



Full wwPDB EM Validation Report ⓘ

Sep 13, 2026 – 03:05 am BST

PDB ID : 29EX / pdb_000029ex
EMDB ID : EMD-57132
Title : Cryo-EM structure of 3-methylcrotonyl- CoA carboxylase (MCC) complex
(BC-engage BCCP state) from Mycobacterium smegmatis
Authors : Yadav, A.; Geibel, S.R.J.
Deposited on : 2026-03-09
Resolution : 2.90 Å(reported)
Based on initial model : .

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:

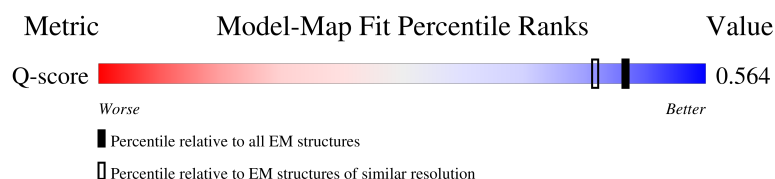
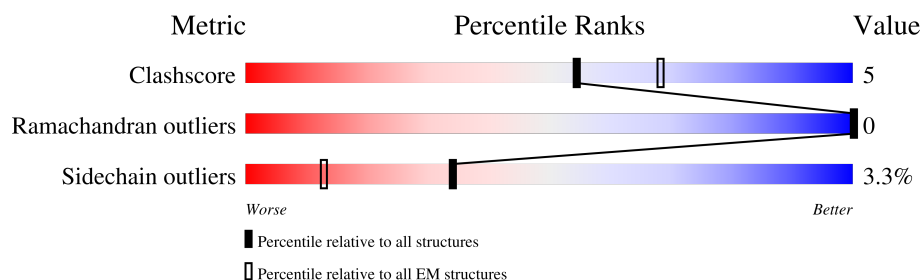
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance

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

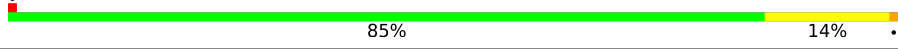
The reported resolution of this entry is 2.90 Å.

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.



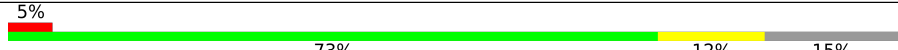
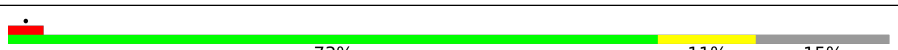
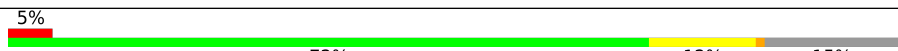
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	D1	513	
1	D2	513	
1	D3	513	
1	D4	513	

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Mol	Chain	Length	Quality of chain
1	D5	513	
1	D6	513	
2	A1	669	
2	A2	669	
2	A3	669	
2	A4	669	
2	A5	669	
2	A6	669	

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	BTN	A2	701	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 48267 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.

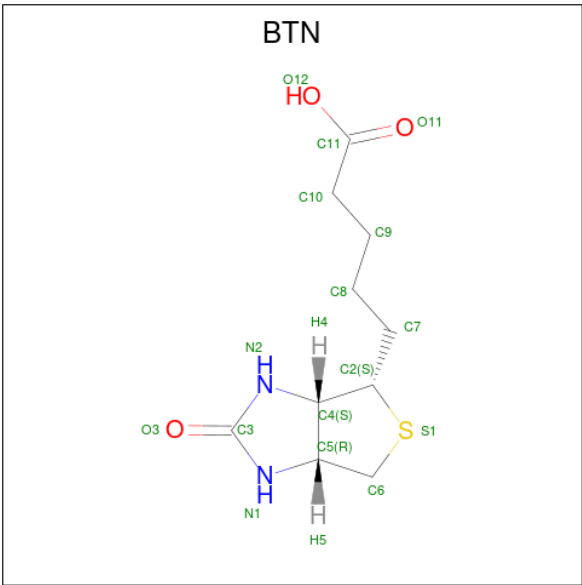
- Molecule 1 is a protein called Carboxyl transferase domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D1	511	Total	C	N	O	S	0	0
			3838	2423	680	717	18		
1	D2	511	Total	C	N	O	S	0	0
			3838	2423	680	717	18		
1	D3	511	Total	C	N	O	S	0	0
			3838	2423	680	717	18		
1	D4	511	Total	C	N	O	S	0	0
			3838	2423	680	717	18		
1	D5	511	Total	C	N	O	S	0	0
			3838	2423	680	717	18		
1	D6	511	Total	C	N	O	S	0	0
			3838	2423	680	717	18		

- Molecule 2 is a protein called biotin carboxylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A1	568	Total	C	N	O	S	0	0
			4195	2623	751	810	11		
2	A2	566	Total	C	N	O	S	0	0
			4181	2613	749	808	11		
2	A3	568	Total	C	N	O	S	0	0
			4195	2623	751	810	11		
2	A4	568	Total	C	N	O	S	0	0
			4195	2623	751	810	11		
2	A5	567	Total	C	N	O	S	0	0
			4188	2618	750	809	11		
2	A6	568	Total	C	N	O	S	0	0
			4195	2623	751	810	11		

- Molecule 3 is BIOTIN (CCD ID: BTN) (formula: $C_{10}H_{16}N_2O_3S$) (labeled as "Ligand of Interest" by depositor).

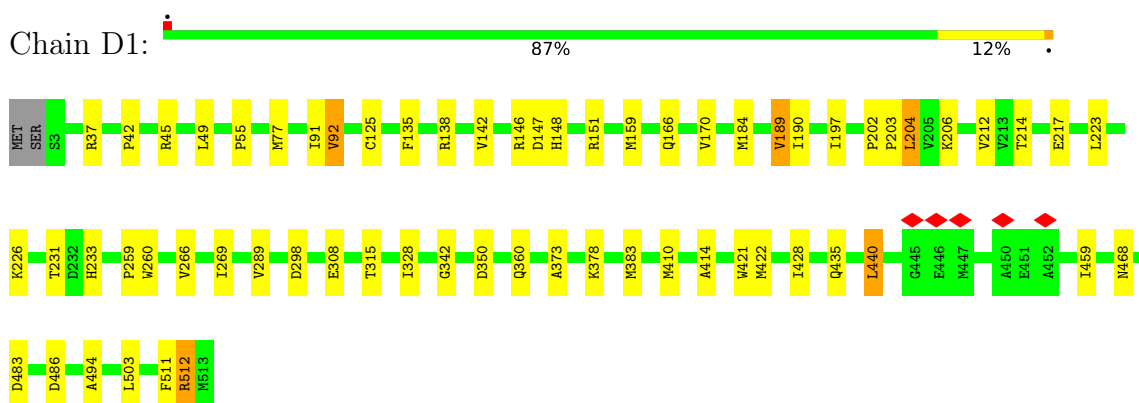


Mol	Chain	Residues	Atoms					AltConf
3	A1	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	A2	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	A3	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	A4	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	A5	1	Total	C	N	O	S	0
			15	10	2	2	1	
3	A6	1	Total	C	N	O	S	0
			15	10	2	2	1	

3 Residue-property plots [i](#)

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

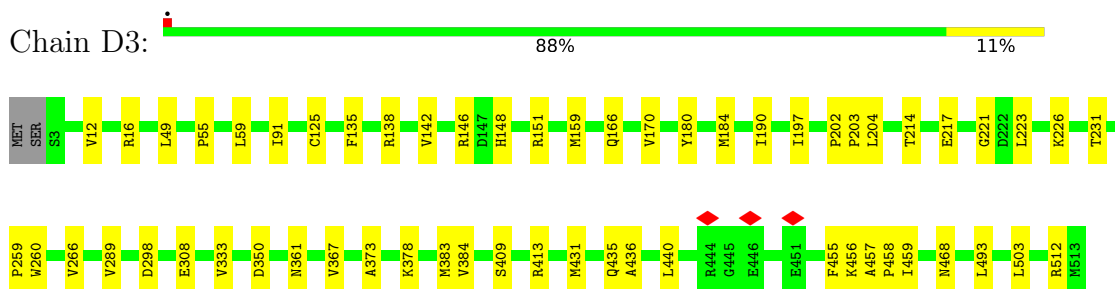
- Molecule 1: Carboxyl transferase domain protein



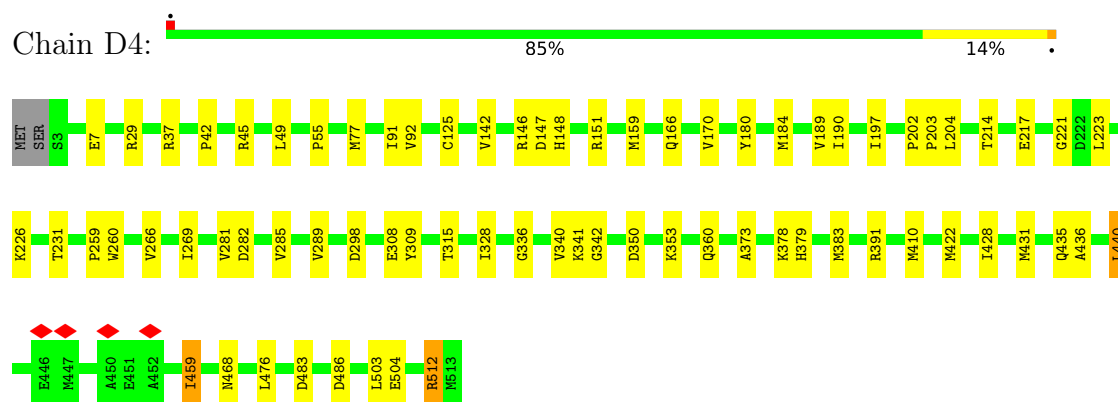
- Molecule 1: Carboxyl transferase domain protein



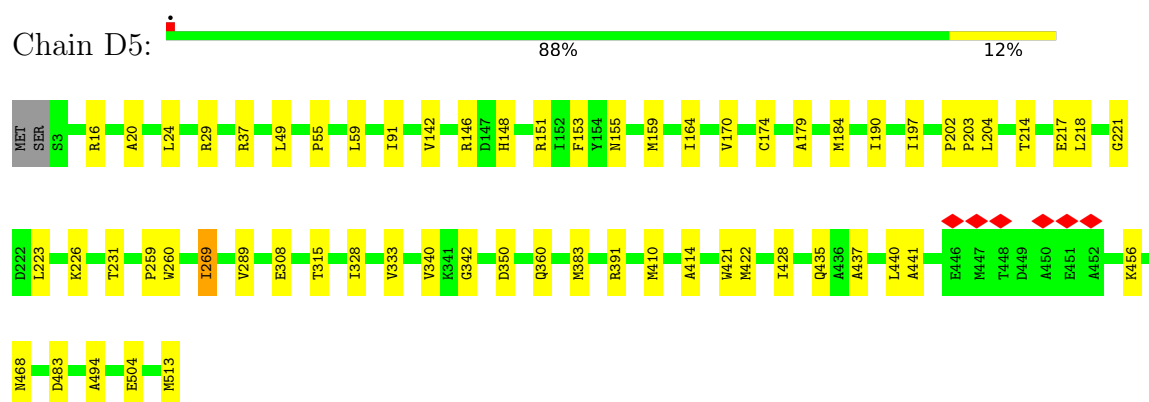
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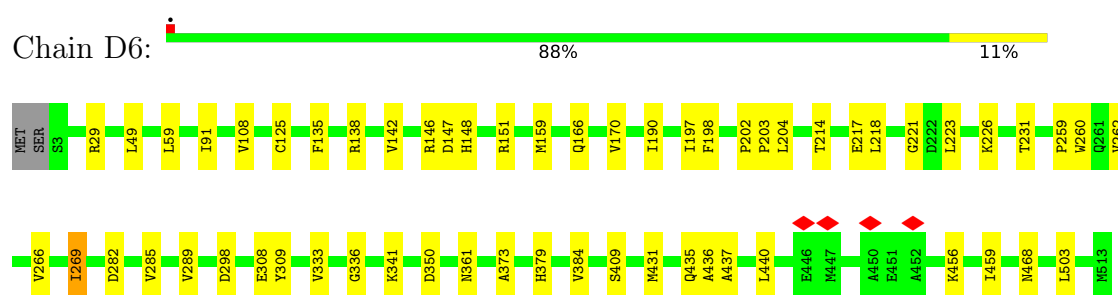
- Molecule 1: Carboxyl transferase domain protein



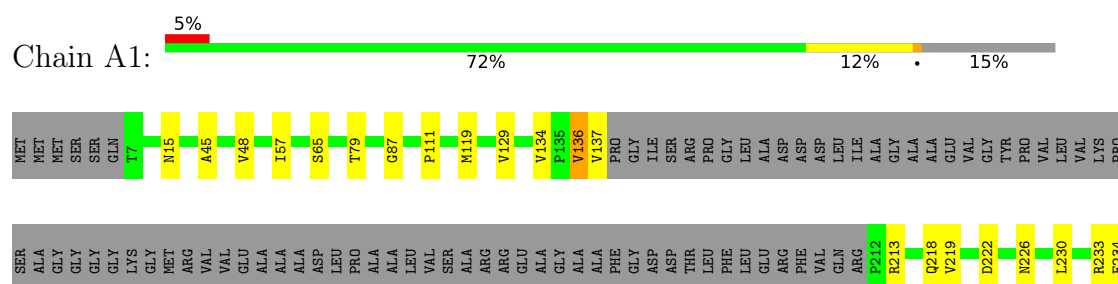
- Molecule 1: Carboxyl transferase domain protein

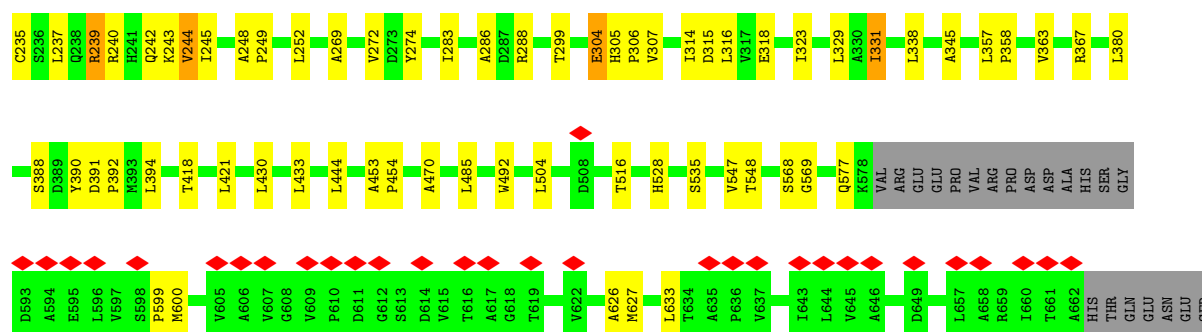


- Molecule 1: Carboxyl transferase domain protein

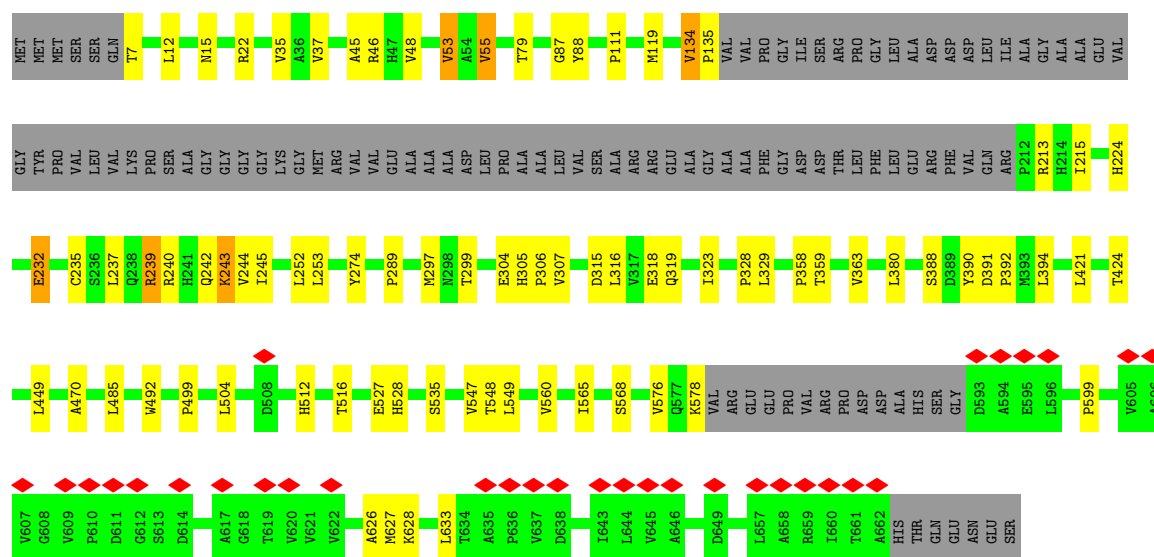
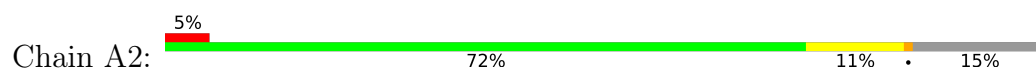


- Molecule 2: biotin carboxylase

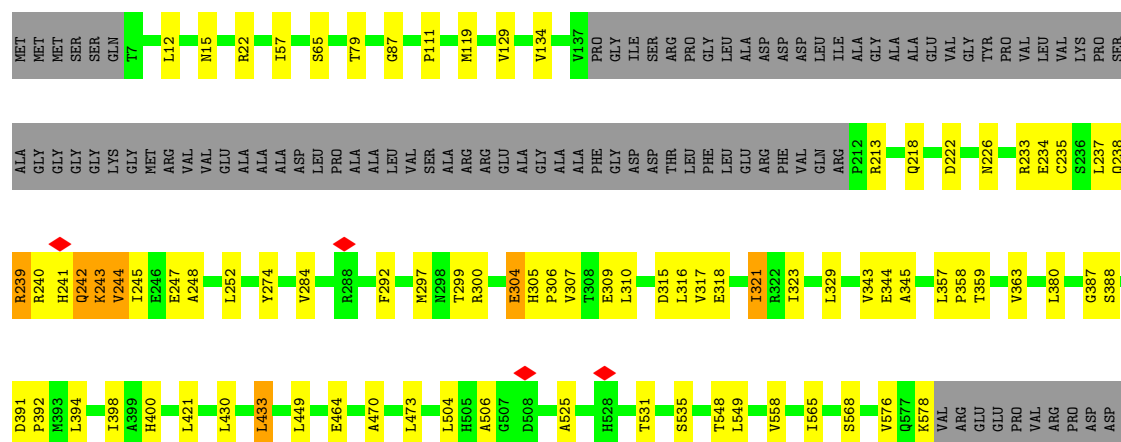
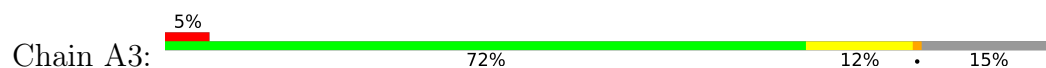


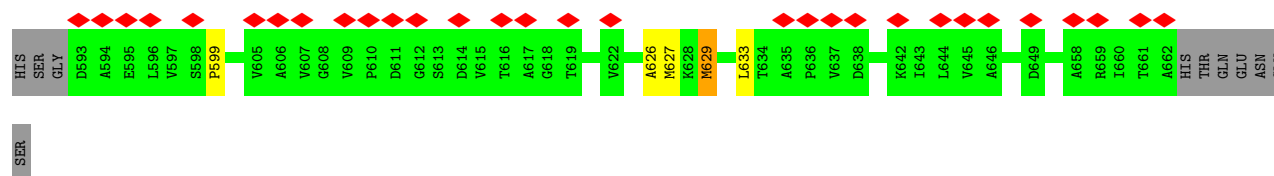


• Molecule 2: biotin carboxylase

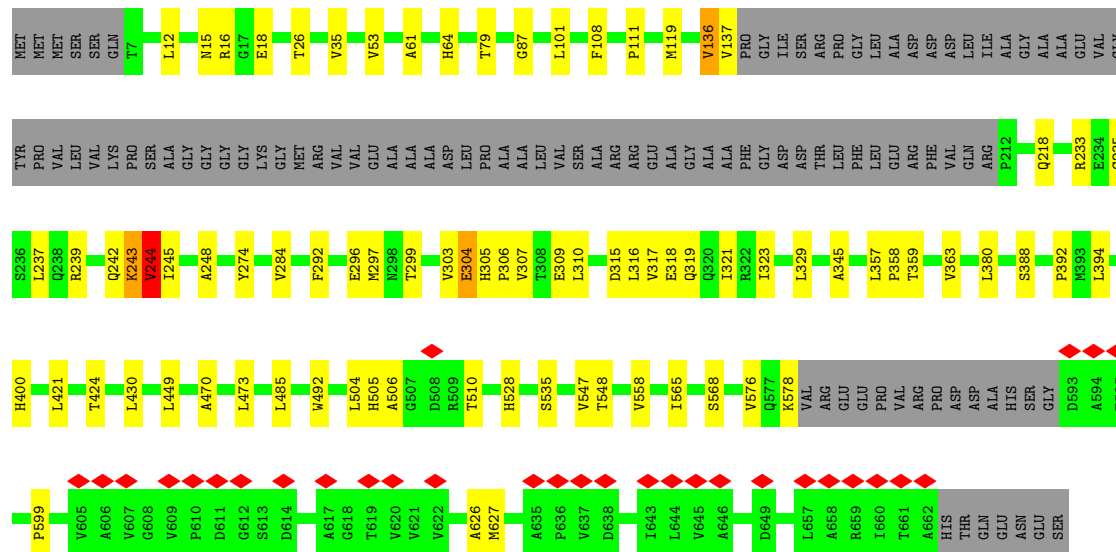
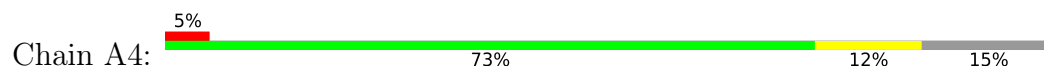


• Molecule 2: biotin carboxylase

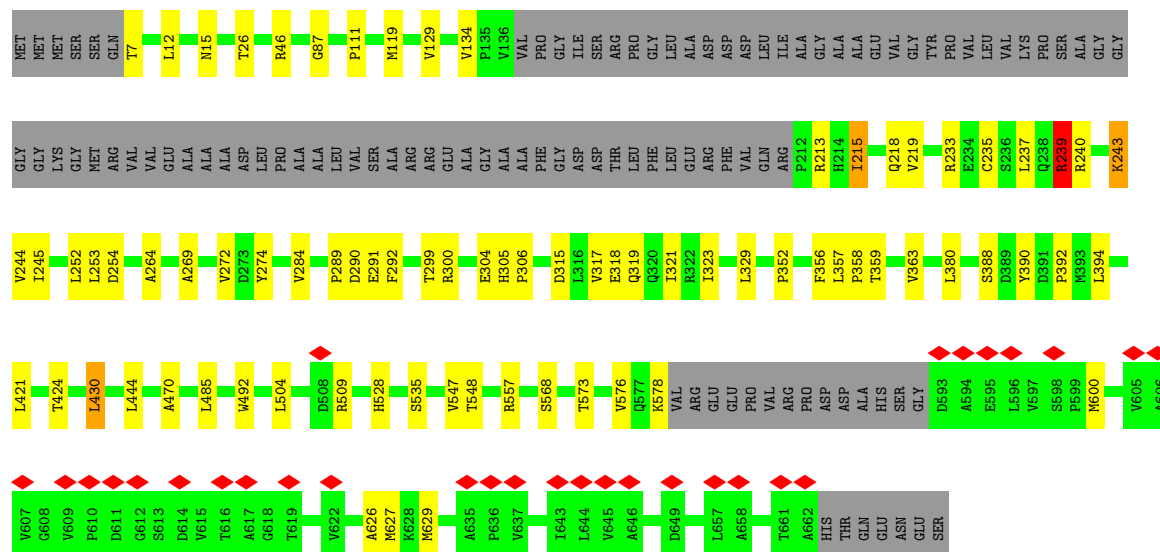
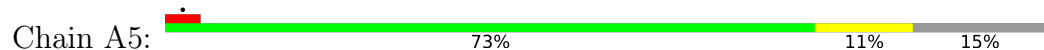




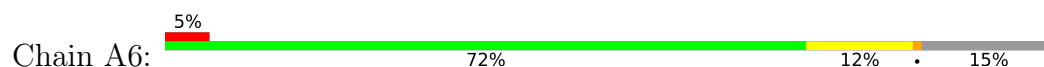
• Molecule 2: biotin carboxylase

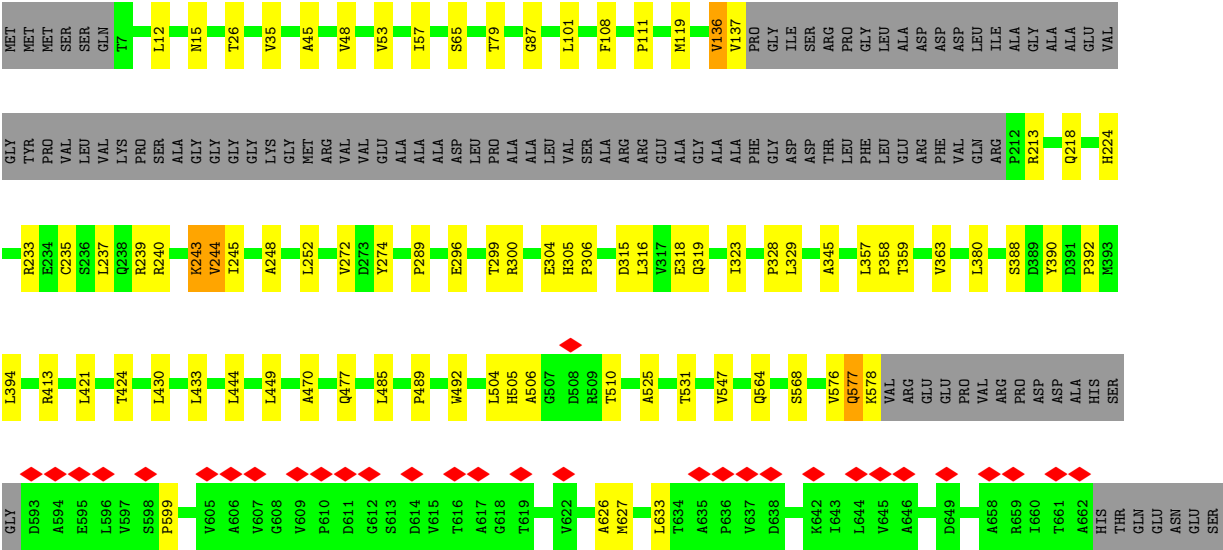


• Molecule 2: biotin carboxylase



• Molecule 2: biotin carboxylase





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	6660	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.389	Depositor
Minimum map value	-0.803	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.144	Depositor
Map size (Å)	353.28, 353.28, 353.28	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1776, 1.1776, 1.1776	Depositor

5 Model quality

5.1 Standard geometry

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

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	D1	0.30	0/3923	0.34	0/5333
1	D2	0.30	0/3923	0.33	0/5333
1	D3	0.30	0/3923	0.34	0/5333
1	D4	0.30	0/3923	0.33	0/5333
1	D5	0.30	0/3923	0.34	0/5333
1	D6	0.30	0/3923	0.33	0/5333
2	A1	0.23	0/4272	0.34	1/5828 (0.0%)
2	A2	0.23	0/4258	0.34	1/5808 (0.0%)
2	A3	0.25	0/4272	0.36	1/5828 (0.0%)
2	A4	0.23	0/4272	0.34	1/5828 (0.0%)
2	A5	0.23	0/4265	0.35	1/5818 (0.0%)
2	A6	0.22	0/4272	0.33	0/5828
All	All	0.27	0/49149	0.34	5/66936 (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
2	A1	0	1
2	A2	0	2
2	A3	0	1
2	A5	0	2
2	A6	0	1
All	All	0	7

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A4	244	VAL	N-CA-C	-5.37	107.38	111.62
2	A2	244	VAL	N-CA-C	-5.14	107.56	111.62
2	A1	244	VAL	N-CA-C	-5.14	107.80	112.12
2	A5	244	VAL	N-CA-C	-5.14	107.80	112.12
2	A3	629	MET	CB-CG-SD	5.10	128.01	112.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A1	239	ARG	Sidechain
2	A2	239	ARG	Sidechain
2	A2	240	ARG	Sidechain
2	A3	240	ARG	Sidechain
2	A5	239	ARG	Sidechain
2	A5	240	ARG	Sidechain
2	A6	240	ARG	Sidechain

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	D1	3838	0	3799	34	0
1	D2	3838	0	3799	33	0
1	D3	3838	0	3799	32	0
1	D4	3838	0	3799	39	0
1	D5	3838	0	3799	36	0
1	D6	3838	0	3799	29	0
2	A1	4195	0	4139	51	0
2	A2	4181	0	4123	57	0
2	A3	4195	0	4139	56	0
2	A4	4195	0	4138	46	0
2	A5	4188	0	4130	44	0
2	A6	4195	0	4139	48	0
3	A1	15	0	15	3	0
3	A2	15	0	15	16	0
3	A3	15	0	15	3	0
3	A4	15	0	15	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A5	15	0	15	1	0
3	A6	15	0	15	1	0
All	All	48267	0	47692	482	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 5.

All (482) 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)
2:A2:628:LYS:NZ	3:A2:701:BTN:C11	2.07	1.16
2:A2:628:LYS:HZ2	3:A2:701:BTN:C11	1.58	1.15
2:A2:391:ASP:HB2	3:A2:701:BTN:H92	1.44	0.96
2:A2:88:TYR:HD1	3:A2:701:BTN:H2	1.36	0.88
2:A2:628:LYS:HZ1	3:A2:701:BTN:C11	1.87	0.87
2:A2:628:LYS:HZ2	3:A2:701:BTN:C10	1.87	0.87
2:A2:628:LYS:NZ	3:A2:701:BTN:C10	2.41	0.82
2:A4:111:PRO:HG3	2:A4:299:THR:HB	1.64	0.80
2:A5:111:PRO:HG3	2:A5:299:THR:HB	1.63	0.80
2:A2:391:ASP:CB	3:A2:701:BTN:H92	2.13	0.79
2:A3:111:PRO:HG3	2:A3:299:THR:HB	1.65	0.78
2:A5:357:LEU:HD23	2:A5:629:MET:HE1	1.66	0.78
2:A6:239:ARG:HB3	2:A6:449:LEU:HD22	1.65	0.77
2:A2:111:PRO:HG3	2:A2:299:THR:HB	1.66	0.77
1:D1:184:MET:HE1	1:D3:384:VAL:HB	1.70	0.74
2:A4:235:CYS:HB3	2:A4:243:LYS:HG2	1.69	0.73
2:A6:111:PRO:HG3	2:A6:299:THR:HB	1.70	0.72
1:D3:440:LEU:HD21	1:D3:459:ILE:HG21	1.70	0.72
1:D1:77:MET:HE3	1:D1:92:VAL:HG13	1.70	0.71
1:D6:440:LEU:HD21	1:D6:459:ILE:HG21	1.71	0.71
2:A2:88:TYR:CD1	3:A2:701:BTN:H2	2.22	0.71
2:A4:303:VAL:CG2	3:A4:701:BTN:H5	2.21	0.71
2:A3:239:ARG:HB3	2:A3:449:LEU:HD22	1.73	0.70
2:A2:213:ARG:HD3	2:A2:252:LEU:HD22	1.73	0.69
1:D5:214:THR:HG22	1:D5:217:GLU:HG2	1.75	0.69
1:D6:214:THR:HG22	1:D6:217:GLU:HG2	1.74	0.69
2:A1:111:PRO:HG3	2:A1:299:THR:HB	1.74	0.69
2:A6:213:ARG:HD3	2:A6:252:LEU:HD22	1.75	0.68
2:A1:213:ARG:HD3	2:A1:252:LEU:HD22	1.76	0.67
2:A5:235:CYS:HB3	2:A5:243:LYS:HG2	1.76	0.67
2:A2:232:GLU:HG2	2:A2:253:LEU:HD12	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A3:358:PRO:HD3	2:A3:629:MET:HE2	1.75	0.67
1:D2:308:GLU:HB3	1:D6:226:LYS:HG2	1.75	0.66
1:D4:180:TYR:HB3	1:D4:184:MET:HE3	1.78	0.65
2:A6:235:CYS:HB3	2:A6:243:LYS:HG2	1.79	0.65
2:A3:237:LEU:HD12	2:A3:245:ILE:HB	1.78	0.65
2:A3:310:LEU:HD23	2:A3:400:HIS:HB2	1.79	0.65
2:A5:380:LEU:HD21	2:A5:394:LEU:HD22	1.79	0.64
2:A1:239:ARG:HH21	2:A1:240:ARG:HB2	1.63	0.64
2:A2:235:CYS:HB3	2:A2:243:LYS:HG2	1.80	0.64
1:D3:226:LYS:HG2	1:D5:308:GLU:HB3	1.81	0.63
2:A6:358:PRO:HB3	2:A6:627:MET:SD	2.38	0.63
1:D3:159:MET:HE2	1:D3:166:GLN:HE22	1.64	0.63
1:D6:159:MET:HE2	1:D6:166:GLN:HE22	1.64	0.63
2:A4:303:VAL:HG21	3:A4:701:BTN:H5	1.81	0.63
2:A4:345:ALA:HB1	2:A4:430:LEU:HD13	1.79	0.63
1:D4:342:GLY:HA3	1:D4:383:MET:HE3	1.80	0.62
2:A1:129:VAL:HG22	2:A1:134:VAL:HB	1.82	0.62
1:D4:308:GLU:HB3	1:D5:226:LYS:HG2	1.80	0.62
2:A2:239:ARG:HB3	2:A2:449:LEU:HD22	1.82	0.62
2:A4:239:ARG:HB3	2:A4:449:LEU:HD22	1.82	0.62
2:A5:388:SER:HB2	2:A5:626:ALA:HB1	1.82	0.61
2:A2:380:LEU:HD21	2:A2:394:LEU:HD22	1.81	0.61
2:A3:358:PRO:HB3	2:A3:627:MET:SD	2.41	0.61
2:A4:310:LEU:HD23	2:A4:400:HIS:HB2	1.83	0.61
2:A5:358:PRO:HB3	2:A5:627:MET:SD	2.41	0.60
2:A3:213:ARG:HD3	2:A3:252:LEU:HD22	1.83	0.60
2:A6:345:ALA:HB1	2:A6:430:LEU:HD13	1.83	0.60
2:A4:388:SER:HB2	2:A4:626:ALA:HB1	1.84	0.60
1:D3:12:VAL:O	1:D3:16:ARG:HG2	2.02	0.60
2:A3:323:ILE:HD11	2:A3:329:LEU:HD21	1.84	0.59
1:D3:55:PRO:HB3	2:A4:492:TRP:HB3	1.83	0.59
2:A5:15:ASN:HD22	2:A5:87:GLY:HA3	1.67	0.59
1:D4:431:MET:HG3	1:D4:436:ALA:HB2	1.85	0.59
2:A1:15:ASN:HD22	2:A1:87:GLY:HA3	1.67	0.59
2:A3:345:ALA:HB1	2:A3:430:LEU:HD13	1.84	0.59
2:A1:345:ALA:HB1	2:A1:430:LEU:HD13	1.84	0.59
2:A3:380:LEU:HD21	2:A3:394:LEU:HD22	1.83	0.59
2:A4:15:ASN:HD22	2:A4:87:GLY:HA3	1.67	0.59
1:D2:214:THR:HG23	1:D2:217:GLU:H	1.68	0.59
1:D4:422:MET:HE1	1:D4:428:ILE:HG21	1.85	0.58
1:D4:55:PRO:HB3	2:A5:492:TRP:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:628:LYS:HZ2	3:A2:701:BTN:C9	2.16	0.58
2:A3:15:ASN:HD22	2:A3:87:GLY:HA3	1.69	0.58
1:D1:55:PRO:HB3	2:A2:492:TRP:HB3	1.86	0.58
2:A2:358:PRO:HB3	2:A2:627:MET:SD	2.44	0.58
2:A6:237:LEU:HD21	2:A6:444:LEU:HD22	1.85	0.58
1:D4:391:ARG:HD2	1:D4:504:GLU:O	2.04	0.57
2:A5:213:ARG:HD3	2:A5:252:LEU:HD22	1.85	0.57
2:A6:15:ASN:HD22	2:A6:87:GLY:HA3	1.68	0.57
1:D1:422:MET:HE1	1:D1:428:ILE:HG21	1.85	0.57
2:A2:88:TYR:CD1	3:A2:701:BTN:H4	2.38	0.57
2:A2:388:SER:HB2	2:A2:626:ALA:HB1	1.85	0.57
1:D1:308:GLU:HB3	1:D2:226:LYS:HG2	1.85	0.57
2:A5:252:LEU:HD11	2:A5:289:PRO:HB3	1.87	0.57
1:D2:12:VAL:O	1:D2:16:ARG:HG2	2.05	0.57
2:A1:237:LEU:HD21	2:A1:444:LEU:HD22	1.86	0.57
2:A4:358:PRO:HB3	2:A4:627:MET:SD	2.44	0.57
1:D2:55:PRO:HB3	2:A1:492:TRP:HB3	1.86	0.57
2:A1:237:LEU:HD12	2:A1:245:ILE:HB	1.87	0.57
2:A3:464:GLU:HG3	2:A3:549:LEU:HD13	1.86	0.57
1:D6:437:ALA:O	1:D6:456:LYS:HD2	2.05	0.56
2:A1:218:GLN:HB2	2:A1:233:ARG:HH12	1.69	0.56
2:A5:237:LEU:HD21	2:A5:444:LEU:HD22	1.87	0.56
2:A6:388:SER:HB2	2:A6:626:ALA:HB1	1.86	0.56
1:D1:315:THR:HG22	1:D1:328:ILE:HG23	1.88	0.56
1:D3:378:LYS:HG3	1:D3:512:ARG:HG2	1.88	0.56
1:D4:373:ALA:HA	1:D6:223:LEU:HD21	1.87	0.56
2:A4:380:LEU:HD21	2:A4:394:LEU:HD22	1.88	0.56
1:D4:214:THR:HG23	1:D4:217:GLU:H	1.69	0.56
1:D4:378:LYS:HG3	1:D4:512:ARG:HG2	1.88	0.56
2:A5:237:LEU:HD12	2:A5:245:ILE:HB	1.86	0.55
1:D1:342:GLY:HA3	1:D1:383:MET:HE3	1.87	0.55
1:D5:159:MET:HB2	1:D5:164:ILE:HD12	1.89	0.55
2:A4:505:HIS:HD2	2:A4:510:THR:HG23	1.72	0.55
1:D3:214:THR:HG22	1:D3:217:GLU:HG2	1.89	0.55
1:D5:142:VAL:O	1:D5:148:HIS:HB3	2.06	0.55
1:D2:190:ILE:HD13	1:D2:221:GLY:HA2	1.88	0.55
2:A3:535:SER:HB3	2:A3:548:THR:HB	1.87	0.55
1:D6:431:MET:HG3	1:D6:436:ALA:HB2	1.89	0.55
2:A2:224:HIS:HD2	2:A2:328:PRO:HB3	1.72	0.55
1:D2:391:ARG:HD3	1:D2:504:GLU:O	2.07	0.55
1:D4:159:MET:HE2	1:D4:166:GLN:HE22	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A6:237:LEU:HD12	2:A6:245:ILE:HB	1.88	0.54
2:A5:300:ARG:NH2	3:A5:701:BTN:H62	2.23	0.54
1:D1:226:LYS:HG2	1:D6:308:GLU:HB3	1.90	0.54
1:D3:135:PHE:HD2	1:D3:138:ARG:HB2	1.73	0.54
2:A2:323:ILE:HD11	2:A2:329:LEU:HD21	1.90	0.54
2:A5:359:THR:HG21	2:A5:424:THR:HB	1.89	0.54
1:D2:422:MET:HE1	1:D2:428:ILE:HG21	1.90	0.54
1:D5:422:MET:HE1	1:D5:428:ILE:HG21	1.90	0.54
2:A1:315:ASP:HB3	2:A1:318:GLU:HB3	1.90	0.54
2:A1:388:SER:HB2	2:A1:626:ALA:HB1	1.90	0.54
2:A3:218:GLN:HB2	2:A3:233:ARG:HH12	1.73	0.54
2:A6:305:HIS:HB2	2:A6:316:LEU:HD12	1.89	0.54
1:D4:184:MET:HE1	1:D6:384:VAL:HG11	1.90	0.53
2:A2:252:LEU:HD11	2:A2:289:PRO:HB3	1.89	0.53
2:A2:628:LYS:NZ	3:A2:701:BTN:H102	2.21	0.53
2:A3:344:GLU:HG3	2:A3:398:ILE:HG13	1.91	0.53
1:D4:360:GLN:HG2	1:D4:410:MET:HB3	1.90	0.53
2:A2:15:ASN:HD22	2:A2:87:GLY:HA3	1.74	0.53
2:A3:244:VAL:HG12	2:A3:430:LEU:HD21	1.91	0.53
2:A1:391:ASP:HB2	3:A1:701:BTN:H81	1.90	0.53
1:D1:206:LYS:HD2	1:D1:212:VAL:HG22	1.89	0.53
2:A4:305:HIS:ND1	2:A4:306:PRO:HD3	2.24	0.53
1:D3:308:GLU:HB3	1:D4:226:LYS:HG2	1.91	0.52
1:D5:328:ILE:HG22	1:D5:410:MET:HE1	1.91	0.52
2:A2:215:ILE:HG21	2:A2:253:LEU:HD11	1.91	0.52
1:D1:135:PHE:HD2	1:D1:138:ARG:HB2	1.75	0.52
2:A1:367:ARG:HH12	2:A1:569:GLY:HA2	1.74	0.52
2:A5:363:VAL:HG21	2:A5:380:LEU:HD22	1.92	0.52
1:D2:142:VAL:O	1:D2:148:HIS:HB3	2.09	0.52
1:D4:223:LEU:HD21	1:D6:373:ALA:HA	1.90	0.52
2:A4:61:ALA:HB3	2:A4:64:HIS:HD2	1.73	0.52
2:A6:323:ILE:HD11	2:A6:329:LEU:HD21	1.91	0.52
2:A1:392:PRO:HD3	2:A1:627:MET:HB3	1.90	0.52
1:D1:360:GLN:HG2	1:D1:410:MET:HB3	1.91	0.52
1:D1:223:LEU:HD21	1:D3:373:ALA:HA	1.91	0.52
1:D6:135:PHE:HD2	1:D6:138:ARG:HB2	1.75	0.52
1:D3:431:MET:HG3	1:D3:436:ALA:HB2	1.92	0.51
2:A4:284:VAL:HG22	2:A4:292:PHE:HB3	1.92	0.51
2:A1:380:LEU:HD21	2:A1:394:LEU:HD22	1.91	0.51
1:D2:360:GLN:HG2	1:D2:410:MET:HB3	1.92	0.51
2:A1:219:VAL:HG11	2:A1:269:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:37:VAL:HG12	2:A2:55:VAL:HG13	1.92	0.51
2:A6:305:HIS:ND1	2:A6:306:PRO:HD3	2.26	0.51
1:D6:190:ILE:HD13	1:D6:221:GLY:HA2	1.93	0.51
2:A1:305:HIS:ND1	2:A1:306:PRO:HD3	2.26	0.51
1:D2:328:ILE:HG22	1:D2:410:MET:HE1	1.93	0.50
2:A6:315:ASP:HB3	2:A6:318:GLU:HB3	1.93	0.50
1:D1:189:VAL:HG13	1:D1:233:HIS:HB2	1.92	0.50
1:D5:391:ARG:HD3	1:D5:504:GLU:O	2.12	0.50
1:D6:190:ILE:HB	1:D6:231:THR:HG21	1.93	0.50
2:A6:380:LEU:HD11	2:A6:394:LEU:HB3	1.93	0.50
1:D4:190:ILE:HB	1:D4:231:THR:HG21	1.93	0.50
1:D5:16:ARG:HH21	1:D5:483:ASP:HB2	1.76	0.50
1:D5:55:PRO:HB3	2:A6:492:TRP:HB3	1.92	0.50
2:A5:315:ASP:HB3	2:A5:318:GLU:HB3	1.92	0.50
1:D1:49:LEU:HD23	1:D1:91:ILE:HD13	1.93	0.50
1:D4:49:LEU:HD23	1:D4:91:ILE:HD13	1.92	0.50
2:A3:235:CYS:HB3	2:A3:243:LYS:HG2	1.93	0.50
2:A2:35:VAL:HG22	2:A2:53:VAL:HG23	1.94	0.50
2:A6:252:LEU:HD11	2:A6:289:PRO:HB3	1.92	0.50
1:D5:190:ILE:HD13	1:D5:221:GLY:HA2	1.94	0.49
1:D2:190:ILE:HB	1:D2:231:THR:HG21	1.93	0.49
1:D4:142:VAL:O	1:D4:148:HIS:HB3	2.12	0.49
1:D5:49:LEU:HD23	1:D5:91:ILE:HD13	1.94	0.49
2:A3:305:HIS:ND1	2:A3:306:PRO:HD3	2.27	0.49
1:D3:146:ARG:O	1:D3:151:ARG:HB2	2.12	0.49
1:D3:190:ILE:HD13	1:D3:221:GLY:HA2	1.94	0.49
1:D5:437:ALA:HB1	1:D5:456:LYS:HD2	1.95	0.49
1:D6:142:VAL:O	1:D6:148:HIS:HB3	2.13	0.49
2:A1:363:VAL:HG21	2:A1:380:LEU:HD22	1.93	0.49
2:A1:600:MET:HE2	2:A1:626:ALA:HB3	1.93	0.49
2:A5:245:ILE:HD11	2:A5:430:LEU:HD12	1.95	0.49
2:A3:129:VAL:HG13	2:A3:134:VAL:HB	1.95	0.49
2:A6:233:ARG:HG2	2:A6:248:ALA:HB2	1.93	0.49
2:A6:390:TYR:O	2:A6:627:MET:HG2	2.11	0.49
1:D1:159:MET:HE2	1:D1:166:GLN:HE22	1.78	0.49
2:A6:505:HIS:HD2	2:A6:510:THR:HG23	1.76	0.49
2:A1:233:ARG:HB3	2:A1:248:ALA:HB2	1.95	0.49
2:A3:111:PRO:HB3	2:A3:274:TYR:CE1	2.48	0.49
2:A6:300:ARG:NH2	3:A6:701:BTN:H62	2.28	0.49
2:A3:359:THR:O	2:A3:627:MET:HE1	2.13	0.49
1:D2:146:ARG:O	1:D2:151:ARG:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:315:ASP:HB3	2:A2:318:GLU:HB3	1.95	0.48
2:A1:119:MET:HE2	2:A1:272:VAL:HG11	1.95	0.48
2:A3:470:ALA:HB2	2:A3:504:LEU:HD11	1.95	0.48
2:A6:45:ALA:HB3	2:A6:48:VAL:HG23	1.95	0.48
1:D5:170:VAL:HG21	1:D5:197:ILE:HD11	1.94	0.48
2:A4:305:HIS:HB2	2:A4:316:LEU:HD12	1.93	0.48
2:A2:237:LEU:HD12	2:A2:245:ILE:HB	1.94	0.48
2:A2:499:PRO:HB3	2:A2:516:THR:HG22	1.96	0.48
2:A2:305:HIS:HB2	2:A2:316:LEU:HD12	1.96	0.48
1:D1:378:LYS:HG3	1:D1:512:ARG:HG2	1.95	0.48
2:A2:363:VAL:HG21	2:A2:380:LEU:HD22	1.95	0.48
1:D2:342:GLY:HA3	1:D2:383:MET:HE3	1.95	0.48
1:D4:315:THR:HG22	1:D4:328:ILE:HG23	1.94	0.48
2:A1:485:LEU:H	2:A1:485:LEU:HD23	1.79	0.48
2:A6:564:GLN:HG2	2:A6:577:GLN:HG2	1.96	0.48
2:A4:237:LEU:HD12	2:A4:245:ILE:HB	1.96	0.48
2:A6:392:PRO:HD3	2:A6:627:MET:HB3	1.95	0.48
1:D2:170:VAL:HB	1:D2:190:ILE:HG13	1.95	0.47
1:D2:49:LEU:HD23	1:D2:91:ILE:HD13	1.96	0.47
2:A3:305:HIS:HB2	2:A3:316:LEU:HD12	1.96	0.47
2:A4:359:THR:HG21	2:A4:424:THR:HB	1.96	0.47
2:A6:380:LEU:HD21	2:A6:394:LEU:HD22	1.96	0.47
2:A1:390:TYR:O	2:A1:627:MET:HG2	2.15	0.47
2:A1:391:ASP:CB	3:A1:701:BTN:H81	2.43	0.47
2:A3:363:VAL:HG21	2:A3:380:LEU:HD22	1.96	0.47
2:A4:111:PRO:HB3	2:A4:274:TYR:CE1	2.50	0.47
2:A3:387:GLY:O	2:A3:627:MET:HE2	2.14	0.47
1:D5:170:VAL:HB	1:D5:190:ILE:HG13	1.95	0.47
2:A2:359:THR:HG21	2:A2:424:THR:HB	1.96	0.47
2:A3:433:LEU:HD21	2:A3:449:LEU:HG	1.97	0.47
1:D2:146:ARG:HA	1:D5:414:ALA:HA	1.96	0.47
2:A1:249:PRO:HB3	2:A1:338:LEU:HD23	1.96	0.47
1:D1:170:VAL:HG21	1:D1:197:ILE:HD11	1.97	0.47
1:D5:190:ILE:HB	1:D5:231:THR:HG21	1.97	0.47
2:A1:380:LEU:HD11	2:A1:394:LEU:HB3	1.96	0.47
2:A3:357:LEU:CD1	2:A3:599:PRO:HB2	2.45	0.47
2:A5:219:VAL:HG11	2:A5:269:ALA:HB2	1.97	0.47
2:A6:506:ALA:HB2	2:A6:576:VAL:HG22	1.97	0.47
1:D2:184:MET:HE2	1:D2:184:MET:HB3	1.80	0.47
1:D3:180:TYR:O	1:D3:184:MET:HG2	2.15	0.46
2:A3:315:ASP:HB3	2:A3:318:GLU:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A3:392:PRO:HD3	2:A3:627:MET:HB3	1.96	0.46
2:A3:421:LEU:HD21	2:A3:568:SER:HB2	1.97	0.46
2:A6:470:ALA:HB2	2:A6:504:LEU:HD11	1.96	0.46
1:D1:146:ARG:O	1:D1:151:ARG:HB2	2.15	0.46
2:A5:357:LEU:CD2	2:A5:629:MET:HE1	2.43	0.46
2:A1:421:LEU:HD21	2:A1:568:SER:HB2	1.98	0.46
2:A6:363:VAL:HG21	2:A6:380:LEU:HD22	1.97	0.46
2:A2:119:MET:HE2	2:A2:297:MET:HB3	1.96	0.46
2:A6:218:GLN:HB2	2:A6:233:ARG:HH12	1.81	0.46
2:A1:600:MET:CE	2:A1:626:ALA:HB3	2.45	0.46
3:A3:701:BTN:H2	3:A3:701:BTN:H92	1.69	0.46
2:A5:317:VAL:O	2:A5:321:ILE:HG12	2.16	0.46
1:D1:373:ALA:HA	1:D3:223:LEU:HD21	1.97	0.46
2:A2:535:SER:HB3	2:A2:548:THR:HB	1.97	0.46
2:A5:390:TYR:O	2:A5:627:MET:HG2	2.16	0.46
2:A6:505:HIS:CD2	2:A6:510:THR:HG23	2.51	0.46
1:D1:142:VAL:O	1:D1:148:HIS:HB3	2.15	0.46
1:D1:483:ASP:HB3	1:D1:486:ASP:HB2	1.98	0.46
2:A2:391:ASP:HB2	3:A2:701:BTN:C9	2.31	0.46
2:A4:303:VAL:HG23	3:A4:701:BTN:H5	1.97	0.46
2:A6:35:VAL:HG13	2:A6:53:VAL:HG13	1.97	0.46
2:A6:111:PRO:HB3	2:A6:274:TYR:CE1	2.51	0.46
1:D1:259:PRO:HG2	1:D1:260:TRP:CE3	2.51	0.46
1:D6:170:VAL:HG21	1:D6:197:ILE:HD11	1.98	0.46
2:A2:305:HIS:ND1	2:A2:306:PRO:HD3	2.30	0.46
2:A2:392:PRO:HD3	2:A2:627:MET:HB3	1.97	0.46
2:A3:392:PRO:HB3	2:A3:627:MET:SD	2.55	0.46
2:A4:535:SER:HB3	2:A4:548:THR:HB	1.98	0.46
3:A2:701:BTN:H101	3:A2:701:BTN:H72	1.49	0.45
2:A3:233:ARG:HG2	2:A3:248:ALA:HB2	1.98	0.45
2:A4:35:VAL:HG13	2:A4:53:VAL:HG13	1.97	0.45
1:D4:170:VAL:HG21	1:D4:197:ILE:HD11	1.98	0.45
2:A5:535:SER:HB3	2:A5:548:THR:HB	1.97	0.45
1:D6:336:GLY:HA3	1:D6:379:HIS:HD2	1.81	0.45
2:A2:380:LEU:HD11	2:A2:394:LEU:HB3	1.99	0.45
2:A4:315:ASP:HB3	2:A4:318:GLU:HB3	1.98	0.45
2:A4:470:ALA:HB2	2:A4:504:LEU:HD11	1.98	0.45
2:A5:215:ILE:HG21	2:A5:253:LEU:HD11	1.97	0.45
1:D4:42:PRO:HA	1:D4:45:ARG:HD2	1.98	0.45
1:D5:153:PHE:HB3	1:D5:184:MET:SD	2.57	0.45
1:D6:282:ASP:HB3	1:D6:285:VAL:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A3:388:SER:HB2	2:A3:626:ALA:HB1	1.99	0.45
2:A3:525:ALA:HB2	2:A3:531:THR:HG22	1.98	0.45
2:A5:380:LEU:HD11	2:A5:394:LEU:HB3	1.98	0.45
2:A1:45:ALA:HB3	2:A1:48:VAL:HG23	1.99	0.45
1:D1:190:ILE:HB	1:D1:231:THR:HG21	1.98	0.45
1:D1:266:VAL:HB	1:D1:298:ASP:HB3	1.99	0.45
1:D4:440:LEU:HD13	1:D4:440:LEU:HA	1.85	0.45
2:A1:535:SER:HB3	2:A1:548:THR:HB	1.99	0.45
2:A5:504:LEU:HD13	2:A5:576:VAL:HG11	1.99	0.45
1:D2:259:PRO:HG2	1:D2:260:TRP:CE3	2.51	0.45
1:D4:266:VAL:HB	1:D4:298:ASP:HB3	1.99	0.45
1:D5:360:GLN:HG2	1:D5:410:MET:HB3	1.97	0.45
2:A1:305:HIS:HB2	2:A1:316:LEU:HD12	1.97	0.45
2:A4:380:LEU:HD11	2:A4:394:LEU:HD13	1.99	0.45
1:D4:336:GLY:HA3	1:D4:379:HIS:HD2	1.81	0.45
1:D4:350:ASP:OD1	1:D4:391:ARG:HG2	2.16	0.45
2:A1:213:ARG:HG3	2:A1:286:ALA:HB2	1.98	0.45
2:A3:380:LEU:HD11	2:A3:394:LEU:HD13	1.99	0.45
2:A4:317:VAL:O	2:A4:321:ILE:HG12	2.16	0.45
2:A4:421:LEU:HD21	2:A4:568:SER:HB2	1.99	0.45
2:A6:119:MET:HE2	2:A6:272:VAL:HG11	1.98	0.45
1:D2:153:PHE:HB3	1:D2:184:MET:SD	2.57	0.45
1:D3:493:LEU:HD23	2:A4:485:LEU:HG	1.99	0.45
1:D4:190:ILE:HD13	1:D4:221:GLY:HA2	1.98	0.45
2:A2:111:PRO:HB3	2:A2:274:TYR:CE1	2.52	0.45
1:D5:155:ASN:O	1:D5:159:MET:HG2	2.18	0.44
1:D1:42:PRO:HA	1:D1:45:ARG:HD2	2.00	0.44
2:A4:233:ARG:HG2	2:A4:248:ALA:HB2	1.99	0.44
2:A5:470:ALA:HB2	2:A5:504:LEU:HD11	2.00	0.44
1:D1:440:LEU:HD12	1:D1:440:LEU:HA	1.90	0.44
1:D3:190:ILE:HB	1:D3:231:THR:HG21	1.99	0.44
1:D5:342:GLY:HA3	1:D5:383:MET:HE3	1.98	0.44
1:D3:259:PRO:HG2	1:D3:260:TRP:CE3	2.51	0.44
1:D5:441:ALA:HB2	1:D5:456:LYS:HD3	1.99	0.44
2:A3:380:LEU:HD11	2:A3:394:LEU:HB3	1.99	0.44
2:A5:392:PRO:HD3	2:A5:627:MET:HB3	1.99	0.44
2:A6:57:ILE:HD12	2:A6:65:SER:O	2.17	0.44
2:A1:235:CYS:HB3	2:A1:243:LYS:HG2	1.99	0.44
2:A1:314:ILE:HD13	2:A1:331:ILE:HD12	2.00	0.44
2:A2:305:HIS:CG	2:A2:306:PRO:HD3	2.53	0.44
2:A4:363:VAL:HG21	2:A4:380:LEU:HD22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A4:380:LEU:HD11	2:A4:394:LEU:HB3	1.99	0.44
1:D2:336:GLY:HA3	1:D2:379:HIS:HD2	1.82	0.44
2:A4:303:VAL:HG21	3:A4:701:BTN:C5	2.46	0.44
2:A5:134:VAL:HG13	2:A5:264:ALA:HB1	1.99	0.44
1:D3:142:VAL:O	1:D3:148:HIS:HB3	2.17	0.44
1:D5:174:CYS:SG	1:D5:179:ALA:HA	2.58	0.44
2:A3:239:ARG:O	2:A3:242:GLN:HB2	2.18	0.44
2:A3:433:LEU:HD12	2:A3:433:LEU:HA	1.73	0.44
2:A3:473:LEU:HD21	2:A3:578:LYS:HD3	1.99	0.44
2:A4:244:VAL:HG12	2:A4:430:LEU:HD21	2.00	0.44
2:A5:421:LEU:HD21	2:A5:568:SER:HB2	1.98	0.44
2:A5:485:LEU:HD23	2:A5:485:LEU:H	1.81	0.44
2:A6:136:VAL:HG12	2:A6:137:VAL:H	1.83	0.44
2:A6:433:LEU:HD12	2:A6:433:LEU:HA	1.90	0.44
2:A6:485:LEU:HD23	2:A6:485:LEU:H	1.83	0.44
1:D2:315:THR:HG22	1:D2:328:ILE:HG23	2.00	0.44
1:D5:146:ARG:O	1:D5:151:ARG:HB2	2.18	0.44
1:D5:315:THR:HG22	1:D5:328:ILE:HG23	2.00	0.44
1:D6:384:VAL:HG22	1:D6:409:SER:HA	2.00	0.44
2:A5:323:ILE:HD11	2:A5:329:LEU:HD21	1.99	0.44
1:D4:259:PRO:HG2	1:D4:260:TRP:CE3	2.53	0.43
1:D6:266:VAL:HB	1:D6:298:ASP:HB3	1.99	0.43
2:A1:111:PRO:HB3	2:A1:274:TYR:CE1	2.53	0.43
1:D6:259:PRO:HG2	1:D6:260:TRP:CE3	2.53	0.43
2:A2:485:LEU:HD23	2:A2:485:LEU:H	1.83	0.43
2:A5:305:HIS:ND1	2:A5:306:PRO:HD3	2.33	0.43
2:A6:421:LEU:HD21	2:A6:568:SER:HB2	2.00	0.43
1:D1:328:ILE:HG22	1:D1:410:MET:HE1	1.99	0.43
2:A5:129:VAL:HG13	2:A5:134:VAL:HB	2.00	0.43
1:D2:170:VAL:HG21	1:D2:197:ILE:HD11	2.00	0.43
2:A3:565:ILE:HD11	2:A3:578:LYS:HD3	2.01	0.43
1:D2:174:CYS:SG	1:D2:179:ALA:HA	2.58	0.43
2:A4:357:LEU:HD13	2:A4:599:PRO:HB2	2.00	0.43
1:D1:214:THR:HG22	1:D1:217:GLU:HG2	2.00	0.43
1:D3:457:ALA:HB3	1:D3:458:PRO:HD3	2.00	0.43
2:A2:470:ALA:HB2	2:A2:504:LEU:HD11	2.01	0.43
2:A3:238:GLN:HB2	2:A3:241:HIS:O	2.19	0.43
2:A6:599:PRO:HD3	2:A6:633:LEU:HD21	2.01	0.43
2:A3:599:PRO:HD3	2:A3:633:LEU:HD21	2.00	0.43
2:A4:136:VAL:HG12	2:A4:137:VAL:H	1.84	0.43
1:D6:49:LEU:HD23	1:D6:91:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:380:LEU:HD11	2:A2:394:LEU:HD13	2.01	0.43
2:A3:358:PRO:HD3	2:A3:629:MET:CE	2.46	0.43
2:A4:119:MET:HE3	2:A4:297:MET:SD	2.59	0.43
1:D4:77:MET:SD	1:D4:92:VAL:HG13	2.59	0.43
2:A1:304:GLU:O	2:A1:307:VAL:HG22	2.18	0.43
2:A4:506:ALA:HB2	2:A4:576:VAL:HG22	2.00	0.43
2:A6:244:VAL:HG12	2:A6:430:LEU:HD21	2.01	0.43
2:A2:421:LEU:HD21	2:A2:568:SER:HB2	2.00	0.42
1:D5:202:PRO:N	1:D5:203:PRO:HD2	2.35	0.42
1:D5:421:TRP:HH2	1:D5:494:ALA:HB2	1.84	0.42
2:A2:315:ASP:O	2:A2:319:GLN:HG2	2.18	0.42
2:A3:391:ASP:HB2	3:A3:701:BTN:H81	2.01	0.42
1:D3:266:VAL:HB	1:D3:298:ASP:HB3	1.99	0.42
1:D6:269:ILE:H	1:D6:269:ILE:HG13	1.62	0.42
2:A2:390:TYR:O	2:A2:627:MET:HG2	2.19	0.42
2:A5:119:MET:HE2	2:A5:272:VAL:HG11	2.01	0.42
2:A5:305:HIS:CG	2:A5:306:PRO:HD3	2.53	0.42
1:D4:159:MET:HE2	1:D4:166:GLN:NE2	2.33	0.42
1:D6:259:PRO:HG3	1:D6:503:LEU:HG	2.01	0.42
2:A1:222:ASP:HA	2:A1:323:ILE:HG23	2.00	0.42
1:D4:459:ILE:HD12	1:D4:459:ILE:HA	1.95	0.42
2:A1:391:ASP:HB2	3:A1:701:BTN:C11	2.49	0.42
2:A1:470:ALA:HB2	2:A1:504:LEU:HD11	2.01	0.42
1:D3:202:PRO:N	1:D3:203:PRO:HD2	2.35	0.42
1:D3:384:VAL:HG22	1:D3:409:SER:HA	2.01	0.42
1:D5:20:ALA:O	1:D5:24:LEU:HD23	2.20	0.42
1:D5:259:PRO:HG2	1:D5:260:TRP:CE3	2.55	0.42
2:A1:599:PRO:HD3	2:A1:633:LEU:HD21	2.02	0.42
2:A5:290:ASP:HB3	2:A5:291:GLU:OE1	2.19	0.42
2:A6:359:THR:HG21	2:A6:424:THR:HB	2.00	0.42
1:D2:202:PRO:N	1:D2:203:PRO:HD2	2.35	0.42
1:D3:49:LEU:HD23	1:D3:91:ILE:HD13	2.02	0.42
1:D6:198:PHE:CD2	1:D6:218:LEU:HD23	2.54	0.42
2:A3:317:VAL:O	2:A3:321:ILE:HD12	2.19	0.42
2:A5:600:MET:CE	2:A5:626:ALA:HB3	2.50	0.42
2:A6:101:LEU:HD12	2:A6:108:PHE:HD1	1.83	0.42
1:D3:456:LYS:HA	1:D3:459:ILE:HG22	2.01	0.42
2:A5:284:VAL:HG22	2:A5:292:PHE:HB3	2.02	0.42
1:D1:259:PRO:HG3	1:D1:503:LEU:HG	2.02	0.42
1:D5:269:ILE:H	1:D5:269:ILE:HG13	1.60	0.42
2:A1:358:PRO:HB3	2:A1:627:MET:SD	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:504:LEU:HD13	2:A2:576:VAL:HG11	2.02	0.42
2:A3:357:LEU:HD23	2:A3:629:MET:HE1	2.01	0.42
2:A3:506:ALA:HB2	2:A3:576:VAL:HG22	2.01	0.42
2:A4:218:GLN:HB2	2:A4:233:ARG:HH12	1.84	0.42
2:A5:352:PRO:HA	2:A5:356:PHE:CD1	2.55	0.42
1:D1:414:ALA:HA	1:D3:146:ARG:HA	2.01	0.42
1:D1:511:PHE:CG	1:D5:513:MET:HE1	2.55	0.42
1:D5:184:MET:HE2	1:D5:184:MET:HB3	1.86	0.42
2:A5:111:PRO:HB3	2:A5:274:TYR:CE1	2.55	0.42
2:A6:316:LEU:HD23	2:A6:316:LEU:HA	1.87	0.42
1:D6:146:ARG:O	1:D6:151:ARG:HB2	2.19	0.41
2:A1:222:ASP:OD1	2:A1:226:ASN:HB2	2.20	0.41
2:A2:391:ASP:CG	3:A2:701:BTN:H92	2.45	0.41
2:A3:222:ASP:OD2	2:A3:226:ASN:HB2	2.20	0.41
2:A4:305:HIS:HD2	2:A4:309:GLU:OE2	2.03	0.41
1:D2:360:GLN:HE21	1:D2:396:THR:HG21	1.84	0.41
2:A1:367:ARG:O	2:A1:418:THR:HA	2.20	0.41
2:A3:300:ARG:NH2	3:A3:701:BTN:H62	2.35	0.41
2:A4:323:ILE:HD11	2:A4:329:LEU:HD21	2.01	0.41
2:A5:218:GLN:HB2	2:A5:233:ARG:HH12	1.83	0.41
2:A5:557:ARG:HE	2:A5:557:ARG:HB2	1.49	0.41
2:A6:477:GLN:HG2	2:A6:489:PRO:HD3	2.02	0.41
2:A6:525:ALA:HB2	2:A6:531:THR:HG22	2.00	0.41
1:D2:29:ARG:HH11	1:D2:29:ARG:HB3	1.86	0.41
1:D4:483:ASP:HB3	1:D4:486:ASP:HB2	2.02	0.41
1:D6:29:ARG:HH11	1:D6:29:ARG:HB3	1.85	0.41
1:D6:202:PRO:N	1:D6:203:PRO:HD2	2.35	0.41
1:D6:309:TYR:O	1:D6:341:LYS:HD2	2.19	0.41
2:A1:433:LEU:HA	2:A1:433:LEU:HD23	1.85	0.41
2:A3:316:LEU:HD23	2:A3:316:LEU:HA	1.92	0.41
1:D4:29:ARG:HB3	1:D4:29:ARG:HH11	1.84	0.41
1:D4:282:ASP:HB3	1:D4:285:VAL:HG23	2.02	0.41
2:A4:304:GLU:O	2:A4:307:VAL:HG22	2.20	0.41
2:A4:315:ASP:O	2:A4:319:GLN:HG2	2.20	0.41
2:A4:392:PRO:HD3	2:A4:627:MET:HB3	2.02	0.41
1:D2:373:ALA:HA	1:D5:223:LEU:HD21	2.03	0.41
2:A1:323:ILE:HD11	2:A1:329:LEU:HD21	2.02	0.41
1:D2:289:VAL:HG21	1:D2:329:ALA:HB1	2.01	0.41
1:D2:367:VAL:HG11	1:D5:204:LEU:HG	2.03	0.41
1:D4:353:LYS:HG2	1:D4:391:ARG:NH2	2.36	0.41
1:D3:226:LYS:HE2	1:D5:308:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:304:GLU:O	2:A2:307:VAL:HG22	2.21	0.41
1:D1:202:PRO:N	1:D1:203:PRO:HD2	2.35	0.41
1:D1:204:LEU:HD22	1:D3:367:VAL:HG11	2.03	0.41
1:D1:421:TRP:HH2	1:D1:494:ALA:HB2	1.85	0.41
1:D3:170:VAL:HG21	1:D3:197:ILE:HD11	2.02	0.41
1:D6:108:VAL:HG21	1:D6:142:VAL:HG13	2.02	0.41
2:A1:57:ILE:HD12	2:A1:65:SER:O	2.21	0.41
2:A1:136:VAL:HG12	2:A1:137:VAL:H	1.86	0.41
2:A1:218:GLN:HB3	2:A1:230:LEU:HB2	2.02	0.41
2:A2:512:HIS:H	2:A2:527:GLU:HG2	1.86	0.41
2:A3:119:MET:HE3	2:A3:297:MET:SD	2.60	0.41
2:A3:234:GLU:HB3	2:A3:247:GLU:HG3	2.03	0.41
2:A4:485:LEU:H	2:A4:485:LEU:HD23	1.86	0.41
2:A5:315:ASP:O	2:A5:319:GLN:HG2	2.20	0.41
1:D3:259:PRO:HG3	1:D3:503:LEU:HG	2.03	0.41
1:D4:7:GLU:HB2	1:D4:281:VAL:HG21	2.02	0.41
1:D5:29:ARG:HH11	1:D5:29:ARG:HB3	1.85	0.41
2:A1:357:LEU:HD22	2:A1:600:MET:SD	2.61	0.41
2:A3:284:VAL:HG22	2:A3:292:PHE:HB3	2.02	0.41
1:D2:269:ILE:H	1:D2:269:ILE:HG13	1.60	0.40
1:D4:309:TYR:O	1:D4:341:LYS:HD2	2.21	0.40
2:A2:45:ALA:HB3	2:A2:48:VAL:HG23	2.03	0.40
2:A2:134:VAL:HG22	2:A2:135:PRO:HD2	2.02	0.40
2:A3:304:GLU:O	2:A3:307:VAL:HG22	2.20	0.40
2:A4:101:LEU:HD12	2:A4:108:PHE:HD1	1.86	0.40
2:A5:239:ARG:HG3	2:A5:356:PHE:CD2	2.56	0.40
1:D4:146:ARG:O	1:D4:151:ARG:HB2	2.21	0.40
1:D4:202:PRO:N	1:D4:203:PRO:HD2	2.35	0.40
2:A1:453:ALA:N	2:A1:454:PRO:HD2	2.36	0.40
2:A3:305:HIS:HD2	2:A3:309:GLU:OE2	2.05	0.40
2:A6:315:ASP:O	2:A6:319:GLN:HG2	2.20	0.40
1:D2:421:TRP:HH2	1:D2:494:ALA:HB2	1.86	0.40
1:D3:159:MET:HE2	1:D3:166:GLN:NE2	2.32	0.40
2:A2:599:PRO:HD3	2:A2:633:LEU:HD21	2.04	0.40
2:A6:224:HIS:ND1	2:A6:328:PRO:HB3	2.36	0.40
2:A6:357:LEU:CD1	2:A6:599:PRO:HB2	2.51	0.40
2:A2:88:TYR:CD1	3:A2:701:BTN:C2	2.99	0.40
2:A3:57:ILE:HD12	2:A3:65:SER:O	2.22	0.40
1:D2:144:PRO:HD2	1:D2:148:HIS:ND1	2.36	0.40
1:D4:259:PRO:HG3	1:D4:503:LEU:HG	2.03	0.40
2:A2:560:VAL:HG22	2:A2:565:ILE:HG23	2.04	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	D1	509/513 (99%)	493 (97%)	16 (3%)	0	100	100
1	D2	509/513 (99%)	491 (96%)	18 (4%)	0	100	100
1	D3	509/513 (99%)	493 (97%)	16 (3%)	0	100	100
1	D4	509/513 (99%)	496 (97%)	13 (3%)	0	100	100
1	D5	509/513 (99%)	490 (96%)	19 (4%)	0	100	100
1	D6	509/513 (99%)	491 (96%)	18 (4%)	0	100	100
2	A1	562/669 (84%)	543 (97%)	19 (3%)	0	100	100
2	A2	560/669 (84%)	546 (98%)	14 (2%)	0	100	100
2	A3	562/669 (84%)	541 (96%)	21 (4%)	0	100	100
2	A4	562/669 (84%)	548 (98%)	14 (2%)	0	100	100
2	A5	561/669 (84%)	548 (98%)	13 (2%)	0	100	100
2	A6	562/669 (84%)	546 (97%)	16 (3%)	0	100	100
All	All	6423/7092 (91%)	6226 (97%)	197 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	D1	392/394 (100%)	378 (96%)	14 (4%)	31	65
1	D2	392/394 (100%)	379 (97%)	13 (3%)	33	67
1	D3	392/394 (100%)	380 (97%)	12 (3%)	35	69
1	D4	392/394 (100%)	378 (96%)	14 (4%)	31	65
1	D5	392/394 (100%)	381 (97%)	11 (3%)	38	72
1	D6	392/394 (100%)	380 (97%)	12 (3%)	35	69
2	A1	425/499 (85%)	412 (97%)	13 (3%)	35	69
2	A2	423/499 (85%)	408 (96%)	15 (4%)	32	66
2	A3	425/499 (85%)	413 (97%)	12 (3%)	38	72
2	A4	425/499 (85%)	408 (96%)	17 (4%)	28	62
2	A5	424/499 (85%)	409 (96%)	15 (4%)	32	66
2	A6	425/499 (85%)	413 (97%)	12 (3%)	38	72
All	All	4899/5358 (91%)	4739 (97%)	160 (3%)	34	67

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D1	37	ARG
1	D1	92	VAL
1	D1	125	CYS
1	D1	147	ASP
1	D1	189	VAL
1	D1	204	LEU
1	D1	269	ILE
1	D1	289	VAL
1	D1	350	ASP
1	D1	435	GLN
1	D1	440	LEU
1	D1	459	ILE
1	D1	468	ASN
1	D1	512	ARG
1	D2	16	ARG
1	D2	59	LEU
1	D2	269	ILE
1	D2	330	ASN
1	D2	333	VAL
1	D2	340	VAL
1	D2	350	ASP
1	D2	435	GLN

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Mol	Chain	Res	Type
1	D2	440	LEU
1	D2	453	GLU
1	D2	455	PHE
1	D2	468	ASN
1	D2	512	ARG
1	D3	59	LEU
1	D3	125	CYS
1	D3	204	LEU
1	D3	289	VAL
1	D3	333	VAL
1	D3	350	ASP
1	D3	361	ASN
1	D3	383	MET
1	D3	413	ARG
1	D3	435	GLN
1	D3	455	PHE
1	D3	468	ASN
1	D4	37	ARG
1	D4	125	CYS
1	D4	147	ASP
1	D4	189	VAL
1	D4	204	LEU
1	D4	269	ILE
1	D4	289	VAL
1	D4	340	VAL
1	D4	435	GLN
1	D4	440	LEU
1	D4	459	ILE
1	D4	468	ASN
1	D4	476	LEU
1	D4	512	ARG
1	D5	37	ARG
1	D5	59	LEU
1	D5	218	LEU
1	D5	269	ILE
1	D5	289	VAL
1	D5	333	VAL
1	D5	340	VAL
1	D5	350	ASP
1	D5	435	GLN
1	D5	440	LEU
1	D5	468	ASN

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Mol	Chain	Res	Type
1	D6	59	LEU
1	D6	125	CYS
1	D6	147	ASP
1	D6	204	LEU
1	D6	262	VAL
1	D6	269	ILE
1	D6	289	VAL
1	D6	333	VAL
1	D6	350	ASP
1	D6	361	ASN
1	D6	435	GLN
1	D6	468	ASN
2	A1	79	THR
2	A1	136	VAL
2	A1	234	GLU
2	A1	242	GLN
2	A1	244	VAL
2	A1	283	ILE
2	A1	288	ARG
2	A1	304	GLU
2	A1	331	ILE
2	A1	516	THR
2	A1	528	HIS
2	A1	547	VAL
2	A1	577	GLN
2	A2	7	THR
2	A2	12	LEU
2	A2	22	ARG
2	A2	46	ARG
2	A2	53	VAL
2	A2	55	VAL
2	A2	79	THR
2	A2	134	VAL
2	A2	232	GLU
2	A2	242	GLN
2	A2	243	LYS
2	A2	528	HIS
2	A2	547	VAL
2	A2	549	LEU
2	A2	578	LYS
2	A3	12	LEU
2	A3	22	ARG

Continued on next page...

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Mol	Chain	Res	Type
2	A3	79	THR
2	A3	239	ARG
2	A3	242	GLN
2	A3	243	LYS
2	A3	244	VAL
2	A3	304	GLU
2	A3	321	ILE
2	A3	343	VAL
2	A3	433	LEU
2	A3	558	VAL
2	A4	12	LEU
2	A4	16	ARG
2	A4	18	GLU
2	A4	26	THR
2	A4	79	THR
2	A4	136	VAL
2	A4	242	GLN
2	A4	243	LYS
2	A4	244	VAL
2	A4	296	GLU
2	A4	304	GLU
2	A4	473	LEU
2	A4	528	HIS
2	A4	547	VAL
2	A4	558	VAL
2	A4	565	ILE
2	A4	578	LYS
2	A5	7	THR
2	A5	12	LEU
2	A5	26	THR
2	A5	46	ARG
2	A5	215	ILE
2	A5	239	ARG
2	A5	243	LYS
2	A5	254	ASP
2	A5	304	GLU
2	A5	430	LEU
2	A5	509	ARG
2	A5	528	HIS
2	A5	547	VAL
2	A5	573	THR
2	A5	578	LYS

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Mol	Chain	Res	Type
2	A6	12	LEU
2	A6	26	THR
2	A6	79	THR
2	A6	136	VAL
2	A6	243	LYS
2	A6	244	VAL
2	A6	296	GLU
2	A6	304	GLU
2	A6	413	ARG
2	A6	547	VAL
2	A6	577	GLN
2	A6	578	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	D1	111	HIS
1	D1	156	GLN
1	D1	272	GLN
1	D1	321	HIS
1	D1	407	ASN
1	D1	462	GLN
1	D2	94	ASN
1	D2	272	GLN
1	D2	360	GLN
1	D2	379	HIS
1	D2	407	ASN
1	D2	435	GLN
1	D2	462	GLN
1	D3	94	ASN
1	D3	166	GLN
1	D3	194	GLN
1	D3	272	GLN
1	D3	361	ASN
1	D3	407	ASN
1	D3	462	GLN
1	D4	194	GLN
1	D4	272	GLN
1	D4	379	HIS
1	D4	407	ASN
1	D4	462	GLN
1	D5	94	ASN

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Mol	Chain	Res	Type
1	D5	321	HIS
1	D5	360	GLN
1	D5	407	ASN
1	D5	462	GLN
1	D5	465	HIS
1	D6	166	GLN
1	D6	193	ASN
1	D6	272	GLN
1	D6	330	ASN
1	D6	361	ASN
1	D6	379	HIS
1	D6	407	ASN
1	D6	462	GLN
2	A1	15	ASN
2	A1	238	GLN
2	A1	241	HIS
2	A2	242	GLN
2	A3	15	ASN
2	A3	214	HIS
2	A3	238	GLN
2	A4	15	ASN
2	A4	64	HIS
2	A4	241	HIS
2	A4	298	ASN
2	A4	302	GLN
2	A4	505	HIS
2	A4	528	HIS
2	A4	564	GLN
2	A4	577	GLN
2	A5	238	GLN
2	A5	241	HIS
2	A6	15	ASN
2	A6	47	HIS
2	A6	224	HIS
2	A6	241	HIS
2	A6	298	ASN
2	A6	505	HIS
2	A6	564	GLN
2	A6	577	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	BTN	A6	701	2	16,16,17	0.51	0	21,21,23	1.31	3 (14%)
3	BTN	A4	701	-	16,16,17	0.51	0	21,21,23	1.20	3 (14%)
3	BTN	A1	701	2	16,16,17	0.53	0	21,21,23	1.28	3 (14%)
3	BTN	A2	701	-	16,16,17	0.54	0	21,21,23	1.26	2 (9%)
3	BTN	A5	701	2	16,16,17	0.52	0	21,21,23	1.30	3 (14%)
3	BTN	A3	701	2	16,16,17	0.53	0	21,21,23	1.13	2 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BTN	A6	701	2	-	0/5/27/28	0/2/2/2
3	BTN	A4	701	-	-	0/5/27/28	0/2/2/2
3	BTN	A1	701	2	-	0/5/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BTN	A2	701	-	-	4/5/27/28	0/2/2/2
3	BTN	A5	701	2	-	0/5/27/28	0/2/2/2
3	BTN	A3	701	2	-	4/5/27/28	0/2/2/2

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A6	701	BTN	C6-S1-C2	-3.70	82.29	89.89
3	A5	701	BTN	C6-S1-C2	-3.63	82.44	89.89
3	A1	701	BTN	C6-S1-C2	-3.46	82.78	89.89
3	A1	701	BTN	C6-C5-C4	-3.25	105.84	108.66
3	A2	701	BTN	C4-C2-S1	3.20	108.25	105.20
3	A4	701	BTN	C6-S1-C2	-3.13	83.46	89.89
3	A6	701	BTN	C6-C5-C4	-3.12	105.95	108.66
3	A5	701	BTN	C6-C5-C4	-3.09	105.98	108.66
3	A4	701	BTN	C6-C5-C4	-3.05	106.01	108.66
3	A2	701	BTN	C6-C5-C4	-2.99	106.06	108.66
3	A6	701	BTN	C2-C4-C5	-2.71	105.79	108.94
3	A5	701	BTN	C2-C4-C5	-2.66	105.86	108.94
3	A3	701	BTN	C4-C2-S1	2.52	107.61	105.20
3	A3	701	BTN	C6-C5-C4	-2.38	106.59	108.66
3	A1	701	BTN	C2-C4-C5	-2.29	106.28	108.94
3	A4	701	BTN	C2-C4-C5	-2.03	106.58	108.94

There are no chirality outliers.

All (8) torsion outliers are listed below:

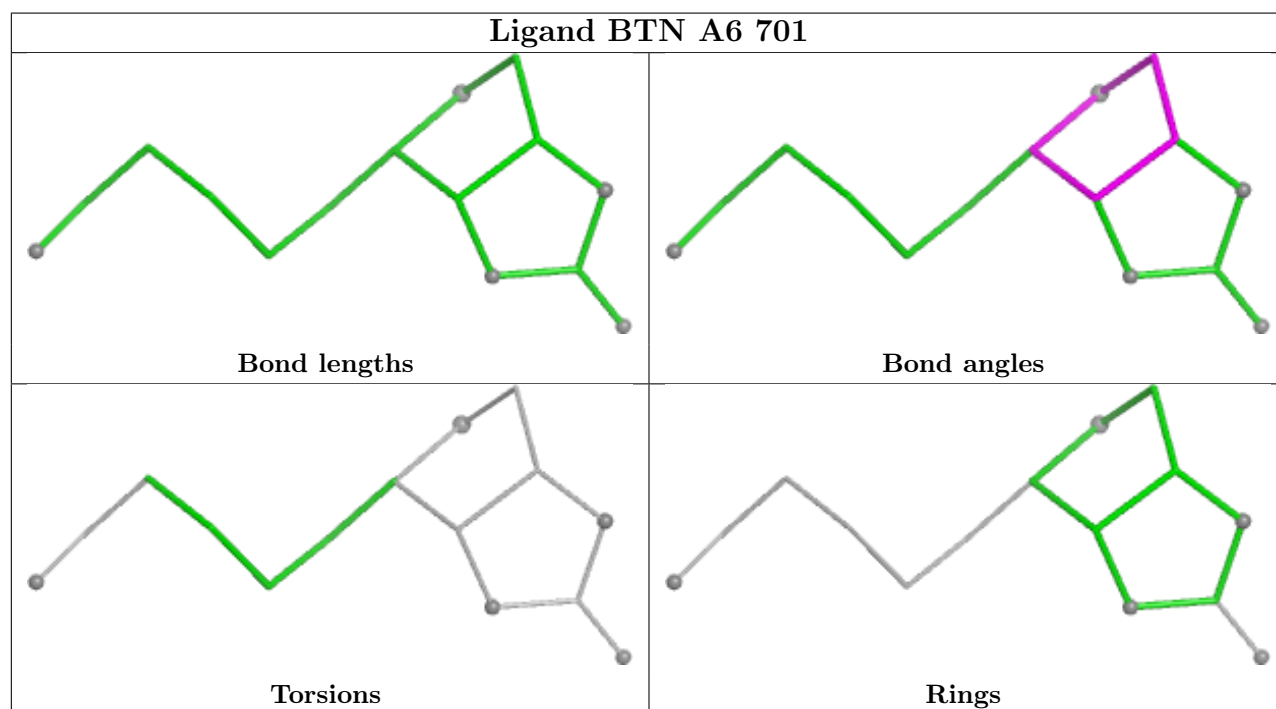
Mol	Chain	Res	Type	Atoms
3	A2	701	BTN	S1-C2-C7-C8
3	A2	701	BTN	C4-C2-C7-C8
3	A3	701	BTN	C2-C7-C8-C9
3	A3	701	BTN	S1-C2-C7-C8
3	A3	701	BTN	C4-C2-C7-C8
3	A2	701	BTN	C7-C8-C9-C10
3	A3	701	BTN	C7-C8-C9-C10
3	A2	701	BTN	C2-C7-C8-C9

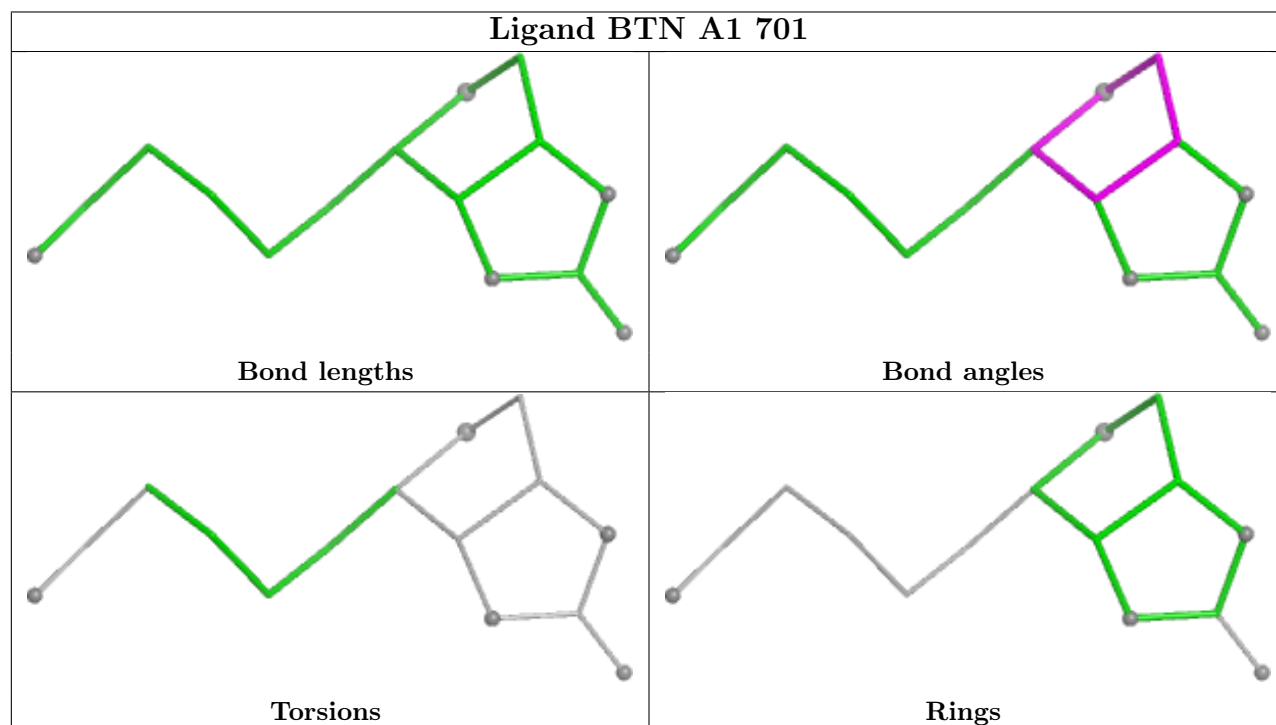
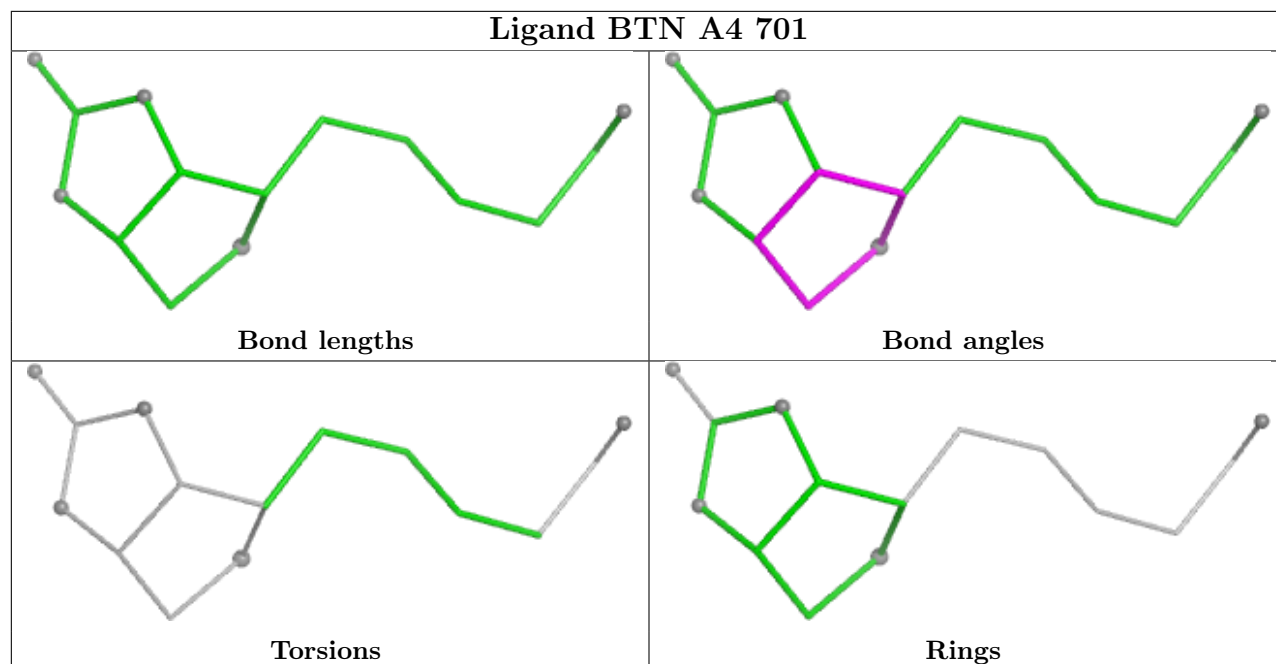
There are no ring outliers.

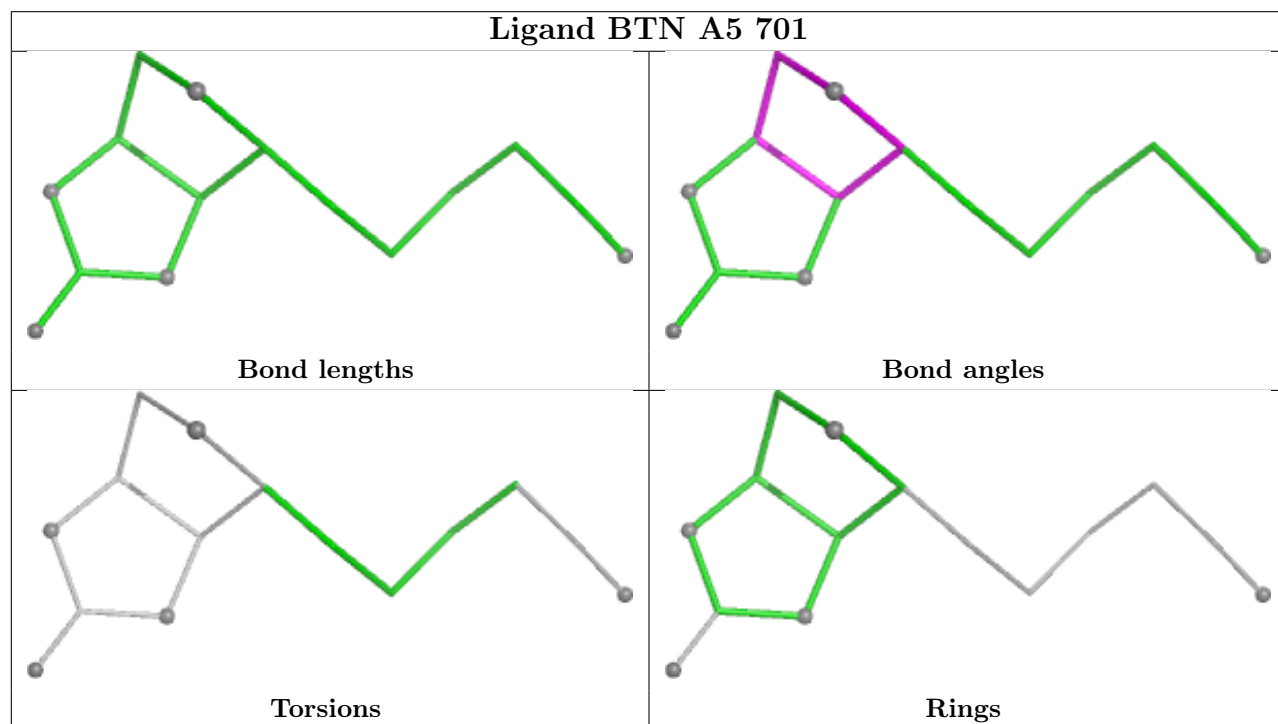
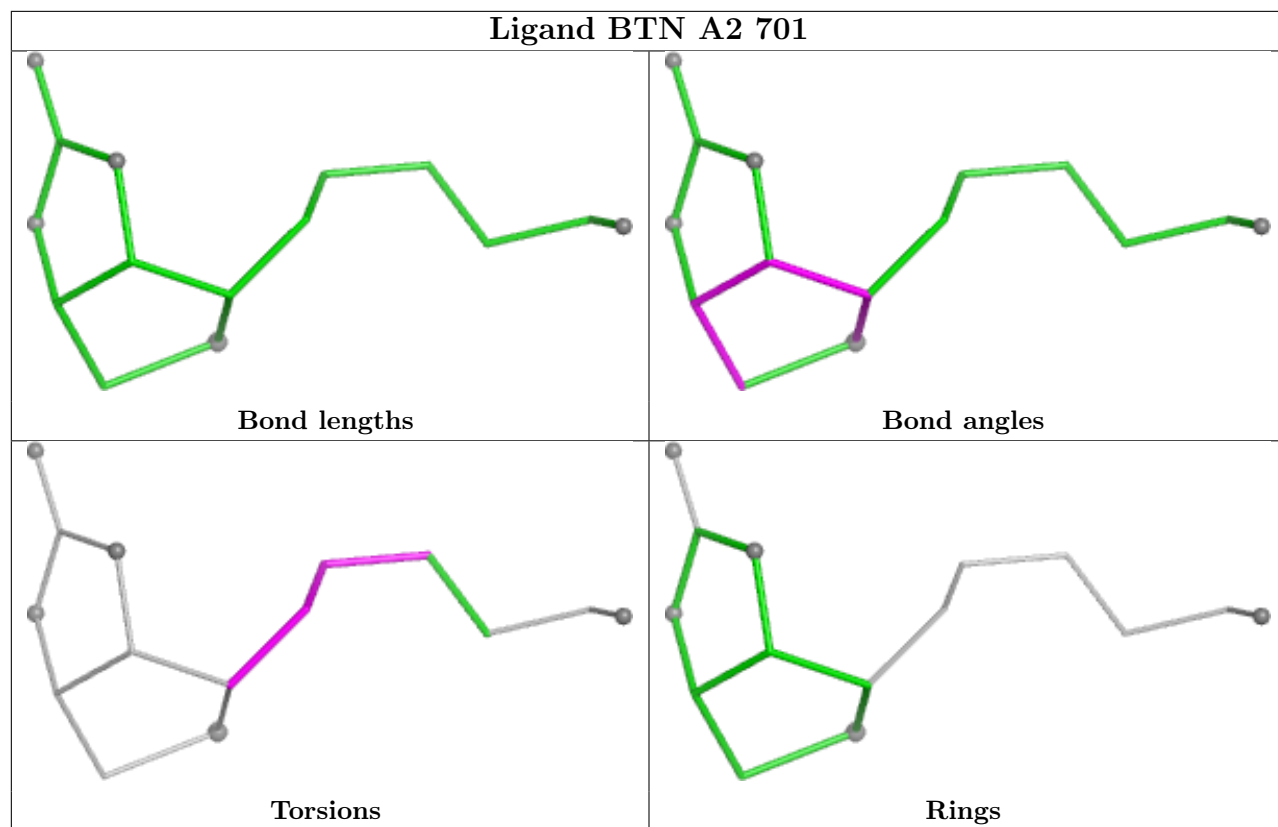
6 monomers are involved in 28 short contacts:

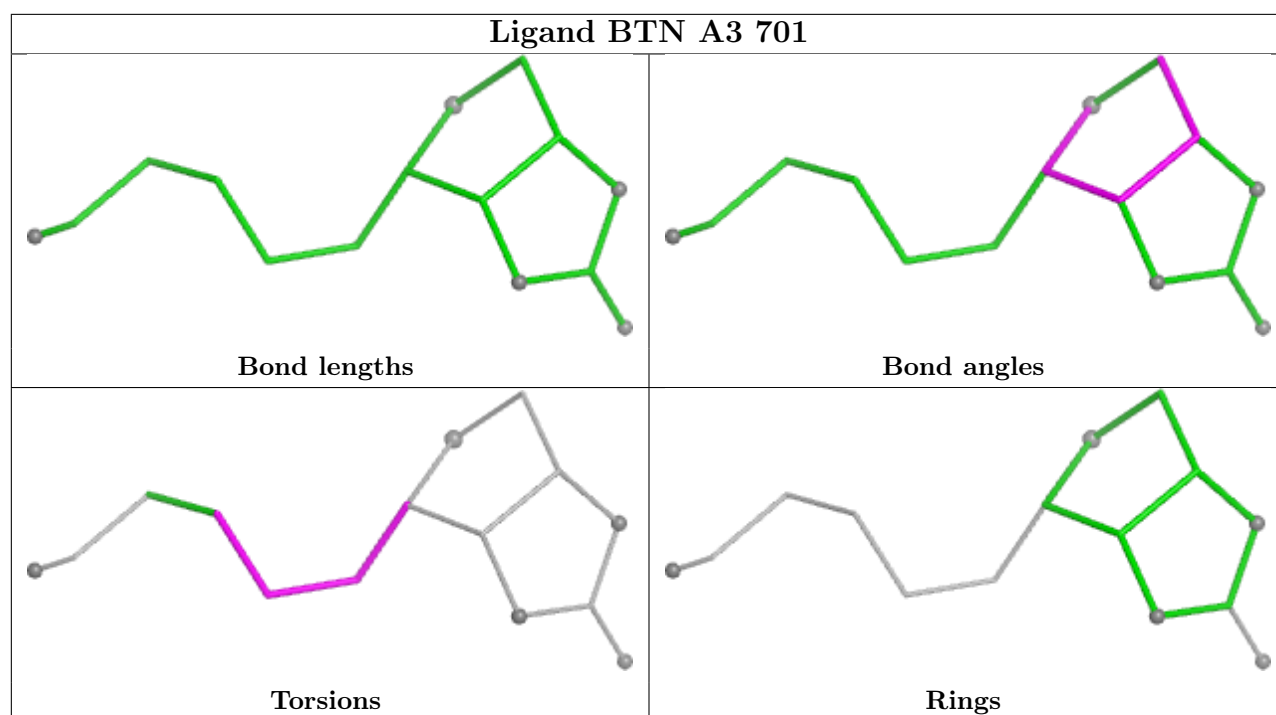
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A6	701	BTN	1	0
3	A4	701	BTN	4	0
3	A1	701	BTN	3	0
3	A2	701	BTN	16	0
3	A5	701	BTN	1	0
3	A3	701	BTN	3	0

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.

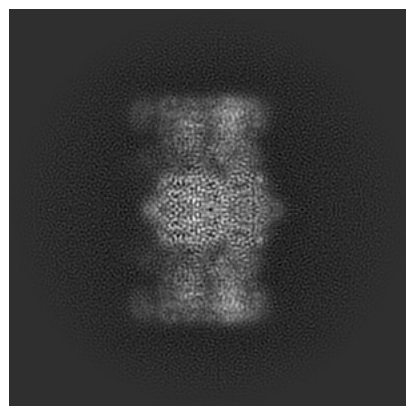
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57132. These allow visual inspection of the internal detail of the map and identification of artifacts.

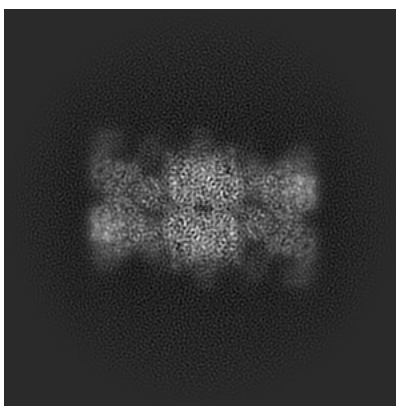
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

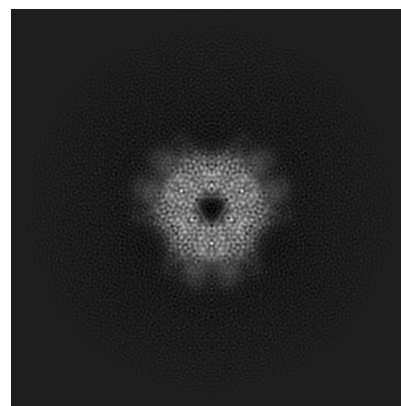
6.1.1 Primary map



X

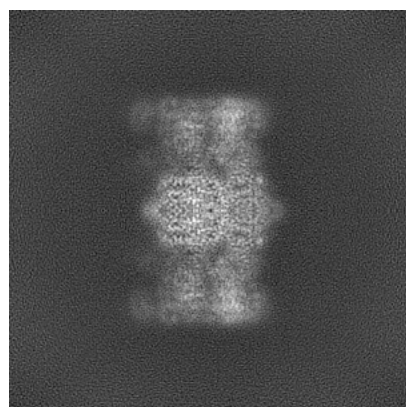


Y

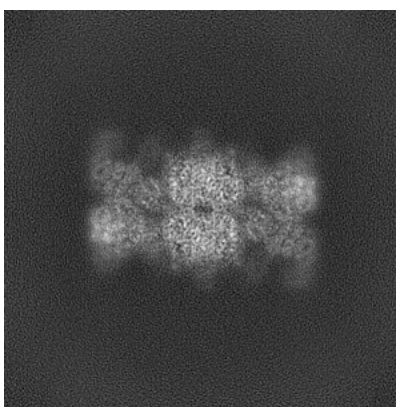


Z

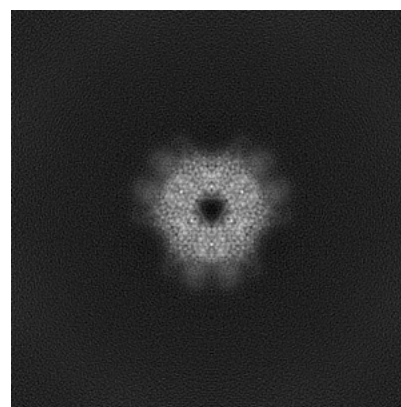
6.1.2 Raw map



X



Y

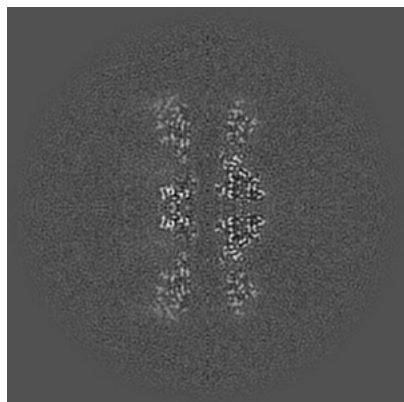


Z

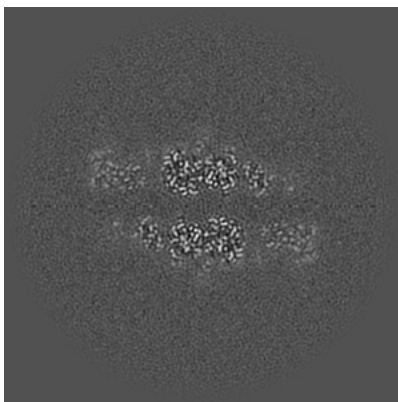
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

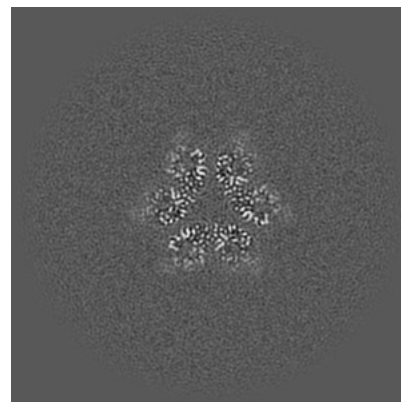
6.2.1 Primary map



X Index: 150

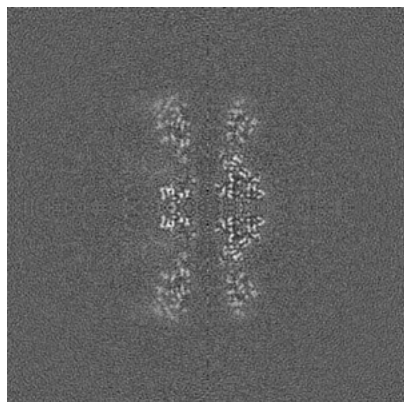


Y Index: 150

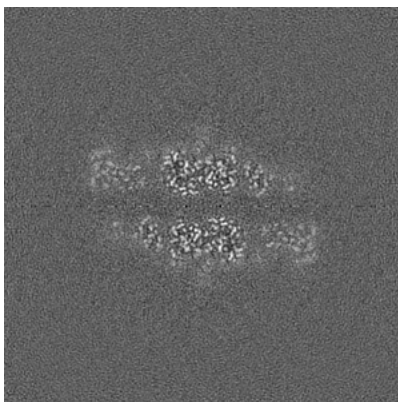


Z Index: 150

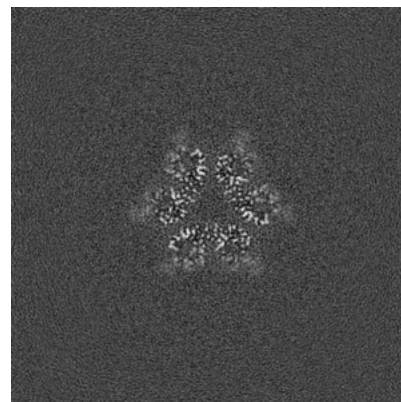
6.2.2 Raw map



X Index: 150



Y Index: 150

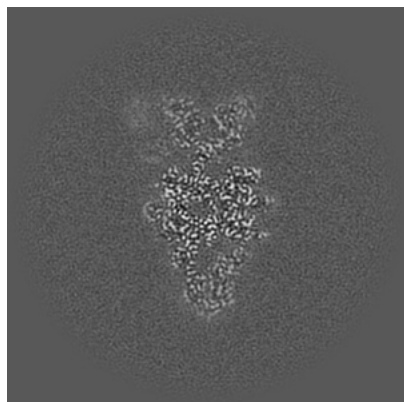


Z Index: 150

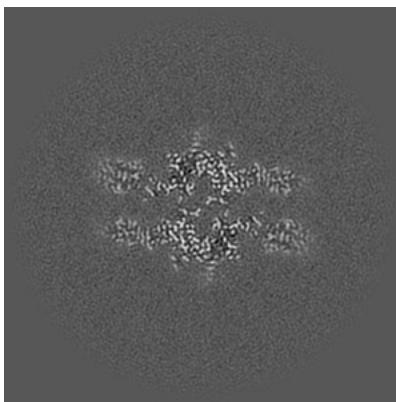
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

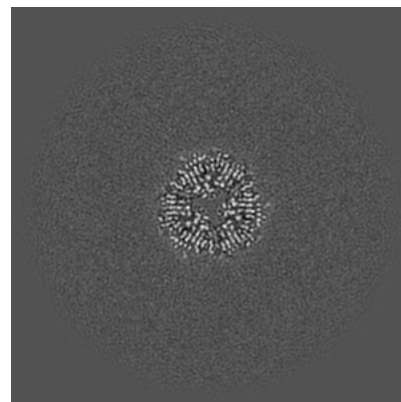
6.3.1 Primary map



X Index: 166

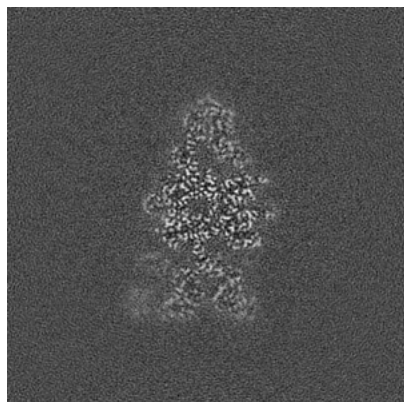


Y Index: 141

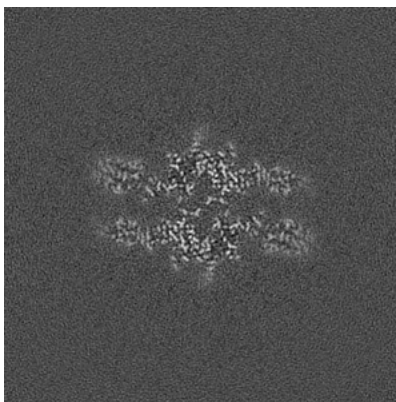


Z Index: 135

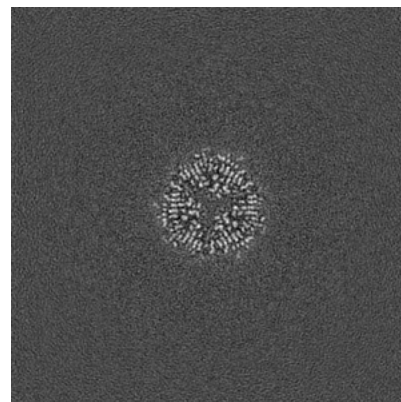
6.3.2 Raw map



X Index: 134



Y Index: 141

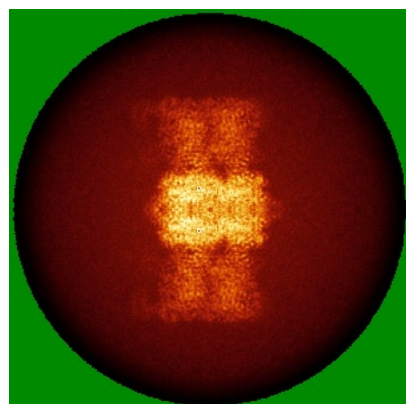


Z Index: 163

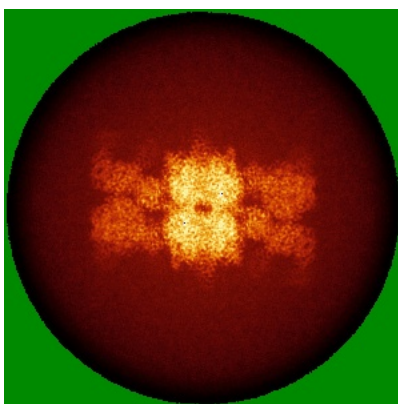
The images above show the largest variance slices of the map in three orthogonal directions.

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

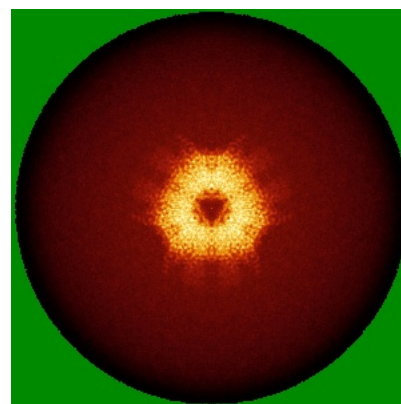
6.4.1 Primary map



X

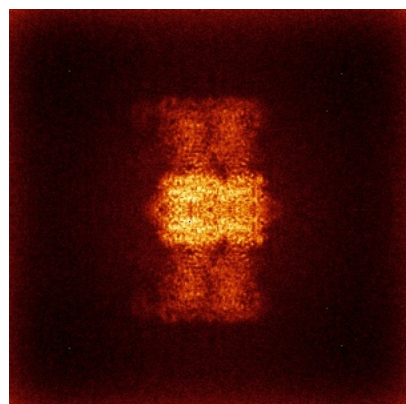


Y

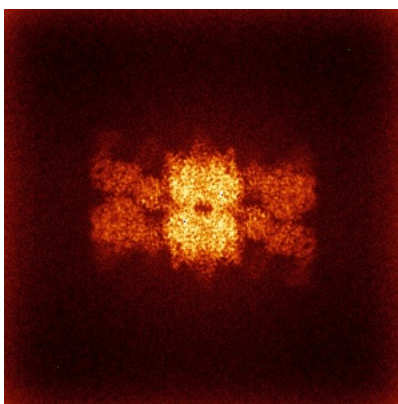


Z

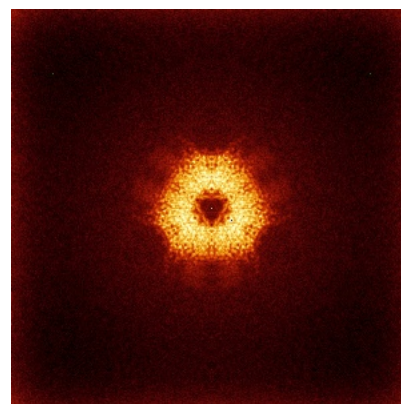
6.4.2 Raw map



X



Y

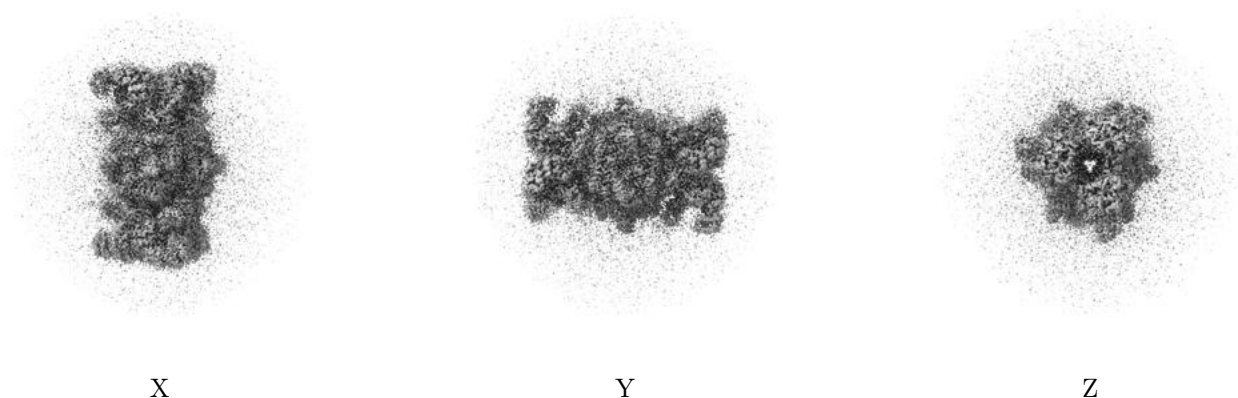


Z

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.

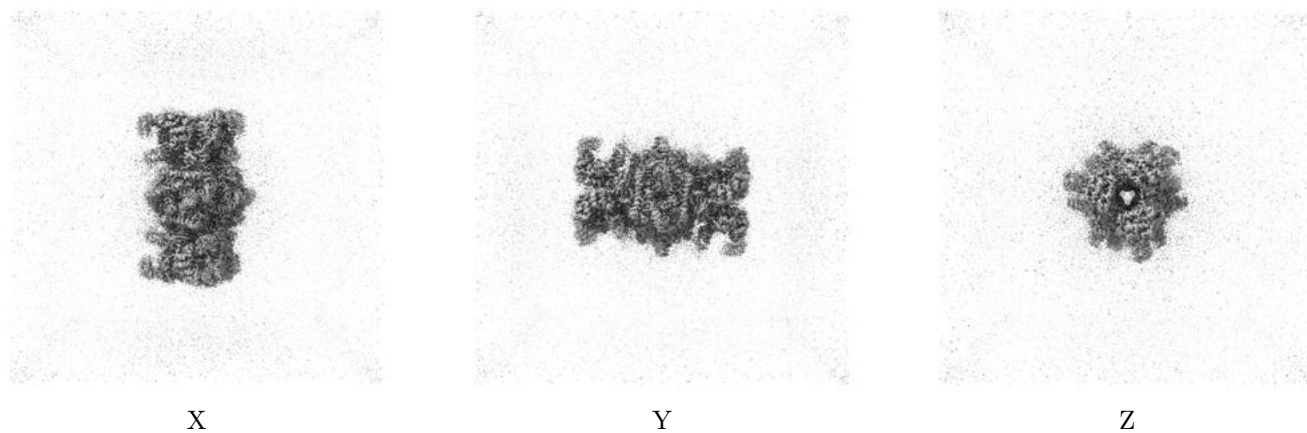
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.144. 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.

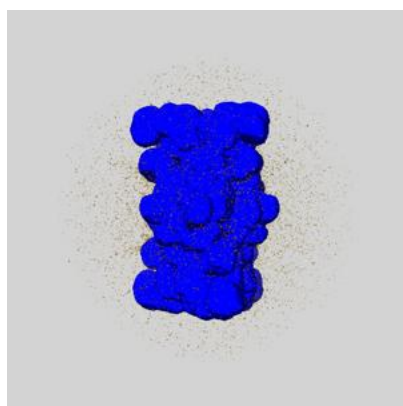
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

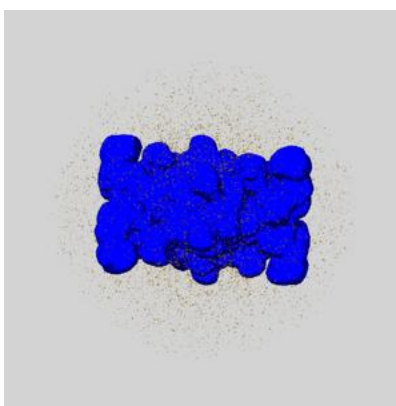
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

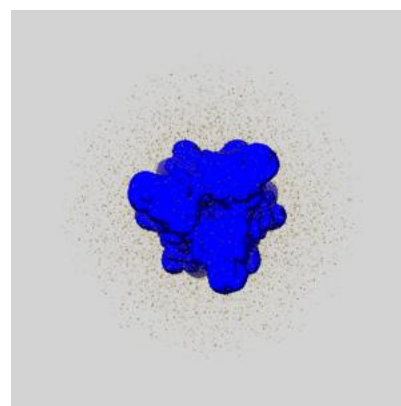
6.6.1 emd_57132_msk_1.map [i](#)



X



Y

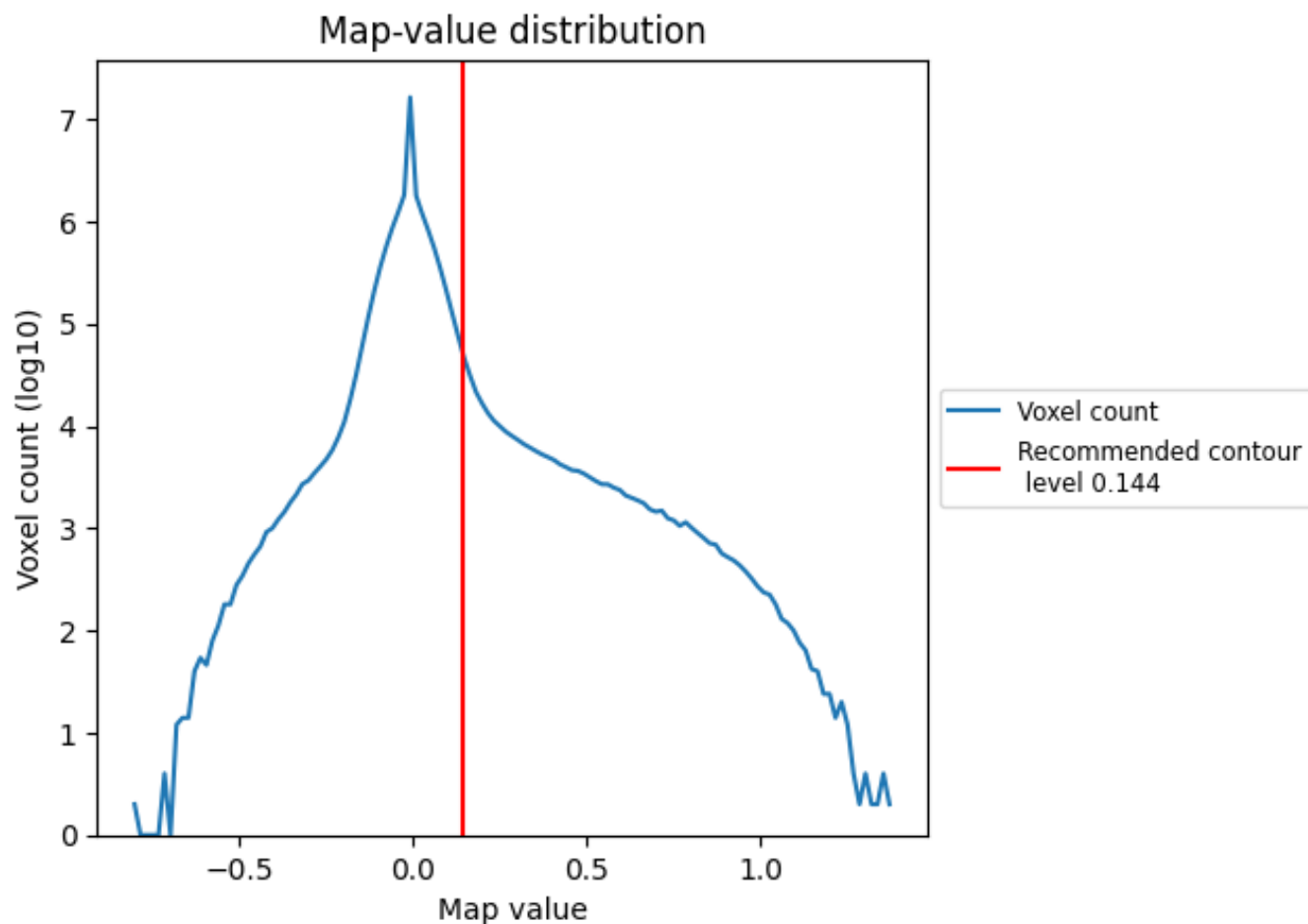


Z

7 Map analysis [i](#)

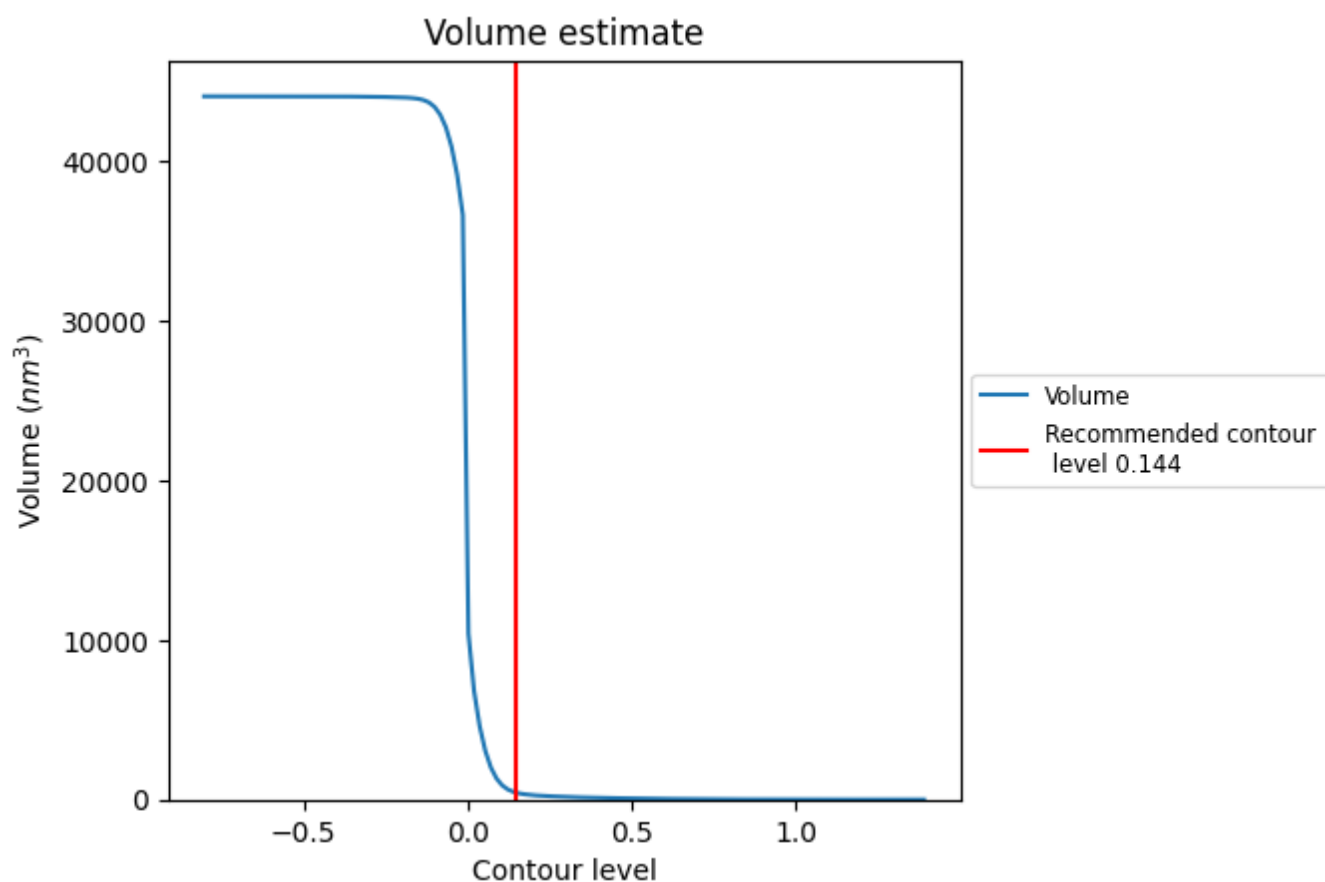
This section contains the results of statistical analysis of the map.

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.

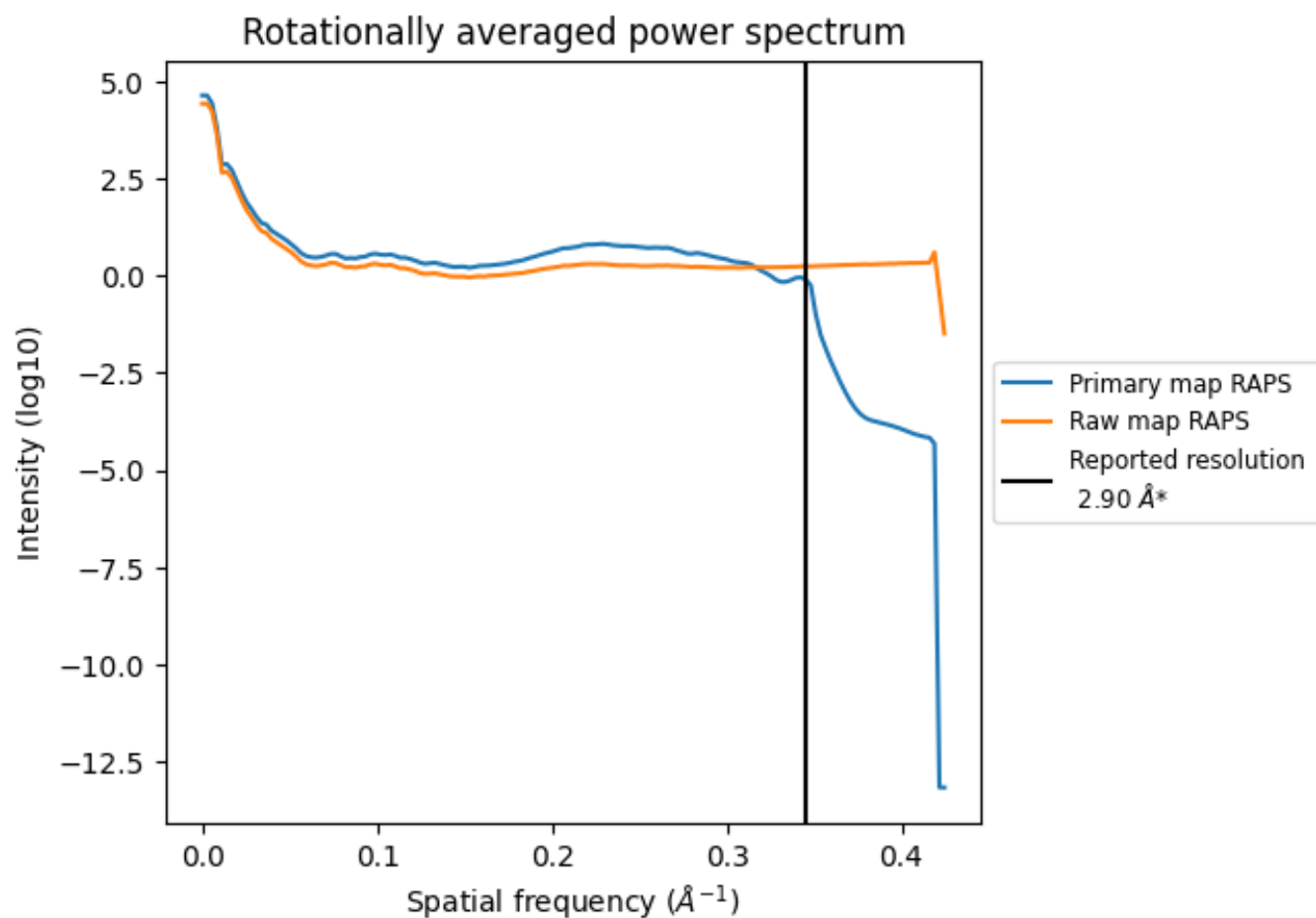
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 456 nm³; this corresponds to an approximate mass of 412 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 ⓘ

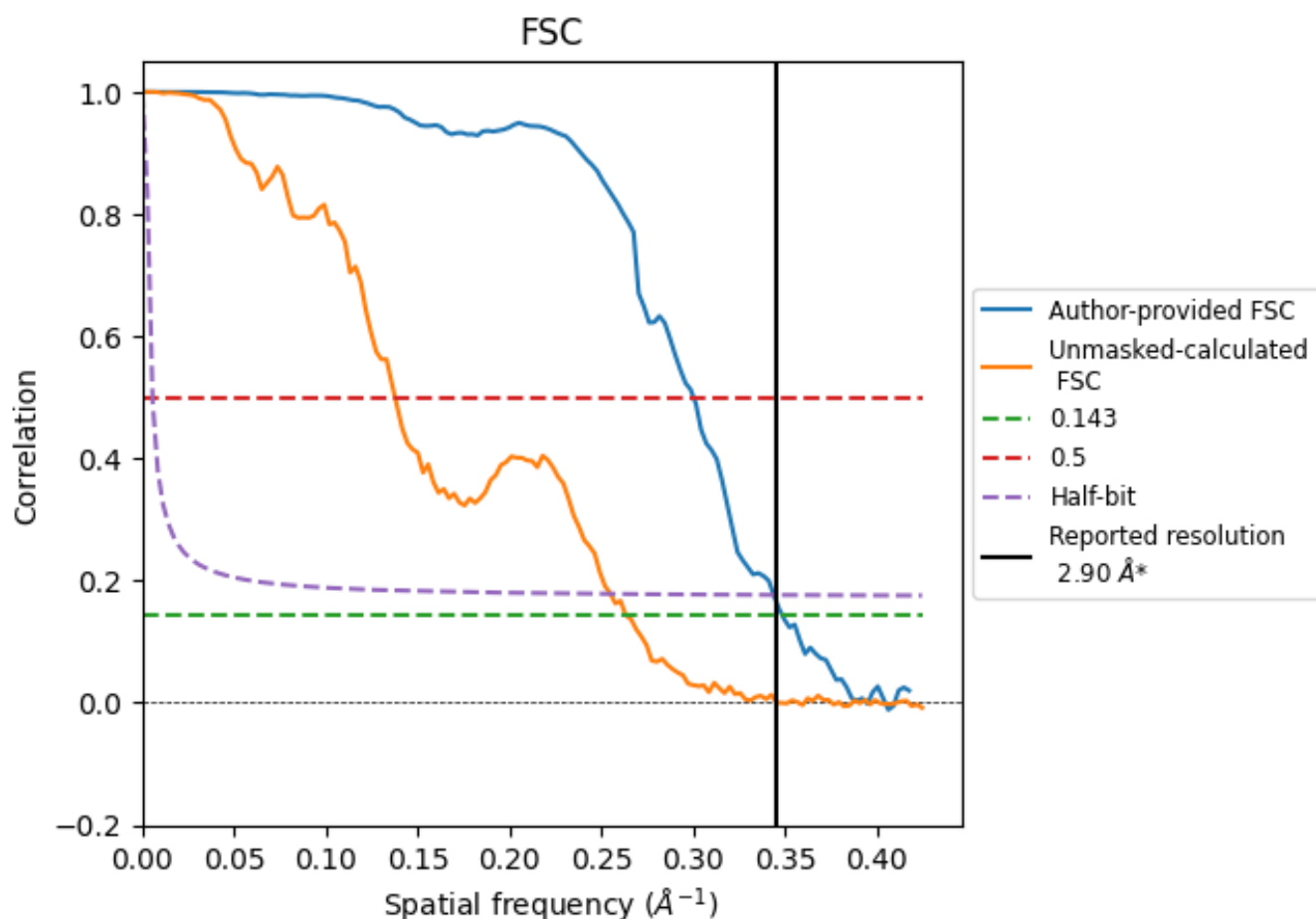


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

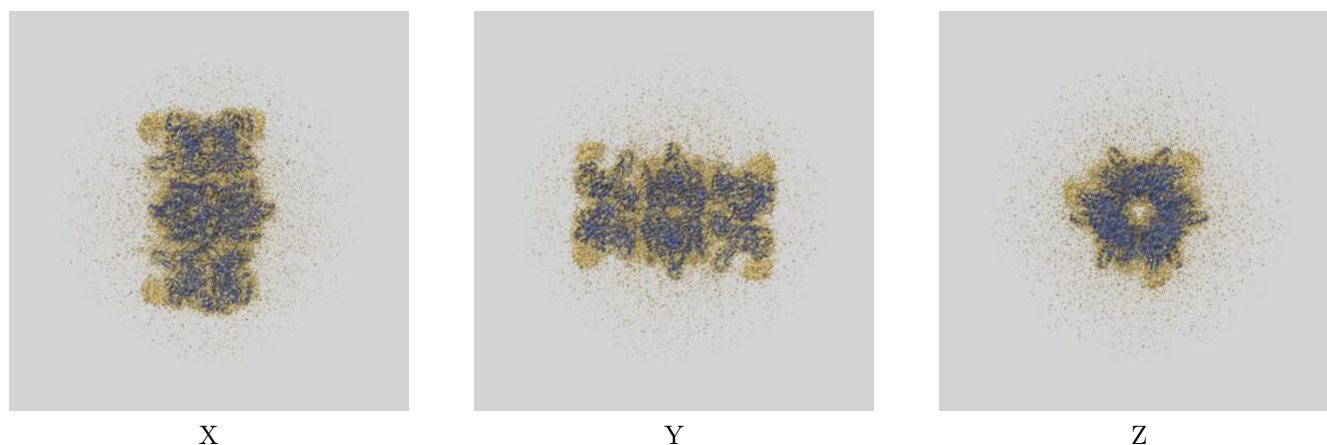
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.87	3.33	2.91
Unmasked-calculated*	3.80	7.27	3.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.80 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

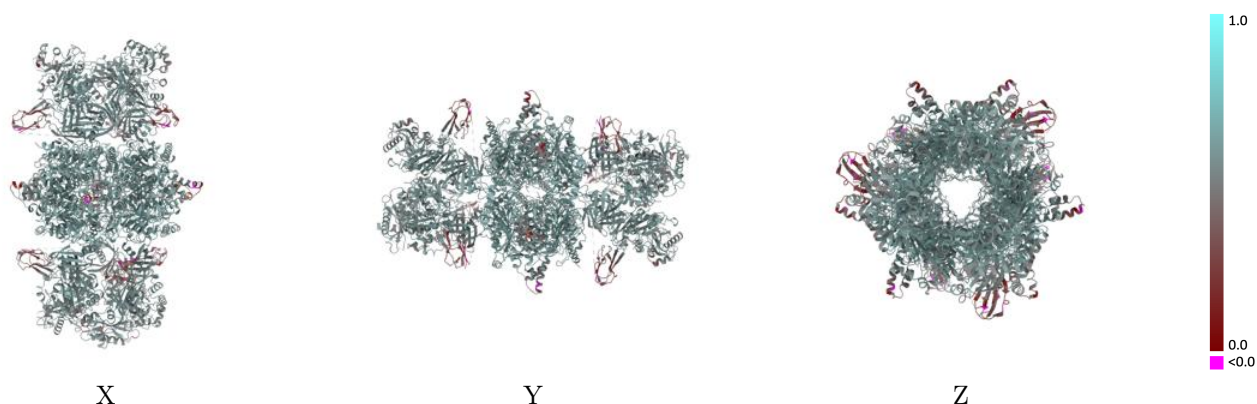
This section contains information regarding the fit between EMDB map EMD-57132 and PDB model 29EX. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



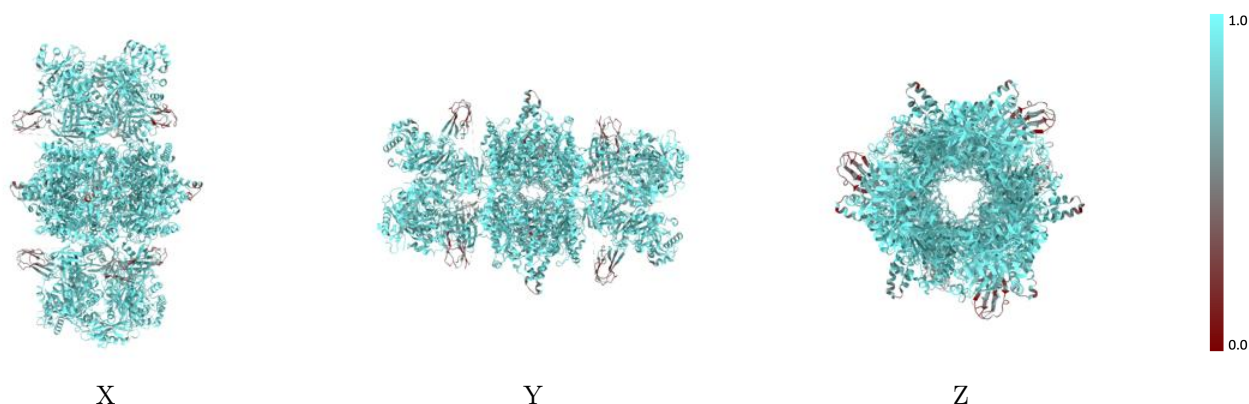
The images above show the 3D surface view of the map at the recommended contour level 0.144 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



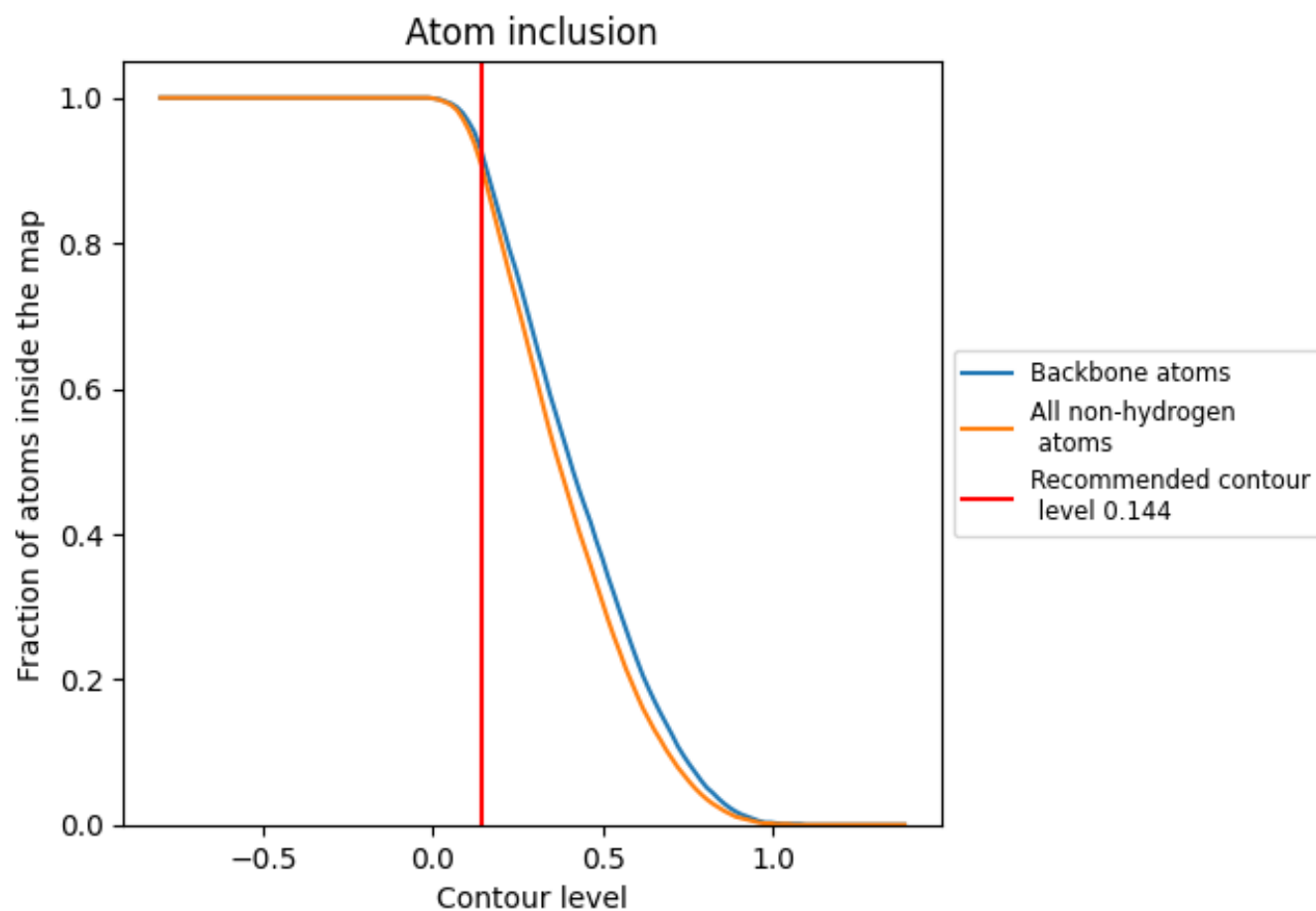
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.144).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 90% 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 (0.144) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9050	0.5640
A1	0.8590	0.5340
A2	0.8570	0.5310
A3	0.8560	0.5320
A4	0.8580	0.5310
A5	0.8600	0.5330
A6	0.8580	0.5330
D1	0.9570	0.5980
D2	0.9610	0.6000
D3	0.9570	0.5980
D4	0.9580	0.5970
D5	0.9540	0.5980
D6	0.9550	0.5980

1.0

0.0

<0.0