Full wwPDB EM Validation Report ⓘ

May 8, 2023 – 09:56 PM EDT

PDB ID	:	7MK9
EMDB ID	:	EMD-23887
Title	:	Complex structure of trailing EC of EC+EC (trailing EC-focused)
Authors	:	Yang, C.; Murakami, K.
Deposited on	:	2021-04-22
Resolution	:	3.54 Å(reported)
Based on initial models	:	3PO2, 5C4J

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:

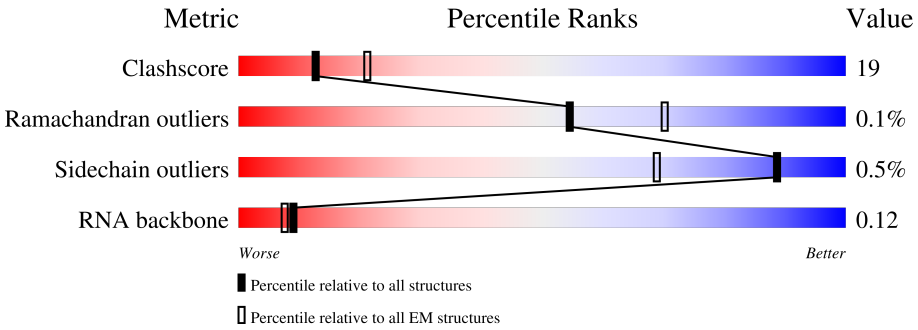
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 3.54 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	N	40	35% 45% 55%
2	O	40	20% 50% 50%
3	A	1733	50% 32% 18%
4	B	1224	5% 57% 38% 5%
5	C	318	48% 35% 17%
6	D	221	30% 48% 29% 24%
7	E	215	62% 37%

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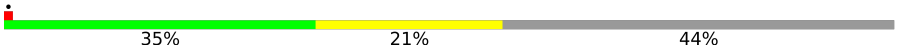
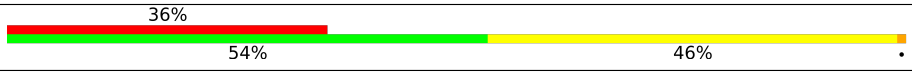
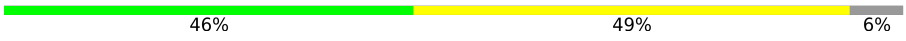
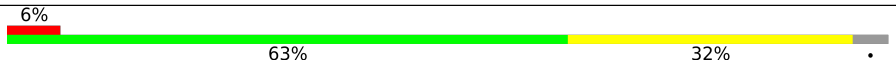
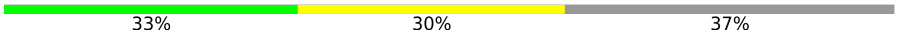
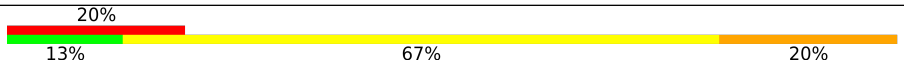
Mol	Chain	Length	Quality of chain
8	F	155	
9	G	171	
10	H	146	
11	I	122	
12	J	70	
13	K	120	
14	L	70	
15	R	15	
16	Q	735	
17	M	400	

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 36122 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 DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	N	40	822	393	162	227	40	0	0

- Molecule 2 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	O	40	827	396	141	250	40	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	1425	11167	7036	1948	2121	62	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	1166	9227	5823	1619	1729	56	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	265	2086	1312	347	414	13	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	D	168	1331	822	237	270	2	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 8 is a protein called DNA-directed RNA polymerases I,II,and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	87	Total	C	N	O	S	0	0
			705	451	119	132	3		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	171	Total	C	N	O	S	0	0
			1335	858	221	248	8		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	135	Total	C	N	O	S	0	0
			1080	679	182	214	5		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	114	Total	C	N	O	S	0	0
			927	571	168	178	10		

- Molecule 12 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	66	Total	C	N	O	S	0	0
			540	345	94	95	6		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	115	Total	C	N	O	S	0	0
			924	593	157	172	2		

- Molecule 14 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 15 is a RNA chain called RNA (5'-R(P*UP*CP*GP*AP*GP*AP*GP*GP*AP*UP*CP*CP*CP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	15	Total	C	N	O	P	0	0
			312	141	56	100	15		

- Molecule 16 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	214	Total	C	N	O	S	0	0
			1619	1017	297	299	6		

- Molecule 17 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	135	Total	C	N	O	S	0	0
			1106	694	197	210	5		

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
18	A	2	Total	Zn	0
			2	2	
18	B	1	Total	Zn	0
			1	1	
18	C	1	Total	Zn	0
			1	1	
18	I	2	Total	Zn	0
			2	2	
18	J	1	Total	Zn	0
			1	1	
18	L	1	Total	Zn	0
			1	1	

- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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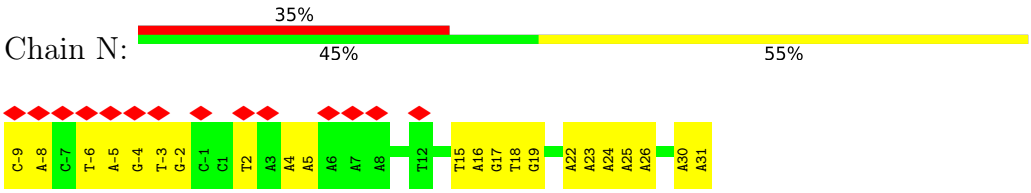
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
19	R	1	1	1	0

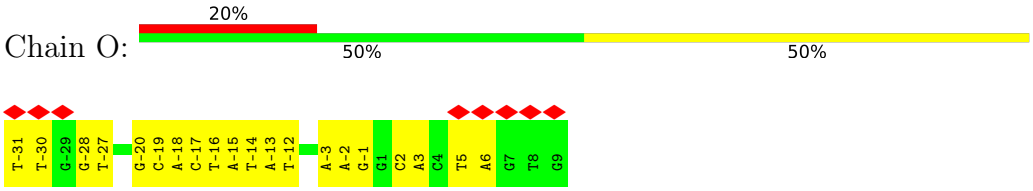
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

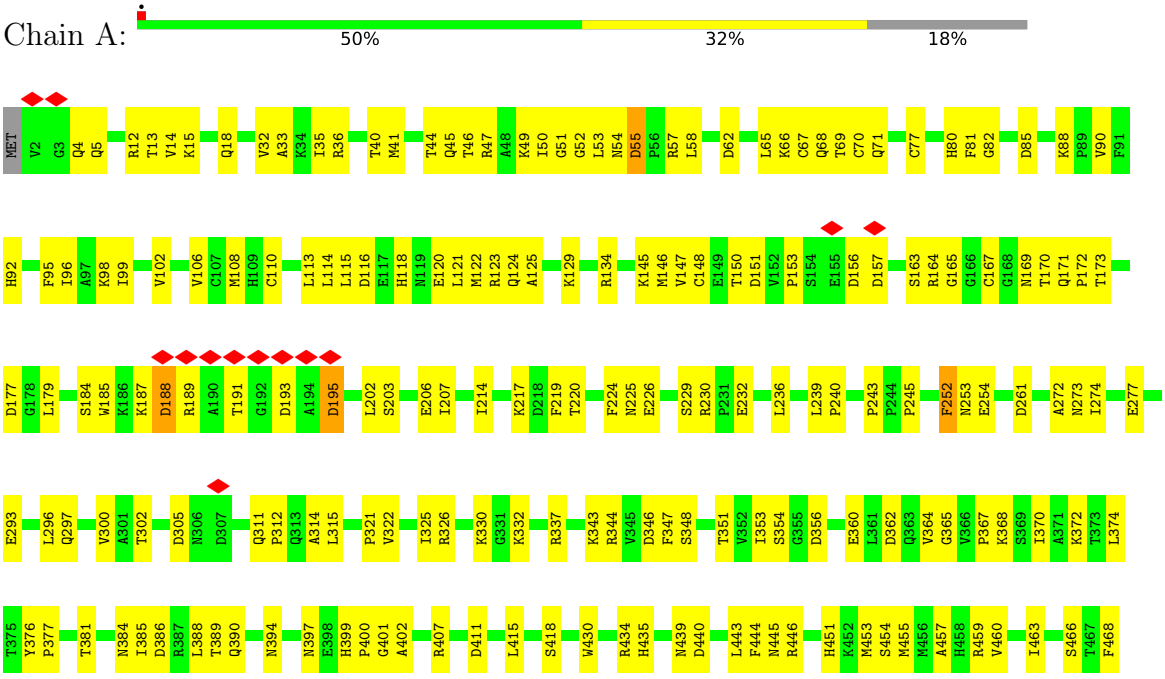
• Molecule 1: DNA (40-MER)

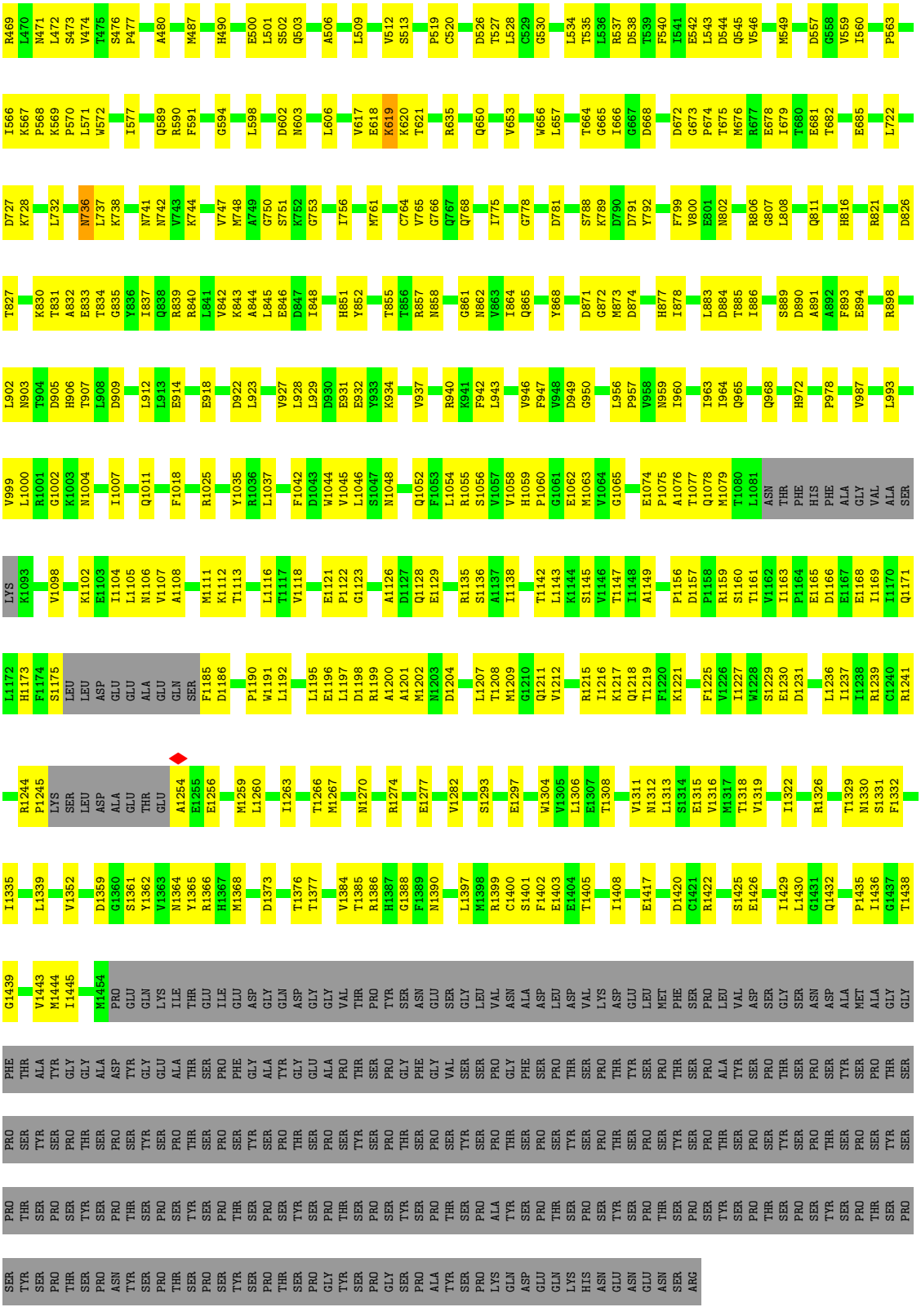


• Molecule 2: DNA (40-MER)



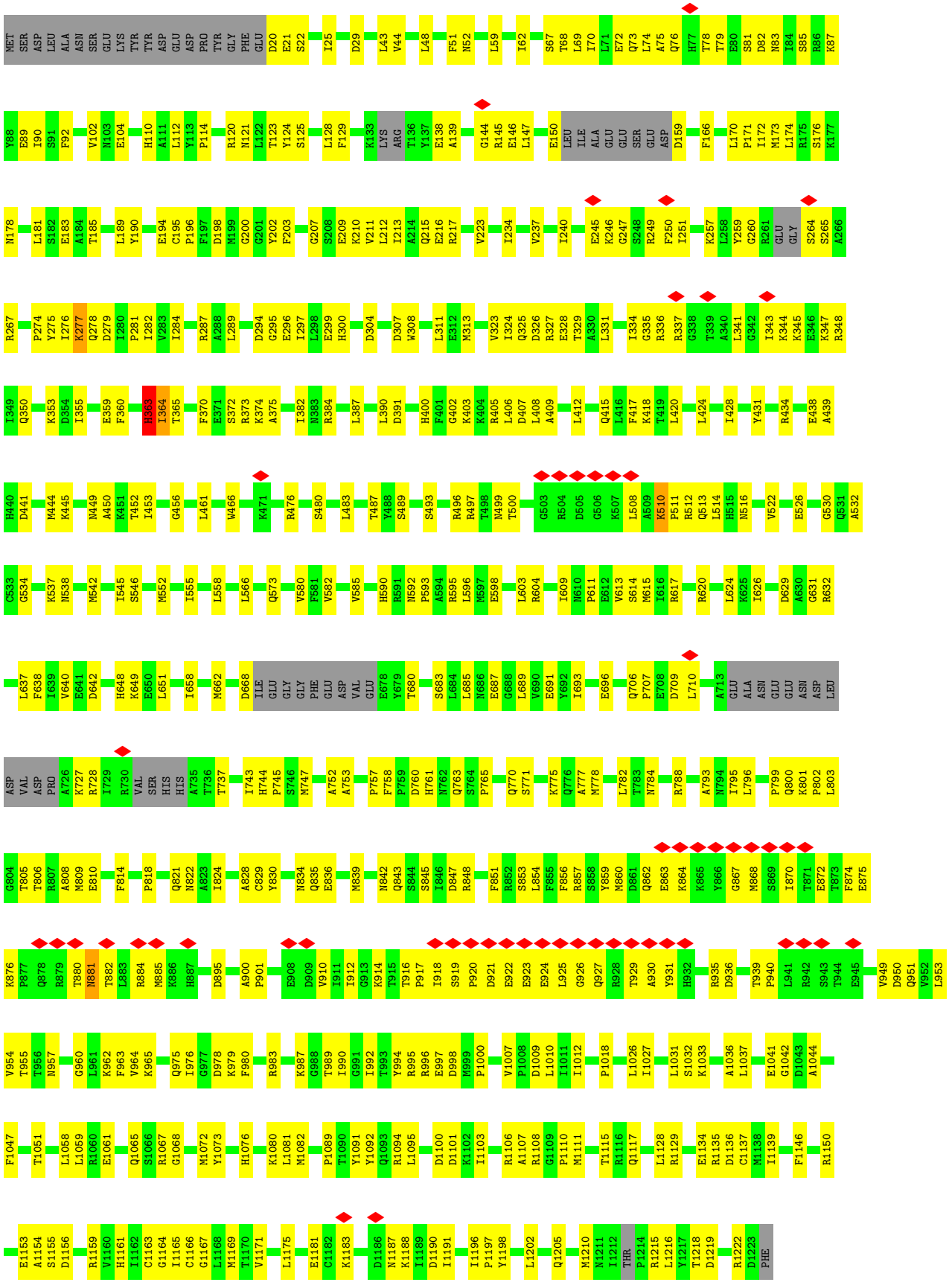
• Molecule 3: DNA-directed RNA polymerase subunit





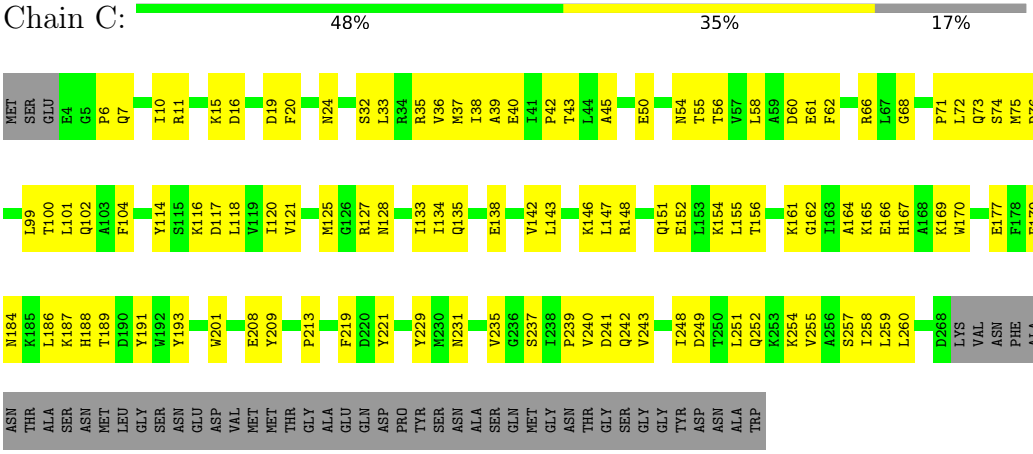
• Molecule 4: DNA-directed RNA polymerase subunit beta

Chain B:



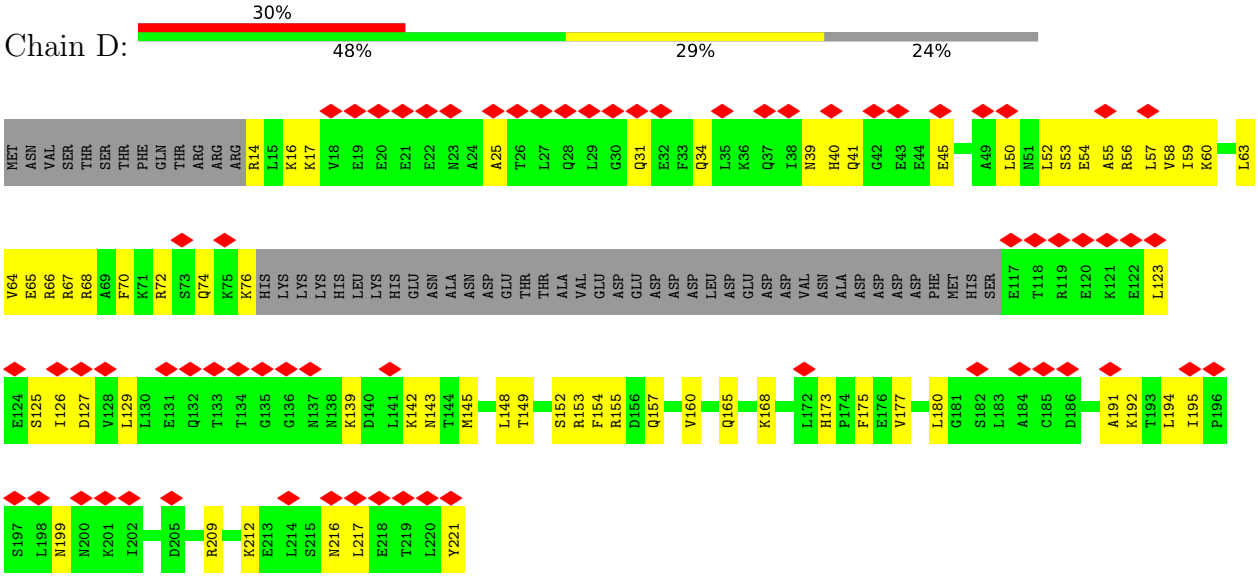
• Molecule 5: DNA-directed RNA polymerase II subunit RPB3

Chain C:



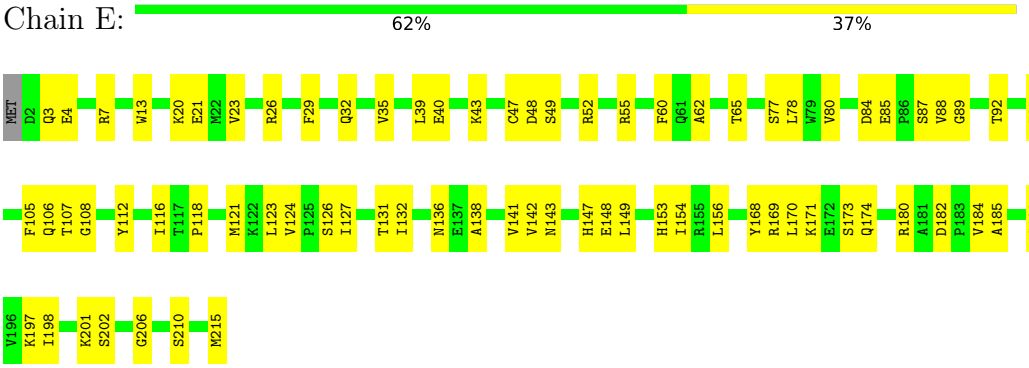
• Molecule 6: DNA-directed RNA polymerase II subunit RPB4

Chain D:



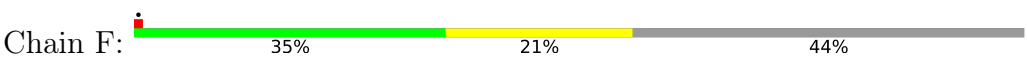
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

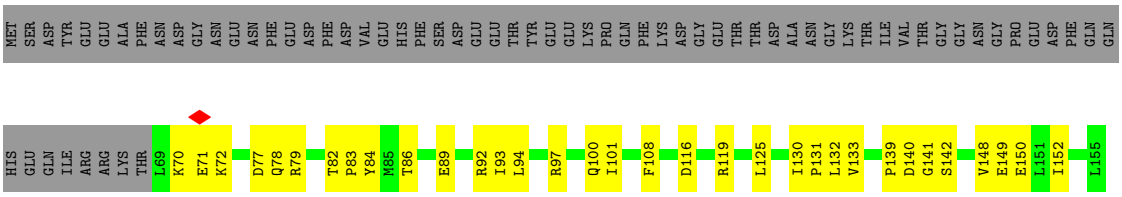
Chain E:



• Molecule 8: DNA-directed RNA polymerases I,II,and III subunit RPABC2

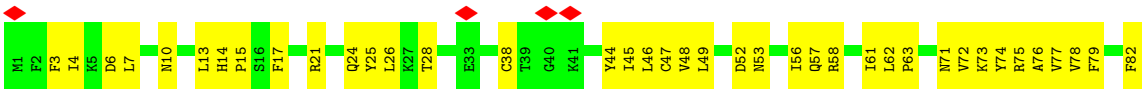
Chain F:

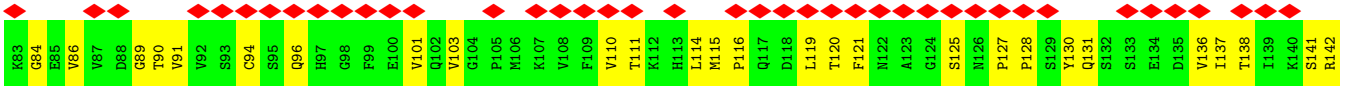


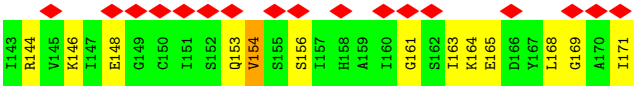


• Molecule 9: DNA-directed RNA polymerase II subunit RPB7

Chain G:

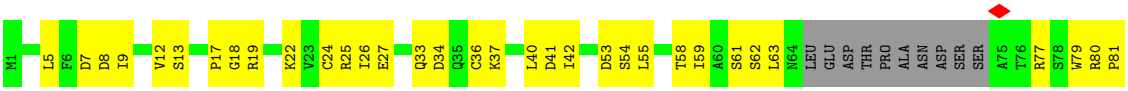






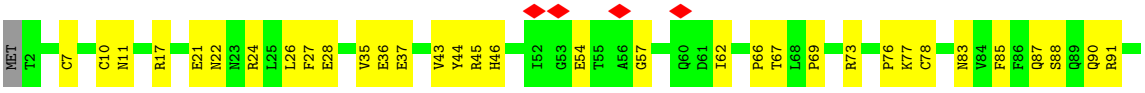
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3

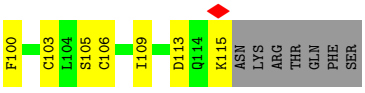
Chain H:



• Molecule 11: DNA-directed RNA polymerase II subunit RPB9

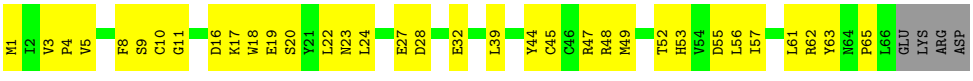
Chain I:





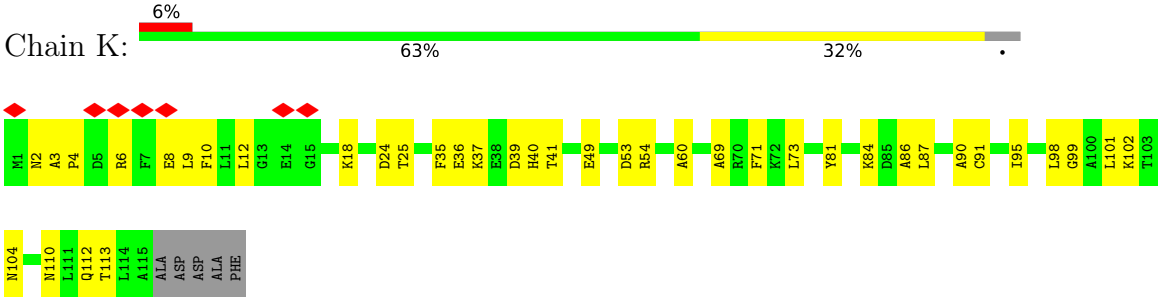
• Molecule 12: DNA-directed RNA polymerases II subunit RPABC5

Chain J:



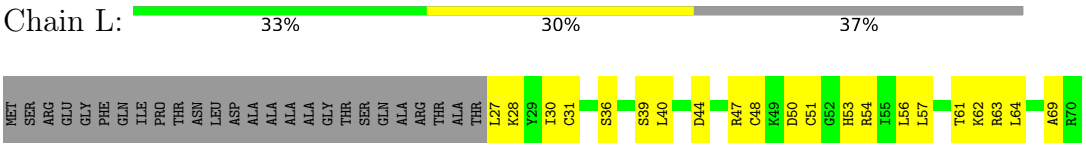
• Molecule 13: DNA-directed RNA polymerase II subunit RPB11

Chain K:



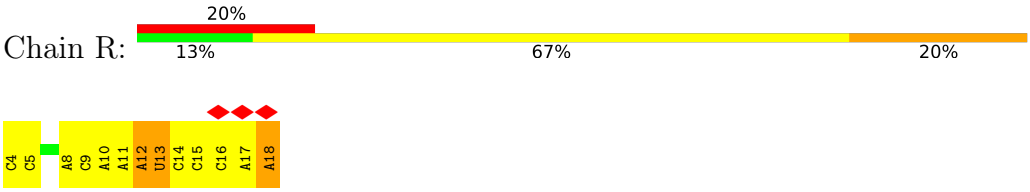
• Molecule 14: DNA-directed RNA polymerases II subunit RPABC4

Chain L:



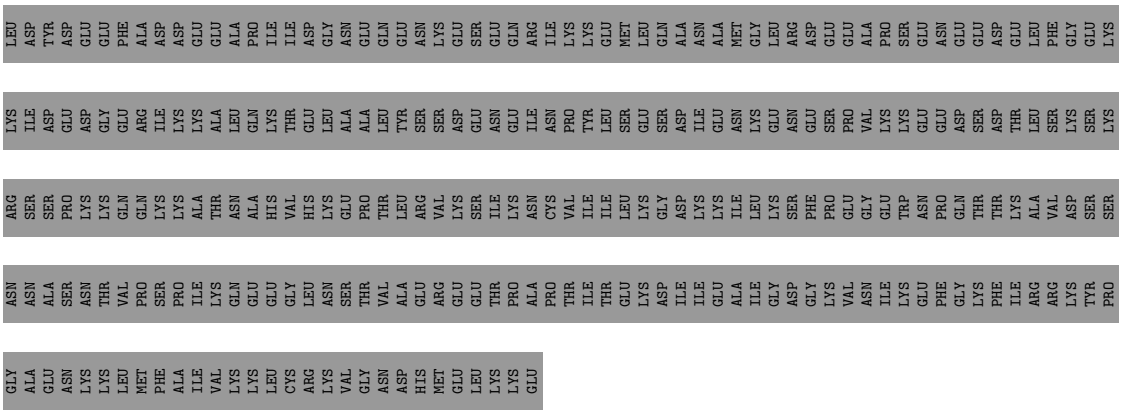
• Molecule 15: RNA (5'-R(P*UP*CP*GP*AP*GP*AP*GP*GP*AP*UP*CP*CP*CP*AP*A)-3')

Chain R:

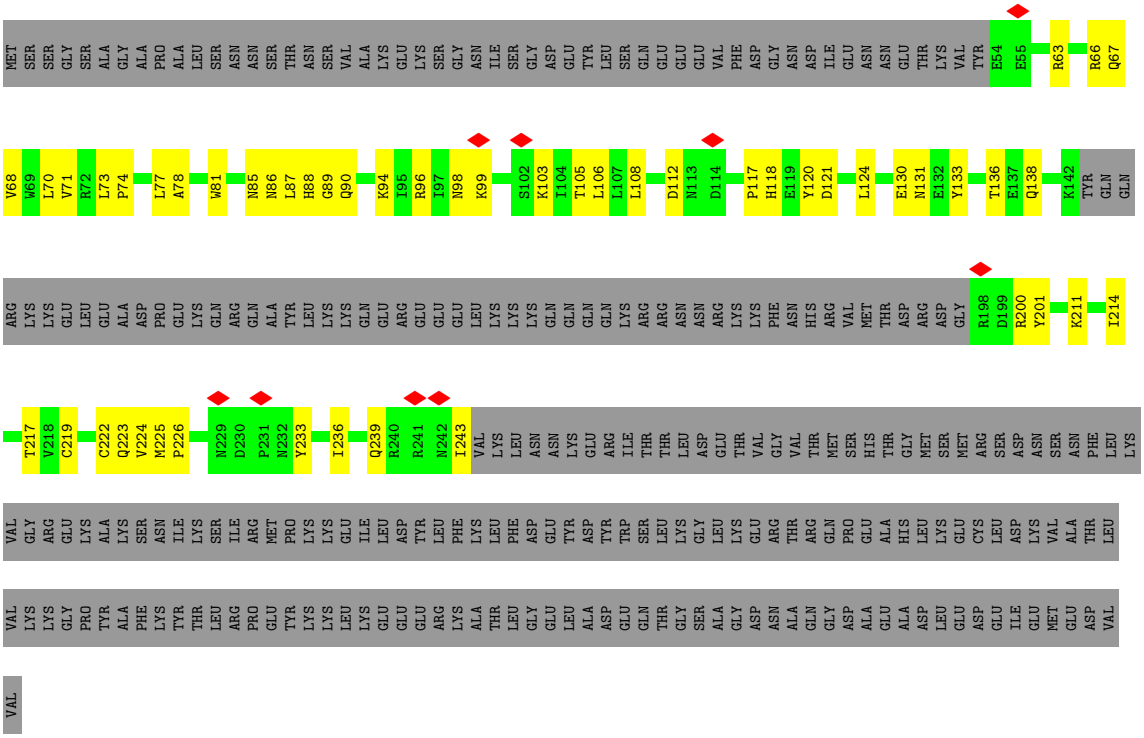


• Molecule 16: Transcription initiation factor IIF subunit alpha

Chain Q:



• Molecule 17: Transcription initiation factor IIF subunit beta



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66261	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.056	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0084	Depositor
Map size (Å)	237.6, 237.6, 237.6	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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	N	0.54	0/926	0.87	0/1425
2	O	0.60	0/925	0.99	0/1429
3	A	0.33	0/11368	0.49	0/15383
4	B	0.34	0/9402	0.52	0/12680
5	C	0.32	0/2124	0.50	0/2879
6	D	0.24	0/1339	0.44	0/1793
7	E	0.32	0/1788	0.45	0/2406
8	F	0.35	0/717	0.51	0/967
9	G	0.29	0/1363	0.49	0/1840
10	H	0.33	0/1097	0.52	0/1484
11	I	0.30	0/945	0.45	0/1273
12	J	0.40	0/549	0.51	0/738
13	K	0.32	0/942	0.48	0/1272
14	L	0.28	0/354	0.57	0/468
15	R	0.58	0/347	0.85	1/536 (0.2%)
16	Q	0.27	0/1648	0.45	1/2226 (0.0%)
17	M	0.25	0/1124	0.47	0/1517
All	All	0.34	0/36958	0.53	2/50316 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	3
4	B	0	3
9	G	0	1
All	All	0	7

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	R	12	A	O5'-P-OP1	-5.83	100.45	105.70
16	Q	421	PRO	N-CA-CB	5.72	110.16	103.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	252	PHE	Peptide
3	A	55	ASP	Peptide
3	A	750	GLY	Peptide
4	B	363	HIS	Peptide
4	B	510	LYS	Peptide
4	B	881	ASN	Peptide
9	G	154	VAL	Peptide

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	N	822	0	449	19	0
2	O	827	0	458	19	0
3	A	11167	0	11188	458	0
4	B	9227	0	9200	393	0
5	C	2086	0	2045	96	0
6	D	1331	0	1344	56	0
7	E	1752	0	1776	63	0
8	F	705	0	731	30	0
9	G	1335	0	1346	56	0
10	H	1080	0	1049	58	0
11	I	927	0	881	33	0
12	J	540	0	553	37	0
13	K	924	0	934	39	0
14	L	352	0	375	20	0
15	R	312	0	165	12	0
16	Q	1619	0	1452	41	0
17	M	1106	0	1099	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	C	1	0	0	0	0
18	I	2	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
19	A	1	0	0	0	0
19	R	1	0	0	0	0
All	All	36122	0	35045	1329	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 19.

All (1329) 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)
4:B:510:LYS:HG3	4:B:511:PRO:HD3	1.45	0.98
14:L:48:CYS:SG	14:L:51:CYS:HB2	2.09	0.93
3:A:110:CYS:HB3	3:A:167:CYS:SG	2.09	0.92
3:A:802:ASN:HD21	3:A:806:ARG:HB2	1.35	0.91
4:B:334:ILE:HA	4:B:347:LYS:HG3	1.52	0.90
4:B:763:GLN:HG2	4:B:765:PRO:HD2	1.53	0.89
3:A:148:CYS:HB2	3:A:171:GLN:HE22	1.41	0.86
14:L:28:LYS:HB2	14:L:39:SER:HA	1.57	0.86
3:A:1266:THR:O	3:A:1270:ASN:HB2	1.76	0.86
3:A:397:ASN:O	13:K:2:ASN:ND2	2.08	0.85
4:B:799:PRO:HB2	4:B:818:PRO:HG2	1.59	0.85
16:Q:105:ALA:HB1	17:M:87:LEU:HD12	1.59	0.84
10:H:55:LEU:HA	10:H:146:ARG:HH12	1.42	0.83
9:G:91:VAL:HG22	9:G:101:VAL:HG22	1.61	0.83
3:A:368:LYS:HZ2	13:K:4:PRO:HD3	1.43	0.81
4:B:542:MET:HE1	4:B:747:MET:HB3	1.63	0.81
3:A:202:LEU:HB3	3:A:207:ILE:HD11	1.62	0.80
4:B:805:THR:OG1	4:B:809:MET:SD	2.39	0.80
4:B:880:THR:HA	4:B:931:TYR:H	1.47	0.79
8:F:125:LEU:HA	8:F:130:ILE:HD11	1.64	0.78
4:B:526:GLU:O	4:B:538:ASN:ND2	2.17	0.78
4:B:75:ALA:HB2	4:B:83:ASN:H	1.48	0.77
8:F:97:ARG:HD2	8:F:100:GLN:HE22	1.49	0.77
3:A:368:LYS:HD3	13:K:3:ALA:HA	1.66	0.77
4:B:1166:CYS:SG	6:D:16:LYS:NZ	2.57	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:246:LYS:HE2	4:B:249:ARG:HD2	1.67	0.76
4:B:829:CYS:HA	4:B:834:ASN:HD21	1.48	0.76
10:H:80:ARG:HD3	10:H:81:PRO:HD2	1.67	0.76
9:G:21:ARG:HH22	9:G:25:TYR:HB2	1.49	0.76
15:R:14:C:O2	15:R:14:C:O2'	2.02	0.76
6:D:153:ARG:HH22	6:D:160:VAL:HA	1.49	0.76
3:A:367:PRO:HB3	3:A:466:SER:HA	1.67	0.76
4:B:85:SER:HB3	4:B:138:GLU:HB3	1.68	0.75
3:A:1430:LEU:HB3	3:A:1432:GLN:HE22	1.51	0.75
16:Q:106:ILE:HG22	17:M:87:LEU:HD11	1.69	0.74
3:A:1420:ASP:OD2	3:A:1422:ARG:NH1	2.21	0.74
12:J:10:CYS:SG	12:J:11:GLY:N	2.60	0.74
4:B:74:LEU:HA	4:B:85:SER:HA	1.69	0.73
14:L:61:THR:HG22	14:L:63:ARG:H	1.50	0.73
4:B:978:ASP:OD2	4:B:1094:ARG:NH2	2.21	0.73
3:A:18:GLN:HB3	4:B:1215:ARG:HB2	1.70	0.72
3:A:1208:THR:OG1	3:A:1211:GLN:OE1	2.07	0.72
5:C:165:LYS:HE2	13:K:9:LEU:HD11	1.69	0.72
6:D:152:SER:HB2	6:D:155:ARG:HH21	1.54	0.72
12:J:1:MET:HA	12:J:57:ILE:HG23	1.69	0.72
3:A:15:LYS:HD3	4:B:1219:ASP:HA	1.72	0.72
3:A:252:PHE:O	3:A:254:GLU:N	2.21	0.72
4:B:842:ASN:ND2	4:B:845:SER:OG	2.21	0.72
3:A:855:THR:OG1	3:A:857:ARG:NH1	2.23	0.72
9:G:47:CYS:SG	9:G:48:VAL:N	2.62	0.72
3:A:40:THR:HG22	3:A:53:LEU:HB2	1.72	0.72
5:C:177:GLU:HB2	5:C:231:ASN:HB3	1.70	0.72
6:D:64:VAL:HG23	6:D:68:ARG:HH22	1.53	0.71
16:Q:375:LEU:HB2	16:Q:387:ILE:HB	1.72	0.71
4:B:384:ARG:HH21	4:B:387:LEU:HD11	1.55	0.71
4:B:806:THR:HG23	4:B:808:ALA:H	1.56	0.71
15:R:13:U:H5"	15:R:14:C:H5"	1.73	0.71
6:D:39:ASN:ND2	6:D:41:GLN:OE1	2.23	0.71
6:D:70:PHE:O	6:D:74:GLN:NE2	2.23	0.71
4:B:190:TYR:HE2	4:B:196:PRO:HD3	1.56	0.70
10:H:81:PRO:O	10:H:87:ARG:NH2	2.24	0.70
3:A:273:ASN:HA	3:A:296:LEU:HD21	1.73	0.70
4:B:287:ARG:NH1	4:B:324:ILE:O	2.23	0.70
4:B:1165:ILE:N	4:B:1190:ASP:OD1	2.17	0.70
4:B:822:ASN:O	12:J:48:ARG:NH2	2.24	0.70
14:L:47:ARG:HH21	14:L:54:ARG:HE	1.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:234:ILE:HG21	4:B:257:LYS:HD2	1.73	0.69
4:B:365:THR:HG21	4:B:370:PHE:HB2	1.73	0.69
14:L:31:CYS:HA	14:L:56:LEU:HA	1.74	0.69
17:M:96:ARG:NH2	17:M:103:LYS:O	2.25	0.69
3:A:1397:LEU:HD23	3:A:1429:ILE:HD11	1.75	0.69
3:A:69:THR:HA	3:A:71:GLN:HE22	1.57	0.69
3:A:1059:HIS:ND1	8:F:86:THR:OG1	2.23	0.69
3:A:871:ASP:OD2	3:A:1366:ARG:NH2	2.25	0.69
4:B:82:ASP:H	4:B:83:ASN:HA	1.57	0.69
4:B:582:VAL:O	4:B:585:VAL:HG12	1.92	0.69
3:A:747:VAL:HG12	3:A:753:GLY:HA3	1.73	0.69
9:G:4:ILE:HD12	9:G:49:LEU:HD11	1.75	0.69
3:A:1136:SER:HB2	3:A:1274:ARG:HH22	1.57	0.69
4:B:44:VAL:HG11	4:B:200:GLY:HA2	1.75	0.69
4:B:611:PRO:HG2	4:B:685:LEU:HD21	1.75	0.69
13:K:95:ILE:HD12	13:K:98:LEU:HD11	1.75	0.69
3:A:365:GLY:HA3	3:A:469:ARG:HB3	1.74	0.68
4:B:510:LYS:O	4:B:512:ARG:N	2.27	0.68
5:C:10:ILE:HD12	5:C:20:PHE:HB3	1.75	0.68
4:B:757:PRO:HD3	4:B:983:ARG:HE	1.59	0.68
3:A:346:ASP:H	4:B:1154:ALA:HB1	1.58	0.68
4:B:526:GLU:OE2	4:B:753:ALA:N	2.20	0.67
3:A:46:THR:O	3:A:47:ARG:NE	2.28	0.67
4:B:706:GLN:HB2	4:B:709:ASP:HB3	1.77	0.67
3:A:883:LEU:HD23	3:A:885:THR:H	1.58	0.67
3:A:821:ARG:HD3	4:B:514:LEU:HB2	1.76	0.67
3:A:830:LYS:NZ	3:A:1079:MET:O	2.28	0.67
3:A:884:ASP:OD2	3:A:1025:ARG:NE	2.27	0.67
4:B:642:ASP:HA	4:B:649:LYS:HE3	1.76	0.67
17:M:124:LEU:HD23	17:M:222:CYS:HB3	1.76	0.67
3:A:311:GLN:HG2	3:A:312:PRO:HD3	1.77	0.67
3:A:788:SER:HB2	11:I:69:PRO:HG3	1.77	0.67
4:B:72:GLU:HA	4:B:87:LYS:HA	1.77	0.66
4:B:839:MET:HG3	4:B:1012:ILE:HG22	1.77	0.66
9:G:148:GLU:H	9:G:161:GLY:HA2	1.60	0.66
3:A:1161:THR:HG22	3:A:1163:ILE:H	1.60	0.66
4:B:210:LYS:NZ	4:B:480:SER:O	2.29	0.66
4:B:365:THR:O	4:B:374:LYS:NZ	2.28	0.66
7:E:136:ASN:HD21	7:E:138:ALA:HB3	1.60	0.66
3:A:868:TYR:HD1	3:A:1058:VAL:HG21	1.60	0.66
3:A:1126:ALA:HA	3:A:1304:TRP:HD1	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:97:VAL:HA	7:E:100:ILE:HD12	1.77	0.66
9:G:153:GLN:HG3	9:G:154:VAL:H	1.60	0.66
3:A:569:LYS:NZ	5:C:221:TYR:O	2.29	0.66
3:A:1159:ARG:HH12	3:A:1186:ASP:HB2	1.60	0.66
4:B:363:HIS:O	4:B:365:THR:N	2.29	0.66
3:A:1107:VAL:HA	3:A:1108:ALA:HB3	1.78	0.65
4:B:864:LYS:H	4:B:872:GLU:HG3	1.60	0.65
5:C:10:ILE:HG21	13:K:112:GLN:HG3	1.79	0.65
3:A:1318:THR:HG22	7:E:141:VAL:HG11	1.78	0.65
4:B:771:SER:O	4:B:775:LYS:NZ	2.29	0.65
4:B:884:ARG:NH2	4:B:936:ASP:O	2.30	0.65
4:B:1161:HIS:HB3	4:B:1191:ILE:HD11	1.77	0.65
3:A:528:LEU:HD11	3:A:619:LYS:HB3	1.76	0.65
3:A:802:ASN:ND2	3:A:807:GLY:O	2.29	0.65
6:D:139:LYS:HA	6:D:142:LYS:HE3	1.78	0.65
6:D:165:GLN:HA	6:D:168:LYS:HE3	1.76	0.65
3:A:1444:MET:HB3	8:F:133:VAL:HG23	1.78	0.65
4:B:172:ILE:HD11	4:B:178:ASN:HB2	1.78	0.65
3:A:81:PHE:HE1	3:A:243:PRO:HD3	1.60	0.65
4:B:48:LEU:O	4:B:52:ASN:ND2	2.27	0.65
5:C:148:ARG:HH12	12:J:65:PRO:HD2	1.61	0.65
3:A:1128:GLN:OE1	3:A:1304:TRP:NE1	2.30	0.65
17:M:138:GLN:HG3	17:M:211:LYS:HB3	1.78	0.65
4:B:173:MET:HB3	4:B:176:SER:HB3	1.79	0.65
10:H:33:GLN:HG3	10:H:36:CYS:H	1.61	0.65
4:B:604:ARG:NH1	4:B:691:GLU:OE2	2.30	0.64
3:A:390:GLN:NE2	3:A:394:ASN:OD1	2.29	0.64
3:A:4:GLN:O	4:B:1159:ARG:NH2	2.31	0.64
4:B:334:ILE:HG13	4:B:335:GLY:H	1.60	0.64
4:B:796:LEU:HA	4:B:853:SER:HA	1.78	0.64
6:D:40:HIS:HB2	9:G:73:LYS:HZ2	1.62	0.64
7:E:124:VAL:HG13	7:E:132:ILE:HB	1.79	0.64
16:Q:376:LEU:HD12	17:M:71:VAL:HG21	1.78	0.64
4:B:822:ASN:OD1	12:J:48:ARG:NH2	2.31	0.64
3:A:226:GLU:HG2	3:A:230:ARG:HE	1.63	0.64
8:F:86:THR:N	8:F:89:GLU:OE2	2.29	0.64
3:A:356:ASP:HB2	3:A:469:ARG:HD2	1.79	0.64
4:B:493:SER:OG	4:B:497:ARG:NH2	2.31	0.64
4:B:1033:LYS:HD2	4:B:1059:LEU:HD11	1.80	0.64
6:D:139:LYS:NZ	6:D:143:ASN:OD1	2.21	0.64
4:B:79:THR:HB	4:B:81:SER:H	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:226:PRO:HG3	17:M:236:ILE:HD11	1.80	0.64
7:E:62:ALA:O	7:E:77:SER:OG	2.15	0.63
3:A:77:CYS:SG	3:A:80:HIS:CE1	2.79	0.63
3:A:567:LYS:HB3	3:A:568:PRO:HD3	1.81	0.63
7:E:169:ARG:NH2	8:F:142:SER:OG	2.31	0.63
9:G:52:ASP:OD1	9:G:53:ASN:N	2.32	0.63
7:E:88:VAL:HG21	7:E:116:ILE:HG12	1.80	0.63
1:N:17:DG:H2"	1:N:18:DT:H5'	1.78	0.63
3:A:826:ASP:OD2	3:A:827:THR:N	2.31	0.63
4:B:980:PHE:HE1	4:B:1094:ARG:HG3	1.64	0.63
4:B:1135:ARG:NH2	4:B:1136:ASP:OD1	2.31	0.63
3:A:1197:LEU:HB2	3:A:1236:LEU:HB3	1.81	0.63
4:B:327:ARG:HG2	16:Q:398:ARG:HH12	1.64	0.63
14:L:40:LEU:HD12	14:L:44:ASP:HB2	1.80	0.63
3:A:959:ASN:OD1	3:A:960:ILE:N	2.32	0.62
3:A:894:GLU:HB2	3:A:898:ARG:HB2	1.81	0.62
4:B:1072:MET:HB3	4:B:1081:LEU:HD12	1.81	0.62
3:A:367:PRO:HG2	3:A:370:ILE:HG12	1.81	0.62
4:B:194:GLU:HA	4:B:784:ASN:HD22	1.65	0.62
4:B:1163:CYS:O	4:B:1167:GLY:N	2.23	0.62
9:G:46:LEU:HB2	9:G:77:VAL:HG13	1.81	0.62
14:L:30:ILE:HB	14:L:57:LEU:HB2	1.82	0.62
4:B:930:ALA:HA	4:B:931:TYR:C	2.20	0.62
4:B:1106:ARG:NH2	4:B:1110:PRO:O	2.32	0.62
10:H:8:ASP:OD1	10:H:9:ILE:N	2.31	0.62
3:A:55:ASP:HA	3:A:58:LEU:HD23	1.81	0.62
3:A:169:ASN:OD1	3:A:170:THR:N	2.31	0.62
4:B:104:GLU:OE2	4:B:110:HIS:HE1	1.82	0.62
3:A:500:GLU:OE2	4:B:1146:PHE:N	2.31	0.62
13:K:8:GLU:HA	13:K:37:LYS:HZ2	1.65	0.62
16:Q:97:GLU:OE2	17:M:96:ARG:NH1	2.32	0.62
3:A:203:SER:O	3:A:206:GLU:HG2	2.00	0.62
3:A:512:VAL:HA	3:A:519:PRO:HA	1.80	0.62
3:A:827:THR:HA	3:A:830:LYS:HG2	1.80	0.62
3:A:1200:ALA:O	3:A:1204:ASP:HB2	2.00	0.62
16:Q:141:ARG:NH1	16:Q:345:GLU:O	2.33	0.62
3:A:526:ASP:OD1	3:A:527:THR:N	2.31	0.61
4:B:334:ILE:HG13	4:B:335:GLY:N	2.16	0.61
3:A:146:MET:O	3:A:171:GLN:N	2.32	0.61
3:A:885:THR:O	3:A:940:ARG:NH1	2.32	0.61
7:E:147:HIS:HE1	7:E:149:LEU:HD13	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:598:LEU:O	10:H:25:ARG:NH2	2.27	0.61
4:B:20:ASP:OD1	4:B:21:GLU:N	2.33	0.61
4:B:1134:GLU:OE1	4:B:1134:GLU:N	2.28	0.61
3:A:834:THR:OG1	3:A:1076:ALA:HB1	2.00	0.61
4:B:795:ILE:O	4:B:854:LEU:N	2.32	0.61
11:I:45:ARG:HE	11:I:46:HIS:H	1.46	0.61
3:A:134:ARG:NH2	3:A:220:THR:O	2.33	0.61
3:A:1044:TRP:O	3:A:1048:ASN:ND2	2.33	0.61
3:A:1385:THR:OG1	3:A:1388:GLY:N	2.31	0.61
4:B:1010:LEU:HD11	4:B:1092:TYR:HE2	1.65	0.61
8:F:116:ASP:OD2	8:F:119:ARG:N	2.30	0.61
12:J:44:TYR:HA	12:J:47:ARG:HB3	1.83	0.61
3:A:789:LYS:NZ	11:I:67:THR:OG1	2.32	0.61
4:B:875:GLU:OE2	4:B:881:ASN:ND2	2.34	0.61
3:A:384:ASN:HB2	3:A:388:LEU:HD13	1.82	0.61
13:K:36:GLU:N	13:K:36:GLU:OE1	2.34	0.61
17:M:223:GLN:NE2	17:M:224:VAL:O	2.33	0.60
3:A:81:PHE:CE1	3:A:243:PRO:HD3	2.35	0.60
4:B:341:LEU:HB3	4:B:344:LYS:HD2	1.82	0.60
16:Q:126:LYS:HD3	17:M:130:GLU:HB2	1.84	0.60
5:C:125:MET:SD	5:C:127:ARG:NE	2.73	0.60
9:G:89:GLY:HA3	9:G:103:VAL:HG22	1.83	0.60
3:A:453:MET:O	3:A:454:SER:OG	2.17	0.60
5:C:162:GLY:HA3	5:C:170:TRP:CE2	2.37	0.60
5:C:240:VAL:O	5:C:243:VAL:HG22	2.01	0.60
3:A:886:ILE:HD11	3:A:943:LEU:HB3	1.84	0.60
4:B:114:PRO:HG3	4:B:181:LEU:HD11	1.84	0.60
4:B:296:GLU:O	4:B:300:HIS:ND1	2.28	0.60
3:A:147:VAL:HA	3:A:170:THR:HA	1.83	0.60
3:A:502:SER:OG	3:A:503:GLN:NE2	2.29	0.60
3:A:115:LEU:HD21	3:A:145:LYS:HD3	1.83	0.60
4:B:1037:LEU:O	12:J:47:ARG:NH1	2.35	0.60
5:C:167:HIS:CE1	5:C:169:LYS:HG3	2.37	0.60
10:H:12:VAL:HG12	10:H:53:ASP:H	1.65	0.60
3:A:148:CYS:HB2	3:A:171:GLN:NE2	2.15	0.60
3:A:840:ARG:NH1	3:A:1384:VAL:O	2.34	0.60
3:A:1142:THR:O	3:A:1145:SER:OG	2.18	0.60
5:C:143:LEU:HD21	5:C:146:LYS:HE3	1.84	0.60
3:A:1113:THR:O	3:A:1330:ASN:ND2	2.35	0.60
3:A:1168:GLU:O	3:A:1171:GLN:NE2	2.35	0.60
3:A:326:ARG:O	3:A:330:LYS:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:209:GLU:OE1	4:B:788:ARG:NH2	2.25	0.59
7:E:168:TYR:HB3	7:E:170:LEU:HD23	1.84	0.59
9:G:84:GLY:HA2	9:G:146:LYS:HD2	1.84	0.59
11:I:78:CYS:SG	11:I:105:SER:OG	2.60	0.59
3:A:905:ASP:OD1	3:A:906:HIS:N	2.35	0.59
4:B:924:GLU:HG2	4:B:925:LEU:HD12	1.83	0.59
4:B:997:GLU:OE1	4:B:997:GLU:N	2.33	0.59
3:A:590:ARG:NH2	3:A:620:LYS:HB3	2.17	0.59
4:B:146:GLU:HG2	4:B:147:LEU:H	1.65	0.59
9:G:154:VAL:O	9:G:156:SER:N	2.34	0.59
9:G:116:PRO:HD2	9:G:119:LEU:HD22	1.83	0.59
3:A:871:ASP:OD1	3:A:872:GLY:N	2.34	0.59
4:B:876:LYS:HB2	4:B:895:ASP:HA	1.83	0.59
10:H:5:LEU:HD11	10:H:61:SER:HB3	1.83	0.59
3:A:589:GLN:HB3	3:A:591:PHE:HE2	1.68	0.59
4:B:295:GLY:HA3	11:I:11:ASN:HB3	1.84	0.59
10:H:99:GLY:HA3	10:H:118:PHE:CD1	2.38	0.59
10:H:135:LEU:HD13	10:H:137:GLN:HB3	1.85	0.59
4:B:510:LYS:HG3	4:B:511:PRO:CD	2.27	0.59
4:B:770:GLN:O	4:B:770:GLN:NE2	2.35	0.59
16:Q:379:GLU:N	16:Q:383:SER:O	2.25	0.59
3:A:33:ALA:H	3:A:82:GLY:HA2	1.67	0.59
3:A:618:GLU:HG3	3:A:620:LYS:H	1.65	0.59
10:H:128:ASN:OD1	10:H:131:ASN:ND2	2.34	0.59
4:B:372:SER:OG	4:B:373:ARG:NH1	2.34	0.59
3:A:32:VAL:O	3:A:57:ARG:NH1	2.35	0.59
4:B:1058:LEU:O	4:B:1061:GLU:HG3	2.02	0.59
5:C:66:ARG:NH2	12:J:3:VAL:O	2.35	0.59
10:H:62:SER:OG	10:H:63:LEU:N	2.36	0.59
10:H:130:ARG:H	10:H:130:ARG:HD3	1.68	0.59
11:I:45:ARG:HE	11:I:46:HIS:N	2.01	0.59
3:A:1054:LEU:HB3	8:F:84:TYR:HE1	1.68	0.58
4:B:79:THR:HG22	4:B:82:ASP:HA	1.85	0.58
6:D:56:ARG:NH2	6:D:154:PHE:O	2.31	0.58
9:G:144:ARG:HB2	9:G:169:GLY:H	1.67	0.58
3:A:1129:GLU:OE1	3:A:1129:GLU:N	2.33	0.58
4:B:687:GLU:OE1	4:B:687:GLU:N	2.26	0.58
3:A:1209:MET:HA	3:A:1212:VAL:HG22	1.85	0.58
4:B:70:ILE:HG22	4:B:89:GLU:HA	1.86	0.58
6:D:123:LEU:HG	6:D:145:MET:HE1	1.85	0.58
3:A:239:LEU:HD12	3:A:240:PRO:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:668:ASP:OD2	16:Q:28:ARG:NH2	2.36	0.58
5:C:239:PRO:HB2	5:C:242:GLN:HG2	1.85	0.58
9:G:56:ILE:HG13	9:G:57:GLN:H	1.68	0.58
10:H:99:GLY:HA3	10:H:118:PHE:HD1	1.68	0.58
2:O:-13:DA:H1'	3:A:835:GLY:HA3	1.86	0.58
4:B:75:ALA:O	4:B:76:GLN:HG2	2.03	0.58
4:B:275:TYR:HB3	4:B:337:ARG:HD2	1.86	0.58
4:B:307:ASP:OD1	4:B:308:TRP:N	2.37	0.58
6:D:40:HIS:HB2	9:G:73:LYS:NZ	2.19	0.58
3:A:473:SER:OG	3:A:650:GLN:OE1	2.18	0.58
3:A:664:THR:OG1	3:A:668:ASP:OD2	2.16	0.58
4:B:412:LEU:HB3	4:B:466:TRP:CZ2	2.39	0.58
9:G:120:THR:OG1	9:G:131:GLN:O	2.22	0.58
3:A:1118:VAL:HB	3:A:1306:LEU:HB2	1.86	0.57
1:N:18:DT:H1'	1:N:19:DG:C8	2.39	0.57
3:A:1390:ASN:HD22	3:A:1402:PHE:HD2	1.52	0.57
4:B:364:ILE:HG22	4:B:585:VAL:HG23	1.84	0.57
4:B:802:PRO:HB3	4:B:1091:TYR:CG	2.39	0.57
5:C:208:GLU:N	5:C:208:GLU:OE1	2.37	0.57
6:D:139:LYS:HZ3	6:D:142:LYS:HB2	1.69	0.57
3:A:68:GLN:NE2	3:A:70:CYS:SG	2.77	0.57
4:B:185:THR:O	4:B:189:LEU:N	2.25	0.57
4:B:194:GLU:N	4:B:194:GLU:OE1	2.38	0.57
4:B:857:ARG:NH1	4:B:859:TYR:OH	2.34	0.57
3:A:12:ARG:HH21	4:B:1218:THR:HG21	1.68	0.57
3:A:440:ASP:H	3:A:460:VAL:HG12	1.70	0.57
3:A:471:ASN:OD1	3:A:472:LEU:N	2.38	0.57
3:A:781:ASP:HB2	3:A:789:LYS:HD2	1.86	0.57
3:A:865:GLN:NE2	3:A:1373:ASP:OD2	2.26	0.57
3:A:1116:LEU:HB3	3:A:1329:THR:HG23	1.87	0.57
4:B:104:GLU:OE2	4:B:110:HIS:CE1	2.58	0.57
5:C:55:THR:HB	5:C:152:GLU:H	1.70	0.57
7:E:123:LEU:HD23	7:E:123:LEU:H	1.70	0.57
8:F:130:ILE:N	8:F:149:GLU:OE2	2.38	0.57
3:A:490:HIS:HB3	4:B:1150:ARG:HH12	1.69	0.57
5:C:179:GLU:HB2	5:C:229:TYR:HB2	1.86	0.57
3:A:243:PRO:HB2	3:A:245:PRO:HD2	1.86	0.57
3:A:557:ASP:HB3	3:A:559:VAL:HG12	1.86	0.57
3:A:816:HIS:HE2	4:B:763:GLN:HA	1.69	0.57
4:B:918:ILE:HG22	4:B:921:ASP:HB2	1.87	0.57
8:F:84:TYR:HE2	8:F:152:ILE:HD11	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:445:ASN:HA	3:A:455:MET:HE1	1.86	0.57
3:A:806:ARG:O	4:B:728:ARG:NH2	2.38	0.57
4:B:420:LEU:HD21	4:B:456:GLY:HA3	1.86	0.57
10:H:98:TYR:OH	10:H:139:ASN:ND2	2.28	0.57
3:A:434:ARG:HD2	3:A:435:HIS:O	2.05	0.57
3:A:761:MET:HE1	4:B:1018:PRO:HA	1.86	0.57
4:B:727:LYS:HB3	4:B:1051:THR:HG21	1.87	0.57
3:A:949:ASP:OD1	3:A:950:GLY:N	2.38	0.56
4:B:487:THR:HG22	4:B:489:SER:H	1.70	0.56
12:J:3:VAL:HG11	12:J:18:TRP:CD2	2.40	0.56
3:A:1191:TRP:HZ3	11:I:43:VAL:HG21	1.70	0.56
3:A:563:PRO:HG3	3:A:570:PRO:HB3	1.87	0.56
3:A:922:ASP:OD1	3:A:923:LEU:N	2.38	0.56
3:A:1161:THR:HG22	3:A:1163:ILE:N	2.20	0.56
3:A:1216:ILE:O	3:A:1219:THR:HG22	2.06	0.56
4:B:1065:GLN:OE1	4:B:1068:GLY:N	2.38	0.56
5:C:114:TYR:N	5:C:117:ASP:OD2	2.35	0.56
5:C:248:ILE:HG21	13:K:102:LYS:HB2	1.87	0.56
3:A:173:THR:OG1	3:A:184:SER:OG	2.24	0.56
3:A:1329:THR:HB	3:A:1335:ILE:HD11	1.88	0.56
4:B:867:GLY:HA3	4:B:868:MET:C	2.25	0.56
5:C:76:ASP:OD2	5:C:128:ASN:N	2.38	0.56
3:A:372:LYS:NZ	13:K:2:ASN:HB2	2.20	0.56
4:B:1156:ASP:HB3	4:B:1198:TYR:H	1.71	0.56
5:C:43:THR:HG23	5:C:170:TRP:HD1	1.70	0.56
6:D:56:ARG:NH1	6:D:155:ARG:HE	2.03	0.56
8:F:84:TYR:CE2	8:F:152:ILE:HD11	2.40	0.56
12:J:8:PHE:H	12:J:49:MET:CE	2.19	0.56
3:A:14:VAL:HG22	4:B:1216:LEU:HD21	1.87	0.56
3:A:385:ILE:O	3:A:389:THR:OG1	2.20	0.56
3:A:741:ASN:OD1	3:A:742:ASN:N	2.39	0.56
4:B:323:VAL:HG13	4:B:324:ILE:HG13	1.88	0.56
4:B:1181:GLU:HG3	4:B:1188:LYS:HE3	1.88	0.56
3:A:179:LEU:HD12	3:A:297:GLN:HE22	1.70	0.56
3:A:451:HIS:CD2	3:A:453:MET:HB2	2.41	0.56
3:A:1335:ILE:HG23	3:A:1339:LEU:HD12	1.88	0.56
2:O:-16:DT:H2"	2:O:-15:DA:C8	2.41	0.56
3:A:1111:MET:SD	3:A:1331:SER:OG	2.52	0.56
3:A:1149:ALA:HB1	11:I:45:ARG:HH22	1.70	0.56
4:B:874:PHE:CE1	4:B:962:LYS:HB3	2.41	0.56
11:I:27:PHE:O	11:I:36:GLU:N	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:82:ASP:N	4:B:83:ASN:HA	2.18	0.56
4:B:872:GLU:HG2	4:B:917:PRO:HD3	1.88	0.56
6:D:191:ALA:HA	6:D:194:LEU:HD12	1.88	0.56
5:C:166:GLU:O	13:K:6:ARG:NH2	2.26	0.55
7:E:202:SER:O	7:E:206:GLY:N	2.33	0.55
3:A:737:LEU:HD11	3:A:741:ASN:HD22	1.71	0.55
3:A:964:ILE:O	3:A:968:GLN:HG3	2.06	0.55
3:A:738:LYS:NZ	5:C:193:TYR:O	2.37	0.55
4:B:287:ARG:NH2	4:B:294:ASP:OD1	2.30	0.55
4:B:805:THR:O	4:B:1044:ALA:N	2.40	0.55
4:B:629:ASP:O	4:B:632:ARG:NH2	2.35	0.55
6:D:148:LEU:O	6:D:152:SER:OG	2.13	0.55
17:M:86:ASN:OD1	17:M:90:GLN:NE2	2.40	0.55
4:B:824:ILE:HD11	12:J:48:ARG:HD2	1.89	0.55
7:E:156:LEU:HD21	7:E:197:LYS:HB2	1.89	0.55
8:F:77:ASP:OD2	8:F:78:GLN:N	2.40	0.55
13:K:8:GLU:HG2	13:K:37:LYS:HZ2	1.72	0.55
3:A:540:PHE:HB3	3:A:571:LEU:HD23	1.89	0.55
4:B:1155:SER:OG	4:B:1156:ASP:N	2.38	0.55
5:C:101:LEU:O	5:C:102:GLN:NE2	2.39	0.55
3:A:874:ASP:O	3:A:878:ILE:HD11	2.07	0.55
3:A:946:VAL:HG23	3:A:947:PHE:H	1.71	0.55
3:A:1192:LEU:HD11	3:A:1239:ARG:HB3	1.87	0.55
5:C:54:ASN:OD1	5:C:55:THR:N	2.39	0.55
5:C:68:GLY:HA3	14:L:69:ALA:HB1	1.88	0.55
5:C:241:ASP:N	5:C:241:ASP:OD1	2.40	0.55
11:I:44:TYR:OH	11:I:46:HIS:ND1	2.40	0.55
7:E:201:LYS:HA	7:E:206:GLY:O	2.07	0.55
9:G:13:LEU:HD12	9:G:26:LEU:HD21	1.89	0.55
15:R:14:C:O2	15:R:14:C:C2'	2.55	0.55
3:A:44:THR:N	3:A:45:GLN:HA	2.22	0.54
3:A:848:ILE:HB	3:A:1065:GLY:HA3	1.90	0.54
3:A:337:ARG:HH21	3:A:839:ARG:CZ	2.20	0.54
3:A:1149:ALA:HB3	3:A:1196:GLU:HB3	1.89	0.54
4:B:277:LYS:HA	4:B:337:ARG:HH21	1.72	0.54
4:B:921:ASP:O	4:B:927:GLN:NE2	2.38	0.54
4:B:1156:ASP:CB	4:B:1198:TYR:H	2.19	0.54
5:C:184:ASN:ND2	5:C:189:THR:O	2.37	0.54
10:H:130:ARG:HB2	10:H:133:ASN:HB3	1.88	0.54
12:J:48:ARG:O	12:J:52:THR:HG22	2.07	0.54
13:K:9:LEU:HG	13:K:10:PHE:CD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:98:LEU:HD12	13:K:99:GLY:N	2.22	0.54
3:A:446:ARG:HD2	3:A:480:ALA:HB2	1.89	0.54
3:A:40:THR:O	3:A:50:ILE:N	2.38	0.54
3:A:535:THR:HG21	3:A:617:VAL:HG23	1.90	0.54
4:B:247:GLY:HA2	4:B:418:LYS:HE2	1.88	0.54
6:D:66:ARG:NH1	6:D:67:ARG:HH21	2.04	0.54
10:H:135:LEU:O	10:H:137:GLN:N	2.40	0.54
3:A:386:ASP:OD1	3:A:386:ASP:N	2.39	0.54
4:B:862:GLN:O	4:B:914:LYS:NZ	2.31	0.54
10:H:145:ARG:O	10:H:146:ARG:HD3	2.08	0.54
3:A:1052:GLN:HG2	3:A:1055:ARG:HH21	1.73	0.54
9:G:46:LEU:HD11	9:G:79:PHE:HB2	1.90	0.54
16:Q:377:SER:OG	17:M:67:GLN:O	2.24	0.54
3:A:918:GLU:OE1	3:A:918:GLU:N	2.35	0.54
5:C:66:ARG:HH22	12:J:5:VAL:HG23	1.73	0.54
5:C:73:GLN:OE1	5:C:75:MET:N	2.36	0.54
8:F:89:GLU:OE1	8:F:89:GLU:N	2.29	0.54
11:I:100:PHE:HB3	11:I:109:ILE:HD11	1.90	0.54
14:L:50:ASP:OD1	14:L:51:CYS:N	2.39	0.54
4:B:620:ARG:NH1	11:I:57:GLY:HA3	2.23	0.54
4:B:863:GLU:HG2	4:B:872:GLU:HB2	1.90	0.54
3:A:530:GLY:HA3	3:A:657:LEU:HD21	1.89	0.54
3:A:682:THR:O	3:A:685:GLU:HG3	2.07	0.54
5:C:50:GLU:HB2	5:C:156:THR:HB	1.89	0.54
7:E:171:LYS:O	7:E:173:SER:N	2.39	0.54
11:I:22:ASN:HB3	11:I:24:ARG:NH1	2.23	0.54
11:I:26:LEU:HD13	11:I:37:GLU:HA	1.90	0.54
12:J:32:GLU:OE1	12:J:32:GLU:N	2.33	0.54
1:N:-5:DA:H2"	1:N:-4:DG:C8	2.42	0.54
3:A:1000:LEU:N	3:A:1011:GLN:OE1	2.36	0.54
4:B:743:ILE:HG13	4:B:744:HIS:N	2.22	0.54
3:A:833:GLU:O	3:A:837:ILE:HD12	2.07	0.53
3:A:1445:ILE:HB	9:G:61:ILE:HD11	1.90	0.53
4:B:487:THR:OG1	4:B:777:ALA:O	2.25	0.53
6:D:125:SER:O	6:D:129:LEU:HG	2.07	0.53
8:F:70:LYS:O	8:F:71:GLU:HG3	2.07	0.53
13:K:12:LEU:HA	13:K:37:LYS:HG3	1.88	0.53
3:A:537:ARG:NH1	3:A:602:ASP:OD2	2.41	0.53
3:A:1319:VAL:HG13	3:A:1322:ILE:HG13	1.89	0.53
4:B:957:ASN:OD1	4:B:960:GLY:N	2.41	0.53
16:Q:98:TYR:CD1	16:Q:100:GLU:HG2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:363:GLY:HA2	16:Q:395:PHE:HA	1.89	0.53
17:M:117:PRO:HG3	17:M:233:TYR:HA	1.91	0.53
3:A:225:ASN:O	3:A:229:SER:N	2.35	0.53
3:A:443:LEU:HB2	3:A:501:LEU:HD11	1.90	0.53
7:E:100:ILE:HG23	7:E:105:PHE:HB2	1.90	0.53
9:G:94:CYS:HB2	9:G:127:PRO:HB2	1.89	0.53
16:Q:28:ARG:HE	16:Q:32:LEU:HD11	1.73	0.53
17:M:67:GLN:HB2	17:M:219:CYS:SG	2.49	0.53
17:M:96:ARG:HE	17:M:105:THR:HG22	1.72	0.53
3:A:1126:ALA:HA	3:A:1304:TRP:CD1	2.42	0.53
4:B:384:ARG:HE	4:B:387:LEU:HD12	1.74	0.53
4:B:1031:LEU:HD21	4:B:1042:GLY:HA3	1.89	0.53
7:E:48:ASP:OD1	7:E:49:SER:N	2.39	0.53
3:A:346:ASP:OD1	3:A:347:PHE:N	2.42	0.53
3:A:1002:GLY:HA3	3:A:1007:ILE:HG21	1.91	0.53
3:A:1430:LEU:HB3	3:A:1432:GLN:NE2	2.23	0.53
4:B:67:SER:HG	4:B:92:PHE:H	1.57	0.53
10:H:95:TYR:CE2	10:H:97:MET:HG2	2.44	0.53
3:A:957:PRO:HG2	3:A:1018:PHE:CD1	2.44	0.53
4:B:245:GLU:N	4:B:246:LYS:HA	2.24	0.53
4:B:580:VAL:HG22	4:B:624:LEU:HD23	1.89	0.53
2:O:-19:DC:H2"	2:O:-18:DA:C8	2.44	0.53
3:A:1359:ASP:OD1	3:A:1359:ASP:N	2.42	0.53
4:B:542:MET:CE	4:B:747:MET:HB3	2.37	0.53
11:I:17:ARG:N	11:I:26:LEU:O	2.37	0.53
3:A:851:HIS:CD2	8:F:139:PRO:HG3	2.44	0.53
4:B:696:GLU:OE1	4:B:696:GLU:N	2.41	0.53
10:H:118:PHE:O	10:H:120:GLY:N	2.42	0.53
4:B:355:ILE:O	4:B:359:GLU:HG3	2.09	0.53
4:B:830:TYR:CZ	4:B:1000:PRO:HD3	2.44	0.53
4:B:1041:GLU:N	16:Q:23:LYS:HZ1	2.06	0.53
3:A:113:LEU:O	3:A:164:ARG:NH2	2.42	0.52
3:A:851:HIS:CE1	3:A:857:ARG:HB2	2.43	0.52
3:A:857:ARG:NH1	8:F:139:PRO:HG2	2.24	0.52
3:A:1074:GLU:HG3	3:A:1075:PRO:HD3	1.91	0.52
7:E:3:GLN:OE1	7:E:4:GLU:HG3	2.09	0.52
3:A:619:LYS:NZ	15:R:18:A:OP2	2.42	0.52
6:D:52:LEU:HD12	6:D:148:LEU:HD23	1.92	0.52
9:G:116:PRO:HA	9:G:164:LYS:HZ3	1.73	0.52
3:A:92:HIS:HB2	3:A:236:LEU:HD23	1.92	0.52
3:A:381:THR:HG1	3:A:384:ASN:H	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:604:ARG:NH2	4:B:613:VAL:O	2.43	0.52
9:G:45:ILE:HG13	9:G:78:VAL:HG12	1.90	0.52
11:I:88:SER:O	11:I:91:ARG:NH1	2.38	0.52
4:B:680:THR:H	4:B:683:SER:HB2	1.74	0.52
4:B:860:MET:HB2	4:B:963:PHE:HE1	1.73	0.52
17:M:73:LEU:HD11	17:M:77:LEU:HD23	1.90	0.52
3:A:69:THR:HA	3:A:71:GLN:NE2	2.24	0.52
4:B:85:SER:O	4:B:87:LYS:N	2.42	0.52
4:B:120:ARG:HG2	4:B:955:THR:HG21	1.92	0.52
4:B:1080:LYS:HG2	5:C:180:TYR:OH	2.10	0.52
5:C:138:GLU:OE1	5:C:138:GLU:N	2.43	0.52
9:G:21:ARG:HH12	9:G:25:TYR:H	1.57	0.52
12:J:20:SER:HA	12:J:23:ASN:HD21	1.74	0.52
3:A:315:LEU:HD23	3:A:315:LEU:H	1.74	0.52
3:A:1166:ASP:HA	3:A:1169:ILE:HD13	1.92	0.52
4:B:546:SER:OG	4:B:631:GLY:N	2.43	0.52
4:B:745:PRO:HB2	4:B:1047:PHE:HD2	1.75	0.52
4:B:1165:ILE:HD12	4:B:1187:ASN:HD22	1.73	0.52
6:D:57:LEU:HD13	6:D:157:GLN:HG2	1.91	0.52
7:E:85:GLU:OE2	7:E:89:GLY:N	2.38	0.52
16:Q:121:PHE:HB2	17:M:131:ASN:HB3	1.92	0.52
3:A:821:ARG:NH2	4:B:534:GLY:HA2	2.25	0.52
7:E:170:LEU:HD12	7:E:174:GLN:HB2	1.92	0.52
13:K:53:ASP:OD1	13:K:54:ARG:N	2.43	0.52
3:A:106:VAL:HG21	3:A:214:ILE:HD12	1.91	0.52
3:A:852:TYR:CD1	3:A:1060:PRO:HB2	2.45	0.52
7:E:180:ARG:N	7:E:215:MET:OXT	2.42	0.52
17:M:73:LEU:HD12	17:M:74:PRO:HD2	1.92	0.52
3:A:566:ILE:HB	10:H:96:VAL:HG23	1.92	0.52
4:B:102:VAL:H	4:B:112:LEU:HD23	1.74	0.52
4:B:129:PHE:HB3	4:B:166:PHE:HA	1.90	0.52
4:B:189:LEU:HD21	4:B:196:PRO:HA	1.91	0.52
5:C:255:VAL:O	5:C:258:ILE:HG22	2.10	0.52
11:I:7:CYS:HB3	11:I:10:CYS:O	2.09	0.52
16:Q:116:THR:HG22	17:M:136:THR:HG22	1.92	0.52
17:M:96:ARG:NH2	17:M:98:ASN:OD1	2.43	0.52
4:B:62:ILE:HD13	4:B:417:PHE:HD2	1.75	0.52
4:B:217:ARG:NE	4:B:407:ASP:OD2	2.35	0.52
4:B:276:ILE:O	4:B:337:ARG:NH2	2.42	0.52
7:E:182:ASP:OD2	7:E:184:VAL:HG12	2.10	0.52
3:A:768:GLN:HE21	3:A:800:VAL:HG21	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:903:ASN:O	3:A:907:THR:OG1	2.28	0.51
3:A:909:ASP:HB3	3:A:912:LEU:HD13	1.92	0.51
3:A:1364:ASN:OD1	3:A:1365:TYR:N	2.43	0.51
3:A:1373:ASP:HA	3:A:1376:THR:HG22	1.92	0.51
4:B:496:ARG:O	4:B:497:ARG:NH1	2.42	0.51
4:B:640:VAL:HA	4:B:651:LEU:HA	1.91	0.51
4:B:1041:GLU:H	16:Q:23:LYS:HZ1	1.57	0.51
4:B:1082:MET:O	5:C:189:THR:OG1	2.20	0.51
16:Q:404:LEU:HB3	16:Q:408:GLU:OE2	2.10	0.51
3:A:1035:TYR:HB3	3:A:1037:LEU:HD23	1.91	0.51
4:B:73:GLN:HA	16:Q:330:ARG:NH2	2.25	0.51
10:H:33:GLN:OE1	10:H:34:ASP:N	2.43	0.51
13:K:110:ASN:HA	13:K:113:THR:HG23	1.93	0.51
17:M:106:LEU:N	17:M:120:TYR:O	2.27	0.51
3:A:589:GLN:HB3	3:A:591:PHE:CE2	2.45	0.51
4:B:29:ASP:HB3	4:B:658:ILE:HD13	1.92	0.51
9:G:116:PRO:HD3	9:G:163:ILE:HG13	1.91	0.51
11:I:113:ASP:OD1	11:I:115:LYS:NZ	2.40	0.51
1:N:17:DG:H2'	1:N:18:DT:C6	2.45	0.51
2:O:-2:DA:H2"	2:O:-1:DG:C8	2.46	0.51
3:A:172:PRO:HG3	3:A:185:TRP:CE2	2.46	0.51
3:A:590:ARG:NH1	3:A:621:THR:OG1	2.43	0.51
3:A:862:ASN:HA	7:E:174:GLN:HB3	1.92	0.51
7:E:96:PHE:CZ	7:E:100:ILE:HD11	2.45	0.51
7:E:118:PRO:HA	7:E:121:MET:HG3	1.92	0.51
3:A:1116:LEU:HD23	3:A:1311:VAL:HA	1.92	0.51
4:B:809:MET:HG3	4:B:814:PHE:HD1	1.76	0.51
4:B:922:GLU:HG2	4:B:926:GLY:HA3	1.92	0.51
7:E:87:SER:OG	7:E:88:VAL:N	2.43	0.51
9:G:10:ASN:HA	9:G:71:ASN:HA	1.91	0.51
16:Q:97:GLU:HA	17:M:99:LYS:HE3	1.92	0.51
16:Q:129:PRO:HA	16:Q:133:PHE:CD1	2.45	0.51
3:A:775:ILE:HD12	3:A:775:ILE:H	1.75	0.51
4:B:171:PRO:HG2	4:B:461:LEU:HD12	1.92	0.51
4:B:867:GLY:HA3	4:B:868:MET:O	2.10	0.51
7:E:40:GLU:OE1	7:E:40:GLU:N	2.43	0.51
3:A:108:MET:SD	3:A:171:GLN:HG3	2.50	0.51
3:A:567:LYS:HE3	10:H:95:TYR:HD1	1.75	0.51
3:A:1215:ARG:O	3:A:1218:GLN:NE2	2.43	0.51
4:B:629:ASP:OD1	4:B:632:ARG:NE	2.36	0.51
4:B:1065:GLN:NE2	4:B:1067:ARG:H	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:137:GLN:OE1	10:H:139:ASN:N	2.44	0.51
6:D:59:ILE:HG13	6:D:60:LYS:HD3	1.92	0.51
3:A:348:SER:HB3	4:B:1128:LEU:HD12	1.93	0.51
3:A:993:LEU:HD21	3:A:1046:LEU:HB3	1.92	0.51
3:A:1199:ARG:HD3	3:A:1236:LEU:HD11	1.93	0.51
3:A:1202:MET:HE3	3:A:1207:LEU:HB3	1.93	0.51
4:B:79:THR:CB	4:B:81:SER:H	2.24	0.51
4:B:406:LEU:HB2	4:B:545:ILE:HD11	1.93	0.51
8:F:93:ILE:HD11	8:F:132:LEU:HG	1.92	0.51
14:L:31:CYS:HB2	14:L:48:CYS:HB3	1.91	0.51
3:A:653:VAL:O	3:A:657:LEU:HD23	2.11	0.51
3:A:1426:GLU:OE2	3:A:1426:GLU:N	2.39	0.51
4:B:391:ASP:OD2	11:I:90:GLN:NE2	2.44	0.51
7:E:180:ARG:NH2	7:E:192:ARG:HB2	2.26	0.51
3:A:1062:GLU:OE1	3:A:1062:GLU:N	2.35	0.50
3:A:1277:GLU:N	3:A:1277:GLU:OE1	2.39	0.50
4:B:344:LYS:HZ2	4:B:347:LYS:HA	1.76	0.50
9:G:96:GLN:HA	9:G:128:PRO:HB2	1.93	0.50
4:B:216:GLU:HG2	4:B:500:THR:HB	1.92	0.50
4:B:546:SER:OG	4:B:632:ARG:N	2.33	0.50
10:H:13:SER:OG	10:H:27:GLU:OE2	2.28	0.50
3:A:1173:HIS:CE1	3:A:1227:ILE:HG23	2.47	0.50
4:B:195:CYS:HB3	4:B:782:LEU:HD22	1.94	0.50
5:C:6:PRO:HG2	13:K:101:LEU:HB2	1.94	0.50
10:H:26:ILE:N	10:H:40:LEU:O	2.38	0.50
3:A:40:THR:HB	3:A:54:ASN:HB2	1.93	0.50
3:A:542:GLU:OE1	3:A:544:ASP:N	2.33	0.50
3:A:802:ASN:ND2	3:A:806:ARG:HB2	2.17	0.50
4:B:526:GLU:OE2	4:B:752:ALA:N	2.45	0.50
7:E:43:LYS:HE3	7:E:47:CYS:HB2	1.94	0.50
7:E:141:VAL:HG13	7:E:142:VAL:HG23	1.94	0.50
10:H:37:LYS:H	10:H:126:GLU:HB2	1.77	0.50
16:Q:390:ASP:OD1	16:Q:391:LYS:N	2.44	0.50
3:A:668:ASP:OD2	3:A:742:ASN:HB2	2.11	0.50
3:A:942:PHE:HD2	3:A:943:LEU:HD22	1.75	0.50
4:B:212:LEU:HD11	4:B:409:ALA:HB2	1.94	0.50
4:B:360:PHE:HE2	4:B:374:LYS:HD2	1.76	0.50
5:C:161:LYS:O	5:C:170:TRP:NE1	2.44	0.50
6:D:31:GLN:O	6:D:34:GLN:NE2	2.44	0.50
16:Q:17:ASN:HB3	16:Q:20:PRO:HD3	1.93	0.50
4:B:604:ARG:NH2	4:B:614:SER:HA	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:835:GLN:OE1	4:B:835:GLN:N	2.39	0.50
4:B:360:PHE:CE2	4:B:374:LYS:HD2	2.46	0.50
4:B:793:ALA:HB3	4:B:856:PHE:HB2	1.94	0.50
4:B:992:ILE:HD11	4:B:994:TYR:CZ	2.47	0.50
8:F:140:ASP:OD1	8:F:141:GLY:N	2.45	0.50
3:A:402:ALA:HA	3:A:434:ARG:HA	1.94	0.50
4:B:121:ASN:HA	4:B:207:GLY:HA3	1.94	0.50
4:B:247:GLY:O	4:B:249:ARG:N	2.44	0.50
4:B:604:ARG:HH22	4:B:614:SER:HA	1.77	0.50
4:B:910:VAL:HA	4:B:940:PRO:HA	1.93	0.50
5:C:73:GLN:OE1	5:C:74:SER:N	2.45	0.50
12:J:9:SER:HB2	12:J:45:CYS:HB2	1.94	0.50
3:A:665:GLY:O	3:A:668:ASP:HB2	2.12	0.49
4:B:582:VAL:HG22	4:B:626:ILE:HB	1.93	0.49
6:D:14:ARG:O	6:D:17:LYS:HG3	2.12	0.49
15:R:12:A:H2'	15:R:13:U:C6	2.47	0.49
3:A:325:ILE:HG13	4:B:1210:MET:CE	2.42	0.49
3:A:864:ILE:HD12	3:A:1377:THR:HG21	1.94	0.49
3:A:877:HIS:CD2	3:A:1056:SER:HA	2.47	0.49
3:A:1157:ASP:OD1	3:A:1160:SER:N	2.45	0.49
4:B:25:ILE:HG23	4:B:29:ASP:HB2	1.94	0.49
4:B:800:GLN:OE1	12:J:53:HIS:HA	2.12	0.49
4:B:900:ALA:HB1	14:L:61:THR:OG1	2.12	0.49
5:C:258:ILE:HD11	13:K:35:PHE:CZ	2.47	0.49
7:E:106:GLN:HG2	7:E:107:THR:HG23	1.93	0.49
2:O:-12:DT:OP2	3:A:332:LYS:NZ	2.45	0.49
3:A:147:VAL:HG23	3:A:170:THR:HG22	1.93	0.49
3:A:1138:ILE:HD11	3:A:1316:VAL:HG12	1.93	0.49
4:B:279:ASP:OD1	4:B:279:ASP:N	2.46	0.49
4:B:325:GLN:O	16:Q:401:TYR:OH	2.30	0.49
4:B:365:THR:HG22	4:B:374:LYS:HZ3	1.78	0.49
4:B:648:HIS:CD2	4:B:648:HIS:H	2.29	0.49
7:E:21:GLU:OE2	7:E:143:ASN:ND2	2.46	0.49
11:I:76:PRO:O	11:I:77:LYS:HD3	2.12	0.49
1:N:17:DG:H2'	1:N:18:DT:H71	1.95	0.49
3:A:35:ILE:HD12	3:A:35:ILE:H	1.77	0.49
5:C:7:GLN:HA	13:K:104:ASN:ND2	2.27	0.49
10:H:95:TYR:HB3	10:H:144:ILE:HB	1.94	0.49
4:B:373:ARG:NE	4:B:566:LEU:HB2	2.28	0.49
11:I:54:GLU:HB2	11:I:100:PHE:CE2	2.48	0.49
3:A:66:LYS:HE2	3:A:69:THR:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:446:ARG:HB2	3:A:487:MET:SD	2.52	0.49
5:C:102:GLN:HE22	5:C:154:LYS:HA	1.78	0.49
6:D:53:SER:O	6:D:57:LEU:HG	2.12	0.49
3:A:808:LEU:O	4:B:728:ARG:NH1	2.46	0.49
4:B:336:ARG:HG3	4:B:337:ARG:H	1.78	0.49
4:B:1171:VAL:HG11	4:B:1191:ILE:HD13	1.94	0.49
4:B:1196:ILE:HD12	4:B:1197:PRO:HD2	1.94	0.49
5:C:146:LYS:HD2	12:J:57:ILE:HD12	1.95	0.49
6:D:216:ASN:OD1	6:D:217:LEU:N	2.46	0.49
3:A:311:GLN:CG	3:A:312:PRO:HD3	2.41	0.49
2:O:2:DC:H2"	2:O:3:DA:C8	2.48	0.49
3:A:5:GLN:HG3	4:B:1175:LEU:HD13	1.95	0.49
3:A:594:GLY:HA3	3:A:603:ASN:HD21	1.77	0.49
3:A:675:THR:HG21	3:A:736:ASN:HB2	1.95	0.49
3:A:1165:GLU:N	3:A:1165:GLU:OE1	2.44	0.49
4:B:123:THR:O	4:B:125:SER:N	2.45	0.49
4:B:327:ARG:HG3	4:B:328:GLU:OE1	2.13	0.49
5:C:35:ARG:HA	5:C:38:ILE:HG22	1.94	0.49
5:C:252:GLN:HB3	13:K:98:LEU:HD13	1.95	0.49
4:B:822:ASN:HA	4:B:1091:TYR:HA	1.94	0.49
6:D:55:ALA:HA	6:D:58:VAL:HG22	1.95	0.49
7:E:20:LYS:HD2	7:E:35:VAL:HA	1.95	0.49
3:A:171:GLN:N	3:A:171:GLN:OE1	2.44	0.48
3:A:232:GLU:OE1	3:A:232:GLU:N	2.43	0.48
3:A:766:GLY:HA2	3:A:799:PHE:HE1	1.78	0.48
3:A:1332:PHE:HA	3:A:1335:ILE:HD13	1.94	0.48
4:B:78:THR:HG23	4:B:79:THR:H	1.78	0.48
8:F:97:ARG:O	8:F:101:ILE:HG12	2.12	0.48
10:H:145:ARG:C	10:H:146:ARG:HD3	2.33	0.48
12:J:8:PHE:H	12:J:49:MET:HE1	1.77	0.48
3:A:509:LEU:HD23	3:A:509:LEU:H	1.78	0.48
4:B:260:GLY:O	4:B:267:ARG:NH2	2.38	0.48
5:C:66:ARG:NH2	12:J:5:VAL:HG23	2.27	0.48
3:A:744:LYS:O	3:A:748:MET:HG3	2.13	0.48
4:B:405:ARG:NE	4:B:629:ASP:OD2	2.38	0.48
5:C:54:ASN:ND2	5:C:60:ASP:OD1	2.23	0.48
5:C:99:LEU:HD11	5:C:120:ILE:HD13	1.94	0.48
5:C:249:ASP:O	5:C:252:GLN:NE2	2.46	0.48
10:H:105:GLU:O	10:H:113:ALA:N	2.41	0.48
3:A:172:PRO:HG3	3:A:185:TRP:CZ2	2.49	0.48
3:A:261:ASP:OD1	3:A:322:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:960:ILE:O	3:A:963:ILE:HG22	2.14	0.48
3:A:972:HIS:O	3:A:972:HIS:ND1	2.47	0.48
3:A:1116:LEU:HG	3:A:1308:THR:HG21	1.96	0.48
4:B:308:TRP:O	4:B:311:LEU:N	2.47	0.48
4:B:868:MET:O	4:B:870:ILE:N	2.47	0.48
11:I:87:GLN:HE22	11:I:91:ARG:NH1	2.11	0.48
13:K:24:ASP:OD1	13:K:25:THR:N	2.46	0.48
2:O:-14:DT:H4'	2:O:-14:DT:OP1	2.13	0.48
3:A:114:LEU:C	3:A:164:ARG:HH22	2.16	0.48
3:A:118:HIS:HA	3:A:123:ARG:NH2	2.29	0.48
3:A:120:GLU:O	3:A:123:ARG:HB2	2.13	0.48
3:A:673:GLY:O	3:A:676:MET:HG3	2.13	0.48
4:B:104:GLU:OE1	4:B:104:GLU:N	2.43	0.48
4:B:980:PHE:CE1	4:B:1094:ARG:HG3	2.46	0.48
3:A:399:HIS:O	3:A:401:GLY:N	2.45	0.48
3:A:1208:THR:H	3:A:1211:GLN:NE2	2.11	0.48
4:B:428:ILE:HA	4:B:445:LYS:HE3	1.96	0.48
4:B:1106:ARG:HH22	4:B:1111:MET:HE1	1.77	0.48
5:C:167:HIS:ND1	5:C:169:LYS:HG3	2.28	0.48
9:G:49:LEU:HG	9:G:76:ALA:HA	1.96	0.48
3:A:118:HIS:HA	3:A:123:ARG:HH22	1.78	0.48
3:A:1443:VAL:HG12	9:G:61:ILE:HD13	1.94	0.48
4:B:400:HIS:HB3	4:B:403:LYS:HZ3	1.78	0.48
4:B:806:THR:H	4:B:809:MET:HE1	1.79	0.48
6:D:67:ARG:NE	6:D:129:LEU:HD22	2.29	0.48
10:H:118:PHE:N	10:H:121:LEU:O	2.39	0.48
3:A:65:LEU:O	3:A:71:GLN:HA	2.13	0.48
3:A:346:ASP:OD2	4:B:1108:ARG:N	2.34	0.48
3:A:1111:MET:C	3:A:1113:THR:H	2.17	0.48
4:B:400:HIS:CE1	4:B:402:GLY:H	2.31	0.48
4:B:444:MET:SD	4:B:445:LYS:N	2.87	0.48
5:C:252:GLN:HB3	13:K:98:LEU:CD1	2.44	0.48
1:N:-6:DT:H2"	1:N:-5:DA:C8	2.48	0.48
3:A:839:ARG:NH2	3:A:1403:GLU:OE2	2.35	0.48
3:A:878:ILE:HA	3:A:956:LEU:O	2.13	0.48
3:A:1254:ALA:N	3:A:1256:GLU:OE2	2.47	0.48
4:B:706:GLN:OE1	4:B:707:PRO:HD2	2.14	0.48
17:M:239:GLN:O	17:M:243:ILE:HG12	2.13	0.48
1:N:22:DA:H2"	1:N:23:DA:OP2	2.14	0.47
3:A:1191:TRP:CZ3	11:I:43:VAL:HG21	2.49	0.47
3:A:1444:MET:HG3	9:G:58:ARG:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:313:MET:HE1	4:B:390:LEU:HD13	1.96	0.47
5:C:148:ARG:N	5:C:151:GLN:OE1	2.23	0.47
9:G:125:SER:HB3	9:G:128:PRO:HA	1.95	0.47
13:K:35:PHE:HD2	13:K:71:PHE:CZ	2.32	0.47
15:R:13:U:H5"	15:R:14:C:C5'	2.43	0.47
3:A:567:LYS:HE2	10:H:95:TYR:HA	1.96	0.47
4:B:124:TYR:O	4:B:172:ILE:HG22	2.14	0.47
6:D:53:SER:OG	6:D:152:SER:HB3	2.13	0.47
3:A:115:LEU:HA	3:A:164:ARG:HH12	1.78	0.47
7:E:108:GLY:N	7:E:131:THR:O	2.35	0.47
15:R:17:A:O5'	15:R:17:A:H8	1.97	0.47
3:A:121:LEU:HD12	3:A:124:GLN:NE2	2.28	0.47
3:A:528:LEU:HD22	3:A:751:SER:HB3	1.95	0.47
3:A:843:LYS:NZ	3:A:1401:SER:O	2.44	0.47
3:A:1156:PRO:HA	3:A:1190:PRO:HB2	1.96	0.47
3:A:1312:ASN:OD1	3:A:1313:LEU:N	2.47	0.47
4:B:190:TYR:CE2	4:B:196:PRO:HD3	2.43	0.47
4:B:522:VAL:HG21	4:B:537:LYS:HB2	1.95	0.47
6:D:64:VAL:HG23	6:D:68:ARG:NH2	2.26	0.47
1:N:2:DT:H5"	1:N:2:DT:H6	1.80	0.47
3:A:217:LYS:O	3:A:220:THR:OG1	2.28	0.47
4:B:211:VAL:HG21	4:B:483:LEU:HD13	1.95	0.47
9:G:131:GLN:HB2	9:G:136:VAL:HG22	1.96	0.47
3:A:33:ALA:HA	3:A:57:ARG:HH22	1.79	0.47
3:A:219:PHE:HB3	3:A:224:PHE:HB2	1.96	0.47
3:A:1077:THR:OG1	3:A:1078:GLN:OE1	2.29	0.47
4:B:20:ASP:OD1	4:B:22:SER:N	2.41	0.47
4:B:277:LYS:HE3	4:B:278:GLN:NE2	2.29	0.47
4:B:604:ARG:NH2	4:B:615:MET:SD	2.87	0.47
4:B:848:ARG:NH1	12:J:8:PHE:O	2.38	0.47
7:E:185:ALA:O	7:E:189:GLY:N	2.47	0.47
11:I:69:PRO:HB2	11:I:85:PHE:CE1	2.50	0.47
16:Q:407:ASP:HB3	16:Q:411:LYS:NZ	2.30	0.47
2:O:-31:DT:H2"	2:O:-30:DT:C6	2.49	0.47
3:A:1102:LYS:O	3:A:1106:ASN:CB	2.63	0.47
6:D:126:ILE:HD13	6:D:145:MET:HG3	1.96	0.47
7:E:32:GLN:O	7:E:35:VAL:HG22	2.15	0.47
8:F:97:ARG:HD2	8:F:100:GLN:NE2	2.25	0.47
9:G:6:ASP:HA	9:G:75:ARG:HA	1.96	0.47
1:N:-9:DC:H2"	1:N:-8:DA:C8	2.49	0.47
3:A:923:LEU:O	3:A:927:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:801:LYS:O	12:J:52:THR:OG1	2.18	0.47
5:C:134:ILE:HG13	5:C:134:ILE:O	2.15	0.47
6:D:139:LYS:HD2	6:D:142:LYS:HD2	1.96	0.47
3:A:679:ILE:HD11	3:A:732:LEU:HB3	1.96	0.47
3:A:1417:GLU:OE1	3:A:1417:GLU:N	2.46	0.47
10:H:17:PRO:HA	10:H:24:CYS:SG	2.54	0.47
3:A:18:GLN:O	4:B:1215:ARG:N	2.48	0.46
3:A:807:GLY:O	4:B:728:ARG:NH1	2.49	0.46
3:A:1102:LYS:O	3:A:1106:ASN:HB3	2.13	0.46
4:B:183:GLU:N	4:B:183:GLU:OE1	2.48	0.46
6:D:56:ARG:HH12	6:D:155:ARG:HE	1.62	0.46
8:F:108:PHE:HE1	8:F:131:PRO:HG3	1.79	0.46
10:H:41:ASP:OD2	10:H:122:LEU:N	2.44	0.46
10:H:102:TYR:CZ	10:H:115:TYR:HB3	2.50	0.46
17:M:73:LEU:HD23	17:M:78:ALA:HA	1.97	0.46
3:A:1159:ARG:HH11	3:A:1185:PHE:HB3	1.81	0.46
4:B:593:PRO:HG2	4:B:617:ARG:NH2	2.30	0.46
4:B:1100:ASP:OD1	4:B:1101:ASP:N	2.49	0.46
5:C:102:GLN:HE22	5:C:154:LYS:HG2	1.81	0.46
3:A:95:PHE:O	3:A:99:ILE:HG13	2.16	0.46
3:A:360:GLU:OE1	3:A:360:GLU:N	2.40	0.46
3:A:891:ALA:HA	3:A:894:GLU:OE2	2.15	0.46
4:B:449:ASN:O	4:B:452:THR:OG1	2.27	0.46
4:B:526:GLU:HB3	4:B:538:ASN:HD22	1.80	0.46
6:D:14:ARG:HB2	6:D:17:LYS:HE2	1.98	0.46
7:E:112:TYR:CE2	7:E:136:ASN:HB2	2.51	0.46
13:K:49:GLU:OE1	13:K:90:ALA:HB1	2.15	0.46
2:O:-19:DC:H2"	2:O:-18:DA:OP2	2.16	0.46
3:A:33:ALA:HB3	3:A:82:GLY:HA3	1.96	0.46
3:A:457:ALA:HB3	3:A:506:ALA:HA	1.98	0.46
3:A:722:LEU:HD12	3:A:799:PHE:CE1	2.51	0.46
4:B:304:ASP:OD2	4:B:307:ASP:N	2.45	0.46
4:B:408:LEU:HG	4:B:409:ALA:H	1.80	0.46
4:B:450:ALA:HA	4:B:453:ILE:HG22	1.96	0.46
9:G:111:THR:HB	9:G:114:LEU:HD13	1.96	0.46
9:G:165:GLU:O	9:G:168:LEU:HB3	2.15	0.46
10:H:116:TYR:HB2	10:H:123:MET:SD	2.55	0.46
3:A:474:VAL:O	3:A:477:PRO:HD2	2.14	0.46
3:A:1042:PHE:O	3:A:1045:VAL:HG12	2.14	0.46
4:B:104:GLU:HG3	14:L:54:ARG:HH12	1.80	0.46
4:B:431:TYR:HD2	4:B:445:LYS:HD2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:181:ASP:OD2	5:C:184:ASN:N	2.49	0.46
10:H:124:ARG:NE	10:H:126:GLU:OE1	2.48	0.46
1:N:15:DT:H2"	1:N:16:DA:C8	2.51	0.46
2:O:-15:DA:H5"	3:A:1386:ARG:HD3	1.96	0.46
3:A:928:LEU:O	3:A:931:GLU:HG3	2.16	0.46
3:A:1293:SER:N	3:A:1297:GLU:O	2.31	0.46
4:B:424:LEU:CD1	4:B:449:ASN:HB3	2.45	0.46
4:B:526:GLU:CB	4:B:538:ASN:HD22	2.28	0.46
4:B:874:PHE:HD1	4:B:962:LYS:HD3	1.81	0.46
5:C:186:LEU:HB3	5:C:188:HIS:CD2	2.51	0.46
12:J:55:ASP:O	12:J:56:LEU:HD23	2.16	0.46
3:A:62:ASP:OD1	3:A:62:ASP:N	2.49	0.46
4:B:246:LYS:NZ	4:B:415:GLN:OE1	2.31	0.46
15:R:16:C:H3'	15:R:16:C:H6	1.80	0.46
17:M:63:ARG:HH22	17:M:66:ARG:NH1	2.13	0.46
3:A:1239:ARG:HH22	3:A:1241:ARG:HH21	1.63	0.46
4:B:1222:ARG:O	4:B:1222:ARG:NE	2.48	0.46
6:D:25:ALA:HA	6:D:175:PHE:HE2	1.80	0.46
17:M:81:TRP:N	17:M:81:TRP:CD1	2.84	0.46
3:A:439:ASN:N	3:A:460:VAL:O	2.33	0.46
3:A:560:ILE:HD11	10:H:79:TRP:O	2.16	0.46
3:A:563:PRO:HA	3:A:572:TRP:NE1	2.31	0.46
4:B:803:LEU:HG	4:B:822:ASN:HD22	1.81	0.46
5:C:71:PRO:HB2	5:C:133:ILE:HD13	1.97	0.46
5:C:91:HIS:HB2	5:C:96:SER:HB2	1.98	0.46
10:H:83:GLN:OE1	13:K:54:ARG:NH2	2.48	0.46
2:O:2:DC:H2"	2:O:3:DA:H8	1.79	0.46
3:A:346:ASP:OD1	4:B:1107:ALA:HA	2.15	0.46
3:A:443:LEU:HD12	3:A:444:PHE:H	1.81	0.46
5:C:35:ARG:HE	13:K:41:THR:HB	1.81	0.46
3:A:50:ILE:HG23	3:A:52:GLY:H	1.81	0.45
4:B:1187:ASN:ND2	4:B:1190:ASP:HB3	2.31	0.45
6:D:56:ARG:HD3	6:D:149:THR:HA	1.97	0.45
6:D:123:LEU:HA	6:D:145:MET:HE2	1.99	0.45
3:A:372:LYS:HD2	13:K:2:ASN:HB3	1.99	0.45
3:A:530:GLY:CA	3:A:657:LEU:HD21	2.45	0.45
3:A:563:PRO:HD2	10:H:79:TRP:CD1	2.51	0.45
4:B:345:LYS:N	4:B:348:ARG:HH21	2.14	0.45
4:B:839:MET:HG2	4:B:1010:LEU:HD12	1.97	0.45
4:B:901:PRO:HA	4:B:949:VAL:HG12	1.97	0.45
5:C:42:PRO:HB3	5:C:161:LYS:HZ1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:56:THR:HG23	5:C:58:LEU:H	1.80	0.45
9:G:21:ARG:NH1	9:G:24:GLN:HB2	2.31	0.45
3:A:85:ASP:O	3:A:273:ASN:ND2	2.47	0.45
3:A:98:LYS:O	3:A:102:VAL:HG23	2.16	0.45
4:B:1065:GLN:HE22	4:B:1067:ARG:HB2	1.82	0.45
5:C:11:ARG:HD3	5:C:19:ASP:HB3	1.98	0.45
5:C:104:PHE:HA	5:C:152:GLU:OE1	2.16	0.45
3:A:1282:VAL:HG12	3:A:1308:THR:HA	1.98	0.45
4:B:247:GLY:C	4:B:249:ARG:H	2.20	0.45
4:B:542:MET:HE1	4:B:747:MET:CB	2.42	0.45
9:G:62:LEU:HD12	9:G:63:PRO:HD2	1.97	0.45
3:A:727:ASP:OD1	3:A:728:LYS:N	2.50	0.45
3:A:737:LEU:HD11	3:A:741:ASN:ND2	2.31	0.45
3:A:826:ASP:HA	4:B:508:LEU:HD11	1.99	0.45
3:A:1116:LEU:H	3:A:1308:THR:HG22	1.82	0.45
3:A:1198:ASP:HB3	3:A:1201:ALA:HB3	1.99	0.45
4:B:976:ILE:O	4:B:990:ILE:HB	2.17	0.45
3:A:1143:LEU:O	3:A:1147:THR:N	2.50	0.45
3:A:1390:ASN:ND2	3:A:1402:PHE:HB3	2.32	0.45
3:A:1399:ARG:NH1	3:A:1408:ILE:HD11	2.32	0.45
4:B:216:GLU:CG	4:B:500:THR:HB	2.46	0.45
4:B:278:GLN:OE1	4:B:335:GLY:HA2	2.17	0.45
4:B:281:PRO:HD2	4:B:284:ILE:HD12	1.99	0.45
4:B:637:LEU:HD12	4:B:693:ILE:HG13	1.98	0.45
4:B:1073:TYR:CE1	4:B:1080:LYS:HD2	2.52	0.45
6:D:152:SER:O	6:D:221:TYR:OH	2.31	0.45
7:E:55:ARG:HB2	7:E:84:ASP:OD1	2.16	0.45
9:G:56:ILE:HG22	9:G:72:VAL:HG22	1.98	0.45
11:I:21:GLU:HG2	11:I:22:ASN:N	2.32	0.45
11:I:28:GLU:HB3	11:I:35:VAL:HG23	1.97	0.45
16:Q:118:LEU:HB3	16:Q:392:VAL:HG22	1.99	0.45
3:A:1330:ASN:OD1	3:A:1331:SER:N	2.50	0.45
4:B:259:TYR:O	4:B:267:ARG:NH2	2.50	0.45
4:B:438:GLU:HA	4:B:439:ALA:HA	1.68	0.45
4:B:1072:MET:HE3	4:B:1073:TYR:H	1.82	0.45
9:G:110:VAL:HG11	9:G:163:ILE:HG12	1.98	0.45
10:H:18:GLY:O	10:H:19:ARG:HG2	2.17	0.45
3:A:1112:LYS:HD2	3:A:1112:LYS:HA	1.85	0.45
4:B:810:GLU:HG3	16:Q:24:ARG:HH22	1.82	0.45
3:A:821:ARG:HH21	4:B:534:GLY:HA2	1.81	0.45
4:B:344:LYS:HZ2	4:B:348:ARG:H	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:363:HIS:HD2	4:B:364:ILE:HG23	1.80	0.45
5:C:11:ARG:NH2	5:C:209:TYR:OH	2.40	0.45
13:K:60:ALA:O	13:K:73:LEU:HD12	2.16	0.45
17:M:200:ARG:HD2	17:M:201:TYR:N	2.32	0.45
1:N:16:DA:H2'	1:N:17:DG:C8	2.52	0.45
3:A:1361:SER:HA	3:A:1362:TYR:HA	1.63	0.45
4:B:1106:ARG:HH22	4:B:1111:MET:CE	2.30	0.45
7:E:92:THR:O	7:E:95:THR:OG1	2.29	0.45
9:G:21:ARG:NH2	9:G:25:TYR:HB2	2.26	0.45
12:J:16:ASP:OD1	12:J:17:LYS:N	2.50	0.45
14:L:31:CYS:HA	14:L:56:LEU:HD23	1.99	0.45
1:N:24:DA:H2"	1:N:25:DA:C8	2.52	0.44
3:A:1329:THR:HG22	3:A:1331:SER:H	1.82	0.44
6:D:54:GLU:HA	6:D:57:LEU:HD12	2.00	0.44
14:L:30:ILE:HA	14:L:36:SER:O	2.16	0.44
16:Q:100:GLU:OE1	17:M:94:LYS:HB3	2.17	0.44
3:A:791:ASP:OD1	3:A:792:TYR:N	2.51	0.44
3:A:868:TYR:CD1	3:A:1058:VAL:HG21	2.45	0.44
4:B:89:GLU:HG3	4:B:159:ASP:OD1	2.17	0.44
4:B:139:ALA:N	4:B:150:GLU:O	2.50	0.44
4:B:995:ARG:HB2	4:B:997:GLU:OE2	2.18	0.44
7:E:180:ARG:HH21	7:E:192:ARG:HB2	1.81	0.44
10:H:7:ASP:OD1	10:H:8:ASP:N	2.51	0.44
10:H:12:VAL:HG21	10:H:26:ILE:HD11	1.99	0.44
12:J:19:GLU:OE1	12:J:19:GLU:N	2.40	0.44
17:M:98:ASN:OD1	17:M:103:LYS:HB3	2.16	0.44
3:A:455:MET:HG3	4:B:1137:CYS:SG	2.58	0.44
4:B:843:GLN:NE2	4:B:847:ASP:OD1	2.50	0.44
5:C:6:PRO:HA	5:C:24:ASN:HB2	1.98	0.44
5:C:142:VAL:HG21	12:J:5:VAL:HG22	1.99	0.44
5:C:148:ARG:HG2	12:J:61:LEU:HG	1.98	0.44
9:G:3:PHE:HE2	9:G:82:PHE:HE2	1.64	0.44
9:G:14:HIS:CG	9:G:15:PRO:HD2	2.52	0.44
9:G:90:THR:OG1	9:G:141:SER:OG	2.25	0.44
10:H:137:GLN:CD	10:H:138:GLU:H	2.20	0.44
12:J:18:TRP:CZ2	12:J:22:LEU:HD21	2.52	0.44
3:A:678:GLU:HA	3:A:681:GLU:HG3	1.99	0.44
3:A:764:CYS:SG	3:A:765:VAL:N	2.90	0.44
4:B:68:THR:HG21	16:Q:334:VAL:HB	2.00	0.44
4:B:1010:LEU:HD11	4:B:1092:TYR:CE2	2.49	0.44
4:B:1032:SER:OG	4:B:1089:PRO:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:40:GLU:N	5:C:40:GLU:OE1	2.51	0.44
5:C:62:PHE:O	5:C:66:ARG:HG3	2.17	0.44
6:D:72:ARG:HB3	6:D:76:LYS:NZ	2.32	0.44
10:H:109:LYS:O	10:H:109:LYS:HD3	2.17	0.44
3:A:928:LEU:HD13	3:A:987:VAL:HG11	2.00	0.44
4:B:1163:CYS:HB3	4:B:1166:CYS:HB2	1.89	0.44
7:E:121:MET:HA	7:E:124:VAL:HG23	1.99	0.44
7:E:169:ARG:NH2	8:F:140:ASP:OD2	2.50	0.44
10:H:135:LEU:HD22	10:H:137:GLN:HB2	1.99	0.44
16:Q:23:LYS:HA	16:Q:23:LYS:HD3	1.87	0.44
3:A:545:GLN:O	3:A:549:MET:HG2	2.17	0.44
3:A:965:GLN:HA	3:A:968:GLN:OE1	2.17	0.44
3:A:1063:MET:SD	3:A:1436:ILE:HD12	2.58	0.44
3:A:1209:MET:HE1	3:A:1229:SER:N	2.33	0.44
3:A:1259:MET:SD	3:A:1260:LEU:N	2.91	0.44
4:B:174:LEU:HA	4:B:174:LEU:HD23	1.73	0.44
4:B:237:VAL:HG12	4:B:257:LYS:HG2	2.00	0.44
4:B:343:ILE:HD12	4:B:343:ILE:H	1.83	0.44
4:B:953:LEU:HD21	4:B:965:LYS:HB2	1.99	0.44
6:D:209:ARG:HA	6:D:212:LYS:NZ	2.33	0.44
9:G:116:PRO:HA	9:G:164:LYS:NZ	2.32	0.44
1:N:4:DA:H5’	1:N:5:DA:H5’	1.99	0.44
2:O:-28:DG:H2’	2:O:-27:DT:H71	2.00	0.44
3:A:890:ASP:O	3:A:893:PHE:HB3	2.18	0.44
4:B:43:LEU:O	4:B:496:ARG:NH2	2.51	0.44
4:B:344:LYS:HA	4:B:348:ARG:HE	1.82	0.44
4:B:803:LEU:HG	4:B:822:ASN:ND2	2.33	0.44
4:B:929:THR:HG23	4:B:931:TYR:HB2	1.99	0.44
5:C:162:GLY:HA3	5:C:170:TRP:CD2	2.53	0.44
7:E:13:TRP:CE3	7:E:39:LEU:HD12	2.52	0.44
7:E:48:ASP:OD1	7:E:52:ARG:HB2	2.18	0.44
7:E:153:HIS:CD2	7:E:184:VAL:HG21	2.52	0.44
7:E:154:ILE:CG2	7:E:197:LYS:HB3	2.48	0.44
14:L:51:CYS:HB3	14:L:53:HIS:ND1	2.33	0.44
16:Q:120:LYS:HB3	16:Q:394:LYS:HA	1.99	0.44
3:A:311:GLN:HG2	3:A:312:PRO:CD	2.46	0.44
3:A:946:VAL:HG23	3:A:947:PHE:N	2.32	0.44
4:B:102:VAL:HB	4:B:112:LEU:HD21	2.00	0.44
4:B:223:VAL:HG22	4:B:240:ILE:HD11	2.00	0.44
4:B:350:GLN:HA	4:B:353:LYS:HG2	1.99	0.44
4:B:689:LEU:HD23	4:B:689:LEU:HA	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:778:MET:HE1	4:B:1094:ARG:HH11	1.83	0.44
4:B:996:ARG:HG3	4:B:1007:VAL:HG11	2.00	0.44
7:E:23:VAL:HG13	7:E:78:LEU:HD21	1.99	0.44
9:G:7:LEU:HD22	9:G:74:TYR:OH	2.18	0.44
9:G:165:GLU:HB3	9:G:168:LEU:HD23	2.00	0.44
16:Q:119:LEU:HD21	16:Q:121:PHE:CE1	2.52	0.44
3:A:337:ARG:HE	3:A:839:ARG:HH22	1.66	0.44
3:A:353:ILE:HG22	3:A:468:PHE:HB2	1.99	0.44
3:A:1207:LEU:CD1	3:A:1211:GLN:HE21	2.31	0.44
3:A:1326:ARG:HA	7:E:148:GLU:OE2	2.18	0.44
4:B:328:GLU:HA	4:B:331:LEU:HD12	2.00	0.44
4:B:882:THR:HB	4:B:885:MET:HB3	2.00	0.44
5:C:148:ARG:HG3	5:C:148:ARG:O	2.17	0.44
6:D:52:LEU:HG	6:D:148:LEU:HA	1.98	0.44
17:M:105:THR:HA	17:M:121:ASP:HA	1.99	0.44
2:O:-3:DA:C2	3:A:252:PHE:CD2	3.06	0.43
3:A:314:ALA:O	3:A:322:VAL:HG12	2.17	0.43
3:A:346:ASP:CG	4:B:1108:ARG:H	2.17	0.43
3:A:368:LYS:NZ	13:K:4:PRO:HD3	2.25	0.43
3:A:543:LEU:HD22	3:A:572:TRP:HZ3	1.83	0.43
4:B:431:TYR:HA	4:B:434:ARG:HB3	2.00	0.43
4:B:573:GLN:N	4:B:573:GLN:OE1	2.51	0.43
6:D:63:LEU:O	6:D:66:ARG:HG3	2.17	0.43
17:M:225:MET:SD	17:M:226:PRO:HD2	2.58	0.43
3:A:513:SER:HB3	3:A:520:CYS:HB3	1.99	0.43
3:A:1293:SER:HB3	3:A:1297:GLU:H	1.83	0.43
4:B:128:LEU:HD11	4:B:170:LEU:HG	2.00	0.43
5:C:187:LYS:HB2	5:C:219:PHE:HE1	1.82	0.43
7:E:88:VAL:HG11	7:E:116:ILE:HG23	1.99	0.43
10:H:96:VAL:HG12	10:H:143:LEU:HD22	2.00	0.43
16:Q:128:ASN:HB3	16:Q:131:THR:OG1	2.18	0.43
16:Q:326:ARG:HD3	16:Q:326:ARG:HA	1.80	0.43
2:O:-2:DA:H2"	2:O:-1:DG:N7	2.33	0.43
3:A:108:MET:C	3:A:110:CYS:H	2.21	0.43
3:A:956:LEU:HD23	3:A:956:LEU:HA	1.87	0.43
4:B:51:PHE:CG	4:B:173:MET:HB2	2.53	0.43
5:C:235:VAL:HG13	5:C:237:SER:H	1.82	0.43
7:E:126:SER:OG	7:E:127:ILE:N	2.51	0.43
9:G:142:ARG:HG3	9:G:171:ILE:HD13	2.00	0.43
12:J:24:LEU:O	12:J:28:ASP:HB2	2.18	0.43
14:L:63:ARG:NH1	14:L:64:LEU:H	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:25:DA:H2"	1:N:26:DA:H8	1.83	0.43
3:A:332:LYS:HD2	3:A:332:LYS:HA	1.79	0.43
3:A:399:HIS:HB3	3:A:400:PRO:HD3	1.99	0.43
3:A:1042:PHE:O	3:A:1046:LEU:HG	2.18	0.43
4:B:530:GLY:C	4:B:532:ALA:H	2.22	0.43
5:C:239:PRO:O	5:C:242:GLN:HB2	2.18	0.43
3:A:115:LEU:N	3:A:164:ARG:HH22	2.15	0.43
3:A:230:ARG:HB3	3:A:232:GLU:OE1	2.19	0.43
3:A:476:SER:OG	3:A:477:PRO:HD3	2.19	0.43
3:A:811:GLN:H	3:A:811:GLN:CD	2.19	0.43
3:A:957:PRO:HG2	3:A:1018:PHE:HD1	1.82	0.43
4:B:198:ASP:OD2	4:B:202:TYR:OH	2.28	0.43
4:B:412:LEU:HB3	4:B:466:TRP:HZ2	1.83	0.43
4:B:651:LEU:HD23	4:B:651:LEU:H	1.84	0.43
4:B:862:GLN:HB3	4:B:963:PHE:HD1	1.83	0.43
4:B:912:ILE:HG13	4:B:939:THR:HB	1.99	0.43
5:C:16:ASP:OD1	5:C:16:ASP:N	2.46	0.43
3:A:116:ASP:HB3	3:A:164:ARG:CZ	2.49	0.43
3:A:778:GLY:HA3	4:B:516:ASN:HB2	2.00	0.43
4:B:203:PHE:N	4:B:210:LYS:O	2.50	0.43
13:K:39:ASP:OD1	13:K:41:THR:HG22	2.19	0.43
3:A:12:ARG:HH21	4:B:1218:THR:CG2	2.31	0.43
3:A:390:GLN:NE2	3:A:390:GLN:O	2.51	0.43
3:A:445:ASN:OD1	3:A:446:ARG:N	2.50	0.43
3:A:943:LEU:HA	3:A:946:VAL:HG22	2.00	0.43
3:A:1400:CYS:HB2	3:A:1405:THR:HG23	2.00	0.43
4:B:69:LEU:HD12	4:B:69:LEU:HA	1.84	0.43
4:B:213:ILE:O	4:B:215:GLN:NE2	2.52	0.43
4:B:709:ASP:OD1	4:B:710:LEU:N	2.48	0.43
6:D:123:LEU:HA	6:D:145:MET:CE	2.48	0.43
3:A:666:ILE:CG1	4:B:1026:LEU:HB3	2.48	0.43
3:A:807:GLY:HA3	4:B:728:ARG:HH22	1.84	0.43
3:A:871:ASP:CG	3:A:873:MET:H	2.22	0.43
3:A:1063:MET:HG3	4:B:1139:ILE:HG22	2.01	0.43
4:B:424:LEU:O	4:B:428:ILE:HG13	2.19	0.43
4:B:595:ARG:O	4:B:598:GLU:HG3	2.18	0.43
4:B:836:GLU:OE1	4:B:836:GLU:N	2.52	0.43
4:B:862:GLN:HB3	4:B:963:PHE:CD1	2.53	0.43
4:B:918:ILE:HA	4:B:919:SER:C	2.39	0.43
5:C:45:ALA:HA	5:C:72:LEU:HD13	2.00	0.43
6:D:55:ALA:O	6:D:59:ILE:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:79:ARG:NH1	8:F:150:GLU:OE1	2.38	0.43
3:A:844:ALA:HB3	3:A:845:LEU:HD12	2.01	0.43
4:B:658:ILE:O	4:B:662:MET:HG2	2.19	0.43
4:B:979:LYS:O	4:B:1095:LEU:HB2	2.19	0.43
5:C:61:GLU:H	5:C:61:GLU:CD	2.22	0.43
5:C:249:ASP:O	5:C:252:GLN:HG3	2.19	0.43
9:G:91:VAL:HG11	9:G:137:ILE:HG12	2.01	0.43
12:J:17:LYS:HB3	12:J:39:LEU:HD21	2.01	0.43
13:K:8:GLU:HG2	13:K:37:LYS:NZ	2.33	0.43
13:K:81:TYR:CE2	13:K:86:ALA:HB2	2.54	0.43
3:A:41:MET:HE3	3:A:47:ARG:HA	2.01	0.43
3:A:146:MET:HB3	3:A:171:GLN:O	2.18	0.43
3:A:842:VAL:O	3:A:846:GLU:HG3	2.19	0.43
3:A:889:SER:HA	3:A:1297:GLU:HG3	2.00	0.43
3:A:1104:ILE:HD12	3:A:1352:VAL:HG22	2.01	0.43
5:C:15:LYS:NZ	5:C:135:GLN:OE1	2.36	0.43
5:C:32:SER:O	5:C:36:VAL:HG13	2.18	0.43
5:C:33:LEU:HB3	5:C:37:MET:HE1	2.01	0.43
7:E:147:HIS:CE1	7:E:149:LEU:HB2	2.54	0.43
3:A:302:THR:HA	3:A:305:ASP:O	2.19	0.42
3:A:857:ARG:HB3	3:A:861:GLY:HA2	1.99	0.42
3:A:1207:LEU:HD21	3:A:1274:ARG:HH21	1.83	0.42
6:D:177:VAL:HA	6:D:180:LEU:HB2	2.01	0.42
3:A:354:SER:OG	3:A:469:ARG:NE	2.52	0.42
3:A:538:ASP:OD1	10:H:22:LYS:HB2	2.18	0.42
3:A:1173:HIS:CD2	3:A:1227:ILE:HG23	2.54	0.42
4:B:499:ASN:OD1	4:B:500:THR:N	2.51	0.42
4:B:923:GLU:HG3	4:B:924:GLU:OE1	2.19	0.42
5:C:101:LEU:HB3	5:C:155:LEU:HB2	2.00	0.42
6:D:63:LEU:HD13	6:D:126:ILE:HG22	2.00	0.42
10:H:42:ILE:HD12	10:H:42:ILE:HA	1.87	0.42
12:J:23:ASN:HB2	12:J:27:GLU:OE2	2.19	0.42
15:R:16:C:C6	15:R:16:C:O5'	2.72	0.42
17:M:108:LEU:HB3	17:M:118:HIS:HA	2.00	0.42
3:A:902:LEU:H	3:A:902:LEU:HD23	1.84	0.42
3:A:1225:PHE:CE2	3:A:1227:ILE:HD11	2.55	0.42
4:B:282:ILE:HD12	4:B:382:ILE:HD13	2.01	0.42
4:B:828:ALA:O	4:B:834:ASN:ND2	2.53	0.42
4:B:919:SER:HA	4:B:920:PRO:HA	1.74	0.42
4:B:954:VAL:O	14:L:56:LEU:HB2	2.19	0.42
6:D:126:ILE:HG13	6:D:127:ASP:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:105:ALA:O	17:M:89:GLY:HA2	2.17	0.42
16:Q:428:LEU:O	16:Q:432:GLY:N	2.52	0.42
3:A:343:LYS:HE3	4:B:1117:GLN:HE21	1.84	0.42
3:A:446:ARG:CD	3:A:480:ALA:HB2	2.49	0.42
3:A:589:GLN:HG3	3:A:606:LEU:HD13	2.01	0.42
3:A:1004:ASN:HD21	3:A:1007:ILE:HG12	1.84	0.42
3:A:1263:ILE:O	3:A:1267:MET:HG2	2.18	0.42
4:B:21:GLU:N	4:B:21:GLU:OE1	2.52	0.42
5:C:11:ARG:HG2	5:C:11:ARG:HH11	1.84	0.42
7:E:198:ILE:HB	7:E:210:SER:OG	2.20	0.42
10:H:5:LEU:HB2	10:H:59:ILE:HG21	2.01	0.42
10:H:118:PHE:HB2	10:H:121:LEU:HB2	2.01	0.42
12:J:4:PRO:HD3	12:J:53:HIS:HD2	1.84	0.42
17:M:133:TYR:HB3	17:M:214:ILE:HD11	2.01	0.42
2:O:5:DT:H2"	2:O:6:DA:C8	2.54	0.42
3:A:207:ILE:HD12	3:A:207:ILE:H	1.85	0.42
3:A:274:ILE:O	3:A:277:GLU:HG3	2.19	0.42
3:A:543:LEU:HD21	3:A:570:PRO:HB2	2.00	0.42
3:A:672:ASP:OD2	3:A:674:PRO:HG2	2.20	0.42
3:A:756:ILE:HD12	3:A:756:ILE:H	1.85	0.42
3:A:914:GLU:OE1	3:A:978:PRO:HB2	2.20	0.42
4:B:51:PHE:CD1	4:B:173:MET:HB2	2.55	0.42
4:B:297:ILE:H	4:B:297:ILE:HD12	1.84	0.42
4:B:839:MET:N	4:B:989:THR:O	2.52	0.42
4:B:1153:GLU:OE1	4:B:1153:GLU:N	2.53	0.42
7:E:4:GLU:HA	7:E:7:ARG:HG2	2.00	0.42
7:E:112:TYR:CD1	7:E:116:ILE:HD11	2.54	0.42
1:N:-3:DT:H2"	1:N:-2:DG:H8	1.84	0.42
2:O:-13:DA:C8	3:A:832:ALA:HA	2.55	0.42
3:A:177:ASP:OD1	3:A:177:ASP:N	2.52	0.42
3:A:362:ASP:N	3:A:362:ASP:OD1	2.53	0.42
3:A:1244:ARG:HA	3:A:1245:PRO:HD3	1.92	0.42
6:D:173:HIS:CD2	6:D:175:PHE:HB3	2.54	0.42
9:G:138:THR:O	9:G:141:SER:HB3	2.20	0.42
11:I:113:ASP:OD2	11:I:115:LYS:HB2	2.19	0.42
14:L:27:LEU:HD11	14:L:62:LYS:NZ	2.35	0.42
3:A:88:LYS:HB3	3:A:293:GLU:OE2	2.19	0.42
3:A:90:VAL:HG21	3:A:300:VAL:HG11	2.01	0.42
3:A:344:ARG:CZ	4:B:1129:ARG:HB2	2.50	0.42
3:A:415:LEU:HA	3:A:418:SER:HB2	2.00	0.42
4:B:954:VAL:HG23	4:B:964:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:987:LYS:HZ3	15:R:12:A:P	2.42	0.42
5:C:183:TRP:CE3	5:C:213:PRO:HD3	2.55	0.42
9:G:115:MET:HG2	9:G:163:ILE:HD11	2.01	0.42
10:H:130:ARG:H	10:H:130:ARG:CD	2.32	0.42
3:A:32:VAL:N	3:A:81:PHE:O	2.51	0.42
3:A:50:ILE:HG13	3:A:51:GLY:H	1.85	0.42
3:A:439:ASN:HA	3:A:460:VAL:H	1.85	0.42
3:A:635:ARG:HA	3:A:635:ARG:HD3	1.89	0.42
3:A:1044:TRP:CD2	3:A:1048:ASN:ND2	2.88	0.42
4:B:144:GLY:HA2	4:B:145:ARG:HA	1.79	0.42
4:B:760:ASP:OD1	4:B:761:HIS:N	2.53	0.42
11:I:28:GLU:HA	11:I:35:VAL:HA	2.02	0.42
15:R:16:C:C6	15:R:16:C:C3'	3.03	0.42
2:O:-3:DA:H2	3:A:252:PHE:CD2	2.37	0.42
3:A:151:ASP:OD1	3:A:163:SER:HA	2.20	0.42
3:A:362:ASP:O	3:A:459:ARG:N	2.46	0.42
3:A:1171:GLN:O	3:A:1175:SER:OG	2.36	0.42
4:B:603:LEU:HB3	4:B:609:ILE:CD1	2.49	0.42
5:C:257:SER:O	5:C:260:LEU:HG	2.19	0.42
6:D:14:ARG:HE	6:D:17:LYS:NZ	2.18	0.42
7:E:106:GLN:OE1	7:E:106:GLN:N	2.43	0.42
8:F:94:LEU:HD21	8:F:125:LEU:HD22	2.02	0.42
9:G:24:GLN:O	9:G:28:THR:HG23	2.20	0.42
17:M:86:ASN:HA	17:M:88:HIS:CE1	2.55	0.42
1:N:30:DA:H2"	1:N:31:DA:C8	2.55	0.42
3:A:252:PHE:HE1	15:R:4:C:N1	2.17	0.42
3:A:444:PHE:CZ	3:A:487:MET:HG2	2.55	0.42
3:A:851:HIS:CG	8:F:139:PRO:HG3	2.55	0.42
3:A:858:ASN:OD1	3:A:862:ASN:N	2.49	0.42
4:B:445:LYS:HE2	4:B:445:LYS:HB2	1.85	0.42
4:B:847:ASP:HB3	5:C:167:HIS:CE1	2.55	0.42
4:B:1036:ALA:O	12:J:47:ARG:HD3	2.19	0.42
5:C:33:LEU:HA	5:C:36:VAL:HG22	2.01	0.42
17:M:68:VAL:N	17:M:217:THR:O	2.53	0.42
2:O:-20:DG:H2"	2:O:-19:DC:C6	2.54	0.41
3:A:1195:LEU:O	3:A:1237:ILE:HA	2.20	0.41
3:A:1315:GLU:OE1	3:A:1315:GLU:N	2.53	0.41
3:A:1384:VAL:O	3:A:1384:VAL:HG23	2.20	0.41
4:B:326:ASP:O	4:B:329:THR:OG1	2.35	0.41
4:B:526:GLU:HG2	4:B:771:SER:OG	2.20	0.41
4:B:638:PHE:CD2	4:B:743:ILE:HG22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:121:PHE:HB2	9:G:130:TYR:CD2	2.55	0.41
10:H:58:THR:HB	10:H:143:LEU:HB2	2.02	0.41
17:M:70:LEU:HD12	17:M:70:LEU:HA	1.92	0.41
3:A:351:THR:HG22	4:B:1103:ILE:HG13	2.01	0.41
3:A:367:PRO:HA	3:A:463:ILE:O	2.19	0.41
3:A:1063:MET:CE	3:A:1436:ILE:HG23	2.50	0.41
3:A:1173:HIS:NE2	3:A:1227:ILE:HG23	2.34	0.41
4:B:998:ASP:HB2	4:B:1076:HIS:CD2	2.55	0.41
5:C:39:ALA:O	5:C:164:ALA:HB3	2.20	0.41
5:C:146:LYS:C	5:C:147:LEU:HD12	2.40	0.41
5:C:148:ARG:NH1	12:J:63:TYR:O	2.54	0.41
5:C:148:ARG:HD3	12:J:61:LEU:O	2.20	0.41
7:E:26:ARG:NH1	7:E:189:GLY:HA3	2.36	0.41
7:E:60:PHE:O	7:E:80:VAL:HG22	2.20	0.41
7:E:171:LYS:O	7:E:171:LYS:HG3	2.20	0.41
8:F:140:ASP:CG	8:F:142:SER:HG	2.23	0.41
13:K:18:LYS:HA	13:K:18:LYS:HD2	1.89	0.41
3:A:1199:ARG:NH1	3:A:1231:ASP:OD1	2.53	0.41
4:B:190:TYR:CE1	12:J:62:ARG:HG3	2.55	0.41
4:B:487:THR:HG22	4:B:489:SER:N	2.34	0.41
4:B:737:THR:HG22	11:I:66:PRO:HB3	2.02	0.41
4:B:1115:THR:HG23	4:B:1117:GLN:H	1.85	0.41
6:D:50:LEU:HD12	6:D:50:LEU:HA	1.91	0.41
8:F:72:LYS:HD3	8:F:72:LYS:HA	1.81	0.41
3:A:41:MET:HA	3:A:49:LYS:HA	2.01	0.41
3:A:332:LYS:HA	3:A:337:ARG:NH1	2.36	0.41
3:A:929:LEU:O	3:A:932:GLU:HG3	2.20	0.41
3:A:1365:TYR:HA	3:A:1368:MET:HE3	2.03	0.41
4:B:289:LEU:HD22	4:B:375:ALA:HB2	2.03	0.41
4:B:1134:GLU:HA	4:B:1137:CYS:SG	2.60	0.41
7:E:136:ASN:ND2	7:E:138:ALA:HB3	2.33	0.41
10:H:26:ILE:HG22	10:H:40:LEU:HB3	2.02	0.41
10:H:54:SER:O	10:H:146:ARG:NH1	2.53	0.41
12:J:3:VAL:HA	12:J:53:HIS:CD2	2.56	0.41
1:N:-3:DT:OP1	4:B:868:MET:N	2.53	0.41
3:A:57:ARG:O	3:A:68:GLN:HB3	2.20	0.41
3:A:153:PRO:HB2	3:A:156:ASP:CG	2.41	0.41
3:A:187:LYS:O	3:A:188:ASP:C	2.59	0.41
3:A:1079:MET:HE2	3:A:1098:VAL:HG23	2.03	0.41
3:A:1121:GLU:HG3	3:A:1123:GLY:H	1.85	0.41
3:A:1217:LYS:HE3	3:A:1221:LYS:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:274:PRO:HA	4:B:275:TYR:HA	1.67	0.41
4:B:441:ASP:OD1	4:B:444:MET:HG3	2.21	0.41
5:C:54:ASN:OD1	5:C:56:THR:HG22	2.20	0.41
5:C:101:LEU:HD13	5:C:118:LEU:HB3	2.02	0.41
5:C:191:TYR:HB3	5:C:201:TRP:NE1	2.35	0.41
6:D:65:GLU:HA	6:D:68:ARG:CZ	2.51	0.41
7:E:43:LYS:HD2	7:E:43:LYS:HA	1.67	0.41
10:H:101:ALA:HB2	10:H:116:TYR:CE1	2.55	0.41
14:L:31:CYS:SG	14:L:48:CYS:CB	3.08	0.41
3:A:13:THR:OG1	3:A:1432:GLN:HG2	2.21	0.41
3:A:364:VAL:HG12	3:A:459:ARG:O	2.21	0.41
3:A:370:ILE:O	3:A:374:LEU:N	2.50	0.41
3:A:407:ARG:HG2	3:A:430:TRP:CE2	2.55	0.41
3:A:534:LEU:HD13	3:A:656:TRP:CD2	2.55	0.41
4:B:251:ILE:H	4:B:251:ILE:HD12	1.84	0.41
4:B:919:SER:H	4:B:923:GLU:HA	1.86	0.41
6:D:152:SER:HB2	6:D:155:ARG:NH2	2.30	0.41
8:F:130:ILE:HB	8:F:148:VAL:HG11	2.01	0.41
17:M:120:TYR:HD2	17:M:226:PRO:HA	1.85	0.41
3:A:451:HIS:HD2	3:A:453:MET:H	1.69	0.41
3:A:1147:THR:HA	3:A:1197:LEU:HD23	2.03	0.41
4:B:295:GLY:O	4:B:299:GLU:HG2	2.21	0.41
4:B:364:ILE:CG2	4:B:585:VAL:HG23	2.48	0.41
4:B:445:LYS:NZ	4:B:449:ASN:OD1	2.37	0.41
4:B:513:GLN:H	4:B:513:GLN:HG3	1.70	0.41
6:D:192:LYS:HG2	6:D:199:ASN:HA	2.02	0.41
7:E:156:LEU:HB2	7:E:195:VAL:O	2.21	0.41
8:F:82:THR:HA	8:F:83:PRO:HD3	1.88	0.41
11:I:62:ILE:HD13	11:I:62:ILE:HA	1.96	0.41
17:M:67:GLN:OE1	17:M:67:GLN:N	2.50	0.41
17:M:121:ASP:OD1	17:M:225:MET:HB3	2.21	0.41
3:A:368:LYS:NZ	13:K:2:ASN:O	2.49	0.41
3:A:549:MET:SD	3:A:577:ILE:HD13	2.60	0.41
4:B:408:LEU:HA	4:B:408:LEU:HD12	1.87	0.41
4:B:757:PRO:HD3	4:B:983:ARG:NE	2.32	0.41
4:B:992:ILE:HD11	4:B:994:TYR:CE2	2.56	0.41
4:B:1164:GLY:N	4:B:1190:ASP:OD1	2.54	0.41
4:B:1202:LEU:HA	4:B:1205:GLN:OE1	2.20	0.41
10:H:12:VAL:CG1	10:H:53:ASP:H	2.32	0.41
11:I:103:CYS:HB3	11:I:106:CYS:SG	2.61	0.41
13:K:40:HIS:H	13:K:40:HIS:CD2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:16:DA:H3'	1:N:17:DG:H8	1.86	0.41
2:O:-17:DC:H2'	2:O:-16:DT:H72	2.03	0.41
3:A:67:CYS:O	3:A:68:GLN:HG3	2.20	0.41
3:A:96:ILE:HD13	3:A:96:ILE:HA	1.93	0.41
3:A:129:LYS:O	3:A:129:LYS:HG3	2.21	0.41
3:A:737:LEU:HD21	3:A:741:ASN:HD22	1.85	0.41
3:A:999:VAL:H	3:A:1011:GLN:CD	2.25	0.41
3:A:1121:GLU:CD	3:A:1122:PRO:HD2	2.42	0.41
3:A:1435:PRO:HA	3:A:1439:GLY:O	2.21	0.41
3:A:1438:THR:OG1	8:F:92:ARG:HD3	2.20	0.41
4:B:247:GLY:O	4:B:250:PHE:CD2	2.74	0.41
4:B:590:HIS:HD2	4:B:592:ASN:N	2.19	0.41
4:B:975:GLN:HG2	4:B:976:ILE:H	1.85	0.41
4:B:1027:ILE:H	4:B:1027:ILE:HD12	1.85	0.41
5:C:254:LYS:O	5:C:257:SER:OG	2.32	0.41
11:I:73:ARG:O	11:I:83:ASN:ND2	2.54	0.41
11:I:76:PRO:HD2	11:I:77:LYS:NZ	2.36	0.41
13:K:84:LYS:O	13:K:87:LEU:HG	2.20	0.41
16:Q:109:GLU:CD	16:Q:109:GLU:H	2.24	0.41
16:Q:376:LEU:HA	16:Q:385:THR:O	2.21	0.41
3:A:376:TYR:CD1	3:A:377:PRO:HD2	2.56	0.41
3:A:890:ASP:O	3:A:893:PHE:N	2.54	0.41
3:A:956:LEU:HD22	3:A:957:PRO:HD2	2.02	0.41
3:A:1104:ILE:HG13	3:A:1105:LEU:N	2.36	0.41
4:B:59:LEU:O	4:B:62:ILE:HG22	2.21	0.41
4:B:313:MET:HE3	4:B:390:LEU:HD22	2.03	0.41
4:B:431:TYR:CD2	4:B:445:LYS:HD2	2.56	0.41
4:B:821:GLN:NE2	4:B:851:PHE:H	2.19	0.41
4:B:963:PHE:CZ	4:B:965:LYS:HD3	2.55	0.41
5:C:259:LEU:HD13	13:K:91:CYS:HB2	2.03	0.41
6:D:195:ILE:HG13	9:G:86:VAL:HG23	2.02	0.41
7:E:29:PHE:N	7:E:65:THR:HG22	2.36	0.41
9:G:91:VAL:HB	9:G:141:SER:HB2	2.03	0.41
3:A:150:THR:O	3:A:165:GLY:N	2.45	0.40
3:A:407:ARG:HG2	3:A:430:TRP:CD2	2.56	0.40
3:A:543:LEU:HA	3:A:546:VAL:HG22	2.02	0.40
4:B:497:ARG:HD3	4:B:497:ARG:HA	1.74	0.40
4:B:758:PHE:CE2	4:B:1044:ALA:HA	2.56	0.40
4:B:950:ASP:OD1	4:B:951:GLN:N	2.55	0.40
16:Q:104:ARG:H	16:Q:383:SER:HB3	1.86	0.40
16:Q:408:GLU:HA	16:Q:411:LYS:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:71:VAL:HG22	17:M:222:CYS:SG	2.61	0.40
3:A:272:ALA:O	3:A:296:LEU:HD11	2.21	0.40
3:A:407:ARG:HB2	3:A:411:ASP:HB2	2.04	0.40
3:A:570:PRO:C	3:A:571:LEU:HD12	2.42	0.40
3:A:1425:SER:O	3:A:1429:ILE:HG12	2.21	0.40
4:B:69:LEU:HB3	4:B:90:ILE:HG13	2.04	0.40
4:B:558:LEU:HD21	4:B:580:VAL:HG11	2.04	0.40
4:B:1169:MET:HE2	4:B:1169:MET:HB3	1.83	0.40
7:E:60:PHE:H	7:E:80:VAL:CG2	2.34	0.40
9:G:38:CYS:HA	9:G:44:TYR:HA	2.02	0.40
17:M:112:ASP:OD1	17:M:118:HIS:NE2	2.54	0.40
3:A:122:MET:HA	3:A:125:ALA:HB3	2.04	0.40
3:A:566:ILE:HD12	10:H:97:MET:HA	2.03	0.40
3:A:1229:SER:OG	3:A:1230:GLU:N	2.55	0.40
4:B:824:ILE:N	4:B:1009:ASP:OD2	2.40	0.40
6:D:39:ASN:HB2	6:D:45:GLU:HB2	2.02	0.40
7:E:106:GLN:O	7:E:131:THR:N	2.47	0.40
9:G:13:LEU:HD21	9:G:17:PHE:O	2.20	0.40
17:M:85:ASN:O	17:M:88:HIS:NE2	2.54	0.40
1:N:22:DA:H2"	1:N:23:DA:C8	2.57	0.40
3:A:156:ASP:OD1	3:A:157:ASP:N	2.51	0.40
3:A:831:THR:HG23	3:A:832:ALA:N	2.36	0.40
3:A:934:LYS:O	3:A:937:VAL:HG12	2.21	0.40
3:A:1135:ARG:HG3	3:A:1282:VAL:HG23	2.02	0.40
3:A:1163:ILE:H	3:A:1163:ILE:HD12	1.86	0.40
14:L:40:LEU:CD1	14:L:44:ASP:HB2	2.51	0.40
3:A:315:LEU:HB2	3:A:321:PRO:HA	2.04	0.40
4:B:552:MET:HA	4:B:555:ILE:HG22	2.03	0.40
4:B:592:ASN:O	4:B:596:LEU:HD13	2.21	0.40
4:B:916:THR:OG1	4:B:935:ARG:HB3	2.22	0.40
5:C:36:VAL:HG11	5:C:251:LEU:HD12	2.04	0.40
5:C:100:THR:OG1	5:C:121:VAL:HG21	2.22	0.40
13:K:8:GLU:OE1	13:K:69:ALA:N	2.39	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	
3	A	1417/1733 (82%)	1266 (89%)	148 (10%)	3 (0%)	47	80
4	B	1150/1224 (94%)	1001 (87%)	147 (13%)	2 (0%)	47	80
5	C	263/318 (83%)	231 (88%)	32 (12%)	0	100	100
6	D	164/221 (74%)	159 (97%)	5 (3%)	0	100	100
7	E	212/215 (99%)	196 (92%)	16 (8%)	0	100	100
8	F	85/155 (55%)	77 (91%)	8 (9%)	0	100	100
9	G	169/171 (99%)	155 (92%)	14 (8%)	0	100	100
10	H	129/146 (88%)	110 (85%)	19 (15%)	0	100	100
11	I	112/122 (92%)	102 (91%)	10 (9%)	0	100	100
12	J	64/70 (91%)	54 (84%)	10 (16%)	0	100	100
13	K	113/120 (94%)	108 (96%)	5 (4%)	0	100	100
14	L	42/70 (60%)	30 (71%)	12 (29%)	0	100	100
16	Q	208/735 (28%)	202 (97%)	6 (3%)	0	100	100
17	M	131/400 (33%)	123 (94%)	8 (6%)	0	100	100
All	All	4259/5700 (75%)	3814 (90%)	440 (10%)	5 (0%)	54	84

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	188	ASP
4	B	364	ILE
3	A	195	ASP
3	A	253	ASN
4	B	363	HIS

5.3.2 Protein sidechains (i)

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
3	A	1235/1520 (81%)	1228 (99%)	7 (1%)	86 94
4	B	1000/1061 (94%)	995 (100%)	5 (0%)	88 95
5	C	233/274 (85%)	232 (100%)	1 (0%)	91 97
6	D	146/200 (73%)	146 (100%)	0	100 100
7	E	196/197 (100%)	196 (100%)	0	100 100
8	F	77/137 (56%)	77 (100%)	0	100 100
9	G	151/152 (99%)	151 (100%)	0	100 100
10	H	118/128 (92%)	115 (98%)	3 (2%)	47 76
11	I	108/116 (93%)	108 (100%)	0	100 100
12	J	61/65 (94%)	61 (100%)	0	100 100
13	K	99/102 (97%)	99 (100%)	0	100 100
14	L	39/57 (68%)	39 (100%)	0	100 100
16	Q	147/641 (23%)	145 (99%)	2 (1%)	67 85
17	M	125/363 (34%)	125 (100%)	0	100 100
All	All	3735/5013 (74%)	3717 (100%)	18 (0%)	89 95

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	36	ARG
3	A	189	ARG
3	A	191	THR
3	A	193	ASP
3	A	195	ASP
3	A	619	LYS
3	A	736	ASN
4	B	264	SER
4	B	265	SER
4	B	277	LYS
4	B	476	ARG

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Mol	Chain	Res	Type
4	B	1183	LYS
5	C	116	LYS
10	H	77	ARG
10	H	130	ARG
10	H	146	ARG
16	Q	330	ARG
16	Q	333	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	68	GLN
3	A	71	GLN
3	A	451	HIS
3	A	768	GLN
3	A	802	ASN
3	A	851	HIS
3	A	1128	GLN
3	A	1171	GLN
3	A	1390	ASN
4	B	110	HIS
4	B	538	ASN
4	B	834	ASN
5	C	102	GLN
6	D	39	ASN
6	D	41	GLN
6	D	74	GLN
6	D	150	ASN
8	F	100	GLN
11	I	87	GLN
11	I	89	GLN
13	K	40	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	R	14/15 (93%)	8 (57%)	0

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	R	5	C
15	R	8	A
15	R	9	C
15	R	10	A
15	R	11	A
15	R	13	U
15	R	15	C
15	R	18	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

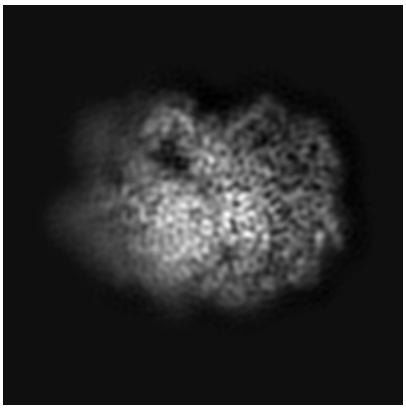
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23887. These allow visual inspection of the internal detail of the map and identification of artifacts.

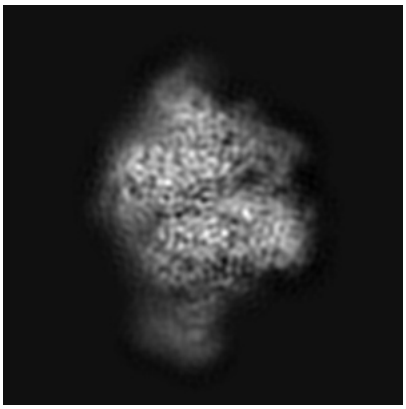
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

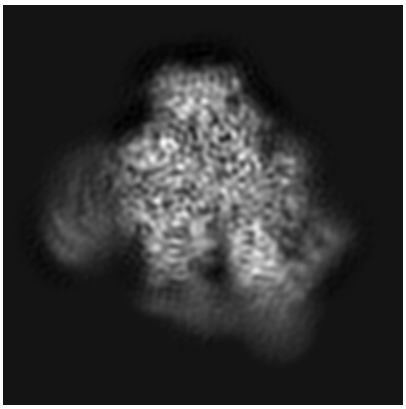
6.1.1 Primary map



X

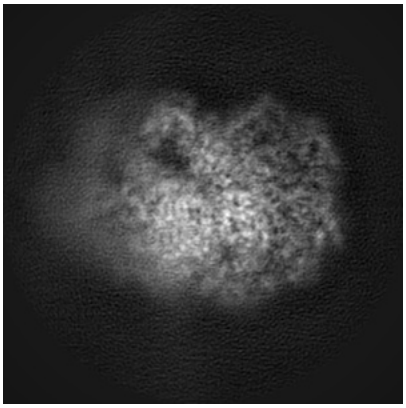


Y

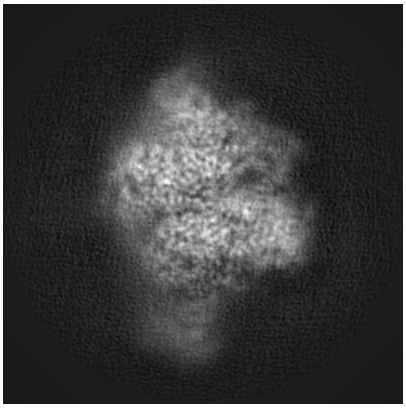


Z

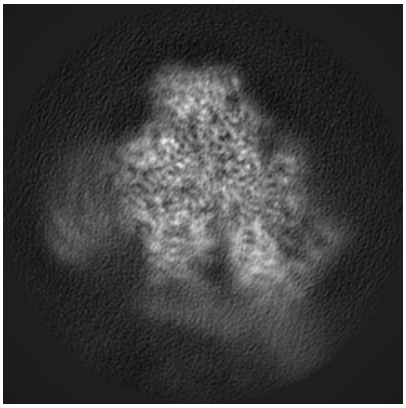
6.1.2 Raw map



X



Y

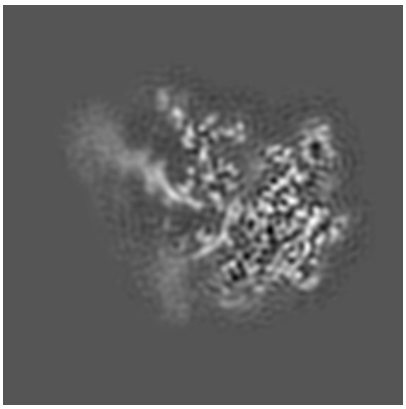


Z

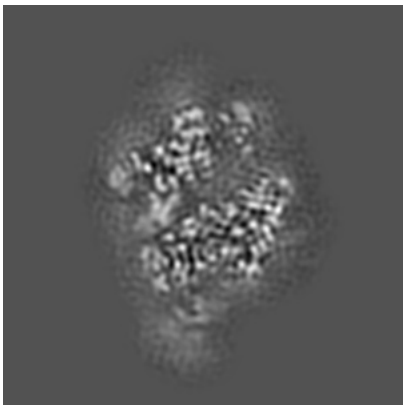
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

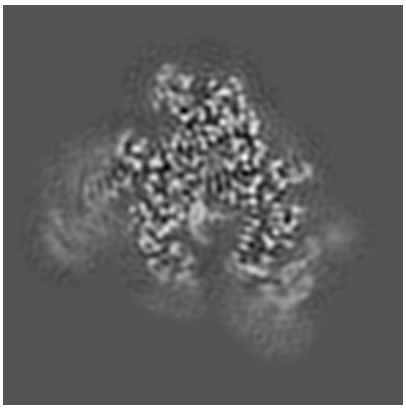
6.2.1 Primary map



X Index: 110

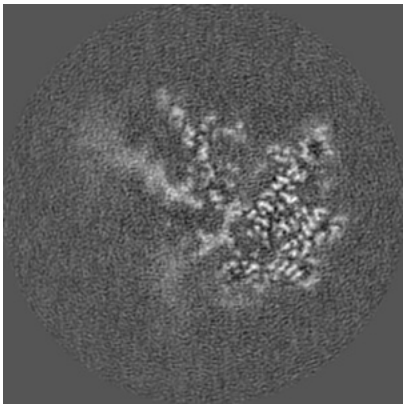


Y Index: 110

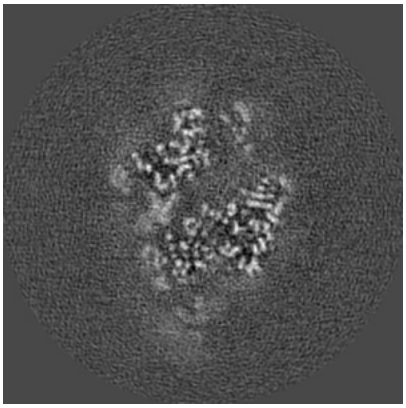


Z Index: 110

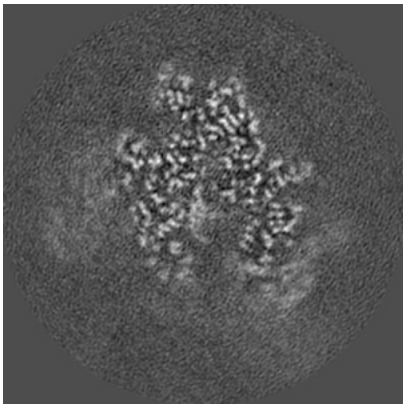
6.2.2 Raw map



X Index: 110



Y Index: 110

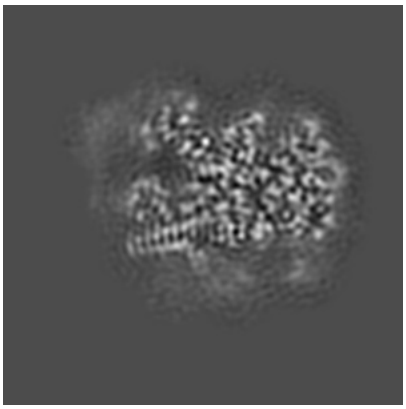


Z Index: 110

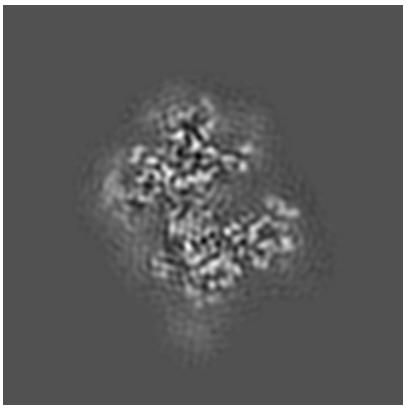
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

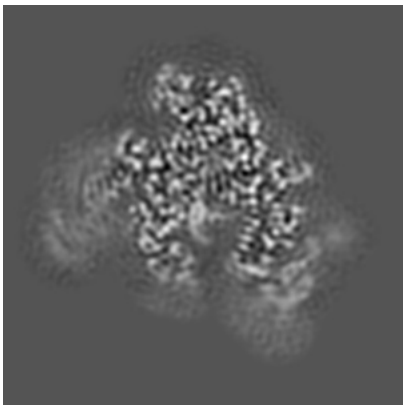
6.3.1 Primary map



X Index: 96

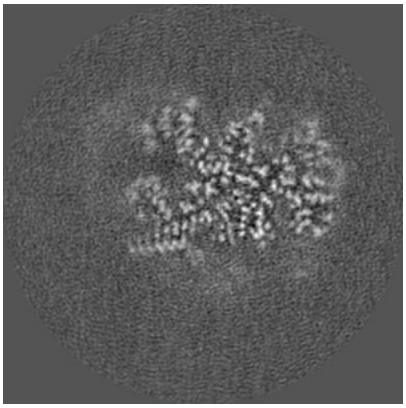


Y Index: 131

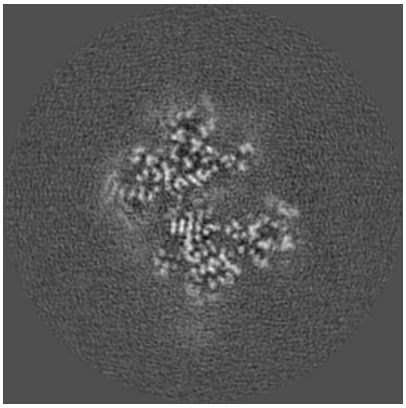


Z Index: 110

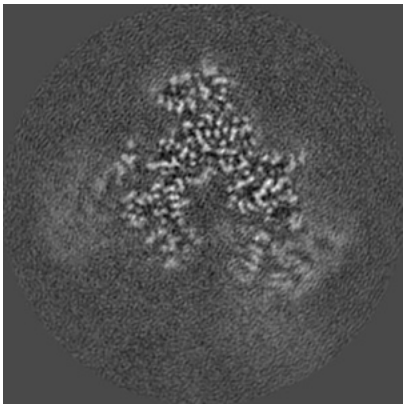
6.3.2 Raw map



X Index: 95



Y Index: 131

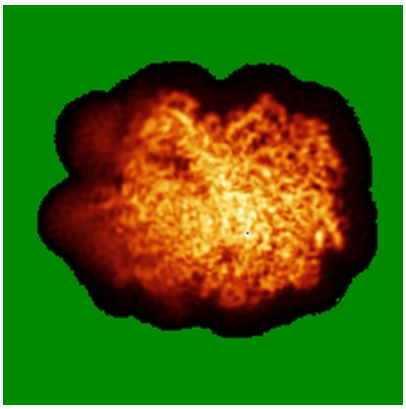


Z Index: 101

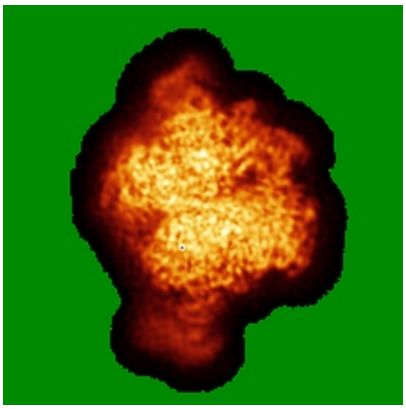
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

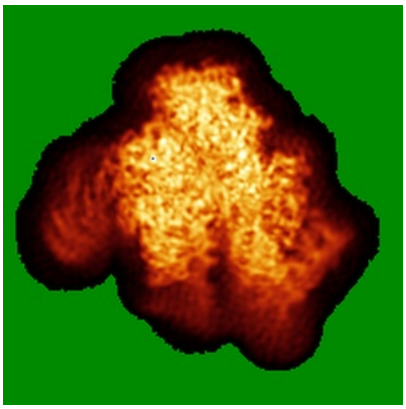
6.4.1 Primary map



X

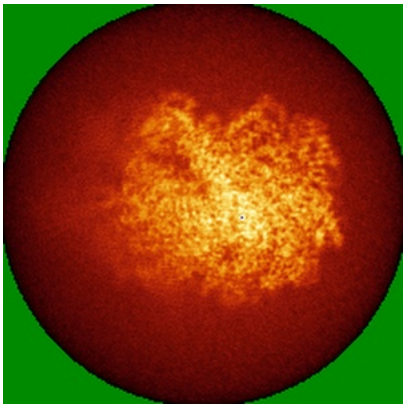


Y

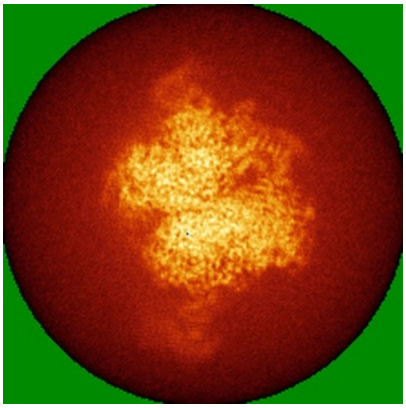


Z

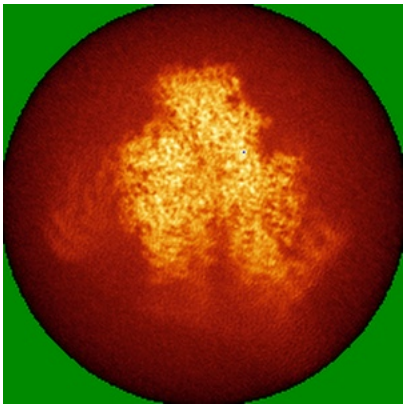
6.4.2 Raw map



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.

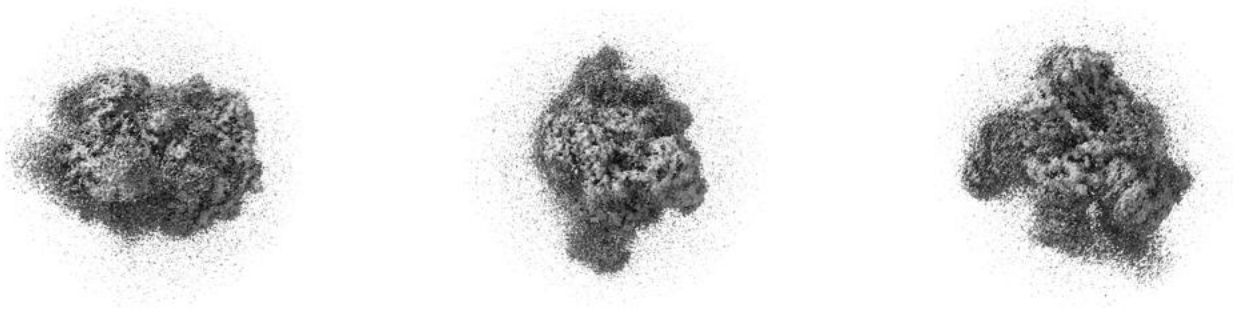
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0084. 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



X Y Z

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.

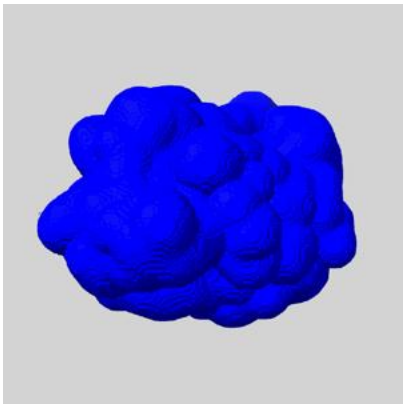
6.6 Mask visualisation

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

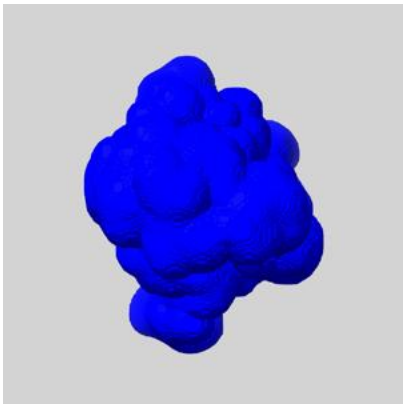
A mask typically either:

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

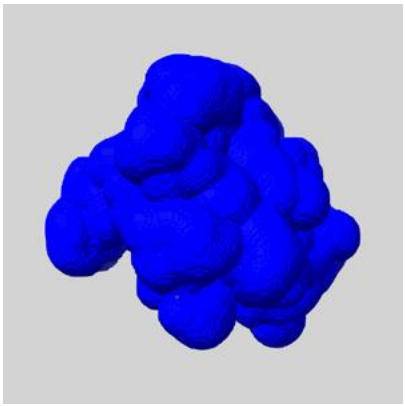
6.6.1 emd_23887_msk_1.map



X



Y

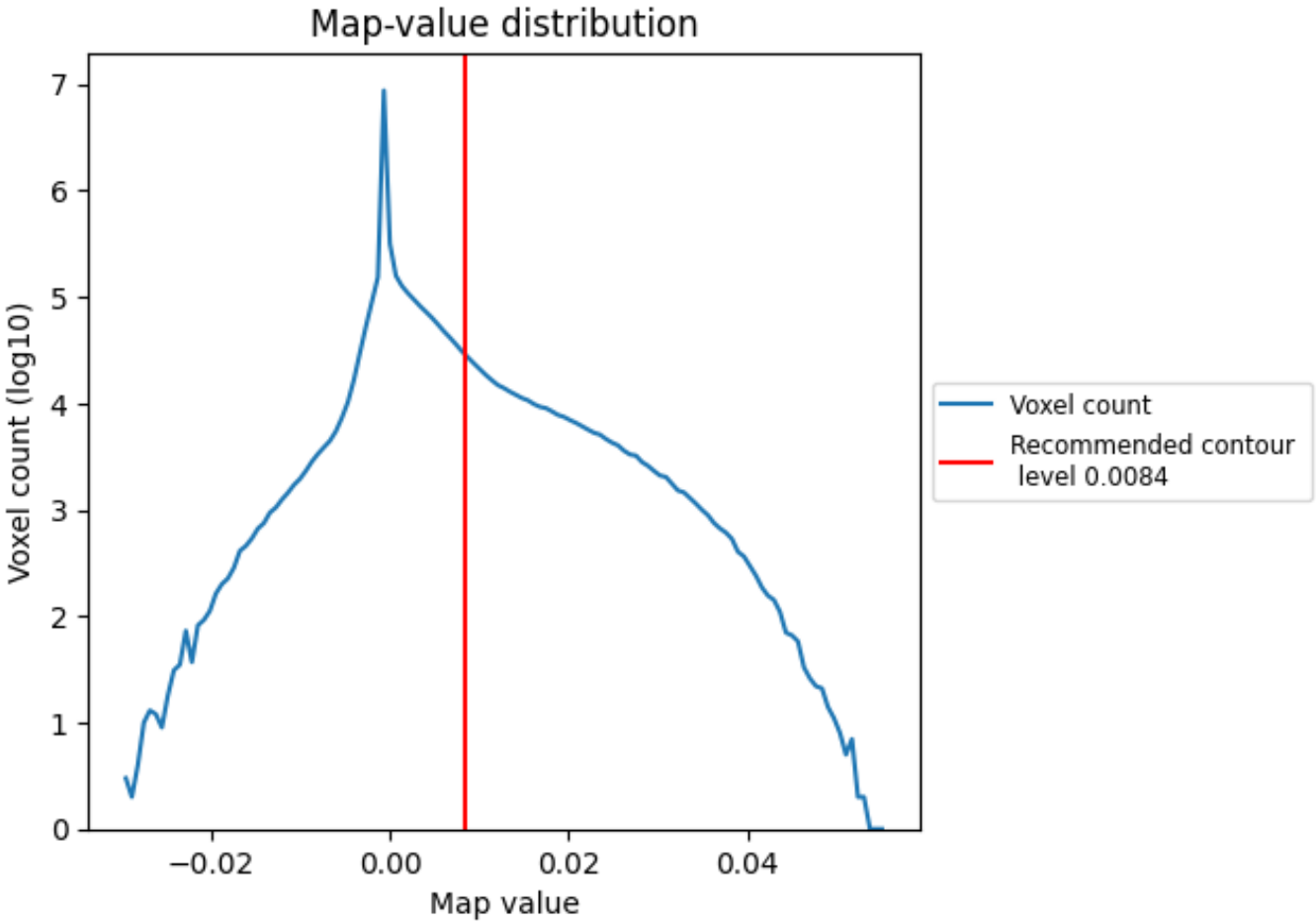


Z

7 Map analysis

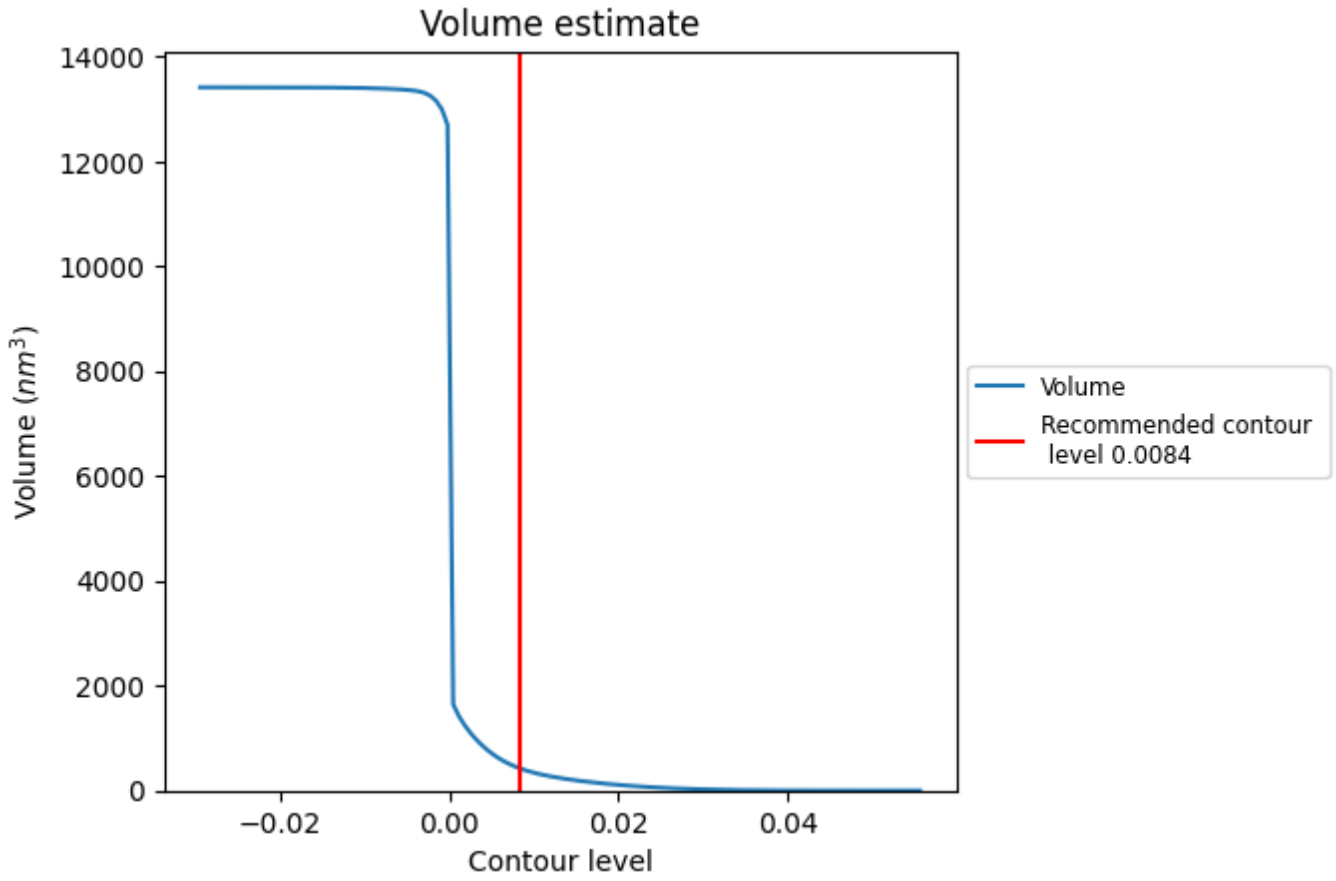
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

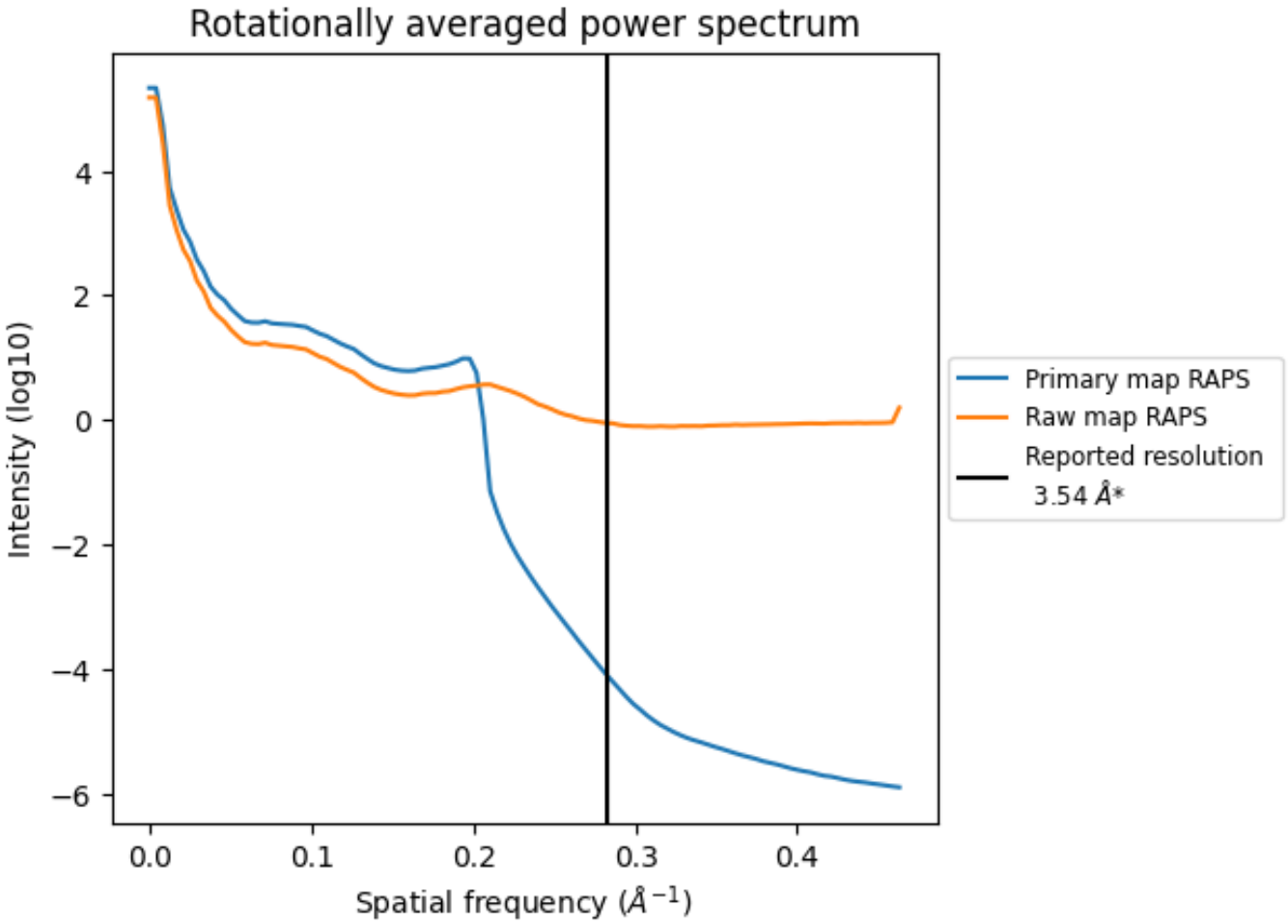
7.2 Volume estimate



The volume at the recommended contour level is 420 nm^3; this corresponds to an approximate mass of 379 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

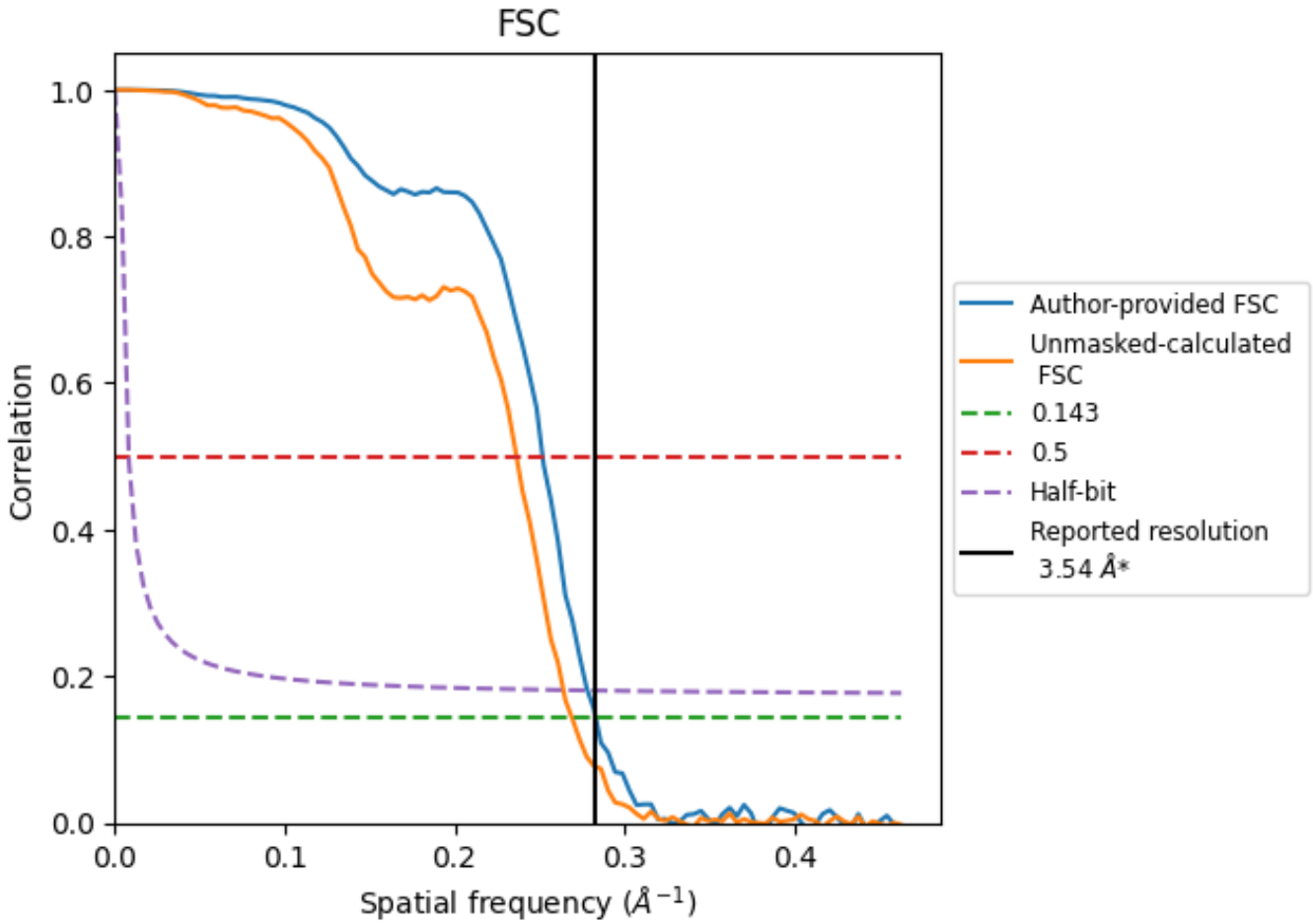


*Reported resolution corresponds to spatial frequency of 0.282 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.282 Å^{-1}

8.2 Resolution estimates (i)

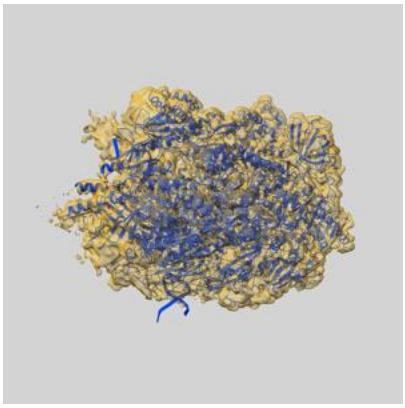
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.54	-	-
Author-provided FSC curve	3.53	3.97	3.59
Unmasked-calculated*	3.72	4.23	3.79

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

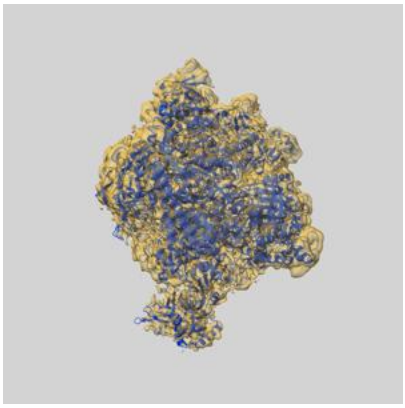
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23887 and PDB model 7MK9. Per-residue inclusion information can be found in section 3 on page 8.

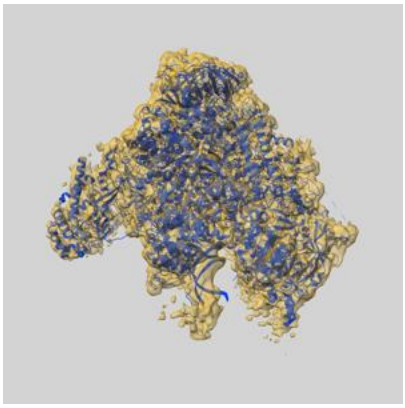
9.1 Map-model overlay



X



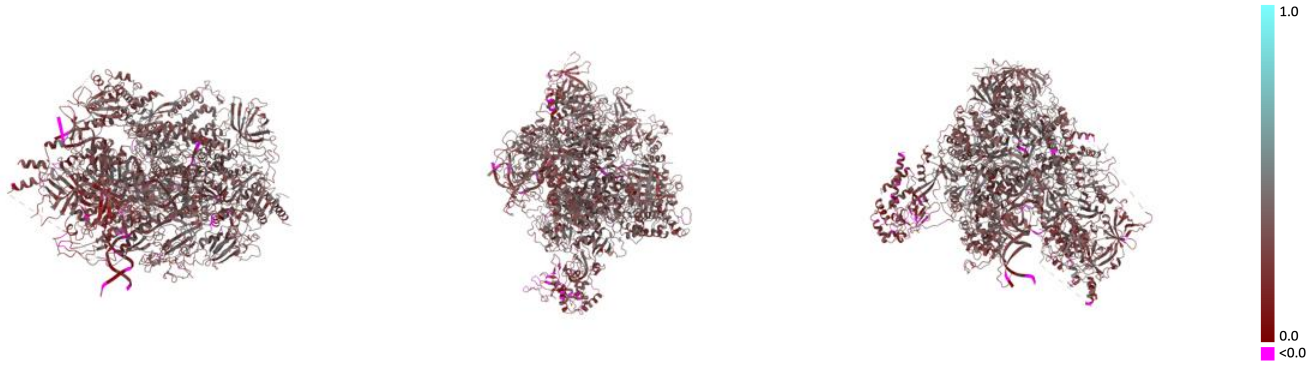
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0084 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.

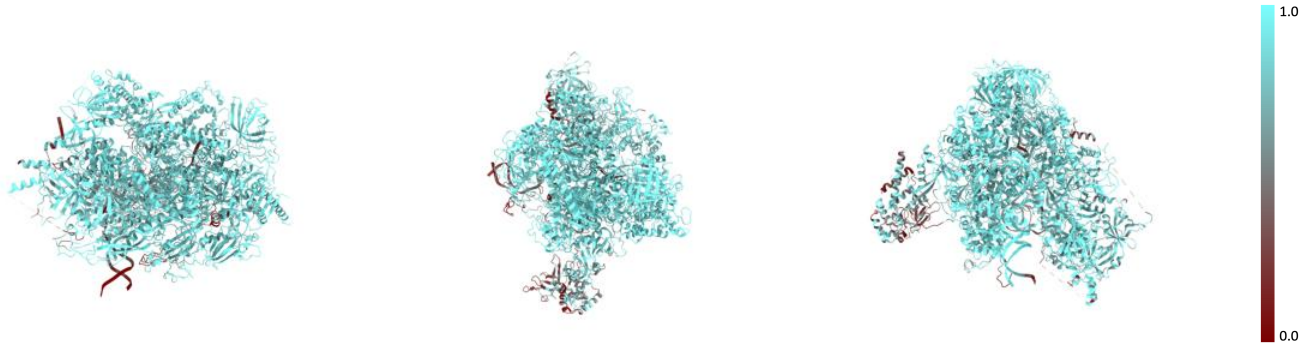
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

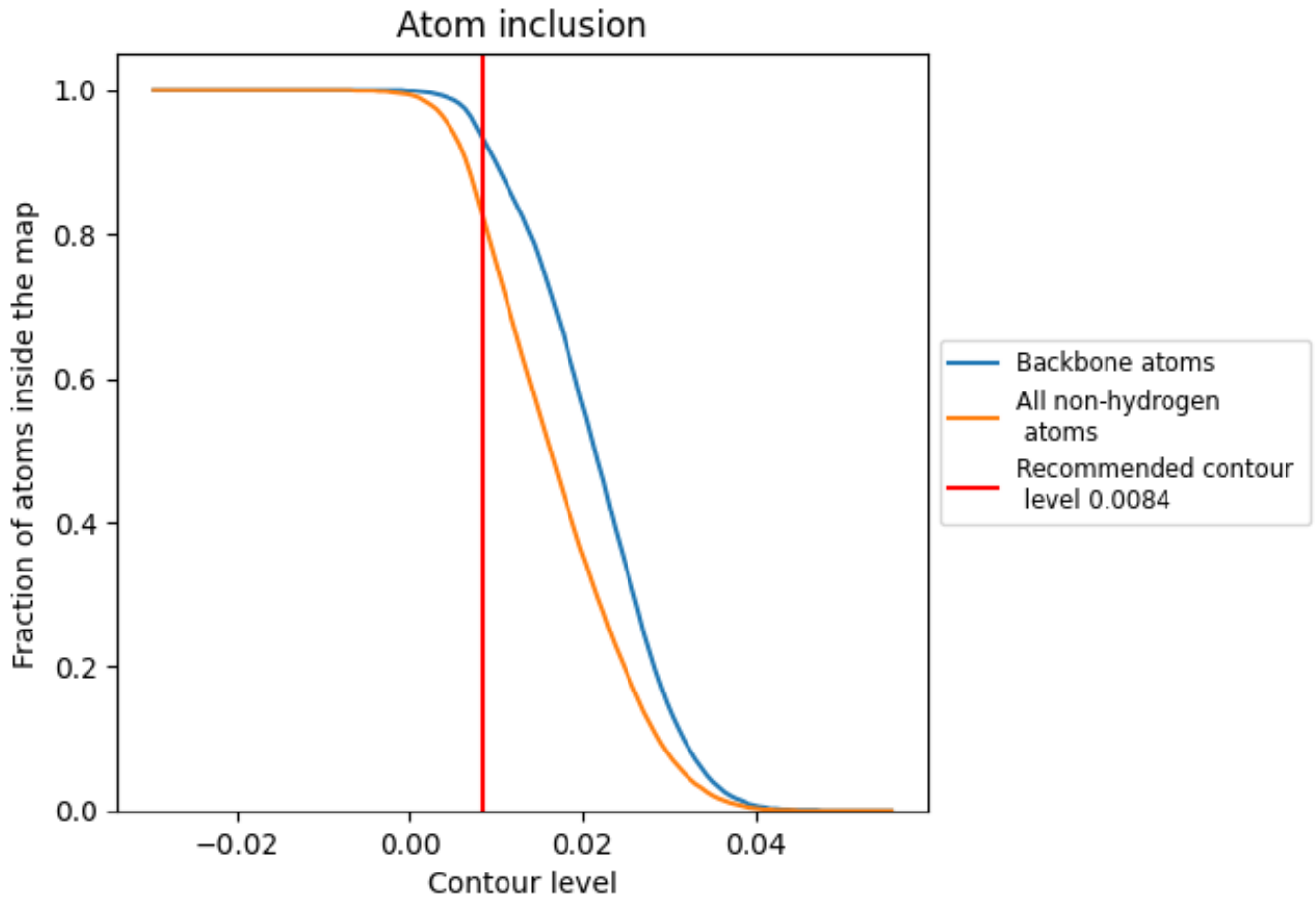
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0084).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 83% 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 (0.0084) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8270	0.3170
A	0.8810	0.3470
B	0.8380	0.3360
C	0.9000	0.3600
D	0.5130	0.1930
E	0.9050	0.3440
F	0.8750	0.3580
G	0.5470	0.1910
H	0.9300	0.3400
I	0.8800	0.3390
J	0.9290	0.3570
K	0.8330	0.3200
L	0.9000	0.3260
M	0.7830	0.2340
N	0.5910	0.1750
O	0.7400	0.2100
Q	0.7520	0.2700
R	0.7440	0.2300