



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 01:53 PM UTC

PDB ID : 8H36 / pdb_00008h36
EMDB ID : EMD-34452
Title : Cryo-EM Structure of the KBTBD2-CUL3-Rbx1-p85a dimeric complex
Authors : Hu, Y.; Mao, Q.; Chen, Z.; Sun, L.
Deposited on : 2022-10-08
Resolution : 4.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
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

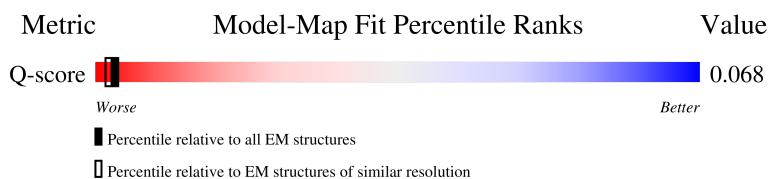
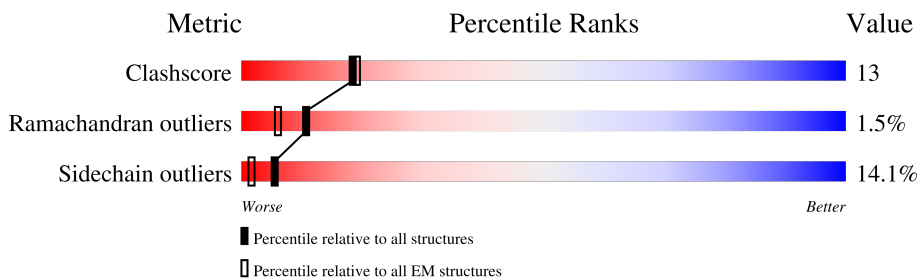
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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	2407 (4.10 - 5.10)

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	D	108	
1	E	108	
2	A	623	
2	B	623	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	724	9%31%18%•48%
3	H	724	16%33%15%•48%
4	C	768	•60%28%5%•6%
4	F	768	•60%28%5%•6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28650 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 E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	89	Total	C	N	O	S	0	0
			737	466	135	127	9		
1	D	89	Total	C	N	O	S	0	0
			737	466	135	127	9		

- Molecule 2 is a protein called Kelch repeat and BTB domain-containing protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	567	Total	C	N	O	S	0	0
			4582	2933	754	857	38		
2	B	564	Total	C	N	O	S	0	0
			4556	2916	751	851	38		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	252	ASP	SER	engineered mutation	UNP Q8IY47
B	252	ASP	SER	engineered mutation	UNP Q8IY47

- Molecule 3 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	379	Total	C	N	O	S	0	0
			3150	1976	560	605	9		
3	H	379	Total	C	N	O	S	0	0
			3150	1976	560	605	9		

- Molecule 4 is a protein called Cullin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	720	Total	C	N	O	S	0	0
			5866	3689	1037	1101	39		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	720	Total	C	N	O	S	0	0
			5866	3689	1037	1101	39		

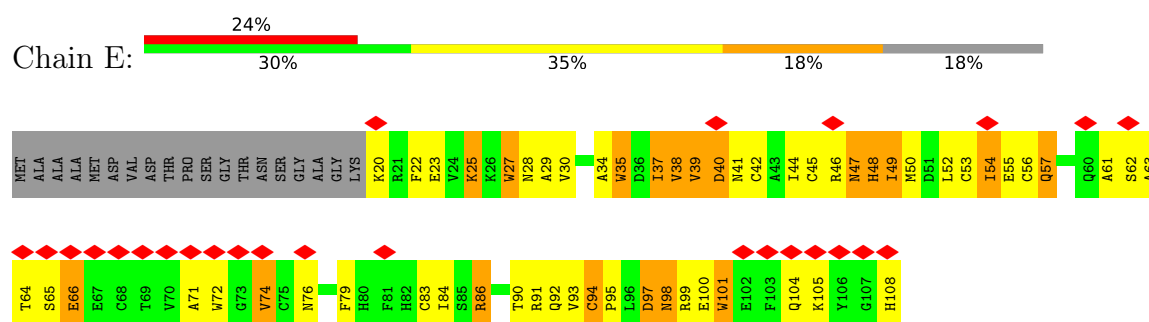
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	E	3	Total	Zn	0
			3	3	
5	D	3	Total	Zn	0
			3	3	

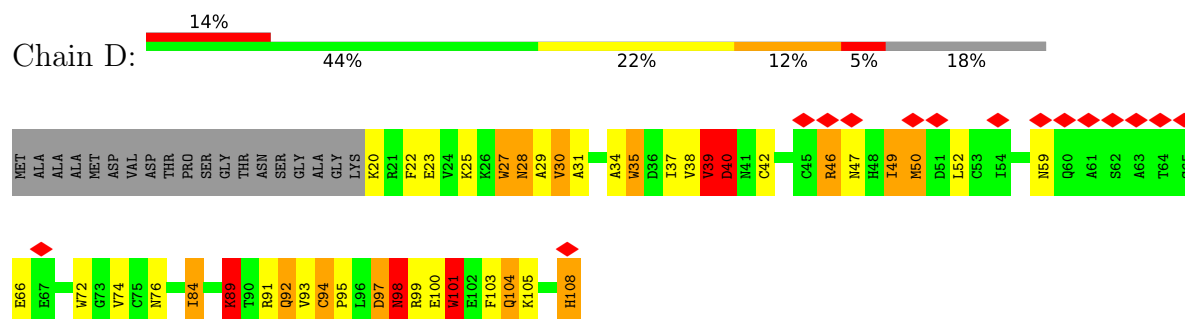
3 Residue-property plots

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.

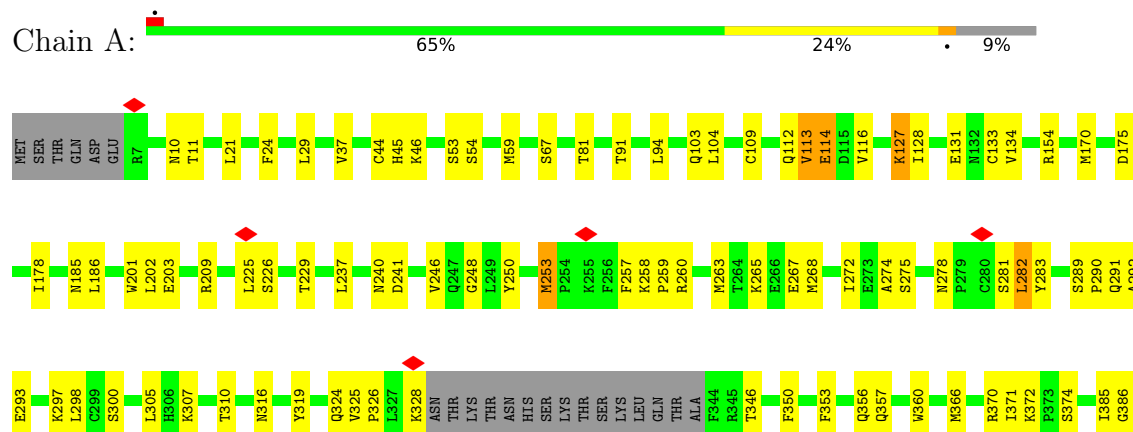
- Molecule 1: E3 ubiquitin-protein ligase RBX1

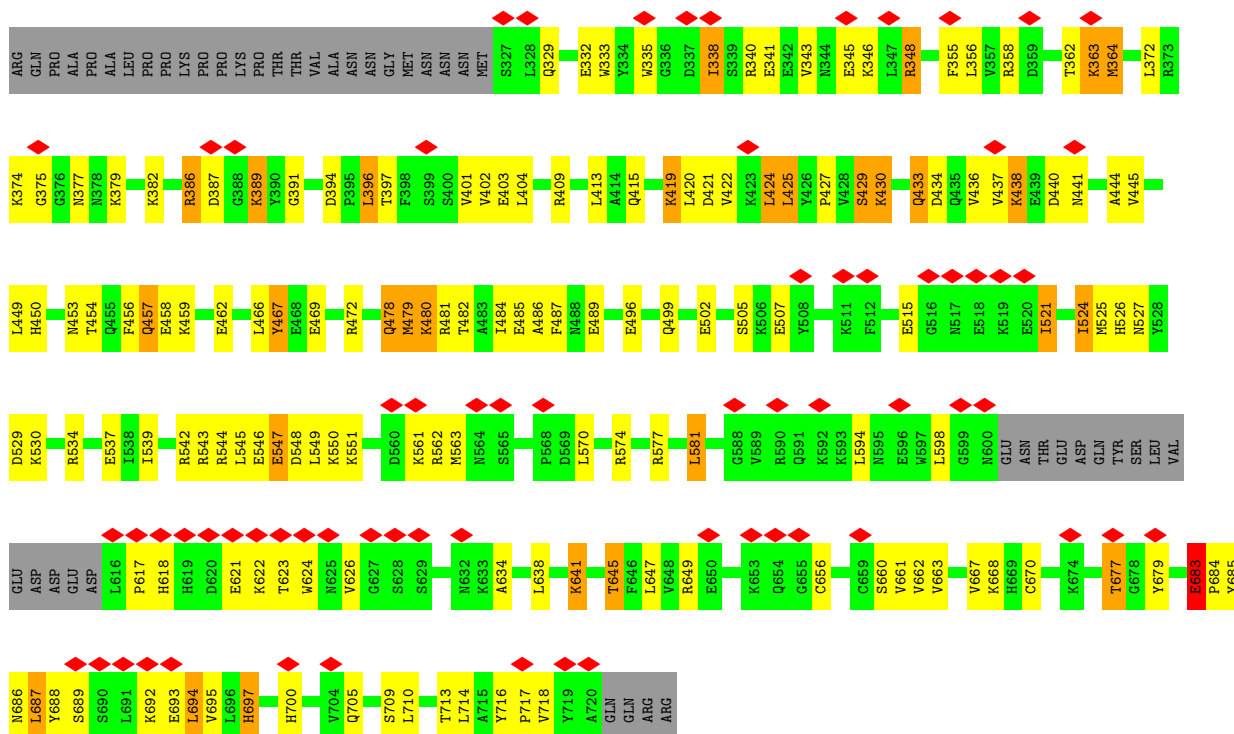


- Molecule 1: E3 ubiquitin-protein ligase RBX1

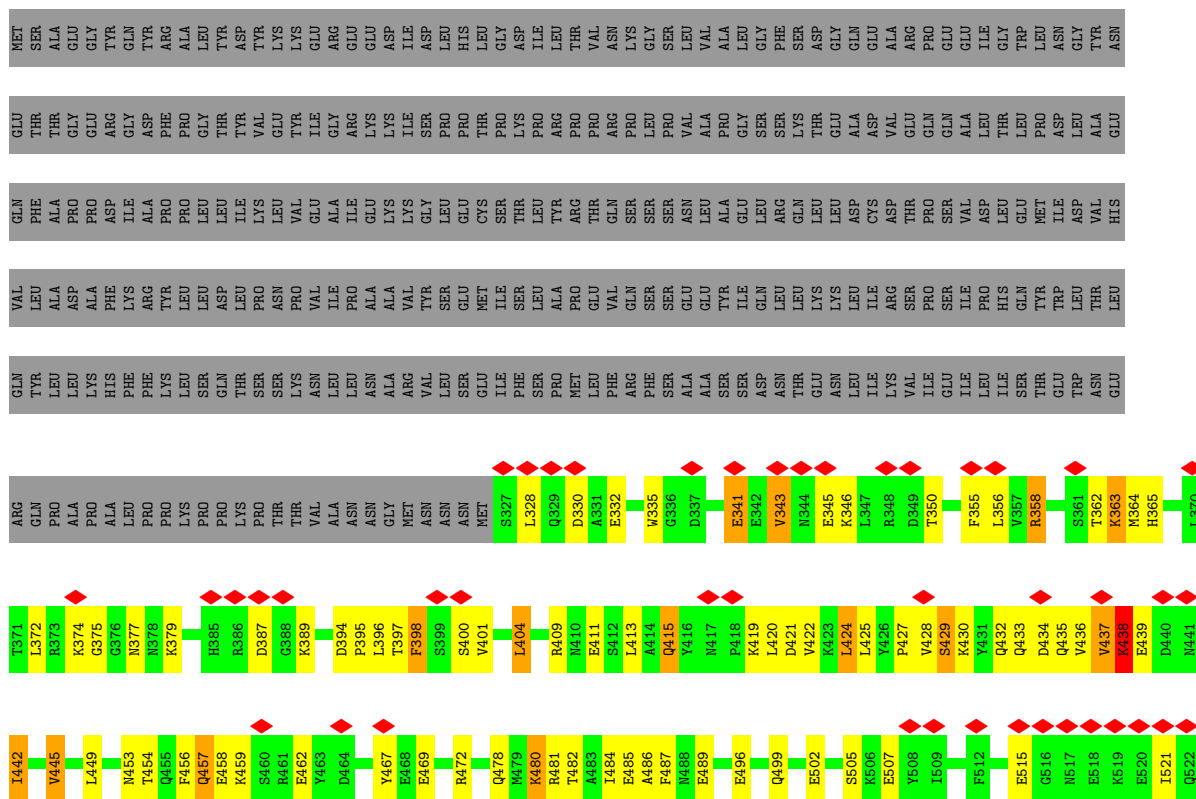
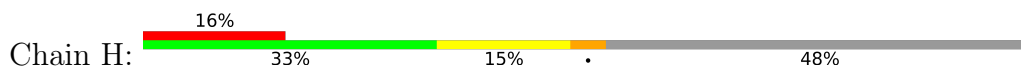


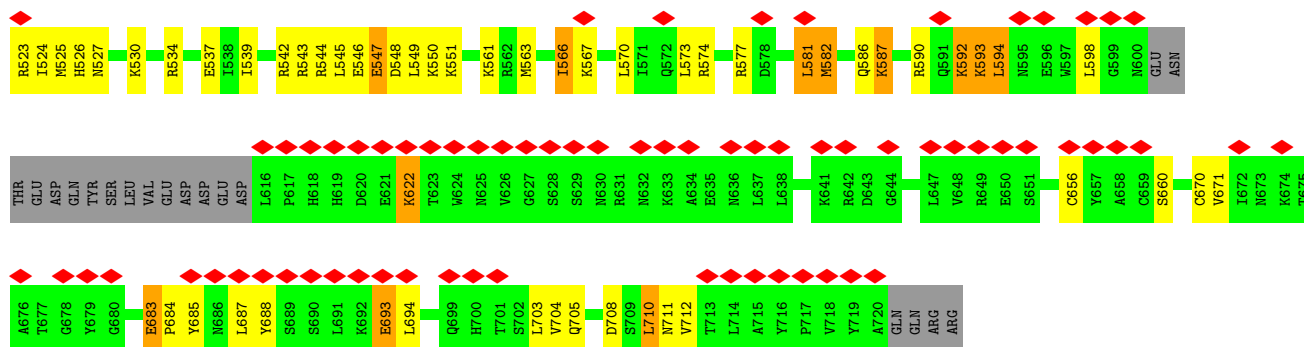
- Molecule 2: Kelch repeat and BTB domain-containing protein 2





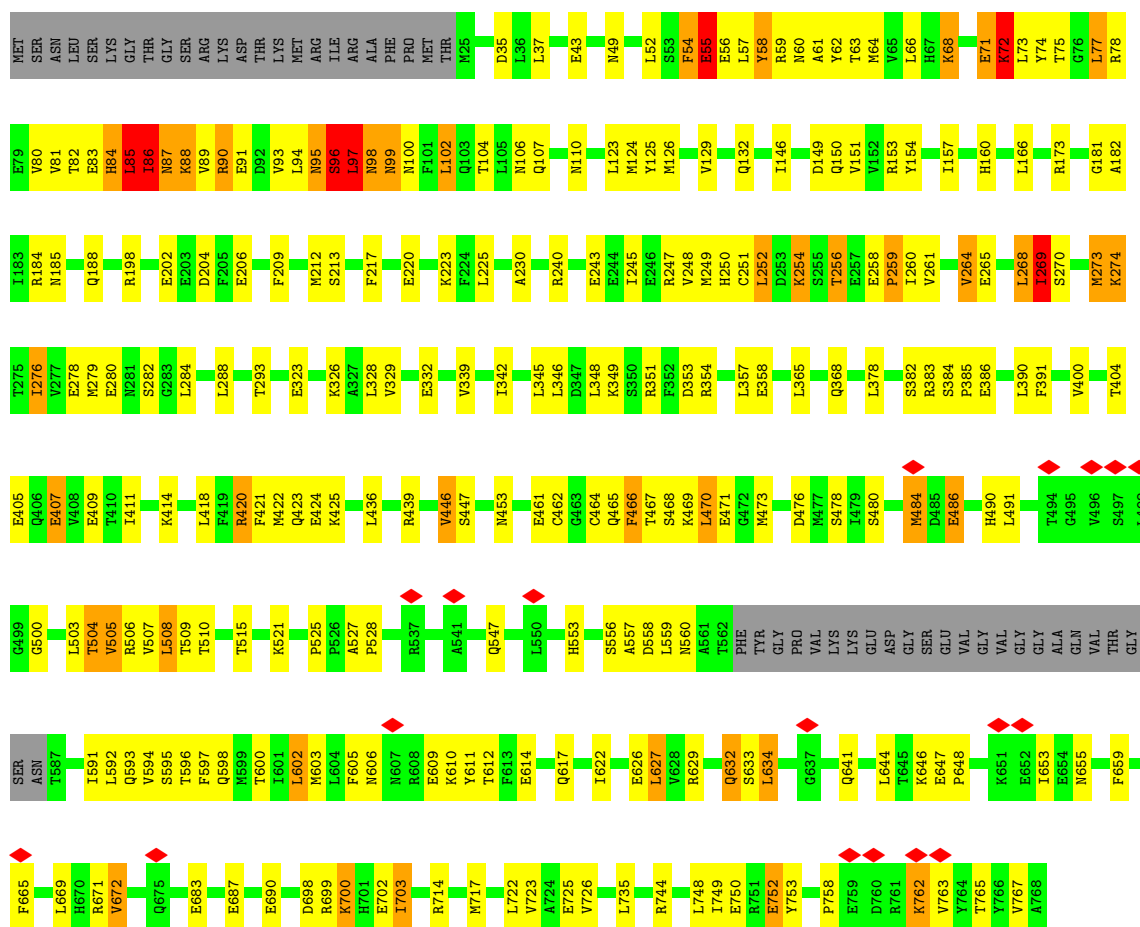
- Molecule 3: Phosphatidylinositol 3-kinase regulatory subunit alpha





• Molecule 4: Cullin-3

Chain C: 60% 28% 5% • 6%



• Molecule 4: Cullin-3

Chain F: 60% 28% 5% • 6%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	333476	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.895	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.001	Depositor
Map size ($\text{\AA}$)	511.488, 511.488, 511.488	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.332, 1.332, 1.332	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	D	0.77	1/759 (0.1%)	0.99	2/1029 (0.2%)
1	E	0.82	1/759 (0.1%)	1.01	1/1029 (0.1%)
2	A	0.41	0/4692	0.57	0/6367
2	B	0.33	0/4665	0.48	2/6330 (0.0%)
3	G	0.79	0/3209	0.97	1/4315 (0.0%)
3	H	0.78	0/3209	0.99	3/4315 (0.1%)
4	C	0.63	15/5959 (0.3%)	0.74	17/8006 (0.2%)
4	F	0.46	1/5959 (0.0%)	0.68	12/8006 (0.1%)
All	All	0.58	18/29211 (0.1%)	0.75	38/39397 (0.1%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	58	TYR	CA-C	-7.73	1.42	1.52
4	C	62	TYR	CA-C	-7.71	1.42	1.52
4	C	54	PHE	CA-C	-7.57	1.42	1.52
4	C	264	VAL	C-O	6.86	1.31	1.24
4	C	55	GLU	CA-C	-6.84	1.44	1.52
4	C	85	LEU	C-O	-6.80	1.15	1.24
4	C	61	ALA	CA-C	-6.71	1.44	1.52
4	C	57	LEU	N-CA	-6.55	1.38	1.46
4	C	63	THR	CA-C	-6.54	1.44	1.52
4	C	55	GLU	N-CA	-5.85	1.39	1.46
1	E	30	VAL	CA-CB	-5.79	1.47	1.54
1	D	30	VAL	CA-CB	-5.64	1.47	1.54
4	C	63	THR	N-CA	-5.49	1.39	1.46
4	C	96	SER	C-O	-5.48	1.17	1.24
4	F	481	ASN	C-O	5.42	1.30	1.24
4	C	59	ARG	CA-C	-5.28	1.46	1.52
4	C	64	MET	CA-C	-5.21	1.45	1.52
4	C	56	GLU	CA-C	-5.04	1.46	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	67	HIS	N-CA-C	-11.57	100.70	112.97
4	C	55	GLU	N-CA-C	-10.55	99.86	111.36
4	F	466	PHE	N-CA-C	-9.53	102.45	114.56
4	F	90	ARG	N-CA-C	-8.43	102.05	111.07
4	C	72	LYS	N-CA-C	-7.47	102.29	111.33
4	C	62	TYR	N-CA-C	-6.69	104.06	111.82
1	D	27	TRP	O-C-N	-6.45	116.04	123.33
4	C	95	ASN	N-CA-C	-6.35	104.40	111.71
4	C	259	PRO	CB-CA-C	-6.30	102.56	113.20
4	C	264	VAL	CB-CA-C	-6.24	103.71	111.70
4	F	69	HIS	N-CA-C	-6.20	103.40	111.71
1	E	27	TRP	O-C-N	-6.14	116.14	123.27
4	F	273	MET	N-CA-C	-6.08	104.56	111.07
3	G	424	LEU	N-CA-C	-5.85	106.38	112.93
3	H	424	LEU	N-CA-C	-5.83	106.39	112.93
4	C	62	TYR	CA-C-N	-5.79	112.57	120.44
4	C	62	TYR	C-N-CA	-5.79	112.57	120.44
1	D	89	LYS	N-CA-C	-5.78	106.27	113.38
4	C	58	TYR	N-CA-C	-5.74	105.16	111.82
4	C	77	LEU	N-CA-C	-5.73	104.03	111.02
4	F	467	THR	N-CA-C	-5.73	105.55	112.54
4	F	276	ILE	N-CA-C	-5.70	106.15	111.45
4	C	762	LYS	N-CA-C	-5.57	107.13	114.04
4	C	97	LEU	CA-C-N	-5.56	112.26	120.38
4	C	97	LEU	C-N-CA	-5.56	112.26	120.38
4	C	84	HIS	O-C-N	5.43	128.77	122.20
4	F	623	PRO	CA-C-N	-5.43	115.98	122.44
4	F	623	PRO	C-N-CA	-5.43	115.98	122.44
4	F	259	PRO	CA-C-N	-5.36	114.19	120.72
4	F	259	PRO	C-N-CA	-5.36	114.19	120.72
2	B	242	LYS	N-CA-C	-5.31	106.06	112.54
2	B	588	PRO	N-CA-C	-5.30	106.16	113.53
4	F	475	ARG	N-CA-C	-5.16	105.57	111.14
3	H	581	LEU	N-CA-C	-5.07	106.94	113.02
3	H	400	SER	N-CA-C	5.05	116.48	108.96
4	C	99	ASN	N-CA-C	5.02	117.43	109.50
4	C	54	PHE	CA-C-N	-5.00	113.19	120.29
4	C	54	PHE	C-N-CA	-5.00	113.19	120.29

There are no chirality outliers.

There are no planarity outliers.

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	D	737	0	686	27	0
1	E	737	0	686	54	0
2	A	4582	0	4481	113	0
2	B	4556	0	4461	110	0
3	G	3150	0	3096	79	0
3	H	3150	0	3096	60	0
4	C	5866	0	5904	163	0
4	F	5866	0	5904	164	0
5	D	3	0	0	0	0
5	E	3	0	0	0	0
All	All	28650	0	28314	747	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 13.

All (747) 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:B:154:ARG:HD3	2:B:357:GLN:NE2	1.43	1.33
2:A:298:LEU:CD2	2:A:591:LEU:HD21	1.76	1.15
2:B:298:LEU:HD23	2:B:591:LEU:HD21	1.26	1.10
4:C:342:ILE:HD13	4:C:391:PHE:CD2	1.88	1.08
2:A:298:LEU:HD23	2:A:591:LEU:HD21	1.14	1.08
4:F:342:ILE:HD13	4:F:391:PHE:CD2	1.88	1.08
2:B:185:ASN:CG	2:B:356:GLN:HE22	1.59	1.08
4:C:342:ILE:CG2	4:C:391:PHE:CD1	2.42	1.03
4:F:342:ILE:CG2	4:F:391:PHE:CD1	2.42	1.02
2:B:154:ARG:CD	2:B:357:GLN:NE2	2.22	1.02
4:F:469:LYS:HE3	1:D:104:GLN:HE22	1.20	1.02
1:D:39:VAL:O	1:D:40:ASP:HB3	1.56	1.01
2:A:154:ARG:HD3	2:A:357:GLN:NE2	1.73	1.01
4:F:342:ILE:HG21	4:F:391:PHE:CG	1.95	1.01
4:C:342:ILE:HG21	4:C:391:PHE:CG	1.95	1.00
4:C:378:LEU:HD23	4:C:422:MET:HG2	1.43	0.99
4:F:378:LEU:HD23	4:F:422:MET:HG2	1.43	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:ILE:HD11	1:E:39:VAL:HG22	1.44	0.99
2:B:154:ARG:HD3	2:B:357:GLN:HE21	0.94	0.98
4:F:342:ILE:HG21	4:F:391:PHE:CD1	2.00	0.96
4:F:469:LYS:HE3	1:D:104:GLN:NE2	1.81	0.95
4:C:342:ILE:HG21	4:C:391:PHE:CD1	2.00	0.95
4:F:768:ALA:HB1	1:D:89:LYS:HB3	1.47	0.93
2:A:154:ARG:HH11	2:A:357:GLN:HE22	1.13	0.93
4:F:342:ILE:HD13	4:F:391:PHE:CG	2.05	0.92
1:E:37:ILE:CD1	1:E:108:HIS:HE1	1.82	0.91
4:C:342:ILE:HD13	4:C:391:PHE:CG	2.05	0.91
2:A:297:LYS:HB3	2:A:592:GLU:OE1	1.70	0.91
2:B:298:LEU:CD2	2:B:591:LEU:HD21	1.99	0.91
1:E:79:PHE:CD2	1:E:84:ILE:HG21	2.06	0.90
4:F:96:SER:HB3	4:F:104:THR:HG21	1.54	0.90
2:A:59:MET:HE1	4:C:54:PHE:HB2	1.56	0.88
3:H:439:GLU:HB2	3:H:445:VAL:HG13	1.56	0.87
2:A:185:ASN:CG	2:A:356:GLN:HE22	1.81	0.87
4:F:506:ARG:HB2	1:D:30:VAL:HG22	1.55	0.86
1:E:71:ALA:CB	1:E:84:ILE:HD11	2.05	0.86
4:C:82:THR:HG22	4:C:146:ILE:HG12	1.58	0.84
2:A:154:ARG:HD3	2:A:357:GLN:HE21	1.39	0.83
4:F:440:LEU:HD13	4:F:477:MET:HG3	1.61	0.82
4:C:217:PHE:HE2	4:C:264:VAL:HG22	1.44	0.82
4:F:378:LEU:HD23	4:F:422:MET:CG	2.08	0.82
4:F:469:LYS:CE	1:D:104:GLN:HE22	1.92	0.82
4:F:342:ILE:HG23	4:F:391:PHE:CD1	2.15	0.81
4:C:378:LEU:HD23	4:C:422:MET:CG	2.08	0.81
2:A:154:ARG:NH1	2:A:357:GLN:NE2	2.29	0.81
2:B:185:ASN:CG	2:B:356:GLN:NE2	2.37	0.81
1:D:34:ALA:HA	1:D:76:ASN:ND2	1.97	0.80
2:A:154:ARG:NH1	2:A:357:GLN:HE22	1.79	0.79
1:E:39:VAL:HG12	1:E:39:VAL:O	1.82	0.79
2:A:298:LEU:HD23	2:A:591:LEU:CD2	2.07	0.79
1:E:71:ALA:HB3	1:E:84:ILE:HD11	1.63	0.79
4:C:342:ILE:HG23	4:C:391:PHE:CD1	2.15	0.79
4:C:86:ILE:HB	4:C:150:GLN:NE2	1.98	0.78
4:C:480:SER:HB2	4:C:506:ARG:HB3	1.66	0.77
4:C:217:PHE:CE2	4:C:264:VAL:HG22	2.19	0.77
4:F:89:VAL:HG11	4:F:151:VAL:HG22	1.66	0.77
4:C:345:LEU:HG	4:C:418:LEU:HD11	1.66	0.76
2:B:154:ARG:HH11	2:B:357:GLN:NE2	1.82	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:345:LEU:HG	4:F:418:LEU:HD11	1.66	0.76
3:H:343:VAL:HG21	3:H:358:ARG:HH11	1.51	0.75
2:B:265:LYS:HD3	2:B:587:TYR:CE1	2.22	0.75
2:A:253:MET:HB3	2:A:258:LYS:HG3	1.69	0.74
4:F:217:PHE:CE2	4:F:264:VAL:HB	2.23	0.74
4:F:93:VAL:HG11	4:F:156:CYS:SG	2.29	0.72
2:B:358:ASN:ND2	2:B:591:LEU:O	2.21	0.72
2:A:29:LEU:HD22	2:B:61:MET:SD	2.30	0.72
1:E:34:ALA:HA	1:E:76:ASN:ND2	2.05	0.72
4:F:342:ILE:HG21	4:F:391:PHE:CB	2.19	0.72
1:E:37:ILE:CD1	1:E:108:HIS:CE1	2.69	0.72
4:C:342:ILE:HG21	4:C:391:PHE:CB	2.19	0.72
4:C:94:LEU:O	4:C:97:LEU:HB2	1.88	0.71
4:C:86:ILE:HB	4:C:150:GLN:HE22	1.55	0.71
2:B:261:LEU:HG	2:B:587:TYR:CE1	2.25	0.71
2:A:297:LYS:HB3	2:A:592:GLU:CD	2.14	0.71
4:C:260:ILE:O	4:C:264:VAL:HG23	1.90	0.71
2:B:266:GLU:HG3	2:B:588:PRO:HG3	1.73	0.71
1:E:45:CYS:HB2	1:E:54:ILE:HG12	1.73	0.71
1:E:37:ILE:HD11	1:E:108:HIS:HE1	1.53	0.71
2:A:185:ASN:CG	2:A:356:GLN:NE2	2.47	0.71
1:E:79:PHE:CD2	1:E:84:ILE:CG2	2.74	0.69
2:A:154:ARG:CD	2:A:357:GLN:NE2	2.53	0.69
2:A:521:SER:HB2	2:A:542:HIS:HA	1.75	0.69
4:C:209:PHE:HE2	4:C:260:ILE:HG13	1.57	0.69
2:A:459:ARG:HB3	2:A:476:GLY:HA2	1.73	0.69
2:B:397:ARG:HB3	2:B:415:LEU:HB2	1.74	0.69
4:F:425:LYS:HZ2	4:F:462:CYS:HB2	1.58	0.69
1:E:37:ILE:HD11	1:E:108:HIS:CE1	2.28	0.68
2:A:372:LYS:HD3	2:A:580:ARG:HH21	1.58	0.68
4:C:323:GLU:HA	4:C:326:LYS:HZ3	1.58	0.68
1:E:52:LEU:HD11	1:E:66:GLU:HG2	1.75	0.68
1:E:71:ALA:HB3	1:E:84:ILE:CD1	2.22	0.68
2:A:240:ASN:ND2	2:A:291:GLN:HG2	2.08	0.68
2:B:436:LEU:O	2:B:455:ARG:NH2	2.26	0.67
3:H:387:ASP:C	3:H:389:LYS:H	2.03	0.67
2:B:372:LYS:HD3	2:B:580:ARG:HH21	1.60	0.67
2:B:185:ASN:ND2	2:B:356:GLN:HE22	1.92	0.67
3:G:453:ASN:HD21	3:G:577:ARG:NH1	1.92	0.66
4:C:622:ILE:HG12	4:C:627:LEU:HD13	1.76	0.66
4:C:342:ILE:HG21	4:C:391:PHE:HB2	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:154:ARG:HH11	2:A:357:GLN:NE2	1.85	0.66
2:B:154:ARG:CD	2:B:357:GLN:HE22	2.07	0.66
2:A:250:TYR:O	2:A:258:LYS:NZ	2.30	0.66
4:C:85:LEU:O	4:C:86:ILE:C	2.39	0.66
2:B:301:PRO:HD2	2:B:360:TRP:HD1	1.61	0.66
1:D:34:ALA:HA	1:D:76:ASN:HD21	1.61	0.65
1:E:79:PHE:HD2	1:E:84:ILE:HG21	1.61	0.65
4:F:622:ILE:HG12	4:F:627:LEU:HD13	1.77	0.65
4:F:66:LEU:C	4:F:68:LYS:H	2.02	0.65
3:G:618:HIS:HA	3:G:624:TRP:HE1	1.60	0.65
4:F:342:ILE:HG21	4:F:391:PHE:HB2	1.77	0.65
2:B:459:ARG:NH1	2:B:498:THR:OG1	2.30	0.64
4:F:504:THR:O	1:D:28:ASN:HA	1.98	0.64
3:G:459:LYS:HB3	3:G:570:LEU:HD13	1.79	0.64
3:G:449:LEU:HD21	3:G:594:LEU:CD2	2.27	0.64
2:A:268:MET:HE1	2:A:588:PRO:HB3	1.79	0.64
4:F:279:MET:O	4:F:280:GLU:HB2	1.98	0.64
4:F:556:SER:HA	4:F:595:SER:HA	1.80	0.64
4:C:89:VAL:HG21	4:C:151:VAL:HG22	1.79	0.64
4:F:258:GLU:HB2	4:F:259:PRO:HD3	1.79	0.64
2:B:570:ARG:HH22	2:B:601:TYR:HB2	1.63	0.63
3:H:459:LYS:HB3	3:H:570:LEU:HD13	1.79	0.63
1:E:44:ILE:CD1	1:E:84:ILE:HG22	2.28	0.63
2:A:436:LEU:O	2:A:455:ARG:NH2	2.31	0.63
4:F:102:LEU:O	4:F:106:ASN:ND2	2.32	0.63
1:E:37:ILE:HD11	1:E:39:VAL:CG2	2.25	0.63
2:A:300:SER:HA	2:A:360:TRP:HE1	1.62	0.62
4:F:264:VAL:HG13	4:F:265:GLU:H	1.64	0.62
3:G:694:LEU:HA	3:G:697:HIS:HB3	1.81	0.62
4:C:102:LEU:O	4:C:106:ASN:ND2	2.32	0.62
2:B:301:PRO:HD2	2:B:360:TRP:CD1	2.34	0.62
3:G:338:ILE:HG13	3:G:358:ARG:HG3	1.81	0.62
2:B:352:TRP:HB3	2:B:363:LYS:HE3	1.82	0.62
4:C:556:SER:HA	4:C:595:SER:HA	1.80	0.62
1:E:79:PHE:HB2	1:E:84:ILE:HG23	1.82	0.62
4:C:269:ILE:HG22	4:C:273:MET:HB2	1.82	0.61
2:B:154:ARG:HH11	2:B:357:GLN:HE22	1.47	0.61
1:E:34:ALA:HA	1:E:76:ASN:HD21	1.65	0.61
3:H:456:PHE:O	3:H:459:LYS:HB2	2.00	0.61
4:F:459:LYS:NZ	4:F:467:THR:HB	2.16	0.61
4:C:90:ARG:O	4:C:91:GLU:C	2.44	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:209:PHE:CE2	4:C:260:ILE:HG13	2.37	0.60
2:A:267:GLU:HG2	2:A:585:LYS:HG2	1.84	0.60
4:C:99:ASN:O	4:C:100:ASN:C	2.44	0.60
2:B:370:ARG:NH1	2:B:386:GLY:O	2.34	0.60
1:E:44:ILE:HD12	1:E:84:ILE:CG2	2.33	0.59
2:A:459:ARG:NH1	2:A:498:THR:OG1	2.35	0.59
3:G:456:PHE:O	3:G:459:LYS:HB2	2.02	0.59
3:H:394:ASP:N	3:H:395:PRO:HD2	2.18	0.59
3:G:547:GLU:HA	3:G:550:LYS:HG2	1.85	0.59
4:C:106:ASN:O	4:C:110:ASN:ND2	2.36	0.59
4:C:703:ILE:HD11	4:C:744:ARG:HD3	1.84	0.59
2:B:535:CYS:SG	2:B:564:ARG:NH1	2.75	0.59
4:F:703:ILE:HD11	4:F:744:ARG:HD3	1.85	0.59
3:G:374:LYS:HZ1	3:G:420:LEU:HA	1.68	0.59
4:F:86:ILE:HA	4:F:150:GLN:HE22	1.66	0.59
2:A:154:ARG:HD3	2:A:357:GLN:HE22	1.63	0.58
4:F:525:PRO:HB2	4:F:528:PRO:HD2	1.85	0.58
2:B:154:ARG:NH1	2:B:357:GLN:NE2	2.49	0.58
2:A:535:CYS:SG	2:A:564:ARG:NH1	2.76	0.58
1:D:72:TRP:HE1	1:D:108:HIS:HA	1.68	0.58
4:F:106:ASN:O	4:F:110:ASN:ND2	2.36	0.58
2:A:397:ARG:NH1	2:A:415:LEU:O	2.36	0.58
4:C:96:SER:O	4:C:99:ASN:N	2.26	0.58
4:F:328:LEU:HD22	4:F:348:LEU:HD21	1.86	0.58
4:F:342:ILE:CD1	4:F:391:PHE:CD2	2.78	0.58
4:C:342:ILE:CD1	4:C:391:PHE:CD2	2.78	0.58
2:B:250:TYR:O	2:B:258:LYS:NZ	2.35	0.57
3:H:547:GLU:HA	3:H:550:LYS:HG2	1.84	0.57
2:B:355:ALA:O	2:B:587:TYR:HD2	1.87	0.57
4:C:328:LEU:HD22	4:C:348:LEU:HD21	1.86	0.57
4:C:525:PRO:HB2	4:C:528:PRO:HD2	1.85	0.57
2:A:185:ASN:ND2	2:A:356:GLN:HE22	2.01	0.57
2:A:201:TRP:O	2:A:209:ARG:NH1	2.38	0.57
2:A:522:ASP:HB3	2:A:541:THR:HB	1.86	0.57
2:B:201:TRP:O	2:B:209:ARG:NH1	2.36	0.57
2:A:396:ARG:HD2	2:A:397:ARG:H	1.68	0.57
2:A:467:PHE:HB3	2:A:472:PHE:HE2	1.69	0.57
4:F:458:LEU:HB3	4:F:467:THR:HG22	1.86	0.57
4:C:345:LEU:CG	4:C:418:LEU:HD11	2.35	0.57
4:F:323:GLU:HA	4:F:326:LYS:HZ3	1.69	0.57
4:C:202:GLU:HA	4:C:206:GLU:HB3	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:93:VAL:HA	4:F:97:LEU:HG	1.87	0.57
1:D:27:TRP:CZ2	1:D:29:ALA:HB2	2.40	0.57
1:E:53:CYS:HB2	1:E:83:CYS:SG	2.46	0.56
4:C:248:VAL:HA	4:C:252:LEU:HB2	1.87	0.56
4:F:202:GLU:HA	4:F:206:GLU:HB3	1.87	0.56
1:E:27:TRP:CZ2	1:E:29:ALA:HB2	2.40	0.56
2:B:392:GLY:HA2	2:B:396:ARG:HG2	1.87	0.56
2:B:353:PHE:HB2	2:B:360:TRP:CZ2	2.41	0.56
4:F:220:GLU:HA	4:F:223:LYS:HG2	1.87	0.56
4:C:557:ALA:HB3	4:C:594:VAL:HG23	1.88	0.56
2:A:297:LYS:O	2:A:592:GLU:HB3	2.06	0.56
4:C:96:SER:O	4:C:98:ASN:N	2.38	0.56
3:H:372:LEU:HD11	3:H:413:LEU:HD13	1.87	0.56
4:F:49:ASN:HA	4:F:52:LEU:HD13	1.88	0.56
2:A:370:ARG:NH1	2:A:386:GLY:O	2.39	0.55
3:H:343:VAL:HG21	3:H:358:ARG:NH1	2.19	0.55
3:H:456:PHE:HE1	3:H:574:ARG:HG2	1.71	0.55
4:F:409:GLU:OE2	4:F:453:ASN:ND2	2.40	0.55
4:C:342:ILE:HG23	4:C:391:PHE:CE1	2.41	0.55
4:C:717:MET:HB3	4:C:722:LEU:HG	1.89	0.55
4:F:717:MET:HB3	4:F:722:LEU:HG	1.89	0.55
4:C:71:GLU:O	4:C:72:LYS:C	2.49	0.55
4:C:612:THR:OG1	4:C:655:ASN:O	2.24	0.55
4:F:100:ASN:HB3	4:F:103:GLN:HB2	1.89	0.55
4:F:342:ILE:HG23	4:F:391:PHE:CE1	2.41	0.55
4:F:480:SER:HB2	4:F:506:ARG:HE	1.71	0.55
4:F:129:VAL:O	4:F:132:GLN:NE2	2.40	0.55
4:F:612:THR:OG1	4:F:655:ASN:O	2.24	0.55
2:B:188:VAL:HG23	2:B:263:MET:HE2	1.89	0.55
4:C:78:ARG:O	4:C:82:THR:HG23	2.06	0.55
4:C:409:GLU:OE2	4:C:453:ASN:ND2	2.40	0.55
2:B:185:ASN:OD1	2:B:356:GLN:NE2	2.40	0.55
3:G:484:ILE:HD11	3:G:542:ARG:HG3	1.89	0.55
4:C:220:GLU:HA	4:C:223:LYS:HG2	1.87	0.55
3:H:496:GLU:HG2	3:H:499:GLN:HE21	1.72	0.55
4:C:365:LEU:HD12	4:C:368:GLN:HE21	1.72	0.54
3:G:449:LEU:HD21	3:G:594:LEU:HD22	1.89	0.54
4:C:58:TYR:OH	4:C:125:TYR:HB2	2.08	0.54
1:E:39:VAL:O	1:E:39:VAL:CG1	2.53	0.54
3:G:496:GLU:HG2	3:G:499:GLN:HE21	1.72	0.54
4:F:259:PRO:HA	4:F:262:LYS:HB2	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:397:ARG:HB3	2:A:415:LEU:HB2	1.89	0.54
4:C:74:TYR:O	4:C:77:LEU:HB3	2.07	0.54
4:C:129:VAL:O	4:C:132:GLN:NE2	2.40	0.54
4:F:557:ALA:HB3	4:F:594:VAL:HG23	1.88	0.54
4:C:86:ILE:O	4:C:87:ASN:C	2.48	0.54
4:C:49:ASN:HA	4:C:52:LEU:HD13	1.88	0.54
4:C:486:GLU:O	4:C:490:HIS:ND1	2.35	0.54
2:A:240:ASN:O	2:A:291:GLN:O	2.25	0.54
2:A:414:PRO:O	2:A:449:TRP:NE1	2.41	0.54
4:F:365:LEU:HD12	4:F:368:GLN:HE21	1.73	0.54
1:E:44:ILE:HD11	1:E:84:ILE:HG22	1.89	0.54
4:C:96:SER:O	4:C:97:LEU:C	2.51	0.54
2:B:267:GLU:HG2	2:B:585:LYS:HG2	1.89	0.54
3:G:679:TYR:HB2	3:G:688:TYR:HB2	1.91	0.53
2:A:94:LEU:HD11	2:A:104:LEU:HD21	1.91	0.53
3:G:456:PHE:HE1	3:G:574:ARG:HG2	1.74	0.53
3:G:374:LYS:NZ	3:G:420:LEU:HA	2.23	0.53
4:C:102:LEU:HD13	4:C:182:ALA:HB1	1.91	0.53
2:B:44:CYS:SG	2:B:45:HIS:N	2.75	0.53
2:B:253:MET:HE2	3:H:534:ARG:HH22	1.73	0.53
3:H:484:ILE:HD11	3:H:542:ARG:HG3	1.89	0.53
1:E:79:PHE:CB	1:E:84:ILE:HG23	2.38	0.53
4:F:345:LEU:CG	4:F:418:LEU:HD11	2.35	0.53
3:G:469:GLU:HA	3:G:472:ARG:HG2	1.91	0.53
4:C:71:GLU:HG2	4:C:72:LYS:HZ2	1.73	0.52
4:F:508:LEU:HD13	4:F:513:TRP:CE2	2.44	0.52
4:C:166:LEU:HD22	4:C:212:MET:HG2	1.91	0.52
2:B:94:LEU:HD11	2:B:104:LEU:HD21	1.91	0.52
3:H:469:GLU:HA	3:H:472:ARG:HG2	1.91	0.52
4:F:102:LEU:HD13	4:F:182:ALA:HB1	1.91	0.52
4:F:472:GLY:HA3	4:F:512:TYR:CZ	2.44	0.52
1:E:94:CYS:HB2	1:E:101:TRP:HB2	1.90	0.52
3:H:487:PHE:HE2	3:H:545:LEU:HG	1.74	0.52
4:F:614:GLU:OE1	4:F:617:GLN:NE2	2.41	0.52
2:B:346:THR:HG22	2:B:369:VAL:HB	1.92	0.52
2:B:524:CYS:SG	2:B:526:ARG:NH1	2.80	0.52
2:B:350:PHE:HD1	2:B:363:LYS:HB2	1.74	0.52
4:F:266:ARG:HG3	4:F:267:GLU:N	2.24	0.52
4:F:378:LEU:HD22	4:F:421:PHE:O	2.10	0.52
4:F:426:ASP:OD2	4:F:699:ARG:NH2	2.42	0.52
3:G:487:PHE:HE2	3:G:545:LEU:HG	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:459:LYS:HZ2	4:F:467:THR:HB	1.73	0.52
2:B:53:SER:OG	2:B:111:LEU:O	2.28	0.52
4:F:606:ASN:HD21	1:D:22:PHE:HD2	1.57	0.52
4:C:240:ARG:NH1	4:C:243:GLU:OE2	2.43	0.52
3:H:432:GLN:HB3	3:H:435:GLN:HB2	1.91	0.52
4:F:240:ARG:NH1	4:F:243:GLU:OE2	2.43	0.52
4:F:441:LEU:HD21	4:F:508:LEU:HD11	1.91	0.52
1:E:63:ALA:HB1	1:E:66:GLU:HA	1.92	0.51
2:B:186:LEU:HB2	2:B:260:ARG:HD3	1.92	0.51
1:E:45:CYS:HB2	1:E:54:ILE:HG23	1.91	0.51
4:C:614:GLU:OE1	4:C:617:GLN:NE2	2.41	0.51
2:B:243:SER:HB2	2:B:292:ALA:HB2	1.92	0.51
2:A:305:LEU:HB3	2:A:325:VAL:HG12	1.93	0.51
4:C:700:LYS:HG2	4:C:744:ARG:HD2	1.93	0.51
2:B:155:MET:HE1	2:B:352:TRP:CZ3	2.45	0.51
4:C:378:LEU:HD22	4:C:421:PHE:O	2.10	0.51
1:E:22:PHE:HD2	4:C:606:ASN:HD21	1.57	0.51
3:G:466:LEU:HD13	3:G:563:MET:HG2	1.93	0.51
2:B:123:TYR:HA	2:B:126:LYS:HE2	1.93	0.51
3:H:437:VAL:O	3:H:438:LYS:C	2.54	0.51
4:F:342:ILE:CG2	4:F:391:PHE:CG	2.76	0.51
4:F:506:ARG:O	1:D:31:ALA:N	2.34	0.51
4:C:90:ARG:O	4:C:94:LEU:HB2	2.11	0.51
4:C:149:ASP:HA	4:C:153:ARG:HB2	1.92	0.51
2:B:274:ALA:O	2:B:284:SER:N	2.38	0.51
3:H:502:GLU:O	3:H:505:SER:OG	2.24	0.51
3:H:543:ARG:HH21	3:H:546:GLU:HG3	1.76	0.51
2:B:226:SER:HB3	2:B:259:PRO:HB3	1.93	0.51
4:F:66:LEU:C	4:F:68:LYS:N	2.66	0.51
4:F:149:ASP:HA	4:F:153:ARG:HB2	1.92	0.51
4:F:166:LEU:HD22	4:F:212:MET:HG2	1.92	0.51
2:B:371:ILE:HB	2:B:388:ASP:HB2	1.93	0.51
2:B:467:PHE:HB3	2:B:472:PHE:HE2	1.75	0.51
2:B:549:TYR:OH	2:B:575:LEU:N	2.40	0.51
3:H:409:ARG:C	3:H:411:GLU:H	2.18	0.51
3:H:449:LEU:HD21	3:H:594:LEU:HG	1.93	0.51
1:D:20:LYS:HE3	1:D:23:GLU:HG2	1.93	0.50
3:G:543:ARG:HH21	3:G:546:GLU:HG3	1.76	0.50
2:A:385:ILE:HG21	2:A:433:VAL:HG21	1.93	0.50
1:E:61:ALA:O	1:E:62:SER:C	2.53	0.50
4:C:97:LEU:HD22	4:C:160:HIS:CD2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:459:ARG:NH2	2:B:473:TYR:O	2.44	0.50
4:C:83:GLU:O	4:C:84:HIS:C	2.52	0.50
2:B:274:ALA:N	2:B:284:SER:O	2.32	0.50
4:C:484:MET:SD	4:C:504:THR:HA	2.52	0.50
4:F:440:LEU:HB3	4:F:477:MET:SD	2.51	0.50
3:H:394:ASP:C	3:H:396:LEU:H	2.20	0.50
4:F:345:LEU:CD2	4:F:418:LEU:HD11	2.42	0.50
2:A:435:THR:OG1	2:A:436:LEU:N	2.41	0.50
4:F:559:LEU:O	4:F:592:LEU:N	2.39	0.50
3:G:457:GLN:O	3:G:458:GLU:C	2.55	0.49
3:G:480:LYS:HB3	3:G:549:LEU:HD21	1.94	0.49
3:H:457:GLN:O	3:H:458:GLU:C	2.55	0.49
3:G:645:THR:HA	3:G:716:TYR:HB2	1.94	0.49
4:F:598:GLN:HG2	4:F:634:LEU:HG	1.94	0.49
2:A:366:MET:HG2	2:A:409:TRP:CZ2	2.47	0.49
3:G:459:LYS:HD2	3:G:570:LEU:HD13	1.95	0.49
4:F:260:ILE:O	4:F:264:VAL:HG12	2.13	0.49
1:E:44:ILE:HD12	1:E:84:ILE:HG23	1.93	0.49
2:B:301:PRO:N	2:B:302:PRO:HD2	2.27	0.49
4:F:273:MET:HG3	4:F:303:PHE:HE2	1.78	0.49
4:F:473:MET:HG3	4:F:513:TRP:CZ2	2.46	0.49
2:A:186:LEU:HB2	2:A:260:ARG:HD3	1.94	0.49
4:C:632:GLN:HG3	4:C:633:SER:N	2.27	0.49
3:H:459:LYS:HA	3:H:462:GLU:HG3	1.93	0.49
2:A:44:CYS:SG	2:A:45:HIS:N	2.84	0.49
2:A:435:THR:O	2:A:455:ARG:NH2	2.38	0.49
2:A:459:ARG:NH1	2:A:475:GLY:O	2.45	0.49
4:C:559:LEU:O	4:C:592:LEU:N	2.39	0.49
2:B:188:VAL:H	2:B:262:GLY:HA3	1.77	0.49
2:B:353:PHE:HB2	2:B:360:TRP:CH2	2.47	0.49
1:E:20:LYS:HE3	1:E:23:GLU:HG2	1.93	0.49
2:A:550:VAL:HG23	2:A:566:HIS:HA	1.95	0.49
4:C:345:LEU:CD2	4:C:418:LEU:HD11	2.42	0.49
2:B:301:PRO:HB2	2:B:360:TRP:HB2	1.94	0.49
4:F:260:ILE:O	4:F:261:VAL:C	2.56	0.49
2:A:21:LEU:HD13	2:B:47:MET:HE3	1.95	0.48
2:A:24:PHE:CD1	2:A:29:LEU:HD12	2.48	0.48
3:H:527:ASN:HA	3:H:530:LYS:HE3	1.94	0.48
2:A:59:MET:CE	4:C:54:PHE:HB2	2.36	0.48
2:B:261:LEU:HG	2:B:587:TYR:CZ	2.48	0.48
3:H:456:PHE:CE1	3:H:574:ARG:HG2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:508:LEU:HD13	4:F:513:TRP:CD2	2.48	0.48
4:F:547:GLN:N	4:F:547:GLN:OE1	2.46	0.48
1:E:22:PHE:HB3	4:C:559:LEU:HD11	1.95	0.48
2:A:226:SER:HB3	2:A:259:PRO:HB3	1.95	0.48
3:G:441:ASN:HD22	3:G:444:ALA:H	1.60	0.48
1:E:71:ALA:HB1	1:E:84:ILE:HD11	1.93	0.48
3:G:450:HIS:O	3:G:453:ASN:HB2	2.14	0.48
4:C:77:LEU:O	4:C:78:ARG:C	2.56	0.48
2:B:399:VAL:HG12	2:B:414:PRO:HA	1.96	0.48
2:B:435:THR:OG1	2:B:436:LEU:N	2.42	0.48
4:F:217:PHE:HB3	4:F:268:LEU:HD12	1.96	0.48
4:C:614:GLU:HA	4:C:617:GLN:HG2	1.96	0.48
1:E:27:TRP:CE2	1:E:29:ALA:HB2	2.49	0.48
2:A:154:ARG:CD	2:A:357:GLN:HE22	2.21	0.48
2:A:427:VAL:HG11	2:A:504:VAL:HG21	1.95	0.48
4:C:86:ILE:HA	4:C:150:GLN:HE22	1.79	0.48
1:E:72:TRP:HB2	1:E:105:LYS:O	2.13	0.48
4:C:107:GLN:HA	4:C:110:ASN:HD21	1.79	0.48
4:C:644:LEU:HD11	4:C:659:PHE:HB3	1.96	0.48
4:F:256:THR:O	4:F:259:PRO:HD2	2.14	0.48
4:C:217:PHE:HA	4:C:220:GLU:HG2	1.96	0.48
4:C:404:THR:OG1	4:C:407:GLU:OE2	2.20	0.48
2:B:301:PRO:CG	2:B:360:TRP:HB2	2.44	0.48
4:F:504:THR:OG1	1:D:27:TRP:O	2.32	0.48
1:D:27:TRP:CE2	1:D:29:ALA:HB2	2.49	0.48
2:A:59:MET:HE1	4:C:54:PHE:CB	2.37	0.47
3:G:453:ASN:ND2	3:G:577:ARG:NH1	2.62	0.47
4:C:89:VAL:HG21	4:C:151:VAL:CG2	2.43	0.47
3:H:566:ILE:HD12	3:H:566:ILE:HA	1.74	0.47
4:F:559:LEU:HD11	1:D:22:PHE:HB3	1.95	0.47
4:F:644:LEU:HD11	4:F:659:PHE:HB3	1.96	0.47
3:G:502:GLU:O	3:G:505:SER:OG	2.24	0.47
4:C:547:GLN:OE1	4:C:547:GLN:N	2.46	0.47
2:B:240:ASN:ND2	2:B:291:GLN:HG2	2.30	0.47
2:B:286:VAL:HG11	2:B:573:TRP:HH2	1.80	0.47
3:H:387:ASP:C	3:H:389:LYS:N	2.72	0.47
4:F:266:ARG:HG3	4:F:267:GLU:H	1.79	0.47
3:G:683:GLU:H	3:G:684:PRO:HD2	1.80	0.47
4:C:386:GLU:OE1	4:C:386:GLU:N	2.44	0.47
4:F:107:GLN:HA	4:F:110:ASN:HD21	1.78	0.47
4:F:258:GLU:O	4:F:261:VAL:HG22	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:605:PHE:HE2	4:F:611:TYR:HB2	1.79	0.47
2:A:113:VAL:HB	2:A:116:VAL:HB	1.96	0.47
3:H:341:GLU:O	3:H:345:GLU:HG2	2.13	0.47
3:H:459:LYS:HD2	3:H:570:LEU:HD13	1.96	0.47
3:H:539:ILE:HD12	3:H:542:ARG:HH21	1.80	0.47
3:H:587:LYS:HA	3:H:587:LYS:HD3	1.56	0.47
4:F:217:PHE:HA	4:F:220:GLU:HG2	1.95	0.47
4:C:81:VAL:O	4:C:84:HIS:HB3	2.15	0.47
2:B:155:MET:HE1	2:B:352:TRP:CH2	2.50	0.47
4:F:90:ARG:HA	4:F:90:ARG:HD3	1.50	0.47
4:F:646:LYS:HE3	4:F:659:PHE:HE1	1.80	0.47
2:A:253:MET:HG2	2:A:258:LYS:HA	1.97	0.47
2:A:274:ALA:HB1	2:A:575:LEU:HD22	1.97	0.47
3:G:482:THR:O	3:G:485:GLU:HG3	2.15	0.47
3:G:663:VAL:HB	3:G:668:LYS:HE2	1.95	0.47
4:C:268:LEU:HD12	4:C:268:LEU:HA	1.70	0.47
2:A:300:SER:HA	2:A:360:TRP:NE1	2.30	0.47
3:G:372:LEU:HB2	3:G:379:LYS:HB2	1.97	0.47
2:B:442:TYR:HB2	2:B:449:TRP:CZ3	2.50	0.47
3:H:413:LEU:HB2	3:H:420:LEU:HB3	1.96	0.47
4:F:614:GLU:HA	4:F:617:GLN:HG2	1.96	0.47
2:A:91:THR:HA	2:B:9:ILE:HD11	1.97	0.47
4:C:605:PHE:HE2	4:C:611:TYR:HB2	1.79	0.47
4:F:264:VAL:O	4:F:265:GLU:C	2.58	0.47
4:C:198:ARG:HH22	4:C:256:THR:HA	1.80	0.46
3:H:544:ARG:O	3:H:547:GLU:HG3	2.15	0.46
4:F:609:GLU:HG3	4:F:610:LYS:H	1.80	0.46
4:F:712:LYS:NZ	4:F:767:VAL:O	2.40	0.46
3:G:480:LYS:HA	3:G:480:LYS:HD3	1.49	0.46
2:B:274:ALA:HB1	2:B:575:LEU:HD22	1.96	0.46
3:H:374:LYS:NZ	3:H:420:LEU:HA	2.31	0.46
3:H:442:ILE:HA	3:H:445:VAL:CG2	2.45	0.46
4:F:326:LYS:HA	4:F:329:VAL:HG22	1.97	0.46
3:G:377:ASN:HB3	3:G:379:LYS:NZ	2.30	0.46
1:D:94:CYS:HB2	1:D:101:TRP:HB2	1.96	0.46
2:A:526:ARG:NH2	2:A:577:ARG:O	2.39	0.46
2:B:102:GLU:OE1	2:B:102:GLU:N	2.41	0.46
4:F:687:GLU:O	4:F:690:GLU:HG3	2.15	0.46
4:C:609:GLU:HG3	4:C:610:LYS:H	1.80	0.46
2:B:586:LEU:HD13	2:B:591:LEU:HD11	1.97	0.46
3:H:482:THR:O	3:H:485:GLU:HG3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:82:THR:O	4:F:86:ILE:HG23	2.16	0.46
4:F:349:LYS:HZ2	4:F:414:LYS:HD2	1.80	0.46
1:E:86:ARG:HE	1:E:86:ARG:HB3	1.44	0.46
2:A:154:ARG:CZ	2:A:357:GLN:NE2	2.79	0.46
4:C:97:LEU:O	4:C:98:ASN:C	2.55	0.46
4:C:349:LYS:HZ1	4:C:414:LYS:HA	1.81	0.46
2:A:297:LYS:O	2:A:592:GLU:CB	2.63	0.46
2:A:431:ILE:HB	2:A:442:TYR:HB3	1.96	0.46
3:G:539:ILE:HD12	3:G:542:ARG:HH21	1.80	0.46
4:C:646:LYS:HE3	4:C:659:PHE:HE1	1.80	0.46
4:C:687:GLU:O	4:C:690:GLU:HG3	2.15	0.46
4:C:749:ILE:HD13	4:C:758:PRO:HD3	1.98	0.46
2:B:250:TYR:CE1	2:B:589:SER:HB2	2.50	0.46
3:H:377:ASN:HB3	3:H:379:LYS:NZ	2.30	0.46
4:F:265:GLU:O	4:F:266:ARG:C	2.58	0.46
3:G:409:ARG:HA	3:G:424:LEU:HB2	1.98	0.46
2:B:416:PRO:HG2	2:B:440:TYR:CD1	2.50	0.46
2:B:459:ARG:HB3	2:B:476:GLY:HA3	1.98	0.46
3:G:524:ILE:HD12	3:G:524:ILE:HA	1.84	0.46
3:G:544:ARG:O	3:G:547:GLU:HG3	2.15	0.46
4:C:486:GLU:HG3	4:C:490:HIS:CE1	2.50	0.46
4:F:349:LYS:HZ1	4:F:414:LYS:HA	1.81	0.46
4:C:71:GLU:O	4:C:74:TYR:N	2.49	0.46
2:B:188:VAL:N	2:B:262:GLY:HA3	2.31	0.46
1:E:25:LYS:HD2	4:C:560:ASN:HD22	1.81	0.45
1:E:41:ASN:HD21	1:E:46:ARG:HG2	1.81	0.45
3:G:481:ARG:HA	3:G:484:ILE:HG22	1.96	0.45
2:B:301:PRO:HG2	2:B:360:TRP:HB2	1.97	0.45
1:E:79:PHE:HB2	1:E:84:ILE:CG2	2.46	0.45
2:B:308:VAL:HG12	2:B:323:GLY:HA3	1.97	0.45
4:F:723:VAL:HA	4:F:726:VAL:HG12	1.98	0.45
1:D:39:VAL:O	1:D:40:ASP:CB	2.42	0.45
2:A:282:LEU:H	2:A:282:LEU:HG	1.52	0.45
2:A:316:ASN:ND2	2:A:585:LYS:O	2.39	0.45
2:B:363:LYS:O	2:B:364:THR:C	2.59	0.45
3:H:372:LEU:HB2	3:H:379:LYS:HB2	1.97	0.45
3:H:438:LYS:HD2	3:H:438:LYS:HA	1.60	0.45
1:E:45:CYS:CB	1:E:54:ILE:HG12	2.43	0.45
4:C:723:VAL:HA	4:C:726:VAL:HG12	1.99	0.45
2:B:261:LEU:HD12	2:B:264:THR:OG1	2.17	0.45
3:H:683:GLU:H	3:H:684:PRO:HD2	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:365:LEU:O	4:F:368:GLN:HG3	2.17	0.45
4:C:326:LYS:HA	4:C:329:VAL:HG22	1.97	0.45
3:H:363:LYS:HD3	3:H:363:LYS:HA	1.68	0.45
4:F:632:GLN:HG3	4:F:633:SER:N	2.30	0.45
2:A:10:ASN:OD1	2:A:11:THR:N	2.50	0.45
3:G:433:GLN:H	3:G:433:GLN:HG3	1.50	0.45
2:B:237:LEU:HB3	2:B:241:ASP:HB2	1.99	0.45
3:H:346:LYS:HD3	3:H:582:MET:HG2	1.99	0.45
1:D:52:LEU:HD13	1:D:52:LEU:HA	1.86	0.45
2:A:307:LYS:HD3	2:A:372:LYS:HE3	1.98	0.45
4:C:254:LYS:H	4:C:254:LYS:HG3	1.53	0.45
2:B:455:ARG:HH22	2:B:459:ARG:H	1.65	0.45
4:F:257:GLU:O	4:F:260:ILE:HG23	2.17	0.45
4:F:386:GLU:OE1	4:F:386:GLU:N	2.44	0.45
3:H:394:ASP:C	3:H:396:LEU:N	2.75	0.45
3:H:415:GLN:H	3:H:415:GLN:HG3	1.44	0.45
4:F:276:ILE:C	4:F:278:GLU:N	2.74	0.45
2:A:406:LYS:HB3	2:A:406:LYS:HE3	1.56	0.45
3:G:425:LEU:HD22	3:G:425:LEU:HA	1.79	0.45
4:C:89:VAL:O	4:C:90:ARG:C	2.60	0.45
4:F:714:ARG:NH1	4:F:725:GLU:OE2	2.50	0.45
2:B:474:ILE:HG23	2:B:499:VAL:HG22	1.99	0.44
2:A:392:GLY:HA3	2:A:395:ASN:HB3	2.00	0.44
4:C:714:ARG:NH1	4:C:725:GLU:OE2	2.50	0.44
2:B:366:MET:HE1	2:B:370:ARG:HB2	1.99	0.44
4:F:93:VAL:CG1	4:F:156:CYS:SG	3.02	0.44
4:F:185:ASN:HA	4:F:188:GLN:HG2	1.99	0.44
4:F:351:ARG:HA	4:F:354:ARG:HG2	2.00	0.44
1:D:94:CYS:HA	1:D:95:PRO:HD3	1.87	0.44
3:H:710:LEU:H	3:H:710:LEU:HG	1.50	0.44
4:F:246:GLU:HA	4:F:249:MET:HE2	2.00	0.44
2:A:170:MET:O	2:A:209:ARG:NH2	2.37	0.44
3:G:456:PHE:CE1	3:G:574:ARG:HG2	2.52	0.44
3:G:457:GLN:HE22	3:G:598:LEU:HA	1.83	0.44
4:C:467:THR:HA	4:C:470:LEU:HB2	2.00	0.44
2:B:572:LEU:HD22	2:B:572:LEU:HA	1.76	0.44
3:H:398:PHE:CD1	3:H:404:LEU:HA	2.53	0.44
3:G:459:LYS:HA	3:G:462:GLU:HG3	2.00	0.44
4:C:365:LEU:O	4:C:368:GLN:HG3	2.17	0.44
2:B:370:ARG:HH21	2:B:400:GLU:HG2	1.83	0.44
2:A:370:ARG:NH2	2:A:398:THR:O	2.38	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:371:ILE:N	2:A:387:GLY:O	2.40	0.44
2:A:374:SER:HB2	2:A:385:ILE:HB	2.00	0.44
3:G:521:ILE:HD12	3:G:521:ILE:HA	1.84	0.44
3:H:622:LYS:HA	3:H:622:LYS:HD3	1.53	0.44
4:F:261:VAL:O	4:F:262:LYS:C	2.60	0.44
4:F:436:LEU:HD23	4:F:439:ARG:HH11	1.82	0.44
1:E:100:GLU:O	1:E:101:TRP:HB3	2.18	0.44
3:G:454:THR:O	3:G:458:GLU:HG2	2.18	0.44
3:G:479:MET:HE3	3:G:479:MET:HB3	1.69	0.44
3:G:529:ASP:OD1	3:G:529:ASP:N	2.50	0.44
4:C:436:LEU:HD23	4:C:439:ARG:HH11	1.82	0.44
2:B:170:MET:O	2:B:209:ARG:NH2	2.38	0.44
4:F:390:LEU:HD13	4:F:390:LEU:HA	1.89	0.44
2:A:290:PRO:HG2	2:A:530:ILE:HD13	2.00	0.44
2:A:307:LYS:HB3	2:A:371:ILE:HG23	2.00	0.44
2:A:521:SER:CB	2:A:542:HIS:HA	2.46	0.44
4:C:274:LYS:HD2	4:C:274:LYS:HA	1.59	0.44
4:C:288:LEU:O	4:C:351:ARG:NH2	2.42	0.44
3:G:419:LYS:HD2	3:G:419:LYS:HA	1.44	0.44
4:C:83:GLU:O	4:C:86:ILE:HG23	2.17	0.44
4:C:351:ARG:HA	4:C:354:ARG:HG2	1.99	0.44
1:E:79:PHE:CG	1:E:84:ILE:CG2	3.00	0.43
2:A:237:LEU:HB3	2:A:241:ASP:HB2	1.99	0.43
4:C:71:GLU:C	4:C:73:LEU:N	2.69	0.43
4:C:466:PHE:HD1	4:C:466:PHE:HA	1.73	0.43
4:C:559:LEU:HD22	4:C:602:LEU:HD23	1.99	0.43
2:B:366:MET:HG2	2:B:409:TRP:CZ2	2.53	0.43
4:F:559:LEU:HD22	4:F:602:LEU:HD23	1.99	0.43
4:F:647:GLU:HB2	4:F:648:PRO:HD3	2.00	0.43
1:E:54:ILE:HA	1:E:57:GLN:HE21	1.83	0.43
1:E:94:CYS:HA	1:E:95:PRO:HD3	1.87	0.43
2:A:297:LYS:CB	2:A:592:GLU:OE1	2.55	0.43
3:G:355:PHE:O	3:G:356:LEU:HB3	2.18	0.43
4:C:86:ILE:CB	4:C:150:GLN:HE22	2.29	0.43
2:B:272:ILE:HD12	2:B:310:THR:HG22	1.99	0.43
2:B:570:ARG:HE	2:B:570:ARG:HA	1.83	0.43
3:H:548:ASP:O	3:H:551:LYS:HG3	2.18	0.43
4:F:622:ILE:HG13	4:F:627:LEU:HB2	2.01	0.43
3:G:438:LYS:HD2	3:G:438:LYS:HA	1.74	0.43
3:G:453:ASN:HD21	3:G:577:ARG:HH12	1.65	0.43
2:B:109:CYS:O	2:B:112:GLN:NE2	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:486:ALA:O	3:H:489:GLU:HG3	2.18	0.43
2:A:305:LEU:H	2:A:305:LEU:HD23	1.84	0.43
3:G:364:MET:H	3:G:364:MET:HG3	1.53	0.43
3:G:486:ALA:O	3:G:489:GLU:HG3	2.18	0.43
4:C:54:PHE:O	4:C:55:GLU:C	2.57	0.43
4:C:349:LYS:HZ2	4:C:414:LYS:HD2	1.83	0.43
4:C:527:ALA:HB3	4:C:528:PRO:HD3	2.00	0.43
2:A:442:TYR:HB2	2:A:449:TRP:CZ3	2.54	0.43
4:C:125:TYR:O	4:C:129:VAL:HG22	2.19	0.43
4:C:423:GLN:HG2	4:C:424:GLU:H	1.83	0.43
4:C:425:LYS:HZ2	4:C:462:CYS:HB2	1.84	0.43
4:F:553:HIS:HA	4:F:597:PHE:CE1	2.53	0.43
4:F:622:ILE:CG1	4:F:627:LEU:HB2	2.49	0.43
1:E:47:ASN:O	1:E:48:HIS:HB2	2.18	0.43
4:C:342:ILE:CG2	4:C:391:PHE:CG	2.76	0.43
2:B:154:ARG:HH11	2:B:357:GLN:CD	2.26	0.43
1:E:74:VAL:C	1:E:76:ASN:H	2.26	0.43
3:G:638:LEU:HD12	3:G:667:VAL:HG13	2.00	0.43
4:C:85:LEU:O	4:C:89:VAL:HG22	2.19	0.43
4:C:647:GLU:HB2	4:C:648:PRO:HD3	2.00	0.43
2:B:265:LYS:HD3	2:B:587:TYR:CD1	2.53	0.43
4:F:500:GLY:HA2	4:F:503:LEU:HD23	2.01	0.43
2:A:462:ALA:HA	2:A:475:GLY:HA3	2.00	0.43
3:G:677:THR:HB	3:G:687:LEU:HB3	2.01	0.43
4:C:503:LEU:HD12	4:C:505:VAL:HG22	2.00	0.43
2:B:154:ARG:NH1	2:B:357:GLN:CD	2.77	0.43
1:E:44:ILE:CD1	1:E:84:ILE:CG2	2.94	0.43
2:A:225:LEU:HB3	2:A:229:THR:HG23	2.01	0.43
3:G:386:ARG:HB3	3:G:387:ASP:H	1.54	0.43
4:C:185:ASN:HA	4:C:188:GLN:HG2	2.00	0.43
4:F:173:ARG:HH12	4:F:213:SER:HA	1.84	0.43
4:F:423:GLN:HG2	4:F:424:GLU:H	1.83	0.43
4:C:87:ASN:O	4:C:88:LYS:C	2.61	0.43
4:C:354:ARG:HA	4:C:357:LEU:HG	2.01	0.43
2:B:352:TRP:HB3	2:B:363:LYS:CE	2.46	0.43
3:H:355:PHE:O	3:H:356:LEU:HB3	2.18	0.43
4:F:525:PRO:HB3	4:F:603:MET:HG3	2.01	0.43
4:F:527:ALA:HB3	4:F:528:PRO:HD3	2.00	0.43
4:C:82:THR:O	4:C:85:LEU:HB2	2.19	0.42
4:C:446:VAL:HG23	4:C:447:SER:H	1.84	0.42
4:C:525:PRO:HB3	4:C:603:MET:HG3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:88:LYS:HA	4:F:88:LYS:HD3	1.61	0.42
4:F:125:TYR:O	4:F:129:VAL:HG22	2.19	0.42
4:F:181:GLY:HA2	4:F:184:ARG:HG2	2.01	0.42
2:A:250:TYR:HD2	2:A:259:PRO:HG2	1.83	0.42
4:C:154:TYR:HB3	4:C:157:ILE:HG22	2.01	0.42
4:C:346:LEU:HD23	4:C:418:LEU:CD1	2.49	0.42
2:A:246:VAL:O	2:A:250:TYR:HB3	2.18	0.42
3:G:389:LYS:HA	3:G:389:LYS:HD3	1.71	0.42
4:C:80:VAL:O	4:C:81:VAL:C	2.61	0.42
4:C:553:HIS:HA	4:C:597:PHE:CE1	2.53	0.42
3:H:459:LYS:HE2	3:H:573:LEU:HD12	2.02	0.42
4:F:446:VAL:HG23	4:F:447:SER:H	1.83	0.42
4:F:490:HIS:O	4:F:493:ALA:HB3	2.19	0.42
4:F:491:LEU:HA	4:F:491:LEU:HD23	1.79	0.42
2:A:537:PHE:HE2	2:A:567:ILE:HG13	1.85	0.42
3:G:391:GLY:HA3	3:G:396:LEU:HA	2.00	0.42
3:G:548:ASP:O	3:G:551:LYS:HG3	2.18	0.42
4:F:404:THR:OG1	4:F:407:GLU:OE2	2.20	0.42
1:D:98:ASN:HD22	1:D:98:ASN:HA	1.71	0.42
2:A:319:TYR:HB3	2:A:350:PHE:CE2	2.54	0.42
2:A:326:PRO:O	2:A:328:LYS:NZ	2.45	0.42
2:A:391:GLY:H	2:A:396:ARG:HG3	1.84	0.42
2:A:554:TYR:HB2	2:A:561:TRP:CE3	2.55	0.42
3:G:382:LYS:HD3	3:G:382:LYS:HA	1.85	0.42
3:G:478:GLN:HE21	3:G:478:GLN:HB3	1.56	0.42
3:G:641:LYS:HA	3:G:641:LYS:HD3	1.58	0.42
2:B:261:LEU:HD11	2:B:590:CYS:SG	2.60	0.42
2:A:519:ARG:HE	2:A:519:ARG:HB3	1.51	0.42
4:C:37:LEU:HD21	4:C:60:ASN:CB	2.50	0.42
4:C:476:ASP:HB3	4:C:508:LEU:HB3	2.01	0.42
4:C:598:GLN:HG2	4:C:634:LEU:HG	2.01	0.42
2:A:257:PHE:CD2	3:G:534:ARG:HD2	2.54	0.42
3:G:697:HIS:HA	3:G:700:HIS:NE2	2.34	0.42
4:C:181:GLY:HA2	4:C:184:ARG:HG2	2.01	0.42
2:B:348:ASN:ND2	2:B:366:MET:O	2.32	0.42
2:B:437:ASN:O	2:B:455:ARG:N	2.40	0.42
4:F:488:ARG:HA	4:F:488:ARG:HD2	1.56	0.42
1:E:52:LEU:HD13	1:E:56:CYS:HB3	2.02	0.42
2:A:127:LYS:HA	2:A:127:LYS:HD3	1.71	0.42
3:G:459:LYS:O	3:G:462:GLU:HG3	2.20	0.42
4:F:346:LEU:HD23	4:F:418:LEU:CD1	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:ASN:OD1	2:B:11:THR:N	2.53	0.42
3:H:409:ARG:HA	3:H:424:LEU:HB2	2.02	0.42
4:F:475:ARG:O	4:F:476:ASP:C	2.62	0.42
2:A:175:ASP:HA	2:A:178:ILE:HG12	2.01	0.42
3:G:333:TRP:HH2	3:G:402:VAL:HA	1.84	0.42
4:C:349:LYS:NZ	4:C:414:LYS:HD2	2.35	0.42
4:C:68:LYS:HD3	4:C:68:LYS:HA	1.76	0.41
2:B:223:ASP:HB2	2:B:257:PHE:HE1	1.84	0.41
4:F:293:THR:HB	4:F:358:GLU:CD	2.46	0.41
1:D:50:MET:H	1:D:50:MET:HG2	1.76	0.41
1:D:84:ILE:HD13	1:D:84:ILE:O	2.20	0.41
1:E:65:SER:O	1:E:66:GLU:C	2.62	0.41
2:A:390:VAL:HA	2:A:396:ARG:HG3	2.02	0.41
2:B:554:TYR:HB2	2:B:561:TRP:CZ3	2.54	0.41
4:F:317:MET:HE2	4:F:317:MET:HB2	2.00	0.41
4:F:354:ARG:HA	4:F:357:LEU:HG	2.01	0.41
3:G:364:MET:HE2	3:G:364:MET:HB2	1.66	0.41
4:C:96:SER:CB	4:C:104:THR:HG21	2.50	0.41
4:C:258:GLU:HB3	4:C:259:PRO:HD3	2.02	0.41
4:C:593:GLN:HE21	4:C:593:GLN:HB3	1.71	0.41
3:H:593:LYS:HD2	3:H:593:LYS:HA	1.35	0.41
4:F:67:HIS:O	4:F:68:LYS:C	2.64	0.41
4:F:154:TYR:HB3	4:F:157:ILE:HG22	2.01	0.41
4:F:257:GLU:O	4:F:261:VAL:HG13	2.20	0.41
4:F:467:THR:HA	4:F:470:LEU:HB2	2.01	0.41
4:F:710:ILE:HG21	4:F:729:GLN:HE22	1.86	0.41
4:F:756:ARG:HA	4:F:764:TYR:CE1	2.54	0.41
2:A:467:PHE:HB3	2:A:472:PHE:CE2	2.53	0.41
4:C:293:THR:HB	4:C:358:GLU:CD	2.45	0.41
3:H:592:LYS:HA	3:H:592:LYS:HD3	1.59	0.41
4:F:262:LYS:O	4:F:263:VAL:C	2.64	0.41
4:F:288:LEU:O	4:F:351:ARG:NH2	2.42	0.41
4:F:752:GLU:H	4:F:752:GLU:HG3	1.55	0.41
1:D:97:ASP:OD1	1:D:97:ASP:N	2.54	0.41
2:A:298:LEU:HD21	2:A:591:LEU:HD21	1.84	0.41
2:A:353:PHE:HB2	2:A:360:TRP:CH2	2.56	0.41
4:C:173:ARG:HH12	4:C:213:SER:HA	1.84	0.41
4:F:464:CYS:HA	4:F:467:THR:OG1	2.20	0.41
4:F:592:LEU:HD23	4:F:672:VAL:HG13	2.02	0.41
1:D:49:ILE:HD12	1:D:49:ILE:HA	1.80	0.41
2:A:114:GLU:H	2:A:114:GLU:HG2	1.48	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:240:ASN:ND2	2:A:291:GLN:CG	2.82	0.41
3:G:430:LYS:H	3:G:430:LYS:HG3	1.56	0.41
4:C:230:ALA:HB2	4:C:276:ILE:HG13	2.01	0.41
4:C:348:LEU:HA	4:C:351:ARG:HG2	2.02	0.41
4:C:592:LEU:HD23	4:C:672:VAL:HG13	2.02	0.41
2:B:97:ASN:OD1	2:B:100:THR:OG1	2.32	0.41
2:B:593:GLU:H	2:B:593:GLU:HG2	1.47	0.41
1:E:97:ASP:N	1:E:97:ASP:OD1	2.54	0.41
3:G:363:LYS:HD2	3:G:363:LYS:HA	1.45	0.41
4:C:339:VAL:HG23	4:C:391:PHE:CD1	2.56	0.41
4:C:500:GLY:HA2	4:C:503:LEU:HD23	2.01	0.41
3:H:534:ARG:HA	3:H:537:GLU:HG2	2.03	0.41
4:F:85:LEU:O	4:F:86:ILE:C	2.64	0.41
4:F:488:ARG:HH12	4:F:502:ASP:HA	1.85	0.41
1:E:37:ILE:HD13	1:E:72:TRP:CH2	2.56	0.41
4:F:123:LEU:HB3	4:F:126:MET:HE2	2.03	0.41
4:F:348:LEU:HA	4:F:351:ARG:HG2	2.02	0.41
1:E:38:VAL:C	1:E:40:ASP:H	2.28	0.41
2:A:459:ARG:HD2	2:A:476:GLY:HA3	2.03	0.41
3:G:467:TYR:HD1	3:G:467:TYR:HA	1.73	0.41
3:G:581:LEU:HD12	3:G:581:LEU:HA	1.84	0.41
3:G:617:PRO:HB2	3:G:717:PRO:HG2	2.02	0.41
3:G:710:LEU:HA	3:G:710:LEU:HD23	1.84	0.41
4:C:84:HIS:O	4:C:85:LEU:C	2.63	0.41
2:B:46:LYS:NZ	2:B:67:SER:O	2.53	0.41
2:B:598:PRO:HA	2:B:599:PRO:HD3	1.90	0.41
3:H:335:TRP:CZ3	3:H:346:LYS:HD2	2.56	0.41
4:C:384:SER:HB2	4:C:385:PRO:HD3	2.03	0.41
2:B:427:VAL:HG21	2:B:471:ILE:HG12	2.02	0.41
3:H:480:LYS:HB3	3:H:549:LEU:HD21	2.03	0.41
4:F:274:LYS:O	4:F:277:VAL:HG22	2.21	0.41
4:F:349:LYS:NZ	4:F:414:LYS:HD2	2.35	0.41
4:F:420:ARG:NH1	4:F:461:GLU:OE2	2.54	0.41
2:A:81:THR:HG21	2:A:103:GLN:HG3	2.04	0.40
2:A:289:SER:HB3	2:A:292:ALA:HB3	2.03	0.40
3:G:624:TRP:HA	3:G:718:VAL:HG12	2.02	0.40
4:C:123:LEU:HB3	4:C:126:MET:HE2	2.03	0.40
4:C:749:ILE:HG21	4:C:758:PRO:HD3	2.03	0.40
2:B:109:CYS:HA	2:B:117:LEU:HD11	2.03	0.40
4:F:560:ASN:HA	4:F:591:ILE:HG13	2.03	0.40
1:E:49:ILE:HD12	1:E:49:ILE:HA	1.66	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:46:LYS:NZ	2:A:67:SER:O	2.54	0.40
2:A:112:GLN:HG2	4:C:124:MET:HE1	2.03	0.40
2:A:202:LEU:HD12	2:A:203:GLU:HG3	2.03	0.40
4:C:558:ASP:OD1	4:C:671:ARG:NH2	2.54	0.40
2:B:417:CYS:HB2	2:B:419:TRP:CZ2	2.56	0.40
3:H:420:LEU:HA	3:H:420:LEU:HD23	1.94	0.40
4:F:384:SER:HB2	4:F:385:PRO:HD3	2.03	0.40
2:A:278:ASN:HD22	2:A:281:SER:H	1.69	0.40
3:G:335:TRP:CG	3:G:335:TRP:O	2.74	0.40
3:G:534:ARG:HA	3:G:537:GLU:HG2	2.02	0.40
3:G:634:ALA:HB2	3:G:649:ARG:HD3	2.03	0.40
4:C:622:ILE:HG13	4:C:627:LEU:HB2	2.03	0.40
4:F:653:ILE:H	4:F:653:ILE:HD13	1.87	0.40
2:A:272:ILE:HD12	2:A:310:THR:HG22	2.03	0.40
3:G:527:ASN:HA	3:G:530:LYS:HE3	2.02	0.40
4:C:245:ILE:HD13	4:C:261:VAL:HG11	2.04	0.40
4:C:420:ARG:NH1	4:C:461:GLU:OE2	2.54	0.40
4:C:560:ASN:HA	4:C:591:ILE:HG13	2.03	0.40
4:C:752:GLU:O	4:C:753:TYR:C	2.65	0.40
2:B:265:LYS:HA	2:B:265:LYS:HD2	1.89	0.40
2:B:273:GLU:OE2	2:B:307:LYS:N	2.55	0.40
2:B:599:PRO:O	2:B:600:THR:C	2.65	0.40
4:F:432:TYR:HE2	4:F:470:LEU:HD21	1.86	0.40
4:F:556:SER:OG	1:D:28:ASN:ND2	2.55	0.40
2:A:442:TYR:OH	2:A:447:ASP:OD1	2.38	0.40
2:A:522:ASP:O	2:A:540:GLU:HA	2.21	0.40
2:A:571:VAL:HA	2:A:597:LYS:HB3	2.03	0.40
3:G:348:ARG:HE	3:G:348:ARG:HB3	1.76	0.40
4:C:553:HIS:HA	4:C:597:PHE:HE1	1.87	0.40
2:B:108:ALA:O	2:B:112:GLN:N	2.53	0.40
3:H:688:TYR:HB3	3:H:693:GLU:HB3	2.03	0.40
4:F:263:VAL:HG23	4:F:264:VAL:H	1.87	0.40
4:F:680:LYS:HE3	4:F:680:LYS:HB3	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	D	87/108 (81%)	61 (70%)	16 (18%)	10 (12%)	0	5
1	E	87/108 (81%)	55 (63%)	19 (22%)	13 (15%)	0	3
2	A	561/623 (90%)	516 (92%)	42 (8%)	3 (0%)	24	63
2	B	558/623 (90%)	518 (93%)	37 (7%)	3 (0%)	24	63
3	G	375/724 (52%)	328 (88%)	43 (12%)	4 (1%)	11	45
3	H	375/724 (52%)	338 (90%)	30 (8%)	7 (2%)	6	32
4	C	716/768 (93%)	648 (90%)	62 (9%)	6 (1%)	16	53
4	F	716/768 (93%)	654 (91%)	56 (8%)	6 (1%)	16	53
All	All	3475/4446 (78%)	3118 (90%)	305 (9%)	52 (2%)	11	38

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	521	SER
4	C	97	LEU
4	C	269	ILE
4	C	270	SER
2	B	592	GLU
3	H	398	PHE
4	F	264	VAL
4	F	280	GLU
1	D	40	ASP
1	E	39	VAL
1	E	66	GLU
1	E	94	CYS
3	G	375	GLY
3	G	683	GLU
4	C	85	LEU
4	C	86	ILE
3	H	375	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	438	LYS
1	D	35	TRP
1	D	92	GLN
1	D	94	CYS
1	E	35	TRP
1	E	57	GLN
1	E	64	THR
1	E	98	ASN
1	E	104	GLN
4	C	87	ASN
3	H	683	GLU
4	F	263	VAL
1	E	40	ASP
1	E	97	ASP
3	G	429	SER
2	B	599	PRO
4	F	262	LYS
1	D	97	ASP
1	D	98	ASN
1	E	48	HIS
1	E	101	TRP
4	F	381	ASN
1	D	46	ARG
3	G	427	PRO
3	H	330	ASP
3	H	429	SER
1	D	39	VAL
1	D	101	TRP
1	E	38	VAL
2	B	248	GLY
3	H	427	PRO
2	A	248	GLY
2	A	599	PRO
4	F	623	PRO
1	D	38	VAL

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	D	78/90 (87%)	51 (65%)	27 (35%)	0	2
1	E	78/90 (87%)	60 (77%)	18 (23%)	1	5
2	A	510/560 (91%)	473 (93%)	37 (7%)	13	34
2	B	507/560 (90%)	479 (94%)	28 (6%)	19	42
3	G	345/654 (53%)	268 (78%)	77 (22%)	1	6
3	H	345/654 (53%)	272 (79%)	73 (21%)	1	6
4	C	652/693 (94%)	557 (85%)	95 (15%)	3	14
4	F	652/693 (94%)	561 (86%)	91 (14%)	3	15
All	All	3167/3994 (79%)	2721 (86%)	446 (14%)	5	15

All (446) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	25	LYS
1	E	28	ASN
1	E	35	TRP
1	E	37	ILE
1	E	42	CYS
1	E	47	ASN
1	E	49	ILE
1	E	50	MET
1	E	54	ILE
1	E	55	GLU
1	E	74	VAL
1	E	86	ARG
1	E	90	THR
1	E	91	ARG
1	E	92	GLN
1	E	93	VAL
1	E	98	ASN
1	E	99	ARG
2	A	37	VAL
2	A	53	SER
2	A	54	SER
2	A	109	CYS
2	A	113	VAL
2	A	114	GLU
2	A	127	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	128	ILE
2	A	131	GLU
2	A	133	CYS
2	A	134	VAL
2	A	253	MET
2	A	263	MET
2	A	265	LYS
2	A	275	SER
2	A	282	LEU
2	A	283	TYR
2	A	293	GLU
2	A	324	GLN
2	A	346	THR
2	A	390	VAL
2	A	396	ARG
2	A	406	LYS
2	A	469	ASP
2	A	470	LYS
2	A	519	ARG
2	A	565	GLN
2	A	568	SER
2	A	569	GLU
2	A	570	ARG
2	A	571	VAL
2	A	572	LEU
2	A	589	SER
2	A	597	LYS
2	A	600	THR
2	A	601	TYR
2	A	602	LEU
3	G	329	GLN
3	G	332	GLU
3	G	338	ILE
3	G	340	ARG
3	G	341	GLU
3	G	343	VAL
3	G	345	GLU
3	G	346	LYS
3	G	348	ARG
3	G	362	THR
3	G	363	LYS
3	G	364	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	386	ARG
3	G	389	LYS
3	G	394	ASP
3	G	396	LEU
3	G	397	THR
3	G	401	VAL
3	G	403	GLU
3	G	404	LEU
3	G	413	LEU
3	G	415	GLN
3	G	419	LYS
3	G	421	ASP
3	G	422	VAL
3	G	425	LEU
3	G	429	SER
3	G	430	LYS
3	G	433	GLN
3	G	434	ASP
3	G	436	VAL
3	G	437	VAL
3	G	438	LYS
3	G	440	ASP
3	G	445	VAL
3	G	457	GLN
3	G	467	TYR
3	G	478	GLN
3	G	479	MET
3	G	480	LYS
3	G	507	GLU
3	G	515	GLU
3	G	521	ILE
3	G	524	ILE
3	G	525	MET
3	G	526	HIS
3	G	547	GLU
3	G	561	LYS
3	G	562	ARG
3	G	581	LEU
3	G	621	GLU
3	G	622	LYS
3	G	623	THR
3	G	626	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	641	LYS
3	G	645	THR
3	G	647	LEU
3	G	656	CYS
3	G	660	SER
3	G	661	VAL
3	G	662	VAL
3	G	670	CYS
3	G	677	THR
3	G	683	GLU
3	G	685	TYR
3	G	686	ASN
3	G	687	LEU
3	G	689	SER
3	G	692	LYS
3	G	693	GLU
3	G	694	LEU
3	G	695	VAL
3	G	697	HIS
3	G	705	GLN
3	G	709	SER
3	G	713	THR
3	G	714	LEU
4	C	35	ASP
4	C	43	GLU
4	C	55	GLU
4	C	66	LEU
4	C	68	LYS
4	C	71	GLU
4	C	72	LYS
4	C	75	THR
4	C	86	ILE
4	C	88	LYS
4	C	90	ARG
4	C	93	VAL
4	C	95	ASN
4	C	96	SER
4	C	97	LEU
4	C	98	ASN
4	C	102	LEU
4	C	204	ASP
4	C	225	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	C	247	ARG
4	C	249	MET
4	C	250	HIS
4	C	251	CYS
4	C	252	LEU
4	C	254	LYS
4	C	256	THR
4	C	265	GLU
4	C	268	LEU
4	C	269	ILE
4	C	273	MET
4	C	274	LYS
4	C	276	ILE
4	C	278	GLU
4	C	279	MET
4	C	280	GLU
4	C	282	SER
4	C	284	LEU
4	C	332	GLU
4	C	353	ASP
4	C	382	SER
4	C	383	ARG
4	C	390	LEU
4	C	400	VAL
4	C	405	GLU
4	C	407	GLU
4	C	411	ILE
4	C	420	ARG
4	C	446	VAL
4	C	464	CYS
4	C	465	GLN
4	C	466	PHE
4	C	468	SER
4	C	469	LYS
4	C	470	LEU
4	C	471	GLU
4	C	473	MET
4	C	478	SER
4	C	484	MET
4	C	486	GLU
4	C	491	LEU
4	C	504	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	C	505	VAL
4	C	507	VAL
4	C	508	LEU
4	C	509	THR
4	C	510	THR
4	C	515	THR
4	C	521	LYS
4	C	596	THR
4	C	600	THR
4	C	602	LEU
4	C	626	GLU
4	C	627	LEU
4	C	629	ARG
4	C	632	GLN
4	C	634	LEU
4	C	641	GLN
4	C	653	ILE
4	C	665	PHE
4	C	669	LEU
4	C	672	VAL
4	C	683	GLU
4	C	698	ASP
4	C	699	ARG
4	C	700	LYS
4	C	702	GLU
4	C	703	ILE
4	C	735	LEU
4	C	748	LEU
4	C	750	GLU
4	C	752	GLU
4	C	762	LYS
4	C	763	VAL
4	C	765	THR
4	C	767	VAL
2	B	19	GLU
2	B	29	LEU
2	B	37	VAL
2	B	114	GLU
2	B	131	GLU
2	B	203	GLU
2	B	243	SER
2	B	253	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	277	GLU
2	B	278	ASN
2	B	280	CYS
2	B	297	LYS
2	B	305	LEU
2	B	328	LYS
2	B	363	LYS
2	B	374	SER
2	B	394	LEU
2	B	397	ARG
2	B	406	LYS
2	B	570	ARG
2	B	571	VAL
2	B	572	LEU
2	B	592	GLU
2	B	593	GLU
2	B	596	TRP
2	B	597	LYS
2	B	600	THR
2	B	601	TYR
3	H	328	LEU
3	H	332	GLU
3	H	341	GLU
3	H	343	VAL
3	H	350	THR
3	H	358	ARG
3	H	362	THR
3	H	363	LYS
3	H	364	MET
3	H	365	HIS
3	H	397	THR
3	H	401	VAL
3	H	404	LEU
3	H	415	GLN
3	H	419	LYS
3	H	421	ASP
3	H	422	VAL
3	H	425	LEU
3	H	428	VAL
3	H	429	SER
3	H	430	LYS
3	H	433	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	434	ASP
3	H	436	VAL
3	H	437	VAL
3	H	438	LYS
3	H	442	ILE
3	H	445	VAL
3	H	453	ASN
3	H	454	THR
3	H	457	GLN
3	H	467	TYR
3	H	478	GLN
3	H	480	LYS
3	H	481	ARG
3	H	507	GLU
3	H	515	GLU
3	H	521	ILE
3	H	523	ARG
3	H	524	ILE
3	H	525	MET
3	H	526	HIS
3	H	547	GLU
3	H	561	LYS
3	H	563	MET
3	H	566	ILE
3	H	567	LYS
3	H	577	ARG
3	H	581	LEU
3	H	582	MET
3	H	586	GLN
3	H	587	LYS
3	H	590	ARG
3	H	592	LYS
3	H	593	LYS
3	H	594	LEU
3	H	598	LEU
3	H	622	LYS
3	H	656	CYS
3	H	660	SER
3	H	670	CYS
3	H	671	VAL
3	H	685	TYR
3	H	687	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	693	GLU
3	H	694	LEU
3	H	703	LEU
3	H	704	VAL
3	H	705	GLN
3	H	708	ASP
3	H	710	LEU
3	H	711	ASN
3	H	712	VAL
4	F	35	ASP
4	F	43	GLU
4	F	55	GLU
4	F	56	GLU
4	F	57	LEU
4	F	68	LYS
4	F	71	GLU
4	F	72	LYS
4	F	77	LEU
4	F	83	GLU
4	F	84	HIS
4	F	86	ILE
4	F	88	LYS
4	F	90	ARG
4	F	91	GLU
4	F	94	LEU
4	F	97	LEU
4	F	98	ASN
4	F	99	ASN
4	F	102	LEU
4	F	204	ASP
4	F	225	LEU
4	F	249	MET
4	F	251	CYS
4	F	252	LEU
4	F	254	LYS
4	F	256	THR
4	F	257	GLU
4	F	260	ILE
4	F	261	VAL
4	F	262	LYS
4	F	264	VAL
4	F	265	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	F	266	ARG
4	F	268	LEU
4	F	269	ILE
4	F	273	MET
4	F	274	LYS
4	F	279	MET
4	F	280	GLU
4	F	282	SER
4	F	284	LEU
4	F	332	GLU
4	F	353	ASP
4	F	383	ARG
4	F	390	LEU
4	F	400	VAL
4	F	405	GLU
4	F	407	GLU
4	F	411	ILE
4	F	420	ARG
4	F	446	VAL
4	F	468	SER
4	F	469	LYS
4	F	470	LEU
4	F	473	MET
4	F	478	SER
4	F	479	ILE
4	F	480	SER
4	F	481	ASN
4	F	486	GLU
4	F	488	ARG
4	F	491	LEU
4	F	492	GLN
4	F	509	THR
4	F	510	THR
4	F	515	THR
4	F	521	LYS
4	F	596	THR
4	F	600	THR
4	F	602	LEU
4	F	627	LEU
4	F	629	ARG
4	F	632	GLN
4	F	634	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	F	641	GLN
4	F	653	ILE
4	F	665	PHE
4	F	669	LEU
4	F	672	VAL
4	F	683	GLU
4	F	701	HIS
4	F	735	LEU
4	F	748	LEU
4	F	750	GLU
4	F	751	ARG
4	F	752	GLU
4	F	757	THR
4	F	761	ARG
4	F	762	LYS
4	F	763	VAL
1	D	25	LYS
1	D	28	ASN
1	D	35	TRP
1	D	37	ILE
1	D	39	VAL
1	D	40	ASP
1	D	42	CYS
1	D	46	ARG
1	D	47	ASN
1	D	49	ILE
1	D	50	MET
1	D	59	ASN
1	D	66	GLU
1	D	74	VAL
1	D	84	ILE
1	D	89	LYS
1	D	91	ARG
1	D	92	GLN
1	D	93	VAL
1	D	98	ASN
1	D	99	ARG
1	D	100	GLU
1	D	101	TRP
1	D	103	PHE
1	D	104	GLN
1	D	105	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	108	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	28	ASN
1	E	41	ASN
1	E	98	ASN
1	E	108	HIS
2	A	71	HIS
2	A	112	GLN
2	A	166	GLN
2	A	185	ASN
2	A	230	GLN
2	A	278	ASN
2	A	356	GLN
2	A	357	GLN
2	A	566	HIS
3	G	365	HIS
3	G	432	GLN
3	G	441	ASN
3	G	450	HIS
3	G	453	ASN
3	G	478	GLN
3	G	564	ASN
3	G	572	GLN
3	G	586	GLN
3	G	591	GLN
3	G	595	ASN
3	G	669	HIS
3	G	686	ASN
3	G	706	HIS
3	G	707	ASN
4	C	84	HIS
4	C	99	ASN
4	C	106	ASN
4	C	110	ASN
4	C	112	HIS
4	C	150	GLN
4	C	163	GLN
4	C	218	GLN
4	C	222	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	C	228	ASN
4	C	281	ASN
4	C	308	ASN
4	C	324	GLN
4	C	343	GLN
4	C	481	ASN
4	C	560	ASN
4	C	606	ASN
4	C	618	GLN
4	C	641	GLN
4	C	657	HIS
2	B	71	HIS
2	B	76	ASN
2	B	112	GLN
2	B	230	GLN
2	B	356	GLN
2	B	357	GLN
2	B	565	GLN
3	H	433	GLN
3	H	435	GLN
3	H	453	ASN
3	H	457	GLN
3	H	478	GLN
3	H	572	GLN
3	H	591	GLN
3	H	595	ASN
3	H	632	ASN
3	H	673	ASN
3	H	700	HIS
3	H	705	GLN
3	H	706	HIS
4	F	69	HIS
4	F	87	ASN
4	F	106	ASN
4	F	110	ASN
4	F	112	HIS
4	F	150	GLN
4	F	163	GLN
4	F	218	GLN
4	F	222	GLN
4	F	228	ASN
4	F	281	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	F	308	ASN
4	F	324	GLN
4	F	343	GLN
4	F	606	ASN
4	F	618	GLN
4	F	641	GLN
4	F	657	HIS
4	F	718	GLN
4	F	719	HIS
1	D	28	ASN
1	D	98	ASN
1	D	104	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

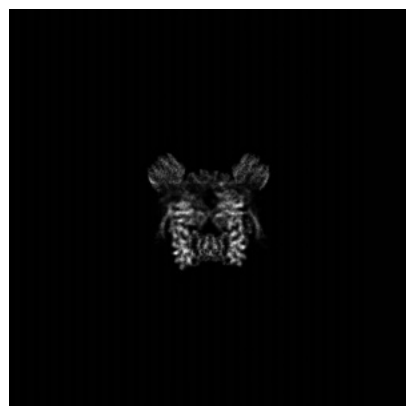
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34452. 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

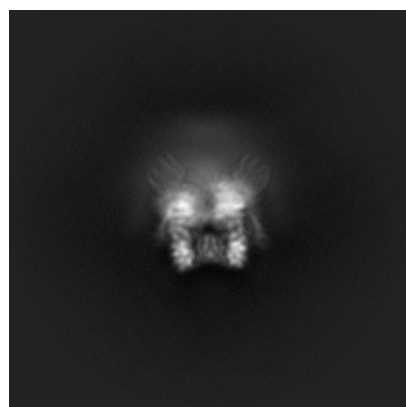


Y

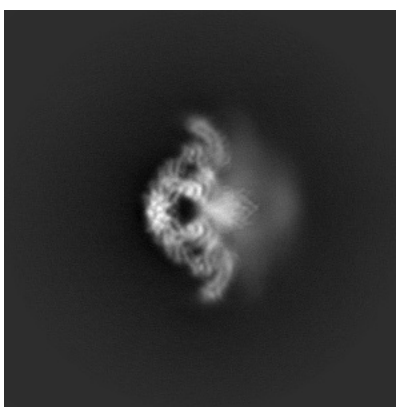


Z

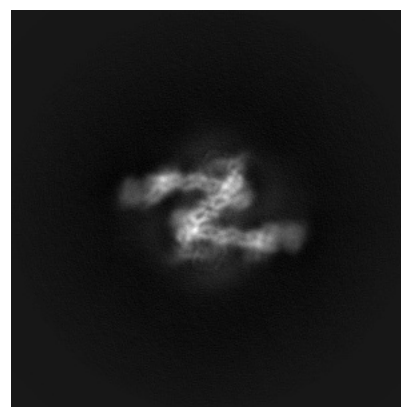
6.1.2 Raw map



X



Y



Z

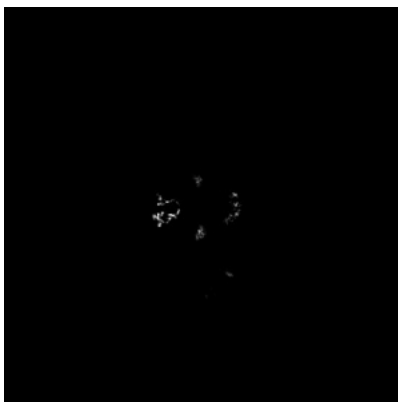
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

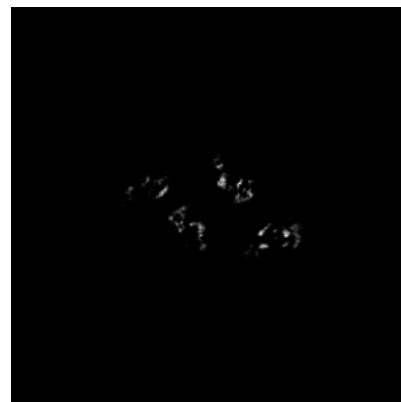
6.2.1 Primary map



X Index: 192

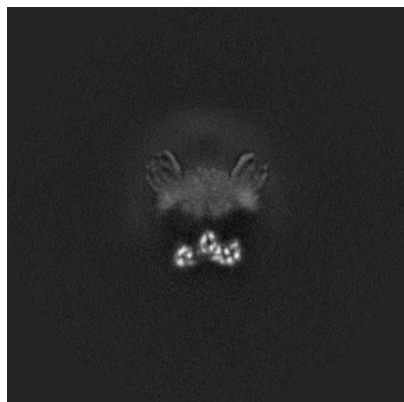


Y Index: 192

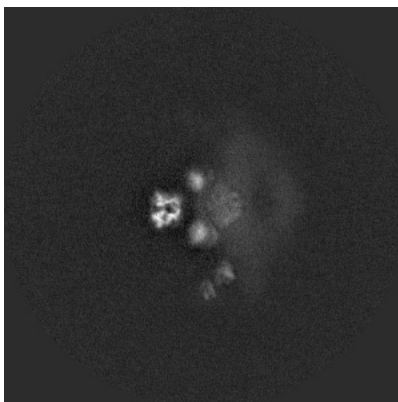


Z Index: 192

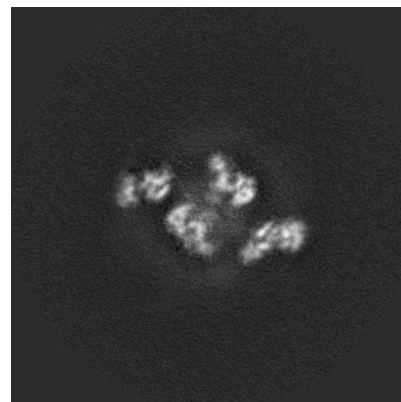
6.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

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

6.3 Largest variance slices [i](#)

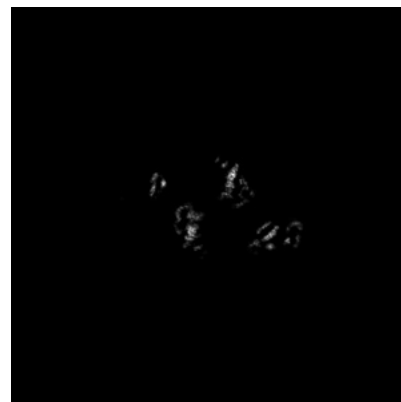
6.3.1 Primary map



X Index: 178



Y Index: 222

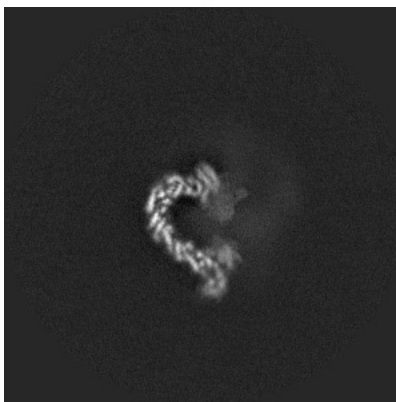


Z Index: 188

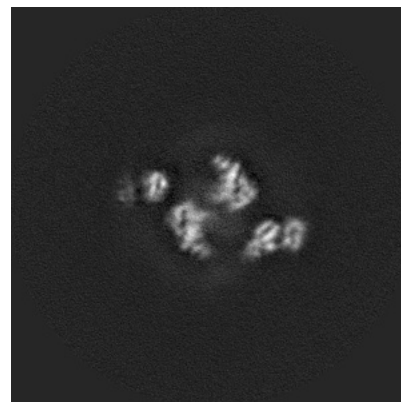
6.3.2 Raw map



X Index: 176



Y Index: 214



Z Index: 188

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

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

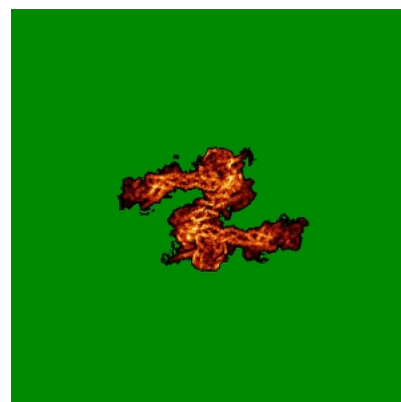
6.4.1 Primary map



X

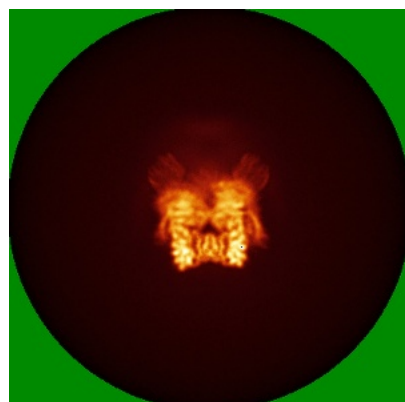


Y



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.

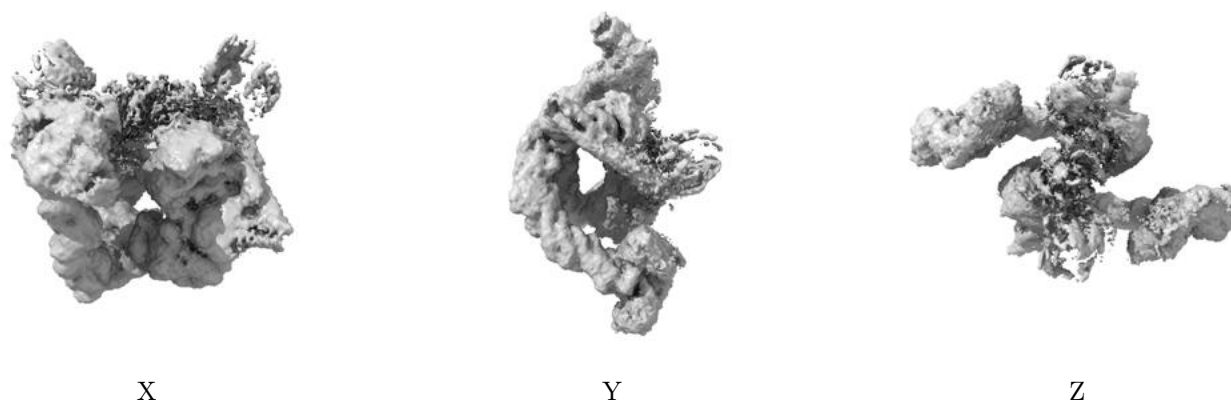
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.001. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

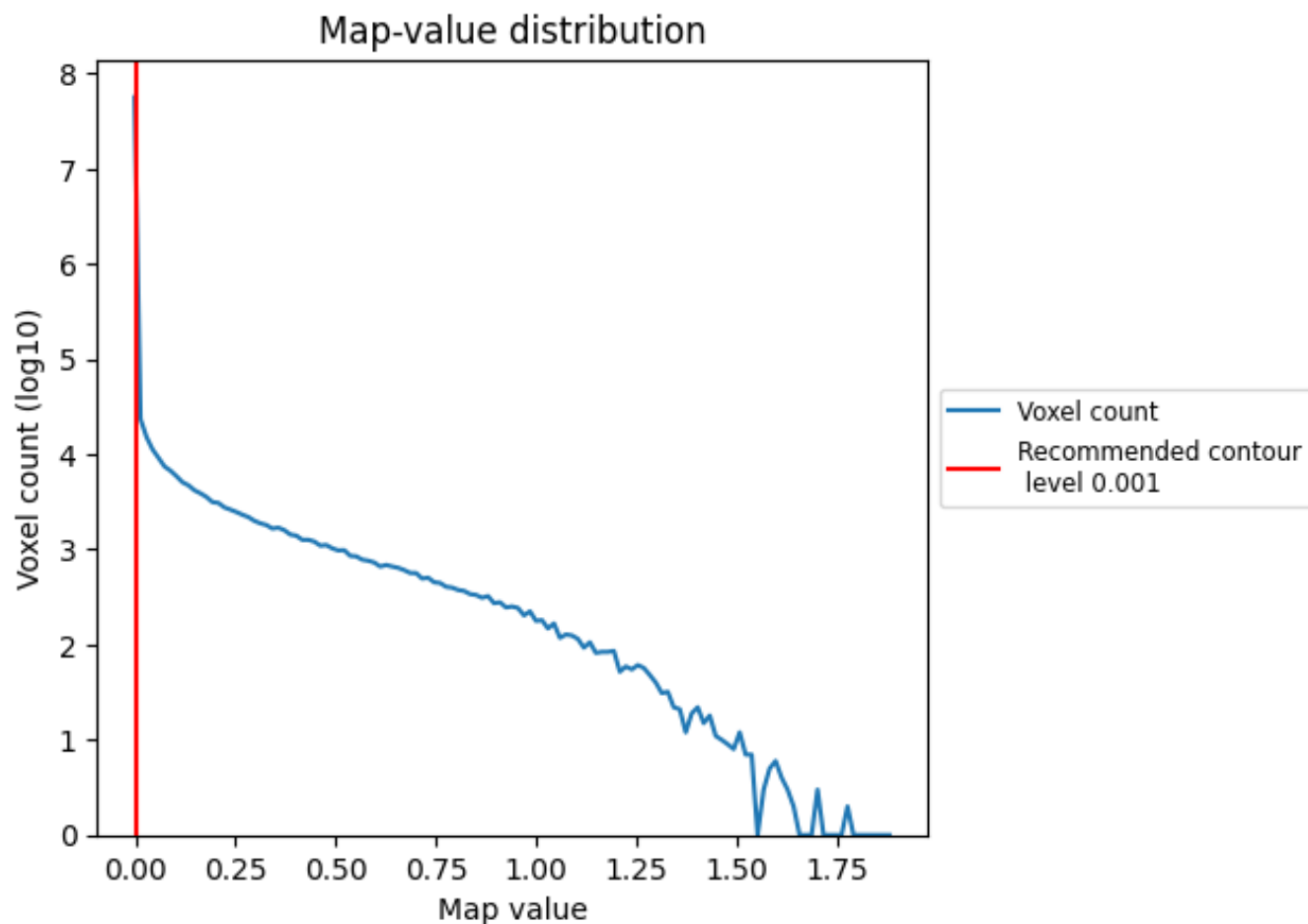
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

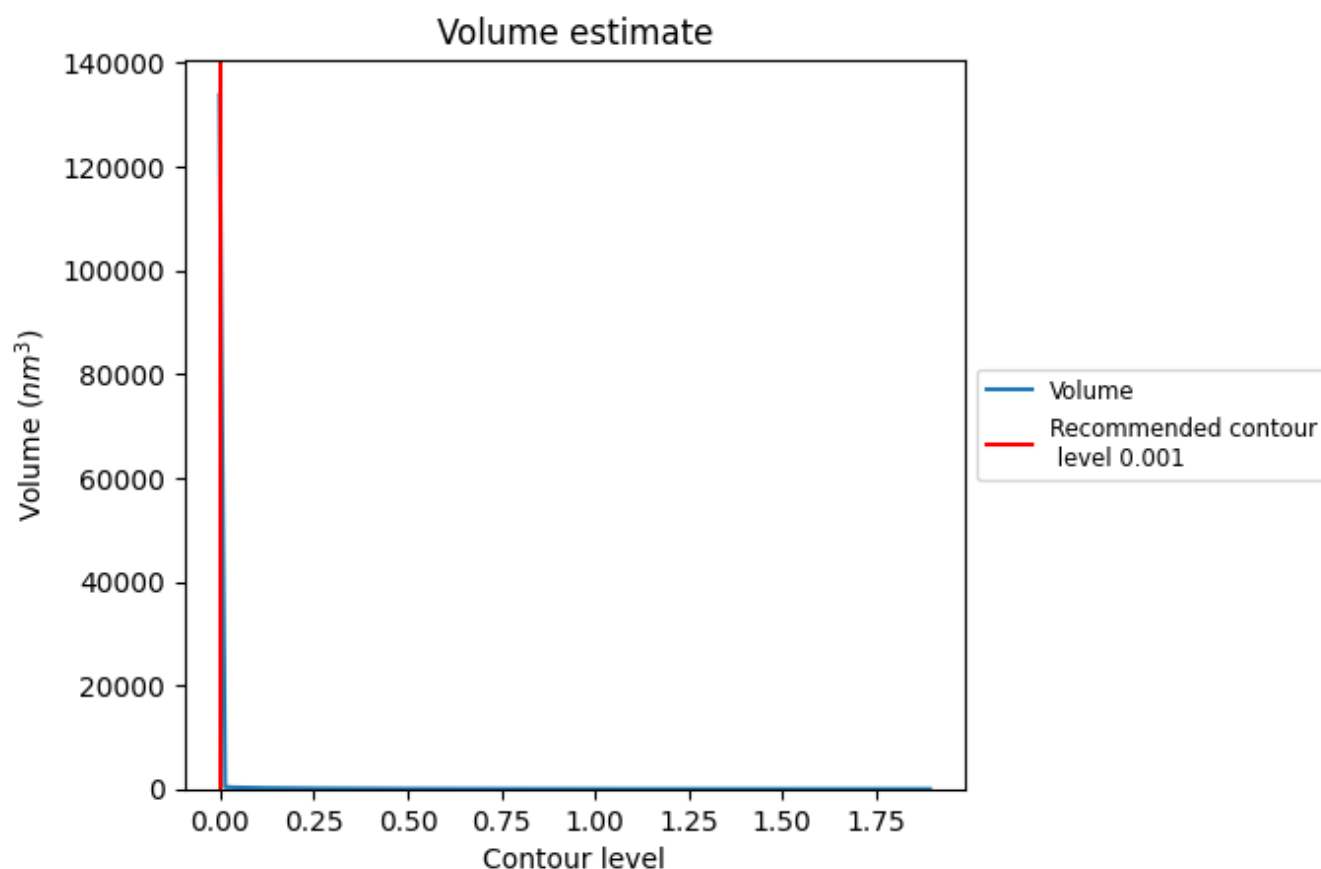
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

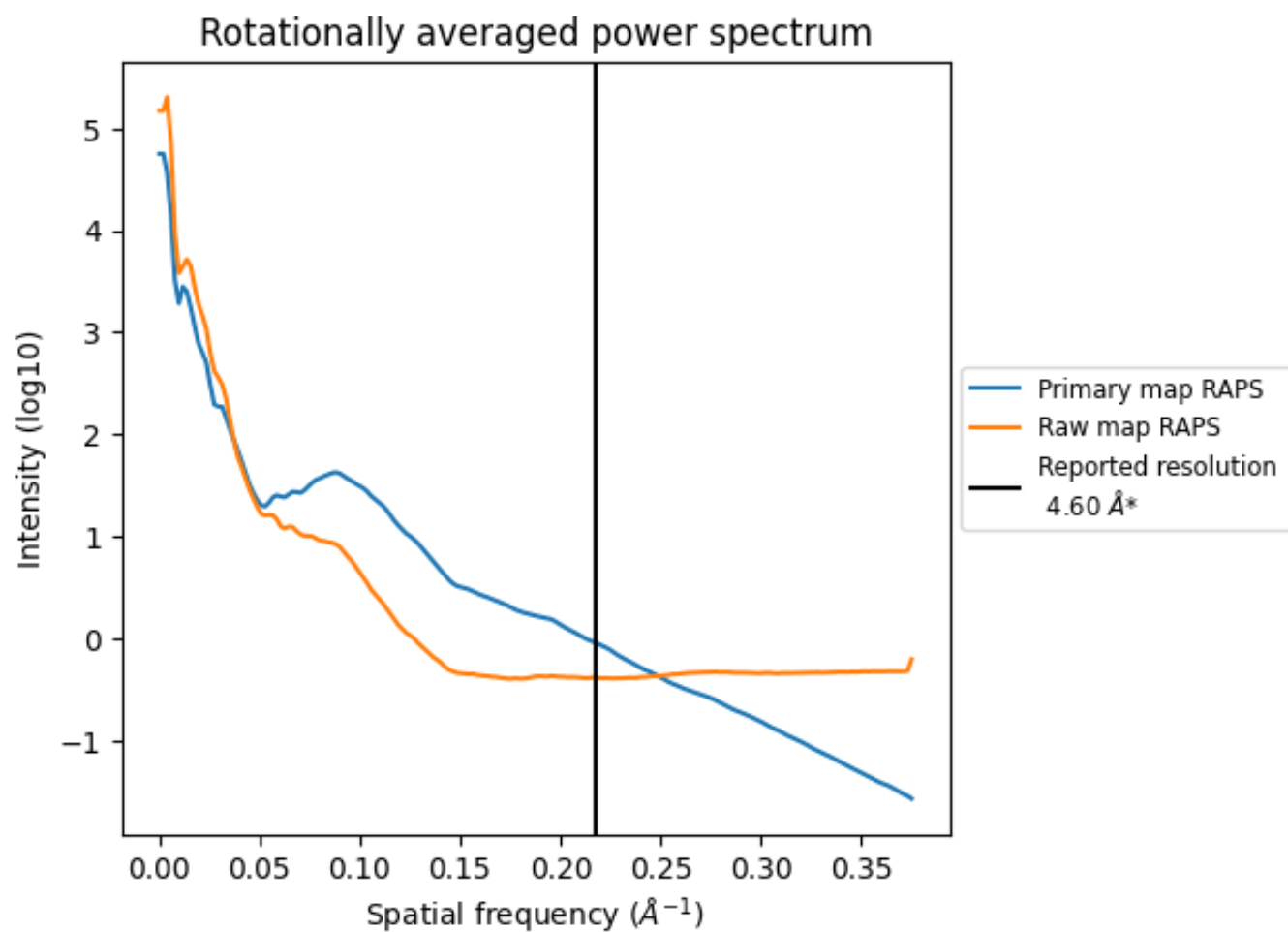
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 108840 nm^3 ; this corresponds to an approximate mass of 98318 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 ⓘ

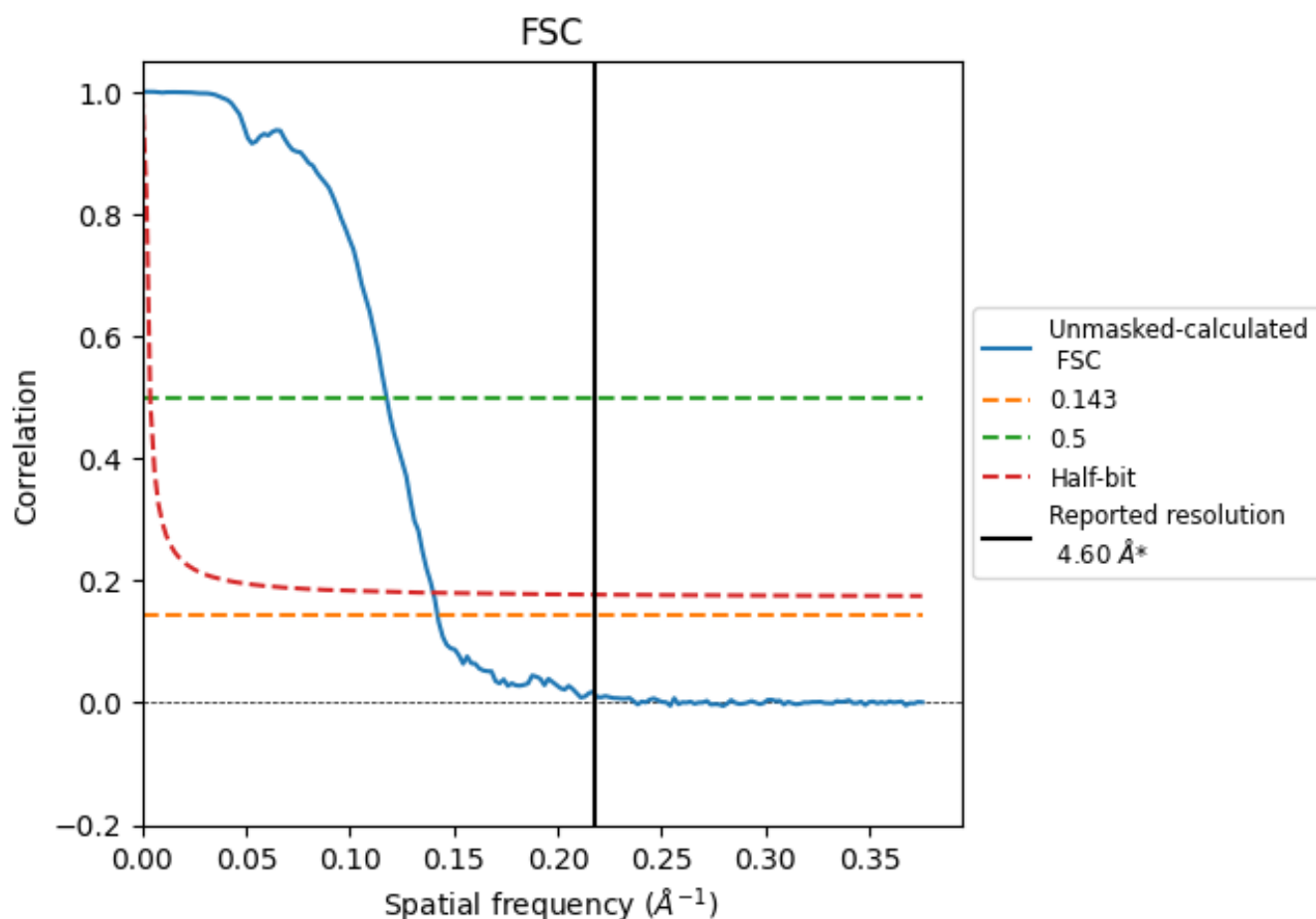


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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 0.217 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

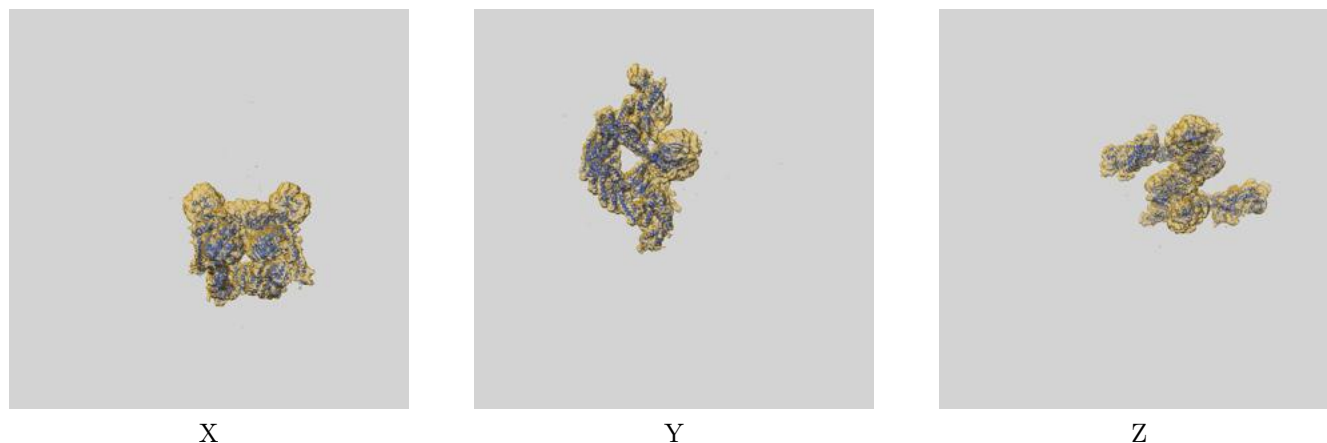
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.03	8.50	7.14

*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 7.03 differs from the reported value 4.6 by more than 10 %

9 Map-model fit [i](#)

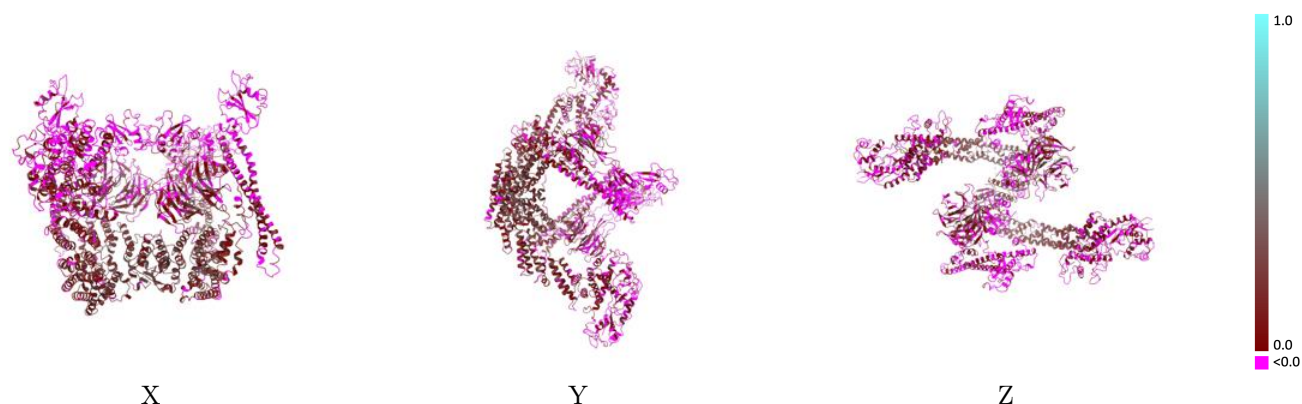
This section contains information regarding the fit between EMDB map EMD-34452 and PDB model 8H36. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



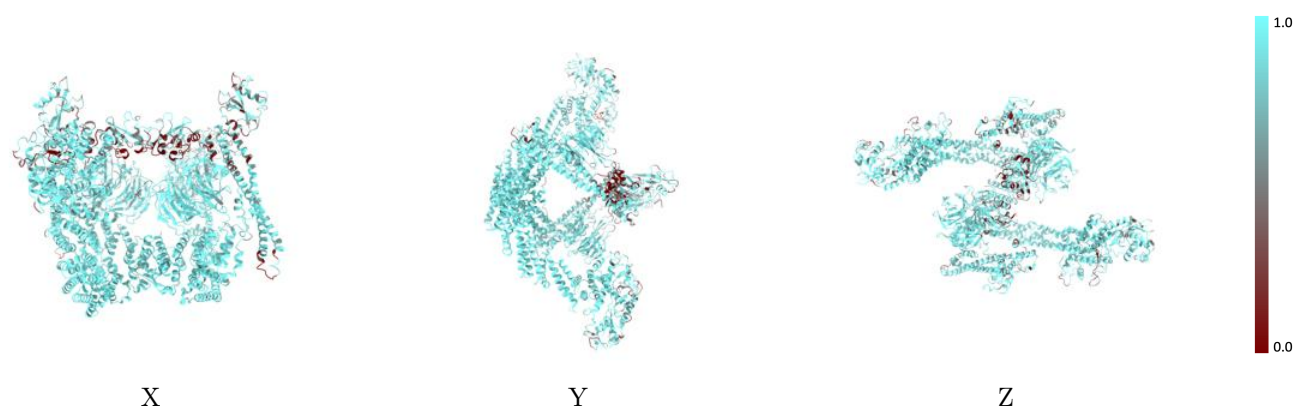
The images above show the 3D surface view of the map at the recommended contour level 0.001 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



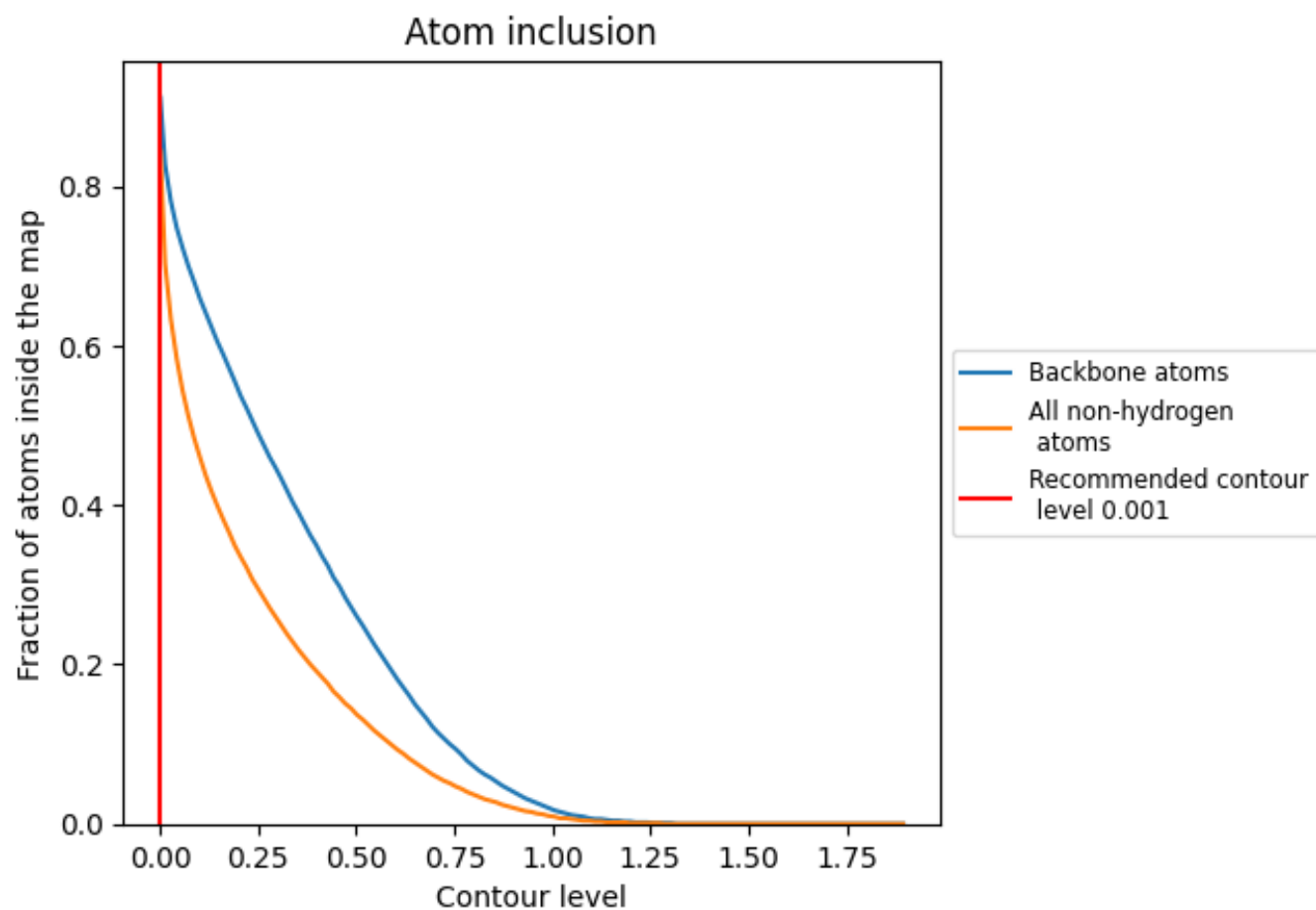
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.001).

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.001) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8440	0.0680
A	0.9110	0.1140
B	0.9120	0.1350
C	0.9070	0.1010
D	0.7410	-0.0200
E	0.6220	-0.0290
F	0.9000	0.0940
G	0.7220	-0.0580
H	0.6260	-0.0360

