



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:06 PM UTC

PDB ID : 6K71 / pdb_00006k71
EMDB ID : EMD-9840
Title : eIF2 - eIF2B complex
Authors : Kashiwagi, K.; Yokoyama, T.; Ito, T.
Deposited on : 2019-06-05
Resolution : 4.30 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:

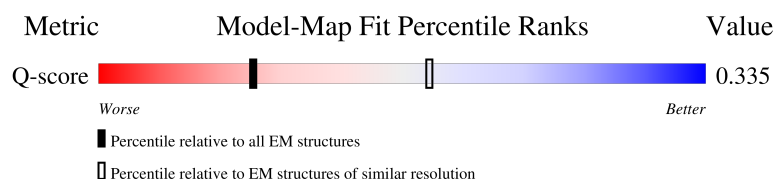
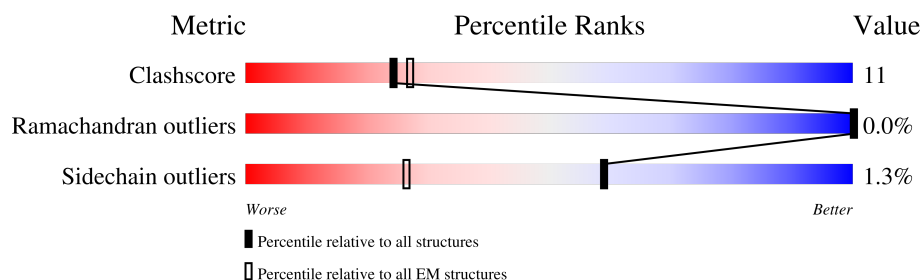
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.30 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.



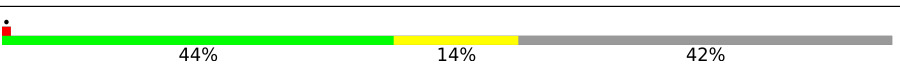
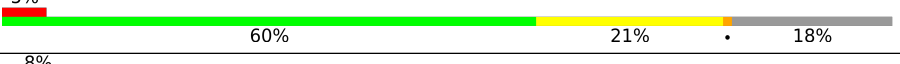
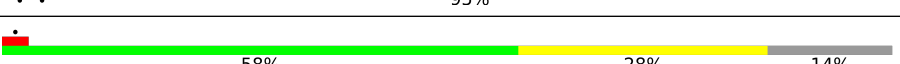
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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	305	
1	B	305	
2	C	351	
2	D	351	

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Mol	Chain	Length	Quality of chain
3	E	452	
3	F	452	
4	G	523	
4	H	523	
5	I	721	
5	J	721	
6	K	315	
7	M	333	
8	P	472	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 32589 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 Translation initiation factor eIF-2B subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	265	Total	C	N	O	S	0	0
			2055	1327	344	374	10		
1	B	265	Total	C	N	O	S	0	0
			2055	1327	344	374	10		

- Molecule 2 is a protein called Translation initiation factor eIF-2B subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	318	Total	C	N	O	S	0	0
			2486	1571	438	462	15		
2	D	318	Total	C	N	O	S	0	0
			2486	1571	438	462	15		

- Molecule 3 is a protein called Translation initiation factor eIF-2B subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	336	Total	C	N	O	S	0	0
			2306	1463	398	432	13		
3	F	332	Total	C	N	O	S	0	0
			2275	1443	393	426	13		

- Molecule 4 is a protein called Translation initiation factor eIF-2B subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	357	Total	C	N	O	S	0	0
			2779	1756	495	514	14		
4	H	357	Total	C	N	O	S	0	0
			2779	1756	495	514	14		

- Molecule 5 is a protein called Translation initiation factor eIF-2B subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	421	Total	C	N	O	S	0	0
			3312	2087	585	625	15		
5	J	588	Total	C	N	O	S	0	0
			4675	2963	812	878	22		

- Molecule 6 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	265	Total	C	N	O	S	0	0
			2139	1350	375	404	10		

- Molecule 7 is a protein called Eukaryotic translation initiation factor 2 subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	16	Total	C	N	O	S	0	0
			145	93	24	27	1		

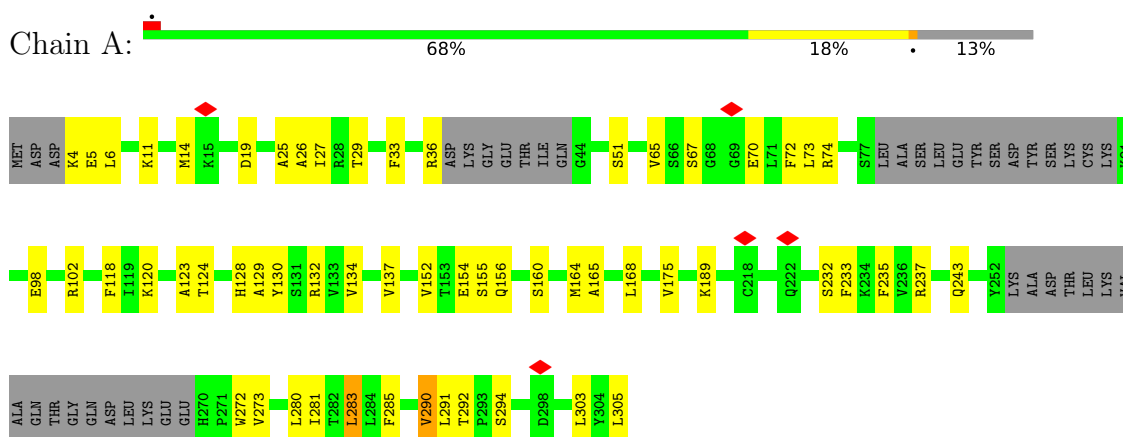
- Molecule 8 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	406	Total	C	N	O	S	0	0
			3097	1974	544	563	16		

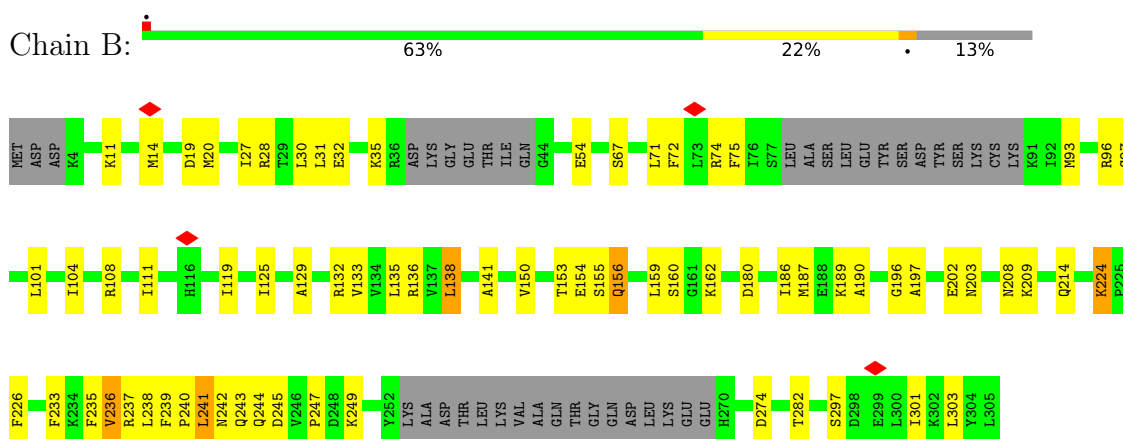
3 Residue-property plots

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.

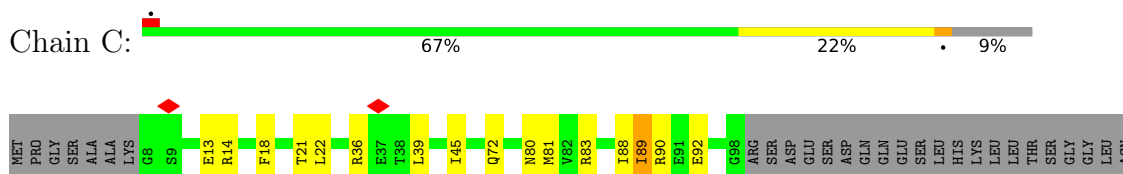
- Molecule 1: Translation initiation factor eIF-2B subunit alpha

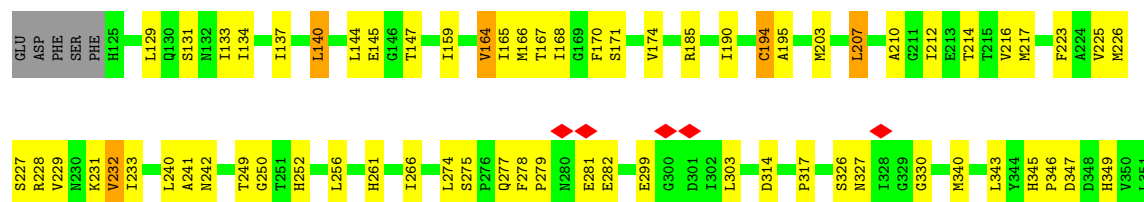


- Molecule 1: Translation initiation factor eIF-2B subunit alpha

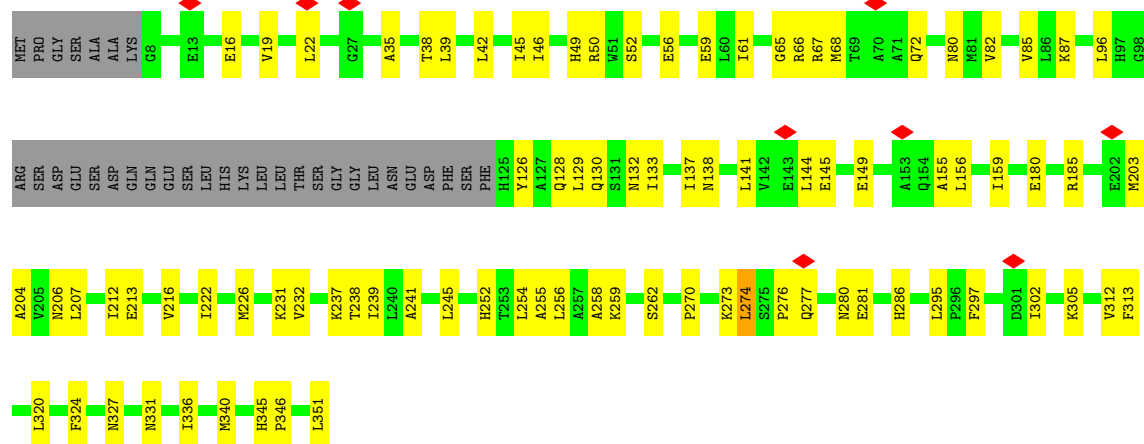


- Molecule 2: Translation initiation factor eIF-2B subunit beta

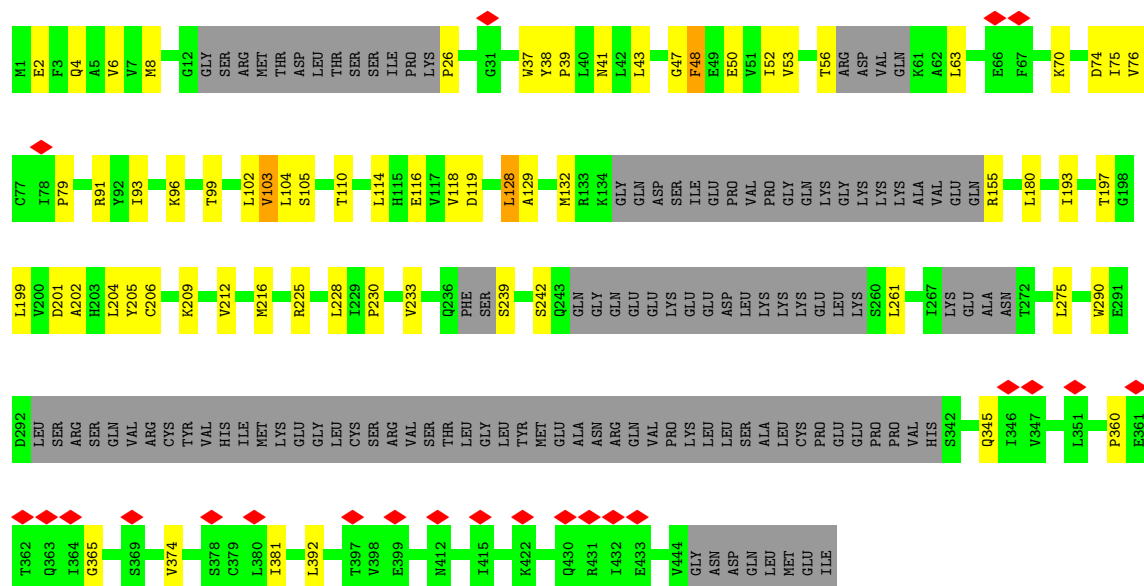




• Molecule 2: Translation initiation factor eIF-2B subunit beta



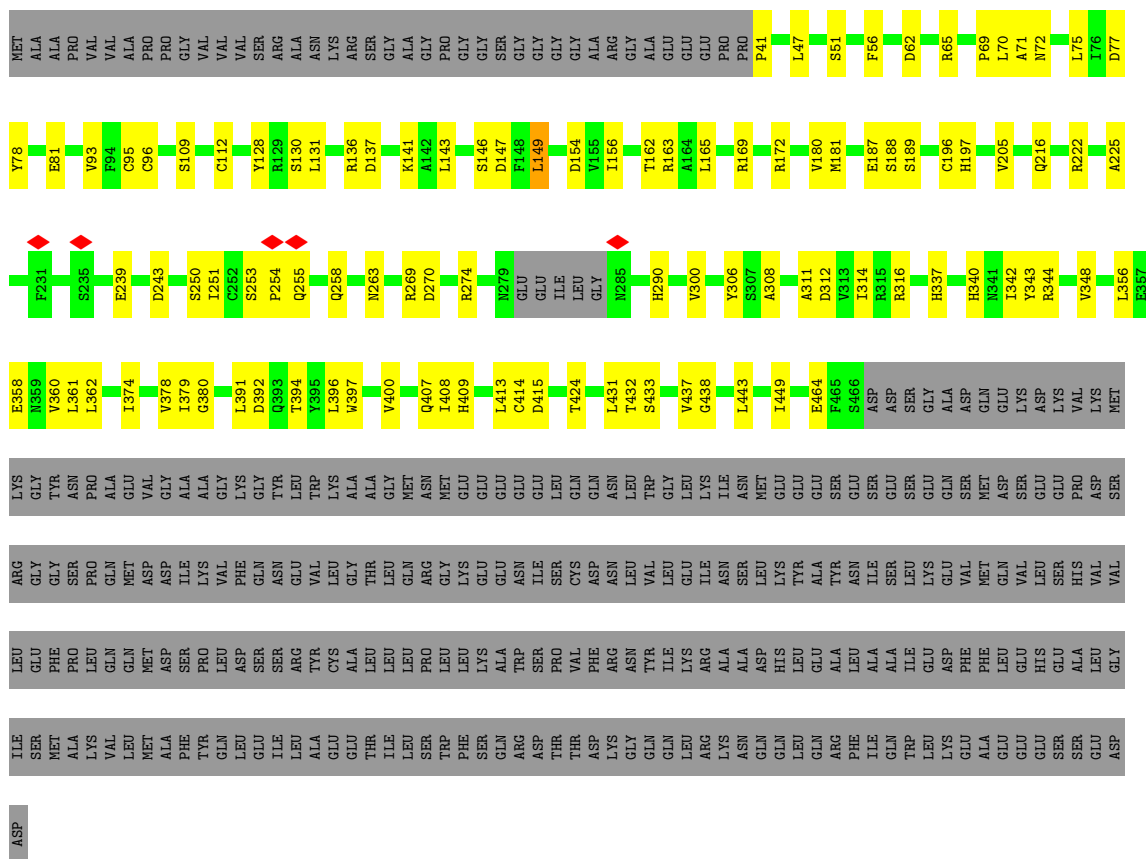
• Molecule 3: Translation initiation factor eIF-2B subunit gamma



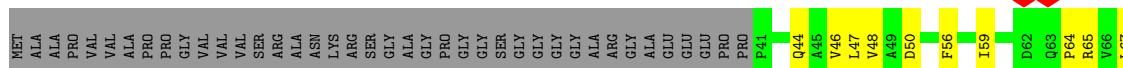
• Molecule 3: Translation initiation factor eIF-2B subunit gamma

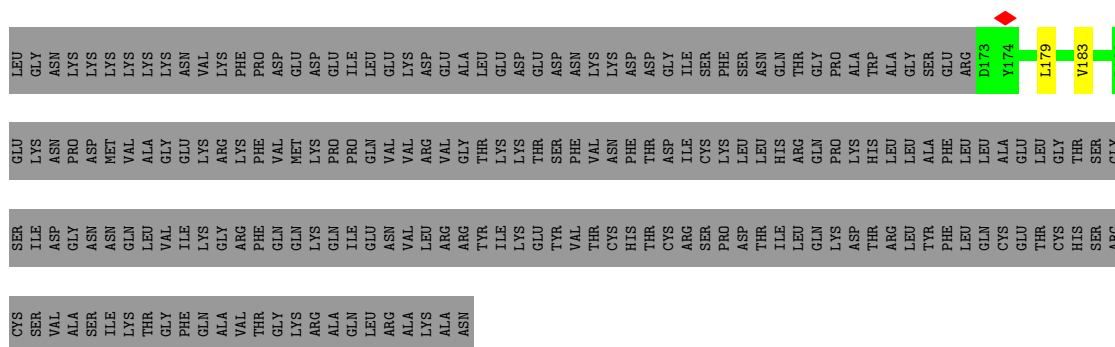


- Molecule 5: Translation initiation factor eIF-2B subunit epsilon

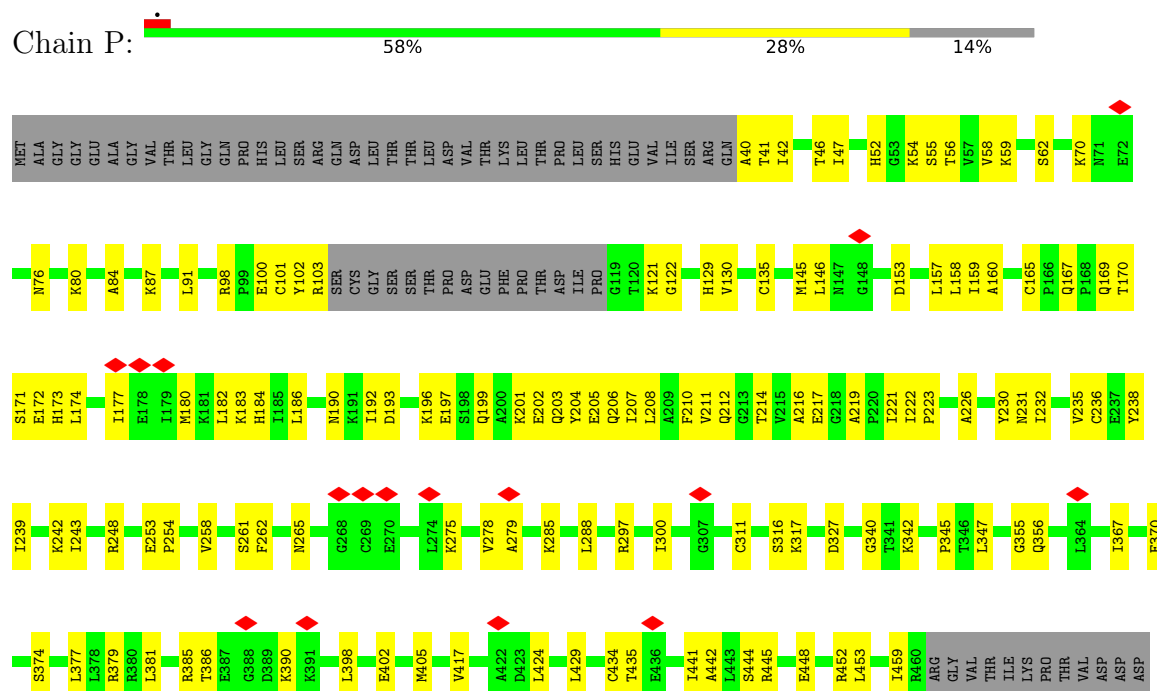


- Molecule 5: Translation initiation factor eIF-2B subunit epsilon





- Molecule 8: Eukaryotic translation initiation factor 2 subunit 3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	82123	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0112	Depositor
Map size (Å)	367.5, 367.5, 367.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.47, 1.47, 1.47	Depositor

5 Model quality

5.1 Standard geometry

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	0.35	0/2087	0.81	2/2818 (0.1%)
1	B	0.36	0/2087	0.84	0/2818
2	C	0.39	0/2533	0.89	3/3426 (0.1%)
2	D	0.37	0/2533	0.84	1/3426 (0.0%)
3	E	0.32	0/2332	0.73	0/3166
3	F	0.32	0/2301	0.76	1/3123 (0.0%)
4	G	0.39	0/2831	0.81	4/3847 (0.1%)
4	H	0.42	0/2831	0.90	2/3847 (0.1%)
5	I	0.34	0/3380	0.76	0/4597
5	J	0.35	0/4767	0.76	1/6467 (0.0%)
6	K	0.34	0/2170	0.91	6/2925 (0.2%)
7	M	0.27	0/147	0.95	0/197
8	P	0.31	0/3145	0.79	1/4246 (0.0%)
All	All	0.36	0/33144	0.81	21/44903 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
2	C	0	2
2	D	0	2
3	E	0	2
3	F	0	4
4	G	0	2
4	H	0	5
5	J	0	4
6	K	0	9
8	P	0	3
All	All	0	40

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	36	ILE	N-CA-C	-6.79	105.72	112.17
8	P	192	ILE	N-CA-C	-6.70	106.77	113.20
6	K	179	ASN	N-CA-C	6.69	118.23	111.07
2	C	194	CYS	CA-C-N	-6.44	115.03	123.34
2	C	194	CYS	C-N-CA	-6.44	115.03	123.34
6	K	242	LEU	N-CA-C	-6.38	105.42	113.72
4	H	509	CYS	N-CA-C	6.21	117.74	110.97
6	K	118	VAL	CA-C-N	6.18	129.98	121.33
6	K	118	VAL	C-N-CA	6.18	129.98	121.33
6	K	115	VAL	N-CA-C	-6.09	105.88	111.67
2	D	312	VAL	N-CA-C	-5.90	107.00	113.43
4	G	247	GLU	CA-C-N	5.80	129.52	120.82
4	G	247	GLU	C-N-CA	5.80	129.52	120.82
5	J	125	SER	N-CA-C	5.79	119.17	111.30
4	H	482	LEU	CA-CB-CG	5.74	136.41	116.30
4	G	367	LEU	CA-CB-CG	5.39	135.18	116.30
6	K	182	ARG	N-CA-C	5.34	117.10	111.28
2	C	45	ILE	N-CA-C	-5.30	106.70	112.80
1	A	291	LEU	CA-C-N	5.11	129.84	121.57
1	A	291	LEU	C-N-CA	5.11	129.84	121.57
4	G	364	ARG	C-N-CD	-5.09	109.39	120.60

There are no chirality outliers.

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	GLN	Peptide
1	A	168	LEU	Peptide
1	A	280	LEU	Peptide
1	B	156	GLN	Peptide
1	B	224	LYS	Peptide
1	B	241	LEU	Peptide
1	B	301	ILE	Peptide
2	C	195	ALA	Peptide
2	C	227	SER	Peptide
2	D	126	TYR	Peptide
2	D	327	ASN	Peptide
3	E	230	PRO	Peptide
3	E	47	GLY	Peptide
3	F	101	VAL	Peptide

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Mol	Chain	Res	Type	Group
3	F	119	ASP	Peptide
3	F	44	GLU	Peptide
3	F	47	GLY	Peptide
4	G	186	TYR	Peptide
4	G	246	GLU	Peptide
4	H	348	GLU	Peptide
4	H	395	LEU	Peptide
4	H	432	VAL	Peptide
4	H	450	ASP	Peptide
4	H	508	PRO	Peptide
5	J	118	ASN	Peptide
5	J	124	THR	Peptide
5	J	249	ILE	Peptide
5	J	314	ILE	Peptide
6	K	115	VAL	Peptide
6	K	124	ASP	Peptide
6	K	156	ALA	Peptide
6	K	168	LEU	Peptide
6	K	172	GLU	Peptide
6	K	202	TYR	Peptide
6	K	223	MET	Peptide
6	K	39	TYR	Peptide
6	K	50	GLU	Peptide
8	P	180	MET	Peptide
8	P	370	GLU	Peptide
8	P	98	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2055	0	2138	30	0
1	B	2055	0	2138	47	0
2	C	2486	0	2500	53	0
2	D	2486	0	2500	55	0
3	E	2306	0	2049	42	0
3	F	2275	0	2014	40	0
4	G	2779	0	2838	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	2779	0	2838	58	0
5	I	3312	0	3283	64	0
5	J	4675	0	4649	97	0
6	K	2139	0	2184	87	0
7	M	145	0	138	23	0
8	P	3097	0	3253	100	0
All	All	32589	0	32522	697	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 11.

All (697) 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)
6:K:178:ASN:ND2	6:K:182:ARG:HD2	1.24	1.50
7:M:179:LEU:CD1	8:P:223:PRO:HG2	1.69	1.20
6:K:178:ASN:CG	6:K:182:ARG:HD2	1.69	1.16
7:M:179:LEU:HD21	8:P:231:ASN:HD21	1.03	1.14
7:M:179:LEU:HD13	8:P:223:PRO:HG2	1.18	1.13
6:K:176:LEU:HA	6:K:180:ILE:HG22	1.26	1.11
6:K:178:ASN:ND2	6:K:182:ARG:CD	2.15	1.09
6:K:176:LEU:HA	6:K:180:ILE:CG2	1.84	1.08
6:K:222:ASN:ND2	6:K:253:GLN:HG2	1.70	1.07
6:K:176:LEU:CD1	6:K:180:ILE:HG21	1.84	1.06
7:M:179:LEU:CD1	8:P:223:PRO:HD2	1.85	1.06
6:K:176:LEU:HD12	6:K:180:ILE:CG2	1.84	1.06
6:K:176:LEU:HD12	6:K:180:ILE:HG21	1.37	1.04
7:M:179:LEU:CD1	8:P:223:PRO:CG	2.34	1.04
6:K:222:ASN:HD22	6:K:253:GLN:HG2	1.21	1.01
6:K:178:ASN:O	6:K:182:ARG:HB2	1.62	0.99
6:K:178:ASN:O	6:K:182:ARG:N	1.98	0.97
7:M:179:LEU:CD1	8:P:223:PRO:CD	2.43	0.97
7:M:179:LEU:HD11	8:P:223:PRO:HD2	1.47	0.96
7:M:179:LEU:HD12	8:P:223:PRO:CG	1.96	0.94
6:K:178:ASN:O	6:K:182:ARG:CB	2.16	0.94
6:K:222:ASN:HD21	6:K:253:GLN:HE21	1.17	0.92
7:M:183:VAL:HG22	8:P:230:TYR:CZ	2.04	0.92
7:M:179:LEU:HD21	8:P:231:ASN:ND2	1.86	0.88
6:K:178:ASN:HD21	6:K:182:ARG:HD2	1.38	0.88
8:P:55:SER:O	8:P:59:LYS:HB2	1.78	0.84
7:M:183:VAL:CG2	8:P:230:TYR:CE2	2.63	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:222:ASN:ND2	6:K:253:GLN:CG	2.44	0.81
7:M:183:VAL:HG22	8:P:230:TYR:CE2	2.14	0.81
4:H:310:GLU:O	4:H:314:LEU:HB2	1.80	0.81
7:M:179:LEU:HD12	8:P:223:PRO:CD	2.10	0.80
7:M:179:LEU:HD13	8:P:223:PRO:CG	2.03	0.80
6:K:176:LEU:HD12	6:K:180:ILE:HG23	1.64	0.79
7:M:179:LEU:HD12	8:P:223:PRO:HG2	1.60	0.78
6:K:222:ASN:HD22	6:K:253:GLN:CG	1.97	0.77
5:I:77:ASP:O	5:I:81:GLU:HB2	1.84	0.77
7:M:179:LEU:CD2	7:M:183:VAL:HG21	2.15	0.76
7:M:179:LEU:HD12	8:P:223:PRO:HD2	1.68	0.76
2:D:96:LEU:HD12	2:D:128:GLN:HE21	1.52	0.75
6:K:178:ASN:OD1	6:K:182:ARG:HB2	1.87	0.75
2:C:36:ARG:HH12	2:C:145:GLU:HB3	1.51	0.74
6:K:176:LEU:HD13	6:K:180:ILE:HG21	1.69	0.74
6:K:210:GLU:HA	6:K:213:ARG:HG2	1.69	0.74
6:K:222:ASN:HD21	6:K:253:GLN:NE2	1.84	0.73
4:G:333:ILE:HG22	4:G:400:LYS:HB3	1.71	0.71
2:C:299:GLU:HG3	2:C:303:LEU:HB2	1.73	0.70
7:M:179:LEU:HD23	7:M:183:VAL:HG21	1.71	0.70
3:E:129:ALA:HB3	3:E:206:CYS:HB2	1.73	0.69
4:H:229:LEU:HD22	4:H:273:MET:HG3	1.74	0.69
5:I:270:ASP:OD2	5:I:274:ARG:NH1	2.26	0.69
6:K:176:LEU:HD13	6:K:180:ILE:HD13	1.76	0.68
7:M:183:VAL:HG21	8:P:230:TYR:CE2	2.29	0.68
2:C:226:MET:SD	2:C:226:MET:N	2.68	0.67
2:C:22:LEU:O	2:C:72:GLN:NE2	2.28	0.67
4:H:518:VAL:HG23	4:H:519:LYS:HG3	1.76	0.66
5:J:256:VAL:O	5:J:260:PHE:HB2	1.94	0.66
1:B:235:PHE:HB3	1:B:237:ARG:HH12	1.60	0.66
6:K:176:LEU:CD1	6:K:180:ILE:HD13	2.26	0.66
4:G:310:GLU:O	4:G:314:LEU:HB2	1.96	0.66
5:J:414:CYS:SG	5:J:415:ASP:N	2.67	0.65
5:J:711:LYS:HA	5:J:715:GLU:HB2	1.78	0.65
5:I:216:GLN:HE22	5:I:225:ALA:H	1.44	0.65
3:F:166:ARG:NH1	3:F:167:LEU:O	2.30	0.65
6:K:196:GLU:HA	6:K:234:ARG:HG2	1.77	0.65
5:J:416:ASN:HB3	5:J:434:GLN:HG2	1.79	0.65
5:I:96:CYS:HB2	5:I:128:TYR:HB2	1.79	0.64
6:K:178:ASN:CG	6:K:182:ARG:CD	2.60	0.64
2:C:92:GLU:HB3	2:C:129:LEU:HD21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:171:SER:HA	8:P:174:LEU:HG	1.78	0.64
5:J:623:PRO:HA	5:J:626:LYS:HG2	1.79	0.64
5:J:675:ILE:HG22	5:J:676:LEU:HG	1.80	0.64
2:D:305:LYS:HE2	4:H:377:VAL:HG13	1.80	0.64
6:K:178:ASN:C	6:K:182:ARG:HB2	2.22	0.64
1:B:247:PRO:HB2	1:B:249:LYS:HG2	1.80	0.64
5:I:344:ARG:HB3	5:I:348:VAL:HG21	1.79	0.64
2:D:159:ILE:O	2:D:185:ARG:NH1	2.31	0.63
2:D:270:PRO:HD2	2:D:273:LYS:HE2	1.80	0.63
1:A:283:LEU:HD21	1:A:290:VAL:HG23	1.79	0.63
2:C:223:PHE:HB3	4:G:421:ALA:HB1	1.79	0.63
8:P:165:CYS:SG	8:P:199:GLN:NE2	2.72	0.63
4:H:220:SER:O	4:H:417:ARG:NH1	2.32	0.63
5:J:184:ILE:HG22	5:J:290:HIS:HB3	1.80	0.63
5:J:361:LEU:HD13	5:J:378:VAL:HG12	1.81	0.63
1:B:187:MET:O	1:B:224:LYS:NZ	2.31	0.62
2:D:128:GLN:OE1	2:D:132:ASN:ND2	2.32	0.62
6:K:176:LEU:CA	6:K:180:ILE:HG22	2.16	0.62
2:D:237:LYS:HD3	2:D:238:THR:HG23	1.79	0.62
4:H:428:ARG:NH2	4:H:496:LEU:O	2.33	0.62
6:K:178:ASN:CG	6:K:182:ARG:HB2	2.25	0.61
6:K:178:ASN:HD22	6:K:182:ARG:HH11	1.46	0.61
1:B:72:PHE:HA	1:B:75:PHE:HB3	1.81	0.61
8:P:221:ILE:HG12	8:P:223:PRO:HD3	1.83	0.61
2:D:66:ARG:HE	2:D:351:LEU:HB3	1.64	0.61
4:G:319:ILE:HD11	4:G:341:LEU:HD11	1.83	0.61
5:I:407:GLN:HB2	5:I:424:THR:HA	1.83	0.61
5:J:612:LEU:HD12	5:J:662:SER:HB3	1.83	0.61
3:F:64:CYS:O	3:F:68:LYS:NZ	2.34	0.61
4:G:405:ALA:HA	4:G:416:SER:HB2	1.81	0.61
2:C:159:ILE:O	2:C:185:ARG:NH1	2.34	0.61
5:J:313:VAL:HG13	5:J:314:ILE:HG13	1.81	0.61
5:J:594:GLN:O	5:J:598:HIS:HB2	2.00	0.61
6:K:111:ILE:HG13	6:K:112:LEU:HG	1.83	0.61
5:J:130:SER:OG	5:J:267:GLN:NE2	2.34	0.60
5:J:344:ARG:HE	5:J:350:LEU:HD11	1.65	0.60
1:B:67:SER:HB3	1:B:236:VAL:HG22	1.82	0.60
3:E:132:MET:HG3	3:E:201:ASP:HA	1.83	0.60
8:P:253:GLU:O	8:P:285:LYS:NZ	2.33	0.60
2:C:256:LEU:HD23	4:G:426:VAL:HG12	1.84	0.60
2:D:297:PHE:HB3	5:J:188:SER:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:207:ALA:HA	6:K:210:GLU:HB2	1.83	0.60
3:F:265:SER:OG	3:F:266:PHE:N	2.35	0.60
2:C:345:HIS:ND1	2:C:347:ASP:OD1	2.34	0.60
4:G:403:LEU:HB3	4:G:436:VAL:HG12	1.82	0.60
4:G:347:GLN:NE2	4:G:375:SER:OG	2.33	0.59
4:H:212:LEU:O	4:H:216:GLN:NE2	2.35	0.59
1:A:98:GLU:OE2	1:A:102:ARG:NH1	2.34	0.59
2:C:240:LEU:HD13	2:C:279:PRO:HG3	1.84	0.59
5:J:92:PHE:HA	5:J:121:ARG:HB2	1.84	0.59
8:P:199:GLN:O	8:P:203:GLN:HB2	2.03	0.59
4:H:513:PRO:HA	4:H:516:LEU:HD13	1.83	0.59
1:A:118:PHE:HB3	2:D:280:ASN:HD22	1.67	0.59
1:B:19:ASP:OD1	1:B:136:ARG:NH2	2.36	0.59
1:B:197:ALA:HA	1:B:208:ASN:HD21	1.67	0.59
5:J:654:LEU:HG	5:J:693:LYS:HB3	1.85	0.59
6:K:192:ARG:HE	6:K:236:VAL:HG11	1.66	0.59
3:E:8:MET:H	3:E:105:SER:HA	1.67	0.59
5:I:414:CYS:SG	5:I:415:ASP:N	2.69	0.59
5:J:414:CYS:HB3	5:J:433:SER:H	1.67	0.59
3:F:32:ASN:ND2	3:F:357:LEU:O	2.34	0.59
8:P:236:CYS:HA	8:P:239:ILE:HG12	1.85	0.59
2:D:66:ARG:HG2	2:D:351:LEU:HD22	1.84	0.59
3:F:170:MET:HG3	3:F:229:ILE:HG13	1.85	0.59
1:B:274:ASP:OD1	1:B:274:ASP:N	2.35	0.58
4:H:188:ARG:NE	4:H:459:ASP:OD2	2.32	0.58
6:K:178:ASN:O	6:K:182:ARG:CA	2.50	0.58
8:P:159:ILE:HG12	8:P:170:THR:HG21	1.85	0.58
4:H:370:ARG:HD2	4:H:374:ARG:HH22	1.69	0.58
5:I:72:ASN:HD21	5:I:380:GLY:HA2	1.68	0.58
2:C:203:MET:O	2:C:207:LEU:HB2	2.03	0.58
2:D:46:ILE:O	2:D:50:ARG:NH2	2.35	0.58
4:G:416:SER:HB3	4:G:420:THR:HG21	1.85	0.58
3:E:155:ARG:N	3:E:197:THR:HG1	2.02	0.58
4:H:205:PRO:HA	4:H:208:VAL:HG22	1.85	0.58
3:F:183:LYS:HB3	5:I:222:ARG:HH12	1.68	0.58
6:K:8:PHE:HE1	6:K:109:TYR:HB2	1.69	0.58
1:B:19:ASP:O	1:B:132:ARG:NH1	2.37	0.57
1:B:202:GLU:HB2	1:B:297:SER:HB3	1.86	0.57
8:P:101:CYS:SG	8:P:121:LYS:NZ	2.77	0.57
1:A:74:ARG:NH1	1:A:303:LEU:O	2.37	0.57
2:D:46:ILE:HA	2:D:49:HIS:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:116:GLU:HA	3:E:119:ASP:HB2	1.86	0.57
4:H:475:ASN:ND2	4:H:477:GLN:OE1	2.37	0.57
6:K:143:LYS:O	6:K:147:TYR:N	2.35	0.57
1:A:154:GLU:O	1:A:160:SER:OG	2.22	0.57
3:E:63:LEU:HD21	3:E:79:PRO:HB3	1.87	0.57
8:P:442:ALA:HB1	8:P:453:LEU:HD11	1.84	0.57
6:K:178:ASN:HD22	6:K:182:ARG:NH1	2.03	0.57
3:E:39:PRO:HA	3:E:114:LEU:HD11	1.87	0.57
4:G:175:SER:O	4:G:185:GLN:NE2	2.37	0.57
4:H:310:GLU:HA	4:H:314:LEU:HD23	1.87	0.57
5:J:426:LYS:NZ	5:J:445:GLU:OE1	2.38	0.57
5:J:581:LEU:O	8:P:385:ARG:NH1	2.38	0.57
1:A:134:VAL:HA	1:A:137:VAL:HG12	1.86	0.57
3:F:1:MET:HG2	4:G:199:PRO:HB2	1.86	0.57
5:J:554:GLN:HG2	5:J:558:LEU:HD23	1.87	0.57
4:G:336:TYR:HD1	4:G:361:VAL:HG23	1.70	0.56
4:H:346:LEU:HD21	4:H:358:VAL:HG21	1.87	0.56
4:G:455:ASN:ND2	4:G:489:TYR:O	2.38	0.56
6:K:126:GLN:HE22	6:K:128:GLU:HB2	1.68	0.56
6:K:257:VAL:HG13	6:K:261:LYS:HD3	1.86	0.56
4:G:409:LEU:HD23	4:G:447:VAL:HA	1.87	0.56
4:H:274:HIS:HA	4:H:277:ILE:HG12	1.87	0.56
7:M:179:LEU:HD22	7:M:183:VAL:HG21	1.87	0.56
8:P:197:GLU:O	8:P:201:LYS:HB2	2.05	0.56
5:J:84:THR:OG1	5:J:118:ASN:ND2	2.38	0.56
8:P:100:GLU:OE1	8:P:103:ARG:N	2.37	0.56
8:P:278:VAL:HA	8:P:340:GLY:HA2	1.86	0.56
5:I:344:ARG:HE	5:I:348:VAL:HG11	1.71	0.56
5:J:374:ILE:HG12	5:J:391:LEU:HB2	1.87	0.56
8:P:441:ILE:HD11	8:P:459:ILE:HG12	1.86	0.56
6:K:34:VAL:O	6:K:44:GLY:N	2.39	0.56
2:D:286:HIS:ND1	2:D:313:PHE:O	2.39	0.56
4:G:388:ILE:HA	4:G:391:ALA:HB2	1.87	0.56
5:I:51:SER:OG	5:I:65:ARG:NH1	2.33	0.56
8:P:40:ALA:N	8:P:129:HIS:O	2.39	0.56
4:H:479:HIS:HB2	4:H:482:LEU:HD22	1.87	0.56
2:D:207:LEU:HD12	2:D:212:ILE:HD12	1.88	0.56
3:F:109:ILE:O	3:F:133:ARG:NH1	2.39	0.55
3:E:110:THR:HA	3:E:275:LEU:HD23	1.88	0.55
3:F:160:VAL:HA	3:F:167:LEU:HA	1.86	0.55
5:I:342:ILE:HD13	5:I:356:LEU:HG	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:385:ILE:HD11	5:J:391:LEU:HD11	1.89	0.55
8:P:167:GLN:HE22	8:P:169:GLN:HB2	1.71	0.55
3:F:38:TYR:HA	3:F:41:ASN:HB2	1.88	0.55
2:D:345:HIS:HD2	2:D:346:PRO:HD2	1.71	0.55
7:M:183:VAL:HG22	8:P:230:TYR:OH	2.06	0.55
5:J:149:LEU:HD23	5:J:251:ILE:HG22	1.88	0.55
1:A:27:ILE:HA	1:A:72:PHE:HE2	1.72	0.55
2:C:39:LEU:HD11	2:C:137:ILE:HG23	1.88	0.55
8:P:87:LYS:HA	8:P:130:VAL:H	1.71	0.55
1:B:125:ILE:HB	1:B:150:VAL:HG22	1.88	0.55
5:I:136:ARG:NH2	5:I:263:ASN:O	2.36	0.55
5:I:180:VAL:HG12	5:I:181:MET:HG3	1.89	0.55
5:J:177:ASN:HB3	5:J:255:GLN:HE22	1.71	0.54
4:G:238:GLN:HA	4:G:297:LYS:HD3	1.88	0.54
8:P:377:LEU:HB2	8:P:379:ARG:HH12	1.71	0.54
4:H:333:ILE:HG22	4:H:400:LYS:HB3	1.90	0.54
8:P:367:ILE:HD12	8:P:434:CYS:HA	1.89	0.54
1:A:67:SER:OG	1:A:235:PHE:O	2.26	0.54
3:E:91:ARG:HG2	3:E:216:MET:HE3	1.89	0.54
5:J:44:GLN:NE2	5:J:143:LEU:O	2.34	0.54
5:J:612:LEU:HD21	5:J:659:LEU:HA	1.90	0.54
2:D:204:ALA:HB1	2:D:216:VAL:HG21	1.90	0.54
4:H:183:LEU:HD22	4:H:184:PRO:HD2	1.90	0.54
5:I:216:GLN:NE2	5:I:225:ALA:O	2.41	0.54
2:D:16:GLU:OE2	2:D:67:ARG:NH1	2.41	0.54
2:D:277:GLN:NE2	2:D:281:GLU:OE2	2.41	0.54
8:P:41:THR:HG22	8:P:130:VAL:HA	1.90	0.54
2:C:249:THR:OG1	2:C:250:GLY:N	2.40	0.54
3:E:104:LEU:HD12	3:E:204:LEU:HD21	1.89	0.54
4:H:502:THR:OG1	4:H:503:GLU:N	2.38	0.54
2:D:46:ILE:HD12	2:D:130:GLN:HG2	1.90	0.53
3:E:93:ILE:HG22	3:E:96:LYS:HB2	1.89	0.53
8:P:297:ARG:NH2	8:P:311:CYS:SG	2.76	0.53
2:C:233:ILE:HB	2:C:266:ILE:HG22	1.90	0.53
3:F:117:VAL:HG13	3:F:129:ALA:HB3	1.88	0.53
5:J:368:ILE:HA	5:J:385:ILE:HG23	1.89	0.53
4:G:437:CYS:HA	4:G:501:ILE:HB	1.90	0.53
8:P:210:PHE:O	8:P:214:THR:OG1	2.27	0.53
1:A:51:SER:HB3	1:A:73:LEU:HD21	1.89	0.53
2:C:89:ILE:HD11	2:C:133:ILE:HG23	1.89	0.53
4:H:223:ASN:HD21	4:H:340:SER:HB2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:239:ILE:HA	2:D:245:LEU:HA	1.89	0.53
5:I:146:SER:HA	5:I:254:PRO:HD3	1.91	0.53
5:J:186:LYS:HB2	5:J:245:LEU:HG	1.90	0.53
2:D:56:GLU:HA	2:D:59:GLU:HG2	1.90	0.53
4:G:170:ARG:HH12	4:G:266:CYS:HA	1.73	0.53
8:P:374:SER:HA	8:P:424:LEU:HA	1.90	0.53
1:B:153:THR:OG1	1:B:180:ASP:OD1	2.24	0.53
4:H:218:LEU:HD12	4:H:219:VAL:HG23	1.90	0.53
5:I:70:LEU:HA	5:I:306:TYR:HE1	1.74	0.53
5:J:589:LEU:HD11	8:P:212:GLN:HG2	1.89	0.53
8:P:91:LEU:HB3	8:P:122:GLY:HA3	1.91	0.53
8:P:177:ILE:HG22	8:P:182:LEU:HD22	1.91	0.53
2:D:324:PHE:HB2	2:D:331:ASN:H	1.73	0.52
4:H:458:ASP:OD1	4:H:458:ASP:N	2.39	0.52
5:I:109:SER:OG	5:I:112:CYS:SG	2.67	0.52
5:I:147:ASP:OD2	5:I:169:ARG:NH1	2.35	0.52
5:J:624:LEU:O	5:J:628:TRP:NE1	2.41	0.52
3:E:103:VAL:HG13	3:E:205:TYR:HB2	1.91	0.52
5:I:47:LEU:HD23	5:I:93:VAL:HG13	1.91	0.52
5:I:70:LEU:HD22	5:I:156:ILE:HD13	1.90	0.52
6:K:21:MET:HG2	6:K:70:CYS:HA	1.91	0.52
2:C:81:MET:HE1	2:C:140:LEU:HD12	1.90	0.52
2:C:88:ILE:HG13	2:C:89:ILE:HD12	1.92	0.52
5:I:396:LEU:HD12	5:I:400:VAL:HG21	1.91	0.52
8:P:202:GLU:OE1	8:P:206:GLN:NE2	2.43	0.52
2:D:130:GLN:HA	2:D:133:ILE:HD12	1.90	0.52
4:H:240:TYR:O	4:H:297:LYS:NZ	2.43	0.52
5:I:141:LYS:HB3	5:I:143:LEU:HD13	1.91	0.52
5:J:65:ARG:NH1	5:J:154:ASP:OD1	2.43	0.52
2:C:314:ASP:OD2	4:G:392:SER:OG	2.26	0.52
3:F:10:VAL:HG22	3:F:84:MET:HG3	1.91	0.52
2:C:299:GLU:O	4:G:374:ARG:NH1	2.43	0.52
3:F:36:ILE:O	3:F:70:LYS:NZ	2.29	0.52
2:C:170:PHE:HD1	2:C:203:MET:HB3	1.74	0.52
2:C:277:GLN:NE2	2:C:281:GLU:OE2	2.41	0.52
2:D:145:GLU:OE1	6:K:67:ARG:NH2	2.43	0.52
5:I:95:CYS:SG	5:I:96:CYS:N	2.83	0.52
5:J:376:ASN:HB2	5:J:393:GLN:HG2	1.92	0.52
3:E:38:TYR:OH	3:E:290:TRP:O	2.20	0.52
6:K:178:ASN:ND2	6:K:182:ARG:NH1	2.58	0.52
1:A:272:TRP:HD1	1:A:273:VAL:HG23	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ALA:HB2	1:B:155:SER:HB2	1.90	0.51
1:B:203:ASN:HB2	1:B:239:PHE:HE1	1.74	0.51
2:C:207:LEU:HD22	2:C:212:ILE:HD13	1.90	0.51
3:E:212:VAL:O	3:E:216:MET:CB	2.57	0.51
2:D:22:LEU:O	2:D:72:GLN:NE2	2.38	0.51
3:F:155:ARG:N	3:F:197:THR:OG1	2.43	0.51
4:G:220:SER:HA	4:G:225:ARG:HE	1.75	0.51
6:K:234:ARG:HE	6:K:235:TYR:H	1.57	0.51
8:P:386:THR:HB	8:P:390:LYS:HB2	1.93	0.51
1:A:128:HIS:CD2	1:A:129:ALA:H	2.28	0.51
2:C:164:VAL:HG22	2:C:229:VAL:HG12	1.91	0.51
6:K:178:ASN:OD1	6:K:182:ARG:CB	2.57	0.51
7:M:179:LEU:HD23	7:M:183:VAL:CG2	2.40	0.51
1:B:74:ARG:HD2	1:B:303:LEU:HG	1.92	0.51
4:H:220:SER:HA	4:H:225:ARG:HE	1.76	0.51
5:J:99:ALA:O	5:J:103:LYS:CB	2.59	0.51
5:J:698:ARG:O	5:J:704:GLN:NE2	2.43	0.51
1:B:108:ARG:HD3	1:B:136:ARG:HG2	1.91	0.51
8:P:211:VAL:HB	8:P:217:GLU:HB3	1.93	0.51
1:B:132:ARG:HE	1:B:133:VAL:HG22	1.75	0.51
6:K:74:ILE:HG12	6:K:88:ARG:HH21	1.75	0.51
1:A:4:LYS:HG3	1:A:6:LEU:H	1.74	0.51
2:D:231:LYS:NZ	2:D:232:VAL:O	2.44	0.51
3:F:32:ASN:ND2	3:F:375:ILE:O	2.44	0.51
5:I:374:ILE:HA	5:I:391:LEU:HD22	1.93	0.51
5:J:131:LEU:HD21	5:J:268:THR:HA	1.93	0.51
8:P:54:LYS:NZ	8:P:135:CYS:O	2.43	0.51
1:B:154:GLU:HG2	1:B:156:GLN:HB3	1.93	0.51
1:B:160:SER:OG	1:B:209:LYS:NZ	2.44	0.51
6:K:58:SER:HB2	6:K:61:LYS:HE3	1.93	0.51
1:B:242:ASN:H	1:B:245:ASP:CG	2.19	0.50
2:D:239:ILE:HB	2:D:274:LEU:HD22	1.93	0.50
1:B:20:MET:SD	1:B:20:MET:N	2.84	0.50
5:J:78:TYR:HB3	5:J:156:ILE:HD13	1.93	0.50
5:J:630:PRO:O	5:J:634:ASN:N	2.38	0.50
6:K:90:VAL:HG13	6:K:93:GLU:HB3	1.92	0.50
8:P:46:THR:HG23	8:P:135:CYS:HB3	1.92	0.50
1:B:196:GLY:O	1:B:208:ASN:ND2	2.44	0.50
4:G:229:LEU:HD11	4:G:260:MET:HE2	1.92	0.50
5:J:172:ARG:NH1	5:J:253:SER:OG	2.45	0.50
6:K:176:LEU:CA	6:K:180:ILE:CG2	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:4:GLN:HA	3:E:50:GLU:HG3	1.93	0.50
3:E:118:VAL:HG13	4:H:198:ILE:HG12	1.92	0.50
4:G:320:SER:OG	4:G:348:GLU:OE2	2.26	0.50
4:H:332:VAL:HG12	4:H:357:ARG:HB3	1.94	0.50
5:J:46:VAL:HG23	5:J:92:PHE:HB2	1.92	0.50
3:E:37:TRP:O	3:E:41:ASN:N	2.43	0.50
5:J:99:ALA:O	5:J:103:LYS:HB2	2.12	0.50
8:P:193:ASP:O	8:P:196:LYS:NZ	2.43	0.50
5:I:343:TYR:N	5:I:360:VAL:O	2.34	0.50
5:J:151:VAL:HG12	5:J:249:ILE:HA	1.94	0.50
1:A:120:LYS:HB3	1:A:123:ALA:HB2	1.93	0.50
2:C:90:ARG:HD2	2:C:345:HIS:CD2	2.47	0.50
3:E:128:LEU:HD11	3:E:228:LEU:HD22	1.94	0.50
1:A:19:ASP:O	1:A:132:ARG:NH1	2.45	0.50
4:G:260:MET:SD	4:G:260:MET:N	2.85	0.50
1:B:30:LEU:HD21	1:B:54:GLU:HB3	1.94	0.49
3:F:1:MET:HA	4:G:199:PRO:HB2	1.94	0.49
5:I:392:ASP:N	5:I:392:ASP:OD1	2.45	0.49
6:K:179:ASN:N	6:K:179:ASN:ND2	2.60	0.49
8:P:208:LEU:O	8:P:212:GLN:NE2	2.44	0.49
3:E:345:GLN:HA	3:E:360:PRO:HB3	1.95	0.49
5:J:47:LEU:HD23	5:J:151:VAL:HG23	1.94	0.49
1:B:190:ALA:HB3	1:B:224:LYS:HZ2	1.77	0.49
3:E:239:SER:O	3:E:242:SER:OG	2.30	0.49
4:G:191:SER:OG	4:G:192:LEU:N	2.44	0.49
4:G:200:SER:OG	4:G:203:ILE:O	2.28	0.49
1:A:6:LEU:HD21	1:A:33:PHE:HB2	1.94	0.49
2:C:217:MET:HE2	2:C:225:VAL:HG21	1.93	0.49
5:J:563:ARG:HD2	8:P:379:ARG:HD3	1.95	0.49
8:P:58:VAL:O	8:P:62:SER:N	2.45	0.49
1:A:70:GLU:HG2	1:A:237:ARG:HD3	1.94	0.49
3:E:2:GLU:O	3:E:99:THR:OG1	2.27	0.49
3:F:67:PHE:O	3:F:72:LYS:NZ	2.45	0.49
5:I:414:CYS:HB3	5:I:432:THR:HA	1.94	0.49
1:A:11:LYS:HA	1:A:14:MET:HG2	1.95	0.49
3:F:232:LEU:HD13	3:F:239:SER:HA	1.95	0.49
5:I:316:ARG:HH22	5:I:337:HIS:CD2	2.31	0.49
5:J:393:GLN:OE1	5:J:410:GLN:NE2	2.44	0.49
8:P:160:ALA:HA	8:P:190:ASN:HB3	1.95	0.49
3:F:208:LYS:HB3	3:F:211:ILE:HG12	1.95	0.49
5:J:180:VAL:HG12	5:J:181:MET:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:575:VAL:HA	5:J:578:ILE:HG22	1.95	0.49
1:A:130:TYR:HA	1:A:164:MET:HE3	1.93	0.49
2:D:213:GLU:OE2	4:H:483:ARG:NH2	2.46	0.49
8:P:76:ASN:O	8:P:80:LYS:NZ	2.40	0.49
8:P:300:ILE:HB	8:P:347:LEU:HD11	1.95	0.49
2:D:302:ILE:HG23	4:H:377:VAL:HG11	1.95	0.48
4:G:234:GLN:HA	4:G:237:ILE:HG22	1.95	0.48
5:I:413:LEU:HD13	5:I:431:LEU:HB2	1.94	0.48
2:C:166:MET:HB3	2:C:232:VAL:HG23	1.96	0.48
2:C:281:GLU:HG2	2:C:282:GLU:HG2	1.94	0.48
5:I:362:LEU:HA	5:I:379:ILE:HB	1.96	0.48
5:J:64:PRO:HG2	5:J:67:LEU:H	1.77	0.48
5:J:129:ARG:NH1	5:J:130:SER:OG	2.47	0.48
6:K:255:MET:HA	6:K:258:ILE:HG22	1.95	0.48
1:B:241:LEU:HD21	4:H:499:LEU:HD11	1.95	0.48
2:C:167:THR:OG1	2:C:168:ILE:N	2.46	0.48
3:F:85:GLY:O	3:F:89:SER:N	2.44	0.48
8:P:434:CYS:SG	8:P:435:THR:N	2.86	0.48
1:A:243:GLN:HE22	1:B:189:LYS:HB3	1.78	0.48
4:G:446:ARG:NH2	4:G:454:SER:OG	2.47	0.48
6:K:32:ALA:H	6:K:46:ILE:HG12	1.79	0.48
2:C:330:GLY:HA3	4:H:447:VAL:HG11	1.95	0.48
3:F:26:PRO:HG2	3:F:56:THR:HG23	1.95	0.48
5:J:70:LEU:HD21	5:J:310:CYS:HA	1.94	0.48
5:J:622:LEU:HA	5:J:625:LEU:HB2	1.96	0.48
1:B:27:ILE:HA	1:B:72:PHE:HE2	1.79	0.48
5:I:431:LEU:HD22	5:I:449:ILE:HB	1.96	0.48
1:A:232:SER:OG	1:A:233:PHE:N	2.47	0.47
2:C:326:SER:OG	2:C:327:ASN:N	2.47	0.47
4:G:226:CYS:SG	4:G:441:TYR:OH	2.66	0.47
4:H:324:TYR:O	4:H:354:ARG:NH2	2.47	0.47
5:J:185:PHE:HB2	5:J:246:ASP:HA	1.96	0.47
8:P:398:LEU:HD11	8:P:417:VAL:HG11	1.94	0.47
2:D:226:MET:HE2	2:D:258:ALA:HA	1.95	0.47
2:D:87:LYS:HG3	2:D:345:HIS:H	1.79	0.47
6:K:33:TYR:HA	6:K:45:MET:HA	1.95	0.47
2:D:52:SER:OG	2:D:56:GLU:OE2	2.31	0.47
4:H:388:ILE:HG13	4:H:422:GLN:HE21	1.79	0.47
4:H:401:VAL:HG13	4:H:434:VAL:HA	1.95	0.47
6:K:126:GLN:OE1	6:K:129:SER:N	2.47	0.47
2:D:241:ALA:HB2	2:D:276:PRO:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:308:ALA:O	5:I:312:ASP:HB2	2.15	0.47
5:J:616:ARG:HD2	5:J:619:ALA:HB3	1.97	0.47
4:G:292:ARG:HE	4:G:295:GLU:HG2	1.80	0.47
5:I:69:PRO:HG2	5:I:397:TRP:NE1	2.29	0.47
5:J:56:PHE:HD2	5:J:65:ARG:HG2	1.80	0.47
6:K:199:CYS:SG	6:K:200:TYR:N	2.88	0.47
1:B:186:ILE:HD12	1:B:189:LYS:HZ3	1.80	0.47
2:D:259:LYS:HG3	2:D:320:LEU:HD11	1.97	0.47
3:E:233:VAL:HG22	3:E:261:LEU:HB3	1.96	0.47
3:F:133:ARG:NH1	3:F:276:ALA:O	2.48	0.47
3:F:211:ILE:O	3:F:215:LEU:HB2	2.14	0.47
4:H:210:LEU:HD23	4:H:263:LEU:HD21	1.97	0.47
4:H:311:LYS:O	4:H:315:ALA:HB3	2.15	0.47
5:J:633:ARG:NH2	5:J:636:ILE:O	2.47	0.47
6:K:133:ARG:HD3	6:K:166:LEU:HD21	1.97	0.47
6:K:178:ASN:ND2	6:K:182:ARG:HH11	2.10	0.47
6:K:178:ASN:HD21	6:K:182:ARG:CD	2.05	0.47
1:B:240:PRO:HA	1:B:245:ASP:HB2	1.96	0.47
2:C:241:ALA:HA	2:C:340:MET:HE1	1.97	0.47
4:G:423:LEU:HA	4:G:426:VAL:HG22	1.95	0.47
5:J:356:LEU:HD12	5:J:360:VAL:HG11	1.97	0.47
5:J:560:THR:HA	5:J:563:ARG:HE	1.80	0.47
6:K:109:TYR:O	6:K:113:ARG:N	2.34	0.47
2:C:346:PRO:O	2:C:349:HIS:ND1	2.48	0.46
2:D:255:ALA:HB1	2:D:320:LEU:HD23	1.96	0.46
4:G:319:ILE:HG13	4:G:345:ILE:HD11	1.97	0.46
4:G:514:VAL:HG23	4:G:517:ARG:HE	1.80	0.46
5:I:188:SER:OG	5:I:189:SER:N	2.47	0.46
5:J:48:VAL:HG12	5:J:134:VAL:HG11	1.97	0.46
5:J:181:MET:SD	5:J:252:CYS:HA	2.55	0.46
1:A:237:ARG:HB2	1:A:305:LEU:HG	1.97	0.46
1:A:292:THR:HG23	1:A:294:SER:H	1.81	0.46
5:I:75:LEU:HD23	5:I:154:ASP:HA	1.97	0.46
1:B:243:GLN:HE22	1:B:244:GLN:HE21	1.61	0.46
2:D:340:MET:SD	2:D:340:MET:N	2.88	0.46
3:E:43:LEU:HD21	4:H:198:ILE:HG22	1.97	0.46
5:J:182:THR:HG22	5:J:288:HIS:HB2	1.96	0.46
3:F:396:VAL:HA	3:F:413:ALA:HB3	1.97	0.46
8:P:145:MET:HB3	8:P:145:MET:HE3	1.85	0.46
1:A:165:ALA:HA	1:A:175:VAL:HG11	1.98	0.46
4:H:311:LYS:O	4:H:315:ALA:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:41:THR:HG23	8:P:42:ILE:HG12	1.98	0.46
8:P:258:VAL:HG22	8:P:356:GLN:H	1.81	0.46
5:J:646:LEU:HA	5:J:649:ILE:HG22	1.97	0.46
6:K:212:LEU:HD13	8:P:275:LYS:HE3	1.98	0.46
8:P:47:ILE:HD11	8:P:157:LEU:HG	1.97	0.46
8:P:316:SER:OG	8:P:317:LYS:N	2.48	0.46
3:E:53:VAL:HG23	3:E:75:ILE:HD11	1.98	0.46
3:E:212:VAL:O	3:E:216:MET:HB3	2.15	0.46
5:I:250:SER:OG	5:I:269:ARG:NH2	2.49	0.46
2:C:210:ALA:HB3	2:C:212:ILE:HD11	1.98	0.46
4:G:443:PHE:HB3	4:G:516:LEU:HD22	1.97	0.46
4:H:405:ALA:HA	4:H:416:SER:HB3	1.96	0.46
5:J:396:LEU:HD11	5:J:400:VAL:HG11	1.97	0.46
5:J:700:ASN:HB3	5:J:703:LEU:HB3	1.98	0.46
1:B:32:GLU:O	1:B:35:LYS:NZ	2.48	0.46
1:B:135:LEU:HA	1:B:138:LEU:HD23	1.98	0.46
2:C:165:ILE:HG13	2:C:231:LYS:HG3	1.98	0.46
2:C:166:MET:HE2	2:C:190:ILE:HD11	1.97	0.46
2:D:203:MET:HE2	2:D:203:MET:HB2	1.89	0.46
2:C:131:SER:HA	2:C:134:ILE:HG22	1.98	0.46
2:D:66:ARG:HA	2:D:66:ARG:HD3	1.72	0.46
3:F:132:MET:HG2	3:F:201:ASP:HA	1.97	0.46
4:G:334:LEU:HB3	4:G:401:VAL:HG23	1.98	0.46
8:P:448:GLU:OE2	8:P:452:ARG:NE	2.48	0.46
2:C:171:SER:HB3	2:C:174:VAL:HG12	1.97	0.45
5:I:128:TYR:OH	5:I:137:ASP:OD2	2.32	0.45
8:P:56:THR:OG1	8:P:226:ALA:O	2.31	0.45
3:F:107:ASP:HB3	3:F:278:TYR:HB2	1.97	0.45
4:H:275:ASN:ND2	4:H:441:TYR:O	2.49	0.45
4:H:282:LYS:O	4:H:286:SER:N	2.49	0.45
5:J:362:LEU:HB3	5:J:366:THR:HG21	1.98	0.45
5:I:437:VAL:HG11	5:I:443:LEU:HD21	1.99	0.45
4:G:311:LYS:O	4:G:315:ALA:CB	2.65	0.45
5:I:130:SER:OG	5:I:131:LEU:N	2.50	0.45
8:P:211:VAL:HA	8:P:216:ALA:HB3	1.98	0.45
2:D:80:ASN:ND2	2:D:274:LEU:O	2.39	0.45
3:F:6:VAL:HG12	3:F:52:ILE:HB	1.98	0.45
5:I:187:GLU:HA	5:I:243:ASP:HB2	1.99	0.45
4:H:326:LYS:HG2	4:H:435:LEU:HD11	1.99	0.45
5:I:255:GLN:HA	5:I:258:GLN:HG2	1.98	0.45
5:J:177:ASN:HB3	5:J:255:GLN:NE2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:144:LEU:HA	2:C:147:THR:HG23	1.99	0.45
4:G:471:VAL:HG12	4:G:473:LEU:H	1.82	0.45
5:I:311:ALA:HA	5:I:314:ILE:HG22	1.99	0.45
1:B:93:MET:HG3	1:B:96:ARG:HD3	1.98	0.45
5:J:616:ARG:HA	5:J:619:ALA:HB3	1.97	0.45
8:P:258:VAL:HG23	8:P:355:GLY:H	1.82	0.45
1:B:203:ASN:HB2	1:B:239:PHE:CE1	2.52	0.45
6:K:133:ARG:HB2	6:K:166:LEU:HD11	1.99	0.45
2:C:18:PHE:HA	2:C:21:THR:HG22	1.99	0.45
3:F:231:TYR:HD2	3:F:233:VAL:HG23	1.82	0.45
4:H:334:LEU:HD23	4:H:398:VAL:HG21	1.98	0.45
8:P:204:TYR:HA	8:P:207:ILE:HG12	1.99	0.45
3:F:223:SER:O	3:F:226:SER:N	2.42	0.44
8:P:238:TYR:HD1	8:P:242:LYS:HG3	1.82	0.44
1:A:152:VAL:HG21	1:A:164:MET:HB3	1.99	0.44
2:C:170:PHE:CD1	2:C:203:MET:HB3	2.52	0.44
5:I:109:SER:HG	5:I:112:CYS:HG	1.58	0.44
3:E:204:LEU:HA	3:E:204:LEU:HD23	1.70	0.44
4:G:172:ASP:OD1	4:G:173:TYR:N	2.51	0.44
5:J:94:PHE:HD2	5:J:134:VAL:HG22	1.81	0.44
1:A:283:LEU:HD22	1:A:285:PHE:CZ	2.53	0.44
4:G:328:SER:OG	4:G:329:ASN:N	2.47	0.44
5:I:75:LEU:HA	5:I:78:TYR:HD2	1.81	0.44
6:K:24:VAL:HG13	6:K:34:VAL:HG12	1.99	0.44
6:K:61:LYS:HG3	6:K:62:LEU:HD22	1.99	0.44
6:K:209:LYS:HE3	8:P:342:LYS:HD3	1.99	0.44
8:P:153:ASP:OD1	8:P:248:ARG:NH2	2.50	0.44
1:B:101:LEU:HA	1:B:104:ILE:HG22	1.99	0.44
3:E:53:VAL:N	3:E:76:VAL:O	2.47	0.44
5:J:403:ALA:HB3	5:J:420:LYS:HA	2.00	0.44
6:K:129:SER:O	6:K:133:ARG:NH1	2.50	0.44
6:K:205:ILE:HB	8:P:342:LYS:HZ1	1.83	0.44
8:P:186:LEU:HA	8:P:219:ALA:HB3	2.00	0.44
4:G:210:LEU:HD11	4:G:228:ALA:HB1	1.98	0.44
5:I:62:ASP:OD2	5:I:433:SER:OG	2.36	0.44
8:P:177:ILE:HA	8:P:182:LEU:HB3	1.99	0.44
1:A:124:THR:OG1	1:A:189:LYS:O	2.33	0.44
1:B:159:LEU:HD23	1:B:162:LYS:HD2	2.00	0.44
2:C:252:HIS:HD2	2:C:317:PRO:HD3	1.82	0.44
5:I:172:ARG:NH2	5:I:253:SER:OG	2.50	0.44
8:P:265:ASN:HD21	8:P:275:LYS:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:4:GLN:O	3:E:102:LEU:N	2.50	0.44
4:G:355:ARG:HH22	4:G:382:PRO:HD2	1.82	0.44
5:J:264:PHE:HD2	8:P:405:MET:HE1	1.83	0.44
5:J:583:TYR:CG	8:P:171:SER:HB2	2.53	0.44
6:K:28:ALA:HB2	6:K:33:TYR:HD1	1.82	0.44
6:K:35:SER:HA	6:K:43:GLU:HA	1.99	0.44
8:P:345:PRO:HB2	8:P:347:LEU:H	1.82	0.44
5:J:604:PRO:HA	5:J:608:MET:HE2	1.99	0.43
6:K:204:GLY:HA2	6:K:207:ALA:HB3	2.00	0.43
3:F:125:ASP:OD1	4:G:209:ARG:NH2	2.51	0.43
8:P:402:GLU:OE2	8:P:445:ARG:NE	2.49	0.43
2:C:226:MET:HE2	2:C:226:MET:HB2	1.74	0.43
5:J:136:ARG:NH2	5:J:264:PHE:HA	2.33	0.43
6:K:9:TYR:HB2	6:K:144:ARG:HH22	1.83	0.43
6:K:226:LYS:HE3	6:K:238:THR:HG21	2.00	0.43
5:J:411:SER:OG	5:J:412:LEU:N	2.52	0.43
1:B:71:LEU:HD22	1:B:233:PHE:HB3	1.99	0.43
2:C:242:ASN:HD21	2:C:278:PHE:HE1	1.67	0.43
3:F:2:GLU:O	3:F:99:THR:OG1	2.27	0.43
5:I:77:ASP:O	5:I:81:GLU:CB	2.60	0.43
5:I:343:TYR:HB2	5:I:361:LEU:HA	2.00	0.43
6:K:189:VAL:O	6:K:189:VAL:HG13	2.17	0.43
6:K:213:ARG:HA	6:K:216:LEU:HB2	2.01	0.43
8:P:205:GLU:HA	8:P:208:LEU:HG	1.99	0.43
8:P:254:PRO:HB2	8:P:288:LEU:HD13	1.99	0.43
8:P:327:ASP:OD1	8:P:327:ASP:N	2.51	0.43
2:C:13:GLU:HG2	2:C:14:ARG:HD3	2.01	0.43
2:D:65:GLY:HA2	2:D:68:MET:HE3	2.01	0.43
3:E:201:ASP:OD2	3:E:225:ARG:NH1	2.52	0.43
3:F:63:LEU:HD21	3:F:79:PRO:HA	2.01	0.43
4:H:486:ASN:OD1	4:H:486:ASN:N	2.50	0.43
6:K:175:VAL:O	6:K:180:ILE:HG22	2.18	0.43
6:K:210:GLU:HG2	6:K:213:ARG:HD3	1.99	0.43
8:P:62:SER:HB2	8:P:84:ALA:HA	2.00	0.43
4:H:203:ILE:HA	4:H:259:TYR:HE1	1.83	0.43
8:P:52:HIS:CE1	8:P:158:LEU:HB3	2.54	0.43
1:B:235:PHE:HB3	1:B:237:ARG:NH1	2.32	0.43
3:E:180:LEU:HD11	5:J:226:PHE:HB2	2.00	0.43
4:G:227:ILE:HA	4:G:230:LEU:HB2	2.00	0.43
5:J:156:ILE:HD11	5:J:321:LEU:HG	2.00	0.43
5:J:654:LEU:HD11	5:J:694:GLY:HA2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:172:GLU:HG2	6:K:175:VAL:HB	2.00	0.43
5:I:71:ALA:HA	5:I:378:VAL:HG11	2.00	0.43
5:J:56:PHE:CG	5:J:59:ILE:HD11	2.54	0.43
5:J:563:ARG:CZ	8:P:379:ARG:HB3	2.48	0.43
3:E:209:LYS:HA	3:E:212:VAL:HG22	2.00	0.42
5:I:162:THR:HA	5:I:165:LEU:HG	2.01	0.42
5:J:75:LEU:HD11	5:J:300:VAL:HG11	2.01	0.42
8:P:261:SER:HA	8:P:279:ALA:HA	2.01	0.42
1:A:5:GLU:OE1	1:A:36:ARG:NH2	2.51	0.42
5:I:149:LEU:HD23	5:I:251:ILE:HD13	2.00	0.42
5:J:588:SER:OG	5:J:591:GLU:OE1	2.33	0.42
2:D:149:GLU:OE2	6:K:64:ARG:NH2	2.52	0.42
2:D:252:HIS:CD2	2:D:256:LEU:HD13	2.55	0.42
6:K:170:GLU:HG2	6:K:171:ASP:H	1.84	0.42
2:D:155:ALA:HB3	2:D:180:GLU:HG2	2.01	0.42
4:H:177:VAL:HB	4:H:485:LEU:HD12	2.01	0.42
4:H:193:THR:HA	4:H:196:MET:HG3	2.01	0.42
2:C:164:VAL:HG11	2:C:228:ARG:HG3	2.00	0.42
3:F:108:LEU:HD22	3:F:204:LEU:HD11	2.01	0.42
1:A:26:ALA:HB2	1:A:65:VAL:HG13	2.00	0.42
3:E:4:GLN:HG2	3:E:50:GLU:HB2	2.02	0.42
3:F:83:ASP:OD1	3:F:83:ASP:N	2.52	0.42
3:F:365:GLY:N	3:F:381:ILE:O	2.53	0.42
4:H:507:ILE:HG13	4:H:515:VAL:HG21	2.01	0.42
5:J:230:LEU:H	5:J:230:LEU:HG	1.73	0.42
5:J:274:ARG:HA	5:J:274:ARG:HD2	1.89	0.42
5:J:397:TRP:HB2	5:J:414:CYS:HA	2.02	0.42
8:P:169:GLN:HA	8:P:172:GLU:HB3	2.02	0.42
1:B:75:PHE:HZ	1:B:97:GLY:HA2	1.83	0.42
1:B:226:PHE:O	1:B:282:THR:N	2.44	0.42
2:D:82:VAL:HA	2:D:85:VAL:HG12	2.02	0.42
2:D:156:LEU:HD12	2:D:156:LEU:HA	1.91	0.42
2:D:156:LEU:HD11	2:D:185:ARG:HD3	2.01	0.42
2:D:259:LYS:HD3	2:D:262:SER:HA	2.02	0.42
2:D:295:LEU:HD13	2:D:295:LEU:HA	1.87	0.42
6:K:7:ARG:HH22	6:K:127:LEU:HD22	1.83	0.42
8:P:429:LEU:HA	8:P:429:LEU:HD12	1.86	0.42
1:B:180:ASP:OD2	1:B:214:GLN:NE2	2.52	0.42
3:F:345:GLN:HA	3:F:360:PRO:HA	2.01	0.42
4:G:249:SER:OG	4:G:288:GLY:O	2.34	0.42
5:I:163:ARG:HH21	5:I:290:HIS:CE1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:167:ASP:O	6:K:169:ASN:N	2.52	0.42
1:B:119:ILE:HD11	1:B:141:ALA:HB1	2.01	0.42
8:P:183:LYS:HG3	8:P:184:HIS:CD2	2.54	0.42
4:G:257:LYS:HE3	6:K:29:GLU:HB2	2.01	0.41
4:H:224:ALA:HA	4:H:227:ILE:HG22	2.02	0.41
5:I:343:TYR:HD2	5:I:361:LEU:HD12	1.84	0.41
5:I:407:GLN:HB3	5:I:409:HIS:HE1	1.85	0.41
6:K:8:PHE:CE1	6:K:109:TYR:HB2	2.51	0.41
2:C:226:MET:HG2	2:C:261:HIS:CD2	2.55	0.41
2:D:222:ILE:HD11	2:D:254:LEU:HD13	2.01	0.41
3:F:105:SER:OG	3:F:107:ASP:O	2.28	0.41
3:F:170:MET:HE2	3:F:229:ILE:HD11	2.02	0.41
3:F:401:GLY:O	3:F:419:ALA:N	2.43	0.41
4:H:176:LYS:HE3	4:H:176:LYS:HB2	1.93	0.41
5:J:271:ASP:N	5:J:271:ASP:OD1	2.50	0.41
8:P:186:LEU:HD12	8:P:222:ILE:HD13	2.03	0.41
8:P:232:ILE:HA	8:P:235:VAL:HB	2.02	0.41
8:P:405:MET:HB2	8:P:444:SER:HB3	2.00	0.41
1:B:28:ARG:HA	1:B:31:LEU:HB2	2.02	0.41
3:E:26:PRO:HG2	3:E:56:THR:HB	2.02	0.41
3:E:193:ILE:HB	5:J:240:VAL:HG12	2.01	0.41
5:I:438:GLY:H	5:I:464:GLU:HG2	1.86	0.41
5:J:573:ASN:OD1	5:J:573:ASN:N	2.50	0.41
6:K:97:LYS:O	6:K:101:LYS:HG2	2.20	0.41
6:K:175:VAL:O	6:K:180:ILE:N	2.46	0.41
2:C:80:ASN:ND2	2:C:83:ARG:HH21	2.19	0.41
2:C:207:LEU:HD12	2:C:214:THR:HB	2.02	0.41
3:E:201:ASP:OD1	3:E:202:ALA:N	2.54	0.41
3:E:365:GLY:N	3:E:381:ILE:O	2.54	0.41
4:G:253:VAL:HB	4:G:284:ILE:HD11	2.02	0.41
4:H:400:LYS:NZ	4:H:435:LEU:HB2	2.35	0.41
6:K:22:VAL:HG23	6:K:36:LEU:HA	2.01	0.41
6:K:167:ASP:HB3	6:K:171:ASP:HA	2.03	0.41
3:E:212:VAL:O	3:E:216:MET:HB2	2.21	0.41
5:I:356:LEU:HD13	5:I:374:ILE:HG23	2.02	0.41
5:I:394:THR:HG21	5:I:408:ILE:HG23	2.02	0.41
2:C:274:LEU:HD22	2:C:275:SER:H	1.84	0.41
2:D:16:GLU:HA	2:D:19:VAL:HG22	2.03	0.41
5:I:41:PRO:HG2	5:I:169:ARG:HE	1.84	0.41
5:I:316:ARG:NH2	5:I:343:TYR:OH	2.53	0.41
5:J:351:GLY:H	5:J:368:ILE:HG23	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:SER:O	1:A:160:SER:OG	2.39	0.41
4:G:204:HIS:HD2	4:G:206:ALA:H	1.69	0.41
5:J:248:HIS:CE1	5:J:299:ARG:HE	2.39	0.41
1:B:11:LYS:HD2	1:B:14:MET:HE3	2.03	0.41
2:C:216:VAL:HB	4:G:484:LEU:HD23	2.03	0.41
4:G:177:VAL:HG11	4:G:485:LEU:HD13	2.02	0.41
4:H:172:ASP:OD1	4:H:173:TYR:N	2.54	0.41
4:H:186:TYR:OH	4:H:265:GLN:OE1	2.28	0.41
4:H:373:LEU:HD23	4:H:373:LEU:HA	1.93	0.41
5:J:50:ASP:OD1	5:J:50:ASP:N	2.53	0.41
5:J:76:ILE:HD11	5:J:105:HIS:CD2	2.55	0.41
5:J:76:ILE:HD11	5:J:105:HIS:HD2	1.86	0.41
8:P:100:GLU:CD	8:P:102:TYR:H	2.29	0.41
8:P:169:GLN:O	8:P:173:HIS:N	2.52	0.41
8:P:207:ILE:HD11	8:P:221:ILE:HD12	2.03	0.41
1:A:25:ALA:O	1:A:29:THR:OG1	2.28	0.41
1:B:108:ARG:HA	1:B:111:ILE:HG12	2.02	0.41
2:C:164:VAL:HG21	2:C:228:ARG:HG3	2.03	0.41
2:D:42:LEU:HD13	2:D:45:ILE:HG21	2.03	0.41
3:E:74:ASP:N	3:E:74:ASP:OD1	2.54	0.41
4:G:499:LEU:HD13	4:G:499:LEU:HA	1.88	0.41
4:H:237:ILE:HD12	4:H:237:ILE:HA	1.96	0.41
5:J:132:GLY:H	5:J:267:GLN:HE21	1.67	0.41
6:K:262:ILE:HD13	6:K:265:LYS:HE3	2.03	0.41
8:P:70:LYS:HD3	8:P:262:PHE:HD1	1.86	0.41
1:B:242:ASN:N	1:B:245:ASP:OD2	2.33	0.40
2:C:194:CYS:SG	2:C:249:THR:HG23	2.61	0.40
3:E:6:VAL:HG12	3:E:52:ILE:HB	2.03	0.40
4:G:170:ARG:NH2	4:G:266:CYS:O	2.54	0.40
4:H:346:LEU:HD12	4:H:346:LEU:HA	1.77	0.40
5:I:56:PHE:H	5:I:65:ARG:HH21	1.68	0.40
5:I:205:VAL:HG13	5:I:239:GLU:HB2	2.04	0.40
5:J:47:LEU:N	5:J:92:PHE:O	2.49	0.40
5:J:211:ARG:HD2	5:J:286:GLN:HG3	2.02	0.40
1:B:108:ARG:HG3	1:B:132:ARG:NH2	2.36	0.40
2:D:138:ASN:HA	2:D:141:LEU:HG	2.03	0.40
3:E:48:PHE:HZ	3:E:114:LEU:HD13	1.87	0.40
3:F:56:THR:O	3:F:63:LEU:N	2.55	0.40
4:H:170:ARG:HH11	4:H:186:TYR:HB3	1.85	0.40
5:I:196:CYS:SG	5:I:197:HIS:N	2.95	0.40
5:J:200:ASN:ND2	5:J:242:TYR:OH	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:183:VAL:HG21	8:P:230:TYR:HE2	1.81	0.40
2:C:89:ILE:HG13	2:C:133:ILE:HG12	2.03	0.40
2:D:129:LEU:HG	2:D:133:ILE:HD11	2.03	0.40
3:E:132:MET:HB3	3:E:199:LEU:HD23	2.03	0.40
3:E:374:VAL:O	3:E:392:LEU:N	2.55	0.40
4:H:333:ILE:HD12	4:H:402:LEU:HD13	2.02	0.40
5:I:340:HIS:HB3	5:I:358:GLU:HA	2.02	0.40
5:J:157:SER:HB2	5:J:297:GLY:HA3	2.03	0.40
2:D:35:ALA:HA	2:D:38:THR:HG22	2.03	0.40
8:P:197:GLU:O	8:P:201:LYS:CB	2.70	0.40
2:D:203:MET:HA	2:D:206:ASN:HB3	2.04	0.40
4:G:204:HIS:CD2	4:G:206:ALA:H	2.39	0.40
4:H:408:LEU:HB2	4:H:443:PHE:CE1	2.57	0.40
5:J:139:ASP:OD2	5:J:261:THR:OG1	2.36	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	257/305 (84%)	233 (91%)	24 (9%)	0	100	100
1	B	257/305 (84%)	227 (88%)	30 (12%)	0	100	100
2	C	314/351 (90%)	274 (87%)	40 (13%)	0	100	100
2	D	314/351 (90%)	283 (90%)	31 (10%)	0	100	100
3	E	320/452 (71%)	251 (78%)	68 (21%)	1 (0%)	36	71
3	F	316/452 (70%)	261 (83%)	55 (17%)	0	100	100
4	G	355/523 (68%)	317 (89%)	38 (11%)	0	100	100
4	H	355/523 (68%)	315 (89%)	40 (11%)	0	100	100
5	I	417/721 (58%)	344 (82%)	73 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	J	580/721 (80%)	493 (85%)	87 (15%)	0	100	100
6	K	263/315 (84%)	197 (75%)	65 (25%)	1 (0%)	30	66
7	M	14/333 (4%)	13 (93%)	1 (7%)	0	100	100
8	P	402/472 (85%)	316 (79%)	86 (21%)	0	100	100
All	All	4164/5824 (72%)	3524 (85%)	638 (15%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	48	PHE
6	K	169	ASN

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	225/260 (86%)	222 (99%)	3 (1%)	61	72
1	B	225/260 (86%)	222 (99%)	3 (1%)	61	72
2	C	270/298 (91%)	264 (98%)	6 (2%)	45	64
2	D	270/298 (91%)	264 (98%)	6 (2%)	45	64
3	E	194/398 (49%)	191 (98%)	3 (2%)	57	70
3	F	190/398 (48%)	189 (100%)	1 (0%)	81	81
4	G	313/444 (70%)	307 (98%)	6 (2%)	50	66
4	H	313/444 (70%)	305 (97%)	8 (3%)	40	60
5	I	376/626 (60%)	374 (100%)	2 (0%)	81	81
5	J	525/626 (84%)	523 (100%)	2 (0%)	84	82
6	K	237/280 (85%)	234 (99%)	3 (1%)	61	72
7	M	16/304 (5%)	16 (100%)	0	100	100
8	P	339/397 (85%)	336 (99%)	3 (1%)	70	76
All	All	3493/5033 (69%)	3447 (99%)	46 (1%)	59	72

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	281	ILE
1	A	283	LEU
1	A	290	VAL
1	B	138	LEU
1	B	236	VAL
1	B	238	LEU
2	C	89	ILE
2	C	140	LEU
2	C	164	VAL
2	C	207	LEU
2	C	232	VAL
2	C	343	LEU
2	D	39	LEU
2	D	61	ILE
2	D	137	ILE
2	D	144	LEU
2	D	274	LEU
2	D	336	ILE
3	E	70	LYS
3	E	103	VAL
3	E	128	LEU
3	F	128	LEU
4	G	212	LEU
4	G	230	LEU
4	G	280	LEU
4	G	367	LEU
4	G	425	LEU
4	G	453	VAL
4	H	263	LEU
4	H	280	LEU
4	H	310	GLU
4	H	359	VAL
4	H	440	THR
4	H	457	LEU
4	H	463	LEU
4	H	500	VAL
5	I	149	LEU
5	I	300	VAL
5	J	127	LEU
5	J	230	LEU
6	K	179	ASN
6	K	180	ILE

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Mol	Chain	Res	Type
6	K	270	ASN
8	P	146	LEU
8	P	243	ILE
8	P	381	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	HIS
1	A	242	ASN
1	B	208	ASN
1	B	244	GLN
2	C	44	GLN
2	C	80	ASN
2	C	132	ASN
2	C	242	ASN
2	C	252	HIS
2	C	260	HIS
2	C	327	ASN
2	D	128	GLN
2	D	132	ASN
2	D	138	ASN
3	F	203	HIS
4	G	274	HIS
4	G	347	GLN
4	H	347	GLN
4	H	455	ASN
4	H	475	ASN
5	I	72	ASN
5	I	216	GLN
5	I	359	ASN
5	I	407	GLN
5	I	410	GLN
5	J	105	HIS
5	J	118	ASN
5	J	168	HIS
5	J	255	GLN
5	J	267	GLN
5	J	359	ASN
5	J	384	HIS
5	J	388	ASN
5	J	398	GLN

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Mol	Chain	Res	Type
6	K	10	GLN
6	K	132	GLN
6	K	155	HIS
6	K	178	ASN
6	K	222	ASN
6	K	253	GLN
6	K	270	ASN
8	P	138	HIS
8	P	184	HIS
8	P	231	ASN
8	P	265	ASN

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](#)

There are no ligands in this entry.

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.

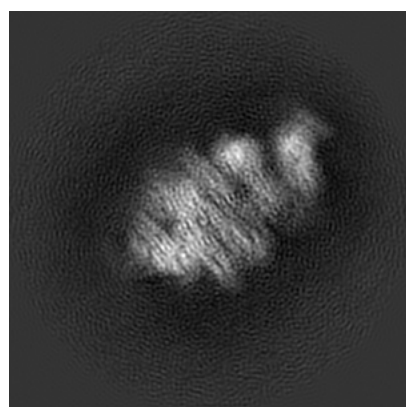
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9840. These allow visual inspection of the internal detail of the map and identification of artifacts.

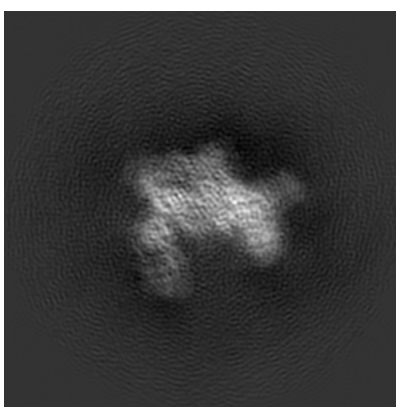
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

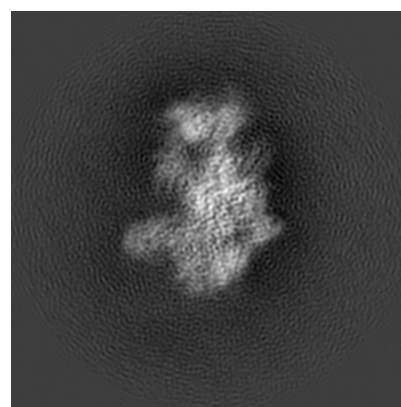
6.1.1 Primary map



X



Y

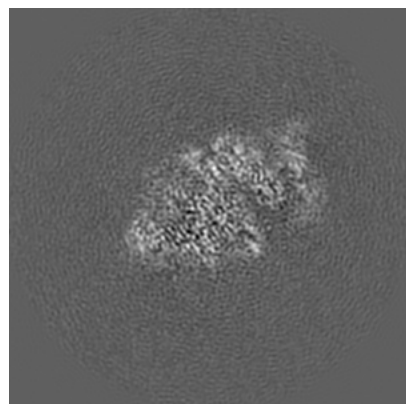


Z

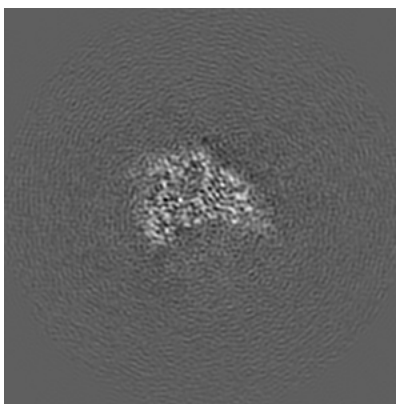
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

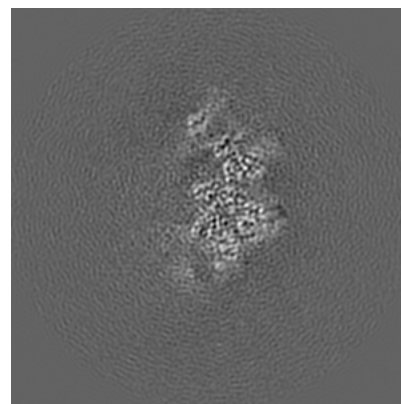
6.2.1 Primary map



X Index: 125



Y Index: 125

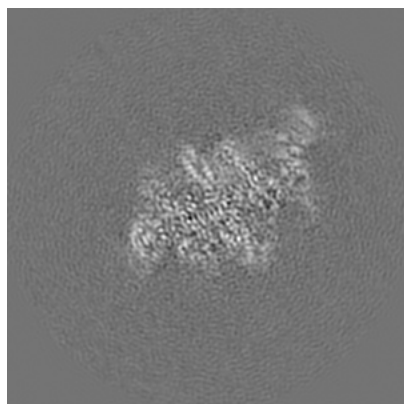


Z Index: 125

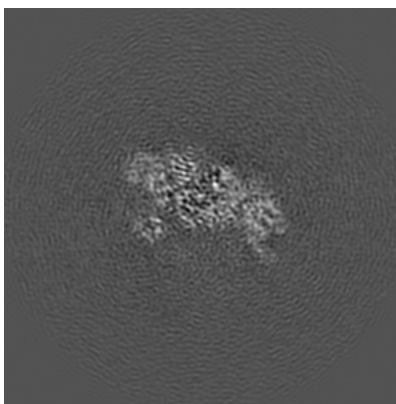
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

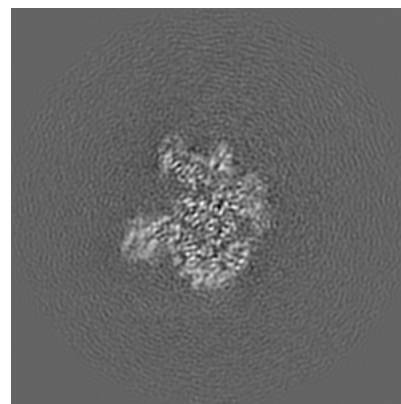
6.3.1 Primary map



X Index: 132



Y Index: 133

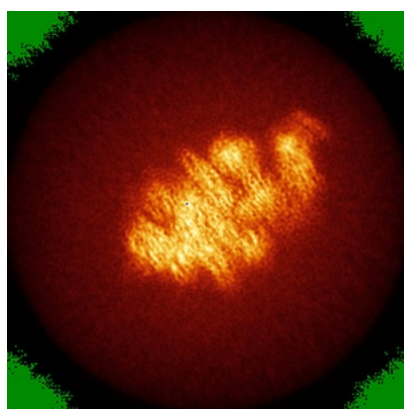


Z Index: 100

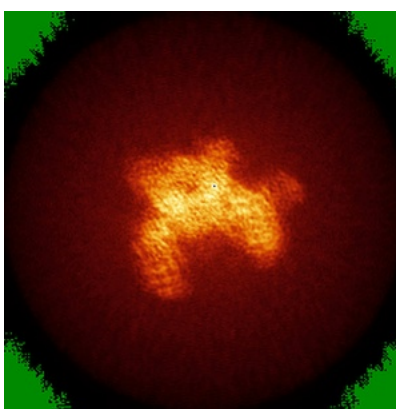
The images above show the largest variance slices of the map in three orthogonal directions.

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

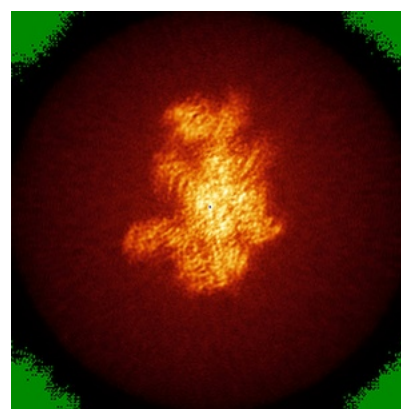
6.4.1 Primary map



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

This section was not generated.

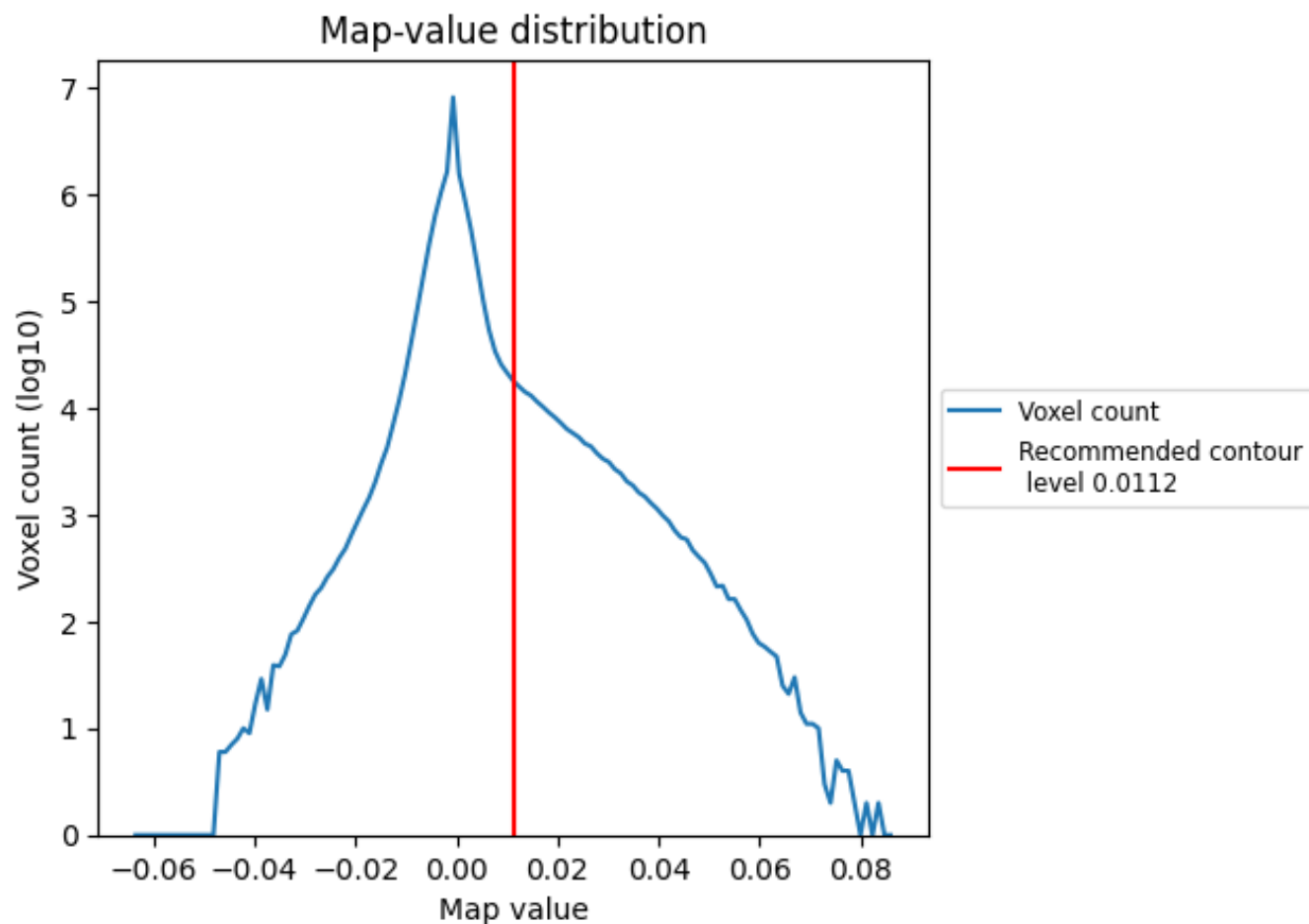
6.6 Mask visualisation

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

7 Map analysis [i](#)

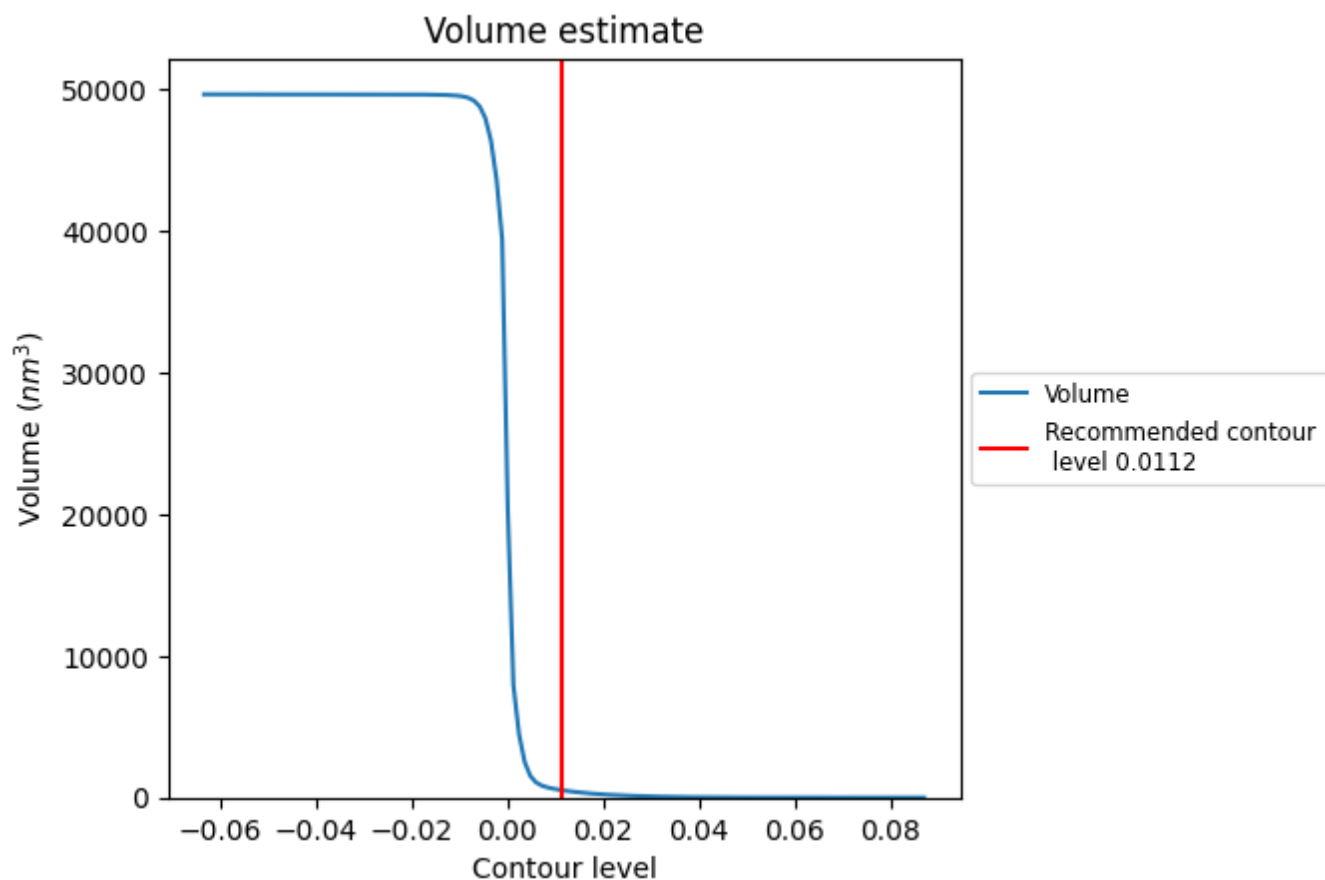
This section contains the results of statistical analysis of the map.

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.

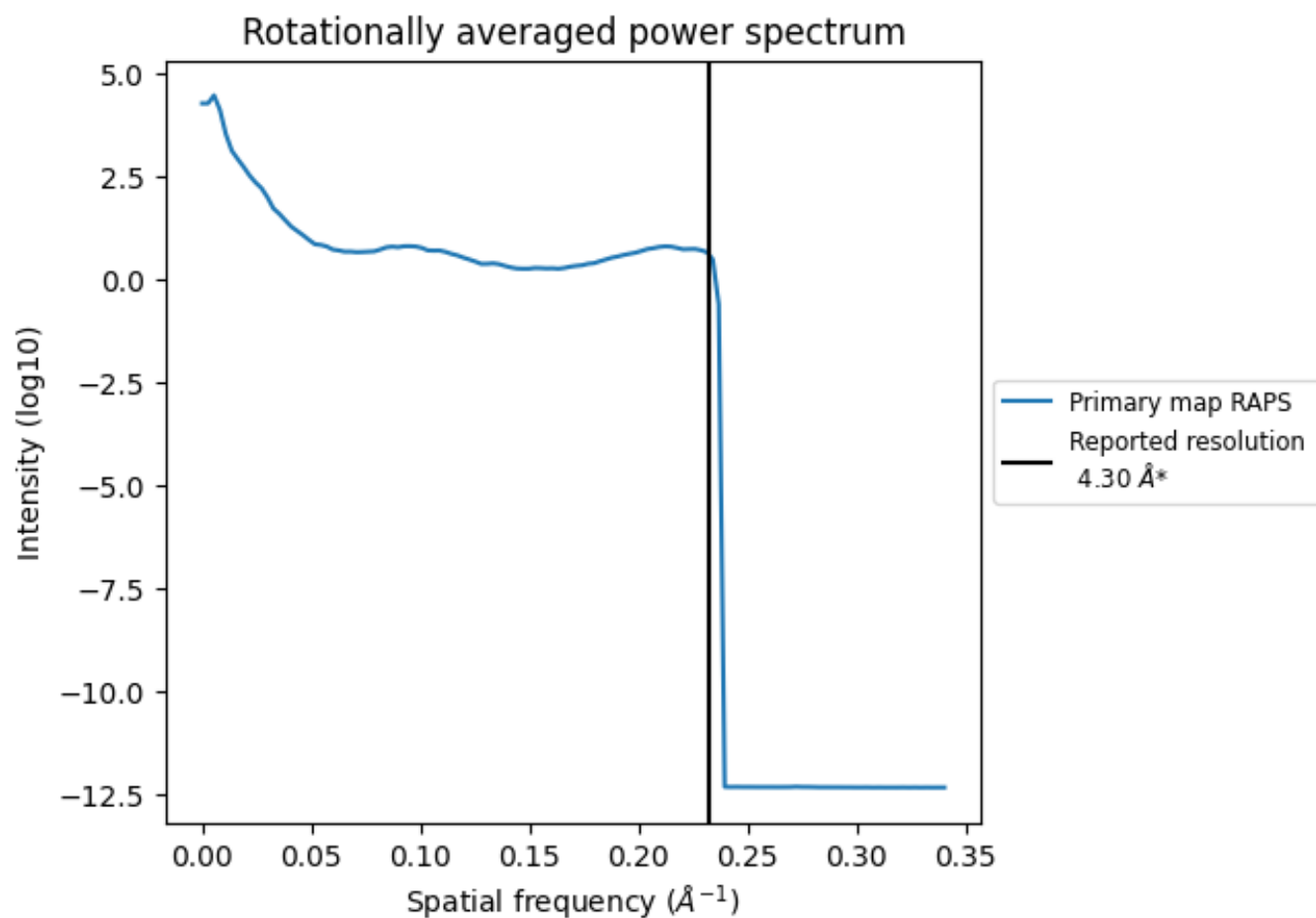
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 526 nm³; this corresponds to an approximate mass of 475 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 ⓘ

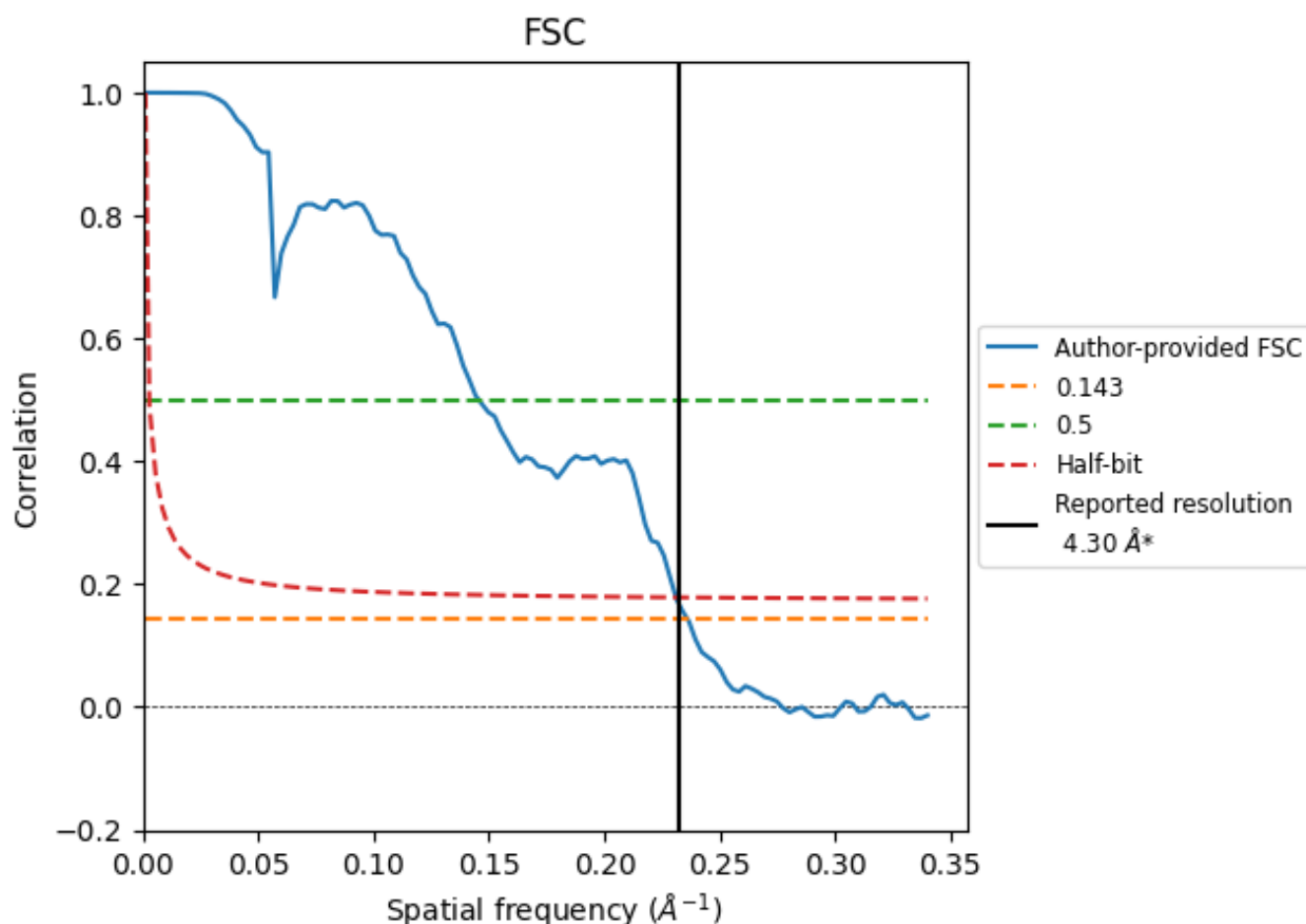


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

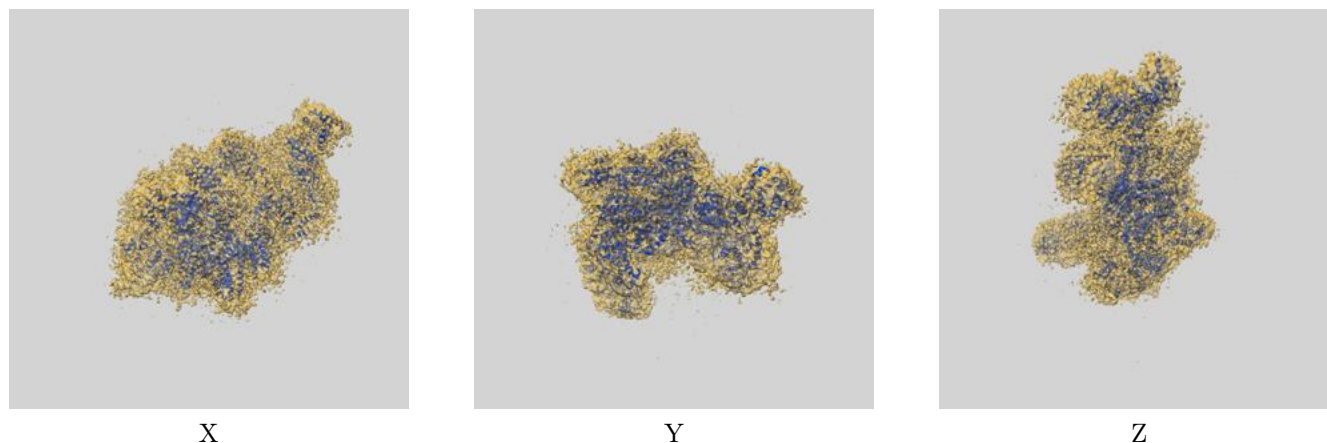
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.24	6.87	4.33
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9840 and PDB model 6K71. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



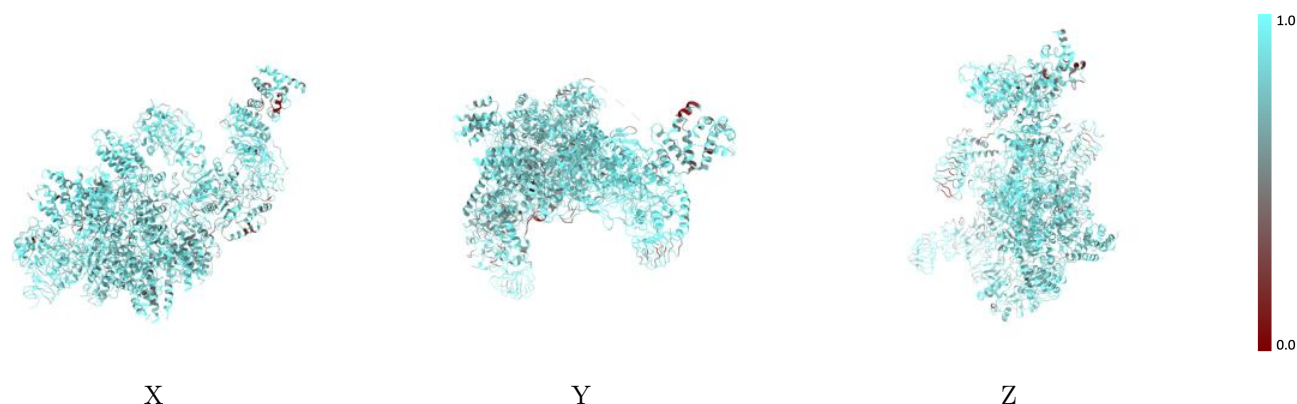
The images above show the 3D surface view of the map at the recommended contour level 0.0112 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



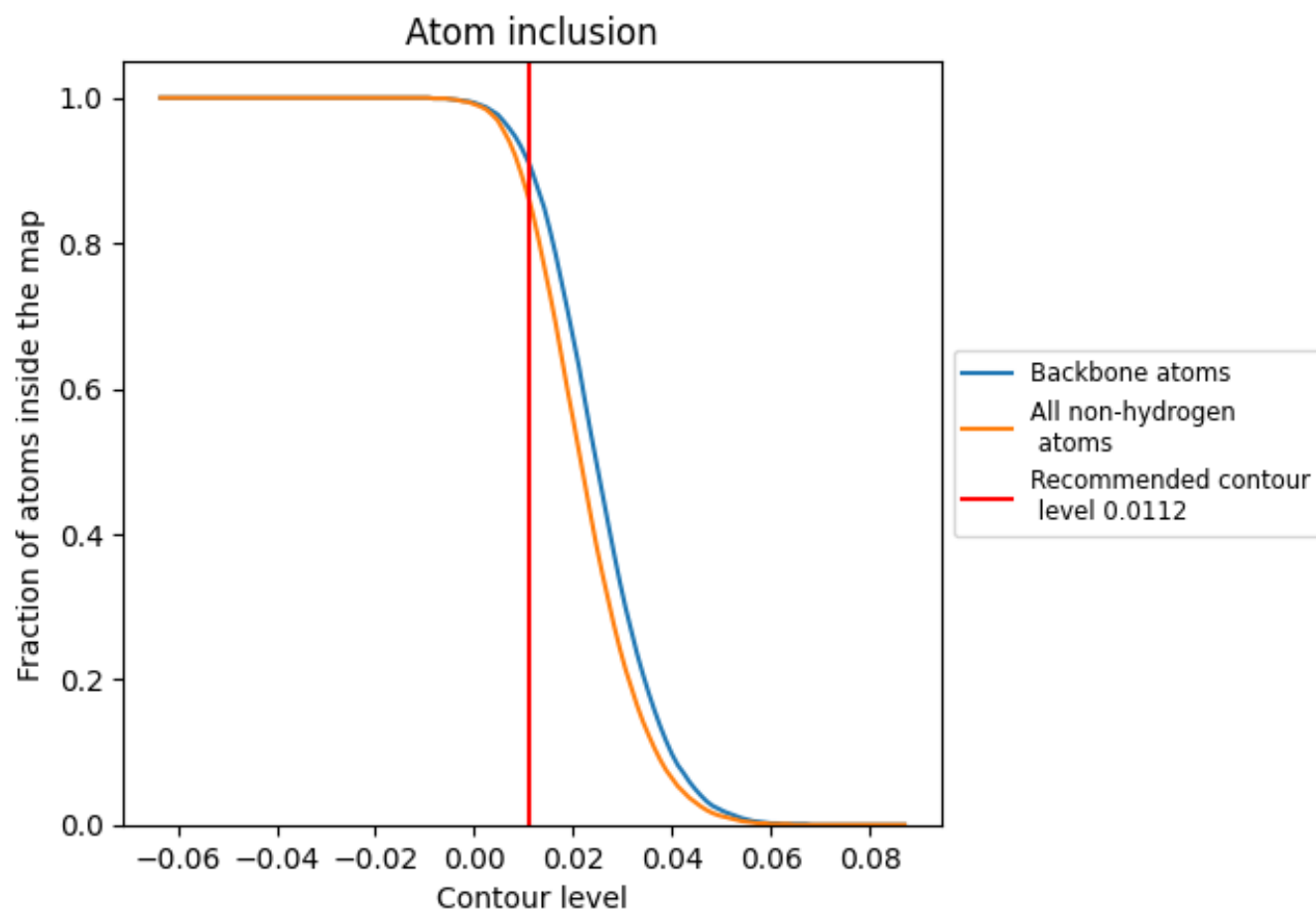
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0112).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 86% 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 (0.0112) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8570	 0.3350
A	 0.8570	 0.3300
B	 0.8770	 0.3250
C	 0.8650	 0.3550
D	 0.8580	 0.3560
E	 0.8910	 0.2970
F	 0.8680	 0.3120
G	 0.8510	 0.3700
H	 0.8930	 0.3480
I	 0.8990	 0.3660
J	 0.8210	 0.3480
K	 0.7290	 0.2960
M	 0.9280	 0.1540
P	 0.8720	 0.2980

