



Full wwPDB EM Validation Report ⓘ

Jun 24, 2024 – 12:13 PM EDT

PDB ID : 8T0Q
EMDB ID : EMD-40945
Title : Open state of lysine 5,6-aminomutase from *Thermoanaerobacter tengcongensis*
Authors : Tian, S.; Voss, P.; Pham, K.; Klose, T.
Deposited on : 2023-06-01
Resolution : 3.06 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.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

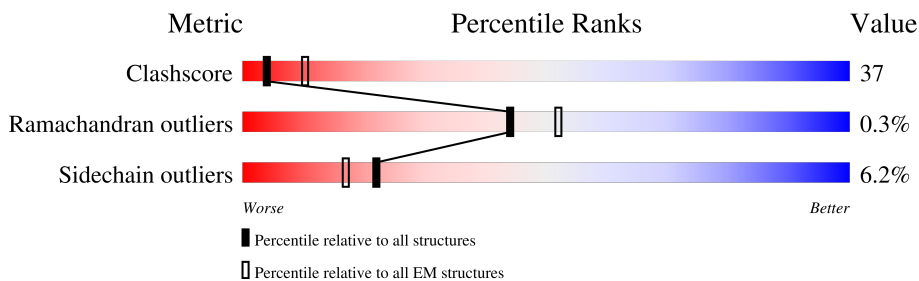
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.06 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	269	
1	B	269	
2	C	532	
2	D	532	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	B12	A	401	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	B12	B	401	-	-	X	-
5	5AD	D	601	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12571 atoms, of which 216 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 D-lysine 5,6-aminomutase beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	257	Total	C	N	O	S	0	0
			1992	1274	331	377	10		
1	B	256	Total	C	N	O	S	0	0
			1983	1269	329	375	10		

- Molecule 2 is a protein called D-lysine 5,6-aminomutase alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	517	Total	C	N	O	S	0	0
			4066	2588	692	764	22		
2	D	517	Total	C	N	O	S	0	0
			4066	2588	692	764	22		

There are 24 discrepancies between the modelled and reference sequences:

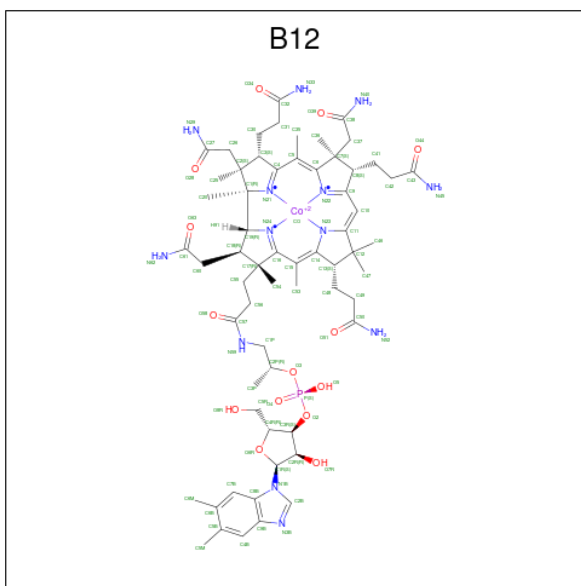
Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	MET	-	initiating methionine	UNP Q8RBT3
C	-10	GLY	-	expression tag	UNP Q8RBT3
C	-9	SER	-	expression tag	UNP Q8RBT3
C	-8	SER	-	expression tag	UNP Q8RBT3
C	-7	HIS	-	expression tag	UNP Q8RBT3
C	-6	HIS	-	expression tag	UNP Q8RBT3
C	-5	HIS	-	expression tag	UNP Q8RBT3
C	-4	HIS	-	expression tag	UNP Q8RBT3
C	-3	HIS	-	expression tag	UNP Q8RBT3
C	-2	HIS	-	expression tag	UNP Q8RBT3
C	-1	SER	-	expression tag	UNP Q8RBT3
C	0	GLN	-	expression tag	UNP Q8RBT3
D	-11	MET	-	initiating methionine	UNP Q8RBT3
D	-10	GLY	-	expression tag	UNP Q8RBT3
D	-9	SER	-	expression tag	UNP Q8RBT3
D	-8	SER	-	expression tag	UNP Q8RBT3
D	-7	HIS	-	expression tag	UNP Q8RBT3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	HIS	-	expression tag	UNP Q8RBT3
D	-5	HIS	-	expression tag	UNP Q8RBT3
D	-4	HIS	-	expression tag	UNP Q8RBT3
D	-3	HIS	-	expression tag	UNP Q8RBT3
D	-2	HIS	-	expression tag	UNP Q8RBT3
D	-1	SER	-	expression tag	UNP Q8RBT3
D	0	GLN	-	expression tag	UNP Q8RBT3

- Molecule 3 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$) (labeled as "Ligand of Interest" by depositor).



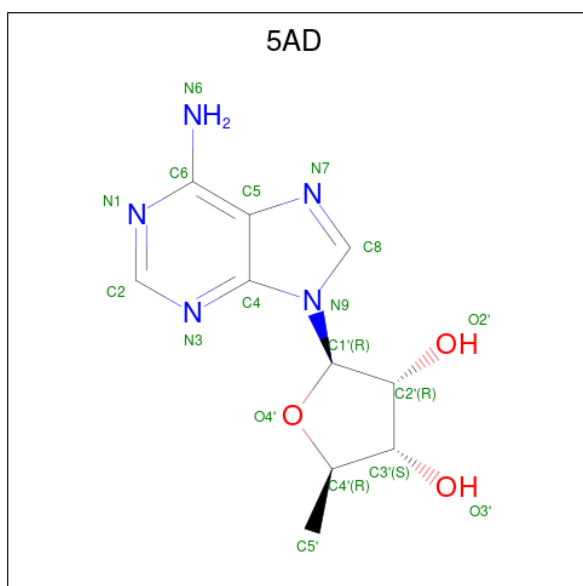
Mol	Chain	Residues	Atoms							AltConf
			Total	C	Co	H	N	O	P	
3	A	1	179	62	1	88	13	14	1	0
3	B	1	179	62	1	88	13	14	1	0

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
4	A	1	23	8	8	1	5	1	0
4	B	1	23	8	8	1	5	1	0

- Molecule 5 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula: $C_{10}H_{13}N_5O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
5	C	1	30	10	12	5	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
5	D	1	30	10	12	5	3	0

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1482472	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57.8	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.240	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.2	Depositor
Map size (\AA)	269.824, 269.824, 269.824	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.054, 1.054, 1.054	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: PLP, B12, 5AD

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	1/2029 (0.0%)	0.48	0/2743
1	B	0.39	1/2020 (0.0%)	0.54	2/2731 (0.1%)
2	C	0.28	0/4134	0.48	1/5579 (0.0%)
2	D	0.26	0/4134	0.47	0/5579
All	All	0.30	2/12317 (0.0%)	0.49	3/16632 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	146	TYR	CB-CG	-7.40	1.40	1.51
1	A	133	HIS	CA-CB	-5.13	1.42	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	GLY	N-CA-C	8.75	134.99	113.10
1	B	221	GLY	N-CA-C	5.94	127.95	113.10
2	C	269	ARG	NE-CZ-NH2	-5.19	117.70	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1992	0	2015	170	0
1	B	1983	0	2007	243	0
2	C	4066	0	4107	202	0
2	D	4066	0	4107	281	0
3	A	91	88	88	31	0
3	B	91	88	87	69	0
4	A	15	8	7	0	0
4	B	15	8	6	2	0
5	C	18	12	13	1	0
5	D	18	12	13	11	0
All	All	12355	216	12450	920	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 37.

All (920) 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)
3:B:401:B12:C14	5:D:601:5AD:H5'1	1.74	1.17
3:B:401:B12:N23	5:D:601:5AD:C5'	2.08	1.16
1:A:127:THR:HG21	1:A:131:ASP:OD1	1.46	1.14
1:B:221:GLY:HA3	3:B:401:B12:C9B	1.81	1.10
3:B:401:B12:N23	5:D:601:5AD:H5'1	1.66	1.07
4:B:402:PLP:O1P	2:D:190:SER:OG	1.73	1.06
1:B:221:GLY:HA3	3:B:401:B12:N3B	1.71	1.04
2:D:200:THR:HG21	2:D:208:TYR:HB2	1.42	1.01
3:A:401:B12:H362	3:A:401:B12:H351	1.43	0.99
2:C:284:ARG:HB3	2:C:330:ILE:HD11	1.42	0.97
3:A:401:B12:H531	3:A:401:B12:H543	1.46	0.96
1:A:163:LEU:HD21	1:A:175:LYS:HG2	1.45	0.96
1:A:127:THR:CG2	1:A:131:ASP:OD1	2.14	0.94
1:A:142:ASN:ND2	2:C:269:ARG:HH11	1.66	0.94
1:A:102:LYS:HE2	1:A:102:LYS:HA	1.51	0.93
1:B:23:LYS:HG2	1:B:24:PRO:HD2	1.49	0.92
3:B:401:B12:C11	5:D:601:5AD:C5'	2.48	0.92
1:A:141:MET:HE2	1:A:185:LEU:HD12	1.48	0.91
1:B:147:ALA:H	2:D:187:THR:HG21	1.35	0.91
2:D:266:ILE:HG21	2:D:478:LEU:HD13	1.52	0.91
2:D:155:TYR:HB3	2:D:406:LEU:HA	1.51	0.91
1:A:73:ASP:OD1	1:A:74:LYS:N	2.03	0.91
1:B:221:GLY:O	1:B:225:ILE:CG1	2.20	0.90
1:B:248:VAL:HG21	3:B:401:B12:HM63	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:LEU:HD23	3:B:401:B12:HM51	1.53	0.89
2:D:411:THR:HB	2:D:414:ILE:HD11	1.55	0.89
1:A:142:ASN:HD22	2:C:269:ARG:NH1	1.69	0.88
1:B:189:THR:HG23	1:B:223:PRO:HG3	1.51	0.88
1:A:126:ALA:HB2	1:A:163:LEU:HB2	1.56	0.88
1:A:122:VAL:HB	1:A:181:ALA:HA	1.56	0.87
2:D:280:GLN:HE21	2:D:284:ARG:HD2	1.40	0.86
3:B:401:B12:H492	3:B:401:B12:H533	1.57	0.86
1:B:140:ILE:HG13	3:B:401:B12:C6M	2.05	0.86
2:D:163:ILE:HD12	2:D:164:TYR:N	1.91	0.86
2:D:397:THR:HG23	2:D:402:GLN:HB2	1.58	0.86
3:B:401:B12:H362	3:B:401:B12:H351	1.58	0.85
3:A:401:B12:H421	3:A:401:B12:H363	1.59	0.85
2:D:409:MET:HG3	2:D:417:PRO:HB3	1.57	0.85
1:A:185:LEU:HD23	1:A:219:ILE:HB	1.58	0.85
1:B:197:ILE:O	1:B:201:THR:HG23	1.78	0.84
3:B:401:B12:N23	5:D:601:5AD:H5'3	1.92	0.84
2:D:116:GLU:OE1	2:D:116:GLU:N	2.09	0.84
3:B:401:B12:H551	3:B:401:B12:O63	1.77	0.83
1:B:139:ALA:HB1	1:B:146:TYR:CD2	2.13	0.83
2:C:146:TYR:OH	2:C:226:GLU:OE1	1.97	0.83
2:C:155:TYR:HB3	2:C:406:LEU:HA	1.60	0.83
2:D:37:VAL:HG12	2:D:41:ARG:HH12	1.42	0.83
1:B:134:THR:OG1	2:D:494:LYS:NZ	2.11	0.83
1:B:140:ILE:HG23	1:B:245:ALA:HA	1.60	0.82
1:B:193:LYS:HD2	1:B:193:LYS:O	1.81	0.81
2:D:41:ARG:HG2	2:D:64:VAL:HG21	1.63	0.80
2:D:146:TYR:OH	2:D:226:GLU:OE1	1.99	0.80
1:B:213:ARG:HD2	1:B:213:ARG:O	1.83	0.79
1:B:246:ASP:OD1	1:B:247:HIS:ND1	2.13	0.79
2:C:296:THR:OG1	2:C:298:GLU:OE1	2.00	0.79
1:B:142:ASN:HD22	2:D:269:ARG:HD2	1.46	0.79
1:B:154:ARG:NH1	2:D:304:THR:OG1	2.15	0.79
1:A:142:ASN:HD22	2:C:269:ARG:HH11	0.86	0.79
1:A:188:GLN:OE1	1:A:199:ASN:ND2	2.15	0.79
1:B:139:ALA:HB1	1:B:146:TYR:HD2	1.47	0.78
1:A:213:ARG:O	1:A:213:ARG:NH1	2.16	0.78
1:A:24:PRO:HG2	1:A:32:GLY:HA2	1.64	0.78
1:B:197:ILE:HD12	1:B:198:LYS:H	1.48	0.77
2:D:343:MET:HB2	2:D:354:GLU:OE1	1.84	0.77
1:B:140:ILE:HG13	3:B:401:B12:HM61	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:267:LEU:HD21	2:D:478:LEU:HD22	1.66	0.77
1:B:104:MET:SD	1:B:109:THR:OG1	2.43	0.76
1:B:141:MET:HE1	1:B:160:ALA:HB1	1.66	0.76
2:C:238:ALA:O	2:C:243:MET:HG2	1.84	0.76
2:D:88:THR:HG23	2:D:90:LEU:H	1.51	0.76
1:B:137:LEU:HD23	1:B:141:MET:HG3	1.66	0.76
1:A:184:LEU:HG	1:A:216:VAL:HG21	1.67	0.76
1:B:128:THR:HG23	1:B:186:VAL:HG23	1.68	0.76
1:A:154:ARG:HD3	2:C:304:THR:HG21	1.66	0.76
1:A:14:ASP:OD1	1:A:16:THR:N	2.17	0.76
1:B:141:MET:CE	1:B:160:ALA:HB1	2.15	0.76
1:B:185:LEU:HD23	3:B:401:B12:C5M	2.15	0.75
1:B:240:GLY:O	1:B:243:THR:HG22	1.86	0.75
1:B:248:VAL:HG21	3:B:401:B12:C6M	2.15	0.75
1:B:191:THR:HG21	1:B:224:ARG:HD2	1.69	0.75
2:D:159:ALA:HB2	2:D:184:ILE:HB	1.68	0.75
2:D:243:MET:HG2	2:D:244:PRO:HD3	1.69	0.75
2:C:496:LEU:HD13	2:C:496:LEU:O	1.86	0.74
2:D:268:PHE:CE2	2:D:300:ASN:HB3	2.23	0.74
3:B:401:B12:H473	3:B:401:B12:H491	1.69	0.74
1:A:44:ASP:OD1	1:A:45:GLY:N	2.21	0.74
1:B:106:MET:HA	1:B:106:MET:CE	2.17	0.74
1:B:187:SER:O	1:B:188:GLN:NE2	2.20	0.74
2:D:83:ASN:HD21	2:D:111:MET:HA	1.53	0.73
2:C:410:LEU:H	2:C:410:LEU:HD23	1.53	0.73
1:B:197:ILE:HD12	1:B:198:LYS:N	2.03	0.73
2:C:154:LEU:HD22	2:C:407:LEU:HD21	1.69	0.73
2:D:155:TYR:HH	2:D:235:CYS:HG	1.30	0.73
1:B:221:GLY:O	1:B:225:ILE:HG13	1.88	0.73
2:D:261:ASP:OD2	2:D:297:GLY:N	2.22	0.73
1:A:240:GLY:O	1:A:243:THR:HG22	1.89	0.73
3:B:401:B12:H302	3:B:401:B12:H353	1.71	0.73
1:B:246:ASP:OD1	1:B:247:HIS:N	2.23	0.72
1:A:36:LEU:HD22	1:B:36:LEU:HD22	1.71	0.72
2:C:442:GLU:OE1	2:D:450:ILE:HB	1.88	0.72
2:D:31:ILE:HD11	2:D:277:MET:O	1.89	0.72
1:A:236:ASP:N	1:A:236:ASP:OD1	2.22	0.72
2:D:45:ARG:NE	2:D:245:GLU:OE2	2.17	0.72
2:D:36:THR:HG23	2:D:278:VAL:HG12	1.72	0.72
1:B:106:MET:HA	1:B:106:MET:HE2	1.73	0.71
1:B:216:VAL:HG11	1:B:264:LEU:HD21	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:303:THR:HG22	2:C:304:THR:HG23	1.71	0.71
2:C:398:ILE:HD13	2:C:433:PHE:HA	1.70	0.71
1:B:221:GLY:HA3	3:B:401:B12:C4B	2.20	0.71
3:B:401:B12:C11	5:D:601:5AD:H5'1	2.17	0.71
2:D:73:LEU:O	2:D:73:LEU:HD13	1.90	0.71
2:C:136:ARG:O	2:C:140:GLU:HG2	1.89	0.71
2:C:150:GLU:HA	2:C:150:GLU:OE2	1.91	0.71
2:C:284:ARG:HB3	2:C:330:ILE:CD1	2.20	0.70
2:D:235:CYS:HA	2:D:257:VAL:O	1.90	0.70
1:A:141:MET:CE	1:A:185:LEU:HD12	2.21	0.70
3:A:401:B12:H262	3:A:401:B12:H601	1.73	0.70
2:D:414:ILE:HG13	2:D:415:HIS:CD2	2.27	0.70
1:A:141:MET:O	1:A:153:GLU:HB2	1.92	0.70
1:B:217:LEU:HD12	1:B:217:LEU:H	1.55	0.70
2:C:409:MET:HG3	2:C:417:PRO:HB3	1.73	0.70
2:D:188:ALA:HA	2:D:269:ARG:HH21	1.56	0.70
1:A:193:LYS:O	1:A:198:LYS:NZ	2.24	0.70
1:A:35:GLN:NE2	1:B:35:GLN:OE1	2.24	0.70
2:C:116:GLU:OE2	2:C:116:GLU:N	2.25	0.70
2:C:84:ALA:CB	2:C:95:ILE:HD13	2.22	0.70
3:B:401:B12:C13	5:D:601:5AD:H5'1	2.22	0.69
1:B:215:LYS:HA	1:B:261:ILE:HD13	1.74	0.69
2:D:174:ALA:HB1	2:D:232:ILE:CD1	2.21	0.69
1:A:215:LYS:O	1:A:261:ILE:HD12	1.92	0.69
2:D:189:GLN:HG2	2:D:192:LEU:HD13	1.75	0.69
2:D:211:GLN:HG3	2:D:249:MET:HG2	1.75	0.69
1:A:62:GLU:HA	1:A:62:GLU:OE2	1.92	0.69
3:A:401:B12:H543	3:A:401:B12:C53	2.23	0.69
3:B:401:B12:H262	3:B:401:B12:C60	2.23	0.69
2:C:37:VAL:HG13	2:C:64:VAL:HG11	1.75	0.69
2:D:239:SER:HA	2:D:243:MET:HE3	1.75	0.68
3:A:401:B12:H471	3:A:401:B12:H492	1.76	0.68
1:B:104:MET:HE1	1:B:108:GLU:C	2.14	0.68
1:A:187:SER:O	1:A:188:GLN:NE2	2.21	0.68
2:D:37:VAL:HG12	2:D:41:ARG:NH1	2.07	0.68
2:C:299:ASP:HB3	2:C:373:MET:SD	2.34	0.68
2:D:279:ASP:OD1	2:D:280:GLN:N	2.26	0.68
2:D:298:GLU:OE1	2:D:298:GLU:HA	1.94	0.67
1:B:198:LYS:HB3	1:B:198:LYS:NZ	2.09	0.67
2:C:411:THR:HB	2:C:414:ILE:HD11	1.76	0.67
1:A:126:ALA:CB	1:A:163:LEU:HB2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:GLU:OE2	1:B:62:GLU:HA	1.93	0.67
1:B:225:ILE:HG13	1:B:225:ILE:O	1.93	0.67
1:B:221:GLY:CA	1:B:225:ILE:HD11	2.24	0.67
2:C:144:LYS:HE3	2:C:145:LYS:N	2.09	0.67
1:B:23:LYS:HG2	1:B:24:PRO:CD	2.23	0.67
2:D:114:LEU:HA	2:D:117:ILE:CD1	2.25	0.67
1:B:35:GLN:O	1:B:36:LEU:HD23	1.95	0.67
1:B:221:GLY:C	1:B:225:ILE:HD11	2.16	0.67
1:B:142:ASN:O	1:B:151:GLY:HA3	1.94	0.67
2:D:91:SER:N	2:D:94:GLU:OE2	2.25	0.66
2:D:360:MET:O	2:D:364:ILE:HG13	1.95	0.66
2:D:442:GLU:OE1	2:D:442:GLU:HA	1.95	0.66
2:C:55:LEU:HD12	2:C:55:LEU:O	1.94	0.66
1:A:112:TYR:HE1	1:A:257:VAL:HG21	1.60	0.66
2:C:438:ASP:N	2:C:438:ASP:OD1	2.29	0.66
2:D:189:GLN:HA	2:D:192:LEU:HD12	1.78	0.66
2:D:165:GLU:N	2:D:165:GLU:OE1	2.28	0.66
2:D:468:GLU:OE1	2:D:482:LYS:NZ	2.27	0.66
1:A:218:LEU:HD12	1:A:235:TYR:CE2	2.30	0.66
1:B:104:MET:HB3	1:B:250:THR:OG1	1.96	0.66
2:C:17:ARG:NH2	2:C:364:ILE:O	2.29	0.66
2:C:249:MET:O	2:C:253:GLU:HG2	1.95	0.66
1:B:154:ARG:HD2	2:D:304:THR:OG1	1.96	0.66
2:D:157:ILE:CG2	2:D:184:ILE:HG12	2.26	0.65
1:A:184:LEU:HG	1:A:216:VAL:CG2	2.26	0.65
2:C:444:TYR:O	2:D:444:TYR:HB2	1.96	0.65
2:D:17:ARG:NH2	2:D:364:ILE:O	2.29	0.65
2:D:162:ASN:OD1	2:D:201:THR:HA	1.96	0.65
2:D:240:GLY:O	2:D:242:CYS:N	2.29	0.65
1:A:105:SER:OG	1:A:108:GLU:OE1	2.08	0.65
2:D:241:LEU:HG	2:D:271:ILE:HD11	1.78	0.65
2:C:373:MET:HB3	2:C:406:LEU:HD23	1.78	0.65
1:B:117:ILE:HG21	1:B:256:MET:CE	2.26	0.65
2:D:104:LEU:HD13	2:D:105:ASP:N	2.10	0.65
1:B:139:ALA:CB	1:B:146:TYR:HD2	2.10	0.65
2:D:258:MET:SD	2:D:287:ASN:ND2	2.69	0.65
2:D:332:GLU:OE1	2:D:332:GLU:N	2.26	0.65
1:B:261:ILE:HD12	1:B:262:PRO:N	2.12	0.64
2:C:157:ILE:HG21	2:C:184:ILE:HD11	1.80	0.64
1:B:248:VAL:O	1:B:252:ILE:HG22	1.97	0.64
2:D:38:SER:HA	2:D:41:ARG:CZ	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:GLY:O	1:B:86:ILE:HG22	1.98	0.64
2:D:287:ASN:HB2	2:D:294:ILE:HD11	1.80	0.64
2:D:343:MET:CE	2:D:354:GLU:HG2	2.27	0.64
4:B:402:PLP:O1P	2:D:190:SER:CB	2.44	0.64
2:C:69:SER:OG	2:C:70:LYS:HG2	1.98	0.64
2:D:18:GLU:OE1	2:D:21:ARG:NH1	2.30	0.64
2:C:12:LEU:HD12	2:C:459:LEU:CD2	2.28	0.64
1:B:28:THR:OG1	1:B:31:ASP:OD2	2.16	0.63
2:D:481:GLY:HA2	2:D:486:ILE:O	1.97	0.63
1:B:261:ILE:HD12	1:B:262:PRO:HD2	1.79	0.63
1:B:256:MET:HG2	1:B:261:ILE:CG2	2.28	0.63
2:D:62:VAL:HA	2:D:65:ASP:OD2	1.97	0.63
2:D:273:MET:CE	2:D:475:PHE:HD1	2.11	0.63
2:C:343:MET:N	2:C:354:GLU:OE2	2.30	0.63
2:C:414:ILE:HG13	2:C:415:HIS:CD2	2.33	0.63
2:C:163:ILE:O	2:C:167:VAL:HG13	1.99	0.63
2:D:139:ARG:NH2	2:D:290:ALA:O	2.32	0.63
2:D:83:ASN:ND2	2:D:111:MET:HA	2.13	0.63
2:D:266:ILE:HD13	2:D:273:MET:HG2	1.81	0.63
1:A:259:ARG:HD3	1:A:261:ILE:HD11	1.81	0.63
1:B:20:THR:HG22	1:B:92:THR:HG21	1.81	0.63
3:B:401:B12:H543	3:B:401:B12:C53	2.27	0.63
2:C:84:ALA:HB1	2:C:95:ILE:HD13	1.81	0.63
2:C:237:TYR:CD1	2:C:259:LEU:HD22	2.34	0.63
2:C:273:MET:CE	2:C:475:PHE:HA	2.29	0.63
1:B:108:GLU:OE1	1:B:108:GLU:N	2.23	0.63
1:B:261:ILE:HD12	1:B:262:PRO:CD	2.29	0.62
2:C:113:ASP:OD1	2:C:114:LEU:N	2.32	0.62
2:C:191:LEU:HD21	2:C:269:ARG:HD2	1.80	0.62
2:C:269:ARG:HB3	2:C:271:ILE:HG13	1.81	0.62
2:D:189:GLN:HA	2:D:192:LEU:CD1	2.29	0.62
2:D:484:ALA:O	2:D:486:ILE:HD12	1.99	0.62
1:B:104:MET:HE1	1:B:109:THR:N	2.15	0.62
1:B:108:GLU:HA	1:B:111:GLU:OE2	1.99	0.62
3:B:401:B12:C11	5:D:601:5AD:H5'2	2.29	0.62
2:D:342:GLU:OE2	2:D:376:THR:N	2.16	0.62
1:B:221:GLY:CA	3:B:401:B12:N3B	2.57	0.62
2:D:38:SER:HA	2:D:41:ARG:NH1	2.15	0.62
2:D:361:VAL:HG12	2:D:370:LEU:CD1	2.30	0.61
1:A:36:LEU:HD13	1:A:59:MET:HE1	1.81	0.61
1:A:185:LEU:HD22	3:A:401:B12:HM51	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:341:PHE:O	2:C:375:PRO:HB3	2.00	0.61
2:D:155:TYR:CD1	2:D:406:LEU:HD13	2.35	0.61
1:A:127:THR:O	1:A:167:VAL:HG22	2.00	0.61
1:A:206:LEU:O	1:A:206:LEU:HD12	2.00	0.61
2:C:341:PHE:HE2	2:C:396:VAL:HG21	1.63	0.61
2:D:341:PHE:HE2	2:D:396:VAL:HG21	1.65	0.61
2:C:385:LYS:HD2	2:D:427:GLU:OE2	2.00	0.61
1:A:73:ASP:OD1	1:A:74:LYS:HG2	2.00	0.61
3:B:401:B12:O28	3:B:401:B12:N33	2.34	0.61
2:D:409:MET:HG3	2:D:417:PRO:CB	2.30	0.61
2:D:273:MET:HE1	2:D:475:PHE:HA	1.81	0.61
1:A:85:LEU:HD12	1:A:86:ILE:N	2.16	0.61
2:C:479:GLU:OE2	2:C:490:ILE:HG13	2.00	0.61
2:D:185:ARG:HD2	2:D:189:GLN:OE1	1.99	0.61
1:A:122:VAL:HG11	1:A:179:VAL:HG12	1.81	0.61
2:C:159:ALA:HB1	2:C:206:GLY:HA2	1.82	0.60
1:B:140:ILE:CG1	3:B:401:B12:HM61	2.29	0.60
2:D:54:ASP:N	2:D:54:ASP:OD1	2.26	0.60
2:C:243:MET:HE1	2:C:280:GLN:HB3	1.84	0.60
2:D:114:LEU:HA	2:D:117:ILE:HD13	1.82	0.60
1:A:36:LEU:HD13	1:A:59:MET:CE	2.32	0.60
1:A:138:ASP:O	1:A:142:ASN:HB2	2.01	0.60
2:C:9:ASP:O	2:C:13:VAL:HG23	2.01	0.60
3:A:401:B12:H361	3:A:401:B12:N40	2.15	0.60
1:A:33:LYS:HD2	2:D:418:PHE:HZ	1.66	0.60
1:B:139:ALA:CB	1:B:146:TYR:CD2	2.84	0.60
2:C:85:MET:HE1	2:C:92:PRO:HD3	1.83	0.60
2:C:435:ASN:O	2:D:349:ASN:HA	2.02	0.60
2:D:123:ASP:OD1	2:D:124:ILE:N	2.34	0.60
1:B:113:ILE:HG23	1:B:117:ILE:CD1	2.32	0.60
3:B:401:B12:H533	3:B:401:B12:C49	2.30	0.60
2:C:167:VAL:HA	2:C:217:MET:CE	2.32	0.60
1:B:189:THR:HA	1:B:223:PRO:HD2	1.82	0.60
2:C:356:ALA:HB2	2:C:451:ILE:HG23	1.84	0.60
2:D:266:ILE:HG12	2:D:273:MET:HA	1.83	0.60
1:A:125:GLY:HA3	1:A:141:MET:HE3	1.84	0.60
1:B:222:GLY:N	3:B:401:B12:N3B	2.49	0.60
2:D:130:GLU:OE1	2:D:130:GLU:HA	2.02	0.60
1:A:102:LYS:HE2	1:A:102:LYS:CA	2.29	0.59
2:C:190:SER:HB2	2:C:240:GLY:HA3	1.83	0.59
1:A:14:ASP:OD1	1:A:16:THR:HG22	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:THR:O	1:B:25:TYR:HB3	2.02	0.59
2:D:469:ILE:O	2:D:473:GLY:N	2.28	0.59
1:A:37:SER:HA	1:A:79:PHE:O	2.02	0.59
1:B:105:SER:HB3	1:B:108:GLU:OE2	2.03	0.59
2:D:181:ILE:HD12	2:D:221:LEU:HD21	1.84	0.59
2:C:233:ARG:HB3	2:C:256:ASP:HB2	1.84	0.59
2:C:273:MET:O	2:C:277:MET:HG2	2.02	0.59
2:D:196:PRO:HG2	2:D:210:THR:HG22	1.84	0.59
1:B:32:GLY:HA3	1:B:85:LEU:H	1.68	0.59
2:D:241:LEU:HG	2:D:271:ILE:CD1	2.33	0.59
2:D:376:THR:HB	2:D:412:GLU:OE2	2.02	0.59
1:A:128:THR:HG23	1:A:186:VAL:HG23	1.85	0.59
1:B:255:GLU:HA	1:B:255:GLU:OE1	2.03	0.59
1:A:21:ARG:HH11	1:A:21:ARG:HB2	1.68	0.59
3:B:401:B12:H353	3:B:401:B12:C30	2.33	0.58
3:B:401:B12:H352	3:B:401:B12:H312	1.84	0.58
1:A:252:ILE:HG22	1:A:256:MET:HE1	1.86	0.58
2:C:31:ILE:HD11	2:C:277:MET:HB3	1.86	0.58
2:D:273:MET:CE	2:D:475:PHE:HA	2.32	0.58
2:D:392:MET:HE2	2:D:392:MET:HA	1.85	0.58
2:D:139:ARG:NH1	2:D:255:LEU:O	2.36	0.58
2:D:409:MET:HB3	2:D:421:ASP:OD1	2.03	0.58
1:A:69:HIS:HA	1:A:78:PHE:O	2.03	0.58
2:C:408:GLY:O	2:C:425:SER:OG	2.16	0.58
2:D:37:VAL:HG21	2:D:68:LYS:NZ	2.18	0.58
1:B:143:MET:SD	2:D:486:ILE:HG12	2.43	0.58
1:B:221:GLY:O	1:B:225:ILE:HG12	2.03	0.58
2:C:277:MET:O	2:C:280:GLN:HG3	2.03	0.58
2:D:91:SER:OG	2:D:94:GLU:HG2	2.03	0.58
2:D:163:ILE:O	2:D:167:VAL:HG22	2.04	0.58
2:C:243:MET:SD	2:C:260:ASN:ND2	2.76	0.58
2:D:233:ARG:HB3	2:D:256:ASP:HB2	1.85	0.58
1:A:21:ARG:HB2	1:A:21:ARG:NH1	2.19	0.58
1:A:252:ILE:O	1:A:256:MET:HE2	2.03	0.58
3:A:401:B12:H301	3:A:401:B12:H203	1.85	0.58
1:B:216:VAL:CG1	1:B:264:LEU:HD21	2.32	0.58
1:A:203:LEU:HD23	1:A:235:TYR:OH	2.04	0.58
1:B:227:HIS:CE1	1:B:237:ALA:HA	2.38	0.58
1:B:249:ALA:O	1:B:253:VAL:HG12	2.04	0.58
2:C:185:ARG:HG3	2:C:209:ALA:HB2	1.86	0.58
2:D:185:ARG:NH2	2:D:239:SER:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:195:VAL:HG11	2:C:249:MET:CE	2.34	0.58
1:B:142:ASN:ND2	2:D:269:ARG:HD2	2.19	0.57
2:D:109:ILE:HG23	2:D:110:PRO:HD2	1.85	0.57
1:A:36:LEU:CD2	1:B:36:LEU:HD22	2.34	0.57
2:D:155:TYR:OH	2:D:235:CYS:SG	2.48	0.57
1:A:215:LYS:HA	1:A:262:PRO:HD2	1.85	0.57
2:D:481:GLY:O	2:D:485:ASP:HA	2.04	0.57
1:B:154:ARG:HH11	2:D:304:THR:HG1	1.46	0.57
2:D:36:THR:HG21	2:D:279:ASP:HB3	1.85	0.57
2:D:63:VAL:O	2:D:67:ILE:HG22	2.04	0.57
1:B:44:ASP:HA	1:B:77:THR:HG21	1.86	0.57
2:C:82:GLY:HA2	2:C:85:MET:HG3	1.85	0.57
2:C:85:MET:CE	2:C:92:PRO:HD3	2.34	0.57
2:C:167:VAL:HA	2:C:217:MET:HE1	1.85	0.57
2:D:260:ASN:HB3	2:D:294:ILE:HG23	1.85	0.57
1:A:215:LYS:O	1:A:261:ILE:HG23	2.05	0.57
1:B:213:ARG:HD2	1:B:213:ARG:C	2.24	0.57
3:B:401:B12:H262	3:B:401:B12:C18	2.34	0.57
2:C:109:ILE:HG23	2:C:110:PRO:HD2	1.87	0.57
2:D:361:VAL:HG12	2:D:370:LEU:HD11	1.86	0.57
1:B:69:HIS:HA	1:B:78:PHE:O	2.05	0.56
1:B:126:ALA:CB	1:B:163:LEU:HB2	2.35	0.56
1:B:157:MET:HE3	1:B:157:MET:HA	1.87	0.56
1:B:256:MET:HG2	1:B:261:ILE:HG21	1.86	0.56
2:D:167:VAL:O	2:D:171:GLN:HG3	2.04	0.56
2:D:217:MET:HE2	2:D:217:MET:HA	1.87	0.56
1:B:193:LYS:NZ	1:B:195:ALA:HA	2.20	0.56
2:C:324:PHE:O	2:C:327:ILE:HG22	2.05	0.56
2:C:375:PRO:HG2	2:C:379:MET:HE1	1.86	0.56
2:D:53:ASN:ND2	2:D:57:VAL:HB	2.19	0.56
1:B:221:GLY:O	1:B:225:ILE:CD1	2.54	0.56
1:A:124:VAL:HG12	1:A:172:PHE:HE1	1.71	0.56
1:A:95:GLN:HA	1:A:95:GLN:OE1	2.06	0.56
2:C:139:ARG:NH2	2:C:290:ALA:O	2.38	0.56
2:C:255:LEU:O	2:C:292:ILE:HG12	2.05	0.56
2:D:51:GLY:C	2:D:59:LEU:HD23	2.26	0.56
2:D:188:ALA:HA	2:D:269:ARG:NH2	2.19	0.56
1:B:123:VAL:CG1	1:B:185:LEU:HD13	2.36	0.56
1:B:221:GLY:O	1:B:225:ILE:HD11	2.06	0.56
3:B:401:B12:H362	3:B:401:B12:C35	2.33	0.56
2:D:83:ASN:O	2:D:86:ILE:HG22	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:HB2	1:A:29:MET:SD	2.46	0.55
1:A:62:GLU:OE1	1:A:86:ILE:HB	2.05	0.55
1:B:105:SER:OG	1:B:106:MET:N	2.39	0.55
1:B:113:ILE:HG23	1:B:117:ILE:HD11	1.88	0.55
2:C:357:GLN:O	2:C:361:VAL:HG23	2.06	0.55
2:D:159:ALA:CB	2:D:184:ILE:HB	2.36	0.55
2:D:243:MET:HG2	2:D:244:PRO:CD	2.36	0.55
1:B:142:ASN:HD22	2:D:269:ARG:CD	2.15	0.55
1:A:36:LEU:HD11	1:A:61:LEU:HD11	1.88	0.55
1:B:113:ILE:HG23	1:B:117:ILE:HG13	1.88	0.55
1:B:19:LEU:O	1:B:91:TYR:HB3	2.06	0.55
1:B:108:GLU:H	1:B:108:GLU:CD	2.05	0.55
2:C:167:VAL:HG12	2:C:217:MET:HE3	1.89	0.55
1:A:135:VAL:HG23	3:A:401:B12:O51	2.06	0.55
1:B:168:PRO:HD2	1:B:171:GLU:OE2	2.06	0.55
1:B:252:ILE:O	1:B:256:MET:HB2	2.07	0.55
3:B:401:B12:C30	3:B:401:B12:C35	2.85	0.55
2:D:117:ILE:HD12	2:D:117:ILE:H	1.71	0.55
1:A:143:MET:CE	2:C:486:ILE:HB	2.37	0.55
1:B:137:LEU:CD2	1:B:141:MET:HG3	2.34	0.55
2:C:468:GLU:O	2:C:472:GLU:HG2	2.07	0.55
2:C:516:ARG:HH11	2:C:516:ARG:HB3	1.72	0.55
1:B:134:THR:OG1	1:B:134:THR:O	2.25	0.55
2:D:287:ASN:CB	2:D:294:ILE:HD11	2.36	0.55
1:A:122:VAL:HG12	1:A:181:ALA:HB2	1.88	0.55
1:B:198:LYS:HB3	1:B:198:LYS:HZ1	1.71	0.55
1:B:207:LEU:H	1:B:207:LEU:HD22	1.72	0.55
2:C:387:HIS:HE1	2:C:428:SER:HB3	1.72	0.55
1:B:50:GLU:OE1	1:B:54:GLN:NE2	2.40	0.55
2:C:155:TYR:CD1	2:C:406:LEU:HD13	2.41	0.55
3:B:401:B12:C53	3:B:401:B12:C48	2.85	0.54
1:A:85:LEU:HD12	1:A:86:ILE:H	1.73	0.54
1:A:253:VAL:O	1:A:257:VAL:HG23	2.07	0.54
1:B:203:LEU:HD12	1:B:235:TYR:OH	2.07	0.54
3:A:401:B12:H312	3:A:401:B12:H251	1.89	0.54
2:D:502:LYS:HE2	2:D:506:TYR:CE2	2.43	0.54
3:B:401:B12:H2P	3:B:401:B12:O58	2.06	0.54
2:C:84:ALA:HB3	2:C:95:ILE:HD13	1.88	0.54
2:C:247:ALA:HA	2:C:258:MET:HE1	1.90	0.54
2:D:23:ILE:HG23	2:D:474:LEU:HB2	1.89	0.54
2:D:104:LEU:HD11	2:D:109:ILE:CD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:PHE:CD1	2:C:419:MET:HE1	2.43	0.54
1:B:143:MET:N	1:B:153:GLU:OE2	2.41	0.54
2:D:162:ASN:HB3	2:D:165:GLU:CD	2.28	0.54
1:A:139:ALA:HB1	1:A:146:TYR:HB2	1.89	0.54
2:C:157:ILE:HG23	2:C:184:ILE:HG12	1.89	0.54
2:D:174:ALA:HB1	2:D:232:ILE:HD12	1.90	0.54
3:A:401:B12:H621	3:A:401:B12:H541	1.72	0.54
1:B:112:TYR:CE1	1:B:253:VAL:HG22	2.43	0.54
3:B:401:B12:H481	3:B:401:B12:H532	1.89	0.54
2:C:272:ASN:HD21	2:C:496:LEU:HD23	1.71	0.54
2:D:105:ASP:HB3	2:D:108:SER:OG	2.08	0.54
2:D:166:ASP:OD2	2:D:207:THR:HG21	2.08	0.54
1:B:210:GLU:OE2	1:B:267:TYR:OH	2.19	0.53
2:C:165:GLU:HA	2:C:165:GLU:OE2	2.07	0.53
3:B:401:B12:C55	3:B:401:B12:H531	2.38	0.53
2:D:53:ASN:OD1	2:D:55:LEU:N	2.22	0.53
1:B:168:PRO:HD2	1:B:171:GLU:CD	2.29	0.53
2:D:235:CYS:HB2	2:D:257:VAL:HB	1.91	0.53
3:A:401:B12:C53	3:A:401:B12:H551	2.38	0.53
2:C:516:ARG:HB3	2:C:516:ARG:NH1	2.24	0.53
2:D:150:GLU:HA	2:D:150:GLU:OE1	2.09	0.53
1:A:239:PHE:HB3	1:A:243:THR:HG21	1.89	0.53
2:C:12:LEU:HD21	2:C:463:TYR:CD2	2.43	0.53
1:A:73:ASP:HB3	1:A:76:PHE:HD2	1.74	0.53
2:D:241:LEU:HD22	2:D:275:ARG:NH2	2.23	0.53
3:B:401:B12:H262	3:B:401:B12:H601	1.90	0.53
2:C:33:ALA:O	2:C:34:HIS:ND1	2.42	0.53
2:D:161:GLY:HA2	2:D:206:GLY:O	2.08	0.53
1:B:180:GLY:HA2	1:B:264:LEU:HB2	1.90	0.52
3:B:401:B12:H312	3:B:401:B12:C35	2.39	0.52
1:A:122:VAL:CB	1:A:181:ALA:HA	2.36	0.52
2:C:397:THR:HG23	2:C:402:GLN:HB2	1.90	0.52
1:B:143:MET:SD	2:D:486:ILE:CD1	2.97	0.52
2:C:362:ARG:NH2	2:C:401:LYS:O	2.30	0.52
2:C:302:LEU:HD12	2:C:340:ALA:HB3	1.91	0.52
1:A:205:GLU:OE1	1:A:205:GLU:HA	2.10	0.52
3:B:401:B12:N24	5:D:601:5AD:H5'3	2.25	0.52
2:C:129:VAL:HG13	2:C:289:PHE:CE2	2.45	0.52
1:A:21:ARG:HH11	1:A:21:ARG:CB	2.22	0.52
1:B:24:PRO:HG2	1:B:32:GLY:HA2	1.91	0.52
2:D:41:ARG:HG3	2:D:41:ARG:HH11	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:166:ASP:O	2:D:170:ALA:N	2.33	0.52
2:C:139:ARG:HD3	2:C:256:ASP:OD1	2.10	0.52
2:C:12:LEU:HD13	2:C:12:LEU:O	2.10	0.52
2:D:282:PHE:HD1	2:D:511:ILE:HD11	1.75	0.52
1:B:113:ILE:HD13	1:B:121:VAL:CG2	2.38	0.52
1:B:117:ILE:HD13	1:B:256:MET:HE2	1.92	0.52
1:B:126:ALA:HB2	1:B:163:LEU:HB2	1.91	0.52
1:B:227:HIS:NE2	1:B:237:ALA:HA	2.25	0.52
3:B:401:B12:O5	3:B:401:B12:O7R	2.26	0.52
2:C:88:THR:OG1	2:C:90:LEU:HD12	2.09	0.52
2:C:174:ALA:HB1	2:C:232:ILE:HD13	1.92	0.52
3:A:401:B12:H362	3:A:401:B12:C35	2.28	0.52
1:B:35:GLN:C	1:B:36:LEU:HD23	2.30	0.52
1:A:126:ALA:HB1	1:A:167:VAL:HG21	1.90	0.51
1:B:131:ASP:OD1	1:B:190:VAL:HB	2.09	0.51
2:D:280:GLN:NE2	2:D:284:ARG:HD2	2.19	0.51
1:A:42:VAL:HG11	1:B:91:TYR:CE2	2.45	0.51
3:A:401:B12:N40	3:A:401:B12:C36	2.72	0.51
3:B:401:B12:H351	3:B:401:B12:H372	1.91	0.51
2:C:247:ALA:HA	2:C:258:MET:CE	2.41	0.51
2:D:80:TYR:CE2	2:D:107:THR:HG22	2.45	0.51
1:A:207:LEU:HD22	1:A:212:ILE:HG13	1.93	0.51
2:C:148:ASP:OD2	2:C:233:ARG:NH2	2.44	0.51
2:C:167:VAL:O	2:C:171:GLN:HG3	2.10	0.51
1:A:42:VAL:HG11	1:B:91:TYR:HE2	1.76	0.51
1:B:193:LYS:O	1:B:193:LYS:CD	2.56	0.51
2:D:163:ILE:HG21	2:D:213:ASN:CG	2.31	0.51
1:B:122:VAL:HB	1:B:181:ALA:HA	1.91	0.51
3:A:401:B12:H353	3:A:401:B12:H302	1.92	0.51
1:B:169:ASN:HD22	1:B:203:LEU:HB2	1.76	0.51
2:D:113:ASP:OD1	2:D:113:ASP:N	2.42	0.51
2:D:363:GLU:OE1	2:D:363:GLU:O	2.29	0.51
2:D:41:ARG:NH1	2:D:41:ARG:HG3	2.26	0.51
2:D:80:TYR:HE2	2:D:107:THR:HG22	1.75	0.51
2:D:279:ASP:OD1	2:D:279:ASP:C	2.50	0.51
1:A:153:GLU:OE1	2:C:488:ARG:NH2	2.41	0.51
1:A:163:LEU:CD2	1:A:175:LYS:HG2	2.31	0.51
1:A:258:LYS:HD2	1:A:258:LYS:O	2.11	0.51
3:B:401:B12:H531	3:B:401:B12:C56	2.41	0.51
2:D:236:ASN:O	2:D:258:MET:HA	2.11	0.51
2:C:12:LEU:HD12	2:C:459:LEU:HG	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:405:HIS:CD2	2:C:407:LEU:HD23	2.45	0.50
1:A:218:LEU:HD12	1:A:235:TYR:HE2	1.76	0.50
2:D:35:THR:HG22	2:D:502:LYS:HE2	1.92	0.50
1:A:196:HIS:CE1	1:A:197:ILE:HG12	2.46	0.50
2:D:104:LEU:HD11	2:D:109:ILE:HD12	1.93	0.50
3:A:401:B12:H492	3:A:401:B12:C47	2.41	0.50
1:B:143:MET:HG2	1:B:153:GLU:CG	2.42	0.50
2:C:239:SER:HA	2:C:243:MET:CG	2.42	0.50
2:C:270:ASP:O	2:C:493:GLY:HA2	2.11	0.50
2:C:332:GLU:OE1	2:C:367:LYS:NZ	2.45	0.50
2:D:148:ASP:OD1	2:D:148:ASP:N	2.39	0.50
2:C:411:THR:CB	2:C:414:ILE:HD11	2.42	0.50
2:C:437:ALA:HB3	2:D:349:ASN:OD1	2.11	0.50
2:D:105:ASP:OD2	2:D:108:SER:HB3	2.11	0.50
2:D:192:LEU:HD23	2:D:194:TYR:CE1	2.47	0.50
1:B:184:LEU:HB2	1:B:218:LEU:HD12	1.94	0.50
1:A:19:LEU:HA	1:A:22:VAL:HG23	1.94	0.50
1:A:32:GLY:O	1:A:84:SER:HA	2.11	0.50
1:B:44:ASP:OD1	1:B:45:GLY:N	2.43	0.50
1:B:123:VAL:HG13	1:B:185:LEU:HD13	1.94	0.50
1:B:220:CYS:HB3	1:B:225:ILE:HD13	1.94	0.50
3:B:401:B12:N33	3:B:401:B12:C27	2.75	0.50
3:B:401:B12:N29	3:B:401:B12:C25	2.73	0.50
2:D:88:THR:OG1	2:D:90:LEU:HD23	2.12	0.50
2:D:267:LEU:HD21	2:D:478:LEU:CD2	2.40	0.50
1:A:91:TYR:CE1	1:B:47:LYS:HG2	2.47	0.50
1:A:154:ARG:NH1	2:C:304:THR:OG1	2.44	0.50
1:B:150:TYR:OH	2:D:303:THR:HG21	2.11	0.50
1:A:208:GLU:OE2	1:A:213:ARG:HG2	2.12	0.50
2:C:344:ASN:OD1	2:C:345:PRO:HD2	2.12	0.50
2:D:32:ASP:OD1	2:D:32:ASP:C	2.50	0.50
1:A:42:VAL:HG21	1:B:91:TYR:CD2	2.47	0.49
1:A:85:LEU:HD22	1:B:59:MET:SD	2.53	0.49
1:B:25:TYR:HD1	1:B:29:MET:HA	1.77	0.49
1:B:189:THR:OG1	1:B:223:PRO:HD3	2.12	0.49
3:B:401:B12:C49	3:B:401:B12:C47	2.89	0.49
2:D:411:THR:HB	2:D:414:ILE:CD1	2.35	0.49
1:B:63:ASN:OD1	1:B:63:ASN:O	2.30	0.49
2:D:343:MET:HE3	2:D:354:GLU:HG2	1.93	0.49
1:A:121:VAL:HG11	1:A:256:MET:HE1	1.94	0.49
1:A:125:GLY:HA2	1:A:185:LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:341:PHE:O	2:D:375:PRO:HB3	2.12	0.49
2:D:356:ALA:HB2	2:D:451:ILE:HG23	1.94	0.49
1:B:249:ALA:HA	1:B:252:ILE:CG2	2.42	0.49
3:B:401:B12:H262	3:B:401:B12:C61	2.42	0.49
2:C:149:LYS:NZ	2:C:179:ASP:OD2	2.29	0.49
2:D:31:ILE:CG1	2:D:278:VAL:HA	2.43	0.49
2:D:221:LEU:HD12	2:D:234:LEU:HD13	1.93	0.49
1:A:40:LEU:HD23	1:B:24:PRO:HA	1.95	0.49
1:A:101:ILE:O	1:A:101:ILE:HG13	2.13	0.49
1:A:140:ILE:HD13	1:A:248:VAL:HG21	1.95	0.49
1:B:152:LEU:HA	1:B:155:TYR:CD1	2.47	0.49
1:A:145:GLY:HA3	1:A:149:HIS:O	2.11	0.49
1:B:36:LEU:HB2	1:B:81:ILE:HB	1.95	0.49
1:B:183:ALA:O	1:B:184:LEU:HD23	2.12	0.49
1:B:239:PHE:HB3	1:B:243:THR:HG21	1.95	0.49
3:B:401:B12:H473	3:B:401:B12:C49	2.39	0.49
2:C:362:ARG:HA	2:C:370:LEU:HD11	1.95	0.49
1:A:182:ASP:O	1:A:216:VAL:HG23	2.12	0.49
1:B:189:THR:HG23	1:B:223:PRO:CG	2.34	0.49
1:B:204:VAL:HA	1:B:207:LEU:HD23	1.95	0.49
2:C:167:VAL:HG12	2:C:217:MET:CE	2.42	0.49
2:D:186:ALA:O	2:D:189:GLN:HB2	2.12	0.49
1:B:18:ASP:OD1	1:B:20:THR:N	2.45	0.49
2:D:91:SER:O	2:D:95:ILE:HG22	2.13	0.49
2:D:196:PRO:HG2	2:D:210:THR:CG2	2.43	0.49
2:D:32:ASP:OD1	2:D:33:ALA:N	2.45	0.48
2:D:185:ARG:HH11	2:D:189:GLN:HB3	1.78	0.48
2:D:298:GLU:HB2	2:D:338:GLY:O	2.13	0.48
1:A:252:ILE:HG22	1:A:256:MET:CE	2.43	0.48
2:D:272:ASN:ND2	2:D:496:LEU:HB2	2.28	0.48
3:A:401:B12:H482	3:A:401:B12:H533	1.95	0.48
1:B:203:LEU:O	1:B:207:LEU:HD22	2.13	0.48
2:C:118:LYS:HD3	2:C:507:PHE:CD1	2.48	0.48
2:C:196:PRO:HG2	2:C:210:THR:HG22	1.94	0.48
1:A:138:ASP:HB2	2:C:191:LEU:HD13	1.94	0.48
1:A:185:LEU:HD22	3:A:401:B12:C5M	2.44	0.48
2:D:409:MET:CG	2:D:417:PRO:HB3	2.36	0.48
1:A:36:LEU:HD22	1:B:36:LEU:CD2	2.42	0.48
1:B:54:GLN:O	1:B:58:LYS:HG3	2.13	0.48
1:B:193:LYS:HZ1	1:B:195:ALA:HA	1.78	0.48
2:D:162:ASN:HB3	2:D:165:GLU:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:MET:HG3	1:B:30:ASN:N	2.29	0.48
2:C:195:VAL:HG11	2:C:249:MET:HE3	1.94	0.48
2:D:87:TYR:CD2	2:D:109:ILE:HD13	2.48	0.48
2:D:233:ARG:HB3	2:D:256:ASP:CB	2.43	0.48
2:D:512:ASP:C	2:D:512:ASP:OD1	2.52	0.48
1:B:213:ARG:NH2	1:B:234:GLY:O	2.47	0.48
1:A:207:LEU:CD1	1:A:218:LEU:HD21	2.44	0.48
2:C:375:PRO:O	2:C:379:MET:HE3	2.14	0.48
1:A:39:THR:HA	1:A:77:THR:O	2.14	0.48
1:B:163:LEU:HD21	1:B:175:LYS:HG2	1.95	0.48
2:C:479:GLU:OE2	2:C:490:ILE:N	2.43	0.48
2:D:6:LEU:HD13	2:D:455:ALA:CB	2.44	0.48
1:B:67:VAL:HG11	2:C:414:ILE:HG21	1.95	0.48
2:D:223:GLU:OE1	2:D:223:GLU:HA	2.14	0.48
1:B:170:GLU:O	1:B:173:VAL:HG12	2.14	0.47
1:B:221:GLY:C	1:B:225:ILE:CD1	2.82	0.47
2:D:256:ASP:OD1	2:D:256:ASP:N	2.47	0.47
1:A:42:VAL:HG13	1:A:43:PRO:HD2	1.96	0.47
1:A:241:PRO:HA	3:A:401:B12:H2R	1.97	0.47
1:B:22:VAL:HG21	1:B:91:TYR:HB2	1.96	0.47
1:B:67:VAL:CG1	2:C:414:ILE:HG21	2.44	0.47
1:B:184:LEU:O	1:B:219:ILE:HD12	2.14	0.47
1:B:221:GLY:C	1:B:225:ILE:CG1	2.82	0.47
3:B:401:B12:O7R	3:B:401:B12:H2B	2.14	0.47
2:D:243:MET:N	2:D:244:PRO:HD2	2.28	0.47
1:A:14:ASP:OD1	1:A:14:ASP:C	2.53	0.47
1:A:224:ARG:NH1	1:A:224:ARG:HG3	2.30	0.47
2:C:36:THR:HA	2:C:498:GLY:O	2.14	0.47
2:D:35:THR:HG21	2:D:506:TYR:CZ	2.49	0.47
2:D:73:LEU:HD12	2:D:500:VAL:HG21	1.96	0.47
2:C:235:CYS:HA	2:C:257:VAL:O	2.14	0.47
1:A:25:TYR:CD2	1:A:29:MET:HA	2.49	0.47
1:B:20:THR:HG22	1:B:92:THR:CG2	2.44	0.47
1:B:23:LYS:CG	1:B:24:PRO:HD2	2.33	0.47
1:B:210:GLU:HG3	1:B:212:ILE:HG12	1.97	0.47
2:D:74:SER:HB2	2:D:501:GLU:O	2.14	0.47
2:D:299:ASP:HB3	2:D:373:MET:SD	2.55	0.47
2:D:405:HIS:CD2	2:D:407:LEU:HD23	2.50	0.47
1:B:113:ILE:HG23	1:B:117:ILE:CG1	2.43	0.47
1:B:215:LYS:CA	1:B:261:ILE:HD13	2.42	0.47
1:B:249:ALA:HA	1:B:252:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:104:LEU:HD21	2:D:109:ILE:HD11	1.97	0.47
2:D:185:ARG:HH11	2:D:185:ARG:HG2	1.80	0.47
1:B:104:MET:HE3	1:B:109:THR:HA	1.96	0.47
1:B:255:GLU:OE1	1:B:258:LYS:HE2	2.15	0.47
2:C:86:ILE:HD11	2:C:116:GLU:HB3	1.96	0.47
2:C:273:MET:HE3	2:C:475:PHE:HD1	1.80	0.47
2:D:14:ASP:C	2:D:14:ASP:OD1	2.53	0.47
1:A:24:PRO:HD3	1:B:55:LEU:HD21	1.97	0.47
1:B:258:LYS:NZ	1:B:259:ARG:HB2	2.30	0.47
2:C:282:PHE:HD1	2:C:511:ILE:HD11	1.79	0.47
2:C:322:GLU:HG3	2:C:335:MET:HE1	1.96	0.47
1:B:210:GLU:OE1	1:B:210:GLU:HA	2.15	0.47
2:C:237:TYR:CE1	2:C:259:LEU:HD22	2.49	0.47
2:C:443:ILE:HG13	2:C:443:ILE:O	2.15	0.47
2:D:155:TYR:OH	2:D:182:ALA:HB2	2.14	0.47
2:C:165:GLU:OE2	2:C:165:GLU:CA	2.62	0.46
2:C:174:ALA:HB1	2:C:232:ILE:CD1	2.46	0.46
2:C:444:TYR:CE2	2:D:444:TYR:HB3	2.50	0.46
2:D:295:ASN:ND2	2:D:371:LYS:HD2	2.30	0.46
1:A:161:TYR:CE1	1:A:179:VAL:HG11	2.51	0.46
1:B:128:THR:CG2	1:B:186:VAL:HG23	2.40	0.46
3:B:401:B12:C53	3:B:401:B12:H481	2.44	0.46
2:C:512:ASP:OD1	2:C:512:ASP:C	2.53	0.46
3:A:401:B12:C35	3:A:401:B12:H372	2.45	0.46
2:C:405:HIS:HD2	2:C:407:LEU:HD23	1.81	0.46
2:D:191:LEU:O	2:D:241:LEU:HD12	2.15	0.46
1:B:246:ASP:OD1	1:B:246:ASP:C	2.53	0.46
2:C:444:TYR:HH	2:D:444:TYR:HD2	1.63	0.46
2:D:204:PHE:HD1	2:D:205:GLY:N	2.13	0.46
1:B:268:LYS:HA	1:B:268:LYS:HE2	1.97	0.46
1:A:228:GLU:OE1	1:A:228:GLU:C	2.54	0.46
3:A:401:B12:H363	3:A:401:B12:C42	2.27	0.46
1:B:103:ALA:HB1	1:B:246:ASP:OD2	2.16	0.46
2:D:140:GLU:C	2:D:140:GLU:OE1	2.54	0.46
1:B:33:LYS:HG2	2:C:418:PHE:CZ	2.50	0.46
1:B:50:GLU:OE2	1:B:50:GLU:C	2.54	0.46
2:C:157:ILE:HD13	2:C:184:ILE:HD11	1.98	0.46
1:B:113:ILE:HD13	1:B:121:VAL:HG21	1.98	0.46
2:C:228:LEU:HD12	2:C:232:ILE:HD11	1.98	0.46
2:C:239:SER:HA	2:C:243:MET:HG2	1.97	0.46
2:C:272:ASN:HD21	2:C:496:LEU:CD2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:ASP:O	2:D:502:LYS:HD2	2.15	0.46
2:D:390:ASP:HA	2:D:393:PHE:HB3	1.98	0.46
1:B:221:GLY:C	1:B:225:ILE:HG12	2.35	0.46
1:A:36:LEU:HA	1:B:35:GLN:O	2.16	0.46
2:C:263:LEU:O	2:C:267:LEU:HG	2.16	0.46
2:D:53:ASN:HD22	2:D:57:VAL:HB	1.79	0.46
2:D:200:THR:HG23	2:D:213:ASN:ND2	2.31	0.46
2:D:511:ILE:HD13	2:D:511:ILE:HA	1.81	0.46
1:A:72:LEU:HD22	2:C:423:ALA:CB	2.46	0.45
1:A:150:TYR:HB3	1:A:154:ARG:HD2	1.97	0.45
1:A:221:GLY:HA3	3:A:401:B12:C4B	2.46	0.45
1:B:123:VAL:HG13	1:B:185:LEU:CD1	2.47	0.45
1:B:134:THR:CG2	1:B:165:SER:HA	2.46	0.45
1:A:188:GLN:O	1:A:222:GLY:HA3	2.16	0.45
1:B:44:ASP:CA	1:B:77:THR:HG21	2.46	0.45
2:C:153:LEU:HD21	2:C:403:ARG:NH2	2.31	0.45
2:C:200:THR:HB	2:C:213:ASN:HD21	1.82	0.45
2:C:202:GLU:C	2:C:202:GLU:OE1	2.55	0.45
2:D:141:GLU:OE1	2:D:142:PHE:N	2.50	0.45
2:D:273:MET:HE1	2:D:475:PHE:HD1	1.81	0.45
3:A:401:B12:H312	3:A:401:B12:C25	2.47	0.45
1:B:108:GLU:HA	1:B:111:GLU:CD	2.36	0.45
1:B:160:ALA:C	1:B:161:TYR:HD1	2.19	0.45
1:B:186:VAL:O	1:B:220:CYS:HA	2.16	0.45
2:C:6:LEU:HD13	2:C:455:ALA:CB	2.47	0.45
1:A:62:GLU:OE2	1:A:62:GLU:CA	2.62	0.45
1:B:39:THR:HG23	1:B:77:THR:O	2.17	0.45
3:B:401:B12:H601	3:B:401:B12:C26	2.47	0.45
2:C:285:VAL:HG22	2:C:515:LEU:HD13	1.98	0.45
2:D:84:ALA:O	2:D:88:THR:HG22	2.17	0.45
2:D:267:LEU:HB2	2:D:268:PHE:HD1	1.81	0.45
1:A:122:VAL:HG12	1:A:181:ALA:CB	2.46	0.45
1:B:144:LYS:O	2:D:269:ARG:NH1	2.50	0.45
2:C:156:VAL:HG11	2:C:178:ALA:HB2	1.99	0.45
2:D:241:LEU:HD22	2:D:275:ARG:CZ	2.47	0.45
2:D:282:PHE:CD1	2:D:511:ILE:HD11	2.50	0.45
1:A:85:LEU:CD1	1:A:87:HIS:H	2.29	0.45
1:A:101:ILE:C	1:A:102:LYS:HD2	2.37	0.45
1:B:215:LYS:HB3	1:B:261:ILE:HD11	1.98	0.45
2:C:36:THR:HG23	2:C:278:VAL:HG11	1.98	0.45
2:C:54:ASP:OD1	2:C:54:ASP:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:272:ASN:ND2	2:D:496:LEU:HD23	2.32	0.45
3:B:401:B12:H351	3:B:401:B12:C37	2.46	0.45
2:C:36:THR:HG22	2:C:499:VAL:HG22	1.99	0.45
2:C:238:ALA:HB2	2:C:258:MET:SD	2.56	0.45
1:A:142:ASN:HD22	2:C:269:ARG:CD	2.30	0.45
2:C:88:THR:CB	2:C:90:LEU:HD12	2.47	0.45
2:C:322:GLU:HG3	2:C:335:MET:CE	2.47	0.45
2:C:516:ARG:NH1	2:C:516:ARG:CB	2.79	0.45
2:D:42:THR:O	2:D:46:LEU:HG	2.17	0.45
2:D:163:ILE:HD12	2:D:163:ILE:C	2.37	0.45
1:A:31:ASP:OD1	1:A:31:ASP:O	2.35	0.45
1:A:35:GLN:O	1:B:36:LEU:HA	2.17	0.45
2:C:12:LEU:HD12	2:C:459:LEU:HD21	1.97	0.45
2:D:31:ILE:HD11	2:D:277:MET:C	2.38	0.45
1:B:137:LEU:HD23	1:B:137:LEU:O	2.17	0.45
2:D:163:ILE:HG21	2:D:213:ASN:OD1	2.17	0.45
1:A:224:ARG:HG3	1:A:224:ARG:HH11	1.82	0.44
1:B:127:THR:HB	1:B:165:SER:O	2.17	0.44
1:B:173:VAL:CG1	1:B:206:LEU:HD21	2.47	0.44
1:B:255:GLU:OE1	1:B:255:GLU:CA	2.63	0.44
1:A:124:VAL:HG12	1:A:172:PHE:CE1	2.52	0.44
1:A:236:ASP:O	1:A:237:ALA:HB3	2.16	0.44
1:B:217:LEU:HD12	1:B:217:LEU:N	2.29	0.44
1:B:222:GLY:N	3:B:401:B12:C2B	2.81	0.44
1:A:124:VAL:HG23	1:A:181:ALA:HB2	1.98	0.44
2:D:79:THR:HG1	2:D:507:PHE:HE1	1.63	0.44
1:A:163:LEU:HD12	1:A:172:PHE:HD1	1.83	0.44
3:B:401:B12:O39	3:B:401:B12:H412	2.17	0.44
2:C:91:SER:HB2	2:C:92:PRO:HD2	1.99	0.44
2:D:291:GLY:HA2	2:D:334:GLN:OE1	2.17	0.44
2:D:344:ASN:OD1	2:D:345:PRO:HD2	2.16	0.44
1:A:114:LYS:HG2	1:A:157:MET:CE	2.47	0.44
1:A:185:LEU:CD2	1:A:219:ILE:HB	2.40	0.44
3:B:401:B12:C35	3:B:401:B12:H372	2.47	0.44
2:D:51:GLY:O	2:D:59:LEU:HD23	2.17	0.44
2:D:335:MET:O	2:D:368:ALA:HB1	2.18	0.44
1:A:106:MET:HG3	1:A:155:TYR:CE1	2.53	0.44
1:B:127:THR:HG23	1:B:187:SER:O	2.17	0.44
1:B:167:VAL:HG13	1:B:171:GLU:OE1	2.18	0.44
2:C:316:ALA:HB1	2:C:466:LEU:HD21	2.00	0.44
1:A:114:LYS:CG	1:A:157:MET:HE2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:TYR:CD1	1:B:29:MET:HA	2.53	0.44
1:B:124:VAL:HG12	1:B:172:PHE:CE1	2.52	0.44
1:B:154:ARG:NH1	2:D:304:THR:HG1	2.08	0.44
1:B:182:ASP:OD1	1:B:182:ASP:C	2.56	0.44
3:B:401:B12:C14	5:D:601:5AD:C5'	2.58	0.44
2:C:121:VAL:HG12	2:C:121:VAL:O	2.17	0.44
2:C:211:GLN:NE2	2:C:253:GLU:OE2	2.43	0.44
2:C:327:ILE:HD12	2:C:327:ILE:HA	1.82	0.44
2:C:435:ASN:ND2	2:D:345:PRO:O	2.45	0.44
2:C:496:LEU:HD13	2:C:496:LEU:C	2.37	0.44
2:D:41:ARG:HG2	2:D:64:VAL:CG2	2.42	0.44
2:D:200:THR:HG23	2:D:213:ASN:HD21	1.81	0.44
1:A:122:VAL:O	1:A:181:ALA:HB1	2.18	0.44
1:B:18:ASP:OD1	1:B:18:ASP:C	2.56	0.44
2:C:11:GLU:C	2:C:11:GLU:OE1	2.56	0.44
2:D:35:THR:HG22	2:D:502:LYS:CE	2.47	0.44
2:D:257:VAL:HG22	2:D:293:ILE:HB	2.00	0.44
1:A:128:THR:O	1:A:199:ASN:ND2	2.49	0.44
2:C:222:ASP:OD2	2:C:254:ARG:NH2	2.51	0.44
2:C:411:THR:HB	2:C:414:ILE:CD1	2.46	0.44
1:A:138:ASP:HB2	2:C:191:LEU:CD1	2.47	0.43
1:B:113:ILE:HD13	1:B:121:VAL:HG23	2.00	0.43
1:B:124:VAL:HG12	1:B:172:PHE:HE1	1.82	0.43
1:B:124:VAL:HG23	1:B:181:ALA:HB2	1.99	0.43
3:B:401:B12:C53	3:B:401:B12:H561	2.48	0.43
2:C:32:ASP:C	2:C:32:ASP:OD1	2.56	0.43
2:D:33:ALA:O	2:D:34:HIS:ND1	2.51	0.43
2:D:85:MET:SD	2:D:92:PRO:HD3	2.57	0.43
2:D:159:ALA:HB1	2:D:206:GLY:HA2	2.00	0.43
2:D:238:ALA:O	2:D:243:MET:HA	2.17	0.43
2:D:266:ILE:HG23	2:D:273:MET:HB2	2.00	0.43
2:D:374:PRO:HD3	2:D:406:LEU:HG	2.00	0.43
1:B:35:GLN:HG2	1:B:36:LEU:N	2.33	0.43
2:C:503:ASP:CG	2:C:504:PRO:HD2	2.38	0.43
2:D:171:GLN:HB3	2:D:224:VAL:HG21	2.01	0.43
1:B:150:TYR:HD2	1:B:154:ARG:NE	2.17	0.43
2:C:12:LEU:HD12	2:C:459:LEU:CG	2.49	0.43
2:D:41:ARG:NE	2:D:245:GLU:OE1	2.52	0.43
2:D:82:GLY:C	2:D:117:ILE:HG23	2.38	0.43
2:D:471:GLN:HA	2:D:471:GLN:OE1	2.17	0.43
1:A:185:LEU:HB3	3:A:401:B12:HM52	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:GLU:C	1:A:232:GLU:OE2	2.56	0.43
1:B:104:MET:CE	1:B:109:THR:HA	2.49	0.43
1:A:111:GLU:OE1	1:A:114:LYS:HD2	2.17	0.43
1:A:252:ILE:CG2	1:A:256:MET:HE1	2.48	0.43
2:C:273:MET:SD	2:C:490:ILE:HA	2.58	0.43
5:C:601:5AD:H8	5:C:601:5AD:H3'	2.00	0.43
2:D:153:LEU:HD21	2:D:403:ARG:NH2	2.34	0.43
2:C:155:TYR:OH	2:C:235:CYS:SG	2.74	0.43
2:D:409:MET:N	2:D:409:MET:SD	2.91	0.43
1:A:119:ARG:HH11	1:A:119:ARG:HB3	1.84	0.43
3:A:401:B12:H2B	3:A:401:B12:O7R	2.18	0.43
1:B:62:GLU:OE2	1:B:62:GLU:CA	2.65	0.43
1:B:201:THR:HG22	1:B:233:LEU:HD22	2.01	0.43
2:C:272:ASN:HD22	2:C:496:LEU:HA	1.83	0.43
2:D:390:ASP:N	2:D:390:ASP:OD1	2.50	0.43
1:B:133:HIS:HD2	1:B:189:THR:HG21	1.83	0.43
3:A:401:B12:H472	3:A:401:B12:H10	1.77	0.43
1:B:108:GLU:HA	1:B:111:GLU:OE1	2.18	0.43
1:B:203:LEU:O	1:B:203:LEU:HD22	2.19	0.43
1:B:215:LYS:HB3	1:B:261:ILE:CD1	2.49	0.43
1:A:249:ALA:O	1:A:253:VAL:HG23	2.19	0.43
1:B:163:LEU:CD2	1:B:175:LYS:HG2	2.49	0.43
2:D:361:VAL:HG12	2:D:370:LEU:HD13	2.01	0.43
1:B:200:LEU:HB3	1:B:235:TYR:CE1	2.54	0.42
1:A:104:MET:CE	1:A:109:THR:HA	2.49	0.42
1:B:14:ASP:OD1	1:B:16:THR:OG1	2.36	0.42
2:D:343:MET:HE1	2:D:354:GLU:HG2	2.01	0.42
1:A:122:VAL:HG11	1:A:179:VAL:CG1	2.49	0.42
1:A:125:GLY:HA3	1:A:141:MET:CE	2.48	0.42
1:A:127:THR:HB	1:A:165:SER:O	2.19	0.42
1:A:142:ASN:ND2	2:C:269:ARG:CD	2.82	0.42
3:B:401:B12:O7R	3:B:401:B12:P	2.77	0.42
2:C:476:LYS:HD3	2:C:476:LYS:HA	1.80	0.42
2:C:477:ALA:HB1	2:C:482:LYS:HG3	2.01	0.42
3:A:401:B12:C47	3:A:401:B12:C49	2.98	0.42
1:B:36:LEU:HD11	1:B:59:MET:HE2	2.00	0.42
1:B:122:VAL:CG1	1:B:181:ALA:HA	2.49	0.42
2:C:144:LYS:HD2	2:C:144:LYS:O	2.19	0.42
2:D:91:SER:O	2:D:94:GLU:HG3	2.20	0.42
2:D:185:ARG:HG2	2:D:185:ARG:NH1	2.35	0.42
1:A:191:THR:HG21	1:A:224:ARG:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ILE:HG13	3:B:401:B12:HM62	1.98	0.42
2:C:391:ALA:O	2:C:395:VAL:HG23	2.20	0.42
2:C:511:ILE:HD13	2:C:511:ILE:HA	1.81	0.42
2:C:443:ILE:HA	2:D:444:TYR:O	2.19	0.42
2:D:249:MET:O	2:D:253:GLU:HG2	2.19	0.42
1:A:128:THR:HB	1:A:169:ASN:OD1	2.19	0.42
1:A:128:THR:CG2	1:A:186:VAL:HG23	2.49	0.42
1:A:142:ASN:O	1:A:151:GLY:HA3	2.19	0.42
1:A:182:ASP:C	1:A:216:VAL:HG23	2.40	0.42
2:D:238:ALA:O	2:D:243:MET:HB2	2.20	0.42
2:D:496:LEU:HD13	2:D:496:LEU:O	2.20	0.42
1:B:200:LEU:N	1:B:200:LEU:HD22	2.35	0.42
1:B:258:LYS:HE3	1:B:258:LYS:HB3	1.72	0.42
2:D:155:TYR:CZ	2:D:182:ALA:HB2	2.55	0.42
2:D:465:LEU:O	2:D:465:LEU:HD12	2.19	0.42
1:A:243:THR:OG1	1:A:244:PHE:N	2.53	0.42
2:D:92:PRO:HA	2:D:95:ILE:CG2	2.50	0.42
2:D:511:ILE:O	2:D:515:LEU:HB2	2.20	0.42
1:A:167:VAL:O	1:A:167:VAL:HG23	2.19	0.42
1:B:173:VAL:HG11	1:B:206:LEU:HD21	2.01	0.42
3:B:401:B12:H302	3:B:401:B12:C35	2.40	0.42
3:B:401:B12:N24	5:D:601:5AD:C5'	2.83	0.42
2:D:113:ASP:O	2:D:117:ILE:CD1	2.68	0.42
2:D:222:ASP:OD2	2:D:254:ARG:NH2	2.41	0.42
2:D:241:LEU:HD23	2:D:241:LEU:HA	1.92	0.42
2:D:267:LEU:O	2:D:488:ARG:NH2	2.32	0.42
1:A:33:LYS:HA	1:A:83:GLY:O	2.20	0.41
1:A:229:LEU:C	1:A:229:LEU:HD23	2.40	0.41
1:B:90:ASP:OD1	1:B:90:ASP:C	2.59	0.41
3:B:401:B12:H531	3:B:401:B12:H561	2.02	0.41
2:C:269:ARG:HA	2:C:269:ARG:HD3	1.29	0.41
1:A:35:GLN:C	1:A:36:LEU:HD23	2.40	0.41
3:A:401:B12:H351	3:A:401:B12:H372	2.01	0.41
2:C:331:PRO:HD2	2:C:334:GLN:NE2	2.35	0.41
2:D:163:ILE:HD12	2:D:164:TYR:H	1.80	0.41
3:B:401:B12:H351	3:B:401:B12:C36	2.27	0.41
2:D:496:LEU:O	2:D:496:LEU:HD22	2.20	0.41
2:D:509:PRO:O	2:D:513:LEU:HG	2.20	0.41
1:A:14:ASP:OD1	1:A:15:THR:N	2.52	0.41
1:B:112:TYR:CE1	1:B:257:VAL:HG21	2.55	0.41
2:C:343:MET:CB	2:C:354:GLU:OE2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:150:GLU:OE1	2:D:150:GLU:CA	2.68	0.41
2:D:212:GLU:OE1	2:D:212:GLU:N	2.53	0.41
2:D:219:LYS:O	2:D:223:GLU:HG2	2.20	0.41
2:D:284:ARG:HB3	2:D:330:ILE:HD11	2.02	0.41
1:A:77:THR:HB	1:A:79:PHE:HE1	1.85	0.41
1:B:32:GLY:O	1:B:85:LEU:N	2.53	0.41
1:B:221:GLY:N	1:B:225:ILE:HD11	2.35	0.41
2:C:12:LEU:HD13	2:C:12:LEU:C	2.40	0.41
2:C:133:ARG:NH2	2:C:518:ASP:HA	2.36	0.41
2:D:163:ILE:HA	2:D:166:ASP:OD2	2.20	0.41
1:A:197:ILE:HD11	1:A:229:LEU:HD11	2.03	0.41
3:A:401:B12:O7R	3:A:401:B12:P	2.79	0.41
1:B:261:ILE:HD12	1:B:261:ILE:C	2.41	0.41
3:B:401:B12:O28	3:B:401:B12:C32	2.68	0.41
3:B:401:B12:C35	3:B:401:B12:C31	2.98	0.41
2:C:91:SER:O	2:C:95:ILE:HG13	2.20	0.41
2:D:30:PHE:CD2	2:D:475:PHE:HZ	2.39	0.41
2:D:152:PRO:HA	2:D:403:ARG:O	2.21	0.41
2:D:237:TYR:HD1	2:D:259:LEU:HB2	1.86	0.41
2:D:392:MET:HA	2:D:392:MET:CE	2.49	0.41
1:A:111:GLU:OE1	1:A:111:GLU:HA	2.20	0.41
1:A:134:THR:CG2	1:A:165:SER:HA	2.51	0.41
1:A:205:GLU:OE1	1:A:205:GLU:CA	2.69	0.41
1:B:32:GLY:O	1:B:84:SER:HA	2.21	0.41
1:B:117:ILE:HG21	1:B:256:MET:HE2	2.01	0.41
1:B:128:THR:HA	1:B:167:VAL:O	2.20	0.41
2:C:268:PHE:CD1	2:C:268:PHE:N	2.88	0.41
2:D:267:LEU:HB2	2:D:268:PHE:CD1	2.55	0.41
2:D:273:MET:O	2:D:273:MET:SD	2.79	0.41
1:A:90:ASP:OD1	1:A:90:ASP:C	2.59	0.41
2:D:490:ILE:HD12	2:D:491:ASP:N	2.36	0.41
1:A:19:LEU:HD22	1:A:91:TYR:HD2	1.84	0.41
3:A:401:B12:H262	3:A:401:B12:H91	1.52	0.41
1:B:169:ASN:ND2	1:B:203:LEU:HB2	2.35	0.41
1:B:171:GLU:H	1:B:171:GLU:HG3	1.72	0.41
2:C:6:LEU:CD2	2:C:451:ILE:HG22	2.51	0.41
2:C:86:ILE:CD1	2:C:116:GLU:HB3	2.51	0.41
2:C:152:PRO:HA	2:C:403:ARG:O	2.20	0.41
2:C:162:ASN:OD1	2:C:201:THR:HA	2.21	0.41
2:C:397:THR:HG21	2:C:405:HIS:ND1	2.36	0.41
2:D:225:SER:OG	2:D:231:TYR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:270:ASP:O	2:D:493:GLY:HA2	2.20	0.41
1:B:112:TYR:CD1	1:B:112:TYR:C	2.94	0.41
2:C:41:ARG:NE	2:C:245:GLU:OE2	2.43	0.41
2:D:70:LYS:HE2	2:D:70:LYS:HB2	1.91	0.41
2:D:215:ARG:HG3	2:D:215:ARG:HH11	1.86	0.41
2:C:349:ASN:HA	2:D:435:ASN:O	2.20	0.40
2:D:104:LEU:HD11	2:D:109:ILE:HD11	2.03	0.40
2:D:195:VAL:O	2:D:195:VAL:HG23	2.21	0.40
2:D:272:ASN:HA	2:D:493:GLY:HA3	2.04	0.40
1:B:73:ASP:OD1	1:B:74:LYS:N	2.49	0.40
1:B:147:ALA:N	2:D:187:THR:HG21	2.18	0.40
2:C:4:SER:HA	2:C:363:GLU:OE2	2.20	0.40
2:C:157:ILE:HG23	2:C:184:ILE:CG1	2.50	0.40
2:C:411:THR:CG2	2:C:414:ILE:HD11	2.51	0.40
2:D:185:ARG:HD3	2:D:209:ALA:HB2	2.02	0.40
1:A:207:LEU:HD11	1:A:218:LEU:HD21	2.02	0.40
1:B:36:LEU:HD11	1:B:59:MET:CE	2.52	0.40
1:B:140:ILE:CD1	3:B:401:B12:HM61	2.51	0.40
1:B:212:ILE:HG22	1:B:215:LYS:NZ	2.36	0.40
2:C:11:GLU:OE1	2:C:12:LEU:N	2.54	0.40
2:C:47:LEU:HD21	2:C:121:VAL:CG1	2.51	0.40
2:C:301:TYR:CD1	2:C:301:TYR:N	2.90	0.40
1:B:104:MET:HE1	1:B:108:GLU:HB2	2.01	0.40
3:B:401:B12:O7R	3:B:401:B12:C2B	2.69	0.40
3:B:401:B12:O39	3:B:401:B12:C8	2.68	0.40
2:C:104:LEU:HG	2:C:105:ASP:N	2.37	0.40
2:D:67:ILE:HD11	2:D:80:TYR:CD1	2.57	0.40
2:D:271:ILE:HG22	2:D:276:THR:OG1	2.21	0.40
2:D:411:THR:HG23	2:D:421:ASP:OD2	2.21	0.40
1:A:29:MET:HG3	1:A:30:ASN:N	2.37	0.40
1:A:146:TYR:CE1	2:C:187:THR:HG23	2.56	0.40
1:B:189:THR:O	1:B:191:THR:HG23	2.21	0.40
2:C:343:MET:HB2	2:C:354:GLU:OE2	2.21	0.40
2:D:160:THR:HG23	2:D:166:ASP:OD1	2.21	0.40
2:D:315:LEU:HD11	2:D:364:ILE:HD12	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	255/269 (95%)	240 (94%)	15 (6%)	0	100	100
1	B	254/269 (94%)	230 (91%)	21 (8%)	3 (1%)	13	40
2	C	515/532 (97%)	499 (97%)	15 (3%)	1 (0%)	47	77
2	D	515/532 (97%)	505 (98%)	9 (2%)	1 (0%)	47	77
All	All	1539/1602 (96%)	1474 (96%)	60 (4%)	5 (0%)	44	70

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	222	GLY
2	D	241	LEU
1	B	145	GLY
1	B	147	ALA
2	C	269	ARG

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	213/224 (95%)	200 (94%)	13 (6%)	18	46
1	B	212/224 (95%)	188 (89%)	24 (11%)	6	21
2	C	429/442 (97%)	415 (97%)	14 (3%)	38	67
2	D	429/442 (97%)	401 (94%)	28 (6%)	17	44
All	All	1283/1332 (96%)	1204 (94%)	79 (6%)	22	46

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	31	ASP
1	A	47	LYS
1	A	131	ASP
1	A	144	LYS
1	A	187	SER
1	A	191	THR
1	A	205	GLU
1	A	227	HIS
1	A	236	ASP
1	A	243	THR
1	A	247	HIS
1	A	267	TYR
1	B	23	LYS
1	B	37	SER
1	B	84	SER
1	B	92	THR
1	B	96	VAL
1	B	104	MET
1	B	106	MET
1	B	114	LYS
1	B	131	ASP
1	B	133	HIS
1	B	134	THR
1	B	143	MET
1	B	169	ASN
1	B	172	PHE
1	B	182	ASP
1	B	187	SER
1	B	193	LYS
1	B	194	ASP
1	B	236	ASP
1	B	246	ASP
1	B	247	HIS
1	B	258	LYS
1	B	261	ILE
1	B	267	TYR
2	C	69	SER
2	C	70	LYS
2	C	115	PHE
2	C	144	LYS
2	C	202	GLU

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Mol	Chain	Res	Type
2	C	207	THR
2	C	219	LYS
2	C	258	MET
2	C	268	PHE
2	C	269	ARG
2	C	324	PHE
2	C	410	LEU
2	C	438	ASP
2	C	444	TYR
2	D	4	SER
2	D	32	ASP
2	D	52	VAL
2	D	54	ASP
2	D	59	LEU
2	D	65	ASP
2	D	70	LYS
2	D	179	ASP
2	D	204	PHE
2	D	222	ASP
2	D	235	CYS
2	D	256	ASP
2	D	261	ASP
2	D	269	ARG
2	D	273	MET
2	D	279	ASP
2	D	335	MET
2	D	342	GLU
2	D	360	MET
2	D	376	THR
2	D	390	ASP
2	D	412	GLU
2	D	428	SER
2	D	435	ASN
2	D	467	LYS
2	D	475	PHE
2	D	507	PHE
2	D	516	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN

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Mol	Chain	Res	Type
1	B	142	ASN
2	C	272	ASN
2	C	387	HIS
2	D	280	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
4	PLP	A	402	1	15,15,16	0.99	1 (6%)	20,22,23	1.03	2 (10%)
3	B12	B	401	-	90,101,101	2.12	30 (33%)	137,166,166	2.35	43 (31%)
4	PLP	B	402	1	15,15,16	1.84	5 (33%)	20,22,23	2.12	5 (25%)
5	5AD	C	601	-	17,20,20	2.34	6 (35%)	15,30,30	2.82	5 (33%)
3	B12	A	401	-	90,101,101	2.74	53 (58%)	137,166,166	2.36	44 (32%)
5	5AD	D	601	-	17,20,20	1.12	2 (11%)	15,30,30	2.47	5 (33%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PLP	A	402	1	-	3/6/6/8	0/1/1/1
3	B12	B	401	-	-	22/52/223/223	0/3/11/11
4	PLP	B	402	1	-	3/6/6/8	0/1/1/1
5	5AD	C	601	-	-	0/0/20/20	0/3/3/3
3	B12	A	401	-	-	16/52/223/223	0/3/11/11
5	5AD	D	601	-	-	0/0/20/20	0/3/3/3

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	B12	C14-N23	-8.15	1.24	1.35
3	B	401	B12	C14-N23	-7.06	1.26	1.35
3	A	401	B12	C16-C15	-5.61	1.29	1.44
5	C	601	5AD	C2'-C1'	-5.53	1.45	1.53
3	B	401	B12	C16-C15	-5.48	1.29	1.44
3	B	401	B12	C19-N24	5.38	1.58	1.48
5	C	601	5AD	C4-N3	-5.19	1.28	1.35
3	B	401	B12	C18-C19	-4.58	1.43	1.53
3	A	401	B12	C1-C2	-4.39	1.48	1.58
3	A	401	B12	C17-C16	-4.39	1.44	1.54
3	B	401	B12	C1-C19	-4.38	1.45	1.55
3	A	401	B12	C2-C3	-4.27	1.44	1.57
3	A	401	B12	C26-C2	-4.23	1.45	1.55
3	A	401	B12	C11-N23	-4.21	1.29	1.37
3	A	401	B12	C36-C7	-4.18	1.47	1.54
3	A	401	B12	C54-C17	-4.17	1.47	1.54
3	A	401	B12	C12-C11	-4.12	1.45	1.52
3	A	401	B12	C4B-C9B	-4.07	1.35	1.41
3	A	401	B12	O6R-C4R	-4.06	1.35	1.45
3	A	401	B12	C7-C8	-4.04	1.44	1.55
3	A	401	B12	C30-C3	-3.96	1.45	1.54
3	A	401	B12	C7B-C8B	-3.87	1.33	1.40
3	A	401	B12	C7-C6	-3.68	1.45	1.54
3	A	401	B12	C12-C13	-3.58	1.44	1.55
3	A	401	B12	C17-C18	-3.57	1.48	1.54
3	B	401	B12	C11-N23	-3.57	1.30	1.37
3	B	401	B12	C17-C18	-3.54	1.48	1.54
3	A	401	B12	C47-C12	-3.53	1.46	1.54
3	A	401	B12	C8-C9	-3.41	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	B12	C3-C4	-3.34	1.43	1.51
3	B	401	B12	C4B-C9B	-3.34	1.36	1.41
3	B	401	B12	C1-C2	-3.32	1.51	1.58
3	A	401	B12	C13-C14	-3.31	1.46	1.52
3	A	401	B12	C10-C11	-3.23	1.28	1.38
3	A	401	B12	C20-C1	-3.22	1.47	1.53
3	A	401	B12	O51-C50	-3.22	1.14	1.24
3	A	401	B12	C48-C13	-3.13	1.47	1.54
3	B	401	B12	C17-C16	-3.11	1.47	1.54
3	A	401	B12	C60-C18	-3.10	1.47	1.54
3	B	401	B12	C9-N22	3.09	1.38	1.30
3	B	401	B12	C26-C2	-3.09	1.48	1.55
3	B	401	B12	C54-C17	-3.07	1.49	1.54
3	B	401	B12	C13-C14	-3.05	1.46	1.52
4	B	402	PLP	C3-C2	3.02	1.43	1.40
3	A	401	B12	C46-C12	-3.01	1.47	1.54
3	A	401	B12	C9B-N3B	-3.00	1.29	1.38
3	A	401	B12	C37-C7	-2.99	1.47	1.56
3	A	401	B12	C2R-C1R	-2.97	1.49	1.53
3	A	401	B12	O6R-C1R	-2.91	1.37	1.41
3	B	401	B12	C12-C13	-2.83	1.47	1.55
4	B	402	PLP	P-O2P	-2.82	1.44	1.54
3	B	401	B12	C55-C17	-2.79	1.48	1.54
3	B	401	B12	C6B-C5B	2.78	1.47	1.40
3	A	401	B12	C55-C17	-2.77	1.48	1.54
3	B	401	B12	C12-C11	-2.77	1.47	1.52
3	A	401	B12	C41-C8	-2.76	1.48	1.54
3	B	401	B12	O6R-C4R	-2.75	1.38	1.45
3	A	401	B12	C3R-C4R	-2.68	1.45	1.52
3	B	401	B12	C6-C5	-2.56	1.29	1.36
5	C	601	5AD	O4'-C1'	-2.56	1.37	1.41
3	A	401	B12	C6-C5	-2.55	1.29	1.36
4	B	402	PLP	P-O3P	-2.52	1.45	1.54
3	A	401	B12	C57-N59	-2.48	1.27	1.33
5	C	601	5AD	C5-N7	-2.48	1.30	1.39
5	C	601	5AD	C3'-C2'	-2.47	1.46	1.53
3	B	401	B12	C10-C11	-2.44	1.30	1.38
3	A	401	B12	P-O4	-2.44	1.42	1.50
3	B	401	B12	C36-C7	-2.41	1.50	1.54
3	B	401	B12	C7B-C8B	-2.35	1.36	1.40
3	A	401	B12	O3-C2P	-2.34	1.39	1.45
3	A	401	B12	C1P-N59	-2.33	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	B12	C5M-C5B	-2.32	1.46	1.51
3	A	401	B12	C2R-C3R	-2.31	1.47	1.52
4	B	402	PLP	C5-C4	2.30	1.43	1.40
3	A	401	B12	C55-C56	-2.29	1.47	1.53
5	C	601	5AD	C2-N1	-2.27	1.29	1.33
5	D	601	5AD	C2'-C1'	-2.26	1.50	1.53
4	A	402	PLP	C2-N1	2.25	1.38	1.33
3	A	401	B12	P-O5	-2.24	1.44	1.55
3	B	401	B12	C55-C56	-2.24	1.47	1.53
3	B	401	B12	C10-C9	2.23	1.45	1.39
3	B	401	B12	C48-C13	-2.22	1.49	1.54
3	A	401	B12	C56-C57	-2.19	1.47	1.51
3	A	401	B12	C9-N22	2.18	1.36	1.30
3	B	401	B12	C8-C9	-2.17	1.46	1.51
3	A	401	B12	P-O2	-2.17	1.54	1.60
3	A	401	B12	C5R-C4R	-2.16	1.44	1.51
3	A	401	B12	C19-N24	2.13	1.52	1.48
3	A	401	B12	C6M-C6B	-2.13	1.46	1.51
5	D	601	5AD	C5-C4	2.12	1.46	1.40
3	B	401	B12	C7-C6	-2.12	1.49	1.54
3	A	401	B12	O58-C57	-2.11	1.19	1.23
3	B	401	B12	C9B-N3B	-2.09	1.32	1.38
3	A	401	B12	C18-C19	-2.09	1.49	1.53
4	B	402	PLP	C4A-C4	-2.08	1.47	1.51
3	A	401	B12	O44-C43	-2.05	1.17	1.24
3	B	401	B12	C2-C3	-2.03	1.51	1.57

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	B12	C20-C1-C19	-10.53	99.21	109.36
3	A	401	B12	C60-C18-C19	-9.64	89.48	114.62
5	C	601	5AD	C1'-N9-C4	-7.05	114.25	126.64
3	A	401	B12	C3P-C2P-C1P	-6.92	97.96	111.39
3	B	401	B12	C1-C19-C18	6.63	132.77	121.88
5	D	601	5AD	C5'-C4'-C3'	-6.57	108.80	115.70
3	B	401	B12	C26-C2-C3	6.29	118.54	107.41
3	A	401	B12	C55-C17-C16	-6.29	104.23	116.65
3	A	401	B12	C26-C2-C3	-6.24	96.38	107.41
4	B	402	PLP	O4P-C5A-C5	-6.03	97.87	109.35
3	B	401	B12	C55-C17-C16	5.94	128.38	116.65
3	B	401	B12	C48-C13-C14	5.81	122.97	108.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	B12	C19-C1-N21	5.61	107.91	102.16
3	A	401	B12	C54-C17-C55	5.59	118.47	109.25
3	B	401	B12	C18-C60-C61	-5.53	100.16	113.97
3	B	401	B12	C2P-C1P-N59	-5.39	104.98	112.93
3	A	401	B12	C13-C14-N23	5.13	116.08	109.10
3	B	401	B12	C20-C1-N21	5.08	118.60	110.27
3	B	401	B12	C17-C18-C19	4.97	109.96	102.36
3	B	401	B12	C54-C17-C18	4.83	120.11	112.98
3	A	401	B12	C31-C30-C3	-4.63	101.37	114.73
5	C	601	5AD	O4'-C1'-C2'	-4.47	100.39	106.93
3	A	401	B12	O8R-C5R-C4R	-4.41	96.17	111.29
5	D	601	5AD	N3-C2-N1	-4.36	121.86	128.68
3	B	401	B12	C18-C17-C16	4.32	105.91	100.67
3	A	401	B12	C7B-C8B-C9B	-4.28	116.31	120.54
3	A	401	B12	C30-C3-C2	-4.16	110.28	119.09
3	B	401	B12	C55-C56-C57	-4.07	102.35	111.23
3	A	401	B12	C25-C2-C1	3.96	119.76	113.78
5	C	601	5AD	N3-C2-N1	-3.95	122.50	128.68
3	A	401	B12	C17-C18-C19	3.93	108.36	102.36
3	A	401	B12	C13-C14-C15	-3.88	118.38	124.32
3	B	401	B12	C54-C17-C16	-3.86	92.38	112.40
3	A	401	B12	O3-C2P-C1P	3.84	114.58	106.92
3	B	401	B12	C4B-C9B-C8B	3.84	125.04	121.10
3	B	401	B12	C25-C2-C26	-3.83	101.96	109.71
3	A	401	B12	C7-C6-N22	3.78	114.85	107.94
4	B	402	PLP	C6-C5-C4	3.78	121.13	118.16
3	A	401	B12	C12-C11-C10	-3.75	118.49	123.37
3	A	401	B12	C18-C17-C16	3.74	105.21	100.67
3	A	401	B12	O3-P-O4	-3.71	95.53	109.47
4	B	402	PLP	C3-C4-C5	-3.71	114.73	118.74
3	A	401	B12	C3R-C2R-C1R	3.64	107.95	99.89
3	B	401	B12	C55-C17-C18	-3.46	104.46	111.15
3	B	401	B12	C12-C11-C10	-3.45	118.88	123.37
3	A	401	B12	C18-C60-C61	-3.38	105.52	113.97
3	A	401	B12	C41-C42-C43	-3.31	101.36	112.59
3	A	401	B12	C47-C12-C46	-3.26	103.84	109.35
5	C	601	5AD	C3'-C2'-C1'	3.10	105.64	100.98
3	B	401	B12	C7B-C8B-C9B	-3.09	117.49	120.54
3	A	401	B12	C7-C6-C5	-3.06	123.25	128.07
3	B	401	B12	C7-C37-C38	-3.02	105.16	114.25
3	A	401	B12	C20-C1-C2	-2.97	108.32	113.28
3	A	401	B12	C8-C9-N22	2.94	116.62	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	B12	C2-C1-N21	2.92	105.84	101.77
3	A	401	B12	C9-C10-C11	-2.92	121.75	125.97
3	A	401	B12	C12-C11-N23	2.91	115.88	111.83
3	A	401	B12	C8-C9-C10	-2.90	117.06	123.32
3	A	401	B12	C49-C48-C13	-2.84	106.53	114.73
3	B	401	B12	C16-C15-C14	-2.83	116.95	121.25
5	C	601	5AD	C4-C5-N7	-2.83	106.45	109.40
3	A	401	B12	C20-C1-C19	2.73	111.99	109.36
3	B	401	B12	C3R-C2R-C1R	2.72	105.92	99.89
3	A	401	B12	O5-P-O3	2.60	117.03	106.78
3	A	401	B12	C55-C17-C18	-2.51	106.30	111.15
3	B	401	B12	C49-C48-C13	2.48	121.89	114.73
3	B	401	B12	C12-C11-N23	2.42	115.21	111.83
3	B	401	B12	C30-C31-C32	-2.40	104.45	112.59
3	B	401	B12	C41-C8-C9	2.39	115.41	111.19
3	B	401	B12	C13-C12-C11	-2.39	98.26	100.97
3	B	401	B12	C60-C18-C17	-2.38	109.98	115.74
3	B	401	B12	C7-C8-C9	2.36	103.93	100.90
3	B	401	B12	C7-C6-N22	2.36	112.25	107.94
3	A	401	B12	O6R-C4R-C3R	2.34	109.89	104.87
3	A	401	B12	C56-C57-N59	-2.34	112.49	116.42
3	B	401	B12	C17-C16-N24	-2.33	107.56	111.15
3	A	401	B12	C55-C56-C57	-2.32	106.18	111.23
3	A	401	B12	C5M-C5B-C6B	-2.30	116.02	120.74
3	A	401	B12	C6M-C6B-C5B	-2.28	116.06	120.74
3	B	401	B12	C1-C2-C3	2.27	104.50	101.60
3	B	401	B12	C1P-N59-C57	-2.27	117.75	122.69
4	B	402	PLP	C4A-C4-C3	2.27	124.34	120.50
4	A	402	PLP	C6-C5-C4	2.27	119.94	118.16
3	A	401	B12	C7-C37-C38	-2.26	107.45	114.25
3	B	401	B12	C48-C49-C50	-2.26	104.93	112.59
3	A	401	B12	C2-C3-C4	2.25	104.19	101.63
5	D	601	5AD	O4'-C1'-C2'	-2.25	103.64	106.93
3	B	401	B12	C13-C14-C15	-2.24	120.89	124.32
3	A	401	B12	C8B-C9B-N3B	-2.23	103.13	107.83
3	A	401	B12	C5M-C5B-C4B	2.22	125.65	120.34
3	B	401	B12	C48-C13-C12	-2.21	110.43	116.63
3	B	401	B12	C35-C5-C6	-2.21	118.92	122.43
5	D	601	5AD	C2-N1-C6	2.20	122.51	118.75
3	A	401	B12	C54-C17-C18	2.19	116.21	112.98
4	B	402	PLP	O2P-P-O4P	-2.18	100.92	106.73
5	D	601	5AD	O3'-C3'-C4'	2.18	115.81	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	B12	C2-C1-C19	-2.14	115.22	118.60
3	A	401	B12	C19-C1-N21	2.13	104.35	102.16
3	B	401	B12	C35-C5-C4	2.13	121.13	116.79
3	B	401	B12	C8-C9-C10	-2.05	118.89	123.32
3	A	401	B12	C48-C13-C12	-2.04	110.92	116.63
3	B	401	B12	C31-C30-C3	-2.02	108.90	114.73
4	A	402	PLP	C5-C6-N1	-2.02	120.45	123.82
3	B	401	B12	C13-C14-N23	2.01	111.84	109.10

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	B12	C25-C2-C26-C27
3	A	401	B12	C16-C17-C55-C56
3	A	401	B12	C54-C17-C55-C56
3	A	401	B12	N59-C1P-C2P-C3P
3	A	401	B12	N59-C1P-C2P-O3
3	A	401	B12	C3R-O2-P-O5
3	B	401	B12	C2-C3-C30-C31
3	B	401	B12	C4-C3-C30-C31
3	B	401	B12	C54-C17-C55-C56
3	B	401	B12	C18-C17-C55-C56
3	B	401	B12	C1P-C2P-O3-P
3	B	401	B12	C3P-C2P-O3-P
3	B	401	B12	C3R-O2-P-O4
3	B	401	B12	C3R-O2-P-O5
4	A	402	PLP	C5A-O4P-P-O2P
4	A	402	PLP	C5A-O4P-P-O3P
4	B	402	PLP	C5A-O4P-P-O2P
4	B	402	PLP	C5A-O4P-P-O3P
3	A	401	B12	O6R-C4R-C5R-O8R
3	A	401	B12	C3R-C4R-C5R-O8R
3	B	401	B12	C2R-C3R-O2-P
3	B	401	B12	C42-C41-C8-C9
3	A	401	B12	C2R-C3R-O2-P
3	A	401	B12	C3R-O2-P-O3
3	A	401	B12	C3-C2-C26-C27
3	A	401	B12	C4R-C3R-O2-P
3	B	401	B12	C3R-O2-P-O3
3	B	401	B12	C55-C56-C57-O58
4	A	402	PLP	C5A-O4P-P-O1P

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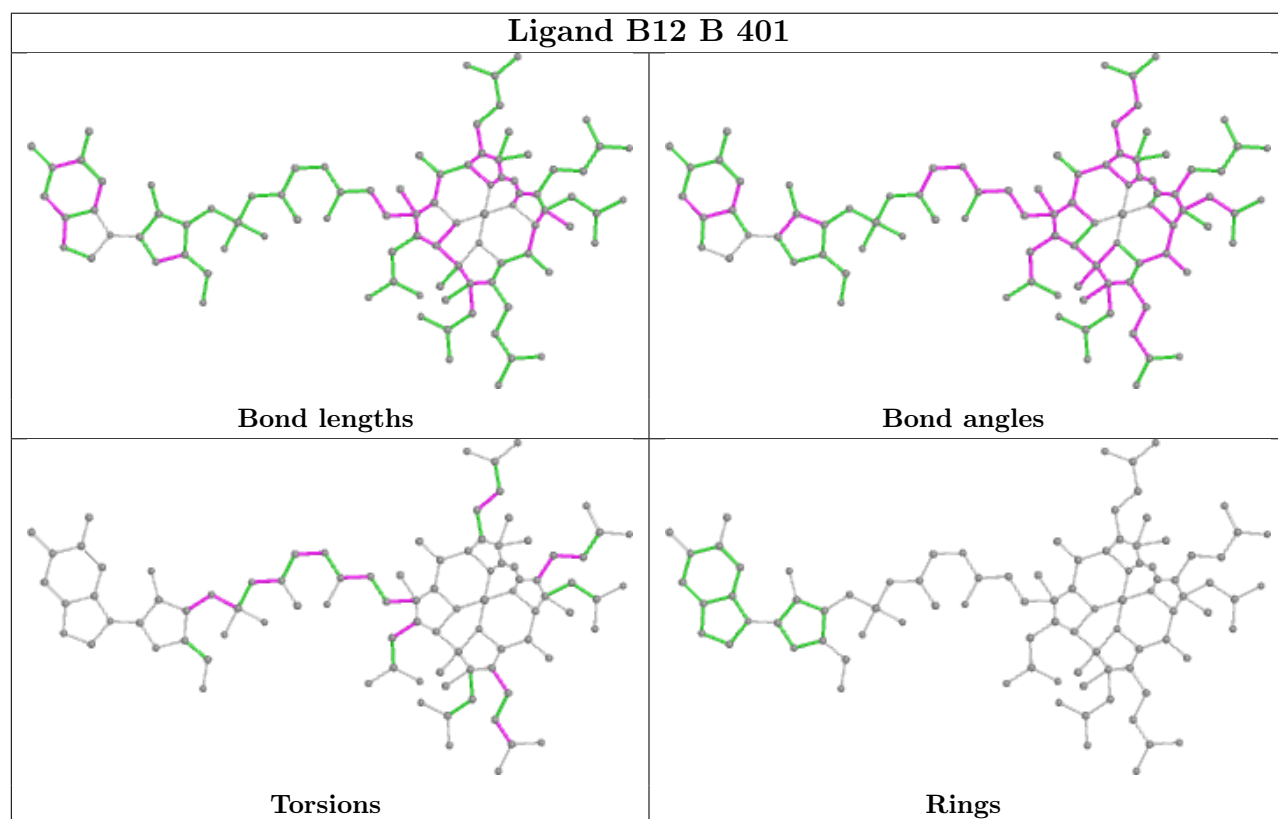
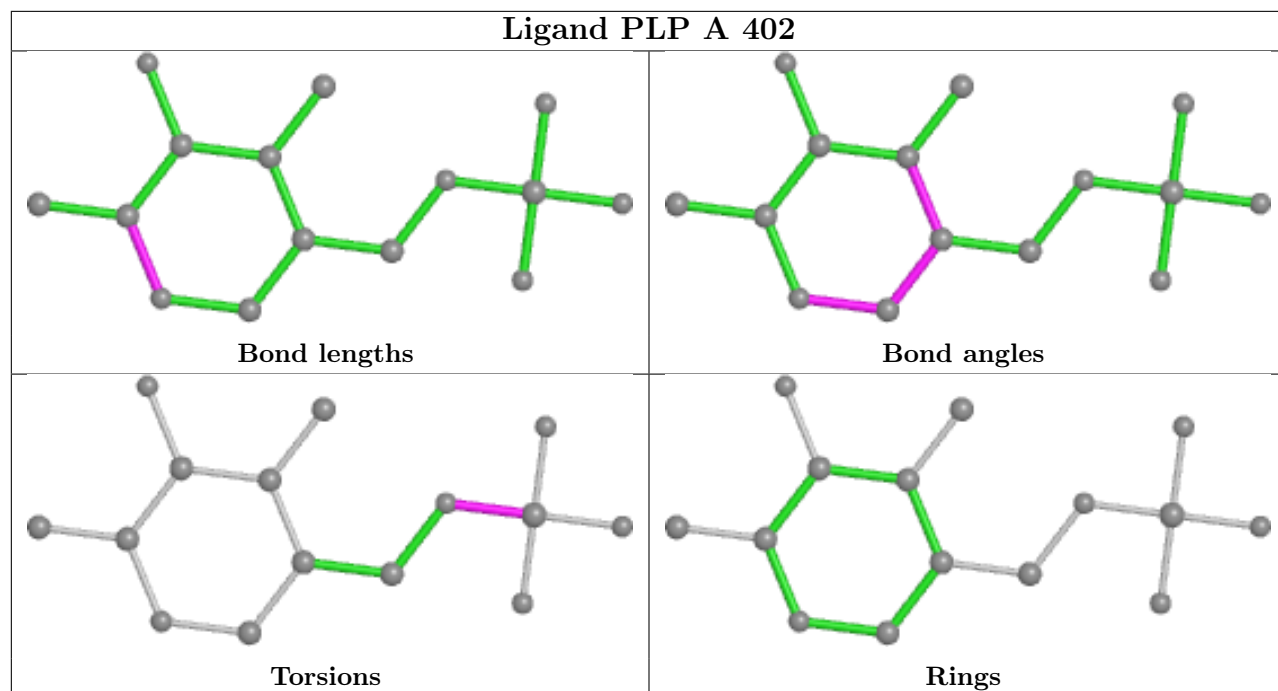
Mol	Chain	Res	Type	Atoms
4	B	402	PLP	C5A-O4P-P-O1P
3	B	401	B12	C55-C56-C57-N59
3	A	401	B12	C3R-O2-P-O4
3	A	401	B12	C18-C17-C55-C56
3	A	401	B12	C18-C60-C61-O63
3	A	401	B12	C18-C60-C61-N62
3	B	401	B12	C2P-C1P-N59-C57
3	B	401	B12	C30-C31-C32-N33
3	B	401	B12	C16-C17-C55-C56
3	B	401	B12	C17-C18-C60-C61
3	B	401	B12	C19-C18-C60-C61
3	B	401	B12	C8-C41-C42-C43
3	B	401	B12	C4R-C3R-O2-P
3	B	401	B12	C13-C48-C49-C50
3	B	401	B12	C30-C31-C32-O34

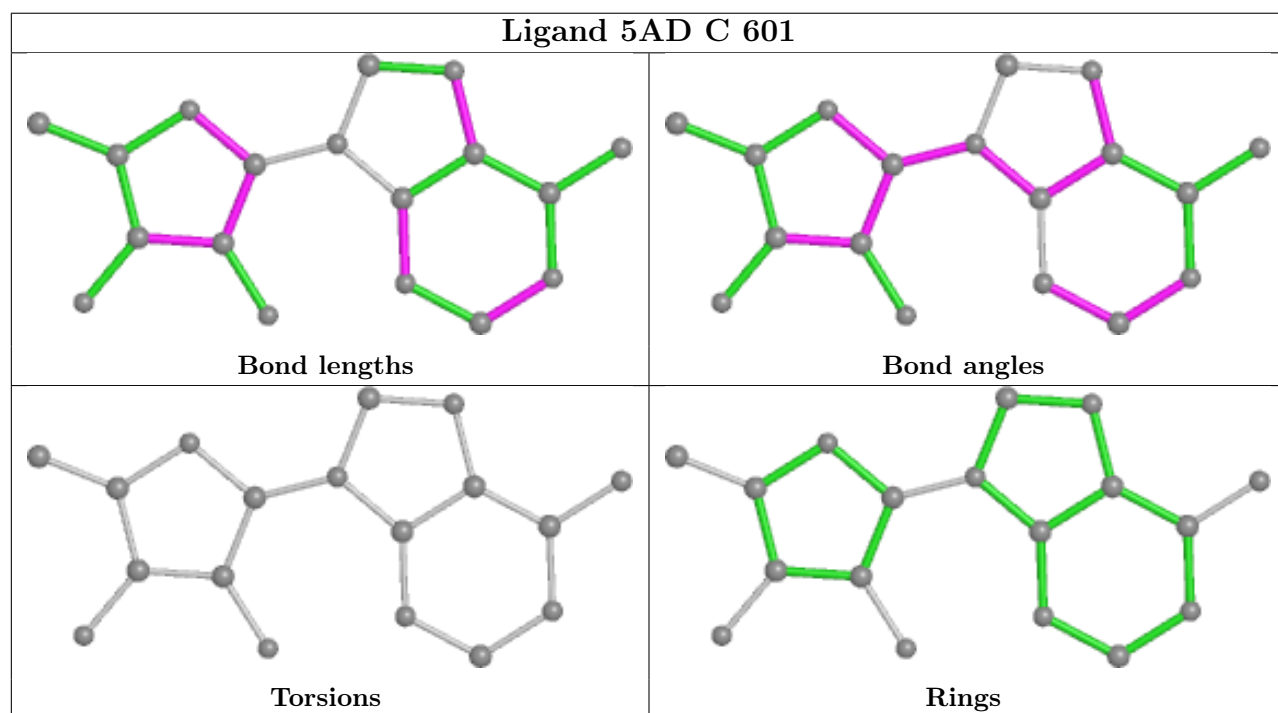
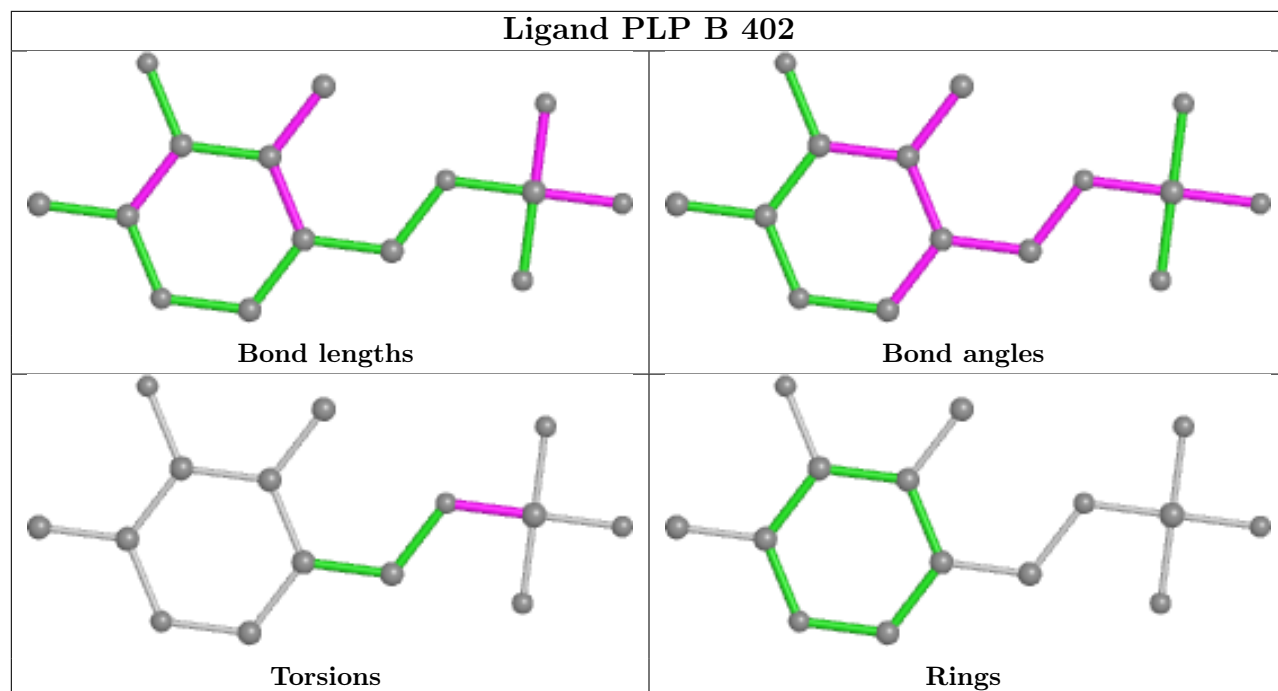
There are no ring outliers.

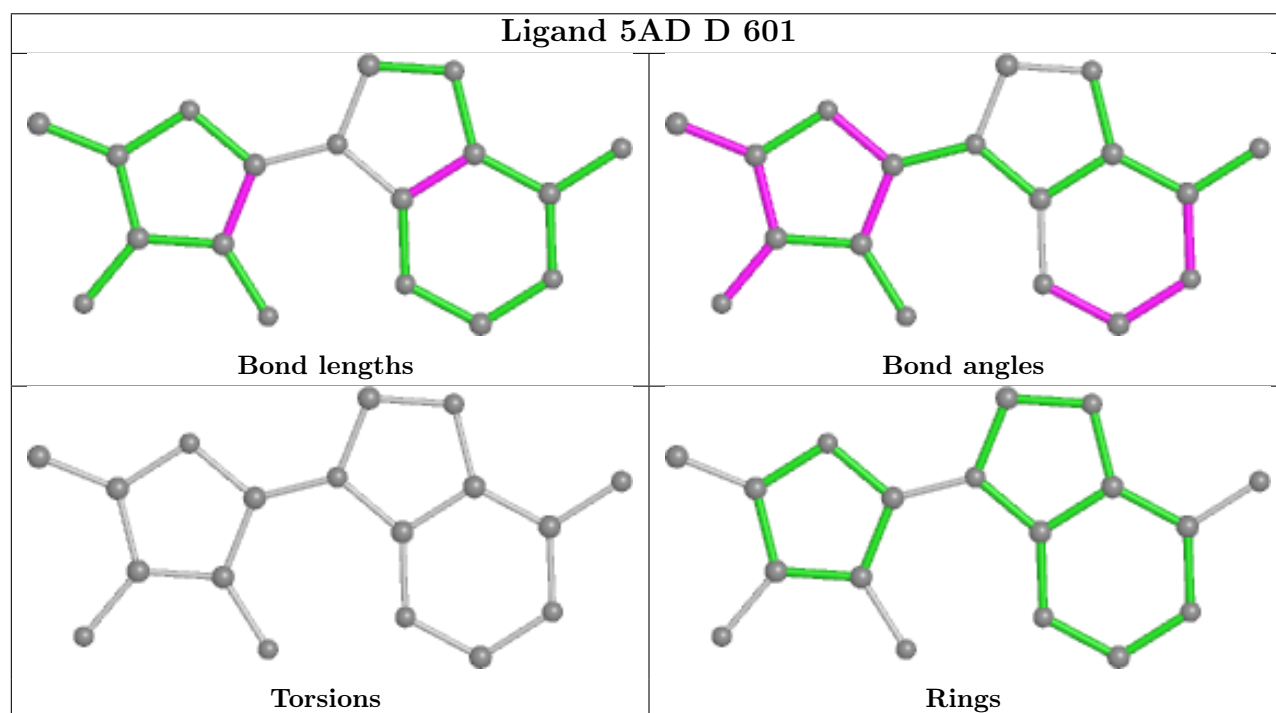
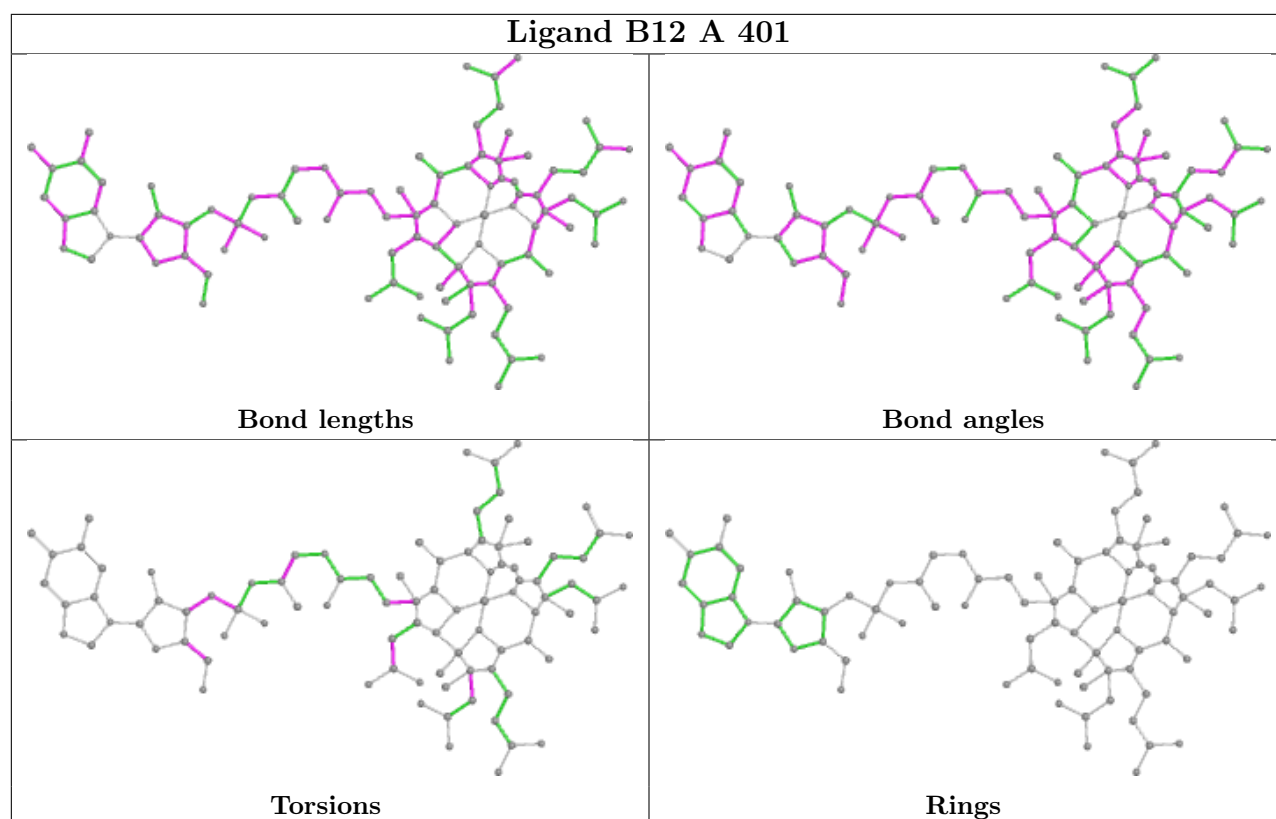
5 monomers are involved in 103 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	B12	69	0
4	B	402	PLP	2	0
5	C	601	5AD	1	0
3	A	401	B12	31	0
5	D	601	5AD	11	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.

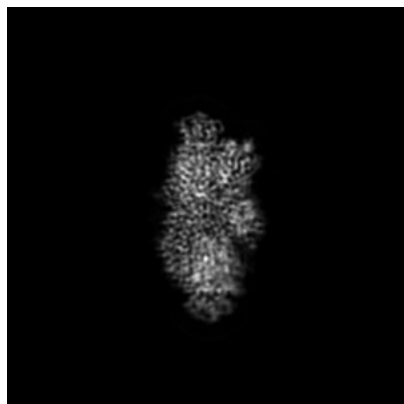
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40945. These allow visual inspection of the internal detail of the map and identification of artifacts.

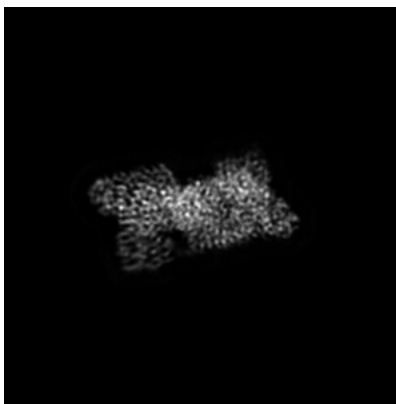
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

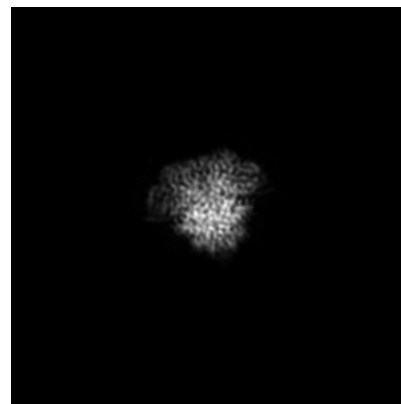
6.1.1 Primary map



X

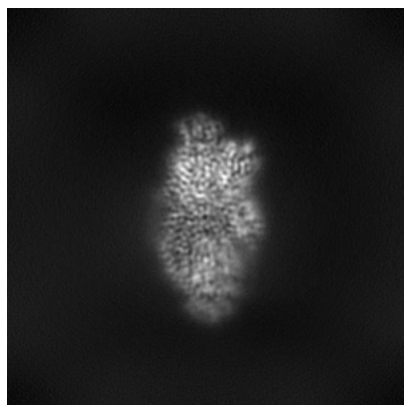


Y

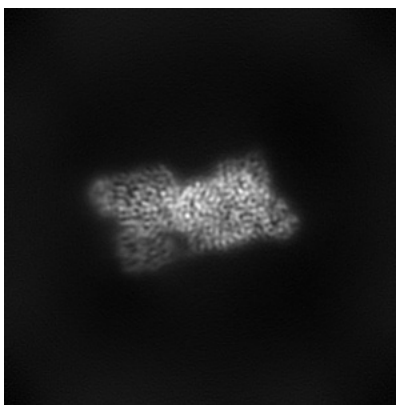


Z

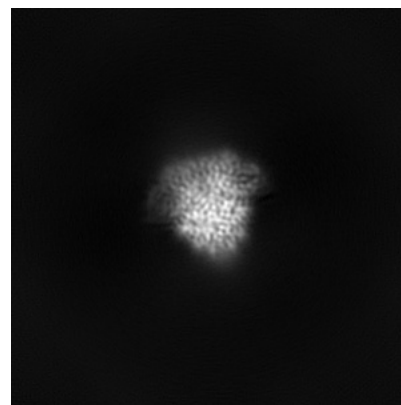
6.1.2 Raw map



X



Y

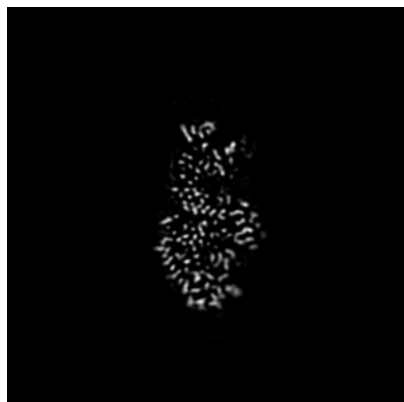


Z

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

6.2 Central slices [i](#)

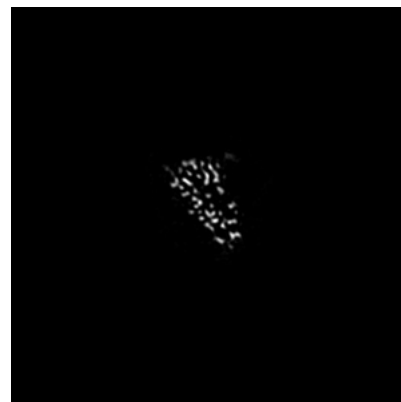
6.2.1 Primary map



X Index: 128

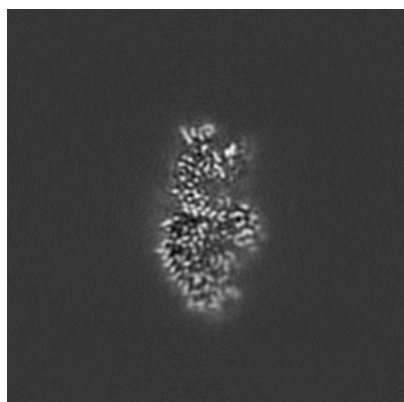


Y Index: 128

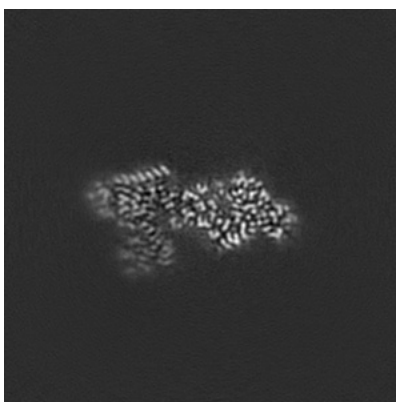


Z Index: 128

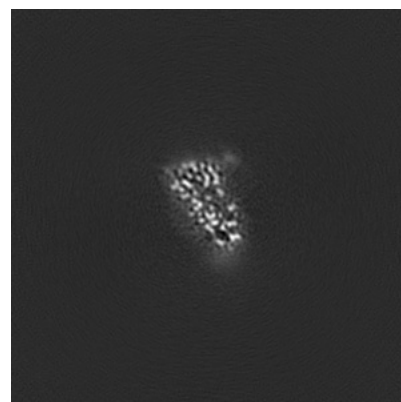
6.2.2 Raw map



X Index: 128



Y Index: 128

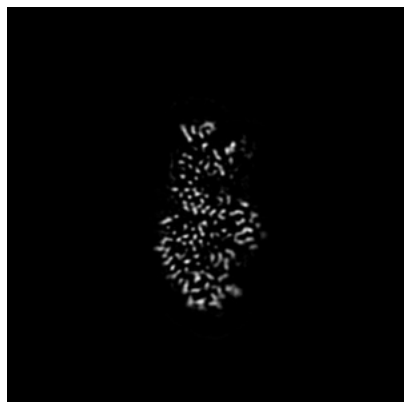


Z Index: 128

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: 128

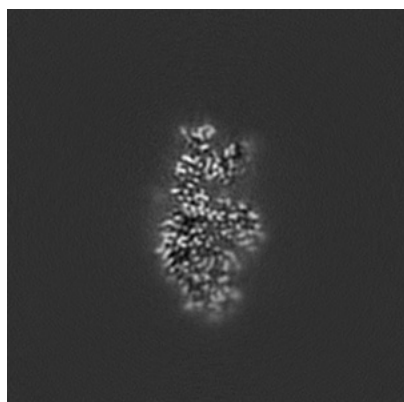


Y Index: 123

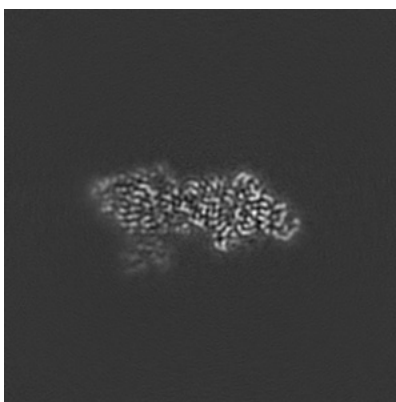


Z Index: 123

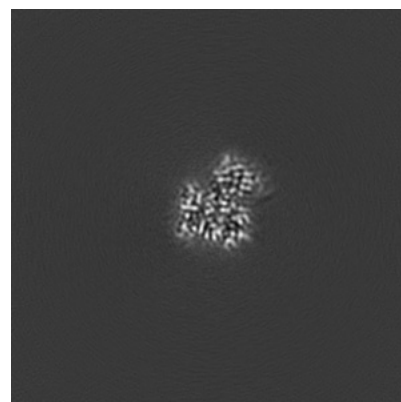
6.3.2 Raw map



X Index: 129



Y Index: 123

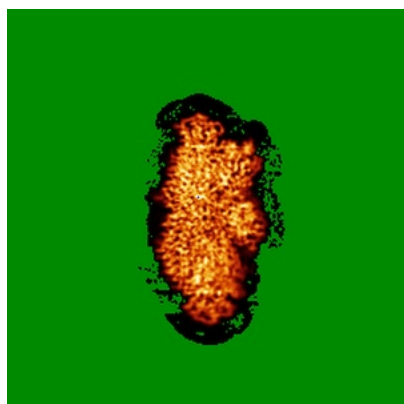


Z Index: 153

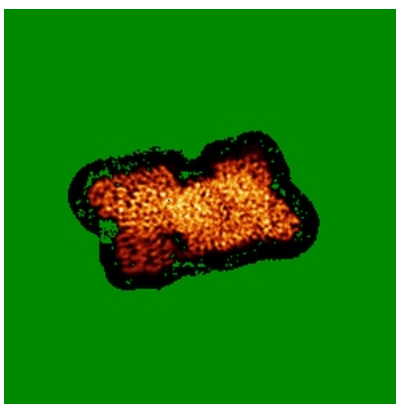
The images above show the largest variance slices of the map in three orthogonal directions.

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

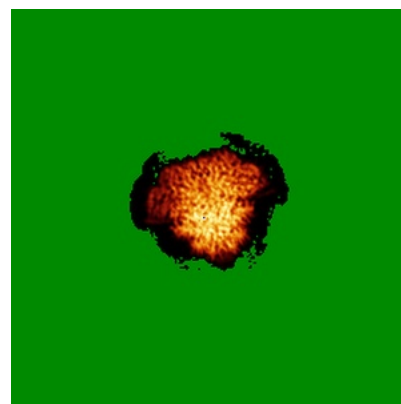
6.4.1 Primary map



X

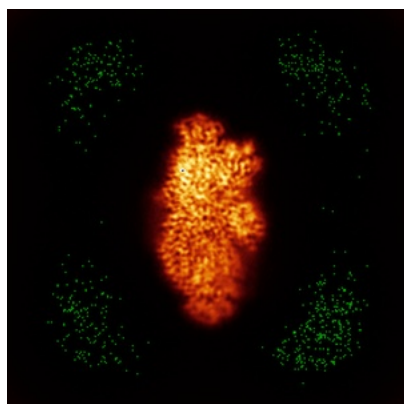


Y

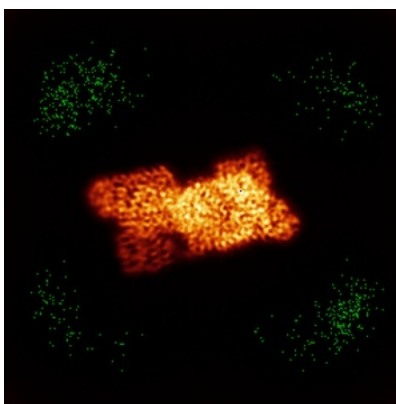


Z

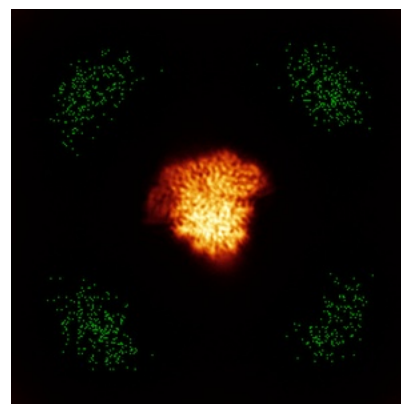
6.4.2 Raw map



X



Y

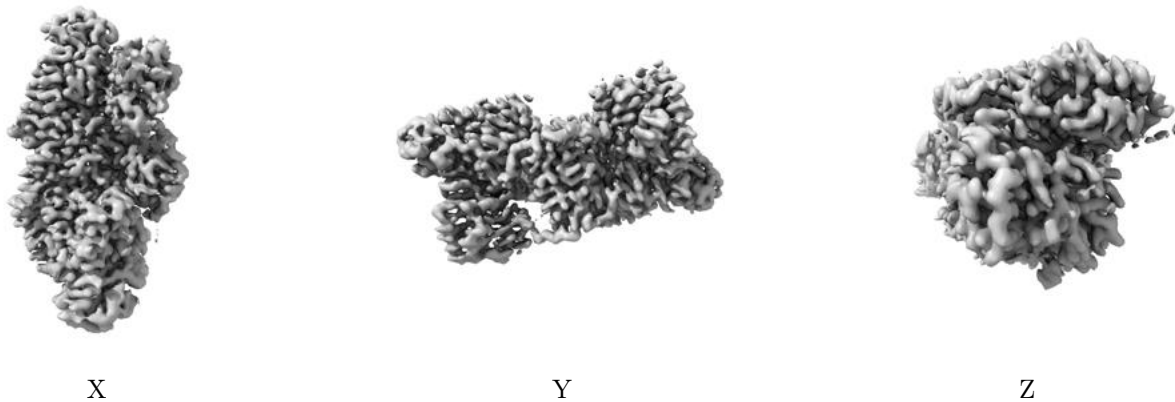


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

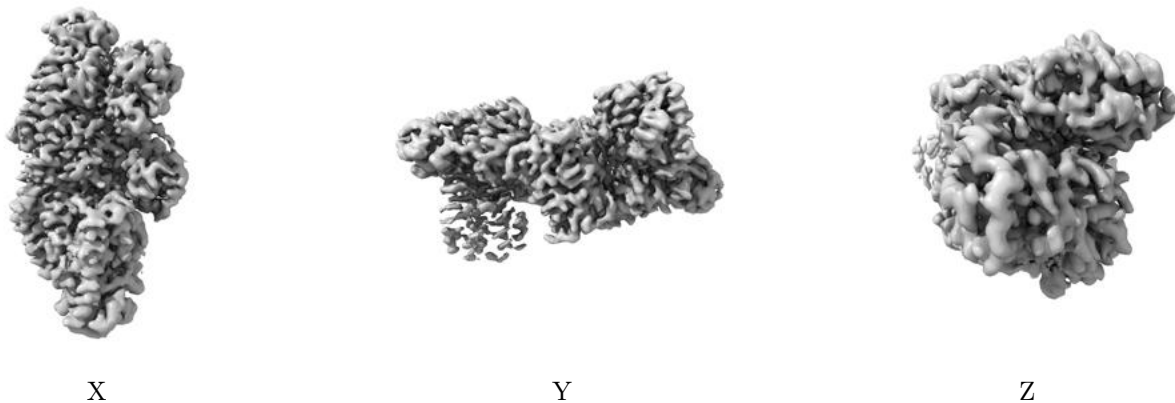
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

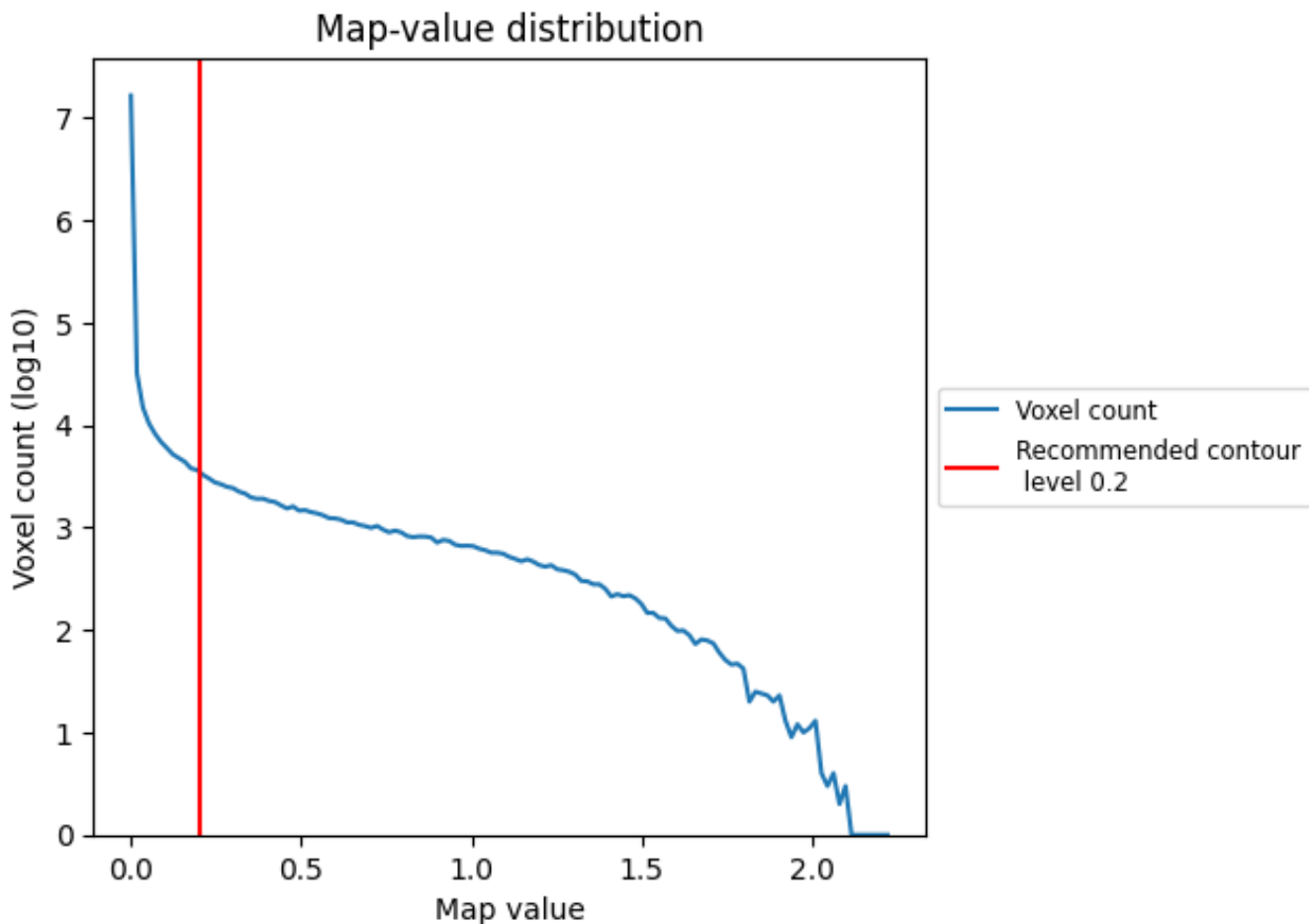
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

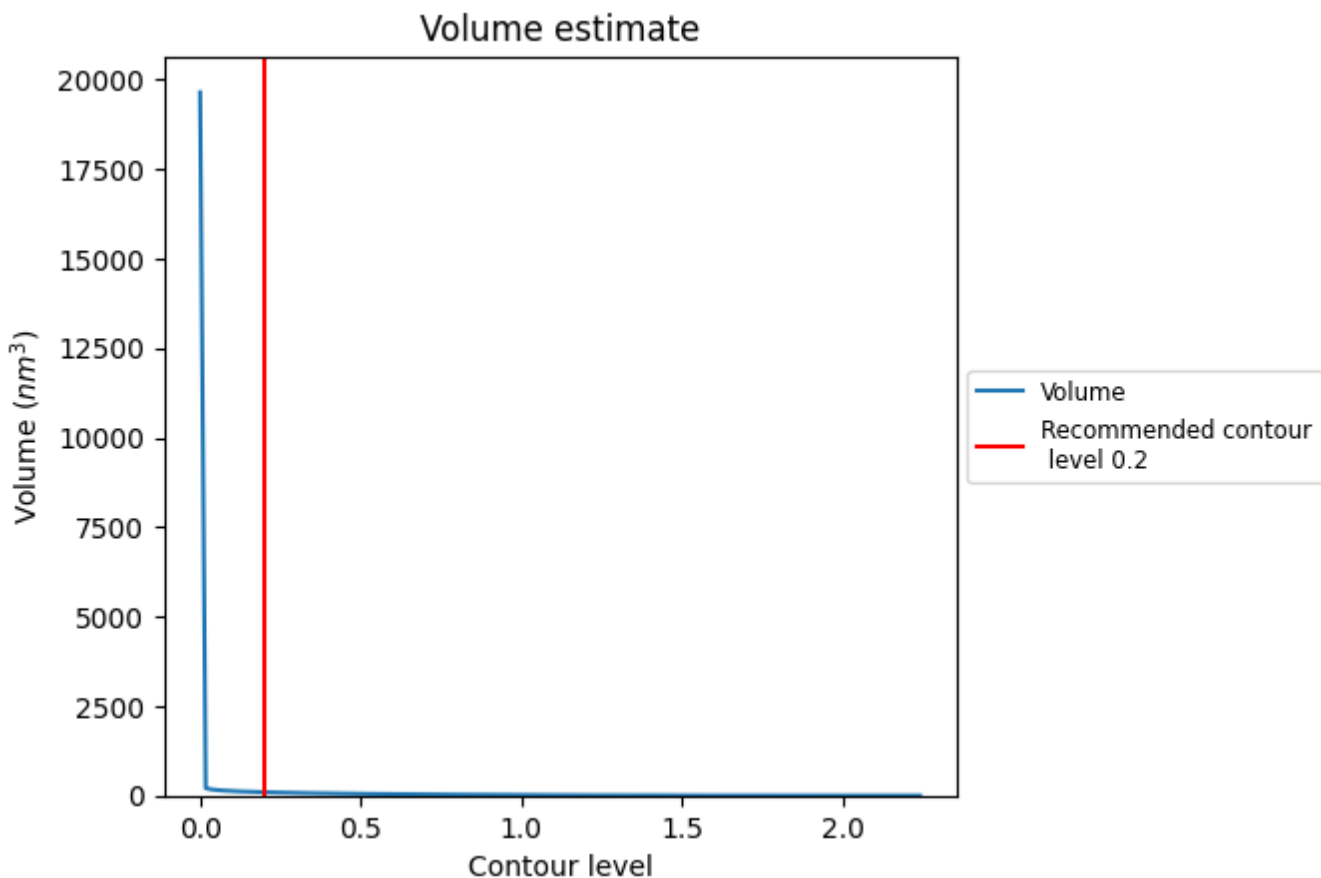
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

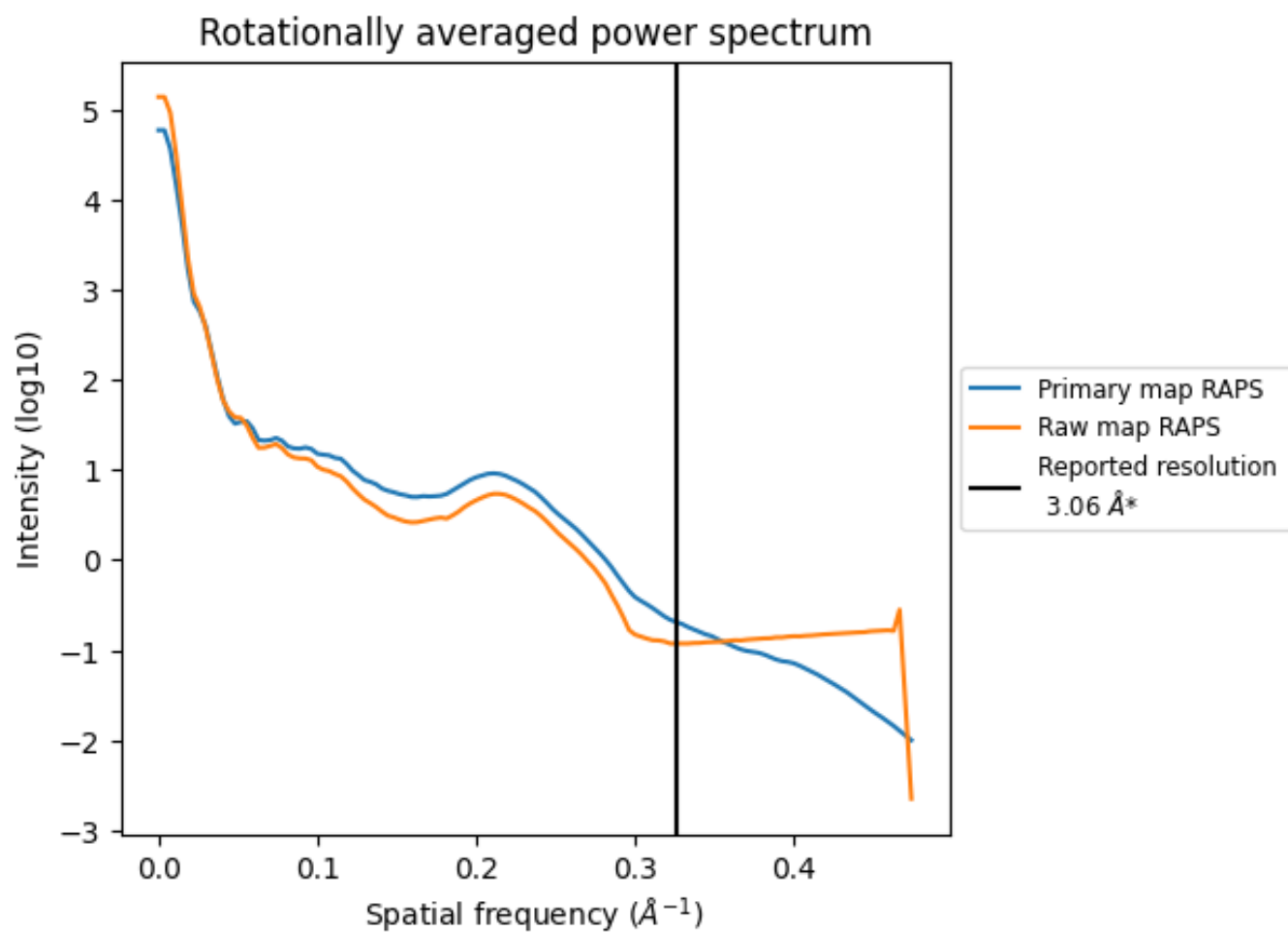
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 93 nm^3 ; this corresponds to an approximate mass of 84 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](#)

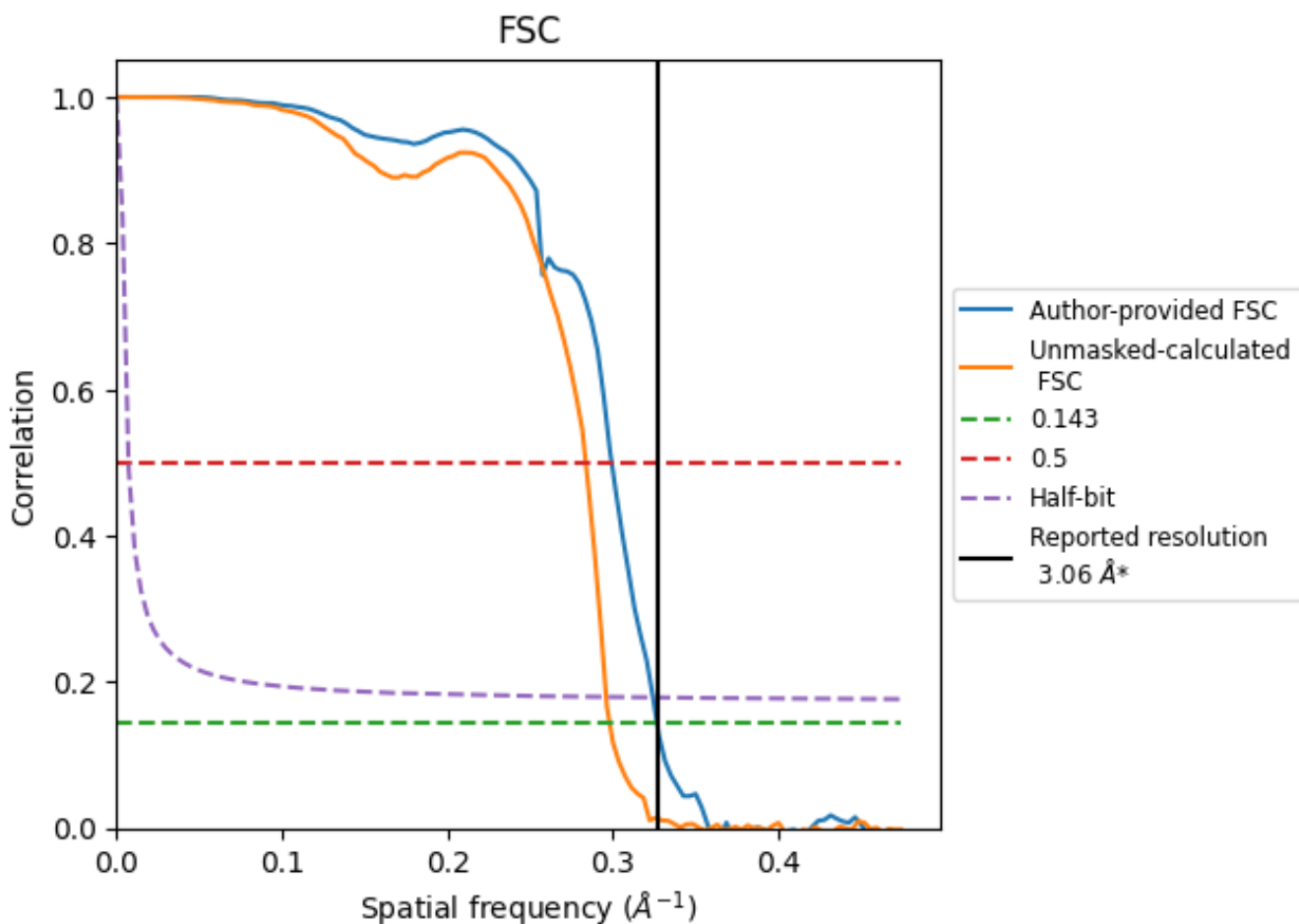


*Reported resolution corresponds to spatial frequency of 0.327 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.327 Å⁻¹

8.2 Resolution estimates [i](#)

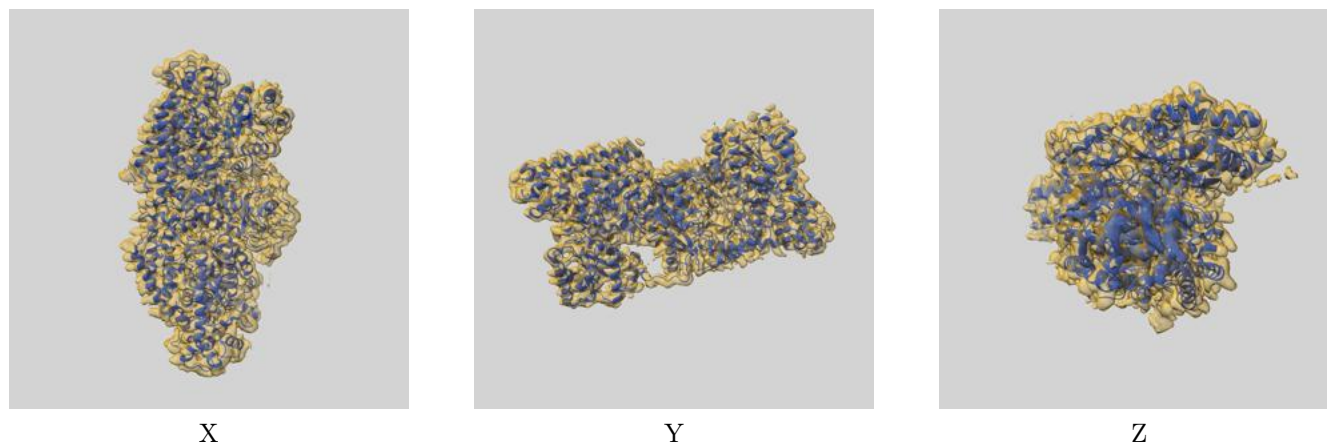
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	3.06	3.34	3.08
Unmasked-calculated*	3.35	3.52	3.38

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

9 Map-model fit [i](#)

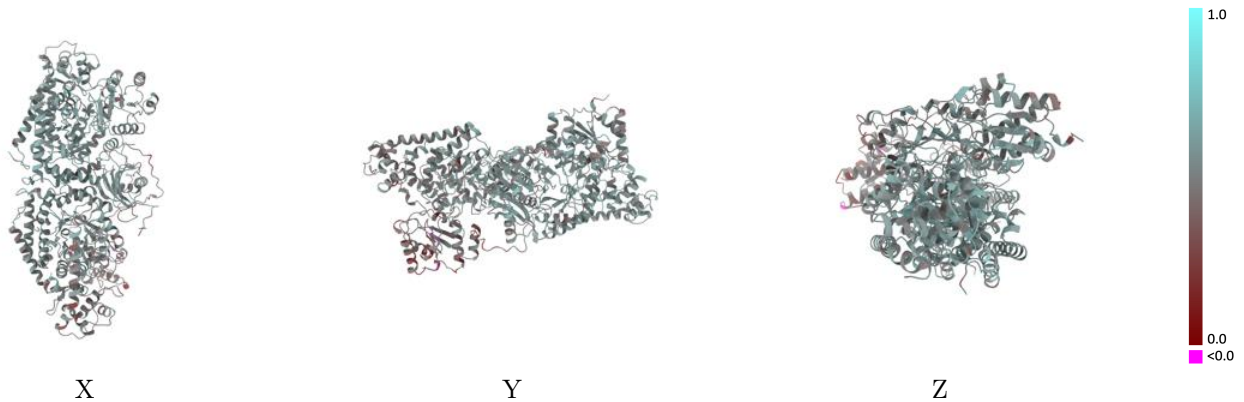
This section contains information regarding the fit between EMDB map EMD-40945 and PDB model 8T0Q. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



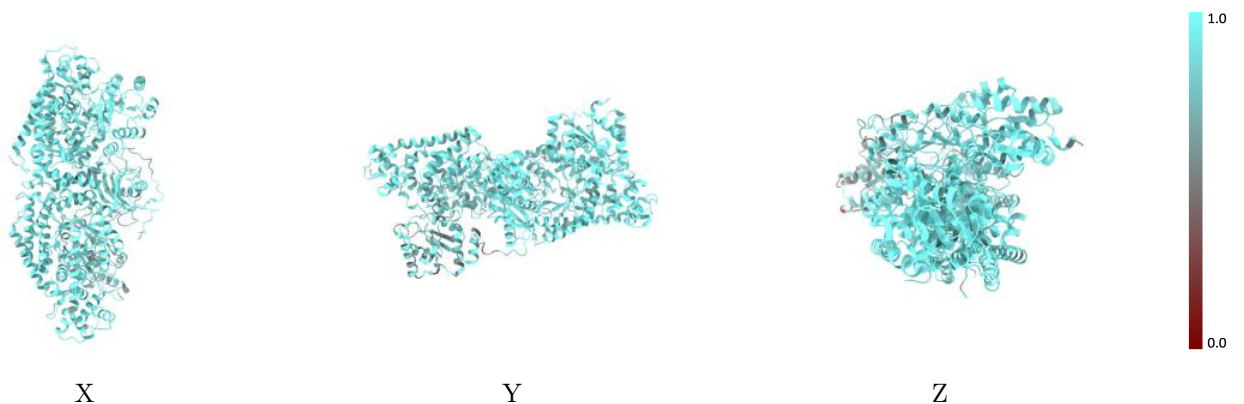
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



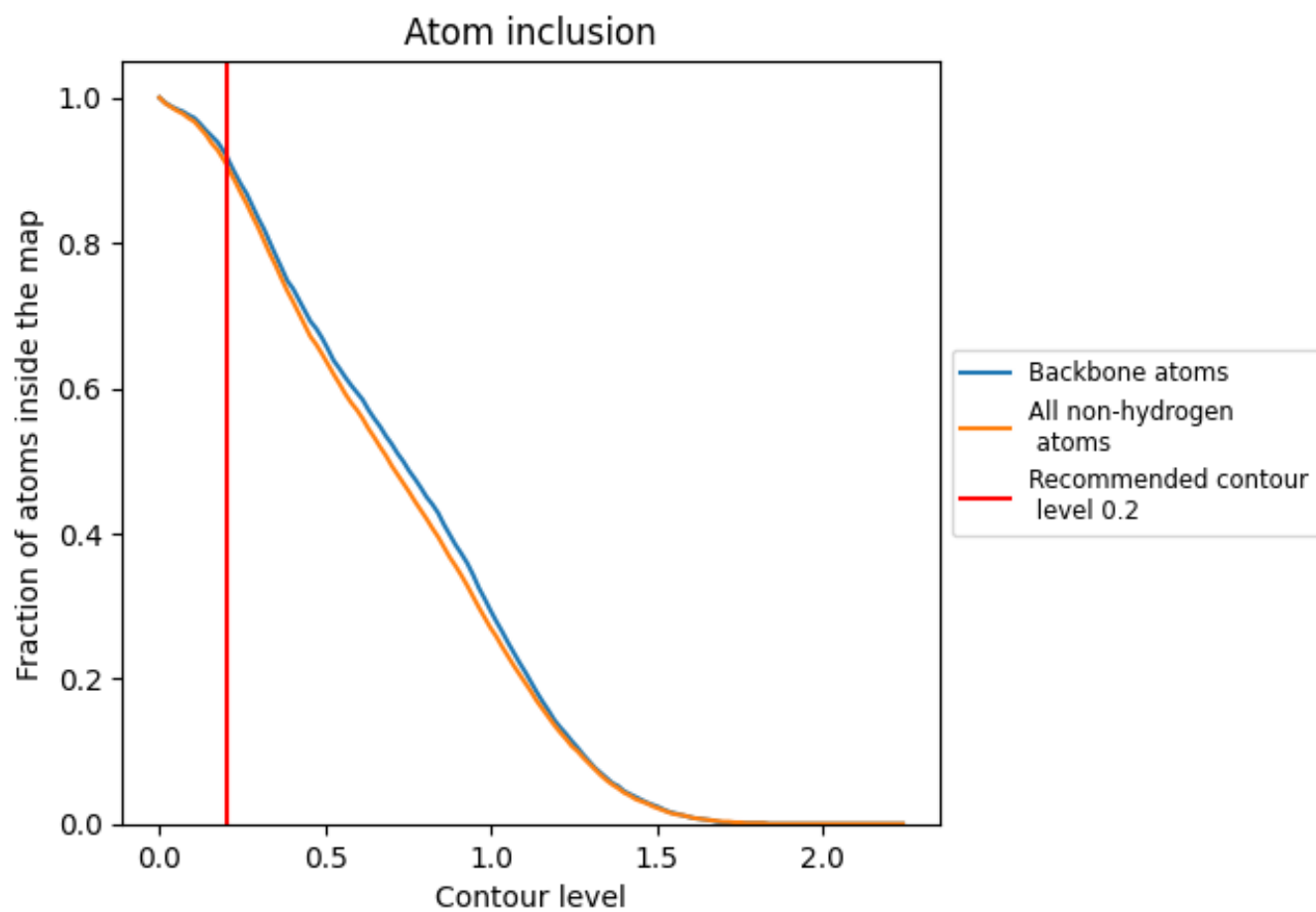
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).










9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

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

Chain	Atom inclusion	Q-score
All	 0.9090	 0.5150
A	 0.9120	 0.5180
B	 0.8000	 0.4410
C	 0.9500	 0.5520
D	 0.9260	 0.5150

