



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 05:04 pm GMT

PDB ID : 5NVU
EMDB ID : EMD-3705
Title : Full length human cytoplasmic dynein-1 in the phi-particle conformation
Authors : Zhang, K.; Foster, H.E.; Carter, A.P.
Deposited on : 2017-05-04
Resolution : 15.00 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

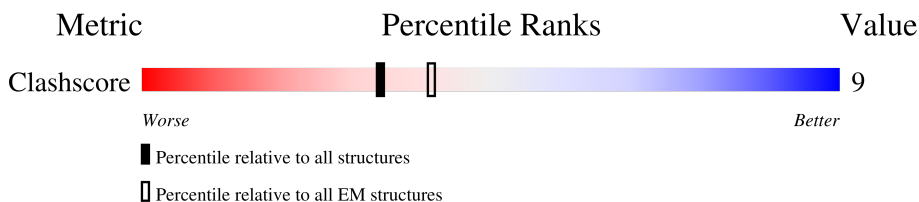
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

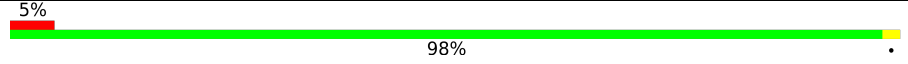
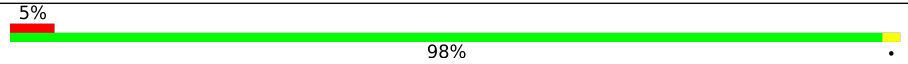
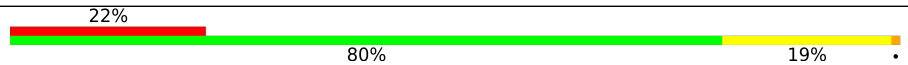
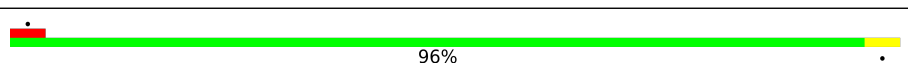
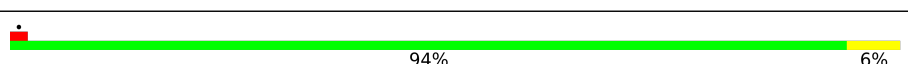
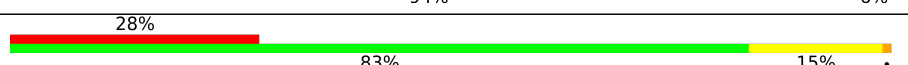
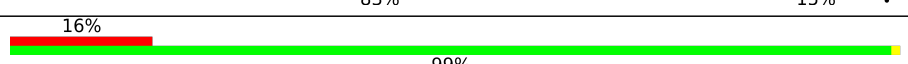
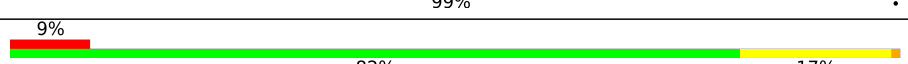
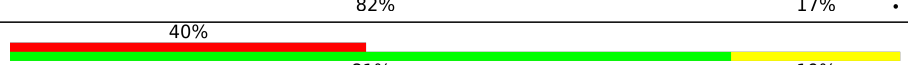
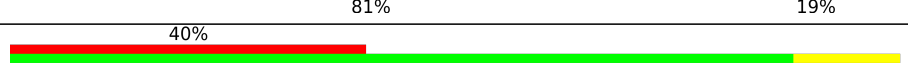
The reported resolution of this entry is 15.00 Å.

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.



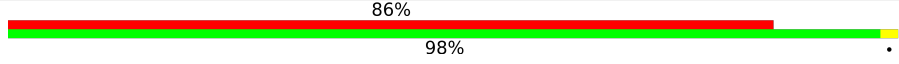
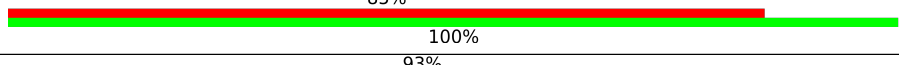
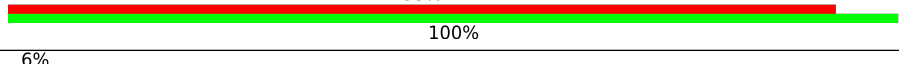
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297

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	3169	 5% 98% .
1	B	3169	 5% 98% .
2	C	932	 22% 80% 19% .
3	D	350	 . 96% .
3	E	350	 . 94% 6% .
4	F	893	 28% 83% 15% .
5	G	298	 16% 99% .
6	H	295	 9% 82% 17% .
7	I	125	 40% 81% 19% .
8	J	124	 40% 88% 12% .

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Mol	Chain	Length	Quality of chain
9	K	85	 <p>74% 98%</p>
9	L	85	 <p>86% 98%</p>
10	M	103	 <p>90% 92% 8%</p>
11	N	104	 <p>97% 89% 11%</p>
12	O	27	 <p>85% 100%</p>
13	P	29	 <p>93% 100%</p>
14	Q	120	 <p>6% 100%</p>
14	R	120	 <p>5% 98%</p>

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 51478 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 Dynein motor domain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	3169	Total	C	N	O	0	0
			15703	9365	3169	3169		
1	B	3169	Total	C	N	O	0	0
			15703	9365	3169	3169		

- Molecule 2 is a protein called Dynein tail heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	C	932	Total	C	N	O	0	0
			4654	2790	932	932		

- Molecule 3 is a protein called Dynein intermediate chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	D	350	Total	C	N	O	0	0
			1723	1023	350	350		
3	E	350	Total	C	N	O	0	0
			1723	1023	350	350		

- Molecule 4 is a protein called Dynein tail heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	F	893	Total	C	N	O	0	0
			4459	2673	893	893		

- Molecule 5 is a protein called Dynein light intermediate chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	G	298	Total	C	N	O	5	0
			1496	890	303	303		

- Molecule 6 is a protein called Dynein light intermediate chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	H	295	1459	869	295	295	0	0

- Molecule 7 is a protein called N-terminal dimerization domain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	I	125	625	375	125	125	0	0

- Molecule 8 is a protein called N-terminal dimerization domain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	J	124	620	372	124	124	0	0

- Molecule 9 is a protein called LC8.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	K	85	421	251	85	85	0	0
9	L	85	421	251	85	85	0	0

- Molecule 10 is a protein called Tctex.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	M	103	507	301	103	103	0	0

- Molecule 11 is a protein called Tctex.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	N	104	513	305	104	104	0	0

- Molecule 12 is a protein called Intermediate chain N-terminus peptides.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	O	27	134	80	27	27	0	0

- Molecule 13 is a protein called Intermediate chain N-terminus peptides.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	P	29	143	85	29	29	0	0

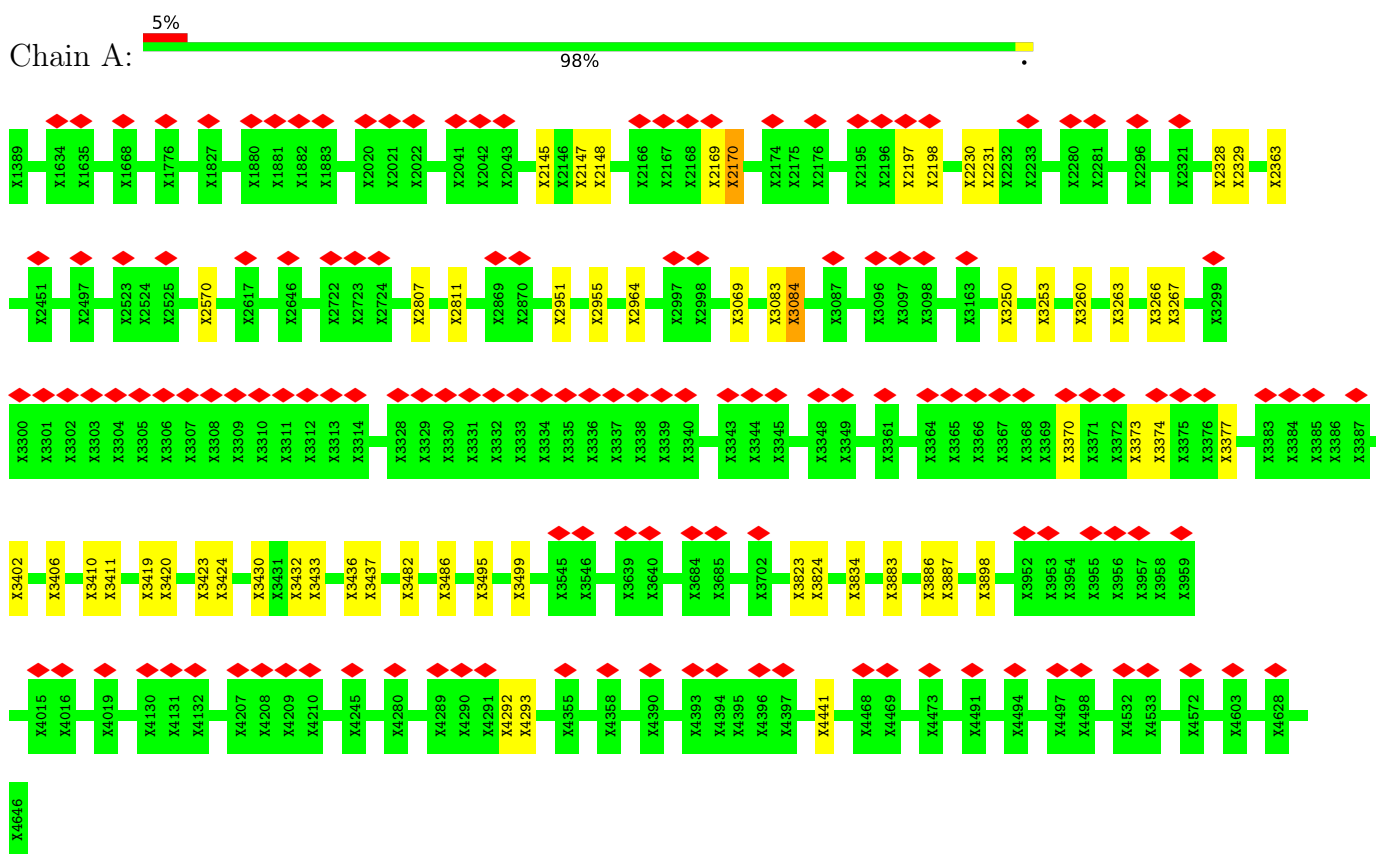
- Molecule 14 is a protein called Robl.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	Q	120	587	347	120	120	0	0
14	R	120	587	347	120	120	0	0

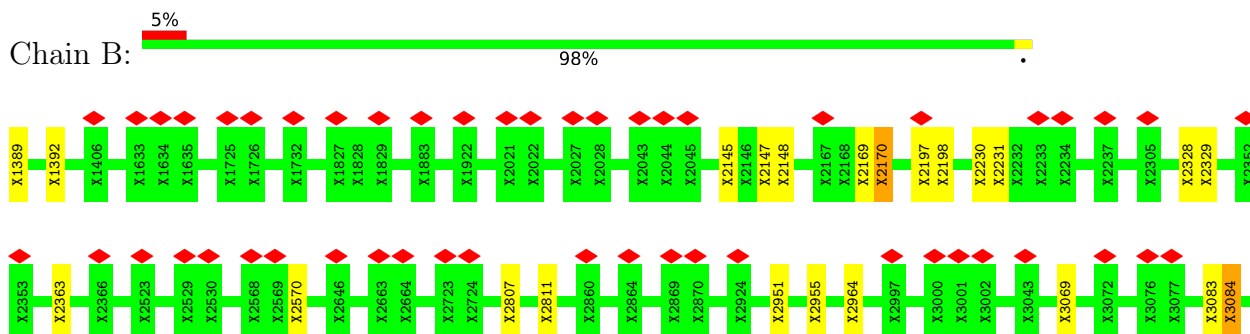
3 Residue-property plots [i](#)

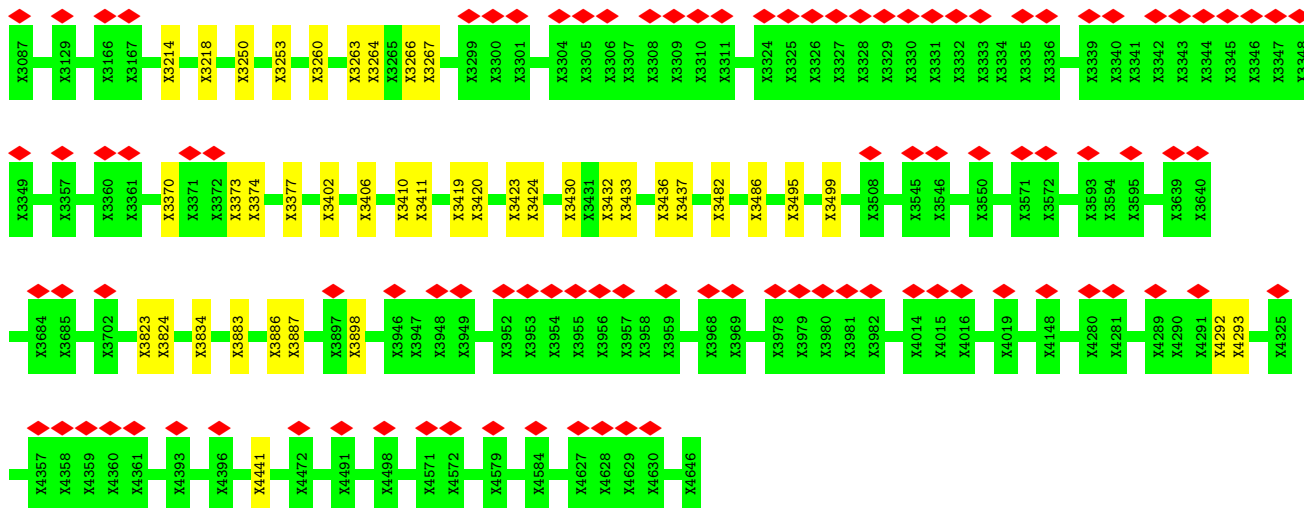
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

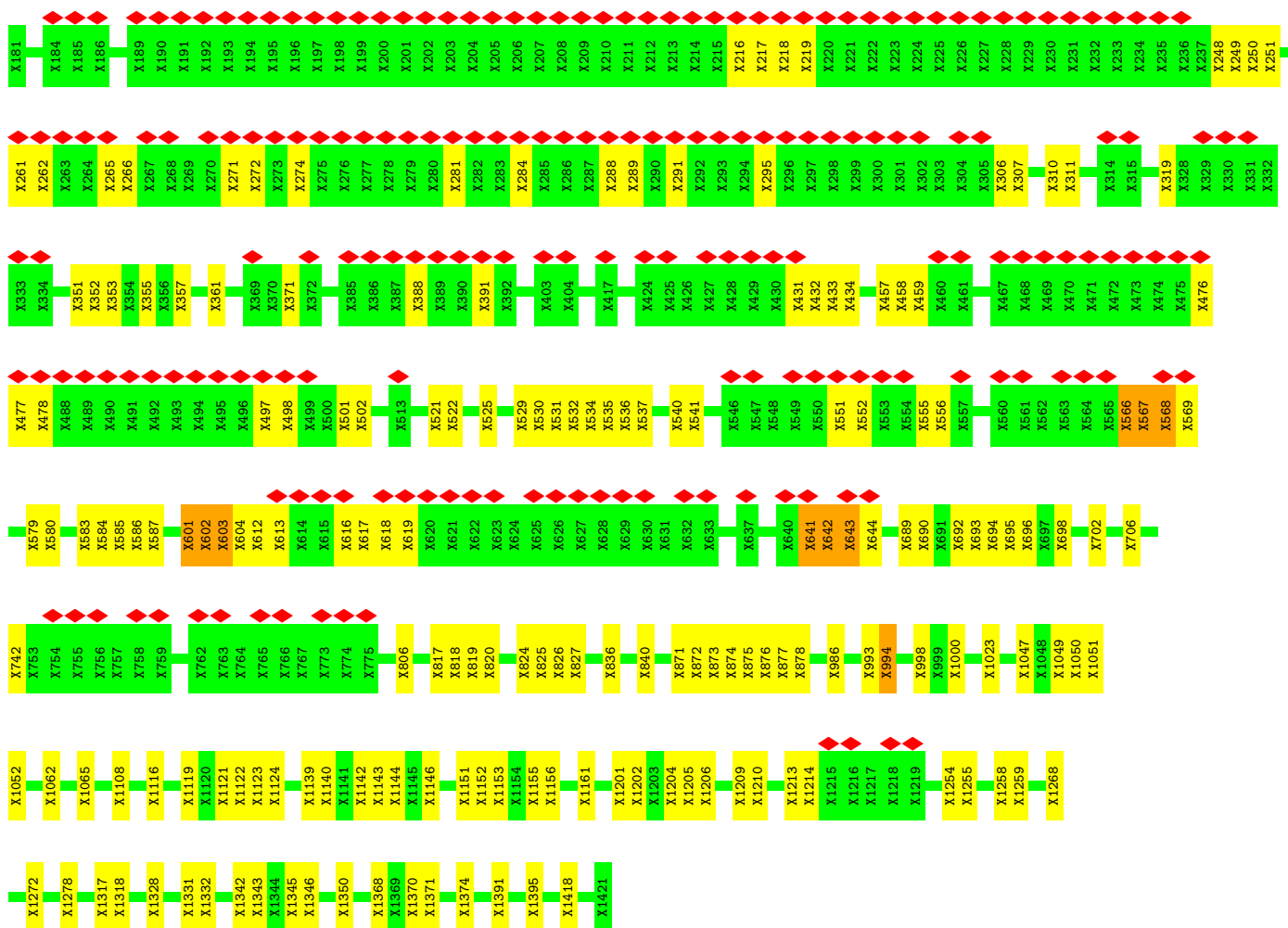
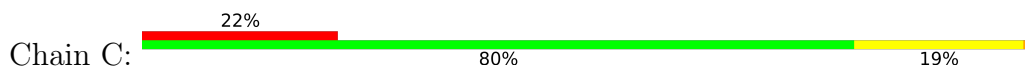


- Molecule 1: Dynein motor domain

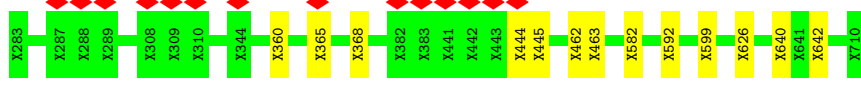




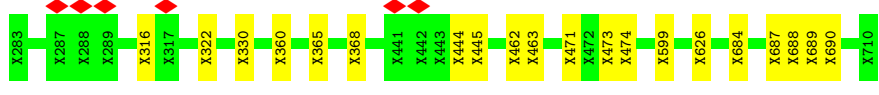
• Molecule 2: Dynein tail heavy chain



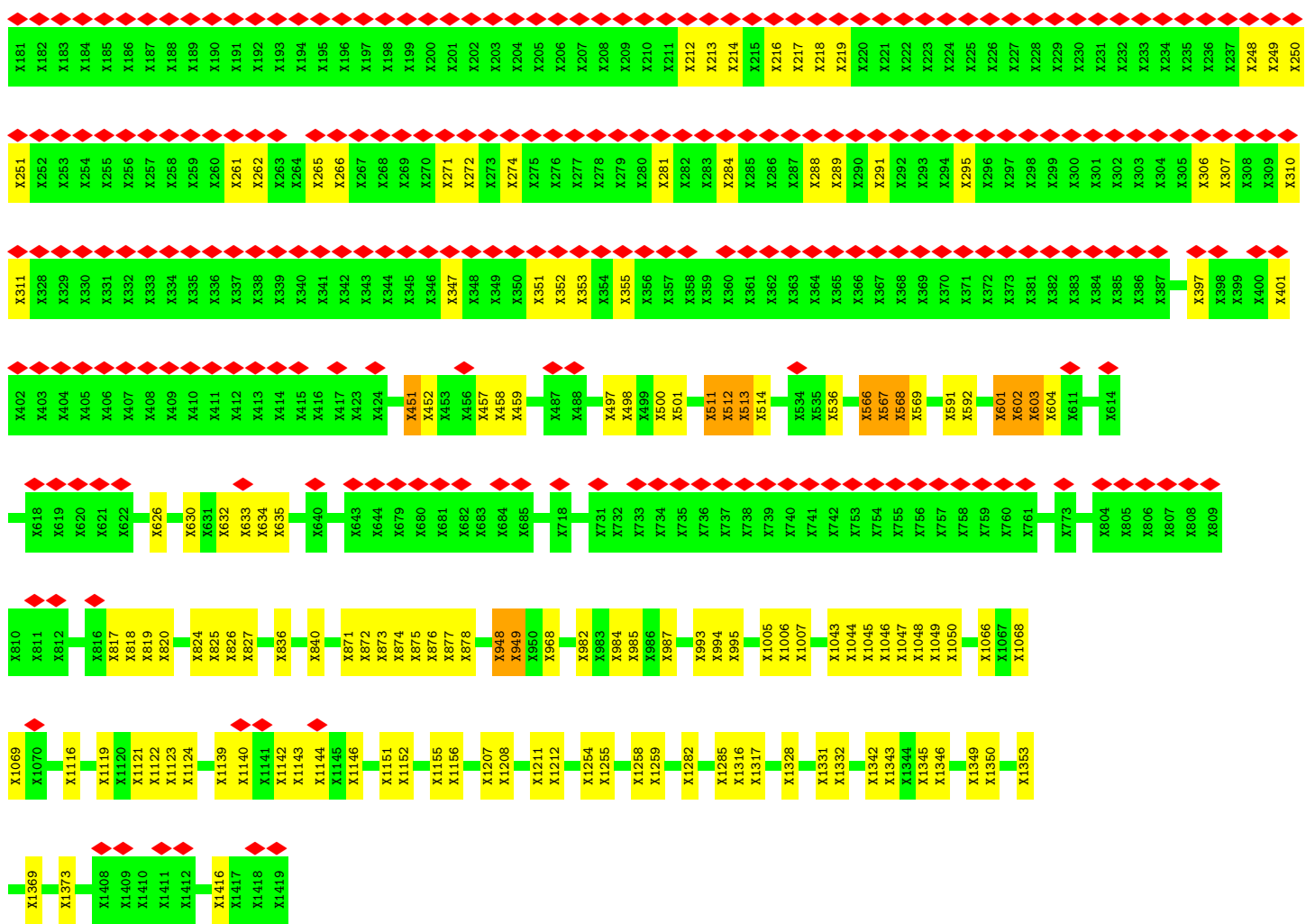
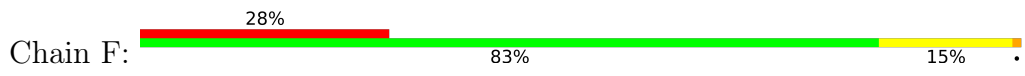
• Molecule 3: Dynein intermediate chain



• Molecule 3: Dynein intermediate chain

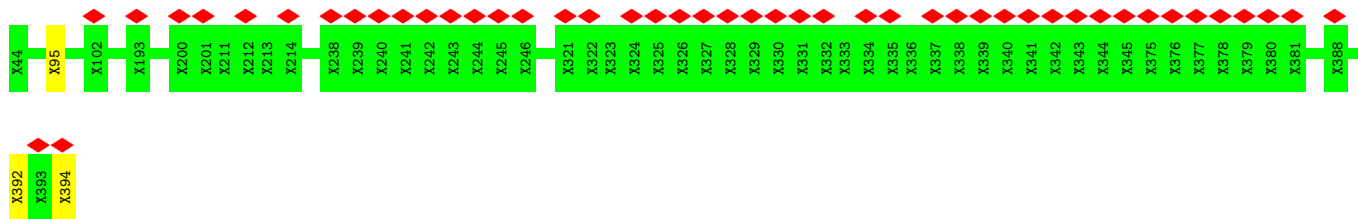


• Molecule 4: Dynein tail heavy chain

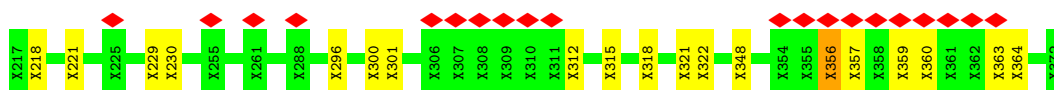
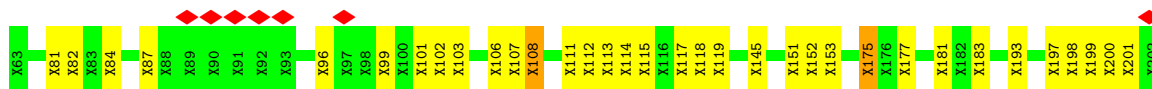
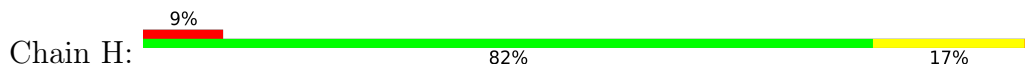


• Molecule 5: Dynein light intermediate chain

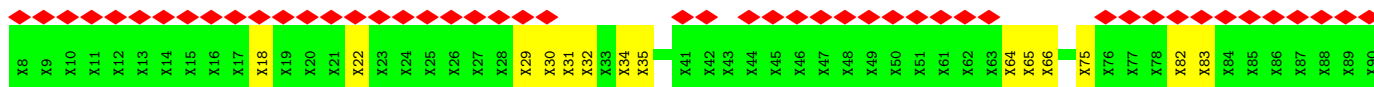
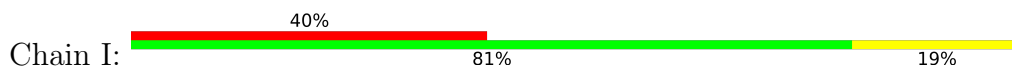




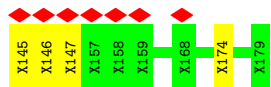
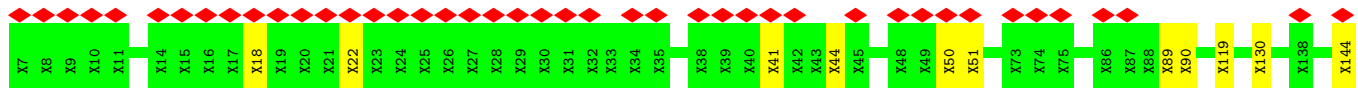
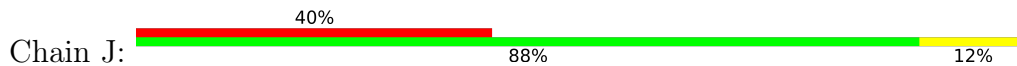
• Molecule 6: Dynein light intermediate chain



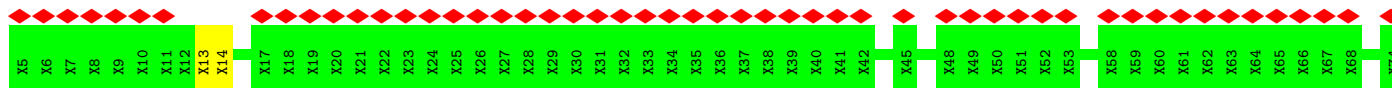
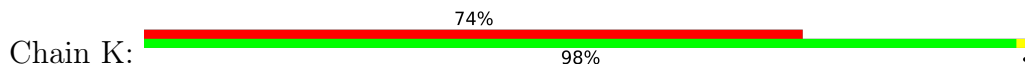
• Molecule 7: N-terminal dimerization domain

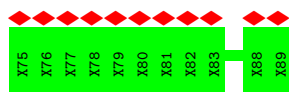


• Molecule 8: N-terminal dimerization domain

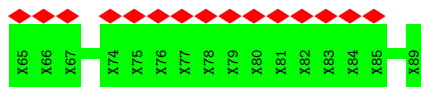
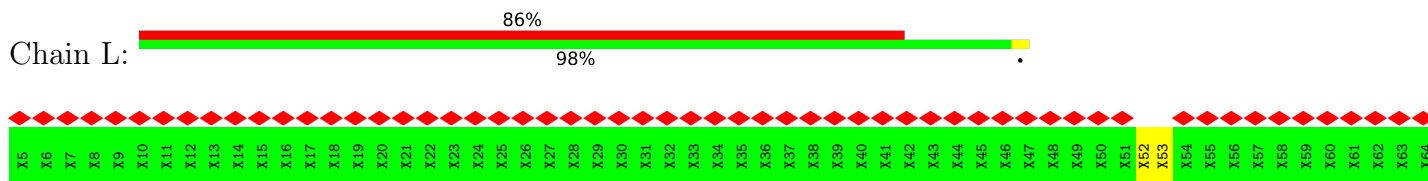


• Molecule 9: LC8

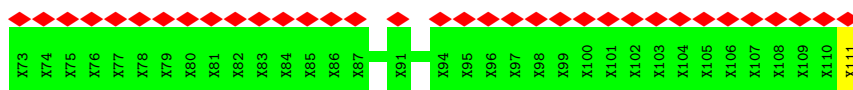
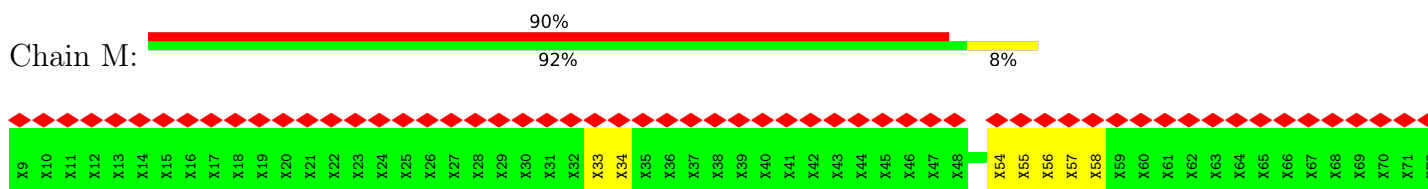




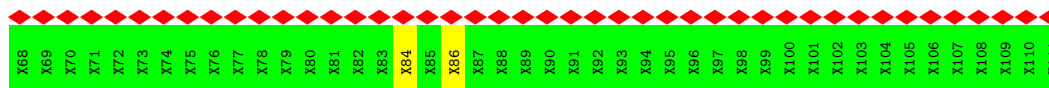
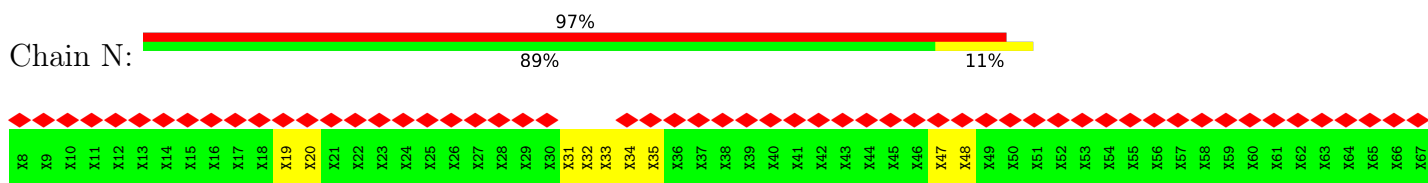
- Molecule 9: LC8



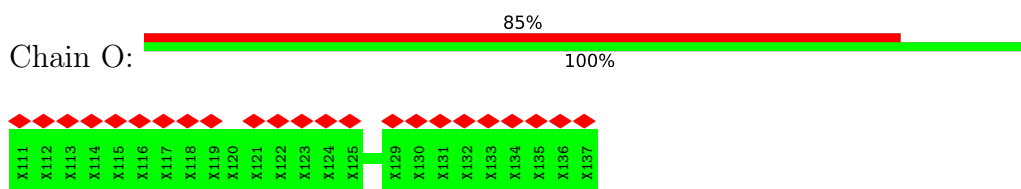
- Molecule 10: Tctex



- Molecule 11: Tctex

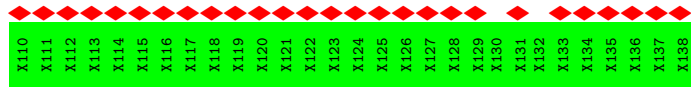


- Molecule 12: Intermediate chain N-terminus peptides

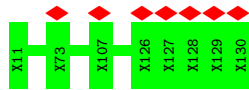


- Molecule 13: Intermediate chain N-terminus peptides

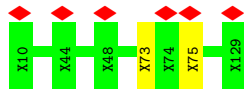




• Molecule 14: Robl



• Molecule 14: Robl



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	28736	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 ($e^-/\text{\AA}^2$)	1.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.439	Depositor
Minimum map value	-0.264	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	792.00006, 792.00006, 792.00006	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.64, 2.64, 2.64	Depositor

5 Model quality i

5.1 Standard geometry i

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	8
2	C	0	11
4	F	0	13
6	H	0	8
All	All	0	48

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2170	UNK	Peptide
1	A	2570	UNK	Peptide
1	A	2964	UNK	Peptide
1	A	3069	UNK	Peptide
1	A	3084	UNK	Peptide
1	A	3834	UNK	Peptide
1	A	3898	UNK	Peptide
1	A	4441	UNK	Peptide
1	B	2170	UNK	Peptide
1	B	2570	UNK	Peptide
1	B	2964	UNK	Peptide
1	B	3069	UNK	Peptide
1	B	3084	UNK	Peptide

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Mol	Chain	Res	Type	Group
1	B	3834	UNK	Peptide
1	B	3898	UNK	Peptide
1	B	4441	UNK	Peptide
2	C	477	UNK	Mainchain
2	C	566	UNK	Mainchain
2	C	567	UNK	Mainchain
2	C	568	UNK	Mainchain
2	C	601	UNK	Mainchain
2	C	602	UNK	Mainchain
2	C	603	UNK	Mainchain
2	C	641	UNK	Mainchain
2	C	642	UNK	Mainchain
2	C	643	UNK	Mainchain
2	C	994	UNK	Peptide
4	F	451	UNK	Mainchain
4	F	511	UNK	Mainchain
4	F	512	UNK	Mainchain
4	F	513	UNK	Mainchain
4	F	566	UNK	Mainchain
4	F	567	UNK	Mainchain
4	F	568	UNK	Mainchain
4	F	601	UNK	Mainchain
4	F	602	UNK	Mainchain
4	F	603	UNK	Mainchain
4	F	948	UNK	Mainchain
4	F	949	UNK	Mainchain
4	F	968	UNK	Peptide
6	H	108	UNK	Mainchain,Peptide
6	H	175	UNK	Mainchain
6	H	218	UNK	Mainchain
6	H	312	UNK	Mainchain
6	H	356	UNK	Mainchain
6	H	84	UNK	Mainchain
6	H	96	UNK	Mainchain

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	15703	0	3145	36	0
1	B	15703	0	3143	43	0
2	C	4654	0	984	212	0
3	D	1723	0	360	9	0
3	E	1723	0	358	48	0
4	F	4459	0	955	152	0
5	G	1496	0	301	2	0
6	H	1459	0	295	48	0
7	I	625	0	146	19	0
8	J	620	0	142	15	0
9	K	421	0	94	1	0
9	L	421	0	95	1	0
10	M	507	0	108	6	0
11	N	513	0	112	7	0
12	O	134	0	30	0	0
13	P	143	0	31	0	0
14	Q	587	0	113	0	0
14	R	587	0	114	2	0
All	All	51478	0	10526	554	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 9.

All (554) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:81:UNK:C	6:H:87:UNK:CB	1.85	1.53
2:C:1161:UNK:CB	2:C:1318:UNK:N	1.74	1.50
2:C:497:UNK:O	2:C:501:UNK:CB	1.66	1.43
2:C:817:UNK:O	2:C:819:UNK:N	1.58	1.37
4:F:817:UNK:O	4:F:819:UNK:N	1.58	1.36
7:I:31:UNK:CB	7:I:34:UNK:CB	2.01	1.35
2:C:1161:UNK:CB	2:C:1318:UNK:CA	2.09	1.31
2:C:689:UNK:O	2:C:693:UNK:CB	1.79	1.30
8:J:18:UNK:O	8:J:22:UNK:CB	1.82	1.27
2:C:522:UNK:CB	3:E:330:UNK:CB	2.12	1.26
1:A:3263:UNK:O	1:A:3266:UNK:CB	1.81	1.26
1:B:3263:UNK:O	1:B:3266:UNK:CB	1.81	1.26
7:I:31:UNK:O	7:I:34:UNK:N	1.67	1.26
2:C:536:UNK:O	2:C:540:UNK:CB	1.87	1.22
2:C:498:UNK:O	2:C:502:UNK:CB	1.88	1.22
2:C:522:UNK:HA	3:E:330:UNK:CB	1.70	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:81:UNK:O	6:H:87:UNK:CB	1.83	1.21
6:H:82:UNK:N	6:H:87:UNK:CB	2.03	1.21
4:F:1282:UNK:O	4:F:1316:UNK:CB	1.88	1.21
4:F:1285:UNK:CB	4:F:1316:UNK:HA	1.68	1.21
2:C:457:UNK:CB	2:C:459:UNK:N	2.04	1.21
2:C:1023:UNK:CB	2:C:1108:UNK:CB	2.19	1.20
4:F:457:UNK:CB	4:F:459:UNK:N	2.04	1.19
8:J:18:UNK:O	8:J:22:UNK:N	1.74	1.19
2:C:584:UNK:CA	3:E:689:UNK:C	1.76	1.18
2:C:1161:UNK:CB	2:C:1317:UNK:C	2.20	1.18
2:C:522:UNK:CA	3:E:330:UNK:CB	2.20	1.17
2:C:457:UNK:HA	2:C:458:UNK:CB	1.72	1.16
4:F:497:UNK:O	4:F:500:UNK:CB	1.93	1.16
4:F:1285:UNK:CB	4:F:1316:UNK:CA	2.22	1.15
6:H:101:UNK:O	6:H:119:UNK:O	1.64	1.15
2:C:319:UNK:CB	2:C:371:UNK:CB	2.24	1.15
4:F:457:UNK:HA	4:F:458:UNK:CB	1.71	1.14
2:C:584:UNK:CA	3:E:690:UNK:N	2.12	1.13
2:C:319:UNK:CB	2:C:371:UNK:CA	2.27	1.12
6:H:145:UNK:CB	6:H:301:UNK:CB	2.28	1.12
4:F:872:UNK:O	4:F:876:UNK:CB	1.99	1.10
2:C:872:UNK:O	2:C:876:UNK:CB	1.99	1.10
2:C:1161:UNK:CB	2:C:1318:UNK:HA	1.81	1.08
2:C:872:UNK:O	2:C:876:UNK:N	1.88	1.06
4:F:872:UNK:O	4:F:876:UNK:N	1.88	1.06
2:C:248:UNK:N	2:C:357:UNK:HA	1.71	1.06
4:F:512:UNK:HA	4:F:536:UNK:CB	1.85	1.05
6:H:359:UNK:O	6:H:360:UNK:O	1.75	1.05
6:H:82:UNK:CA	6:H:87:UNK:CB	2.35	1.04
2:C:537:UNK:O	2:C:541:UNK:N	1.89	1.04
2:C:698:UNK:CB	3:E:471:UNK:CB	2.35	1.04
6:H:107:UNK:HA	6:H:112:UNK:O	1.58	1.04
4:F:873:UNK:O	4:F:877:UNK:N	1.93	1.02
2:C:580:UNK:CB	3:E:684:UNK:CB	2.38	1.01
2:C:873:UNK:O	2:C:877:UNK:N	1.93	1.01
6:H:152:UNK:C	6:H:153:UNK:H2	1.74	1.00
4:F:1046:UNK:O	4:F:1050:UNK:CB	2.10	1.00
6:H:82:UNK:HA	6:H:87:UNK:CB	1.89	1.00
2:C:692:UNK:C	3:E:473:UNK:C	2.41	0.99
4:F:311:UNK:CB	4:F:347:UNK:C	2.40	0.99
2:C:1047:UNK:O	2:C:1051:UNK:CB	2.12	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:271:UNK:O	4:F:274:UNK:N	1.97	0.97
1:B:1389:UNK:O	4:F:1353:UNK:C	2.10	0.96
2:C:271:UNK:O	2:C:274:UNK:N	1.97	0.96
4:F:311:UNK:CB	4:F:347:UNK:O	2.12	0.96
2:C:695:UNK:C	3:E:474:UNK:CB	2.18	0.96
8:J:18:UNK:O	8:J:22:UNK:CA	2.12	0.96
6:H:315:UNK:CB	6:H:322:UNK:O	2.13	0.96
4:F:512:UNK:CA	4:F:536:UNK:CB	2.42	0.96
6:H:193:UNK:O	6:H:221:UNK:O	1.82	0.96
2:C:281:UNK:O	2:C:284:UNK:CA	2.16	0.93
2:C:537:UNK:O	2:C:541:UNK:CB	2.17	0.93
4:F:632:UNK:O	4:F:635:UNK:N	2.01	0.93
2:C:1350:UNK:CB	2:C:1418:UNK:CB	2.46	0.93
4:F:281:UNK:O	4:F:284:UNK:CA	2.16	0.92
2:C:585:UNK:C	3:E:689:UNK:CB	2.43	0.92
4:F:1350:UNK:CB	4:F:1416:UNK:CB	2.46	0.92
2:C:319:UNK:CB	2:C:371:UNK:C	2.48	0.91
4:F:497:UNK:O	4:F:500:UNK:CA	2.19	0.91
6:H:106:UNK:O	6:H:113:UNK:HA	1.69	0.90
4:F:632:UNK:O	4:F:634:UNK:N	2.04	0.90
1:A:3083:UNK:HA	1:A:3084:UNK:C	2.02	0.90
2:C:319:UNK:CB	2:C:371:UNK:HA	2.01	0.90
7:I:31:UNK:O	7:I:34:UNK:CA	2.19	0.90
1:B:3083:UNK:HA	1:B:3084:UNK:C	2.02	0.89
1:B:3263:UNK:O	1:B:3266:UNK:CA	2.19	0.89
2:C:584:UNK:N	3:E:687:UNK:C	2.36	0.88
2:C:431:UNK:O	2:C:433:UNK:N	2.06	0.88
3:E:365:UNK:HA	3:E:444:UNK:CB	2.03	0.88
8:J:144:UNK:O	8:J:146:UNK:N	2.06	0.88
2:C:431:UNK:O	2:C:434:UNK:N	2.06	0.88
1:A:3263:UNK:O	1:A:3266:UNK:CA	2.20	0.88
3:E:445:UNK:CB	3:E:463:UNK:CB	2.52	0.88
1:B:3263:UNK:C	1:B:3266:UNK:CB	2.52	0.88
4:F:1285:UNK:CB	4:F:1316:UNK:N	2.36	0.88
4:F:311:UNK:CB	4:F:347:UNK:CB	2.50	0.87
3:D:445:UNK:CB	3:D:463:UNK:CB	2.52	0.87
1:A:3263:UNK:C	1:A:3266:UNK:CB	2.52	0.87
2:C:281:UNK:O	2:C:284:UNK:N	2.08	0.87
8:J:144:UNK:O	8:J:145:UNK:C	2.21	0.87
2:C:536:UNK:O	2:C:540:UNK:N	2.08	0.87
3:D:365:UNK:HA	3:D:444:UNK:CB	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:199:UNK:O	6:H:200:UNK:CB	2.23	0.87
2:C:583:UNK:N	3:E:688:UNK:N	2.22	0.87
4:F:281:UNK:O	4:F:284:UNK:N	2.07	0.85
8:J:18:UNK:C	8:J:22:UNK:CB	2.55	0.85
2:C:534:UNK:O	2:C:536:UNK:N	2.10	0.83
4:F:281:UNK:O	4:F:284:UNK:CB	2.26	0.83
2:C:281:UNK:O	2:C:284:UNK:CB	2.26	0.83
4:F:457:UNK:CB	4:F:459:UNK:CB	2.56	0.83
2:C:457:UNK:CB	2:C:459:UNK:CB	2.56	0.83
2:C:1342:UNK:O	2:C:1345:UNK:CB	2.26	0.83
4:F:1044:UNK:O	4:F:1048:UNK:N	2.11	0.83
6:H:102:UNK:O	6:H:118:UNK:HA	1.79	0.83
4:F:1342:UNK:O	4:F:1345:UNK:CB	2.26	0.82
2:C:248:UNK:O	2:C:251:UNK:N	2.13	0.82
2:C:584:UNK:N	3:E:688:UNK:N	2.21	0.82
7:I:31:UNK:O	7:I:34:UNK:CB	2.28	0.82
4:F:248:UNK:O	4:F:251:UNK:N	2.13	0.81
2:C:817:UNK:O	2:C:818:UNK:C	2.29	0.81
2:C:612:UNK:H	2:C:613:UNK:C	1.94	0.81
2:C:817:UNK:C	2:C:819:UNK:N	2.43	0.81
4:F:817:UNK:O	4:F:818:UNK:C	2.29	0.81
4:F:512:UNK:CB	4:F:536:UNK:HA	2.11	0.80
2:C:476:UNK:O	2:C:478:UNK:N	2.15	0.80
2:C:586:UNK:N	3:E:689:UNK:CB	2.45	0.80
2:C:319:UNK:CB	2:C:371:UNK:O	2.29	0.80
4:F:982:UNK:CB	5:G:95:UNK:CB	2.60	0.80
4:F:836:UNK:O	4:F:840:UNK:CB	2.30	0.80
4:F:497:UNK:O	4:F:500:UNK:N	2.14	0.80
4:F:512:UNK:CB	4:F:536:UNK:CA	2.59	0.79
2:C:836:UNK:O	2:C:840:UNK:CB	2.31	0.79
8:J:50:UNK:O	8:J:51:UNK:O	2.01	0.78
4:F:824:UNK:O	4:F:827:UNK:N	2.16	0.78
7:I:115:UNK:CB	8:J:119:UNK:CB	2.61	0.78
1:B:1392:UNK:N	4:F:1353:UNK:O	2.17	0.78
4:F:497:UNK:C	4:F:500:UNK:CB	2.61	0.78
4:F:497:UNK:HA	4:F:500:UNK:CB	2.14	0.78
2:C:824:UNK:O	2:C:827:UNK:N	2.16	0.78
2:C:1209:UNK:O	2:C:1213:UNK:N	2.16	0.78
4:F:632:UNK:O	4:F:633:UNK:C	2.32	0.77
4:F:817:UNK:C	4:F:819:UNK:N	2.43	0.77
2:C:248:UNK:H2	2:C:357:UNK:HA	1.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1005:UNK:O	4:F:1007:UNK:CB	2.33	0.77
2:C:551:UNK:O	2:C:555:UNK:N	2.17	0.77
1:A:3263:UNK:O	1:A:3267:UNK:N	2.18	0.76
3:E:365:UNK:CA	3:E:444:UNK:CB	2.63	0.76
4:F:216:UNK:O	4:F:219:UNK:N	2.18	0.76
4:F:497:UNK:O	4:F:501:UNK:N	2.18	0.76
2:C:873:UNK:O	2:C:877:UNK:CB	2.34	0.76
1:B:3263:UNK:O	1:B:3267:UNK:N	2.18	0.76
2:C:216:UNK:O	2:C:219:UNK:N	2.18	0.76
2:C:319:UNK:N	2:C:371:UNK:CB	2.49	0.76
2:C:587:UNK:CB	3:E:689:UNK:O	2.33	0.76
3:D:365:UNK:CA	3:D:444:UNK:CB	2.63	0.76
4:F:1316:UNK:O	4:F:1317:UNK:N	2.19	0.76
2:C:431:UNK:O	2:C:432:UNK:C	2.33	0.76
2:C:457:UNK:CA	2:C:458:UNK:CB	2.57	0.75
4:F:271:UNK:O	4:F:274:UNK:CA	2.35	0.75
4:F:873:UNK:O	4:F:877:UNK:CB	2.34	0.75
2:C:696:UNK:N	3:E:474:UNK:CB	2.50	0.75
2:C:534:UNK:C	2:C:536:UNK:N	2.50	0.75
2:C:271:UNK:O	2:C:274:UNK:CA	2.35	0.75
4:F:872:UNK:O	4:F:876:UNK:CA	2.34	0.75
7:I:65:UNK:CB	7:I:75:UNK:CB	2.65	0.75
2:C:872:UNK:O	2:C:876:UNK:CA	2.35	0.74
6:H:103:UNK:CB	6:H:117:UNK:O	2.35	0.74
2:C:248:UNK:CB	2:C:361:UNK:N	2.48	0.74
1:B:1392:UNK:CA	4:F:1353:UNK:O	2.35	0.74
2:C:248:UNK:CA	2:C:357:UNK:HA	2.18	0.73
6:H:81:UNK:O	6:H:87:UNK:CA	2.36	0.73
2:C:531:UNK:HA	2:C:532:UNK:CB	2.18	0.73
6:H:107:UNK:HA	6:H:112:UNK:C	2.18	0.73
7:I:144:UNK:O	7:I:145:UNK:C	2.33	0.73
4:F:1044:UNK:O	4:F:1048:UNK:CB	2.37	0.72
2:C:583:UNK:O	3:E:689:UNK:CB	2.37	0.72
1:A:3433:UNK:O	1:A:3437:UNK:N	2.23	0.72
1:B:3433:UNK:O	1:B:3437:UNK:N	2.23	0.72
4:F:512:UNK:CB	4:F:536:UNK:CB	2.68	0.72
4:F:291:UNK:O	4:F:295:UNK:N	2.24	0.71
1:A:3263:UNK:HA	1:A:3266:UNK:CB	2.21	0.71
1:B:3263:UNK:HA	1:B:3266:UNK:CB	2.21	0.71
2:C:695:UNK:HA	3:E:471:UNK:CB	2.21	0.70
2:C:529:UNK:O	2:C:532:UNK:HA	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:291:UNK:O	2:C:295:UNK:N	2.24	0.70
6:H:152:UNK:C	6:H:153:UNK:N	2.53	0.70
2:C:580:UNK:CB	3:E:684:UNK:O	2.40	0.70
2:C:271:UNK:O	2:C:274:UNK:HA	1.92	0.69
2:C:536:UNK:O	2:C:540:UNK:CA	2.39	0.69
2:C:1121:UNK:O	2:C:1124:UNK:N	2.25	0.69
2:C:616:UNK:O	2:C:619:UNK:N	2.26	0.69
4:F:1121:UNK:O	4:F:1124:UNK:N	2.25	0.69
6:H:107:UNK:CB	6:H:111:UNK:HA	2.22	0.69
2:C:1210:UNK:O	2:C:1214:UNK:CB	2.42	0.68
6:H:106:UNK:O	6:H:114:UNK:N	2.27	0.68
2:C:689:UNK:O	2:C:693:UNK:N	2.26	0.68
4:F:1255:UNK:O	4:F:1259:UNK:N	2.27	0.68
2:C:306:UNK:O	2:C:310:UNK:N	2.27	0.68
2:C:1391:UNK:O	2:C:1395:UNK:N	2.27	0.68
4:F:1207:UNK:O	4:F:1211:UNK:N	2.27	0.68
6:H:107:UNK:CB	6:H:111:UNK:C	2.72	0.68
2:C:497:UNK:C	2:C:501:UNK:CB	2.67	0.67
2:C:583:UNK:N	3:E:687:UNK:C	2.56	0.67
4:F:213:UNK:N	4:F:214:UNK:CB	2.28	0.67
4:F:271:UNK:O	4:F:274:UNK:HA	1.92	0.67
4:F:306:UNK:O	4:F:310:UNK:N	2.27	0.67
2:C:694:UNK:C	3:E:471:UNK:C	2.73	0.67
4:F:1285:UNK:CB	4:F:1316:UNK:H2	2.08	0.67
2:C:580:UNK:HA	3:E:684:UNK:O	1.93	0.67
4:F:497:UNK:C	4:F:500:UNK:N	2.57	0.67
3:D:445:UNK:O	3:D:462:UNK:CB	2.42	0.67
4:F:1285:UNK:CB	4:F:1316:UNK:CB	2.72	0.67
2:C:281:UNK:O	2:C:284:UNK:C	2.42	0.67
3:E:445:UNK:O	3:E:462:UNK:CB	2.43	0.67
2:C:1255:UNK:O	2:C:1259:UNK:N	2.27	0.67
4:F:281:UNK:O	4:F:284:UNK:C	2.42	0.66
1:B:3419:UNK:O	1:B:3423:UNK:CB	2.43	0.66
1:A:3419:UNK:O	1:A:3423:UNK:CB	2.43	0.66
1:A:3402:UNK:O	1:A:3406:UNK:N	2.28	0.66
1:B:3402:UNK:O	1:B:3406:UNK:N	2.29	0.66
4:F:948:UNK:O	4:F:949:UNK:CB	2.40	0.66
4:F:212:UNK:C	4:F:214:UNK:CB	2.74	0.66
2:C:583:UNK:C	3:E:687:UNK:C	2.74	0.66
6:H:107:UNK:CA	6:H:112:UNK:O	2.41	0.66
2:C:497:UNK:O	2:C:501:UNK:CA	2.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1161:UNK:HA	2:C:1317:UNK:CB	2.26	0.65
1:B:3260:UNK:CB	1:B:3430:UNK:CB	2.74	0.65
4:F:632:UNK:C	4:F:634:UNK:N	2.59	0.65
4:F:1005:UNK:O	4:F:1006:UNK:C	2.43	0.65
2:C:1049:UNK:O	2:C:1052:UNK:N	2.29	0.65
1:A:3260:UNK:CB	1:A:3430:UNK:CB	2.74	0.65
2:C:476:UNK:C	2:C:478:UNK:N	2.57	0.65
4:F:351:UNK:C	4:F:353:UNK:N	2.58	0.65
8:J:144:UNK:C	8:J:146:UNK:N	2.52	0.65
2:C:817:UNK:O	2:C:820:UNK:N	2.30	0.64
4:F:351:UNK:O	4:F:352:UNK:C	2.45	0.64
4:F:817:UNK:O	4:F:820:UNK:N	2.30	0.64
2:C:351:UNK:C	2:C:353:UNK:N	2.58	0.64
2:C:583:UNK:N	3:E:687:UNK:CA	2.32	0.64
2:C:692:UNK:C	3:E:473:UNK:O	2.34	0.64
6:H:101:UNK:O	6:H:119:UNK:C	2.45	0.64
2:C:351:UNK:O	2:C:352:UNK:C	2.45	0.64
1:A:3432:UNK:O	1:A:3436:UNK:N	2.31	0.64
4:F:1152:UNK:O	4:F:1156:UNK:CB	2.45	0.64
1:B:3432:UNK:O	1:B:3436:UNK:N	2.31	0.63
2:C:1152:UNK:O	2:C:1156:UNK:CB	2.45	0.63
6:H:200:UNK:C	6:H:201:UNK:N	2.61	0.63
2:C:537:UNK:O	2:C:541:UNK:CA	2.46	0.63
1:A:3263:UNK:CA	1:A:3266:UNK:CB	2.77	0.63
2:C:1062:UNK:O	2:C:1065:UNK:N	2.32	0.63
4:F:817:UNK:O	4:F:819:UNK:CA	2.45	0.63
1:B:3263:UNK:O	1:B:3266:UNK:C	2.47	0.63
1:B:3420:UNK:O	1:B:3424:UNK:N	2.32	0.63
2:C:817:UNK:O	2:C:819:UNK:CA	2.45	0.62
1:A:3420:UNK:O	1:A:3424:UNK:N	2.32	0.62
2:C:616:UNK:O	2:C:617:UNK:C	2.48	0.62
1:A:3250:UNK:O	1:A:3253:UNK:CB	2.48	0.62
2:C:431:UNK:C	2:C:433:UNK:N	2.62	0.62
6:H:107:UNK:CB	6:H:111:UNK:CA	2.78	0.62
2:C:690:UNK:O	3:E:473:UNK:HA	1.99	0.62
2:C:1342:UNK:O	2:C:1346:UNK:N	2.33	0.62
4:F:457:UNK:CA	4:F:458:UNK:CB	2.56	0.62
4:F:1116:UNK:O	4:F:1119:UNK:N	2.32	0.62
1:A:3263:UNK:O	1:A:3266:UNK:C	2.47	0.62
1:B:3250:UNK:O	1:B:3253:UNK:CB	2.48	0.62
10:M:54:UNK:C	10:M:56:UNK:H2	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:457:UNK:CB	4:F:459:UNK:CA	2.78	0.62
4:F:1342:UNK:O	4:F:1346:UNK:N	2.33	0.62
2:C:457:UNK:CB	2:C:459:UNK:CA	2.78	0.61
4:F:262:UNK:O	4:F:266:UNK:N	2.33	0.61
4:F:1285:UNK:HA	4:F:1316:UNK:CB	2.30	0.61
2:C:689:UNK:O	2:C:693:UNK:CA	2.47	0.61
2:C:692:UNK:O	3:E:473:UNK:C	2.48	0.61
1:B:3263:UNK:CA	1:B:3266:UNK:CB	2.77	0.61
2:C:262:UNK:O	2:C:266:UNK:N	2.33	0.61
2:C:1116:UNK:O	2:C:1119:UNK:N	2.32	0.61
4:F:1285:UNK:CA	4:F:1316:UNK:CB	2.79	0.61
4:F:1254:UNK:O	4:F:1258:UNK:CB	2.49	0.61
2:C:1254:UNK:O	2:C:1258:UNK:CB	2.49	0.61
4:F:497:UNK:CA	4:F:500:UNK:CB	2.79	0.61
4:F:1151:UNK:O	4:F:1155:UNK:N	2.34	0.60
2:C:1151:UNK:O	2:C:1155:UNK:N	2.34	0.60
2:C:694:UNK:O	3:E:471:UNK:CB	2.50	0.60
2:C:1350:UNK:CB	2:C:1418:UNK:C	2.79	0.60
2:C:1140:UNK:O	2:C:1144:UNK:N	2.35	0.60
4:F:1350:UNK:CB	4:F:1416:UNK:C	2.79	0.60
4:F:248:UNK:O	4:F:249:UNK:C	2.48	0.60
6:H:106:UNK:O	6:H:113:UNK:CA	2.46	0.60
2:C:1121:UNK:O	2:C:1122:UNK:C	2.50	0.60
2:C:1350:UNK:CB	2:C:1418:UNK:CA	2.80	0.60
4:F:626:UNK:O	4:F:630:UNK:N	2.34	0.60
4:F:1282:UNK:C	4:F:1316:UNK:CB	2.79	0.60
2:C:319:UNK:CA	2:C:371:UNK:CB	2.79	0.59
2:C:583:UNK:CA	3:E:687:UNK:C	2.42	0.59
3:D:599:UNK:HA	3:D:626:UNK:O	2.02	0.59
2:C:248:UNK:O	2:C:249:UNK:C	2.48	0.59
4:F:1121:UNK:O	4:F:1122:UNK:C	2.50	0.59
8:J:144:UNK:O	8:J:147:UNK:N	2.35	0.59
4:F:1282:UNK:O	4:F:1316:UNK:N	2.36	0.59
1:A:3419:UNK:O	1:A:3423:UNK:N	2.36	0.59
2:C:1161:UNK:CB	2:C:1318:UNK:CB	2.81	0.59
4:F:1350:UNK:CB	4:F:1416:UNK:CA	2.80	0.59
1:B:3419:UNK:O	1:B:3423:UNK:N	2.36	0.59
4:F:397:UNK:O	4:F:401:UNK:N	2.35	0.59
4:F:874:UNK:O	4:F:878:UNK:N	2.35	0.59
2:C:248:UNK:HA	2:C:357:UNK:HA	1.84	0.59
4:F:1140:UNK:O	4:F:1144:UNK:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:580:UNK:CA	3:E:684:UNK:O	2.51	0.59
3:E:599:UNK:HA	3:E:626:UNK:O	2.02	0.59
4:F:824:UNK:O	4:F:825:UNK:C	2.50	0.59
2:C:307:UNK:O	2:C:311:UNK:N	2.36	0.58
4:F:1152:UNK:O	4:F:1156:UNK:N	2.36	0.58
4:F:1255:UNK:O	4:F:1259:UNK:CB	2.52	0.58
2:C:1391:UNK:O	2:C:1395:UNK:CB	2.52	0.58
8:J:130:UNK:CB	8:J:174:UNK:CB	2.81	0.58
2:C:874:UNK:O	2:C:878:UNK:N	2.35	0.58
2:C:824:UNK:O	2:C:825:UNK:C	2.50	0.58
4:F:568:UNK:O	4:F:569:UNK:C	2.51	0.58
4:F:307:UNK:O	4:F:311:UNK:N	2.37	0.58
2:C:641:UNK:O	2:C:642:UNK:C	2.51	0.58
2:C:1152:UNK:O	2:C:1156:UNK:N	2.36	0.58
2:C:1201:UNK:O	2:C:1205:UNK:N	2.37	0.58
2:C:583:UNK:C	3:E:689:UNK:CB	2.80	0.57
4:F:216:UNK:O	4:F:217:UNK:C	2.52	0.57
4:F:281:UNK:O	4:F:284:UNK:O	2.22	0.57
1:A:3370:UNK:O	1:A:3374:UNK:N	2.38	0.57
2:C:281:UNK:O	2:C:284:UNK:O	2.22	0.57
6:H:82:UNK:HA	6:H:87:UNK:C	2.33	0.57
2:C:566:UNK:O	2:C:567:UNK:C	2.51	0.57
2:C:643:UNK:O	2:C:644:UNK:C	2.52	0.57
2:C:1255:UNK:O	2:C:1259:UNK:CB	2.51	0.57
4:F:603:UNK:O	4:F:604:UNK:C	2.51	0.57
2:C:1202:UNK:O	2:C:1206:UNK:CB	2.52	0.57
8:J:41:UNK:O	8:J:44:UNK:CB	2.53	0.57
1:B:3370:UNK:O	1:B:3374:UNK:N	2.38	0.57
2:C:216:UNK:O	2:C:217:UNK:C	2.52	0.57
2:C:601:UNK:O	2:C:602:UNK:C	2.52	0.57
4:F:351:UNK:O	4:F:353:UNK:N	2.38	0.57
2:C:251:UNK:CB	2:C:357:UNK:CB	2.82	0.57
4:F:451:UNK:O	4:F:452:UNK:C	2.51	0.57
4:F:1068:UNK:HA	4:F:1069:UNK:C	2.34	0.57
2:C:1139:UNK:O	2:C:1143:UNK:N	2.38	0.56
4:F:567:UNK:O	4:F:568:UNK:C	2.51	0.56
4:F:1139:UNK:O	4:F:1143:UNK:N	2.38	0.56
4:F:511:UNK:O	4:F:512:UNK:C	2.51	0.56
4:F:1043:UNK:O	4:F:1047:UNK:CB	2.53	0.56
7:I:144:UNK:O	7:I:146:UNK:N	2.38	0.56
2:C:351:UNK:O	2:C:353:UNK:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:512:UNK:O	4:F:513:UNK:C	2.51	0.56
2:C:603:UNK:O	2:C:604:UNK:C	2.51	0.56
1:A:3482:UNK:O	1:A:3486:UNK:N	2.39	0.56
2:C:567:UNK:O	2:C:568:UNK:C	2.51	0.56
2:C:1023:UNK:CA	2:C:1108:UNK:CB	2.83	0.56
4:F:602:UNK:O	4:F:603:UNK:C	2.51	0.56
4:F:1369:UNK:O	4:F:1373:UNK:CB	2.54	0.56
6:H:181:UNK:O	6:H:183:UNK:N	2.39	0.56
2:C:871:UNK:O	2:C:875:UNK:N	2.39	0.56
4:F:871:UNK:O	4:F:875:UNK:N	2.39	0.56
1:B:3482:UNK:O	1:B:3486:UNK:N	2.39	0.55
4:F:498:UNK:C	4:F:500:UNK:N	2.58	0.55
2:C:1370:UNK:O	2:C:1374:UNK:CB	2.54	0.55
4:F:513:UNK:O	4:F:514:UNK:C	2.52	0.55
2:C:587:UNK:N	3:E:689:UNK:CB	2.70	0.55
2:C:602:UNK:O	2:C:603:UNK:C	2.52	0.55
2:C:552:UNK:O	2:C:556:UNK:N	2.39	0.55
7:I:29:UNK:O	7:I:30:UNK:C	2.53	0.55
1:A:3886:UNK:C	1:A:3887:UNK:N	2.70	0.55
2:C:288:UNK:O	2:C:289:UNK:C	2.53	0.55
2:C:568:UNK:O	2:C:569:UNK:C	2.52	0.55
4:F:1282:UNK:O	4:F:1316:UNK:CA	2.55	0.55
2:C:873:UNK:O	2:C:877:UNK:CA	2.55	0.54
6:H:103:UNK:CA	6:H:117:UNK:O	2.54	0.54
4:F:288:UNK:O	4:F:289:UNK:C	2.53	0.54
4:F:566:UNK:O	4:F:567:UNK:C	2.52	0.54
6:H:151:UNK:O	6:H:153:UNK:N	2.40	0.54
7:I:18:UNK:O	7:I:22:UNK:N	2.41	0.54
4:F:873:UNK:O	4:F:877:UNK:CA	2.55	0.54
2:C:612:UNK:CB	2:C:613:UNK:CB	2.85	0.54
4:F:1045:UNK:O	4:F:1049:UNK:CB	2.56	0.54
1:B:3886:UNK:C	1:B:3887:UNK:N	2.70	0.54
2:C:642:UNK:O	2:C:643:UNK:C	2.52	0.54
4:F:281:UNK:C	4:F:284:UNK:N	2.71	0.54
2:C:531:UNK:CA	2:C:532:UNK:CB	2.86	0.54
4:F:311:UNK:CB	4:F:347:UNK:CA	2.86	0.54
2:C:281:UNK:C	2:C:284:UNK:N	2.71	0.53
4:F:601:UNK:O	4:F:602:UNK:C	2.52	0.53
2:C:1153:UNK:CB	2:C:1278:UNK:CB	2.86	0.53
2:C:993:UNK:O	2:C:994:UNK:C	2.57	0.53
2:C:1350:UNK:CB	2:C:1418:UNK:O	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1316:UNK:C	4:F:1317:UNK:N	2.70	0.53
1:B:2145:UNK:O	1:B:2148:UNK:N	2.42	0.53
2:C:551:UNK:O	2:C:555:UNK:CB	2.57	0.53
4:F:1350:UNK:CB	4:F:1416:UNK:O	2.57	0.53
1:A:2145:UNK:O	1:A:2148:UNK:N	2.42	0.53
4:F:1044:UNK:O	4:F:1048:UNK:CA	2.57	0.53
2:C:1202:UNK:O	2:C:1206:UNK:N	2.42	0.52
3:D:365:UNK:CB	3:D:444:UNK:CB	2.87	0.52
3:E:365:UNK:CB	3:E:444:UNK:CB	2.87	0.52
2:C:998:UNK:C	2:C:1000:UNK:N	2.71	0.52
6:H:363:UNK:O	6:H:364:UNK:CB	2.58	0.52
4:F:457:UNK:CA	4:F:459:UNK:N	2.72	0.52
4:F:497:UNK:O	4:F:500:UNK:C	2.57	0.52
4:F:984:UNK:O	4:F:985:UNK:C	2.58	0.52
2:C:612:UNK:N	2:C:613:UNK:CB	2.73	0.51
2:C:616:UNK:O	2:C:618:UNK:N	2.42	0.51
2:C:742:UNK:HA	2:C:806:UNK:CB	2.40	0.51
6:H:114:UNK:O	6:H:115:UNK:CB	2.58	0.51
1:B:1389:UNK:O	4:F:1353:UNK:O	2.27	0.51
2:C:986:UNK:CB	6:H:102:UNK:CB	2.88	0.51
6:H:102:UNK:O	6:H:118:UNK:CA	2.55	0.51
7:I:98:UNK:O	7:I:116:UNK:CB	2.59	0.51
2:C:612:UNK:CA	2:C:613:UNK:CB	2.89	0.51
6:H:229:UNK:O	6:H:230:UNK:CB	2.58	0.51
6:H:200:UNK:C	6:H:201:UNK:H2	2.24	0.51
1:B:3495:UNK:O	1:B:3499:UNK:N	2.44	0.51
6:H:348:UNK:CB	6:H:364:UNK:O	2.59	0.51
7:I:64:UNK:HA	7:I:75:UNK:O	2.11	0.51
1:A:3495:UNK:O	1:A:3499:UNK:N	2.44	0.50
1:B:4292:UNK:O	1:B:4293:UNK:C	2.59	0.50
1:A:3263:UNK:O	1:A:3266:UNK:N	2.45	0.50
1:A:3883:UNK:O	1:A:3887:UNK:N	2.45	0.50
1:B:3263:UNK:O	1:B:3266:UNK:N	2.45	0.50
6:H:108:UNK:N	6:H:112:UNK:O	2.45	0.50
6:H:152:UNK:CA	6:H:153:UNK:H2	2.25	0.50
1:A:4292:UNK:O	1:A:4293:UNK:C	2.58	0.50
7:I:99:UNK:O	7:I:100:UNK:CB	2.60	0.50
2:C:457:UNK:CA	2:C:459:UNK:N	2.72	0.49
2:C:1049:UNK:O	2:C:1050:UNK:C	2.60	0.49
1:B:3883:UNK:O	1:B:3887:UNK:N	2.45	0.49
2:C:536:UNK:C	2:C:540:UNK:CB	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:31:UNK:O	7:I:35:UNK:N	2.45	0.49
1:A:3373:UNK:O	1:A:3377:UNK:N	2.46	0.49
2:C:871:UNK:O	2:C:875:UNK:CB	2.60	0.49
4:F:984:UNK:O	4:F:987:UNK:N	2.45	0.49
4:F:1328:UNK:O	4:F:1331:UNK:CB	2.61	0.49
6:H:103:UNK:HA	6:H:117:UNK:O	2.12	0.49
1:B:1389:UNK:N	4:F:1349:UNK:O	2.46	0.49
6:H:359:UNK:C	6:H:360:UNK:O	2.58	0.48
1:B:3373:UNK:O	1:B:3377:UNK:N	2.46	0.48
4:F:871:UNK:O	4:F:875:UNK:CB	2.61	0.48
4:F:1066:UNK:C	4:F:1068:UNK:H	2.26	0.48
14:R:73:UNK:C	14:R:75:UNK:N	2.75	0.48
2:C:616:UNK:C	2:C:618:UNK:N	2.76	0.48
2:C:1328:UNK:O	2:C:1331:UNK:CB	2.61	0.48
4:F:281:UNK:HA	4:F:284:UNK:CB	2.43	0.48
1:A:2147:UNK:O	1:A:2363:UNK:N	2.46	0.48
2:C:1268:UNK:O	2:C:1272:UNK:N	2.46	0.48
11:N:33:UNK:C	11:N:35:UNK:N	2.73	0.48
4:F:272:UNK:C	4:F:274:UNK:N	2.73	0.48
4:F:512:UNK:N	4:F:536:UNK:CB	2.76	0.48
2:C:248:UNK:C	2:C:250:UNK:N	2.76	0.48
1:B:2147:UNK:O	1:B:2363:UNK:N	2.47	0.47
2:C:281:UNK:HA	2:C:284:UNK:CB	2.44	0.47
2:C:1342:UNK:O	2:C:1345:UNK:CA	2.62	0.47
6:H:175:UNK:C	6:H:177:UNK:N	2.75	0.47
1:B:3823:UNK:O	1:B:3824:UNK:CB	2.61	0.47
2:C:272:UNK:C	2:C:274:UNK:N	2.73	0.47
3:E:360:UNK:HA	3:E:368:UNK:O	2.15	0.47
4:F:248:UNK:C	4:F:250:UNK:N	2.76	0.47
2:C:261:UNK:O	2:C:265:UNK:N	2.48	0.47
10:M:55:UNK:O	10:M:57:UNK:N	2.48	0.47
2:C:579:UNK:O	3:E:687:UNK:CA	2.63	0.47
4:F:261:UNK:O	4:F:265:UNK:N	2.48	0.47
9:K:13:UNK:O	9:K:14:UNK:C	2.63	0.47
10:M:33:UNK:O	10:M:34:UNK:C	2.61	0.47
2:C:1204:UNK:O	2:C:1205:UNK:C	2.63	0.47
1:A:3823:UNK:O	1:A:3824:UNK:CB	2.61	0.47
2:C:585:UNK:N	3:E:689:UNK:N	2.19	0.47
3:D:360:UNK:HA	3:D:368:UNK:O	2.15	0.46
4:F:1342:UNK:O	4:F:1345:UNK:CA	2.62	0.46
2:C:352:UNK:O	2:C:355:UNK:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:993:UNK:O	4:F:994:UNK:C	2.61	0.46
2:C:693:UNK:N	3:E:473:UNK:C	2.79	0.46
4:F:352:UNK:O	4:F:355:UNK:N	2.49	0.46
7:I:31:UNK:O	7:I:32:UNK:C	2.63	0.46
7:I:82:UNK:O	7:I:83:UNK:CB	2.62	0.46
1:A:2951:UNK:O	1:A:2955:UNK:N	2.49	0.46
2:C:824:UNK:O	2:C:826:UNK:N	2.49	0.46
4:F:591:UNK:O	4:F:592:UNK:C	2.64	0.46
1:B:2169:UNK:HA	1:B:2170:UNK:CB	2.45	0.46
1:B:2951:UNK:O	1:B:2955:UNK:N	2.49	0.46
2:C:587:UNK:CB	3:E:689:UNK:C	2.93	0.46
2:C:530:UNK:C	2:C:532:UNK:HA	2.46	0.45
1:A:3250:UNK:O	1:A:3253:UNK:N	2.50	0.45
4:F:824:UNK:O	4:F:826:UNK:N	2.49	0.45
1:A:2169:UNK:HA	1:A:2170:UNK:CB	2.46	0.45
4:F:216:UNK:C	4:F:218:UNK:N	2.79	0.45
6:H:356:UNK:N	6:H:357:UNK:CA	2.79	0.45
2:C:1161:UNK:CA	2:C:1317:UNK:CB	2.93	0.45
2:C:824:UNK:C	2:C:826:UNK:N	2.80	0.45
11:N:33:UNK:O	11:N:34:UNK:C	2.64	0.45
1:B:3250:UNK:O	1:B:3253:UNK:N	2.49	0.45
6:H:197:UNK:O	6:H:198:UNK:CB	2.64	0.45
2:C:521:UNK:O	2:C:525:UNK:N	2.50	0.44
1:B:2197:UNK:HA	1:B:2198:UNK:CB	2.48	0.44
2:C:1209:UNK:O	2:C:1213:UNK:CB	2.66	0.44
1:A:2230:UNK:O	1:A:2231:UNK:C	2.66	0.44
1:B:2230:UNK:O	1:B:2231:UNK:C	2.66	0.44
4:F:824:UNK:C	4:F:826:UNK:N	2.79	0.43
2:C:702:UNK:O	2:C:706:UNK:N	2.51	0.43
2:C:522:UNK:HA	3:E:330:UNK:CA	2.44	0.43
6:H:99:UNK:CB	6:H:103:UNK:O	2.66	0.43
9:L:52:UNK:HA	9:L:53:UNK:HA	1.76	0.43
2:C:534:UNK:O	2:C:535:UNK:CB	2.61	0.43
7:I:146:UNK:HA	7:I:147:UNK:HA	1.80	0.43
14:R:73:UNK:O	14:R:75:UNK:N	2.51	0.43
8:J:89:UNK:C	8:J:90:UNK:O	2.67	0.43
1:A:2328:UNK:O	1:A:2329:UNK:C	2.67	0.43
11:N:31:UNK:O	11:N:32:UNK:C	2.67	0.43
2:C:612:UNK:N	2:C:613:UNK:C	2.72	0.42
2:C:1142:UNK:O	2:C:1146:UNK:N	2.52	0.42
4:F:1142:UNK:O	4:F:1146:UNK:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3410:UNK:O	1:A:3411:UNK:C	2.67	0.42
1:B:3410:UNK:O	1:B:3411:UNK:C	2.67	0.42
1:A:2197:UNK:HA	1:A:2198:UNK:CB	2.48	0.42
2:C:289:UNK:C	2:C:291:UNK:N	2.81	0.42
2:C:692:UNK:O	3:E:474:UNK:N	2.52	0.42
1:B:2328:UNK:O	1:B:2329:UNK:C	2.67	0.42
1:A:3420:UNK:O	1:A:3424:UNK:CB	2.67	0.42
2:C:216:UNK:C	2:C:218:UNK:N	2.79	0.42
11:N:33:UNK:O	11:N:35:UNK:N	2.52	0.42
1:B:3420:UNK:O	1:B:3424:UNK:CB	2.67	0.42
2:C:612:UNK:N	2:C:613:UNK:CA	2.83	0.42
2:C:583:UNK:CA	3:E:688:UNK:N	2.74	0.42
2:C:1121:UNK:C	2:C:1123:UNK:N	2.81	0.42
2:C:1328:UNK:O	2:C:1332:UNK:N	2.53	0.42
2:C:497:UNK:O	2:C:501:UNK:N	2.53	0.41
10:M:54:UNK:O	10:M:56:UNK:N	2.35	0.41
4:F:1208:UNK:O	4:F:1212:UNK:CB	2.68	0.41
4:F:1328:UNK:O	4:F:1332:UNK:N	2.53	0.41
11:N:19:UNK:O	11:N:20:UNK:C	2.69	0.41
2:C:388:UNK:O	2:C:391:UNK:CB	2.68	0.41
4:F:289:UNK:C	4:F:291:UNK:N	2.81	0.41
10:M:55:UNK:O	10:M:56:UNK:C	2.69	0.41
4:F:1121:UNK:C	4:F:1123:UNK:N	2.81	0.41
1:B:3264:UNK:C	1:B:3266:UNK:N	2.78	0.41
1:A:2807:UNK:O	1:A:2811:UNK:N	2.54	0.41
4:F:1343:UNK:HA	4:F:1346:UNK:CB	2.51	0.41
5:G:392:UNK:C	5:G:394:UNK:N	2.84	0.41
8:J:89:UNK:O	8:J:90:UNK:O	2.38	0.41
1:B:2807:UNK:O	1:B:2811:UNK:N	2.54	0.41
6:H:318:UNK:O	6:H:321:UNK:N	2.53	0.41
7:I:144:UNK:C	7:I:146:UNK:N	2.81	0.41
10:M:58:UNK:O	10:M:111:UNK:O	2.38	0.41
11:N:84:UNK:C	11:N:86:UNK:N	2.83	0.41
2:C:248:UNK:H2	2:C:357:UNK:CA	2.25	0.40
2:C:1343:UNK:HA	2:C:1346:UNK:CB	2.51	0.40
3:D:640:UNK:C	3:D:642:UNK:N	2.84	0.40
7:I:66:UNK:O	7:I:94:UNK:HA	2.21	0.40
8:J:50:UNK:O	8:J:51:UNK:C	2.67	0.40
2:C:1368:UNK:O	2:C:1371:UNK:N	2.54	0.40
3:D:582:UNK:HA	3:D:592:UNK:O	2.21	0.40
11:N:47:UNK:O	11:N:48:UNK:C	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:296:UNK:O	6:H:300:UNK:N	2.54	0.40
1:B:3214:UNK:O	1:B:3218:UNK:N	2.55	0.40
3:E:316:UNK:O	3:E:322:UNK:HA	2.21	0.40
3:E:599:UNK:CA	3:E:626:UNK:O	2.70	0.40
4:F:994:UNK:HA	4:F:995:UNK:HA	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	F	29
2	C	27
1	A	14
1	B	14
7	I	7
8	J	7
5	G	3
3	D	3
3	E	3
6	H	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	1161:UNK	C	1190:UNK	N	65.65
1	F	1161:UNK	C	1190:UNK	N	65.10
1	C	1354:UNK	C	1356:UNK	N	52.82
1	F	1354:UNK	C	1356:UNK	N	52.47
1	C	1389:UNK	C	1391:UNK	N	50.97
1	F	1388:UNK	C	1390:UNK	N	50.26
1	C	1070:UNK	C	1103:UNK	N	45.07
1	F	1009:UNK	C	1039:UNK	N	43.38
1	F	1223:UNK	C	1254:UNK	N	41.42
1	C	1223:UNK	C	1254:UNK	N	40.65
1	F	950:UNK	C	968:UNK	N	39.06
1	F	1070:UNK	C	1103:UNK	N	35.87
1	C	950:UNK	C	968:UNK	N	34.77
1	F	311:UNK	C	328:UNK	N	33.44
1	C	1010:UNK	C	1012:UNK	N	32.93
1	G	73:UNK	C	89:UNK	N	29.12
1	F	474:UNK	C	484:UNK	N	28.56
1	C	1025:UNK	C	1033:UNK	N	25.99
1	F	514:UNK	C	519:UNK	N	21.59
1	F	718:UNK	C	728:UNK	N	21.33
1	C	514:UNK	C	519:UNK	N	20.21
1	I	51:UNK	C	61:UNK	N	19.81
1	J	78:UNK	C	82:UNK	N	19.13
1	J	51:UNK	C	61:UNK	N	18.63
1	C	767:UNK	C	773:UNK	N	18.57
1	F	644:UNK	C	679:UNK	N	18.32

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	417:UNK	C	419:UNK	N	18.30
1	F	569:UNK	C	576:UNK	N	17.15
1	C	787:UNK	C	804:UNK	N	17.11
1	C	718:UNK	C	728:UNK	N	16.76
1	F	742:UNK	C	753:UNK	N	16.70
1	A	2389:UNK	C	2408:UNK	N	16.60
1	B	2389:UNK	C	2408:UNK	N	16.60
1	F	417:UNK	C	423:UNK	N	16.51
1	C	374:UNK	C	381:UNK	N	16.27
1	A	4361:UNK	C	4379:UNK	N	16.15
1	B	4361:UNK	C	4379:UNK	N	16.15
1	F	530:UNK	C	534:UNK	N	15.31
1	G	201:UNK	C	211:UNK	N	15.26
1	F	373:UNK	C	381:UNK	N	15.18
1	D	383:UNK	C	441:UNK	N	14.69
1	E	383:UNK	C	441:UNK	N	14.69
1	A	4595:UNK	C	4603:UNK	N	14.62
1	B	4595:UNK	C	4603:UNK	N	14.62
1	C	604:UNK	C	612:UNK	N	14.39
1	C	237:UNK	C	248:UNK	N	14.35
1	F	237:UNK	C	248:UNK	N	14.35
1	F	604:UNK	C	611:UNK	N	13.86
1	I	119:UNK	C	125:UNK	N	13.52
1	A	1987:UNK	C	1996:UNK	N	13.18
1	B	1987:UNK	C	1996:UNK	N	13.18
1	C	569:UNK	C	576:UNK	N	13.17
1	C	887:UNK	C	915:UNK	N	13.07
1	F	887:UNK	C	915:UNK	N	13.07
1	J	90:UNK	C	94:UNK	N	12.85
1	C	1285:UNK	C	1316:UNK	N	12.77
1	C	478:UNK	C	488:UNK	N	12.61
1	A	4498:UNK	C	4502:UNK	N	12.60
1	B	4498:UNK	C	4502:UNK	N	12.60
1	C	532:UNK	C	534:UNK	N	12.54
1	C	853:UNK	C	862:UNK	N	12.53
1	F	853:UNK	C	862:UNK	N	12.53
1	F	787:UNK	C	804:UNK	N	12.30
1	A	4545:UNK	C	4557:UNK	N	12.27
1	B	4545:UNK	C	4557:UNK	N	12.27
1	F	767:UNK	C	773:UNK	N	12.24
1	F	453:UNK	C	456:UNK	N	12.10
1	J	119:UNK	C	125:UNK	N	11.74

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	319:UNK	C	328:UNK	N	11.38
1	I	78:UNK	C	82:UNK	N	11.27
1	A	2115:UNK	C	2128:UNK	N	10.73
1	B	2115:UNK	C	2128:UNK	N	10.73
1	C	644:UNK	C	679:UNK	N	9.60
1	C	742:UNK	C	753:UNK	N	9.45
1	A	1768:UNK	C	1775:UNK	N	8.82
1	B	1768:UNK	C	1775:UNK	N	8.82
1	J	147:UNK	C	157:UNK	N	8.69
1	I	90:UNK	C	94:UNK	N	8.37
1	H	179:UNK	C	181:UNK	N	7.77
1	A	3974:UNK	C	3978:UNK	N	7.61
1	B	3974:UNK	C	3978:UNK	N	7.61
1	G	345:UNK	C	375:UNK	N	7.49
1	I	148:UNK	C	157:UNK	N	7.15
1	I	66:UNK	C	73:UNK	N	7.13
1	C	454:UNK	C	456:UNK	N	6.88
1	D	566:UNK	C	573:UNK	N	6.80
1	E	566:UNK	C	573:UNK	N	6.80
1	D	605:UNK	C	621:UNK	N	6.16
1	E	605:UNK	C	621:UNK	N	6.16
1	J	66:UNK	C	73:UNK	N	6.08
1	A	4401:UNK	C	4403:UNK	N	5.96
1	B	4401:UNK	C	4403:UNK	N	5.96
1	J	99:UNK	C	114:UNK	N	5.31
1	I	100:UNK	C	114:UNK	N	5.09
1	F	1285:UNK	C	1316:UNK	N	4.77
1	A	3895:UNK	C	3897:UNK	N	3.73
1	B	3895:UNK	C	3897:UNK	N	3.73
1	A	3846:UNK	C	3849:UNK	N	3.32
1	B	3846:UNK	C	3849:UNK	N	3.32
1	F	543:UNK	C	545:UNK	N	3.27
1	B	4562:UNK	C	4563:UNK	N	3.05
1	A	4562:UNK	C	4563:UNK	N	3.04
1	A	3886:UNK	C	3887:UNK	N	2.70
1	B	3886:UNK	C	3887:UNK	N	2.70
1	F	1316:UNK	C	1317:UNK	N	2.70
1	H	200:UNK	C	201:UNK	N	2.61
1	H	152:UNK	C	153:UNK	N	2.53
1	F	213:UNK	C	214:UNK	N	2.10
1	C	804:UNK	C	805:UNK	N	1.05
1	F	804:UNK	C	805:UNK	N	1.05

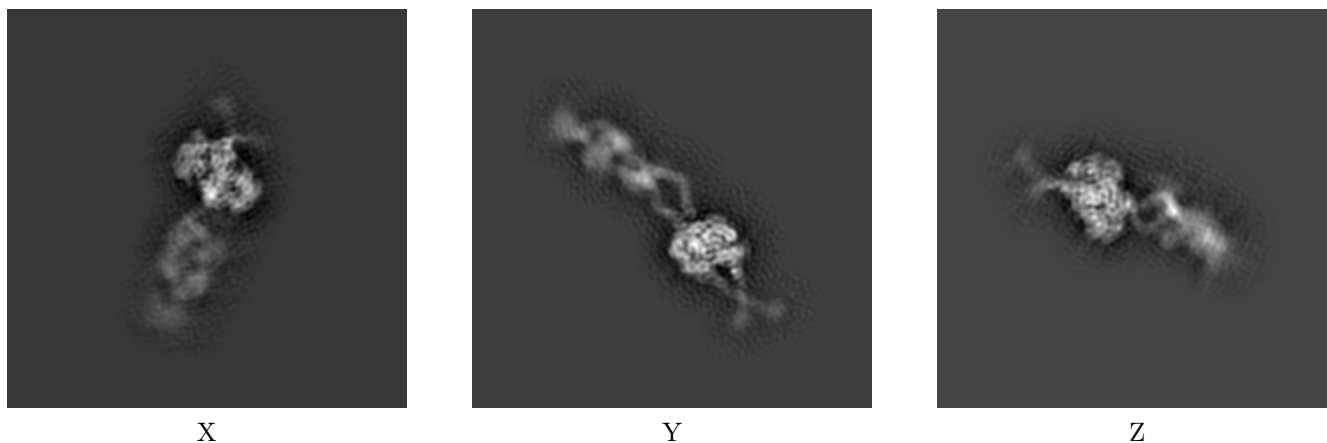
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3705. 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](#)

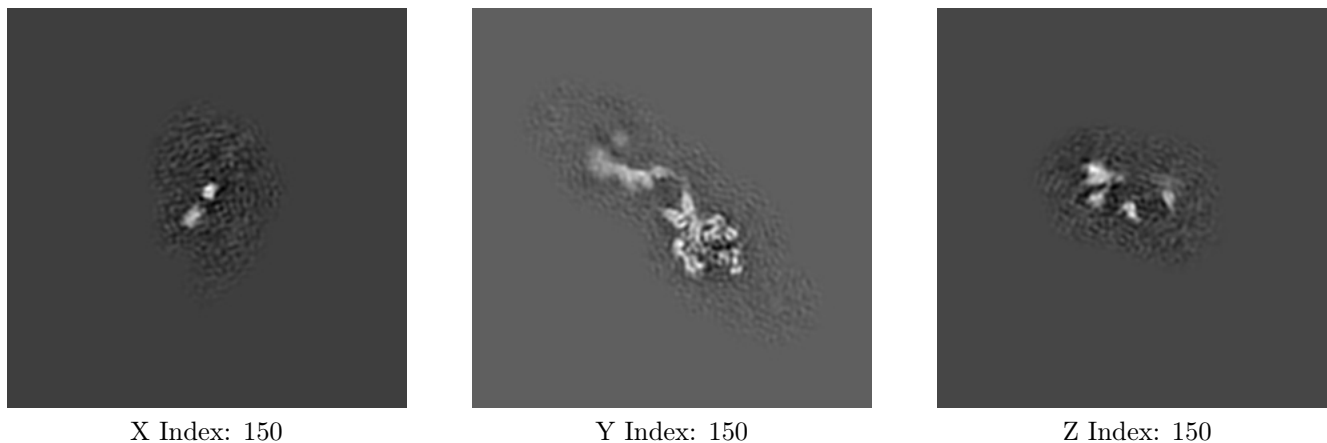
6.1.1 Primary map



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

6.2 Central slices [i](#)

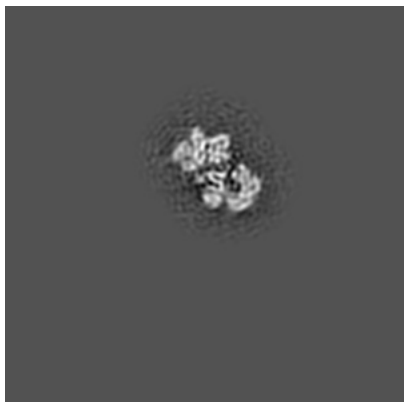
6.2.1 Primary map



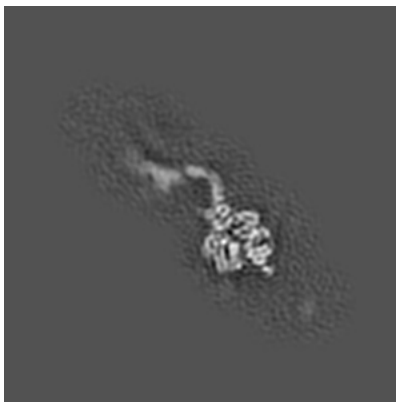
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

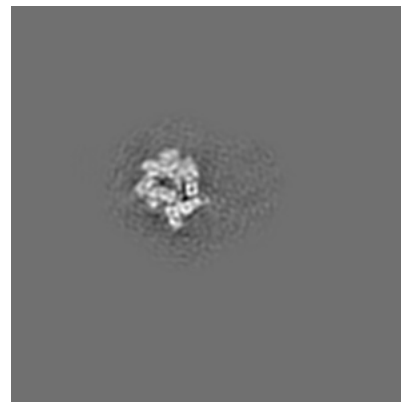
6.3.1 Primary map



X Index: 116



Y Index: 154



Z Index: 169

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

6.4 Orthogonal surface views [i](#)

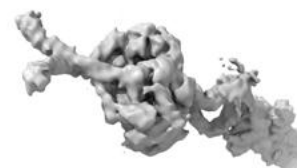
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

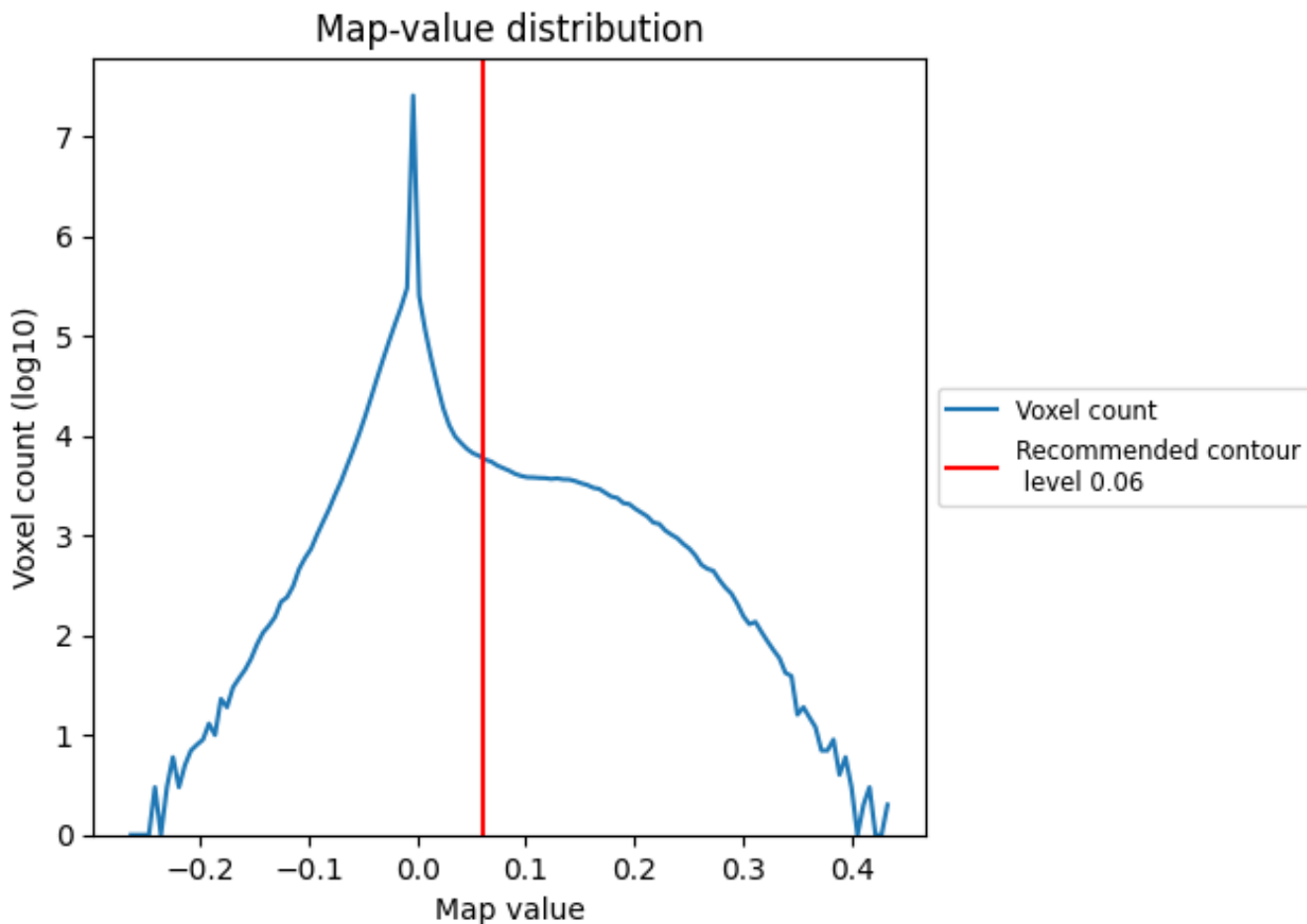
6.5 Mask visualisation

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

7 Map analysis [i](#)

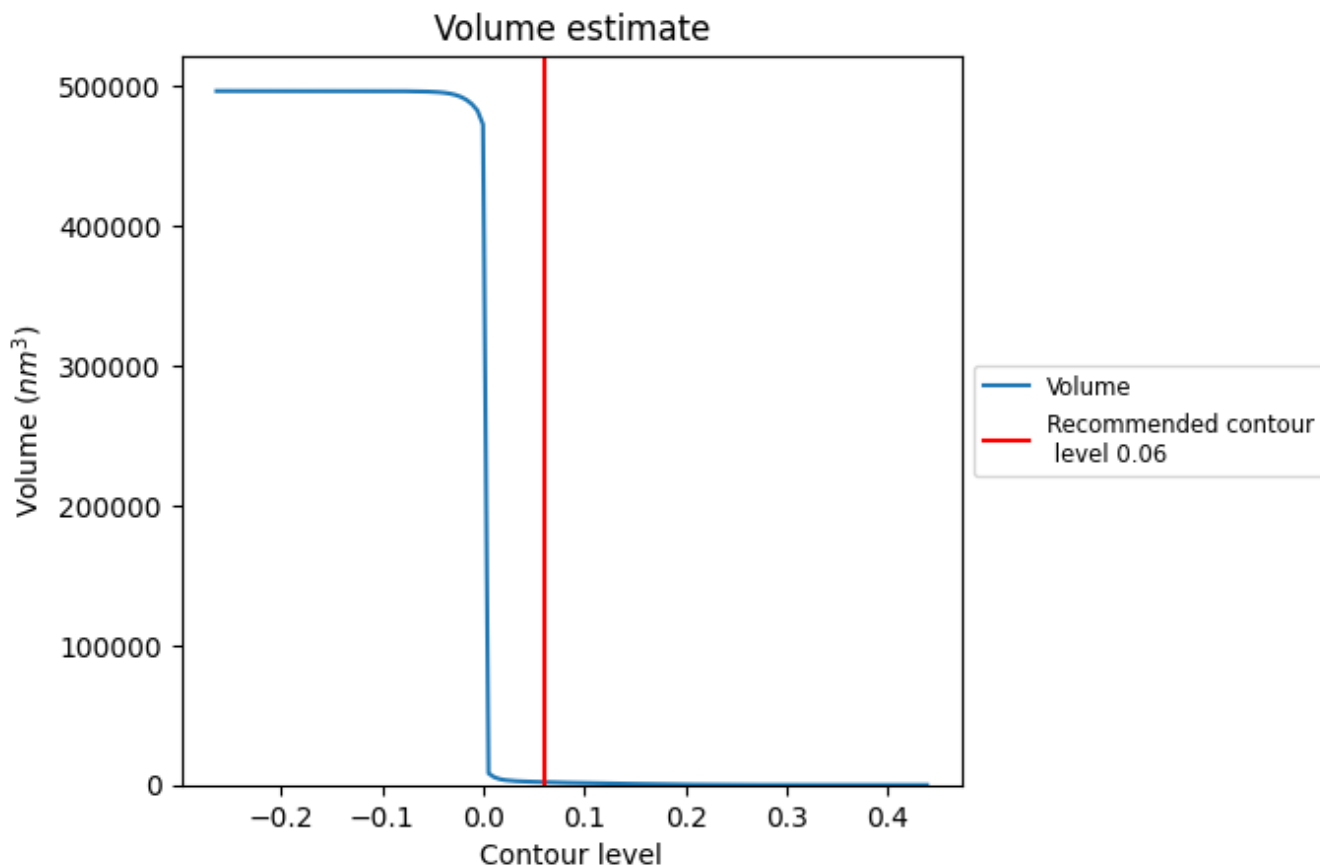
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

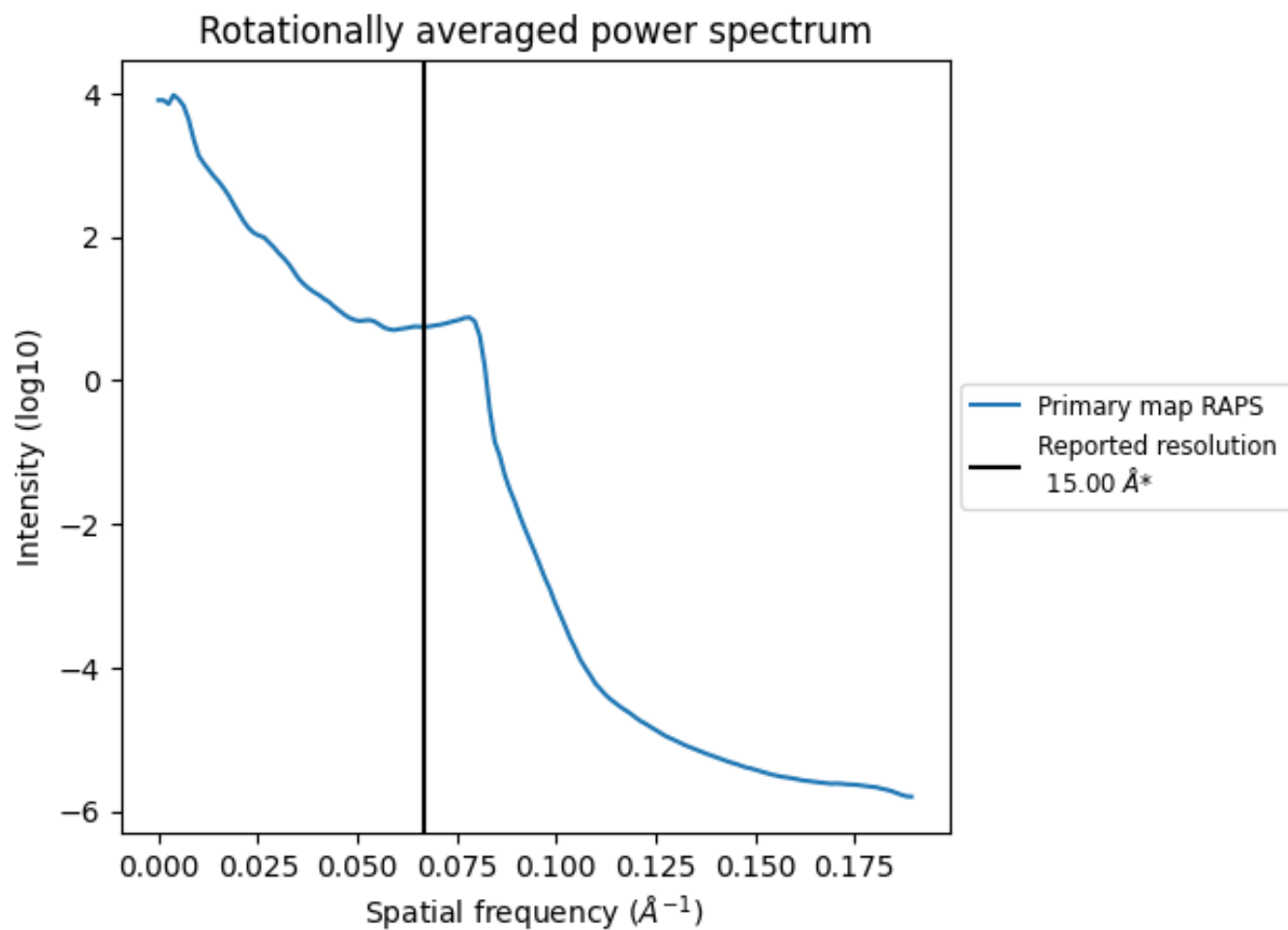
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2029 nm^3 ; this corresponds to an approximate mass of 1832 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.067\AA^{-1}

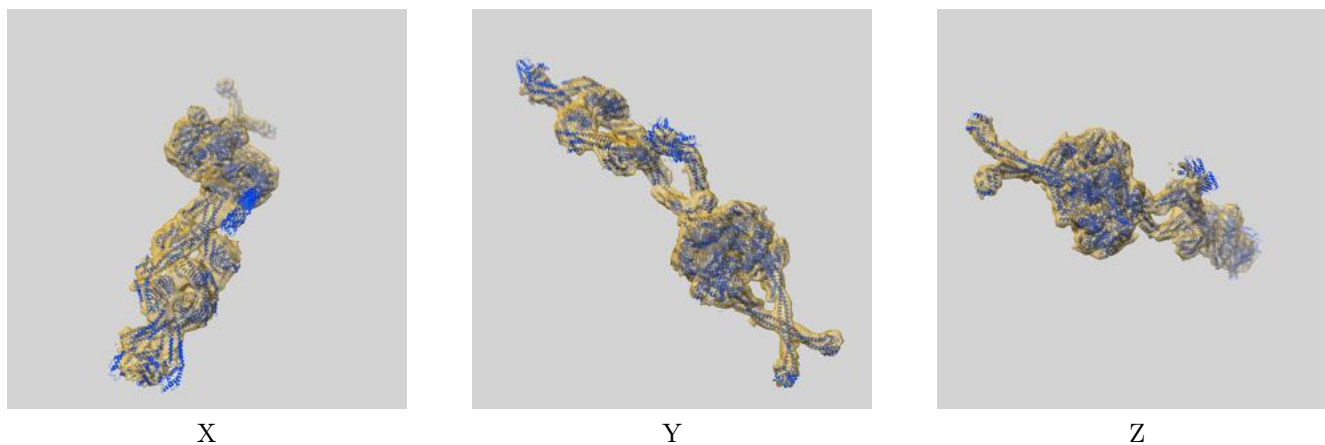
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

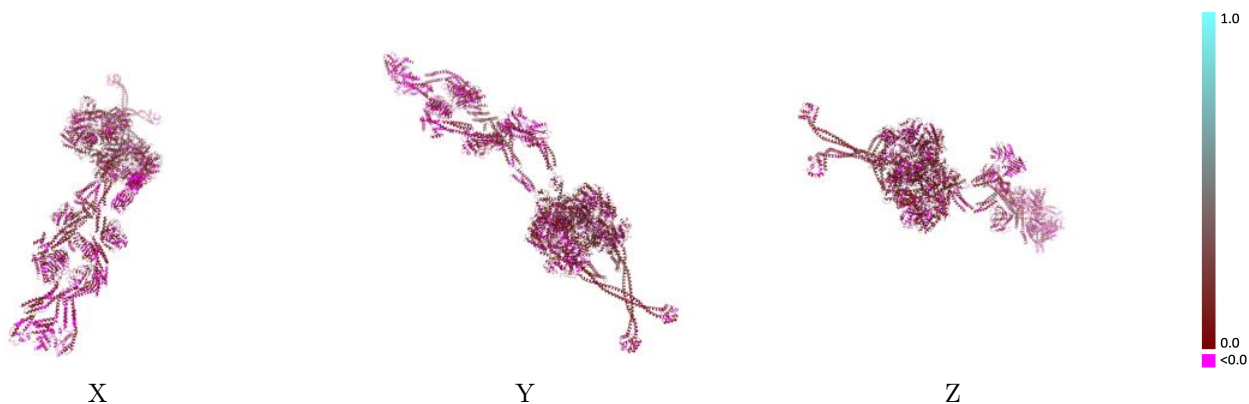
This section contains information regarding the fit between EMDB map EMD-3705 and PDB model 5NVU. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



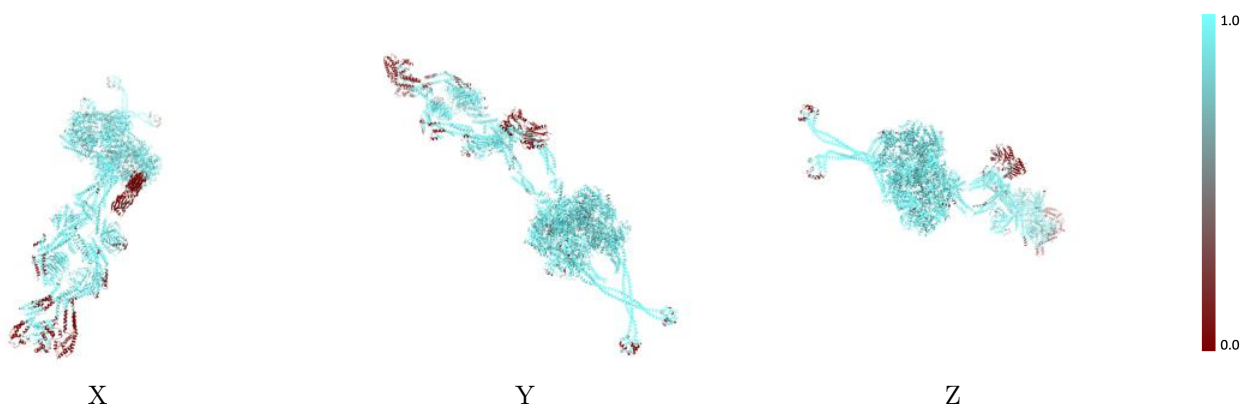
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



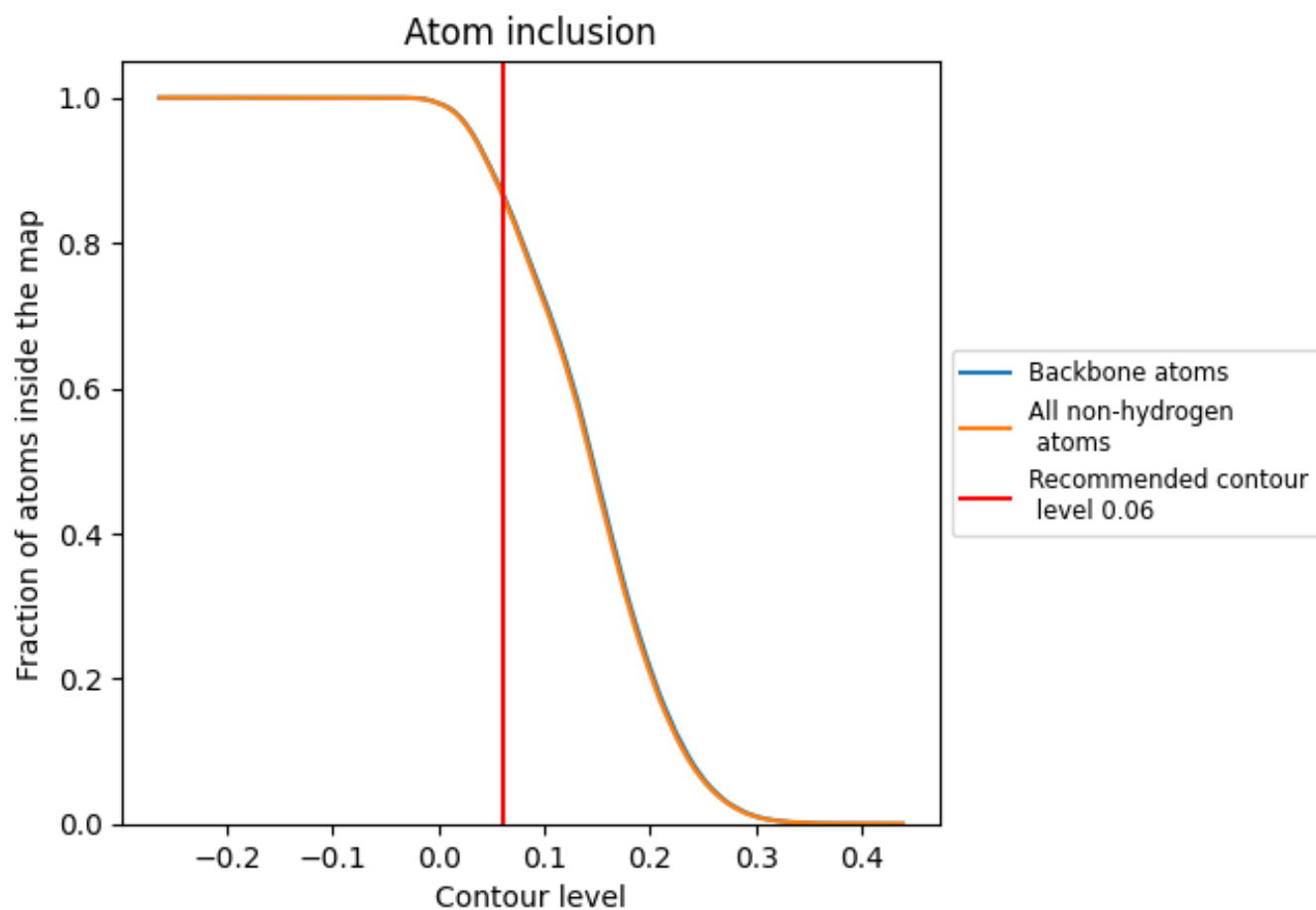
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8666	 0.0870
A	 0.9490	 0.1130
B	 0.9464	 0.1010
C	 0.7813	 0.0960
D	 0.9524	 0.0450
E	 0.9855	 0.0560
F	 0.7174	 0.0540
G	 0.8430	 0.0480
H	 0.9088	 0.0750
I	 0.5984	 0.0040
J	 0.5823	 0.0010
K	 0.2542	 -0.0000
L	 0.1330	 0.0370
M	 0.1045	 0.0240
N	 0.0273	 -0.0050
O	 0.1716	 -0.0240
P	 0.0629	 -0.0020
Q	 0.9319	 0.0530
R	 0.9250	 0.0480

