:HE2	1:B:783:MET:HA	1.86	0.56
1:B:124:ARG:NH2	1:B:126:ASP:OD2	2.38	0.56
1:A:45:ARG:NE	1:A:71:ASP:OD2	2.35	0.55
1:C:542:ARG:CZ	1:C:631:ARG:HH22	2.18	0.55
1:A:927:SER:OG	1:A:930:GLU:OE1	2.21	0.55
1:C:1040:GLN:O	1:C:1042:PRO:HD3	2.06	0.55
1:C:1121:ILE:HD11	1:C:1141:SER:HB3	1.87	0.55
1:A:640:GLN:HE21	1:A:675:ARG:HB2	1.69	0.55
1:A:644:ARG:HE	1:A:908:THR:CG2	2.11	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1160:VAL:HG12	1:A:1175:LEU:HG	1.86	0.55
1:B:586:ASP:OD2	1:B:845:TYR:OH	2.24	0.55
1:B:741:LYS:HD2	1:B:771:HIS:CD2	2.41	0.55
1:B:641:MET:HE3	1:B:671:MET:SD	2.46	0.55
1:C:1125:VAL:HG11	1:C:1157:VAL:HG11	1.87	0.55
1:A:126:ASP:OD1	1:A:127:PHE:N	2.39	0.55
1:B:942:ARG:NH2	1:D:1146:GLU:OE1	2.39	0.55
1:B:959:PHE:HE2	1:B:964:ARG:HH11	1.53	0.55
1:C:1116:MET:HE3	1:C:1116:MET:HA	1.89	0.55
1:D:607:TRP:HZ2	1:D:627:LEU:HB2	1.72	0.55
1:B:864:ASN:HB3	1:B:866:ILE:HD12	1.88	0.54
1:D:832:PHE:O	1:D:836:GLU:HG2	2.07	0.54
1:A:385:ARG:HG3	1:A:386:SER:H	1.71	0.54
1:D:571:ARG:HD3	1:D:608:GLY:HA3	1.88	0.54
1:A:761:ASP:OD1	1:A:762:ARG:N	2.40	0.54
1:C:935:ALA:HB3	1:C:966:LYS:HE3	1.89	0.54
1:D:507:VAL:O	1:D:508:MET:C	2.49	0.54
1:A:817:THR:HG21	1:A:822:LEU:HD12	1.90	0.54
1:A:1015:ASP:OD1	1:A:1015:ASP:N	2.40	0.54
1:C:498:GLN:HG2	1:C:1085:ARG:HH11	1.72	0.54
1:B:547:ARG:NH1	1:B:548:GLU:OE2	2.40	0.54
1:A:1133:LYS:HG3	1:C:969:LYS:HZ1	1.73	0.54
1:C:1070:ARG:HA	1:C:1070:ARG:NH1	2.22	0.54
1:C:1069:ASN:O	1:C:1070:ARG:HD2	2.09	0.53
1:A:817:THR:HG22	1:A:823:ASP:HA	1.91	0.53
1:C:574:HIS:CE1	1:C:582:VAL:HB	2.44	0.53
1:B:209:SER:O	1:B:213:LEU:N	2.42	0.53
1:B:1069:ASN:OD1	1:B:1070:ARG:N	2.35	0.53
1:C:644:ARG:HB2	1:C:647:ASN:O	2.09	0.53
1:A:192:ILE:HB	1:A:206:VAL:HG22	1.90	0.53
1:B:567:ASP:HB3	1:B:604:MET:SD	2.48	0.53
1:C:998:HIS:HD2	1:C:1021:LYS:HG2	1.74	0.53
1:A:995:VAL:HG23	1:A:1000:GLU:HA	1.89	0.53
1:C:606:ASN:OD1	1:C:607:TRP:N	2.38	0.53
1:A:646:ALA:HB3	1:A:653:ASN:HD22	1.73	0.53
1:C:900:MET:HA	1:C:928:ARG:HH21	1.74	0.53
1:A:881:MET:HE1	1:A:883:LEU:HD12	1.90	0.53
1:A:390:ASP:OD1	1:A:391:THR:N	2.40	0.53
1:C:1003:THR:OG1	1:C:1006:ASP:OD2	2.25	0.52
1:A:43:ALA:HA	1:A:66:ILE:HD11	1.90	0.52
1:B:282:HIS:O	1:B:282:HIS:ND1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:890:VAL:HG22	1:B:922:VAL:HG11	1.90	0.52
1:D:919:GLN:HA	1:D:922:VAL:HG12	1.91	0.52
1:B:743:MET:SD	1:B:743:MET:N	2.80	0.52
1:C:631:ARG:HD2	1:C:639:PHE:HE2	1.73	0.52
1:B:629:GLU:O	1:B:633:LEU:HD23	2.10	0.52
1:B:959:PHE:CE2	1:B:964:ARG:HD2	2.45	0.52
1:C:501:LEU:HD22	1:C:1078:PHE:CD1	2.43	0.52
1:A:900:MET:HA	1:A:900:MET:HE2	1.91	0.52
1:B:343:ASP:OD2	1:B:346:HIS:ND1	2.36	0.52
1:C:501:LEU:HD13	1:C:1078:PHE:HB2	1.92	0.52
1:C:1107:ASP:OD1	1:C:1108:VAL:N	2.43	0.52
1:D:1135:GLN:HE22	1:D:1137:LEU:HB3	1.73	0.52
1:A:197:TYR:O	1:A:202:ARG:NH1	2.42	0.52
1:D:677:PHE:HB3	1:D:703:ALA:HB3	1.92	0.52
1:B:641:MET:HB2	1:B:671:MET:SD	2.50	0.52
1:D:679:SER:HB3	1:D:909:PRO:HD2	1.92	0.52
1:B:149:MET:HE2	1:B:149:MET:N	2.25	0.52
1:D:506:HIS:HA	1:D:1089:VAL:HG13	1.92	0.52
1:B:574:HIS:HB3	1:B:580:THR:HA	1.92	0.51
1:B:616:MET:HE2	1:B:616:MET:HA	1.92	0.51
1:C:1013:TYR:HB3	1:C:1016:VAL:HG22	1.90	0.51
1:D:743:MET:SD	1:D:743:MET:N	2.82	0.51
1:C:616:MET:HE3	1:C:616:MET:HA	1.91	0.51
1:D:769:HIS:NE2	1:D:795:ASP:OD1	2.41	0.51
1:B:385:ARG:HG3	1:B:386:SER:H	1.75	0.51
1:B:1012:MET:HE3	1:B:1012:MET:HA	1.92	0.51
2:B:2002:BTI:H102	1:D:613:ASP:OD2	2.11	0.51
1:D:900:MET:SD	1:D:901:LEU:HG	2.51	0.51
1:D:907:VAL:HG12	1:D:908:THR:N	2.26	0.51
1:B:263:ARG:NH1	1:B:336:THR:OG1	2.40	0.51
1:B:393:ARG:HH22	1:B:1086:SER:HB2	1.76	0.51
1:B:888:LYS:HA	1:B:891:LYS:HZ3	1.74	0.51
1:C:731:VAL:HG11	1:C:763:PHE:CE1	2.46	0.51
1:B:402:GLY:H	1:B:405:ILE:HB	1.76	0.51
1:D:1158:ARG:HH12	1:D:1178:GLU:HB2	1.76	0.51
1:A:40:VAL:HG22	1:A:113:ALA:HB3	1.93	0.50
1:B:395:GLU:OE1	1:B:454:GLY:HA3	2.11	0.50
1:B:1070:ARG:NH1	1:B:1070:ARG:HA	2.24	0.50
1:A:575:GLN:HA	1:A:580:THR:HB	1.93	0.50
1:B:644:ARG:HE	1:B:908:THR:HG21	1.75	0.50
1:C:583:ARG:HH21	1:C:1031:ASP:HA	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:LEU:HD22	1:B:323:ILE:HD11	1.93	0.50
1:B:552:GLY:HA2	1:B:555:ARG:HE	1.76	0.50
1:A:907:VAL:HG12	1:A:908:THR:N	2.25	0.50
1:D:604:MET:HE2	1:D:604:MET:HA	1.94	0.50
1:A:680:LEU:O	1:A:682:TYR:N	2.43	0.50
1:A:1053:GLU:OE1	1:A:1056:LYS:HG3	2.12	0.50
1:A:1058:LEU:HD21	4:A:1203:ACO:H1B	1.94	0.50
1:B:51:ARG:NH2	1:B:343:ASP:OD1	2.44	0.50
1:A:374:ILE:O	1:A:430:ILE:HD12	2.12	0.49
1:C:680:LEU:HA	1:C:905:ILE:HD11	1.94	0.49
1:A:936:GLU:HB3	1:A:969:LYS:HZ1	1.77	0.49
1:A:239:ILE:H	3:A:1202:ANP:HN62	1.59	0.49
1:A:724:MET:HE2	1:A:762:ARG:HH11	1.76	0.49
1:A:951:TYR:O	1:A:978:PRO:HG2	2.12	0.49
1:D:636:ASN:OD1	1:D:637:ILE:HD12	2.12	0.49
1:D:1006:ASP:OD1	1:D:1007:VAL:N	2.46	0.49
1:A:465:VAL:HG22	1:A:487:LEU:HD23	1.95	0.49
1:B:465:VAL:HG22	1:B:487:LEU:HD21	1.94	0.49
1:D:724:MET:HE3	1:D:724:MET:HA	1.94	0.49
1:C:580:THR:HG22	1:C:614:VAL:HG11	1.94	0.49
1:B:378:VAL:HG13	1:B:426:LEU:HB2	1.94	0.49
1:B:827:PRO:HD2	1:B:830:ARG:HH21	1.78	0.49
1:A:285:PRO:O	1:A:288:ARG:HG3	2.11	0.49
1:A:970:ASP:OD1	1:A:970:ASP:N	2.45	0.49
1:B:94:GLN:HA	1:B:97:LEU:HD12	1.95	0.49
1:B:740:ILE:HB	1:B:770:ILE:HD12	1.95	0.49
1:A:87:GLY:HA2	1:A:90:LEU:HD13	1.95	0.49
1:B:267:ILE:HD13	1:B:476:VAL:HG11	1.95	0.49
1:C:530:PRO:HB2	1:C:593:TYR:CE2	2.48	0.49
1:A:243:ARG:O	1:A:314:VAL:N	2.41	0.49
1:C:584:THR:OG1	1:C:621:GLU:OE1	2.21	0.49
1:C:844:LEU:HD22	1:C:1036:ARG:HA	1.95	0.49
1:C:731:VAL:HG11	1:C:763:PHE:HE1	1.79	0.48
1:C:908:THR:HB	1:C:909:PRO:HD3	1.94	0.48
1:C:1022:ASP:OD1	1:C:1023:PHE:N	2.47	0.48
1:B:543:ASP:OD1	1:B:544:ILE:N	2.46	0.48
1:B:310:VAL:HG22	1:B:325:VAL:HG22	1.94	0.48
1:A:400:GLY:H	1:A:450:PHE:HE1	1.61	0.48
1:A:504:LEU:HD23	1:A:1042:PRO:HG3	1.95	0.48
4:A:1203:ACO:H2A	1:B:77:ARG:HH12	1.78	0.48
1:B:680:LEU:HD13	1:B:955:PRO:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:921:MET:HE1	1:C:927:SER:C	2.37	0.48
1:D:1095:MET:O	1:D:1096:LYS:HE2	2.13	0.48
1:A:91:ALA:HB3	1:A:94:GLN:HB2	1.95	0.48
1:A:265:CYS:SG	1:A:276:GLU:HG3	2.53	0.48
1:A:97:LEU:HA	1:A:121:LEU:HD21	1.95	0.48
1:D:543:ASP:OD1	1:D:544:ILE:N	2.46	0.48
1:B:278:ALA:HB2	1:B:335:VAL:HG12	1.94	0.48
1:B:987:LEU:H	1:B:987:LEU:HD23	1.79	0.48
1:C:796:VAL:HG11	1:C:810:MET:HA	1.95	0.48
1:B:41:MET:HE3	1:B:114:VAL:HG12	1.94	0.48
1:B:313:LEU:O	1:B:321:TYR:N	2.43	0.48
1:B:540:GLY:N	1:B:636:ASN:OD1	2.46	0.48
1:B:644:ARG:CD	1:B:908:THR:HG21	2.44	0.48
1:B:285:PRO:HA	1:B:288:ARG:HG2	1.96	0.47
1:C:567:ASP:HB2	1:C:601:LEU:HD11	1.96	0.47
1:A:384:ALA:HB2	1:A:491:ARG:HH12	1.79	0.47
1:A:746:LEU:HD11	1:A:865:GLU:HG2	1.95	0.47
1:B:701:GLU:HG3	1:B:737:ILE:HB	1.96	0.47
1:C:1069:ASN:OD1	1:C:1070:ARG:N	2.39	0.47
1:A:613:ASP:OD2	2:C:1900:BTI:H102	2.13	0.47
1:A:265:CYS:SG	1:A:273:LYS:HD2	2.54	0.47
1:A:1133:LYS:HG3	1:C:969:LYS:NZ	2.28	0.47
1:B:679:SER:HB3	1:B:909:PRO:HD2	1.95	0.47
1:C:1033:LEU:HD23	1:C:1033:LEU:H	1.78	0.47
1:A:77:ARG:O	4:B:2001:ACO:N6A	2.47	0.47
1:A:1038:PHE:HD2	1:A:1039:LEU:HD12	1.80	0.47
1:D:1130:LYS:HD2	1:D:1155:GLY:O	2.15	0.47
1:A:494:GLN:NE2	1:A:496:ARG:HE	2.13	0.47
1:A:570:PHE:O	1:A:574:HIS:NE2	2.46	0.47
1:B:574:HIS:CE1	1:B:582:VAL:HB	2.49	0.47
1:C:1112:ILE:HD12	1:C:1175:LEU:HD21	1.96	0.47
1:B:624:TRP:NE1	1:B:1009:SER:OG	2.41	0.47
1:A:607:TRP:CE3	1:A:641:MET:HE2	2.50	0.47
1:A:1129:ALA:H	1:A:1157:VAL:HG22	1.80	0.47
1:C:609:GLY:HA2	1:C:649:VAL:HG13	1.97	0.47
1:A:178:HIS:NE2	1:A:182:GLU:OE2	2.48	0.47
1:C:571:ARG:HG3	1:C:607:TRP:O	2.15	0.47
1:D:644:ARG:HE	1:D:908:THR:CG2	2.20	0.47
1:D:771:HIS:ND1	1:D:795:ASP:OD2	2.40	0.47
1:D:1038:PHE:HD2	1:D:1039:LEU:HD12	1.80	0.47
1:A:205:ARG:HD2	1:A:219:ARG:NH2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:ARG:HD2	1:A:1052:LEU:HD21	1.95	0.46
1:A:278:ALA:HB3	1:A:279:PRO:HD3	1.96	0.46
1:B:99:ILE:O	1:B:103:ILE:HG12	2.15	0.46
1:D:987:LEU:H	1:D:987:LEU:HD23	1.80	0.46
1:A:677:PHE:HE2	1:A:907:VAL:HG11	1.80	0.46
1:B:504:LEU:HD22	1:B:1042:PRO:HD3	1.98	0.46
1:B:581:ARG:HG2	1:B:848:PHE:CE2	2.51	0.46
1:B:599:SER:HA	1:B:637:ILE:HD11	1.96	0.46
1:A:269:ARG:HG2	1:A:270:ARG:NH1	2.30	0.46
1:A:494:GLN:OE1	1:A:496:ARG:HG3	2.15	0.46
1:A:524:PRO:HA	1:A:1036:ARG:HH12	1.79	0.46
1:B:116:PRO:HD2	1:B:117:GLY:H	1.80	0.46
1:B:447:LEU:HD22	1:B:459:ILE:HD12	1.97	0.46
1:B:1128:GLY:H	1:B:1157:VAL:HG13	1.79	0.46
1:C:896:GLU:OE1	1:C:896:GLU:N	2.46	0.46
1:D:909:PRO:O	1:D:913:ILE:HG12	2.15	0.46
1:C:742:ASP:OD2	1:C:747:LEU:HB2	2.15	0.46
1:A:490:LEU:C	1:A:491:ARG:HD3	2.41	0.46
1:A:1098:MET:SD	1:A:1099:HIS:N	2.89	0.46
1:A:440:ALA:O	1:A:466:LEU:HD11	2.16	0.46
1:A:907:VAL:O	1:A:911:SER:N	2.28	0.46
1:B:817:THR:HG21	1:B:822:LEU:HB2	1.97	0.46
1:C:680:LEU:HD13	1:C:955:PRO:HA	1.98	0.46
1:D:662:PHE:HA	1:D:1008:LEU:HD21	1.98	0.46
1:A:604:MET:O	1:A:640:GLN:N	2.48	0.46
1:A:1001:GLU:CD	1:A:1001:GLU:H	2.24	0.46
1:B:569:THR:HG21	1:B:834:TYR:OH	2.16	0.46
1:B:852:ALA:HA	1:B:855:LYS:NZ	2.30	0.46
1:D:1162:VAL:HG13	1:D:1166:MET:HE2	1.97	0.46
1:B:852:ALA:HA	1:B:855:LYS:HZ2	1.81	0.46
1:B:671:MET:HG2	1:B:674:PHE:CZ	2.51	0.46
1:B:1036:ARG:HG3	1:B:1037:LEU:N	2.31	0.46
1:D:607:TRP:CZ2	1:D:627:LEU:HB2	2.49	0.46
1:A:443:MET:O	1:A:447:LEU:HG	2.17	0.45
1:A:724:MET:HE2	1:A:762:ARG:NH1	2.31	0.45
1:B:243:ARG:O	1:B:314:VAL:HG12	2.16	0.45
1:D:1096:LYS:HB2	1:D:1098:MET:HE3	1.98	0.45
1:A:100:PRO:C	1:A:104:LYS:HZ2	2.24	0.45
1:A:277:ILE:HG13	1:A:279:PRO:HD2	1.98	0.45
1:B:571:ARG:NE	1:B:605:GLU:OE2	2.31	0.45
1:B:731:VAL:HG11	1:B:763:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:907:VAL:CG1	1:D:908:THR:H	2.29	0.45
1:B:192:ILE:HG12	1:B:238:PHE:HB2	1.99	0.45
1:B:571:ARG:HH11	1:B:575:GLN:HE22	1.64	0.45
1:B:760:ARG:NH2	1:B:790:GLY:O	2.50	0.45
1:A:176:SER:HB2	1:A:179:GLU:HG2	1.98	0.45
1:A:207:VAL:HG11	1:A:213:LEU:HD13	1.98	0.45
1:A:571:ARG:HG3	1:A:607:TRP:O	2.17	0.45
1:B:1133:LYS:HG2	1:B:1153:MET:HA	1.97	0.45
1:D:743:MET:HE2	1:D:907:VAL:HG22	1.97	0.45
1:A:380:THR:HG22	1:A:380:THR:O	2.17	0.45
1:B:906:LYS:HA	1:B:910:SER:OG	2.17	0.45
1:C:804:MET:HE3	1:C:804:MET:HB3	1.91	0.45
1:A:253:GLN:HE22	1:A:354:GLY:HA2	1.81	0.45
1:C:856:SER:OG	1:C:857:GLY:N	2.50	0.45
1:B:390:ASP:OD1	1:B:391:THR:N	2.50	0.45
1:D:1058:LEU:H	1:D:1058:LEU:HG	1.59	0.45
1:A:496:ARG:HD3	1:A:1052:LEU:HD11	1.99	0.45
1:A:523:SER:O	1:A:1036:ARG:NH1	2.48	0.45
1:B:1013:TYR:HB2	1:B:1016:VAL:HG12	1.98	0.45
1:D:760:ARG:NH1	1:D:766:LEU:O	2.50	0.45
1:D:921:MET:O	1:D:925:GLY:N	2.50	0.45
1:D:801:MET:HE3	1:D:801:MET:HB3	1.89	0.44
1:A:380:THR:O	1:A:390:ASP:N	2.36	0.44
1:A:571:ARG:HD3	1:A:608:GLY:HA3	1.99	0.44
1:A:883:LEU:HD22	1:A:886:LYS:HD2	1.98	0.44
1:C:508:MET:HE2	1:C:508:MET:HB2	1.79	0.44
1:C:543:ASP:OD1	1:C:544:ILE:N	2.49	0.44
1:C:603:SER:OG	1:C:640:GLN:OE1	2.34	0.44
1:A:850:CYS:HB3	1:A:872:THR:HG22	1.99	0.44
1:D:574:HIS:HB3	1:D:580:THR:HA	2.00	0.44
1:D:1160:VAL:HG12	1:D:1175:LEU:HB3	1.98	0.44
1:A:177:LEU:HB2	1:A:217:TYR:CE2	2.52	0.44
1:A:583:ARG:HH21	1:A:1031:ASP:HA	1.82	0.44
1:A:1115:PRO:HB2	1:C:920:PHE:HE1	1.81	0.44
1:A:1119:LYS:NZ	1:A:1120:VAL:O	2.51	0.44
1:B:1119:LYS:HG3	1:B:1167:THR:HG22	1.98	0.44
1:C:1068:LEU:HD22	1:C:1072:GLY:HA2	1.98	0.44
1:C:754:MET:SD	1:C:755:LEU:N	2.91	0.44
1:C:833:ASP:OD1	1:C:834:TYR:N	2.51	0.44
1:A:408:ASP:HB2	1:A:428:LYS:HE2	2.00	0.44
1:B:69:GLU:HG2	1:B:70:GLN:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:CYS:SG	1:B:136:VAL:HG13	2.57	0.44
1:B:279:PRO:HG2	1:B:372:CYS:HA	2.00	0.44
1:B:567:ASP:HA	1:B:796:VAL:O	2.18	0.44
1:B:680:LEU:HA	1:B:905:ILE:HD11	1.99	0.44
1:B:849:ASP:OD1	1:B:850:CYS:N	2.51	0.44
1:C:498:GLN:HE22	1:C:1087:ILE:HD13	1.83	0.44
1:C:502:HIS:HA	1:C:1087:ILE:HG12	1.99	0.44
1:D:500:LEU:HD22	1:D:1052:LEU:HD22	2.00	0.44
1:D:1043:LYS:HB2	1:D:1043:LYS:HE2	1.38	0.43
1:A:406:ARG:HD2	1:B:403:MET:O	2.17	0.43
1:A:908:THR:HG23	1:A:909:PRO:N	2.27	0.43
1:B:961:GLU:HG2	1:B:962:PRO:HD3	2.00	0.43
1:D:918:ALA:HA	1:D:921:MET:HE2	2.00	0.43
1:A:633:LEU:O	1:A:634:ILE:HD13	2.18	0.43
1:A:820:THR:HG22	1:A:822:LEU:H	1.83	0.43
1:A:436:HIS:HB3	1:A:437:PRO:HD3	2.01	0.43
1:B:677:PHE:HB2	1:B:703:ALA:HB3	1.99	0.43
1:C:650:GLY:HA2	1:C:1013:TYR:OH	2.18	0.43
1:C:1138:CYS:SG	1:C:1139:VAL:N	2.92	0.43
1:D:506:HIS:HA	1:D:1089:VAL:CG1	2.49	0.43
1:D:961:GLU:HG2	1:D:962:PRO:HD3	2.00	0.43
1:A:403:MET:HB2	1:A:442:LYS:HE2	2.00	0.43
1:A:921:MET:HE1	1:A:927:SER:C	2.43	0.43
1:B:824:THR:HG22	1:B:826:VAL:HG23	2.00	0.43
1:C:686:MET:SD	1:C:730:LEU:HD21	2.59	0.43
1:D:644:ARG:HB2	1:D:647:ASN:O	2.18	0.43
1:A:494:GLN:HB3	4:A:1203:ACO:O5A	2.18	0.43
1:B:897:ALA:HA	1:B:900:MET:HE3	2.00	0.43
2:B:2002:BTI:N3	1:D:908:THR:OG1	2.51	0.43
1:D:533:PRO:HG2	1:D:596:HIS:CD2	2.53	0.43
1:A:66:ILE:HD12	1:A:86:ILE:HD13	2.01	0.43
1:A:241:LYS:HB3	1:A:316:ARG:HH11	1.84	0.43
1:B:280:ALA:HB1	1:B:283:LEU:HD23	2.00	0.43
1:C:574:HIS:HB3	1:C:580:THR:HA	2.01	0.43
1:C:624:TRP:NE1	1:C:1009:SER:OG	2.42	0.43
1:D:614:VAL:HG23	1:D:618:PHE:HD2	1.83	0.43
1:D:616:MET:HE2	1:D:616:MET:HA	2.01	0.43
1:B:126:ASP:O	1:B:129:GLN:HG3	2.19	0.43
1:B:330:GLN:HG3	1:B:332:GLU:OE1	2.19	0.43
1:B:678:ASP:N	1:B:686:MET:HE1	2.33	0.43
1:A:41:MET:O	1:A:114:VAL:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:PHE:HB2	1:B:190:PRO:HD3	2.00	0.43
2:C:1900:BTI:HN2	2:C:1900:BTI:H73	1.70	0.43
1:D:585:HIS:O	1:D:589:LYS:HG2	2.19	0.43
1:D:775:THR:HA	1:D:804:MET:O	2.19	0.43
1:A:428:LYS:HE2	1:A:428:LYS:HB3	1.67	0.43
1:A:859:SER:O	1:A:860:ASP:HB2	2.19	0.43
4:A:1203:ACO:HH33	1:B:79:LYS:HG3	2.00	0.43
1:B:545:LEU:HD23	1:B:545:LEU:HA	1.81	0.43
1:B:1143:MET:SD	1:B:1144:LYS:HE3	2.59	0.43
1:D:854:MET:SD	1:D:871:TYR:HE2	2.42	0.43
1:B:126:ASP:OD1	1:B:126:ASP:N	2.50	0.42
1:C:775:THR:HA	1:C:804:MET:O	2.19	0.42
1:C:1121:ILE:HD11	1:C:1141:SER:CB	2.49	0.42
1:A:278:ALA:HB2	1:A:335:VAL:HB	2.01	0.42
1:A:309:THR:O	1:A:326:ASN:N	2.47	0.42
1:C:501:LEU:CD2	1:C:1078:PHE:CG	2.95	0.42
1:C:687:LEU:HA	1:C:690:MET:CE	2.49	0.42
1:C:1133:LYS:H	1:C:1154:GLU:CD	2.27	0.42
1:D:608:GLY:HA2	1:D:642:LEU:HB3	2.01	0.42
1:A:381:GLU:HA	1:A:389:PRO:HA	2.01	0.42
1:A:1063:LEU:HD21	1:A:1079:GLU:HB2	2.01	0.42
1:B:583:ARG:NH2	1:B:1031:ASP:HA	2.35	0.42
1:B:1070:ARG:HA	1:B:1070:ARG:HH11	1.84	0.42
1:C:1153:MET:SD	1:C:1177:ILE:HG21	2.59	0.42
1:A:849:ASP:OD1	1:D:855:LYS:HE3	2.19	0.42
1:A:852:ALA:O	1:A:855:LYS:NZ	2.52	0.42
1:D:619:LEU:HB3	1:D:621:GLU:OE1	2.19	0.42
1:A:1130:LYS:HD2	1:A:1155:GLY:O	2.18	0.42
2:B:2002:BTI:HN2	2:B:2002:BTI:H73	1.74	0.42
1:C:827:PRO:HD2	1:C:830:ARG:HH21	1.84	0.42
1:D:616:MET:HB3	1:D:1016:VAL:HG11	2.01	0.42
1:D:726:LEU:O	1:D:730:LEU:HD23	2.19	0.42
1:A:524:PRO:HA	1:A:1036:ARG:NH1	2.35	0.42
1:B:323:ILE:HG22	1:B:324:GLU:HG2	2.01	0.42
1:B:457:THR:OG1	1:B:458:ASN:N	2.53	0.42
1:C:870:GLN:O	1:C:870:GLN:HG2	2.19	0.42
1:A:312:PHE:HE1	1:A:322:PHE:HD1	1.66	0.42
1:A:376:CYS:SG	1:A:443:MET:HE3	2.59	0.42
1:A:908:THR:OG1	2:C:1900:BTI:H63	2.18	0.42
1:B:1131:VAL:HG11	1:B:1137:LEU:HD21	2.02	0.42
1:C:783:MET:HE2	1:C:783:MET:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:GLY:N	1:A:677:PHE:O	2.53	0.42
1:A:1030:LEU:HD23	1:A:1030:LEU:HA	1.86	0.42
1:B:280:ALA:HB1	1:B:283:LEU:HB2	2.01	0.42
1:B:315:ASP:OD1	1:B:316:ARG:NH1	2.53	0.42
1:B:677:PHE:HZ	1:B:705:SER:HB3	1.84	0.42
1:B:771:HIS:HE1	1:B:807:GLN:NE2	2.17	0.42
1:C:959:PHE:HE2	1:C:964:ARG:HD2	1.83	0.42
1:B:104:LYS:HG2	1:B:107:LYS:HZ2	1.84	0.41
2:B:2002:BTI:H103	2:B:2002:BTI:H72	1.73	0.41
1:D:1096:LYS:HB2	1:D:1098:MET:CE	2.50	0.41
1:D:497:ALA:HA	1:D:1052:LEU:HD21	2.02	0.41
1:D:930:GLU:OE1	1:D:930:GLU:N	2.51	0.41
1:A:363:ARG:HB2	1:A:366:ASN:HB2	2.02	0.41
1:A:196:ALA:O	1:A:202:ARG:NH2	2.53	0.41
1:A:290:ARG:NH2	1:A:294:ASP:OD1	2.53	0.41
1:A:871:TYR:OH	1:A:891:LYS:NZ	2.39	0.41
1:B:1049:GLU:OE1	1:B:1059:HIS:NE2	2.54	0.41
1:C:566:MET:HG3	1:C:603:SER:O	2.21	0.41
1:A:631:ARG:NH2	1:A:634:ILE:O	2.45	0.41
1:A:1047:GLU:OE1	1:A:1060:ILE:N	2.53	0.41
1:B:644:ARG:HD3	1:B:908:THR:HG21	2.01	0.41
1:C:585:HIS:CD2	1:C:1034:ASN:HA	2.56	0.41
1:D:725:GLY:O	1:D:729:GLU:OE1	2.39	0.41
1:A:401:GLU:HG3	1:B:407:LEU:O	2.20	0.41
1:B:614:VAL:HG23	1:B:618:PHE:HD2	1.86	0.41
1:B:731:VAL:HG11	1:B:763:PHE:HE1	1.85	0.41
1:B:863:GLU:OE1	1:B:863:GLU:N	2.53	0.41
1:C:501:LEU:HD23	1:C:501:LEU:HA	1.81	0.41
1:D:1107:ASP:OD1	1:D:1108:VAL:N	2.54	0.41
1:B:373:ALA:HA	1:B:431:ALA:O	2.20	0.41
1:D:595:ALA:HB2	1:D:634:ILE:HD13	2.03	0.41
1:A:248:GLN:NE2	1:A:263:ARG:HH12	2.19	0.41
1:A:435:ASP:CG	1:A:437:PRO:HD2	2.46	0.41
1:B:123:GLU:OE2	1:B:328:ARG:HD3	2.21	0.41
1:B:566:MET:HG2	1:B:603:SER:O	2.21	0.41
1:B:680:LEU:HA	1:B:680:LEU:HD23	1.88	0.41
1:C:724:MET:HE1	1:C:759:LEU:HA	2.03	0.41
1:D:1050:VAL:HG12	1:D:1052:LEU:H	1.86	0.41
1:A:350:HIS:O	1:A:353:GLU:HB3	2.20	0.41
1:B:644:ARG:HB2	1:B:647:ASN:O	2.21	0.41
1:B:775:THR:HA	1:B:804:MET:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:520:ALA:HB3	1:C:847:ALA:HA	2.01	0.41
1:C:640:GLN:NE2	1:C:675:ARG:HD2	2.29	0.41
1:D:499:LYS:HB3	1:D:499:LYS:HE3	1.58	0.41
1:A:253:GLN:NE2	1:A:354:GLY:HA2	2.36	0.41
1:A:335:VAL:HG12	1:A:430:ILE:HD11	2.01	0.41
1:A:375:GLN:HE21	1:A:430:ILE:HD13	1.86	0.41
1:B:53:PHE:CE2	1:B:80:ALA:HB2	2.56	0.41
1:B:116:PRO:HD2	1:B:117:GLY:N	2.35	0.41
1:B:640:GLN:HE21	1:B:675:ARG:CG	2.34	0.41
1:B:817:THR:CG2	1:B:822:LEU:HB2	2.51	0.41
1:B:897:ALA:HA	1:B:900:MET:HG2	2.03	0.41
1:C:859:SER:OG	1:C:860:ASP:N	2.51	0.41
1:D:621:GLU:HG3	1:D:1031:ASP:HB2	2.03	0.41
1:A:609:GLY:HA3	1:A:644:ARG:HH12	1.85	0.40
1:A:1135:GLN:HE21	1:A:1151:SER:HB2	1.85	0.40
1:D:579:ALA:O	1:D:581:ARG:HD2	2.21	0.40
1:D:1120:VAL:HG21	1:D:1162:VAL:HG11	2.02	0.40
1:A:335:VAL:O	1:A:339:ILE:HG12	2.22	0.40
1:C:498:GLN:HE22	1:C:1087:ILE:CD1	2.33	0.40
1:C:1095:MET:HB3	1:C:1097:GLU:OE1	2.21	0.40
1:D:907:VAL:O	1:D:911:SER:N	2.30	0.40
1:A:901:LEU:HD11	1:A:948:LEU:HD21	2.03	0.40
1:A:1119:LYS:NZ	1:A:1121:ILE:HD13	2.37	0.40
1:A:1119:LYS:HE3	1:A:1119:LYS:HB3	1.95	0.40
1:B:278:ALA:HB3	1:B:279:PRO:HD3	2.03	0.40
1:B:573:ALA:HA	1:B:576:SER:OG	2.21	0.40
1:B:771:HIS:CE1	1:B:807:GLN:NE2	2.89	0.40
1:C:772:THR:HG21	1:C:783:MET:HE3	2.02	0.40
1:C:991:GLU:O	1:C:995:VAL:HG23	2.21	0.40
1:A:88:ARG:NH1	1:A:88:ARG:HB2	2.36	0.40
1:A:434:LYS:HE2	1:A:434:LYS:HB3	1.85	0.40
1:B:309:THR:OG1	1:B:326:ASN:HB2	2.21	0.40
1:C:534:ILE:HD13	1:C:534:ILE:HA	1.93	0.40
1:C:686:MET:O	1:C:690:MET:HG3	2.21	0.40
1:C:942:ARG:HD2	1:C:946:GLU:HG2	2.03	0.40
1:A:798:ALA:O	1:A:802:SER:HB3	2.22	0.40
1:A:1132:ALA:HA	1:A:1154:GLU:CD	2.47	0.40
1:B:447:LEU:HD23	1:B:447:LEU:HA	1.89	0.40
1:B:859:SER:OG	1:B:860:ASP:N	2.54	0.40
1:C:903:ASP:OD1	1:C:903:ASP:N	2.54	0.40
1:C:961:GLU:HG2	1:C:962:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:701:GLU:OE2	1:D:739:CYS: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	1144/1178 (97%)	1067 (93%)	76 (7%)	1 (0%)	48	78
1	B	1145/1178 (97%)	1067 (93%)	77 (7%)	1 (0%)	48	78
1	C	682/1178 (58%)	614 (90%)	64 (9%)	4 (1%)	21	52
1	D	682/1178 (58%)	645 (95%)	35 (5%)	2 (0%)	36	65
All	All	3653/4712 (78%)	3393 (93%)	252 (7%)	8 (0%)	44	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1095	MET
1	C	1042	PRO
1	A	495	ASN
1	C	908	THR
1	D	1099	HIS
1	C	533	PRO
1	C	1041	GLY
1	B	804	MET

5.3.2 Protein sidechains [i](#)

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	942/968 (97%)	942 (100%)	0	100	100
1	B	943/968 (97%)	942 (100%)	1 (0%)	88	88
1	C	564/968 (58%)	537 (95%)	27 (5%)	23	48
1	D	564/968 (58%)	539 (96%)	25 (4%)	25	50
All	All	3013/3872 (78%)	2960 (98%)	53 (2%)	51	67

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1144	LYS
1	C	496	ARG
1	C	498	GLN
1	C	500	LEU
1	C	502	HIS
1	C	506	HIS
1	C	508	MET
1	C	513	THR
1	C	519	LYS
1	C	521	SER
1	C	525	THR
1	C	528	VAL
1	C	532	VAL
1	C	907	VAL
1	C	910	SER
1	C	1036	ARG
1	C	1037	LEU
1	C	1038	PHE
1	C	1040	GLN
1	C	1043	LYS
1	C	1048	PHE
1	C	1049	GLU
1	C	1051	GLU
1	C	1053	GLU
1	C	1054	ARG
1	C	1056	LYS
1	C	1067	ASP
1	C	1144	LYS
1	D	495	ASN
1	D	496	ARG

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Mol	Chain	Res	Type
1	D	499	LYS
1	D	500	LEU
1	D	501	LEU
1	D	507	VAL
1	D	508	MET
1	D	1043	LYS
1	D	1047	GLU
1	D	1049	GLU
1	D	1051	GLU
1	D	1052	LEU
1	D	1053	GLU
1	D	1056	LYS
1	D	1057	THR
1	D	1058	LEU
1	D	1059	HIS
1	D	1065	VAL
1	D	1068	LEU
1	D	1074	ARG
1	D	1079	GLU
1	D	1084	LEU
1	D	1085	ARG
1	D	1087	ILE
1	D	1088	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	GLN
1	A	463	GLN
1	A	560	HIS
1	A	640	GLN
1	A	899	GLN
1	A	1135	GLN
1	B	94	GLN
1	B	436	HIS
1	B	470	GLN
1	B	498	GLN
1	B	771	HIS
1	B	879	HIS
1	B	898	ASN
1	C	498	GLN
1	C	506	HIS

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Mol	Chain	Res	Type
1	C	898	ASN
1	C	923	GLN
1	C	934	GLN
1	C	1040	GLN
1	C	1059	HIS
1	C	1081	ASN
1	D	498	GLN
1	D	502	HIS
1	D	510	ASN
1	D	721	GLN
1	D	807	GLN
1	D	870	GLN
1	D	873	ASN
1	D	1073	GLN
1	D	1075	GLN
1	D	1083	GLN
1	D	1135	GLN

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 [i](#)

8 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
2	BTI	D	1900	1	15,16,16	6.44	11 (73%)	20,21,21	2.82	9 (45%)
2	BTI	C	1900	1	15,16,16	6.42	11 (73%)	20,21,21	2.99	10 (50%)
4	ACO	A	1203	-	51,53,53	0.31	0	73,79,79	0.49	1 (1%)
3	ANP	B	2003	-	33,33,33	3.61	14 (42%)	45,52,52	3.19	12 (26%)
2	BTI	A	1201	1	15,16,16	6.43	11 (73%)	20,21,21	3.01	9 (45%)
4	ACO	B	2001	-	51,53,53	0.40	0	73,79,79	0.48	1 (1%)
3	ANP	A	1202	-	33,33,33	3.59	15 (45%)	45,52,52	3.22	11 (24%)
2	BTI	B	2002	1	15,16,16	6.47	11 (73%)	20,21,21	3.15	10 (50%)

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
2	BTI	D	1900	1	-	3/6/27/27	0/2/2/2
2	BTI	C	1900	1	-	5/6/27/27	0/2/2/2
4	ACO	A	1203	-	-	15/51/67/67	0/3/3/3
3	ANP	B	2003	-	-	6/18/38/38	0/3/3/3
2	BTI	A	1201	1	-	3/6/27/27	0/2/2/2
4	ACO	B	2001	-	-	18/51/67/67	0/3/3/3
3	ANP	A	1202	-	-	4/18/38/38	0/3/3/3
2	BTI	B	2002	1	-	4/6/27/27	0/2/2/2

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1900	BTI	C6-S1	-13.19	1.44	1.81
2	D	1900	BTI	C6-S1	-13.17	1.44	1.81
2	B	2002	BTI	C6-S1	-13.17	1.44	1.81
2	A	1201	BTI	C6-S1	-13.16	1.44	1.81
2	B	2002	BTI	C3-N3	12.53	1.58	1.35
2	D	1900	BTI	C3-N3	12.44	1.58	1.35
2	A	1201	BTI	C3-N3	12.42	1.58	1.35
2	C	1900	BTI	C3-N3	12.32	1.57	1.35
3	A	1202	ANP	C2'-C3'	-11.21	1.23	1.53
3	B	2003	ANP	C2'-C3'	-11.14	1.23	1.53
2	D	1900	BTI	C3-N2	8.80	1.51	1.35
2	C	1900	BTI	C3-N2	8.78	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2002	BTI	C3-N2	8.75	1.51	1.35
2	A	1201	BTI	C3-N2	8.69	1.51	1.35
3	B	2003	ANP	PA-O3A	8.23	1.68	1.59
2	A	1201	BTI	C5-N3	-8.23	1.33	1.46
2	B	2002	BTI	C5-N3	-8.23	1.33	1.46
2	C	1900	BTI	C5-N3	-8.17	1.34	1.46
2	D	1900	BTI	C5-N3	-8.08	1.34	1.46
3	A	1202	ANP	PA-O3A	7.87	1.68	1.59
2	C	1900	BTI	C2-S1	-7.74	1.70	1.82
2	A	1201	BTI	C2-S1	-7.71	1.70	1.82
2	D	1900	BTI	C2-S1	-7.67	1.70	1.82
2	B	2002	BTI	C2-S1	-7.63	1.70	1.82
2	B	2002	BTI	C6-C5	5.62	1.65	1.53
3	B	2003	ANP	O3'-C3'	5.62	1.56	1.43
3	A	1202	ANP	O3'-C3'	5.60	1.56	1.43
2	D	1900	BTI	C6-C5	5.59	1.64	1.53
2	A	1201	BTI	C6-C5	5.56	1.64	1.53
2	C	1900	BTI	C6-C5	5.48	1.64	1.53
3	B	2003	ANP	O4'-C1'	-5.41	1.29	1.42
3	A	1202	ANP	O4'-C1'	-5.41	1.29	1.42
3	B	2003	ANP	PB-O3A	5.22	1.65	1.59
3	A	1202	ANP	PB-O1B	5.17	1.54	1.46
3	A	1202	ANP	PB-O3A	4.93	1.65	1.59
3	B	2003	ANP	PB-O1B	4.88	1.53	1.46
3	B	2003	ANP	C2'-C1'	4.68	1.68	1.53
3	B	2003	ANP	PG-N3B	4.39	1.74	1.63
3	A	1202	ANP	C2'-C1'	4.36	1.67	1.53
3	A	1202	ANP	PG-N3B	4.35	1.74	1.63
2	B	2002	BTI	C7-C2	3.94	1.63	1.52
3	A	1202	ANP	C5'-C4'	-3.87	1.39	1.51
2	D	1900	BTI	C7-C2	3.82	1.62	1.52
2	D	1900	BTI	C4-N2	-3.81	1.38	1.45
2	B	2002	BTI	C4-N2	-3.79	1.38	1.45
3	B	2003	ANP	C5'-C4'	-3.78	1.40	1.51
2	A	1201	BTI	C4-N2	-3.77	1.38	1.45
2	C	1900	BTI	C4-N2	-3.73	1.38	1.45
2	A	1201	BTI	C2-C4	-3.70	1.43	1.53
2	A	1201	BTI	C7-C2	3.69	1.62	1.52
2	D	1900	BTI	C2-C4	-3.68	1.43	1.53
2	B	2002	BTI	C2-C4	-3.66	1.43	1.53
2	C	1900	BTI	C2-C4	-3.65	1.43	1.53
2	C	1900	BTI	C7-C2	3.63	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1202	ANP	C3'-C4'	3.54	1.62	1.53
3	B	2003	ANP	C3'-C4'	3.45	1.61	1.53
3	A	1202	ANP	C5-C4	-3.28	1.33	1.39
2	D	1900	BTI	C5-C4	3.25	1.65	1.55
2	C	1900	BTI	C5-C4	3.25	1.65	1.55
2	A	1201	BTI	C5-C4	3.20	1.64	1.55
2	B	2002	BTI	C5-C4	3.17	1.64	1.55
3	A	1202	ANP	O4'-C4'	3.11	1.51	1.45
3	B	2003	ANP	PB-O2B	-3.07	1.48	1.56
3	A	1202	ANP	PB-O2B	-3.02	1.48	1.56
3	B	2003	ANP	C5-C4	-2.99	1.33	1.39
3	B	2003	ANP	O4'-C4'	2.94	1.51	1.45
3	B	2003	ANP	C6-N6	2.53	1.40	1.34
2	B	2002	BTI	O3-C3	-2.34	1.18	1.23
2	D	1900	BTI	O3-C3	-2.22	1.18	1.23
2	A	1201	BTI	O3-C3	-2.21	1.18	1.23
3	A	1202	ANP	C6-N6	2.20	1.39	1.34
2	C	1900	BTI	O3-C3	-2.16	1.18	1.23
3	A	1202	ANP	C5-N7	-2.08	1.35	1.39

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1202	ANP	C1'-N9-C8	-13.04	98.16	127.09
3	B	2003	ANP	C1'-N9-C8	-12.89	98.48	127.09
3	B	2003	ANP	C4-N9-C1'	10.79	151.87	126.63
3	A	1202	ANP	C4-N9-C1'	10.76	151.80	126.63
2	A	1201	BTI	C6-S1-C2	7.49	105.55	89.98
2	D	1900	BTI	C6-S1-C2	7.35	105.28	89.98
2	C	1900	BTI	C6-S1-C2	7.04	104.62	89.98
2	B	2002	BTI	C6-S1-C2	6.96	104.46	89.98
3	A	1202	ANP	N3-C2-N1	-5.76	119.86	128.58
3	B	2003	ANP	N3-C2-N1	-5.68	119.98	128.58
2	D	1900	BTI	C4-C5-N3	5.33	108.35	102.43
2	C	1900	BTI	C4-C5-N3	5.23	108.24	102.43
2	A	1201	BTI	C4-C5-N3	5.23	108.23	102.43
3	A	1202	ANP	N9-C8-N7	-5.21	106.55	113.94
2	B	2002	BTI	C5-C4-N2	5.16	108.51	102.68
2	B	2002	BTI	C8-C7-C2	-5.16	102.19	114.04
3	B	2003	ANP	N9-C8-N7	-5.14	106.64	113.94
2	B	2002	BTI	C4-C5-N3	5.05	108.03	102.43
2	A	1201	BTI	C5-C4-N2	4.86	108.17	102.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1900	BTI	C5-C4-N2	4.82	108.12	102.68
2	D	1900	BTI	C5-C4-N2	4.74	108.02	102.68
3	A	1202	ANP	C5-C4-N3	-4.44	120.61	126.72
3	B	2003	ANP	C5-C4-N3	-4.37	120.70	126.72
2	B	2002	BTI	O11-C11-C10	-4.21	91.06	126.30
2	B	2002	BTI	C4-N2-C3	-4.10	107.47	112.56
3	A	1202	ANP	C4-N9-C8	4.09	110.03	105.74
2	C	1900	BTI	O11-C11-C10	-3.96	93.15	126.30
2	C	1900	BTI	C4-N2-C3	-3.94	107.67	112.56
2	A	1201	BTI	C4-N2-C3	-3.91	107.70	112.56
2	D	1900	BTI	C4-N2-C3	-3.78	107.87	112.56
3	B	2003	ANP	C4-N9-C8	3.73	109.66	105.74
2	A	1201	BTI	C8-C7-C2	-3.71	105.52	114.04
3	A	1202	ANP	C4'-O4'-C1'	-3.54	101.64	109.47
2	C	1900	BTI	C8-C7-C2	-3.47	106.07	114.04
2	A	1201	BTI	O11-C11-C10	-3.39	97.93	126.30
3	A	1202	ANP	N3-C4-N9	3.37	132.90	127.17
3	B	2003	ANP	C2-N3-C4	3.29	119.87	111.83
3	A	1202	ANP	C2-N3-C4	3.26	119.80	111.83
3	A	1202	ANP	O4'-C1'-N9	3.19	114.22	108.09
3	B	2003	ANP	C5-N7-C8	3.10	108.32	103.45
2	D	1900	BTI	C5-N3-C3	-3.08	107.86	112.38
2	A	1201	BTI	C5-N3-C3	-3.02	107.95	112.38
2	C	1900	BTI	C5-N3-C3	-3.01	107.97	112.38
2	B	2002	BTI	C5-N3-C3	-2.96	108.03	112.38
3	A	1202	ANP	C5-N7-C8	2.89	107.99	103.45
3	B	2003	ANP	N3-C4-N9	2.83	131.98	127.17
3	B	2003	ANP	C3'-C2'-C1'	2.76	106.67	101.46
4	A	1203	ACO	P2A-O6A-CCP	-2.67	106.60	121.12
4	B	2001	ACO	P2A-O6A-CCP	-2.57	107.10	121.12
2	B	2002	BTI	C6-C5-N3	-2.57	109.88	113.18
2	B	2002	BTI	C2-C4-C5	-2.36	106.00	108.89
2	C	1900	BTI	C6-C5-C4	-2.33	105.37	109.06
2	A	1201	BTI	C6-C5-N3	-2.30	110.22	113.18
2	B	2002	BTI	C6-C5-C4	-2.25	105.51	109.06
3	B	2003	ANP	C4-C5-N7	-2.20	108.06	110.58
2	C	1900	BTI	C2-C4-C5	-2.19	106.22	108.89
3	B	2003	ANP	N6-C6-N1	-2.17	113.54	118.38
2	D	1900	BTI	C6-C5-C4	-2.16	105.64	109.06
2	C	1900	BTI	C6-C5-N3	-2.13	110.44	113.18
2	D	1900	BTI	C6-C5-N3	-2.12	110.44	113.18
2	A	1201	BTI	C6-C5-C4	-2.08	105.77	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1900	BTI	C2-C4-C5	-2.04	106.39	108.89
2	D	1900	BTI	C8-C7-C2	-2.03	109.37	114.04

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	BTI	S1-C2-C7-C8
2	A	1201	BTI	C4-C2-C7-C8
2	B	2002	BTI	C9-C10-C11-O11
2	B	2002	BTI	S1-C2-C7-C8
2	B	2002	BTI	C4-C2-C7-C8
2	C	1900	BTI	C9-C10-C11-O11
2	C	1900	BTI	S1-C2-C7-C8
2	C	1900	BTI	C4-C2-C7-C8
2	D	1900	BTI	S1-C2-C7-C8
2	D	1900	BTI	C4-C2-C7-C8
3	A	1202	ANP	PB-N3B-PG-O1G
3	A	1202	ANP	PG-N3B-PB-O1B
3	B	2003	ANP	PB-N3B-PG-O1G
3	B	2003	ANP	O4'-C4'-C5'-O5'
3	B	2003	ANP	C3'-C4'-C5'-O5'
4	A	1203	ACO	CCP-O6A-P2A-O3A
4	A	1203	ACO	CCP-O6A-P2A-O4A
4	A	1203	ACO	C9P-CAP-CBP-CCP
4	A	1203	ACO	C9P-CAP-CBP-CEP
4	A	1203	ACO	N8P-C9P-CAP-OAP
4	B	2001	ACO	C5B-O5B-P1A-O1A
4	B	2001	ACO	CCP-O6A-P2A-O3A
4	B	2001	ACO	CCP-O6A-P2A-O4A
4	B	2001	ACO	C9P-CAP-CBP-CCP
4	B	2001	ACO	C9P-CAP-CBP-CEP
4	B	2001	ACO	N8P-C9P-CAP-OAP
4	B	2001	ACO	O-C-S1P-C2P
4	A	1203	ACO	C4B-C3B-O3B-P3B
4	A	1203	ACO	S1P-C2P-C3P-N4P
4	A	1203	ACO	C3B-C4B-C5B-O5B
4	A	1203	ACO	C2B-C3B-O3B-P3B
4	B	2001	ACO	CH3-C-S1P-C2P
4	A	1203	ACO	O9P-C9P-CAP-OAP
4	B	2001	ACO	O9P-C9P-CAP-OAP
4	B	2001	ACO	P1A-O3A-P2A-O6A

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Mol	Chain	Res	Type	Atoms
4	A	1203	ACO	C9P-CAP-CBP-CDP
4	B	2001	ACO	C9P-CAP-CBP-CDP
2	A	1201	BTI	C11-C10-C9-C8
2	C	1900	BTI	C2-C7-C8-C9
4	B	2001	ACO	C3P-C2P-S1P-C
4	A	1203	ACO	CCP-O6A-P2A-O5A
4	B	2001	ACO	CCP-O6A-P2A-O5A
4	B	2001	ACO	OAP-CAP-CBP-CCP
2	D	1900	BTI	C2-C7-C8-C9
3	B	2003	ANP	C4'-C5'-O5'-PA
3	A	1202	ANP	O4'-C4'-C5'-O5'
4	A	1203	ACO	O4B-C4B-C5B-O5B
3	B	2003	ANP	PB-O3A-PA-O2A
4	A	1203	ACO	C3B-O3B-P3B-O7A
4	B	2001	ACO	S1P-C2P-C3P-N4P
3	A	1202	ANP	C4'-C5'-O5'-PA
4	A	1203	ACO	OAP-CAP-CBP-CDP
4	B	2001	ACO	OAP-CAP-CBP-CDP
2	C	1900	BTI	C11-C10-C9-C8
4	B	2001	ACO	O9P-C9P-CAP-CBP
4	B	2001	ACO	N8P-C9P-CAP-CBP
3	B	2003	ANP	PB-O3A-PA-O1A
2	B	2002	BTI	C2-C7-C8-C9

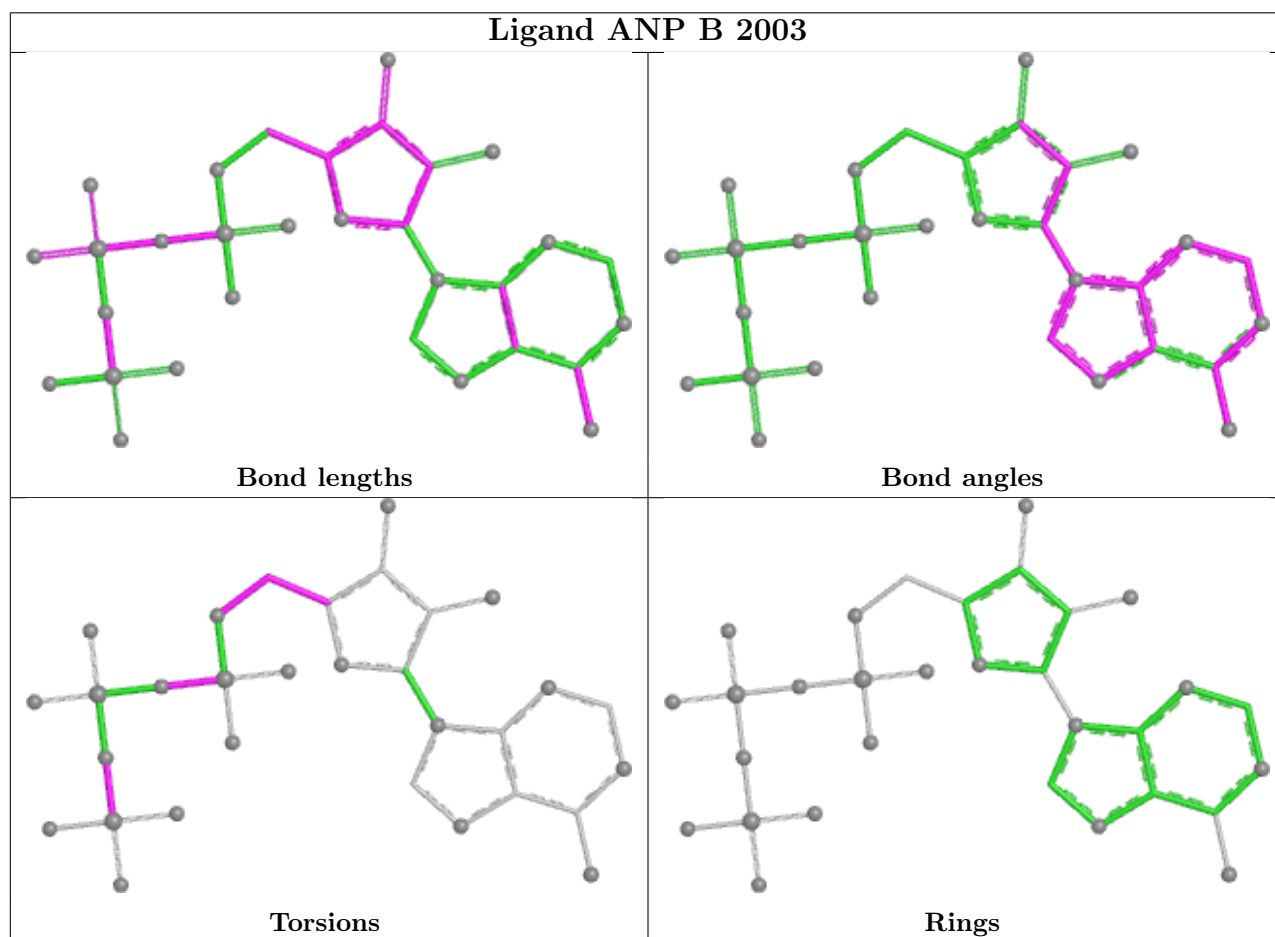
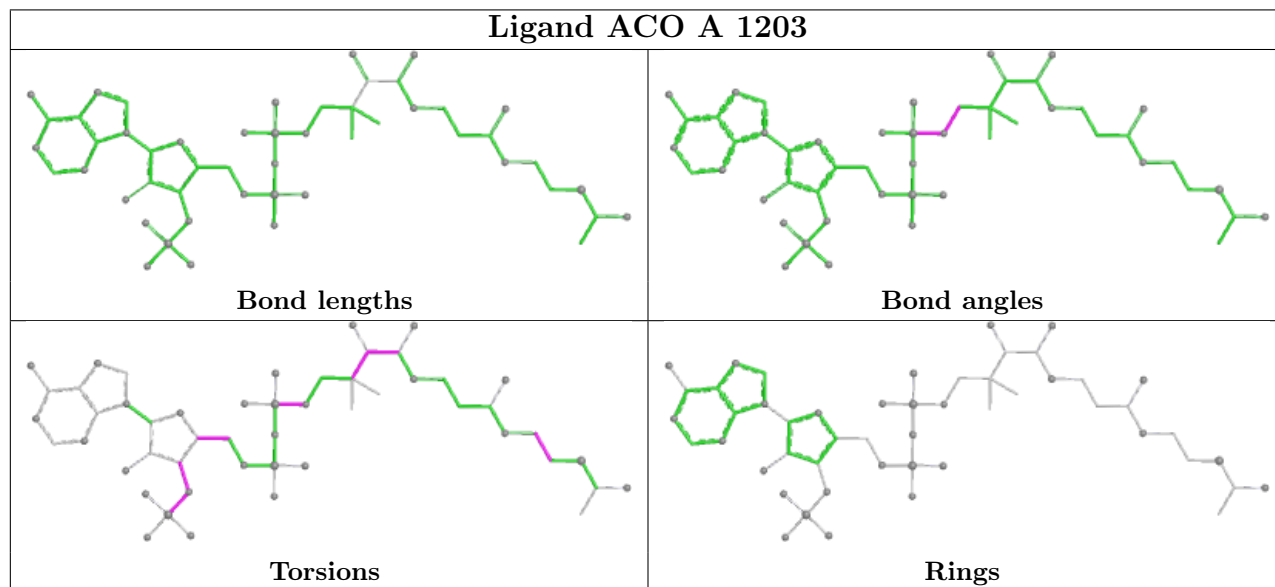
There are no ring outliers.

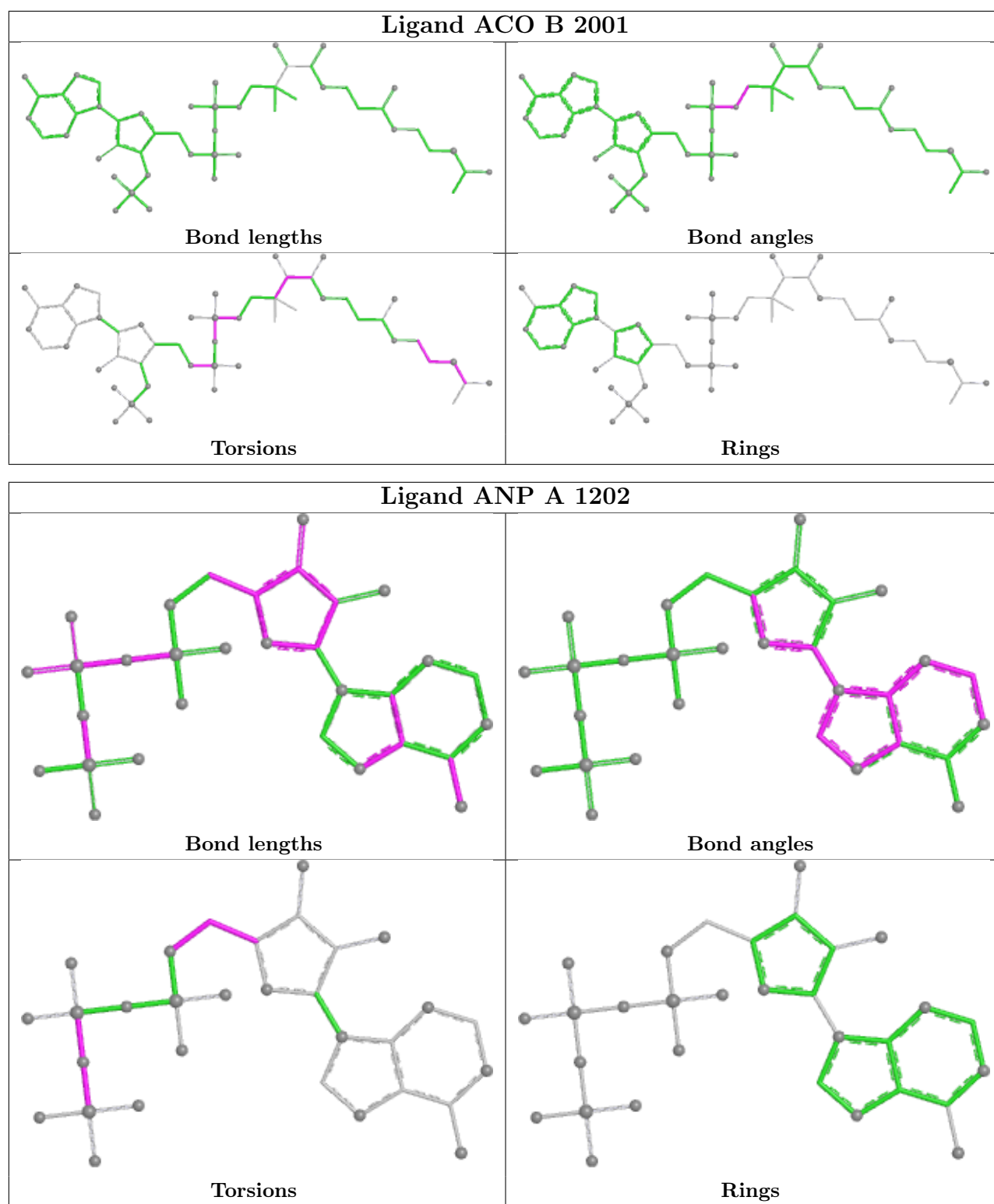
5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1900	BTI	3	0
4	A	1203	ACO	4	0
4	B	2001	ACO	2	0
3	A	1202	ANP	1	0
2	B	2002	BTI	5	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

There are no chain breaks in this entry.

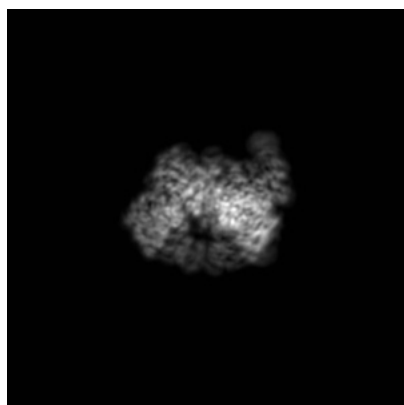
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32775. These allow visual inspection of the internal detail of the map and identification of artifacts.

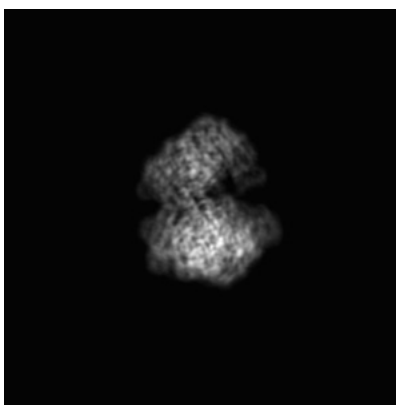
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

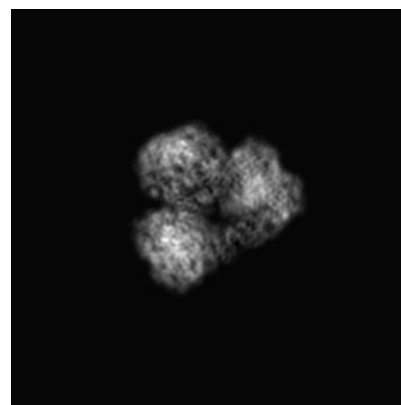
6.1.1 Primary map



X



Y

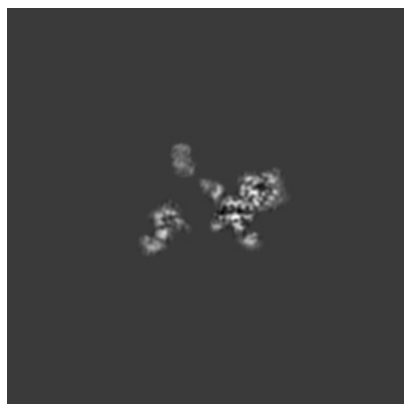


Z

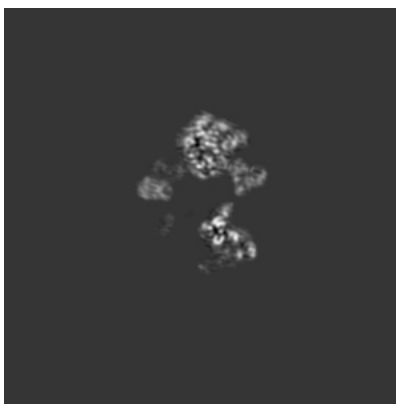
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

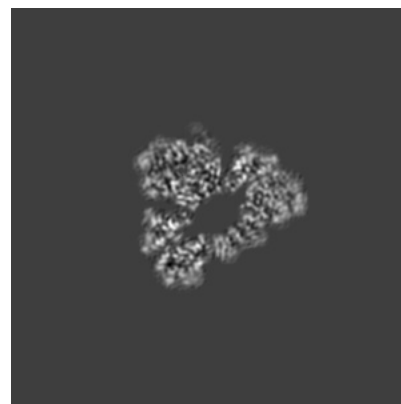
6.2.1 Primary map



X Index: 156



Y Index: 156

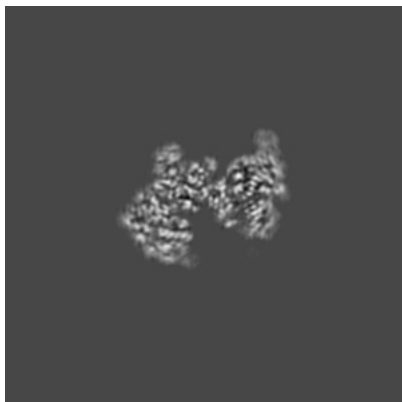


Z Index: 156

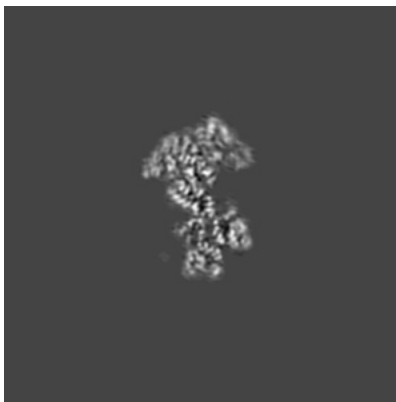
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

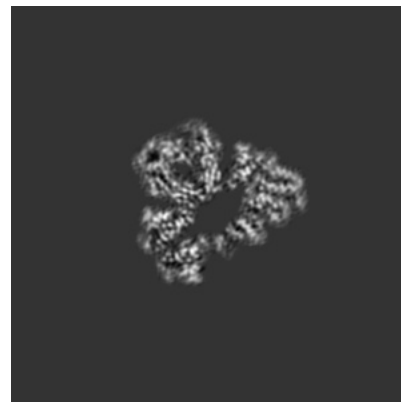
6.3.1 Primary map



X Index: 129



Y Index: 180

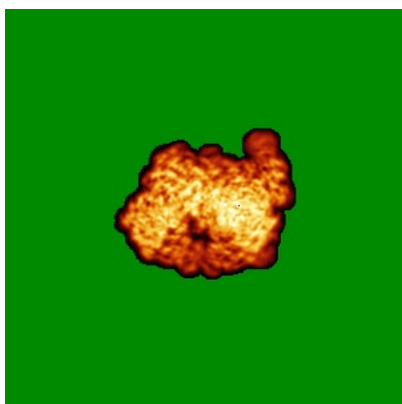


Z Index: 159

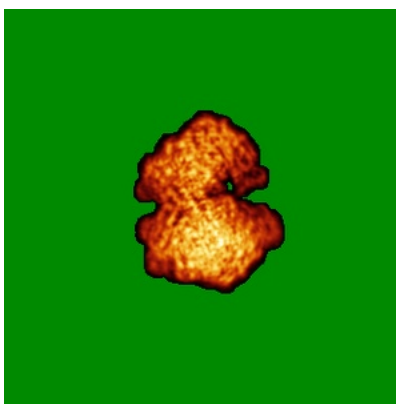
The images above show the largest variance slices of the map in three orthogonal directions.

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

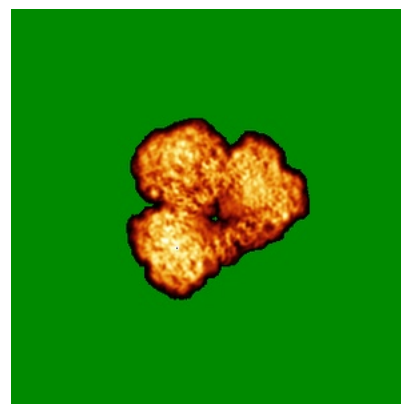
6.4.1 Primary map



X



Y

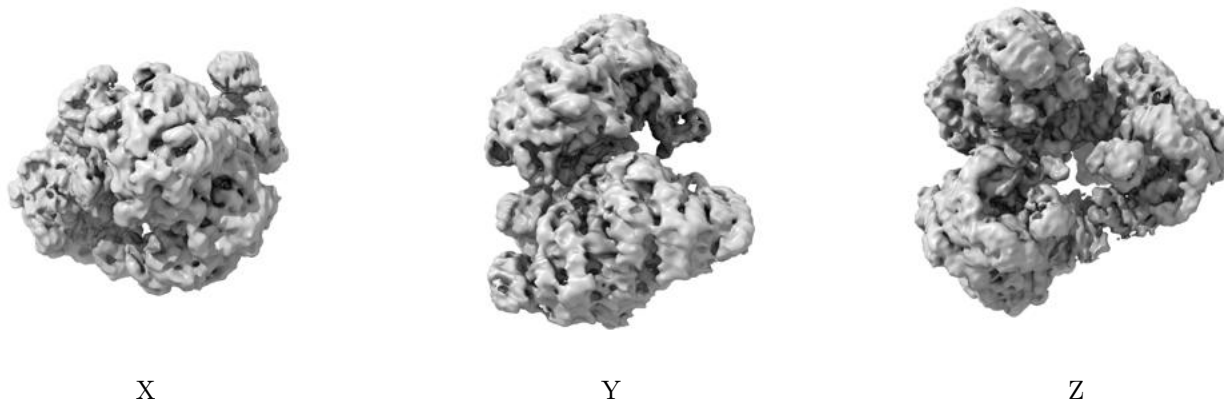


Z

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 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

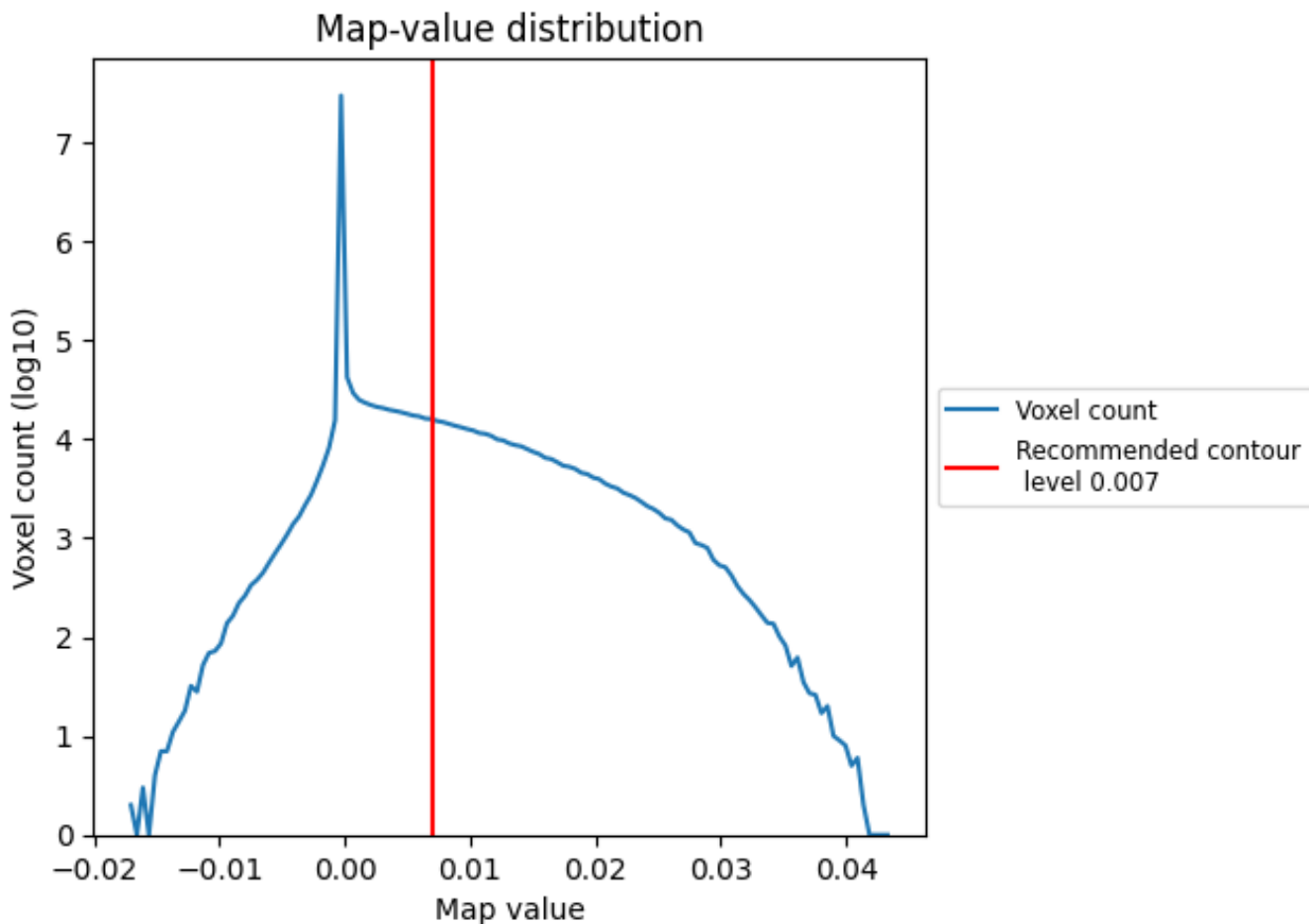
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

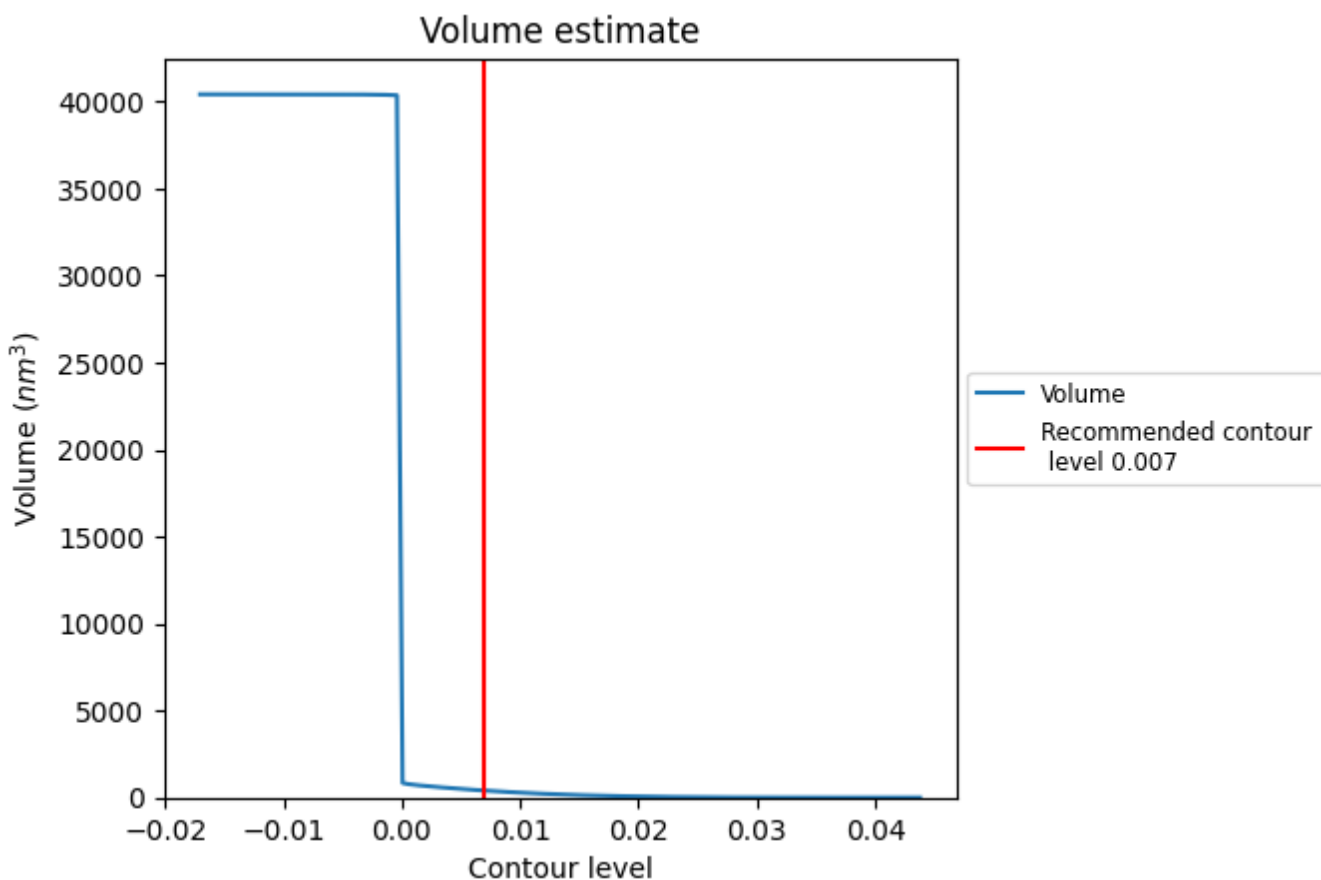
This section contains the results of statistical analysis of the map.

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.

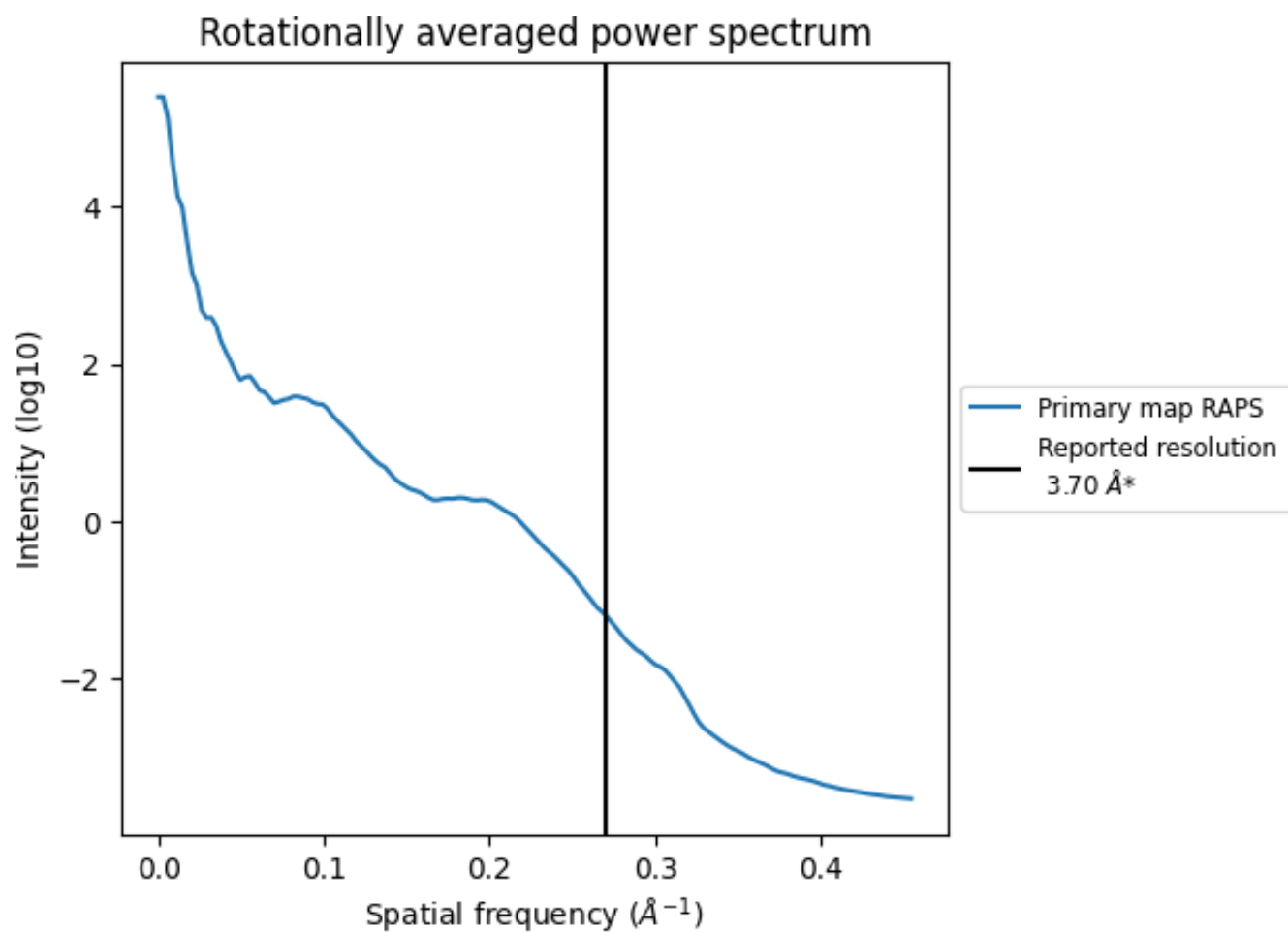
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 401 nm³; this corresponds to an approximate mass of 362 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

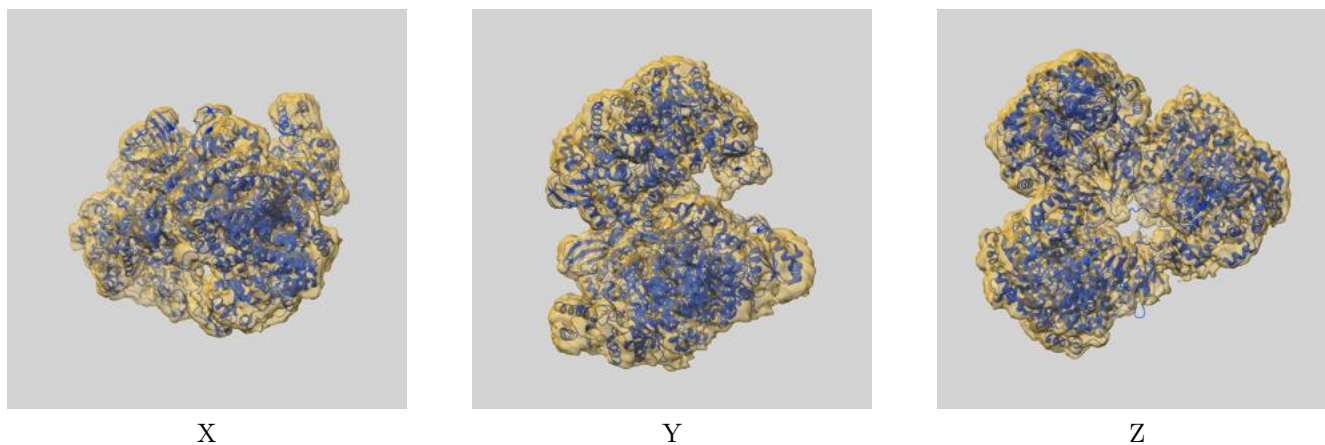
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32775 and PDB model 7WTB. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



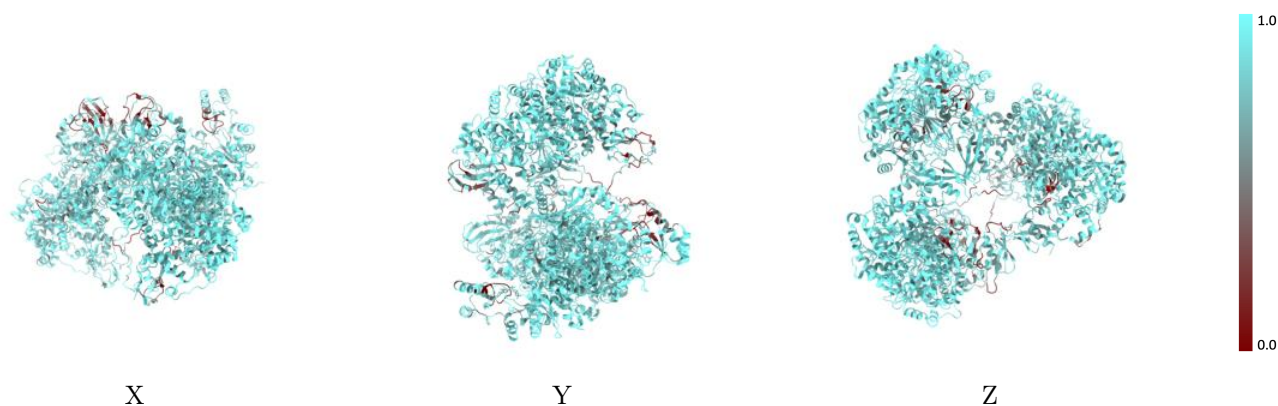
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



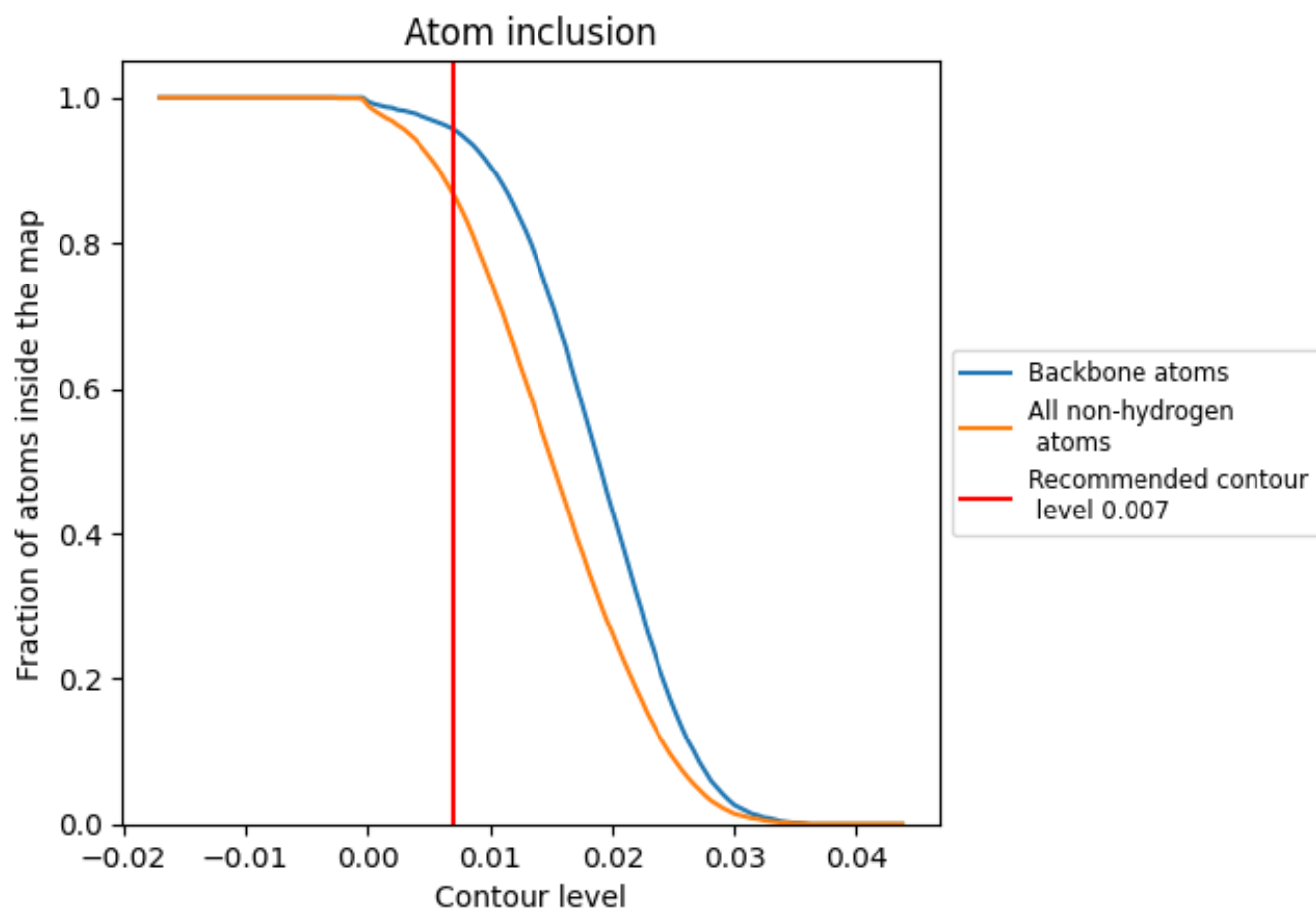
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).











9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 87% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8670	 0.3130
A	 0.8790	 0.3210
B	 0.8720	 0.3150
C	 0.8710	 0.3130
D	 0.8350	 0.2970

