



Full wwPDB EM Validation Report ⓘ

Apr 29, 2026 – 01:19 am BST

PDB ID : 29HH / pdb_000029hh
EMDB ID : EMD-57179
Title : Cryo-EM structure of the CUL1-RBX1-SKP1-FBXO22 SCF ubiquitination ligase in complex with NSD2, UNC10088 and Bach1
Authors : Amann, S.J.; Robertson, K.C.; Grishkovskaya, I.; Liu, T.; James, L.I.; Brown, N.B.; Haselbach, D.
Deposited on : 2026-03-11
Resolution : 4.20 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.dev132
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) : 2.49

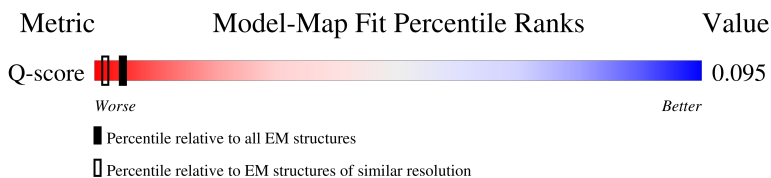
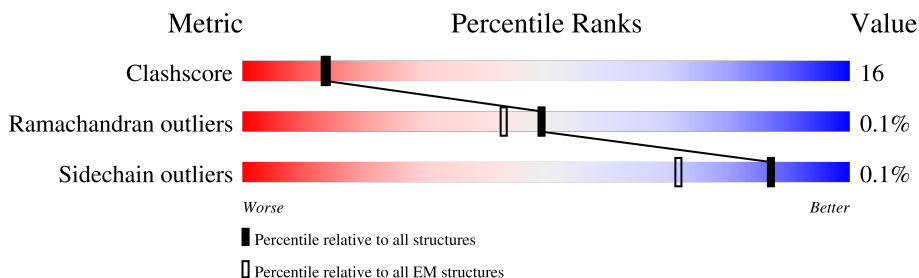
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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.



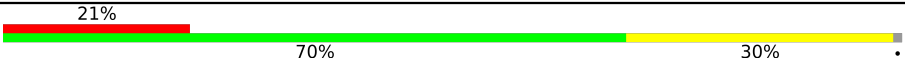
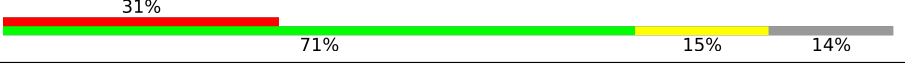
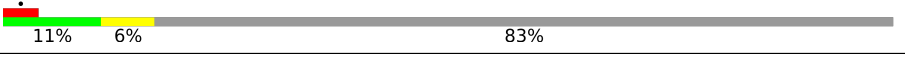
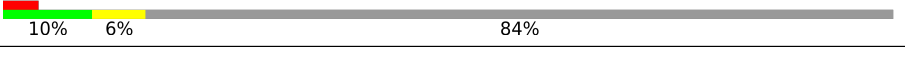
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	403	<div> <div>22%</div> <div>59%</div> <div>34%</div> <div>7%</div> </div>
2	B	1365	<div> <div>5%</div> <div>7%</div> <div>90%</div> </div>
3	C	163	<div> <div>9%</div> <div>66%</div> <div>33%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	776	
5	E	108	
6	G	736	
6	H	736	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 14314 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 F-box only protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	376	Total	C	N	O	S	0	0
			2911	1853	504	537	17		

- Molecule 2 is a protein called Histone-lysine N-methyltransferase NSD2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	136	Total	C	N	O	S	0	0
			1084	698	187	194	5		

- Molecule 3 is a protein called S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	163	Total	C	N	O	S	0	0
			1308	820	211	270	7		

- Molecule 4 is a protein called Cullin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	772	Total	C	N	O	S	0	0
			6274	3969	1081	1195	29		

- Molecule 5 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	93	Total	C	N	O	S	0	0
			759	479	140	131	9		

- Molecule 6 is a protein called Transcription regulator protein BACH1.

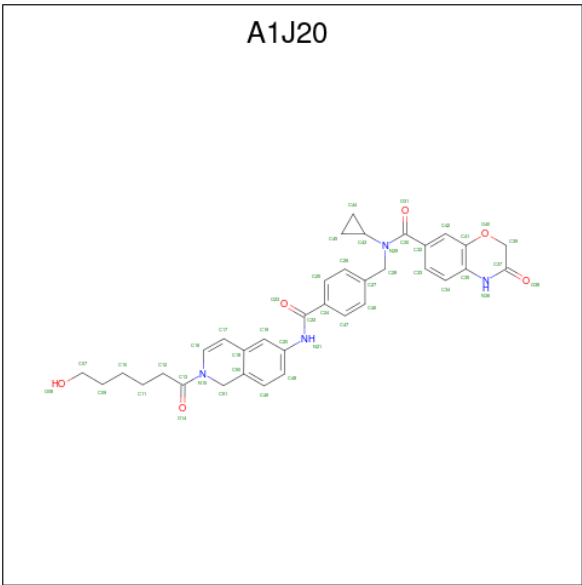
Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	122	Total	C	N	O	S	0	0
			972	621	162	184	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	121	961	612	161	183	5	0	0

- Molecule 7 is {N}-cyclopropyl- {N}-[[4-[[2-(6-oxidanylhexanoyl)-1 {H}-isoquinolin-6-yl]carbamoyl]phenyl]methyl]-3-oxidanylidene-4 {H}-1,4-benzoxazine-7-carboxamide (CCD ID: A1J20) (formula: C₃₅H₃₆N₄O₆) (labeled as "Ligand of Interest" by depositor).

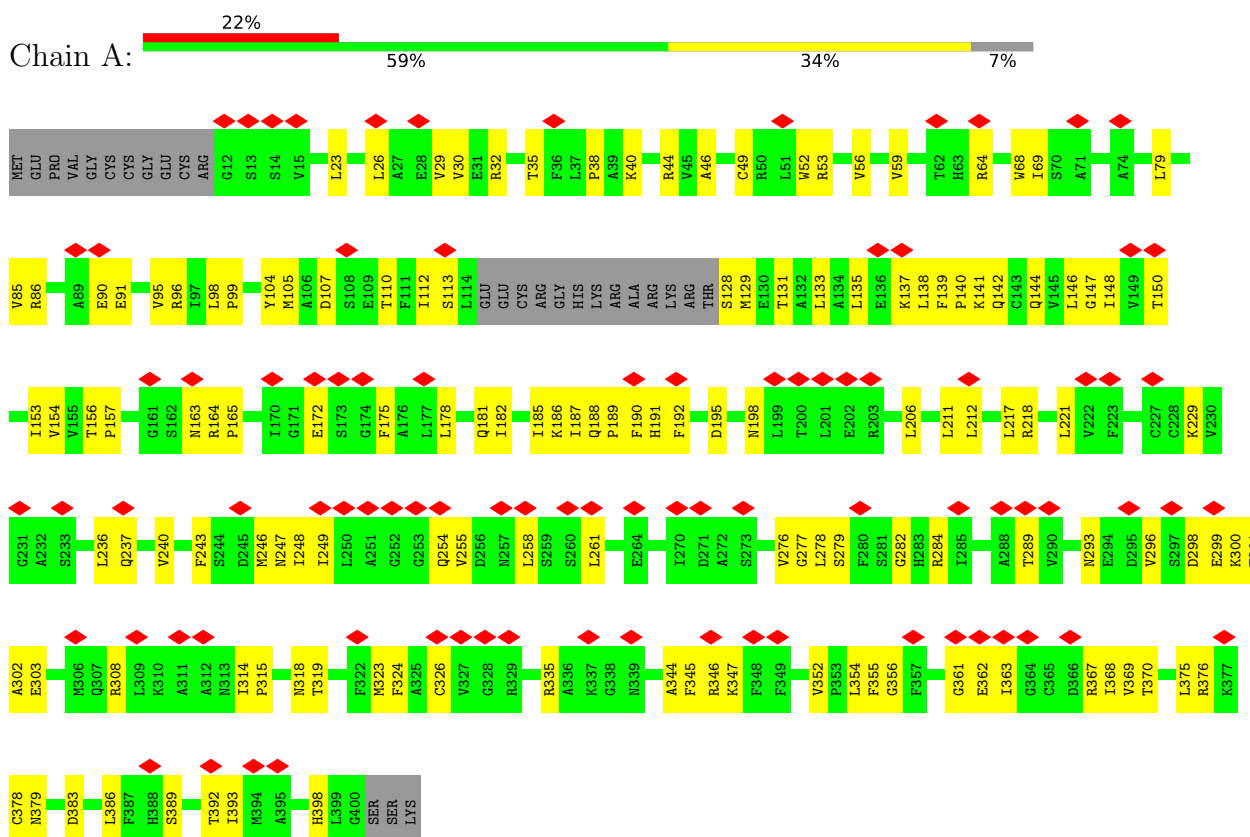


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	A	1	45	35	4	6	0

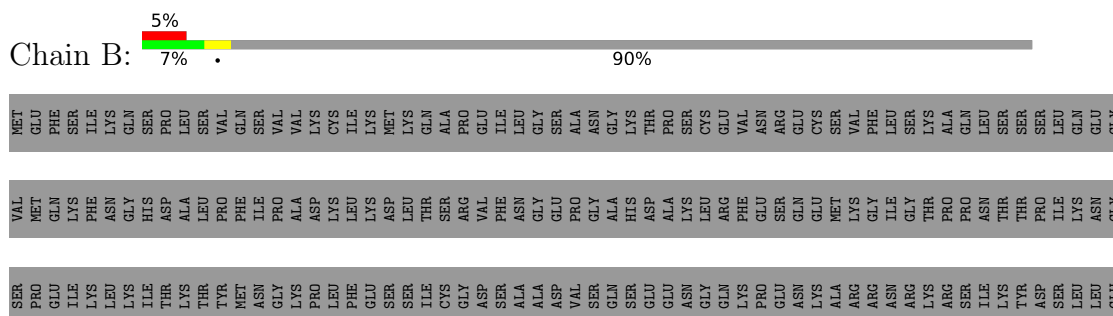
3 Residue-property plots

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

• Molecule 1: F-box only protein 22

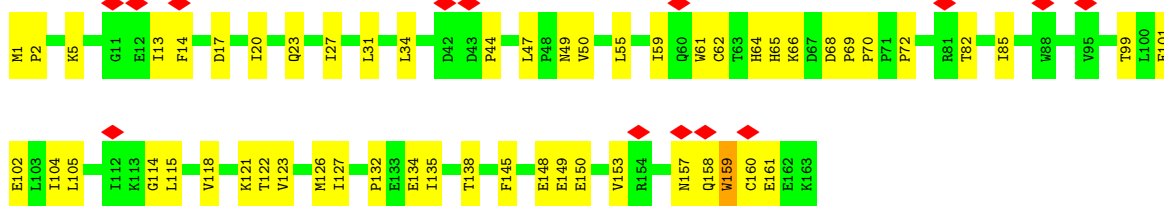


• Molecule 2: Histone-lysine N-methyltransferase NSD2

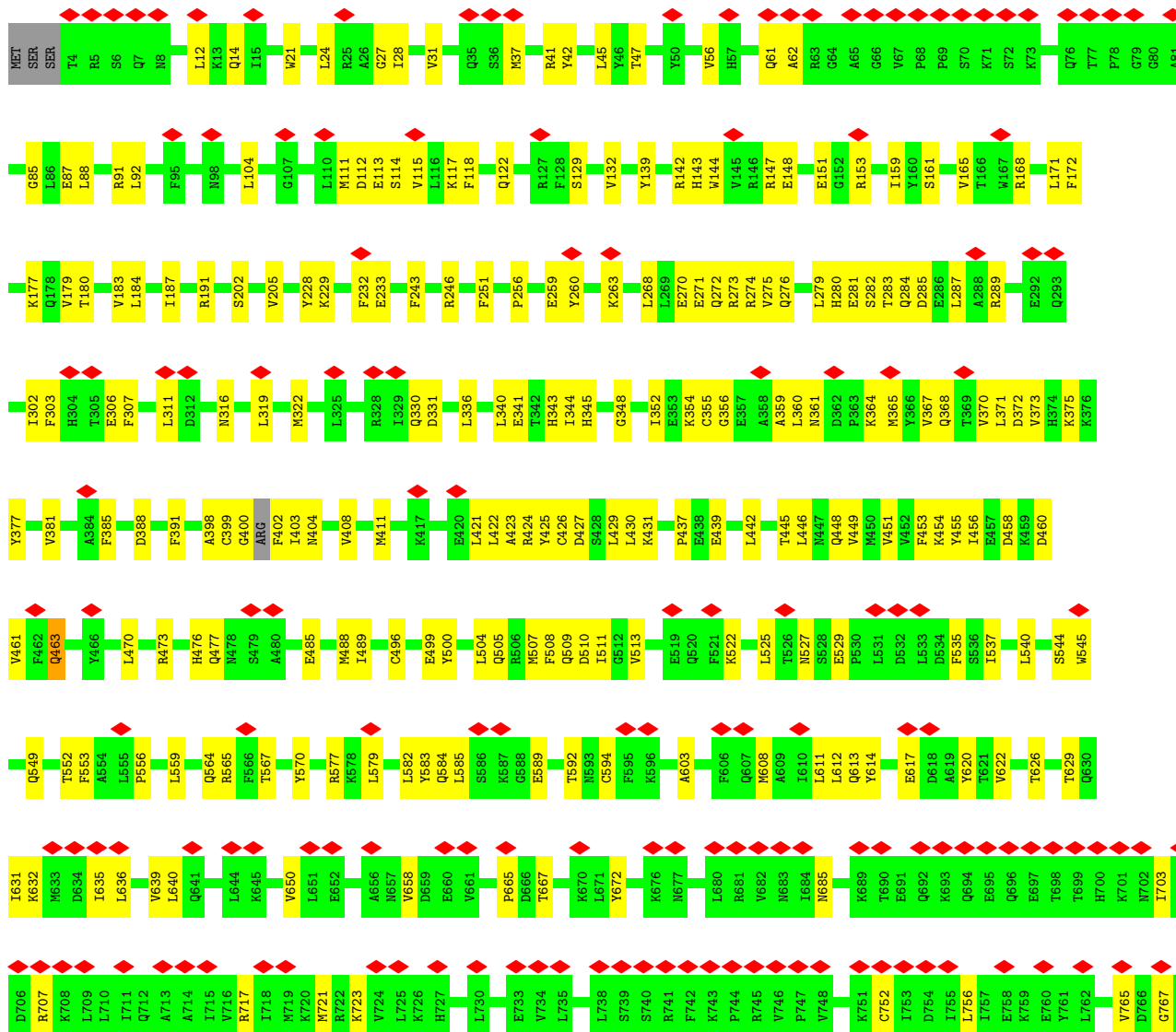


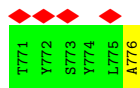


- Molecule 3: S-phase kinase-associated protein 1

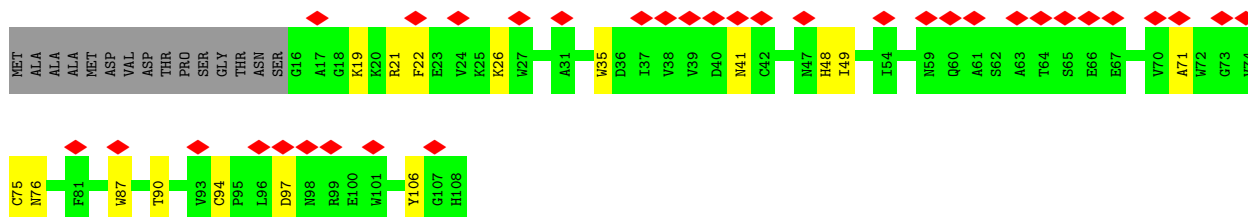


- Molecule 4: Cullin-1

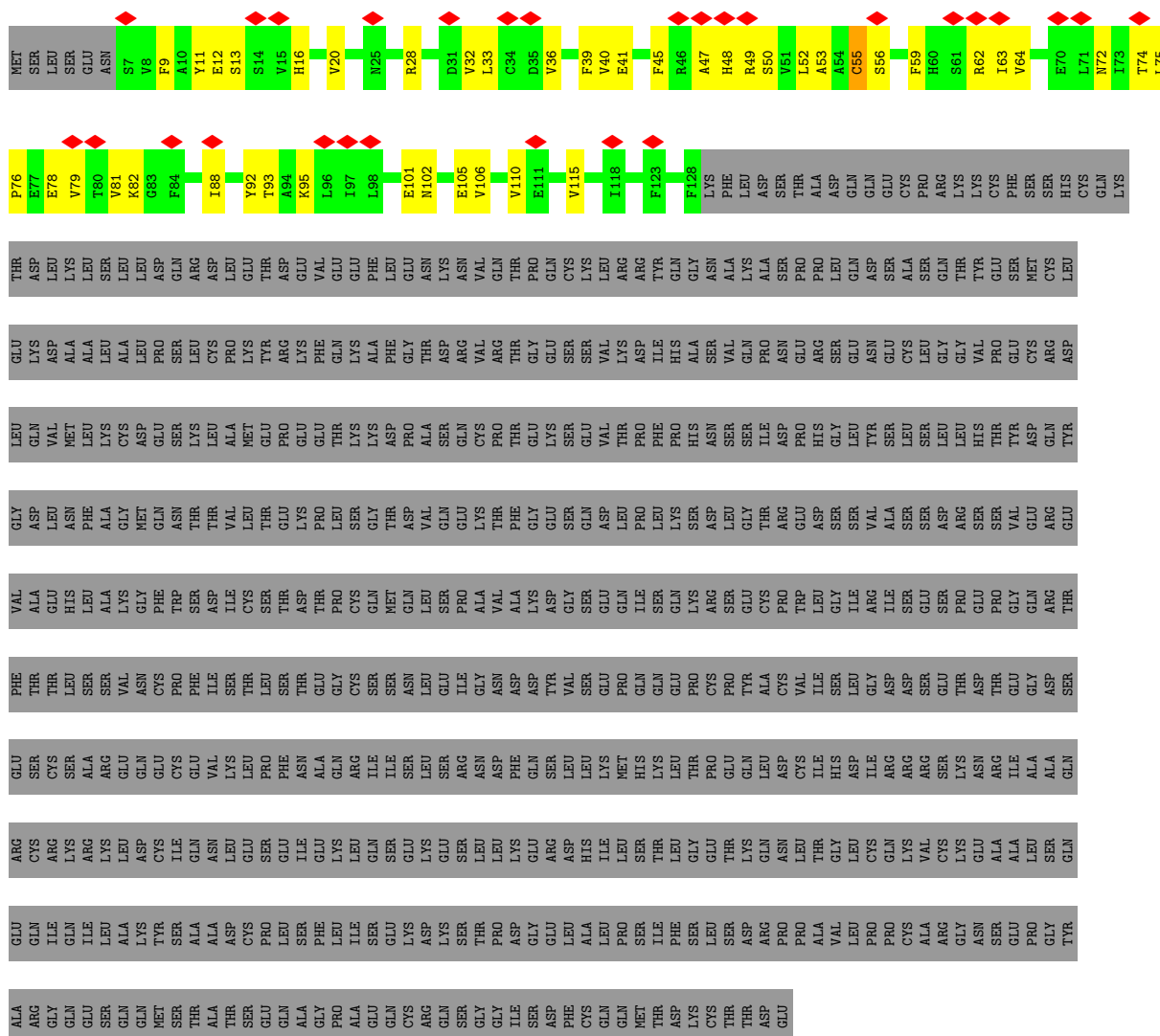




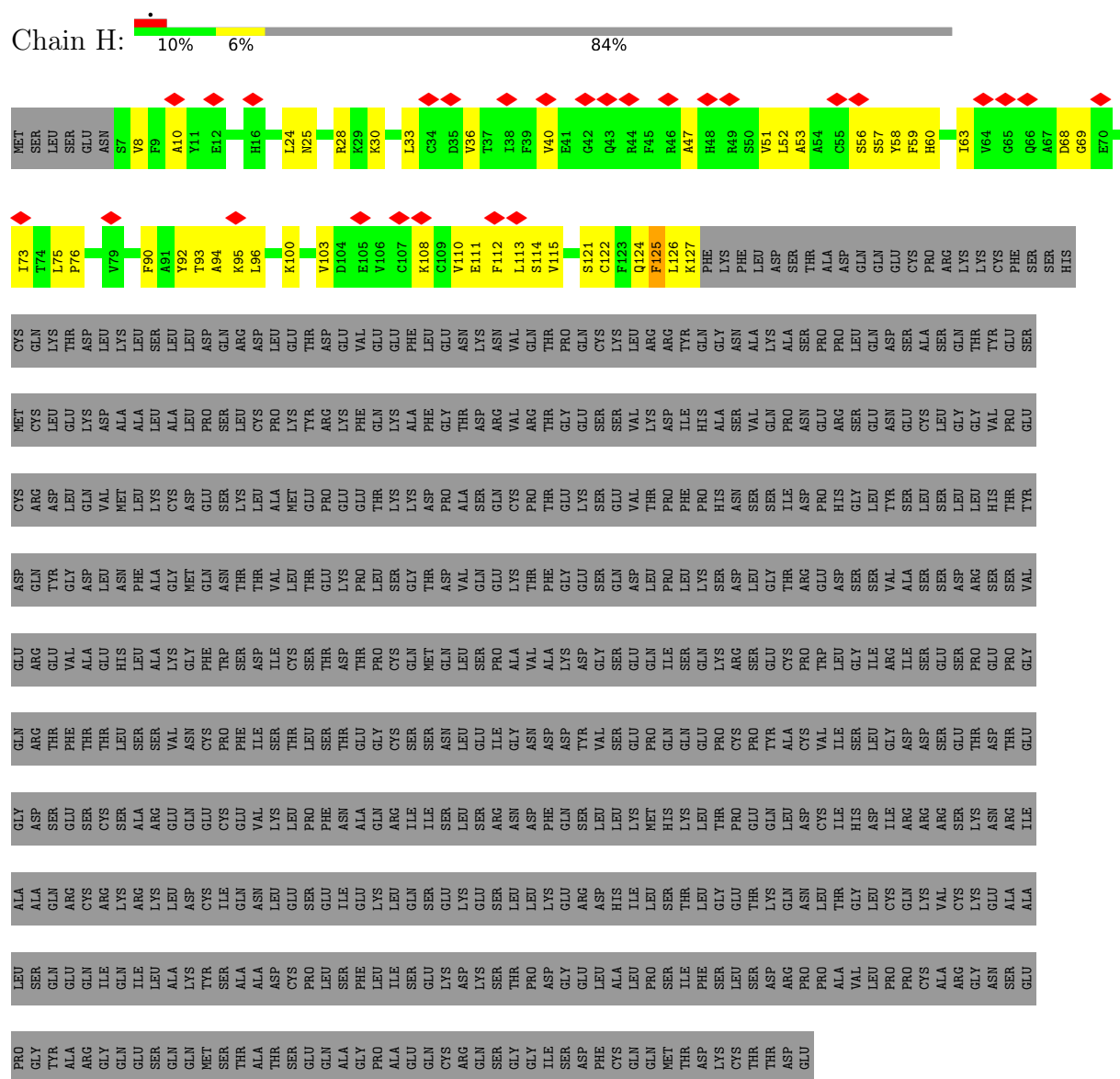
• Molecule 5: E3 ubiquitin-protein ligase RBX1



• Molecule 6: Transcription regulator protein BACH1



● Molecule 6: Transcription regulator protein BACH1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73358	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.733	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	228.23999, 228.23999, 228.23999	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.951, 0.951, 0.951	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1J20

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	0.23	0/2966	0.62	0/4017
2	B	0.20	0/1113	0.52	0/1500
3	C	0.22	0/1331	0.55	1/1801 (0.1%)
4	D	0.23	0/6381	0.55	0/8593
5	E	0.22	0/781	0.59	1/1057 (0.1%)
6	G	0.25	0/990	0.62	0/1337
6	H	0.22	0/978	0.60	0/1321
All	All	0.23	0/14540	0.57	2/19626 (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
4	D	0	1
6	G	0	1
6	H	0	2
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	19	LYS	CB-CA-C	-5.62	110.08	116.54
3	C	159	TRP	N-CA-C	-5.12	107.06	113.15

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	632	LYS	Peptide
6	G	55	CYS	Peptide
6	H	114	SER	Peptide
6	H	125	PHE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2911	0	2929	113	0
2	B	1084	0	1040	43	0
3	C	1308	0	1281	49	0
4	D	6274	0	6305	172	0
5	E	759	0	718	12	0
6	G	972	0	961	42	0
6	H	961	0	952	40	0
7	A	45	0	0	2	0
All	All	14314	0	14186	449	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 16.

All (449) 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)
7:A:501:A1J20:C50	7:A:501:A1J20:C51	1.75	1.61
1:A:229:LYS:CE	2:B:272:GLU:OE1	1.84	1.24
1:A:229:LYS:HE3	2:B:272:GLU:OE1	0.96	1.12
1:A:326:CYS:HB2	1:A:362:GLU:OE2	1.64	0.96
2:B:291:GLU:O	2:B:294:CYS:SG	2.23	0.96
4:D:617:GLU:HB2	4:D:620:TYR:HE1	1.30	0.93
2:B:289:GLN:HG2	2:B:292:LYS:HE2	1.54	0.89
2:B:343:LYS:HG3	2:B:358:GLN:HE21	1.42	0.84
1:A:326:CYS:CB	1:A:362:GLU:OE2	2.25	0.83
1:A:187:ILE:HG22	1:A:278:LEU:HD11	1.60	0.83
2:B:335:MET:HE1	2:B:343:LYS:HD3	1.62	0.81
4:D:614:TYR:HA	4:D:620:TYR:CE2	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:TRP:HB2	1:A:175:PHE:HE2	1.46	0.77
1:A:229:LYS:HE3	2:B:272:GLU:CD	2.07	0.76
4:D:552:THR:HG22	4:D:553:PHE:H	1.50	0.76
4:D:617:GLU:HB2	4:D:620:TYR:CE1	2.18	0.76
4:D:356:GLY:HA2	4:D:359:ALA:HB3	1.67	0.76
1:A:254:GLN:HG2	1:A:361:GLY:HA3	1.68	0.75
4:D:613:GLN:HG3	4:D:629:THR:HG22	1.69	0.74
6:H:52:LEU:O	6:H:56:SER:HB2	1.85	0.74
1:A:379:ASN:HB3	1:A:383:ASP:HA	1.71	0.72
3:C:145:PHE:HE1	3:C:150:GLU:HA	1.54	0.72
2:B:239:MET:HE2	2:B:267:PHE:HZ	1.55	0.72
1:A:323:MET:HE1	1:A:392:THR:HG23	1.72	0.71
3:C:101:PHE:HA	3:C:104:ILE:HG12	1.71	0.71
4:D:104:LEU:HD13	4:D:171:LEU:HA	1.73	0.70
6:H:108:LYS:HA	6:H:111:GLU:HG2	1.73	0.70
2:B:229:LYS:HB3	2:B:280:SER:HB2	1.74	0.70
6:G:63:ILE:HG22	6:G:64:VAL:H	1.56	0.70
4:D:504:LEU:HA	4:D:507:MET:HE3	1.74	0.69
1:A:240:VAL:HA	1:A:243:PHE:CE1	2.28	0.69
1:A:110:THR:HG21	1:A:172:GLU:HG2	1.73	0.69
4:D:272:GLN:HA	4:D:284:GLN:HE22	1.56	0.69
3:C:145:PHE:HD1	3:C:149:GLU:HB2	1.59	0.68
6:G:81:VAL:HG23	6:G:82:LYS:HD2	1.75	0.68
1:A:299:GLU:HA	1:A:302:ALA:HB3	1.75	0.68
2:B:259:ALA:HA	2:B:279:LYS:HZ3	1.59	0.68
1:A:56:VAL:HA	1:A:59:VAL:HG12	1.76	0.67
4:D:275:VAL:HG23	4:D:279:LEU:HD22	1.77	0.67
4:D:270:GLU:O	4:D:273:ARG:HG3	1.95	0.66
4:D:564:GLN:NE2	4:D:565:ARG:HG2	2.11	0.66
6:G:106:VAL:O	6:G:110:VAL:HG23	1.96	0.65
2:B:226:VAL:HB	2:B:281:LEU:HD11	1.78	0.65
2:B:289:GLN:HE22	2:B:293:LEU:HG	1.61	0.65
4:D:582:LEU:HD22	4:D:584:GLN:HE22	1.62	0.65
1:A:38:PRO:HB3	1:A:96:ARG:CZ	2.26	0.65
1:A:206:LEU:HG	1:A:212:LEU:HD11	1.79	0.65
4:D:61:GLN:HG3	4:D:62:ALA:H	1.60	0.65
4:D:24:LEU:O	4:D:28:ILE:HD12	1.96	0.64
1:A:99:PRO:HB3	1:A:178:LEU:HD12	1.80	0.64
1:A:68:TRP:HB2	1:A:175:PHE:CE2	2.31	0.64
6:G:40:VAL:HG12	6:G:41:GLU:OE1	1.97	0.64
6:G:28:ARG:HH22	6:G:47:ALA:HA	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:279:LYS:H	2:B:279:LYS:HD2	1.61	0.63
1:A:367:ARG:HH22	1:A:375:LEU:N	1.96	0.63
4:D:367:VAL:HG11	4:D:425:TYR:CD1	2.33	0.63
4:D:717:ARG:O	4:D:721:MET:HG3	1.99	0.63
6:G:110:VAL:HG13	6:G:115:VAL:HG12	1.81	0.62
1:A:293:ASN:HB3	1:A:296:VAL:HG23	1.80	0.62
1:A:249:ILE:HD11	1:A:369:VAL:H	1.64	0.62
1:A:278:LEU:HD12	1:A:279:SER:H	1.65	0.62
4:D:445:THR:O	4:D:448:GLN:HG3	2.00	0.61
1:A:98:LEU:HD12	1:A:99:PRO:HD2	1.82	0.61
6:G:9:PHE:HD2	6:H:96:LEU:HD12	1.64	0.61
4:D:271:GLU:O	4:D:275:VAL:HG12	2.01	0.61
6:H:60:HIS:HA	6:H:63:ILE:HG12	1.82	0.61
1:A:140:PRO:HD3	3:C:159:TRP:CD2	2.36	0.61
1:A:157:PRO:HG2	1:A:163:ASN:HB3	1.83	0.61
1:A:376:ARG:HG3	6:H:10:ALA:HB3	1.82	0.61
4:D:273:ARG:HD2	4:D:274:ARG:N	2.15	0.61
4:D:549:GLN:NE2	4:D:584:GLN:OE1	2.31	0.61
4:D:364:LYS:NZ	4:D:368:GLN:HB2	2.17	0.60
4:D:570:TYR:CE2	4:D:579:LEU:HD11	2.36	0.60
1:A:229:LYS:CE	2:B:272:GLU:CD	2.72	0.60
4:D:113:GLU:O	4:D:117:LYS:HG3	2.02	0.60
4:D:368:GLN:HA	4:D:371:LEU:HG	1.84	0.60
4:D:205:VAL:HG23	4:D:228:TYR:CE1	2.36	0.60
2:B:345:THR:C	2:B:356:ASN:HD21	2.10	0.60
2:B:289:GLN:NE2	2:B:293:LEU:HG	2.16	0.59
4:D:765:VAL:HG12	4:D:767:GLY:H	1.67	0.59
1:A:128:SER:O	1:A:129:MET:HE2	2.02	0.59
1:A:40:LYS:HE2	3:C:157:ASN:O	2.01	0.59
1:A:363:ILE:HG23	1:A:386:LEU:HD21	1.84	0.59
3:C:114:GLY:O	3:C:118:VAL:HG23	2.03	0.59
3:C:145:PHE:HE1	3:C:150:GLU:CA	2.16	0.59
6:H:30:LYS:O	6:H:30:LYS:HD3	2.02	0.59
1:A:300:LYS:O	1:A:303:GLU:HB3	2.02	0.59
4:D:311:LEU:HB3	4:D:343:HIS:CD2	2.37	0.59
4:D:437:PRO:HG2	4:D:442:LEU:HD21	1.85	0.58
2:B:225:LEU:HB3	2:B:284:PHE:HB3	1.84	0.58
2:B:238:CYS:HB3	2:B:264:VAL:HB	1.85	0.58
4:D:485:GLU:O	4:D:489:ILE:HD12	2.03	0.58
4:D:280:HIS:CE1	4:D:282:SER:H	2.21	0.58
4:D:525:LEU:HA	4:D:529:GLU:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:9:PHE:CD2	6:G:11:TYR:HB2	2.39	0.58
6:G:11:TYR:HE2	6:G:13:SER:HB2	1.69	0.58
3:C:17:ASP:HB3	3:C:20:ILE:HD13	1.85	0.57
4:D:340:LEU:HG	4:D:344:ILE:HD11	1.86	0.57
6:H:122:CYS:HA	6:H:125:PHE:HE1	1.70	0.57
4:D:37:MET:HE1	4:D:45:LEU:HD12	1.86	0.57
1:A:319:THR:HG23	1:A:352:VAL:HG23	1.85	0.57
1:A:323:MET:HB3	1:A:356:GLY:HA3	1.87	0.57
4:D:388:ASP:HB3	4:D:391:PHE:HD2	1.69	0.57
4:D:507:MET:HB3	4:D:545:TRP:CZ2	2.39	0.57
4:D:148:GLU:HG3	4:D:153:ARG:HH11	1.69	0.56
4:D:183:VAL:HG11	4:D:232:PHE:HE1	1.70	0.56
4:D:614:TYR:HA	4:D:620:TYR:HE2	1.67	0.56
4:D:355:CYS:HB3	4:D:365:MET:HE2	1.87	0.56
1:A:206:LEU:HD11	1:A:243:PHE:HB3	1.88	0.56
4:D:559:LEU:HD23	4:D:583:TYR:CZ	2.41	0.56
4:D:522:LYS:HA	4:D:525:LEU:HG	1.87	0.56
4:D:143:HIS:O	4:D:147:ARG:HG2	2.06	0.56
6:G:102:ASN:O	6:G:106:VAL:HG12	2.05	0.56
1:A:140:PRO:HA	3:C:160:CYS:SG	2.46	0.56
4:D:496:CYS:HB2	4:D:500:TYR:HD2	1.71	0.56
1:A:367:ARG:HH12	1:A:375:LEU:C	2.14	0.56
4:D:408:VAL:HA	4:D:411:MET:HE2	1.86	0.56
6:G:50:SER:HB3	6:H:33:LEU:HD12	1.88	0.56
6:G:56:SER:HA	6:G:115:VAL:HG23	1.88	0.56
2:B:259:ALA:HA	2:B:279:LYS:NZ	2.21	0.56
6:H:51:VAL:HG11	6:H:92:TYR:CE1	2.40	0.56
1:A:362:GLU:OE1	1:A:389:SER:HA	2.06	0.55
3:C:70:PRO:HB2	3:C:72:PRO:HD2	1.87	0.55
6:H:28:ARG:HB2	6:H:92:TYR:HE2	1.71	0.55
1:A:49:CYS:HB3	1:A:52:TRP:CD1	2.41	0.55
4:D:446:LEU:HD12	4:D:488:MET:SD	2.46	0.55
2:B:236:TRP:CD2	2:B:237:PRO:HD2	2.41	0.55
6:G:39:PHE:HB2	6:G:72:ASN:OD1	2.05	0.55
6:H:112:PHE:CD2	6:H:113:LEU:HG	2.41	0.55
4:D:458:ASP:CG	4:D:707:ARG:HH22	2.15	0.55
4:D:553:PHE:CB	4:D:631:ILE:HD11	2.37	0.55
4:D:367:VAL:HG11	4:D:425:TYR:CG	2.42	0.54
1:A:144:GLN:HG2	1:A:189:PRO:HG2	1.90	0.54
3:C:61:TRP:CD2	3:C:115:LEU:HD12	2.43	0.54
4:D:553:PHE:HZ	4:D:583:TYR:HB3	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:76:PRO:HG2	6:G:79:VAL:HG22	1.90	0.54
1:A:191:HIS:ND1	1:A:276:VAL:HB	2.23	0.54
4:D:556:PRO:HB3	4:D:612:LEU:HD23	1.89	0.54
6:G:28:ARG:NH2	6:G:47:ALA:HA	2.21	0.54
6:H:122:CYS:HA	6:H:125:PHE:CE1	2.43	0.54
4:D:311:LEU:HB3	4:D:343:HIS:CG	2.43	0.54
6:G:45:PHE:CE2	6:G:47:ALA:HB2	2.43	0.54
1:A:318:ASN:H	1:A:398:HIS:HE1	1.55	0.54
6:H:58:TYR:CE2	6:H:113:LEU:HD22	2.42	0.54
4:D:340:LEU:O	4:D:344:ILE:HG13	2.07	0.54
4:D:589:GLU:HB2	5:E:26:LYS:HB3	1.89	0.53
6:H:58:TYR:CD2	6:H:113:LEU:HB3	2.43	0.53
1:A:324:PHE:O	1:A:393:ILE:HG12	2.09	0.53
1:A:367:ARG:HH22	1:A:375:LEU:H	1.56	0.53
2:B:279:LYS:HD2	2:B:279:LYS:N	2.24	0.53
4:D:423:ALA:HA	4:D:426:CYS:SG	2.49	0.53
4:D:508:PHE:O	4:D:511:ILE:HG22	2.09	0.53
5:E:87:TRP:HA	5:E:90:THR:HG1	1.74	0.53
2:B:244:PRO:HB2	2:B:348:TYR:CD2	2.44	0.53
4:D:183:VAL:O	4:D:187:ILE:HG13	2.09	0.53
4:D:251:PHE:CE2	4:D:260:TYR:HA	2.44	0.53
4:D:427:ASP:O	4:D:431:LYS:HG3	2.08	0.53
6:H:24:LEU:HD13	6:H:51:VAL:HG22	1.91	0.53
6:H:121:SER:HA	6:H:124:GLN:NE2	2.24	0.53
1:A:64:ARG:HH11	1:A:284:ARG:NH1	2.07	0.52
1:A:318:ASN:H	1:A:398:HIS:CE1	2.27	0.52
3:C:20:ILE:HG23	3:C:62:CYS:HB3	1.90	0.52
4:D:451:VAL:O	4:D:454:LYS:HG2	2.10	0.52
4:D:496:CYS:HB2	4:D:500:TYR:CD2	2.45	0.52
3:C:5:LYS:HD2	3:C:13:ILE:CG2	2.40	0.52
1:A:289:THR:H	1:A:368:ILE:HG22	1.75	0.52
2:B:358:GLN:NE2	2:B:359:VAL:HG23	2.23	0.52
4:D:460:ASP:HA	4:D:463:GLN:HG3	1.91	0.52
6:G:11:TYR:CE2	6:G:13:SER:HB2	2.45	0.52
3:C:23:GLN:NE2	3:C:65:HIS:NE2	2.56	0.52
3:C:61:TRP:CG	3:C:115:LEU:HD12	2.45	0.52
4:D:451:VAL:HA	4:D:454:LYS:HE3	1.92	0.51
1:A:69:ILE:HD11	1:A:91:GLU:HG3	1.93	0.51
4:D:114:SER:HA	4:D:117:LYS:NZ	2.26	0.51
4:D:276:GLN:HB2	4:D:284:GLN:OE1	2.11	0.51
4:D:470:LEU:HA	4:D:473:ARG:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:101:PHE:O	3:C:105:LEU:HD23	2.11	0.51
4:D:151:GLU:OE2	4:D:153:ARG:HG2	2.11	0.51
1:A:148:ILE:HG23	1:A:255:VAL:HG21	1.93	0.51
4:D:168:ARG:HA	4:D:172:PHE:HB3	1.92	0.51
4:D:202:SER:HA	4:D:205:VAL:HG12	1.91	0.51
1:A:335:ARG:NE	1:A:335:ARG:HA	2.26	0.50
4:D:319:LEU:HD12	4:D:322:MET:HE3	1.93	0.50
4:D:129:SER:HA	4:D:132:VAL:HG12	1.93	0.50
4:D:399:CYS:O	4:D:403:ILE:HB	2.10	0.50
6:G:53:ALA:HA	6:G:59:PHE:HB2	1.93	0.50
3:C:99:THR:HA	3:C:102:GLU:HG3	1.94	0.50
4:D:272:GLN:HG3	4:D:284:GLN:NE2	2.26	0.50
4:D:87:GLU:OE2	4:D:91:ARG:HD2	2.11	0.50
1:A:185:ILE:O	1:A:186:LYS:HE2	2.11	0.50
1:A:240:VAL:HA	1:A:243:PHE:HE1	1.76	0.50
2:B:322:TRP:O	2:B:326:ILE:HG12	2.12	0.50
4:D:567:THR:HA	4:D:570:TYR:HB3	1.92	0.50
6:H:28:ARG:HB2	6:H:92:TYR:CE2	2.47	0.50
6:H:100:LYS:HE3	6:H:127:LYS:NZ	2.26	0.50
1:A:32:ARG:O	1:A:35:THR:HG22	2.12	0.50
1:A:164:ARG:HA	1:A:346:ARG:NH1	2.26	0.50
4:D:184:LEU:HA	4:D:187:ILE:HD12	1.93	0.50
6:G:78:GLU:HG3	6:G:79:VAL:HG13	1.94	0.50
4:D:636:LEU:O	4:D:640:LEU:HG	2.12	0.49
6:H:53:ALA:O	6:H:57:SER:HB3	2.12	0.49
1:A:314:ILE:HD11	1:A:370:THR:HG22	1.94	0.49
4:D:360:LEU:HD12	4:D:361:ASN:N	2.28	0.49
4:D:12:LEU:HD12	4:D:14:GLN:H	1.77	0.49
4:D:161:SER:O	4:D:165:VAL:HG23	2.12	0.49
4:D:280:HIS:HE1	4:D:282:SER:HB2	1.77	0.49
4:D:552:THR:CG2	4:D:553:PHE:H	2.24	0.49
4:D:650:VAL:HG22	4:D:672:TYR:CE1	2.47	0.49
1:A:163:ASN:O	1:A:165:PRO:HD3	2.13	0.49
1:A:278:LEU:HD12	1:A:279:SER:N	2.26	0.49
1:A:315:PRO:HB2	1:A:398:HIS:NE2	2.28	0.49
4:D:37:MET:HE3	4:D:41:ARG:HG3	1.95	0.49
1:A:133:LEU:HD23	1:A:137:LYS:HD2	1.95	0.49
2:B:236:TRP:HE1	2:B:267:PHE:HB2	1.77	0.49
3:C:31:LEU:HD13	3:C:34:LEU:HD11	1.94	0.49
3:C:31:LEU:HA	3:C:34:LEU:HG	1.94	0.49
3:C:132:PRO:HA	3:C:135:ILE:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LYS:HB3	1:A:188:GLN:HE21	1.77	0.48
1:A:105:MET:HA	1:A:148:ILE:O	2.13	0.48
4:D:187:ILE:O	4:D:191:ARG:HG2	2.14	0.48
7:A:501:A1J20:C17	2:B:275:TRP:HD1	2.25	0.48
4:D:505:GLN:O	4:D:509:GLN:HG2	2.12	0.48
2:B:337:VAL:O	2:B:341:LYS:HG3	2.14	0.48
4:D:21:TRP:CZ3	4:D:88:LEU:HD12	2.49	0.48
6:G:39:PHE:HD2	6:G:74:THR:HG22	1.78	0.48
1:A:296:VAL:HG13	1:A:301:THR:OG1	2.14	0.48
6:H:36:VAL:HG13	6:H:47:ALA:HB3	1.95	0.48
4:D:622:VAL:HG23	4:D:667:THR:O	2.13	0.48
4:D:354:LYS:HD3	4:D:354:LYS:N	2.29	0.48
4:D:535:PHE:CE2	4:D:537:ILE:HD11	2.49	0.48
5:E:21:ARG:HB3	5:E:22:PHE:HD2	1.78	0.48
1:A:138:LEU:HA	3:C:161:GLU:OE2	2.14	0.48
2:B:225:LEU:CB	2:B:284:PHE:HB3	2.44	0.48
4:D:114:SER:HA	4:D:117:LYS:HZ1	1.78	0.48
6:G:28:ARG:HD2	6:G:92:TYR:CZ	2.49	0.47
1:A:107:ASP:HA	1:A:150:THR:O	2.14	0.47
1:A:164:ARG:HG2	1:A:346:ARG:HH12	1.79	0.47
3:C:47:LEU:HB3	3:C:50:VAL:HB	1.96	0.47
3:C:145:PHE:CD1	3:C:149:GLU:HB2	2.44	0.47
1:A:182:ILE:CG2	1:A:185:ILE:HB	2.44	0.47
6:H:51:VAL:HG11	6:H:92:TYR:HE1	1.79	0.47
3:C:122:THR:O	3:C:126:MET:HG2	2.14	0.47
1:A:195:ASP:HB3	1:A:198:ASN:OD1	2.15	0.47
1:A:261:LEU:HD23	1:A:261:LEU:O	2.15	0.47
4:D:592:THR:HG22	5:E:22:PHE:CE1	2.50	0.47
6:H:52:LEU:O	6:H:56:SER:CB	2.57	0.47
1:A:190:PHE:CZ	1:A:277:GLY:HA3	2.50	0.47
1:A:247:ASN:O	1:A:367:ARG:HD3	2.15	0.47
1:A:308:ARG:NH1	1:A:308:ARG:HB3	2.29	0.47
1:A:345:PHE:CD2	1:A:354:LEU:HD12	2.50	0.47
2:B:358:GLN:N	2:B:358:GLN:OE1	2.47	0.47
4:D:316:ASN:HA	4:D:319:LEU:HB3	1.97	0.47
4:D:439:GLU:HA	4:D:442:LEU:HD12	1.96	0.47
4:D:448:GLN:HA	4:D:451:VAL:HG23	1.97	0.47
4:D:499:GLU:HG2	4:D:500:TYR:N	2.29	0.47
6:H:58:TYR:CD2	6:H:113:LEU:HD22	2.49	0.47
3:C:17:ASP:HB3	3:C:20:ILE:CD1	2.45	0.47
4:D:421:LEU:HA	4:D:424:ARG:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:279:LYS:H	2:B:279:LYS:CD	2.26	0.47
3:C:82:THR:O	3:C:121:LYS:HD2	2.14	0.47
6:G:39:PHE:CD2	6:G:74:THR:HG22	2.49	0.47
3:C:158:GLN:C	3:C:160:CYS:H	2.23	0.46
4:D:316:ASN:HA	4:D:319:LEU:CB	2.45	0.46
1:A:246:MET:SD	1:A:248:ILE:HG23	2.55	0.46
4:D:179:VAL:O	4:D:183:VAL:HG23	2.16	0.46
1:A:110:THR:HA	1:A:113:SER:OG	2.15	0.46
6:H:59:PHE:HZ	6:H:73:ILE:HD11	1.80	0.46
6:H:125:PHE:CE2	6:H:126:LEU:HD23	2.49	0.46
1:A:85:VAL:HG22	1:A:135:LEU:HD21	1.96	0.46
3:C:145:PHE:CE1	3:C:150:GLU:HA	2.43	0.46
4:D:330:GLN:CG	6:G:62:ARG:HH22	2.29	0.46
1:A:40:LYS:HZ2	1:A:44:ARG:HG3	1.80	0.46
4:D:425:TYR:CZ	4:D:429:LEU:HD21	2.51	0.46
4:D:476:HIS:O	4:D:477:GLN:HG2	2.15	0.46
4:D:552:THR:HG22	4:D:553:PHE:N	2.23	0.46
1:A:99:PRO:HG3	3:C:159:TRP:HH2	1.79	0.46
4:D:229:LYS:HA	4:D:233:GLU:HG2	1.98	0.46
4:D:85:GLY:HA3	4:D:144:TRP:CZ3	2.51	0.46
4:D:111:MET:HE1	4:D:113:GLU:HG3	1.97	0.46
4:D:461:VAL:HG22	4:D:703:ILE:HD13	1.97	0.46
6:H:93:THR:HG22	6:H:95:LYS:O	2.16	0.46
1:A:156:THR:HB	1:A:355:PHE:CZ	2.50	0.46
1:A:248:ILE:O	1:A:367:ARG:HG2	2.16	0.46
4:D:56:VAL:O	4:D:56:VAL:HG13	2.16	0.46
4:D:367:VAL:HG21	4:D:425:TYR:CD2	2.51	0.46
1:A:131:THR:O	1:A:135:LEU:HD23	2.16	0.46
3:C:134:GLU:O	3:C:138:THR:HG23	2.16	0.46
6:G:13:SER:HB3	6:H:94:ALA:HB1	1.98	0.46
6:G:88:ILE:HG12	6:G:92:TYR:CE2	2.51	0.46
6:G:101:GLU:HG2	6:G:102:ASN:N	2.31	0.46
4:D:184:LEU:HD23	4:D:187:ILE:HD12	1.98	0.45
4:D:303:PHE:HA	4:D:306:GLU:HB2	1.97	0.45
4:D:243:PHE:HA	4:D:246:ARG:NH1	2.32	0.45
4:D:251:PHE:CE2	4:D:263:LYS:HD2	2.51	0.45
1:A:191:HIS:CE1	1:A:276:VAL:HB	2.51	0.45
3:C:65:HIS:HA	3:C:68:ASP:OD1	2.16	0.45
3:C:69:PRO:HB2	3:C:70:PRO:HD2	1.99	0.45
5:E:48:HIS:CG	5:E:49:ILE:H	2.35	0.45
1:A:79:LEU:H	1:A:79:LEU:HD23	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:VAL:HB	2:B:281:LEU:CD1	2.46	0.45
2:B:337:VAL:HA	2:B:340:ARG:HG2	1.99	0.45
4:D:21:TRP:HZ3	4:D:88:LEU:HD12	1.82	0.45
5:E:71:ALA:HB3	5:E:76:ASN:ND2	2.32	0.45
6:H:40:VAL:HG22	6:H:75:LEU:H	1.81	0.45
2:B:291:GLU:HA	2:B:294:CYS:SG	2.56	0.45
4:D:111:MET:SD	4:D:113:GLU:HG3	2.56	0.45
4:D:460:ASP:O	4:D:463:GLN:HG3	2.17	0.45
4:D:553:PHE:HB3	4:D:631:ILE:HD11	1.98	0.45
6:G:13:SER:OG	6:G:16:HIS:HB2	2.16	0.45
6:H:59:PHE:CE2	6:H:63:ILE:HG21	2.52	0.45
3:C:5:LYS:HD3	3:C:14:PHE:O	2.17	0.45
1:A:221:LEU:HD11	1:A:278:LEU:HB3	1.97	0.45
3:C:99:THR:O	3:C:102:GLU:HG3	2.17	0.45
1:A:141:LYS:HE3	1:A:142:GLN:NE2	2.32	0.44
1:A:146:LEU:HD11	1:A:276:VAL:HG21	1.99	0.44
2:B:335:MET:HE3	2:B:340:ARG:HA	1.98	0.44
3:C:5:LYS:HB3	3:C:44:PRO:HB3	1.98	0.44
6:H:90:PHE:CD1	6:H:96:LEU:HD21	2.51	0.44
2:B:267:PHE:HB3	2:B:328:GLN:OE1	2.18	0.44
4:D:177:LYS:O	4:D:180:THR:HG22	2.17	0.44
6:H:103:VAL:HG21	6:H:126:LEU:HD11	1.99	0.44
2:B:289:GLN:HE22	2:B:293:LEU:CG	2.29	0.44
4:D:268:LEU:O	4:D:272:GLN:OE1	2.35	0.44
1:A:69:ILE:O	1:A:175:PHE:HD2	2.01	0.44
3:C:49:ASN:OD1	4:D:47:THR:HG23	2.17	0.44
4:D:355:CYS:SG	4:D:365:MET:HE2	2.58	0.44
6:G:110:VAL:HG13	6:G:115:VAL:CG1	2.47	0.44
1:A:104:TYR:CZ	1:A:147:GLY:HA3	2.52	0.44
2:B:343:LYS:CG	2:B:358:GLN:HE21	2.21	0.44
4:D:510:ASP:HA	4:D:513:VAL:HG22	1.99	0.44
5:E:87:TRP:HA	5:E:90:THR:OG1	2.18	0.44
6:G:16:HIS:O	6:G:20:VAL:HG23	2.18	0.44
1:A:185:ILE:HD13	1:A:282:GLY:HA3	2.00	0.44
2:B:244:PRO:HB2	2:B:348:TYR:HD2	1.82	0.44
4:D:427:ASP:O	4:D:430:LEU:HG	2.18	0.44
4:D:635:ILE:O	4:D:639:VAL:HG23	2.17	0.44
6:G:79:VAL:HG12	6:G:105:GLU:OE1	2.18	0.44
4:D:330:GLN:HG3	4:D:331:ASP:N	2.33	0.44
5:E:71:ALA:C	5:E:76:ASN:HD21	2.25	0.44
4:D:61:GLN:HG3	4:D:62:ALA:N	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:118:PHE:CE1	4:D:122:GLN:HG3	2.53	0.43
4:D:139:TYR:O	4:D:142:ARG:HG2	2.18	0.43
6:G:52:LEU:O	6:G:56:SER:CB	2.66	0.43
4:D:205:VAL:HG21	4:D:279:LEU:O	2.18	0.43
4:D:285:ASP:O	4:D:289:ARG:HB3	2.18	0.43
4:D:367:VAL:O	4:D:370:VAL:HG12	2.19	0.43
4:D:112:ASP:O	4:D:115:VAL:HG22	2.18	0.43
6:H:110:VAL:HG22	6:H:115:VAL:HB	1.99	0.43
1:A:26:LEU:HD23	1:A:29:VAL:HG21	2.00	0.43
3:C:5:LYS:HD3	3:C:5:LYS:HA	1.76	0.43
4:D:540:LEU:HD23	4:D:545:TRP:HB3	2.00	0.43
3:C:85:ILE:O	3:C:85:ILE:HG13	2.19	0.43
4:D:307:PHE:CE1	4:D:336:LEU:HG	2.53	0.43
4:D:348:GLY:O	4:D:352:ILE:HG23	2.19	0.43
6:G:28:ARG:HH21	6:G:48:HIS:CE1	2.37	0.43
4:D:381:VAL:O	4:D:385:PHE:HB2	2.19	0.43
4:D:626:THR:HG23	4:D:631:ILE:O	2.18	0.43
6:G:32:VAL:HG12	6:G:33:LEU:HD13	2.00	0.43
6:H:28:ARG:CZ	6:H:47:ALA:HA	2.48	0.43
1:A:153:ILE:HG13	1:A:154:VAL:N	2.34	0.43
1:A:298:ASP:OD2	1:A:300:LYS:HE2	2.19	0.43
2:B:287:GLU:N	2:B:287:GLU:OE1	2.52	0.43
3:C:20:ILE:H	3:C:20:ILE:HD12	1.84	0.43
4:D:341:GLU:HG2	4:D:398:ALA:HB2	2.01	0.43
4:D:371:LEU:HD12	4:D:372:ASP:OD2	2.19	0.42
6:H:25:ASN:HA	6:H:92:TYR:CE2	2.54	0.42
1:A:236:LEU:O	1:A:240:VAL:HG22	2.19	0.42
1:A:344:ALA:HA	1:A:347:LYS:HG2	2.01	0.42
4:D:527:ASN:C	4:D:527:ASN:HD22	2.27	0.42
4:D:544:SER:HB2	4:D:545:TRP:CD1	2.54	0.42
4:D:622:VAL:HB	4:D:665:PRO:O	2.18	0.42
4:D:723:LYS:CE	4:D:776:ALA:HA	2.49	0.42
1:A:319:THR:HG23	1:A:352:VAL:CG2	2.48	0.42
3:C:149:GLU:O	3:C:153:VAL:HG13	2.19	0.42
4:D:275:VAL:HG13	4:D:284:GLN:OE1	2.19	0.42
4:D:584:GLN:HG2	4:D:585:LEU:N	2.32	0.42
5:E:75:CYS:HB2	5:E:106:TYR:OH	2.20	0.42
6:G:28:ARG:HA	6:G:28:ARG:NE	2.34	0.42
1:A:26:LEU:O	1:A:30:VAL:HG23	2.18	0.42
1:A:46:ALA:HB1	1:A:53:ARG:HA	2.02	0.42
2:B:291:GLU:C	2:B:294:CYS:HG	2.04	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:40:VAL:HG13	6:G:75:LEU:HD12	2.01	0.42
1:A:23:LEU:HB3	1:A:52:TRP:CH2	2.55	0.42
6:G:63:ILE:HG22	6:G:64:VAL:N	2.30	0.42
1:A:323:MET:HE3	1:A:324:PHE:N	2.35	0.42
4:D:37:MET:HE2	4:D:42:TYR:HA	2.02	0.42
6:G:9:PHE:CD2	6:H:96:LEU:HD12	2.51	0.42
4:D:27:GLY:O	4:D:31:VAL:HG23	2.20	0.42
4:D:372:ASP:HA	4:D:375:LYS:HE2	2.00	0.42
4:D:454:LYS:HG3	4:D:455:TYR:CD1	2.55	0.42
6:G:93:THR:HG22	6:G:95:LYS:HB3	2.02	0.42
3:C:27:ILE:O	3:C:31:LEU:HD23	2.19	0.42
6:H:28:ARG:CB	6:H:92:TYR:HE2	2.32	0.42
6:H:68:ASP:OD2	6:H:69:GLY:N	2.53	0.42
1:A:181:GLN:OE1	1:A:181:GLN:O	2.38	0.42
4:D:427:ASP:HA	4:D:430:LEU:CD2	2.49	0.42
6:G:13:SER:H	6:H:94:ALA:HB1	1.84	0.42
1:A:86:ARG:HE	1:A:90:GLU:HG3	1.85	0.42
1:A:303:GLU:HG2	1:A:347:LYS:NZ	2.35	0.42
2:B:239:MET:HE2	2:B:267:PHE:CZ	2.44	0.42
3:C:64:HIS:C	3:C:66:LYS:H	2.27	0.41
1:A:139:PHE:CD2	3:C:159:TRP:CZ2	3.08	0.41
5:E:94:CYS:HA	5:E:97:ASP:O	2.19	0.41
1:A:326:CYS:N	1:A:362:GLU:OE2	2.53	0.41
4:D:272:GLN:HG3	4:D:284:GLN:HE21	1.85	0.41
4:D:280:HIS:HB3	4:D:283:THR:OG1	2.20	0.41
4:D:608:MET:HA	4:D:611:LEU:HG	2.02	0.41
6:H:110:VAL:HA	6:H:115:VAL:HG23	2.02	0.41
1:A:378:CYS:SG	6:H:8:VAL:HG23	2.60	0.41
4:D:92:LEU:HD23	4:D:159:ILE:HD11	2.02	0.41
4:D:280:HIS:CG	4:D:281:GLU:N	2.88	0.41
4:D:373:VAL:HB	4:D:377:TYR:CE2	2.54	0.41
1:A:191:HIS:CE1	1:A:258:LEU:HD21	2.55	0.41
4:D:453:PHE:HA	4:D:456:ILE:HG12	2.01	0.41
4:D:612:LEU:HD12	4:D:612:LEU:HA	1.80	0.41
6:G:36:VAL:CG2	6:G:49:ARG:HE	2.33	0.41
1:A:237:GLN:HA	1:A:240:VAL:HG22	2.01	0.41
3:C:55:LEU:O	3:C:59:ILE:HG13	2.20	0.41
2:B:252:LEU:HD23	2:B:260:ARG:HH11	1.86	0.41
1:A:140:PRO:HB2	1:A:142:GLN:OE1	2.21	0.41
1:A:300:LYS:HE2	1:A:300:LYS:HB2	1.90	0.41
3:C:50:VAL:HG12	3:C:55:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:85:ILE:HG22	3:C:118:VAL:HG13	2.02	0.41
4:D:256:PRO:HG2	4:D:259:GLU:HG2	2.02	0.41
4:D:400:GLY:O	4:D:404:ASN:HB3	2.20	0.41
4:D:422:LEU:HD11	4:D:449:VAL:HG13	2.03	0.41
4:D:442:LEU:O	4:D:446:LEU:HD23	2.20	0.41
4:D:275:VAL:HG11	4:D:287:LEU:HD23	2.03	0.41
4:D:577:ARG:HG3	5:E:35:TRP:CE3	2.56	0.41
4:D:658:VAL:O	4:D:658:VAL:HG23	2.21	0.41
1:A:112:ILE:HD12	1:A:112:ILE:HA	1.86	0.40
1:A:211:LEU:HA	1:A:217:LEU:HD13	2.03	0.40
3:C:1:MET:N	3:C:2:PRO:HA	2.36	0.40
4:D:345:HIS:ND1	4:D:402:PHE:CE2	2.90	0.40
6:G:11:TYR:CG	6:G:12:GLU:N	2.89	0.40
1:A:91:GLU:O	1:A:95:VAL:HG23	2.20	0.40
1:A:218:ARG:HA	1:A:248:ILE:HG21	2.03	0.40
1:A:192:PHE:HE2	1:A:206:LEU:HD13	1.86	0.40
3:C:123:VAL:O	3:C:127:ILE:HD12	2.21	0.40
3:C:148:GLU:HG2	3:C:149:GLU:N	2.37	0.40
2:B:346:PHE:HD1	2:B:356:ASN:ND2	2.19	0.40
4:D:302:ILE:HD12	4:D:302:ILE:H	1.87	0.40
4:D:463:GLN:HE21	4:D:463:GLN:HB2	1.71	0.40
4:D:603:ALA:HA	4:D:685:ASN:OD1	2.21	0.40
4:D:752:CYS:O	4:D:756:LEU:HG	2.21	0.40
6:G:55:CYS:O	6:G:115:VAL:HG23	2.21	0.40
1:A:40:LYS:HZ2	1:A:44:ARG:CG	2.35	0.40
4:D:594:CYS:HB2	5:E:21:ARG:HA	2.04	0.40
4:D:631:ILE:HD12	4:D:631:ILE:H	1.87	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	372/403 (92%)	349 (94%)	23 (6%)	0	100	100
2	B	132/1365 (10%)	128 (97%)	4 (3%)	0	100	100
3	C	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
4	D	770/776 (99%)	735 (96%)	35 (4%)	0	100	100
5	E	91/108 (84%)	78 (86%)	12 (13%)	1 (1%)	11	45
6	G	120/736 (16%)	108 (90%)	12 (10%)	0	100	100
6	H	119/736 (16%)	110 (92%)	8 (7%)	1 (1%)	16	52
All	All	1765/4287 (41%)	1662 (94%)	101 (6%)	2 (0%)	49	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	41	ASN
6	H	76	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	321/344 (93%)	321 (100%)	0	100	100
2	B	109/1173 (9%)	108 (99%)	1 (1%)	70	75
3	C	150/150 (100%)	150 (100%)	0	100	100
4	D	694/698 (99%)	693 (100%)	1 (0%)	88	88
5	E	79/90 (88%)	79 (100%)	0	100	100
6	G	111/663 (17%)	111 (100%)	0	100	100
6	H	110/663 (17%)	110 (100%)	0	100	100
All	All	1574/3781 (42%)	1572 (100%)	2 (0%)	87	88

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	216	HIS
4	D	463	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	188	GLN
1	A	257	ASN
2	B	247	HIS
2	B	356	ASN
4	D	48	HIS
4	D	76	GLN
4	D	98	ASN
4	D	143	HIS
4	D	192	ASN
4	D	253	GLN
4	D	254	GLN
4	D	343	HIS
4	D	509	GLN
4	D	527	ASN
4	D	538	GLN
4	D	712	GLN
5	E	41	ASN
5	E	76	ASN
5	E	77	HIS
6	G	102	ASN
6	G	117	ASN
6	H	27	GLN
6	H	43	GLN
6	H	48	HIS
6	H	60	HIS
6	H	116	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
7	A1J20	A	501	-	49,50,50	6.33	35 (71%)	61,70,70	3.00	22 (36%)

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
7	A1J20	A	501	-	-	5/34/54/54	0/6/6/6

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	501	A1J20	C42-C41	17.08	1.70	1.38
7	A	501	A1J20	C37-N36	13.23	1.49	1.35
7	A	501	A1J20	C49-C50	11.88	1.59	1.39
7	A	501	A1J20	C35-N36	11.74	1.60	1.39
7	A	501	A1J20	C19-C18	11.33	1.60	1.40
7	A	501	A1J20	C51-C50	10.96	1.75	1.51
7	A	501	A1J20	C51-N15	10.11	1.60	1.46
7	A	501	A1J20	C47-C24	9.01	1.54	1.39
7	A	501	A1J20	C18-C50	8.96	1.50	1.41
7	A	501	A1J20	C26-C25	8.53	1.54	1.38
7	A	501	A1J20	O38-C37	8.38	1.40	1.23
7	A	501	A1J20	C34-C33	-8.28	1.23	1.38
7	A	501	A1J20	C46-C27	7.37	1.54	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	501	A1J20	C48-C20	-7.37	1.26	1.39
7	A	501	A1J20	C13-N15	7.03	1.49	1.35
7	A	501	A1J20	C33-C32	-6.81	1.27	1.39
7	A	501	A1J20	O40-C39	-6.62	1.27	1.43
7	A	501	A1J20	C30-N29	6.20	1.48	1.34
7	A	501	A1J20	C35-C41	5.74	1.52	1.40
7	A	501	A1J20	C22-N21	4.50	1.47	1.35
7	A	501	A1J20	C34-C35	4.49	1.47	1.39
7	A	501	A1J20	C19-C20	-3.97	1.33	1.39
7	A	501	A1J20	C25-C24	-3.60	1.33	1.39
7	A	501	A1J20	C32-C30	3.26	1.55	1.50
7	A	501	A1J20	C20-N21	3.18	1.48	1.41
7	A	501	A1J20	C49-C48	-3.03	1.33	1.38
7	A	501	A1J20	C18-C17	-2.86	1.38	1.44
7	A	501	A1J20	C28-C27	2.73	1.56	1.51
7	A	501	A1J20	C47-C46	-2.68	1.33	1.38
7	A	501	A1J20	C26-C27	-2.63	1.33	1.38
7	A	501	A1J20	C24-C22	2.58	1.55	1.50
7	A	501	A1J20	O40-C41	-2.50	1.34	1.37
7	A	501	A1J20	C44-C43	2.40	1.54	1.48
7	A	501	A1J20	C45-C43	2.21	1.53	1.48
7	A	501	A1J20	C12-C13	2.07	1.55	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	501	A1J20	O40-C41-C42	8.02	129.38	117.05
7	A	501	A1J20	C33-C32-C42	7.53	128.15	119.24
7	A	501	A1J20	C35-N36-C37	-7.08	115.72	124.49
7	A	501	A1J20	C32-C42-C41	-6.34	111.18	119.61
7	A	501	A1J20	C19-C18-C50	-5.46	113.58	118.86
7	A	501	A1J20	C42-C41-C35	-5.22	114.28	120.54
7	A	501	A1J20	C17-C16-N15	5.18	127.31	122.43
7	A	501	A1J20	C48-C20-C19	5.14	125.75	119.65
7	A	501	A1J20	C18-C17-C16	5.05	127.48	120.93
7	A	501	A1J20	C34-C35-N36	4.98	128.35	119.84
7	A	501	A1J20	C49-C50-C18	-4.38	112.65	118.19
7	A	501	A1J20	C39-O40-C41	3.90	127.56	115.61
7	A	501	A1J20	C34-C33-C32	3.63	125.00	120.78
7	A	501	A1J20	C19-C18-C17	3.61	129.94	122.91
7	A	501	A1J20	C33-C34-C35	3.38	126.18	119.64
7	A	501	A1J20	O40-C39-C37	3.32	123.70	114.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	501	A1J20	C51-C50-C49	3.31	128.72	119.76
7	A	501	A1J20	C34-C35-C41	-2.99	115.21	119.05
7	A	501	A1J20	O40-C41-C35	-2.72	116.34	121.58
7	A	501	A1J20	C20-N21-C22	-2.50	120.08	126.58
7	A	501	A1J20	C41-C35-N36	-2.32	116.44	118.56
7	A	501	A1J20	C18-C19-C20	2.08	121.74	119.28

There are no chirality outliers.

All (5) torsion outliers are listed below:

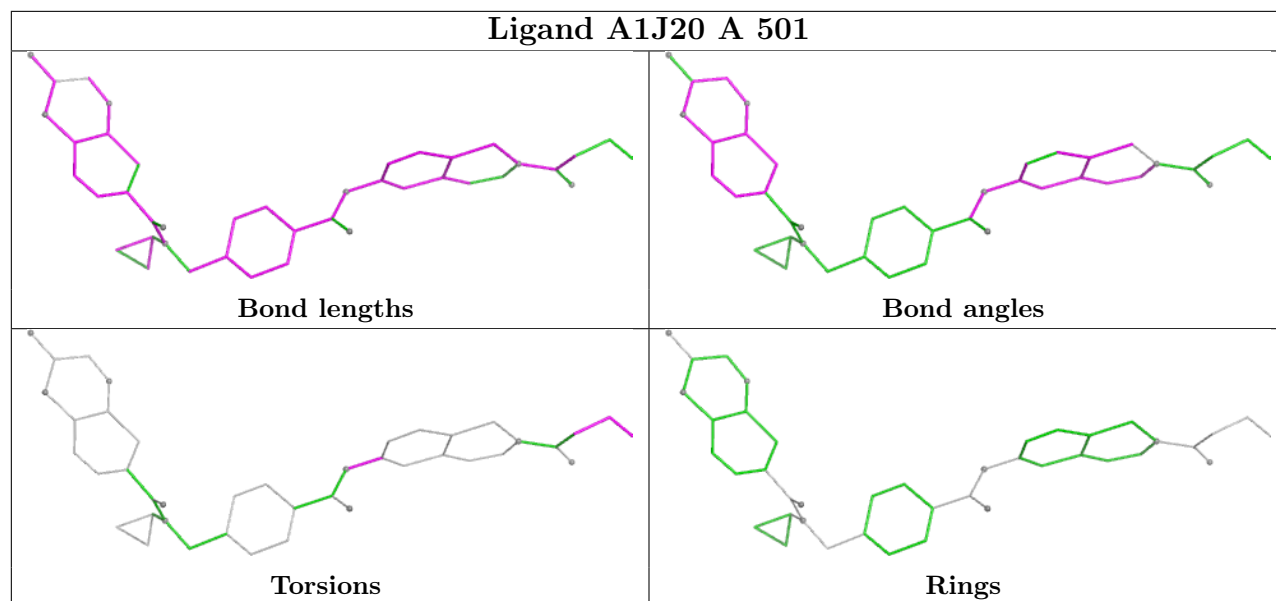
Mol	Chain	Res	Type	Atoms
7	A	501	A1J20	C10-C11-C12-C13
7	A	501	A1J20	C19-C20-N21-C22
7	A	501	A1J20	C48-C20-N21-C22
7	A	501	A1J20	C09-C10-C11-C12
7	A	501	A1J20	O08-C07-C09-C10

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	501	A1J20	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57179. These allow visual inspection of the internal detail of the map and identification of artifacts.

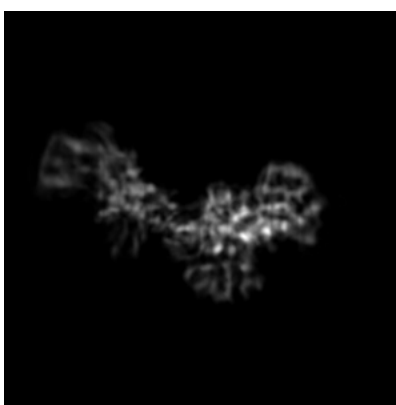
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

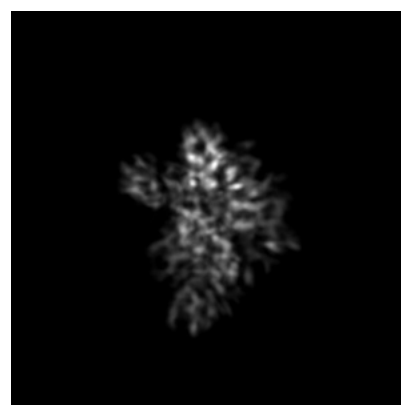
6.1.1 Primary map



X



Y



Z

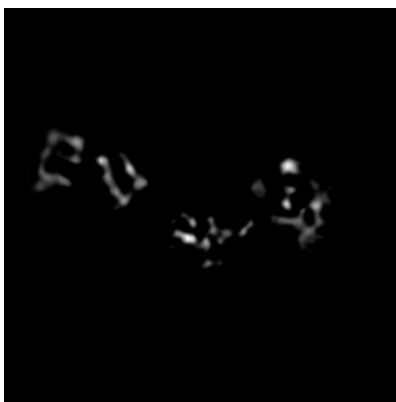
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 120



Y Index: 120



Z Index: 120

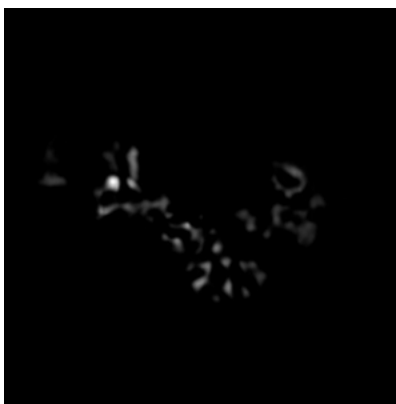
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 109



Y Index: 134



Z Index: 135

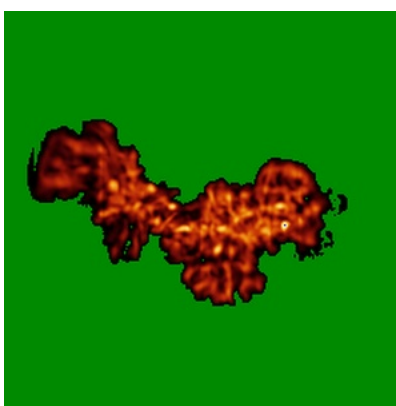
The images above show the largest variance slices of the map in three orthogonal directions.

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

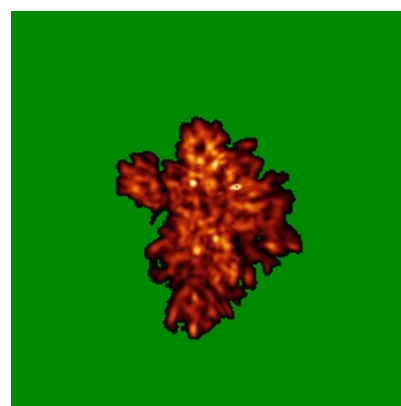
6.4.1 Primary map



X



Y

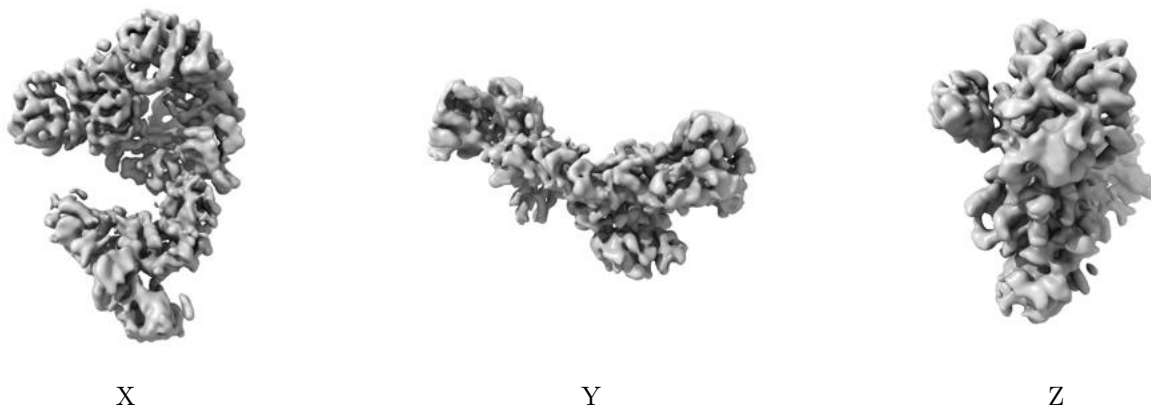


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

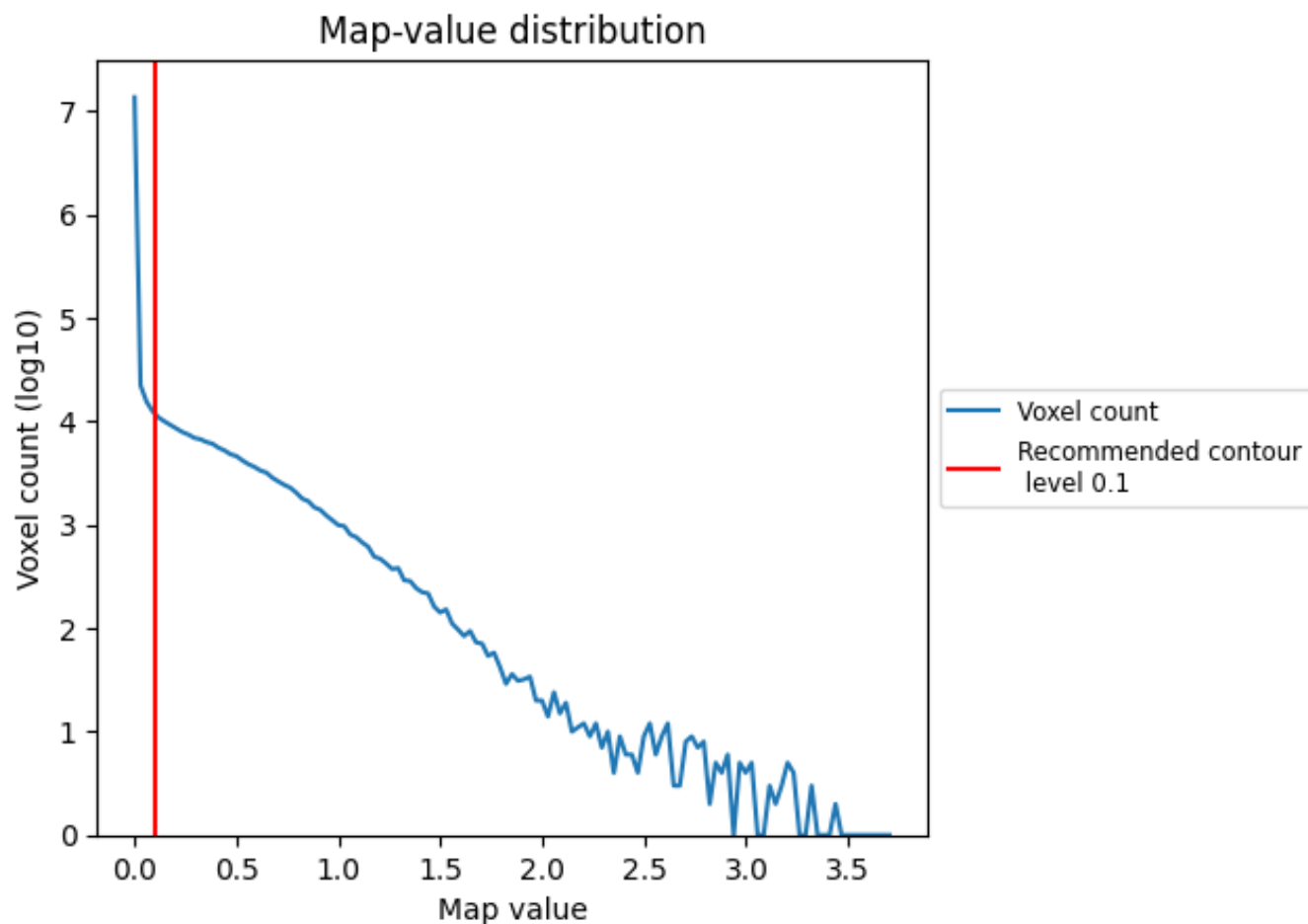
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

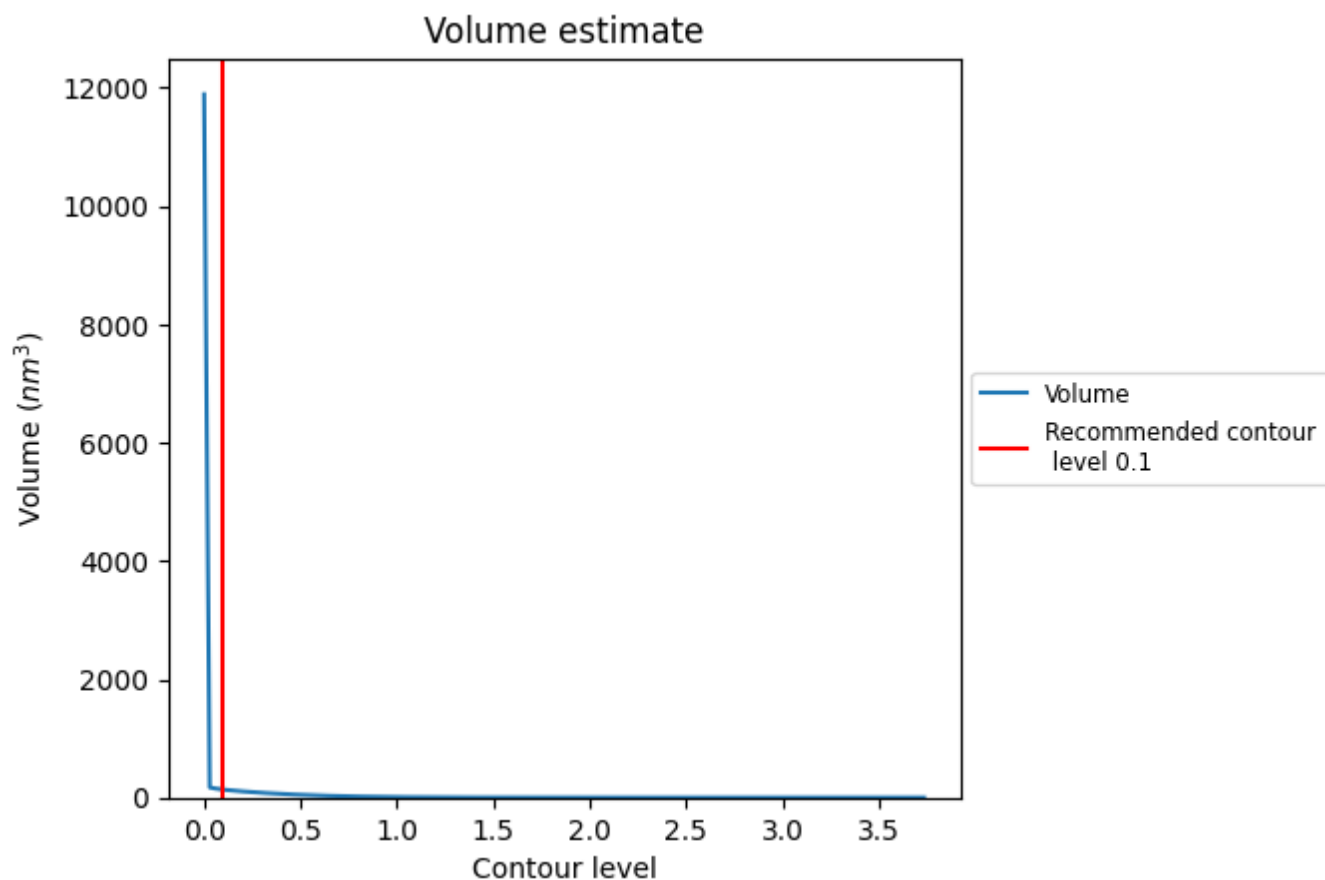
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

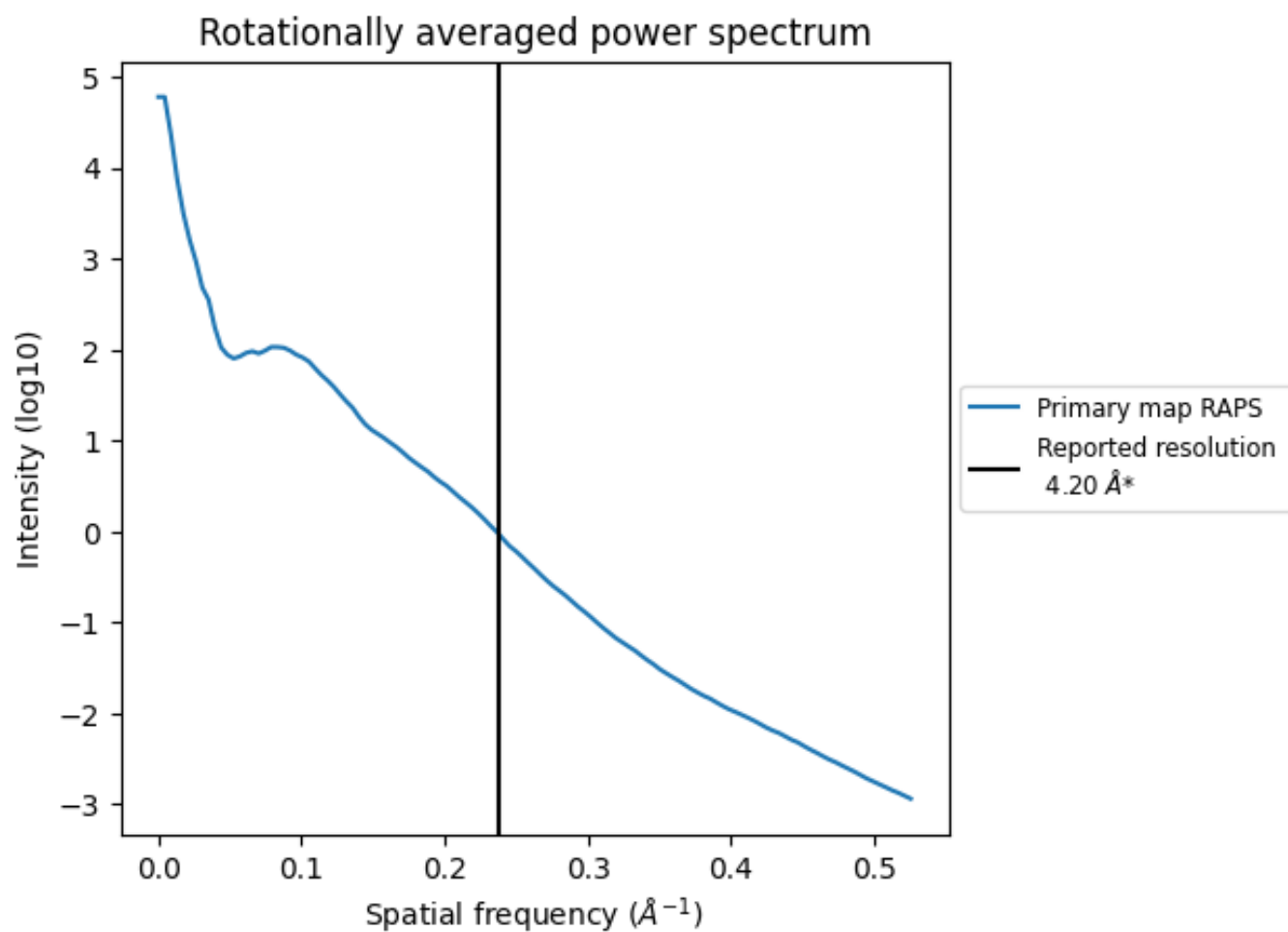
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 135 nm^3 ; this corresponds to an approximate mass of 122 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 0.238 Å⁻¹

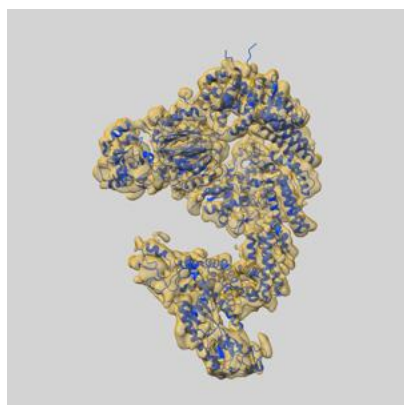
8 Fourier-Shell correlation ⓘ

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

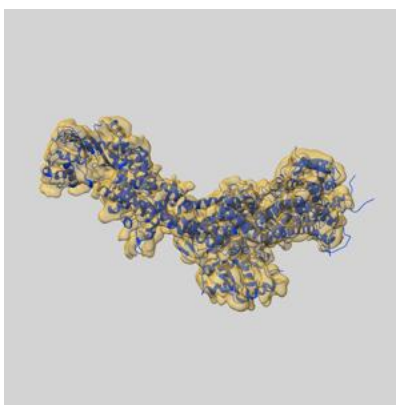
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-57179 and PDB model 29HH. Per-residue inclusion information can be found in section [3](#) on page [6](#).

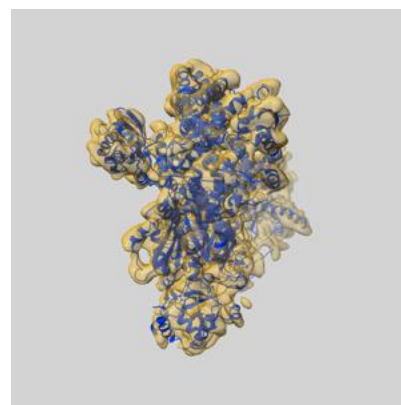
9.1 Map-model overlay [i](#)



X



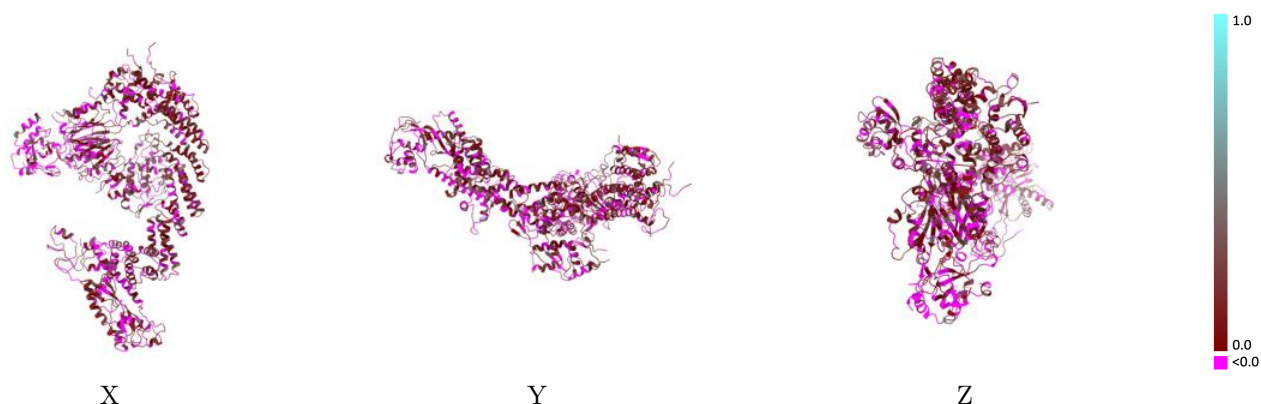
Y



Z

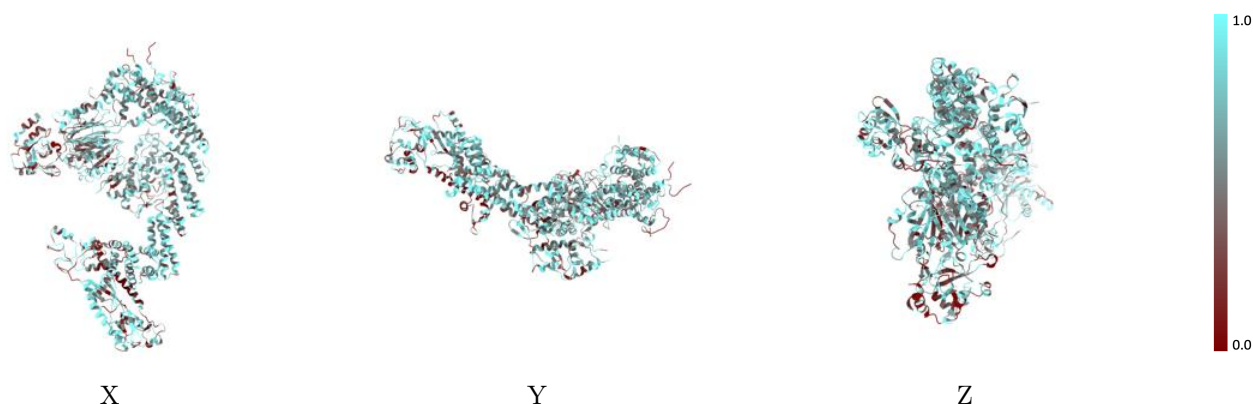
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



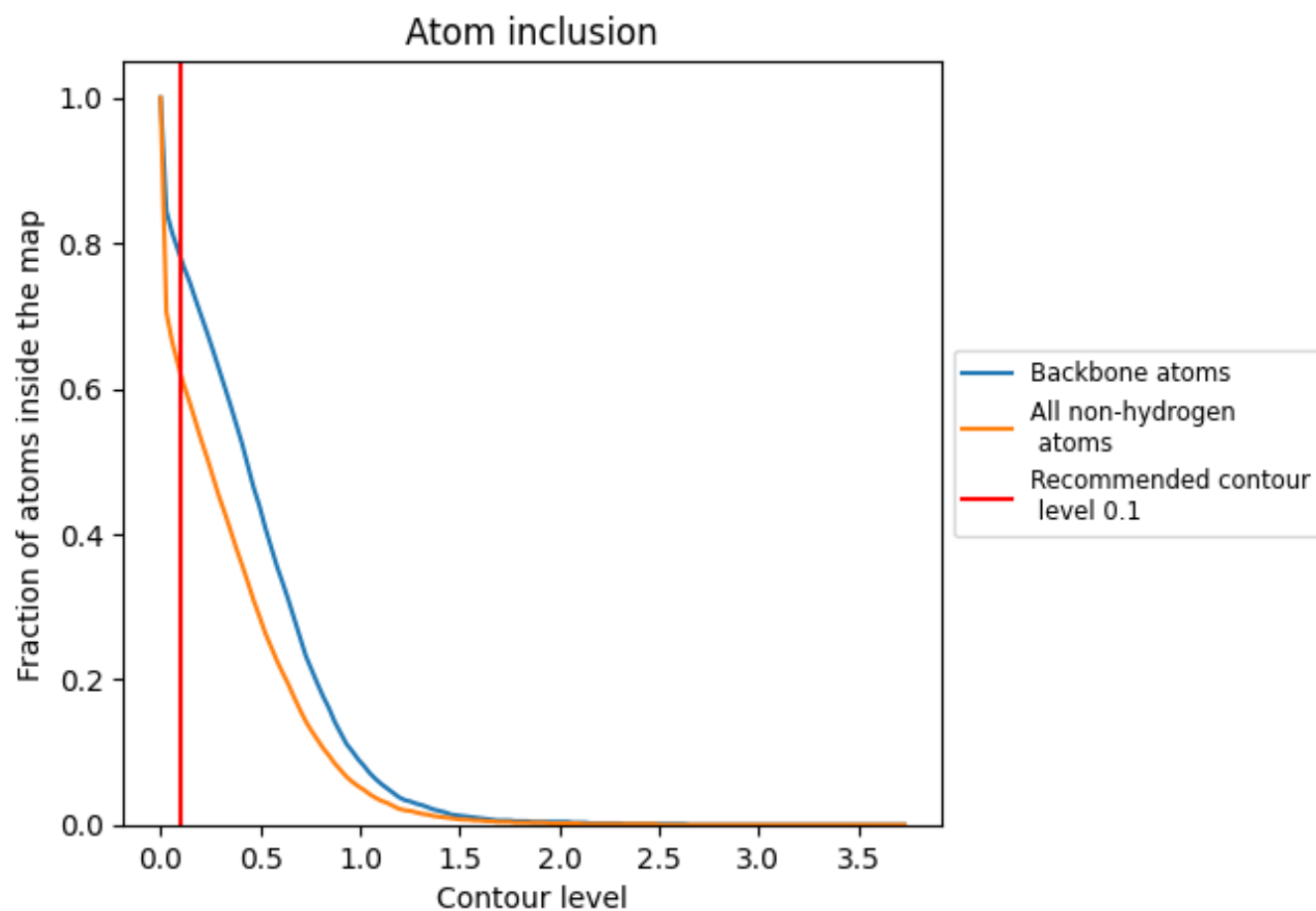
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion ⓘ



At the recommended contour level, 78% of all backbone atoms, 62% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6200	<div></div> 0.0950
A	<div></div> 0.6260	<div></div> 0.0890
B	<div></div> 0.4510	<div></div> -0.0220
C	<div></div> 0.6980	<div></div> 0.1460
D	<div></div> 0.6290	<div></div> 0.1030
E	<div></div> 0.5630	<div></div> 0.0890
G	<div></div> 0.6130	<div></div> 0.1010
H	<div></div> 0.6700	<div></div> 0.1170

1.0

0.0

<0.0