



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:45 PM UTC

PDB ID : 7KZN / pdb_00007kzn
EMDB ID : EMD-23083
Title : Outer dynein arm core subcomplex from *C. reinhardtii*
Authors : Walton, T.; Wu, H.; Brown, A.B.
Deposited on : 2020-12-10
Resolution : 4.00 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

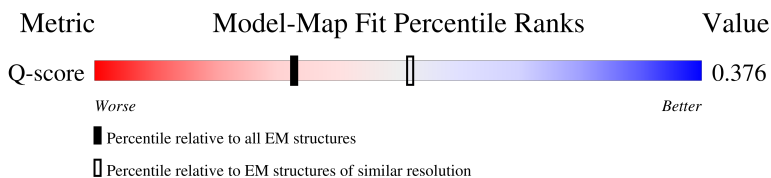
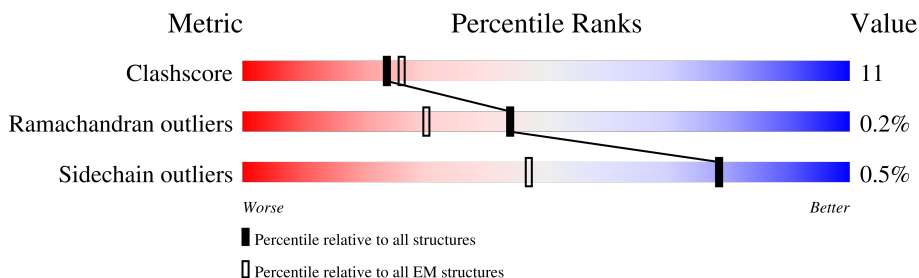
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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.



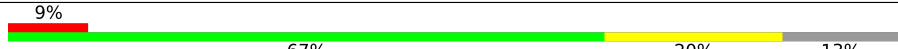
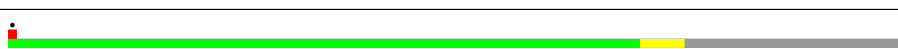
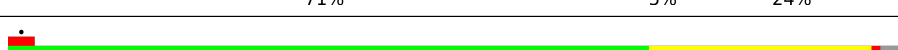
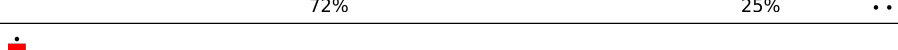
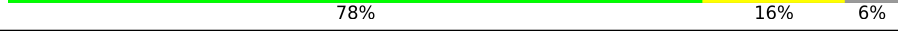
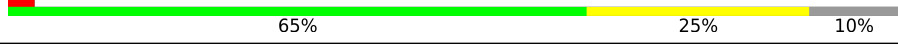
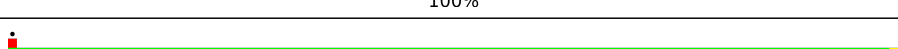
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	4503	 6% 7% 93%
2	B	4568	 11% 85%
3	C	4485	 17% 5% 78%
4	D	683	 47% 19% 33%

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Mol	Chain	Length	Quality of chain
5	E	567	
6	F	136	
7	G	159	
8	H	120	
9	I	105	
10	J	100	
11	K	91	
11	L	91	
11	M	91	
11	N	91	
12	O	117	
13	P	103	
14	X	121	
15	Y	168	
16	Z	184	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 31205 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 Heavy chain alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	315	Total	C	N	O	0	0
			1544	914	315	315		

- Molecule 2 is a protein called Flagellar outer dynein arm heavy chain beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	683	Total	C	N	O	S	0	0
			5028	3180	878	946	24		

- Molecule 3 is a protein called Dynein gamma chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	965	Total	C	N	O	S	0	0
			7293	4574	1296	1386	37		

- Molecule 4 is a protein called Dynein, 78 kDa intermediate chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	456	Total	C	N	O	S	0	0
			3609	2297	610	678	24		

- Molecule 5 is a protein called Dynein, 70 kDa intermediate chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	474	Total	C	N	O	S	0	0
			3697	2332	623	725	17		

- Molecule 6 is a protein called Flagellar outer dynein arm light chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	100	Total	C	N	O	0	0
			495	295	100	100		

- Molecule 7 is a protein called Dynein 18 kDa light chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	138	Total	C	N	O	S	0	0
			1089	677	183	220	9		

- Molecule 8 is a protein called Dynein 11 kDa light chain, flagellar outer arm.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	91	Total	C	N	O	0	0
			451	269	91	91		

- Molecule 9 is a protein called Dynein light chain roadblock LC7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	103	Total	C	N	O	S	0	0
			827	525	148	153	1		

- Molecule 10 is a protein called Dynein light chain roadblock LC7b.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	94	Total	C	N	O	S	0	0
			741	466	133	140	2		

- Molecule 11 is a protein called Dynein 8 kDa light chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	82	Total	C	N	O	S	0	0
			671	433	112	122	4		
11	L	82	Total	C	N	O	S	0	0
			671	433	112	122	4		
11	M	82	Total	C	N	O	S	0	0
			671	433	112	122	4		
11	N	82	Total	C	N	O		0	0
			407	243	82	82			

- Molecule 12 is a protein called Dynein light chain 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	O	97	Total	C	N	O	0	0
			481	286	97	98		

- Molecule 13 is a protein called Dynein light chain 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	98	Total	C	N	O	S	0	0
			805	523	128	146	8		

- Molecule 14 is a protein called DC1.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	X	121	Total	C	N	O	0	0
			605	363	121	121		

- Molecule 15 is a protein called DC2.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	Y	168	Total	C	N	O	0	0
			840	504	168	168		

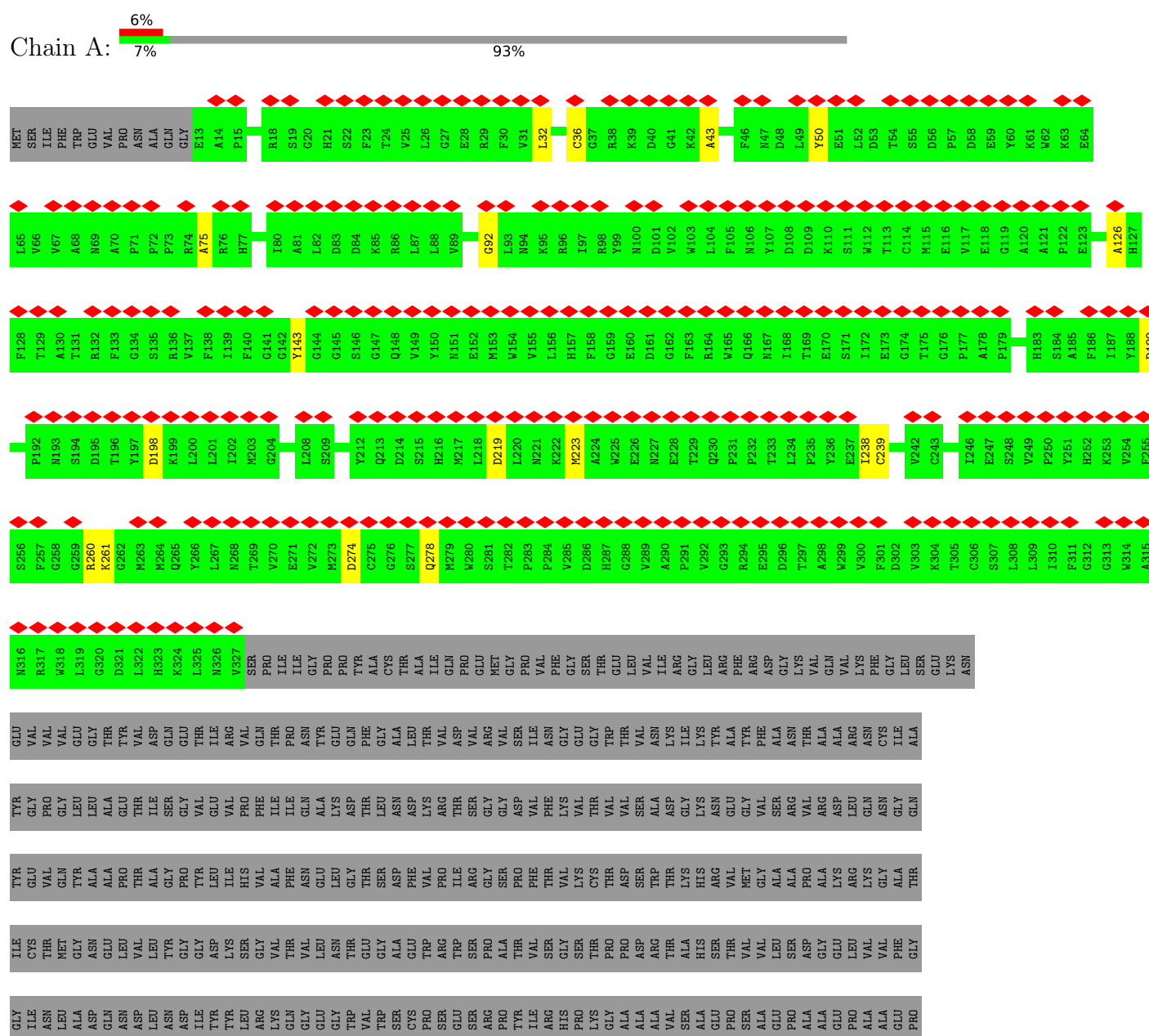
- Molecule 16 is a protein called Outer dynein arm-docking complex protein DC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Z	157	Total	C	N	O	S	0	0
			1280	798	221	252	9		

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: Heavy chain alpha







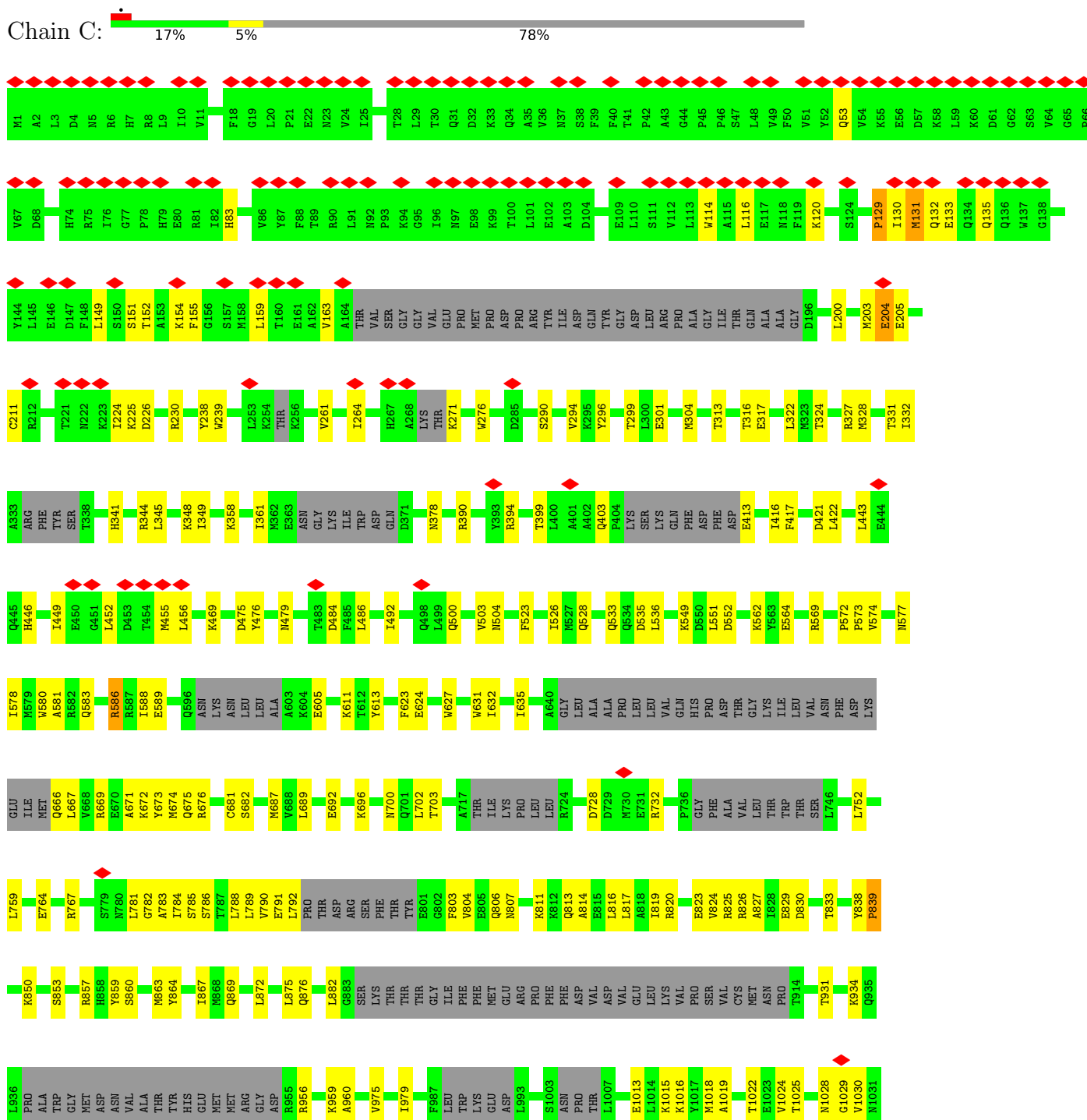








- Molecule 3: Dynein gamma chain, flagellar outer arm



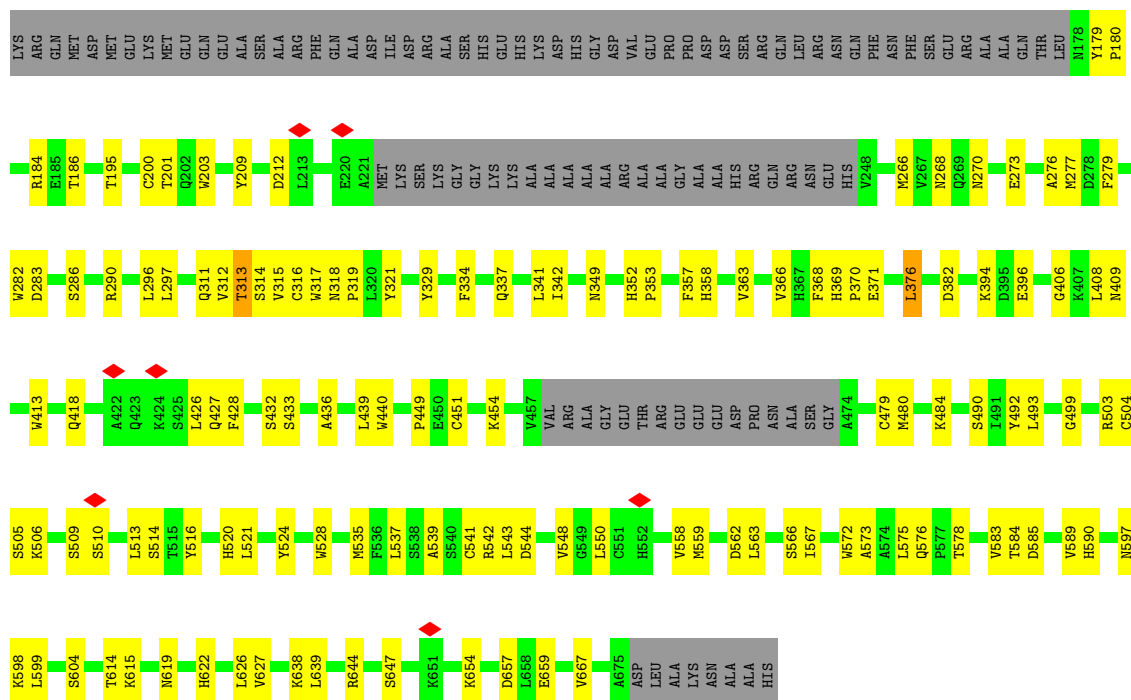




- Molecule 4: Dynein, 78 kDa intermediate chain, flagellar outer arm

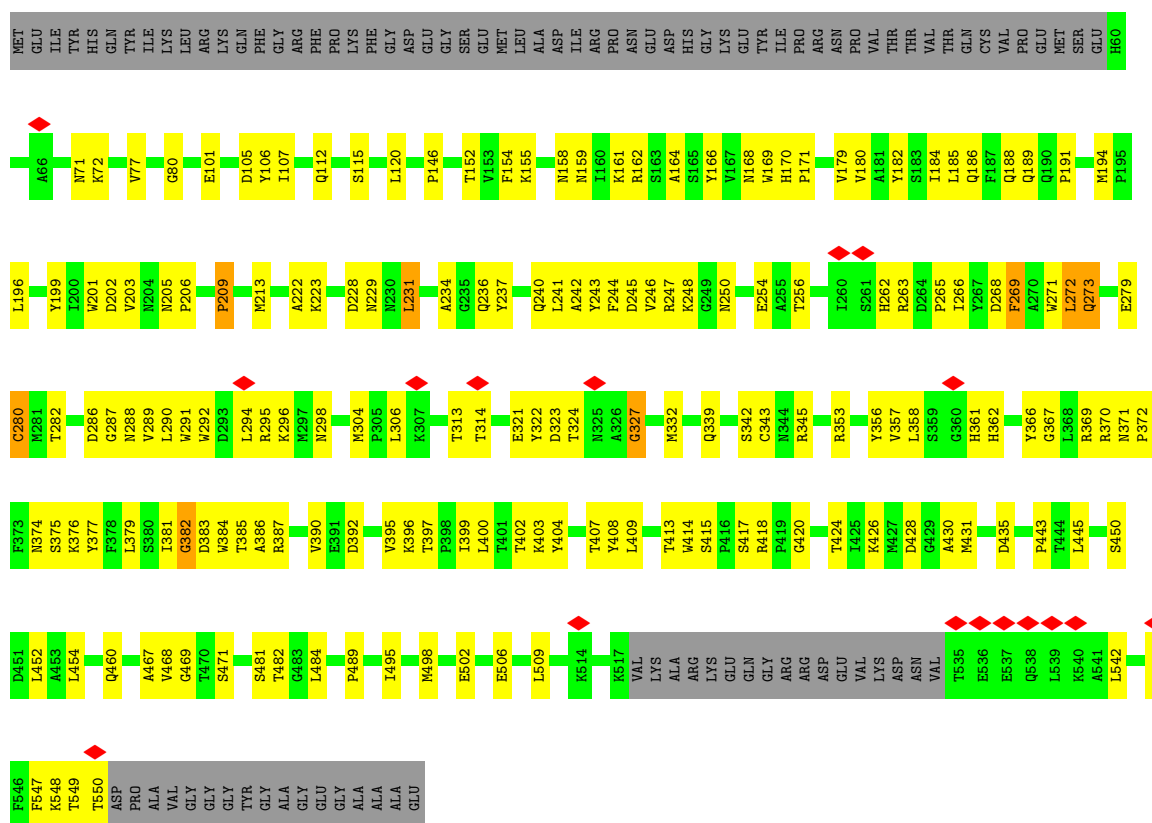
Chain D:

[illegible]

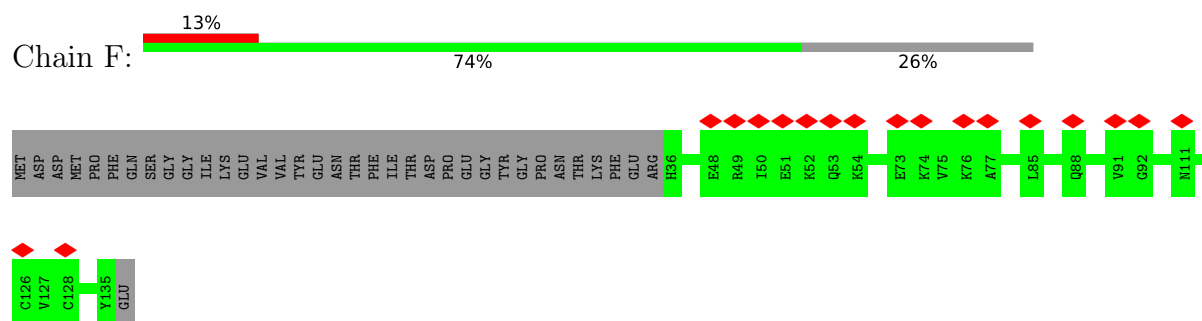


- Molecule 5: Dynein, 70 kDa intermediate chain, flagellar outer arm

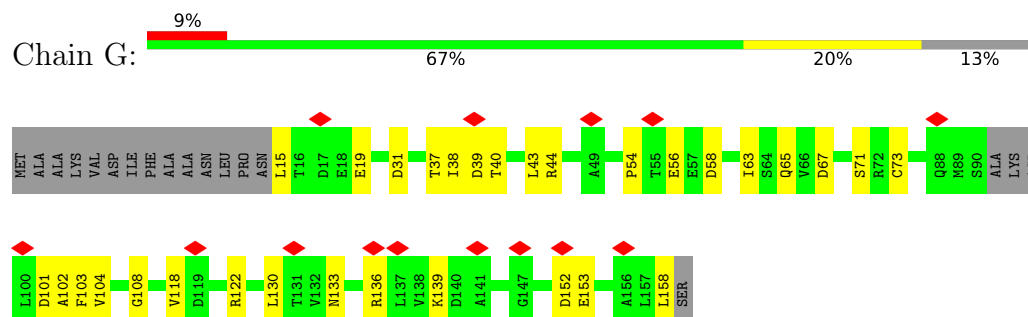
Chain E: 53% 29% 16%



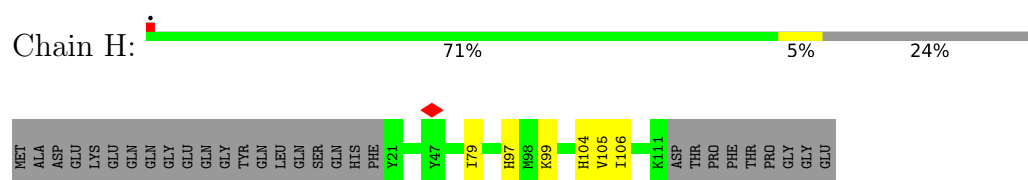
- Molecule 6: Flagellar outer dynein arm light chain 2



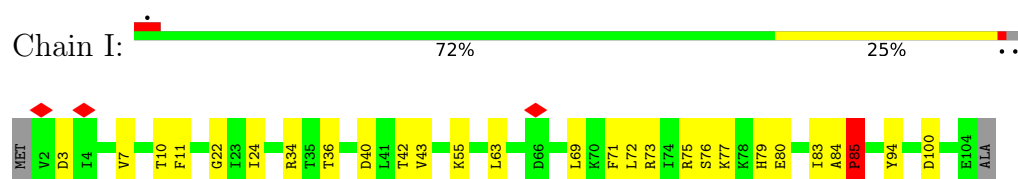
- Molecule 7: Dynein 18 kDa light chain, flagellar outer arm



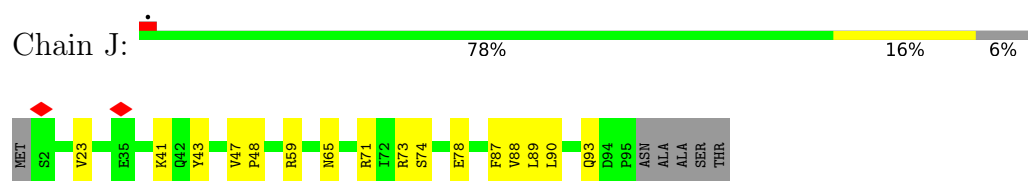
- Molecule 8: Dynein 11 kDa light chain, flagellar outer arm



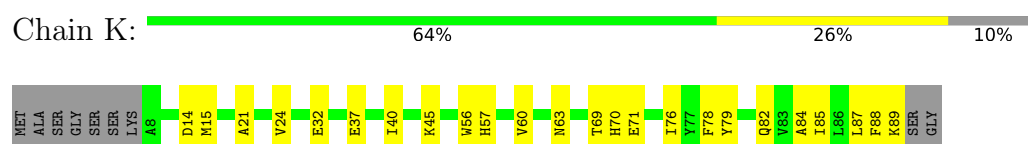
- Molecule 9: Dynein light chain roadblock LC7a



- Molecule 10: Dynein light chain roadblock LC7b

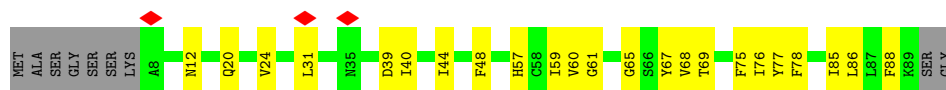


- Molecule 11: Dynein 8 kDa light chain, flagellar outer arm



- Molecule 11: Dynein 8 kDa light chain, flagellar outer arm

Chain L: 



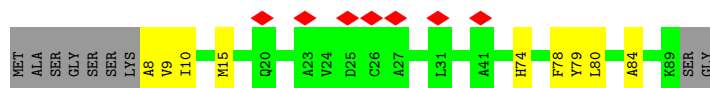
- Molecule 11: Dynein 8 kDa light chain, flagellar outer arm

Chain M: 



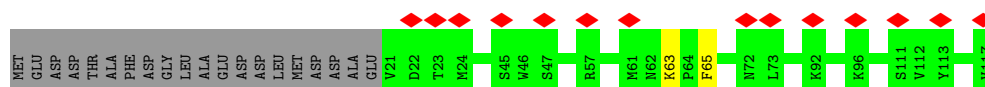
- Molecule 11: Dynein 8 kDa light chain, flagellar outer arm

Chain N: 



- Molecule 12: Dynein light chain 9

Chain O: 



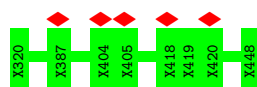
- Molecule 13: Dynein light chain 10

Chain P: 

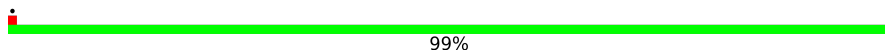


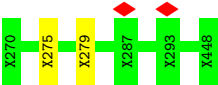
- Molecule 14: DC1

Chain X: 

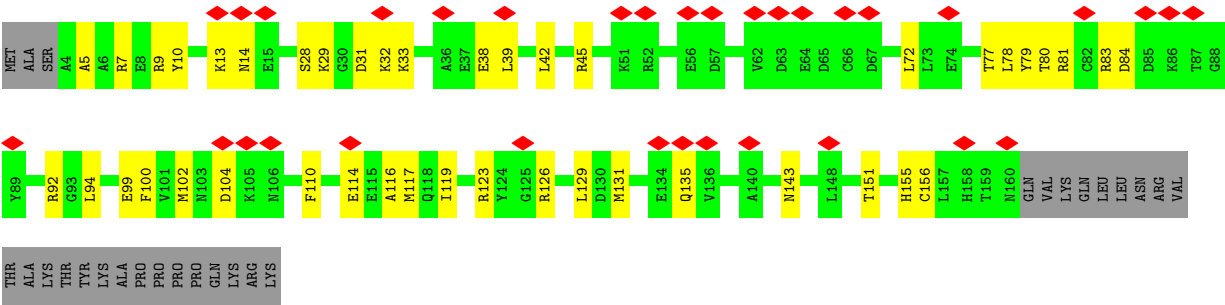


- Molecule 15: DC2

Chain Y: 



• Molecule 16: Outer dynein arm-docking complex protein DC3



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=0°, rise=82 Å, axial sym=C1	Depositor
Number of segments used	485694	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	61.48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.150	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0125	Depositor
Map size (Å)	353.6, 353.6, 353.6	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	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	0.13	0/1543	0.40	0/2140
2	B	0.39	0/5090	0.75	3/6881 (0.0%)
3	C	0.41	0/7381	0.75	5/9958 (0.1%)
4	D	0.67	1/3699 (0.0%)	1.02	7/5023 (0.1%)
5	E	0.64	0/3784	1.01	7/5152 (0.1%)
6	F	0.18	0/494	0.60	0/687
7	G	0.27	0/1098	0.60	0/1471
8	H	0.20	0/450	0.42	0/626
9	I	0.50	0/840	0.89	1/1133 (0.1%)
10	J	0.52	0/752	0.76	0/1019
11	K	0.41	0/687	0.74	0/926
11	L	0.44	0/687	0.80	0/926
11	M	0.37	0/687	0.81	0/926
11	N	0.16	0/406	0.42	0/565
12	O	0.21	0/480	0.66	0/666
13	P	0.49	0/823	0.95	0/1108
16	Z	0.23	0/1299	0.55	0/1745
All	All	0.46	1/30200 (0.0%)	0.80	23/40952 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	314	SER	CA-CB	-5.44	1.44	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	129	PRO	CA-N-CD	-8.06	100.72	112.00
3	C	455	MET	CB-CG-SD	-6.99	91.72	112.70
3	C	586	ARG	CA-CB-CG	6.88	127.85	114.10
2	B	603	ARG	CB-CG-CD	6.84	127.04	111.30
4	D	184	ARG	N-CA-CB	6.46	122.09	111.62
9	I	85	PRO	N-CA-C	6.20	125.25	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	313	THR	CB-CA-C	6.12	120.64	109.99
3	C	586	ARG	CB-CA-C	5.80	121.50	109.95
5	E	327	GLY	N-CA-C	5.72	124.01	112.34
5	E	382	GLY	CA-C-N	-5.46	112.25	122.73
5	E	382	GLY	C-N-CA	-5.46	112.25	122.73
4	D	479	CYS	CA-C-N	-5.26	112.56	121.18
4	D	479	CYS	C-N-CA	-5.26	112.56	121.18
2	B	628	TRP	N-CA-C	-5.24	105.57	111.28
4	D	426	LEU	N-CA-C	-5.15	101.36	109.50
3	C	131	MET	N-CA-CB	5.12	117.65	110.12
4	D	311	GLN	N-CA-CB	-5.11	102.09	110.68
5	E	280	CYS	N-CA-C	5.07	116.00	108.60
4	D	376	LEU	CB-CG-CD1	5.06	125.89	110.70
5	E	372	PRO	CA-C-N	5.01	131.11	121.54
5	E	372	PRO	C-N-CA	5.01	131.11	121.54
2	B	589	TRP	CA-CB-CG	5.01	123.11	113.60
5	E	272	LEU	N-CA-C	-5.01	102.66	110.42

There are no chirality outliers.

There are no planarity outliers.

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	1544	0	701	10	0
2	B	5028	0	4588	124	0
3	C	7293	0	6812	149	0
4	D	3609	0	3534	94	0
5	E	3697	0	3534	136	0
6	F	495	0	221	0	0
7	G	1089	0	1072	22	0
8	H	451	0	204	3	0
9	I	827	0	841	21	0
10	J	741	0	750	14	0
11	K	671	0	654	20	0
11	L	671	0	654	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	M	671	0	654	24	0
11	N	407	0	192	5	0
12	O	481	0	230	1	0
13	P	805	0	801	20	0
14	X	605	0	129	0	0
15	Y	840	0	181	1	0
16	Z	1280	0	1239	25	0
All	All	31205	0	26991	633	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 (633) 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)
8:H:79:ILE:O	8:H:105:VAL:HA	1.63	0.99
2:B:382:MET:O	2:B:386:VAL:HG23	1.69	0.92
2:B:503:GLU:HG2	4:D:510:SER:HB2	1.56	0.88
4:D:200:CYS:HG	13:P:89:TYR:HH	1.23	0.84
2:B:627:LEU:HG	2:B:631:MET:HE2	1.61	0.82
11:M:61:GLY:O	11:M:84:ALA:HB3	1.80	0.80
4:D:200:CYS:SG	13:P:89:TYR:OH	2.41	0.79
4:D:318:ASN:HD21	4:D:321:TYR:HB2	1.49	0.78
4:D:520:HIS:H	4:D:542:ARG:HD2	1.49	0.76
2:B:743:GLN:HE22	5:E:263:ARG:HD2	1.51	0.74
5:E:168:ASN:ND2	5:E:222:ALA:O	2.21	0.73
3:C:819:ILE:HG21	5:E:205:ASN:HB3	1.71	0.73
3:C:813:GLN:O	3:C:816:LEU:HB2	1.89	0.72
5:E:286:ASP:OD2	5:E:288:ASN:ND2	2.23	0.72
5:E:158:ASN:ND2	5:E:199:TYR:OH	2.23	0.71
5:E:266:ILE:HG22	5:E:268:ASP:H	1.55	0.71
4:D:319:PRO:HG2	4:D:370:PRO:HA	1.72	0.70
11:K:15:MET:HE3	11:K:76:ILE:HD11	1.72	0.70
3:C:666:GLN:HG2	3:C:667:LEU:HD23	1.74	0.70
5:E:101:GLU:OE1	9:I:34:ARG:NH2	2.24	0.70
5:E:162:ARG:HD3	5:E:196:LEU:HD22	1.74	0.70
3:C:569:ARG:NH1	4:D:614:THR:OG1	2.24	0.69
16:Z:99:GLU:HA	16:Z:102:MET:HE2	1.73	0.69
4:D:282:TRP:O	4:D:638:LYS:NZ	2.23	0.69
4:D:436:ALA:HB3	4:D:454:LYS:HA	1.75	0.69
4:D:503:ARG:NH1	4:D:514:SER:OG	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:596:ARG:NE	5:E:404:TYR:OH	2.24	0.69
13:P:62:LYS:HG3	13:P:63:LYS:HD3	1.75	0.69
5:E:304:MET:SD	5:E:353:ARG:NH2	2.65	0.68
13:P:74:LYS:HE3	13:P:95:ARG:HD3	1.75	0.67
5:E:414:TRP:CD1	5:E:420:GLY:HA2	2.28	0.67
16:Z:151:THR:O	16:Z:155:HIS:ND1	2.24	0.67
2:B:590:VAL:HG11	2:B:635:ARG:HB3	1.76	0.67
2:B:619:GLU:HA	2:B:622:ARG:HG2	1.77	0.67
4:D:286:SER:O	4:D:290:ARG:NH1	2.28	0.67
4:D:598:LYS:O	4:D:598:LYS:NZ	2.28	0.66
3:C:784:ILE:HG12	3:C:820:ARG:HD3	1.77	0.66
4:D:349:ASN:ND2	4:D:352:HIS:O	2.29	0.66
5:E:375:SER:OG	5:E:376:LYS:N	2.27	0.66
4:D:195:THR:HG22	13:P:81:THR:HG22	1.78	0.66
2:B:349:GLN:NE2	2:B:353:ASN:OD1	2.29	0.66
5:E:332:MET:HG3	5:E:342:SER:HB2	1.76	0.66
7:G:15:LEU:N	7:G:19:GLU:OE2	2.29	0.66
3:C:696:LYS:O	3:C:700:ASN:ND2	2.28	0.66
11:L:68:VAL:HG23	11:M:57:HIS:HB3	1.78	0.66
5:E:454:LEU:HB3	5:E:468:VAL:HG11	1.78	0.65
9:I:84:ALA:O	9:I:94:TYR:HA	1.96	0.65
5:E:454:LEU:HD13	5:E:468:VAL:HG11	1.77	0.65
5:E:399:ILE:HG12	5:E:400:LEU:HD12	1.79	0.65
9:I:72:LEU:HB3	9:I:83:ILE:HB	1.78	0.65
4:D:418:GLN:HB2	4:D:427:GLN:HB2	1.78	0.65
2:B:392:ASN:HA	2:B:395:PHE:HD2	1.60	0.65
5:E:321:GLU:HG2	5:E:370:ARG:H	1.61	0.65
3:C:816:LEU:HD23	5:E:205:ASN:HD21	1.62	0.65
4:D:266:MET:HE3	10:J:71:ARG:HE	1.62	0.64
5:E:452:LEU:HB3	5:E:471:SER:HB3	1.80	0.64
2:B:418:PHE:O	2:B:422:ASP:HB2	1.98	0.64
7:G:99:THR:O	7:G:103:PHE:CB	2.45	0.64
11:K:60:VAL:HG22	11:K:85:ILE:HG12	1.79	0.64
4:D:583:VAL:HG22	4:D:589:VAL:HG22	1.80	0.63
7:G:44:ARG:NH1	7:G:54:PRO:O	2.30	0.63
3:C:586:ARG:HH21	4:D:520:HIS:CG	2.15	0.63
11:K:45:LYS:HG3	11:K:56:TRP:HB2	1.81	0.63
11:N:10:ILE:HA	11:N:78:PHE:HA	1.80	0.63
4:D:283:ASP:OD1	4:D:644:ARG:NH1	2.31	0.63
7:G:99:THR:O	7:G:103:PHE:HB2	1.97	0.63
7:G:136:ARG:HA	7:G:139:LYS:HE2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:76:SER:HB3	9:I:79:HIS:H	1.63	0.63
11:K:78:PHE:HB2	11:K:85:ILE:HB	1.81	0.63
16:Z:114:GLU:HA	16:Z:117:MET:HE2	1.80	0.63
3:C:1029:GLY:O	7:G:65:GLN:NE2	2.32	0.62
3:C:573:PRO:O	3:C:577:ASN:ND2	2.32	0.62
4:D:203:TRP:HB2	10:J:59:ARG:HE	1.63	0.62
2:B:506:ARG:HH22	2:B:540:VAL:HG12	1.64	0.62
2:B:743:GLN:OE1	5:E:263:ARG:NH2	2.33	0.62
4:D:212:ASP:CG	13:P:20:LEU:HG	2.25	0.62
3:C:469:LYS:NZ	3:C:484:ASP:OD2	2.33	0.62
3:C:476:TYR:O	3:C:479:ASN:ND2	2.33	0.62
4:D:451:CYS:SG	4:D:454:LYS:NZ	2.73	0.62
11:L:67:TYR:HD2	11:M:45:LYS:HD3	1.65	0.62
3:C:226:ASP:H	3:C:230:ARG:HH12	1.48	0.62
3:C:417:PHE:O	3:C:421:ASP:HB2	1.99	0.62
4:D:408:LEU:O	4:D:409:ASN:ND2	2.32	0.62
1:A:274:ASP:O	1:A:278:GLN:N	2.33	0.61
2:B:798:ILE:HG22	2:B:802:MET:HE1	1.83	0.61
2:B:147:GLU:OE2	3:C:154:LYS:NZ	2.34	0.61
2:B:627:LEU:HG	2:B:631:MET:CE	2.31	0.60
3:C:669:ARG:NH2	3:C:692:GLU:OE2	2.34	0.60
5:E:418:ARG:HD3	5:E:484:LEU:HD13	1.83	0.60
3:C:838:TYR:HD1	3:C:839:PRO:HD2	1.65	0.60
2:B:321:PHE:HB3	2:B:324:ILE:HD12	1.84	0.60
2:B:526:PHE:HB2	2:B:603:ARG:HH21	1.67	0.60
2:B:235:THR:O	2:B:239:PHE:HB2	2.01	0.60
16:Z:42:LEU:HA	16:Z:45:ARG:HD2	1.83	0.60
2:B:322:LYS:HA	2:B:325:MET:HE3	1.84	0.60
3:C:789:LEU:H	3:C:875:LEU:HD21	1.65	0.60
5:E:481:SER:OG	5:E:482:THR:N	2.33	0.60
5:E:262:HIS:HB2	5:E:290:LEU:HD13	1.82	0.59
2:B:155:PHE:HZ	3:C:152:THR:HG22	1.68	0.59
4:D:654:LYS:HG3	4:D:657:ASP:HB2	1.83	0.59
5:E:185:LEU:O	5:E:189:GLN:NE2	2.36	0.59
3:C:574:VAL:HG11	3:C:631:TRP:HB2	1.84	0.59
11:M:55:THR:OG1	11:M:89:LYS:NZ	2.35	0.59
5:E:385:THR:OG1	5:E:387:ARG:NE	2.35	0.59
3:C:129:PRO:HD2	3:C:130:ILE:H	1.67	0.59
11:L:57:HIS:HB2	11:L:88:PHE:CE1	2.38	0.59
16:Z:10:TYR:HA	16:Z:13:LYS:HG2	1.83	0.59
2:B:591:ARG:HH21	2:B:693:LEU:HD21	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:823:GLU:O	3:C:827:ALA:N	2.36	0.58
4:D:575:LEU:HD11	4:D:644:ARG:HB2	1.85	0.58
8:H:99:LYS:HA	8:H:104:HIS:HA	1.84	0.58
10:J:47:VAL:HG11	10:J:90:LEU:HD11	1.85	0.58
5:E:164:ALA:HB3	5:E:469:GLY:HA3	1.85	0.58
16:Z:79:TYR:O	16:Z:83:ARG:NH2	2.36	0.58
3:C:572:PRO:HB2	3:C:674:MET:HE1	1.85	0.58
5:E:379:LEU:HB2	5:E:414:TRP:CZ3	2.39	0.58
7:G:71:SER:OG	7:G:73:CYS:O	2.21	0.58
11:L:61:GLY:HA3	11:M:64:PHE:HA	1.86	0.58
2:B:424:PHE:HA	2:B:427:ARG:HD3	1.85	0.58
3:C:781:LEU:HD21	3:C:824:VAL:HG21	1.84	0.58
4:D:342:ILE:HG23	4:D:357:PHE:HB2	1.85	0.58
4:D:639:LEU:O	4:D:644:ARG:NH2	2.37	0.58
5:E:418:ARG:HD3	5:E:484:LEU:HA	1.84	0.58
3:C:931:THR:HA	3:C:934:LYS:HZ3	1.68	0.58
3:C:116:LEU:HD12	3:C:163:VAL:HB	1.87	0.57
2:B:348:MET:HA	2:B:351:ILE:HD12	1.84	0.57
5:E:379:LEU:HB2	5:E:414:TRP:CH2	2.40	0.57
2:B:319:ASP:O	2:B:322:LYS:NZ	2.37	0.57
3:C:1030:VAL:HA	7:G:65:GLN:HE22	1.69	0.57
3:C:394:ARG:NH1	3:C:413:GLU:OE1	2.38	0.57
16:Z:131:MET:O	16:Z:155:HIS:NE2	2.37	0.57
2:B:324:ILE:O	2:B:327:THR:HB	2.04	0.57
2:B:729:SER:OG	2:B:730:ALA:N	2.37	0.57
4:D:201:THR:HG1	4:D:203:TRP:CD1	2.23	0.57
3:C:1041:HIS:O	3:C:1045:ASN:N	2.31	0.57
3:C:869:GLN:OE1	3:C:956:ARG:NH1	2.34	0.57
4:D:366:VAL:HB	4:D:376:LEU:HD11	1.85	0.57
3:C:120:LYS:HB3	3:C:159:LEU:HD21	1.86	0.56
2:B:251:HIS:NE2	2:B:285:GLU:OE1	2.38	0.56
3:C:341:HIS:O	3:C:345:LEU:HB2	2.06	0.56
4:D:503:ARG:HB3	4:D:514:SER:HB2	1.86	0.56
16:Z:92:ARG:NH2	16:Z:156:CYS:SG	2.76	0.56
2:B:526:PHE:HB2	2:B:603:ARG:NH2	2.20	0.56
3:C:131:MET:O	3:C:135:GLN:N	2.37	0.56
5:E:107:ILE:HG21	9:I:3:ASP:HB3	1.88	0.56
5:E:289:VAL:HB	5:E:306:LEU:HD13	1.87	0.56
2:B:624:TYR:O	2:B:628:TRP:HB2	2.04	0.56
4:D:619:ASN:ND2	4:D:622:HIS:O	2.39	0.56
5:E:243:TYR:HD2	5:E:254:GLU:HB2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:384:TRP:HB3	5:E:408:TYR:HA	1.88	0.56
3:C:676:ARG:HG3	3:C:689:LEU:HD21	1.87	0.56
2:B:147:GLU:OE2	2:B:151:ASN:ND2	2.38	0.55
2:B:768:LEU:O	2:B:772:LYS:N	2.38	0.55
7:G:44:ARG:NH1	7:G:56:GLU:OE2	2.27	0.55
3:C:225:LYS:HB2	3:C:344:ARG:HH22	1.71	0.55
3:C:230:ARG:HG3	3:C:348:LYS:HE3	1.88	0.55
5:E:168:ASN:OD1	5:E:179:VAL:HB	2.06	0.55
5:E:168:ASN:HD22	5:E:223:LYS:HA	1.72	0.55
5:E:180:VAL:HG21	5:E:201:TRP:HE1	1.71	0.55
3:C:784:ILE:HG23	3:C:817:LEU:HD22	1.87	0.55
3:C:358:LYS:NZ	3:C:475:ASP:OD1	2.40	0.55
3:C:792:LEU:HD21	3:C:882:LEU:HD13	1.88	0.55
5:E:120:LEU:HD11	9:I:73:ARG:HH11	1.71	0.55
5:E:72:LYS:HA	11:K:69:THR:HA	1.89	0.55
16:Z:28:SER:N	16:Z:38:GLU:OE1	2.37	0.55
2:B:649:THR:HG22	2:B:653:LYS:HE2	1.89	0.55
4:D:428:PHE:HB2	4:D:440:TRP:HB2	1.89	0.55
4:D:504:CYS:SG	4:D:505:SER:N	2.80	0.55
13:P:42:VAL:HG21	13:P:92:VAL:HG11	1.88	0.55
3:C:296:TYR:HE2	3:C:332:ILE:HG21	1.72	0.55
2:B:211:GLN:OE1	2:B:253:GLN:NE2	2.40	0.54
5:E:345:ARG:HA	5:E:353:ARG:HE	1.72	0.54
11:L:76:ILE:O	11:L:86:LEU:HA	2.08	0.54
5:E:374:ASN:HD21	5:E:489:PRO:HB2	1.71	0.54
5:E:450:SER:OG	5:E:452:LEU:N	2.40	0.54
3:C:132:GLN:O	3:C:135:GLN:HB2	2.07	0.54
5:E:112:GLN:O	5:E:115:SER:OG	2.22	0.54
5:E:361:HIS:HE1	5:E:383:ASP:H	1.55	0.54
7:G:37:THR:HB	7:G:73:CYS:HB3	1.89	0.54
5:E:213:MET:HE2	5:E:244:PHE:HB3	1.89	0.54
9:I:69:LEU:HA	10:J:74:SER:HA	1.89	0.54
5:E:366:TYR:H	5:E:382:GLY:HA3	1.71	0.54
9:I:85:PRO:HA	9:I:94:TYR:HA	1.90	0.54
2:B:443:ARG:NH2	2:B:533:GLU:O	2.41	0.53
2:B:647:ALA:O	2:B:650:SER:OG	2.27	0.53
11:M:76:ILE:HB	11:M:87:LEU:HB2	1.89	0.53
2:B:630:GLU:O	2:B:633:GLU:HB2	2.08	0.53
3:C:830:ASP:O	3:C:833:THR:OG1	2.22	0.53
4:D:329:TYR:HD2	4:D:341:LEU:HD23	1.72	0.53
3:C:500:GLN:NE2	3:C:504:ASN:OD1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:503:ARG:HD2	4:D:550:LEU:HD11	1.89	0.53
2:B:381:ARG:HH12	2:B:431:MET:HG3	1.74	0.53
4:D:369:HIS:HE1	4:D:371:GLU:HB3	1.73	0.53
2:B:134:PRO:HA	2:B:137:GLN:HG3	1.89	0.53
3:C:328:MET:O	3:C:331:THR:OG1	2.26	0.53
2:B:330:LEU:HA	2:B:333:LYS:HB2	1.89	0.53
2:B:682:ARG:HH11	5:E:188:GLN:HG2	1.73	0.53
9:I:76:SER:OG	10:J:65:ASN:OD1	2.27	0.53
13:P:13:LEU:HD21	13:P:95:ARG:HH11	1.72	0.53
13:P:21:VAL:HG12	13:P:90:ILE:HG22	1.89	0.53
2:B:685:ARG:HH12	5:E:265:PRO:HG3	1.73	0.52
2:B:743:GLN:HA	2:B:746:ALA:HB3	1.90	0.52
3:C:301:GLU:HA	3:C:304:MET:HE2	1.91	0.52
3:C:675:GLN:HB2	3:C:689:LEU:HD23	1.91	0.52
3:C:864:TYR:HA	3:C:867:ILE:HD12	1.91	0.52
3:C:503:VAL:HG21	3:C:536:LEU:HD11	1.90	0.52
5:E:245:ASP:OD1	5:E:246:VAL:N	2.41	0.52
5:E:386:ALA:O	5:E:402:THR:OG1	2.27	0.52
5:E:80:GLY:HA2	11:K:79:TYR:CE2	2.45	0.52
7:G:39:ASP:OD1	7:G:40:THR:N	2.39	0.52
9:I:11:PHE:CE2	9:I:34:ARG:HD2	2.44	0.52
11:L:67:TYR:CD2	11:M:45:LYS:HD3	2.45	0.52
16:Z:29:LYS:HE2	16:Z:31:ASP:HB2	1.92	0.52
16:Z:39:LEU:HD11	16:Z:94:LEU:HD21	1.92	0.52
16:Z:7:ARG:HH21	16:Z:123:ARG:HB2	1.75	0.52
3:C:316:THR:OG1	3:C:317:GLU:OE1	2.28	0.52
2:B:64:LEU:CB	2:B:75:THR:O	2.57	0.52
2:B:380:LEU:HD12	2:B:381:ARG:HG3	1.92	0.52
2:B:560:LEU:HD22	2:B:624:TYR:HE1	1.75	0.52
11:K:71:GLU:HG2	11:K:89:LYS:HB3	1.92	0.52
4:D:334:PHE:O	4:D:337:GLN:NE2	2.43	0.51
4:D:510:SER:HB3	4:D:513:LEU:HD23	1.91	0.51
5:E:272:LEU:HD11	5:E:291:TRP:HZ3	1.75	0.51
10:J:48:PRO:HG3	10:J:88:VAL:HG11	1.92	0.51
16:Z:13:LYS:NZ	16:Z:14:ASN:OD1	2.43	0.51
1:A:219:ASP:O	1:A:223:MET:HA	2.10	0.51
2:B:799:LYS:HA	2:B:802:MET:HE2	1.92	0.51
3:C:781:LEU:HB3	3:C:867:ILE:HD11	1.92	0.51
3:C:203:MET:HE2	3:C:271:LYS:NZ	2.26	0.51
3:C:823:GLU:O	3:C:826:ARG:HB2	2.09	0.51
3:C:826:ARG:O	3:C:829:GLU:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:31:LEU:HD12	11:L:40:ILE:HD13	1.93	0.51
3:C:204:GLU:HG2	3:C:205:GLU:N	2.25	0.51
3:C:785:SER:HB2	3:C:867:ILE:HA	1.93	0.51
4:D:382:ASP:OD1	4:D:382:ASP:N	2.36	0.51
2:B:327:THR:HG23	5:E:542:LEU:HD11	1.93	0.51
3:C:580:TRP:HZ3	3:C:623:PHE:HE2	1.58	0.51
3:C:239:TRP:HZ3	3:C:290:SER:HA	1.77	0.50
9:I:7:VAL:O	9:I:10:THR:OG1	2.23	0.50
5:E:280:CYS:SG	5:E:292:TRP:HB2	2.51	0.50
16:Z:110:PHE:O	16:Z:143:ASN:ND2	2.43	0.50
2:B:507:ARG:HD3	4:D:509:SER:HB3	1.94	0.50
3:C:803:PHE:O	3:C:806:GLN:HB2	2.10	0.50
16:Z:29:LYS:HE3	16:Z:33:LYS:HE3	1.92	0.50
2:B:515:ALA:HB1	2:B:528:LEU:HD21	1.94	0.50
11:M:25:ASP:HA	11:M:28:THR:HG22	1.93	0.50
2:B:813:ASN:O	2:B:816:LYS:HG2	2.11	0.50
3:C:669:ARG:HH12	3:C:692:GLU:HG3	1.77	0.50
5:E:169:TRP:NE1	5:E:460:GLN:OE1	2.44	0.50
2:B:296:LYS:NZ	5:E:549:THR:O	2.44	0.50
3:C:791:GLU:OE2	3:C:813:GLN:NE2	2.44	0.50
4:D:499:GLY:HA2	4:D:521:LEU:O	2.12	0.50
2:B:499:VAL:O	2:B:503:GLU:HB2	2.12	0.50
3:C:129:PRO:O	3:C:133:GLU:N	2.42	0.50
2:B:520:THR:HG22	2:B:521:THR:HG23	1.93	0.49
2:B:566:LEU:HD11	5:E:407:THR:H	1.77	0.49
3:C:578:ILE:HD11	3:C:627:TRP:HB2	1.93	0.49
3:C:671:ALA:O	3:C:675:GLN:NE2	2.44	0.49
9:I:55:LYS:NZ	11:K:32:GLU:O	2.45	0.49
2:B:525:THR:O	2:B:529:LEU:CB	2.60	0.49
3:C:959:LYS:HE2	7:G:158:LEU:HA	1.94	0.49
5:E:287:GLY:O	5:E:289:VAL:N	2.41	0.49
5:E:272:LEU:HD11	5:E:291:TRP:CZ3	2.47	0.49
2:B:625:ASP:O	2:B:629:GLU:HB2	2.12	0.49
2:B:506:ARG:NH2	2:B:540:VAL:HG12	2.27	0.49
4:D:539:ALA:HB1	4:D:567:ILE:HG21	1.92	0.49
2:B:134:PRO:HA	2:B:137:GLN:HE21	1.77	0.49
2:B:166:MET:HG2	2:B:167:LYS:HD3	1.94	0.49
2:B:264:LYS:HA	2:B:267:GLU:HB2	1.94	0.49
4:D:542:ARG:NH1	4:D:544:ASP:OD2	2.45	0.49
4:D:544:ASP:OD1	4:D:544:ASP:N	2.43	0.49
2:B:544:ASP:O	2:B:547:LYS:NZ	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:812:LEU:HA	2:B:815:ILE:HG22	1.95	0.49
3:C:1019:ALA:HA	3:C:1022:THR:HG22	1.94	0.49
5:E:236:GLN:OE1	5:E:240:GLN:HB2	2.12	0.49
9:I:75:ARG:NH1	9:I:76:SER:O	2.46	0.49
9:I:75:ARG:HG2	9:I:80:GLU:HG3	1.95	0.49
11:M:40:ILE:HB	11:M:60:VAL:HG11	1.94	0.49
16:Z:126:ARG:NH2	16:Z:135:GLN:O	2.39	0.49
1:A:238:ILE:HA	1:A:261:LYS:HA	1.95	0.49
5:E:381:ILE:HD11	5:E:424:THR:HA	1.94	0.49
2:B:385:ARG:HH12	2:B:428:CYS:HB2	1.77	0.49
4:D:597:ASN:OD1	4:D:598:LYS:N	2.44	0.49
5:E:384:TRP:HA	5:E:409:LEU:HB2	1.95	0.49
3:C:782:GLY:O	3:C:786:SER:OG	2.31	0.49
3:C:789:LEU:N	3:C:875:LEU:HD21	2.28	0.48
3:C:675:GLN:N	3:C:675:GLN:OE1	2.46	0.48
9:I:24:ILE:HD11	9:I:42:THR:HG23	1.94	0.48
15:Y:275:UNK:O	15:Y:279:UNK:CB	2.61	0.48
3:C:224:ILE:HD13	3:C:238:TYR:CZ	2.49	0.48
2:B:323:PRO:HA	2:B:326:HIS:ND1	2.28	0.48
2:B:563:VAL:HG13	2:B:593:LEU:HD22	1.95	0.48
3:C:361:ILE:HG12	3:C:378:ASN:HB3	1.95	0.48
4:D:368:PHE:CD1	4:D:376:LEU:HD13	2.49	0.48
7:G:152:ASP:OD1	7:G:153:GLU:N	2.46	0.48
16:Z:78:LEU:HA	16:Z:81:ARG:HD3	1.95	0.48
1:A:75:ALA:HB1	1:A:92:GLY:HA3	1.95	0.48
11:N:79:TYR:HA	11:N:84:ALA:HA	1.95	0.48
13:P:51:LYS:HA	13:P:54:GLN:HB2	1.94	0.48
16:Z:5:ALA:O	16:Z:9:ARG:NH1	2.46	0.48
2:B:678:PRO:N	5:E:188:GLN:HE22	2.12	0.48
3:C:583:GLN:NE2	4:D:543:LEU:HD13	2.28	0.48
5:E:146:PRO:HB2	5:E:445:LEU:HD22	1.95	0.48
7:G:99:THR:O	7:G:103:PHE:HB3	2.14	0.48
5:E:154:PHE:CZ	5:E:203:VAL:HG22	2.49	0.48
9:I:40:ASP:HA	9:I:43:VAL:HG22	1.96	0.48
2:B:592:GLY:O	5:E:362:HIS:NE2	2.46	0.48
3:C:611:LYS:HA	3:C:611:LYS:HD2	1.70	0.48
3:C:1028:ASN:HD21	3:C:1048:LYS:HE3	1.79	0.48
3:C:1060:GLN:HA	3:C:1063:HIS:HB3	1.95	0.48
9:I:76:SER:OG	9:I:77:LYS:N	2.47	0.48
2:B:326:HIS:O	2:B:329:MET:HG2	2.14	0.48
2:B:234:LEU:HD13	2:B:237:LEU:HD22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:864:TYR:O	3:C:867:ILE:HB	2.13	0.48
13:P:45:TYR:CD2	13:P:51:LYS:HG3	2.49	0.48
2:B:254:LEU:HD12	2:B:255:THR:HG23	1.95	0.47
2:B:632:THR:HA	2:B:635:ARG:HG3	1.95	0.47
5:E:324:THR:HG22	5:E:376:LYS:HD3	1.95	0.47
2:B:816:LYS:O	2:B:820:LYS:HG2	2.14	0.47
2:B:822:THR:HA	2:B:825:ILE:HD12	1.95	0.47
3:C:551:LEU:HD11	3:C:613:TYR:HB2	1.96	0.47
11:K:57:HIS:HB2	11:K:88:PHE:CE1	2.49	0.47
11:M:58:CYS:HB2	11:M:87:LEU:HD13	1.95	0.47
2:B:380:LEU:O	2:B:383:THR:OG1	2.25	0.47
4:D:615:LYS:O	4:D:627:VAL:HA	2.14	0.47
5:E:162:ARG:NH1	5:E:194:MET:SD	2.82	0.47
4:D:537:LEU:HD23	4:D:572:TRP:CE2	2.49	0.47
5:E:342:SER:HB3	5:E:356:TYR:HB2	1.97	0.47
2:B:687:THR:O	2:B:691:LEU:HB3	2.13	0.47
3:C:876:GLN:HG3	3:C:960:ALA:HB1	1.95	0.47
5:E:272:LEU:HD21	5:E:291:TRP:CZ3	2.49	0.47
1:A:189:PRO:HA	1:A:198:ASP:HA	1.97	0.47
1:A:239:CYS:N	1:A:260:ARG:O	2.43	0.47
3:C:226:ASP:O	3:C:230:ARG:NH1	2.48	0.47
3:C:313:THR:O	3:C:316:THR:OG1	2.27	0.47
3:C:322:LEU:HD21	3:C:349:ILE:HD11	1.96	0.47
3:C:578:ILE:HD12	3:C:624:GLU:HA	1.97	0.47
4:D:598:LYS:HG3	4:D:599:LEU:HD12	1.96	0.47
5:E:294:LEU:O	5:E:296:LYS:N	2.47	0.47
5:E:426:LYS:HE3	5:E:430:ALA:HB3	1.97	0.47
4:D:584:THR:OG1	4:D:585:ASP:N	2.47	0.47
5:E:306:LEU:O	5:E:313:THR:OG1	2.32	0.47
5:E:418:ARG:NH1	5:E:435:ASP:OD2	2.48	0.47
7:G:31:ASP:HB2	7:G:38:ILE:HD13	1.97	0.47
11:L:59:ILE:HG22	11:M:66:SER:HB2	1.97	0.47
11:M:60:VAL:HA	11:M:84:ALA:O	2.15	0.47
4:D:428:PHE:O	4:D:439:LEU:HD12	2.14	0.47
5:E:231:LEU:HA	5:E:244:PHE:O	2.14	0.47
5:E:241:LEU:HD11	5:E:282:THR:HG21	1.96	0.47
3:C:790:VAL:HG22	3:C:875:LEU:HD22	1.97	0.47
5:E:248:LYS:HD3	5:E:250:ASN:HD21	1.80	0.47
3:C:574:VAL:HB	3:C:674:MET:HE3	1.97	0.46
5:E:77:VAL:HG21	11:K:84:ALA:HB2	1.96	0.46
2:B:525:THR:O	2:B:529:LEU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:647:SER:OG	4:D:659:GLU:OE1	2.33	0.46
11:M:24:VAL:HG22	11:M:78:PHE:HE1	1.81	0.46
13:P:59:GLN:HB3	13:P:63:LYS:HZ1	1.80	0.46
2:B:649:THR:O	2:B:652:GLU:HG3	2.15	0.46
3:C:581:ALA:HB2	3:C:623:PHE:HD2	1.81	0.46
1:A:36:CYS:HA	1:A:43:ALA:HA	1.98	0.46
2:B:274:TYR:HA	2:B:277:PHE:HD2	1.81	0.46
5:E:152:THR:HG21	5:E:206:PRO:HG3	1.96	0.46
5:E:323:ASP:HB3	5:E:327:GLY:HA2	1.97	0.46
5:E:414:TRP:HB3	5:E:415:SER:H	1.57	0.46
2:B:115:PRO:HG2	2:B:116:LEU:HD12	1.97	0.46
3:C:783:ALA:HA	3:C:786:SER:HG	1.80	0.46
11:N:9:VAL:O	11:N:79:TYR:N	2.49	0.46
2:B:122:ILE:HA	2:B:126:VAL:HG22	1.97	0.46
3:C:672:LYS:NZ	3:C:687:MET:O	2.44	0.46
5:E:105:ASP:OD1	5:E:106:TYR:N	2.48	0.46
10:J:59:ARG:HG3	10:J:65:ASN:O	2.16	0.46
11:L:77:TYR:HD1	11:L:86:LEU:HD12	1.80	0.46
11:M:59:ILE:O	11:M:85:ILE:HA	2.15	0.46
2:B:128:MET:SD	2:B:129:PRO:HD3	2.55	0.46
2:B:742:GLN:O	2:B:746:ALA:N	2.47	0.46
3:C:449:ILE:HD13	3:C:523:PHE:HE1	1.80	0.46
7:G:104:VAL:HA	7:G:108:GLY:HA3	1.96	0.46
13:P:55:MET:O	13:P:59:GLN:HG2	2.15	0.46
16:Z:84:ASP:OD1	16:Z:84:ASP:N	2.48	0.46
2:B:570:TYR:OH	5:E:428:ASP:OD2	2.33	0.46
3:C:261:VAL:HA	3:C:264:ILE:HD12	1.98	0.46
4:D:186:THR:OG1	11:L:65:GLY:HA2	2.15	0.46
4:D:484:LYS:HG2	4:D:492:TYR:HB3	1.98	0.46
4:D:528:TRP:CH2	4:D:550:LEU:HD13	2.51	0.46
5:E:291:TRP:H	5:E:291:TRP:CD1	2.33	0.46
11:K:56:TRP:HA	11:K:88:PHE:O	2.15	0.46
11:L:77:TYR:CD1	11:L:86:LEU:HD12	2.50	0.46
3:C:239:TRP:HB3	3:C:294:VAL:HG22	1.98	0.46
3:C:324:THR:HG22	3:C:327:ARG:HH22	1.81	0.46
4:D:315:VAL:HG11	4:D:626:LEU:HD12	1.97	0.46
5:E:155:LYS:NZ	5:E:159:ASN:O	2.48	0.46
11:K:76:ILE:HB	11:K:87:LEU:HD23	1.98	0.46
11:L:24:VAL:HG22	11:L:78:PHE:CE1	2.51	0.46
11:M:28:THR:O	11:M:32:GLU:HG2	2.17	0.45
2:B:499:VAL:O	2:B:503:GLU:CB	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:266:MET:HG3	10:J:71:ARG:NH2	2.30	0.45
4:D:562:ASP:OD1	4:D:563:LEU:N	2.49	0.45
7:G:63:ILE:O	7:G:67:ASP:N	2.39	0.45
9:I:63:LEU:HD11	10:J:43:TYR:HE1	1.82	0.45
2:B:633:GLU:O	2:B:636:THR:OG1	2.29	0.45
5:E:241:LEU:HB2	5:E:256:THR:HB	1.99	0.45
3:C:443:LEU:HD11	3:C:452:LEU:HD22	1.99	0.45
3:C:492:ILE:HD13	3:C:492:ILE:HA	1.85	0.45
3:C:850:LYS:O	3:C:853:SER:OG	2.31	0.45
3:C:1041:HIS:NE2	7:G:58:ASP:OD2	2.40	0.45
4:D:490:SER:OG	4:D:505:SER:OG	2.25	0.45
4:D:573:ALA:HB1	4:D:575:LEU:HD23	1.98	0.45
2:B:164:GLY:O	2:B:168:GLY:N	2.49	0.45
2:B:687:THR:O	2:B:691:LEU:CB	2.64	0.45
3:C:422:LEU:HB3	3:C:476:TYR:CG	2.51	0.45
4:D:342:ILE:HD11	4:D:376:LEU:HD21	1.99	0.45
4:D:413:TRP:CZ3	4:D:433:SER:HB2	2.51	0.45
5:E:164:ALA:HA	5:E:182:TYR:HA	1.98	0.45
5:E:392:ASP:O	5:E:396:LYS:NZ	2.33	0.45
2:B:280:LEU:O	2:B:284:VAL:HG23	2.16	0.45
4:D:394:LYS:O	4:D:396:GLU:N	2.48	0.45
4:D:558:VAL:HG23	4:D:559:MET:HG3	1.99	0.45
13:P:31:LYS:O	13:P:35:MET:HB2	2.17	0.45
3:C:752:LEU:HD23	3:C:752:LEU:HA	1.68	0.45
4:D:576:GLN:NE2	4:D:578:THR:OG1	2.50	0.45
11:K:57:HIS:O	11:K:87:LEU:HA	2.16	0.45
11:K:79:TYR:OH	11:K:82:GLN:OE1	2.35	0.45
3:C:564:GLU:N	3:C:564:GLU:OE1	2.49	0.45
5:E:369:ARG:HH21	5:E:413:THR:HG21	1.82	0.45
11:K:14:ASP:N	11:K:14:ASP:OD1	2.48	0.45
11:M:57:HIS:HB2	11:M:88:PHE:CE1	2.50	0.45
3:C:1052:VAL:HA	3:C:1055:LYS:NZ	2.32	0.45
4:D:541:CYS:HA	4:D:566:SER:HB2	1.99	0.45
11:M:47:GLU:HG2	11:M:50:ARG:NH1	2.32	0.45
2:B:216:LEU:HA	2:B:216:LEU:HD23	1.73	0.45
4:D:516:TYR:CZ	4:D:548:VAL:HG11	2.52	0.45
10:J:78:GLU:HB3	10:J:93:GLN:O	2.17	0.45
3:C:811:LYS:O	3:C:814:ALA:HB3	2.17	0.44
3:C:825:ARG:HE	3:C:864:TYR:HE2	1.64	0.44
4:D:277:MET:HE2	4:D:277:MET:HB3	1.82	0.44
9:I:100:ASP:OD1	9:I:100:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:391:LYS:HA	2:B:391:LYS:HD2	1.80	0.44
3:C:120:LYS:HG2	3:C:159:LEU:HD11	1.99	0.44
5:E:272:LEU:HD13	5:E:322:TYR:CE2	2.51	0.44
16:Z:77:THR:O	16:Z:80:THR:OG1	2.29	0.44
3:C:211:CYS:SG	3:C:276:TRP:NE1	2.90	0.44
3:C:589:GLU:OE1	3:C:613:TYR:OH	2.24	0.44
3:C:804:VAL:O	3:C:807:ASN:HB2	2.17	0.44
11:L:39:ASP:N	11:L:39:ASP:OD1	2.47	0.44
16:Z:32:LYS:HG3	16:Z:72:LEU:HD13	1.99	0.44
2:B:510:ALA:HA	2:B:513:ILE:HG22	1.98	0.44
3:C:224:ILE:HG13	3:C:344:ARG:NH2	2.33	0.44
3:C:225:LYS:HA	3:C:344:ARG:HH12	1.82	0.44
3:C:789:LEU:HD23	3:C:875:LEU:HD11	1.98	0.44
2:B:807:ASP:O	2:B:811:VAL:HG23	2.16	0.44
3:C:860:SER:HA	3:C:863:MET:HE2	1.99	0.44
5:E:361:HIS:CE1	5:E:383:ASP:H	2.33	0.44
13:P:45:TYR:HB2	13:P:52:CYS:SG	2.57	0.44
2:B:453:LYS:O	2:B:455:LYS:N	2.51	0.44
2:B:622:ARG:O	2:B:625:ASP:HB2	2.18	0.44
5:E:545:GLU:HA	5:E:548:LYS:HD2	2.00	0.44
5:E:356:TYR:HB3	5:E:358:LEU:HD12	1.98	0.44
2:B:239:PHE:HD2	2:B:240:TRP:HD1	1.65	0.44
3:C:129:PRO:HD2	3:C:130:ILE:N	2.31	0.44
3:C:669:ARG:O	3:C:673:TYR:N	2.51	0.44
11:N:15:MET:HA	11:N:74:HIS:HA	2.00	0.44
3:C:296:TYR:O	3:C:299:THR:OG1	2.33	0.44
12:O:63:LYS:O	12:O:65:PHE:N	2.51	0.44
2:B:266:LEU:HB3	2:B:274:TYR:CZ	2.53	0.43
2:B:330:LEU:HB3	5:E:542:LEU:HD22	1.99	0.43
3:C:149:LEU:O	3:C:152:THR:OG1	2.30	0.43
4:D:276:ALA:O	4:D:279:PHE:HB3	2.18	0.43
5:E:199:TYR:CE2	5:E:209:PRO:HG3	2.53	0.43
5:E:399:ILE:HG23	5:E:400:LEU:H	1.82	0.43
2:B:266:LEU:HB3	2:B:274:TYR:CE1	2.52	0.43
2:B:457:LEU:HD22	2:B:511:ILE:HG23	2.00	0.43
2:B:517:ASP:OD1	2:B:517:ASP:N	2.48	0.43
2:B:520:THR:HG21	5:E:402:THR:HA	1.99	0.43
3:C:728:ASP:OD1	3:C:732:ARG:NH1	2.51	0.43
4:D:212:ASP:OD2	13:P:20:LEU:HG	2.18	0.43
4:D:318:ASN:HA	4:D:368:PHE:HD2	1.83	0.43
5:E:71:ASN:O	11:K:70:HIS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:366:TYR:H	5:E:382:GLY:CA	2.31	0.43
5:E:395:VAL:O	5:E:397:THR:N	2.50	0.43
11:M:44:ILE:HG22	11:M:87:LEU:HD11	2.00	0.43
2:B:464:ILE:HD13	2:B:508:LEU:HD12	1.99	0.43
3:C:857:ARG:HD2	3:C:857:ARG:HA	1.80	0.43
2:B:820:LYS:HA	2:B:823:GLN:HG3	2.00	0.43
3:C:500:GLN:HG2	3:C:535:ASP:OD2	2.18	0.43
3:C:1024:VAL:HG13	3:C:1044:LYS:NZ	2.33	0.43
5:E:273:GLN:HE21	5:E:273:GLN:HB3	1.53	0.43
11:M:80:LEU:HD12	11:M:80:LEU:HA	1.81	0.43
3:C:446:HIS:HD2	3:C:526:ILE:HG12	1.84	0.43
5:E:377:TYR:CD1	5:E:390:VAL:HG22	2.53	0.43
5:E:381:ILE:HD13	5:E:381:ILE:HG21	1.79	0.43
1:A:219:ASP:O	1:A:223:MET:CA	2.67	0.43
2:B:293:ASP:O	2:B:296:LYS:HG2	2.18	0.43
3:C:399:THR:HB	3:C:403:GLN:HE22	1.83	0.43
3:C:528:GLN:HE22	3:C:533:GLN:HG3	1.84	0.43
3:C:1015:LYS:HA	3:C:1015:LYS:HD3	1.78	0.43
16:Z:32:LYS:O	16:Z:72:LEU:N	2.52	0.43
2:B:68:ASP:O	2:B:70:LYS:N	2.51	0.43
5:E:272:LEU:CG	5:E:291:TRP:HZ3	2.32	0.43
16:Z:100:PHE:O	16:Z:104:ASP:N	2.52	0.43
3:C:486:LEU:HD23	3:C:486:LEU:HA	1.88	0.43
3:C:872:LEU:O	3:C:876:GLN:HG2	2.19	0.43
3:C:1013:GLU:HA	3:C:1016:LYS:HE3	2.01	0.43
4:D:352:HIS:CD2	4:D:353:PRO:HD2	2.53	0.43
5:E:77:VAL:HG13	11:K:63:ASN:H	1.84	0.43
2:B:583:TYR:HB3	2:B:642:TRP:CZ3	2.53	0.43
4:D:357:PHE:O	4:D:358:HIS:ND1	2.52	0.43
5:E:247:ARG:HG3	5:E:248:LYS:NZ	2.34	0.43
5:E:417:SER:O	5:E:417:SER:OG	2.29	0.43
5:E:547:PHE:HA	5:E:550:THR:HG23	2.00	0.43
2:B:693:LEU:HA	2:B:693:LEU:HD23	1.78	0.42
3:C:53:GLN:HA	3:C:83:HIS:HA	2.01	0.42
3:C:394:ARG:HH12	3:C:416:ILE:HG21	1.84	0.42
4:D:406:GLY:HA3	4:D:449:PRO:HG3	2.01	0.42
10:J:87:PHE:HE1	10:J:89:LEU:HB2	1.84	0.42
11:L:60:VAL:HG12	11:L:85:ILE:HG23	2.01	0.42
4:D:268:ASN:O	4:D:268:ASN:ND2	2.52	0.42
5:E:199:TYR:CZ	5:E:209:PRO:HG3	2.54	0.42
8:H:97:HIS:HA	8:H:106:ILE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:71:PHE:CD1	10:J:73:ARG:HB2	2.54	0.42
3:C:203:MET:HE2	3:C:271:LYS:HZ3	1.84	0.42
4:D:490:SER:HA	4:D:506:LYS:HD3	1.99	0.42
5:E:184:ILE:HD12	5:E:191:PRO:HG3	2.00	0.42
5:E:228:ASP:OD1	5:E:229:ASN:N	2.52	0.42
2:B:729:SER:N	2:B:732:ASP:OD2	2.52	0.42
4:D:535:MET:HE3	4:D:667:VAL:HG21	2.01	0.42
11:L:69:THR:O	11:L:69:THR:OG1	2.37	0.42
2:B:637:ARG:HA	2:B:637:ARG:HD3	1.77	0.42
4:D:209:TYR:CZ	13:P:94:GLY:HA2	2.54	0.42
5:E:169:TRP:HZ3	5:E:467:ALA:HB2	1.85	0.42
5:E:414:TRP:HD1	5:E:420:GLY:HA2	1.82	0.42
7:G:130:LEU:HD11	7:G:133:ASN:ND2	2.34	0.42
9:I:22:GLY:HA2	9:I:36:THR:HG21	2.01	0.42
2:B:475:PHE:HE1	2:B:493:ASP:HB3	1.85	0.42
2:B:594:MET:HE1	2:B:631:MET:HE3	2.02	0.42
5:E:502:GLU:O	5:E:506:GLU:HG3	2.19	0.42
7:G:101:ASP:OD1	7:G:102:ALA:N	2.52	0.42
11:K:21:ALA:HA	11:K:24:VAL:HG22	2.00	0.42
2:B:385:ARG:HH22	2:B:428:CYS:HB3	1.84	0.42
2:B:389:THR:O	2:B:393:TYR:HB2	2.20	0.42
3:C:632:ILE:O	3:C:635:ILE:HG22	2.19	0.42
3:C:975:VAL:O	3:C:979:ILE:HD12	2.20	0.42
4:D:296:LEU:HA	4:D:638:LYS:O	2.20	0.42
5:E:430:ALA:O	5:E:431:MET:HE2	2.20	0.42
11:M:37:GLU:OE1	11:M:60:VAL:HG13	2.19	0.42
2:B:583:TYR:HB3	2:B:642:TRP:CH2	2.54	0.42
3:C:759:LEU:HD12	3:C:759:LEU:HA	1.82	0.42
3:C:764:GLU:O	3:C:767:ARG:HG3	2.19	0.42
3:C:859:TYR:O	3:C:863:MET:HG2	2.19	0.42
4:D:313:THR:HG23	4:D:363:VAL:O	2.19	0.42
5:E:269:PHE:HE2	5:E:271:TRP:CZ2	2.37	0.42
5:E:403:LYS:HZ1	5:E:443:PRO:HD2	1.84	0.42
11:L:12:ASN:HB2	11:L:75:PHE:HE2	1.84	0.42
3:C:789:LEU:HA	3:C:813:GLN:OE1	2.19	0.42
4:D:493:LEU:HD21	4:D:550:LEU:HD11	2.01	0.42
11:N:8:ALA:HA	11:N:80:LEU:HA	2.01	0.42
4:D:316:CYS:SG	4:D:317:TRP:N	2.93	0.41
4:D:516:TYR:CE2	4:D:548:VAL:HG11	2.55	0.41
4:D:598:LYS:HA	4:D:598:LYS:HD2	1.88	0.41
5:E:166:TYR:HE1	5:E:168:ASN:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:118:VAL:O	7:G:122:ARG:HG3	2.20	0.41
11:L:44:ILE:O	11:L:48:PHE:HB2	2.20	0.41
2:B:583:TYR:CE2	2:B:682:ARG:HD3	2.55	0.41
2:B:597:ILE:HG23	2:B:628:TRP:NE1	2.35	0.41
3:C:1028:ASN:ND2	3:C:1048:LYS:HE3	2.36	0.41
4:D:480:MET:SD	4:D:524:TYR:HA	2.60	0.41
5:E:376:LYS:HD2	5:E:376:LYS:HA	1.90	0.41
7:G:43:LEU:HD12	7:G:43:LEU:HA	1.84	0.41
3:C:549:LYS:O	3:C:552:ASP:HB3	2.19	0.41
3:C:562:LYS:HA	3:C:623:PHE:HZ	1.86	0.41
4:D:318:ASN:HB3	4:D:368:PHE:CE2	2.55	0.41
4:D:590:HIS:HB3	4:D:604:SER:HA	2.02	0.41
5:E:186:GLN:O	5:E:189:GLN:NE2	2.42	0.41
5:E:234:ALA:HB3	5:E:242:ALA:HB3	2.03	0.41
5:E:236:GLN:HB3	5:E:237:TYR:H	1.63	0.41
5:E:371:ASN:HB3	5:E:414:TRP:CH2	2.55	0.41
2:B:762:LEU:O	2:B:766:LYS:N	2.53	0.41
4:D:615:LYS:HE2	4:D:615:LYS:HB2	1.78	0.41
5:E:506:GLU:HA	5:E:509:LEU:HG	2.02	0.41
11:L:20:GLN:O	11:L:24:VAL:HG23	2.20	0.41
13:P:57:LYS:HB3	13:P:70:VAL:HG23	2.03	0.41
3:C:605:GLU:CD	3:C:605:GLU:H	2.27	0.41
3:C:1015:LYS:HA	3:C:1018:MET:HB2	2.03	0.41
5:E:495:ILE:HA	5:E:498:MET:HG2	2.03	0.41
2:B:543:HIS:HA	2:B:546:GLU:OE1	2.20	0.41
3:C:732:ARG:NH1	3:C:732:ARG:HB2	2.35	0.41
5:E:161:LYS:O	5:E:184:ILE:HD11	2.19	0.41
5:E:371:ASN:N	5:E:377:TYR:O	2.53	0.41
11:M:55:THR:O	11:M:89:LYS:NZ	2.52	0.41
16:Z:116:ALA:HA	16:Z:119:ILE:HG22	2.02	0.41
4:D:432:SER:OG	4:D:433:SER:N	2.53	0.41
5:E:342:SER:OG	5:E:343:CYS:N	2.53	0.41
11:M:19:MET:HE3	11:M:19:MET:HB3	1.89	0.41
13:P:92:VAL:HG13	13:P:96:THR:OG1	2.20	0.41
2:B:155:PHE:HE1	3:C:155:PHE:HE2	1.68	0.41
2:B:522:ILE:O	2:B:556:TYR:OH	2.25	0.41
2:B:738:ASP:HA	2:B:741:ARG:HH11	1.85	0.41
3:C:702:LEU:HA	3:C:702:LEU:HD23	1.93	0.41
5:E:154:PHE:HZ	5:E:203:VAL:HG22	1.85	0.41
5:E:243:TYR:CD2	5:E:254:GLU:HB2	2.53	0.41
11:K:40:ILE:HG22	11:K:60:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:O	1:A:50:TYR:N	2.51	0.41
3:C:456:LEU:HD23	3:C:456:LEU:HA	1.94	0.41
3:C:788:LEU:HD12	3:C:788:LEU:HA	1.92	0.41
3:C:1025:THR:HA	3:C:1028:ASN:ND2	2.35	0.41
4:D:408:LEU:HA	4:D:408:LEU:HD23	1.87	0.41
5:E:272:LEU:HD13	5:E:322:TYR:HE2	1.86	0.41
5:E:339:GLN:HB3	5:E:357:VAL:HG23	2.02	0.41
10:J:41:LYS:HA	10:J:41:LYS:HD2	1.86	0.41
2:B:273:TYR:HB3	2:B:277:PHE:CE2	2.55	0.41
4:D:179:TYR:HA	4:D:180:PRO:HD3	2.01	0.41
3:C:390:ARG:HH22	3:C:421:ASP:N	2.19	0.40
3:C:703:THR:O	3:C:703:THR:OG1	2.36	0.40
5:E:202:ASP:OD1	5:E:203:VAL:N	2.54	0.40
16:Z:129:LEU:HD21	16:Z:135:GLN:HB2	2.02	0.40
2:B:152:LEU:HD12	2:B:152:LEU:HA	1.91	0.40
3:C:151:SER:O	3:C:154:LYS:HG3	2.20	0.40
3:C:681:CYS:SG	3:C:682:SER:N	2.95	0.40
4:D:520:HIS:CE1	4:D:542:ARG:HH21	2.39	0.40
5:E:367:GLY:HA3	5:E:381:ILE:HG22	2.04	0.40
11:M:53:ASN:HD22	11:M:89:LYS:HE2	1.86	0.40
1:A:126:ALA:H	1:A:143:TYR:H	1.69	0.40
2:B:756:LYS:HA	2:B:759:ARG:HG2	2.03	0.40
10:J:23:VAL:O	10:J:87:PHE:HB2	2.21	0.40
11:K:37:GLU:OE1	11:K:37:GLU:N	2.54	0.40
11:L:24:VAL:HG22	11:L:78:PHE:HE1	1.86	0.40
11:M:40:ILE:HG21	11:M:60:VAL:HG21	2.04	0.40
5:E:286:ASP:O	5:E:314:THR:HA	2.21	0.40
3:C:588:ILE:HD12	3:C:588:ILE:HA	1.91	0.40
3:C:785:SER:O	3:C:785:SER:OG	2.28	0.40
4:D:408:LEU:HD22	4:D:432:SER:HB3	2.03	0.40
5:E:170:HIS:HA	5:E:171:PRO:HD3	1.87	0.40
5:E:304:MET:O	5:E:306:LEU:HD12	2.21	0.40
13:P:20:LEU:HA	13:P:20:LEU:HD13	1.81	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	313/4503 (7%)	279 (89%)	34 (11%)	0	100	100
2	B	647/4568 (14%)	615 (95%)	31 (5%)	1 (0%)	43	75
3	C	925/4485 (21%)	858 (93%)	65 (7%)	2 (0%)	43	75
4	D	450/683 (66%)	387 (86%)	63 (14%)	0	100	100
5	E	470/567 (83%)	371 (79%)	94 (20%)	5 (1%)	11	44
6	F	98/136 (72%)	94 (96%)	4 (4%)	0	100	100
7	G	134/159 (84%)	125 (93%)	9 (7%)	0	100	100
8	H	89/120 (74%)	77 (86%)	12 (14%)	0	100	100
9	I	101/105 (96%)	89 (88%)	11 (11%)	1 (1%)	12	45
10	J	92/100 (92%)	81 (88%)	11 (12%)	0	100	100
11	K	80/91 (88%)	73 (91%)	7 (9%)	0	100	100
11	L	80/91 (88%)	72 (90%)	8 (10%)	0	100	100
11	M	80/91 (88%)	73 (91%)	7 (9%)	0	100	100
11	N	80/91 (88%)	68 (85%)	12 (15%)	0	100	100
12	O	95/117 (81%)	92 (97%)	3 (3%)	0	100	100
13	P	96/103 (93%)	89 (93%)	7 (7%)	0	100	100
16	Z	155/184 (84%)	136 (88%)	19 (12%)	0	100	100
All	All	3985/16194 (25%)	3579 (90%)	397 (10%)	9 (0%)	44	75

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	625	ASP
5	E	298	ASN
9	I	85	PRO
5	E	295	ARG
3	C	114	TRP

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Mol	Chain	Res	Type
5	E	269	PHE
5	E	231	LEU
5	E	209	PRO
3	C	839	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	463/3998 (12%)	459 (99%)	4 (1%)	70	76
3	C	701/3945 (18%)	699 (100%)	2 (0%)	86	85
4	D	401/584 (69%)	397 (99%)	4 (1%)	68	76
5	E	400/489 (82%)	398 (100%)	2 (0%)	81	82
7	G	121/136 (89%)	121 (100%)	0	100	100
9	I	90/91 (99%)	90 (100%)	0	100	100
10	J	83/87 (95%)	83 (100%)	0	100	100
11	K	70/76 (92%)	70 (100%)	0	100	100
11	L	70/76 (92%)	70 (100%)	0	100	100
11	M	70/76 (92%)	70 (100%)	0	100	100
13	P	86/90 (96%)	85 (99%)	1 (1%)	63	73
16	Z	138/162 (85%)	138 (100%)	0	100	100
All	All	2693/9810 (28%)	2680 (100%)	13 (0%)	78	82

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	124	GLN
2	B	627	LEU
2	B	628	TRP
2	B	629	GLU
3	C	200	LEU
3	C	204	GLU

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Mol	Chain	Res	Type
4	D	270	ASN
4	D	273	GLU
4	D	297	LEU
4	D	312	VAL
5	E	273	GLN
5	E	279	GLU
13	P	20	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	429	HIS
2	B	477	GLN
2	B	549	HIS
3	C	439	GLN
3	C	500	GLN
3	C	504	ASN
3	C	528	GLN
3	C	577	ASN
3	C	593	GLN
3	C	780	ASN
3	C	810	GLN
3	C	1028	ASN
4	D	252	GLN
5	E	158	ASN
5	E	205	ASN
5	E	273	GLN
5	E	374	ASN
7	G	53	ASN
7	G	65	GLN
7	G	68	GLN
10	J	42	GLN
13	P	5	GLN
16	Z	96	ASN
16	Z	160	ASN

5.3.3 RNA ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
15	Y	3
14	X	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	396:UNK	C	403:UNK	N	28.65
1	Y	387:UNK	C	394:UNK	N	22.26
1	Y	420:UNK	C	424:UNK	N	12.82
1	X	345:UNK	C	348:UNK	N	10.08
1	Y	281:UNK	C	284:UNK	N	6.72

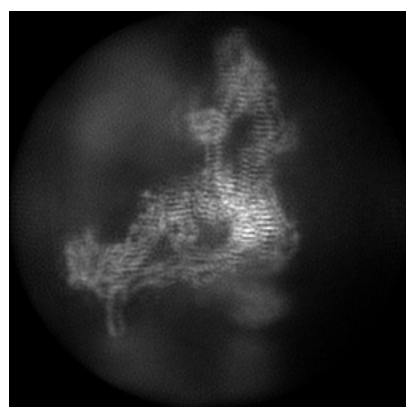
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23083. These allow visual inspection of the internal detail of the map and identification of artifacts.

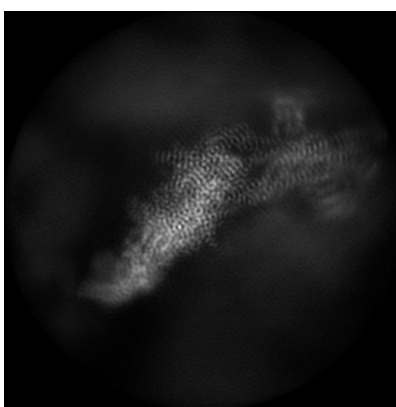
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

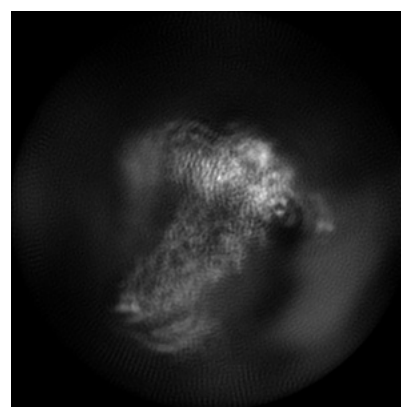
6.1.1 Primary map



X



Y

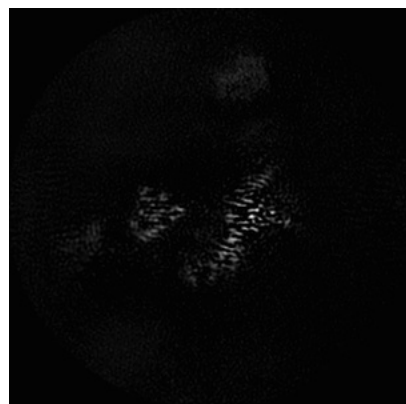


Z

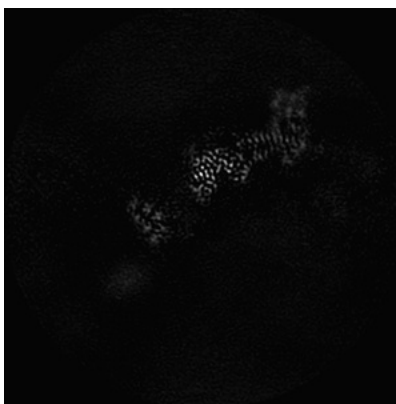
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

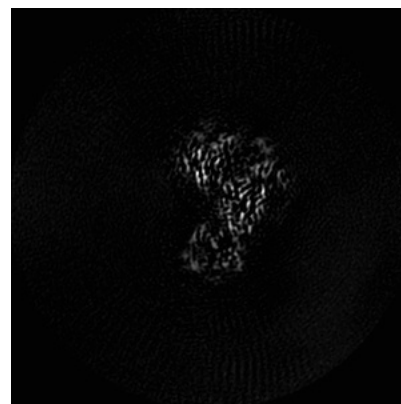
6.2.1 Primary map



X Index: 130



Y Index: 130

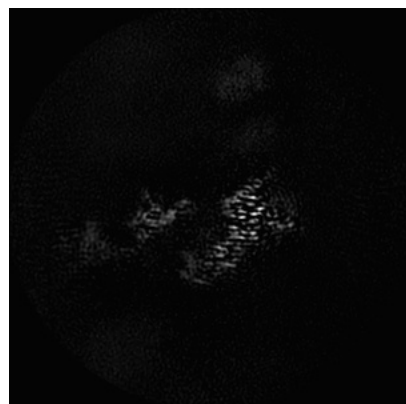


Z Index: 130

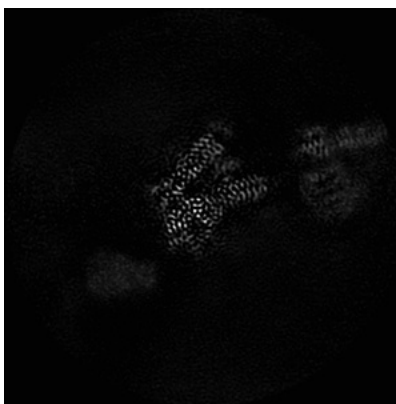
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

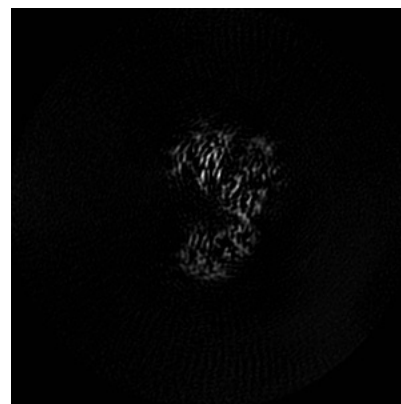
6.3.1 Primary map



X Index: 127



Y Index: 152

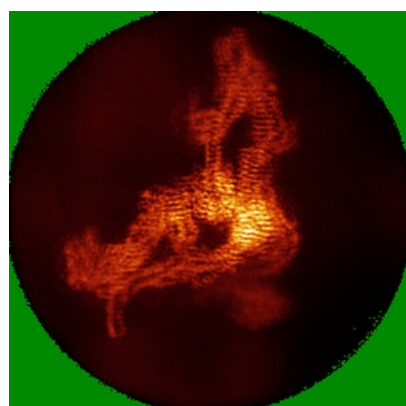


Z Index: 126

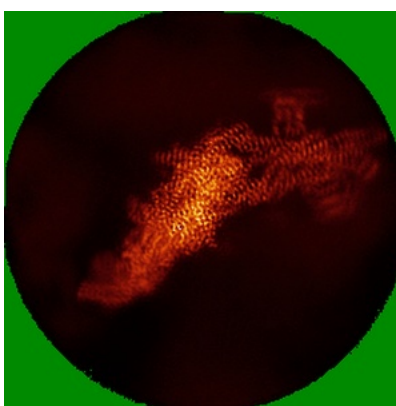
The images above show the largest variance slices of the map in three orthogonal directions.

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

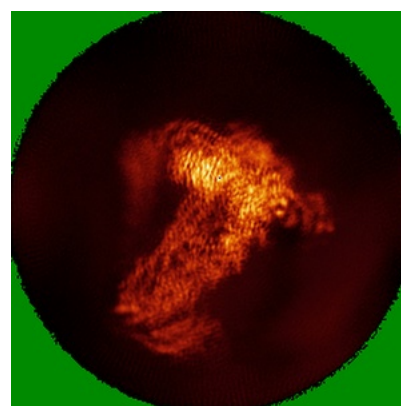
6.4.1 Primary map



X



Y

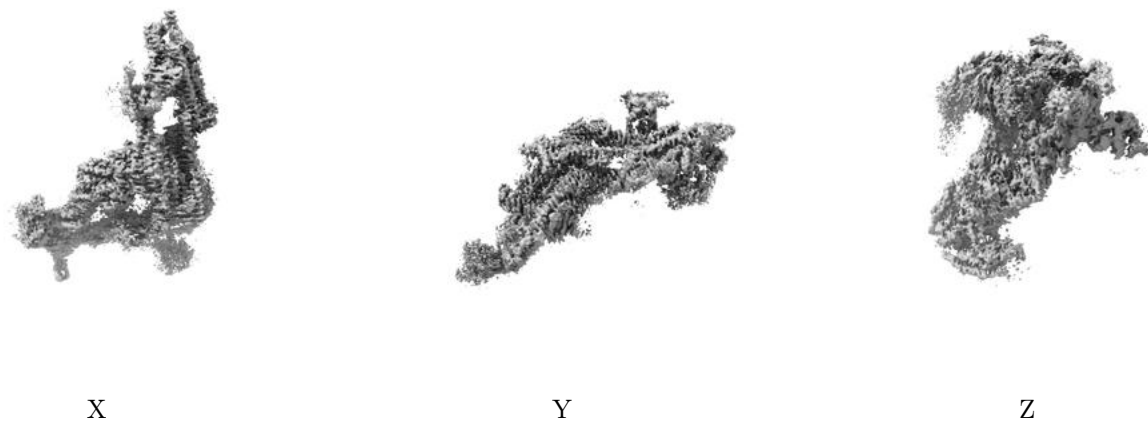


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

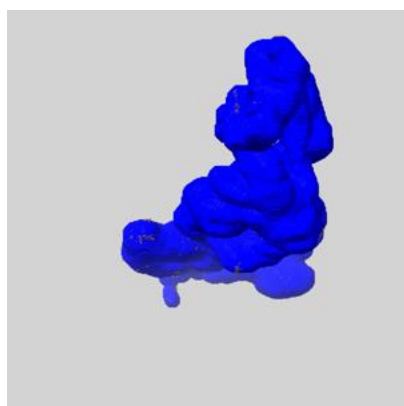
6.6 Mask visualisation [i](#)

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

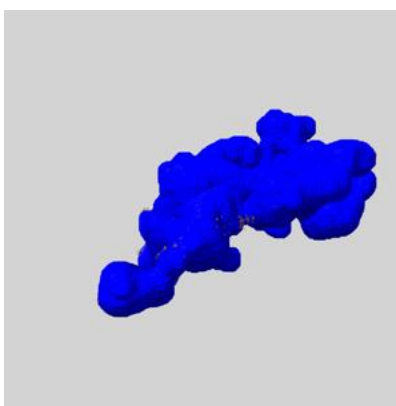
A mask typically either:

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

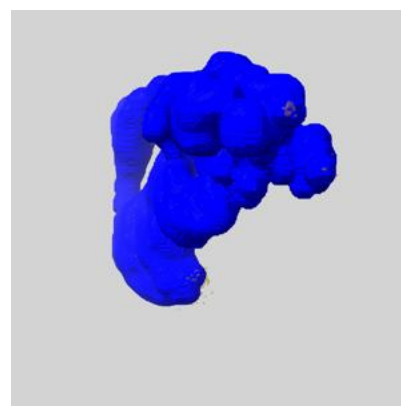
6.6.1 emd_23083_msk_1.map [i](#)



X



Y

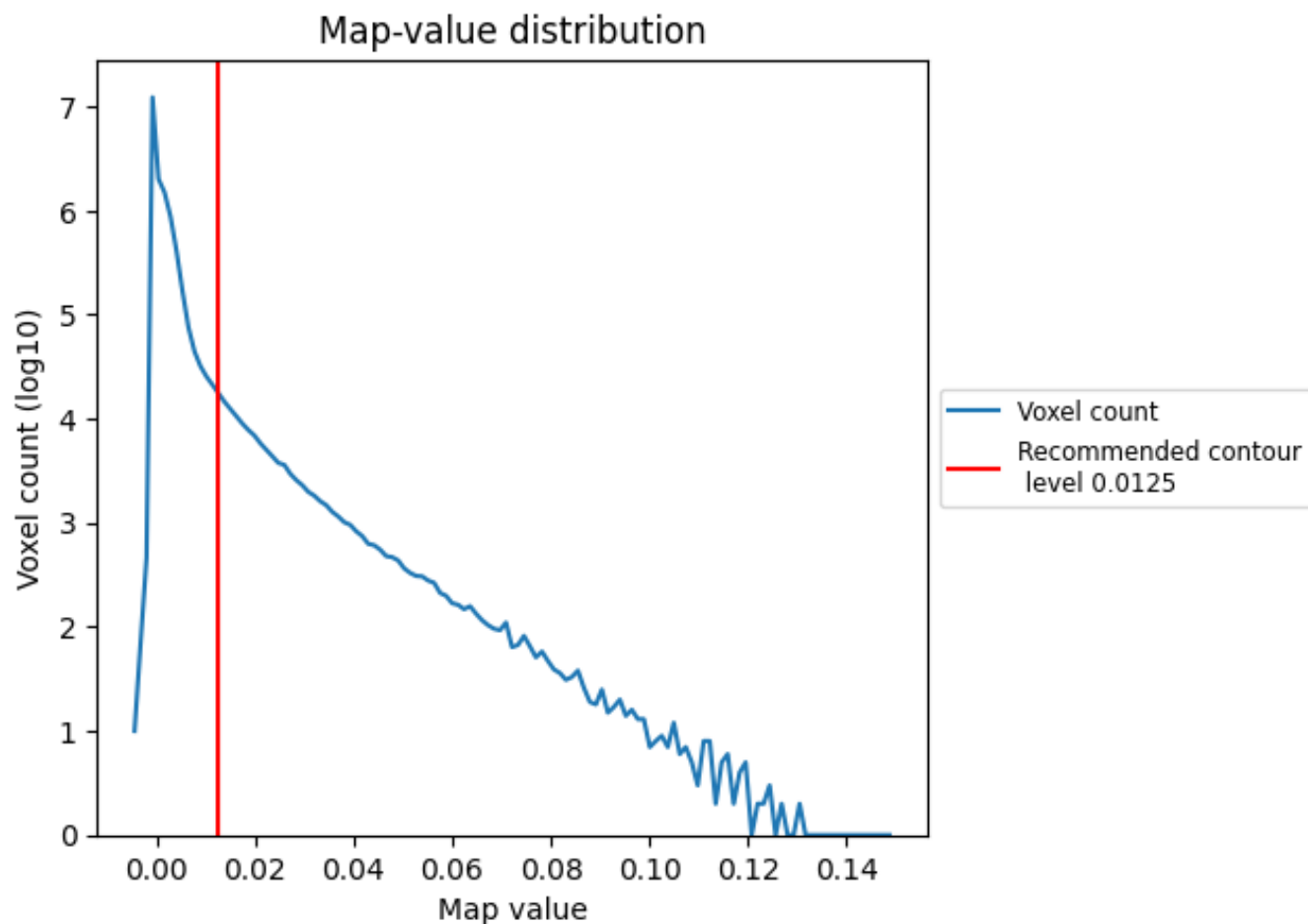


Z

7 Map analysis [i](#)

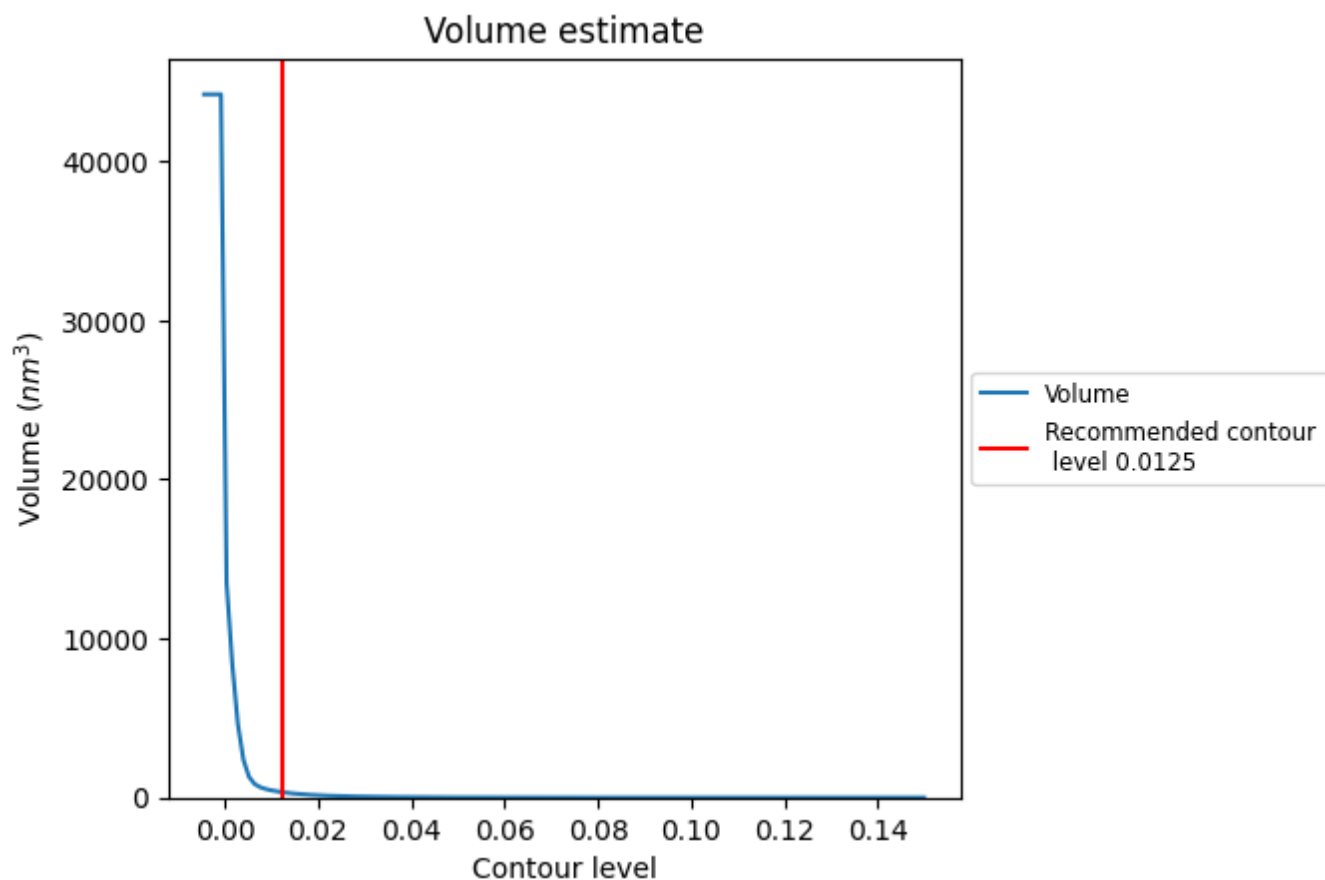
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

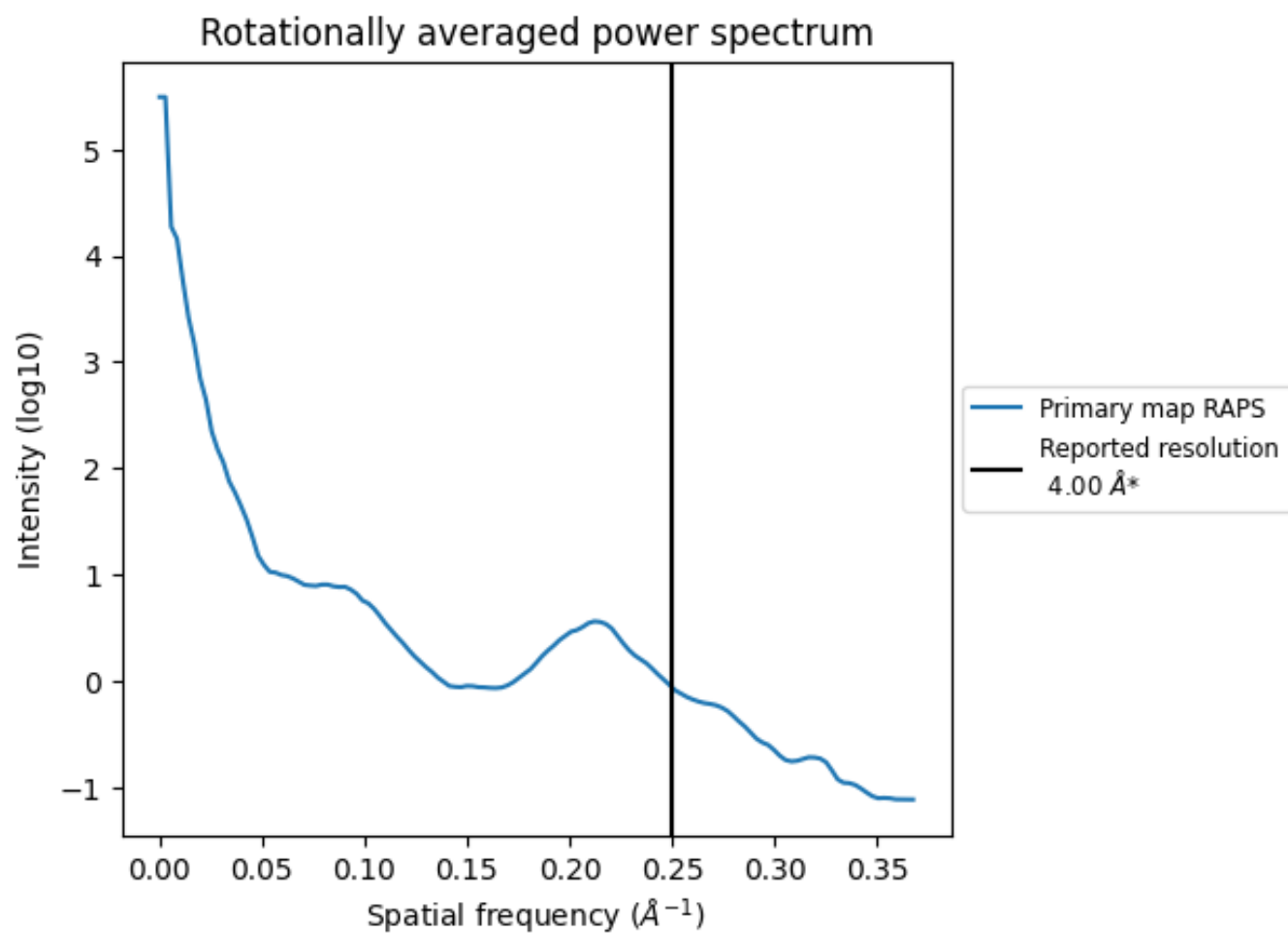
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 330 nm³; this corresponds to an approximate mass of 298 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 0.250 Å⁻¹

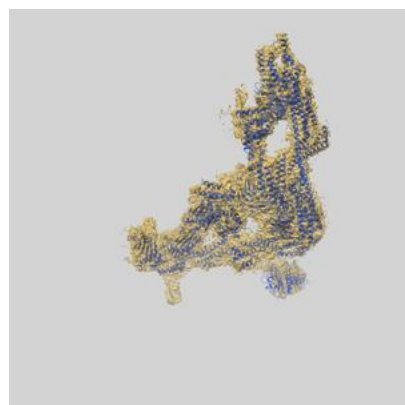
8 Fourier-Shell correlation ⓘ

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

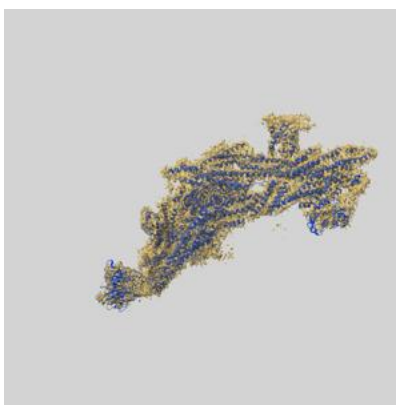
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23083 and PDB model 7KZN. Per-residue inclusion information can be found in section [3](#) on page [7](#).

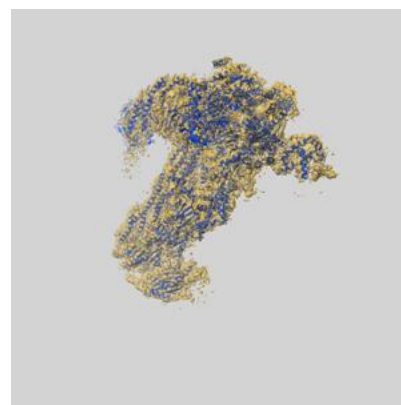
9.1 Map-model overlay [i](#)



X



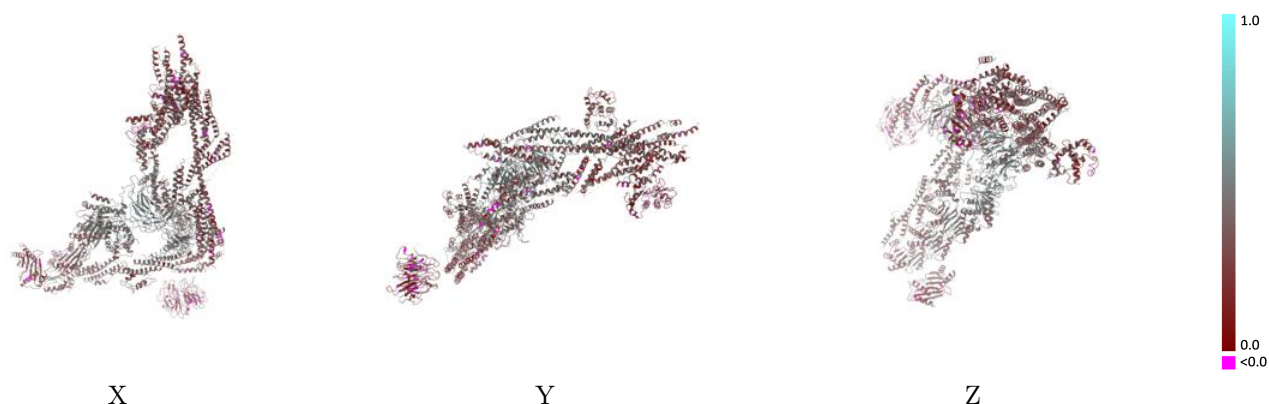
Y



Z

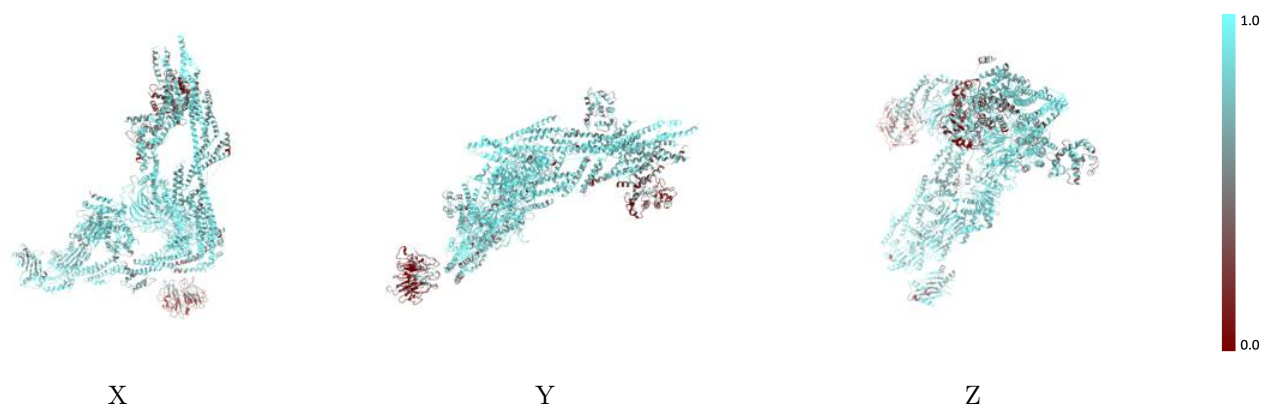
The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



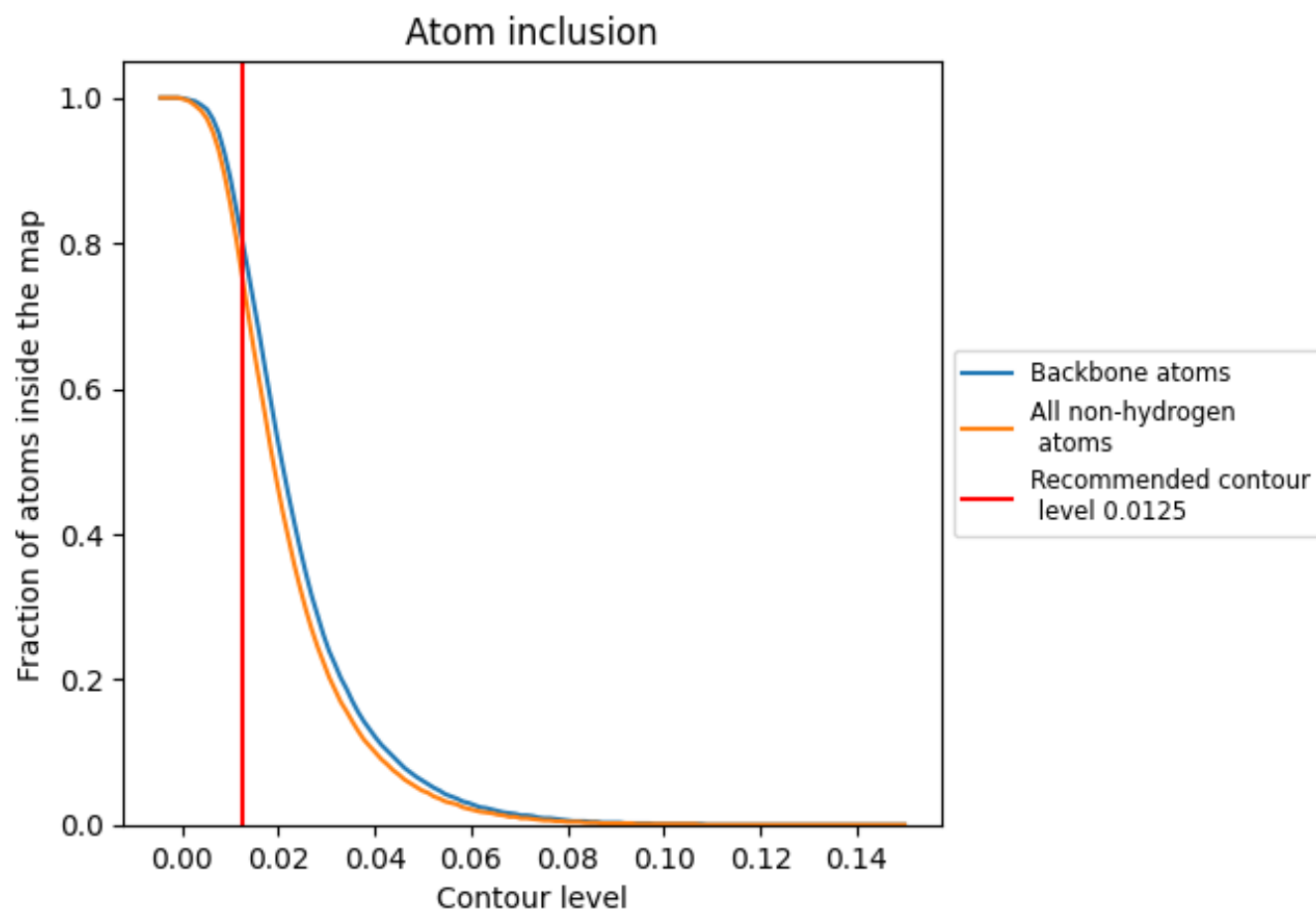
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0125).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 76% 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 (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7550	 0.3760
A	 0.2160	 0.2390
B	 0.6780	 0.3280
C	 0.7650	 0.3780
D	 0.8840	 0.4800
E	 0.8440	 0.4280
F	 0.7310	 0.2340
G	 0.7040	 0.3780
H	 0.9200	 0.3880
I	 0.8290	 0.4610
J	 0.8890	 0.4840
K	 0.8310	 0.4030
L	 0.7850	 0.3470
M	 0.8430	 0.3440
N	 0.8620	 0.3230
O	 0.7800	 0.2730
P	 0.7850	 0.4020
X	 0.8350	 0.3370
Y	 0.8840	 0.3590
Z	 0.6070	 0.2890

