



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:22 PM UTC

PDB ID : 8H38 / pdb_00008h38
EMDB ID : EMD-34455
Title : Cryo-EM Structure of the KBTBD2-CRL3 N8-CSN(mutate) complex
Authors : Hu, Y.; Mao, Q.; Chen, Z.; Sun, L.
Deposited on : 2022-10-08
Resolution : 4.25 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

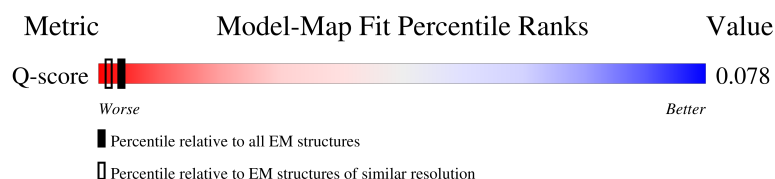
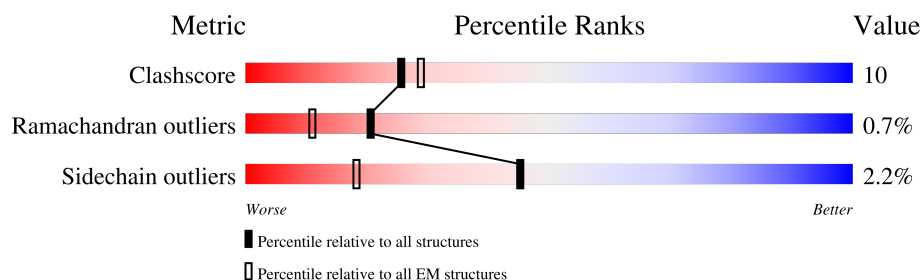
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.25 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	4654 (3.75 - 4.75)

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	527	
2	B	443	
3	C	423	
4	D	406	

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Mol	Chain	Length	Quality of chain
5	E	334	
6	F	327	
7	G	264	
8	H	209	
9	I	623	
9	M	623	
10	L	768	
11	R	108	
12	N	76	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 37306 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 COP9 signalosome complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	412	Total	C	N	O	S	0	0
			3296	2088	574	612	22		

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q13098
A	2	ARG	-	expression tag	UNP Q13098
A	3	ASP	-	expression tag	UNP Q13098
A	4	SER	-	expression tag	UNP Q13098
A	5	SER	-	expression tag	UNP Q13098
A	6	ALA	-	expression tag	UNP Q13098
A	7	PRO	-	expression tag	UNP Q13098
A	8	SER	-	expression tag	UNP Q13098
A	9	SER	-	expression tag	UNP Q13098
A	10	ALA	-	expression tag	UNP Q13098
A	11	SER	-	expression tag	UNP Q13098
A	12	SER	-	expression tag	UNP Q13098
A	13	SER	-	expression tag	UNP Q13098
A	14	VAL	-	expression tag	UNP Q13098
A	15	THR	-	expression tag	UNP Q13098
A	16	ASP	-	expression tag	UNP Q13098
A	17	LEU	-	expression tag	UNP Q13098
A	18	TYR	-	expression tag	UNP Q13098
A	19	CYS	-	expression tag	UNP Q13098
A	20	THR	-	expression tag	UNP Q13098
A	21	PRO	-	expression tag	UNP Q13098
A	22	HIS	-	expression tag	UNP Q13098
A	23	SER	-	expression tag	UNP Q13098
A	24	SER	-	expression tag	UNP Q13098
A	25	ARG	-	expression tag	UNP Q13098
A	26	SER	-	expression tag	UNP Q13098
A	27	ASP	-	expression tag	UNP Q13098
A	28	LEU	-	expression tag	UNP Q13098

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Chain	Residue	Modelled	Actual	Comment	Reference
A	29	VAL	-	expression tag	UNP Q13098
A	30	LEU	-	expression tag	UNP Q13098
A	31	PRO	-	expression tag	UNP Q13098
A	32	GLY	-	expression tag	UNP Q13098
A	33	THR	-	expression tag	UNP Q13098
A	34	ALA	-	expression tag	UNP Q13098
A	35	GLY	-	expression tag	UNP Q13098
A	36	ASP	-	expression tag	UNP Q13098
A	37	PHE	-	expression tag	UNP Q13098
A	38	SER	-	expression tag	UNP Q13098
A	39	LEU	-	expression tag	UNP Q13098
A	40	SER	-	expression tag	UNP Q13098
A	41	ALA	-	expression tag	UNP Q13098
A	42	SER	-	expression tag	UNP Q13098
A	43	LEU	-	expression tag	UNP Q13098
A	44	SER	-	expression tag	UNP Q13098
A	45	ALA	-	expression tag	UNP Q13098
A	46	CYS	-	expression tag	UNP Q13098
A	47	THR	-	expression tag	UNP Q13098
A	48	LEU	-	expression tag	UNP Q13098
A	49	LEU	-	expression tag	UNP Q13098
A	50	TYR	-	expression tag	UNP Q13098
A	51	GLU	-	expression tag	UNP Q13098
A	?	-	ARG	deletion	UNP Q13098
A	?	-	SER	deletion	UNP Q13098
A	?	-	SER	deletion	UNP Q13098
A	?	-	LEU	deletion	UNP Q13098

- Molecule 2 is a protein called COP9 signalosome complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	420	Total	C	N	O	S	0	0
			3430	2173	587	655	15		

- Molecule 3 is a protein called COP9 signalosome complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	407	Total	C	N	O	S	0	0
			3235	2059	543	606	27		

- Molecule 4 is a protein called COP9 signalosome complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	406	Total	C	N	O	S	0	0
			3251	2047	566	622	16		

- Molecule 5 is a protein called COP9 signalosome complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	309	Total	C	N	O	S	0	0
			2452	1563	408	467	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	138	ALA	HIS	engineered mutation	UNP Q92905

- Molecule 6 is a protein called COP9 signalosome complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	288	Total	C	N	O	S	0	0
			2279	1452	379	433	15		

- Molecule 7 is a protein called COP9 signalosome complex subunit 7b.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	214	Total	C	N	O	S	0	0
			1692	1072	287	327	6		

- Molecule 8 is a protein called COP9 signalosome complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	177	Total	C	N	O	S	0	0
			1411	903	245	259	4		

- Molecule 9 is a protein called Kelch repeat and BTB domain-containing protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	557	Total	C	N	O	S	0	0
			4505	2879	746	842	38		
9	M	564	Total	C	N	O	S	0	0
			4557	2911	758	850	38		

- Molecule 10 is a protein called Cullin-3.

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

- Molecule 11 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	89	Total	C	N	O	S	0	0
			737	466	135	127	9		

- Molecule 12 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	76	Total	C	N	O	S	0	0
			591	372	102	115	2		

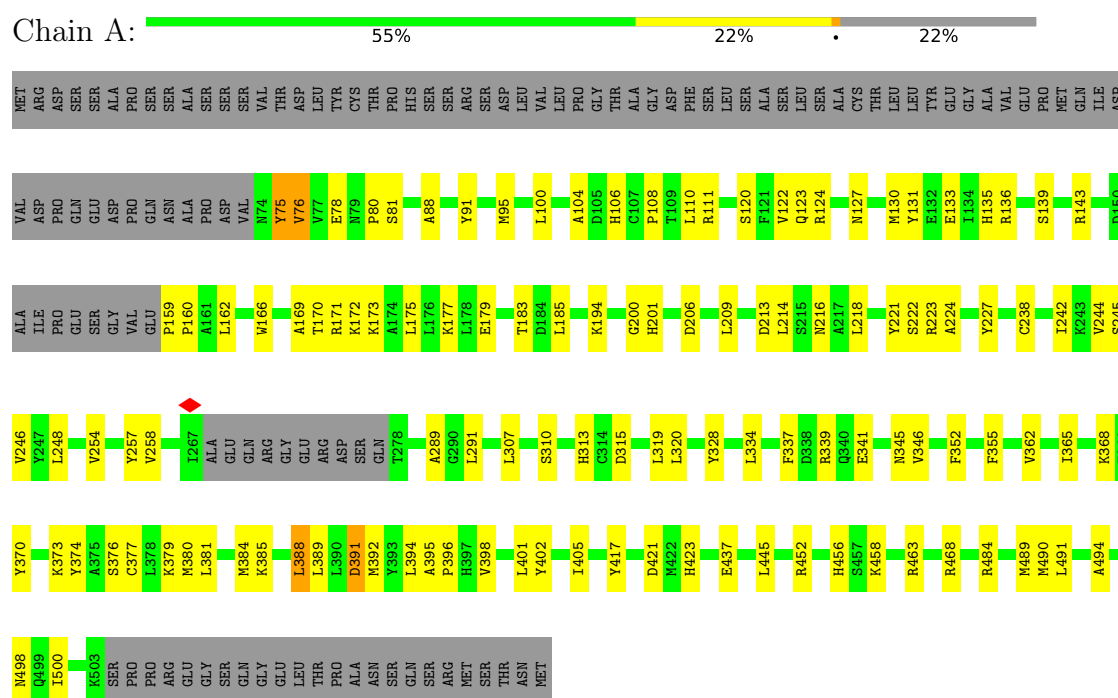
- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
13	E	1	Total	Zn	0
			1	1	
13	R	3	Total	Zn	0
			3	3	

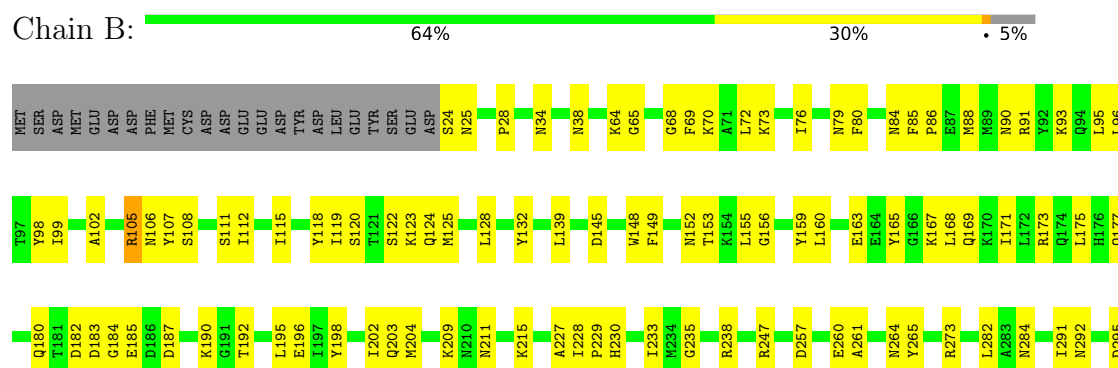
3 Residue-property plots

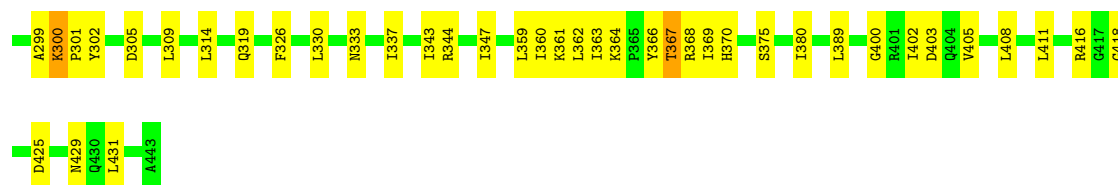
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: COP9 signalosome complex subunit 1



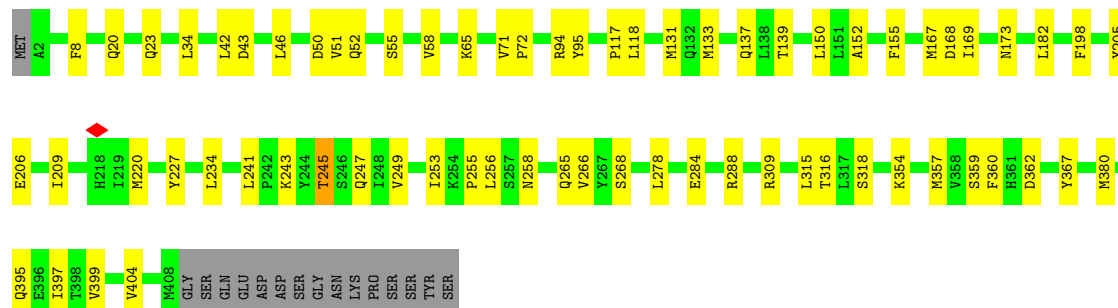
• Molecule 2: COP9 signalosome complex subunit 2





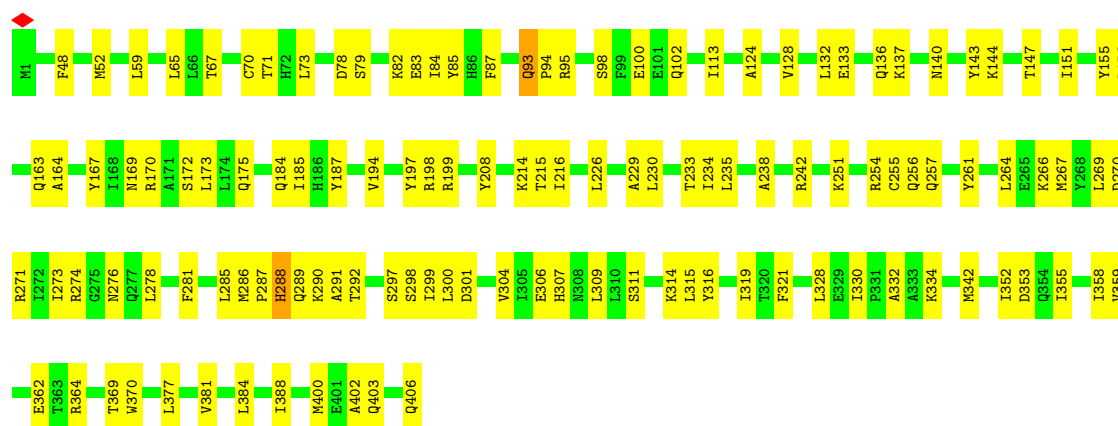
• Molecule 3: COP9 signalosome complex subunit 3

Chain C: 80% 16%



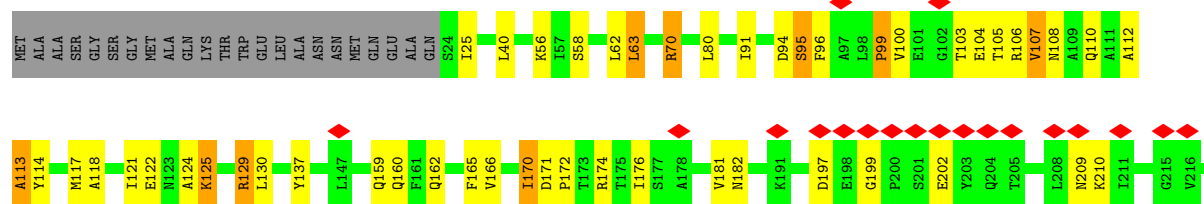
• Molecule 4: COP9 signalosome complex subunit 4

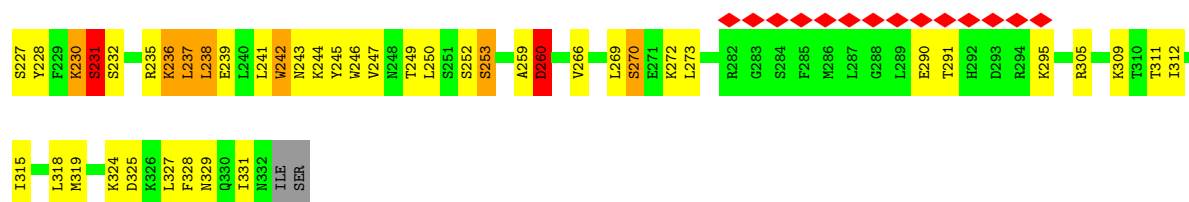
Chain D: 69% 30%



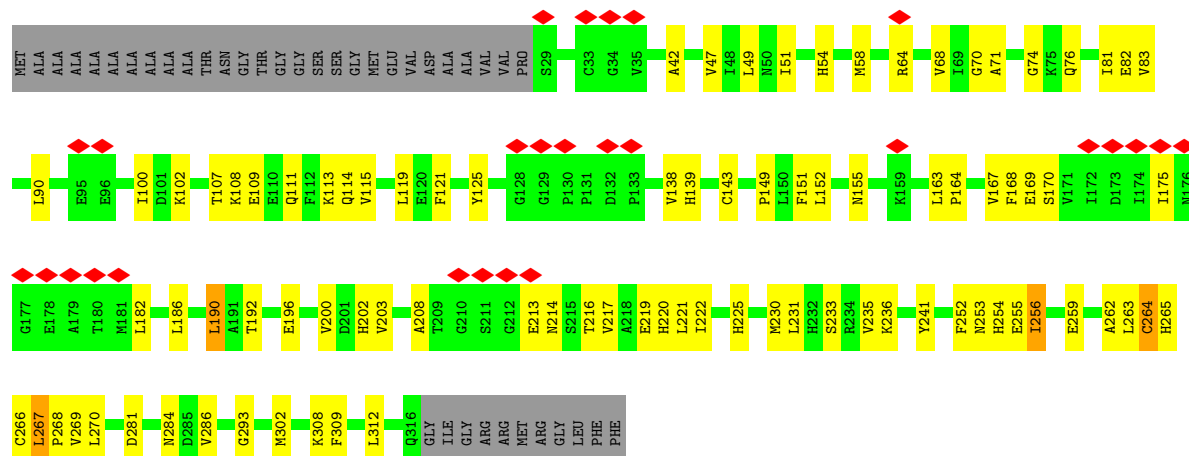
• Molecule 5: COP9 signalosome complex subunit 5

Chain E: 10% 64% 23% 5% 7%

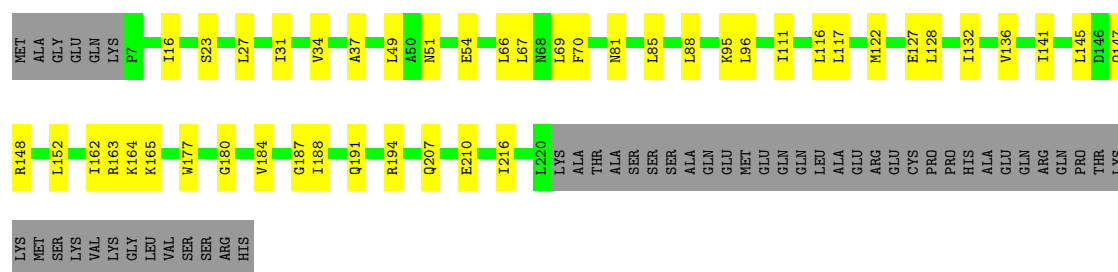




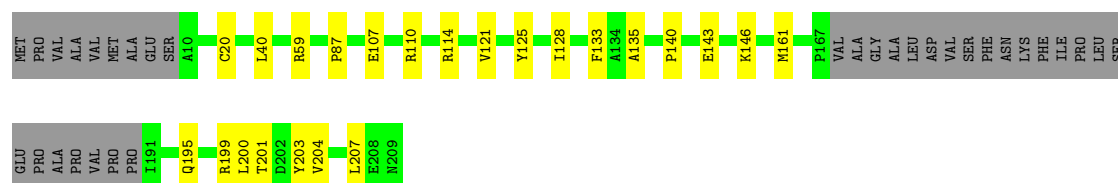
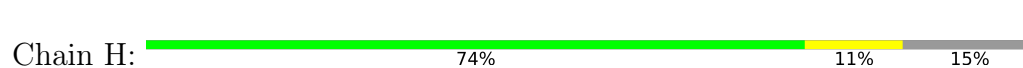
• Molecule 6: COP9 signalosome complex subunit 6



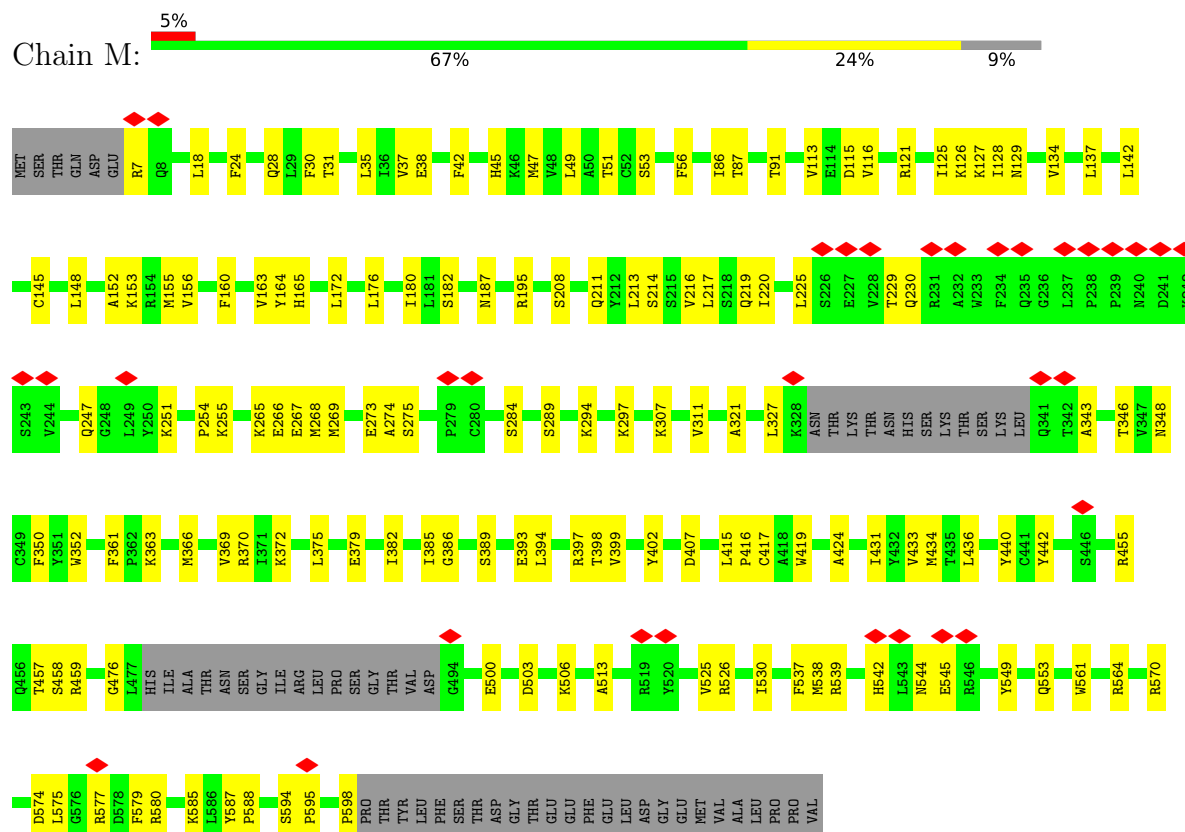
• Molecule 7: COP9 signalosome complex subunit 7b



• Molecule 8: COP9 signalosome complex subunit 8

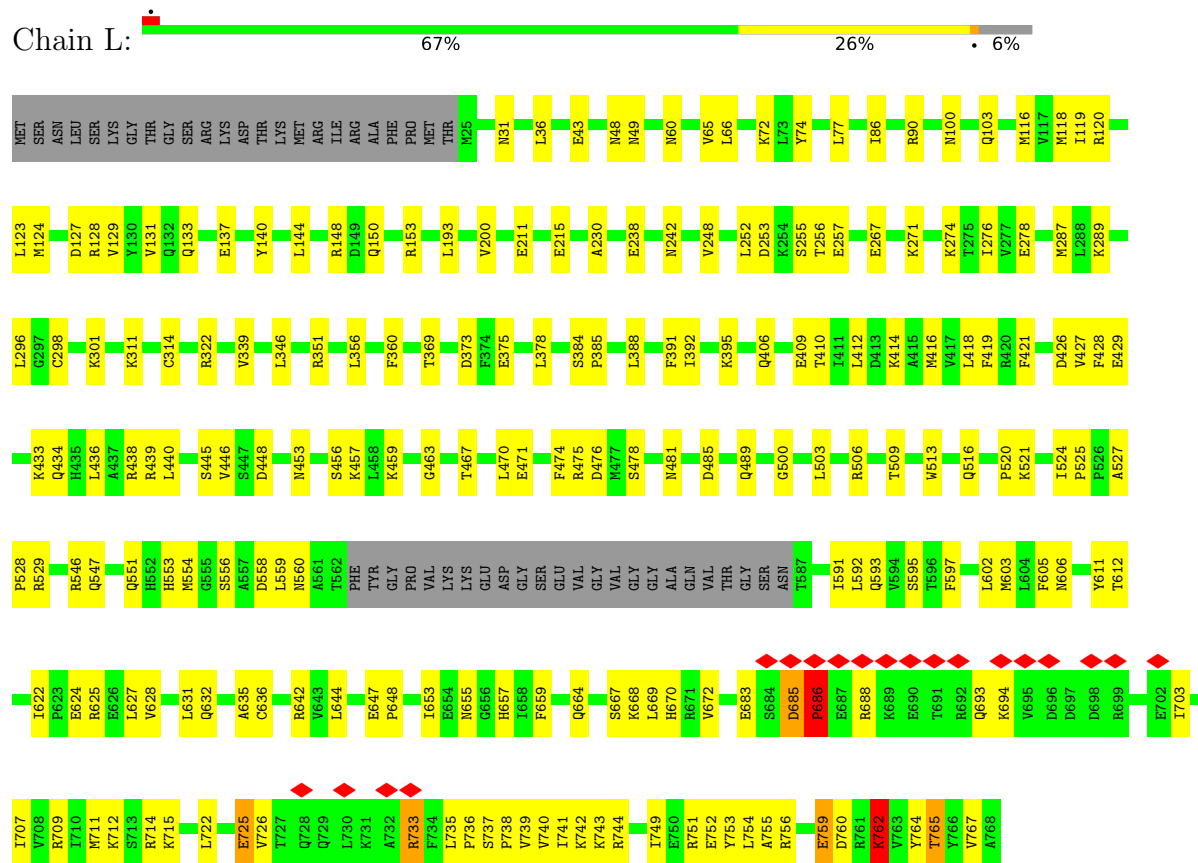


• Molecule 9: Kelch repeat and BTB domain-containing protein 2



- Molecule 10: Cullin-3

Chain L:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	146505	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 ($e^-/\text{\AA}^2$)	53	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	1.577	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.001	Depositor
Map size (Å)	451.00803, 451.00803, 451.00803	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.088, 2.088, 2.088	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A	0.23	0/3352	0.41	0/4520
2	B	0.22	0/3489	0.45	0/4696
3	C	0.17	0/3294	0.38	1/4448 (0.0%)
4	D	0.13	0/3303	0.40	0/4460
5	E	0.74	0/2505	0.96	3/3384 (0.1%)
6	F	0.46	1/2326 (0.0%)	0.54	0/3153
7	G	0.10	0/1713	0.27	0/2318
8	H	0.10	0/1445	0.30	0/1965
9	I	0.10	0/4611	0.31	0/6253
9	M	0.12	0/4664	0.33	0/6324
10	L	0.22	0/5959	0.39	0/8006
11	R	0.37	0/759	0.58	0/1029
12	N	0.69	0/596	0.81	0/800
All	All	0.29	1/38016 (0.0%)	0.46	4/51356 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	264	CYS	C-O	6.65	1.31	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	245	THR	CB-CA-C	-7.14	107.29	115.79
5	E	95	SER	CA-C-N	-5.08	113.00	121.94
5	E	95	SER	C-N-CA	-5.08	113.00	121.94
5	E	125	LYS	N-CA-C	-5.03	105.93	111.71

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	A	3296	0	3336	87	0
2	B	3430	0	3459	86	0
3	C	3235	0	3257	50	0
4	D	3251	0	3253	88	0
5	E	2452	0	2426	64	0
6	F	2279	0	2263	66	0
7	G	1692	0	1730	33	0
8	H	1411	0	1395	17	0
9	I	4505	0	4409	87	0
9	M	4557	0	4473	97	0
10	L	5866	0	5904	147	0
11	R	737	0	686	32	0
12	N	591	0	616	15	0
13	E	1	0	0	0	0
13	R	3	0	0	0	0
All	All	37306	0	37207	769	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 10.

All (769) 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)
5:E:114:TYR:HA	5:E:117:MET:HB3	1.49	0.92
10:L:346:LEU:HD11	10:L:414:LYS:HG3	1.54	0.89
5:E:99:PRO:HG3	6:F:114:GLN:HB3	1.57	0.87
12:N:8:LEU:HB2	12:N:71:LEU:HD11	1.57	0.85
4:D:73:LEU:HD13	4:D:85:TYR:HE1	1.48	0.78
10:L:556:SER:HA	10:L:595:SER:HA	1.65	0.78
4:D:362:GLU:HB3	4:D:364:ARG:HH12	1.49	0.76
9:M:217:LEU:HD13	9:M:225:LEU:HD11	1.67	0.76
5:E:80:LEU:O	5:E:95:SER:HA	1.89	0.73
10:L:412:LEU:HD13	10:L:457:LYS:HE2	1.69	0.73
3:C:255:PRO:O	9:M:544:ASN:ND2	2.22	0.72
5:E:124:ALA:HB1	5:E:129:ARG:HB2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:MET:HE3	6:F:302:MET:HG3	1.71	0.72
5:E:210:LYS:NZ	10:L:715:LYS:HE2	2.05	0.72
9:I:205:ASN:HB3	9:I:209:ARG:HG3	1.71	0.72
4:D:133:GLU:HG2	10:L:547:GLN:HE21	1.54	0.71
3:C:137:GLN:HG2	3:C:168:ASP:HB3	1.70	0.71
1:A:468:ARG:HH12	6:F:281:ASP:HB3	1.55	0.71
5:E:237:LEU:HG	6:F:49:LEU:HD13	1.73	0.70
4:D:352:ILE:HG23	4:D:359:VAL:HG22	1.72	0.70
3:C:284:GLU:OE1	3:C:288:ARG:NH1	2.24	0.70
10:L:624:GLU:HG3	10:L:625:ARG:H	1.56	0.70
10:L:476:ASP:HB2	10:L:513:TRP:HE1	1.55	0.69
9:I:348:ASN:ND2	9:I:366:MET:O	2.25	0.69
2:B:180:GLN:HG3	2:B:185:GLU:HA	1.75	0.69
4:D:238:ALA:HA	4:D:242:ARG:HD3	1.75	0.69
4:D:384:LEU:HD12	6:F:263:LEU:HD22	1.74	0.69
10:L:416:MET:SD	10:L:457:LYS:NZ	2.66	0.69
5:E:315:ILE:HD13	8:H:203:TYR:HB3	1.76	0.68
5:E:238:LEU:HG	5:E:239:GLU:N	2.07	0.68
11:R:94:CYS:HB2	11:R:101:TRP:HB2	1.75	0.68
1:A:120:SER:HA	1:A:123:GLN:HE21	1.58	0.68
9:M:415:LEU:HD23	9:M:417:CYS:H	1.57	0.68
9:I:128:ILE:HG12	9:I:136:LEU:HD21	1.75	0.67
7:G:162:ILE:HG22	7:G:164:LYS:H	1.60	0.67
1:A:127:ASN:HD21	1:A:130:MET:HB2	1.58	0.67
2:B:264:ASN:OD1	10:L:475:ARG:NH2	2.27	0.67
10:L:253:ASP:OD1	10:L:256:THR:HB	1.94	0.67
9:I:434:MET:HE2	9:I:455:ARG:HE	1.60	0.67
7:G:117:LEU:HA	7:G:122:MET:HB3	1.77	0.67
9:I:305:LEU:HD21	9:I:323:GLY:HA3	1.76	0.67
3:C:51:VAL:HG22	3:C:52:GLN:H	1.60	0.66
6:F:217:VAL:HB	6:F:221:LEU:HD23	1.76	0.66
6:F:208:ALA:HA	6:F:219:GLU:HB2	1.77	0.66
4:D:175:GLN:HE22	4:D:184:GLN:HG2	1.61	0.66
10:L:525:PRO:HB2	10:L:528:PRO:HD2	1.78	0.65
5:E:325:ASP:OD1	5:E:329:ASN:ND2	2.29	0.65
9:M:187:ASN:ND2	9:M:587:TYR:OH	2.28	0.65
1:A:139:SER:HA	1:A:160:PRO:HD2	1.79	0.65
1:A:388:LEU:HB2	1:A:394:LEU:HD23	1.77	0.65
4:D:274:ARG:HH21	4:D:276:ASN:HD21	1.45	0.65
4:D:384:LEU:HD21	6:F:259:GLU:HB3	1.79	0.64
8:H:140:PRO:HG2	8:H:143:GLU:OE2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:331:ILE:HD11	7:G:180:GLY:HA3	1.79	0.64
10:L:49:ASN:HD22	10:L:118:MET:HE1	1.63	0.64
10:L:632:GLN:HB2	10:L:636:CYS:HB3	1.78	0.64
2:B:228:ILE:HD13	10:L:471:GLU:HB3	1.79	0.64
4:D:70:CYS:HA	4:D:73:LEU:HD12	1.79	0.63
11:R:52:LEU:HD12	11:R:56:CYS:HB3	1.79	0.63
4:D:288:HIS:ND1	4:D:289:GLN:OE1	2.30	0.63
6:F:139:HIS:HE2	6:F:170:SER:HB3	1.63	0.63
9:I:436:LEU:O	9:I:455:ARG:NH2	2.32	0.63
12:N:43:LEU:HA	12:N:69:LEU:HB2	1.80	0.63
5:E:95:SER:HB2	5:E:137:TYR:CE1	2.34	0.63
11:R:42:CYS:HB3	11:R:45:CYS:SG	2.39	0.63
9:M:297:LYS:HZ1	9:M:595:PRO:HD3	1.64	0.63
1:A:468:ARG:HH22	6:F:281:ASP:HA	1.64	0.63
9:I:64:LEU:HD23	9:I:66:GLU:H	1.64	0.63
11:R:51:ASP:O	11:R:57:GLN:NE2	2.32	0.63
9:M:127:LYS:O	9:M:129:ASN:ND2	2.33	0.62
5:E:318:LEU:HB2	6:F:286:VAL:HG11	1.81	0.62
12:N:41:GLN:HG2	12:N:69:LEU:HD11	1.81	0.62
4:D:352:ILE:HG12	4:D:359:VAL:HG13	1.81	0.62
10:L:683:GLU:O	10:L:688:ARG:NH1	2.32	0.62
9:I:91:THR:HG23	9:I:93:ASN:H	1.64	0.62
10:L:248:VAL:HG23	10:L:252:LEU:HD12	1.82	0.62
1:A:362:VAL:HA	1:A:365:ILE:HD12	1.82	0.61
10:L:622:ILE:HG12	10:L:627:LEU:HD22	1.81	0.61
1:A:258:VAL:HG11	1:A:289:ALA:HB2	1.82	0.61
2:B:260:GLU:O	2:B:264:ASN:ND2	2.33	0.61
9:M:225:LEU:O	9:M:230:GLN:NE2	2.33	0.61
9:M:393:GLU:HG3	9:M:394:LEU:H	1.65	0.61
2:B:73:LYS:HG3	2:B:115:ILE:HD11	1.82	0.61
5:E:230:LYS:O	5:E:231:SER:HB3	2.00	0.61
1:A:494:ALA:O	1:A:498:ASN:ND2	2.32	0.61
10:L:90:ARG:NH2	10:L:150:GLN:OE1	2.34	0.61
3:C:367:TYR:O	6:F:284:ASN:ND2	2.33	0.61
4:D:132:LEU:HD22	4:D:144:LYS:HG2	1.82	0.61
2:B:65:GLY:O	2:B:69:PHE:N	2.22	0.61
9:M:350:PHE:HD2	9:M:363:LYS:HB2	1.66	0.61
5:E:95:SER:HB2	5:E:137:TYR:HE1	1.65	0.61
10:L:433:LYS:HA	10:L:470:LEU:HD21	1.82	0.61
4:D:358:ILE:HD13	7:G:148:ARG:HG3	1.83	0.60
7:G:66:LEU:HD11	7:G:88:LEU:HD21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:539:ARG:HH22	9:M:577:ARG:HD3	1.66	0.60
4:D:235:LEU:HD22	4:D:299:ILE:HG23	1.84	0.60
9:M:269:MET:HE3	9:M:530:ILE:HD12	1.83	0.60
9:I:431:ILE:HB	9:I:442:TYR:HB3	1.83	0.60
10:L:66:LEU:HD11	9:M:142:LEU:HG	1.82	0.60
9:M:213:LEU:HA	9:M:216:VAL:HG12	1.83	0.60
9:I:133:CYS:HB3	9:I:159:LYS:HZ3	1.66	0.60
9:M:254:PRO:O	9:M:255:LYS:HG2	2.02	0.60
9:I:151:SER:HA	9:I:154:ARG:HE	1.65	0.60
1:A:122:VAL:HG13	1:A:127:ASN:HD22	1.66	0.60
1:A:183:THR:HG23	9:M:7:ARG:HH11	1.66	0.60
10:L:129:VAL:O	10:L:133:GLN:NE2	2.35	0.60
2:B:76:ILE:HG12	2:B:88:MET:HG2	1.83	0.59
9:I:201:TRP:O	9:I:209:ARG:NH2	2.35	0.59
9:M:434:MET:HE2	9:M:455:ARG:HE	1.66	0.59
4:D:136:GLN:HA	10:L:521:LYS:HD2	1.84	0.59
9:I:525:VAL:HA	9:I:538:MET:HG2	1.82	0.59
10:L:559:LEU:HD22	10:L:602:LEU:HD22	1.83	0.59
6:F:100:ILE:HD11	6:F:138:VAL:HG13	1.84	0.59
10:L:120:ARG:O	10:L:124:MET:N	2.35	0.59
10:L:628:VAL:HG13	10:L:653:ILE:HD12	1.84	0.59
2:B:300:LYS:NZ	11:R:40:ASP:OD2	2.35	0.59
9:I:273:GLU:HA	9:I:283:TYR:HB3	1.85	0.59
9:I:390:VAL:HG12	9:I:393:GLU:HG3	1.83	0.59
2:B:300:LYS:H	2:B:301:PRO:HD2	1.67	0.59
4:D:362:GLU:HB3	4:D:364:ARG:NH1	2.17	0.59
8:H:195:GLN:HB3	8:H:199:ARG:HH21	1.68	0.59
5:E:291:THR:O	5:E:295:LYS:HG2	2.03	0.59
4:D:198:ARG:O	4:D:199:ARG:NE	2.29	0.58
5:E:110:GLN:HB3	5:E:113:ALA:HB2	1.84	0.58
9:I:155:MET:HG3	9:I:159:LYS:HD3	1.85	0.58
6:F:163:LEU:HD12	6:F:164:PRO:HD2	1.85	0.58
2:B:211:ASN:OD1	2:B:247:ARG:NH1	2.36	0.58
4:D:384:LEU:O	4:D:388:ILE:HG13	2.03	0.58
5:E:210:LYS:CE	10:L:715:LYS:HE2	2.33	0.58
1:A:490:MET:HG3	3:C:167:MET:HG2	1.85	0.58
2:B:96:LEU:HA	2:B:99:ILE:HD12	1.86	0.58
9:M:214:SER:O	9:M:251:LYS:NZ	2.36	0.58
9:M:455:ARG:NH1	9:M:500:GLU:OE2	2.37	0.58
1:A:394:LEU:HG	1:A:398:VAL:HB	1.85	0.58
5:E:319:MET:HG2	8:H:200:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:ASN:HD21	2:B:291:ILE:HG23	1.69	0.58
9:M:265:LYS:HB2	9:M:585:LYS:HB3	1.85	0.58
9:I:302:PRO:HG2	9:I:305:LEU:HB3	1.86	0.57
11:R:72:TRP:HB2	11:R:105:LYS:HB3	1.86	0.57
3:C:51:VAL:HA	3:C:55:SER:HB3	1.84	0.57
7:G:16:ILE:HG12	7:G:49:LEU:HD11	1.84	0.57
10:L:429:GLU:HB3	10:L:433:LYS:HE2	1.86	0.57
1:A:170:THR:OG1	9:I:345:ARG:NH2	2.38	0.57
9:M:397:ARG:HD3	9:M:415:LEU:HB3	1.86	0.57
1:A:490:MET:HG2	3:C:167:MET:HE3	1.87	0.57
4:D:100:GLU:H	4:D:137:LYS:HE3	1.70	0.57
10:L:463:GLY:O	10:L:467:THR:OG1	2.22	0.57
2:B:367:THR:HG23	2:B:411:LEU:HB2	1.86	0.57
4:D:254:ARG:HA	4:D:257:GLN:HG2	1.85	0.57
9:I:382:ILE:HB	9:I:402:TYR:HB3	1.86	0.57
9:M:37:VAL:HG12	9:M:38:GLU:HG2	1.87	0.57
10:L:503:LEU:HD13	11:R:27:TRP:HB3	1.86	0.57
4:D:400:MET:SD	4:D:403:GLN:NE2	2.78	0.57
9:M:28:GLN:NE2	9:M:31:THR:OG1	2.38	0.57
9:I:555:ASP:HB3	9:I:558:LEU:HB2	1.86	0.56
1:A:307:LEU:HD13	1:A:345:ASN:HB3	1.86	0.56
1:A:352:PHE:HA	1:A:355:PHE:HB2	1.87	0.56
2:B:106:ASN:HD22	10:L:446:VAL:H	1.53	0.56
4:D:388:ILE:HG12	6:F:256:ILE:HG12	1.87	0.56
6:F:192:THR:HG23	6:F:196:GLU:HB2	1.86	0.56
10:L:635:ALA:O	10:L:642:ARG:NH1	2.39	0.56
1:A:123:GLN:HB3	1:A:131:TYR:HE2	1.71	0.56
9:I:186:LEU:HD13	9:I:194:VAL:HG11	1.87	0.56
9:I:459:ARG:HB3	9:I:476:GLY:HA3	1.88	0.56
2:B:403:ASP:HB3	2:B:408:LEU:HB3	1.87	0.56
4:D:84:ILE:HA	4:D:87:PHE:HB3	1.86	0.56
4:D:185:ILE:HG13	4:D:216:ILE:HD11	1.88	0.56
2:B:366:TYR:HD2	2:B:367:THR:H	1.54	0.56
5:E:25:ILE:CG2	5:E:231:SER:HA	2.35	0.56
9:M:436:LEU:O	9:M:455:ARG:NH2	2.38	0.56
2:B:38:ASN:OD1	10:L:670:HIS:NE2	2.38	0.56
9:I:265:LYS:HB3	9:I:585:LYS:HD3	1.88	0.56
4:D:281:PHE:HD2	4:D:300:LEU:HD13	1.71	0.55
9:M:459:ARG:HB3	9:M:476:GLY:HA3	1.87	0.55
2:B:375:SER:OG	2:B:380:ILE:O	2.22	0.55
6:F:241:TYR:OH	6:F:253:ASN:ND2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:258:ASN:HB2	9:M:544:ASN:ND2	2.21	0.55
9:I:374:SER:OG	9:I:385:ILE:O	2.23	0.55
10:L:339:VAL:HA	10:L:391:PHE:HD1	1.71	0.55
2:B:425:ASP:OD1	2:B:429:ASN:ND2	2.39	0.55
3:C:209:ILE:HG12	3:C:220:MET:HE1	1.88	0.55
6:F:225:HIS:HB2	7:G:188:ILE:HG21	1.88	0.55
9:M:553:GLN:HB2	9:M:564:ARG:HB2	1.87	0.55
1:A:201:HIS:CE1	1:A:223:ARG:HD2	2.41	0.55
10:L:43:GLU:OE2	10:L:48:ASN:ND2	2.33	0.55
9:I:366:MET:HE1	9:I:370:ARG:HE	1.72	0.55
9:M:431:ILE:HB	9:M:442:TYR:HB3	1.88	0.55
1:A:162:LEU:HD12	1:A:166:TRP:HE1	1.71	0.55
9:M:153:LYS:HE2	9:M:180:ILE:HA	1.87	0.55
1:A:245:SER:HB2	1:A:254:VAL:HG23	1.89	0.55
3:C:198:PHE:HB2	3:C:234:LEU:HD13	1.88	0.55
4:D:352:ILE:HG22	4:D:353:ASP:H	1.71	0.55
9:I:172:LEU:HD22	9:I:176:LEU:HD23	1.89	0.55
2:B:183:ASP:OD2	2:B:184:GLY:N	2.40	0.54
2:B:195:LEU:HD13	2:B:229:PRO:HB3	1.90	0.54
1:A:213:ASP:HB3	1:A:216:ASN:HB2	1.90	0.54
1:A:484:ARG:NH1	3:C:206:GLU:OE1	2.39	0.54
9:I:275:SER:OG	9:I:574:ASP:O	2.21	0.54
10:L:644:LEU:HD11	10:L:659:PHE:HB3	1.89	0.54
2:B:192:THR:HA	2:B:195:LEU:HD12	1.87	0.54
5:E:305:ARG:O	5:E:309:LYS:HG2	2.07	0.54
7:G:31:ILE:HD13	7:G:67:LEU:HD22	1.89	0.54
9:M:30:PHE:O	9:M:45:HIS:NE2	2.41	0.54
5:E:247:VAL:HG22	6:F:230:MET:HE2	1.88	0.54
9:I:45:HIS:HB2	9:I:48:VAL:HG22	1.90	0.54
9:I:385:ILE:HA	9:I:399:VAL:HG12	1.89	0.54
10:L:559:LEU:O	10:L:592:LEU:N	2.30	0.54
2:B:187:ASP:HB2	2:B:190:LYS:HB2	1.90	0.54
6:F:264:CYS:O	6:F:268:PRO:HD2	2.07	0.54
9:M:348:ASN:ND2	9:M:366:MET:O	2.41	0.54
3:C:354:LYS:HB2	8:H:161:MET:HE2	1.89	0.54
9:M:126:LYS:NZ	9:M:407:ASP:OD2	2.41	0.54
9:I:254:PRO:O	9:I:255:LYS:HG2	2.08	0.53
9:M:370:ARG:NH1	9:M:386:GLY:O	2.38	0.53
2:B:132:TYR:CD2	2:B:155:LEU:HD13	2.44	0.53
4:D:256:GLN:HA	4:D:261:TYR:CG	2.43	0.53
10:L:749:ILE:HG22	10:L:756:ARG:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ASP:HB2	2:B:405:VAL:HG22	1.91	0.53
2:B:93:LYS:HA	2:B:96:LEU:HD12	1.91	0.53
2:B:163:GLU:OE1	2:B:165:TYR:OH	2.24	0.53
10:L:500:GLY:HA2	10:L:503:LEU:HD23	1.90	0.53
2:B:90:ASN:HA	2:B:93:LYS:HD2	1.90	0.53
9:I:455:ARG:HD2	9:I:500:GLU:OE1	2.08	0.53
4:D:175:GLN:NE2	4:D:184:GLN:HG2	2.24	0.53
9:M:289:SER:HG	9:M:294:LYS:H	1.56	0.53
1:A:218:LEU:O	1:A:222:SER:N	2.35	0.53
9:I:53:SER:OG	9:I:111:LEU:O	2.24	0.53
10:L:506:ARG:HB2	11:R:30:VAL:HG22	1.91	0.53
3:C:253:ILE:HA	3:C:256:LEU:HB2	1.91	0.53
6:F:217:VAL:HG22	8:H:204:VAL:HG11	1.91	0.53
10:L:356:LEU:HD12	10:L:360:PHE:HB2	1.89	0.53
9:M:195:ARG:HD3	9:M:229:THR:HG21	1.91	0.53
9:M:297:LYS:HB3	9:M:594:SER:HB2	1.90	0.53
2:B:165:TYR:HB3	2:B:204:MET:HE1	1.91	0.53
5:E:171:ASP:HB3	5:E:182:ASN:HB3	1.90	0.53
6:F:151:PHE:HD2	6:F:168:PHE:HB2	1.72	0.53
6:F:267:LEU:HD21	7:G:177:TRP:CE3	2.43	0.53
10:L:148:ARG:HH11	10:L:200:VAL:HG21	1.73	0.53
2:B:431:LEU:HD11	5:E:270:SER:HA	1.91	0.53
1:A:166:TRP:HB2	9:I:345:ARG:HH22	1.74	0.52
10:L:314:CYS:HB3	10:L:369:THR:HG21	1.91	0.52
10:L:739:VAL:HA	10:L:742:LYS:HE3	1.90	0.52
3:C:8:PHE:HB2	3:C:34:LEU:HD11	1.91	0.52
3:C:95:TYR:O	3:C:173:ASN:ND2	2.36	0.52
5:E:237:LEU:HD13	6:F:200:VAL:HG13	1.91	0.52
9:I:62:SER:OG	9:I:66:GLU:OE2	2.27	0.52
9:I:535:CYS:SG	9:I:564:ARG:NH1	2.82	0.52
2:B:122:SER:OG	2:B:123:LYS:N	2.43	0.52
4:D:269:LEU:HD22	4:D:271:ARG:HH22	1.75	0.52
10:L:375:GLU:HA	10:L:421:PHE:HB3	1.91	0.52
5:E:250:LEU:HD21	5:E:328:PHE:HE2	1.75	0.52
9:I:399:VAL:HG13	9:I:415:LEU:HG	1.92	0.52
9:I:476:GLY:O	9:I:496:SER:N	2.43	0.52
10:L:378:LEU:HD13	10:L:418:LEU:HG	1.92	0.52
11:R:54:ILE:HD11	11:R:86:ARG:HH22	1.74	0.52
10:L:735:LEU:N	10:L:736:PRO:HD2	2.25	0.52
9:M:321:ALA:HB3	9:M:375:LEU:HD11	1.92	0.52
12:N:36:ILE:HD13	12:N:74:ARG:HH12	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLU:HG3	1:A:108:PRO:HG2	1.90	0.52
6:F:231:LEU:O	6:F:235:VAL:HG23	2.10	0.52
10:L:144:LEU:HD12	10:L:193:LEU:HA	1.92	0.52
4:D:78:ASP:HA	4:D:82:LYS:NZ	2.24	0.52
10:L:527:ALA:HB3	10:L:528:PRO:HD3	1.92	0.51
10:L:605:PHE:HZ	10:L:659:PHE:HD2	1.55	0.51
10:L:669:LEU:HB2	10:L:672:VAL:HB	1.91	0.51
10:L:553:HIS:O	10:L:554:MET:HE2	2.10	0.51
10:L:764:TYR:O	10:L:765:THR:C	2.54	0.51
9:M:275:SER:OG	9:M:574:ASP:O	2.28	0.51
2:B:107:TYR:HB2	10:L:445:SER:HB2	1.93	0.51
6:F:309:PHE:HA	6:F:312:LEU:CD2	2.41	0.51
10:L:546:ARG:HH21	11:R:35:TRP:HE1	1.59	0.51
1:A:437:GLU:OE1	1:A:458:LYS:NZ	2.44	0.51
1:A:491:LEU:HD23	3:C:167:MET:HG3	1.92	0.51
2:B:95:LEU:HA	2:B:98:TYR:HB2	1.93	0.51
5:E:181:VAL:HB	6:F:202:HIS:CD2	2.46	0.51
10:L:434:GLN:HE21	10:L:438:ARG:HH11	1.56	0.51
10:L:664:GLN:O	10:L:667:SER:OG	2.27	0.51
3:C:397:ILE:HG21	6:F:308:LYS:HB3	1.93	0.51
10:L:559:LEU:HD11	11:R:22:PHE:HB3	1.92	0.51
9:M:35:LEU:HB2	9:M:42:PHE:HB2	1.92	0.51
2:B:165:TYR:HA	2:B:168:LEU:HB3	1.91	0.51
8:H:143:GLU:HB2	8:H:146:LYS:HE3	1.93	0.51
10:L:120:ARG:HG3	10:L:140:TYR:HB2	1.91	0.51
10:L:478:SER:HA	10:L:481:ASN:HD21	1.76	0.51
10:L:524:ILE:O	10:L:529:ARG:NE	2.44	0.51
3:C:167:MET:SD	3:C:167:MET:N	2.84	0.50
10:L:553:HIS:HA	10:L:597:PHE:CE1	2.46	0.50
9:M:47:MET:O	9:M:51:THR:HG23	2.11	0.50
9:M:352:TRP:O	9:M:361:PHE:N	2.43	0.50
9:M:570:ARG:HA	9:M:598:PRO:HB3	1.92	0.50
5:E:209:ASN:O	10:L:715:LYS:NZ	2.44	0.50
9:M:53:SER:HA	9:M:113:VAL:HG22	1.92	0.50
9:M:208:SER:O	9:M:211:GLN:NE2	2.44	0.50
9:M:397:ARG:HE	9:M:417:CYS:C	2.20	0.50
1:A:169:ALA:HA	1:A:172:LYS:HE3	1.92	0.50
4:D:266:LYS:HA	4:D:271:ARG:HH21	1.77	0.50
9:I:301:PRO:HG3	9:I:360:TRP:CE2	2.46	0.50
3:C:315:LEU:O	3:C:360:PHE:N	2.44	0.50
1:A:214:LEU:HB3	1:A:248:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:740:VAL:HA	10:L:743:LYS:HZ3	1.76	0.50
11:R:47:ASN:ND2	11:R:57:GLN:OE1	2.44	0.50
3:C:241:LEU:O	3:C:243:LYS:NZ	2.45	0.50
4:D:124:ALA:O	4:D:128:VAL:HG23	2.12	0.50
9:I:17:LEU:HD22	9:M:18:LEU:HD13	1.93	0.50
2:B:72:LEU:HD22	2:B:91:ARG:HB3	1.92	0.50
2:B:265:TYR:HB3	2:B:273:ARG:HB3	1.93	0.50
10:L:287:MET:HE3	10:L:296:LEU:HD22	1.93	0.50
1:A:209:LEU:HD11	1:A:244:VAL:HG22	1.94	0.50
2:B:238:ARG:NH2	2:B:257:ASP:OD1	2.36	0.50
4:D:328:LEU:HB2	4:D:330:ILE:HG12	1.94	0.50
4:D:48:PHE:HZ	4:D:65:LEU:HB3	1.76	0.50
10:L:322:ARG:NE	10:L:373:ASP:OD1	2.44	0.50
10:L:714:ARG:HH22	10:L:753:TYR:C	2.19	0.50
4:D:230:LEU:HD13	4:D:264:LEU:HD13	1.94	0.49
9:I:232:ALA:O	9:I:235:GLN:NE2	2.45	0.49
9:I:297:LYS:HB3	9:I:594:SER:HB2	1.94	0.49
10:L:289:LYS:O	10:L:351:ARG:NH2	2.44	0.49
9:I:13:TYR:OH	9:M:91:THR:O	2.23	0.49
9:I:548:LYS:NZ	9:I:549:TYR:O	2.44	0.49
10:L:36:LEU:HD11	10:L:60:ASN:HD22	1.77	0.49
10:L:553:HIS:HA	10:L:597:PHE:HE1	1.77	0.49
1:A:95:MET:HE3	1:A:319:LEU:HA	1.94	0.49
2:B:34:ASN:ND2	10:L:668:LYS:O	2.43	0.49
6:F:252:PHE:CE2	6:F:254:HIS:HA	2.47	0.49
9:I:366:MET:HE1	9:I:370:ARG:NE	2.27	0.49
10:L:657:HIS:HD2	10:L:659:PHE:CE1	2.30	0.49
1:A:206:ASP:OD1	1:A:221:TYR:OH	2.30	0.49
1:A:346:VAL:HG13	1:A:352:PHE:HD2	1.77	0.49
1:A:388:LEU:HD13	1:A:398:VAL:HG21	1.94	0.49
7:G:69:LEU:HD13	7:G:85:LEU:HD11	1.94	0.49
9:I:350:PHE:HD2	9:I:363:LYS:HB2	1.78	0.49
10:L:707:ILE:HB	10:L:711:MET:HE1	1.94	0.49
1:A:76:VAL:HG13	1:A:106:HIS:HA	1.95	0.49
1:A:423:HIS:CE1	1:A:458:LYS:HB2	2.47	0.49
3:C:55:SER:HA	3:C:58:VAL:HB	1.93	0.49
3:C:209:ILE:HA	3:C:220:MET:HE1	1.93	0.49
4:D:301:ASP:HA	4:D:304:VAL:HB	1.94	0.49
10:L:738:PRO:HA	10:L:741:ILE:HG22	1.94	0.49
1:A:456:HIS:HA	3:C:357:MET:HE2	1.95	0.49
2:B:227:ALA:HA	10:L:459:LYS:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:52:MET:O	4:D:95:ARG:NH1	2.45	0.49
1:A:339:ARG:NH1	1:A:370:TYR:O	2.38	0.49
3:C:395:GLN:O	3:C:399:VAL:HG23	2.13	0.49
6:F:143:CYS:HA	6:F:149:PRO:HG3	1.95	0.49
9:I:397:ARG:HB3	9:I:415:LEU:HB2	1.94	0.49
11:R:20:LYS:HE3	11:R:23:GLU:HG2	1.95	0.49
2:B:416:ARG:HG2	2:B:418:GLY:H	1.77	0.49
4:D:234:ILE:HA	4:D:242:ARG:HH21	1.78	0.49
10:L:558:ASP:HB2	11:R:26:LYS:HB2	1.95	0.49
1:A:374:TYR:HA	1:A:377:CYS:HB3	1.94	0.49
9:I:47:MET:HG3	9:M:24:PHE:HD2	1.77	0.49
9:M:273:GLU:OE2	9:M:307:LYS:N	2.45	0.49
7:G:136:VAL:HG22	7:G:141:ILE:HG13	1.94	0.48
1:A:417:TYR:HD1	2:B:402:ILE:HB	1.78	0.48
3:C:265:GLN:O	3:C:268:SER:OG	2.27	0.48
6:F:54:HIS:CE1	6:F:68:VAL:HB	2.48	0.48
10:L:77:LEU:HD22	10:L:123:LEU:HD13	1.94	0.48
10:L:612:THR:OG1	10:L:655:ASN:O	2.30	0.48
2:B:314:LEU:HD11	2:B:337:ILE:HD12	1.95	0.48
3:C:318:SER:HA	3:C:357:MET:HA	1.94	0.48
5:E:107:VAL:HG11	12:N:74:ARG:HG3	1.95	0.48
5:E:210:LYS:HZ1	10:L:715:LYS:HE2	1.78	0.48
10:L:429:GLU:OE2	10:L:433:LYS:NZ	2.42	0.48
3:C:43:ASP:OD1	3:C:43:ASP:N	2.45	0.48
10:L:551:GLN:NE2	11:R:30:VAL:O	2.43	0.48
10:L:647:GLU:HB2	10:L:648:PRO:HD3	1.94	0.48
6:F:108:LYS:HA	6:F:111:GLN:HB2	1.95	0.48
10:L:36:LEU:HD11	10:L:60:ASN:ND2	2.29	0.48
10:L:520:PRO:HG3	10:L:553:HIS:CE1	2.48	0.48
10:L:606:ASN:HD21	11:R:22:PHE:HB2	1.78	0.48
4:D:155:TYR:HB3	4:D:164:ALA:HB2	1.96	0.48
4:D:172:SER:HA	4:D:175:GLN:HB3	1.94	0.48
7:G:51:ASN:HA	7:G:54:GLU:HG2	1.94	0.48
10:L:238:GLU:O	10:L:242:ASN:ND2	2.35	0.48
10:L:657:HIS:CD2	10:L:659:PHE:CE1	3.01	0.48
10:L:751:ARG:HG2	10:L:752:GLU:H	1.78	0.48
10:L:476:ASP:OD2	10:L:509:THR:OG1	2.29	0.48
9:M:115:ASP:OD1	9:M:116:VAL:N	2.46	0.48
9:M:419:TRP:HZ3	9:M:433:VAL:HG13	1.78	0.48
9:I:228:VAL:HA	9:I:231:ARG:HD3	1.96	0.48
10:L:267:GLU:O	10:L:271:LYS:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ARG:HB2	1:A:159:PRO:HG3	1.94	0.48
3:C:266:VAL:HG21	3:C:278:LEU:HD22	1.96	0.48
4:D:93:GLN:HB3	4:D:94:PRO:HD3	1.95	0.48
10:L:438:ARG:NH2	10:L:516:GLN:OE1	2.46	0.48
9:M:152:ALA:O	9:M:156:VAL:N	2.32	0.48
1:A:194:LYS:HG2	1:A:227:TYR:HD1	1.79	0.48
1:A:445:LEU:HD22	3:C:309:ARG:HH21	1.78	0.48
6:F:42:ALA:HB3	6:F:82:GLU:HA	1.95	0.47
9:I:425:VAL:HB	9:I:466:ALA:HB2	1.95	0.47
9:M:35:LEU:HD12	9:M:86:ILE:HD11	1.96	0.47
4:D:309:LEU:HD22	4:D:342:MET:SD	2.54	0.47
9:M:385:ILE:HA	9:M:399:VAL:HG12	1.96	0.47
1:A:175:LEU:O	1:A:179:GLU:HG2	2.14	0.47
2:B:105:ARG:H	2:B:105:ARG:HG2	1.36	0.47
9:M:274:ALA:N	9:M:284:SER:O	2.46	0.47
1:A:384:MET:O	1:A:388:LEU:HG	2.15	0.47
4:D:67:THR:OG1	4:D:102:GLN:NE2	2.37	0.47
4:D:147:THR:O	4:D:151:ILE:HG13	2.14	0.47
5:E:210:LYS:HE2	10:L:715:LYS:HE2	1.96	0.47
6:F:217:VAL:HA	6:F:220:HIS:HB3	1.96	0.47
4:D:226:LEU:HD21	4:D:255:CYS:SG	2.54	0.47
5:E:209:ASN:HD22	10:L:715:LYS:HE3	1.78	0.47
7:G:23:SER:HA	7:G:27:LEU:HB2	1.96	0.47
9:I:515:ILE:HG12	9:I:538:MET:HE1	1.97	0.47
10:L:440:LEU:HD11	10:L:474:PHE:CE1	2.50	0.47
1:A:104:ALA:HB1	1:A:111:ARG:HG3	1.97	0.47
2:B:120:SER:HA	2:B:128:LEU:HD11	1.95	0.47
4:D:238:ALA:HB3	4:D:306:GLU:HB3	1.97	0.47
6:F:107:THR:HG22	6:F:111:GLN:HE21	1.80	0.47
9:I:287:CYS:N	9:I:296:TYR:O	2.37	0.47
9:I:553:GLN:HB2	9:I:564:ARG:HB2	1.97	0.47
10:L:556:SER:HB2	10:L:593:GLN:HE21	1.80	0.47
9:M:455:ARG:NH1	9:M:457:THR:O	2.48	0.47
11:R:39:VAL:HA	11:R:49:ILE:HG21	1.97	0.47
2:B:80:PHE:HB3	2:B:118:TYR:HE2	1.80	0.47
10:L:65:VAL:HG11	10:L:129:VAL:HG11	1.97	0.47
10:L:459:LYS:HB3	10:L:471:GLU:OE2	2.15	0.47
9:M:182:SER:HB3	9:M:219:GLN:HB3	1.96	0.47
6:F:70:GLY:HA3	6:F:125:TYR:CZ	2.50	0.47
10:L:703:ILE:HB	10:L:744:ARG:HD2	1.97	0.47
1:A:380:MET:HB3	1:A:384:MET:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:560:ASN:HA	10:L:591:ILE:HA	1.98	0.46
5:E:290:GLU:H	5:E:290:GLU:CD	2.24	0.46
7:G:194:ARG:HD3	8:H:201:THR:HG21	1.97	0.46
10:L:503:LEU:CD1	11:R:27:TRP:HB3	2.45	0.46
2:B:111:SER:O	2:B:115:ILE:HG12	2.14	0.46
4:D:251:LYS:HA	4:D:251:LYS:HD3	1.82	0.46
3:C:131:MET:SD	3:C:139:THR:HG21	2.55	0.46
4:D:194:VAL:O	4:D:198:ARG:HG2	2.16	0.46
4:D:59:LEU:HD11	4:D:98:SER:HB3	1.96	0.46
5:E:259:ALA:O	5:E:260:ASP:C	2.58	0.46
11:R:60:GLN:H	11:R:60:GLN:HG2	1.58	0.46
5:E:56:LYS:HA	5:E:227:SER:O	2.16	0.46
5:E:114:TYR:HB2	12:N:42:ARG:HB2	1.96	0.46
2:B:145:ASP:HA	2:B:148:TRP:HB3	1.98	0.46
2:B:282:LEU:HD22	2:B:343:ILE:HG12	1.96	0.46
4:D:169:ASN:HB3	11:R:39:VAL:HG11	1.98	0.46
6:F:58:MET:HG3	6:F:68:VAL:HG12	1.96	0.46
10:L:124:MET:HA	10:L:127:ASP:HB2	1.97	0.46
9:M:137:LEU:HD22	9:M:156:VAL:HG11	1.97	0.46
12:N:6:LYS:HA	12:N:12:GLU:HA	1.98	0.46
1:A:75:TYR:HB2	1:A:76:VAL:H	1.55	0.46
1:A:173:LYS:O	1:A:177:LYS:HG2	2.16	0.46
5:E:99:PRO:HG2	5:E:112:ALA:O	2.16	0.46
5:E:239:GLU:HG2	5:E:243:ASN:HD21	1.81	0.46
9:M:382:ILE:HB	9:M:402:TYR:HB3	1.98	0.46
1:A:310:SER:O	1:A:313:HIS:ND1	2.35	0.46
4:D:132:LEU:HD11	4:D:147:THR:HB	1.98	0.46
4:D:377:LEU:HD13	6:F:266:CYS:HB2	1.98	0.46
9:I:422:SER:OG	9:I:434:MET:O	2.25	0.46
9:I:382:ILE:O	9:I:402:TYR:N	2.43	0.45
10:L:74:TYR:OH	10:L:137:GLU:OE2	2.33	0.45
9:M:217:LEU:HA	9:M:220:ILE:HG22	1.98	0.45
8:H:20:CYS:HB3	8:H:40:LEU:HG	1.98	0.45
9:I:549:TYR:OH	9:I:575:LEU:N	2.45	0.45
9:M:172:LEU:HD22	9:M:176:LEU:HD23	1.98	0.45
4:D:170:ARG:HA	4:D:173:LEU:HG	1.98	0.45
10:L:124:MET:O	10:L:128:ARG:HG2	2.16	0.45
5:E:99:PRO:HD3	6:F:115:VAL:HG13	1.97	0.45
9:M:415:LEU:HD22	9:M:417:CYS:O	2.16	0.45
9:M:458:SER:O	9:M:459:ARG:NH1	2.43	0.45
9:M:513:ALA:HB3	9:M:561:TRP:HZ3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ALA:HB3	1:A:396:PRO:HD3	1.99	0.45
2:B:88:MET:HB3	2:B:88:MET:HE3	1.85	0.45
4:D:278:LEU:HA	4:D:300:LEU:HD21	1.98	0.45
9:I:84:ILE:HA	9:I:87:THR:HG22	1.99	0.45
9:I:171:GLN:O	9:I:171:GLN:HG2	2.16	0.45
1:A:468:ARG:HH12	6:F:281:ASP:CB	2.28	0.45
2:B:238:ARG:O	2:B:257:ASP:HB3	2.17	0.45
6:F:262:ALA:O	6:F:265:HIS:HB2	2.16	0.45
10:L:453:ASN:O	10:L:456:SER:OG	2.27	0.45
10:L:722:LEU:HA	10:L:725:GLU:HB2	1.98	0.45
9:I:379:GLU:HG3	9:I:379:GLU:O	2.16	0.45
4:D:273:ILE:HG12	4:D:307:HIS:HD2	1.82	0.45
5:E:227:SER:C	5:E:228:TYR:HD2	2.24	0.45
5:E:238:LEU:O	5:E:239:GLU:C	2.59	0.45
8:H:125:TYR:CD2	8:H:128:ILE:HD12	2.52	0.45
9:I:220:ILE:HD13	9:I:260:ARG:HH22	1.80	0.45
10:L:436:LEU:HD23	10:L:439:ARG:HD2	1.99	0.45
12:N:71:LEU:H	12:N:71:LEU:HG	1.50	0.45
6:F:175:ILE:HD11	6:F:182:LEU:HD11	1.99	0.45
7:G:207:GLN:HA	7:G:210:GLU:HG2	1.99	0.45
1:A:254:VAL:O	1:A:258:VAL:HG23	2.17	0.45
3:C:117:PRO:HG2	3:C:152:ALA:HB2	1.97	0.45
4:D:84:ILE:HG13	4:D:87:PHE:HD2	1.82	0.45
10:L:31:ASN:OD1	10:L:72:LYS:NZ	2.50	0.45
10:L:116:MET:HA	10:L:119:ILE:HB	2.00	0.45
1:A:337:PHE:CD2	1:A:341:GLU:HG2	2.53	0.44
1:A:398:VAL:HA	1:A:401:LEU:HB2	1.97	0.44
2:B:64:LYS:HG2	2:B:102:ALA:HB3	1.99	0.44
2:B:198:TYR:O	2:B:202:ILE:HG12	2.17	0.44
3:C:404:VAL:HG11	7:G:216:ILE:HG21	1.99	0.44
4:D:402:ALA:O	4:D:406:GLN:NE2	2.50	0.44
5:E:118:ALA:HB2	12:N:44:ILE:HD11	1.99	0.44
9:I:318:ILE:HB	9:I:353:PHE:HB3	1.99	0.44
9:I:399:VAL:HG23	9:I:412:VAL:HG23	1.99	0.44
9:M:266:GLU:HB2	9:M:268:MET:HE3	1.99	0.44
9:M:503:ASP:HB3	9:M:506:LYS:HB2	1.99	0.44
1:A:391:ASP:HB3	1:A:394:LEU:HB3	2.00	0.44
1:A:463:ARG:NH1	3:C:362:ASP:OD2	2.50	0.44
3:C:94:ARG:HD3	3:C:133:MET:HE1	1.99	0.44
3:C:247:GLN:O	3:C:249:VAL:N	2.50	0.44
4:D:297:SER:O	4:D:301:ASP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:233:SER:O	6:F:236:LYS:HG2	2.17	0.44
9:I:321:ALA:HB3	9:I:375:LEU:HD11	2.00	0.44
9:M:87:THR:O	9:M:91:THR:HG22	2.16	0.44
1:A:315:ASP:OD2	9:I:396:ARG:HB2	2.17	0.44
4:D:364:ARG:HB2	4:D:369:THR:HG1	1.83	0.44
1:A:80:PRO:O	1:A:81:SER:OG	2.29	0.44
1:A:490:MET:CG	3:C:167:MET:HG2	2.46	0.44
4:D:163:GLN:O	4:D:167:TYR:N	2.50	0.44
6:F:76:GLN:HG3	6:F:81:ILE:HG12	1.98	0.44
10:L:436:LEU:HA	10:L:439:ARG:HH11	1.81	0.44
10:L:525:PRO:HB3	10:L:603:MET:HG3	1.99	0.44
9:M:311:VAL:HB	9:M:375:LEU:HB3	2.00	0.44
2:B:305:ASP:O	2:B:309:LEU:N	2.47	0.44
6:F:152:LEU:HD12	6:F:167:VAL:HG22	1.99	0.44
6:F:268:PRO:O	6:F:269:VAL:C	2.61	0.44
7:G:37:ALA:O	7:G:95:LYS:NZ	2.51	0.44
8:H:110:ARG:HE	8:H:114:ARG:HH12	1.65	0.44
10:L:754:LEU:HD23	10:L:756:ARG:HB2	1.99	0.44
9:M:163:VAL:HG12	9:M:165:HIS:H	1.82	0.44
11:R:48:HIS:HD2	11:R:50:MET:HG2	1.81	0.44
1:A:133:GLU:OE2	1:A:136:ARG:NH2	2.46	0.44
4:D:140:ASN:O	4:D:143:TYR:N	2.48	0.44
5:E:312:ILE:HD13	8:H:207:LEU:HB2	2.00	0.44
6:F:169:GLU:HB3	6:F:186:LEU:HD11	2.00	0.44
9:I:413:SER:HB3	9:I:442:TYR:HE1	1.82	0.44
10:L:631:LEU:HD11	10:L:659:PHE:CE2	2.52	0.44
9:M:267:GLU:HG2	9:M:530:ILE:HG13	2.00	0.44
3:C:316:THR:HA	3:C:359:SER:HA	1.98	0.44
6:F:71:ALA:HB1	6:F:121:PHE:HE1	1.83	0.44
7:G:163:ARG:HD2	7:G:165:LYS:HE2	1.99	0.44
1:A:334:LEU:HD23	1:A:405:ILE:HG12	1.99	0.44
5:E:242:TRP:O	5:E:243:ASN:C	2.60	0.44
9:I:20:GLN:HB3	9:I:24:PHE:CE2	2.52	0.44
9:M:49:LEU:HB3	9:M:56:PHE:CD2	2.53	0.44
9:M:128:ILE:HG23	9:M:155:MET:HE3	2.00	0.44
2:B:153:THR:HG21	2:B:196:GLU:HG2	1.99	0.44
4:D:364:ARG:HB2	4:D:369:THR:OG1	2.17	0.44
5:E:327:LEU:HD12	7:G:184:VAL:HG11	2.00	0.44
9:M:370:ARG:NH2	9:M:398:THR:O	2.48	0.44
11:R:94:CYS:O	11:R:96:LEU:N	2.51	0.44
2:B:115:ILE:O	2:B:119:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:LEU:O	3:C:46:LEU:HG	2.18	0.43
3:C:118:LEU:HD13	8:H:59:ARG:HD2	2.00	0.43
9:I:286:VAL:HA	9:I:297:LYS:HA	2.00	0.43
10:L:230:ALA:HB2	10:L:276:ILE:HG12	1.99	0.43
10:L:274:LYS:O	10:L:278:GLU:HG2	2.17	0.43
2:B:295:ASP:OD2	11:R:96:LEU:HD21	2.18	0.43
4:D:285:LEU:HB3	4:D:290:LYS:N	2.33	0.43
9:I:45:HIS:ND1	9:I:90:TYR:OH	2.36	0.43
9:M:247:GLN:O	9:M:251:LYS:HB2	2.18	0.43
1:A:291:LEU:HD22	1:A:320:LEU:HD22	2.00	0.43
2:B:108:SER:O	2:B:112:ILE:HG12	2.19	0.43
5:E:62:LEU:HD23	6:F:203:VAL:HG22	2.01	0.43
10:L:485:ASP:O	10:L:489:GLN:HG2	2.19	0.43
9:M:134:VAL:HB	9:M:160:PHE:CE1	2.53	0.43
2:B:235:GLY:HA2	2:B:261:ALA:HA	2.01	0.43
11:R:44:ILE:HB	11:R:83:CYS:HB3	2.00	0.43
2:B:70:LYS:HG2	2:B:107:TYR:OH	2.19	0.43
2:B:122:SER:OG	2:B:124:GLN:NE2	2.51	0.43
4:D:208:TYR:HB3	4:D:229:ALA:HB2	2.00	0.43
5:E:96:PHE:HZ	5:E:117:MET:HG2	1.82	0.43
6:F:47:VAL:HG21	6:F:83:VAL:HG12	2.00	0.43
9:I:366:MET:HE3	9:I:400:GLU:HB3	1.99	0.43
10:L:631:LEU:HD11	10:L:659:PHE:HE2	1.84	0.43
1:A:238:CYS:HA	1:A:257:TYR:HD2	1.83	0.43
10:L:395:LYS:HA	10:L:395:LYS:HD3	1.79	0.43
5:E:311:THR:HG21	6:F:293:GLY:HA3	2.00	0.43
10:L:100:ASN:HB3	10:L:103:GLN:HB3	1.99	0.43
10:L:737:SER:O	10:L:740:VAL:HG22	2.19	0.43
10:L:440:LEU:HD11	10:L:474:PHE:HE1	1.84	0.43
10:L:709:ARG:HH12	10:L:736:PRO:HA	1.84	0.43
4:D:83:GLU:OE1	4:D:83:GLU:N	2.43	0.43
5:E:236:LYS:HE2	5:E:236:LYS:HB2	1.35	0.43
9:I:434:MET:HE2	9:I:455:ARG:NE	2.31	0.43
10:L:416:MET:HA	10:L:419:PHE:HB3	2.01	0.43
9:M:137:LEU:HB2	9:M:156:VAL:HG21	2.01	0.43
1:A:91:TYR:HE2	1:A:320:LEU:HA	1.84	0.43
1:A:242:ILE:HA	1:A:254:VAL:HG22	2.01	0.43
1:A:242:ILE:O	1:A:246:VAL:HG23	2.18	0.43
1:A:368:LYS:HG2	1:A:373:LYS:HE2	1.99	0.43
1:A:368:LYS:HA	1:A:373:LYS:NZ	2.33	0.43
1:A:385:LYS:HB2	1:A:402:TYR:HE2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:67:THR:O	4:D:71:THR:HG23	2.18	0.43
9:I:301:PRO:HB2	9:I:302:PRO:HD3	2.01	0.43
9:I:397:ARG:HG2	9:I:417:CYS:C	2.44	0.43
9:M:268:MET:HE1	9:M:588:PRO:HG3	2.00	0.43
9:M:346:THR:HG22	9:M:369:VAL:HB	2.01	0.43
2:B:149:PHE:CD1	2:B:175:LEU:HD22	2.54	0.42
4:D:214:LYS:HG3	4:D:215:THR:H	1.83	0.42
4:D:352:ILE:HG22	4:D:353:ASP:N	2.34	0.42
6:F:100:ILE:HB	6:F:102:LYS:HE2	2.01	0.42
9:I:353:PHE:HB2	9:I:360:TRP:CH2	2.53	0.42
10:L:733:ARG:H	10:L:733:ARG:HD3	1.83	0.42
9:M:128:ILE:HG13	9:M:155:MET:HG2	2.00	0.42
11:R:49:ILE:HD12	11:R:49:ILE:HA	1.91	0.42
1:A:185:LEU:HD13	1:A:200:GLY:HA3	2.00	0.42
2:B:292:ASN:ND2	2:B:319:GLN:HE22	2.17	0.42
7:G:81:ASN:HB3	7:G:85:LEU:HG	2.00	0.42
9:I:30:PHE:HB3	9:M:47:MET:HA	2.00	0.42
10:L:426:ASP:OD1	10:L:427:VAL:N	2.52	0.42
9:M:379:GLU:O	9:M:379:GLU:HG3	2.19	0.42
9:M:526:ARG:HB2	9:M:537:PHE:HB3	2.00	0.42
1:A:381:LEU:HG	1:A:402:TYR:CE2	2.54	0.42
2:B:326:PHE:O	2:B:330:LEU:HG	2.19	0.42
2:B:359:LEU:HD21	2:B:389:LEU:HD23	2.00	0.42
4:D:82:LYS:HE2	4:D:113:ILE:HG21	2.01	0.42
10:L:211:GLU:O	10:L:215:GLU:HG2	2.19	0.42
10:L:685:ASP:O	10:L:686:PRO:C	2.62	0.42
1:A:376:SER:HA	1:A:379:LYS:HG2	2.01	0.42
2:B:400:GLY:HA3	2:B:411:LEU:HA	2.02	0.42
3:C:50:ASP:CG	3:C:51:VAL:H	2.27	0.42
3:C:243:LYS:HA	3:C:243:LYS:HD3	1.80	0.42
10:L:153:ARG:HH21	10:L:200:VAL:HG13	1.84	0.42
4:D:264:LEU:HA	4:D:267:MET:HB3	2.02	0.42
4:D:381:VAL:HG22	6:F:263:LEU:HD23	2.00	0.42
10:L:388:LEU:O	10:L:392:ILE:HD12	2.19	0.42
1:A:135:HIS:NE2	1:A:162:LEU:HB3	2.34	0.42
1:A:179:GLU:O	1:A:183:THR:N	2.48	0.42
2:B:65:GLY:O	2:B:68:GLY:N	2.53	0.42
2:B:139:LEU:HB2	2:B:148:TRP:HB2	2.01	0.42
2:B:343:ILE:O	2:B:347:ILE:N	2.52	0.42
6:F:64:ARG:HA	6:F:64:ARG:HD3	1.83	0.42
7:G:122:MET:HG2	7:G:128:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:275:SER:N	9:M:575:LEU:O	2.52	0.42
9:M:416:PRO:HG2	9:M:440:TYR:CE1	2.55	0.42
1:A:88:ALA:HB2	1:A:100:LEU:HD21	2.02	0.42
2:B:160:LEU:HG	2:B:203:GLN:HB2	2.02	0.42
2:B:169:GLN:O	2:B:173:ARG:HG3	2.20	0.42
3:C:205:TYR:HB3	3:C:227:TYR:HB2	2.02	0.42
5:E:118:ALA:HB3	12:N:49:GLN:OE1	2.20	0.42
5:E:241:LEU:HD22	6:F:200:VAL:HB	2.02	0.42
5:E:249:THR:C	5:E:324:LYS:HZ3	2.28	0.42
5:E:327:LEU:O	5:E:331:ILE:HB	2.19	0.42
7:G:34:VAL:O	7:G:95:LYS:NZ	2.53	0.42
7:G:122:MET:HE2	7:G:127:GLU:HB2	2.01	0.42
2:B:230:HIS:HB3	2:B:233:ILE:HD12	2.00	0.42
3:C:150:LEU:HA	3:C:155:PHE:HE1	1.85	0.42
4:D:311:SER:HA	4:D:314:LYS:HG2	2.02	0.42
6:F:51:ILE:HG12	6:F:125:TYR:CD1	2.55	0.42
9:I:539:ARG:HH22	9:I:577:ARG:HD3	1.84	0.42
10:L:503:LEU:HD11	11:R:27:TRP:HE3	1.85	0.42
10:L:693:GLN:NE2	10:L:694:LYS:HG3	2.35	0.42
2:B:24:SER:OG	2:B:25:ASN:N	2.51	0.42
2:B:79:ASN:HB3	2:B:84:ASN:HB3	2.02	0.42
3:C:20:GLN:HB3	3:C:23:GLN:HB2	2.01	0.42
5:E:252:SER:O	5:E:253:SER:HB3	2.20	0.42
7:G:116:LEU:HD13	7:G:132:ILE:HD11	2.00	0.42
10:L:410:THR:O	10:L:414:LYS:HG2	2.20	0.42
4:D:330:ILE:HB	4:D:334:LYS:HD3	2.02	0.42
10:L:749:ILE:HA	10:L:755:ALA:O	2.20	0.42
2:B:159:TYR:CE2	2:B:167:LYS:HB2	2.55	0.41
2:B:209:LYS:O	2:B:209:LYS:HG3	2.19	0.41
3:C:243:LYS:HA	3:C:245:THR:HG23	2.01	0.41
10:L:712:LYS:HA	10:L:712:LYS:HD3	1.76	0.41
9:M:145:CYS:O	9:M:148:LEU:N	2.53	0.41
9:M:389:SER:OG	9:M:398:THR:OG1	2.22	0.41
11:R:84:ILE:HG12	11:R:101:TRP:NE1	2.34	0.41
1:A:171:ARG:HA	1:A:171:ARG:HH11	1.85	0.41
2:B:299:ALA:HB3	2:B:302:TYR:HD2	1.85	0.41
3:C:42:LEU:HD22	3:C:65:LYS:HE2	2.01	0.41
3:C:182:LEU:HD21	3:C:220:MET:HB2	2.03	0.41
4:D:315:LEU:HD21	7:G:136:VAL:HG11	2.02	0.41
5:E:170:ILE:H	5:E:170:ILE:HG12	1.72	0.41
7:G:70:PHE:CE1	7:G:96:LEU:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:187:GLY:O	7:G:191:GLN:HG2	2.21	0.41
9:I:222:ILE:HG12	9:I:257:PHE:HB2	2.01	0.41
9:I:435:THR:HG22	9:I:438:LEU:O	2.19	0.41
10:L:298:CYS:HA	10:L:301:LYS:HE3	2.01	0.41
10:L:740:VAL:HG12	10:L:743:LYS:HZ3	1.83	0.41
9:M:137:LEU:HG	9:M:176:LEU:HD21	2.02	0.41
2:B:125:MET:HA	2:B:128:LEU:HB2	2.02	0.41
4:D:156:LEU:HD22	4:D:197:TYR:CD2	2.56	0.41
4:D:214:LYS:HG3	4:D:215:THR:N	2.36	0.41
5:E:25:ILE:HG23	5:E:231:SER:HA	2.01	0.41
6:F:264:CYS:C	6:F:266:CYS:N	2.78	0.41
8:H:107:GLU:HG2	8:H:110:ARG:HH22	1.85	0.41
10:L:434:GLN:NE2	10:L:438:ARG:HH11	2.17	0.41
9:M:372:LYS:NZ	9:M:580:ARG:HE	2.17	0.41
1:A:108:PRO:C	1:A:110:LEU:H	2.26	0.41
4:D:173:LEU:HD11	11:R:39:VAL:HG13	2.03	0.41
9:I:18:LEU:HD12	9:I:18:LEU:HA	1.89	0.41
9:I:159:LYS:O	9:I:163:VAL:HG22	2.21	0.41
9:I:289:SER:HG	9:I:294:LYS:H	1.65	0.41
10:L:385:PRO:HB3	10:L:428:PHE:HB2	2.03	0.41
9:M:525:VAL:HA	9:M:538:MET:HG2	2.01	0.41
4:D:286:MET:HE1	4:D:292:THR:HA	2.03	0.41
5:E:246:TRP:O	5:E:247:VAL:C	2.63	0.41
9:I:24:PHE:CG	9:I:30:PHE:HE2	2.38	0.41
9:I:134:VAL:HG21	9:I:169:PHE:HA	2.02	0.41
9:I:470:LYS:NZ	9:I:503:ASP:OD2	2.45	0.41
10:L:86:ILE:O	10:L:90:ARG:HB3	2.21	0.41
10:L:124:MET:HE3	10:L:124:MET:HB3	1.98	0.41
10:L:762:LYS:HB3	10:L:762:LYS:HE3	1.45	0.41
9:M:121:ARG:O	9:M:125:ILE:HG12	2.21	0.41
11:R:41:ASN:HA	11:R:48:HIS:HA	2.03	0.41
1:A:201:HIS:HB2	1:A:224:ALA:HB2	2.02	0.41
4:D:172:SER:HB2	4:D:187:TYR:OH	2.20	0.41
4:D:233:THR:O	4:D:242:ARG:NE	2.48	0.41
6:F:109:GLU:HG2	6:F:113:LYS:NZ	2.36	0.41
8:H:87:PRO:HG3	8:H:135:ALA:HB1	2.01	0.41
8:H:121:VAL:HG11	8:H:133:PHE:HD1	1.84	0.41
9:I:102:GLU:HG3	9:I:135:ARG:HH12	1.85	0.41
10:L:406:GLN:O	10:L:409:GLU:HG3	2.21	0.41
10:L:605:PHE:CZ	10:L:659:PHE:HD2	2.36	0.41
9:M:424:ALA:HA	9:M:433:VAL:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:539:ARG:HH21	9:M:579:PHE:HE1	1.69	0.41
11:R:77:HIS:HB2	11:R:101:TRP:HZ3	1.84	0.41
1:A:124:ARG:HG2	9:I:345:ARG:HA	2.02	0.41
1:A:328:TYR:CE1	1:A:394:LEU:HD22	2.55	0.41
1:A:452:ARG:HG3	1:A:463:ARG:NH2	2.35	0.41
2:B:152:ASN:O	2:B:156:GLY:N	2.45	0.41
5:E:250:LEU:HD22	5:E:324:LYS:HD3	2.03	0.41
6:F:221:LEU:HD12	7:G:188:ILE:HG23	2.02	0.41
6:F:264:CYS:O	6:F:267:LEU:N	2.46	0.41
9:M:28:GLN:HG2	9:M:31:THR:HG21	2.02	0.41
9:M:160:PHE:O	9:M:164:TYR:N	2.54	0.41
12:N:36:ILE:HG13	12:N:71:LEU:HB2	2.01	0.41
3:C:380:MET:SD	8:H:203:TYR:CE1	3.13	0.41
4:D:185:ILE:HD13	4:D:185:ILE:HA	1.93	0.41
6:F:74:GLY:HA2	6:F:119:LEU:HD22	2.02	0.41
9:I:205:ASN:ND2	9:I:206:THR:H	2.18	0.41
10:L:311:LYS:HB3	10:L:311:LYS:HE3	1.87	0.41
9:M:352:TRP:HE3	9:M:361:PHE:HB2	1.86	0.41
12:N:17:ILE:HD12	12:N:26:ILE:HG12	2.02	0.41
2:B:155:LEU:HD23	2:B:171:ILE:HD11	2.02	0.41
2:B:177:GLN:HA	2:B:180:GLN:OE1	2.21	0.41
4:D:319:ILE:HG13	7:G:147:GLN:OE1	2.21	0.41
4:D:370:TRP:NE1	5:E:329:ASN:OD1	2.46	0.41
5:E:114:TYR:CD2	12:N:70:VAL:HB	2.56	0.41
5:E:159:GLN:HE21	5:E:159:GLN:HB3	1.55	0.41
6:F:155:ASN:HB3	6:F:164:PRO:HB2	2.03	0.41
9:I:213:LEU:HA	9:I:216:VAL:HG12	2.01	0.41
9:I:390:VAL:HG13	9:I:392:GLY:H	1.86	0.41
9:M:539:ARG:HD3	9:M:549:TYR:CZ	2.56	0.41
12:N:26:ILE:HB	12:N:43:LEU:HD11	2.03	0.41
2:B:211:ASN:O	2:B:215:LYS:HG2	2.20	0.41
2:B:344:ARG:O	2:B:347:ILE:HG22	2.21	0.41
4:D:316:TYR:HE1	7:G:145:LEU:HD22	1.86	0.41
4:D:321:PHE:HB3	4:D:332:ALA:HB1	2.02	0.41
5:E:318:LEU:HD22	6:F:286:VAL:HB	2.02	0.41
10:L:127:ASP:O	10:L:131:VAL:HG22	2.20	0.41
9:M:542:HIS:HB2	9:M:545:GLU:HB2	2.02	0.41
1:A:388:LEU:HG	1:A:388:LEU:H	1.66	0.40
2:B:370:HIS:CE1	4:D:355:ILE:HG12	2.56	0.40
5:E:63:LEU:HD23	5:E:63:LEU:HA	1.85	0.40
6:F:221:LEU:HB3	7:G:188:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:38:PRO:HA	12:N:41:GLN:HB2	2.03	0.40
5:E:70:ARG:HG2	5:E:172:PRO:CB	2.51	0.40
7:G:95:LYS:HB2	7:G:95:LYS:HE3	1.89	0.40
10:L:722:LEU:HG	10:L:726:VAL:HG13	2.02	0.40
11:R:84:ILE:HG12	11:R:101:TRP:HE1	1.86	0.40
1:A:500:ILE:HG13	3:C:169:ILE:HG21	2.03	0.40
5:E:272:LYS:HB2	5:E:272:LYS:HE2	1.65	0.40
6:F:190:LEU:HD13	6:F:190:LEU:HA	1.83	0.40
6:F:222:ILE:HA	6:F:225:HIS:HB3	2.03	0.40
10:L:86:ILE:HG23	10:L:90:ARG:HD2	2.04	0.40
10:L:255:SER:O	10:L:257:GLU:N	2.55	0.40
2:B:416:ARG:HG2	2:B:418:GLY:N	2.36	0.40
7:G:111:ILE:O	7:G:152:LEU:N	2.47	0.40
9:M:327:LEU:HG	9:M:343:ALA:HB1	2.03	0.40
2:B:85:PHE:N	2:B:86:PRO:HD2	2.36	0.40
2:B:333:ASN:O	2:B:337:ILE:HG12	2.21	0.40
4:D:267:MET:SD	4:D:307:HIS:CG	3.14	0.40
10:L:605:PHE:HE1	10:L:611:TYR:HB2	1.87	0.40
11:R:80:HIS:O	11:R:84:ILE:HG22	2.21	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	406/527 (77%)	386 (95%)	20 (5%)	0	100	100
2	B	418/443 (94%)	384 (92%)	30 (7%)	4 (1%)	12	47
3	C	405/423 (96%)	385 (95%)	19 (5%)	1 (0%)	43	77
4	D	404/406 (100%)	373 (92%)	24 (6%)	7 (2%)	7	35
5	E	307/334 (92%)	265 (86%)	35 (11%)	7 (2%)	5	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	286/327 (88%)	270 (94%)	15 (5%)	1 (0%)	36	71
7	G	212/264 (80%)	209 (99%)	3 (1%)	0	100	100
8	H	173/209 (83%)	172 (99%)	1 (1%)	0	100	100
9	I	551/623 (88%)	514 (93%)	37 (7%)	0	100	100
9	M	558/623 (90%)	531 (95%)	27 (5%)	0	100	100
10	L	716/768 (93%)	649 (91%)	60 (8%)	7 (1%)	12	47
11	R	87/108 (81%)	67 (77%)	19 (22%)	1 (1%)	11	45
12	N	74/76 (97%)	63 (85%)	8 (11%)	3 (4%)	2	18
All	All	4597/5131 (90%)	4268 (93%)	298 (6%)	31 (1%)	20	55

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	79	SER
4	D	287	PRO
4	D	288	HIS
4	D	291	ALA
5	E	231	SER
5	E	253	SER
5	E	260	ASP
10	L	685	ASP
11	R	40	ASP
10	L	765	THR
2	B	182	ASP
2	B	300	LYS
4	D	93	GLN
5	E	113	ALA
10	L	384	SER
10	L	448	ASP
10	L	686	PRO
10	L	759	GLU
12	N	35	GLY
4	D	298	SER
2	B	28	PRO
2	B	367	THR
4	D	270	ASP
5	E	242	TRP
10	L	762	LYS
12	N	72	ALA

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Mol	Chain	Res	Type
3	C	72	PRO
6	F	270	LEU
12	N	71	LEU
5	E	99	PRO
5	E	199	GLY

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	360/458 (79%)	354 (98%)	6 (2%)	53	67
2	B	382/405 (94%)	374 (98%)	8 (2%)	47	65
3	C	363/377 (96%)	362 (100%)	1 (0%)	86	84
4	D	347/347 (100%)	347 (100%)	0	100	100
5	E	264/282 (94%)	223 (84%)	41 (16%)	2	13
6	F	255/276 (92%)	247 (97%)	8 (3%)	35	56
7	G	187/229 (82%)	187 (100%)	0	100	100
8	H	147/173 (85%)	147 (100%)	0	100	100
9	I	501/560 (90%)	501 (100%)	0	100	100
9	M	507/560 (90%)	507 (100%)	0	100	100
10	L	652/693 (94%)	645 (99%)	7 (1%)	65	73
11	R	78/90 (87%)	73 (94%)	5 (6%)	16	38
12	N	64/66 (97%)	49 (77%)	15 (23%)	1	5
All	All	4107/4516 (91%)	4016 (98%)	91 (2%)	45	64

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	TYR
1	A	76	VAL
1	A	388	LEU

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Mol	Chain	Res	Type
1	A	389	LEU
1	A	391	ASP
1	A	392	MET
2	B	105	ARG
2	B	360	ILE
2	B	361	LYS
2	B	362	LEU
2	B	363	ILE
2	B	364	LYS
2	B	368	ARG
2	B	369	ILE
3	C	71	VAL
5	E	40	LEU
5	E	58	SER
5	E	63	LEU
5	E	70	ARG
5	E	91	ILE
5	E	94	ASP
5	E	100	VAL
5	E	103	THR
5	E	104	GLU
5	E	105	THR
5	E	106	ARG
5	E	107	VAL
5	E	108	ASN
5	E	121	ILE
5	E	122	GLU
5	E	125	LYS
5	E	129	ARG
5	E	130	LEU
5	E	160	GLN
5	E	162	GLN
5	E	165	PHE
5	E	166	VAL
5	E	170	ILE
5	E	174	ARG
5	E	176	ILE
5	E	197	ASP
5	E	202	GLU
5	E	230	LYS
5	E	231	SER
5	E	232	SER

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Mol	Chain	Res	Type
5	E	235	ARG
5	E	236	LYS
5	E	237	LEU
5	E	238	LEU
5	E	244	LYS
5	E	245	TYR
5	E	260	ASP
5	E	266	VAL
5	E	269	LEU
5	E	270	SER
5	E	273	LEU
6	F	90	LEU
6	F	190	LEU
6	F	213	GLU
6	F	214	ASN
6	F	216	THR
6	F	255	GLU
6	F	256	ILE
6	F	267	LEU
10	L	686	PRO
10	L	725	GLU
10	L	733	ARG
10	L	759	GLU
10	L	760	ASP
10	L	762	LYS
10	L	767	VAL
11	R	60	GLN
11	R	66	GLU
11	R	67	GLU
11	R	70	VAL
11	R	99	ARG
12	N	6	LYS
12	N	7	THR
12	N	9	THR
12	N	11	LYS
12	N	13	ILE
12	N	33	LYS
12	N	34	GLU
12	N	39	GLN
12	N	42	ARG
12	N	44	ILE
12	N	69	LEU

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Mol	Chain	Res	Type
12	N	70	VAL
12	N	71	LEU
12	N	73	LEU
12	N	74	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	123	GLN
1	A	127	ASN
1	A	423	HIS
1	A	467	GLN
1	A	501	HIS
2	B	124	GLN
2	B	169	GLN
2	B	176	HIS
2	B	284	ASN
2	B	292	ASN
3	C	261	HIS
3	C	297	GLN
3	C	374	HIS
4	D	72	HIS
4	D	138	GLN
4	D	240	GLN
4	D	256	GLN
4	D	360	HIS
4	D	406	GLN
5	E	159	GLN
5	E	182	ASN
5	E	243	ASN
5	E	248	ASN
6	F	50	ASN
6	F	111	GLN
6	F	141	GLN
6	F	202	HIS
6	F	232	HIS
6	F	253	ASN
7	G	53	GLN
7	G	98	HIS
7	G	124	ASN
7	G	208	GLN

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Mol	Chain	Res	Type
8	H	23	GLN
9	I	69	GLN
9	I	150	GLN
9	I	205	ASN
9	I	356	GLN
9	I	357	GLN
10	L	49	ASN
10	L	60	ASN
10	L	87	ASN
10	L	132	GLN
10	L	163	GLN
10	L	228	ASN
10	L	286	HIS
10	L	481	ASN
10	L	492	GLN
10	L	593	GLN
10	L	606	ASN
10	L	618	GLN
10	L	657	HIS
10	L	718	GLN
10	L	729	GLN
9	M	20	GLN
9	M	27	GLN
9	M	76	ASN
9	M	129	ASN
9	M	150	GLN
9	M	187	ASN
9	M	230	GLN
9	M	235	GLN
11	R	47	ASN
11	R	57	GLN
11	R	98	ASN
11	R	104	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

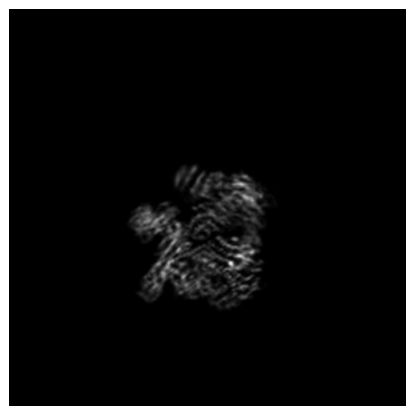
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34455. These allow visual inspection of the internal detail of the map and identification of artifacts.

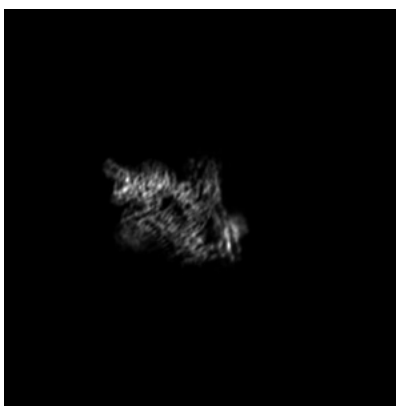
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

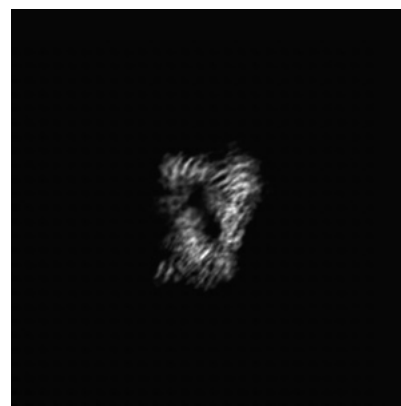
6.1.1 Primary map



X

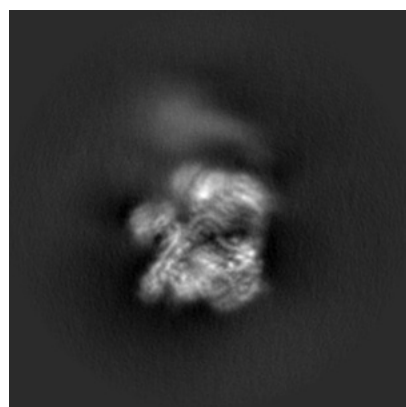


Y

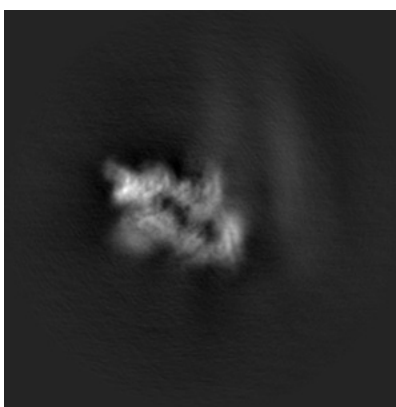


Z

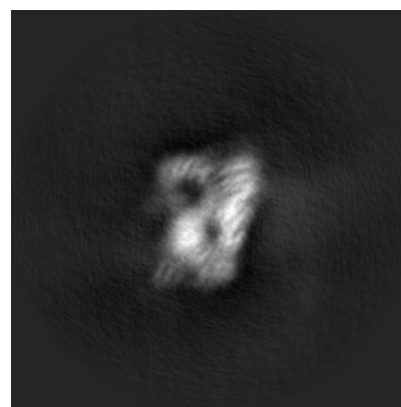
6.1.2 Raw map



X



Y



Z

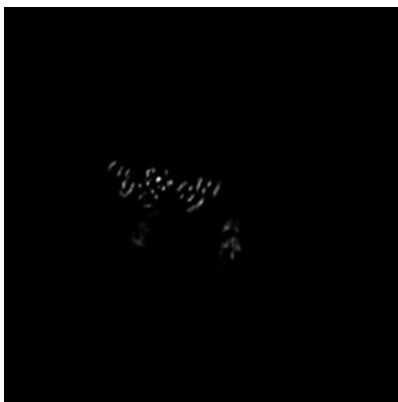
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

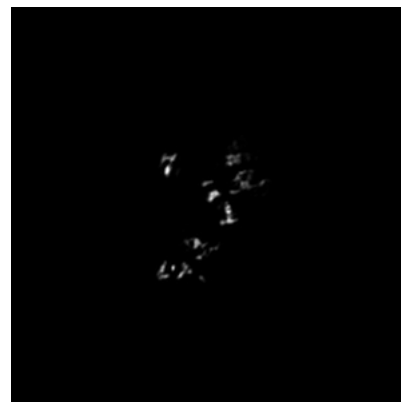
6.2.1 Primary map



X Index: 108

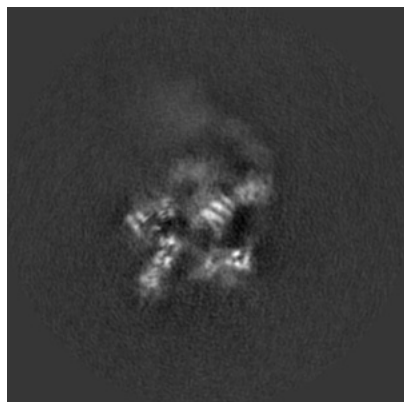


Y Index: 108

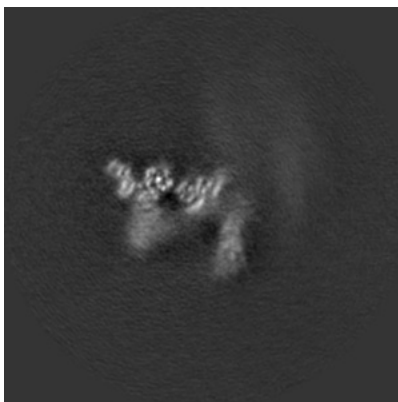


Z Index: 108

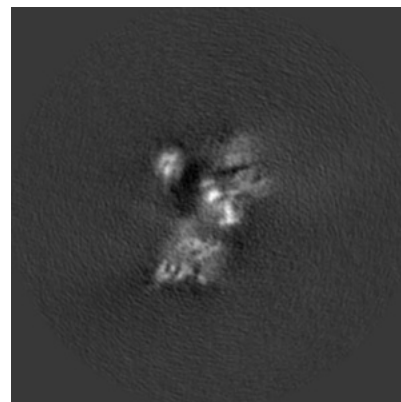
6.2.2 Raw map



X Index: 108



Y Index: 108



Z Index: 108

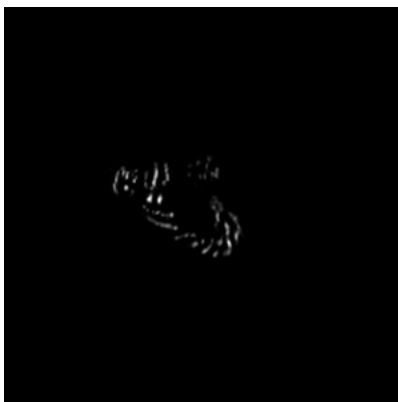
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

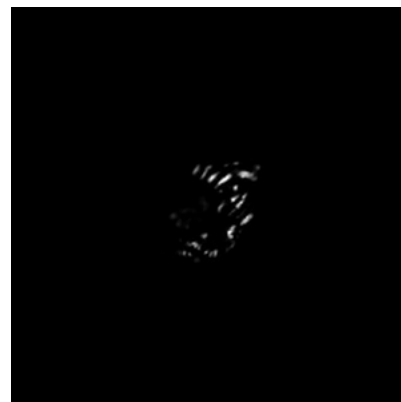
6.3.1 Primary map



X Index: 120

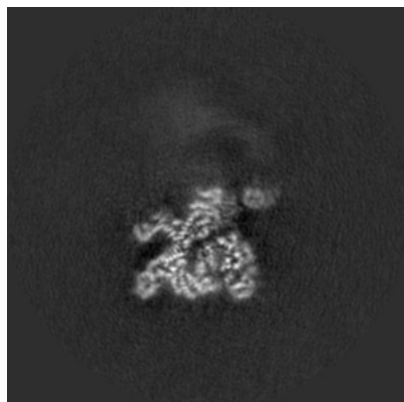


Y Index: 126

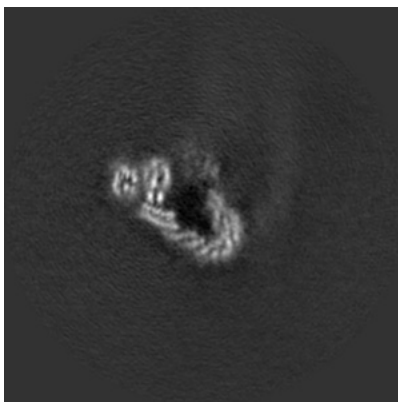


Z Index: 82

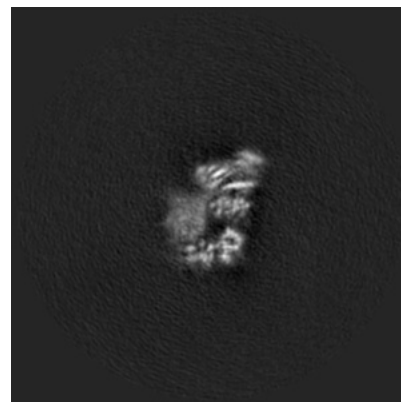
6.3.2 Raw map



X Index: 117



Y Index: 127

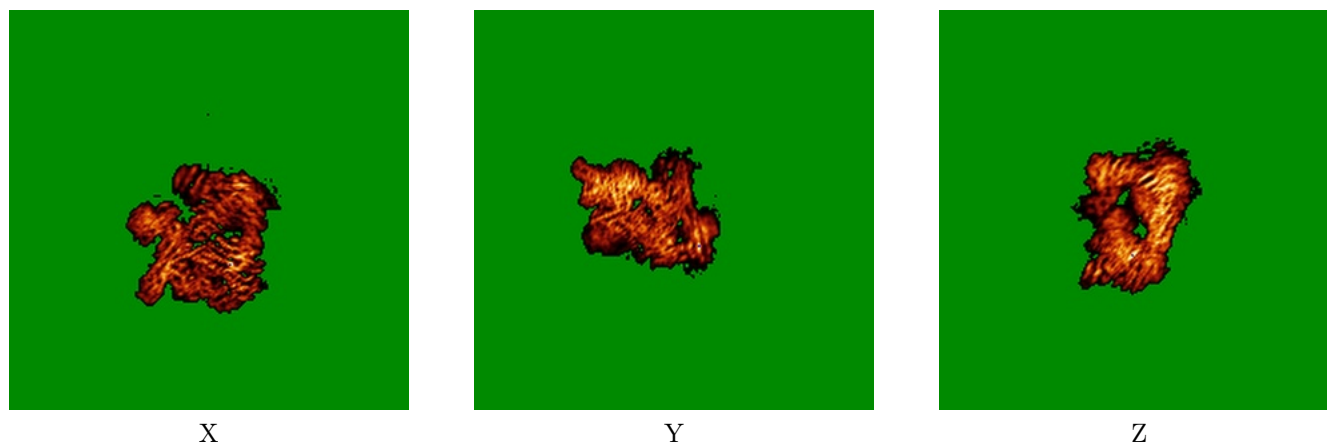


Z Index: 78

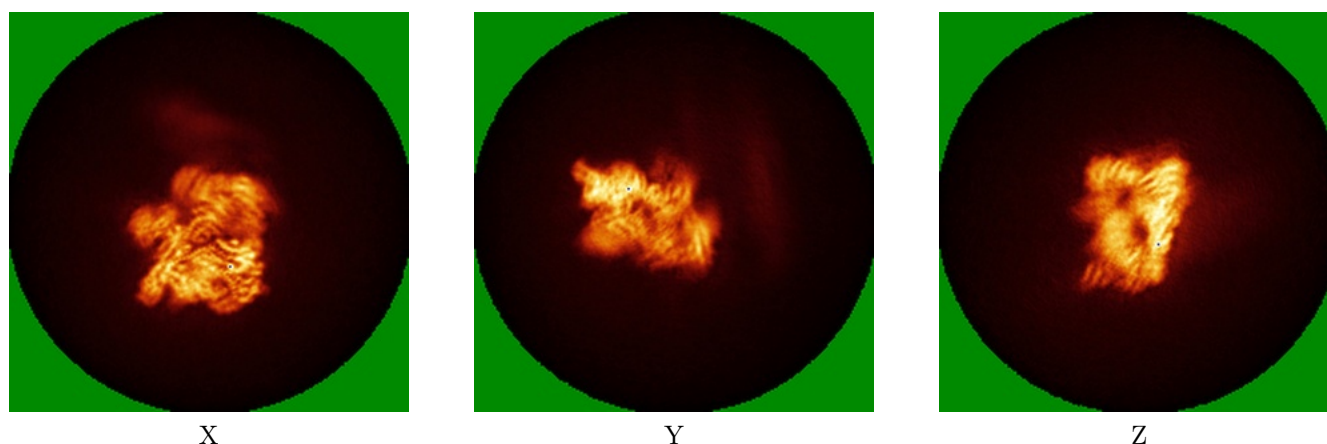
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

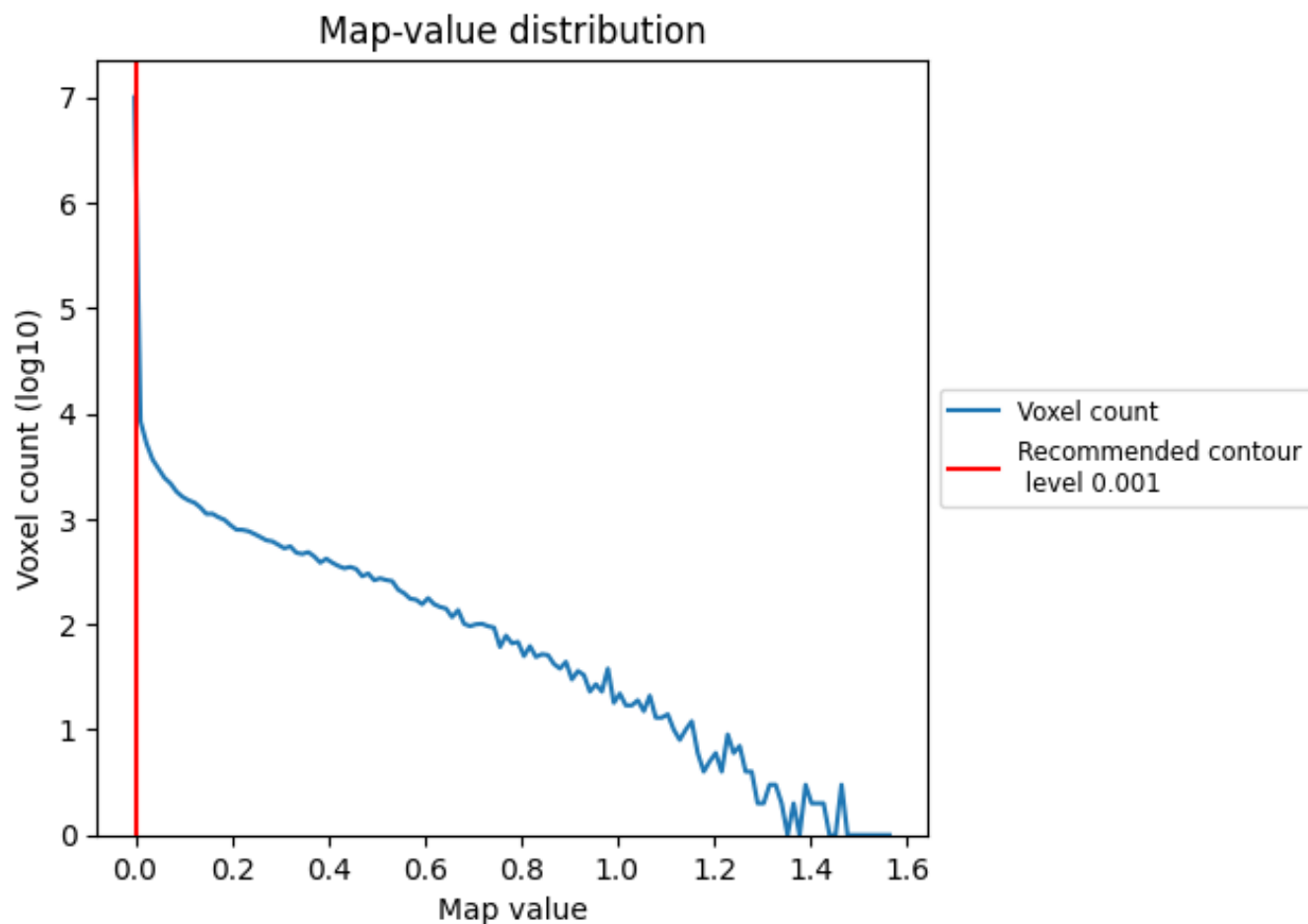
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

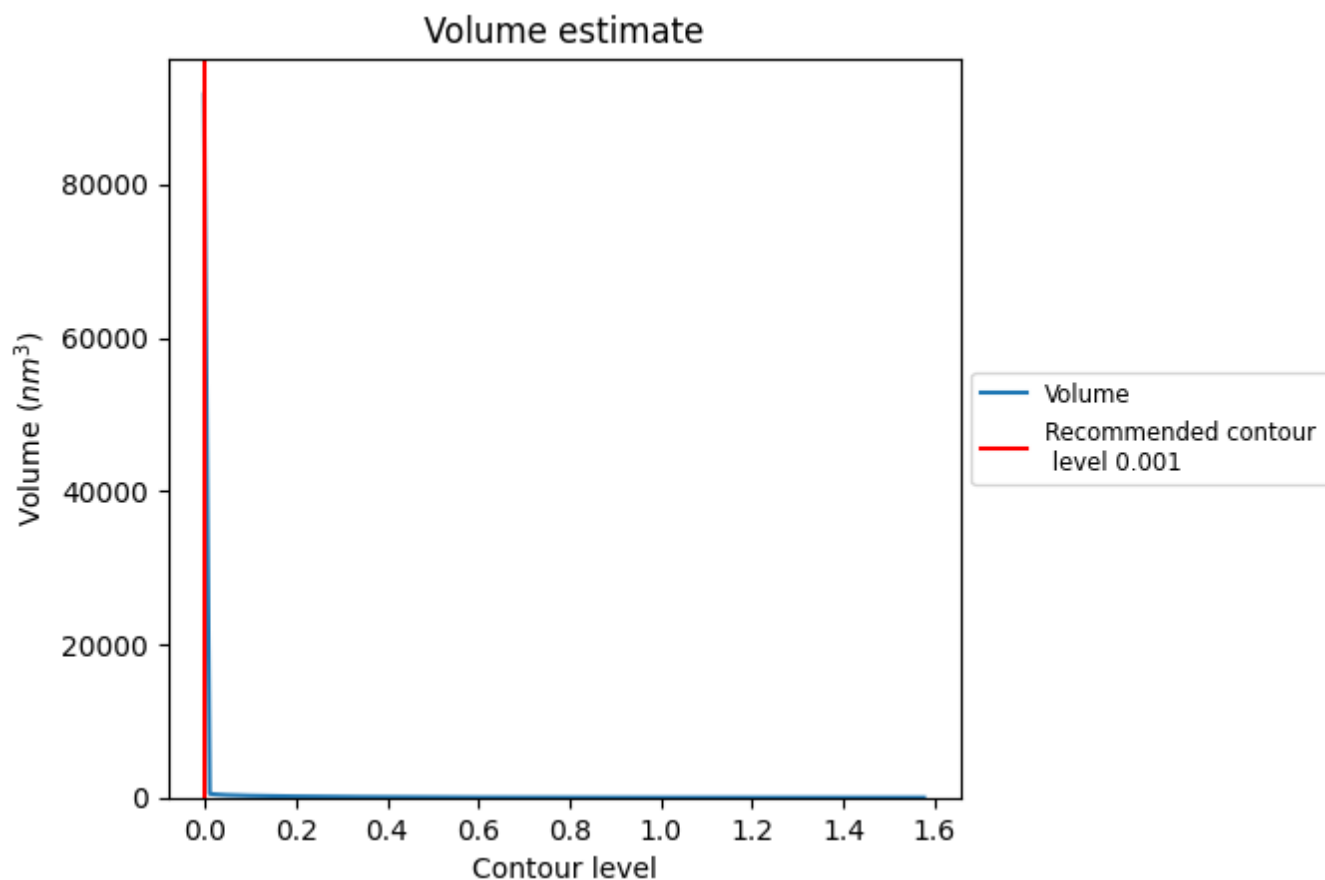
This section contains the results of statistical analysis of the map.

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.

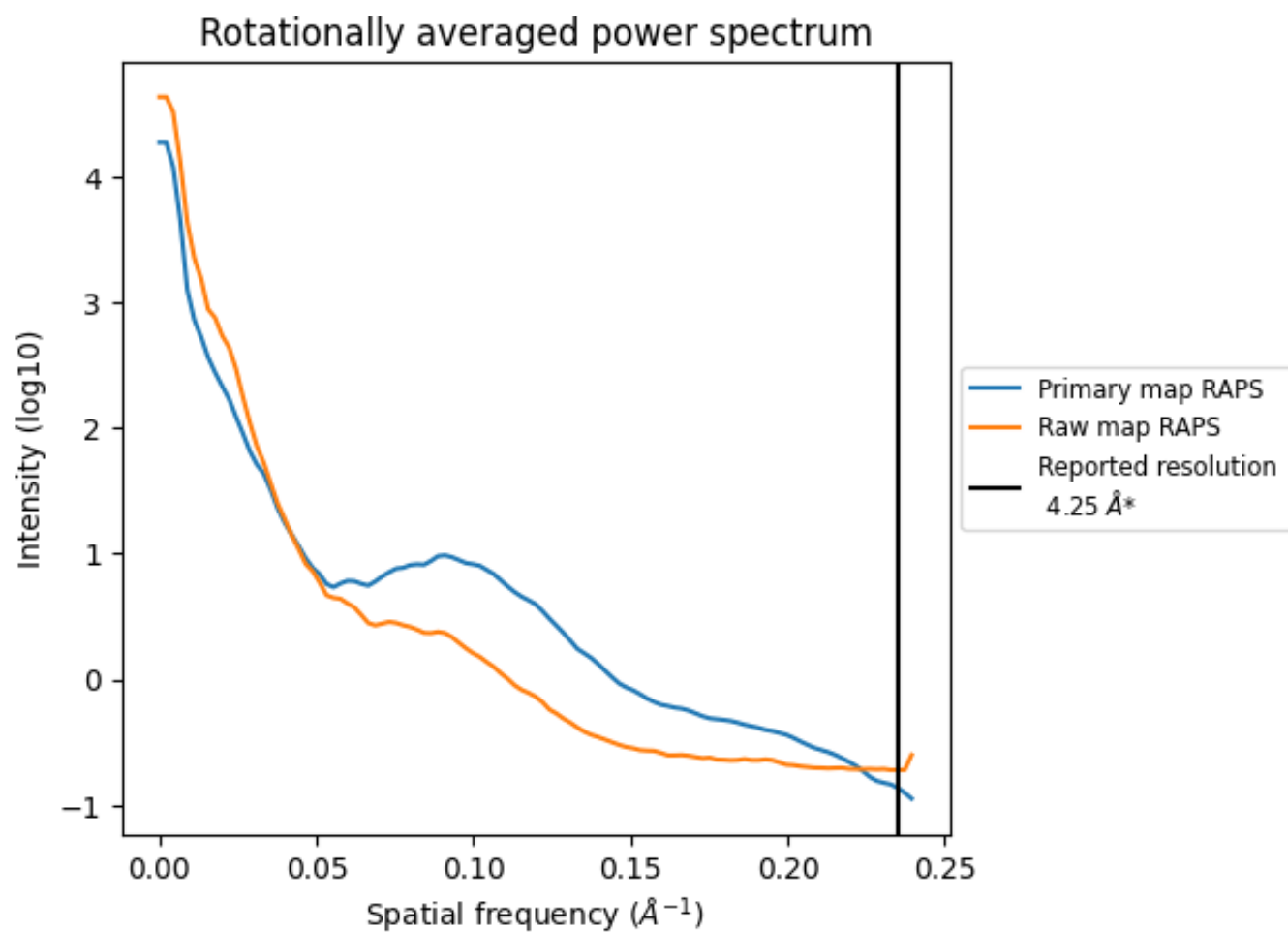
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 72988 nm^3 ; this corresponds to an approximate mass of 65932 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 ⓘ

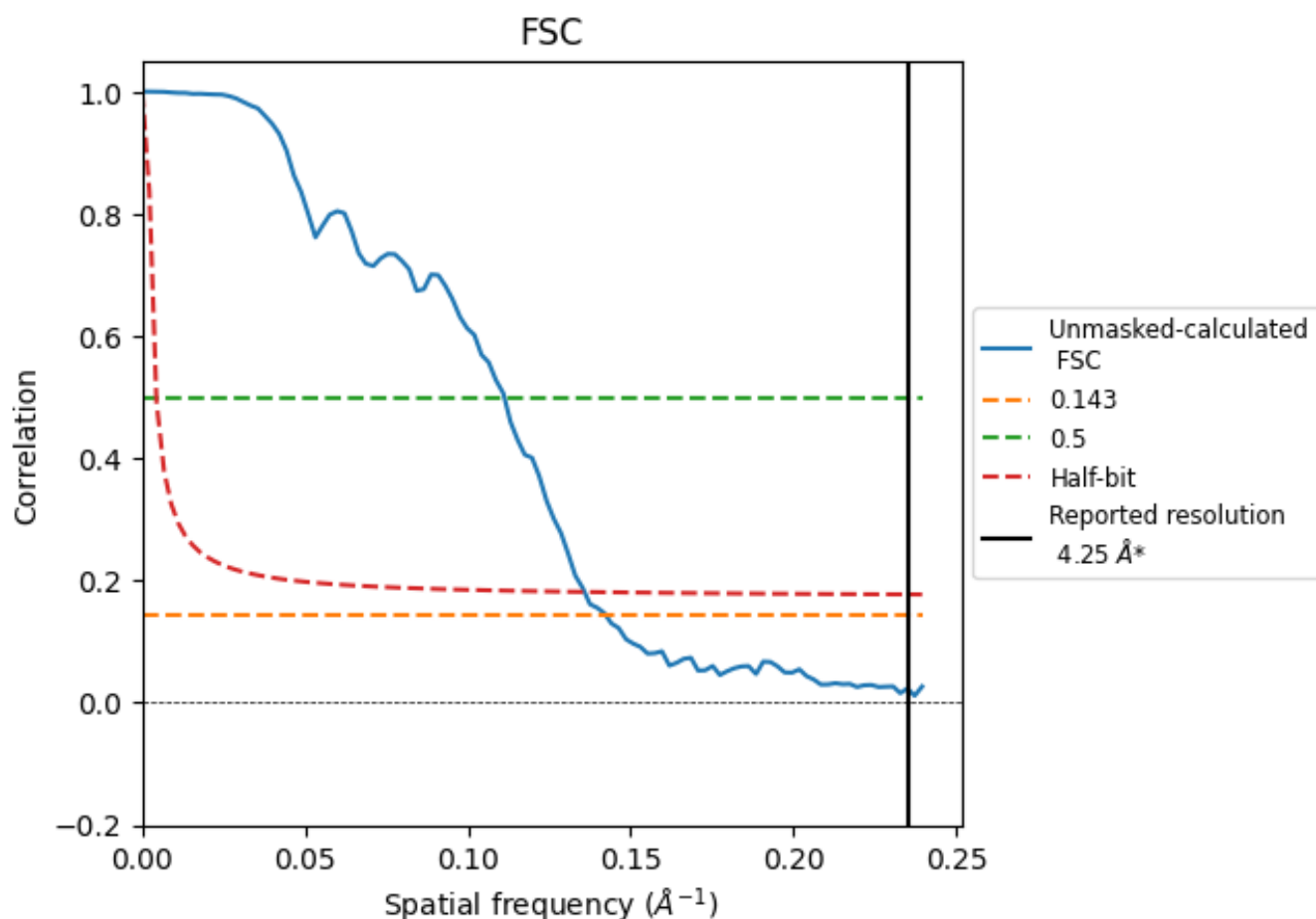


*Reported resolution corresponds to spatial frequency of 0.235 Å⁻¹

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 $0.235 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

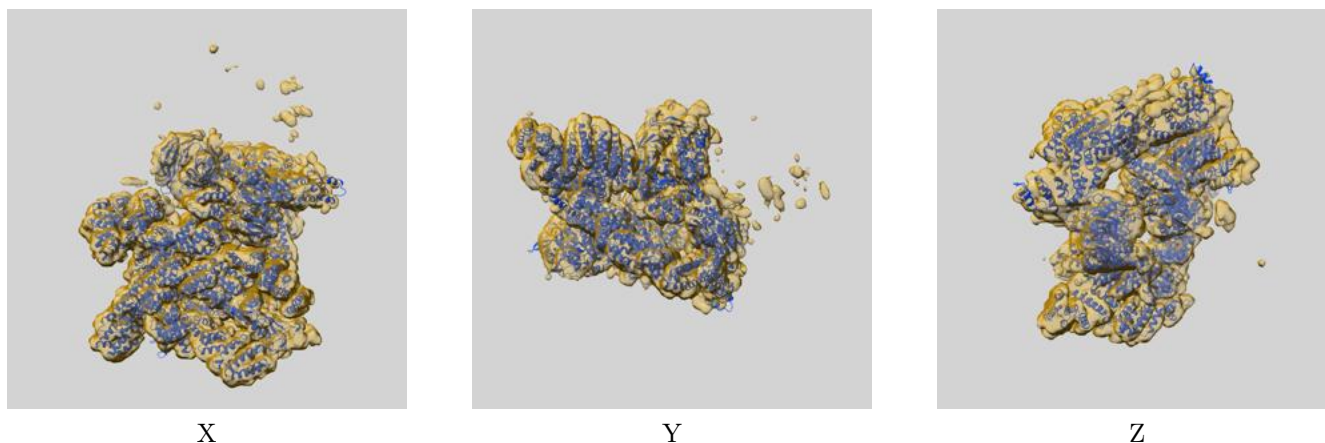
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.25	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.02	8.99	7.36

*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 7.02 differs from the reported value 4.25 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34455 and PDB model 8H38. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



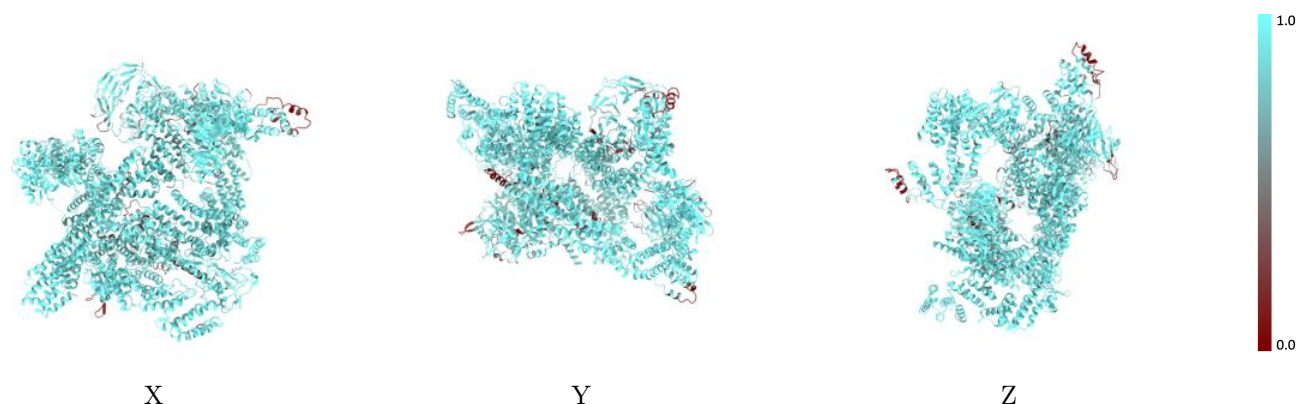
The images above show the 3D surface view of the map at the recommended contour level 0.001 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



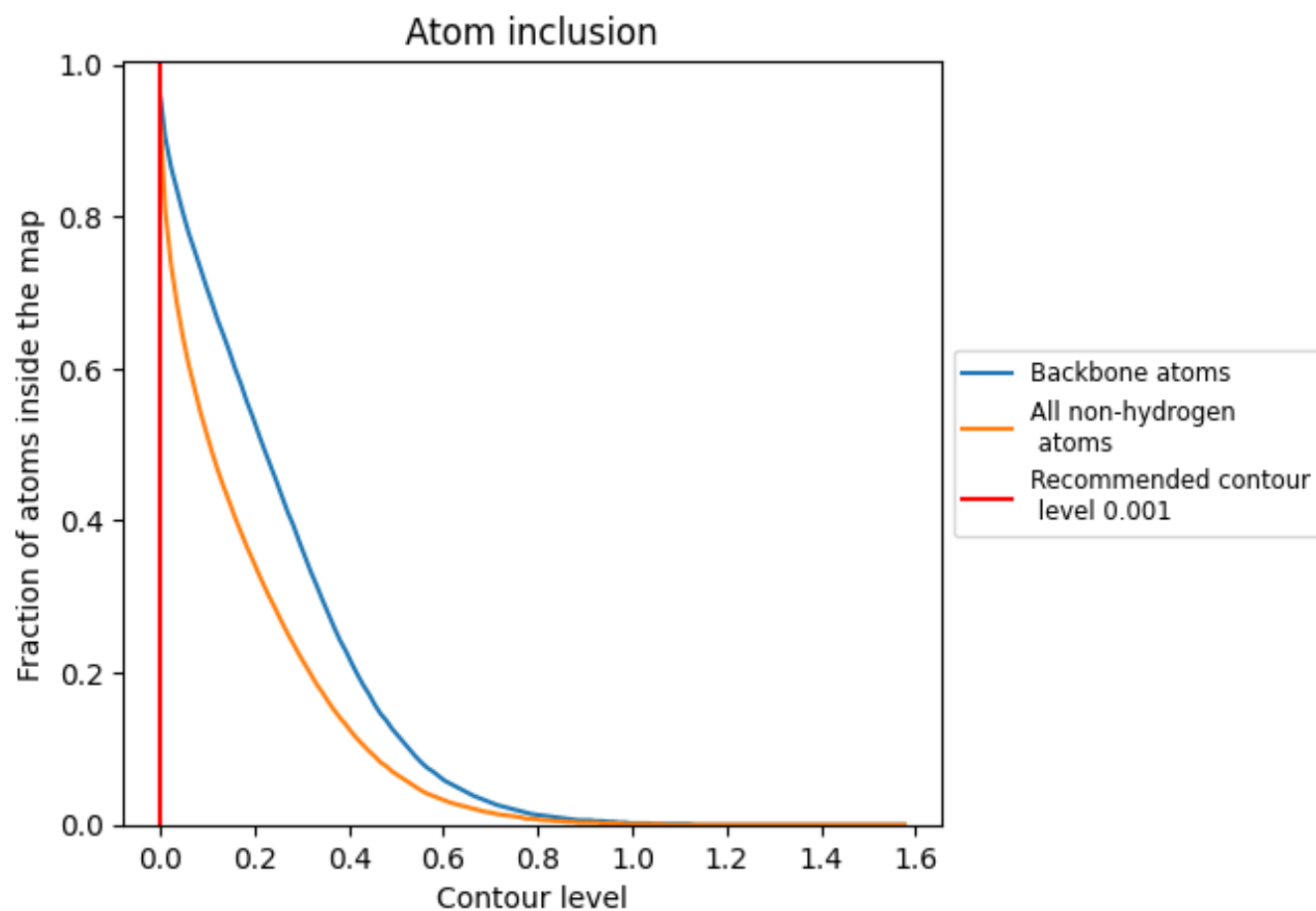
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 96% of all backbone atoms, 92% 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	 0.9200	 0.0780
A	 0.9670	 0.1080
B	 0.9650	 0.1280
C	 0.9640	 0.1260
D	 0.9650	 0.1220
E	 0.8340	 0.0210
F	 0.8830	 0.0690
G	 0.9730	 0.1350
H	 0.9760	 0.1340
I	 0.8320	 0.0110
L	 0.9320	 0.0790
M	 0.9010	 0.0250
N	 0.7900	 -0.0380
R	 0.9460	 0.0970

