



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 04:57 PM UTC

PDB ID : 6POE / pdb_00006poe
EMDB ID : EMD-20413
Title : Structure of ACLY in complex with CoA
Authors : Wei, X.; Marmorstein, R.
Deposited on : 2019-07-03
Resolution : 3.50 Å (reported)
Based on initial model : 3MWD

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:

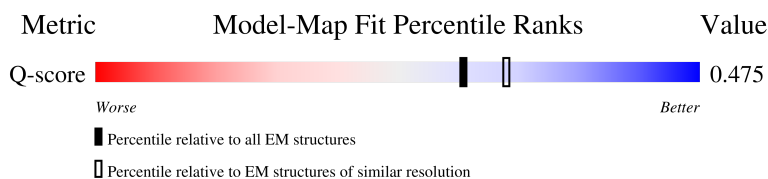
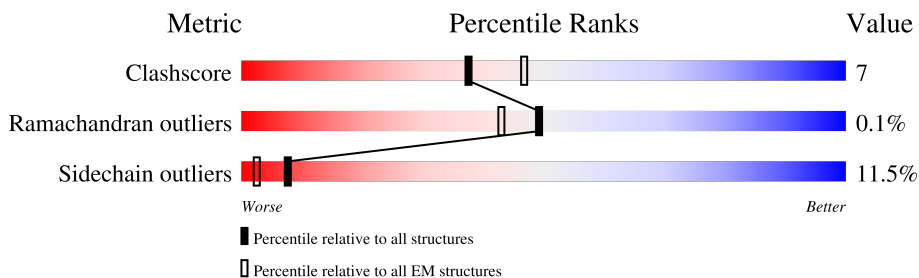
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.50 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	13950 (3.00 - 4.00)

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	
1	B	1101	
1	C	1101	
1	D	1101	

2 Entry composition [i](#)

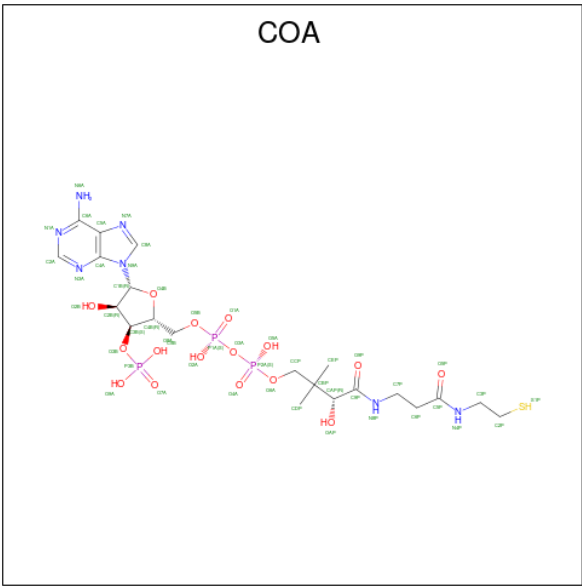
There are 3 unique types of molecules in this entry. The entry contains 31812 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S		
1	A	1021	Total 7906	5064	1340	1458	44	2	0
1	B	1021	Total 7903	5061	1340	1458	44	2	0
1	C	1021	Total 7902	5061	1339	1458	44	2	0
1	D	1021	Total 7906	5064	1340	1458	44	2	0

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
2	B	1	Total 48	21	7	16	3	1	0
2	B	1	Total 48	21	7	16	3	1	0

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Mol	Chain	Residues	Atoms						AltConf
2	C	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	
2	C	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	

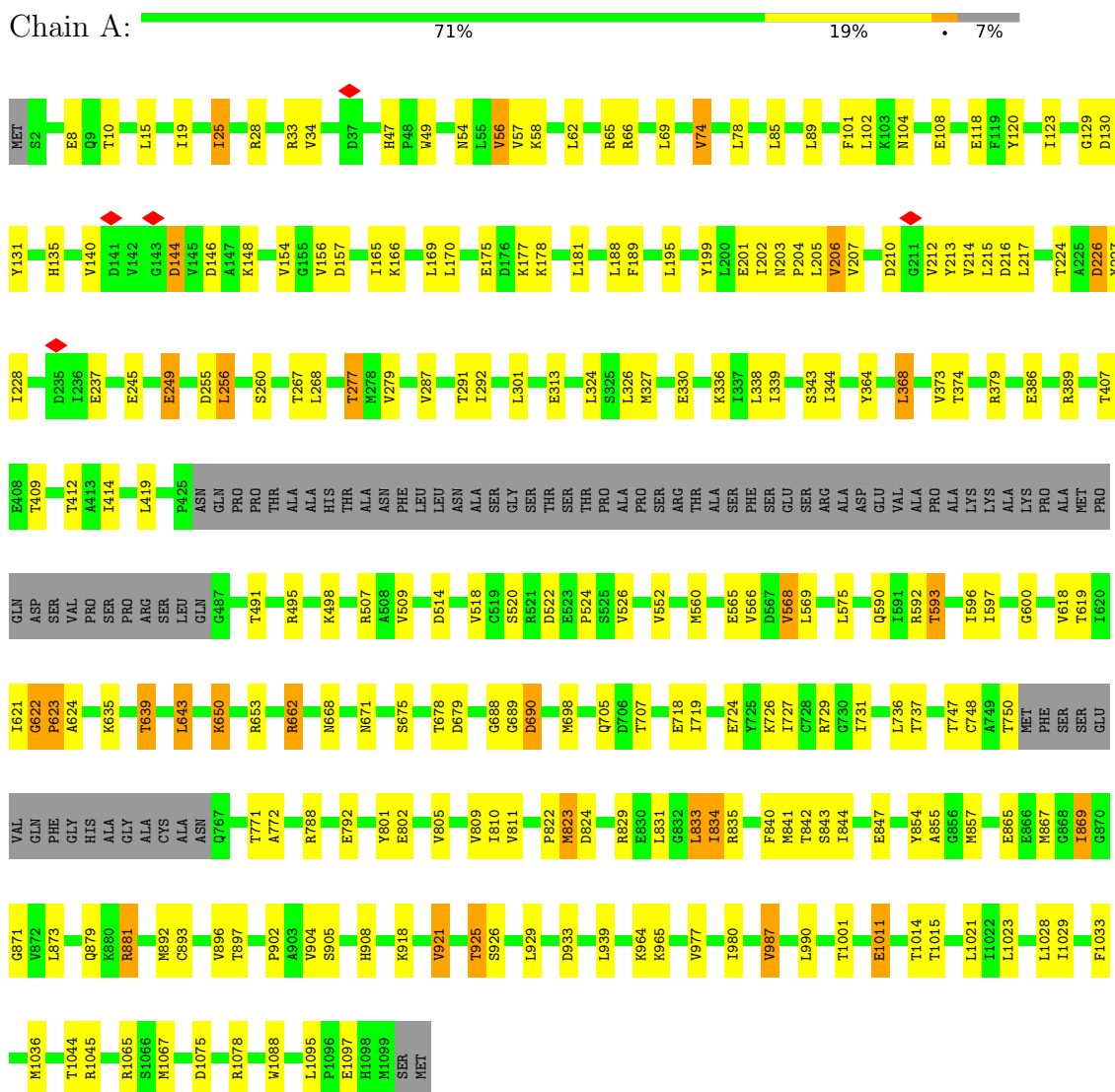
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	O	0
			1	1	
3	C	2	Total	O	0
			2	2	

3 Residue-property plots

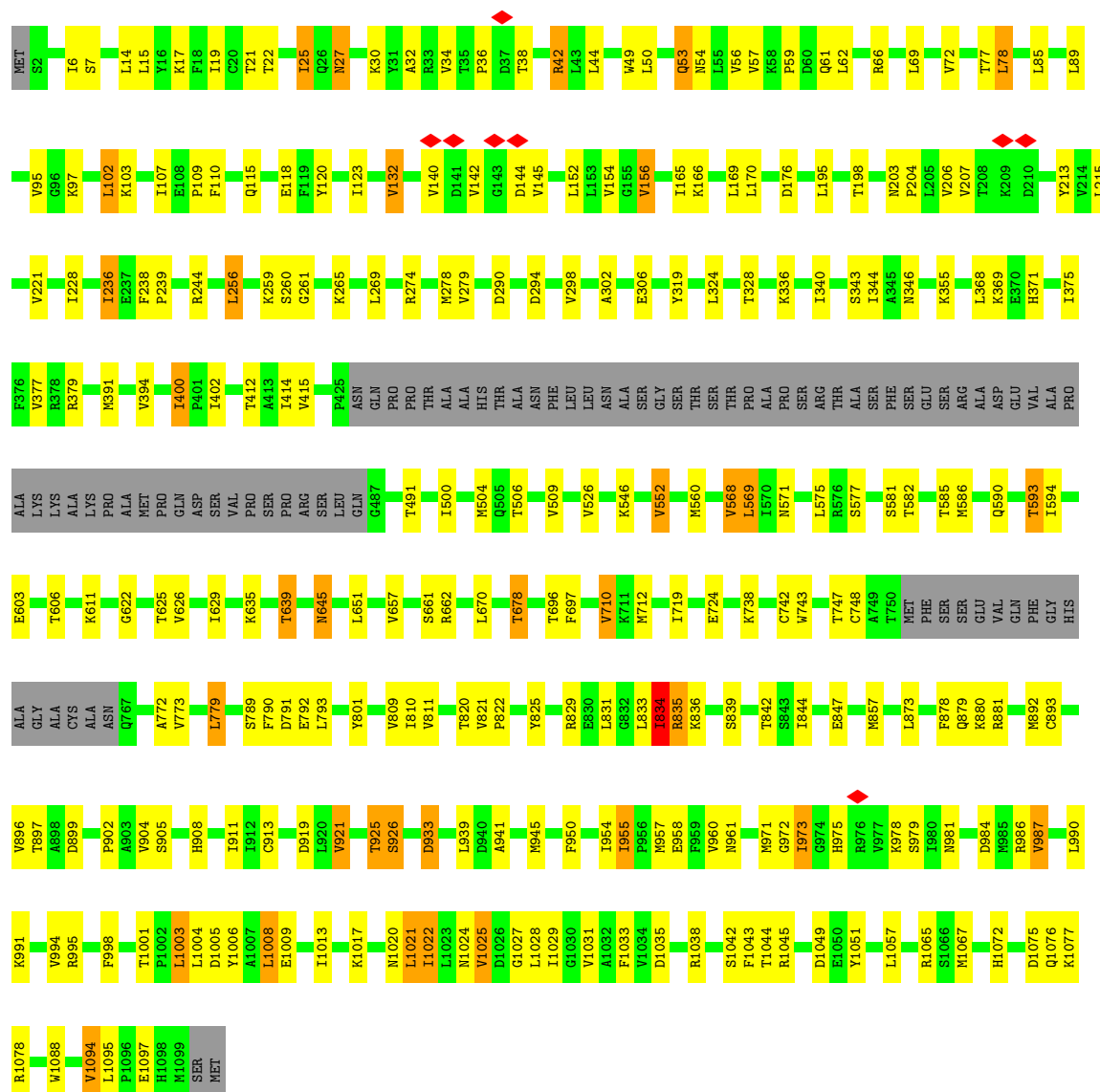
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: ATP-citrate synthase

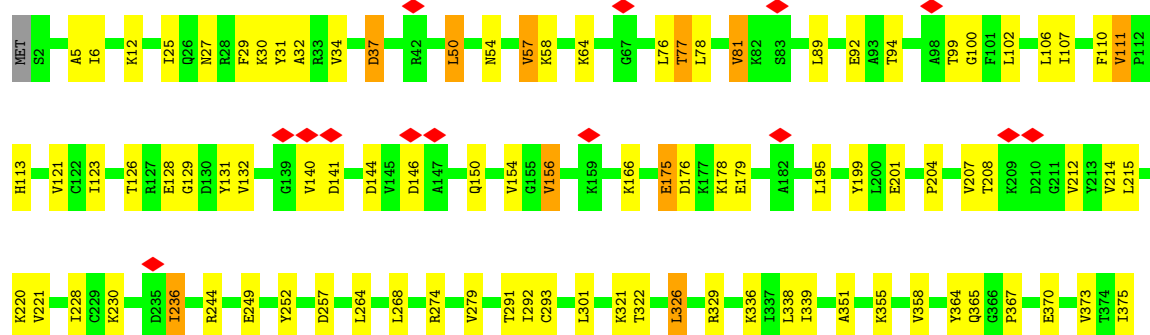


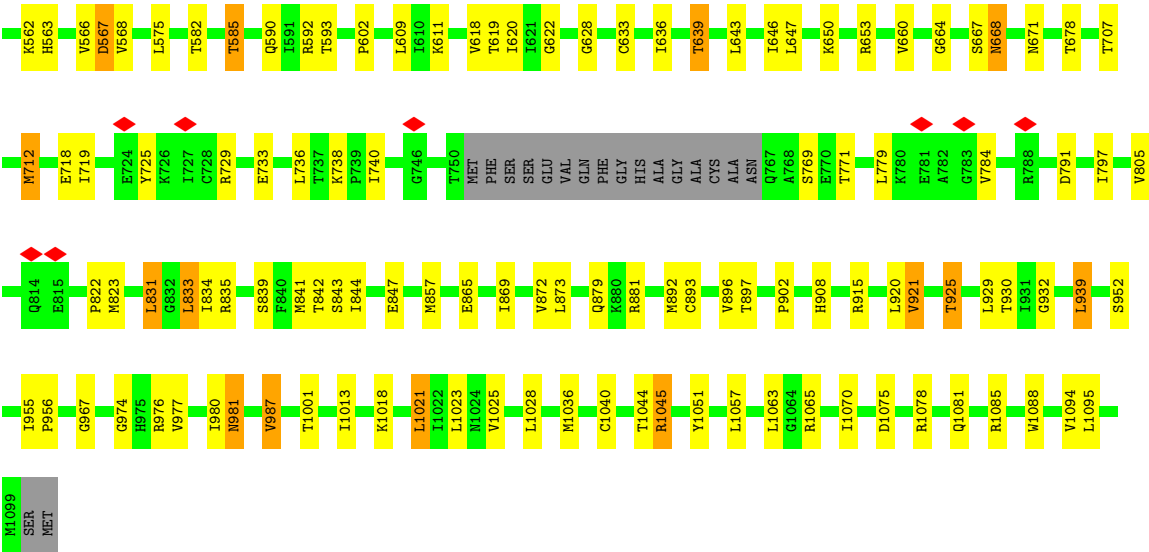
• Molecule 1: ATP-citrate synthase





• Molecule 1: ATP-citrate synthase





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	129563	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.114	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	191.4, 191.4, 191.4	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86999995, 0.86999995, 0.86999995	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COA

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	0.31	0/8083	0.54	4/10942 (0.0%)
1	B	0.32	0/8080	0.55	6/10938 (0.1%)
1	C	0.30	0/8079	0.50	0/10938
1	D	0.29	0/8083	0.54	2/10942 (0.0%)
All	All	0.31	0/32325	0.53	12/43760 (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	B	0	2
1	C	0	1
1	D	0	3
All	All	0	6

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	981	ASN	CA-C-N	9.46	131.17	122.37
1	D	981	ASN	C-N-CA	9.46	131.17	122.37
1	A	622	GLY	CA-C-N	9.00	131.09	119.84
1	A	622	GLY	C-N-CA	9.00	131.09	119.84
1	B	834	ILE	CA-C-N	6.56	134.07	121.54
1	B	834	ILE	C-N-CA	6.56	134.07	121.54
1	B	1094	VAL	CA-C-N	6.06	129.30	120.51
1	B	1094	VAL	C-N-CA	6.06	129.30	120.51
1	A	833	LEU	CA-C-N	-5.69	117.13	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	833	LEU	C-N-CA	-5.69	117.13	123.16
1	B	833	LEU	CA-C-N	-5.27	112.48	121.97
1	B	833	LEU	C-N-CA	-5.27	112.48	121.97

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	622	GLY	Peptide
1	B	834	ILE	Peptide
1	C	622	GLY	Peptide
1	D	622	GLY	Peptide
1	D	952	SER	Peptide
1	D	967	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7906	0	7956	132	0
1	B	7903	0	7947	141	0
1	C	7902	0	7945	118	0
1	D	7906	0	7956	128	0
2	B	96	0	64	0	0
2	C	96	0	64	2	0
3	A	1	0	0	0	0
3	C	2	0	0	0	0
All	All	31812	0	31932	477	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 7.

All (477) 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:A:623:PRO:HB2	1:A:690:ASP:OD2	1.27	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ILE:HD12	1:A:28:ARG:HD2	1.35	1.07
1:A:25:ILE:HD12	1:A:28:ARG:CD	1.89	1.02
1:A:623:PRO:CB	1:A:690:ASP:OD2	2.05	1.02
1:D:43:LEU:O	1:D:47:HIS:HB2	1.67	0.94
1:C:834:ILE:HD13	1:D:834:ILE:HD13	1.50	0.93
1:C:834:ILE:CD1	1:D:834:ILE:HD13	2.00	0.92
1:D:48:PRO:O	1:D:51:LEU:HB3	1.76	0.86
1:A:596:ILE:H	1:A:622:GLY:HA2	1.44	0.81
1:A:25:ILE:HD12	1:A:28:ARG:NE	1.94	0.81
1:C:834:ILE:HD13	1:D:834:ILE:CD1	2.10	0.81
1:B:994:VAL:HG21	1:B:1004:LEU:CD2	2.11	0.79
1:B:995:ARG:HH12	1:B:1008:LEU:HD12	1.49	0.77
1:A:842:THR:HG21	1:C:902:PRO:HG3	1.66	0.76
1:B:842:THR:HG21	1:D:902:PRO:HG3	1.68	0.74
1:A:902:PRO:HG3	1:C:842:THR:HG21	1.70	0.74
1:A:624:ALA:O	1:A:689:GLY:N	2.21	0.73
1:A:118:GLU:HA	1:A:205:LEU:O	1.89	0.72
1:D:65:ARG:O	1:D:69:LEU:HB2	1.90	0.72
1:C:835:ARG:HB2	1:D:822:PRO:CG	2.19	0.71
1:B:995:ARG:HH12	1:B:1008:LEU:CD1	2.03	0.70
1:B:995:ARG:NH1	1:B:1008:LEU:CD1	2.55	0.69
1:C:921:VAL:O	1:C:925:THR:HB	1.92	0.69
1:A:596:ILE:HD12	1:A:623:PRO:HD3	1.74	0.68
1:B:995:ARG:NH1	1:B:1008:LEU:HD11	2.08	0.68
1:D:1018:LYS:HB2	1:D:1021:LEU:HD22	1.75	0.68
1:C:831:LEU:HG	1:C:833:LEU:HD23	1.77	0.66
1:C:833:LEU:HD12	1:C:833:LEU:O	1.95	0.66
1:B:921:VAL:O	1:B:925:THR:HB	1.96	0.66
1:A:560:MET:SD	1:A:590:GLN:NE2	2.70	0.65
1:A:624:ALA:O	1:A:688:GLY:HA2	1.96	0.65
1:B:994:VAL:CG2	1:B:1004:LEU:CD2	2.75	0.64
1:B:994:VAL:HG21	1:B:1004:LEU:HD21	1.78	0.64
1:D:497:THR:O	1:D:521:ARG:NH2	2.31	0.64
1:A:596:ILE:H	1:A:622:GLY:CA	2.11	0.64
1:B:50:LEU:HB3	1:B:78:LEU:HD21	1.79	0.63
1:A:25:ILE:HD12	1:A:28:ARG:HE	1.63	0.63
1:A:25:ILE:CD1	1:A:28:ARG:HD2	2.22	0.63
1:A:203:ASN:O	1:A:216:ASP:HB2	1.99	0.63
1:A:921:VAL:O	1:A:925:THR:HB	1.99	0.62
1:C:626:VAL:HG13	1:C:639:THR:HG22	1.81	0.62
1:C:199:TYR:O	1:C:219:ALA:HA	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:964:LYS:HE3	2:C:1201:COA:O7A	1.99	0.62
1:C:834:ILE:HD11	1:D:834:ILE:HD13	1.80	0.62
1:D:27:ASN:HD21	1:D:109:PRO:HB2	1.66	0.61
1:D:375:ILE:O	1:D:402:ILE:HA	2.00	0.61
1:D:367:PRO:HA	1:D:370:GLU:HG2	1.83	0.60
1:D:521:ARG:NH1	1:D:633:CYS:O	2.34	0.60
1:A:56:VAL:HG12	1:A:74:VAL:HA	1.84	0.60
1:A:690:ASP:OD1	1:A:690:ASP:N	2.35	0.60
1:B:206:VAL:HG23	1:B:213:TYR:HB2	1.84	0.60
1:D:712:MET:HE1	1:D:797:ILE:HG23	1.84	0.60
1:A:25:ILE:CD1	1:A:28:ARG:HE	2.15	0.60
1:B:204:PRO:HG2	1:B:215:LEU:HD12	1.84	0.59
1:B:896:VAL:HG21	1:B:990:LEU:HD11	1.84	0.59
1:D:567:ASP:N	1:D:567:ASP:OD1	2.35	0.59
1:B:933:ASP:OD1	1:B:933:ASP:N	2.35	0.59
1:C:576:ARG:NH2	2:C:1201:COA:O8A	2.36	0.59
1:A:65:ARG:NH1	1:A:140:VAL:O	2.35	0.58
1:B:902:PRO:HG3	1:D:842:THR:HG21	1.85	0.58
1:A:58:LYS:NZ	1:A:215:LEU:O	2.36	0.58
1:C:728:CYS:SG	1:C:732:LYS:NZ	2.77	0.58
1:A:596:ILE:N	1:A:622:GLY:HA2	2.16	0.58
1:A:896:VAL:HG21	1:A:990:LEU:HD11	1.85	0.57
1:A:25:ILE:CD1	1:A:28:ARG:NE	2.65	0.57
1:B:941:ALA:HB1	1:B:971:MET:HG3	1.87	0.57
1:D:1044:THR:OG1	1:D:1045:ARG:N	2.38	0.57
1:A:662:ARG:NH2	1:A:690:ASP:O	2.38	0.57
1:B:955:ILE:HG22	1:B:958:GLU:H	1.70	0.57
1:B:991:LYS:HG3	1:B:1028:LEU:HD11	1.87	0.57
1:B:847:GLU:OE2	1:C:1088:TRP:NE1	2.37	0.57
1:A:1011:GLU:O	1:A:1015:THR:OG1	2.21	0.56
1:D:529:MET:HB2	1:D:552:VAL:HG22	1.87	0.56
1:D:921:VAL:O	1:D:925:THR:HB	2.05	0.56
1:C:933:ASP:OD1	1:C:933:ASP:N	2.38	0.56
1:D:230:LYS:HA	1:D:233:TRP:HB2	1.86	0.56
1:D:340:ILE:HD13	1:D:357:ILE:HD12	1.86	0.56
1:A:879:GLN:OE1	1:C:1078:ARG:NH2	2.37	0.56
1:B:59:PRO:O	1:B:66:ARG:NH1	2.37	0.56
1:A:841:MET:HB3	1:C:1079:LEU:HD13	1.88	0.56
1:D:831:LEU:HB3	1:D:833:LEU:HD23	1.88	0.56
1:B:994:VAL:CG2	1:B:1004:LEU:HD21	2.36	0.56
1:C:920:LEU:HD11	1:C:1070:ILE:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:ILE:HB	1:C:402:ILE:HG12	1.88	0.55
1:D:563:HIS:O	1:D:590:GLN:NE2	2.39	0.55
1:D:668:ASN:OD1	1:D:668:ASN:N	2.38	0.55
1:A:364:TYR:O	1:A:368:LEU:HB2	2.06	0.55
1:B:789:SER:OG	1:B:790:PHE:N	2.39	0.55
1:B:156:VAL:HG13	1:B:611:LYS:HD3	1.89	0.55
1:B:1038:ARG:NH2	1:B:1049:ASP:OD1	2.40	0.55
1:D:667:SER:O	1:D:671:ASN:ND2	2.40	0.55
1:B:582:THR:HG22	1:B:586:MET:HE2	1.88	0.55
1:B:879:GLN:OE1	1:D:1078:ARG:NH2	2.40	0.55
1:D:58:LYS:NZ	1:D:216:ASP:OD1	2.39	0.55
1:D:270:ASN:HD22	1:D:300:GLU:HA	1.70	0.55
1:A:705:GLN:HE22	1:A:737:THR:H	1.55	0.54
1:C:166:LYS:HZ2	1:C:178:LYS:HE2	1.73	0.54
1:C:584:GLU:O	1:C:587:ASN:ND2	2.40	0.54
1:C:92:GLU:HA	1:C:100:GLY:O	2.06	0.54
1:D:278:MET:HG3	1:D:323:ILE:HG13	1.88	0.54
1:B:328:THR:O	1:B:371:HIS:NE2	2.38	0.54
1:B:972:GLY:O	1:B:1024:ASN:HB2	2.07	0.54
1:C:204:PRO:HG2	1:C:215:LEU:HD13	1.89	0.54
1:A:129:GLY:HA2	1:A:156:VAL:HG13	1.90	0.54
1:B:742:CYS:SG	1:B:743:TRP:N	2.81	0.54
1:C:719:ILE:HG22	1:C:772:ALA:HB2	1.90	0.54
1:B:1051:TYR:OH	1:D:1078:ARG:NH1	2.41	0.54
1:D:974:GLY:HA2	1:D:1021:LEU:HA	1.89	0.53
1:D:980:ILE:O	1:D:981:ASN:ND2	2.42	0.53
1:D:1023:LEU:HD23	1:D:1028:LEU:HD12	1.90	0.53
1:A:1088:TRP:NE1	1:D:847:GLU:OE2	2.39	0.53
1:C:244:ARG:NH2	1:C:268:LEU:O	2.41	0.53
1:D:653:ARG:O	1:D:653:ARG:NH1	2.41	0.53
1:A:847:GLU:OE2	1:D:1088:TRP:NE1	2.38	0.53
1:B:509:VAL:HG13	1:B:526:VAL:HG21	1.89	0.53
1:C:835:ARG:HB2	1:D:822:PRO:HG2	1.89	0.53
1:B:54:ASN:HB3	1:B:110:PHE:HB3	1.90	0.53
1:B:994:VAL:HG21	1:B:1004:LEU:HD22	1.90	0.53
1:C:207:VAL:HG22	1:C:212:VAL:HG23	1.90	0.53
1:D:833:LEU:HD12	1:D:833:LEU:O	2.08	0.53
1:A:343:SER:O	1:A:379:ARG:NH1	2.41	0.53
1:B:987:VAL:HB	1:B:1028:LEU:HD13	1.91	0.53
1:B:1006:TYR:CD1	1:B:1006:TYR:C	2.85	0.53
1:A:822:PRO:HG2	1:B:835:ARG:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LYS:HA	1:A:170:LEU:HB2	1.91	0.53
1:A:865:GLU:OE1	1:A:881:ARG:NH1	2.41	0.53
1:C:893:CYS:O	1:C:897:THR:OG1	2.24	0.53
1:B:972:GLY:O	1:B:1024:ASN:CB	2.57	0.53
1:B:343:SER:O	1:B:379:ARG:NH1	2.42	0.53
1:A:58:LYS:NZ	1:A:216:ASP:OD1	2.40	0.52
1:D:865:GLU:OE2	1:D:881:ARG:NH2	2.39	0.52
1:A:624:ALA:O	1:A:688:GLY:CA	2.56	0.52
1:B:57:VAL:HG22	1:B:107:ILE:HG12	1.91	0.52
1:B:941:ALA:CB	1:B:971:MET:HG3	2.39	0.52
1:D:417:MET:HB3	1:D:424:ILE:HG12	1.91	0.52
1:D:514:ASP:HB3	1:D:643:LEU:HD22	1.92	0.52
1:B:375:ILE:HB	1:B:402:ILE:HG12	1.90	0.52
1:B:880:LYS:HD2	1:B:1042:SER:HB2	1.92	0.52
1:B:957:MET:O	1:B:961:ASN:ND2	2.38	0.52
1:C:408:GLU:OE2	1:C:676:ARG:NH1	2.43	0.52
1:D:54:ASN:HD22	1:D:110:PHE:HB3	1.75	0.52
1:D:120:TYR:HB3	1:D:135:HIS:HB3	1.92	0.52
1:D:522:ASP:OD1	1:D:522:ASP:N	2.42	0.52
1:D:650:LYS:O	1:D:653:ARG:NH1	2.43	0.52
1:B:30:LYS:HE3	1:B:109:PRO:HG2	1.91	0.51
1:B:825:TYR:OH	1:B:829:ARG:NH1	2.43	0.51
1:B:132:VAL:HG13	1:B:152:LEU:HB3	1.93	0.51
1:D:375:ILE:HB	1:D:402:ILE:HG12	1.91	0.51
1:B:1088:TRP:NE1	1:C:847:GLU:OE2	2.40	0.51
1:C:567:ASP:OD1	1:C:567:ASP:N	2.43	0.51
1:A:596:ILE:HD12	1:A:623:PRO:CD	2.40	0.51
1:D:378:ARG:NH2	1:D:409:THR:O	2.43	0.51
1:A:256:LEU:O	1:A:260:SER:HB3	2.11	0.51
1:D:707:THR:O	1:D:738:LYS:NZ	2.44	0.51
1:B:61:GLN:OE1	1:B:103:LYS:N	2.42	0.51
1:B:61:GLN:HE22	1:B:102:LEU:HA	1.75	0.51
1:D:92:GLU:HA	1:D:100:GLY:O	2.10	0.51
1:A:509:VAL:HG13	1:A:526:VAL:HG21	1.91	0.50
1:B:324:LEU:O	1:B:328:THR:OG1	2.28	0.50
1:D:389:ARG:NH1	1:D:393:GLU:OE1	2.41	0.50
1:A:623:PRO:O	1:A:690:ASP:CG	2.55	0.50
1:C:677:THR:HB	1:C:798:GLN:HB2	1.94	0.50
1:B:391:MET:HG3	1:B:402:ILE:HG21	1.93	0.50
1:B:747:THR:OG1	1:B:748:CYS:N	2.44	0.50
1:C:123:ILE:HG23	1:C:132:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:707:THR:O	1:C:738:LYS:NZ	2.44	0.50
1:D:487:GLY:O	1:D:592:ARG:NH2	2.44	0.50
1:A:698:MET:HE2	1:A:727:ILE:HD13	1.92	0.50
1:A:857:MET:HE1	1:A:881:ARG:HD2	1.93	0.50
1:A:987:VAL:HG22	1:A:1028:LEU:HD13	1.94	0.50
1:C:521:ARG:NH1	1:C:633:CYS:O	2.41	0.50
1:A:731:ILE:HG13	1:A:736:LEU:HB2	1.94	0.50
1:B:881:ARG:NH1	1:C:1099:MET:O	2.44	0.50
1:C:918:LYS:HD3	1:D:932:GLY:HA3	1.93	0.50
1:D:177:LYS:HG2	1:D:207:VAL:HG21	1.93	0.50
1:A:327:MET:HE1	1:A:338:LEU:HB2	1.93	0.49
1:C:77:THR:O	1:C:81:VAL:HB	2.12	0.49
1:C:522:ASP:OD1	1:C:522:ASP:N	2.45	0.49
1:D:58:LYS:HB3	1:D:66:ARG:HD2	1.94	0.49
1:A:268:LEU:HD21	1:A:326:LEU:HD13	1.94	0.49
1:B:165:ILE:HG23	1:B:169:LEU:HD12	1.93	0.49
1:C:697:PHE:N	1:C:723:GLU:OE2	2.45	0.49
1:D:987:VAL:HG22	1:D:1028:LEU:HD13	1.93	0.49
1:A:498:LYS:NZ	1:A:524:PRO:O	2.41	0.49
1:B:176:ASP:OD1	1:B:176:ASP:N	2.45	0.49
1:D:893:CYS:O	1:D:897:THR:OG1	2.28	0.49
1:A:144:ASP:N	1:A:144:ASP:OD1	2.42	0.49
1:B:986:ARG:HE	1:B:1025:VAL:HG21	1.76	0.49
1:D:268:LEU:HD11	1:D:326:LEU:HD22	1.95	0.49
1:B:57:VAL:HG11	1:B:85:LEU:HD11	1.95	0.49
1:A:56:VAL:HG23	1:A:108:GLU:HB3	1.94	0.49
1:D:417:MET:HE3	1:D:424:ILE:HG23	1.94	0.49
1:B:645:ASN:OD1	1:B:645:ASN:N	2.45	0.49
1:D:740:ILE:HB	1:D:784:VAL:HG22	1.95	0.49
1:A:747:THR:HA	1:A:772:ALA:HB3	1.95	0.49
1:B:950:PHE:HD1	1:B:1006:TYR:CD2	2.31	0.49
1:D:278:MET:HE1	1:D:357:ILE:HG21	1.94	0.49
1:A:277:THR:HG23	1:A:339:ILE:HB	1.94	0.48
1:A:324:LEU:HD22	1:A:368:LEU:HD11	1.94	0.48
1:A:847:GLU:OE1	1:D:1085:ARG:NH1	2.47	0.48
1:B:1078:ARG:NH1	1:D:1051:TYR:OH	2.46	0.48
1:C:842:THR:O	1:C:842:THR:OG1	2.31	0.48
1:D:375:ILE:HD13	1:D:400:ILE:HD12	1.96	0.48
1:B:960:VAL:HG11	1:B:1013:ILE:HG21	1.95	0.48
1:A:893:CYS:O	1:A:897:THR:OG1	2.29	0.48
1:C:351:ALA:O	1:C:355:LYS:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:VAL:HB	1:C:394:VAL:HG21	1.95	0.48
1:D:156:VAL:HB	1:D:611:LYS:HB2	1.95	0.48
1:D:388:LEU:HG	1:D:404:VAL:HB	1.95	0.48
1:A:249:GLU:HG3	1:A:326:LEU:HD21	1.95	0.48
1:A:1011:GLU:HA	1:A:1014:THR:HG22	1.94	0.48
1:A:1023:LEU:HD23	1:A:1028:LEU:HD12	1.95	0.48
1:A:386:GLU:OE2	1:A:389:ARG:NH2	2.47	0.47
1:A:653:ARG:NH1	1:A:679:ASP:O	2.44	0.47
1:C:802:GLU:HA	1:C:805:VAL:HG12	1.95	0.47
1:D:736:LEU:HD12	1:D:740:ILE:HD11	1.95	0.47
1:C:27:ASN:HA	1:C:30:LYS:HD2	1.95	0.47
1:D:636:ILE:O	1:D:639:THR:OG1	2.31	0.47
1:A:1078:ARG:NH2	1:C:879:GLN:OE1	2.47	0.47
1:D:63:ILE:O	1:D:66:ARG:NH1	2.47	0.47
1:C:111:VAL:HG22	1:C:113:HIS:HB3	1.94	0.47
1:C:509:VAL:HG13	1:C:526:VAL:HG21	1.96	0.47
1:A:33:ARG:HE	1:A:104:ASN:HD21	1.62	0.47
1:A:224:THR:OG1	1:A:600:GLY:O	2.31	0.47
1:A:15:LEU:O	1:A:19:ILE:HB	2.14	0.47
1:B:661:SER:OG	1:B:662:ARG:N	2.48	0.47
1:C:291:THR:HG21	1:C:412:THR:HB	1.95	0.47
1:A:495:ARG:NH2	1:A:520:SER:O	2.44	0.47
1:A:925:THR:HG23	1:C:925:THR:HG23	1.97	0.47
1:B:582:THR:HG23	1:B:594:ILE:HG21	1.97	0.47
1:B:1029:ILE:O	1:B:1033:PHE:HB2	2.14	0.47
1:C:274:ARG:HB2	1:C:336:LYS:HA	1.96	0.47
1:C:338:LEU:HB3	1:C:375:ILE:HG12	1.95	0.47
1:C:407:THR:OG1	1:C:676:ARG:NH2	2.46	0.47
1:C:653:ARG:NH2	1:C:679:ASP:O	2.48	0.47
1:C:662:ARG:HH21	1:C:693:PRO:HG3	1.80	0.47
1:D:32:ALA:HB3	1:D:107:ILE:HB	1.96	0.47
1:D:291:THR:HG21	1:D:412:THR:HB	1.95	0.47
1:A:771:THR:OG1	1:A:772:ALA:N	2.48	0.47
1:B:265:LYS:NZ	1:B:306:GLU:OE1	2.47	0.47
1:B:569:LEU:HD21	1:B:571:ASN:HD22	1.80	0.47
1:B:38:THR:HA	1:B:42:ARG:HH21	1.78	0.47
1:C:908:HIS:CE1	1:D:908:HIS:HE1	2.33	0.47
1:D:582:THR:HA	1:D:585:THR:HG22	1.96	0.47
1:D:199:TYR:O	1:D:219:ALA:HA	2.14	0.47
1:D:367:PRO:O	1:D:371:HIS:HB2	2.15	0.47
1:B:972:GLY:HA2	1:B:1027:GLY:HA3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:THR:O	1:A:842:THR:OG1	2.34	0.46
1:C:5:ALA:HA	1:C:220:LYS:HA	1.98	0.46
1:A:843:SER:HB3	1:D:1094:VAL:HG23	1.97	0.46
1:B:377:VAL:HG21	1:B:391:MET:HG2	1.98	0.46
1:A:980:ILE:HD12	1:A:1015:THR:HG21	1.97	0.46
1:C:398:THR:HG23	1:C:400:ILE:H	1.80	0.46
1:C:920:LEU:HD11	1:C:1070:ILE:HG12	1.98	0.46
1:D:244:ARG:NH1	1:D:245:GLU:O	2.47	0.46
1:D:274:ARG:NH2	1:D:334:ASP:OD2	2.48	0.46
1:D:336:LYS:NZ	1:D:371:HIS:O	2.40	0.46
1:D:121:VAL:HB	1:D:202:ILE:HG13	1.98	0.46
1:D:123:ILE:HD11	1:D:188:LEU:HD13	1.97	0.46
1:D:170:LEU:HB2	1:D:178:LYS:HE3	1.97	0.46
1:B:256:LEU:HA	1:B:259:LYS:HZ2	1.81	0.46
1:B:340:ILE:O	1:B:377:VAL:HA	2.16	0.46
1:D:343:SER:OG	1:D:344:ILE:N	2.48	0.46
1:D:892:MET:HE3	1:D:892:MET:HB2	1.73	0.46
1:A:170:LEU:O	1:A:178:LYS:NZ	2.38	0.46
1:C:57:VAL:HB	1:C:107:ILE:HG22	1.98	0.46
1:C:697:PHE:HB2	1:C:723:GLU:HG2	1.97	0.46
1:B:925:THR:HG23	1:D:925:THR:HG23	1.98	0.46
1:C:146:ASP:OD1	1:C:146:ASP:N	2.49	0.46
1:A:662:ARG:NH1	1:A:718:GLU:OE2	2.47	0.45
1:B:120:TYR:HD1	1:B:203:ASN:HB2	1.81	0.45
1:D:58:LYS:HD3	1:D:66:ARG:HE	1.81	0.45
1:C:31:TYR:HB2	1:C:106:LEU:HD11	1.98	0.45
1:A:47:HIS:HD2	1:A:49:TRP:HE1	1.63	0.45
1:A:188:LEU:HD11	1:A:202:ILE:HG13	1.99	0.45
1:B:568:VAL:HB	1:B:593:THR:HG23	1.98	0.45
1:D:628:GLY:H	1:D:636:ILE:HB	1.81	0.45
1:B:635:LYS:NZ	1:B:639:THR:O	2.40	0.45
1:B:25:ILE:H	1:B:25:ILE:HG13	1.38	0.45
1:B:1044:THR:OG1	1:B:1045:ARG:N	2.45	0.45
1:C:984:ASP:HB2	1:C:986:ARG:HD2	1.99	0.45
1:B:6:ILE:HD11	1:B:236:ILE:HD12	1.98	0.45
1:B:15:LEU:O	1:B:19:ILE:HB	2.17	0.45
1:D:268:LEU:HD21	1:D:326:LEU:HD13	1.99	0.45
1:A:635:LYS:HG3	1:A:639:THR:HG23	1.99	0.45
1:B:978:LYS:HG3	1:B:984:ASP:HA	1.98	0.45
1:C:529:MET:HB2	1:C:552:VAL:HG22	1.98	0.45
1:D:915:ARG:NH1	1:D:1081:GLN:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ILE:HG23	1:A:169:LEU:HD23	1.98	0.45
1:B:1094:VAL:HG23	1:C:843:SER:HB3	2.00	0.45
1:C:176:ASP:OD1	1:C:176:ASP:N	2.40	0.45
1:C:230:LYS:HE3	1:C:230:LYS:HB2	1.80	0.45
1:B:913:CYS:SG	1:B:926:SER:OG	2.61	0.44
1:B:21:THR:OG1	1:B:22:THR:N	2.51	0.44
1:B:603:GLU:HA	1:B:606:THR:HG22	1.99	0.44
1:D:225:ALA:HB2	1:D:602:PRO:HB3	1.98	0.44
1:B:32:ALA:HB3	1:B:107:ILE:HB	1.98	0.44
1:C:1045:ARG:HA	1:C:1045:ARG:HD3	1.70	0.44
1:D:5:ALA:HA	1:D:220:LYS:HA	1.98	0.44
1:A:206:VAL:HG23	1:A:213:TYR:HB2	1.99	0.44
1:A:291:THR:HG21	1:A:412:THR:HG21	1.99	0.44
1:B:747:THR:HA	1:B:772:ALA:HB3	1.99	0.44
1:C:375:ILE:O	1:C:402:ILE:HA	2.18	0.44
1:C:867:MET:HB2	1:C:871:GLY:HA3	2.00	0.44
1:D:553:PHE:HZ	1:D:562:LYS:HD3	1.82	0.44
1:A:498:LYS:HD3	1:A:565:GLU:HG3	1.99	0.44
1:A:892:MET:HB2	1:A:892:MET:HE3	1.80	0.44
1:C:355:LYS:HA	1:C:358:VAL:HG22	1.98	0.44
1:D:338:LEU:HB3	1:D:375:ILE:HG13	1.99	0.44
1:B:278:MET:HG3	1:B:319:TYR:HE1	1.82	0.44
1:C:911:ILE:HG23	1:C:1076:GLN:HG3	2.00	0.44
1:A:726:LYS:HG2	1:A:729:ARG:HH21	1.82	0.44
1:A:933:ASP:OD1	1:A:933:ASP:N	2.41	0.44
1:C:582:THR:HG22	1:C:594:ILE:HG21	2.00	0.44
1:D:94:THR:HB	1:D:99:THR:HB	2.00	0.44
1:A:867:MET:HB2	1:A:871:GLY:HA3	2.00	0.43
1:B:49:TRP:HB2	1:B:53:GLN:HE22	1.82	0.43
1:C:257:ASP:HB2	1:C:264:LEU:HB2	1.98	0.43
1:D:857:MET:HE3	1:D:857:MET:HB2	1.87	0.43
1:A:203:ASN:HA	1:A:204:PRO:HA	1.71	0.43
1:A:1044:THR:OG1	1:A:1045:ARG:N	2.51	0.43
1:B:6:ILE:HD12	1:B:6:ILE:HA	1.86	0.43
1:B:400:ILE:H	1:B:400:ILE:HG12	1.56	0.43
1:B:569:LEU:HD22	1:B:585:THR:HG21	2.00	0.43
1:B:724:GLU:HB3	1:B:779:LEU:HD11	2.00	0.43
1:B:1031:VAL:O	1:B:1035:ASP:HB2	2.19	0.43
1:B:1065:ARG:HA	1:B:1065:ARG:HD3	1.72	0.43
1:C:329:ARG:HA	1:C:329:ARG:HD3	1.89	0.43
1:D:355:LYS:HA	1:D:358:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ILE:HG21	1:A:301:LEU:HD13	2.00	0.43
1:C:321:LYS:HG2	1:C:364:TYR:HE2	1.83	0.43
1:A:207:VAL:HG22	1:A:212:VAL:HG22	2.00	0.43
1:A:908:HIS:CE1	1:B:908:HIS:HE1	2.36	0.43
1:C:236:ILE:HD13	1:C:236:ILE:HA	1.85	0.43
1:C:835:ARG:HH22	1:D:514:ASP:CG	2.26	0.43
1:D:545:HIS:H	1:D:546:LYS:HZ2	1.66	0.43
1:D:664:GLY:O	1:D:667:SER:OG	2.35	0.43
1:B:1078:ARG:NH2	1:D:879:GLN:OE1	2.51	0.43
1:A:146:ASP:OD1	1:A:146:ASP:N	2.51	0.43
1:B:995:ARG:NH1	1:B:1008:LEU:HD12	2.22	0.43
1:A:8:GLU:OE2	1:A:66:ARG:NH2	2.40	0.43
1:C:76:LEU:HB2	1:C:81:VAL:HG23	2.00	0.43
1:C:249:GLU:HA	1:C:252:TYR:HB3	2.00	0.43
1:C:394:VAL:HA	1:C:397:THR:HG22	2.00	0.43
1:D:1065:ARG:HD3	1:D:1065:ARG:HA	1.76	0.43
1:C:892:MET:HE3	1:C:892:MET:HB2	1.83	0.43
1:D:791:ASP:OD1	1:D:791:ASP:N	2.47	0.43
1:A:1067:MET:HG2	1:C:1063:LEU:HD21	2.01	0.43
1:B:995:ARG:HH11	1:B:1008:LEU:HD11	1.82	0.43
1:C:144:ASP:OD1	1:C:144:ASP:N	2.45	0.43
1:B:577:SER:O	1:B:581:SER:OG	2.32	0.43
1:B:710:VAL:O	1:B:738:LYS:NZ	2.50	0.43
1:B:893:CYS:O	1:B:897:THR:OG1	2.29	0.43
1:C:54:ASN:HB3	1:C:110:PHE:HB3	2.01	0.43
1:C:568:VAL:HB	1:C:593:THR:HG23	2.01	0.43
1:A:202:ILE:HG23	1:A:214:VAL:HG13	2.00	0.42
1:B:899:ASP:OD2	1:B:1072:HIS:NE2	2.52	0.42
1:C:12:LYS:NZ	1:C:214:VAL:O	2.52	0.42
1:C:37:ASP:OD1	1:C:37:ASP:N	2.51	0.42
1:C:365:GLN:OE1	1:C:398:THR:OG1	2.29	0.42
1:D:288:TYR:OH	1:D:411:MET:O	2.36	0.42
1:B:324:LEU:HD22	1:B:368:LEU:HD21	2.00	0.42
1:B:340:ILE:HB	1:B:377:VAL:HG12	2.01	0.42
1:C:126:THR:HG23	1:C:129:GLY:H	1.83	0.42
1:C:175:GLU:HA	1:C:178:LYS:HD3	2.01	0.42
1:A:57:VAL:HG21	1:A:85:LEU:HD11	2.02	0.42
1:B:274:ARG:HB2	1:B:336:LYS:HA	2.00	0.42
1:D:253:ILE:HD13	1:D:253:ILE:HA	1.92	0.42
1:D:275:ILE:HA	1:D:337:ILE:HG23	2.00	0.42
1:D:725:TYR:OH	1:D:769:SER:O	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:939:LEU:HD12	1:D:1057:LEU:HD22	2.01	0.42
1:A:834:ILE:HD13	1:A:834:ILE:HA	1.75	0.42
1:B:878:PHE:HB3	1:B:1043:PHE:HZ	1.85	0.42
1:A:85:LEU:HB3	1:A:89:LEU:HD12	2.01	0.42
1:A:368:LEU:HG	1:A:373:VAL:HG21	2.02	0.42
1:C:141:ASP:OD1	1:C:141:ASP:N	2.52	0.42
1:A:120:TYR:HB3	1:A:135:HIS:HB3	2.01	0.42
1:A:330:GLU:O	1:A:336:LYS:NZ	2.41	0.42
1:A:568:VAL:HB	1:A:593:THR:HG23	2.02	0.42
1:A:747:THR:OG1	1:A:748:CYS:N	2.50	0.42
1:A:1065:ARG:HD3	1:A:1065:ARG:HA	1.78	0.42
1:B:238:PHE:HA	1:B:239:PRO:HD3	1.93	0.42
1:C:712:MET:HE3	1:C:712:MET:HB2	1.87	0.42
1:C:886:SER:OG	1:C:1036:MET:SD	2.66	0.42
1:A:650:LYS:HE3	1:A:650:LYS:HB2	1.91	0.42
1:C:322:THR:O	1:C:326:LEU:HB2	2.19	0.42
1:D:323:ILE:HD13	1:D:323:ILE:HA	1.87	0.42
1:A:102:LEU:HD23	1:A:102:LEU:HA	1.89	0.42
1:A:1029:ILE:O	1:A:1033:PHE:HB2	2.19	0.42
1:B:269:LEU:N	1:B:302:ALA:O	2.48	0.42
1:C:94:THR:HA	1:C:99:THR:HA	2.00	0.42
1:C:156:VAL:O	1:C:611:LYS:NZ	2.50	0.42
1:C:1040:CYS:SG	1:C:1041:GLY:N	2.92	0.42
1:D:340:ILE:HB	1:D:377:VAL:HG12	2.02	0.42
1:B:546:LYS:HB2	1:B:546:LYS:HE2	1.81	0.42
1:B:629:ILE:HD13	1:B:651:LEU:HD13	2.02	0.42
1:C:64:LYS:HA	1:C:64:LYS:HD3	1.83	0.42
1:D:339:ILE:HA	1:D:376:PHE:O	2.20	0.42
1:A:522:ASP:OD1	1:A:522:ASP:N	2.49	0.42
1:A:869:ILE:HG12	1:C:869:ILE:HG12	2.02	0.42
1:B:166:LYS:HA	1:B:170:LEU:HB2	2.02	0.42
1:B:1003:LEU:HD13	1:B:1003:LEU:HA	1.81	0.42
1:C:50:LEU:HD13	1:C:50:LEU:HA	1.95	0.42
1:C:411:MET:HE1	1:C:666:MET:HE1	2.02	0.42
1:C:620:ILE:HG22	1:C:694:GLY:HA3	2.02	0.42
1:B:355:LYS:HD3	1:B:355:LYS:HA	1.92	0.41
1:B:504:MET:HE1	1:B:552:VAL:HG21	2.02	0.41
1:C:6:ILE:HD11	1:C:236:ILE:HG23	2.02	0.41
1:C:643:LEU:HD12	1:C:643:LEU:HA	1.91	0.41
1:D:355:LYS:HA	1:D:355:LYS:HD2	1.92	0.41
1:B:27:ASN:HA	1:B:30:LYS:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:SER:OG	1:B:344:ILE:N	2.53	0.41
1:B:945:MET:HE3	1:B:945:MET:HB2	1.91	0.41
1:B:1008:LEU:N	1:B:1008:LEU:HD23	2.35	0.41
1:B:1067:MET:HG2	1:D:1063:LEU:HD21	2.02	0.41
1:A:227:TYR:O	1:C:961:ASN:ND2	2.46	0.41
1:A:514:ASP:HB3	1:A:643:LEU:HD13	2.01	0.41
1:B:36:PRO:HG3	1:B:89:LEU:HG	2.02	0.41
1:B:560:MET:O	1:B:590:GLN:NE2	2.51	0.41
1:D:956:PRO:HB2	1:D:1013:ILE:HD12	2.02	0.41
1:B:696:THR:OG1	1:B:697:PHE:N	2.52	0.41
1:C:367:PRO:HA	1:C:370:GLU:HB3	2.02	0.41
1:A:123:ILE:HD13	1:A:189:PHE:HD1	1.85	0.41
1:A:177:LYS:O	1:A:181:LEU:HB2	2.20	0.41
1:A:344:ILE:HB	1:A:668:ASN:HB3	2.02	0.41
1:A:965:LYS:HB2	1:A:965:LYS:HE3	1.88	0.41
1:B:97:LYS:HE2	1:B:97:LYS:HB3	1.91	0.41
1:B:857:MET:HE3	1:B:857:MET:HB2	1.91	0.41
1:C:50:LEU:HD11	1:C:107:ILE:HD12	2.03	0.41
1:C:628:GLY:H	1:C:636:ILE:HB	1.85	0.41
1:D:324:LEU:O	1:D:328:THR:OG1	2.38	0.41
1:A:823:MET:N	1:B:834:ILE:O	2.54	0.41
1:A:835:ARG:HB2	1:B:822:PRO:HG2	2.02	0.41
1:C:292:ILE:HG21	1:C:301:LEU:HD13	2.02	0.41
1:A:592:ARG:HA	1:A:618:VAL:HG12	2.03	0.41
1:A:671:ASN:O	1:A:675:SER:OG	2.35	0.41
1:B:260:SER:OG	1:B:261:GLY:N	2.51	0.41
1:B:625:THR:OG1	1:B:626:VAL:N	2.54	0.41
1:B:973:ILE:HG22	1:B:1022:ILE:C	2.46	0.41
1:D:365:GLN:HG2	1:D:398:THR:HG23	2.03	0.41
1:A:148:LYS:HB3	1:A:148:LYS:HE2	1.86	0.41
1:A:623:PRO:O	1:A:690:ASP:OD2	2.39	0.41
1:A:802:GLU:HA	1:A:805:VAL:HG12	2.03	0.41
1:A:918:LYS:HA	1:A:918:LYS:HD2	1.91	0.41
1:B:670:LEU:HD23	1:B:670:LEU:HA	1.92	0.41
1:B:712:MET:HE3	1:B:712:MET:HB2	1.95	0.41
1:C:123:ILE:HA	1:C:131:TYR:O	2.21	0.41
1:D:76:LEU:HD22	1:D:80:GLY:HA3	2.03	0.41
1:D:354:PHE:HA	1:D:357:ILE:HG12	2.03	0.41
1:D:729:ARG:O	1:D:733:GLU:HB2	2.21	0.41
1:D:920:LEU:HD11	1:D:1070:ILE:HG23	2.03	0.41
1:A:840:PHE:O	1:A:842:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:LEU:HD21	1:C:925:THR:HG21	2.02	0.41
1:B:801:TYR:HE1	1:B:810:ILE:HG21	1.86	0.41
1:D:643:LEU:HD12	1:D:646:ILE:HB	2.02	0.41
1:A:854:TYR:HB3	1:A:855:ALA:H	1.73	0.40
1:B:17:LYS:HB2	1:B:17:LYS:HE3	1.84	0.40
1:B:919:ASP:N	1:B:919:ASP:OD1	2.54	0.40
1:C:377:VAL:HG11	1:C:391:MET:HG2	2.03	0.40
1:D:516:ASP:OD2	1:D:525:SER:OG	2.37	0.40
1:D:841:MET:HE2	1:D:841:MET:HB3	1.85	0.40
1:A:199:TYR:OH	1:A:201:GLU:OE1	2.29	0.40
1:C:32:ALA:HB3	1:C:107:ILE:HG13	2.03	0.40
1:B:244:ARG:H	1:B:244:ARG:HG3	1.61	0.40
1:B:1075:ASP:OD2	1:D:843:SER:N	2.54	0.40
1:C:383:ASN:ND2	1:C:386:GLU:OE1	2.39	0.40
1:D:317:TYR:HB2	1:D:359:ARG:HH12	1.86	0.40
1:D:546:LYS:H	1:D:546:LYS:HG2	1.70	0.40
1:B:657:VAL:HG21	1:B:678:THR:HG21	2.04	0.40
1:B:925:THR:HG21	1:D:929:LEU:HD21	2.03	0.40
1:B:994:VAL:O	1:B:998:PHE:HB2	2.20	0.40
1:A:801:TYR:HE1	1:A:810:ILE:HG21	1.86	0.40
1:B:892:MET:HE3	1:B:892:MET:HB2	1.84	0.40
1:B:911:ILE:HG23	1:B:1076:GLN:HG3	2.04	0.40
1:C:925:THR:HG22	1:D:929:LEU:HD13	2.03	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	1017/1101 (92%)	940 (92%)	76 (8%)	1 (0%)	48 79
1	B	1017/1101 (92%)	945 (93%)	69 (7%)	3 (0%)	36 67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	1017/1101 (92%)	947 (93%)	69 (7%)	1 (0%)	48 79
1	D	1017/1101 (92%)	936 (92%)	80 (8%)	1 (0%)	48 79
All	All	4068/4404 (92%)	3768 (93%)	294 (7%)	6 (0%)	49 79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	623	PRO
1	B	835	ARG
1	B	1021	LEU
1	D	835	ARG
1	B	975	HIS
1	C	835	ARG

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	842/909 (93%)	752 (89%)	90 (11%)	6 27
1	B	841/909 (92%)	743 (88%)	98 (12%)	5 24
1	C	841/909 (92%)	747 (89%)	94 (11%)	6 25
1	D	842/909 (93%)	736 (87%)	106 (13%)	4 21
All	All	3366/3636 (93%)	2978 (88%)	388 (12%)	8 24

All (388) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	25	ILE
1	A	34	VAL
1	A	54	ASN
1	A	56	VAL
1	A	62	LEU

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Mol	Chain	Res	Type
1	A	69	LEU
1	A	74	VAL
1	A	78	LEU
1	A	101	PHE
1	A	130	ASP
1	A	131	TYR
1	A	144	ASP
1	A	154	VAL
1	A	157	ASP
1	A	175	GLU
1	A	195	LEU
1	A	206	VAL
1	A	210	ASP
1	A	217	LEU
1	A	226[A]	ASP
1	A	226[B]	ASP
1	A	228	ILE
1	A	237	GLU
1	A	245	GLU
1	A	249	GLU
1	A	255	ASP
1	A	256	LEU
1	A	267	THR
1	A	277	THR
1	A	279	VAL
1	A	287	VAL
1	A	313	GLU
1	A	368	LEU
1	A	374	THR
1	A	407	THR
1	A	409	THR
1	A	414	ILE
1	A	419	LEU
1	A	491	THR
1	A	507	ARG
1	A	518	VAL
1	A	552	VAL
1	A	566	VAL
1	A	568	VAL
1	A	569	LEU
1	A	575	LEU
1	A	593	THR

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Mol	Chain	Res	Type
1	A	597	ILE
1	A	619	THR
1	A	621	ILE
1	A	639	THR
1	A	643	LEU
1	A	650	LYS
1	A	662	ARG
1	A	678	THR
1	A	690	ASP
1	A	707	THR
1	A	719	ILE
1	A	724	GLU
1	A	750	THR
1	A	788	ARG
1	A	792	GLU
1	A	809	VAL
1	A	811	VAL
1	A	823	MET
1	A	824	ASP
1	A	829	ARG
1	A	831	LEU
1	A	833	LEU
1	A	834	ILE
1	A	844	ILE
1	A	869	ILE
1	A	873	LEU
1	A	881	ARG
1	A	904	VAL
1	A	905	SER
1	A	921	VAL
1	A	925	THR
1	A	926	SER
1	A	939	LEU
1	A	977	VAL
1	A	987	VAL
1	A	1001	THR
1	A	1011	GLU
1	A	1021	LEU
1	A	1036	MET
1	A	1075	ASP
1	A	1095	LEU
1	A	1097	GLU

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Mol	Chain	Res	Type
1	B	7	SER
1	B	14	LEU
1	B	25	ILE
1	B	27	ASN
1	B	34	VAL
1	B	42	ARG
1	B	44	LEU
1	B	53	GLN
1	B	56	VAL
1	B	62	LEU
1	B	69	LEU
1	B	72	VAL
1	B	77	THR
1	B	78	LEU
1	B	95	VAL
1	B	102	LEU
1	B	115	GLN
1	B	118	GLU
1	B	123	ILE
1	B	132	VAL
1	B	140	VAL
1	B	142	VAL
1	B	144	ASP
1	B	145	VAL
1	B	154	VAL
1	B	156	VAL
1	B	195	LEU
1	B	198	THR
1	B	207	VAL
1	B	221	VAL
1	B	228	ILE
1	B	236	ILE
1	B	256	LEU
1	B	279	VAL
1	B	290	ASP
1	B	294	ASP
1	B	298	VAL
1	B	346	ASN
1	B	369	LYS
1	B	394	VAL
1	B	400	ILE
1	B	412	THR

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Mol	Chain	Res	Type
1	B	414	ILE
1	B	415	VAL
1	B	491	THR
1	B	500	ILE
1	B	506	THR
1	B	552	VAL
1	B	568	VAL
1	B	569	LEU
1	B	575	LEU
1	B	593	THR
1	B	639	THR
1	B	645	ASN
1	B	678	THR
1	B	710	VAL
1	B	719	ILE
1	B	773	VAL
1	B	779	LEU
1	B	791	ASP
1	B	792	GLU
1	B	793	LEU
1	B	809	VAL
1	B	811	VAL
1	B	820	THR
1	B	821	VAL
1	B	831	LEU
1	B	836	LYS
1	B	839	SER
1	B	844	ILE
1	B	873	LEU
1	B	904	VAL
1	B	905	SER
1	B	921	VAL
1	B	925	THR
1	B	926	SER
1	B	933	ASP
1	B	939	LEU
1	B	954	ILE
1	B	955	ILE
1	B	973	ILE
1	B	979	SER
1	B	981	ASN
1	B	987	VAL

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Mol	Chain	Res	Type
1	B	1001	THR
1	B	1003	LEU
1	B	1005	ASP
1	B	1008	LEU
1	B	1009	GLU
1	B	1017	LYS
1	B	1020	ASN
1	B	1021	LEU
1	B	1022	ILE
1	B	1025	VAL
1	B	1057	LEU
1	B	1077	LYS
1	B	1095	LEU
1	B	1097	GLU
1	C	25	ILE
1	C	29	PHE
1	C	34	VAL
1	C	37	ASP
1	C	50	LEU
1	C	57	VAL
1	C	58	LYS
1	C	77	THR
1	C	78	LEU
1	C	81	VAL
1	C	89	LEU
1	C	102	LEU
1	C	111	VAL
1	C	121	VAL
1	C	128	GLU
1	C	140	VAL
1	C	150	GLN
1	C	154	VAL
1	C	156	VAL
1	C	175	GLU
1	C	179	GLU
1	C	195	LEU
1	C	201	GLU
1	C	208	THR
1	C	221	VAL
1	C	228	ILE
1	C	236	ILE
1	C	279	VAL

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Mol	Chain	Res	Type
1	C	293	CYS
1	C	326	LEU
1	C	339	ILE
1	C	373	VAL
1	C	377	VAL
1	C	414	ILE
1	C	415	VAL
1	C	516	ASP
1	C	518	VAL
1	C	558	ASP
1	C	567	ASP
1	C	568	VAL
1	C	569	LEU
1	C	575	LEU
1	C	593	THR
1	C	597	ILE
1	C	601	ILE
1	C	645	ASN
1	C	678	THR
1	C	707	THR
1	C	710	VAL
1	C	716	LEU
1	C	719	ILE
1	C	750	THR
1	C	788	ARG
1	C	792	GLU
1	C	793	LEU
1	C	809	VAL
1	C	810	ILE
1	C	811	VAL
1	C	823	MET
1	C	829	ARG
1	C	833	LEU
1	C	834	ILE
1	C	836	LYS
1	C	839	SER
1	C	842	THR
1	C	844	ILE
1	C	848	ARG
1	C	866	GLU
1	C	869	ILE
1	C	873	LEU

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Mol	Chain	Res	Type
1	C	896	VAL
1	C	897	THR
1	C	905	SER
1	C	920	LEU
1	C	921	VAL
1	C	925	THR
1	C	933	ASP
1	C	939	LEU
1	C	954	ILE
1	C	955	ILE
1	C	964	LYS
1	C	977	VAL
1	C	981	ASN
1	C	985	MET
1	C	986	ARG
1	C	987	VAL
1	C	1001	THR
1	C	1014	THR
1	C	1022	ILE
1	C	1025	VAL
1	C	1028	LEU
1	C	1033	PHE
1	C	1040	CYS
1	C	1045	ARG
1	D	22	THR
1	D	34	VAL
1	D	43	LEU
1	D	47	HIS
1	D	50	LEU
1	D	63	ILE
1	D	77	THR
1	D	78	LEU
1	D	79	ASP
1	D	91	GLN
1	D	92	GLU
1	D	94	THR
1	D	95	VAL
1	D	97	LYS
1	D	99	THR
1	D	106	LEU
1	D	111	VAL
1	D	123	ILE

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Mol	Chain	Res	Type
1	D	128	GLU
1	D	132	VAL
1	D	140	VAL
1	D	141	ASP
1	D	142	VAL
1	D	153	LEU
1	D	154	VAL
1	D	156	VAL
1	D	168	HIS
1	D	177	LYS
1	D	188	LEU
1	D	200	LEU
1	D	202	ILE
1	D	205	LEU
1	D	228	ILE
1	D	229	CYS
1	D	242	PHE
1	D	259	LYS
1	D	267	THR
1	D	274	ARG
1	D	275	ILE
1	D	290	ASP
1	D	323	ILE
1	D	327	MET
1	D	328	THR
1	D	334	ASP
1	D	337	ILE
1	D	339	ILE
1	D	350	VAL
1	D	363	ASP
1	D	368	LEU
1	D	371	HIS
1	D	385	GLN
1	D	495	ARG
1	D	497	THR
1	D	504	MET
1	D	506	THR
1	D	513	LEU
1	D	522	ASP
1	D	526	VAL
1	D	542	TYR
1	D	546	LYS

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Mol	Chain	Res	Type
1	D	566	VAL
1	D	567	ASP
1	D	568	VAL
1	D	575	LEU
1	D	585	THR
1	D	593	THR
1	D	609	LEU
1	D	618	VAL
1	D	619	THR
1	D	620	ILE
1	D	639	THR
1	D	647	LEU
1	D	660	VAL
1	D	668	ASN
1	D	678	THR
1	D	712	MET
1	D	718	GLU
1	D	719	ILE
1	D	771	THR
1	D	779	LEU
1	D	805	VAL
1	D	823	MET
1	D	831	LEU
1	D	833	LEU
1	D	839	SER
1	D	844	ILE
1	D	869	ILE
1	D	872	VAL
1	D	873	LEU
1	D	896	VAL
1	D	921	VAL
1	D	925	THR
1	D	930	THR
1	D	939	LEU
1	D	955	ILE
1	D	976	ARG
1	D	977	VAL
1	D	987	VAL
1	D	1001	THR
1	D	1021	LEU
1	D	1025	VAL
1	D	1036	MET

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Mol	Chain	Res	Type
1	D	1040	CYS
1	D	1045	ARG
1	D	1075	ASP
1	D	1095	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	47	HIS
1	A	54	ASN
1	A	104	ASN
1	A	161	ASN
1	A	203	ASN
1	A	332	HIS
1	A	545	HIS
1	A	638	ASN
1	A	668	ASN
1	A	705	GLN
1	A	777	GLN
1	A	807	ASN
1	A	814	GLN
1	A	908	HIS
1	A	961	ASN
1	B	26	GLN
1	B	47	HIS
1	B	53	GLN
1	B	135	HIS
1	B	346	ASN
1	B	403	HIS
1	B	571	ASN
1	B	777	GLN
1	B	850	GLN
1	B	908	HIS
1	B	988	GLN
1	C	113	HIS
1	C	150	GLN
1	C	270	ASN
1	C	299	ASN
1	C	346	ASN
1	C	545	HIS
1	C	587	ASN

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Mol	Chain	Res	Type
1	C	638	ASN
1	C	705	GLN
1	C	850	GLN
1	C	888	GLN
1	C	900	HIS
1	C	988	GLN
1	C	1086	HIS
1	D	27	ASN
1	D	54	ASN
1	D	75	ASN
1	D	150	GLN
1	D	346	ASN
1	D	385	GLN
1	D	645	ASN
1	D	671	ASN
1	D	767	GLN
1	D	776	ASN
1	D	888	GLN
1	D	908	HIS
1	D	961	ASN
1	D	981	ASN
1	D	988	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](#)

4 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	COA	C	1202	-	47,50,50	2.97	19 (40%)	69,75,75	1.95	12 (17%)
2	COA	B	1201	-	47,50,50	3.07	20 (42%)	69,75,75	1.91	13 (18%)
2	COA	C	1201	-	47,50,50	3.01	19 (40%)	69,75,75	1.93	11 (15%)
2	COA	B	1202	-	47,50,50	3.01	19 (40%)	69,75,75	1.98	14 (20%)

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	COA	C	1202	-	-	20/48/64/64	0/3/3/3
2	COA	B	1201	-	-	18/48/64/64	0/3/3/3
2	COA	C	1201	-	-	13/48/64/64	0/3/3/3
2	COA	B	1202	-	-	11/48/64/64	0/3/3/3

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	COA	O4B-C1B	9.17	1.63	1.42
2	C	1202	COA	O4B-C1B	9.14	1.63	1.42
2	C	1201	COA	O4B-C1B	9.00	1.62	1.42
2	B	1202	COA	O4B-C1B	8.69	1.62	1.42
2	B	1201	COA	C9P-N8P	6.83	1.49	1.33
2	B	1202	COA	C9P-N8P	6.82	1.49	1.33
2	C	1201	COA	C9P-N8P	6.79	1.49	1.33
2	B	1202	COA	C2B-C1B	-6.71	1.32	1.53
2	C	1202	COA	C9P-N8P	6.67	1.49	1.33
2	C	1201	COA	C2B-C1B	-6.62	1.32	1.53
2	B	1201	COA	C2B-C1B	-6.52	1.33	1.53
2	C	1202	COA	C2B-C1B	-6.42	1.33	1.53
2	B	1201	COA	P2A-O3A	6.16	1.66	1.59
2	C	1201	COA	O4B-C4B	-6.14	1.31	1.45
2	C	1202	COA	O4B-C4B	-6.08	1.31	1.45
2	B	1202	COA	O4B-C4B	-6.04	1.31	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	COA	O4B-C4B	-5.94	1.31	1.45
2	B	1201	COA	C5P-N4P	5.49	1.46	1.33
2	C	1201	COA	C5P-N4P	5.47	1.46	1.33
2	B	1202	COA	C5P-N4P	5.40	1.46	1.33
2	C	1201	COA	P2A-O3A	5.18	1.65	1.59
2	C	1202	COA	C5P-N4P	5.15	1.45	1.33
2	C	1202	COA	C6A-N6A	5.04	1.47	1.34
2	B	1201	COA	C6A-N6A	5.04	1.47	1.34
2	C	1201	COA	C6A-N6A	4.92	1.46	1.34
2	B	1202	COA	P2A-O3A	4.88	1.64	1.59
2	B	1202	COA	C6A-N6A	4.87	1.46	1.34
2	B	1201	COA	P1A-O3A	4.79	1.64	1.59
2	C	1202	COA	P2A-O3A	4.61	1.64	1.59
2	B	1202	COA	CCP-CBP	4.32	1.59	1.52
2	B	1201	COA	CCP-CBP	4.03	1.59	1.52
2	C	1201	COA	P1A-O3A	4.00	1.63	1.59
2	B	1202	COA	C5A-C4A	-3.89	1.32	1.39
2	B	1202	COA	P1A-O3A	3.89	1.63	1.59
2	C	1202	COA	CCP-CBP	3.80	1.58	1.52
2	C	1202	COA	P1A-O3A	3.74	1.63	1.59
2	C	1201	COA	CCP-CBP	3.74	1.58	1.52
2	C	1201	COA	C5A-C4A	-3.73	1.32	1.39
2	C	1202	COA	C5A-C4A	-3.71	1.32	1.39
2	B	1201	COA	C5A-C4A	-3.39	1.33	1.39
2	B	1202	COA	O9P-C9P	-3.02	1.17	1.23
2	B	1201	COA	P3B-O3B	3.02	1.64	1.59
2	C	1202	COA	C8A-N9A	-2.99	1.32	1.37
2	B	1202	COA	C8A-N9A	-2.98	1.32	1.37
2	C	1202	COA	P3B-O3B	2.96	1.64	1.59
2	C	1201	COA	C8A-N9A	-2.88	1.32	1.37
2	B	1202	COA	C6P-C5P	2.83	1.57	1.51
2	C	1202	COA	O9P-C9P	-2.80	1.18	1.23
2	B	1201	COA	C6P-C5P	2.78	1.56	1.51
2	B	1202	COA	OAP-CAP	-2.77	1.37	1.42
2	C	1201	COA	C6P-C5P	2.76	1.56	1.51
2	B	1202	COA	P3B-O3B	2.73	1.64	1.59
2	C	1202	COA	OAP-CAP	-2.72	1.37	1.42
2	B	1201	COA	O9P-C9P	-2.72	1.18	1.23
2	C	1201	COA	O9P-C9P	-2.71	1.18	1.23
2	C	1201	COA	P3B-O3B	2.69	1.64	1.59
2	B	1202	COA	C5A-N7A	-2.69	1.34	1.39
2	C	1201	COA	OAP-CAP	-2.56	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1201	COA	C5A-N7A	-2.56	1.34	1.39
2	C	1202	COA	C5A-N7A	-2.50	1.34	1.39
2	B	1201	COA	C8A-N9A	-2.46	1.33	1.37
2	C	1202	COA	O2B-C2B	2.45	1.49	1.43
2	C	1202	COA	C6P-C5P	2.44	1.56	1.51
2	B	1201	COA	OAP-CAP	-2.42	1.38	1.42
2	C	1201	COA	O3B-C3B	-2.35	1.36	1.44
2	B	1201	COA	O2B-C2B	2.34	1.48	1.43
2	B	1202	COA	O3B-C3B	-2.32	1.36	1.44
2	C	1201	COA	O2B-C2B	2.29	1.48	1.43
2	B	1201	COA	C5A-N7A	-2.27	1.34	1.39
2	C	1202	COA	O5P-C5P	-2.23	1.18	1.23
2	B	1202	COA	O2B-C2B	2.19	1.48	1.43
2	B	1201	COA	O3B-C3B	-2.19	1.36	1.44
2	C	1202	COA	O3B-C3B	-2.19	1.36	1.44
2	B	1202	COA	O5P-C5P	-2.16	1.19	1.23
2	B	1201	COA	P2A-O6A	2.03	1.67	1.59
2	C	1201	COA	O5P-C5P	-2.03	1.19	1.23
2	B	1201	COA	P1A-O5B	2.03	1.67	1.59

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1202	COA	N6A-C6A-N1A	-7.40	101.90	118.38
2	B	1201	COA	N6A-C6A-N1A	-7.38	101.94	118.38
2	C	1201	COA	N6A-C6A-N1A	-7.16	102.43	118.38
2	C	1202	COA	N6A-C6A-N1A	-6.90	103.01	118.38
2	C	1202	COA	N3A-C2A-N1A	-6.10	119.35	128.58
2	B	1202	COA	N3A-C2A-N1A	-6.08	119.38	128.58
2	B	1201	COA	N3A-C2A-N1A	-5.94	119.59	128.58
2	C	1201	COA	N3A-C2A-N1A	-5.92	119.62	128.58
2	B	1201	COA	C5A-C6A-N6A	5.83	137.73	123.29
2	B	1202	COA	C5A-C6A-N6A	5.78	137.60	123.29
2	C	1201	COA	C5A-C6A-N6A	5.62	137.21	123.29
2	C	1202	COA	C5A-C6A-N6A	5.39	136.62	123.29
2	C	1202	COA	C5A-C4A-N3A	-4.87	120.02	126.72
2	C	1201	COA	C5A-C4A-N3A	-4.63	120.34	126.72
2	B	1202	COA	C5A-C4A-N3A	-4.57	120.42	126.72
2	B	1201	COA	C5A-C4A-N3A	-4.56	120.44	126.72
2	B	1202	COA	N9A-C8A-N7A	-4.37	107.73	113.94
2	C	1202	COA	N9A-C8A-N7A	-4.31	107.83	113.94
2	C	1201	COA	N9A-C8A-N7A	-4.26	107.89	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	COA	N9A-C8A-N7A	-4.13	108.08	113.94
2	C	1202	COA	C2A-N3A-C4A	3.56	120.51	111.83
2	B	1202	COA	C2A-N3A-C4A	3.43	120.21	111.83
2	B	1201	COA	C2A-N3A-C4A	3.40	120.13	111.83
2	C	1201	COA	C2A-N3A-C4A	3.37	120.07	111.83
2	C	1202	COA	N3A-C4A-N9A	3.14	132.51	127.17
2	B	1202	COA	C5A-N7A-C8A	2.86	107.94	103.45
2	C	1202	COA	C5A-N7A-C8A	2.78	107.82	103.45
2	C	1201	COA	N3A-C4A-N9A	2.76	131.86	127.17
2	C	1201	COA	C5A-N7A-C8A	2.74	107.76	103.45
2	B	1201	COA	C5A-N7A-C8A	2.72	107.72	103.45
2	B	1202	COA	CAP-C9P-N8P	2.67	121.55	116.48
2	B	1202	COA	C6P-C5P-N4P	2.62	121.12	116.34
2	B	1202	COA	N3A-C4A-N9A	2.59	131.57	127.17
2	B	1201	COA	N3A-C4A-N9A	2.57	131.53	127.17
2	C	1202	COA	C4A-N9A-C8A	2.53	108.40	105.74
2	C	1202	COA	C6P-C5P-N4P	2.41	120.74	116.34
2	C	1201	COA	C4A-N9A-C8A	2.33	108.18	105.74
2	B	1202	COA	C4A-N9A-C8A	2.30	108.16	105.74
2	C	1201	COA	CAP-C9P-N8P	2.22	120.70	116.48
2	C	1202	COA	C3P-N4P-C5P	-2.15	118.82	122.82
2	B	1201	COA	C6P-C5P-N4P	2.14	120.23	116.34
2	B	1202	COA	C4A-C5A-N7A	-2.12	108.15	110.58
2	B	1201	COA	CAP-C9P-N8P	2.10	120.47	116.48
2	C	1202	COA	C1B-N9A-C8A	-2.08	122.47	127.09
2	B	1201	COA	C4A-N9A-C8A	2.07	107.92	105.74
2	B	1201	COA	C5A-C4A-N9A	2.03	108.03	105.81
2	B	1201	COA	C4A-C5A-N7A	-2.03	108.26	110.58
2	C	1201	COA	C6P-C5P-N4P	2.03	120.04	116.34
2	B	1202	COA	C5A-C4A-N9A	2.02	108.01	105.81
2	B	1202	COA	O5P-C5P-N4P	-2.00	119.10	123.03

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1201	COA	C5B-O5B-P1A-O3A
2	B	1201	COA	CCP-O6A-P2A-O3A
2	B	1201	COA	CCP-O6A-P2A-O4A
2	B	1201	COA	CCP-O6A-P2A-O5A
2	B	1201	COA	CEP-CBP-CCP-O6A
2	B	1201	COA	CAP-CBP-CCP-O6A

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Mol	Chain	Res	Type	Atoms
2	B	1201	COA	OAP-CAP-CBP-CCP
2	B	1201	COA	C9P-CAP-CBP-CCP
2	B	1201	COA	OAP-CAP-CBP-CDP
2	B	1201	COA	C9P-CAP-CBP-CDP
2	B	1201	COA	OAP-CAP-CBP-CEP
2	B	1201	COA	C9P-CAP-CBP-CEP
2	B	1202	COA	C5B-O5B-P1A-O1A
2	B	1202	COA	CBP-CCP-O6A-P2A
2	B	1202	COA	CDP-CBP-CCP-O6A
2	B	1202	COA	CEP-CBP-CCP-O6A
2	B	1202	COA	CAP-CBP-CCP-O6A
2	B	1202	COA	C5P-C6P-C7P-N8P
2	C	1201	COA	C3B-C4B-C5B-O5B
2	C	1201	COA	P2A-O3A-P1A-O5B
2	C	1201	COA	N8P-C9P-CAP-OAP
2	C	1201	COA	C5P-C6P-C7P-N8P
2	C	1201	COA	S1P-C2P-C3P-N4P
2	C	1202	COA	C5B-O5B-P1A-O1A
2	C	1202	COA	C5B-O5B-P1A-O3A
2	C	1202	COA	OAP-CAP-CBP-CCP
2	C	1202	COA	C9P-CAP-CBP-CCP
2	C	1202	COA	OAP-CAP-CBP-CDP
2	C	1202	COA	C9P-CAP-CBP-CDP
2	C	1202	COA	C9P-CAP-CBP-CEP
2	C	1201	COA	O4B-C4B-C5B-O5B
2	C	1201	COA	O9P-C9P-CAP-OAP
2	B	1201	COA	C4B-C5B-O5B-P1A
2	C	1202	COA	C2B-C3B-O3B-P3B
2	C	1202	COA	OAP-CAP-CBP-CEP
2	B	1202	COA	N8P-C9P-CAP-OAP
2	B	1202	COA	C3B-C4B-C5B-O5B
2	B	1202	COA	O4B-C4B-C5B-O5B
2	B	1201	COA	C3B-C4B-C5B-O5B
2	B	1202	COA	O9P-C9P-CAP-OAP
2	B	1201	COA	CDP-CBP-CCP-O6A
2	C	1201	COA	CEP-CBP-CCP-O6A
2	C	1202	COA	CEP-CBP-CCP-O6A
2	C	1202	COA	CAP-CBP-CCP-O6A
2	B	1202	COA	C5B-O5B-P1A-O3A
2	C	1201	COA	C5B-O5B-P1A-O3A
2	C	1202	COA	C5B-O5B-P1A-O2A
2	C	1202	COA	CCP-O6A-P2A-O4A

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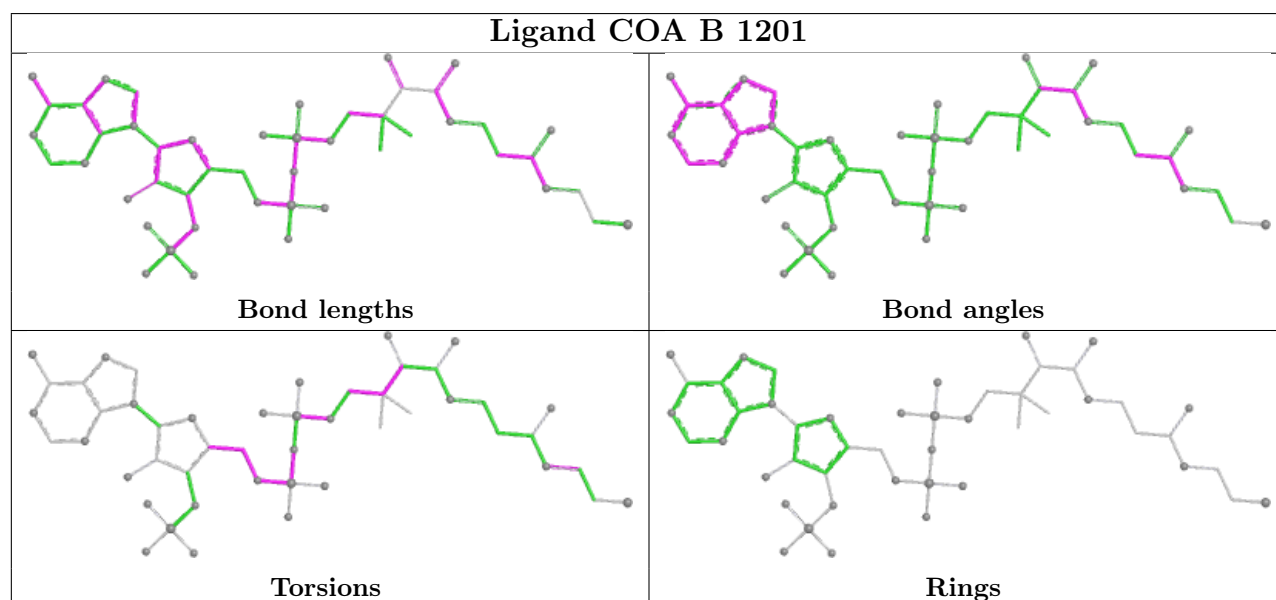
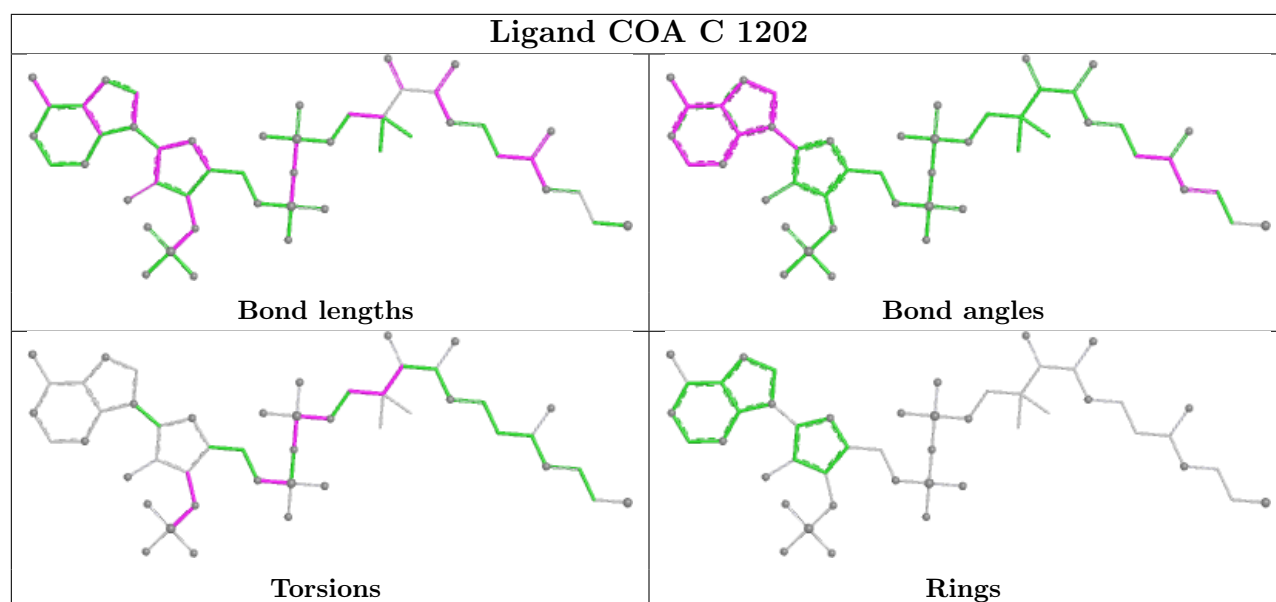
Mol	Chain	Res	Type	Atoms
2	B	1201	COA	P2A-O3A-P1A-O2A
2	C	1201	COA	P1A-O3A-P2A-O5A
2	C	1202	COA	P1A-O3A-P2A-O5A
2	C	1202	COA	C4B-C3B-O3B-P3B
2	C	1202	COA	C3B-O3B-P3B-O7A
2	B	1201	COA	P2A-O3A-P1A-O1A
2	C	1201	COA	P1A-O3A-P2A-O4A
2	C	1202	COA	P1A-O3A-P2A-O4A
2	C	1202	COA	C3B-O3B-P3B-O8A
2	C	1202	COA	C3B-O3B-P3B-O9A
2	C	1201	COA	CDP-CBP-CCP-O6A
2	C	1202	COA	CDP-CBP-CCP-O6A
2	C	1201	COA	C3B-O3B-P3B-O7A
2	B	1201	COA	C2P-C3P-N4P-C5P

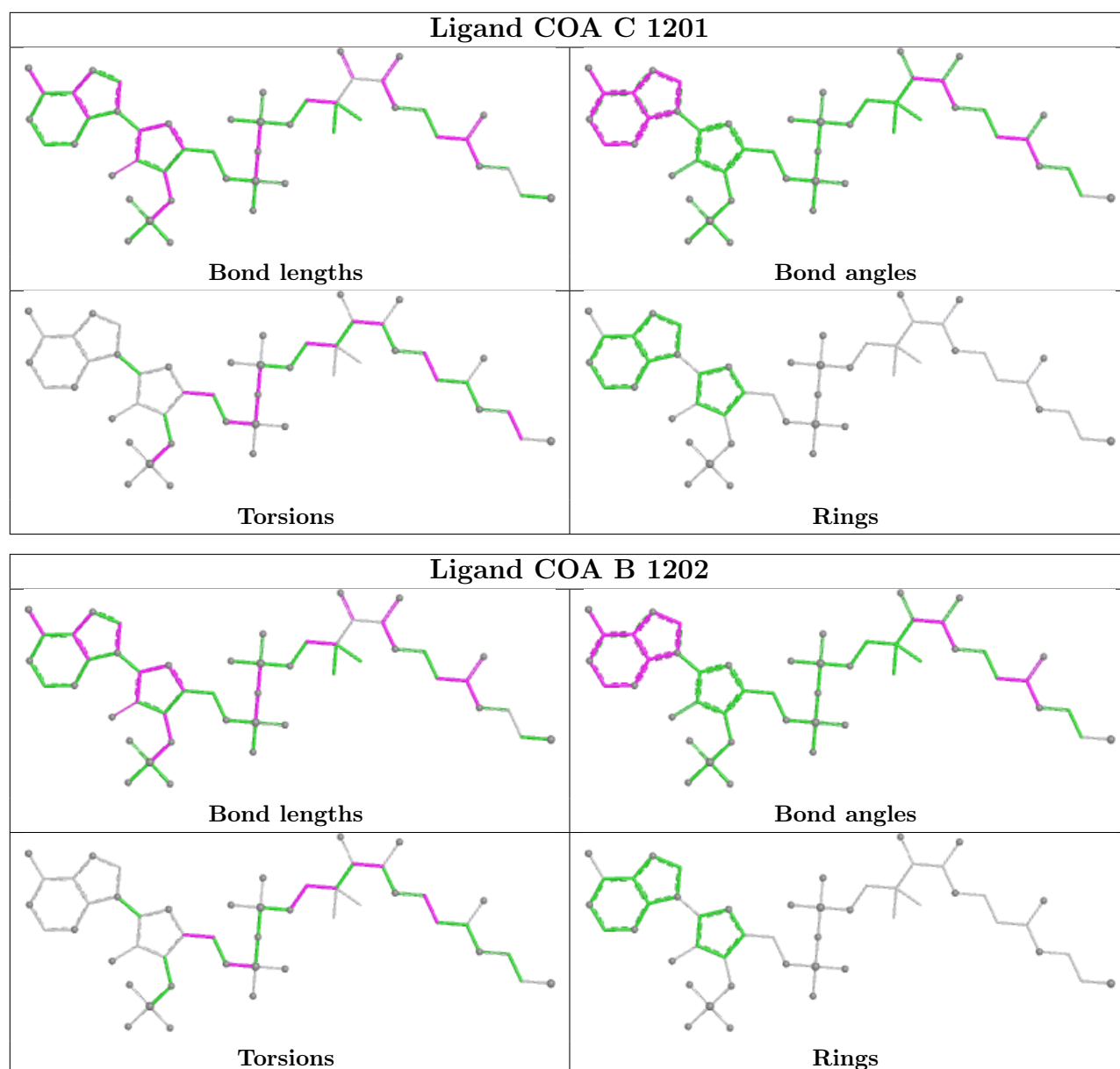
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1201	COA	2	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.

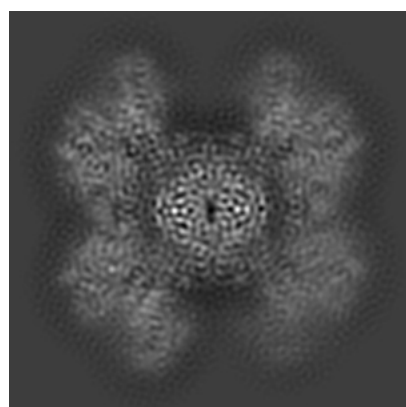
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20413. These allow visual inspection of the internal detail of the map and identification of artifacts.

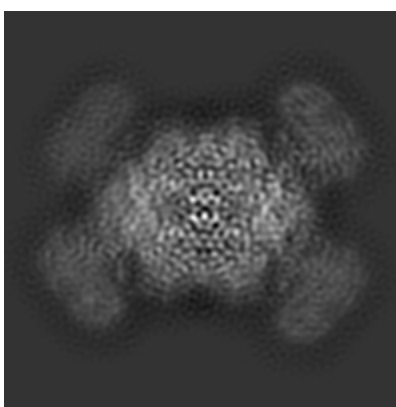
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

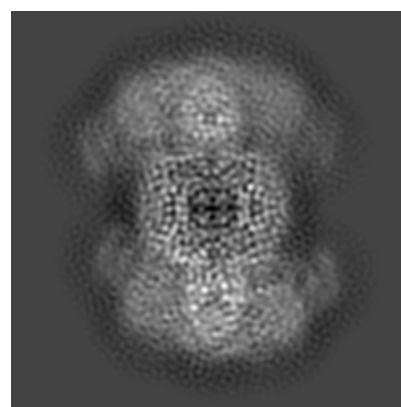
6.1.1 Primary map



X



Y

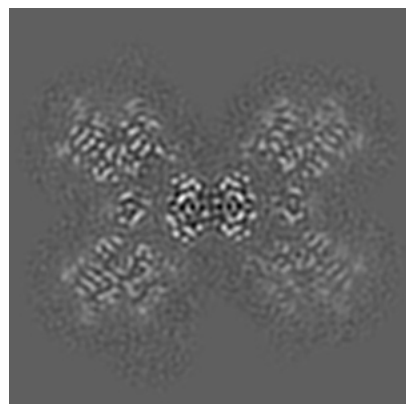


Z

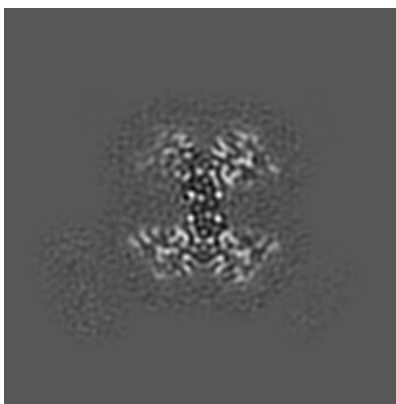
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

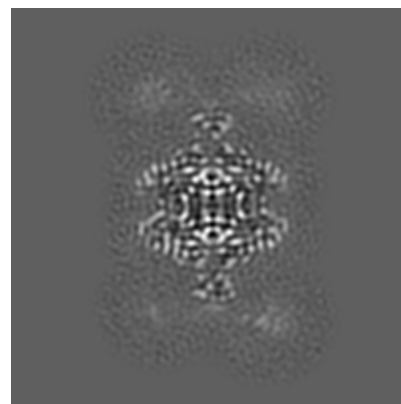
6.2.1 Primary map



X Index: 110



Y Index: 110

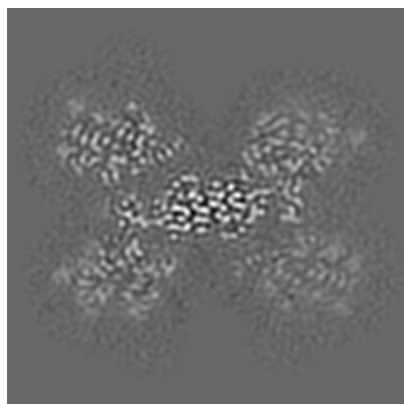


Z Index: 110

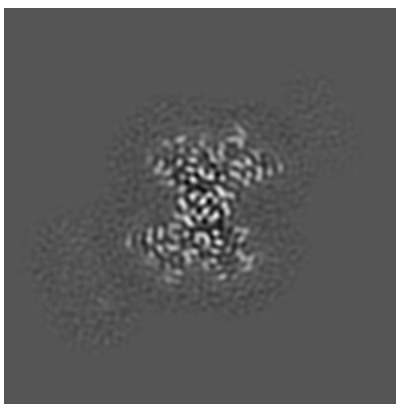
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

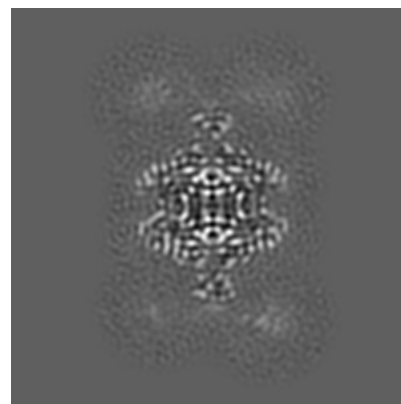
6.3.1 Primary map



X Index: 115



Y Index: 104

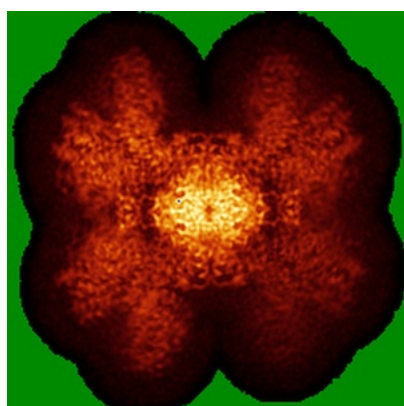


Z Index: 110

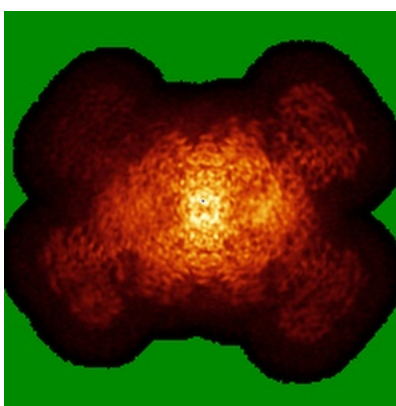
The images above show the largest variance slices of the map in three orthogonal directions.

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

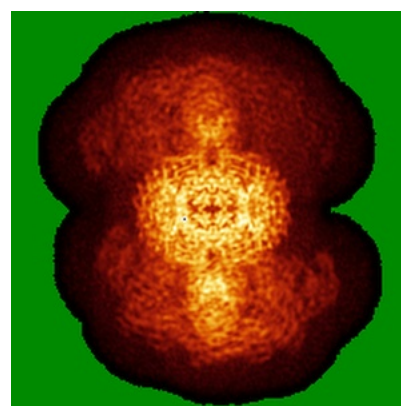
6.4.1 Primary map



X



Y

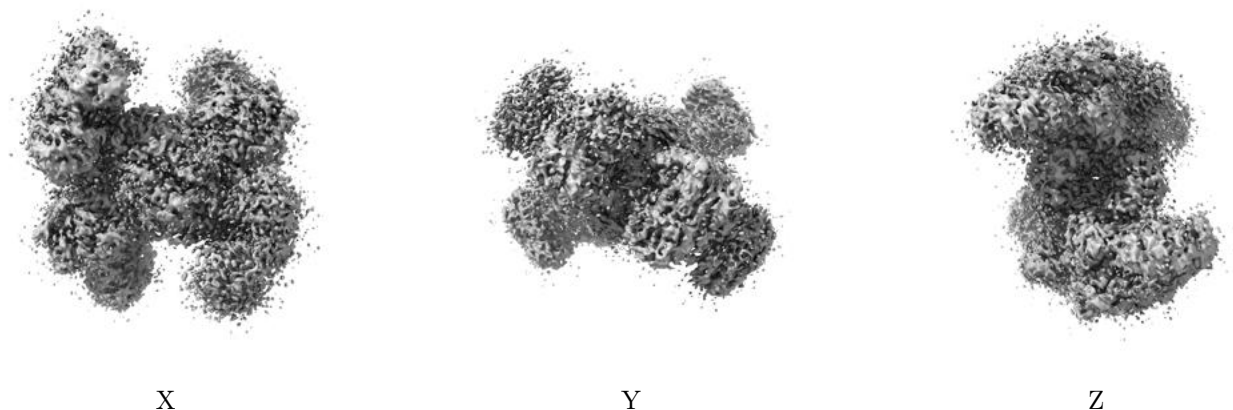


Z

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

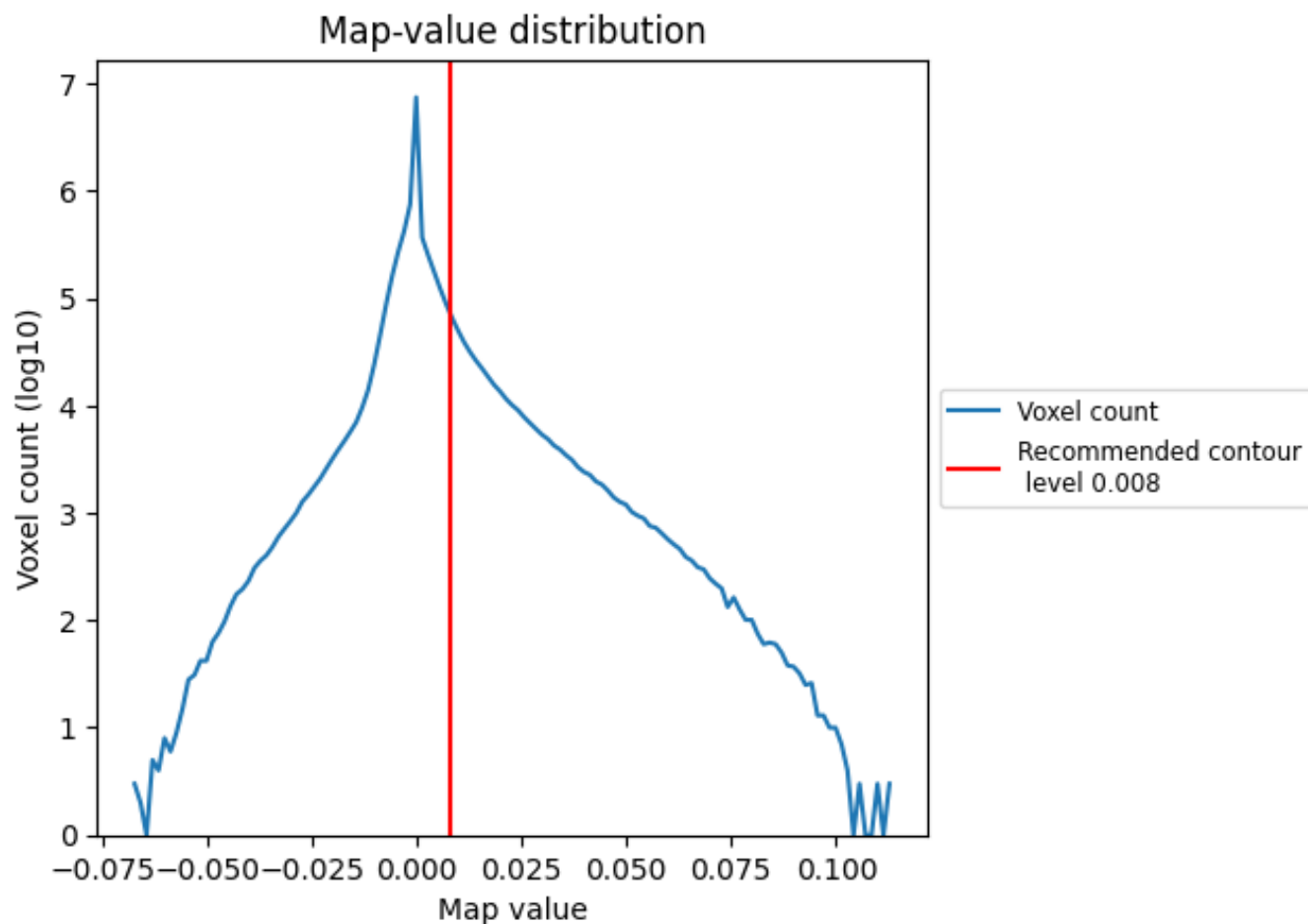
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

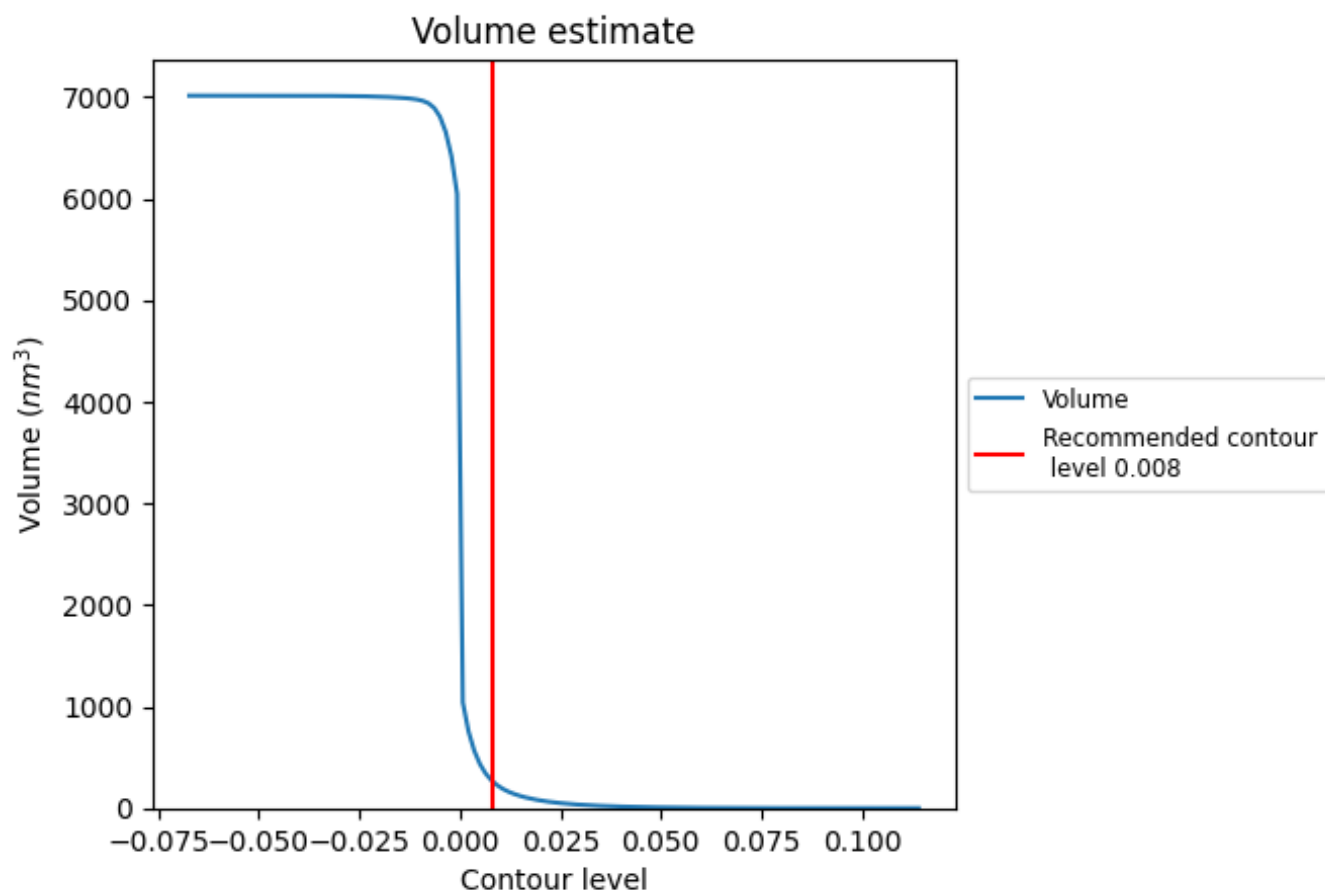
This section contains the results of statistical analysis of the map.

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.

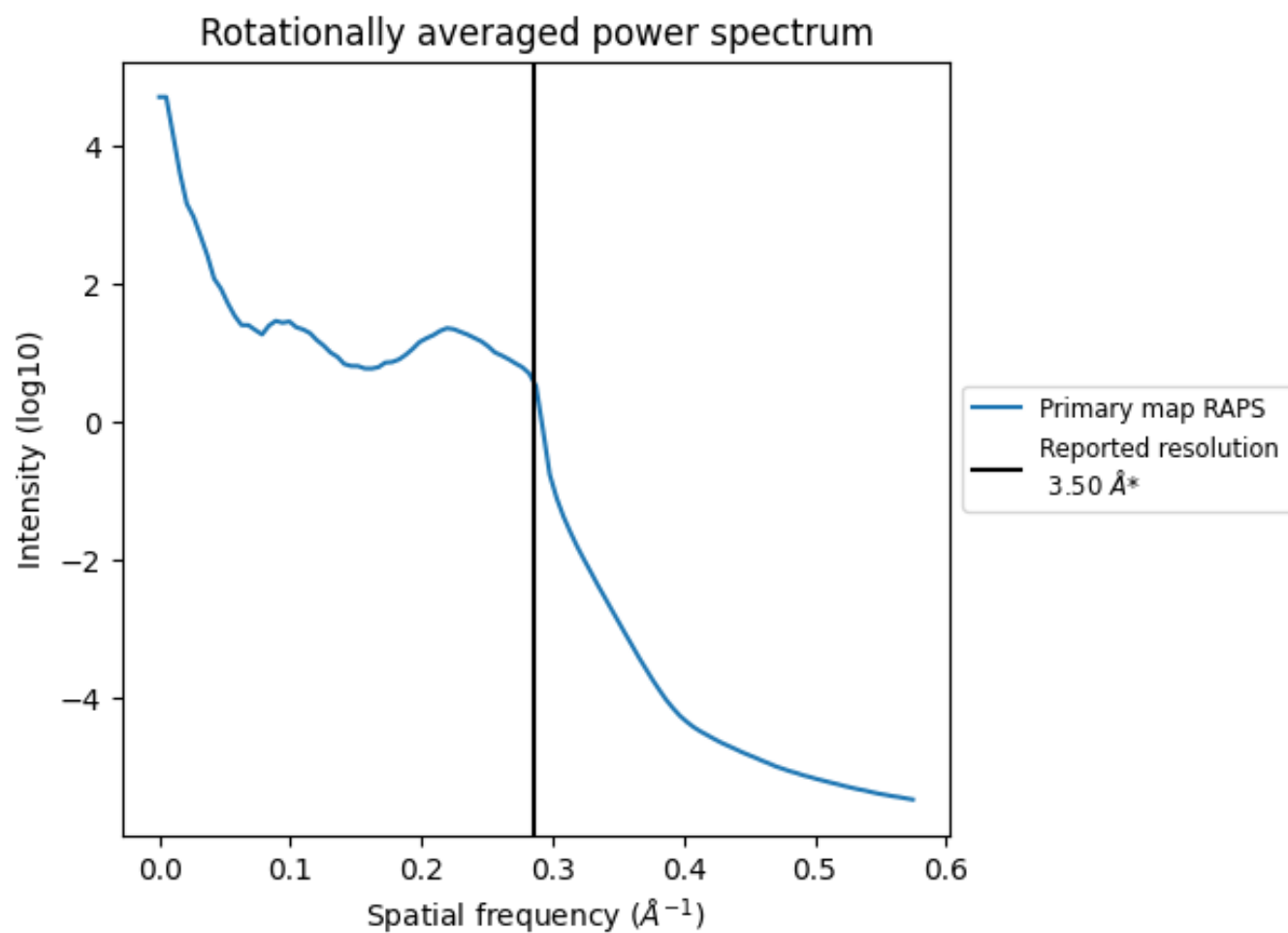
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 270 nm^3 ; this corresponds to an approximate mass of 244 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 0.286 Å⁻¹

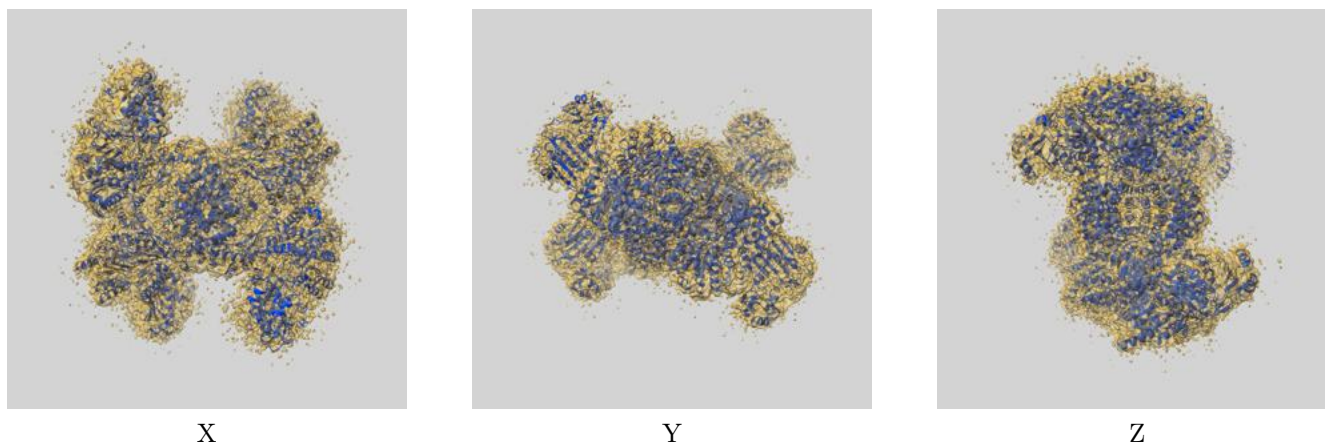
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

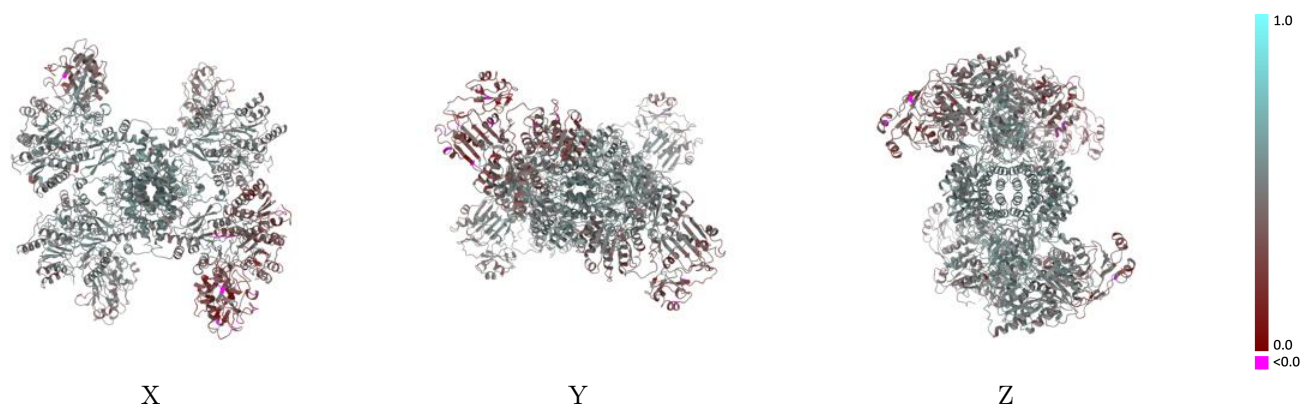
This section contains information regarding the fit between EMDB map EMD-20413 and PDB model 6POE. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



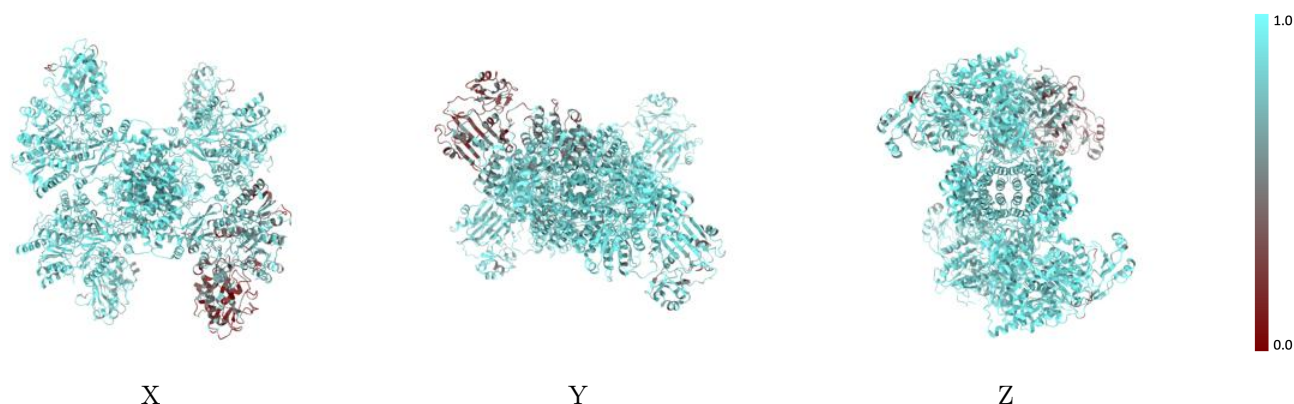
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



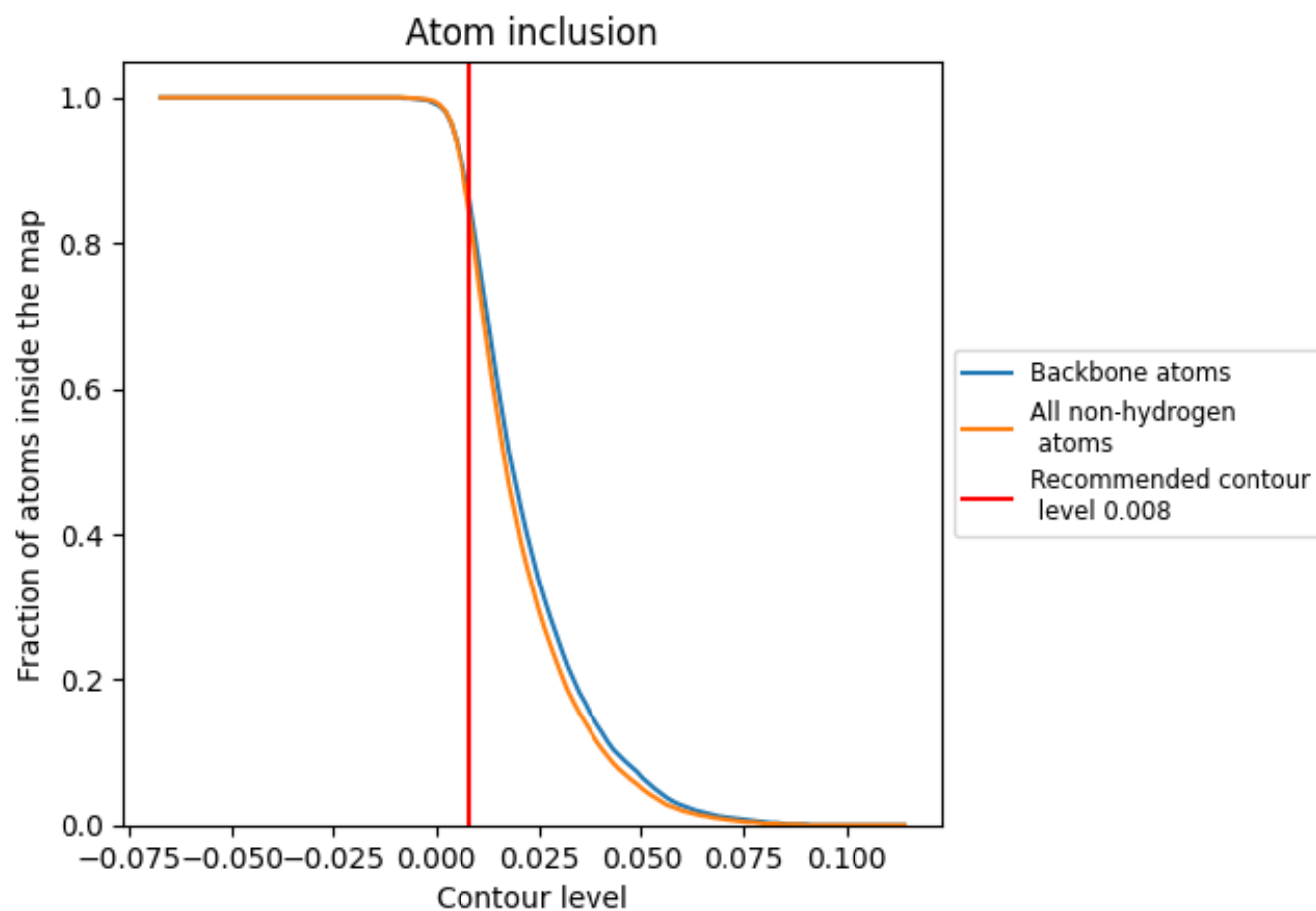
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8430	0.4750
A	0.9020	0.5010
B	0.8990	0.5030
C	0.8730	0.4740
D	0.7100	0.4200

