



Full wwPDB EM Validation Report ⓘ

Nov 2, 2024 – 09:04 pm GMT

PDB ID : 6GYM
EMDB ID : EMD-0092
Title : Structure of a yeast closed complex with distorted DNA (CCdist)
Authors : Dienemann, C.; Schwalb, B.; Schilbach, S.; Cramer, P.
Deposited on : 2018-06-30
Resolution : 6.70 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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

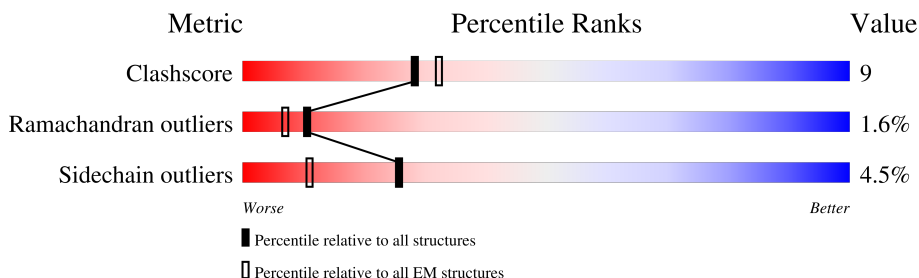
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.70 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.








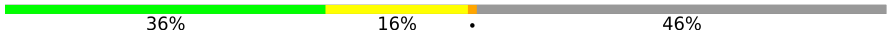





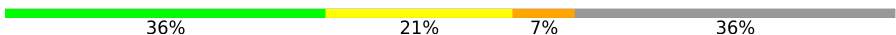




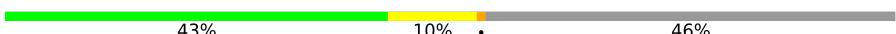




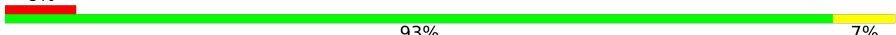
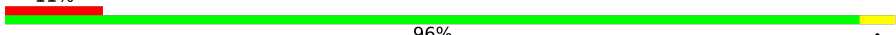
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	0	778	<div> <div>11%</div> <div>76%</div> <div>13%</div> <div>10%</div> </div>
2	1	641	<div> <div>15%</div> <div>70%</div> <div>6%</div> <div>23%</div> </div>
3	2	462	<div> <div>23%</div> <div>83%</div> <div>15%</div> </div>
4	3	321	<div> <div>5%</div> <div>37%</div> <div>6%</div> <div>57%</div> </div>
5	4	338	<div> <div>6%</div> <div>84%</div> <div>12%</div> </div>
6	5	72	<div> <div>54%</div> <div>78%</div> <div>14%</div> <div>8%</div> </div>
7	6	461	<div> <div>61%</div> <div>11%</div> <div>27%</div> </div>
8	7	843	<div> <div>36%</div> <div>12%</div> <div>52%</div> </div>

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Mol	Chain	Length	Quality of chain
9	A	1733	
10	B	1224	
11	C	318	
12	D	221	
13	E	215	
14	F	155	
15	G	171	
16	H	146	
17	I	122	
18	J	70	
19	K	120	
20	L	70	
21	M	345	
22	O	240	
23	Q	735	
24	R	400	
25	U	171	
26	V	122	
27	W	332	
28	X	328	
29	Z	43	
30	N	75	
31	T	75	

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 63012 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 General transcription and DNA repair factor IIIH helicase subunit XPD,General transcription and DNA repair factor IIIH helicase subunit XPD,DNA repair helicase RAD3,DNA repair helicase RAD3,General transcription and DNA repair factor IIIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	698	Total	C	N	O	S	0	0
			4844	3051	856	907	30		

- Molecule 2 is a protein called General transcription and DNA repair factor IIIH subunit TFB1,General transcription and DNA repair factor IIIH subunit TFB1,RNA polymerase II transcription factor B subunit 1,General transcription and DNA repair factor IIIH subunit TFB1,RNA polymerase II transcription factor B subunit 1,General transcription and DNA repair factor IIIH subunit TFB1,General transcription and DNA repair factor IIIH subunit TFB1,General transcription and DNA repair factor IIIH subunit TFB1,RNA polymerase II transcription factor B subunit 1,General transcription and DNA repair factor IIIH subunit TFB1,RNA polymerase II transcription factor B subunit 1,General transcription and DNA repair factor IIIH subunit TFB1,General transcription and DNA repair factor IIIH subunit TFB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	491	Total	C	N	O	S	0	0
			3060	1893	570	590	7		

- Molecule 3 is a protein called General transcription and DNA repair factor IIIH subunit TFB2,General transcription and DNA repair factor IIIH subunit TFB2,General transcription and DNA repair factor IIIH subunit TFB2,General transcription and DNA repair factor IIIH subunit TFB2,General transcription and DNA repair factor IIIH subunit TFB2,General transcription and DNA repair factor IIIH subunit TFB2,General transcription and DNA repair factor IIIH subunit TFB2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	2	395	Total	C	N	O	0	0
			2160	1317	413	430		

- Molecule 4 is a protein called RNA polymerase II transcription factor B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	138	Total	C	N	O	S	0	0
			860	533	160	160	7		

- Molecule 5 is a protein called General transcription and DNA repair factor IIH subunit TFB4,General transcription and DNA repair factor IIH subunit TFB4,RNA polymerase II transcription factor B subunit 4,General transcription and DNA repair factor IIH subunit TFB4,General transcription and DNA repair factor IIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	297	Total 1474	C 876	N 297	O 297	S 4	0	0

- Molecule 6 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	66	Total	C	N	O	S	0	0
			498	314	89	93	2		

- [illegible]

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	335	Total	C	N	O	S	0	0
			2197	1355	399	422	21		

- Molecule 8 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB,General transcription and DNA repair factor IIH helicase subunit XPB,DNA repair helicase RAD25,General transcription and DNA repair factor IIH helicase subunit XPB,DNA repair helicase RAD25,General transcription and DNA repair factor IIH helicase subunit XPB,General transcription and DNA repair factor IIH helicase subunit XPB,DNA repair helicase RAD25,General transcription and DNA repair factor IIH helicase subunit XPB,DNA repair helicase RAD25,General transcription and DNA repair factor IIH helicase subunit XPB,DNA repair helicase RAD25,General transcription and DNA repair factor IIH helicase subunit XPB,DNA repair helicase RAD25,General transcription and DNA repair factor IIH helicase subunit XPB,DNA repair helicase RAD25,General transcription and DNA repair factor IIH helicase subunit XPB,General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	408	Total	C	N	O	S	0	0
			3148	2000	557	572	19		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	1398	Total	C	N	O	S	0	0
			10997	6931	1927	2078	61		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	1152	Total	C	N	O	S	0	0
			9178	5807	1608	1708	55		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	262	Total	C	N	O	S	0	0
			2061	1299	343	406	13		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	157	Total	C	N	O	S	0	0
			1253	779	220	252	2		

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	213	Total	C	N	O	S	0	0
			1744	1107	308	318	11		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	83	Total	C	N	O	S	0	0
			670	428	114	125	3		

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	136	Total	C	N	O	S	0	0
			1089	686	184	215	4		

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

- Molecule 18 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 19 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	112	Total	C	N	O	S	0	0
			904	580	154	168	2		

- Molecule 20 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 21 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	279	Total	C	N	O	S	0	0
			2175	1382	373	403	17		

- Molecule 22 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	180	Total	C	N	O	S	0	0
			1416	921	242	247	6		

- Molecule 23 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	148	Total	C	N	O	S	0	0
			1144	733	195	212	4		

- Molecule 24 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	190	Total	C	N	O	S	0	0
			1303	812	238	246	7		

- Molecule 25 is a protein called Transcription initiation factor IIA large subunit, Transcription initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	92	Total	C	N	O	S	0	0
			757	474	130	150	3		

- Molecule 26 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	100	Total	C	N	O	S	0	0
			782	492	130	156	4		

- Molecule 27 is a protein called Transcription initiation factor IIE subunit alpha, Transcription initiation factor IIE subunit alpha, Transcription initiation factor IIE subunit alpha, Transcription initiation factor IIE subunit alpha, Transcription initiation factor IIE subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	258	Total	C	N	O	S	0	0
			1825	1147	321	351	6		

- Molecule 28 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	160	Total	C	N	O	S	0	0
			1004	620	184	196	4		

- Molecule 29 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	Z	43	Total	C	N	O	0	0
			215	129	43	43		

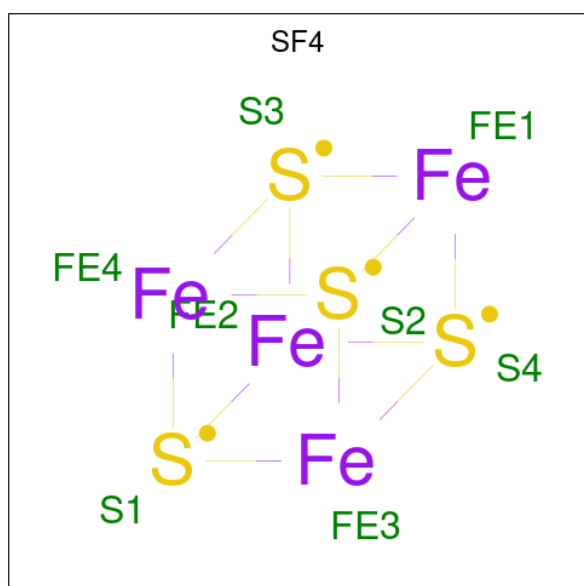
- Molecule 30 is a DNA chain called non-template DNA (HIS4).

Mol	Chain	Residues	Atoms					AltConf	Trace
30	N	75	Total	C	N	O	P	0	0
			1531	736	281	439	75		

- Molecule 31 is a DNA chain called Template DNA (HIS4).

Mol	Chain	Residues	Atoms					AltConf	Trace
31	T	75	Total	C	N	O	P	0	0
			1524	735	273	441	75		

- Molecule 32 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
32	0	1	Total	Fe	S	0
			8	4	4	

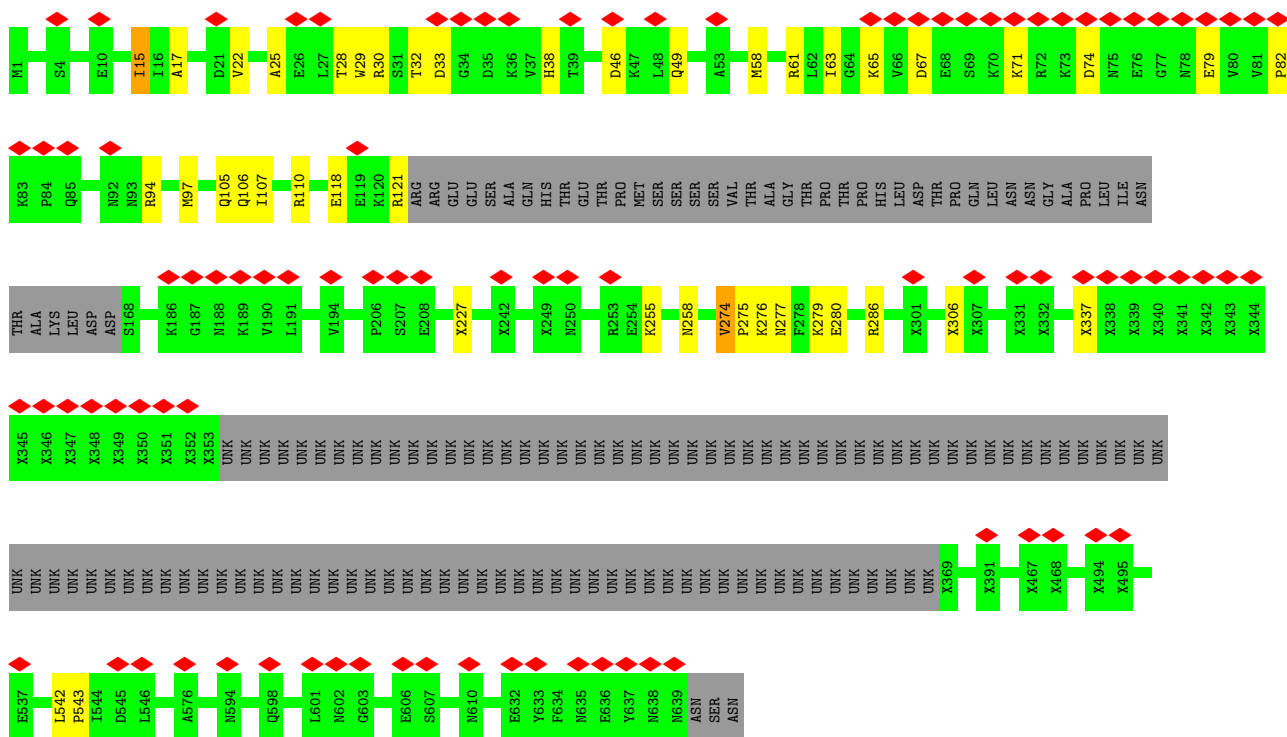
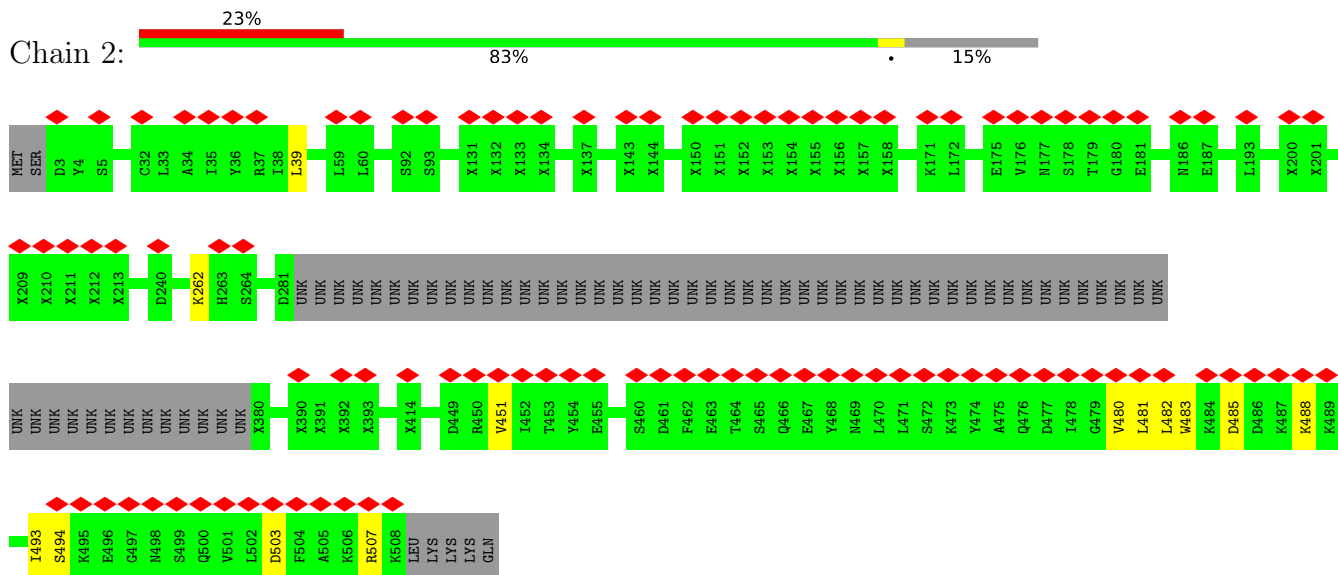
- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
33	3	2	Total 2	Zn 2	0
33	4	1	Total 1	Zn 1	0
33	6	3	Total 3	Zn 3	0
33	A	2	Total 2	Zn 2	0
33	B	1	Total 1	Zn 1	0
33	C	1	Total 1	Zn 1	0
33	I	2	Total 2	Zn 2	0
33	J	1	Total 1	Zn 1	0
33	L	1	Total 1	Zn 1	0
33	M	1	Total 1	Zn 1	0
33	W	1	Total 1	Zn 1	0

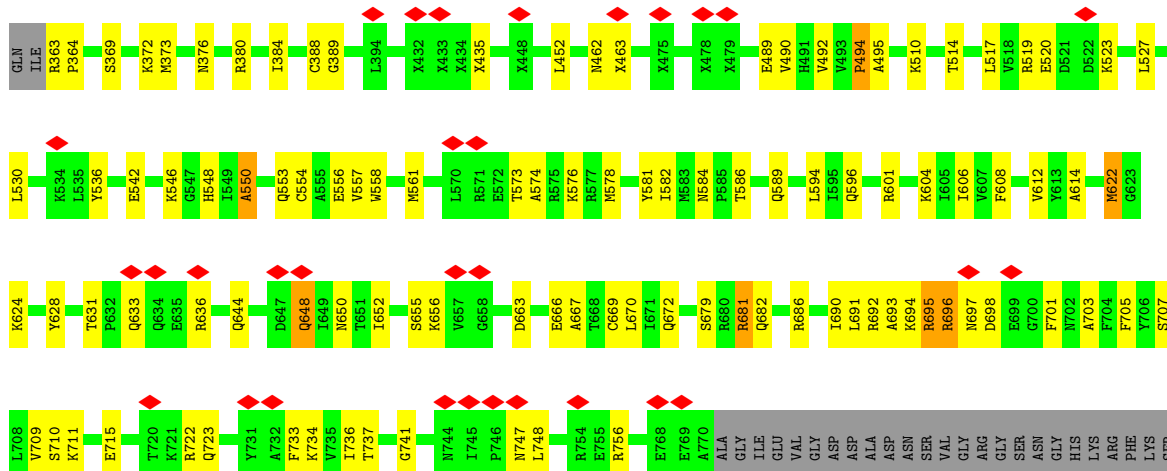
- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
34	A	1	Total 1	Mg 1	0

Chain 1:  15% 70% 6% 9%

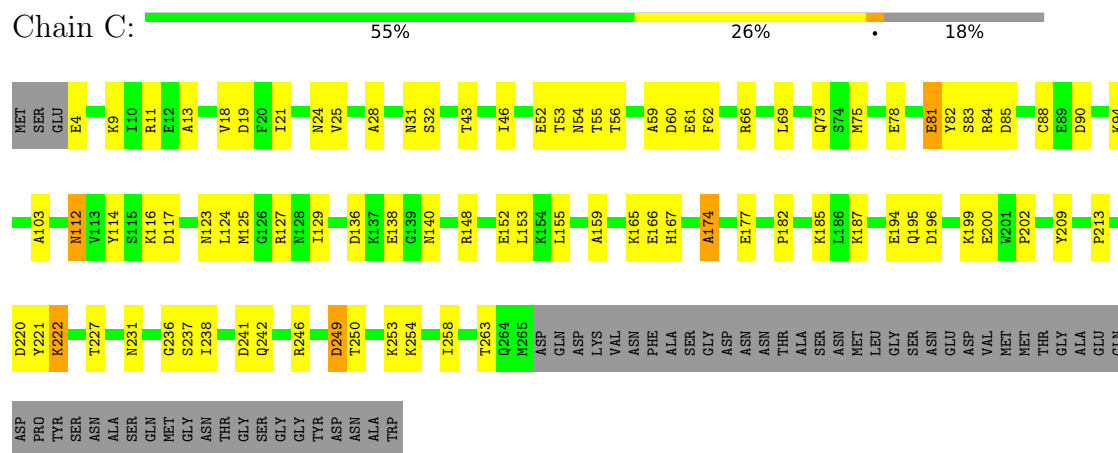
[illegible]

- Molecule 4: RNA polymerase II transcription factor B subunit 3

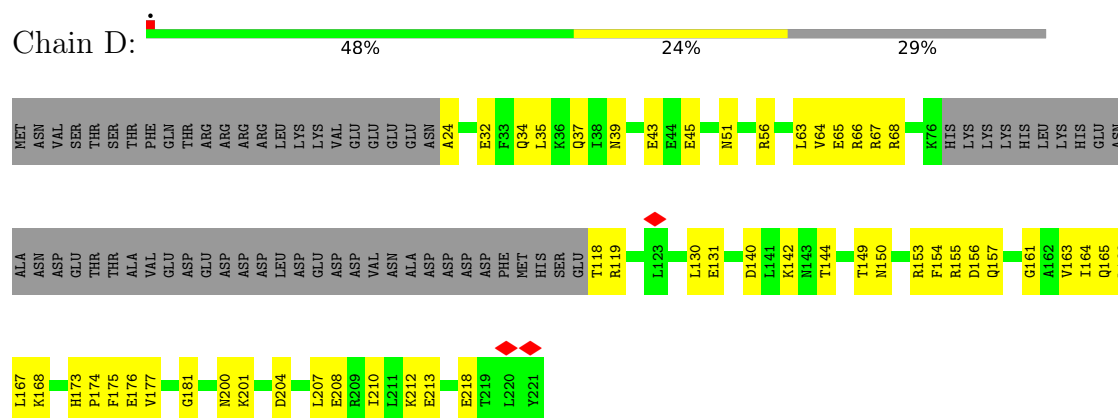


Chain A: 59% 20% • 19%

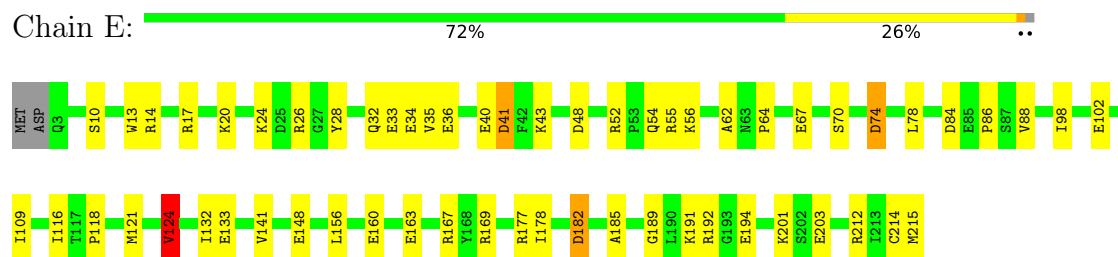




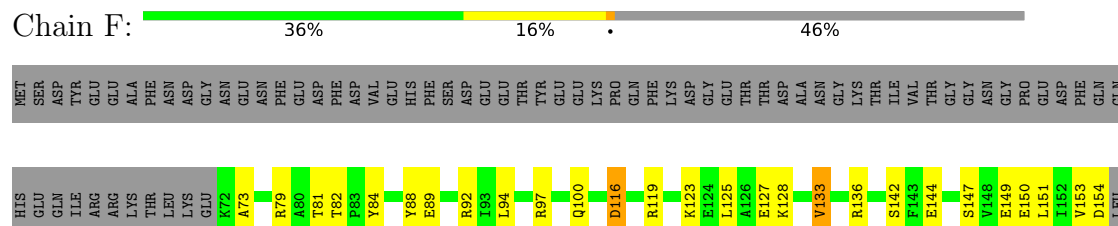
- Molecule 12: DNA-directed RNA polymerase II subunit RPB4



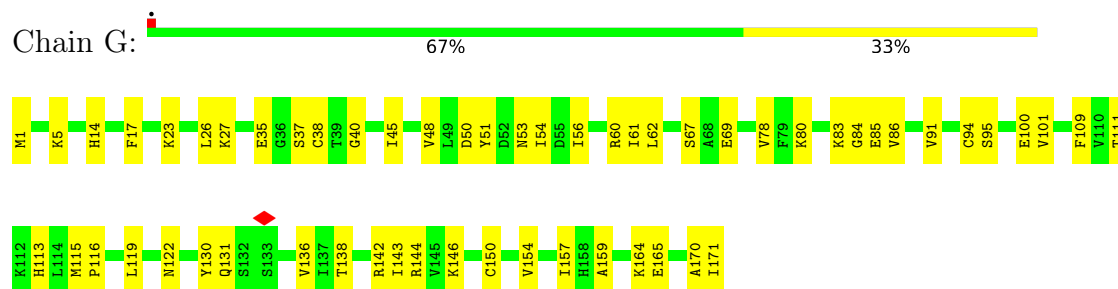
- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC1



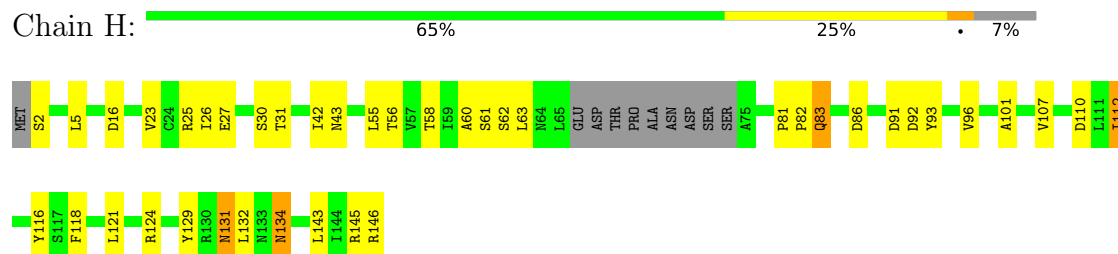
- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC2



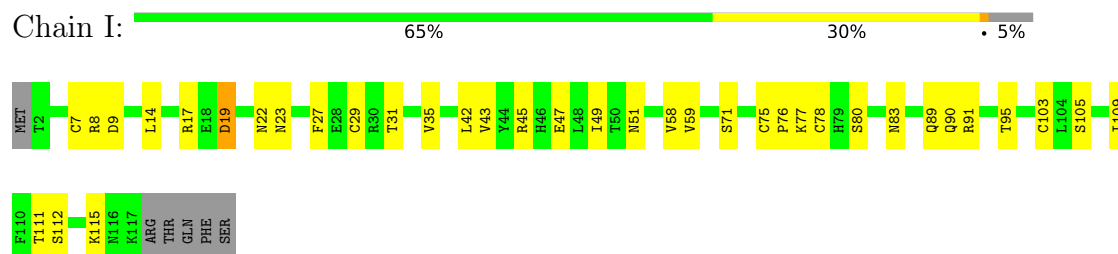
- Molecule 15: DNA-directed RNA polymerase II subunit RPB7



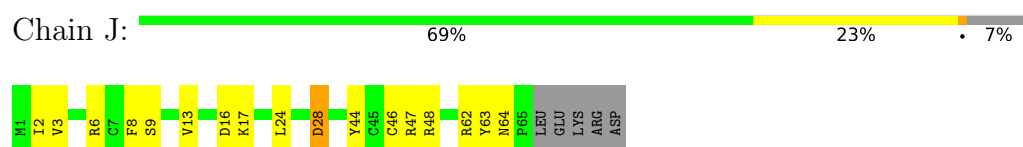
- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC3



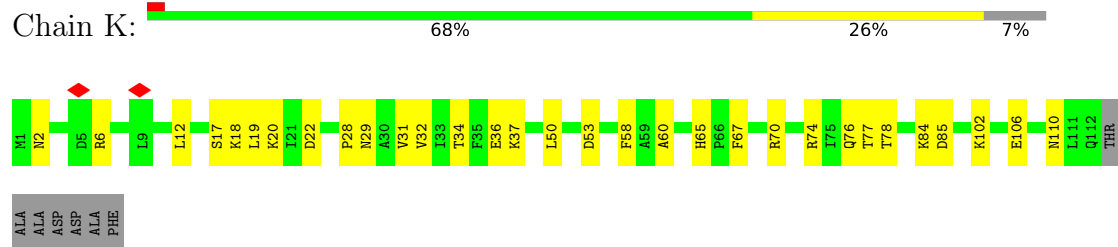
- Molecule 17: DNA-directed RNA polymerase II subunit RPB9



- Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC5

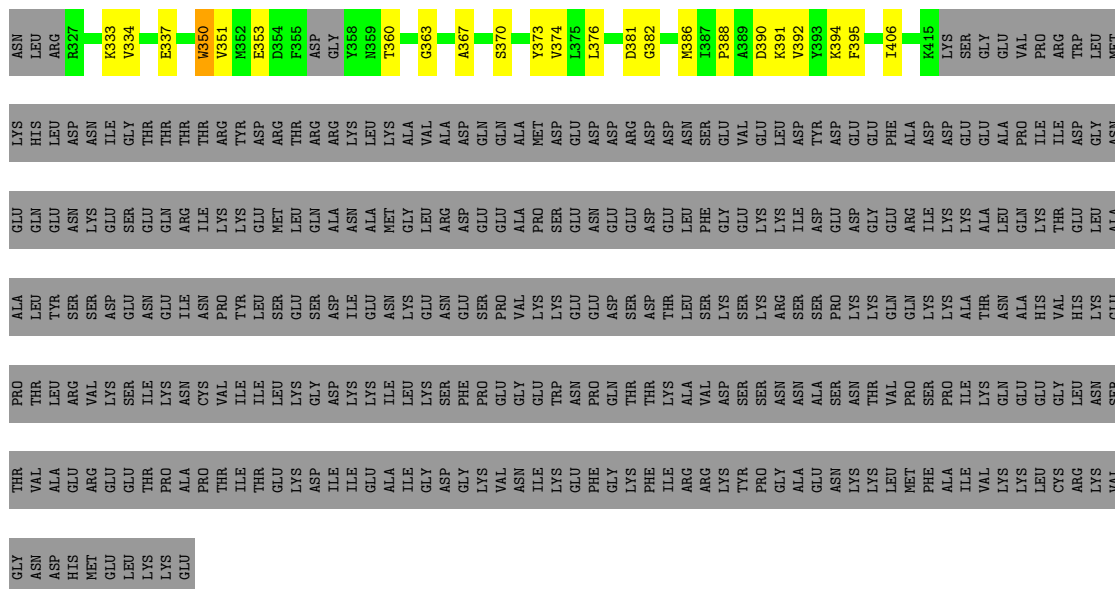


- Molecule 19: DNA-directed RNA polymerase II subunit RPB11

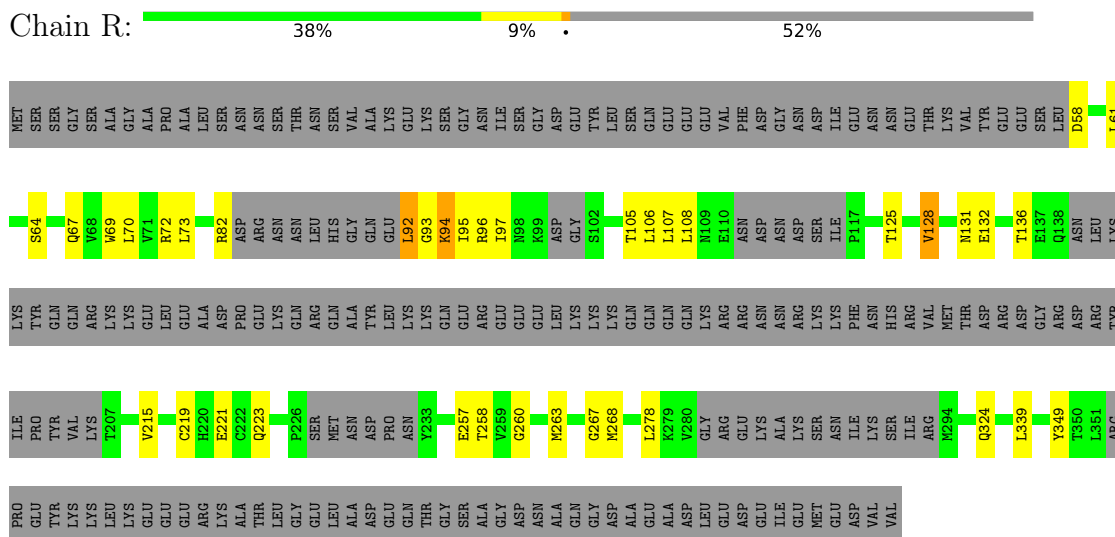


- Molecule 20: DNA-directed RNA polymerases I, II, and III subunit RPABC4

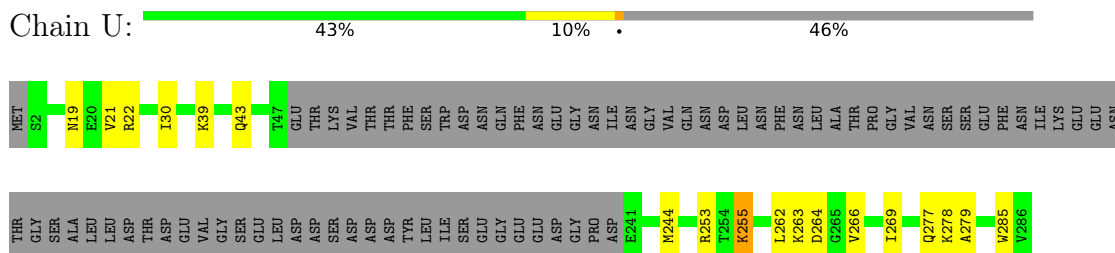




- Molecule 24: Transcription initiation factor IIF subunit beta

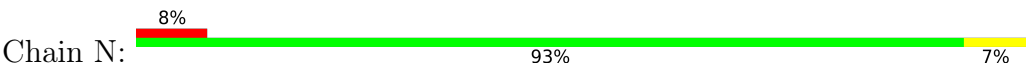


● Molecule 25: Transcription initiation factor IIA large subunit, Transcription initiation factor IIA large subunit

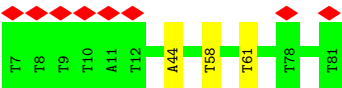
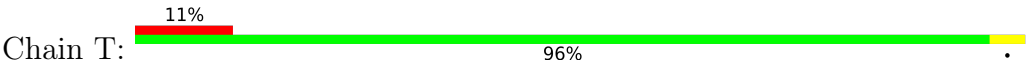


- Molecule 26: Transcription initiation factor IIA subunit 2





• Molecule 31: Template DNA (HIS4)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	60000	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 ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.034	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0057	Depositor
Map size (Å)	479.5, 479.5, 479.5	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.25	0/4739	0.42	0/6431
2	1	0.25	0/2238	0.40	0/3039
3	2	0.24	0/1631	0.39	0/2243
4	3	0.25	0/870	0.43	0/1190
5	4	0.25	0/1367	0.51	2/1900 (0.1%)
6	5	0.23	0/502	0.46	0/677
7	6	0.24	0/1996	0.42	0/2713
8	7	0.24	0/2980	0.40	0/4019
9	A	0.27	0/11192	0.44	0/15128
10	B	0.28	0/9357	0.44	0/12618
11	C	0.28	0/2099	0.43	0/2845
12	D	0.24	0/1262	0.39	0/1693
13	E	0.29	1/1780 (0.1%)	0.41	0/2395
14	F	0.29	0/682	0.43	0/922
15	G	0.27	0/1368	0.46	0/1844
16	H	0.28	0/1107	0.47	0/1499
17	I	0.27	0/962	0.46	0/1295
18	J	0.30	0/541	0.47	0/727
19	K	0.27	0/922	0.42	0/1244
20	L	0.27	0/360	0.51	0/478
21	M	0.26	0/2204	0.46	0/2963
22	O	0.28	0/1443	0.46	0/1942
23	Q	0.26	0/1168	0.44	0/1579
24	R	0.25	0/1312	0.44	0/1777
25	U	0.26	0/766	0.46	0/1032
26	V	0.26	0/789	0.44	0/1066
27	W	0.26	0/1551	0.42	0/2096
28	X	0.25	0/1014	0.44	0/1388
30	N	0.54	0/1719	0.92	0/2638
31	T	0.57	0/1709	0.92	0/2621
All	All	0.29	1/61630 (0.0%)	0.48	2/84002 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E	124	VAL	C-N	5.04	1.43	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	4	260	PRO	N-CA-CB	6.07	110.59	103.30
5	4	265	PRO	N-CA-CB	5.94	110.43	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	4844	0	4244	59	0
2	1	3060	0	2056	24	0
3	2	2160	0	1075	6	0
4	3	860	0	623	13	0
5	4	1474	0	641	2	0
6	5	498	0	506	6	0
7	6	2197	0	1740	29	0
8	7	3148	0	2999	61	0
9	A	10997	0	11083	246	0
10	B	9178	0	9196	213	0
11	C	2061	0	2030	64	0
12	D	1253	0	1275	31	0
13	E	1744	0	1772	38	0
14	F	670	0	690	17	0
15	G	1340	0	1357	38	0
16	H	1089	0	1062	27	0
17	I	944	0	900	18	0
18	J	532	0	543	14	0
19	K	904	0	911	24	0
20	L	358	0	381	19	0
21	M	2175	0	2286	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	O	1416	0	1493	33	0
23	Q	1144	0	1034	27	0
24	R	1303	0	1110	31	0
25	U	757	0	747	15	0
26	V	782	0	790	11	0
27	W	1825	0	1545	38	0
28	X	1004	0	731	18	0
29	Z	215	0	47	3	0
30	N	1531	0	848	4	0
31	T	1524	0	850	5	0
32	0	8	0	0	1	0
33	3	2	0	0	0	0
33	4	1	0	0	0	0
33	6	3	0	0	0	0
33	A	2	0	0	0	0
33	B	1	0	0	0	0
33	C	1	0	0	0	0
33	I	2	0	0	0	0
33	J	1	0	0	0	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	W	1	0	0	0	0
34	A	1	0	0	0	0
All	All	63012	0	56565	1045	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 (1045) 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)
10:B:875:GLU:OE2	10:B:934:LYS:NZ	1.91	1.02
14:F:123:LYS:NZ	14:F:127:GLU:OE2	1.95	0.98
13:E:56:LYS:NZ	13:E:84:ASP:OD2	1.97	0.95
18:J:13:VAL:O	18:J:17:LYS:NZ	2.05	0.90
9:A:362:ASP:OD2	9:A:459:ARG:NH1	2.05	0.88
13:E:56:LYS:H	13:E:56:LYS:HZ3	1.21	0.85
1:O:603:ARG:NH1	1:O:627:PHE:O	2.10	0.84
9:A:434:ARG:NH1	9:A:435:HIS:O	2.11	0.84
13:E:55:ARG:NH1	13:E:84:ASP:OD1	2.11	0.83
16:H:2:SER:N	16:H:61:SER:HG	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:617:ARG:HH12	10:B:619:ILE:HG12	1.42	0.83
1:0:603:ARG:HH12	1:0:628:GLN:HA	1.43	0.83
9:A:41:MET:SD	9:A:257:ARG:NH1	2.52	0.82
9:A:1155:ASP:O	9:A:1241:ARG:NH1	2.12	0.82
14:F:81:THR:OG1	14:F:136:ARG:NH1	2.12	0.82
9:A:1199:ARG:NH1	9:A:1233:ASP:O	2.13	0.82
11:C:148:ARG:NH1	18:J:63:TYR:O	2.12	0.82
9:A:217:LYS:O	9:A:217:LYS:NZ	2.14	0.81
10:B:649:LYS:NZ	10:B:735:ALA:O	2.14	0.81
27:W:44:LYS:NZ	27:W:49:ILE:O	2.14	0.80
10:B:404:LYS:O	10:B:405:ARG:NH1	2.13	0.80
1:0:607:SER:O	1:0:668:ARG:NH1	2.14	0.80
13:E:17:ARG:HH12	13:E:36:GLU:HA	1.46	0.80
9:A:134:ARG:NH1	9:A:221:SER:O	2.15	0.80
10:B:512:ARG:NH1	10:B:533:CYS:O	2.14	0.80
14:F:128:LYS:NZ	14:F:151:LEU:O	2.14	0.79
9:A:446:ARG:NH1	9:A:447:GLN:O	2.16	0.79
9:A:1258:HIS:O	9:A:1262:LYS:NZ	2.16	0.79
12:D:150:ASN:O	15:G:142:ARG:NH1	2.17	0.78
23:Q:121:PHE:O	23:Q:394:LYS:NZ	2.16	0.78
10:B:445:LYS:NZ	24:R:267:GLY:O	2.17	0.78
12:D:200:ASN:OD1	12:D:201:LYS:NZ	2.16	0.78
9:A:1441:PHE:O	14:F:92:ARG:NH1	2.17	0.77
10:B:186:GLU:OE2	18:J:62:ARG:NH1	2.17	0.77
25:U:263:LYS:HZ3	25:U:278:LYS:NZ	1.83	0.77
1:0:594:ARG:NH1	7:6:241:THR:O	2.17	0.77
12:D:131:GLU:OE1	12:D:142:LYS:NZ	2.17	0.77
10:B:771:SER:O	10:B:775:LYS:NZ	2.17	0.77
9:A:1157:ASP:OD2	9:A:1160:SER:N	2.16	0.76
24:R:94:LYS:NZ	24:R:107:LEU:O	2.17	0.76
7:6:137:LEU:O	7:6:139:LYS:NZ	2.19	0.76
10:B:99:LYS:NZ	10:B:178:ASN:O	2.17	0.76
9:A:1365:TYR:HB3	9:A:1366:ARG:HH12	1.51	0.75
27:W:187:LYS:NZ	27:W:190:ASP:OD2	2.17	0.75
9:A:1055:ARG:NH1	14:F:154:ASP:O	2.19	0.75
10:B:210:LYS:NZ	10:B:461:LEU:O	2.19	0.74
10:B:361:LEU:O	10:B:374:LYS:NZ	2.18	0.74
15:G:115:MET:O	15:G:164:LYS:NZ	2.20	0.74
8:7:604:LYS:NZ	8:7:650:ASN:OD1	2.18	0.74
20:L:53:HIS:O	20:L:54:ARG:NH1	2.21	0.74
10:B:104:GLU:OE2	10:B:110:HIS:NE2	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:1060:ARG:NH1	11:C:200:GLU:O	2.21	0.74
21:M:163:LEU:O	21:M:166:LYS:NZ	2.19	0.73
19:K:36:GLU:OE1	19:K:70:ARG:NH1	2.22	0.73
12:D:65:GLU:OE2	12:D:68:ARG:NH1	2.22	0.73
12:D:67:ARG:HH11	12:D:130:LEU:HD21	1.54	0.73
14:F:116:ASP:OD2	14:F:119:ARG:N	2.15	0.73
13:E:182:ASP:OD2	13:E:185:ALA:N	2.21	0.73
25:U:263:LYS:NZ	25:U:277:GLN:OE1	2.22	0.72
10:B:879:ARG:NH1	10:B:885:MET:SD	2.62	0.72
9:A:879:GLU:OE2	9:A:962:ARG:NH2	2.22	0.72
9:A:1198:ASP:OD2	9:A:1201:ALA:N	2.22	0.72
14:F:97:ARG:NH1	14:F:100:GLN:OE1	2.23	0.72
25:U:263:LYS:HZ3	25:U:278:LYS:HZ2	1.36	0.71
9:A:940:ARG:HG2	9:A:944:ARG:HH12	1.55	0.71
7:6:197:LYS:O	7:6:201:LYS:NZ	2.21	0.71
1:0:685:ARG:HA	1:0:688:ARG:HH11	1.54	0.70
9:A:974:ASP:H	9:A:977:LYS:HZ1	1.38	0.70
10:B:657:HIS:HD2	10:B:660:LYS:HZ1	1.38	0.70
9:A:852:TYR:OH	14:F:89:GLU:OE2	2.08	0.70
15:G:35:GLU:OE2	15:G:48:VAL:N	2.23	0.70
9:A:974:ASP:O	9:A:977:LYS:NZ	2.22	0.69
13:E:14:ARG:NH1	13:E:141:VAL:O	2.23	0.69
10:B:1106:ARG:HH11	10:B:1126:GLY:HA2	1.56	0.69
12:D:208:GLU:O	12:D:212:LYS:NZ	2.22	0.69
28:X:257:GLU:O	28:X:261:LYS:NZ	2.26	0.69
13:E:17:ARG:NH1	13:E:35:VAL:O	2.27	0.68
16:H:92:ASP:OD2	16:H:145:ARG:NH1	2.27	0.67
4:3:34:CYS:O	4:3:61:LYS:NZ	2.26	0.67
23:Q:117:HIS:NE2	23:Q:390:ASP:OD2	2.28	0.67
1:0:345:ARG:NH2	1:0:354:GLU:OE2	2.27	0.67
1:0:372:LYS:HB3	1:0:375:ARG:HH11	1.58	0.67
10:B:798:TYR:OH	11:C:66:ARG:NH1	2.27	0.67
9:A:434:ARG:HH12	9:A:437:MET:H	1.43	0.67
10:B:620:ARG:NH1	17:I:89:GLN:OE1	2.28	0.67
19:K:36:GLU:HB3	19:K:37:LYS:HZ3	1.58	0.67
10:B:23:ALA:O	10:B:654:ARG:NH1	2.29	0.66
9:A:1420:ASP:OD2	9:A:1422:ARG:NH1	2.29	0.66
13:E:56:LYS:NZ	13:E:56:LYS:H	1.92	0.66
11:C:196:ASP:OD2	11:C:199:LYS:N	2.29	0.65
14:F:79:ARG:NH1	14:F:150:GLU:OE2	2.29	0.65
8:7:548:HIS:HB2	8:7:697:ASN:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:975:GLN:N	10:B:978:ASP:OD2	2.29	0.65
10:B:27:ALA:N	10:B:708:GLU:OE2	2.30	0.64
10:B:799:PRO:HB2	10:B:818:PRO:HG2	1.77	0.64
10:B:895:ASP:OD2	20:L:42:ARG:NH2	2.28	0.64
8:7:696:ARG:NE	8:7:698:ASP:OD2	2.31	0.64
11:C:114:TYR:N	11:C:117:ASP:OD2	2.29	0.64
9:A:843:LYS:NZ	9:A:1401:SER:O	2.25	0.63
27:W:144:ARG:HH12	27:W:146:GLU:HB2	1.63	0.63
10:B:494:HIS:HD2	10:B:497:ARG:HH11	1.47	0.63
3:2:483:TRP:NE1	6:5:36:ASP:OD2	2.32	0.62
26:V:78:PHE:HB2	26:V:113:ILE:HB	1.80	0.62
2:1:49:GLN:HB3	27:W:413:PHE:HB3	1.81	0.62
8:7:691:LEU:HD23	8:7:694:LYS:HZ1	1.64	0.62
10:B:277:LYS:HG3	10:B:338:GLY:HA2	1.80	0.62
1:0:497:ILE:O	1:0:499:LYS:NZ	2.33	0.62
9:A:982:THR:N	9:A:985:ASP:OD2	2.22	0.62
11:C:54:ASN:HB3	20:L:60:ARG:HH12	1.64	0.62
16:H:93:TYR:HA	16:H:145:ARG:HB3	1.81	0.62
10:B:25:ILE:HA	10:B:655:LYS:HE3	1.81	0.61
20:L:31:CYS:SG	20:L:32:ALA:N	2.72	0.61
8:7:644:GLN:NE2	8:7:666:GLU:OE2	2.33	0.61
1:0:156:CYS:SG	1:0:157:GLU:N	2.73	0.61
3:2:503:ASP:HB3	3:2:507:ARG:HH12	1.65	0.61
10:B:959:ASP:OD1	10:B:959:ASP:N	2.33	0.61
13:E:192:ARG:NH1	13:E:215:MET:OXT	2.34	0.61
9:A:1283:VAL:HB	9:A:1307:GLU:HB2	1.82	0.61
10:B:1053:GLU:OE2	10:B:1067:ARG:NH2	2.25	0.61
12:D:56:ARG:HH22	12:D:155:ARG:HE	1.48	0.61
8:7:672:GLN:HE21	8:7:722:ARG:NH1	1.99	0.61
9:A:974:ASP:H	9:A:977:LYS:NZ	1.98	0.61
10:B:304:ASP:OD2	10:B:307:ASP:N	2.34	0.61
10:B:654:ARG:HA	10:B:654:ARG:HH11	1.64	0.61
21:M:267:LYS:HZ1	21:M:270:ALA:HA	1.66	0.61
8:7:388:CYS:H	8:7:692:ARG:HD3	1.64	0.61
10:B:614:SER:HB3	10:B:627:PHE:HB2	1.83	0.61
16:H:16:ASP:HB3	16:H:25:ARG:HB3	1.82	0.60
16:H:118:PHE:HB2	16:H:121:LEU:HB2	1.83	0.60
1:0:684:ARG:HH21	1:0:687:SER:HB2	1.67	0.60
9:A:1430:LEU:HB2	9:A:1432:GLN:HE22	1.66	0.60
9:A:433:GLU:OE2	10:B:1108:ARG:NH2	2.35	0.60
10:B:649:LYS:HZ2	10:B:738:PHE:HD2	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1281:ARG:NE	9:A:1309:ASP:OD2	2.32	0.60
25:U:255:LYS:NZ	31:T:61:DT:O5'	2.35	0.60
9:A:913:LEU:HA	9:A:979:SER:H	1.66	0.60
9:A:1118:VAL:HB	9:A:1306:LEU:HB2	1.81	0.60
10:B:101:MET:HG3	10:B:169:ARG:NH1	2.16	0.60
10:B:924:GLU:H	10:B:928:ARG:HD2	1.67	0.60
13:E:163:GLU:OE2	13:E:167:ARG:NE	2.35	0.60
13:E:191:LYS:N	13:E:194:GLU:OE2	2.31	0.60
25:U:39:LYS:NZ	25:U:43:GLN:OE1	2.29	0.60
21:M:241:ARG:O	21:M:245:HIS:ND1	2.35	0.59
8:7:376:ASN:HD21	8:7:380:ARG:HB3	1.67	0.59
8:7:369:SER:HB3	8:7:384:ILE:HD13	1.83	0.59
8:7:656:LYS:NZ	8:7:686:ARG:HH21	2.01	0.59
9:A:999:VAL:H	9:A:1011:GLN:HE22	1.49	0.59
10:B:277:LYS:HZ2	10:B:339:THR:N	2.01	0.59
8:7:601:ARG:NH2	8:7:669:CYS:SG	2.75	0.59
9:A:326:ARG:HG2	9:A:1406:VAL:HG11	1.84	0.59
9:A:346:ASP:OD2	10:B:1108:ARG:N	2.36	0.59
13:E:24:LYS:NZ	13:E:32:GLN:OE1	2.36	0.59
24:R:67:GLN:HB3	24:R:219:CYS:HB2	1.83	0.59
15:G:116:PRO:HD3	15:G:164:LYS:HA	1.85	0.59
23:Q:105:ALA:H	24:R:92:LEU:HD23	1.68	0.59
10:B:1187:ASN:HD21	10:B:1190:ASP:H	1.51	0.59
10:B:617:ARG:NH1	10:B:619:ILE:HG12	2.17	0.59
16:H:58:THR:HB	16:H:143:LEU:HB2	1.85	0.58
16:H:101:ALA:HA	16:H:116:TYR:HA	1.84	0.58
1:O:542:PRO:HB3	1:O:626:PRO:HA	1.85	0.58
10:B:1171:VAL:HG22	10:B:1182:CYS:HB2	1.85	0.58
11:C:19:ASP:HB2	11:C:231:ASN:HD22	1.68	0.58
11:C:194:GLU:HG2	11:C:195:GLN:HE21	1.68	0.58
22:O:91:ASN:ND2	22:O:105:ARG:O	2.36	0.58
8:7:672:GLN:NE2	8:7:686:ARG:HH12	2.01	0.58
10:B:1060:ARG:NH1	11:C:202:PRO:HD3	2.18	0.58
14:F:82:THR:HG22	14:F:84:TYR:H	1.67	0.58
9:A:434:ARG:NH1	9:A:437:MET:HG3	2.19	0.58
10:B:657:HIS:CD2	10:B:660:LYS:HZ1	2.21	0.58
22:O:235:SER:HB3	22:O:238:ARG:HH12	1.69	0.58
9:A:130:ASP:OD2	9:A:133:LYS:N	2.27	0.58
9:A:1095:THR:HB	9:A:1100:ARG:HH21	1.67	0.58
12:D:66:ARG:NH1	15:G:35:GLU:OE1	2.37	0.58
22:O:107:ARG:NH2	26:V:66:LEU:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:U:262:LEU:HB2	25:U:279:ALA:HB3	1.86	0.58
9:A:807:GLY:HA3	10:B:728:ARG:HH21	1.68	0.58
9:A:890:ASP:HA	9:A:940:ARG:HH12	1.68	0.58
9:A:269:ILE:HG12	9:A:299:HIS:HB3	1.86	0.57
9:A:407:ARG:HH11	9:A:413:ILE:HD11	1.67	0.57
22:O:68:GLN:O	22:O:127:LYS:NZ	2.28	0.57
9:A:940:ARG:HG2	9:A:944:ARG:NH1	2.19	0.57
11:C:112:ASN:OD1	11:C:112:ASN:N	2.38	0.57
10:B:969:ARG:NH1	11:C:61:GLU:OE1	2.22	0.57
10:B:1165:ILE:HD12	10:B:1185:CYS:HB2	1.87	0.57
15:G:27:LYS:NZ	15:G:51:TYR:O	2.27	0.57
13:E:20:LYS:HB3	13:E:35:VAL:HG22	1.86	0.57
2:1:61:ARG:NH1	27:W:410:GLU:H	2.02	0.57
10:B:906:SER:OG	10:B:909:ASP:OD2	2.19	0.57
9:A:1038:THR:H	9:A:1041:ALA:HB3	1.68	0.57
22:O:171:ARG:HA	22:O:239:LYS:HZ3	1.69	0.57
9:A:390:GLN:O	9:A:394:ASN:ND2	2.37	0.57
9:A:1224:LEU:HD11	9:A:1240:CYS:HB3	1.86	0.57
11:C:125:MET:HB2	11:C:127:ARG:NH1	2.20	0.57
9:A:228:PHE:HE1	10:B:1215:ARG:HH11	1.52	0.57
9:A:353:ILE:HD11	9:A:485:ASP:HB2	1.87	0.57
9:A:985:ASP:OD1	9:A:985:ASP:N	2.38	0.57
11:C:9:LYS:HB3	11:C:21:ILE:HB	1.86	0.57
27:W:149:CYS:SG	27:W:150:SER:N	2.78	0.57
9:A:1309:ASP:OD1	9:A:1309:ASP:N	2.36	0.56
10:B:1112:GLN:HE21	10:B:1119:VAL:HA	1.70	0.56
10:B:89:GLU:HB3	10:B:135:ARG:HB2	1.86	0.56
10:B:593:PRO:HB2	10:B:617:ARG:HE	1.71	0.56
22:O:95:ASN:N	22:O:95:ASN:OD1	2.36	0.56
23:Q:376:LEU:HB2	24:R:69:TRP:HB2	1.87	0.56
1:0:471:ARG:HA	1:0:471:ARG:HH11	1.70	0.56
10:B:824:ILE:N	10:B:1009:ASP:OD2	2.20	0.56
9:A:618:GLU:H	9:A:621:THR:HB	1.68	0.56
15:G:94:CYS:SG	15:G:95:SER:N	2.78	0.56
25:U:244:MET:HB3	26:V:113:ILE:HA	1.87	0.56
9:A:1192:LEU:HD11	9:A:1239:ARG:HB3	1.88	0.56
9:A:351:THR:OG1	9:A:352:VAL:N	2.36	0.56
9:A:494:SER:N	10:B:1149:GLU:OE2	2.39	0.56
10:B:494:HIS:HA	10:B:497:ARG:NH1	2.20	0.56
1:0:494:PRO:HB2	1:0:699:GLN:HE22	1.70	0.56
1:0:669:VAL:HG21	1:0:679:MET:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:532:ARG:NH1	9:A:536:LEU:HD21	2.21	0.56
10:B:277:LYS:NZ	10:B:337:ARG:O	2.31	0.56
23:Q:102:PRO:HA	24:R:94:LYS:HA	1.88	0.56
23:Q:122:GLN:HB2	23:Q:394:LYS:HE3	1.88	0.56
7:6:211:GLN:HE21	7:6:243:ASP:HB3	1.70	0.55
8:7:705:PHE:HE2	8:7:723:GLN:HE22	1.52	0.55
11:C:148:ARG:NH1	18:J:64:ASN:HA	2.22	0.55
2:1:110:ARG:HG3	2:1:286:ARG:HH11	1.71	0.55
9:A:217:LYS:NZ	9:A:221:SER:OG	2.40	0.55
9:A:557:ASP:N	9:A:557:ASP:OD1	2.40	0.55
9:A:946:VAL:HG13	13:E:201:LYS:HB3	1.88	0.55
9:A:1289:ARG:NH1	9:A:1326:ARG:NH1	2.55	0.55
10:B:373:ARG:HG3	10:B:566:LEU:HD23	1.88	0.55
13:E:33:GLU:HA	13:E:36:GLU:HB2	1.88	0.55
22:O:171:ARG:HG2	22:O:239:LYS:HZ3	1.72	0.55
9:A:1444:MET:HB2	14:F:133:VAL:HG13	1.88	0.55
10:B:760:ASP:OD1	10:B:760:ASP:N	2.39	0.55
16:H:134:ASN:N	16:H:134:ASN:OD1	2.39	0.55
24:R:125:THR:HB	24:R:221:GLU:HB3	1.88	0.55
9:A:117:GLU:HA	9:A:122:MET:HG2	1.88	0.55
10:B:402:GLY:O	10:B:405:ARG:NH1	2.37	0.55
8:7:690:ILE:HG22	8:7:694:LYS:NZ	2.22	0.55
9:A:951:GLU:O	9:A:954:TRP:NE1	2.37	0.55
10:B:106:ASP:N	10:B:106:ASP:OD1	2.40	0.55
2:1:286:ARG:NH2	2:1:306:UNK:O	2.40	0.55
9:A:434:ARG:NH1	9:A:437:MET:H	2.04	0.55
9:A:606:LEU:HG	9:A:613:ILE:HD13	1.88	0.55
11:C:73:GLN:NE2	11:C:237:SER:O	2.40	0.55
15:G:143:ILE:HA	15:G:170:ALA:HA	1.88	0.55
7:6:403:CYS:HA	7:6:436:PHE:HA	1.88	0.54
9:A:107:CYS:SG	9:A:108:MET:N	2.80	0.54
11:C:138:GLU:OE1	11:C:140:ASN:ND2	2.40	0.54
17:I:7:CYS:SG	17:I:8:ARG:N	2.80	0.54
1:0:364:LYS:HZ2	1:0:370:GLU:H	1.54	0.54
5:4:289:CYS:SG	5:4:290:SER:N	2.77	0.54
6:5:5:ARG:NH1	6:5:33:GLU:OE2	2.36	0.54
8:7:561:MET:SD	8:7:584:ASN:ND2	2.80	0.54
9:A:365:GLY:HA3	9:A:469:ARG:HB2	1.89	0.54
17:I:17:ARG:NH1	17:I:35:VAL:HG21	2.21	0.54
9:A:312:PRO:HB3	21:M:98:LYS:HA	1.90	0.54
9:A:390:GLN:HA	9:A:393:ARG:NH1	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:497:THR:HA	9:A:500:GLU:HB2	1.89	0.54
10:B:750:GLY:H	10:B:753:ALA:HB3	1.73	0.54
19:K:20:LYS:HB2	19:K:34:THR:HB	1.90	0.54
10:B:884:ARG:HG3	10:B:935:ARG:HE	1.72	0.54
2:1:107:ILE:HG23	2:1:110:ARG:HH11	1.72	0.54
9:A:1063:MET:HG3	10:B:1139:ILE:HG22	1.89	0.54
9:A:1150:SER:HA	9:A:1195:LEU:HA	1.90	0.54
13:E:214:CYS:SG	13:E:215:MET:N	2.81	0.54
27:W:144:ARG:HH11	27:W:155:PRO:HG3	1.73	0.54
8:7:556:GLU:HG2	8:7:707:SER:HB3	1.89	0.54
9:A:526:ASP:OD1	9:A:526:ASP:N	2.41	0.54
9:A:1111:MET:SD	9:A:1111:MET:N	2.81	0.54
10:B:165:VAL:HG11	10:B:448:ILE:HD12	1.89	0.54
4:3:59:CYS:SG	4:3:60:ASP:N	2.81	0.54
10:B:979:LYS:NZ	10:B:1097:HIS:HD2	2.06	0.54
21:M:34:ILE:HG22	21:M:45:CYS:HA	1.90	0.54
9:A:260:ASP:OD1	9:A:260:ASP:N	2.39	0.54
9:A:466:SER:OG	19:K:2:ASN:ND2	2.41	0.54
10:B:496:ARG:NH2	10:B:540:SER:O	2.41	0.54
11:C:52:GLU:HG2	11:C:53:THR:HG23	1.89	0.54
28:X:273:GLU:N	28:X:276:ARG:HH11	2.06	0.54
1:0:712:MET:O	1:0:716:ASN:ND2	2.41	0.53
2:1:227:UNK:O	7:6:212:ASN:ND2	2.38	0.53
7:6:406:CYS:SG	7:6:407:GLN:N	2.80	0.53
9:A:61:ILE:HA	9:A:74:MET:HB3	1.90	0.53
10:B:778:MET:HA	10:B:1096:ARG:HH12	1.72	0.53
10:B:822:ASN:O	18:J:48:ARG:NH1	2.41	0.53
10:B:957:ASN:OD1	10:B:961:LEU:N	2.41	0.53
19:K:12:LEU:HB2	19:K:18:LYS:NZ	2.23	0.53
3:2:503:ASP:HB3	3:2:507:ARG:NH1	2.23	0.53
9:A:518:LYS:NZ	9:A:624:SER:O	2.30	0.53
10:B:635:ARG:HH12	10:B:637:LEU:HD21	1.73	0.53
12:D:32:GLU:O	12:D:37:GLN:NE2	2.41	0.53
15:G:45:ILE:HA	15:G:78:VAL:HG12	1.90	0.53
9:A:862:ASN:OD1	9:A:862:ASN:N	2.41	0.53
12:D:39:ASN:HD21	12:D:43:GLU:HB2	1.74	0.53
22:O:205:LEU:HB2	22:O:213:VAL:HB	1.90	0.53
12:D:51:ASN:HD22	12:D:181:GLY:HA3	1.74	0.53
23:Q:141:ARG:HG2	23:Q:350:TRP:HB3	1.91	0.53
25:U:19:ASN:HA	25:U:22:ARG:NH1	2.24	0.53
12:D:37:GLN:HB3	15:G:5:LYS:NZ	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:169:ARG:NH1	14:F:142:SER:OG	2.42	0.53
21:M:124:ASN:OD1	21:M:124:ASN:N	2.42	0.53
10:B:1163:CYS:SG	10:B:1164:GLY:N	2.82	0.53
15:G:84:GLY:HA2	15:G:146:LYS:NZ	2.23	0.53
28:X:260:VAL:HB	28:X:261:LYS:NZ	2.24	0.53
2:1:49:GLN:HB2	2:1:61:ARG:HB3	1.91	0.53
8:7:631:THR:HB	8:7:636:ARG:HE	1.73	0.53
9:A:849:MET:SD	9:A:849:MET:N	2.82	0.53
9:A:51:GLY:HA2	9:A:57:ARG:HH12	1.73	0.53
9:A:544:ASP:N	9:A:544:ASP:OD1	2.41	0.53
11:C:69:LEU:O	18:J:6:ARG:NE	2.42	0.53
13:E:28:TYR:HA	13:E:64:PRO:HA	1.90	0.53
17:I:90:GLN:O	17:I:91:ARG:NH1	2.42	0.53
10:B:996:ARG:NH2	11:C:174:ALA:O	2.42	0.53
13:E:109:ILE:HG12	13:E:133:GLU:HB2	1.91	0.53
14:F:94:LEU:HD21	14:F:125:LEU:HD22	1.91	0.53
19:K:12:LEU:HB2	19:K:18:LYS:HZ1	1.74	0.53
22:O:196:ARG:HG2	22:O:203:VAL:HG13	1.91	0.53
1:0:234:PHE:HB2	1:0:458:ILE:HA	1.90	0.52
1:0:716:ASN:ND2	7:6:267:SER:O	2.41	0.52
27:W:6:ASP:OD1	27:W:6:ASP:N	2.41	0.52
1:0:257:LEU:HB3	1:0:343:LYS:NZ	2.23	0.52
1:0:468:MET:SD	1:0:468:MET:N	2.83	0.52
10:B:793:ALA:HB3	10:B:856:PHE:HB2	1.91	0.52
22:O:109:PRO:HD3	22:O:138:LYS:NZ	2.24	0.52
23:Q:100:GLU:HA	24:R:96:ARG:HA	1.90	0.52
9:A:1207:LEU:HD21	9:A:1274:ARG:HD3	1.91	0.52
17:I:103:CYS:SG	17:I:105:SER:OG	2.67	0.52
18:J:44:TYR:HA	18:J:47:ARG:HB2	1.91	0.52
10:B:918:ILE:HD13	10:B:935:ARG:HB2	1.92	0.52
9:A:443:LEU:HG	9:A:501:LEU:HD21	1.91	0.52
10:B:249:ARG:NH1	10:B:418:LYS:HG2	2.25	0.52
11:C:165:LYS:O	19:K:6:ARG:NH2	2.41	0.52
9:A:261:ASP:HB3	9:A:322:VAL:HG13	1.90	0.52
10:B:232:SER:O	10:B:261:ARG:NH1	2.42	0.52
11:C:82:TYR:HB3	11:C:84:ARG:NH1	2.25	0.52
27:W:179:ILE:HD12	27:W:182:ILE:HD12	1.92	0.52
8:7:690:ILE:HG22	8:7:694:LYS:HZ2	1.75	0.52
9:A:216:VAL:HG13	9:A:226:GLU:OE2	2.10	0.52
9:A:252:PHE:HB3	9:A:256:GLN:HB2	1.90	0.52
9:A:512:VAL:HG22	9:A:519:PRO:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1173:HIS:NE2	9:A:1228:TRP:O	2.42	0.52
24:R:94:LYS:HZ2	24:R:94:LYS:HB2	1.75	0.52
24:R:105:THR:OG1	24:R:106:LEU:N	2.42	0.52
27:W:144:ARG:NH1	27:W:146:GLU:HB2	2.25	0.52
9:A:761:MET:HA	9:A:804:TYR:HB2	1.92	0.52
10:B:87:LYS:HB2	10:B:137:TYR:HB2	1.92	0.52
10:B:604:ARG:NH2	10:B:611:PRO:O	2.41	0.52
10:B:1076:HIS:O	11:C:31:ASN:ND2	2.38	0.52
4:3:65:LYS:HZ2	15:G:165:GLU:HA	1.73	0.52
8:7:490:VAL:H	8:7:514:THR:HB	1.74	0.52
9:A:314:ALA:HA	21:M:96:ILE:HA	1.91	0.52
9:A:408:ASP:OD1	9:A:430:TRP:NE1	2.43	0.52
8:7:519:ARG:HA	8:7:681:ARG:HG3	1.92	0.51
10:B:331:LEU:HB3	10:B:349:ILE:HG13	1.92	0.51
15:G:60:ARG:NH2	15:G:69:GLU:OE1	2.42	0.51
26:V:61:THR:HB	26:V:86:THR:HB	1.93	0.51
9:A:265:LYS:HZ1	9:A:302:THR:HB	1.74	0.51
9:A:473:SER:OG	9:A:650:GLN:NE2	2.43	0.51
10:B:75:ALA:HB3	10:B:85:SER:HA	1.91	0.51
1:0:257:LEU:HB3	1:0:343:LYS:HZ3	1.76	0.51
13:E:177:ARG:O	13:E:212:ARG:NH1	2.43	0.51
16:H:2:SER:N	16:H:61:SER:OG	2.42	0.51
19:K:36:GLU:HB3	19:K:37:LYS:NZ	2.25	0.51
23:Q:121:PHE:HB2	24:R:131:ASN:HB3	1.92	0.51
30:N:41:DG:O6	31:T:44:DA:N6	2.43	0.51
1:0:345:ARG:HG3	1:0:359:PHE:HE1	1.75	0.51
17:I:29:CYS:SG	17:I:31:THR:OG1	2.68	0.51
19:K:28:PRO:O	19:K:76:GLN:NE2	2.44	0.51
2:1:255:LYS:HD3	2:1:258:ASN:HD22	1.75	0.51
9:A:1396:ALA:N	9:A:1419:ASP:OD2	2.41	0.51
8:7:656:LYS:HZ1	8:7:686:ARG:HH21	1.56	0.51
9:A:54:ASN:OD1	9:A:54:ASN:N	2.43	0.51
10:B:217:ARG:NH1	10:B:407:ASP:OD1	2.44	0.51
10:B:484:ASN:OD1	10:B:484:ASN:N	2.41	0.51
16:H:56:THR:OG1	16:H:146:ARG:NH1	2.43	0.51
17:I:58:VAL:HG11	17:I:109:ILE:HD11	1.93	0.51
19:K:17:SER:H	19:K:20:LYS:NZ	2.09	0.51
23:Q:353:GLU:HG2	23:Q:360:THR:HA	1.91	0.51
10:B:1106:ARG:NH2	10:B:1110:PRO:O	2.44	0.51
17:I:111:THR:OG1	17:I:112:SER:N	2.44	0.51
7:6:254:LEU:HD13	7:6:261:VAL:HG21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1100:ARG:HH12	9:A:1330:ASN:HD21	1.59	0.51
10:B:22:SER:O	10:B:654:ARG:NH2	2.44	0.51
10:B:898:LEU:HB2	20:L:58:LYS:HZ1	1.76	0.51
27:W:144:ARG:NH1	27:W:155:PRO:HG3	2.26	0.51
9:A:562:THR:O	9:A:576:GLN:NE2	2.44	0.51
9:A:991:LYS:NZ	9:A:1023:ARG:HD3	2.26	0.51
13:E:40:GLU:HA	13:E:43:LYS:HE2	1.93	0.51
19:K:29:ASN:ND2	19:K:77:THR:OG1	2.43	0.51
24:R:72:ARG:HB3	24:R:223:GLN:HG3	1.92	0.51
27:W:143:ASP:OD1	27:W:143:ASP:N	2.41	0.51
10:B:373:ARG:HB2	10:B:567:GLU:OE2	2.12	0.50
8:7:622:MET:SD	8:7:622:MET:N	2.85	0.50
9:A:1044:TRP:O	9:A:1048:ASN:ND2	2.44	0.50
21:M:123:ASP:N	21:M:123:ASP:OD1	2.44	0.50
8:7:672:GLN:HE22	8:7:686:ARG:HH22	1.60	0.50
9:A:4:GLN:HE22	10:B:1159:ARG:H	1.59	0.50
10:B:842:ASN:ND2	10:B:845:SER:OG	2.43	0.50
11:C:220:ASP:HA	11:C:222:LYS:NZ	2.27	0.50
12:D:66:ARG:NH2	15:G:35:GLU:OE2	2.40	0.50
28:X:143:LEU:HA	28:X:176:GLY:HA3	1.92	0.50
7:6:393:PRO:HA	7:6:425:SER:HA	1.94	0.50
8:7:557:VAL:HG21	8:7:594:LEU:HD11	1.92	0.50
9:A:875:ALA:HB2	9:A:1366:ARG:HG3	1.93	0.50
20:L:40:LEU:HD13	20:L:44:ASP:HB3	1.93	0.50
22:O:73:THR:HG22	22:O:122:VAL:HG22	1.92	0.50
27:W:193:ARG:NH1	28:X:283:LEU:O	2.36	0.50
7:6:200:ARG:HG3	7:6:201:LYS:HZ2	1.75	0.50
9:A:112:LYS:NZ	9:A:165:GLY:HA3	2.24	0.50
23:Q:363:GLY:HA2	23:Q:395:PHE:HA	1.93	0.50
8:7:558:TRP:HB3	8:7:711:LYS:HE2	1.94	0.50
9:A:9:ALA:HB3	10:B:1193:GLN:HE21	1.77	0.50
10:B:601:ARG:NH2	10:B:691:GLU:OE1	2.44	0.50
26:V:53:LYS:NZ	26:V:54:ASP:OD1	2.41	0.50
9:A:804:TYR:OH	9:A:816:HIS:NE2	2.44	0.50
28:X:260:VAL:HB	28:X:261:LYS:HZ2	1.77	0.50
8:7:573:THR:OG1	8:7:574:ALA:N	2.45	0.50
10:B:494:HIS:CD2	10:B:497:ARG:HH11	2.28	0.50
10:B:848:ARG:HH12	18:J:9:SER:C	2.14	0.50
10:B:891:ASP:OD1	10:B:891:ASP:N	2.45	0.50
15:G:100:GLU:HA	15:G:109:PHE:HA	1.93	0.50
16:H:110:ASP:HB3	16:H:129:TYR:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:553:VAL:HB	9:A:556:TRP:HB2	1.94	0.50
11:C:250:THR:HA	11:C:253:LYS:HD2	1.94	0.50
13:E:48:ASP:OD1	13:E:52:ARG:N	2.45	0.49
15:G:119:LEU:HD11	15:G:130:TYR:HB3	1.92	0.49
15:G:150:CYS:HA	15:G:159:ALA:HA	1.94	0.49
22:O:102:VAL:HB	22:O:115:ILE:HB	1.94	0.49
9:A:946:VAL:HG22	13:E:201:LYS:HD2	1.94	0.49
11:C:78:GLU:OE2	11:C:246:ARG:NE	2.45	0.49
11:C:116:LYS:NZ	11:C:140:ASN:HA	2.27	0.49
13:E:192:ARG:HG2	13:E:215:MET:OXT	2.12	0.49
10:B:101:MET:HG3	10:B:169:ARG:HH12	1.75	0.49
16:H:30:SER:OG	16:H:31:THR:N	2.45	0.49
21:M:321:ASP:OD1	21:M:321:ASP:N	2.44	0.49
28:X:218:ASP:HA	28:X:221:ILE:HD12	1.94	0.49
9:A:1199:ARG:O	9:A:1203:ASN:ND2	2.45	0.49
9:A:1227:ILE:HD13	9:A:1239:ARG:NH1	2.28	0.49
10:B:276:ILE:HA	10:B:338:GLY:HA3	1.93	0.49
10:B:336:ARG:HD2	10:B:348:ARG:HH11	1.77	0.49
21:M:102:THR:OG1	21:M:103:ASP:N	2.46	0.49
22:O:104:MET:HB3	22:O:113:ALA:HB3	1.95	0.49
13:E:98:ILE:O	13:E:102:GLU:N	2.43	0.49
15:G:91:VAL:HG22	15:G:101:VAL:HG22	1.94	0.49
16:H:131:ASN:OD1	16:H:131:ASN:N	2.44	0.49
22:O:196:ARG:NH2	30:N:24:DT:OP1	2.43	0.49
1:O:259:ARG:NH2	1:O:394:GLU:O	2.45	0.49
9:A:255:SER:HB3	21:M:86:LEU:HD11	1.95	0.49
10:B:1040:ASN:N	10:B:1040:ASN:OD1	2.45	0.49
19:K:106:GLU:O	19:K:110:ASN:ND2	2.46	0.49
21:M:54:ASP:HB2	21:M:55:LYS:NZ	2.27	0.49
22:O:98:ARG:NH2	31:T:58:DT:OP1	2.45	0.49
28:X:251:ASN:HD21	28:X:253:LYS:NZ	2.11	0.49
1:O:613:ASP:O	1:O:618:ARG:NH1	2.44	0.49
9:A:483:ASP:N	9:A:483:ASP:OD1	2.46	0.49
9:A:385:ILE:O	9:A:389:THR:OG1	2.30	0.49
9:A:925:LEU:HD23	9:A:928:LEU:HD12	1.94	0.49
10:B:827:ILE:HG22	10:B:1014:PRO:HG3	1.95	0.49
10:B:843:GLN:NE2	10:B:847:ASP:OD1	2.46	0.49
9:A:25:GLU:HA	9:A:28:ARG:HD2	1.94	0.49
9:A:358:ASN:N	9:A:358:ASN:OD1	2.45	0.49
9:A:896:ARG:HD2	9:A:1030:ARG:NH1	2.27	0.49
10:B:896:ASP:HA	20:L:42:ARG:HH22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:982:SER:OG	10:B:983:ARG:N	2.45	0.49
9:A:18:GLN:O	10:B:1215:ARG:N	2.45	0.48
9:A:1146:VAL:HG23	9:A:1197:LEU:HD22	1.95	0.48
10:B:882:THR:HG23	10:B:934:LYS:HG3	1.95	0.48
16:H:62:SER:OG	16:H:63:LEU:N	2.42	0.48
3:2:480:VAL:HG23	3:2:493:ILE:HD12	1.95	0.48
4:3:53:GLN:HB3	4:3:62:ILE:HD13	1.96	0.48
7:6:175:ARG:NH1	7:6:176:ASN:OD1	2.46	0.48
9:A:888:GLY:O	9:A:940:ARG:NH2	2.47	0.48
10:B:64:CYS:HA	10:B:67:SER:HB3	1.93	0.48
18:J:16:ASP:OD1	18:J:16:ASP:N	2.44	0.48
22:O:71:VAL:HG13	22:O:124:THR:HB	1.94	0.48
1:0:37:ASN:OD1	1:0:37:ASN:N	2.46	0.48
1:0:69:ILE:HB	1:0:205:ILE:HG23	1.96	0.48
9:A:98:LYS:HD3	9:A:98:LYS:HA	1.69	0.48
9:A:182:VAL:HA	9:A:201:VAL:HA	1.95	0.48
21:M:113:ALA:O	21:M:117:ASN:ND2	2.47	0.48
1:0:510:PHE:O	1:0:546:TYR:OH	2.31	0.48
9:A:7:SER:HB2	10:B:1175:LEU:HD22	1.95	0.48
10:B:442:PHE:HB2	24:R:278:LEU:HB2	1.96	0.48
10:B:1135:ARG:NH1	10:B:1139:ILE:HD11	2.27	0.48
17:I:49:ILE:HG22	17:I:51:ASN:HD21	1.77	0.48
9:A:390:GLN:HE21	9:A:394:ASN:HD21	1.59	0.48
11:C:241:ASP:N	11:C:241:ASP:OD1	2.46	0.48
12:D:175:PHE:HE1	15:G:1:MET:HG3	1.79	0.48
28:X:187:HIS:HA	28:X:214:TRP:HB2	1.95	0.48
3:2:482:LEU:HD11	3:2:494:SER:HB3	1.96	0.48
7:6:269:GLN:HB3	7:6:274:LYS:NZ	2.29	0.48
12:D:64:VAL:O	12:D:68:ARG:N	2.45	0.48
9:A:119:ASN:HD21	9:A:121:LEU:HB2	1.78	0.48
9:A:843:LYS:NZ	9:A:1402:PHE:HA	2.29	0.48
10:B:1155:SER:OG	10:B:1156:ASP:OD1	2.32	0.48
9:A:226:GLU:HB3	9:A:230:ARG:HH21	1.79	0.48
9:A:818:MET:HG2	10:B:514:LEU:HD23	1.96	0.48
11:C:13:ALA:HA	11:C:18:VAL:HG22	1.96	0.48
17:I:76:PRO:HB2	17:I:77:LYS:HE2	1.95	0.48
19:K:29:ASN:ND2	19:K:78:THR:O	2.47	0.48
4:3:31:ASN:HB3	4:3:34:CYS:HB2	1.96	0.48
8:7:672:GLN:HE21	8:7:722:ARG:HH12	1.60	0.48
10:B:287:ARG:NH1	10:B:325:GLN:O	2.47	0.48
10:B:348:ARG:HA	10:B:351:TYR:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:1156:ASP:OD1	10:B:1156:ASP:N	2.46	0.48
15:G:86:VAL:HA	15:G:146:LYS:HA	1.96	0.48
7:6:154:ILE:HD13	7:6:197:LYS:NZ	2.29	0.48
8:7:612:VAL:HG13	8:7:628:TYR:HB2	1.94	0.48
9:A:567:LYS:HZ2	16:H:91:ASP:HA	1.79	0.48
10:B:210:LYS:NZ	10:B:462:ALA:O	2.36	0.48
12:D:63:LEU:HD13	12:D:130:LEU:HD13	1.95	0.48
13:E:10:SER:HA	13:E:13:TRP:HB3	1.96	0.48
17:I:75:CYS:H	17:I:80:SER:H	1.61	0.48
19:K:58:PHE:HE2	19:K:74:ARG:HB3	1.78	0.48
21:M:269:ILE:HG12	21:M:272:LYS:HD2	1.96	0.48
9:A:265:LYS:HD3	9:A:268:ASP:OD2	2.14	0.47
9:A:345:VAL:HG21	10:B:1150:ARG:HD2	1.96	0.47
21:M:272:LYS:HB3	21:M:272:LYS:HZ3	1.79	0.47
28:X:251:ASN:HD21	28:X:253:LYS:HG2	1.79	0.47
29:Z:3:UNK:O	29:Z:15:UNK:N	2.47	0.47
9:A:333:GLU:OE1	10:B:1129:ARG:NH2	2.47	0.47
10:B:579:ARG:HA	10:B:589:VAL:HG12	1.96	0.47
11:C:54:ASN:ND2	11:C:60:ASP:OD1	2.46	0.47
21:M:267:LYS:HZ1	21:M:270:ALA:CA	2.26	0.47
9:A:481:ASP:N	9:A:481:ASP:OD1	2.47	0.47
9:A:884:ASP:OD1	9:A:884:ASP:N	2.46	0.47
12:D:118:THR:OG1	12:D:119:ARG:N	2.46	0.47
1:0:520:ARG:NH1	1:0:550:ILE:HA	2.30	0.47
8:7:494:PRO:HB3	8:7:523:LYS:HB2	1.96	0.47
11:C:11:ARG:NH1	11:C:209:TYR:OH	2.47	0.47
11:C:75:MET:SD	11:C:246:ARG:NH2	2.87	0.47
20:L:47:ARG:HH12	20:L:49:LYS:HG2	1.77	0.47
4:3:65:LYS:HZ2	15:G:165:GLU:HG2	1.79	0.47
7:6:176:ASN:HA	7:6:206:GLY:HA3	1.97	0.47
27:W:167:GLU:HB2	27:W:168:LYS:HZ2	1.79	0.47
9:A:294:SER:HA	9:A:297:GLN:HB3	1.96	0.47
9:A:806:ARG:HD2	10:B:728:ARG:HA	1.95	0.47
10:B:116:GLU:HG3	20:L:55:ILE:HD11	1.95	0.47
7:6:209:SER:OG	7:6:212:ASN:ND2	2.48	0.47
9:A:45:GLN:NE2	21:M:85:PRO:O	2.48	0.47
9:A:960:ILE:HD12	9:A:1025:ARG:HG3	1.96	0.47
10:B:95:ILE:HD11	10:B:128:LEU:HD23	1.95	0.47
13:E:20:LYS:NZ	13:E:34:GLU:O	2.32	0.47
22:O:71:VAL:HB	22:O:158:GLN:HB2	1.95	0.47
22:O:172:LEU:HD13	22:O:193:LEU:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Q:388:PRO:HB2	24:R:82:ARG:NH1	2.29	0.47
27:W:13:LEU:HB3	27:W:29:LEU:HD21	1.96	0.47
1:0:440:LEU:HD13	1:0:444:ILE:HD12	1.97	0.47
1:0:569:ILE:HA	1:0:599:LEU:HB2	1.96	0.47
4:3:65:LYS:NZ	15:G:165:GLU:HG2	2.30	0.47
7:6:362:VAL:HA	7:6:369:MET:HA	1.97	0.47
8:7:389:GLY:H	8:7:692:ARG:HB3	1.80	0.47
8:7:581:TYR:HE1	8:7:710:SER:H	1.63	0.47
9:A:711:ARG:NE	17:I:95:THR:O	2.48	0.47
10:B:238:ALA:HB3	10:B:256:VAL:HB	1.97	0.47
15:G:113:HIS:HB3	27:W:118:GLU:OE2	2.15	0.47
20:L:32:ALA:HB2	20:L:55:ILE:HB	1.97	0.47
21:M:142:LEU:HD23	21:M:146:VAL:HG11	1.97	0.47
27:W:144:ARG:HE	27:W:148:LEU:HD21	1.80	0.47
1:0:441:ASP:HB3	1:0:444:ILE:HG13	1.97	0.47
1:0:532:ILE:HG22	1:0:533:THR:HG23	1.97	0.47
8:7:589:GLN:HE22	8:7:756:ARG:HH21	1.62	0.47
10:B:487:THR:OG1	10:B:488:TYR:N	2.48	0.47
10:B:881:ASN:O	10:B:933:SER:OG	2.32	0.47
10:B:954:VAL:HG22	10:B:964:VAL:HB	1.97	0.47
10:B:984:HIS:NE2	10:B:1028:GLU:OE1	2.44	0.47
11:C:59:ALA:HB3	11:C:62:PHE:HB2	1.96	0.47
9:A:172:PRO:HB3	9:A:185:TRP:CD2	2.50	0.46
10:B:249:ARG:NH2	10:B:414:ALA:O	2.48	0.46
10:B:278:GLN:HB2	10:B:337:ARG:HH21	1.79	0.46
10:B:834:ASN:HA	10:B:838:SER:HB2	1.97	0.46
13:E:156:LEU:HD23	13:E:160:GLU:HB3	1.97	0.46
16:H:5:LEU:H	16:H:60:ALA:HA	1.80	0.46
8:7:554:CYS:HB2	8:7:733:PHE:HA	1.97	0.46
9:A:148:CYS:SG	9:A:164:ARG:NH2	2.88	0.46
9:A:446:ARG:O	9:A:449:SER:OG	2.33	0.46
9:A:1138:ILE:HG21	9:A:1316:VAL:HG13	1.98	0.46
16:H:5:LEU:O	16:H:134:ASN:ND2	2.47	0.46
19:K:22:ASP:O	19:K:32:VAL:N	2.47	0.46
22:O:133:LYS:HD2	22:O:137:ARG:HH21	1.80	0.46
27:W:149:CYS:HB3	27:W:154:GLU:H	1.81	0.46
9:A:883:LEU:HD13	9:A:943:LEU:HD13	1.95	0.46
9:A:1151:GLU:OE1	17:I:45:ARG:NH2	2.48	0.46
9:A:1267:MET:HA	9:A:1271:ILE:HD12	1.97	0.46
11:C:55:THR:OG1	11:C:152:GLU:O	2.31	0.46
22:O:144:GLN:HG3	22:O:150:ALA:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:274:VAL:HG13	2:1:280:GLU:HB2	1.96	0.46
23:Q:99:ASN:N	24:R:97:ILE:O	2.48	0.46
23:Q:101:PHE:O	24:R:95:ILE:N	2.48	0.46
23:Q:138:ARG:HH12	24:R:58:ASP:HA	1.79	0.46
13:E:54:GLN:HA	13:E:56:LYS:HZ1	1.81	0.46
23:Q:117:HIS:HD2	23:Q:391:LYS:HB2	1.81	0.46
3:2:485:ASP:OD2	3:2:488:LYS:HE2	2.15	0.46
9:A:175:ARG:HB2	9:A:182:VAL:HG13	1.96	0.46
9:A:745:GLN:O	9:A:749:ALA:N	2.45	0.46
9:A:855:THR:HG23	9:A:866:PHE:HA	1.98	0.46
10:B:657:HIS:HD2	10:B:660:LYS:NZ	2.11	0.46
10:B:1158:PHE:HD1	10:B:1160:VAL:HG22	1.81	0.46
11:C:125:MET:HB2	11:C:127:ARG:HH12	1.80	0.46
11:C:238:ILE:HG21	11:C:246:ARG:NH1	2.31	0.46
12:D:210:ILE:HA	12:D:213:GLU:HB2	1.98	0.46
7:6:155:ASP:HB2	7:6:298:LYS:NZ	2.31	0.46
7:6:243:ASP:OD2	7:6:247:ILE:HD12	2.16	0.46
9:A:809:THR:HG23	9:A:812:GLU:OE2	2.16	0.46
9:A:1157:ASP:O	9:A:1241:ARG:NH2	2.47	0.46
10:B:239:GLU:HG2	10:B:255:GLN:HG2	1.97	0.46
10:B:494:HIS:HD2	10:B:497:ARG:NH1	2.11	0.46
10:B:770:GLN:HE21	10:B:985:GLY:H	1.63	0.46
10:B:866:TYR:HB2	10:B:870:ILE:HB	1.98	0.46
15:G:1:MET:HG2	15:G:85:GLU:OE2	2.15	0.46
27:W:29:LEU:HD12	27:W:32:ILE:HD12	1.98	0.46
8:7:672:GLN:HE22	8:7:686:ARG:HH12	1.62	0.46
9:A:1100:ARG:HA	9:A:1103:GLU:OE2	2.16	0.46
9:A:1141:THR:HG22	9:A:1273:LEU:HD12	1.98	0.46
9:A:1348:LEU:HD23	9:A:1372:VAL:HG13	1.98	0.46
10:B:487:THR:HG23	10:B:490:SER:H	1.81	0.46
13:E:26:ARG:HH12	13:E:189:GLY:HA3	1.81	0.46
27:W:186:LEU:HB3	27:W:187:LYS:NZ	2.31	0.46
1:0:538:VAL:HA	1:0:598:LEU:HB3	1.98	0.46
1:0:603:ARG:NH1	1:0:628:GLN:HA	2.23	0.46
8:7:633:GLN:HA	8:7:636:ARG:HB2	1.98	0.46
9:A:512:VAL:HA	9:A:519:PRO:HA	1.97	0.46
10:B:422:LYS:NZ	10:B:426:LYS:HE2	2.31	0.46
25:U:263:LYS:NZ	25:U:278:LYS:NZ	2.60	0.46
1:0:526:LEU:HD22	1:0:621:LEU:HD21	1.98	0.45
12:D:173:HIS:HB3	12:D:176:GLU:HG3	1.97	0.45
27:W:187:LYS:HA	27:W:190:ASP:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:111:ARG:NH2	32:0:801:SF4:S2	2.86	0.45
1:0:238:HIS:NE2	1:0:664:GLN:OE1	2.49	0.45
7:6:221:LEU:HD13	7:6:230:ARG:HB3	1.97	0.45
8:7:490:VAL:HG23	8:7:514:THR:HB	1.98	0.45
9:A:212:LYS:HA	9:A:232:GLU:OE2	2.16	0.45
9:A:900:ASP:OD2	9:A:906:HIS:N	2.46	0.45
9:A:1366:ARG:N	9:A:1366:ARG:HH11	2.14	0.45
13:E:118:PRO:HA	13:E:121:MET:HB2	1.98	0.45
27:W:95:ILE:HG22	27:W:99:LYS:HE2	1.97	0.45
1:0:618:ARG:HH22	1:0:675:ASP:HB3	1.82	0.45
1:0:643:ARG:HG2	1:0:649:ARG:HH11	1.81	0.45
9:A:377:PRO:HA	9:A:433:GLU:HA	1.99	0.45
9:A:977:LYS:H	9:A:1036:ARG:NH1	2.15	0.45
11:C:103:ALA:HB3	11:C:153:LEU:HB3	1.98	0.45
11:C:185:LYS:O	11:C:187:LYS:NZ	2.48	0.45
12:D:140:ASP:O	12:D:144:THR:N	2.47	0.45
22:O:66:THR:O	22:O:68:GLN:NE2	2.47	0.45
25:U:30:ILE:HB	26:V:33:GLU:OE2	2.16	0.45
2:1:58:MET:SD	2:1:94:ARG:NH2	2.89	0.45
7:6:133:SER:H	7:6:136:MET:HG2	1.81	0.45
9:A:563:PRO:HA	9:A:576:GLN:HE22	1.81	0.45
9:A:843:LYS:HZ3	9:A:1402:PHE:HA	1.81	0.45
10:B:328:GLU:HA	10:B:331:LEU:HB2	1.99	0.45
21:M:167:SER:O	21:M:169:GLU:N	2.46	0.45
26:V:76:TRP:N	26:V:115:ALA:O	2.46	0.45
9:A:514:PRO:O	9:A:1364:ASN:ND2	2.50	0.45
10:B:581:PHE:O	10:B:626:ILE:N	2.47	0.45
10:B:1034:VAL:HG22	10:B:1059:LEU:HD13	1.98	0.45
10:B:1103:ILE:O	10:B:1122:ARG:NH2	2.44	0.45
12:D:37:GLN:HB3	15:G:5:LYS:HZ2	1.80	0.45
17:I:83:ASN:N	17:I:83:ASN:OD1	2.49	0.45
22:O:69:ASN:HB2	31:T:61:DT:H1'	1.98	0.45
24:R:260:GLY:HA2	24:R:263:MET:HB2	1.99	0.45
1:0:406:ALA:O	1:0:410:SER:OG	2.34	0.45
6:5:16:ILE:HD13	6:5:19:LEU:HD12	1.99	0.45
9:A:51:GLY:N	9:A:57:ARG:HH12	2.14	0.45
9:A:789:LYS:HE2	9:A:789:LYS:HB3	1.86	0.45
9:A:1062:GLU:OE1	14:F:88:TYR:OH	2.34	0.45
10:B:279:ASP:OD1	10:B:279:ASP:N	2.50	0.45
11:C:4:GLU:O	11:C:24:ASN:ND2	2.50	0.45
13:E:124:VAL:HG13	13:E:132:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:I:78:CYS:SG	17:I:105:SER:OG	2.65	0.45
23:Q:138:ARG:HH12	24:R:58:ASP:CA	2.30	0.45
1:O:471:ARG:O	1:O:474:ASN:ND2	2.49	0.45
9:A:112:LYS:HZ2	9:A:165:GLY:HA3	1.81	0.45
9:A:547:LEU:HB3	19:K:60:ALA:HB2	1.98	0.45
10:B:287:ARG:HH12	10:B:325:GLN:NE2	2.15	0.45
10:B:756:ILE:HG12	10:B:770:GLN:HG2	1.98	0.45
2:1:105:GLN:NE2	27:W:416:VAL:O	2.50	0.45
4:3:28:PHE:HA	4:3:39:CYS:HA	1.99	0.45
1:O:197:ARG:HG3	1:O:221:ARG:NH1	2.31	0.45
2:1:67:ASP:OD1	2:1:67:ASP:N	2.50	0.45
2:1:79:GLU:OE2	2:1:82:PRO:HA	2.17	0.45
8:7:553:GLN:HB3	8:7:734:LYS:NZ	2.31	0.45
9:A:51:GLY:CA	9:A:57:ARG:HH12	2.30	0.45
9:A:267:ALA:O	9:A:271:LYS:NZ	2.43	0.45
9:A:532:ARG:HH12	9:A:536:LEU:HD21	1.80	0.45
10:B:759:PRO:HD2	10:B:1046:PRO:HA	1.98	0.45
11:C:177:GLU:HB2	11:C:231:ASN:HB3	1.99	0.45
11:C:196:ASP:OD2	11:C:199:LYS:HG2	2.17	0.45
19:K:50:LEU:HA	19:K:53:ASP:OD2	2.17	0.45
2:1:106:GLN:O	2:1:286:ARG:NH1	2.49	0.45
8:7:734:LYS:HE2	8:7:736:ILE:HD11	1.99	0.45
9:A:386:ASP:OD1	9:A:386:ASP:N	2.50	0.45
16:H:112:ILE:HG23	16:H:132:LEU:HD12	1.98	0.45
24:R:339:LEU:HA	24:R:349:TYR:HA	1.98	0.45
1:O:44:SER:HB2	1:O:670:LEU:HB2	1.98	0.44
1:O:535:ASP:OD1	1:O:535:ASP:N	2.49	0.44
8:7:576:LYS:HB2	8:7:576:LYS:NZ	2.32	0.44
9:A:451:HIS:HA	9:A:1074:GLU:OE2	2.16	0.44
10:B:233:PRO:HA	10:B:261:ARG:HD3	2.00	0.44
10:B:1065:GLN:HG3	10:B:1067:ARG:H	1.82	0.44
15:G:27:LYS:HE2	15:G:54:ILE:HD12	1.99	0.44
22:O:109:PRO:HD3	22:O:138:LYS:HZ1	1.82	0.44
24:R:61:LEU:HD11	24:R:64:SER:HB3	1.98	0.44
24:R:94:LYS:HD2	24:R:107:LEU:HD23	1.99	0.44
9:A:211:PHE:HB3	9:A:232:GLU:HG2	1.98	0.44
9:A:598:LEU:HD21	16:H:124:ARG:HD2	1.99	0.44
11:C:249:ASP:O	11:C:253:LYS:N	2.50	0.44
14:F:128:LYS:HD3	14:F:149:GLU:HA	1.97	0.44
15:G:131:GLN:HG2	15:G:136:VAL:HG13	1.99	0.44
21:M:44:VAL:HA	21:M:51:VAL:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:542:GLU:O	8:7:546:LYS:NZ	2.51	0.44
9:A:347:PHE:HA	9:A:374:LEU:HD22	1.99	0.44
9:A:418:SER:O	9:A:422:GLY:N	2.46	0.44
9:A:1167:GLU:HA	9:A:1170:ILE:HB	2.00	0.44
10:B:223:VAL:HG22	10:B:240:ILE:HD12	1.99	0.44
10:B:642:ASP:HA	10:B:649:LYS:HA	1.99	0.44
10:B:847:ASP:OD2	11:C:167:HIS:HA	2.17	0.44
11:C:82:TYR:HB2	11:C:85:ASP:OD2	2.18	0.44
15:G:144:ARG:HB2	15:G:171:ILE:HG12	2.00	0.44
17:I:14:LEU:HB3	17:I:27:PHE:HB3	2.00	0.44
25:U:263:LYS:HZ3	25:U:278:LYS:HG2	1.83	0.44
1:0:36:GLY:HA2	1:0:455:SER:H	1.82	0.44
9:A:265:LYS:HA	9:A:268:ASP:OD2	2.17	0.44
9:A:794:PRO:HA	9:A:797:LYS:HB2	2.00	0.44
10:B:100:PRO:O	10:B:180:TYR:OH	2.31	0.44
11:C:185:LYS:C	11:C:187:LYS:HZ2	2.21	0.44
1:0:540:PHE:HB3	1:0:602:ALA:HB2	2.00	0.44
8:7:520:GLU:HB2	8:7:681:ARG:NH1	2.32	0.44
9:A:787:PHE:HB3	9:A:791:ASP:OD2	2.18	0.44
9:A:847:ASP:OD1	9:A:847:ASP:N	2.46	0.44
15:G:122:ASN:HB2	15:G:131:GLN:HG3	1.99	0.44
20:L:31:CYS:HB3	20:L:36:SER:H	1.82	0.44
22:O:163:SER:HB3	22:O:213:VAL:HG13	2.00	0.44
23:Q:127:ILE:HB	23:Q:128:ASN:H	1.64	0.44
27:W:115:LYS:HE2	27:W:115:LYS:HB3	1.86	0.44
28:X:272:ALA:O	28:X:276:ARG:NE	2.51	0.44
7:6:128:LEU:N	7:6:170:GLY:O	2.44	0.44
9:A:840:ARG:NH1	9:A:1106:ASN:OD1	2.32	0.44
10:B:46:GLN:HE22	10:B:496:ARG:NH1	2.15	0.44
10:B:557:PHE:HA	10:B:560:GLU:OE2	2.17	0.44
10:B:657:HIS:HA	10:B:660:LYS:HZ1	1.83	0.44
10:B:924:GLU:HA	10:B:928:ARG:HB3	1.98	0.44
2:1:94:ARG:NH2	2:1:97:MET:SD	2.91	0.44
6:5:21:LEU:HD23	6:5:31:VAL:HG21	2.00	0.44
8:7:606:ILE:HG12	8:7:652:ILE:HD11	1.99	0.44
8:7:672:GLN:HG2	8:7:722:ARG:HH12	1.83	0.44
11:C:148:ARG:HH12	18:J:64:ASN:HA	1.81	0.44
17:I:19:ASP:OD2	17:I:23:ASN:N	2.51	0.44
2:1:46:ASP:N	2:1:63:ILE:O	2.50	0.44
16:H:55:LEU:HA	16:H:146:ARG:OXT	2.18	0.44
21:M:177:LEU:HD22	21:M:207:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:608:PHE:HE2	8:7:670:LEU:HB3	1.82	0.44
9:A:622:VAL:HG23	9:A:629:LEU:HD22	2.00	0.44
9:A:1420:ASP:OD2	9:A:1422:ARG:HG2	2.17	0.44
11:C:136:ASP:OD2	11:C:140:ASN:N	2.41	0.44
20:L:32:ALA:HB3	20:L:53:HIS:HD2	1.82	0.44
20:L:47:ARG:NH2	20:L:48:CYS:O	2.51	0.44
22:O:65:PRO:HA	22:O:164:CYS:HB3	1.99	0.44
22:O:91:ASN:OD1	25:U:285:TRP:NE1	2.51	0.44
23:Q:126:LYS:HD2	24:R:128:VAL:HG21	1.99	0.44
8:7:679:SER:HB2	8:7:682:GLN:HB2	1.99	0.43
13:E:67:GLU:HA	13:E:70:SER:HB3	1.99	0.43
15:G:23:LYS:HG3	15:G:56:ILE:HD12	1.99	0.43
21:M:88:ASP:N	21:M:88:ASP:OD1	2.48	0.43
6:5:33:GLU:H	6:5:41:LEU:HB3	1.83	0.43
9:A:128:ILE:HG22	9:A:130:ASP:H	1.81	0.43
9:A:883:LEU:H	9:A:952:ALA:HB1	1.83	0.43
9:A:1200:ALA:HA	9:A:1203:ASN:HD22	1.82	0.43
10:B:109:THR:HG21	24:R:263:MET:HG3	1.99	0.43
21:M:54:ASP:HB2	21:M:55:LYS:HZ2	1.82	0.43
7:6:251:ILE:HG12	7:6:276:LEU:HD13	2.00	0.43
9:A:219:PHE:HE1	9:A:226:GLU:HG2	1.83	0.43
9:A:408:ASP:OD1	9:A:408:ASP:N	2.51	0.43
9:A:1194:ARG:HE	9:A:1237:ILE:HD12	1.83	0.43
10:B:218:SER:HA	10:B:404:LYS:HA	1.99	0.43
10:B:249:ARG:HH12	10:B:418:LYS:HG2	1.84	0.43
10:B:360:PHE:O	10:B:374:LYS:NZ	2.49	0.43
1:0:356:PRO:HG2	1:0:416:PHE:HB3	2.00	0.43
9:A:66:LYS:HA	21:M:20:ILE:HD11	2.01	0.43
10:B:70:ILE:HD11	23:Q:333:LYS:HB2	2.00	0.43
10:B:637:LEU:HD12	10:B:693:ILE:HD13	2.01	0.43
11:C:54:ASN:HB3	20:L:60:ARG:NH1	2.32	0.43
12:D:37:GLN:O	12:D:45:GLU:N	2.45	0.43
12:D:204:ASP:HA	12:D:207:LEU:HD12	2.01	0.43
8:7:363:ARG:HA	8:7:364:PRO:HD3	1.90	0.43
9:A:51:GLY:H	9:A:55:ASP:HB3	1.82	0.43
9:A:731:ARG:HD3	9:A:731:ARG:HA	1.88	0.43
10:B:120:ARG:NH2	10:B:957:ASN:O	2.51	0.43
12:D:167:LEU:HD22	12:D:177:VAL:HB	2.00	0.43
22:O:75:THR:HB	22:O:154:ASP:OD2	2.19	0.43
22:O:235:SER:O	22:O:238:ARG:NH1	2.52	0.43
1:0:197:ARG:HG3	1:0:221:ARG:HH12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:622:MET:O	8:7:624:LYS:NZ	2.52	0.43
9:A:113:LEU:HD21	9:A:218:ASP:HB3	2.00	0.43
9:A:896:ARG:NH1	9:A:1030:ARG:HH12	2.16	0.43
10:B:345:LYS:NZ	10:B:345:LYS:H	2.17	0.43
10:B:698:GLU:HA	10:B:701:ILE:HD11	2.00	0.43
11:C:127:ARG:HB3	11:C:129:ILE:HG12	2.00	0.43
16:H:110:ASP:O	16:H:129:TYR:N	2.51	0.43
27:W:176:MET:HA	27:W:179:ILE:HG22	1.99	0.43
9:A:243:PRO:HB2	9:A:245:PRO:HD2	2.00	0.43
9:A:1151:GLU:OE2	17:I:42:LEU:HB2	2.19	0.43
10:B:521:LEU:O	10:B:540:SER:N	2.50	0.43
10:B:1060:ARG:NH2	11:C:199:LYS:O	2.52	0.43
11:C:82:TYR:HB3	11:C:84:ARG:HH12	1.84	0.43
1:0:259:ARG:HH22	1:0:397:THR:HB	1.83	0.43
5:4:212:VAL:N	5:4:234:VAL:O	2.52	0.43
9:A:949:ASP:OD1	9:A:949:ASP:N	2.52	0.43
10:B:1161:HIS:HE1	10:B:1193:GLN:HE21	1.67	0.43
11:C:238:ILE:HB	11:C:242:GLN:HB2	2.01	0.43
16:H:26:ILE:HG13	16:H:42:ILE:HD12	2.00	0.43
18:J:6:ARG:HA	18:J:13:VAL:HA	2.00	0.43
24:R:94:LYS:HB2	24:R:107:LEU:HB3	2.00	0.43
27:W:59:ALA:CA	27:W:62:ARG:HH11	2.32	0.43
29:Z:4:UNK:HA	29:Z:14:UNK:HA	2.00	0.43
2:1:17:ALA:N	2:1:28:THR:O	2.49	0.43
8:7:372:LYS:NZ	8:7:536:TYR:HB2	2.33	0.43
9:A:145:LYS:HZ1	9:A:149:GLU:HG3	1.84	0.43
9:A:1191:TRP:NE1	9:A:1256:GLU:OE1	2.52	0.43
10:B:784:ASN:OD1	10:B:784:ASN:N	2.43	0.43
10:B:848:ARG:HH22	10:B:996:ARG:NH1	2.16	0.43
11:C:124:LEU:HB3	11:C:127:ARG:H	1.83	0.43
26:V:62:VAL:HG22	26:V:85:VAL:HG22	2.01	0.43
26:V:87:VAL:O	26:V:104:SER:N	2.51	0.43
28:X:268:LEU:O	28:X:270:GLN:NE2	2.52	0.43
1:0:364:LYS:HZ3	1:0:370:GLU:HA	1.84	0.43
1:0:440:LEU:HB2	1:0:441:ASP:H	1.72	0.43
9:A:540:PHE:HB3	9:A:571:LEU:HD23	2.01	0.43
9:A:567:LYS:HA	9:A:568:PRO:HA	1.92	0.43
10:B:355:ILE:HA	10:B:359:GLU:HG2	2.01	0.43
9:A:452:LYS:HB2	9:A:452:LYS:NZ	2.34	0.42
11:C:249:ASP:OD1	11:C:249:ASP:N	2.52	0.42
23:Q:373:TYR:HB3	24:R:70:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:U:255:LYS:NZ	31:T:61:DT:H3'	2.34	0.42
9:A:198:GLU:HB3	9:A:200:ARG:NH1	2.33	0.42
10:B:761:HIS:HB2	10:B:1024:ALA:HB2	2.01	0.42
10:B:1037:LEU:HD21	18:J:44:TYR:HD1	1.84	0.42
18:J:28:ASP:OD1	18:J:28:ASP:N	2.52	0.42
21:M:129:ALA:O	21:M:133:ILE:N	2.46	0.42
29:Z:30:UNK:N	29:Z:42:UNK:O	2.52	0.42
1:0:74:ARG:HG2	1:0:78:GLU:OE2	2.19	0.42
2:1:15:ILE:HG21	2:1:30:ARG:HH11	1.85	0.42
4:3:28:PHE:CB	4:3:37:ARG:HH11	2.33	0.42
4:3:29:LEU:N	4:3:38:ILE:O	2.52	0.42
9:A:1144:LYS:HB3	9:A:1268:LEU:HB3	2.01	0.42
9:A:1290:LYS:HE3	9:A:1298:TYR:HB3	2.01	0.42
10:B:125:SER:HA	10:B:172:ILE:HG12	2.01	0.42
10:B:341:LEU:H	10:B:341:LEU:HG	1.70	0.42
10:B:969:ARG:NH1	11:C:59:ALA:HB1	2.35	0.42
12:D:174:PRO:HA	12:D:177:VAL:HG22	2.01	0.42
13:E:62:ALA:HB3	13:E:78:LEU:HB3	2.01	0.42
19:K:65:HIS:HD2	19:K:67:PHE:HB2	1.84	0.42
27:W:137:VAL:HG23	27:W:138:GLN:HE21	1.84	0.42
7:6:129:THR:HB	7:6:234:ILE:HA	2.00	0.42
8:7:589:GLN:HB3	8:7:748:LEU:HD13	2.01	0.42
8:7:663:ASP:OD2	8:7:693:ALA:HB2	2.20	0.42
9:A:198:GLU:OE1	9:A:200:ARG:NH2	2.41	0.42
9:A:381:THR:HG23	9:A:383:TYR:H	1.84	0.42
9:A:592:ASP:OD2	9:A:604:GLY:N	2.53	0.42
9:A:635:ARG:HA	9:A:635:ARG:HD3	1.87	0.42
10:B:653:VAL:HB	10:B:689:LEU:HD13	2.00	0.42
10:B:1100:ASP:O	10:B:1122:ARG:NH2	2.48	0.42
11:C:81:GLU:OE2	11:C:94:LYS:HB3	2.18	0.42
28:X:193:LEU:HD23	28:X:196:LEU:HD12	2.01	0.42
28:X:209:ASP:OD1	28:X:209:ASP:N	2.49	0.42
9:A:443:LEU:HD23	9:A:443:LEU:HA	1.86	0.42
9:A:881:GLN:NE2	9:A:959:ASN:OD1	2.45	0.42
9:A:1122:PRO:HD3	9:A:1323:ASP:OD2	2.20	0.42
10:B:764:SER:HA	10:B:767:ASN:HD22	1.85	0.42
20:L:53:HIS:C	20:L:54:ARG:HH11	2.19	0.42
22:O:116:PHE:HB2	22:O:120:LYS:HB2	2.01	0.42
23:Q:120:LYS:HG2	24:R:132:GLU:HG2	2.02	0.42
25:U:269:ILE:HD13	26:V:108:VAL:HG21	2.01	0.42
27:W:123:MET:HG3	27:W:157:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:63:LEU:HD21	4:3:68:PHE:HZ	1.84	0.42
8:7:490:VAL:HG12	8:7:527:LEU:HD13	2.01	0.42
10:B:122:LEU:O	10:B:206:ASN:N	2.50	0.42
10:B:899:ILE:C	20:L:58:LYS:HZ3	2.22	0.42
11:C:254:LYS:HE3	11:C:254:LYS:HB2	1.91	0.42
11:C:258:ILE:HG23	19:K:19:LEU:HD11	2.01	0.42
15:G:84:GLY:HA2	15:G:146:LYS:HZ3	1.83	0.42
27:W:9:VAL:HG22	27:W:189:ILE:HD13	2.01	0.42
8:7:494:PRO:HD3	8:7:527:LEU:HD21	2.02	0.42
9:A:350:ARG:NE	9:A:486:GLU:OE1	2.53	0.42
9:A:824:LEU:HD11	10:B:765:PRO:HB3	2.01	0.42
9:A:1349:TYR:OH	13:E:203:GLU:OE2	2.22	0.42
10:B:1133:MET:HA	10:B:1136:ASP:OD2	2.19	0.42
10:B:1156:ASP:OD2	10:B:1198:TYR:N	2.52	0.42
14:F:123:LYS:HD2	14:F:123:LYS:HA	1.89	0.42
16:H:23:VAL:HA	16:H:43:ASN:HA	2.01	0.42
16:H:81:PRO:HA	16:H:82:PRO:HD3	1.94	0.42
2:1:29:TRP:HB3	2:1:38:HIS:HB2	2.02	0.42
4:3:65:LYS:NZ	15:G:165:GLU:HA	2.35	0.42
9:A:871:ASP:OD2	9:A:873:MET:HB2	2.19	0.42
10:B:603:LEU:HB3	10:B:608:ASP:HB2	2.02	0.42
10:B:852:ARG:NH2	20:L:70:ARG:O	2.44	0.42
16:H:25:ARG:HG2	16:H:27:GLU:OE2	2.19	0.42
21:M:316:LEU:HD12	21:M:316:LEU:HA	1.93	0.42
22:O:108:GLU:O	22:O:138:LYS:NZ	2.36	0.42
22:O:114:LEU:HD12	22:O:122:VAL:HB	2.02	0.42
22:O:169:PRO:HD2	22:O:240:MET:OXT	2.19	0.42
8:7:462:ASN:HB3	8:7:463:UNK:H	1.47	0.42
9:A:24:PRO:HB2	9:A:28:ARG:NH2	2.34	0.42
9:A:88:LYS:HD3	9:A:89:PRO:HD2	2.01	0.42
11:C:185:LYS:HE2	11:C:213:PRO:HB3	2.02	0.42
21:M:215:ARG:HA	21:M:215:ARG:HD3	1.77	0.42
23:Q:123:SER:O	23:Q:125:LYS:N	2.53	0.42
28:X:277:LYS:HA	28:X:277:LYS:HD3	1.90	0.42
9:A:898:ARG:NH2	9:A:900:ASP:OD1	2.53	0.42
9:A:991:LYS:NZ	9:A:994:GLN:HE22	2.18	0.42
9:A:1217:LYS:HZ1	9:A:1226:VAL:H	1.67	0.42
10:B:890:TYR:OH	10:B:936:ASP:OD2	2.37	0.42
10:B:977:GLY:HA3	10:B:1099:VAL:HB	2.02	0.42
12:D:67:ARG:NH1	12:D:130:LEU:HD21	2.28	0.42
12:D:161:GLY:HA2	12:D:164:ILE:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:W:69:ILE:HA	27:W:87:TYR:HA	2.01	0.42
1:O:487:LEU:HD22	1:O:489:LYS:NZ	2.35	0.41
10:B:806:THR:HG23	10:B:1045:SER:HA	2.02	0.41
11:C:46:ILE:HA	11:C:159:ALA:HA	2.02	0.41
13:E:74:ASP:N	13:E:74:ASP:OD1	2.51	0.41
21:M:34:ILE:H	21:M:34:ILE:HG13	1.79	0.41
9:A:66:LYS:HZ3	21:M:20:ILE:HG12	1.85	0.41
9:A:346:ASP:HB3	10:B:1107:ALA:HA	2.01	0.41
11:C:221:TYR:H	11:C:222:LYS:HE2	1.85	0.41
21:M:191:GLU:O	21:M:194:SER:OG	2.36	0.41
1:O:594:ARG:HH12	7:6:242:THR:HA	1.85	0.41
8:7:510:LYS:NZ	8:7:530:LEU:O	2.53	0.41
9:A:1204:ASP:OD2	9:A:1205:LYS:HG3	2.21	0.41
10:B:356:LEU:HA	10:B:360:PHE:HB3	2.02	0.41
10:B:496:ARG:HE	10:B:539:LEU:HB2	1.85	0.41
15:G:14:HIS:HB3	15:G:17:PHE:HD2	1.86	0.41
15:G:37:SER:OG	15:G:38:CYS:N	2.53	0.41
1:O:234:PHE:HD2	1:O:458:ILE:HG12	1.84	0.41
2:1:118:GLU:HG2	2:1:121:ARG:HH21	1.85	0.41
8:7:596:GLN:HE22	8:7:747:ASN:HB2	1.85	0.41
9:A:886:ILE:HD11	9:A:1298:TYR:HE1	1.86	0.41
9:A:1201:ALA:HA	9:A:1204:ASP:HB3	2.03	0.41
12:D:56:ARG:NH2	12:D:154:PHE:O	2.54	0.41
18:J:24:LEU:HD22	18:J:28:ASP:OD2	2.21	0.41
24:R:268:MET:H	24:R:268:MET:HG2	1.63	0.41
26:V:109:ASP:OD1	26:V:109:ASP:N	2.51	0.41
27:W:9:VAL:HG13	27:W:95:ILE:HD11	2.03	0.41
7:6:138:GLU:OE1	7:6:145:ARG:NH2	2.53	0.41
8:7:435:UNK:HA	8:7:452:LEU:H	1.85	0.41
8:7:550:ALA:HB1	8:7:703:ALA:HB2	2.01	0.41
8:7:582:ILE:HG21	8:7:614:ALA:HB1	2.02	0.41
9:A:407:ARG:NH1	9:A:413:ILE:HD11	2.34	0.41
9:A:547:LEU:HD23	9:A:547:LEU:HA	1.90	0.41
10:B:260:GLY:O	10:B:267:ARG:NH2	2.47	0.41
10:B:310:MET:HB2	10:B:390:LEU:HD11	2.03	0.41
10:B:796:LEU:HB3	10:B:799:PRO:HG3	2.02	0.41
12:D:163:VAL:HA	12:D:166:LEU:HB2	2.02	0.41
14:F:79:ARG:HA	14:F:144:GLU:OE2	2.20	0.41
23:Q:103:LEU:N	24:R:93:GLY:O	2.53	0.41
9:A:555:ASP:OD1	9:A:555:ASP:N	2.53	0.41
10:B:336:ARG:HD2	10:B:348:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:400:HIS:CE1	10:B:403:LYS:HZ3	2.38	0.41
11:C:28:ALA:O	11:C:32:SER:N	2.51	0.41
15:G:40:GLY:HA2	15:G:157:ILE:HD11	2.02	0.41
27:W:4:PRO:HD2	27:W:7:ASP:OD2	2.21	0.41
2:1:279:LYS:HD3	2:1:279:LYS:HA	1.90	0.41
9:A:369:SER:OG	19:K:2:ASN:ND2	2.54	0.41
10:B:486:TYR:HD1	10:B:486:TYR:HA	1.76	0.41
10:B:898:LEU:HB2	20:L:58:LYS:NZ	2.36	0.41
10:B:1059:LEU:HD12	10:B:1059:LEU:HA	1.87	0.41
20:L:55:ILE:H	20:L:55:ILE:HG12	1.59	0.41
21:M:199:LYS:O	21:M:201:LYS:N	2.52	0.41
27:W:90:LYS:HE2	27:W:92:PRO:HG2	2.02	0.41
30:N:27:DA:H2'	30:N:28:DA:C4	2.55	0.41
1:0:73:SER:HB3	1:0:78:GLU:HB2	2.01	0.41
9:A:452:LYS:HZ3	10:B:1140:ALA:CB	2.34	0.41
10:B:137:TYR:HB3	10:B:148:LYS:HA	2.03	0.41
12:D:24:ALA:HB2	15:G:83:LYS:HD2	2.02	0.41
27:W:179:ILE:HG13	27:W:183:ILE:HG23	2.02	0.41
7:6:234:ILE:HD12	7:6:263:VAL:HG22	2.02	0.41
8:7:693:ALA:HA	8:7:695:ARG:HH21	1.85	0.41
9:A:1263:ILE:O	9:A:1267:MET:N	2.48	0.41
9:A:1277:GLU:O	9:A:1312:ASN:ND2	2.50	0.41
9:A:1329:THR:HG22	9:A:1331:SER:H	1.85	0.41
9:A:1443:VAL:HG12	15:G:61:ILE:HD12	2.02	0.41
10:B:89:GLU:O	10:B:135:ARG:N	2.47	0.41
10:B:121:ASN:OD1	10:B:121:ASN:N	2.54	0.41
10:B:234:ILE:HG12	10:B:257:LYS:HB3	2.03	0.41
10:B:582:VAL:HA	10:B:626:ILE:HB	2.02	0.41
11:C:116:LYS:HZ3	11:C:140:ASN:HA	1.84	0.41
13:E:88:VAL:HB	13:E:116:ILE:HG23	2.02	0.41
15:G:1:MET:N	15:G:80:LYS:O	2.41	0.41
16:H:92:ASP:N	16:H:92:ASP:OD1	2.52	0.41
19:K:102:LYS:HG2	19:K:106:GLU:OE2	2.20	0.41
21:M:84:ASN:HD21	21:M:86:LEU:HD12	1.85	0.41
21:M:125:GLU:H	21:M:125:GLU:HG3	1.69	0.41
21:M:171:ILE:H	21:M:171:ILE:HG13	1.64	0.41
21:M:267:LYS:HD2	21:M:267:LYS:HA	1.75	0.41
22:O:68:GLN:HA	22:O:127:LYS:HZ2	1.85	0.41
23:Q:374:VAL:HA	23:Q:388:PRO:HA	2.03	0.41
1:0:251:ASP:OD1	1:0:436:ARG:NE	2.54	0.41
2:1:33:ASP:OD1	2:1:33:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:188:ASN:HB3	7:6:191:ASP:OD2	2.21	0.41
9:A:62:ASP:O	9:A:64:ASN:N	2.54	0.41
9:A:332:LYS:HD3	9:A:332:LYS:HA	1.90	0.41
9:A:353:ILE:H	9:A:353:ILE:HG13	1.54	0.41
9:A:1420:ASP:OD1	9:A:1420:ASP:N	2.54	0.41
10:B:187:SER:HA	10:B:190:TYR:HB2	2.03	0.41
12:D:168:LYS:HA	12:D:168:LYS:HD3	1.86	0.41
27:W:90:LYS:HA	27:W:90:LYS:HD2	1.83	0.41
1:0:77:SER:HB3	2:1:337:UNK:HA	2.03	0.40
2:1:46:ASP:OD2	2:1:65:LYS:HA	2.22	0.40
6:5:32:LEU:N	6:5:41:LEU:O	2.53	0.40
7:6:352:CYS:HB3	7:6:366:CYS:HB3	2.03	0.40
8:7:648:GLN:HE21	8:7:648:GLN:HB2	1.70	0.40
9:A:1257:ASP:OD1	9:A:1257:ASP:N	2.55	0.40
10:B:549:THR:OG1	10:B:628:THR:OG1	2.39	0.40
10:B:919:SER:HA	10:B:920:PRO:HD3	1.97	0.40
11:C:166:GLU:HA	19:K:6:ARG:HB3	2.03	0.40
19:K:84:LYS:H	19:K:84:LYS:HG3	1.52	0.40
10:B:179:CYS:SG	10:B:180:TYR:N	2.94	0.40
10:B:709:ASP:OD1	10:B:709:ASP:N	2.55	0.40
16:H:83:GLN:N	16:H:86:ASP:OD2	2.50	0.40
27:W:18:ARG:NH2	28:X:249:GLY:H	2.19	0.40
8:7:578:MET:HG2	8:7:715:GLU:OE2	2.21	0.40
9:A:36:ARG:H	9:A:36:ARG:HE	1.70	0.40
9:A:203:SER:HB2	9:A:206:GLU:HG3	2.02	0.40
9:A:290:GLU:HA	9:A:293:GLU:HB3	2.03	0.40
9:A:1005:GLU:O	9:A:1009:ASN:N	2.55	0.40
10:B:58:THR:HA	10:B:61:ASP:OD2	2.21	0.40
10:B:193:LYS:HB3	10:B:787:VAL:HG21	2.03	0.40
13:E:41:ASP:OD1	13:E:41:ASP:N	2.52	0.40
25:U:19:ASN:HA	25:U:22:ARG:HH12	1.87	0.40
4:3:29:LEU:HG	4:3:40:GLU:OE2	2.21	0.40
9:A:670:ILE:HD13	9:A:805:LEU:HD21	2.04	0.40
9:A:830:LYS:O	9:A:834:THR:OG1	2.35	0.40
10:B:568:ASP:OD1	10:B:568:ASP:N	2.54	0.40
10:B:861:ASP:OD1	10:B:862:GLN:N	2.53	0.40
10:B:929:THR:O	10:B:929:THR:OG1	2.34	0.40
11:C:185:LYS:HA	11:C:187:LYS:NZ	2.37	0.40
19:K:17:SER:H	19:K:20:LYS:HZ3	1.69	0.40
23:Q:381:ASP:OD1	23:Q:382:GLY:N	2.54	0.40
27:W:98:ILE:HG23	28:X:263:TRP:HH2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:278:LEU:O	28:X:282:GLY:N	2.44	0.40
30:N:26:DT:H2'	30:N:27:DA:C8	2.57	0.40
1:0:114:LEU:HD21	1:0:196:VAL:HG21	2.04	0.40
9:A:1003:LYS:HB3	9:A:1003:LYS:HE2	1.85	0.40
9:A:1031:VAL:O	9:A:1036:ARG:N	2.52	0.40
10:B:542:MET:HG3	10:B:747:MET:HB3	2.04	0.40
21:M:295:ALA:HA	21:M:298:VAL:HG12	2.03	0.40
23:Q:114:MET:HB3	24:R:136:THR:HB	2.03	0.40
24:R:257:GLU:HB3	24:R:258:THR:H	1.73	0.40
27:W:183:ILE:HA	27:W:186:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	659/778 (85%)	578 (88%)	71 (11%)	10 (2%)	8	40
2	1	316/641 (49%)	293 (93%)	16 (5%)	7 (2%)	5	29
3	2	284/462 (62%)	263 (93%)	18 (6%)	3 (1%)	12	47
4	3	136/321 (42%)	114 (84%)	20 (15%)	2 (2%)	8	40
5	4	274/338 (81%)	244 (89%)	23 (8%)	7 (3%)	4	25
6	5	64/72 (89%)	57 (89%)	6 (9%)	1 (2%)	8	38
7	6	289/461 (63%)	257 (89%)	27 (9%)	5 (2%)	7	37
8	7	361/843 (43%)	330 (91%)	23 (6%)	8 (2%)	5	29
9	A	1386/1733 (80%)	1253 (90%)	112 (8%)	21 (2%)	8	40
10	B	1136/1224 (93%)	1034 (91%)	87 (8%)	15 (1%)	10	43
11	C	260/318 (82%)	235 (90%)	21 (8%)	4 (2%)	8	40
12	D	153/221 (69%)	143 (94%)	9 (6%)	1 (1%)	19	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	E	211/215 (98%)	194 (92%)	15 (7%)	2 (1%)	14	51
14	F	81/155 (52%)	71 (88%)	9 (11%)	1 (1%)	11	44
15	G	169/171 (99%)	148 (88%)	20 (12%)	1 (1%)	22	60
16	H	132/146 (90%)	110 (83%)	21 (16%)	1 (1%)	16	55
17	I	114/122 (93%)	91 (80%)	20 (18%)	3 (3%)	4	25
18	J	63/70 (90%)	55 (87%)	7 (11%)	1 (2%)	8	38
19	K	110/120 (92%)	105 (96%)	5 (4%)	0	100	100
20	L	43/70 (61%)	36 (84%)	4 (9%)	3 (7%)	1	11
21	M	273/345 (79%)	238 (87%)	25 (9%)	10 (4%)	2	20
22	O	178/240 (74%)	165 (93%)	12 (7%)	1 (1%)	22	60
23	Q	140/735 (19%)	124 (89%)	12 (9%)	4 (3%)	3	23
24	R	176/400 (44%)	150 (85%)	24 (14%)	2 (1%)	12	47
25	U	88/171 (52%)	81 (92%)	5 (6%)	2 (2%)	5	28
26	V	96/122 (79%)	94 (98%)	1 (1%)	1 (1%)	13	49
27	W	196/332 (59%)	181 (92%)	12 (6%)	3 (2%)	8	40
28	X	158/328 (48%)	127 (80%)	26 (16%)	5 (3%)	3	21
All	All	7546/11154 (68%)	6771 (90%)	651 (9%)	124 (2%)	10	38

All (124) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	275	PRO
5	4	87	TYR
5	4	88	PRO
5	4	263	VAL
9	A	47	ARG
21	M	269	ILE
23	Q	127	ILE
24	R	324	GLN
27	W	77	PRO
1	0	573	THR
3	2	39	LEU
4	3	124	ILE
7	6	244	PRO
9	A	474	VAL
10	B	364	ILE

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Mol	Chain	Res	Type
10	B	1046	PRO
20	L	50	ASP
21	M	158	HIS
21	M	268	GLU
23	Q	406	ILE
24	R	215	VAL
25	U	255	LYS
28	X	206	SER
1	0	155	LEU
1	0	277	VAL
1	0	565	LYS
2	1	74	ASP
2	1	277	ASN
2	1	543	PRO
5	4	115	TYR
5	4	305	CYS
7	6	451	CYS
8	7	550	ALA
9	A	67	CYS
9	A	167	CYS
9	A	286	HIS
9	A	407	ARG
9	A	449	SER
10	B	277	LYS
10	B	866	TYR
10	B	933	SER
11	C	90	ASP
13	E	86	PRO
16	H	83	GLN
17	I	115	LYS
18	J	3	VAL
21	M	273	SER
28	X	152	SER
28	X	216	GLN
28	X	251	ASN
1	0	473	LEU
1	0	611	ASP
2	1	25	ALA
5	4	240	SER
7	6	267	SER
8	7	495	ALA
8	7	655	SER

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Mol	Chain	Res	Type
8	7	696	ARG
8	7	741	GLY
9	A	63	ARG
9	A	567	LYS
9	A	569	LYS
9	A	853	ASP
9	A	905	ASP
9	A	1221	LYS
10	B	792	MET
10	B	830	TYR
10	B	868	MET
10	B	1165	ILE
15	G	50	ASP
17	I	9	ASP
17	I	47	GLU
20	L	45	ALA
21	M	163	LEU
21	M	164	LYS
21	M	200	THR
23	Q	367	ALA
23	Q	370	SER
25	U	264	ASP
27	W	412	GLU
1	0	471	ARG
1	0	606	VAL
3	2	451	VAL
7	6	356	VAL
8	7	489	GLU
8	7	494	PRO
8	7	667	ALA
9	A	35	ILE
9	A	50	ILE
9	A	68	GLN
9	A	958	VAL
10	B	124	TYR
10	B	323	VAL
11	C	174	ALA
12	D	156	ASP
13	E	124	VAL
20	L	59	ALA
21	M	168	MET
21	M	325	ASP

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Mol	Chain	Res	Type
22	O	147	GLY
26	V	6	TYR
1	0	34	VAL
1	0	432	ASN
3	2	262	LYS
6	5	35	LEU
9	A	599	SER
9	A	1107	VAL
10	B	343	ILE
10	B	705	MET
14	F	73	ALA
11	C	182	PRO
21	M	304	VAL
28	X	232	VAL
2	1	542	LEU
4	3	23	SER
9	A	61	ILE
9	A	948	VAL
10	B	292	ILE
11	C	236	GLY
2	1	274	VAL
7	6	332	THR
27	W	76	PRO
5	4	299	ILE
10	B	1012	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	
1	0	413/676 (61%)	396 (96%)	17 (4%)	26	47
2	1	179/341 (52%)	174 (97%)	5 (3%)	38	57
3	2	53/273 (19%)	52 (98%)	1 (2%)	52	69
4	3	53/303 (18%)	50 (94%)	3 (6%)	17	38
5	4	4/276 (1%)	4 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	5	53/66 (80%)	53 (100%)	0	100	100
7	6	173/378 (46%)	172 (99%)	1 (1%)	84	88
8	7	315/695 (45%)	304 (96%)	11 (4%)	31	51
9	A	1221/1520 (80%)	1160 (95%)	61 (5%)	20	41
10	B	1000/1061 (94%)	948 (95%)	52 (5%)	19	40
11	C	230/274 (84%)	217 (94%)	13 (6%)	17	38
12	D	139/200 (70%)	132 (95%)	7 (5%)	20	41
13	E	195/197 (99%)	190 (97%)	5 (3%)	41	59
14	F	73/137 (53%)	69 (94%)	4 (6%)	18	39
15	G	152/152 (100%)	145 (95%)	7 (5%)	23	44
16	H	119/128 (93%)	114 (96%)	5 (4%)	25	46
17	I	110/116 (95%)	105 (96%)	5 (4%)	23	45
18	J	60/65 (92%)	56 (93%)	4 (7%)	13	34
19	K	97/102 (95%)	95 (98%)	2 (2%)	48	66
20	L	40/57 (70%)	33 (82%)	7 (18%)	1	8
21	M	245/299 (82%)	225 (92%)	20 (8%)	9	28
22	O	152/205 (74%)	150 (99%)	2 (1%)	65	77
23	Q	109/641 (17%)	99 (91%)	10 (9%)	7	23
24	R	107/363 (30%)	102 (95%)	5 (5%)	22	44
25	U	84/154 (54%)	81 (96%)	3 (4%)	30	50
26	V	90/108 (83%)	86 (96%)	4 (4%)	24	45
27	W	161/244 (66%)	157 (98%)	4 (2%)	42	61
28	X	62/295 (21%)	62 (100%)	0	100	100
All	All	5689/9326 (61%)	5431 (96%)	258 (4%)	26	45

All (258) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	115	CYS
1	0	165	ILE
1	0	191	CYS
1	0	199	MET
1	0	254	THR
1	0	367	THR

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Mol	Chain	Res	Type
1	0	375	ARG
1	0	410	SER
1	0	411	THR
1	0	416	PHE
1	0	440	LEU
1	0	466	LEU
1	0	522	TYR
1	0	578	GLU
1	0	619	THR
1	0	647	ARG
1	0	678	VAL
2	1	15	ILE
2	1	22	VAL
2	1	32	THR
2	1	71	LYS
2	1	276	LYS
3	2	481	LEU
4	3	47	PHE
4	3	59	CYS
4	3	72	ILE
7	6	291	LEU
8	7	373	MET
8	7	492	VAL
8	7	517	LEU
8	7	586	THR
8	7	622	MET
8	7	648	GLN
8	7	681	ARG
8	7	695	ARG
8	7	701	PHE
8	7	709	VAL
8	7	737	THR
9	A	26	GLU
9	A	36	ARG
9	A	69	THR
9	A	70	CYS
9	A	77	CYS
9	A	81	PHE
9	A	147	VAL
9	A	182	VAL
9	A	245	PRO
9	A	260	ASP

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Mol	Chain	Res	Type
9	A	263	THR
9	A	270	LEU
9	A	308	ILE
9	A	351	THR
9	A	353	ILE
9	A	358	ASN
9	A	381	THR
9	A	385	ILE
9	A	386	ASP
9	A	444	PHE
9	A	450	LEU
9	A	452	LYS
9	A	468	PHE
9	A	470	LEU
9	A	475	THR
9	A	476	SER
9	A	489	LEU
9	A	526	ASP
9	A	557	ASP
9	A	573	SER
9	A	592	ASP
9	A	629	LEU
9	A	658	LEU
9	A	756	ILE
9	A	786	HIS
9	A	834	THR
9	A	862	ASN
9	A	884	ASP
9	A	906	HIS
9	A	913	LEU
9	A	960	ILE
9	A	976	THR
9	A	982	THR
9	A	985	ASP
9	A	1058	VAL
9	A	1110	ASN
9	A	1111	MET
9	A	1144	LYS
9	A	1159	ARG
9	A	1195	LEU
9	A	1223	ASP
9	A	1259	MET

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Mol	Chain	Res	Type
9	A	1276	VAL
9	A	1309	ASP
9	A	1311	VAL
9	A	1330	ASN
9	A	1334	ASP
9	A	1341	ILE
9	A	1364	ASN
9	A	1384	VAL
9	A	1450	LEU
10	B	59	LEU
10	B	69	LEU
10	B	86	ARG
10	B	97	VAL
10	B	121	ASN
10	B	199	MET
10	B	217	ARG
10	B	276	ILE
10	B	306	ASN
10	B	309	GLN
10	B	341	LEU
10	B	398	ARG
10	B	425	THR
10	B	484	ASN
10	B	486	TYR
10	B	487	THR
10	B	527	THR
10	B	568	ASP
10	B	602	THR
10	B	604	ARG
10	B	609	ILE
10	B	616	ILE
10	B	624	LEU
10	B	653	VAL
10	B	664	THR
10	B	668	ASP
10	B	690	VAL
10	B	755	ILE
10	B	760	ASP
10	B	806	THR
10	B	854	LEU
10	B	891	ASP
10	B	941	LEU

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Mol	Chain	Res	Type
10	B	950	ASP
10	B	953	LEU
10	B	959	ASP
10	B	964	VAL
10	B	1007	VAL
10	B	1009	ASP
10	B	1022	THR
10	B	1040	ASN
10	B	1048	THR
10	B	1090	THR
10	B	1099	VAL
10	B	1103	ILE
10	B	1147	LEU
10	B	1160	VAL
10	B	1163	CYS
10	B	1170	THR
10	B	1175	LEU
10	B	1185	CYS
10	B	1194	ILE
11	C	25	VAL
11	C	43	THR
11	C	56	THR
11	C	81	GLU
11	C	83	SER
11	C	88	CYS
11	C	112	ASN
11	C	123	ASN
11	C	155	LEU
11	C	222	LYS
11	C	227	THR
11	C	249	ASP
11	C	263	THR
12	D	34	GLN
12	D	35	LEU
12	D	149	THR
12	D	153	ARG
12	D	157	GLN
12	D	165	GLN
12	D	218	GLU
13	E	41	ASP
13	E	74	ASP
13	E	148	GLU

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Mol	Chain	Res	Type
13	E	178	ILE
13	E	182	ASP
14	F	116	ASP
14	F	133	VAL
14	F	147	SER
14	F	153	VAL
15	G	26	LEU
15	G	53	ASN
15	G	62	LEU
15	G	67	SER
15	G	111	THR
15	G	138	THR
15	G	154	VAL
16	H	96	VAL
16	H	107	VAL
16	H	112	ILE
16	H	131	ASN
16	H	134	ASN
17	I	19	ASP
17	I	22	ASN
17	I	43	VAL
17	I	59	VAL
17	I	71	SER
18	J	2	ILE
18	J	8	PHE
18	J	28	ASP
18	J	46	CYS
19	K	31	VAL
19	K	85	ASP
20	L	31	CYS
20	L	40	LEU
20	L	43	THR
20	L	53	HIS
20	L	54	ARG
20	L	55	ILE
20	L	61	THR
21	M	36	GLU
21	M	43	VAL
21	M	88	ASP
21	M	120	ASP
21	M	123	ASP
21	M	124	ASN

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Mol	Chain	Res	Type
21	M	142	LEU
21	M	177	LEU
21	M	185	VAL
21	M	188	THR
21	M	196	ILE
21	M	198	VAL
21	M	199	LYS
21	M	203	PHE
21	M	267	LYS
21	M	269	ILE
21	M	275	ILE
21	M	279	VAL
21	M	304	VAL
21	M	321	ASP
22	O	95	ASN
22	O	124	THR
23	Q	109	GLU
23	Q	130	VAL
23	Q	135	LEU
23	Q	137	VAL
23	Q	334	VAL
23	Q	337	GLU
23	Q	350	TRP
23	Q	351	VAL
23	Q	386	MET
23	Q	392	VAL
24	R	73	LEU
24	R	92	LEU
24	R	94	LYS
24	R	108	LEU
24	R	128	VAL
25	U	21	VAL
25	U	253	ARG
25	U	266	VAL
26	V	9	LEU
26	V	56	THR
26	V	59	LYS
26	V	69	TYR
27	W	6	ASP
27	W	27	LEU
27	W	37	VAL
27	W	156	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	224	ASN
1	0	577	GLN
1	0	628	GLN
1	0	699	GLN
2	1	49	GLN
2	1	105	GLN
2	1	182	GLN
2	1	258	ASN
3	2	498	ASN
6	5	11	GLN
6	5	22	GLN
7	6	184	GLN
7	6	211	GLN
7	6	212	ASN
7	6	249	GLN
7	6	269	GLN
7	6	302	ASN
8	7	491	HIS
8	7	508	HIS
8	7	584	ASN
8	7	589	GLN
8	7	596	GLN
8	7	644	GLN
8	7	648	GLN
8	7	672	GLN
8	7	682	GLN
8	7	767	ASN
9	A	92	HIS
9	A	253	ASN
9	A	297	GLN
9	A	394	ASN
9	A	589	GLN
9	A	611	GLN
9	A	650	GLN
9	A	654	ASN
9	A	698	GLN
9	A	760	GLN
9	A	906	HIS
9	A	953	ASN
9	A	968	GLN
9	A	994	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	1203	ASN
9	A	1330	ASN
9	A	1432	GLN
10	B	47	GLN
10	B	325	GLN
10	B	433	GLN
10	B	657	HIS
10	B	767	ASN
10	B	770	GLN
10	B	842	ASN
10	B	843	GLN
10	B	862	GLN
10	B	1097	HIS
10	B	1112	GLN
10	B	1187	ASN
10	B	1193	GLN
11	C	73	GLN
11	C	102	GLN
11	C	195	GLN
11	C	206	ASN
11	C	231	ASN
12	D	34	GLN
12	D	157	GLN
12	D	165	GLN
12	D	216	ASN
13	E	61	GLN
13	E	63	ASN
15	G	24	GLN
15	G	96	GLN
16	H	83	GLN
17	I	12	ASN
17	I	22	ASN
17	I	51	ASN
17	I	116	ASN
18	J	53	HIS
19	K	2	ASN
19	K	29	ASN
19	K	65	HIS
19	K	92	ASN
19	K	96	ASN
19	K	110	ASN
19	K	112	GLN

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Mol	Chain	Res	Type
21	M	90	ASN
21	M	91	ASN
21	M	114	GLN
21	M	117	ASN
26	V	84	GLN
28	X	251	ASN
28	X	270	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 17 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	SF4	0	801	-	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	SF4	0	801	-	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	801	SF4	1	0

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
27	W	2
2	1	2
3	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	373:UNK	C	407:UNK	N	84.71
1	1	394:UNK	C	465:UNK	N	82.85
1	W	289:UNK	C	349:UNK	N	45.78
1	2	419:UNK	C	433:LEU	N	13.35
1	1	519:UNK	C	537:GLU	N	11.39

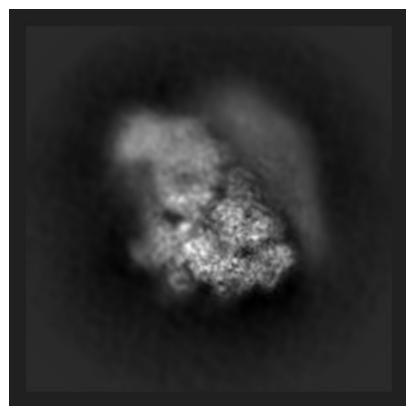
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0092. These allow visual inspection of the internal detail of the map and identification of artifacts.

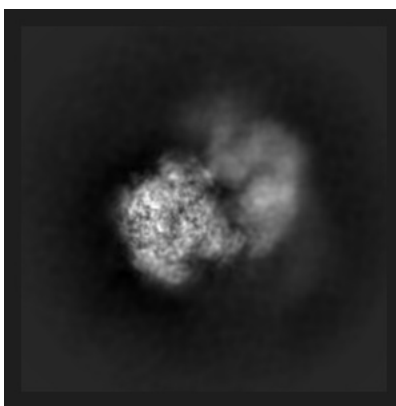
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

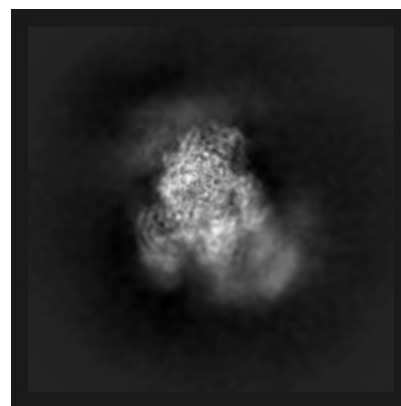
6.1.1 Primary map



X

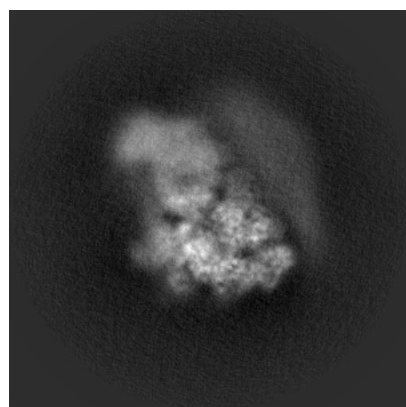


Y

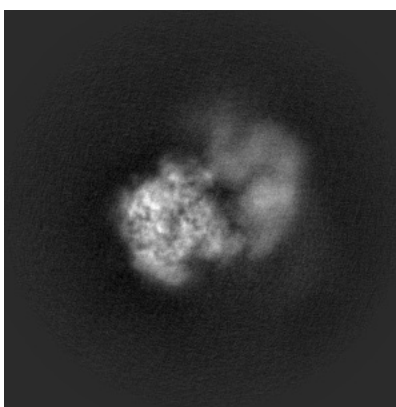


Z

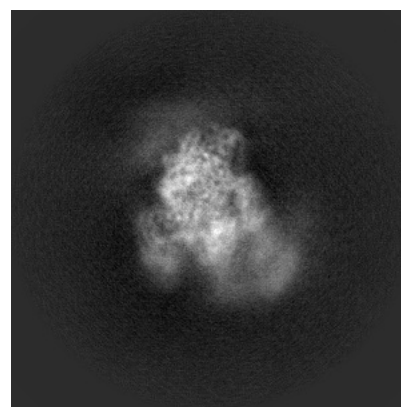
6.1.2 Raw map



X



Y

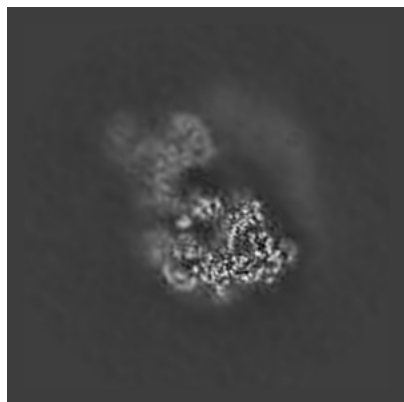


Z

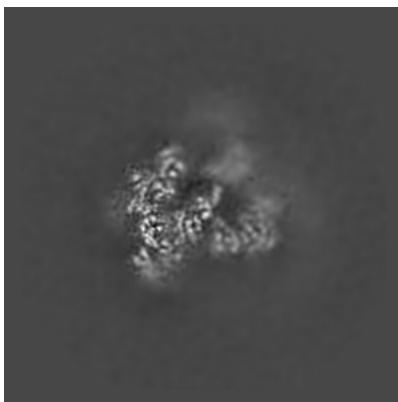
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

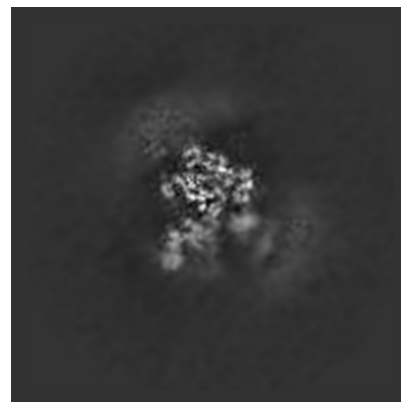
6.2.1 Primary map



X Index: 175

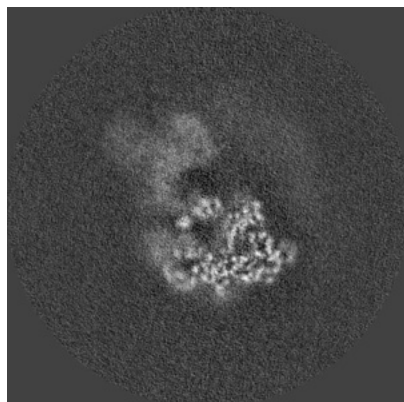


Y Index: 175

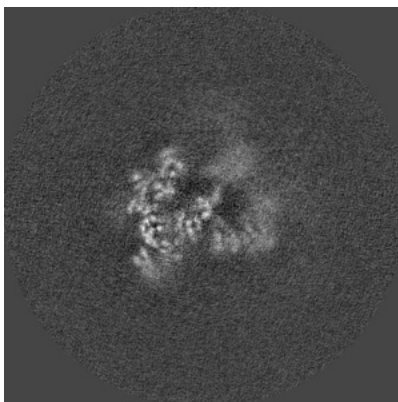


Z Index: 175

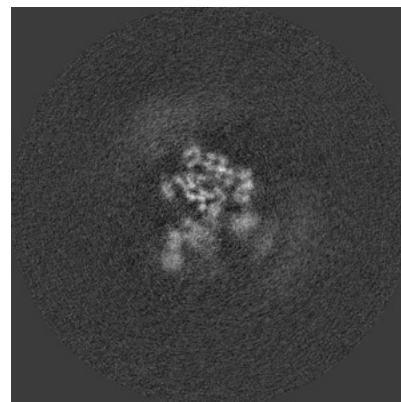
6.2.2 Raw map



X Index: 175



Y Index: 175

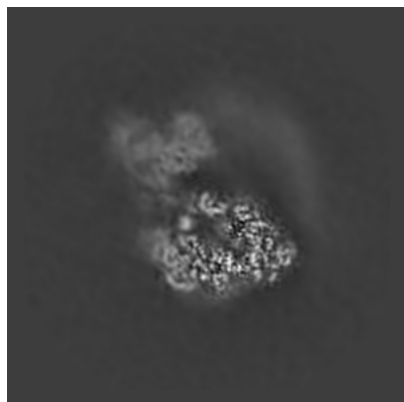


Z Index: 175

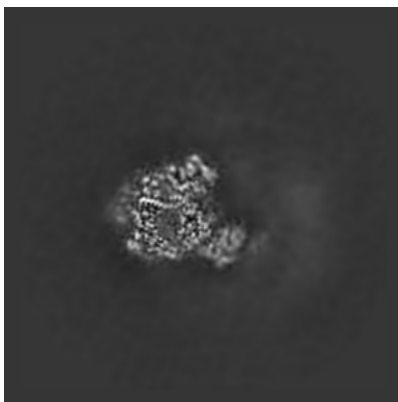
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

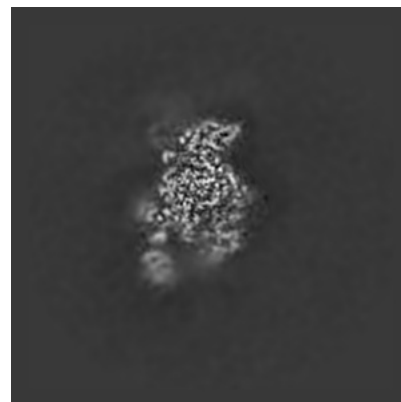
6.3.1 Primary map



X Index: 180

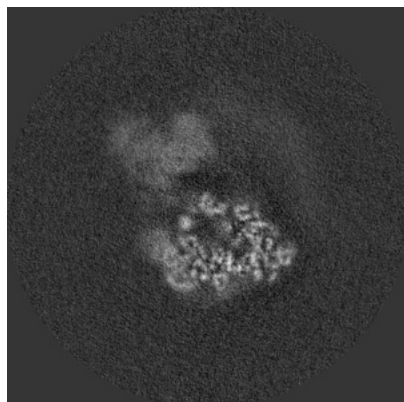


Y Index: 194

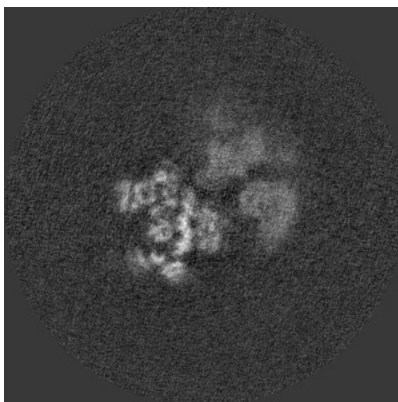


Z Index: 129

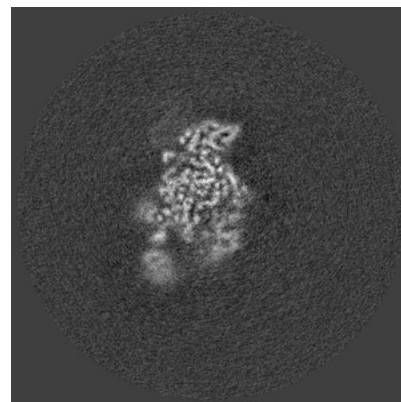
6.3.2 Raw map



X Index: 180



Y Index: 152

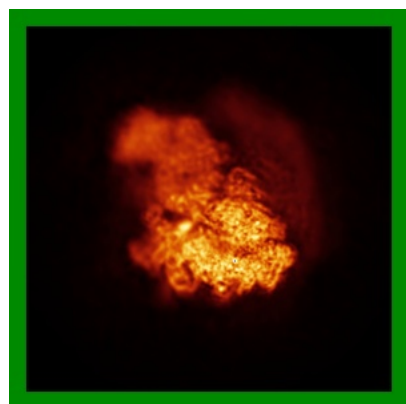


Z Index: 129

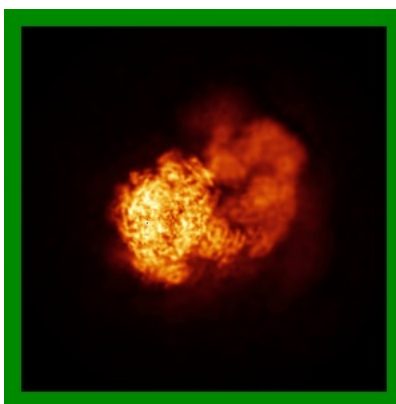
The images above show the largest variance slices of the map in three orthogonal directions.

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

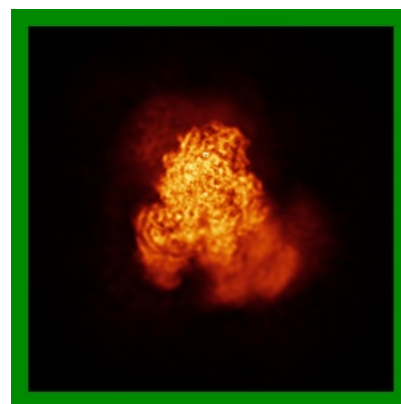
6.4.1 Primary map



X

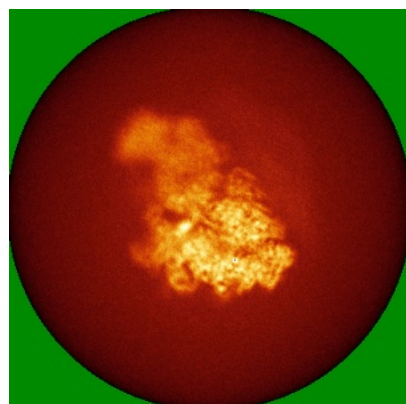


Y

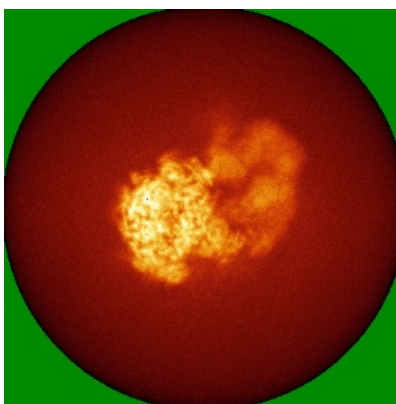


Z

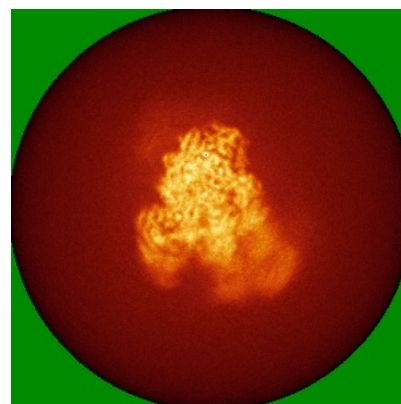
6.4.2 Raw map



X



Y

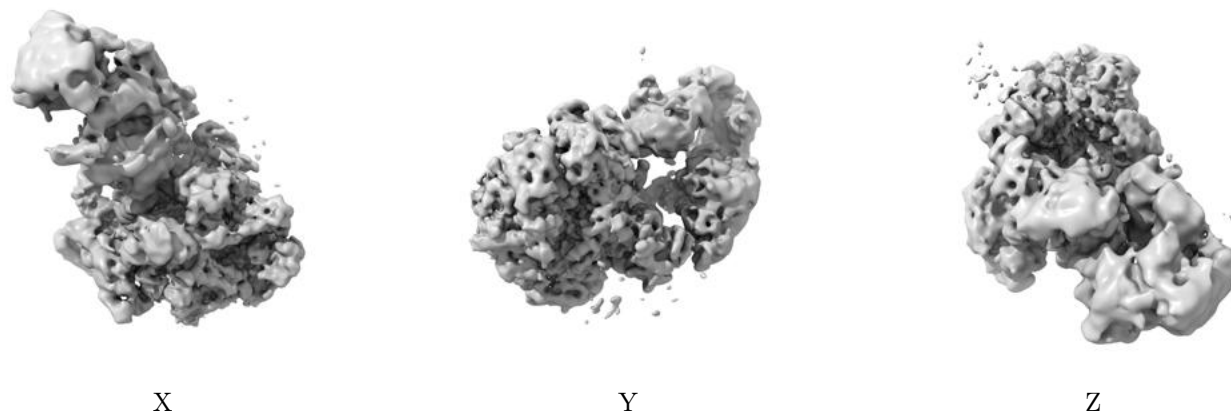


Z

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 0.0057. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

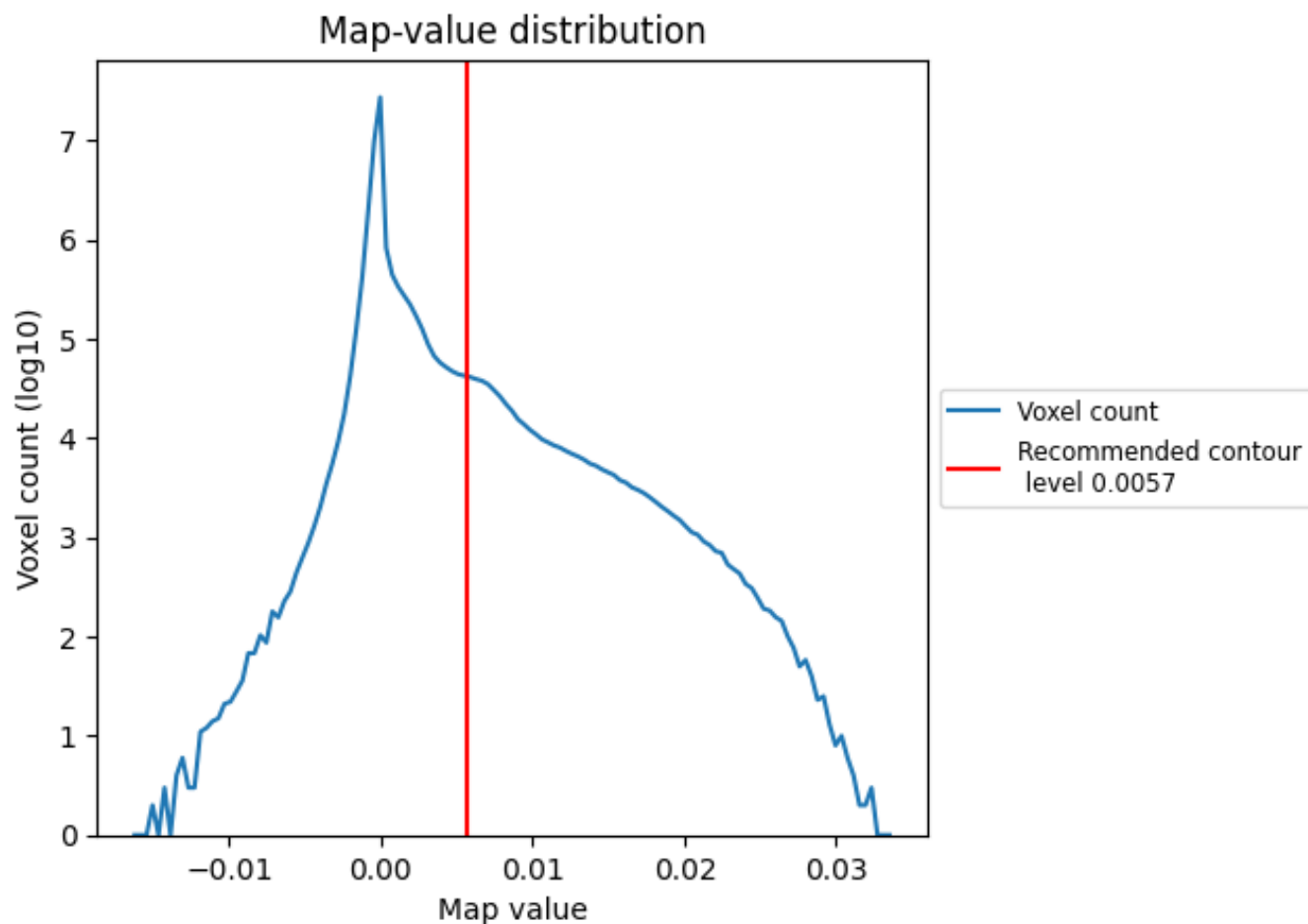
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

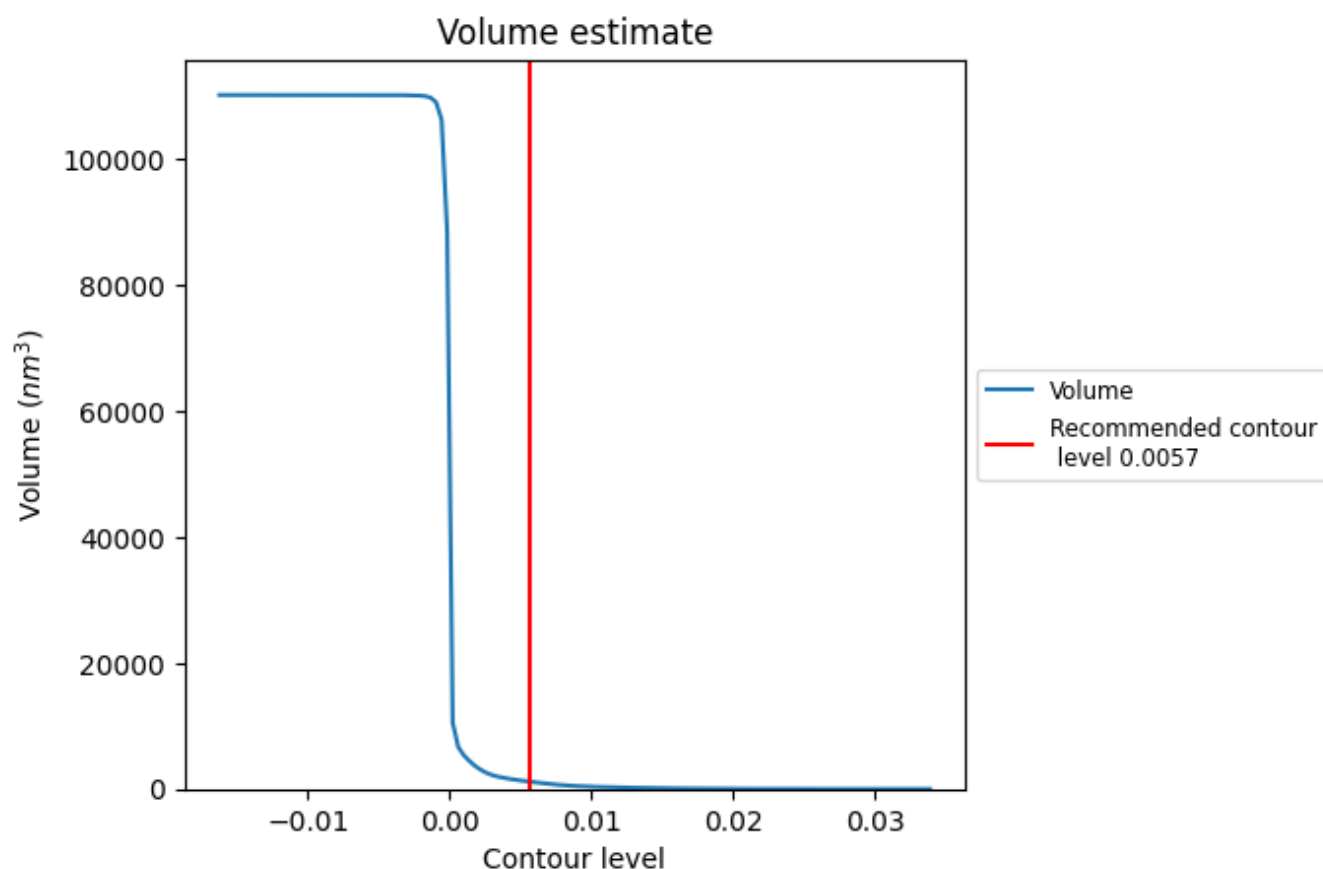
This section contains the results of statistical analysis of the map.

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.

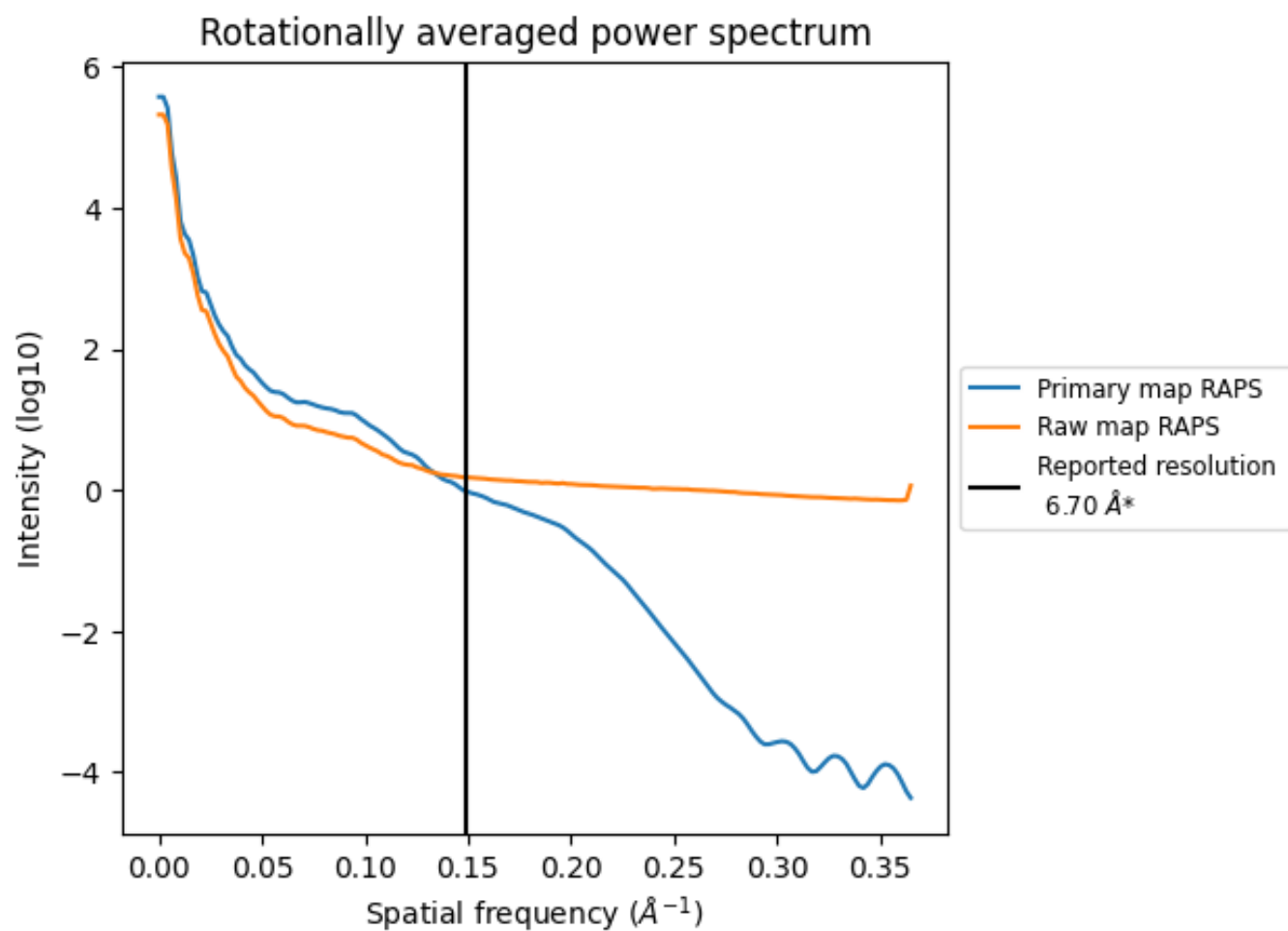
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1149 nm^3 ; this corresponds to an approximate mass of 1038 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 ⓘ

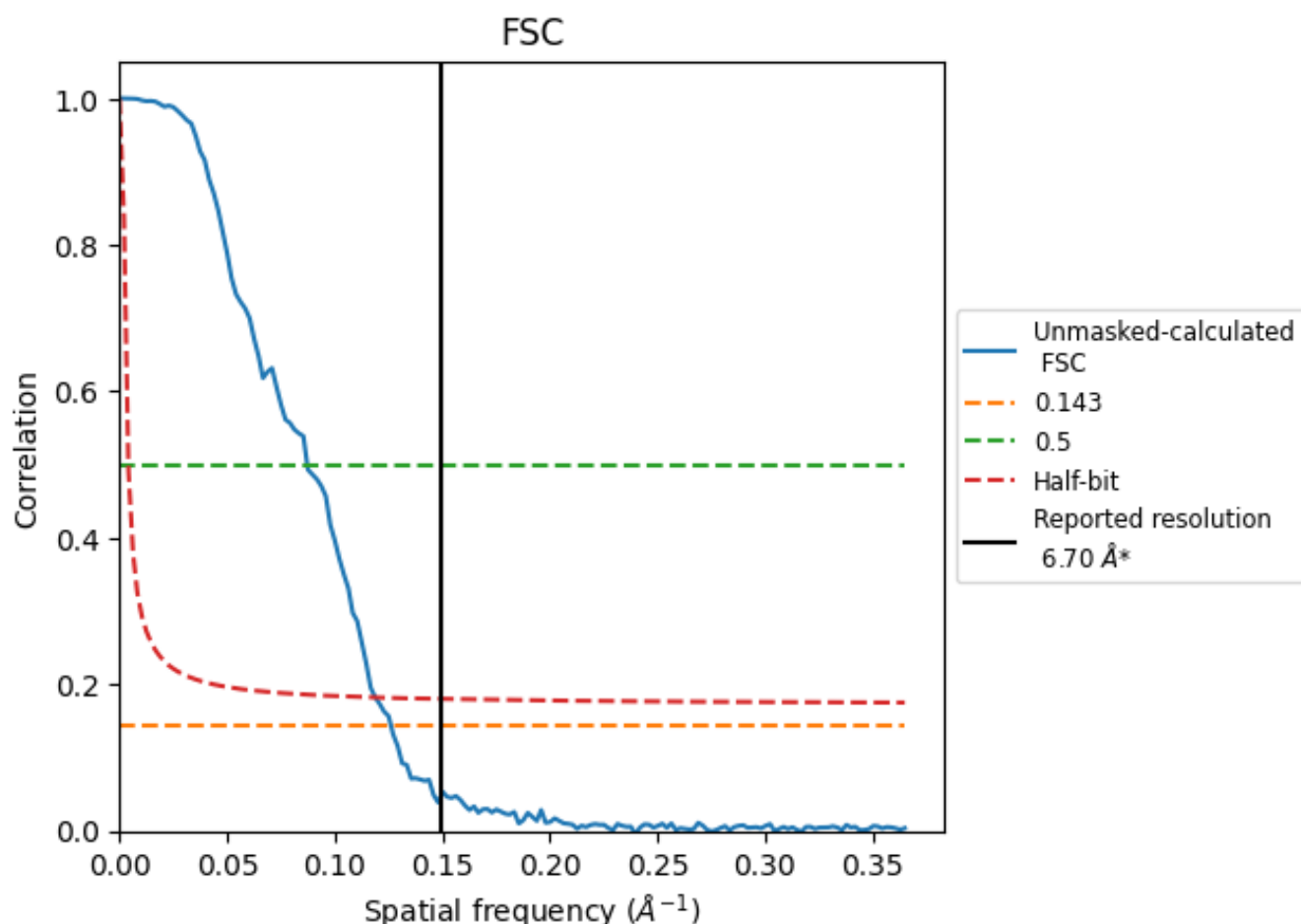


*Reported resolution corresponds to spatial frequency of 0.149 Å⁻¹

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 0.149 \AA^{-1}

8.2 Resolution estimates [i](#)

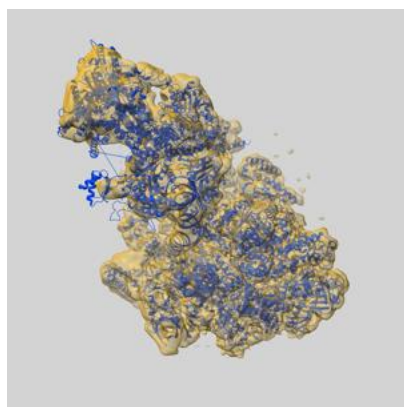
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.92	11.45	8.41

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.92 differs from the reported value 6.7 by more than 10 %

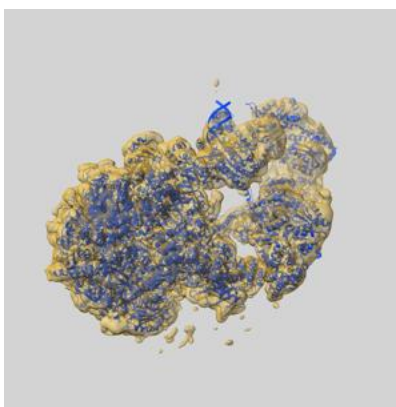
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0092 and PDB model 6GYM. Per-residue inclusion information can be found in section [3](#) on page [11](#).

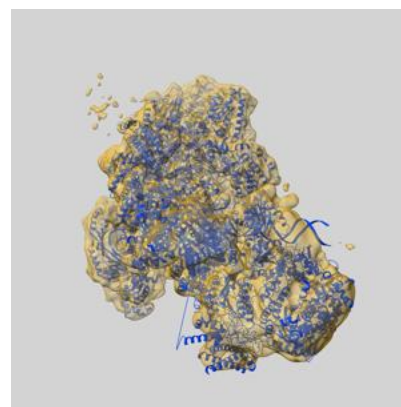
9.1 Map-model overlay [i](#)



X



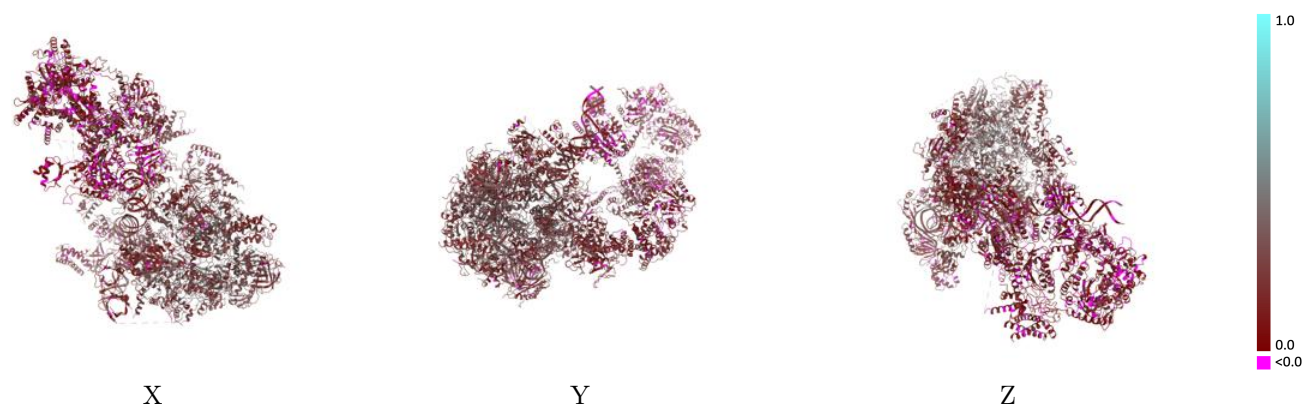
Y



Z

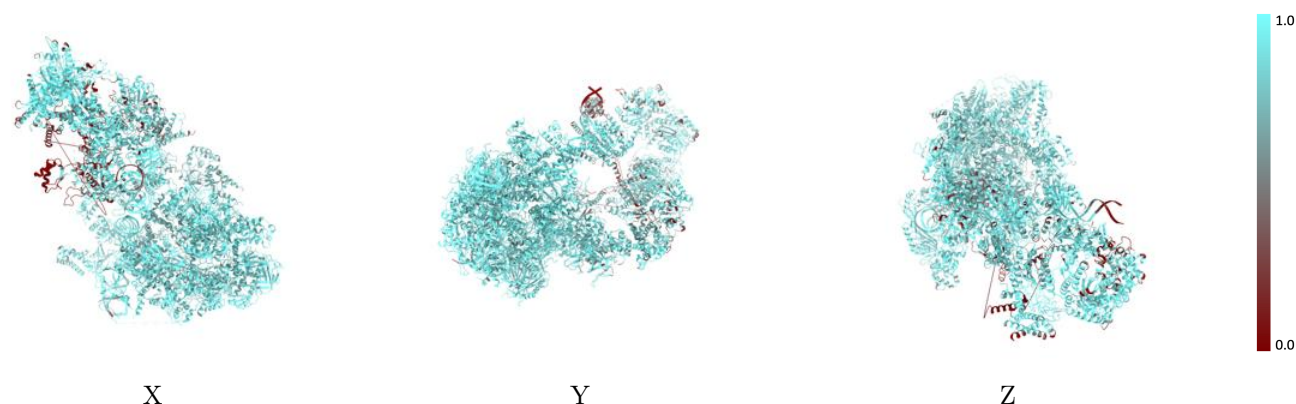
The images above show the 3D surface view of the map at the recommended contour level 0.0057 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



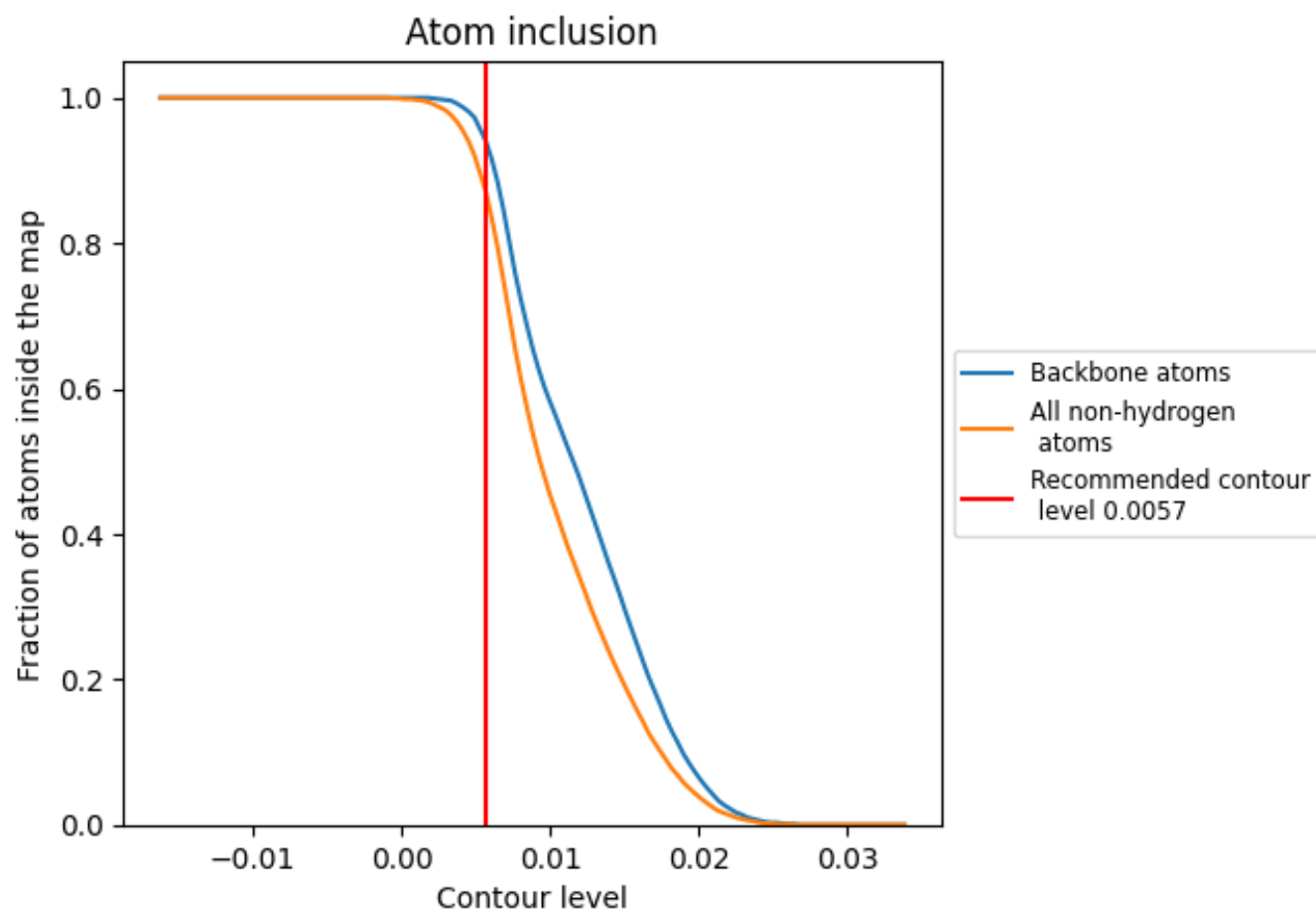
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0057).

































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% 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 (0.0057) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8700	 0.2190
0	 0.7850	 0.1370
1	 0.7310	 0.1470
2	 0.6780	 0.0910
3	 0.8210	 0.1930
4	 0.9190	 0.1090
5	 0.3860	 0.0900
6	 0.8950	 0.1170
7	 0.8840	 0.0870
A	 0.9050	 0.2860
B	 0.9110	 0.3130
C	 0.9380	 0.3170
D	 0.7890	 0.1930
E	 0.9320	 0.2430
F	 0.9220	 0.3170
G	 0.8560	 0.2310
H	 0.9290	 0.2770
I	 0.9340	 0.2420
J	 0.9380	 0.2870
K	 0.9190	 0.2910
L	 0.9310	 0.3010
M	 0.8540	 0.2270
N	 0.9010	 0.2050
O	 0.9290	 0.1820
Q	 0.9420	 0.2200
R	 0.9580	 0.2400
T	 0.8690	 0.2040
U	 0.9110	 0.1450
V	 0.8890	 0.1250
W	 0.7540	 0.1640
X	 0.9430	 0.2180
Z	 0.9630	 0.1140

