



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:02 AM UTC

PDB ID : 5NW4 / pdb_00005nw4
EMDB ID : EMD-3706
Title : Human cytoplasmic dynein-1 bound to dynactin and an N-terminal construct of BICD2
Authors : Zhang, K.; Foster, H.E.; Carter, A.P.
Deposited on : 2017-05-05
Resolution : 8.70 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:

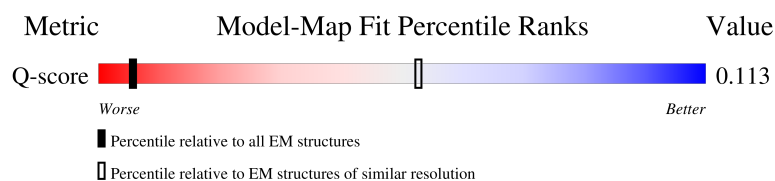
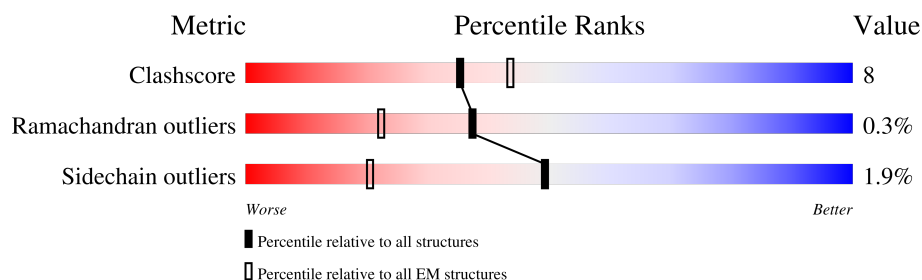
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 8.70 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	282 (8.20 - 9.20)

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	B	889	
2	D	341	
3	C	350	
4	A	922	

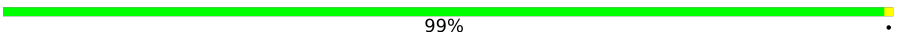
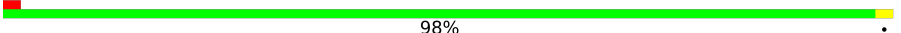
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Mol	Chain	Length	Quality of chain
5	1	125	
6	2	124	
7	R	120	
7	S	120	
8	E	295	
9	F	298	
10	G	376	
10	H	376	
10	O	376	
10	P	376	
10	Q	376	
10	T	376	
10	U	376	
10	W	376	
11	V	396	
12	X	417	
13	Y	286	
14	Z	293	
15	a	571	
16	b	602	
17	c	130	
17	d	130	
18	e	174	
18	f	174	
19	g	190	

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Mol	Chain	Length	Quality of chain
20	h	222	 71%26%
21	i	243	 99%
22	j	52	 98%
23	k	48	 75%15%6%
24	l	71	 55%34%10%
25	m	31	 81%10%10%
26	n	20	 10%65%25%5%5%
27	o	53	 100%
28	5	275	 12%81%19%
28	6	275	 5%80%20%

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 66297 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 heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	B	889	Total	C	N	O	0	0
			4439	2661	889	889		

- Molecule 2 is a protein called dynein intermediate chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	341	Total	C	N	O	0	0
			1680	998	341	341		

- Molecule 3 is a protein called dynein intermediate chain.

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

- Molecule 4 is a protein called dynein heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	A	922	Total	C	N	O	0	0
			4604	2760	922	922		

- Molecule 5 is a protein called dynein N-terminal dimerization domain.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	1	125	Total	C	N	O	0	0
			625	375	125	125		

- Molecule 6 is a protein called dynein N-terminal dimerization domain.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	2	124	Total	C	N	O	0	0
			620	372	124	124		

- Molecule 7 is a protein called Robl.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	R	120	Total	C	N	O	0	0
			587	347	120	120		
7	S	120	Total	C	N	O	0	0
			587	347	120	120		

- Molecule 8 is a protein called dynein light intermediate chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	E	295	Total	C	N	O	0	0
			1459	869	295	295		

- Molecule 9 is a protein called dynein light intermediate chain.

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

- Molecule 10 is a protein called Arp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		
10	H	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		
10	O	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		
10	P	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		
10	Q	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		
10	T	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		
10	U	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		
10	W	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	97	GLU	ASP	conflict	UNP F2Z5G5

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Chain	Residue	Modelled	Actual	Comment	Reference
H	97	GLU	ASP	conflict	UNP F2Z5G5
O	97	GLU	ASP	conflict	UNP F2Z5G5
P	97	GLU	ASP	conflict	UNP F2Z5G5
Q	97	GLU	ASP	conflict	UNP F2Z5G5
T	97	GLU	ASP	conflict	UNP F2Z5G5
U	97	GLU	ASP	conflict	UNP F2Z5G5
W	97	GLU	ASP	conflict	UNP F2Z5G5

- Molecule 11 is a protein called beta-actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	370	Total	C	N	O	S	0	0
			2885	1827	486	550	22		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	-20	MET	-	initiating methionine	UNP I3LVD5
V	-19	SER	-	expression tag	UNP I3LVD5
V	-18	VAL	-	expression tag	UNP I3LVD5
V	-17	ARG	-	expression tag	UNP I3LVD5
V	-16	SER	-	expression tag	UNP I3LVD5
V	-15	ALA	-	expression tag	UNP I3LVD5
V	-14	ARG	-	expression tag	UNP I3LVD5
V	-13	ARG	-	expression tag	UNP I3LVD5
V	-12	ALA	-	expression tag	UNP I3LVD5
V	-11	SER	-	expression tag	UNP I3LVD5
V	-10	ALA	-	expression tag	UNP I3LVD5
V	-9	SER	-	expression tag	UNP I3LVD5
V	-8	ALA	-	expression tag	UNP I3LVD5
V	-7	GLU	-	expression tag	UNP I3LVD5
V	-6	ALA	-	expression tag	UNP I3LVD5
V	-5	GLU	-	expression tag	UNP I3LVD5
V	-4	LEU	-	expression tag	UNP I3LVD5
V	-3	LEU	-	expression tag	UNP I3LVD5
V	-2	GLN	-	expression tag	UNP I3LVD5
V	-1	THR	-	expression tag	UNP I3LVD5
V	0	MET	-	expression tag	UNP I3LVD5
V	1	GLY	-	expression tag	UNP I3LVD5
V	2	ASP	-	expression tag	UNP I3LVD5
V	10	VAL	ILE	conflict	UNP I3LVD5

- Molecule 12 is a protein called Arp11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	369	Total	C	N	O	S	0	0
			2879	1857	486	520	16		

- Molecule 13 is a protein called Capping protein (Actin filament) muscle Z-line, alpha 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Y	275	Total	C	N	O	S	0	0
			2242	1415	393	429	5		

- Molecule 14 is a protein called F-actin capping protein beta subunit variant II.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Z	270	Total	C	N	O	S	0	0
			2137	1333	373	420	11		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	-15	MET	-	initiating methionine	UNP D2JYW4
Z	-14	ASP	-	expression tag	UNP D2JYW4
Z	-13	THR	-	expression tag	UNP D2JYW4
Z	-12	GLU	-	expression tag	UNP D2JYW4
Z	-11	LEU	-	expression tag	UNP D2JYW4
Z	-10	ALA	-	expression tag	UNP D2JYW4
Z	-9	SER	-	expression tag	UNP D2JYW4
Z	-8	PRO	-	expression tag	UNP D2JYW4
Z	-7	GLY	-	expression tag	UNP D2JYW4
Z	-6	PRO	-	expression tag	UNP D2JYW4
Z	-5	LEU	-	expression tag	UNP D2JYW4
Z	-4	LEU	-	expression tag	UNP D2JYW4
Z	-3	LEU	-	expression tag	UNP D2JYW4
Z	-2	GLY	-	expression tag	UNP D2JYW4
Z	-1	LYS	-	expression tag	UNP D2JYW4
Z	0	TYR	-	expression tag	UNP D2JYW4
Z	1	ARG	-	expression tag	UNP D2JYW4

- Molecule 15 is a protein called dynactin shoulder complex.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	a	571	Total	C	N	O	0	0
			2855	1713	571	571		

- Molecule 16 is a protein called dynactin shoulder complex.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	b	602	Total	C	N	O	0	0
			3010	1806	602	602		

- Molecule 17 is a protein called dynactin shoulder complex.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	c	65	Total	C	N	O	0	0
			323	193	65	65		
17	d	65	Total	C	N	O	0	0
			323	193	65	65		

- Molecule 18 is a protein called dynactin shoulder complex.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	e	87	Total	C	N	O	0	0
			435	261	87	87		
18	f	87	Total	C	N	O	0	0
			435	261	87	87		

- Molecule 19 is a protein called Dynactin 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	g	169	Total	C	N	O	0	0
			831	493	169	169		

- Molecule 20 is a protein called Dynactin subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	h	165	Total	C	N	O	0	0
			812	482	165	165		

- Molecule 21 is a protein called dynactin pointed end p62.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	i	243	Total	C	N	O	0	0
			1215	729	243	243		

- Molecule 22 is a protein called p150.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	j	52	Total	C	N	O	0	0
			260	156	52	52		

- Molecule 23 is a protein called Dynactin.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	k	48	Total	C	N	O	S	0	0
			341	216	58	66	1		

- Molecule 24 is a protein called Dynactin.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	l	71	Total	C	N	O	S	0	0
			517	324	93	99	1		

- Molecule 25 is a protein called Dynactin.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	m	31	Total	C	N	O	S	0	0
			179	112	34	32	1		

- Molecule 26 is a protein called Dynactin.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	n	20	Total	C	N	O	S	0	0
			127	80	23	23	1		

- Molecule 27 is a protein called dynactin p150.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	o	53	Total	C	N	O	0	0
			265	159	53	53		

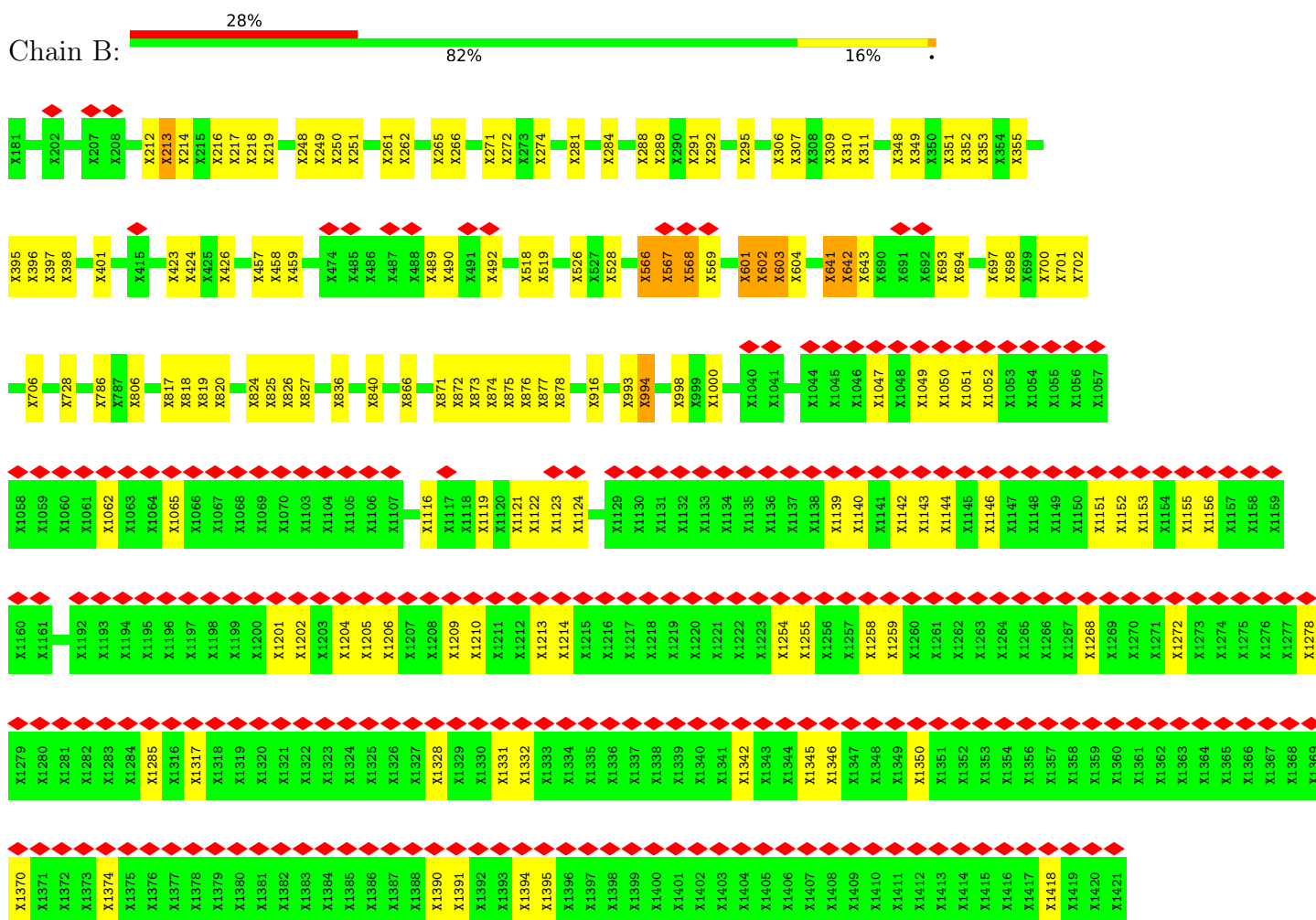
- Molecule 28 is a protein called BICD2N.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	5	275	Total	C	N	O	0	0
			1375	825	275	275		
28	6	275	Total	C	N	O	0	0
			1375	825	275	275		

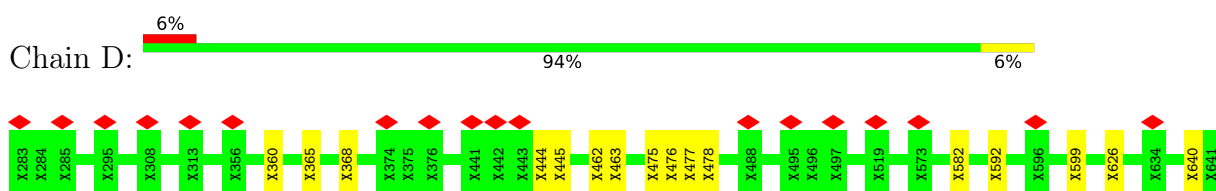
3 Residue-property plots

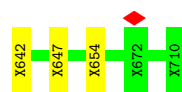
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

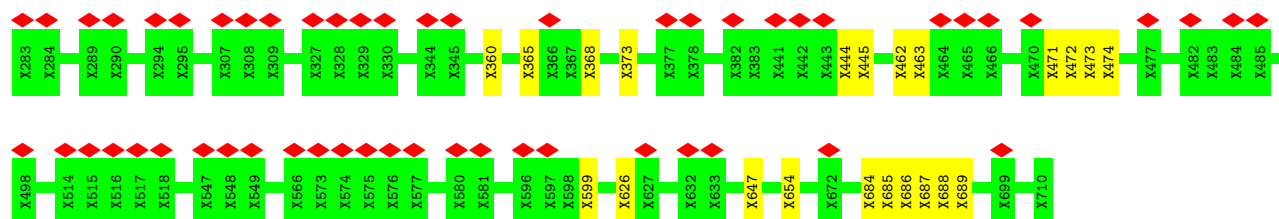


• Molecule 2: dynein intermediate chain

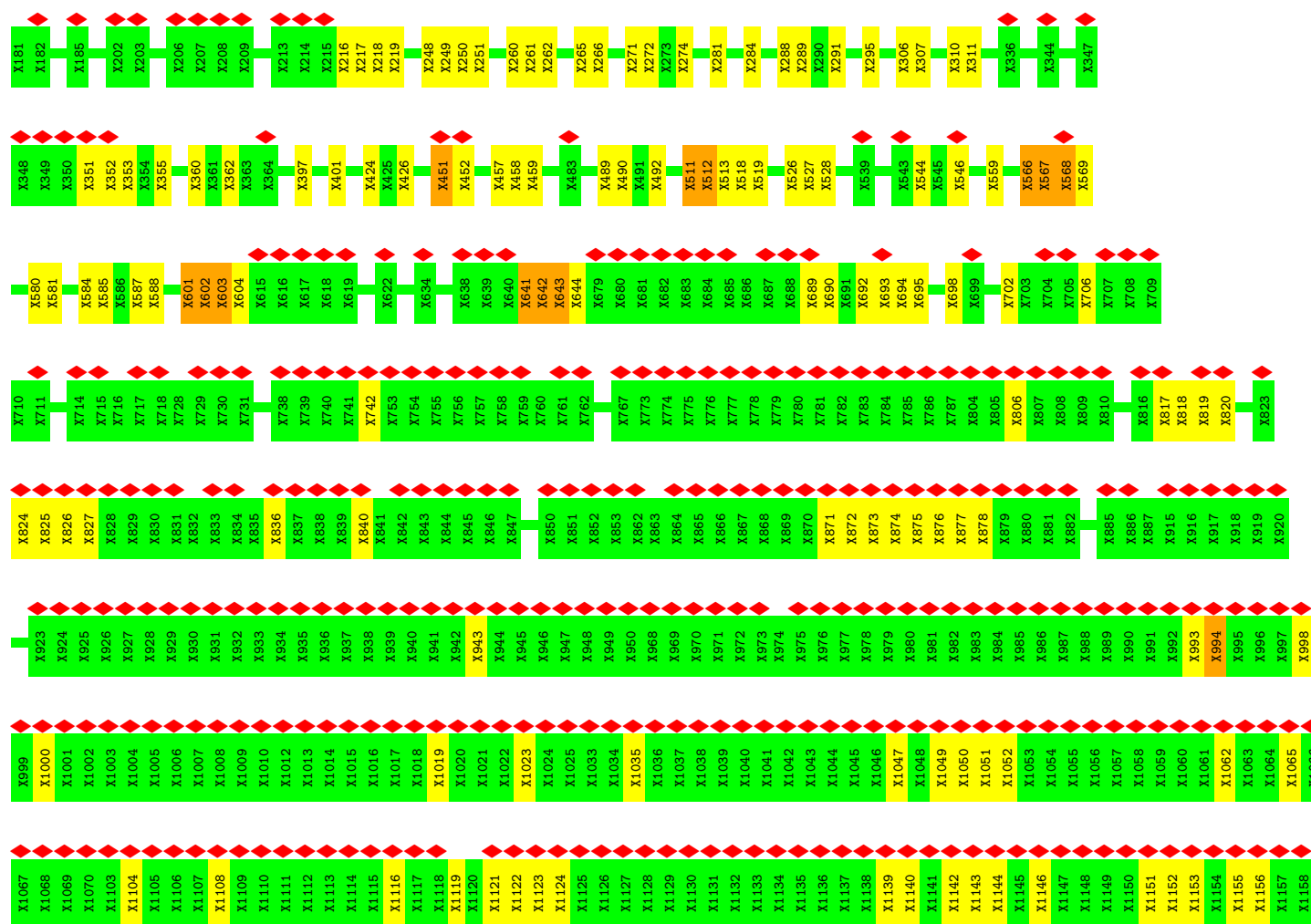
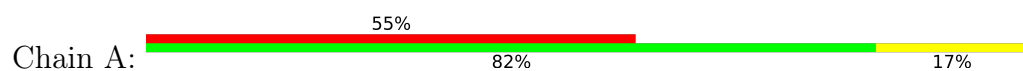


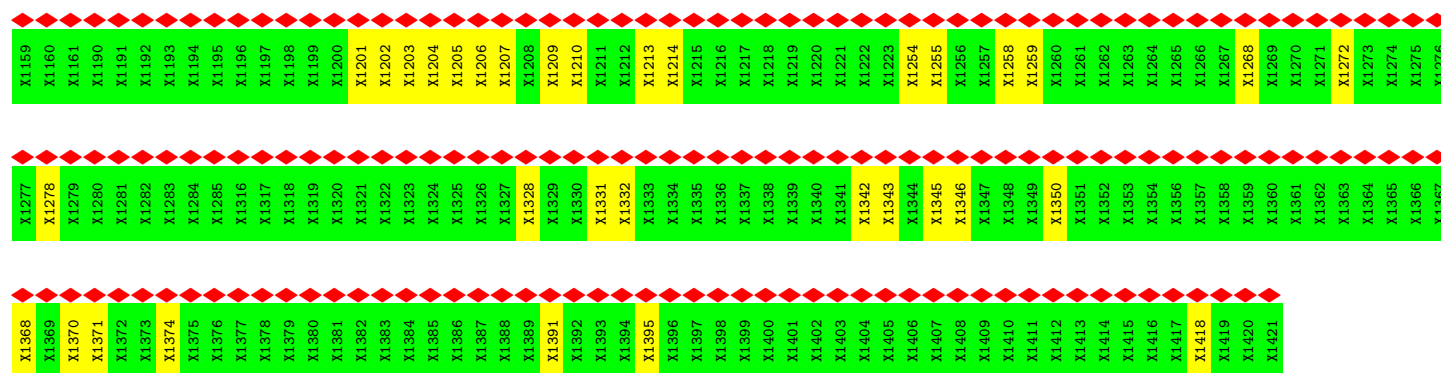


- Molecule 3: dynein intermediate chain

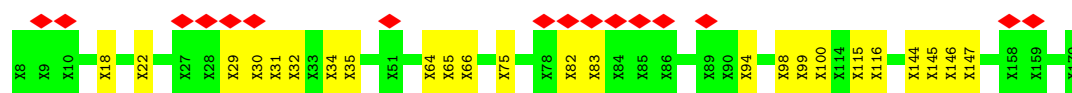
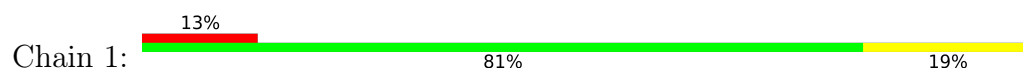


- Molecule 4: dynein heavy chain

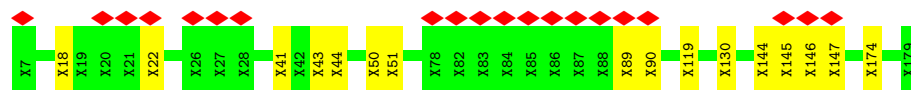
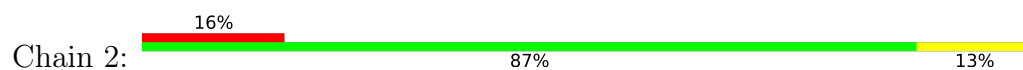




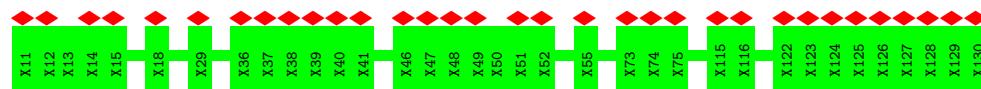
• Molecule 5: dynein N-terminal dimerization domain



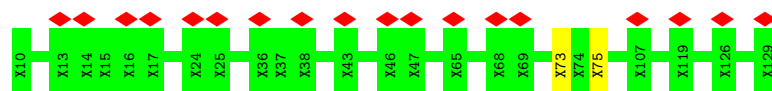
• Molecule 6: dynein N-terminal dimerization domain



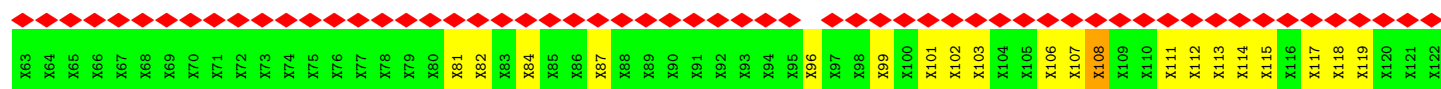
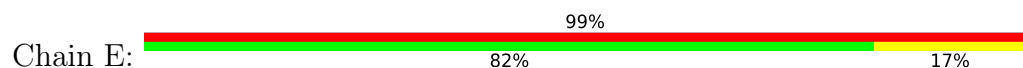
• Molecule 7: Robl

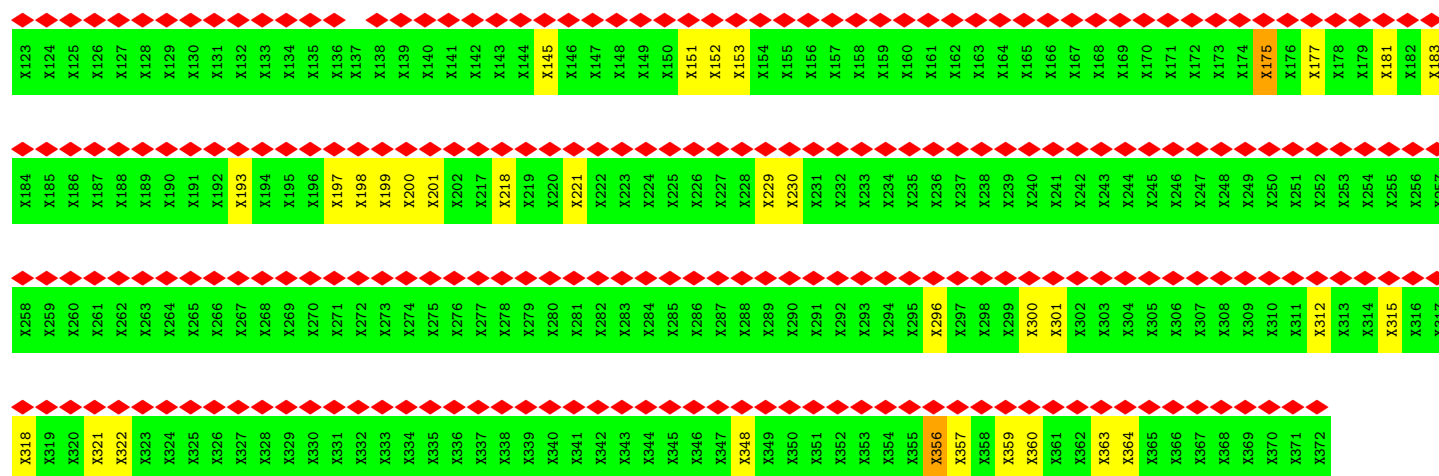


• Molecule 7: Robl

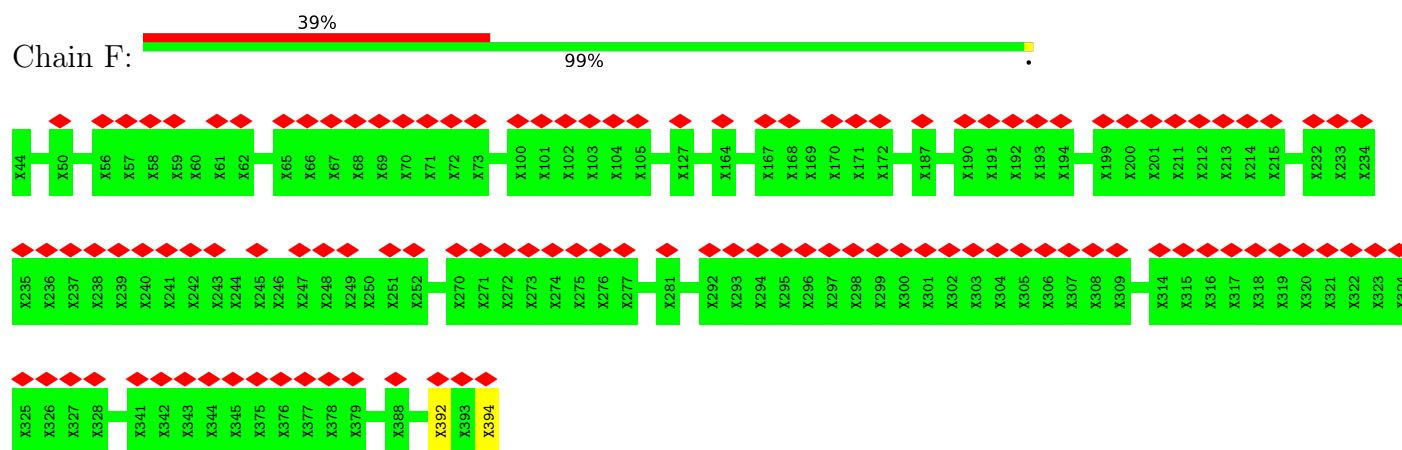


• Molecule 8: dynein light intermediate chain

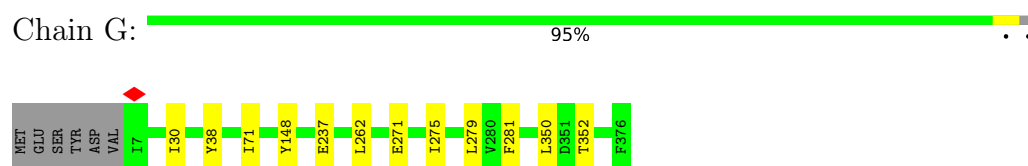




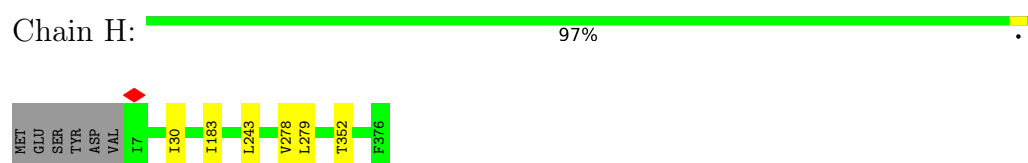
• Molecule 9: dynein light intermediate chain



• Molecule 10: Arp1



• Molecule 10: Arp1



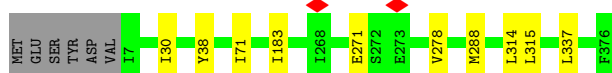
• Molecule 10: Arp1





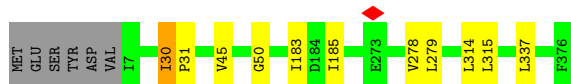
- Molecule 10: Arp1

Chain P: 96%



- Molecule 10: Arp1

Chain Q: 95%



- Molecule 10: Arp1

Chain T: 96%



- Molecule 10: Arp1

Chain U: 93% 5%



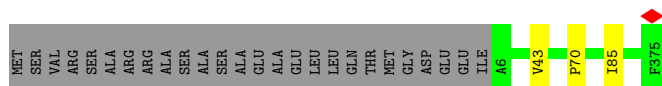
- Molecule 10: Arp1

Chain W: 93% 5%



- Molecule 11: beta-actin

Chain V: 93% 7%



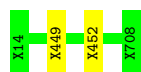
- Molecule 12: Arp11

[illegible]



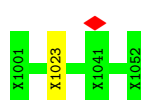
- Molecule 21: dynactin pointed end p62

Chain i: 99%



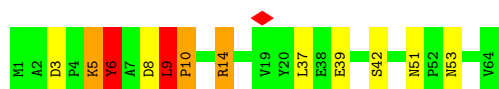
- Molecule 22: p150

Chain j: 98%



- Molecule 23: Dynactin

Chain k: 75% 15% 6%



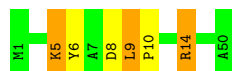
- Molecule 24: Dynactin

Chain l: 55% 34% 10%



- Molecule 25: Dynactin

Chain m: 81% 10% 10%



- Molecule 26: Dynactin

Chain n: 10% 65% 25% 5% 5%



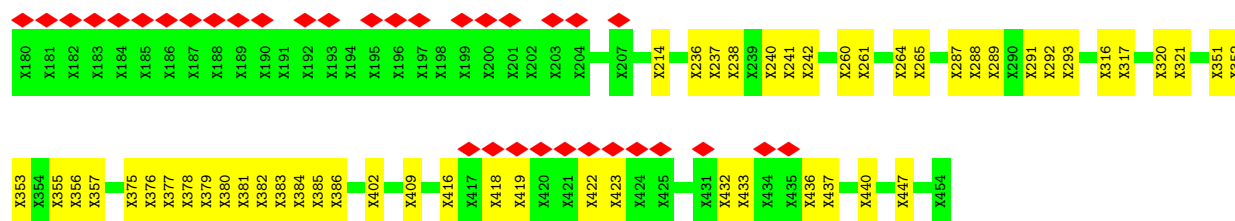
- Molecule 27: dynactin p150

Chain o:  100%

There are no outlier residues recorded for this chain.

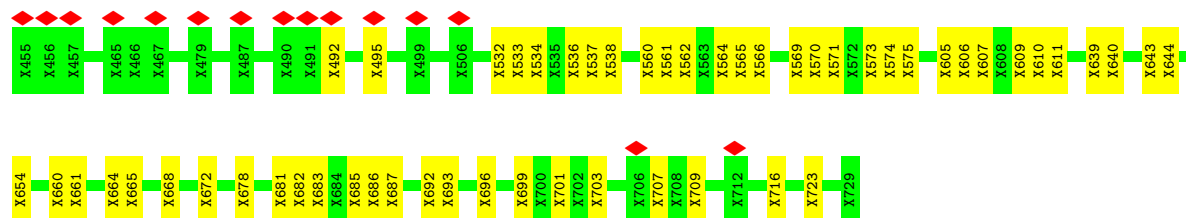
- Molecule 28: BICD2N

Chain 5:  12% 81% 19%



- Molecule 28: BICD2N

Chain 6:  5% 80% 20%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78671	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	0.473	Depositor
Minimum map value	-0.203	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	964.80005, 964.80005, 964.80005	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.68, 2.68, 2.68	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$
10	G	0.54	0/3026	0.77	0/4086
10	H	0.55	0/3026	0.76	0/4086
10	O	0.55	0/3026	0.77	0/4086
10	P	0.55	0/3026	0.76	0/4086
10	Q	0.55	0/3026	0.77	0/4086
10	T	0.55	0/3026	0.76	0/4086
10	U	0.55	0/3026	0.77	0/4086
10	W	0.55	0/3026	0.79	2/4086 (0.0%)
11	V	0.55	0/2948	0.77	0/3991
12	X	0.57	0/2939	0.81	1/3987 (0.0%)
13	Y	0.57	0/2294	0.84	0/3106
14	Z	0.55	0/2173	0.80	1/2935 (0.0%)
19	g	0.51	0/830	1.20	14/1152 (1.2%)
20	h	0.52	0/811	1.23	6/1126 (0.5%)
23	k	0.76	2/347 (0.6%)	1.05	4/473 (0.8%)
24	l	0.67	0/525	0.96	2/708 (0.3%)
25	m	0.66	0/181	1.02	1/249 (0.4%)
26	n	0.70	0/130	0.98	0/179
All	All	0.56	2/37386 (0.0%)	0.81	31/50594 (0.1%)

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	B	0	10
4	A	0	13
8	E	0	8
10	U	0	1
15	a	0	1
16	b	0	2
All	All	0	35

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	k	9	LEU	C-N	5.26	1.41	1.34
23	k	10	PRO	N-CD	5.16	1.54	1.47

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	h	83	PHE	CA-C-N	9.68	131.94	119.84
20	h	83	PHE	C-N-CA	9.68	131.94	119.84
20	h	71	PRO	CA-C-N	9.55	128.90	118.97
20	h	71	PRO	C-N-CA	9.55	128.90	118.97
14	Z	253	PRO	CA-N-CD	-9.23	99.08	112.00
19	g	36	HIS	CA-C-N	8.12	128.13	119.76
19	g	36	HIS	C-N-CA	8.12	128.13	119.76
19	g	71	THR	CA-C-N	7.81	129.60	119.84
19	g	71	THR	C-N-CA	7.81	129.60	119.84
19	g	76	LYS	CA-C-N	6.88	127.29	119.93
19	g	76	LYS	C-N-CA	6.88	127.29	119.93
25	m	5	LYS	N-CA-C	6.79	118.48	111.14
24	l	5	LYS	N-CA-C	6.76	118.44	111.14
23	k	5	LYS	N-CA-C	6.42	118.08	111.14
19	g	167	LEU	CA-C-N	6.28	125.69	118.85
19	g	167	LEU	C-N-CA	6.28	125.69	118.85
19	g	133	ILE	CA-C-N	5.92	125.89	120.03
19	g	133	ILE	C-N-CA	5.92	125.89	120.03
24	l	6	TYR	N-CA-C	5.86	118.09	110.53
23	k	6	TYR	N-CA-C	5.48	117.60	110.53
10	W	41	ARG	CA-C-N	-5.34	114.26	119.76
10	W	41	ARG	C-N-CA	-5.34	114.26	119.76
19	g	30	GLY	CA-C-N	5.32	125.08	119.76
19	g	30	GLY	C-N-CA	5.32	125.08	119.76
20	h	149	CYS	CA-C-N	5.30	126.47	119.84
20	h	149	CYS	C-N-CA	5.30	126.47	119.84
23	k	9	LEU	CA-C-N	-5.30	113.17	119.05
23	k	9	LEU	C-N-CA	-5.30	113.17	119.05
19	g	152	ARG	CA-C-N	5.29	126.45	119.84
19	g	152	ARG	C-N-CA	5.29	126.45	119.84
12	X	242	PRO	N-CA-C	5.07	116.89	110.70

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	451	UNK	Mainchain
4	A	511	UNK	Mainchain
4	A	512	UNK	Mainchain
4	A	566	UNK	Mainchain
4	A	567	UNK	Mainchain
4	A	568	UNK	Mainchain
4	A	601	UNK	Mainchain
4	A	602	UNK	Mainchain
4	A	603	UNK	Mainchain
4	A	641	UNK	Mainchain
4	A	642	UNK	Mainchain
4	A	643	UNK	Mainchain
4	A	994	UNK	Peptide
1	B	213	UNK	Mainchain
1	B	566	UNK	Mainchain
1	B	567	UNK	Mainchain
1	B	568	UNK	Mainchain
1	B	601	UNK	Mainchain
1	B	602	UNK	Mainchain
1	B	603	UNK	Mainchain
1	B	641	UNK	Mainchain
1	B	642	UNK	Mainchain
1	B	994	UNK	Peptide
8	E	108	UNK	Peptide,Mainchain
8	E	175	UNK	Mainchain
8	E	218	UNK	Mainchain
8	E	312	UNK	Mainchain
8	E	356	UNK	Mainchain
8	E	84	UNK	Mainchain
8	E	96	UNK	Mainchain
10	U	375	THR	Peptide
15	a	442	UNK	Peptide
16	b	270	UNK	Peptide
16	b	271	UNK	Peptide

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	B	4439	0	944	176	0
2	D	1680	0	353	31	0
3	C	1723	0	359	44	0
4	A	4604	0	977	181	0
5	1	625	0	147	19	0
6	2	620	0	142	16	0
7	R	587	0	113	0	0
7	S	587	0	114	2	0
8	E	1459	0	295	46	0
9	F	1496	0	300	1	0
10	G	2957	0	2952	10	0
10	H	2957	0	2952	3	0
10	O	2957	0	2952	2	0
10	P	2957	0	2952	4	0
10	Q	2957	0	2952	8	0
10	T	2957	0	2952	22	0
10	U	2957	0	2952	27	0
10	W	2957	0	2952	30	0
11	V	2885	0	2856	2	0
12	X	2879	0	2969	19	0
13	Y	2242	0	2169	74	0
14	Z	2137	0	2122	75	0
15	a	2855	0	585	13	0
16	b	3010	0	619	12	0
17	c	323	0	76	3	0
17	d	323	0	77	10	0
18	e	435	0	93	0	0
18	f	435	0	93	0	0
19	g	831	0	374	11	0
20	h	812	0	344	6	0
21	i	1215	0	285	2	0
22	j	260	0	57	1	0
23	k	341	0	310	7	0
24	l	517	0	490	50	0
25	m	179	0	155	4	0
26	n	127	0	103	6	0
27	o	265	0	57	0	0
28	5	1375	0	277	56	0
28	6	1375	0	277	52	0
All	All	66297	0	41748	858	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 8.

All (858) 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)
1:B:292:UNK:CB	10:T:350:LEU:HD23	1.26	1.59
1:B:866:UNK:CB	1:B:998:UNK:CB	1.78	1.58
3:C:472:UNK:C	4:A:694:UNK:CB	1.82	1.55
1:B:1285:UNK:CB	1:B:1317:UNK:CB	1.80	1.55
1:B:212:UNK:C	1:B:214:UNK:CB	1.81	1.53
3:C:688:UNK:CB	4:A:559:UNK:C	1.86	1.52
24:l:66:THR:HG21	24:l:83:TYR:CD1	1.44	1.51
8:E:81:UNK:C	8:E:87:UNK:CB	1.85	1.50
1:B:292:UNK:N	10:T:350:LEU:CD2	1.74	1.50
1:B:292:UNK:CA	10:T:350:LEU:CD2	1.89	1.49
1:B:289:UNK:CB	10:T:346:ILE:HG21	1.43	1.46
28:5:447:UNK:CB	28:6:723:UNK:CB	1.95	1.44
1:B:292:UNK:N	10:T:350:LEU:HD21	1.10	1.40
1:B:698:UNK:HA	2:D:478:UNK:C	1.51	1.40
3:C:688:UNK:CB	4:A:559:UNK:CA	2.00	1.39
3:C:687:UNK:CA	4:A:585:UNK:HA	1.44	1.37
20:h:32:GLN:N	28:6:707:UNK:CB	1.85	1.36
5:1:31:UNK:CB	5:1:34:UNK:CB	2.01	1.36
1:B:698:UNK:CB	2:D:477:UNK:O	1.74	1.35
4:A:817:UNK:O	4:A:819:UNK:N	1.58	1.35
1:B:817:UNK:O	1:B:819:UNK:N	1.58	1.34
3:C:688:UNK:CB	4:A:559:UNK:CB	2.02	1.33
14:Z:251:ASP:CG	14:Z:255:PHE:HE2	1.36	1.30
4:A:689:UNK:O	4:A:693:UNK:CB	1.79	1.28
1:B:698:UNK:HA	2:D:478:UNK:CA	1.63	1.28
5:1:31:UNK:O	5:1:34:UNK:N	1.67	1.27
6:2:18:UNK:O	6:2:22:UNK:CB	1.82	1.26
28:5:316:UNK:O	28:5:320:UNK:N	1.68	1.26
1:B:292:UNK:CA	10:T:350:LEU:HD23	1.59	1.23
28:6:692:UNK:O	28:6:696:UNK:N	1.70	1.23
8:E:81:UNK:O	8:E:87:UNK:CB	1.83	1.22
1:B:213:UNK:N	1:B:214:UNK:CB	1.79	1.22
14:Z:251:ASP:O	14:Z:255:PHE:CD2	1.94	1.21
8:E:82:UNK:N	8:E:87:UNK:CB	2.03	1.21
1:B:457:UNK:CB	1:B:459:UNK:N	2.04	1.20
1:B:698:UNK:CA	2:D:478:UNK:HA	1.72	1.20
3:C:688:UNK:CB	4:A:559:UNK:O	1.88	1.19
6:2:18:UNK:O	6:2:22:UNK:N	1.74	1.19
4:A:457:UNK:CB	4:A:459:UNK:N	2.04	1.19
10:U:183:ILE:HD11	10:U:278:VAL:CG2	1.72	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:474:UNK:N	4:A:695:UNK:N	1.67	1.19
3:C:687:UNK:CA	4:A:585:UNK:CA	2.18	1.18
24:l:66:THR:HG22	24:l:83:TYR:HA	1.23	1.17
4:A:457:UNK:HA	4:A:458:UNK:CB	1.72	1.16
4:A:518:UNK:CB	4:A:519:UNK:N	2.09	1.15
1:B:518:UNK:CB	1:B:519:UNK:N	2.09	1.15
4:A:518:UNK:C	4:A:519:UNK:CB	2.24	1.15
1:B:457:UNK:HA	1:B:458:UNK:CB	1.71	1.15
14:Z:253:PRO:HD2	14:Z:254:LYS:H	1.08	1.15
1:B:518:UNK:CB	1:B:519:UNK:H2	1.60	1.15
8:E:101:UNK:O	8:E:119:UNK:O	1.64	1.14
13:Y:162:GLN:HG3	14:Z:243:LEU:CD2	1.77	1.14
1:B:518:UNK:C	1:B:519:UNK:CB	2.24	1.14
4:A:518:UNK:CB	4:A:519:UNK:H2	1.60	1.13
1:B:292:UNK:CB	10:T:350:LEU:CD2	2.18	1.11
24:l:66:THR:CG2	24:l:83:TYR:HD1	1.63	1.11
1:B:872:UNK:O	1:B:876:UNK:CB	1.99	1.11
14:Z:245:SER:HB2	14:Z:248:VAL:HG23	1.31	1.11
8:E:145:UNK:CB	8:E:301:UNK:CB	2.28	1.11
14:Z:251:ASP:CG	14:Z:255:PHE:CE2	2.28	1.10
10:U:183:ILE:HD11	10:U:278:VAL:HG21	1.26	1.10
14:Z:245:SER:CB	14:Z:248:VAL:HG23	1.82	1.10
24:l:67:LYS:HE3	24:l:67:LYS:HA	1.34	1.10
24:l:66:THR:CG2	24:l:83:TYR:CD1	2.34	1.09
4:A:872:UNK:O	4:A:876:UNK:CB	1.99	1.09
1:B:698:UNK:N	2:D:478:UNK:HA	1.65	1.08
1:B:212:UNK:O	1:B:214:UNK:CB	2.00	1.08
14:Z:245:SER:OG	14:Z:248:VAL:CG2	2.02	1.07
17:d:66:UNK:CB	17:d:74:UNK:O	2.03	1.07
13:Y:93:LYS:HE3	13:Y:122:GLU:OE2	1.51	1.07
1:B:291:UNK:C	10:T:350:LEU:HD21	1.85	1.06
1:B:872:UNK:O	1:B:876:UNK:N	1.88	1.06
4:A:872:UNK:O	4:A:876:UNK:N	1.88	1.06
1:B:292:UNK:HA	10:T:350:LEU:HD22	1.32	1.06
4:A:248:UNK:CB	4:A:360:UNK:CB	2.33	1.06
1:B:698:UNK:CB	2:D:477:UNK:C	2.32	1.05
3:C:685:UNK:O	4:A:580:UNK:O	1.74	1.05
8:E:82:UNK:CA	8:E:87:UNK:CB	2.35	1.04
10:W:41:ARG:HH12	10:W:72:ARG:HD2	1.22	1.04
14:Z:250:PRO:O	14:Z:253:PRO:CD	2.05	1.04
10:W:43:LYS:HA	12:X:275:ASN:HB3	1.39	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:806:UNK:N	28:5:214:UNK:CB	2.20	1.03
8:E:359:UNK:O	8:E:360:UNK:O	1.75	1.03
14:Z:251:ASP:O	14:Z:255:PHE:HD2	1.38	1.03
28:5:317:UNK:O	28:5:321:UNK:N	1.90	1.03
1:B:292:UNK:HA	10:T:350:LEU:CD2	1.81	1.03
1:B:698:UNK:HA	2:D:478:UNK:HA	1.30	1.03
1:B:698:UNK:N	2:D:477:UNK:O	1.91	1.03
1:B:289:UNK:CB	10:T:346:ILE:CG2	2.36	1.03
28:6:571:UNK:O	28:6:575:UNK:N	1.92	1.02
8:E:82:UNK:HA	8:E:87:UNK:CB	1.89	1.02
1:B:873:UNK:O	1:B:877:UNK:N	1.93	1.02
13:Y:162:GLN:HG3	14:Z:243:LEU:HD21	1.37	1.01
8:E:107:UNK:HA	8:E:112:UNK:O	1.58	1.01
4:A:873:UNK:O	4:A:877:UNK:N	1.93	1.01
8:E:152:UNK:C	8:E:153:UNK:H2	1.74	1.00
10:W:41:ARG:NH1	10:W:72:ARG:HD2	1.75	1.00
1:B:291:UNK:CB	10:T:350:LEU:HD11	1.92	0.99
17:d:38:UNK:N	17:d:73:UNK:O	1.93	0.99
28:5:288:UNK:O	28:5:292:UNK:N	1.94	0.99
28:5:261:UNK:O	28:5:265:UNK:N	1.95	0.99
1:B:1285:UNK:C	1:B:1317:UNK:CB	2.35	0.98
6:2:18:UNK:O	6:2:22:UNK:CA	2.12	0.98
4:A:271:UNK:O	4:A:274:UNK:N	1.97	0.98
4:A:1047:UNK:O	4:A:1051:UNK:CB	2.12	0.98
1:B:1047:UNK:O	1:B:1051:UNK:CB	2.12	0.98
1:B:271:UNK:O	1:B:274:UNK:N	1.97	0.97
8:E:193:UNK:O	8:E:221:UNK:O	1.82	0.97
14:Z:245:SER:OG	14:Z:248:VAL:HG21	1.62	0.97
28:5:353:UNK:O	28:5:357:UNK:N	1.98	0.97
13:Y:168:PHE:O	13:Y:199:TYR:CD1	2.18	0.96
8:E:315:UNK:CB	8:E:322:UNK:O	2.13	0.96
10:W:45:VAL:H	12:X:275:ASN:HD21	1.12	0.95
1:B:698:UNK:CA	2:D:477:UNK:O	2.14	0.95
10:U:185:ILE:HD11	10:U:261:LEU:HG	1.45	0.95
14:Z:251:ASP:OD1	14:Z:255:PHE:CE2	2.19	0.95
14:Z:251:ASP:OD1	14:Z:255:PHE:HE2	1.48	0.95
10:W:45:VAL:N	12:X:275:ASN:HD21	1.65	0.95
10:U:183:ILE:CD1	10:U:278:VAL:HG21	1.95	0.95
24:l:66:THR:CG2	24:l:83:TYR:HA	1.96	0.94
28:5:419:UNK:O	28:5:423:UNK:N	2.01	0.94
1:B:281:UNK:O	1:B:284:UNK:CA	2.16	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:h:32:GLN:CA	28:6:707:UNK:CB	2.46	0.94
4:A:281:UNK:O	4:A:284:UNK:CA	2.17	0.93
1:B:698:UNK:CA	2:D:478:UNK:CA	2.35	0.93
1:B:700:UNK:CB	1:B:786:UNK:CB	2.46	0.93
3:C:473:UNK:N	4:A:694:UNK:CB	0.82	0.93
4:A:1350:UNK:CB	4:A:1418:UNK:CB	2.46	0.93
3:C:472:UNK:CA	4:A:694:UNK:CB	2.45	0.93
1:B:1350:UNK:CB	1:B:1418:UNK:CB	2.47	0.92
3:C:473:UNK:C	4:A:695:UNK:N	2.32	0.92
13:Y:93:LYS:NZ	13:Y:122:GLU:OE1	2.01	0.92
28:5:289:UNK:O	28:5:293:UNK:N	2.03	0.92
8:E:106:UNK:O	8:E:113:UNK:HA	1.69	0.92
1:B:518:UNK:O	1:B:519:UNK:CB	2.18	0.91
13:Y:93:LYS:CE	13:Y:122:GLU:OE2	2.19	0.91
10:W:45:VAL:H	12:X:275:ASN:ND2	1.68	0.91
28:6:605:UNK:O	28:6:609:UNK:N	2.02	0.91
1:B:698:UNK:CA	2:D:478:UNK:C	2.47	0.91
15:a:442:UNK:HA	15:a:443:UNK:CB	1.99	0.91
10:W:47:VAL:HG21	12:X:232:ASN:HB2	1.53	0.91
14:Z:250:PRO:O	14:Z:253:PRO:CG	2.19	0.91
10:W:57:PHE:C	10:W:58:ILE:HD12	1.95	0.91
19:g:180:SER:CB	28:6:701:UNK:CB	2.49	0.90
1:B:292:UNK:CA	10:T:350:LEU:HD22	1.87	0.90
1:B:309:UNK:HA	1:B:348:UNK:CA	2.02	0.90
4:A:518:UNK:O	4:A:519:UNK:CB	2.18	0.90
28:5:353:UNK:O	28:5:357:UNK:CB	2.20	0.90
24:l:66:THR:HB	24:l:69:LEU:HG	1.52	0.90
1:B:1285:UNK:CA	1:B:1317:UNK:CB	2.50	0.89
5:1:31:UNK:O	5:1:34:UNK:CA	2.19	0.89
28:5:288:UNK:O	28:5:292:UNK:CB	2.20	0.89
20:h:32:GLN:H	28:6:707:UNK:CB	1.71	0.89
3:C:365:UNK:HA	3:C:444:UNK:CB	2.03	0.89
14:Z:253:PRO:HD2	14:Z:254:LYS:N	1.86	0.88
13:Y:93:LYS:NZ	13:Y:122:GLU:CD	2.32	0.88
13:Y:162:GLN:CG	14:Z:243:LEU:CD2	2.52	0.87
28:5:409:UNK:CB	28:6:685:UNK:CB	2.51	0.87
3:C:445:UNK:CB	3:C:463:UNK:CB	2.52	0.87
2:D:445:UNK:CB	2:D:463:UNK:CB	2.52	0.87
6:2:144:UNK:O	6:2:145:UNK:C	2.21	0.87
6:2:144:UNK:O	6:2:146:UNK:N	2.06	0.87
13:Y:162:GLN:CG	14:Z:243:LEU:HD21	2.03	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:UNK:O	1:B:284:UNK:N	2.07	0.86
4:A:281:UNK:O	4:A:284:UNK:N	2.08	0.86
1:B:697:UNK:C	2:D:478:UNK:HA	2.06	0.86
2:D:365:UNK:HA	2:D:444:UNK:CB	2.03	0.86
8:E:199:UNK:O	8:E:200:UNK:CB	2.23	0.86
10:W:43:LYS:CA	12:X:275:ASN:HB3	2.06	0.85
14:Z:251:ASP:CB	14:Z:255:PHE:HE2	1.88	0.85
28:5:381:UNK:O	28:5:385:UNK:N	2.07	0.85
28:5:380:UNK:O	28:5:384:UNK:N	2.09	0.85
19:g:153:PRO:O	19:g:154:GLN:O	1.94	0.85
10:Q:50:GLY:HA2	24:l:62:LYS:HD3	1.59	0.84
14:Z:251:ASP:CB	14:Z:255:PHE:CE2	2.61	0.84
6:2:18:UNK:C	6:2:22:UNK:CB	2.55	0.84
4:A:457:UNK:CB	4:A:459:UNK:CB	2.56	0.84
28:5:378:UNK:O	28:5:382:UNK:N	2.10	0.84
4:A:1342:UNK:O	4:A:1345:UNK:CB	2.26	0.83
10:U:352:THR:HG21	24:l:63:ARG:HA	1.60	0.83
3:C:687:UNK:N	4:A:584:UNK:CB	2.40	0.83
17:d:38:UNK:O	17:d:73:UNK:N	2.11	0.83
4:A:281:UNK:O	4:A:284:UNK:CB	2.26	0.83
23:k:8:ASP:C	23:k:10:PRO:HD3	2.03	0.83
1:B:281:UNK:O	1:B:284:UNK:CB	2.26	0.83
1:B:457:UNK:CB	1:B:459:UNK:CB	2.56	0.83
1:B:1342:UNK:O	1:B:1345:UNK:CB	2.26	0.83
10:U:183:ILE:HD11	10:U:278:VAL:HG23	1.61	0.83
14:Z:251:ASP:C	14:Z:255:PHE:CD2	2.56	0.83
3:C:688:UNK:CB	4:A:559:UNK:HA	2.08	0.82
1:B:289:UNK:CB	10:T:346:ILE:HD13	2.08	0.82
1:B:817:UNK:C	1:B:819:UNK:N	2.43	0.82
14:Z:253:PRO:CD	14:Z:254:LYS:H	1.91	0.82
1:B:248:UNK:O	1:B:251:UNK:N	2.13	0.82
1:B:694:UNK:CB	2:D:475:UNK:O	2.27	0.82
10:U:185:ILE:HD11	10:U:261:LEU:CG	2.09	0.82
8:E:102:UNK:O	8:E:118:UNK:HA	1.79	0.81
14:Z:250:PRO:O	14:Z:253:PRO:HG2	1.80	0.81
28:5:402:UNK:CB	28:6:678:UNK:CB	2.58	0.81
4:A:248:UNK:O	4:A:251:UNK:N	2.13	0.81
16:b:240:UNK:HA	16:b:241:UNK:CB	2.10	0.81
5:1:31:UNK:O	5:1:34:UNK:CB	2.28	0.81
28:6:693:UNK:HA	28:6:696:UNK:CB	2.10	0.81
1:B:817:UNK:O	1:B:818:UNK:C	2.29	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:817:UNK:C	4:A:819:UNK:N	2.43	0.81
10:U:352:THR:HG21	24:l:64:VAL:H	1.45	0.81
4:A:817:UNK:O	4:A:818:UNK:C	2.29	0.81
10:W:56:ILE:HG22	10:W:58:ILE:CD1	2.10	0.80
14:Z:251:ASP:C	14:Z:255:PHE:HD2	1.89	0.80
14:Z:252:ASN:N	14:Z:253:PRO:HD3	1.95	0.80
4:A:518:UNK:O	4:A:519:UNK:CA	2.30	0.80
1:B:518:UNK:O	1:B:519:UNK:CA	2.30	0.80
13:Y:168:PHE:O	13:Y:199:TYR:CE1	2.34	0.80
1:B:291:UNK:C	10:T:350:LEU:CD2	2.52	0.79
28:6:682:UNK:O	28:6:686:UNK:N	2.15	0.79
5:1:115:UNK:CB	6:2:119:UNK:CB	2.61	0.79
6:2:50:UNK:O	6:2:51:UNK:O	2.01	0.79
13:Y:162:GLN:HG3	14:Z:243:LEU:HD23	1.61	0.79
1:B:824:UNK:O	1:B:827:UNK:N	2.16	0.79
4:A:836:UNK:O	4:A:840:UNK:CB	2.31	0.79
4:A:260:UNK:HA	10:T:96:LYS:NZ	1.97	0.79
1:B:214:UNK:O	1:B:216:UNK:N	2.15	0.79
3:C:686:UNK:CB	4:A:587:UNK:CB	2.61	0.79
24:l:67:LYS:HE3	24:l:67:LYS:CA	2.11	0.79
1:B:1209:UNK:O	1:B:1213:UNK:N	2.16	0.78
1:B:836:UNK:O	1:B:840:UNK:CB	2.31	0.78
4:A:1209:UNK:O	4:A:1213:UNK:N	2.16	0.78
19:g:180:SER:HA	28:6:701:UNK:CB	2.14	0.78
4:A:824:UNK:O	4:A:827:UNK:N	2.16	0.78
4:A:260:UNK:HA	10:T:96:LYS:HZ3	1.48	0.78
14:Z:250:PRO:C	14:Z:253:PRO:HD3	2.09	0.77
20:h:31:SER:C	28:6:707:UNK:CB	2.57	0.77
10:G:237:GLU:OE2	28:6:492:UNK:O	2.03	0.77
13:Y:168:PHE:CD2	13:Y:200:GLU:HG3	2.19	0.77
28:5:260:UNK:O	28:5:264:UNK:N	2.17	0.77
10:W:45:VAL:N	12:X:275:ASN:ND2	2.28	0.77
10:G:237:GLU:OE1	28:6:495:UNK:CB	2.32	0.77
4:A:216:UNK:O	4:A:219:UNK:N	2.18	0.77
28:5:237:UNK:O	28:5:241:UNK:N	2.18	0.77
2:D:365:UNK:CA	2:D:444:UNK:CB	2.63	0.77
10:U:352:THR:CG2	24:l:63:ARG:HA	2.14	0.76
1:B:216:UNK:O	1:B:219:UNK:N	2.18	0.76
1:B:873:UNK:O	1:B:877:UNK:CB	2.34	0.76
5:1:144:UNK:O	5:1:145:UNK:C	2.33	0.76
3:C:473:UNK:HA	4:A:690:UNK:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:365:UNK:CA	3:C:444:UNK:CB	2.63	0.76
10:W:56:ILE:CG2	10:W:58:ILE:HD11	2.16	0.76
28:5:380:UNK:O	28:5:384:UNK:CB	2.34	0.75
1:B:526:UNK:C	1:B:528:UNK:H	1.99	0.75
4:A:872:UNK:O	4:A:876:UNK:CA	2.35	0.75
4:A:873:UNK:O	4:A:877:UNK:CB	2.34	0.75
28:6:570:UNK:O	28:6:574:UNK:N	2.20	0.75
5:1:65:UNK:CB	5:1:75:UNK:CB	2.65	0.75
28:5:352:UNK:O	28:5:356:UNK:N	2.20	0.75
19:g:180:SER:CA	28:6:701:UNK:CB	2.64	0.75
28:6:560:UNK:O	28:6:564:UNK:N	2.19	0.75
1:B:271:UNK:O	1:B:274:UNK:CA	2.35	0.75
8:E:103:UNK:CB	8:E:117:UNK:O	2.35	0.75
28:6:692:UNK:O	28:6:696:UNK:CB	2.35	0.74
1:B:872:UNK:O	1:B:876:UNK:CA	2.34	0.74
10:Q:50:GLY:CA	24:l:62:LYS:HD3	2.17	0.74
28:5:423:UNK:CB	28:6:699:UNK:CB	2.65	0.74
4:A:271:UNK:O	4:A:274:UNK:CA	2.35	0.74
28:5:317:UNK:O	28:5:321:UNK:CB	2.35	0.74
1:B:701:UNK:CB	2:D:478:UNK:O	2.36	0.74
10:U:352:THR:CG2	24:l:64:VAL:H	2.00	0.74
4:A:526:UNK:C	4:A:528:UNK:H	1.99	0.74
28:5:382:UNK:O	28:5:386:UNK:N	2.21	0.74
10:W:56:ILE:HG22	10:W:58:ILE:HD11	1.68	0.73
1:B:309:UNK:CB	1:B:349:UNK:O	2.30	0.73
3:C:685:UNK:HA	4:A:581:UNK:HA	1.69	0.73
8:E:81:UNK:O	8:E:87:UNK:CA	2.36	0.73
10:U:376:PHE:C	24:l:71:PHE:HB2	2.14	0.73
17:d:37:UNK:HA	17:d:73:UNK:O	1.88	0.73
14:Z:251:ASP:HB2	14:Z:255:PHE:CE2	2.24	0.73
4:A:1019:UNK:CB	4:A:1104:UNK:CB	2.68	0.72
1:B:518:UNK:O	1:B:519:UNK:HA	1.89	0.72
8:E:107:UNK:HA	8:E:112:UNK:C	2.18	0.72
4:A:518:UNK:O	4:A:519:UNK:HA	1.89	0.72
17:c:67:UNK:O	17:c:73:UNK:HA	1.89	0.72
28:5:287:UNK:O	28:5:291:UNK:N	2.23	0.72
4:A:457:UNK:CA	4:A:458:UNK:CB	2.57	0.71
1:B:291:UNK:O	1:B:295:UNK:N	2.24	0.71
28:5:416:UNK:CB	28:6:692:UNK:CB	2.68	0.71
15:a:244:UNK:O	15:a:248:UNK:N	2.24	0.71
28:5:236:UNK:O	28:5:240:UNK:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:152:UNK:C	8:E:153:UNK:N	2.53	0.70
15:a:265:UNK:CB	15:a:467:UNK:CB	2.69	0.70
13:Y:168:PHE:HA	13:Y:199:TYR:CE1	2.26	0.70
4:A:291:UNK:O	4:A:295:UNK:N	2.24	0.70
28:6:561:UNK:O	28:6:565:UNK:N	2.24	0.70
28:6:640:UNK:O	28:6:644:UNK:N	2.25	0.70
13:Y:168:PHE:CA	13:Y:199:TYR:CE1	2.74	0.70
28:6:533:UNK:O	28:6:537:UNK:N	2.25	0.70
1:B:1121:UNK:O	1:B:1124:UNK:N	2.25	0.70
3:C:685:UNK:C	4:A:580:UNK:O	2.39	0.70
24:l:69:LEU:HD22	24:l:69:LEU:O	1.92	0.69
28:6:570:UNK:O	28:6:574:UNK:CB	2.40	0.69
1:B:271:UNK:O	1:B:274:UNK:HA	1.92	0.69
4:A:1023:UNK:O	4:A:1108:UNK:C	2.32	0.69
4:A:271:UNK:O	4:A:274:UNK:HA	1.92	0.69
10:W:58:ILE:HD12	10:W:58:ILE:N	2.06	0.69
13:Y:168:PHE:C	13:Y:199:TYR:CE1	2.71	0.69
24:l:66:THR:HB	24:l:69:LEU:CG	2.22	0.69
13:Y:124:CYS:SG	13:Y:224:THR:HG23	2.31	0.69
4:A:1121:UNK:O	4:A:1124:UNK:N	2.25	0.69
8:E:107:UNK:CB	8:E:111:UNK:HA	2.22	0.69
20:h:32:GLN:CB	28:6:707:UNK:CB	2.71	0.69
14:Z:253:PRO:CD	14:Z:254:LYS:N	2.55	0.69
4:A:544:UNK:C	4:A:546:UNK:H	2.05	0.69
4:A:689:UNK:O	4:A:693:UNK:N	2.26	0.69
28:5:381:UNK:O	28:5:385:UNK:CB	2.41	0.69
14:Z:250:PRO:C	14:Z:253:PRO:CD	2.66	0.68
14:Z:252:ASN:N	14:Z:253:PRO:CD	2.56	0.68
24:l:69:LEU:O	24:l:69:LEU:HD13	1.93	0.68
1:B:1391:UNK:O	1:B:1395:UNK:N	2.27	0.68
14:Z:250:PRO:O	14:Z:253:PRO:HD2	1.91	0.68
28:6:681:UNK:O	28:6:685:UNK:N	2.27	0.68
1:B:306:UNK:O	1:B:310:UNK:N	2.27	0.68
8:E:106:UNK:O	8:E:114:UNK:N	2.27	0.68
10:P:337:LEU:HD12	25:m:5:LYS:CB	2.23	0.68
10:W:47:VAL:HG23	12:X:231:PHE:O	1.94	0.68
4:A:1391:UNK:O	4:A:1395:UNK:N	2.27	0.68
1:B:1210:UNK:O	1:B:1214:UNK:CB	2.42	0.67
4:A:1210:UNK:O	4:A:1214:UNK:CB	2.42	0.67
4:A:1255:UNK:O	4:A:1259:UNK:N	2.27	0.67
13:Y:93:LYS:CE	13:Y:122:GLU:CD	2.66	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:118:LYS:O	13:Y:122:GLU:HG3	1.94	0.67
1:B:457:UNK:CA	1:B:458:UNK:CB	2.56	0.67
1:B:1255:UNK:O	1:B:1259:UNK:N	2.27	0.67
2:D:445:UNK:O	2:D:462:UNK:CB	2.43	0.67
4:A:281:UNK:O	4:A:284:UNK:C	2.42	0.67
6:2:144:UNK:C	6:2:146:UNK:N	2.52	0.67
3:C:473:UNK:CA	4:A:695:UNK:N	2.39	0.67
4:A:306:UNK:O	4:A:310:UNK:N	2.27	0.67
8:E:107:UNK:CB	8:E:111:UNK:C	2.72	0.67
1:B:281:UNK:O	1:B:284:UNK:C	2.42	0.67
3:C:445:UNK:O	3:C:462:UNK:CB	2.43	0.67
4:A:544:UNK:O	4:A:546:UNK:N	2.27	0.66
10:U:352:THR:HG21	24:l:64:VAL:N	2.11	0.66
1:B:698:UNK:HA	2:D:478:UNK:O	1.95	0.66
3:C:472:UNK:CB	4:A:694:UNK:CB	2.73	0.65
28:6:661:UNK:O	28:6:665:UNK:N	2.29	0.65
4:A:1049:UNK:O	4:A:1052:UNK:N	2.29	0.65
28:6:692:UNK:O	28:6:696:UNK:CA	2.43	0.65
28:6:703:UNK:O	28:6:707:UNK:N	2.29	0.65
10:U:121:ARG:HE	10:U:375:THR:HG21	1.61	0.65
1:B:351:UNK:C	1:B:353:UNK:N	2.58	0.65
1:B:1049:UNK:O	1:B:1052:UNK:N	2.30	0.65
1:B:817:UNK:O	1:B:819:UNK:CA	2.45	0.65
17:c:66:UNK:HA	17:c:74:UNK:O	1.96	0.65
19:g:156:GLN:O	19:g:158:LEU:N	2.26	0.65
4:A:362:UNK:CB	4:A:424:UNK:CB	2.75	0.65
1:B:351:UNK:O	1:B:352:UNK:C	2.45	0.64
1:B:817:UNK:O	1:B:820:UNK:N	2.30	0.64
4:A:351:UNK:C	4:A:353:UNK:N	2.58	0.64
8:E:101:UNK:O	8:E:119:UNK:C	2.45	0.64
1:B:1152:UNK:O	1:B:1156:UNK:CB	2.45	0.64
4:A:1152:UNK:O	4:A:1156:UNK:CB	2.45	0.64
10:U:375:THR:HG23	10:U:376:PHE:H	1.62	0.64
8:E:106:UNK:O	8:E:113:UNK:CA	2.46	0.64
4:A:817:UNK:O	4:A:819:UNK:CA	2.45	0.63
14:Z:245:SER:CB	14:Z:248:VAL:CG2	2.59	0.63
4:A:351:UNK:O	4:A:352:UNK:C	2.45	0.63
4:A:817:UNK:O	4:A:820:UNK:N	2.30	0.63
8:E:200:UNK:C	8:E:201:UNK:N	2.61	0.63
4:A:1062:UNK:O	4:A:1065:UNK:N	2.32	0.63
1:B:1062:UNK:O	1:B:1065:UNK:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:107:UNK:CA	8:E:112:UNK:O	2.41	0.63
13:Y:153:THR:HG22	13:Y:180:THR:HG22	1.81	0.63
13:Y:198:TYR:HB2	14:Z:235:LYS:HG2	1.81	0.63
1:B:518:UNK:CA	1:B:519:UNK:H2	2.12	0.62
3:C:686:UNK:O	4:A:585:UNK:C	2.43	0.62
4:A:518:UNK:CA	4:A:519:UNK:H2	2.12	0.62
28:5:238:UNK:O	28:5:242:UNK:N	2.32	0.62
28:5:351:UNK:O	28:5:355:UNK:N	2.33	0.62
1:B:728:UNK:N	1:B:916:UNK:CB	2.63	0.62
1:B:1342:UNK:O	1:B:1346:UNK:N	2.33	0.62
4:A:1023:UNK:O	4:A:1108:UNK:O	2.17	0.62
24:l:56:TYR:CZ	24:l:60:LYS:HD3	2.34	0.62
1:B:248:UNK:O	1:B:249:UNK:C	2.48	0.62
4:A:248:UNK:O	4:A:249:UNK:C	2.48	0.62
24:l:67:LYS:CE	24:l:68:GLY:H	2.13	0.62
14:Z:251:ASP:C	14:Z:253:PRO:CD	2.73	0.62
4:A:262:UNK:O	4:A:266:UNK:N	2.33	0.62
4:A:689:UNK:O	4:A:693:UNK:CA	2.47	0.62
4:A:518:UNK:CB	4:A:519:UNK:CB	2.78	0.61
4:A:1342:UNK:O	4:A:1346:UNK:N	2.33	0.61
4:A:1116:UNK:O	4:A:1119:UNK:N	2.32	0.61
1:B:213:UNK:CB	1:B:214:UNK:H2	1.87	0.61
1:B:457:UNK:CB	1:B:459:UNK:CA	2.78	0.61
1:B:518:UNK:CB	1:B:519:UNK:CB	2.78	0.61
8:E:107:UNK:CB	8:E:111:UNK:CA	2.78	0.61
1:B:262:UNK:O	1:B:266:UNK:N	2.33	0.61
1:B:1116:UNK:O	1:B:1119:UNK:N	2.32	0.61
1:B:1151:UNK:O	1:B:1155:UNK:N	2.34	0.61
1:B:1254:UNK:O	1:B:1258:UNK:CB	2.49	0.61
4:A:457:UNK:CB	4:A:459:UNK:CA	2.78	0.61
28:6:534:UNK:O	28:6:538:UNK:CB	2.49	0.61
4:A:1254:UNK:O	4:A:1258:UNK:CB	2.49	0.61
28:6:668:UNK:O	28:6:672:UNK:N	2.34	0.61
4:A:1151:UNK:O	4:A:1155:UNK:N	2.34	0.60
10:G:350:LEU:HD13	14:Z:265:VAL:HG22	1.80	0.60
28:5:377:UNK:O	28:5:381:UNK:N	2.33	0.60
4:A:1140:UNK:O	4:A:1144:UNK:N	2.35	0.60
4:A:1350:UNK:CB	4:A:1418:UNK:C	2.79	0.60
28:6:606:UNK:O	28:6:610:UNK:N	2.34	0.60
23:k:8:ASP:CA	23:k:10:PRO:HD3	2.31	0.60
1:B:1350:UNK:CB	1:B:1418:UNK:CA	2.80	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1390:UNK:O	1:B:1394:UNK:CB	2.49	0.60
1:B:1140:UNK:O	1:B:1144:UNK:N	2.35	0.60
28:5:316:UNK:O	28:5:320:UNK:CB	2.50	0.60
1:B:874:UNK:O	1:B:878:UNK:N	2.35	0.59
1:B:397:UNK:O	1:B:401:UNK:N	2.35	0.59
1:B:824:UNK:O	1:B:825:UNK:C	2.50	0.59
13:Y:168:PHE:HD2	13:Y:200:GLU:HG3	1.65	0.59
1:B:1121:UNK:O	1:B:1122:UNK:C	2.50	0.59
1:B:1350:UNK:CB	1:B:1418:UNK:C	2.79	0.59
4:A:397:UNK:O	4:A:401:UNK:N	2.35	0.59
6:2:144:UNK:O	6:2:147:UNK:N	2.35	0.59
3:C:599:UNK:HA	3:C:626:UNK:O	2.03	0.59
4:A:1350:UNK:CB	4:A:1418:UNK:CA	2.80	0.59
1:B:395:UNK:O	1:B:396:UNK:C	2.50	0.59
4:A:248:UNK:CA	4:A:360:UNK:CB	2.81	0.59
8:E:82:UNK:HA	8:E:87:UNK:C	2.33	0.59
17:d:35:UNK:HA	17:d:75:UNK:O	2.02	0.59
4:A:874:UNK:O	4:A:878:UNK:N	2.35	0.59
4:A:567:UNK:O	4:A:568:UNK:C	2.51	0.58
10:U:185:ILE:HG23	10:U:185:ILE:O	2.02	0.58
4:A:424:UNK:O	4:A:426:UNK:N	2.36	0.58
6:2:130:UNK:CB	6:2:174:UNK:CB	2.81	0.58
10:W:43:LYS:C	12:X:275:ASN:HB3	2.24	0.58
2:D:599:UNK:HA	2:D:626:UNK:O	2.02	0.58
4:A:1255:UNK:O	4:A:1259:UNK:CB	2.51	0.58
24:l:67:LYS:HE2	24:l:68:GLY:H	1.67	0.58
1:B:281:UNK:O	1:B:284:UNK:O	2.22	0.58
1:B:1201:UNK:O	1:B:1205:UNK:N	2.37	0.58
4:A:824:UNK:O	4:A:825:UNK:C	2.50	0.58
13:Y:26:PRO:HB2	13:Y:172:ARG:HD3	1.85	0.58
13:Y:27:GLY:HA3	13:Y:170:ASN:ND2	2.19	0.58
13:Y:168:PHE:O	13:Y:199:TYR:HD1	1.82	0.58
24:l:69:LEU:HD22	24:l:69:LEU:C	2.28	0.58
4:A:1152:UNK:O	4:A:1156:UNK:N	2.36	0.58
4:A:1202:UNK:O	4:A:1206:UNK:CB	2.52	0.58
4:A:1391:UNK:O	4:A:1395:UNK:CB	2.52	0.58
10:G:271:GLU:OE2	13:Y:266:ARG:NH1	2.36	0.58
1:B:307:UNK:O	1:B:311:UNK:N	2.36	0.58
1:B:1255:UNK:O	1:B:1259:UNK:CB	2.51	0.58
4:A:603:UNK:O	4:A:604:UNK:C	2.51	0.58
28:5:289:UNK:O	28:5:293:UNK:CB	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1202:UNK:O	1:B:1206:UNK:CB	2.52	0.58
1:B:1391:UNK:O	1:B:1395:UNK:CB	2.52	0.58
4:A:601:UNK:O	4:A:602:UNK:C	2.51	0.58
4:A:602:UNK:O	4:A:603:UNK:C	2.51	0.58
28:6:532:UNK:O	28:6:536:UNK:N	2.37	0.58
1:B:424:UNK:O	1:B:426:UNK:N	2.36	0.58
4:A:307:UNK:O	4:A:311:UNK:N	2.37	0.58
1:B:568:UNK:O	1:B:569:UNK:C	2.51	0.57
1:B:216:UNK:O	1:B:217:UNK:C	2.52	0.57
1:B:1152:UNK:O	1:B:1156:UNK:N	2.36	0.57
4:A:943:UNK:CB	4:A:1035:UNK:N	2.67	0.57
14:Z:239:ILE:O	14:Z:243:LEU:HG	2.04	0.57
28:5:288:UNK:O	28:5:292:UNK:CA	2.51	0.57
4:A:216:UNK:O	4:A:217:UNK:C	2.52	0.57
24:l:66:THR:HB	24:l:69:LEU:CD1	2.34	0.57
10:U:182:ARG:C	10:U:183:ILE:HG13	2.28	0.57
1:B:306:UNK:HA	1:B:349:UNK:CB	2.35	0.57
1:B:694:UNK:O	2:D:477:UNK:O	2.22	0.57
4:A:1201:UNK:O	4:A:1205:UNK:N	2.37	0.57
19:g:153:PRO:O	19:g:154:GLN:C	2.48	0.57
4:A:281:UNK:O	4:A:284:UNK:O	2.22	0.57
1:B:566:UNK:O	1:B:567:UNK:C	2.52	0.57
4:A:566:UNK:O	4:A:567:UNK:C	2.51	0.57
4:A:1121:UNK:O	4:A:1122:UNK:C	2.50	0.57
1:B:806:UNK:H	28:5:214:UNK:CB	2.16	0.57
4:A:351:UNK:O	4:A:353:UNK:N	2.38	0.57
4:A:568:UNK:O	4:A:569:UNK:C	2.51	0.57
14:Z:143:LYS:HB3	14:Z:180:ASN:HB2	1.85	0.57
24:l:66:THR:HG22	24:l:83:TYR:CA	2.15	0.57
4:A:511:UNK:O	4:A:512:UNK:C	2.51	0.56
5:1:144:UNK:O	5:1:146:UNK:N	2.38	0.56
28:5:353:UNK:O	28:5:357:UNK:CA	2.53	0.56
3:C:473:UNK:CB	4:A:692:UNK:C	2.84	0.56
4:A:1370:UNK:O	4:A:1374:UNK:CB	2.54	0.56
13:Y:93:LYS:CE	13:Y:122:GLU:OE1	2.54	0.56
13:Y:121:ARG:NE	13:Y:154:ILE:HG12	2.20	0.56
15:a:64:UNK:O	15:a:270:UNK:CB	2.53	0.56
1:B:602:UNK:O	1:B:603:UNK:C	2.51	0.56
4:A:1139:UNK:O	4:A:1143:UNK:N	2.38	0.56
13:Y:40:LEU:HB3	13:Y:46:LEU:HD11	1.86	0.56
15:a:265:UNK:CB	15:a:467:UNK:HA	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:419:UNK:HA	28:5:422:UNK:CB	2.35	0.56
1:B:351:UNK:O	1:B:353:UNK:N	2.38	0.56
16:b:271:UNK:CB	16:b:272:UNK:HA	2.35	0.56
1:B:567:UNK:O	1:B:568:UNK:C	2.51	0.56
1:B:871:UNK:O	1:B:875:UNK:N	2.39	0.56
1:B:1370:UNK:O	1:B:1374:UNK:CB	2.54	0.56
4:A:451:UNK:O	4:A:452:UNK:C	2.51	0.56
4:A:871:UNK:O	4:A:875:UNK:N	2.39	0.56
13:Y:79:HIS:CD2	13:Y:155:ILE:HG21	2.40	0.56
13:Y:167:ASN:HB3	13:Y:169:TRP:CD1	2.40	0.56
28:5:237:UNK:O	28:5:241:UNK:CB	2.54	0.56
1:B:1139:UNK:O	1:B:1143:UNK:N	2.38	0.56
4:A:642:UNK:O	4:A:643:UNK:C	2.52	0.56
6:2:41:UNK:O	6:2:44:UNK:CB	2.53	0.56
8:E:181:UNK:O	8:E:183:UNK:N	2.39	0.56
3:C:688:UNK:C	4:A:559:UNK:CB	2.83	0.56
24:l:67:LYS:HE2	24:l:68:GLY:N	2.21	0.56
1:B:603:UNK:O	1:B:604:UNK:C	2.52	0.56
8:E:103:UNK:CA	8:E:117:UNK:O	2.54	0.56
10:U:121:ARG:NE	10:U:375:THR:HG21	2.21	0.56
3:C:471:UNK:CB	4:A:698:UNK:CB	2.83	0.55
3:C:684:UNK:C	4:A:584:UNK:CB	2.81	0.55
4:A:643:UNK:O	4:A:644:UNK:C	2.52	0.55
5:1:29:UNK:O	5:1:30:UNK:C	2.53	0.55
10:U:352:THR:HG21	24:l:63:ARG:CA	2.33	0.55
13:Y:243:ILE:HG23	14:Z:187:MET:HE1	1.88	0.55
28:5:433:UNK:HA	28:5:436:UNK:CB	2.36	0.55
28:6:562:UNK:O	28:6:566:UNK:N	2.39	0.55
16:b:41:UNK:CA	16:b:42:UNK:CB	2.84	0.55
4:A:641:UNK:O	4:A:642:UNK:C	2.51	0.55
28:5:316:UNK:O	28:5:320:UNK:CA	2.53	0.55
10:W:47:VAL:CG2	12:X:232:ASN:HB2	2.33	0.55
1:B:642:UNK:O	1:B:643:UNK:C	2.52	0.55
13:Y:168:PHE:HA	13:Y:199:TYR:CZ	2.42	0.55
10:H:352:THR:HG21	13:Y:278:LYS:CB	2.37	0.55
1:B:288:UNK:O	1:B:289:UNK:C	2.53	0.54
1:B:601:UNK:O	1:B:602:UNK:C	2.52	0.54
4:A:512:UNK:O	4:A:513:UNK:C	2.51	0.54
1:B:641:UNK:O	1:B:642:UNK:C	2.52	0.54
26:n:2:ALA:O	26:n:3:ASP:HB2	2.08	0.54
5:1:18:UNK:O	5:1:22:UNK:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:352:THR:CG2	24:l:63:ARG:CA	2.86	0.54
24:l:67:LYS:CA	24:l:67:LYS:CE	2.85	0.54
4:A:518:UNK:C	4:A:519:UNK:CA	2.86	0.54
15:a:442:UNK:CB	15:a:445:UNK:CB	2.86	0.54
1:B:1153:UNK:CB	1:B:1278:UNK:CB	2.86	0.54
4:A:281:UNK:C	4:A:284:UNK:N	2.71	0.54
14:Z:108:ARG:HD3	14:Z:117:SER:HB3	1.89	0.54
19:g:153:PRO:C	19:g:154:GLN:O	2.51	0.54
1:B:873:UNK:O	1:B:877:UNK:CA	2.55	0.54
3:C:471:UNK:CB	4:A:695:UNK:HA	2.37	0.54
4:A:288:UNK:O	4:A:289:UNK:C	2.53	0.54
14:Z:251:ASP:C	14:Z:253:PRO:HD3	2.33	0.54
10:W:190:VAL:HG22	10:W:261:LEU:HD23	1.90	0.54
1:B:281:UNK:C	1:B:284:UNK:N	2.71	0.53
8:E:151:UNK:O	8:E:153:UNK:N	2.40	0.53
4:A:873:UNK:O	4:A:877:UNK:CA	2.55	0.53
4:A:1153:UNK:CB	4:A:1278:UNK:CB	2.86	0.53
13:Y:198:TYR:CZ	13:Y:200:GLU:HB2	2.42	0.53
16:b:41:UNK:N	16:b:42:UNK:CB	2.72	0.53
1:B:518:UNK:C	1:B:519:UNK:CA	2.86	0.53
14:Z:96:LEU:HG	14:Z:210:ILE:HD11	1.90	0.53
24:l:61:ASP:N	24:l:61:ASP:OD1	2.41	0.53
1:B:395:UNK:O	1:B:398:UNK:N	2.41	0.53
3:C:365:UNK:CB	3:C:444:UNK:CB	2.87	0.53
4:A:1202:UNK:O	4:A:1206:UNK:N	2.42	0.53
4:A:1350:UNK:CB	4:A:1418:UNK:O	2.57	0.53
12:X:128:LEU:HD13	12:X:136:ALA:HB3	1.90	0.53
1:B:1202:UNK:O	1:B:1206:UNK:N	2.42	0.53
13:Y:118:LYS:HG2	13:Y:145:ALA:HB1	1.90	0.53
14:Z:66:ARG:HD3	14:Z:71:TYR:CE2	2.44	0.53
4:A:993:UNK:O	4:A:994:UNK:C	2.57	0.53
13:Y:237:ASN:OD1	14:Z:246:VAL:HG21	2.09	0.52
14:Z:100:ALA:HB2	14:Z:210:ILE:HD13	1.91	0.52
28:6:534:UNK:O	28:6:538:UNK:N	2.42	0.52
1:B:1350:UNK:CB	1:B:1418:UNK:O	2.57	0.52
28:5:317:UNK:O	28:5:321:UNK:CA	2.57	0.52
28:5:418:UNK:O	28:5:422:UNK:N	2.42	0.52
1:B:993:UNK:O	1:B:994:UNK:C	2.57	0.52
4:A:998:UNK:C	4:A:1000:UNK:N	2.71	0.52
26:n:8:ASP:C	26:n:10:PRO:HD3	2.34	0.52
1:B:526:UNK:O	1:B:528:UNK:N	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:229:UNK:O	8:E:230:UNK:CB	2.58	0.52
14:Z:61:LEU:HD22	14:Z:71:TYR:CD2	2.44	0.52
4:A:526:UNK:O	4:A:528:UNK:N	2.39	0.52
1:B:457:UNK:CA	1:B:459:UNK:N	2.72	0.52
28:6:683:UNK:O	28:6:687:UNK:N	2.43	0.52
8:E:363:UNK:O	8:E:364:UNK:CB	2.58	0.52
13:Y:237:ASN:OD1	14:Z:246:VAL:CG2	2.58	0.52
14:Z:50:ALA:HB2	14:Z:61:LEU:HD21	1.90	0.52
8:E:102:UNK:O	8:E:118:UNK:CA	2.55	0.52
17:d:37:UNK:CA	17:d:73:UNK:O	2.57	0.52
17:d:38:UNK:O	17:d:73:UNK:CB	2.58	0.52
16:b:240:UNK:CA	16:b:241:UNK:CB	2.84	0.51
23:k:9:LEU:N	23:k:10:PRO:CD	2.73	0.51
28:5:260:UNK:O	28:5:264:UNK:CB	2.57	0.51
2:D:365:UNK:CB	2:D:444:UNK:CB	2.87	0.51
24:l:67:LYS:CE	24:l:68:GLY:N	2.73	0.51
1:B:998:UNK:C	1:B:1000:UNK:N	2.71	0.51
4:A:457:UNK:CA	4:A:459:UNK:N	2.72	0.51
4:A:1023:UNK:CB	4:A:1104:UNK:O	2.57	0.51
5:1:98:UNK:O	5:1:116:UNK:CB	2.59	0.51
16:b:280:UNK:O	16:b:284:UNK:N	2.43	0.51
14:Z:144:ILE:HG23	14:Z:178:GLN:O	2.11	0.51
1:B:698:UNK:CA	2:D:477:UNK:C	2.82	0.51
4:A:742:UNK:HA	4:A:806:UNK:CB	2.40	0.51
10:W:45:VAL:HB	12:X:275:ASN:HD21	1.75	0.51
10:W:337:LEU:HD12	24:l:5:LYS:CB	2.40	0.51
4:A:489:UNK:O	4:A:490:UNK:C	2.59	0.51
23:k:9:LEU:N	23:k:10:PRO:HD3	2.25	0.51
5:1:64:UNK:HA	5:1:75:UNK:O	2.11	0.51
8:E:114:UNK:O	8:E:115:UNK:CB	2.58	0.51
4:A:272:UNK:C	4:A:274:UNK:N	2.73	0.51
16:b:283:UNK:O	16:b:287:UNK:N	2.43	0.51
10:W:185:ILE:HD11	10:W:261:LEU:HD21	1.92	0.50
13:Y:67:ILE:HB	13:Y:70:TYR:CD1	2.46	0.50
10:Q:337:LEU:HD12	23:k:5:LYS:CB	2.40	0.50
10:U:151:GLY:HA2	24:l:59:PHE:HE1	1.76	0.50
13:Y:258:LEU:HD12	14:Z:148:TRP:HB2	1.93	0.50
13:Y:39:LEU:HD21	14:Z:32:VAL:CG2	2.42	0.50
7:S:73:UNK:C	7:S:75:UNK:N	2.75	0.50
24:l:69:LEU:CD1	24:l:69:LEU:H	2.25	0.50
3:C:685:UNK:CB	4:A:580:UNK:O	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:l:70:ASP:OD2	24:l:74:ARG:HD3	2.11	0.50
13:Y:93:LYS:HZ2	13:Y:122:GLU:CD	2.17	0.50
17:c:65:UNK:O	17:c:76:UNK:N	2.44	0.50
24:l:8:ASP:C	24:l:10:PRO:HD3	2.37	0.50
10:W:72:ARG:NH2	12:X:277:GLU:OE2	2.45	0.50
13:Y:192:LEU:O	13:Y:209:HIS:HA	2.12	0.50
28:6:533:UNK:O	28:6:537:UNK:CB	2.60	0.50
1:B:489:UNK:O	1:B:490:UNK:C	2.59	0.50
1:B:1049:UNK:O	1:B:1050:UNK:C	2.60	0.50
4:A:1049:UNK:O	4:A:1050:UNK:C	2.60	0.50
8:E:348:UNK:CB	8:E:364:UNK:O	2.59	0.50
4:A:248:UNK:HA	4:A:360:UNK:CB	2.42	0.49
10:W:58:ILE:CD1	10:W:58:ILE:N	2.73	0.49
28:5:238:UNK:O	28:5:242:UNK:CB	2.60	0.49
5:1:31:UNK:O	5:1:35:UNK:N	2.45	0.49
5:1:99:UNK:O	5:1:100:UNK:CB	2.60	0.49
15:a:265:UNK:CB	15:a:467:UNK:CA	2.90	0.49
1:B:1328:UNK:O	1:B:1331:UNK:CB	2.61	0.49
8:E:108:UNK:N	8:E:112:UNK:O	2.45	0.49
8:E:200:UNK:C	8:E:201:UNK:H2	2.24	0.49
19:g:156:GLN:C	19:g:158:LEU:H	2.17	0.49
28:5:378:UNK:CB	28:6:654:UNK:CB	2.91	0.49
4:A:871:UNK:O	4:A:875:UNK:CB	2.60	0.49
8:E:103:UNK:HA	8:E:117:UNK:O	2.13	0.49
1:B:871:UNK:O	1:B:875:UNK:CB	2.61	0.49
10:W:315:LEU:HD11	24:l:14:ARG:CB	2.42	0.49
28:6:561:UNK:O	28:6:565:UNK:CB	2.60	0.49
4:A:1328:UNK:O	4:A:1331:UNK:CB	2.61	0.49
13:Y:64:PRO:HB3	13:Y:75:LEU:HD23	1.94	0.49
13:Y:93:LYS:NZ	13:Y:122:GLU:OE2	2.43	0.49
13:Y:131:TYR:CG	13:Y:229:ILE:HG21	2.47	0.49
16:b:470:UNK:O	16:b:474:UNK:N	2.46	0.49
28:5:433:UNK:O	28:5:437:UNK:N	2.46	0.49
1:B:694:UNK:O	2:D:477:UNK:N	2.46	0.48
28:6:660:UNK:O	28:6:664:UNK:N	2.45	0.48
1:B:1268:UNK:O	1:B:1272:UNK:N	2.46	0.48
3:C:373:UNK:CB	4:A:580:UNK:HA	2.43	0.48
10:G:281:PHE:CD2	14:Z:230:GLU:OE2	2.67	0.48
11:V:43:VAL:HG21	12:X:156:PRO:HG2	1.93	0.48
10:U:332:ALA:O	24:l:47:HIS:HA	2.13	0.48
28:6:571:UNK:O	28:6:575:UNK:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1268:UNK:O	4:A:1272:UNK:N	2.46	0.48
8:E:175:UNK:C	8:E:177:UNK:N	2.75	0.48
13:Y:198:TYR:OH	13:Y:200:GLU:HB3	2.14	0.48
28:5:440:UNK:CB	28:6:716:UNK:CB	2.91	0.48
3:C:685:UNK:CA	4:A:580:UNK:O	2.62	0.48
1:B:291:UNK:C	10:T:350:LEU:HD22	2.42	0.48
10:U:185:ILE:HD11	10:U:261:LEU:CD1	2.43	0.48
13:Y:259:ARG:NH2	14:Z:148:TRP:CH2	2.82	0.48
15:a:242:UNK:C	15:a:244:UNK:N	2.76	0.48
17:d:37:UNK:C	17:d:73:UNK:O	2.59	0.48
28:5:432:UNK:O	28:5:436:UNK:N	2.47	0.48
4:A:281:UNK:HA	4:A:284:UNK:CB	2.44	0.47
4:A:1342:UNK:O	4:A:1345:UNK:CA	2.62	0.47
16:b:290:UNK:O	16:b:294:UNK:N	2.46	0.47
1:B:281:UNK:HA	1:B:284:UNK:CB	2.44	0.47
1:B:694:UNK:C	2:D:477:UNK:N	2.77	0.47
1:B:1342:UNK:O	1:B:1345:UNK:CA	2.62	0.47
15:a:456:UNK:HA	15:a:459:UNK:CB	2.44	0.47
4:A:248:UNK:C	4:A:250:UNK:N	2.76	0.47
3:C:473:UNK:N	4:A:694:UNK:C	2.48	0.47
10:Q:315:LEU:HD11	23:k:14:ARG:CB	2.45	0.47
13:Y:75:LEU:N	13:Y:142:THR:OG1	2.46	0.47
25:m:9:LEU:N	25:m:10:PRO:CD	2.78	0.47
28:6:639:UNK:O	28:6:643:UNK:N	2.48	0.47
1:B:261:UNK:O	1:B:265:UNK:N	2.48	0.47
3:C:360:UNK:HA	3:C:368:UNK:O	2.15	0.47
3:C:689:UNK:CB	4:A:588:UNK:CB	2.93	0.47
13:Y:171:GLY:HA3	14:Z:239:ILE:CG2	2.45	0.47
28:5:352:UNK:O	28:5:356:UNK:CB	2.63	0.47
10:G:148:TYR:CE1	14:Z:265:VAL:HG11	2.50	0.47
2:D:360:UNK:HA	2:D:368:UNK:O	2.15	0.47
5:1:82:UNK:O	5:1:83:UNK:CB	2.62	0.47
24:l:9:LEU:N	24:l:10:PRO:CD	2.78	0.47
3:C:688:UNK:CA	4:A:559:UNK:CB	2.89	0.47
10:P:315:LEU:HD11	25:m:14:ARG:CB	2.44	0.47
28:5:433:UNK:CB	28:6:709:UNK:CB	2.92	0.47
13:Y:197:HIS:CE1	13:Y:199:TYR:HB3	2.50	0.46
15:a:242:UNK:O	15:a:245:UNK:N	2.49	0.46
1:B:272:UNK:C	1:B:274:UNK:N	2.73	0.46
4:A:261:UNK:O	4:A:265:UNK:N	2.48	0.46
14:Z:173:VAL:HG21	14:Z:224:ILE:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:315:LEU:HD11	24:l:14:ARG:HB3	1.97	0.46
14:Z:148:TRP:CZ2	14:Z:173:VAL:HG13	2.51	0.46
28:6:560:UNK:O	28:6:564:UNK:CB	2.64	0.46
4:A:1204:UNK:O	4:A:1205:UNK:C	2.63	0.46
12:X:128:LEU:HD11	12:X:133:ILE:HG13	1.98	0.46
13:Y:117:LEU:HG	13:Y:121:ARG:CZ	2.46	0.46
28:6:569:UNK:O	28:6:573:UNK:N	2.49	0.46
1:B:248:UNK:C	1:B:250:UNK:N	2.76	0.46
1:B:423:UNK:O	1:B:424:UNK:CB	2.64	0.46
1:B:1204:UNK:O	1:B:1205:UNK:C	2.63	0.46
10:U:371:ILE:O	10:U:375:THR:HG22	2.16	0.46
1:B:352:UNK:O	1:B:355:UNK:N	2.49	0.46
11:V:70:PRO:HG3	11:V:85:ILE:HD12	1.97	0.46
17:d:39:UNK:HA	17:d:72:UNK:HA	1.98	0.46
1:B:489:UNK:O	1:B:492:UNK:N	2.49	0.46
10:W:45:VAL:CB	12:X:275:ASN:HD21	2.29	0.46
14:Z:134:ILE:HB	14:Z:150:SER:HB2	1.97	0.46
4:A:352:UNK:O	4:A:355:UNK:N	2.49	0.45
10:U:308:LYS:HG2	24:l:39:GLU:HB2	1.97	0.45
16:b:41:UNK:HA	16:b:42:UNK:CB	2.46	0.45
24:l:3:ASP:N	24:l:6:TYR:OH	2.49	0.45
5:1:31:UNK:O	5:1:32:UNK:C	2.63	0.45
10:H:352:THR:HG21	13:Y:278:LYS:HB3	1.97	0.45
10:O:11:PRO:HG2	10:O:348:ALA:HB1	1.98	0.45
14:Z:261:GLU:O	14:Z:265:VAL:HG23	2.16	0.45
8:E:152:UNK:CA	8:E:153:UNK:H2	2.25	0.45
13:Y:131:TYR:CD2	13:Y:229:ILE:HG21	2.51	0.45
14:Z:72:ARG:HB2	14:Z:79:TYR:CE2	2.51	0.45
4:A:824:UNK:O	4:A:826:UNK:N	2.49	0.45
8:E:356:UNK:N	8:E:357:UNK:CA	2.79	0.45
19:g:156:GLN:C	19:g:158:LEU:N	2.75	0.45
28:6:606:UNK:O	28:6:610:UNK:CB	2.64	0.45
4:A:489:UNK:O	4:A:492:UNK:N	2.49	0.45
13:Y:75:LEU:HG	13:Y:141:CYS:C	2.41	0.45
13:Y:252:ASP:O	13:Y:256:LYS:HB2	2.17	0.45
20:h:72:PRO:CB	20:h:101:ALA:HB2	2.46	0.45
10:Q:50:GLY:HA3	24:l:62:LYS:HD3	1.96	0.45
13:Y:121:ARG:HB3	13:Y:154:ILE:HG12	1.98	0.45
13:Y:121:ARG:HE	13:Y:154:ILE:HG12	1.82	0.45
13:Y:168:PHE:C	13:Y:199:TYR:HE1	2.24	0.45
14:Z:108:ARG:NH1	14:Z:117:SER:OG	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Z:251:ASP:C	14:Z:253:PRO:HD2	2.42	0.45
8:E:197:UNK:O	8:E:198:UNK:CB	2.64	0.45
1:B:824:UNK:O	1:B:826:UNK:N	2.49	0.45
3:C:685:UNK:O	4:A:581:UNK:O	2.34	0.45
17:d:37:UNK:HA	17:d:74:UNK:HA	1.98	0.45
24:l:56:TYR:O	24:l:60:LYS:HB2	2.17	0.45
1:B:824:UNK:C	1:B:826:UNK:N	2.80	0.45
4:A:216:UNK:C	4:A:218:UNK:N	2.79	0.45
10:W:185:ILE:HD13	10:W:268:ILE:HD11	1.99	0.45
13:Y:129:ARG:HG2	13:Y:141:CYS:SG	2.57	0.45
14:Z:251:ASP:C	14:Z:255:PHE:CE2	2.94	0.44
25:m:8:ASP:C	25:m:10:PRO:HD3	2.41	0.44
1:B:216:UNK:C	1:B:218:UNK:N	2.79	0.44
1:B:693:UNK:O	2:D:476:UNK:CB	2.45	0.44
4:A:824:UNK:C	4:A:826:UNK:N	2.80	0.44
13:Y:246:ASN:O	13:Y:250:MET:N	2.47	0.44
3:C:685:UNK:O	4:A:581:UNK:C	2.65	0.44
10:T:331:SER:HA	26:n:13:ALA:HB2	1.99	0.44
13:Y:269:ILE:HD11	14:Z:107:TYR:HD1	1.81	0.44
14:Z:156:VAL:HG21	14:Z:213:ILE:HD11	1.99	0.44
1:B:702:UNK:O	1:B:706:UNK:N	2.51	0.44
3:C:472:UNK:N	4:A:694:UNK:CB	2.80	0.44
28:5:376:UNK:O	28:5:380:UNK:N	2.51	0.44
4:A:518:UNK:CB	4:A:519:UNK:CA	2.93	0.44
4:A:1209:UNK:O	4:A:1213:UNK:CB	2.66	0.44
8:E:99:UNK:CB	8:E:103:UNK:O	2.66	0.44
19:g:136:ASN:CB	19:g:155:PRO:N	2.80	0.44
7:S:73:UNK:O	7:S:75:UNK:N	2.51	0.43
10:Q:45:VAL:HG11	24:l:71:PHE:HD2	1.83	0.43
10:T:262:LEU:HB3	10:T:275:ILE:HD12	2.01	0.43
4:A:289:UNK:C	4:A:291:UNK:N	2.81	0.43
4:A:526:UNK:C	4:A:528:UNK:N	2.72	0.43
5:1:146:UNK:HA	5:1:147:UNK:HA	1.79	0.43
13:Y:59:MET:HE3	13:Y:78:GLU:HA	1.98	0.43
13:Y:237:ASN:CG	14:Z:246:VAL:HG21	2.44	0.43
13:Y:28:GLU:O	13:Y:32:VAL:N	2.47	0.43
24:l:56:TYR:CE2	24:l:60:LYS:HD3	2.53	0.43
24:l:67:LYS:HE3	24:l:68:GLY:H	1.82	0.43
10:T:332:ALA:N	26:n:12:ILE:O	2.52	0.43
10:U:315:LEU:CD1	24:l:44:SER:HB2	2.49	0.43
13:Y:168:PHE:HB3	13:Y:199:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:38:TYR:CD1	10:P:71:ILE:HG23	2.53	0.43
13:Y:32:VAL:O	13:Y:36:VAL:HG23	2.19	0.43
28:6:607:UNK:O	28:6:611:UNK:CB	2.66	0.43
1:B:291:UNK:CB	10:T:350:LEU:CD1	2.80	0.43
4:A:702:UNK:O	4:A:706:UNK:N	2.51	0.43
13:Y:177:TRP:CZ2	13:Y:192:LEU:HD11	2.54	0.43
13:Y:198:TYR:CZ	13:Y:200:GLU:CB	3.02	0.43
1:B:213:UNK:O	1:B:214:UNK:O	2.30	0.43
16:b:271:UNK:CB	16:b:272:UNK:CA	2.96	0.43
1:B:1209:UNK:O	1:B:1213:UNK:CB	2.66	0.42
4:A:544:UNK:C	4:A:546:UNK:N	2.75	0.42
10:O:315:LEU:HG	10:O:330:ILE:HD12	2.01	0.42
28:5:379:UNK:O	28:5:383:UNK:N	2.53	0.42
5:1:144:UNK:C	5:1:146:UNK:N	2.81	0.42
12:X:364:LEU:HD11	21:i:449:UNK:HA	2.01	0.42
1:B:289:UNK:C	1:B:291:UNK:N	2.81	0.42
3:C:473:UNK:N	4:A:695:UNK:N	2.63	0.42
14:Z:181:LYS:O	14:Z:182:SER:OG	2.33	0.42
15:a:442:UNK:CB	15:a:445:UNK:N	2.82	0.42
8:E:318:UNK:O	8:E:321:UNK:N	2.53	0.42
12:X:365:GLN:HE22	21:i:452:UNK:C	2.32	0.42
13:Y:38:LEU:HD23	14:Z:8:CYS:SG	2.59	0.42
4:A:1121:UNK:C	4:A:1123:UNK:N	2.81	0.42
4:A:1142:UNK:O	4:A:1146:UNK:N	2.52	0.42
14:Z:156:VAL:HG22	14:Z:167:TYR:CD1	2.55	0.42
15:a:258:UNK:O	15:a:262:UNK:N	2.52	0.42
1:B:1142:UNK:O	1:B:1146:UNK:N	2.52	0.42
6:2:89:UNK:C	6:2:90:UNK:O	2.67	0.42
13:Y:181:ILE:HD12	13:Y:181:ILE:N	2.33	0.42
13:Y:237:ASN:ND2	14:Z:246:VAL:HG21	2.35	0.42
14:Z:61:LEU:HD22	14:Z:71:TYR:CG	2.54	0.42
10:W:42:PRO:HD3	10:W:55:ASP:HB3	2.02	0.41
24:l:69:LEU:HD13	24:l:69:LEU:H	1.85	0.41
28:5:375:UNK:O	28:5:379:UNK:N	2.53	0.41
28:5:379:UNK:O	28:5:383:UNK:CB	2.68	0.41
5:1:66:UNK:O	5:1:94:UNK:HA	2.21	0.41
13:Y:128:LEU:HB2	13:Y:229:ILE:HD11	2.02	0.41
1:B:1328:UNK:O	1:B:1332:UNK:N	2.53	0.41
10:G:38:TYR:CD1	10:G:71:ILE:HG23	2.56	0.41
4:A:1328:UNK:O	4:A:1332:UNK:N	2.54	0.41
10:U:262:LEU:HB3	10:U:275:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1121:UNK:C	1:B:1123:UNK:N	2.81	0.41
4:A:1343:UNK:HA	4:A:1346:UNK:CB	2.51	0.41
28:6:682:UNK:O	28:6:686:UNK:CB	2.68	0.41
13:Y:118:LYS:HA	13:Y:121:ARG:HD2	2.03	0.41
14:Z:148:TRP:CD1	14:Z:175:LEU:CD2	3.04	0.41
23:k:3:ASP:N	23:k:6:TYR:OH	2.54	0.41
10:G:262:LEU:HB3	10:G:275:ILE:HD12	2.03	0.41
10:U:342:ILE:HD13	24:l:50:VAL:HG21	2.03	0.41
1:B:518:UNK:CB	1:B:519:UNK:CA	2.93	0.41
4:A:527:UNK:O	4:A:528:UNK:CB	2.68	0.41
6:2:50:UNK:O	6:2:51:UNK:C	2.67	0.41
9:F:392:UNK:C	9:F:394:UNK:N	2.84	0.41
10:G:237:GLU:CD	28:6:495:UNK:CB	2.93	0.41
14:Z:173:VAL:HG11	14:Z:228:LEU:HD11	2.03	0.41
6:2:89:UNK:O	6:2:90:UNK:O	2.38	0.41
10:H:243:LEU:HD13	10:P:288:MET:HE2	2.03	0.41
10:Q:30:ILE:HG23	10:Q:31:PRO:HD2	2.03	0.41
16:b:285:UNK:HA	22:j:1023:UNK:HA	2.03	0.41
28:5:381:UNK:O	28:5:385:UNK:CA	2.68	0.41
2:D:582:UNK:HA	2:D:592:UNK:O	2.22	0.40
8:E:296:UNK:O	8:E:300:UNK:N	2.54	0.40
10:G:352:THR:HG21	14:Z:261:GLU:HA	2.03	0.40
10:W:46:ARG:HG3	10:W:47:VAL:H	1.86	0.40
4:A:1368:UNK:O	4:A:1371:UNK:N	2.54	0.40
10:W:45:VAL:CA	12:X:275:ASN:HD21	2.33	0.40
26:n:9:LEU:N	26:n:10:PRO:CD	2.84	0.40
2:D:647:UNK:O	2:D:654:UNK:HA	2.22	0.40
3:C:647:UNK:O	3:C:654:UNK:HA	2.22	0.40
6:2:43:UNK:O	6:2:44:UNK:C	2.68	0.40
28:5:287:UNK:O	28:5:291:UNK:CB	2.69	0.40
28:5:380:UNK:O	28:5:384:UNK:CA	2.69	0.40
2:D:640:UNK:C	2:D:642:UNK:N	2.84	0.40
4:A:1203:UNK:O	4:A:1207:UNK:N	2.55	0.40
13:Y:198:TYR:CB	14:Z:235:LYS:HG2	2.48	0.40
26:n:9:LEU:N	26:n:10:PRO:HD3	2.36	0.40
2:D:599:UNK:CA	2:D:626:UNK:O	2.70	0.40
10:Q:185:ILE:O	10:Q:185:ILE:HG23	2.21	0.40
15:a:51:UNK:O	15:a:55:UNK:N	2.55	0.40
19:g:136:ASN:CB	19:g:154:GLN:C	2.94	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	
10	G	368/376 (98%)	350 (95%)	18 (5%)	0	100	100
10	H	368/376 (98%)	348 (95%)	20 (5%)	0	100	100
10	O	368/376 (98%)	347 (94%)	21 (6%)	0	100	100
10	P	368/376 (98%)	347 (94%)	21 (6%)	0	100	100
10	Q	368/376 (98%)	346 (94%)	22 (6%)	0	100	100
10	T	368/376 (98%)	341 (93%)	27 (7%)	0	100	100
10	U	368/376 (98%)	344 (94%)	24 (6%)	0	100	100
10	W	368/376 (98%)	347 (94%)	21 (6%)	0	100	100
11	V	368/396 (93%)	350 (95%)	18 (5%)	0	100	100
12	X	363/417 (87%)	331 (91%)	31 (8%)	1 (0%)	36	72
13	Y	273/286 (96%)	258 (94%)	15 (6%)	0	100	100
14	Z	268/293 (92%)	257 (96%)	11 (4%)	0	100	100
19	g	167/190 (88%)	145 (87%)	16 (10%)	6 (4%)	2	20
20	h	163/222 (73%)	146 (90%)	16 (10%)	1 (1%)	21	59
23	k	44/48 (92%)	40 (91%)	3 (7%)	1 (2%)	5	28
24	l	67/71 (94%)	58 (87%)	8 (12%)	1 (2%)	8	40
25	m	27/31 (87%)	24 (89%)	2 (7%)	1 (4%)	2	20
26	n	18/20 (90%)	15 (83%)	1 (6%)	2 (11%)	0	5
All	All	4702/4982 (94%)	4394 (93%)	295 (6%)	13 (0%)	37	72

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	g	67	PRO
19	g	72	PRO
19	g	154	GLN
23	k	9	LEU

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Mol	Chain	Res	Type
24	l	9	LEU
25	m	9	LEU
26	n	3	ASP
26	n	9	LEU
19	g	68	ASP
19	g	120	ILE
12	X	387	TRP
19	g	114	ILE
20	h	41	ILE

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	
10	G	318/324 (98%)	316 (99%)	2 (1%)	78	83
10	H	318/324 (98%)	314 (99%)	4 (1%)	61	74
10	O	318/324 (98%)	313 (98%)	5 (2%)	55	70
10	P	318/324 (98%)	313 (98%)	5 (2%)	55	70
10	Q	318/324 (98%)	313 (98%)	5 (2%)	55	70
10	T	318/324 (98%)	315 (99%)	3 (1%)	70	79
10	U	318/324 (98%)	312 (98%)	6 (2%)	50	67
10	W	318/324 (98%)	314 (99%)	4 (1%)	61	74
11	V	313/333 (94%)	313 (100%)	0	100	100
12	X	322/363 (89%)	318 (99%)	4 (1%)	63	75
13	Y	245/254 (96%)	238 (97%)	7 (3%)	37	58
14	Z	242/262 (92%)	236 (98%)	6 (2%)	42	63
23	k	31/41 (76%)	24 (77%)	7 (23%)	1	6
24	l	49/60 (82%)	37 (76%)	12 (24%)	1	4
25	m	7/16 (44%)	5 (71%)	2 (29%)	0	2
26	n	8/16 (50%)	7 (88%)	1 (12%)	4	16
All	All	3761/3937 (96%)	3688 (98%)	73 (2%)	49	67

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	G	30	ILE
10	G	279	LEU
10	H	30	ILE
10	H	183	ILE
10	H	278	VAL
10	H	279	LEU
10	O	183	ILE
10	O	271	GLU
10	O	278	VAL
10	O	279	LEU
10	O	304	SER
10	P	30	ILE
10	P	183	ILE
10	P	271	GLU
10	P	278	VAL
10	P	314	LEU
10	Q	30	ILE
10	Q	183	ILE
10	Q	278	VAL
10	Q	279	LEU
10	Q	314	LEU
10	T	80	VAL
10	T	183	ILE
10	T	278	VAL
10	U	80	VAL
10	U	183	ILE
10	U	197	TYR
10	U	271	GLU
10	U	273	GLU
10	U	278	VAL
10	W	53	GLU
10	W	58	ILE
10	W	183	ILE
10	W	279	LEU
12	X	44	LYS
12	X	274	ASP
12	X	277	GLU
12	X	328	GLU
13	Y	28	GLU
13	Y	73	GLN
13	Y	148	ILE
13	Y	200	GLU

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Mol	Chain	Res	Type
13	Y	243	ILE
13	Y	249	THR
13	Y	258	LEU
14	Z	118	SER
14	Z	144	ILE
14	Z	150	SER
14	Z	235	LYS
14	Z	245	SER
14	Z	268	GLN
23	k	6	TYR
23	k	14	ARG
23	k	37	LEU
23	k	39	GLU
23	k	42	SER
23	k	51	ASN
23	k	53	ASN
24	l	6	TYR
24	l	14	ARG
24	l	37	LEU
24	l	39	GLU
24	l	42	SER
24	l	51	ASN
24	l	53	ASN
24	l	61	ASP
24	l	67	LYS
24	l	69	LEU
24	l	77	LYS
24	l	78	THR
25	m	6	TYR
25	m	14	ARG
26	n	3	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
10	G	16	ASN
10	G	77	HIS
10	G	116	ASN
10	G	178	HIS
10	H	37	ASN
10	O	116	ASN
10	P	37	ASN

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Mol	Chain	Res	Type
10	Q	37	ASN
10	Q	206	HIS
10	T	98	GLN
10	U	77	HIS
11	V	78	ASN
11	V	128	ASN
11	V	246	GLN
11	V	275	HIS
10	W	37	ASN
12	X	379	ASN
13	Y	41	ASN
13	Y	79	HIS
13	Y	84	ASN
13	Y	197	HIS
14	Z	45	GLN
14	Z	178	GLN
14	Z	196	GLN
14	Z	209	HIS
14	Z	264	GLN
23	k	47	HIS
23	k	51	ASN
24	l	47	HIS
24	l	51	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
4	A	29
1	B	28
21	i	12
5	1	7
6	2	7
16	b	5
15	a	5
2	D	4
9	F	3
17	c	3
17	d	3
3	C	3
8	E	3
18	e	2
18	f	2
25	m	1
23	k	1
24	l	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b	363:UNK	C	401:UNK	N	98.24
1	b	167:UNK	C	201:UNK	N	96.90
1	a	166:UNK	C	201:UNK	N	95.47
1	a	362:UNK	C	401:UNK	N	81.15
1	a	625:UNK	C	701:UNK	N	68.30
1	b	634:UNK	C	701:UNK	N	67.11
1	i	467:UNK	C	508:UNK	N	67.04
1	B	1161:UNK	C	1190:UNK	N	65.65
1	A	1161:UNK	C	1190:UNK	N	65.65
1	i	40:UNK	C	155:UNK	N	62.15
1	e	38:UNK	C	42:UNK	N	56.21
1	f	38:UNK	C	42:UNK	N	55.17
1	B	1354:UNK	C	1356:UNK	N	52.82

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1354:UNK	C	1356:UNK	N	52.82
1	A	1389:UNK	C	1391:UNK	N	50.96
1	B	1388:UNK	C	1390:UNK	N	49.88
1	B	1070:UNK	C	1103:UNK	N	48.63
1	A	1070:UNK	C	1103:UNK	N	46.27
1	B	1223:UNK	C	1254:UNK	N	40.65
1	A	1223:UNK	C	1254:UNK	N	40.65
1	i	359:UNK	C	415:UNK	N	40.33
1	a	741:UNK	C	801:UNK	N	35.77
1	B	1009:UNK	C	1039:UNK	N	34.70
1	B	950:UNK	C	968:UNK	N	33.29
1	A	1010:UNK	C	1012:UNK	N	32.93
1	A	950:UNK	C	968:UNK	N	32.02
1	b	768:UNK	C	801:UNK	N	29.90
1	F	73:UNK	C	89:UNK	N	29.12
1	i	193:UNK	C	282:UNK	N	28.74
1	A	417:UNK	C	424:UNK	N	27.41
1	m	20:TYR	C	40:ALA	N	26.28
1	a	553:UNK	C	601:UNK	N	26.08
1	A	1025:UNK	C	1033:UNK	N	25.99
1	b	553:UNK	C	602:UNK	N	25.48
1	i	160:UNK	C	181:UNK	N	25.09
1	A	513:UNK	C	518:UNK	N	23.25
1	i	620:UNK	C	703:UNK	N	23.12
1	k	20:TYR	C	37:LEU	N	22.89
1	l	20:TYR	C	37:LEU	N	22.79
1	B	514:UNK	C	518:UNK	N	22.23
1	c	41:UNK	C	64:UNK	N	22.15
1	d	41:UNK	C	64:UNK	N	22.14
1	B	643:UNK	C	690:UNK	N	19.92
1	1	51:UNK	C	61:UNK	N	19.81
1	B	604:UNK	C	614:UNK	N	19.40
1	2	78:UNK	C	82:UNK	N	19.13
1	2	51:UNK	C	61:UNK	N	18.63
1	A	767:UNK	C	773:UNK	N	18.57
1	A	474:UNK	C	483:UNK	N	18.20
1	A	604:UNK	C	615:UNK	N	17.58
1	B	417:UNK	C	423:UNK	N	17.31
1	d	94:UNK	C	96:UNK	N	17.25
1	c	94:UNK	C	96:UNK	N	17.13
1	A	787:UNK	C	804:UNK	N	17.11
1	A	718:UNK	C	728:UNK	N	16.76

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	e	62:UNK	C	64:UNK	N	16.54
1	f	62:UNK	C	64:UNK	N	16.50
1	B	374:UNK	C	381:UNK	N	16.45
1	A	374:UNK	C	381:UNK	N	16.26
1	A	1285:UNK	C	1316:UNK	N	15.91
1	B	767:UNK	C	773:UNK	N	15.86
1	d	78:UNK	C	80:UNK	N	15.76
1	c	78:UNK	C	80:UNK	N	15.75
1	F	201:UNK	C	211:UNK	N	15.26
1	D	383:UNK	C	441:UNK	N	14.69
1	C	383:UNK	C	441:UNK	N	14.69
1	A	569:UNK	C	576:UNK	N	14.66
1	B	530:UNK	C	534:UNK	N	14.54
1	i	535:UNK	C	580:UNK	N	14.47
1	B	569:UNK	C	576:UNK	N	14.41
1	B	237:UNK	C	248:UNK	N	14.35
1	A	237:UNK	C	248:UNK	N	14.35
1	1	119:UNK	C	125:UNK	N	13.52
1	i	611:UNK	C	615:UNK	N	13.18
1	A	887:UNK	C	915:UNK	N	13.07
1	2	90:UNK	C	94:UNK	N	12.85
1	A	853:UNK	C	862:UNK	N	12.53
1	B	853:UNK	C	862:UNK	N	11.88
1	2	119:UNK	C	125:UNK	N	11.74
1	1	78:UNK	C	82:UNK	N	11.27
1	B	887:UNK	C	915:UNK	N	10.57
1	B	474:UNK	C	485:UNK	N	10.44
1	B	718:UNK	C	728:UNK	N	9.90
1	A	454:UNK	C	456:UNK	N	9.51
1	B	787:UNK	C	806:UNK	N	9.46
1	A	742:UNK	C	753:UNK	N	9.45
1	B	742:UNK	C	753:UNK	N	8.96
1	A	644:UNK	C	679:UNK	N	8.72
1	2	147:UNK	C	157:UNK	N	8.69
1	1	90:UNK	C	94:UNK	N	8.37
1	i	421:UNK	C	423:UNK	N	8.18
1	i	597:UNK	C	601:UNK	N	7.90
1	E	179:UNK	C	181:UNK	N	7.77
1	F	345:UNK	C	375:UNK	N	7.49
1	B	319:UNK	C	328:UNK	N	7.18
1	1	148:UNK	C	157:UNK	N	7.15
1	1	66:UNK	C	73:UNK	N	7.13

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	682:UNK	C	692:UNK	N	7.12
1	i	586:UNK	C	588:UNK	N	7.02
1	D	566:UNK	C	573:UNK	N	6.80
1	C	566:UNK	C	573:UNK	N	6.80
1	B	454:UNK	C	456:UNK	N	6.61
1	D	605:UNK	C	621:UNK	N	6.16
1	C	605:UNK	C	621:UNK	N	6.16
1	2	66:UNK	C	73:UNK	N	6.08
1	2	99:UNK	C	114:UNK	N	5.31
1	A	529:UNK	C	534:UNK	N	5.14
1	1	100:UNK	C	114:UNK	N	5.10
1	A	319:UNK	C	328:UNK	N	4.82
1	i	298:UNK	C	300:UNK	N	4.19
1	B	1285:UNK	C	1316:UNK	N	3.74
1	B	518:UNK	C	519:UNK	N	3.05
1	A	518:UNK	C	519:UNK	N	3.04
1	E	200:UNK	C	201:UNK	N	2.61
1	E	152:UNK	C	153:UNK	N	2.53
1	A	483:UNK	C	484:UNK	N	1.61
1	B	544:UNK	C	545:UNK	N	1.11
1	A	804:UNK	C	805:UNK	N	1.05
1	B	213:UNK	C	214:UNK	N	0.56

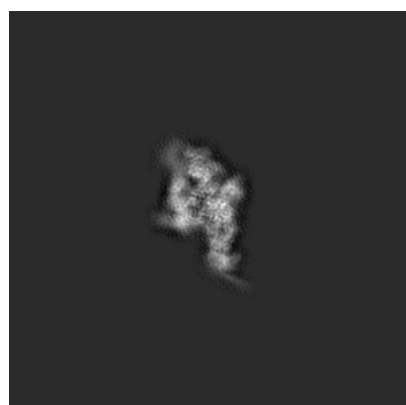
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3706. These allow visual inspection of the internal detail of the map and identification of artifacts.

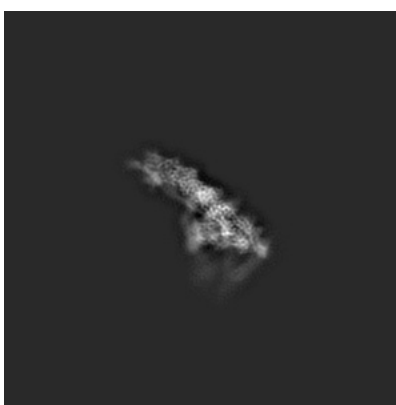
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

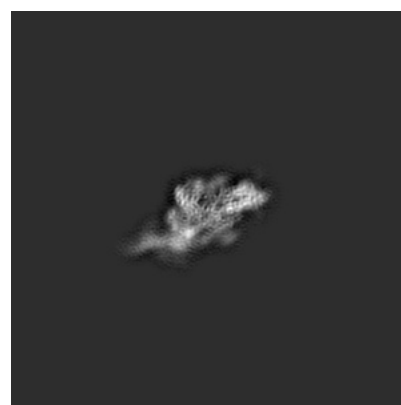
6.1.1 Primary map



X



Y



Z

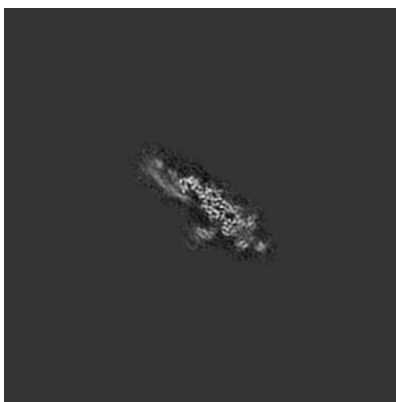
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 180



Y Index: 180

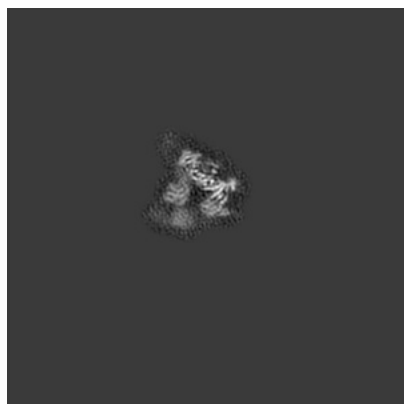


Z Index: 180

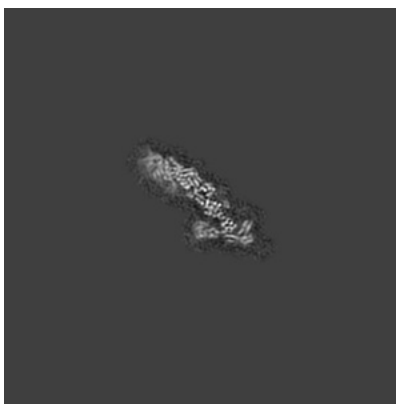
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

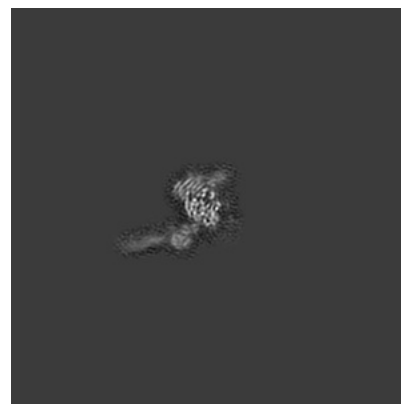
6.3.1 Primary map



X Index: 158



Y Index: 186

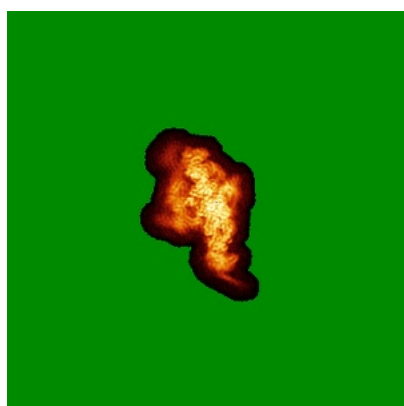


Z Index: 197

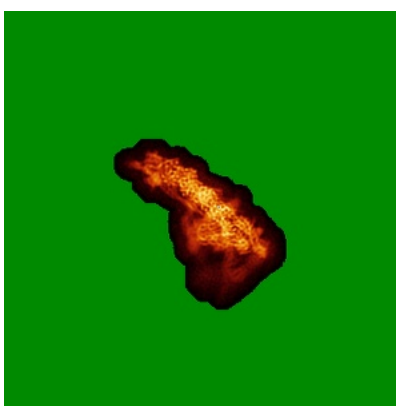
The images above show the largest variance slices of the map in three orthogonal directions.

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

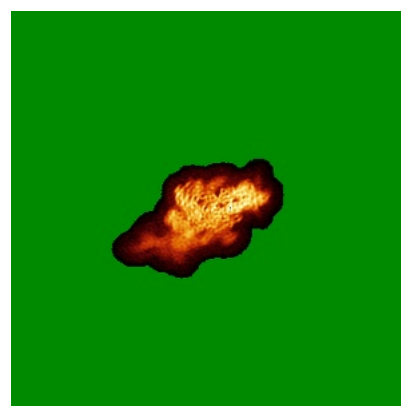
6.4.1 Primary map



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 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

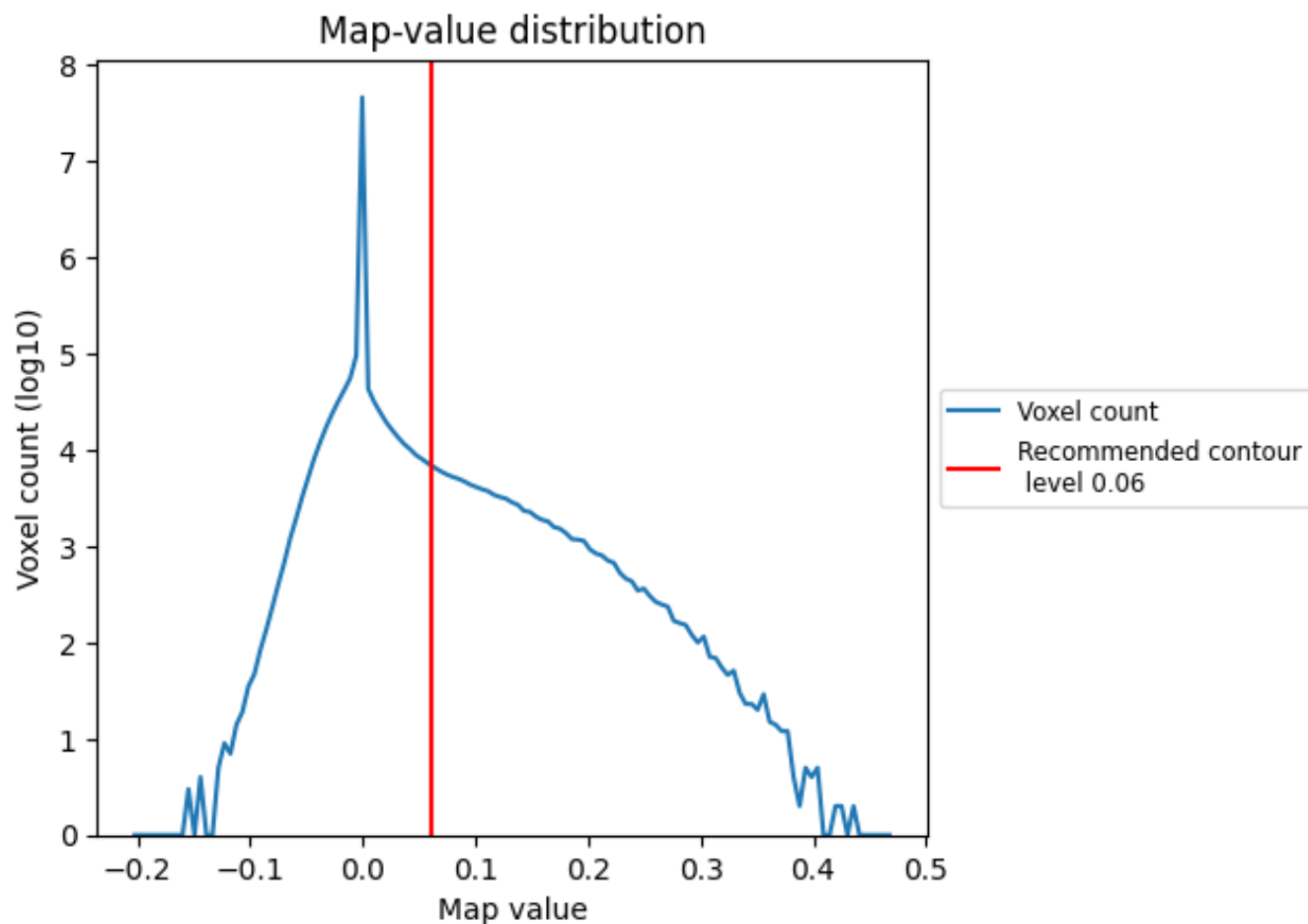
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

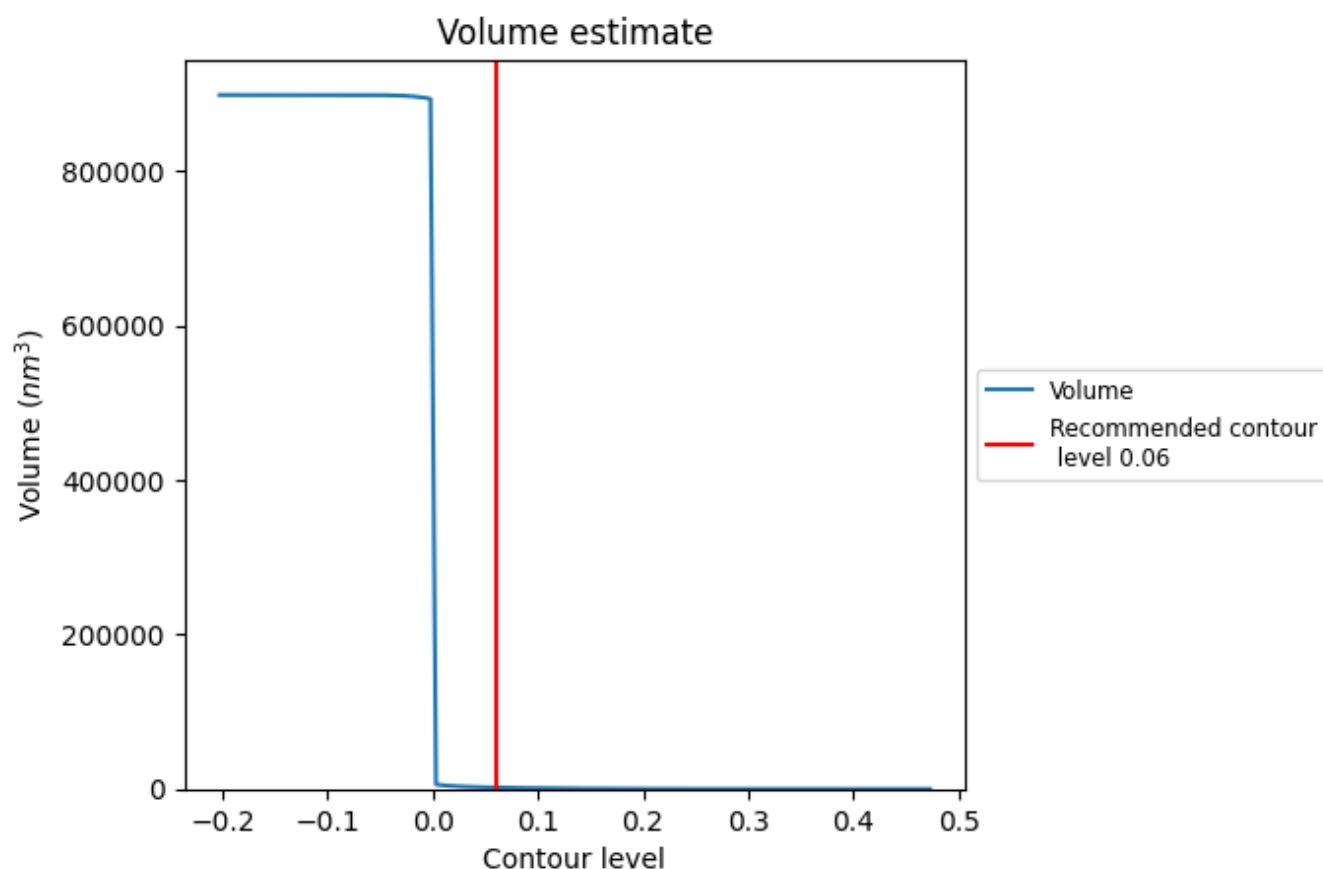
This section contains the results of statistical analysis of the map.

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.

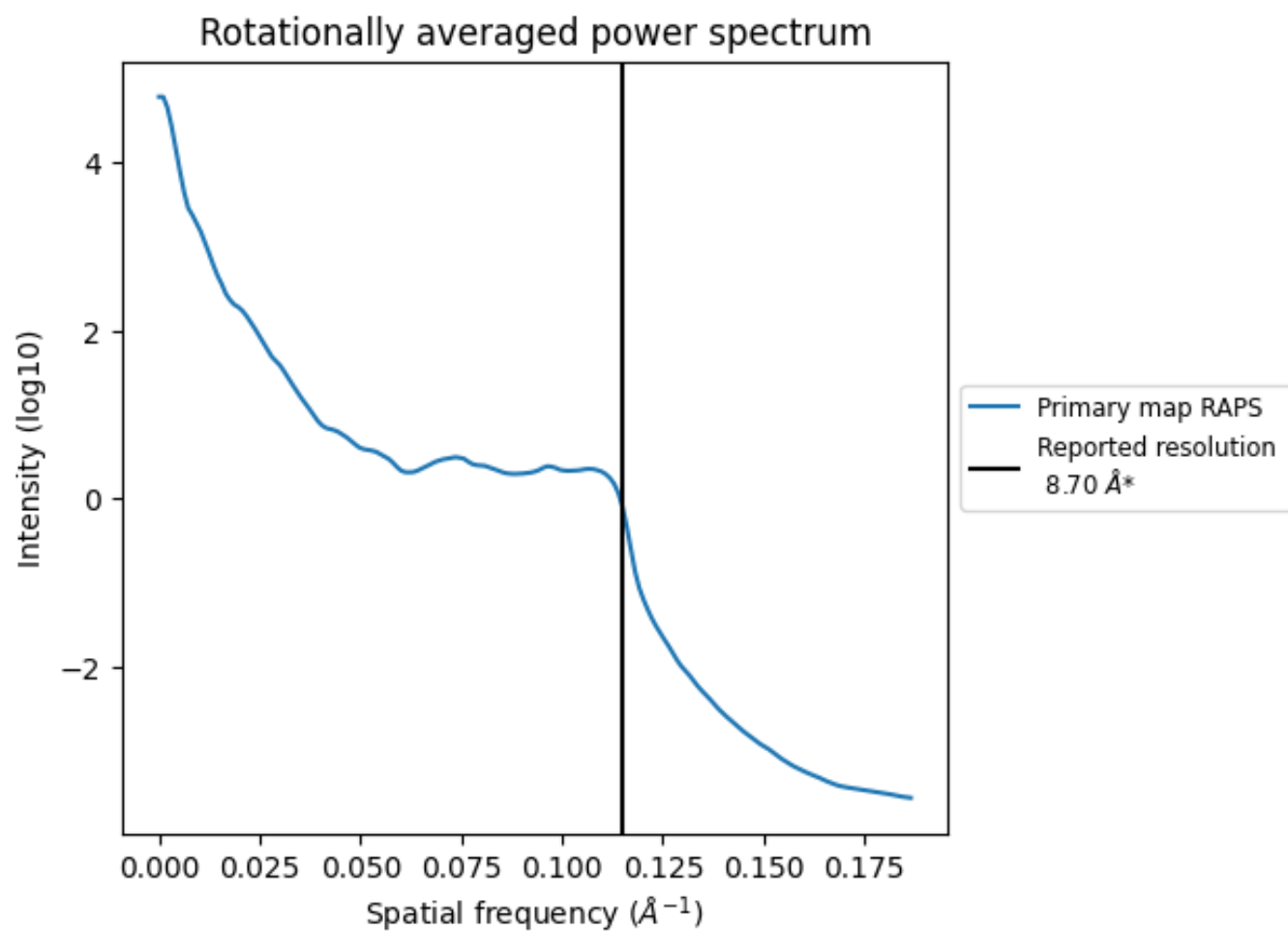
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1849 nm³; this corresponds to an approximate mass of 1670 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 ⓘ

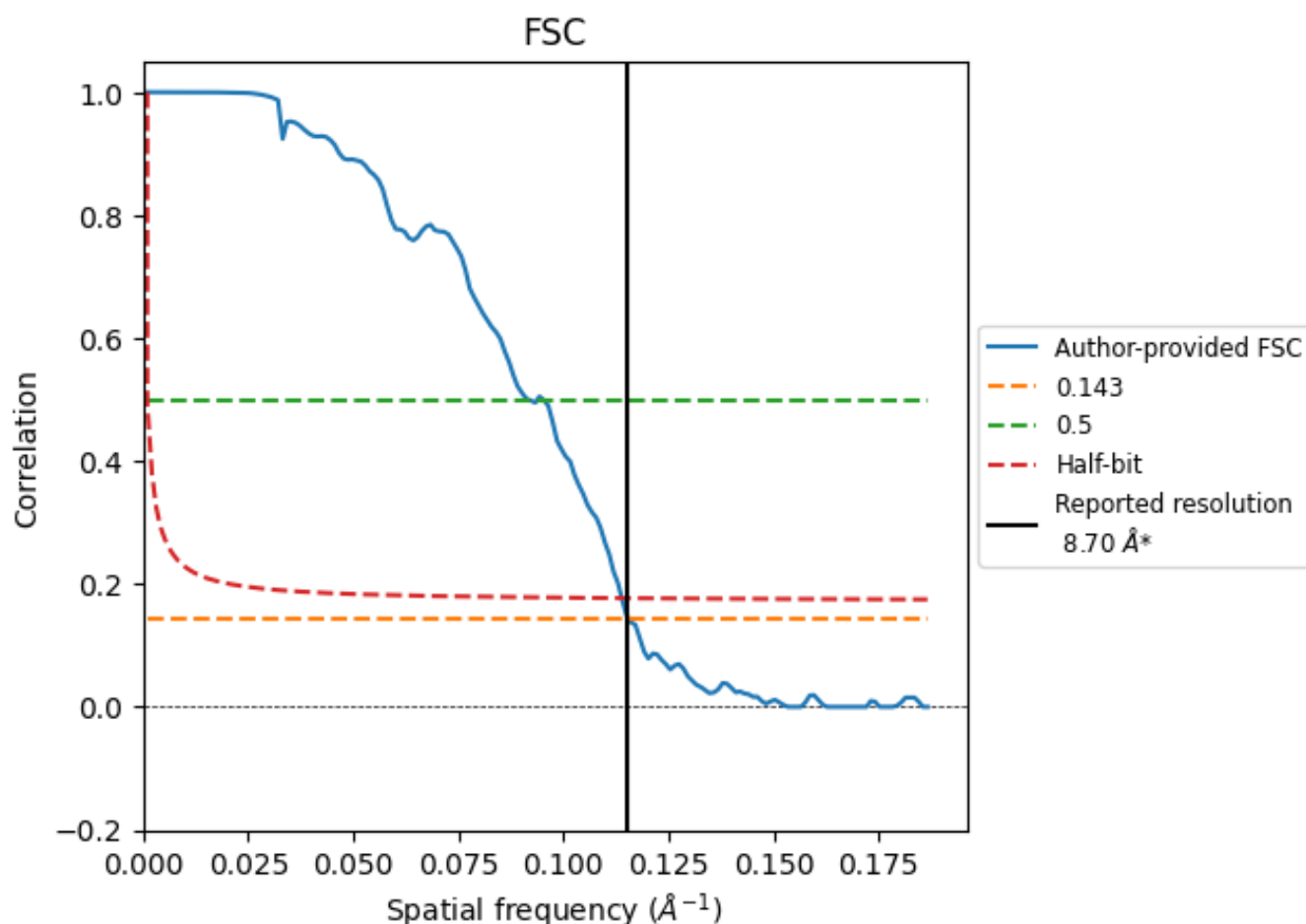


*Reported resolution corresponds to spatial frequency of 0.115 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.115 Å⁻¹

8.2 Resolution estimates [i](#)

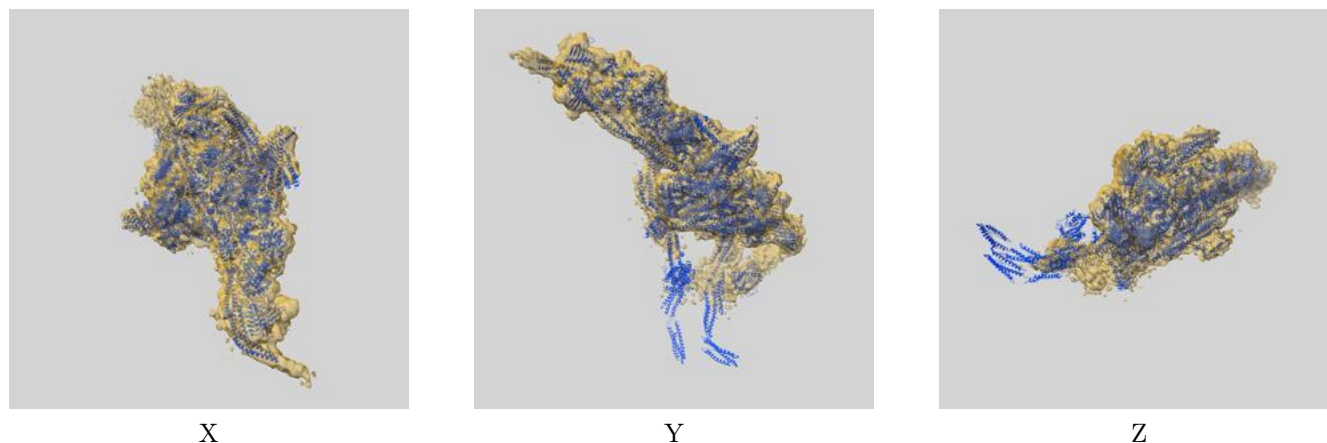
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.70	-	-
Author-provided FSC curve	8.65	10.92	8.78
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3706 and PDB model 5NW4. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



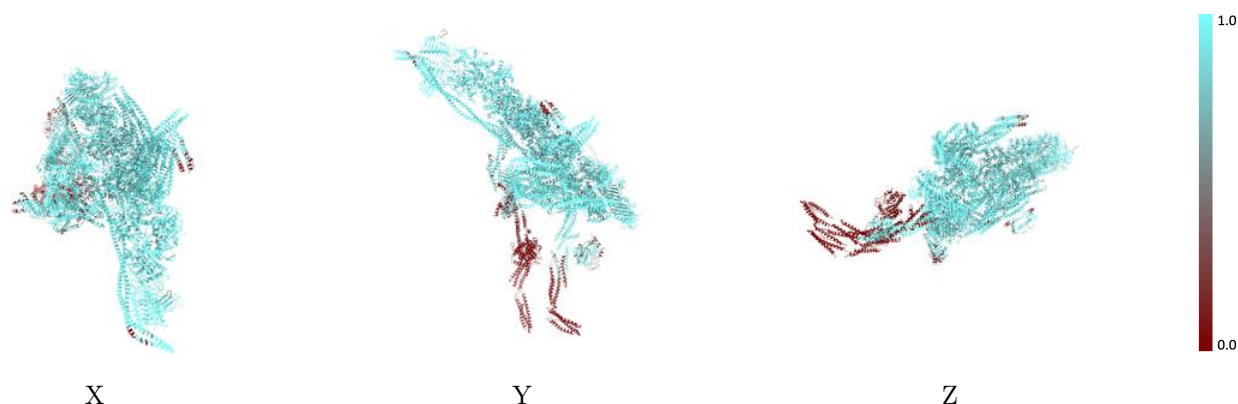
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



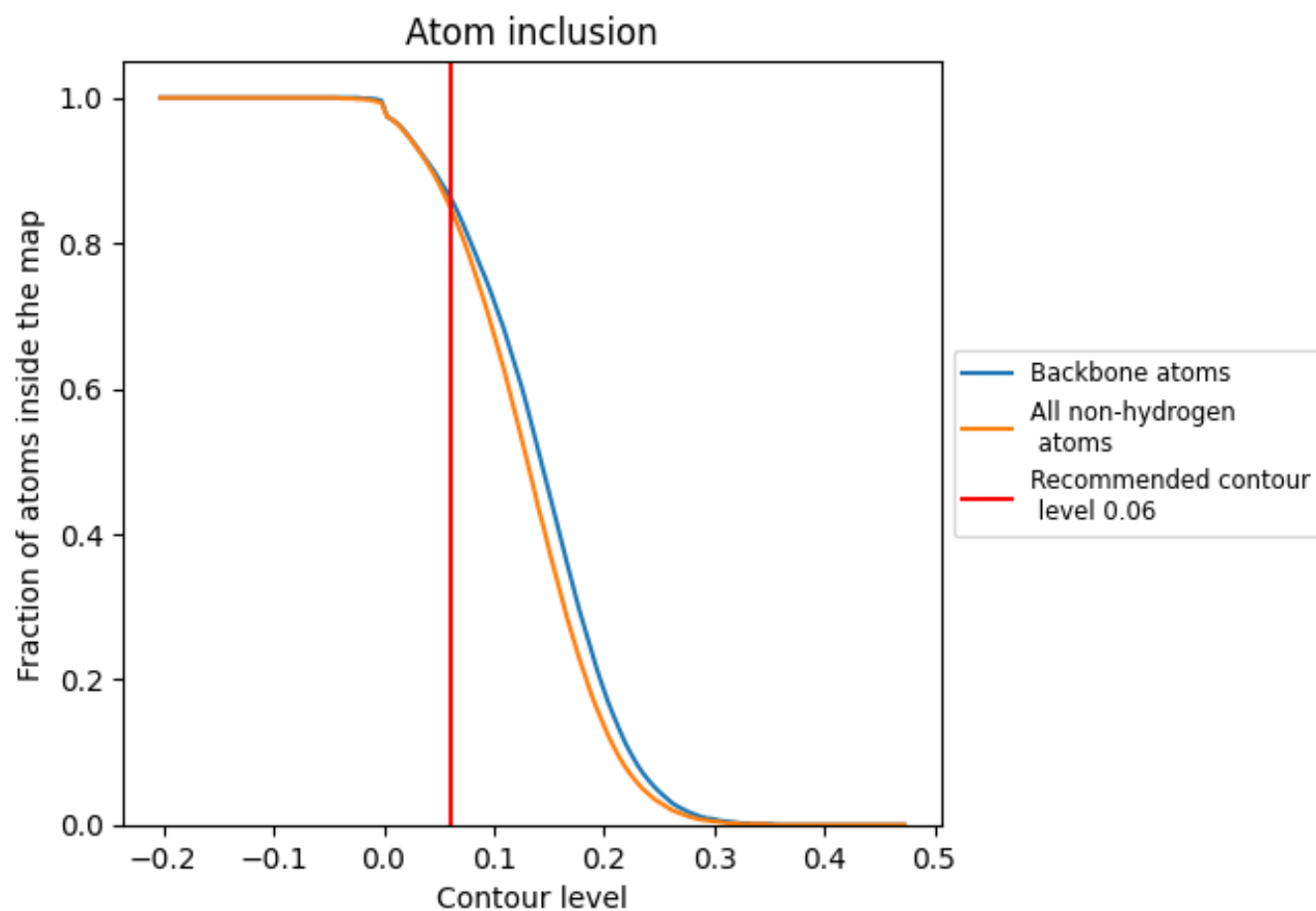
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 86% of all backbone atoms, 85% 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	 0.8510	 0.1130
1	 0.8820	 0.1180
2	 0.8470	 0.1060
5	 0.8730	 0.1620
6	 0.9400	 0.1530
A	 0.4530	 0.0490
B	 0.7040	 0.1350
C	 0.8310	 0.0370
D	 0.9240	 0.0580
E	 0.0070	 -0.0030
F	 0.6190	 0.0340
G	 0.9310	 0.1070
H	 0.9350	 0.1130
O	 0.8870	 0.1060
P	 0.9040	 0.1120
Q	 0.8940	 0.1140
R	 0.6630	 0.0470
S	 0.8380	 0.0580
T	 0.9030	 0.1120
U	 0.9260	 0.1170
V	 0.9510	 0.1170
W	 0.9410	 0.1070
X	 0.9510	 0.1140
Y	 0.9630	 0.1140
Z	 0.9500	 0.1220
a	 0.9920	 0.1980
b	 0.9970	 0.1830
c	 1.0000	 0.1760
d	 0.9850	 0.1680
e	 0.5660	 -0.0230
f	 0.9770	 0.2270
g	 0.9480	 0.1260
h	 0.9990	 0.1300
i	 0.9990	 0.1780
j	 0.9620	 0.1570



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Chain	Atom inclusion	Q-score
k	 0.9200	 0.1810
l	 0.9700	 0.1570
m	 0.9600	 0.1750
n	 0.8950	 0.1690
o	 0.9930	 0.1850