



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:10 PM UTC

PDB ID : 8P4B / pdb_00008p4b
EMDB ID : EMD-17404
Title : Structural insights into human co-transcriptional capping - structure 2
Authors : Garg, G.; Dienemann, C.; Farnung, L.; Schwarz, J.; Linden, A.; Urlaub, H.; Cramer, P.
Deposited on : 2023-05-20
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

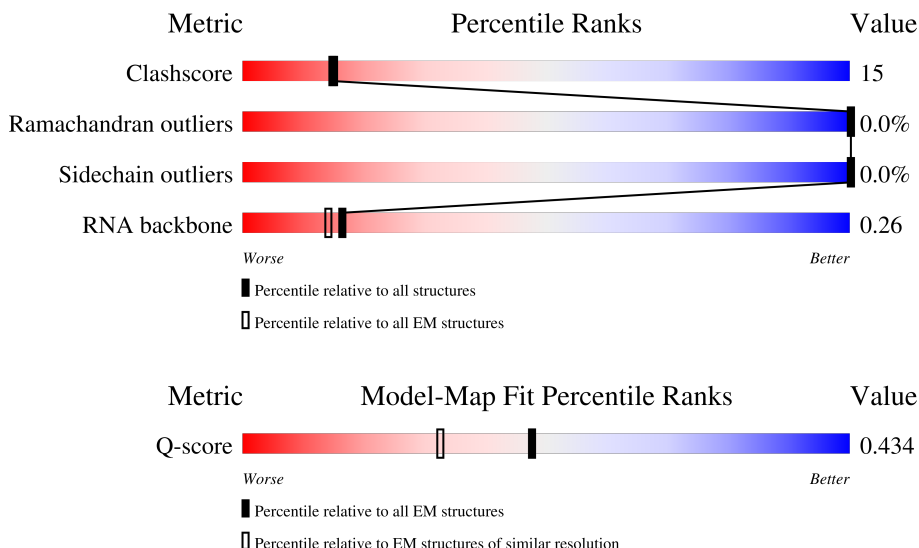
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



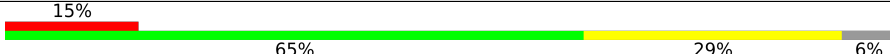
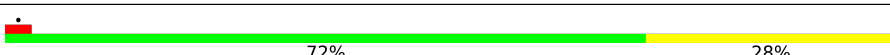
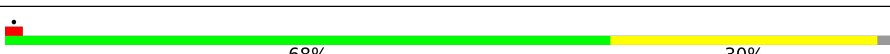
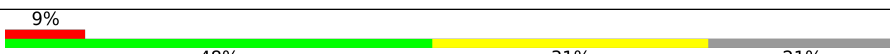
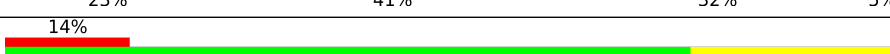
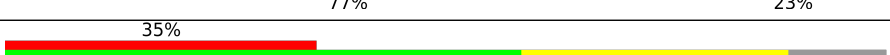
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1970	
2	B	1174	
3	C	275	

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Mol	Chain	Length	Quality of chain
4	E	210	
5	F	127	
6	H	150	
7	I	125	
8	J	67	
9	K	117	
10	L	58	
11	N	24	
12	P	22	
13	T	35	
14	D	142	
15	G	172	
16	M	597	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 35383 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1410	Total	C	N	O	S	0	0
			11166	7029	2001	2067	69		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1132	Total	C	N	O	S	0	0
			9052	5725	1592	1671	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	263	Total	C	N	O	S	0	0
			2115	1324	365	420	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	82	Total	C	N	O	S	0	0
			657	418	113	121	5		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	117	Total	C	N	O	S	0	0
			949	587	169	182	11		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 10 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 11 is a DNA chain called DNA (5'-D(P*AP*GP*CP*GP*GP*CP*GP*GP*AP*G P*CP*CP*AP*GP*CP*AP*GP*GP*GP*AP*GP*CP*TP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	24	Total	C	N	O	P	0	0
			503	234	105	140	24		

- Molecule 12 is a RNA chain called RNA (5'-R(P*GP*UP*AP*AP*CP*CP*GP*GP*AP*G P*AP*GP*GP*GP*AP*AP*CP*CP*CP*AP*CP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	22	Total	C	N	O	P	0	0
			475	212	92	149	22		

- Molecule 13 is a DNA chain called DNA (35-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	35	Total	C	N	O	P	0	0
			711	337	122	217	35		

- Molecule 14 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	126	Total	C	N	O	S	0	0
			1004	630	170	200	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	171	Total	C	N	O	S	0	0
			1333	866	214	245	8		

- Molecule 16 is a protein called mRNA-capping enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	333	Total	C	N	O	S	0	0
			2662	1698	460	484	20		

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

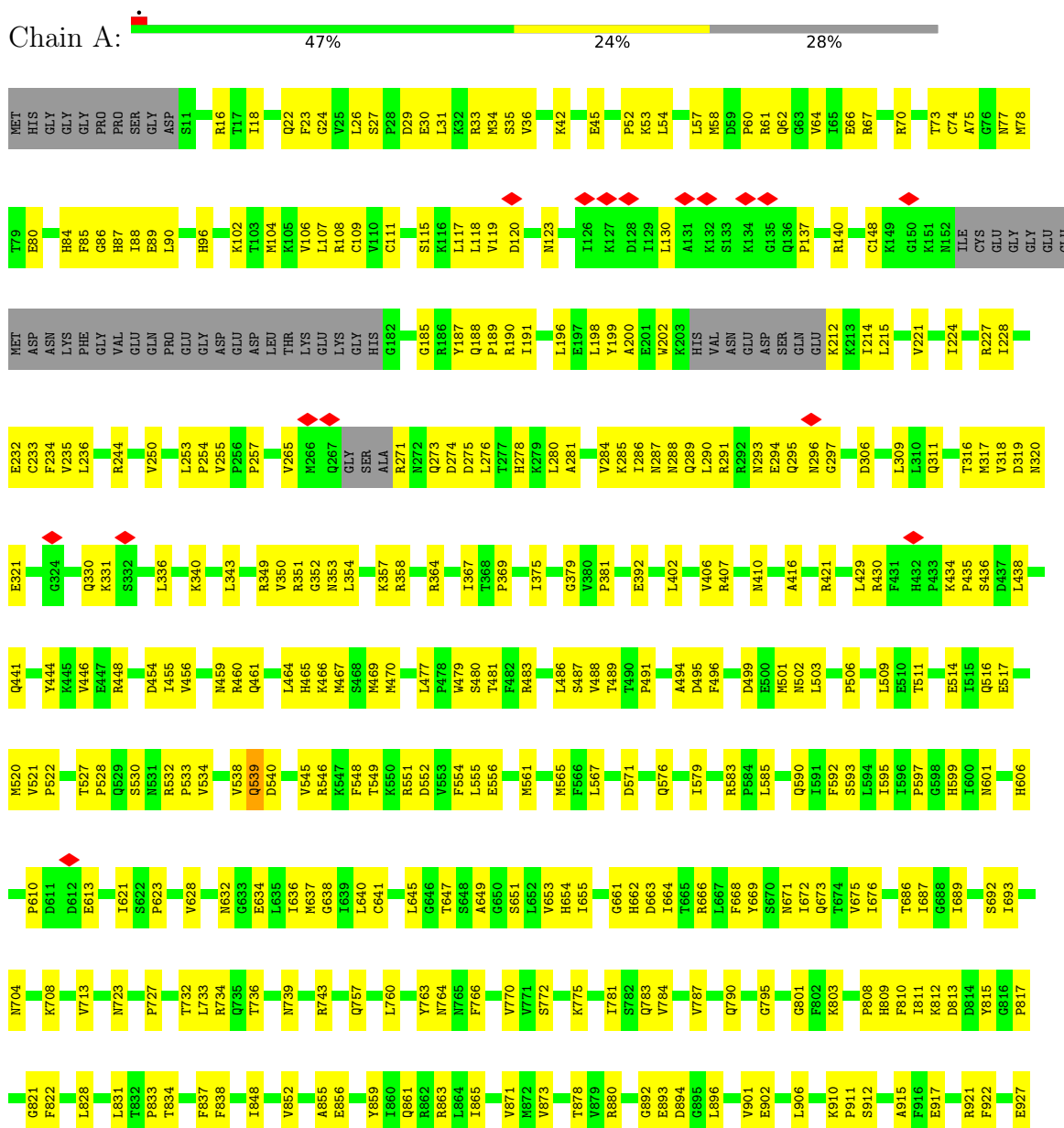
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

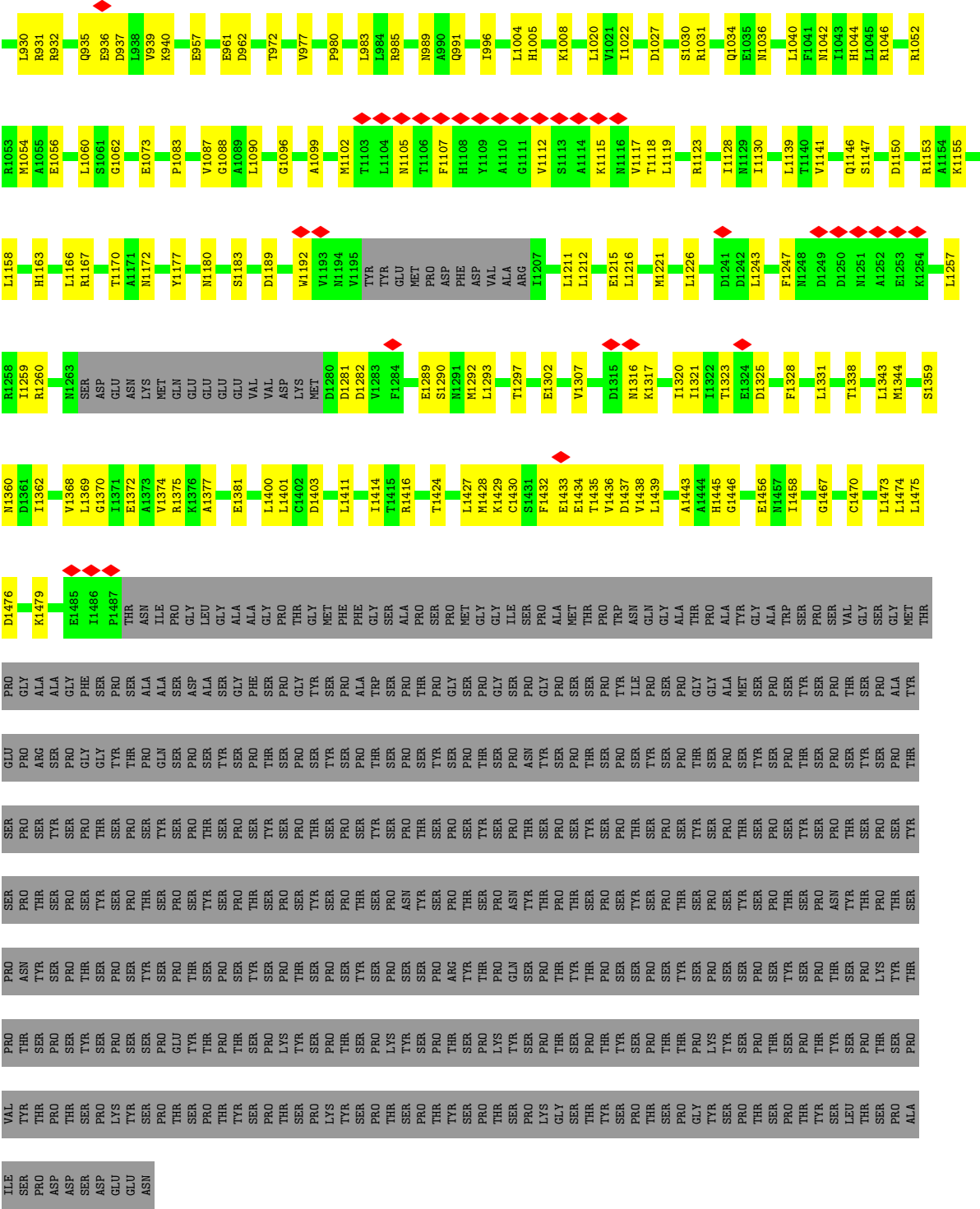
Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Mg	0
			1	1	

3 Residue-property plots

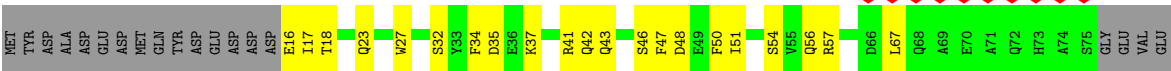
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

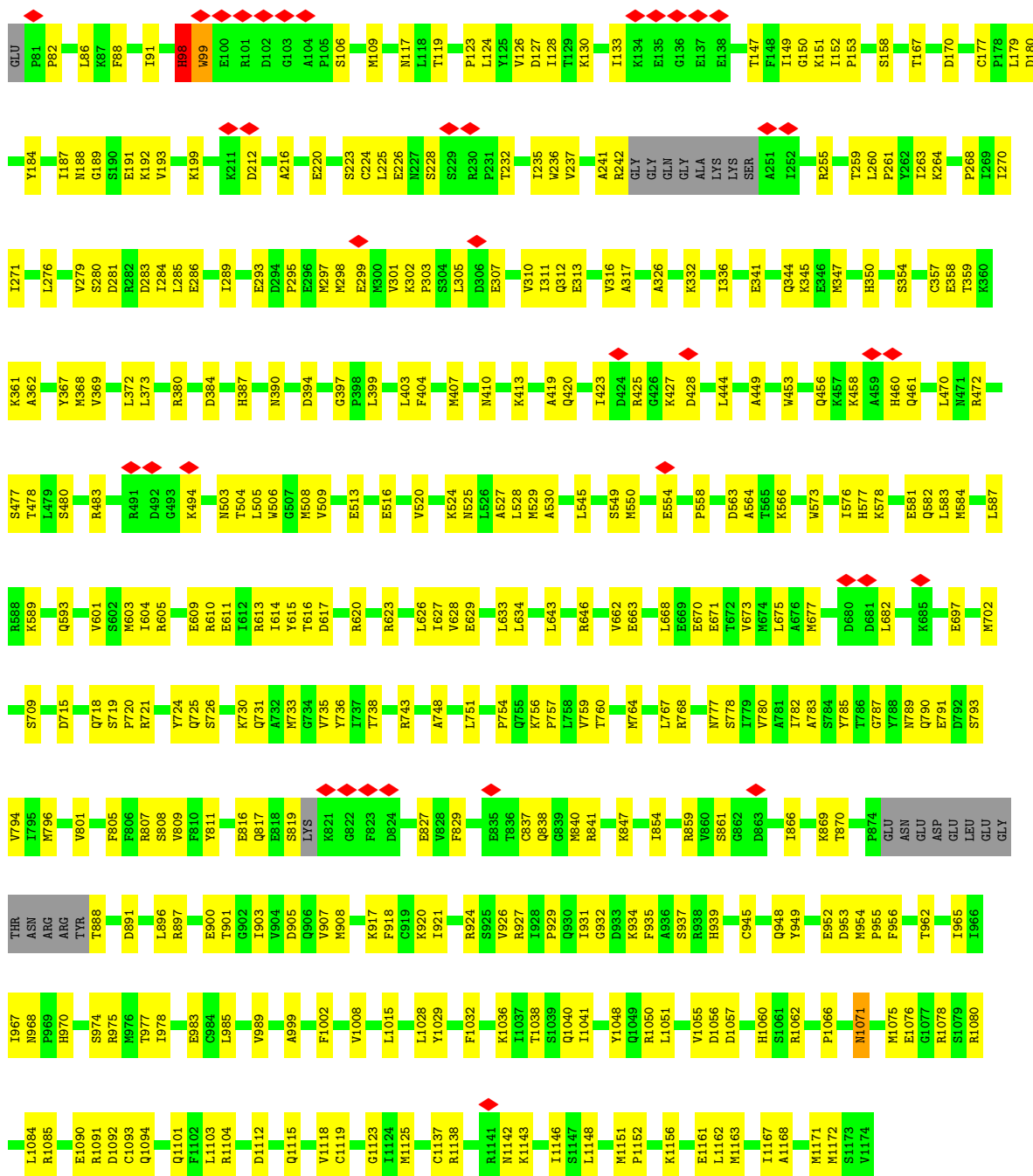
• Molecule 1: DNA-directed RNA polymerase II subunit RPB1





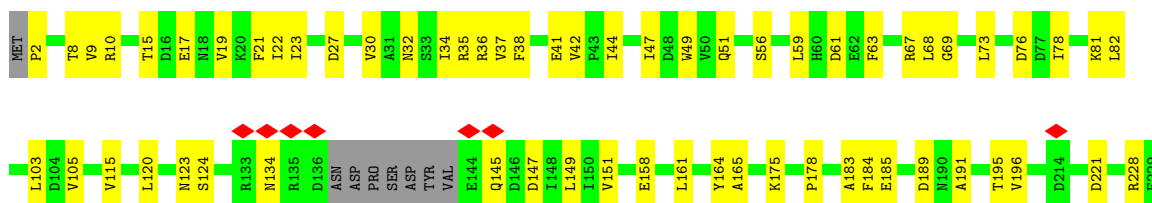
● Molecule 2: DNA-directed RNA polymerase subunit beta

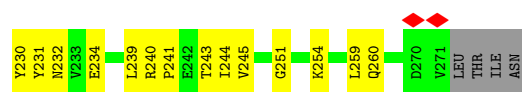




• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

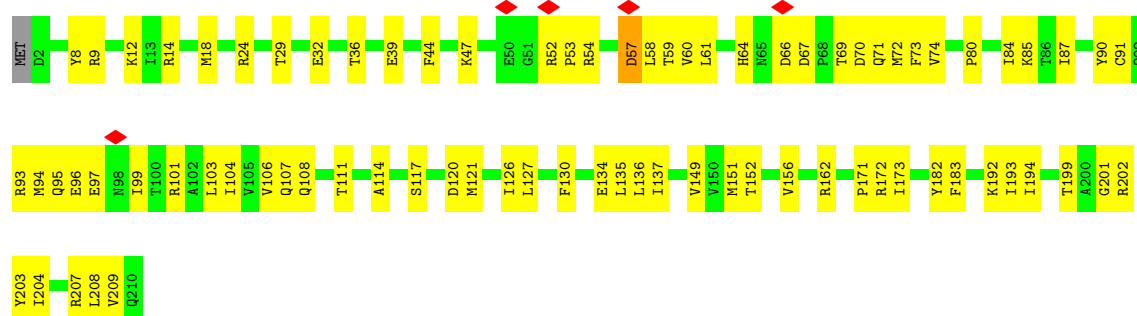
Chain C: 68% 28%





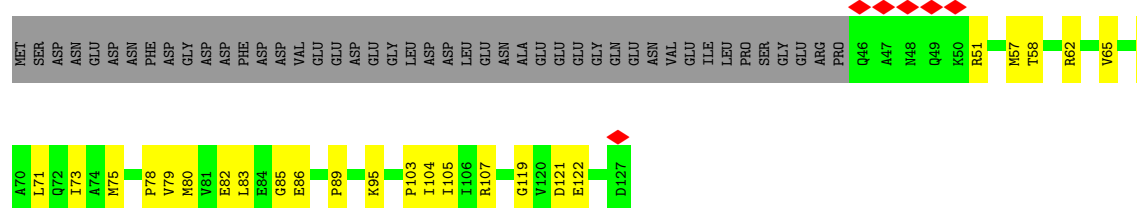
• Molecule 4: DNA-directed RNA polymerase II subunit E

Chain E: 61% 38%



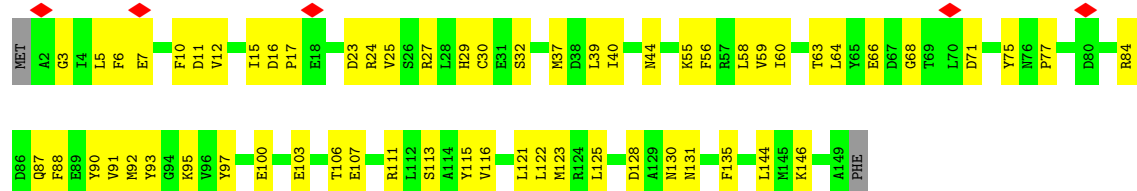
• Molecule 5: DNA-directed RNA polymerase II subunit F

Chain F: 5% 45% 20% 35%



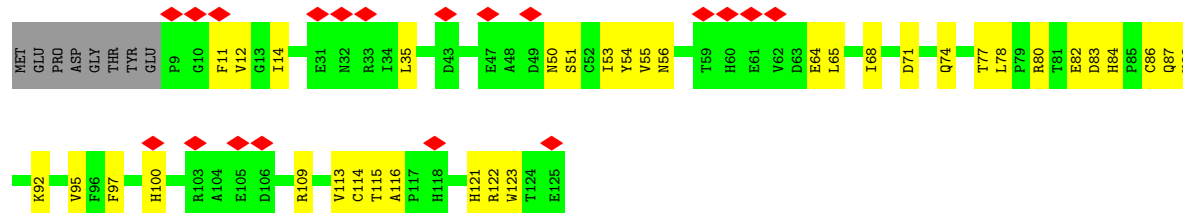
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 58% 41%

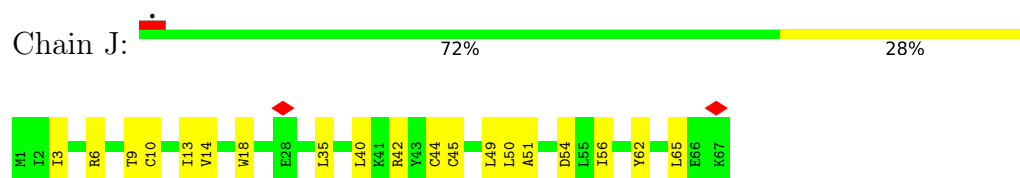


• Molecule 7: DNA-directed RNA polymerase II subunit RPB9

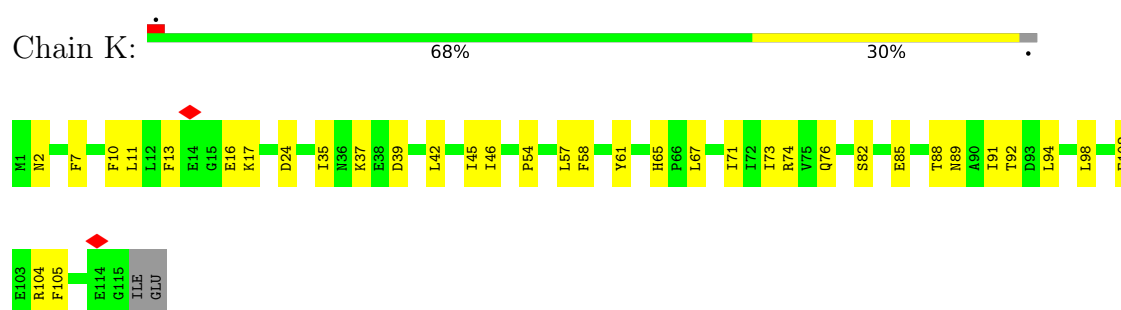
Chain I: 15% 65% 29% 6%



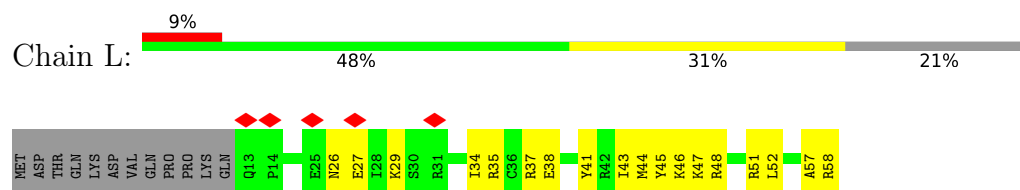
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



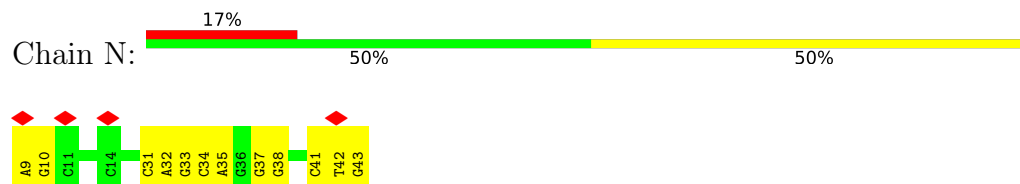
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11-a



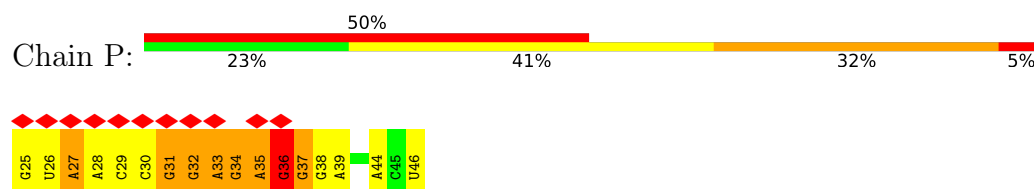
- Molecule 10: RNA polymerase II subunit K



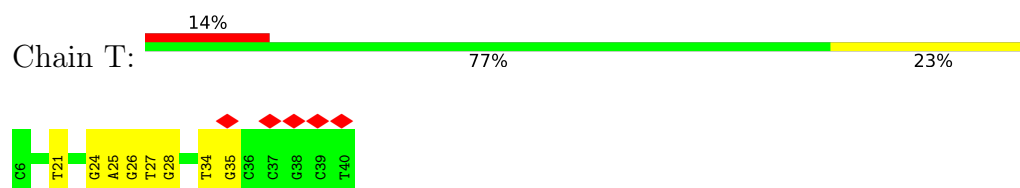
- Molecule 11: DNA (5'-D(P*AP*GP*CP*GP*GP*CP*GP*GP*AP*GP*CP*CP*AP*GP*CP*AP*GP*GP*GP*AP*GP*CP*TP*G)-3')



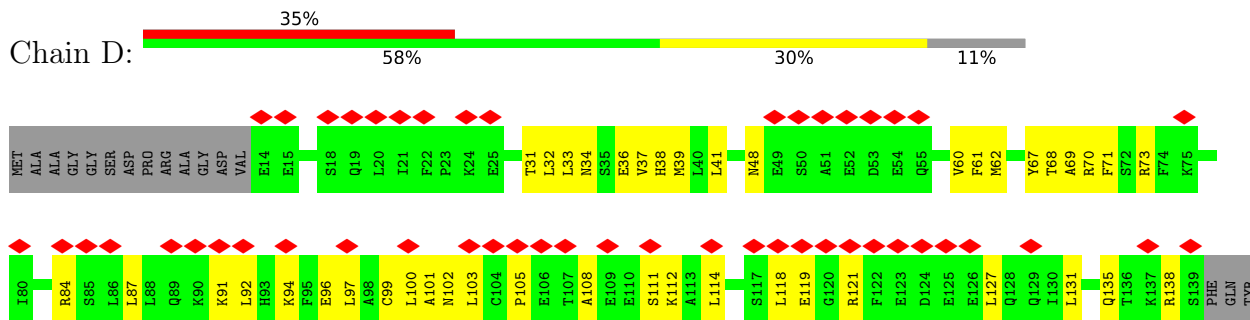
- Molecule 12: RNA (5'-R(P*GP*UP*AP*AP*CP*CP*GP*GP*AP*GP*AP*GP*GP*GP*AP*AP*CP*CP*CP*AP*CP*U)-3')



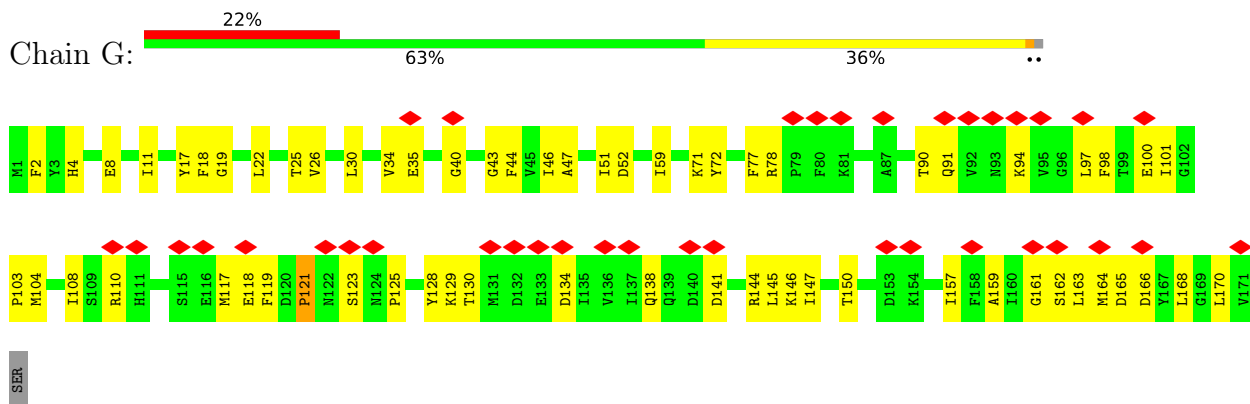
- Molecule 13: DNA (35-MER)



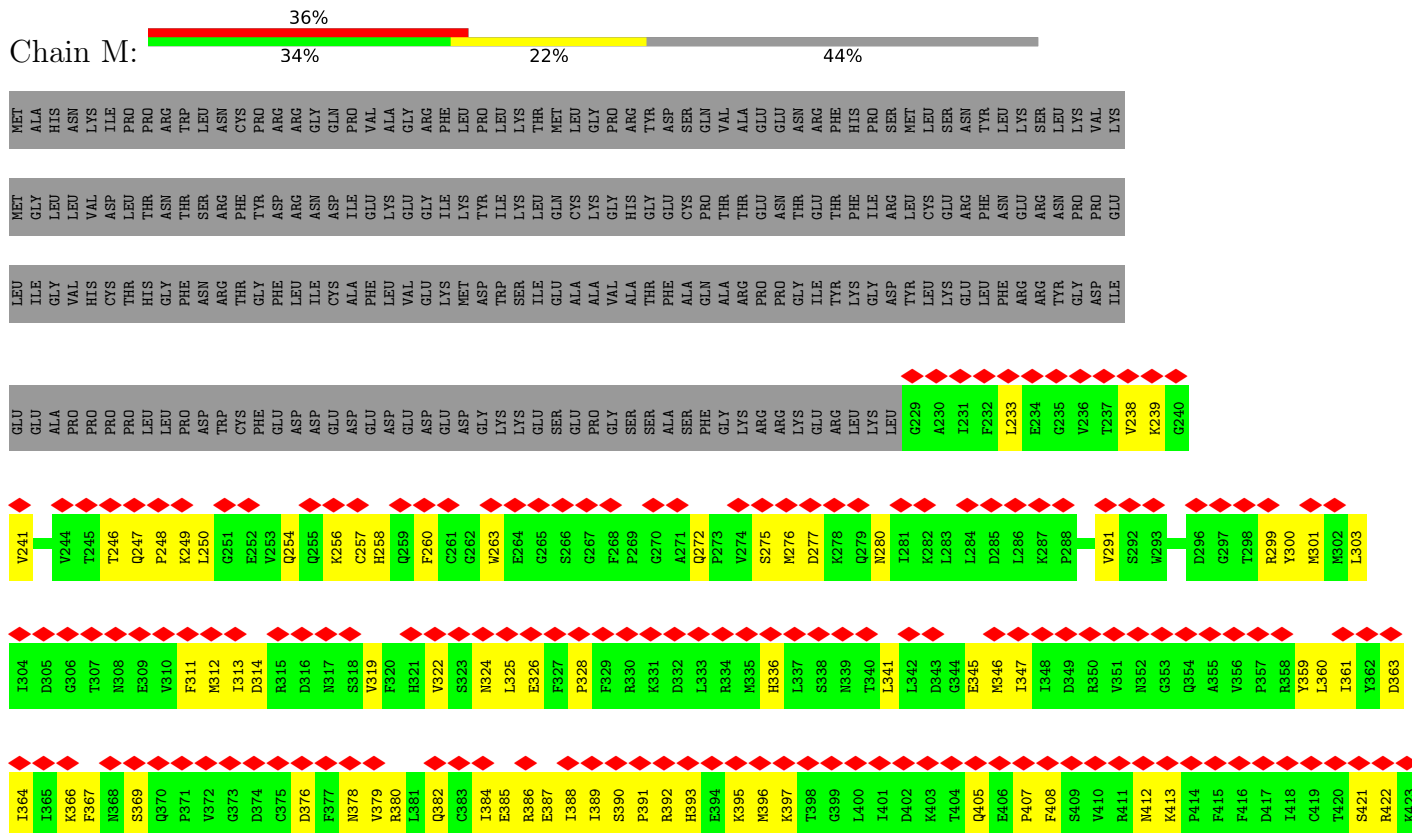
Chain D:

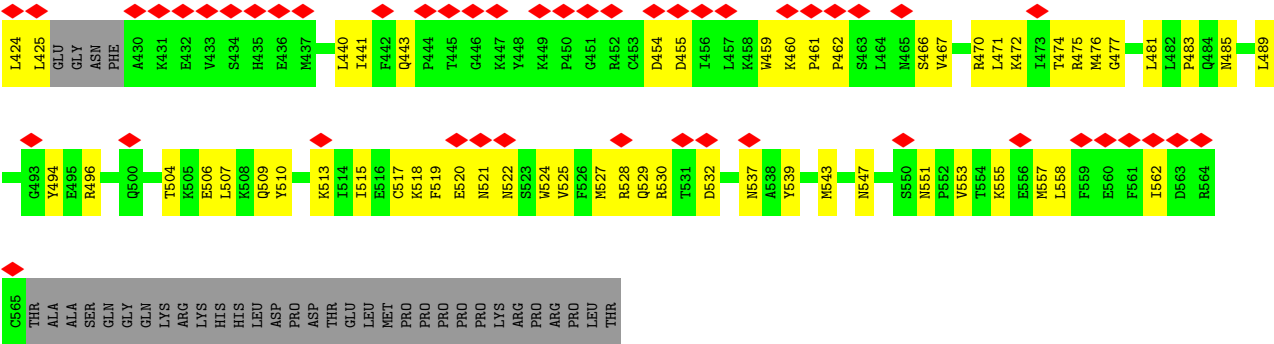


Chain G:



Chain M:





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21150	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.038	Depositor
Minimum map value	-0.013	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00683	Depositor
Map size (Å)	315.0, 315.0, 315.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.15	0/11369	0.40	0/15347
2	B	0.15	0/9232	0.39	3/12462 (0.0%)
3	C	0.14	0/2158	0.34	0/2931
4	E	0.16	0/1751	0.47	0/2366
5	F	0.14	0/667	0.33	0/901
6	H	0.15	0/1207	0.38	0/1628
7	I	0.16	0/972	0.43	0/1316
8	J	0.13	0/542	0.39	1/730 (0.1%)
9	K	0.14	0/939	0.34	0/1271
10	L	0.18	0/394	0.61	0/524
11	N	0.14	0/566	0.25	0/871
12	P	0.28	0/532	0.64	2/828 (0.2%)
13	T	0.18	0/793	0.35	0/1221
14	D	0.13	0/1017	0.36	0/1368
15	G	0.17	0/1364	0.43	1/1853 (0.1%)
16	M	0.17	0/2718	0.44	0/3662
All	All	0.16	0/36221	0.40	7/49279 (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
1	A	0	2
2	B	0	1
4	E	0	1
All	All	0	4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	36	G	C2'-C3'-O3'	6.74	119.61	109.50
2	B	98	HIS	CA-C-N	5.76	132.54	121.54
2	B	98	HIS	C-N-CA	5.76	132.54	121.54
12	P	36	G	C4'-C3'-O3'	5.27	117.31	109.40
8	J	14	VAL	N-CA-C	-5.20	108.22	113.47
15	G	121	PRO	CA-N-CD	-5.07	104.91	112.00
2	B	99	TRP	N-CA-CB	5.02	118.98	110.49

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	538	VAL	Peptide
1	A	539	GLN	Peptide
2	B	98	HIS	Peptide
4	E	57	ASP	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	A	11166	0	11318	373	0
2	B	9052	0	9080	286	0
3	C	2115	0	2057	62	0
4	E	1720	0	1737	60	0
5	F	657	0	684	21	0
6	H	1186	0	1147	49	0
7	I	949	0	879	25	0
8	J	533	0	554	15	0
9	K	920	0	942	28	0
10	L	388	0	393	18	0
11	N	503	0	267	9	0
12	P	475	0	240	31	0
13	T	711	0	395	8	0
14	D	1004	0	980	39	0
15	G	1333	0	1321	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	M	2662	0	2653	106	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	35383	0	34647	1041	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 15.

All (1041) 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)
12:P:27:A:N6	16:M:254:GLN:HE22	1.17	1.40
12:P:27:A:N6	16:M:254:GLN:NE2	1.70	1.33
12:P:27:A:H62	16:M:254:GLN:NE2	1.46	0.96
12:P:25:G:OP1	12:P:25:G:N2	1.99	0.95
12:P:27:A:H61	16:M:254:GLN:NE2	1.48	0.87
2:B:819:SER:H	2:B:827:GLU:HB2	1.42	0.85
2:B:407:MET:HE1	2:B:444:LEU:HG	1.61	0.83
3:C:19:VAL:HG23	3:C:241:PRO:HB2	1.60	0.83
12:P:37:G:H8	12:P:37:G:H5''	1.44	0.83
14:D:87:LEU:HD22	14:D:97:LEU:HG	1.61	0.82
2:B:549:SER:HG	2:B:577:HIS:HE2	1.21	0.82
2:B:260:LEU:HD12	2:B:261:PRO:HD2	1.61	0.82
15:G:11:ILE:HD11	15:G:26:VAL:HG13	1.60	0.82
12:P:35:A:OP2	12:P:35:A:H3'	1.80	0.82
1:A:340:LYS:HG3	1:A:1436:VAL:HG11	1.62	0.80
1:A:42:LYS:O	1:A:288:ASN:ND2	2.14	0.78
1:A:770:VAL:HG21	1:A:781:ILE:HD11	1.64	0.78
2:B:179:LEU:HD22	2:B:768:ARG:HE	1.48	0.78
12:P:27:A:H61	16:M:254:GLN:HE22	0.79	0.78
1:A:255:VAL:HG23	1:A:280:LEU:HD13	1.65	0.78
16:M:518:LYS:HD3	16:M:527:MET:HE2	1.65	0.78
10:L:26:ASN:HD21	10:L:44:MET:HE1	1.48	0.78
2:B:403:LEU:HD23	2:B:407:MET:HE2	1.66	0.78
2:B:603:MET:HG3	2:B:614:ILE:HG12	1.67	0.76
2:B:268:PRO:HG2	2:B:271:ILE:HD12	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:480:SER:OG	2:B:525:ASN:ND2	2.18	0.76
2:B:380:ARG:HD2	2:B:609:GLU:HG3	1.68	0.76
1:A:686:THR:HG21	2:B:1041:ILE:HA	1.67	0.75
1:A:576:GLN:O	1:A:590:GLN:NE2	2.20	0.75
1:A:760:LEU:HD22	1:A:764:ASN:HD22	1.51	0.75
1:A:64:VAL:HG11	1:A:78:MET:HA	1.67	0.74
2:B:32:SER:HB3	2:B:643:LEU:HD21	1.68	0.74
1:A:34:MET:HA	2:B:1138:ARG:HG3	1.69	0.74
14:D:33:LEU:HD11	14:D:101:ALA:HB3	1.70	0.74
16:M:474:THR:HB	16:M:476:MET:HE3	1.70	0.73
1:A:576:GLN:HA	6:H:75:TYR:HB2	1.69	0.73
2:B:907:VAL:HG22	2:B:921:ILE:HG12	1.71	0.73
16:M:518:LYS:HE3	16:M:525:VAL:HG23	1.70	0.73
1:A:760:LEU:HD11	1:A:781:ILE:HG21	1.72	0.72
12:P:35:A:H3'	12:P:35:A:P	2.29	0.72
4:E:80:PRO:HA	4:E:107:GLN:HB2	1.72	0.72
2:B:354:SER:HG	2:B:357:CYS:HG	1.38	0.71
2:B:847:LYS:HA	10:L:51:ARG:HH22	1.54	0.71
9:K:24:ASP:OD2	9:K:74:ARG:NH1	2.23	0.71
2:B:866:ILE:HD11	2:B:896:LEU:HD12	1.72	0.71
2:B:838:GLN:HE21	2:B:888:THR:N	1.88	0.70
4:E:85:LYS:NZ	11:N:41:DC:OP2	2.24	0.70
2:B:270:ILE:HG12	2:B:305:LEU:HD23	1.72	0.70
1:A:549:THR:HG21	1:A:640:LEU:HD12	1.72	0.70
1:A:931:ARG:HD2	1:A:939:VAL:HG11	1.72	0.70
2:B:896:LEU:HD21	2:B:900:GLU:HB3	1.72	0.70
4:E:24:ARG:NE	4:E:183:PHE:O	2.25	0.70
2:B:119:THR:HG23	2:B:187:ILE:HG12	1.74	0.69
2:B:458:LYS:HB2	2:B:461:GLN:HB2	1.74	0.69
12:P:35:A:H4'	12:P:36:G:H2'	1.74	0.69
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.26	0.69
16:M:378:ASN:O	16:M:382:GLN:NE2	2.26	0.69
1:A:233:CYS:SG	1:A:244:ARG:NH1	2.65	0.69
14:D:37:VAL:HG21	15:G:2:PHE:HD2	1.58	0.69
2:B:91:ILE:HD11	2:B:124:LEU:HD12	1.73	0.69
2:B:344:GLN:NE2	2:B:354:SER:O	2.25	0.69
1:A:291:ARG:O	1:A:294:GLU:HG3	1.93	0.69
1:A:592:PHE:HA	1:A:595:ILE:HD12	1.75	0.69
2:B:760:THR:OG1	2:B:764:MET:SD	2.49	0.69
1:A:1372:GLU:HG3	4:E:193:ILE:HD13	1.75	0.68
2:B:311:ILE:HG23	2:B:316:VAL:HG23	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:520:GLU:HG2	16:M:521:ASN:H	1.59	0.68
1:A:1212:LEU:HB3	1:A:1259:ILE:HB	1.75	0.68
1:A:636:ILE:HG22	1:A:637:MET:HG2	1.75	0.68
1:A:808:PRO:HB2	2:B:675:LEU:HD13	1.76	0.68
2:B:298:MET:HA	2:B:301:VAL:HG12	1.76	0.68
2:B:953:ASP:OD1	3:C:36:ARG:NH2	2.23	0.68
1:A:381:PRO:HB3	1:A:480:SER:HA	1.75	0.68
1:A:487:SER:OG	1:A:673:GLN:NE2	2.27	0.68
1:A:902:GLU:OE2	1:A:985:ARG:NH2	2.25	0.68
2:B:425:ARG:HG3	2:B:427:LYS:HG2	1.76	0.68
12:P:37:G:H5''	12:P:37:G:C8	2.28	0.68
3:C:47:ILE:HA	3:C:165:ALA:HA	1.75	0.67
7:I:65:LEU:O	7:I:122:ARG:NH1	2.28	0.67
1:A:296:ASN:OD1	1:A:297:GLY:N	2.28	0.67
4:E:120:ASP:OD1	4:E:121:MET:N	2.28	0.67
15:G:144:ARG:HB3	15:G:168:LEU:HD12	1.77	0.67
2:B:153:PRO:HD2	2:B:444:LEU:HD13	1.77	0.67
2:B:748:ALA:HB3	2:B:811:TYR:HB2	1.76	0.66
1:A:863:ARG:HG2	1:A:1414:ILE:HG22	1.77	0.66
7:I:115:THR:HG22	7:I:116:ALA:H	1.59	0.66
1:A:517:GLU:OE1	5:F:62:ARG:NH1	2.29	0.66
3:C:67:ARG:NH1	8:J:3:ILE:O	2.29	0.66
4:E:9:ARG:HG3	4:E:136:LEU:HD21	1.77	0.66
1:A:196:LEU:HD22	1:A:311:GLN:HE22	1.58	0.66
1:A:1212:LEU:HD22	1:A:1259:ILE:HD12	1.77	0.66
8:J:40:LEU:HD11	8:J:49:LEU:HD12	1.78	0.66
1:A:1170:THR:HA	1:A:1216:LEU:HA	1.77	0.66
12:P:31:G:N3	12:P:31:G:H2'	2.10	0.66
3:C:69:GLY:HA3	10:L:57:ALA:HB1	1.77	0.66
1:A:320:ASN:ND2	1:A:336:LEU:O	2.27	0.66
1:A:1099:ALA:HA	1:A:1102:MET:HE3	1.78	0.66
1:A:111:CYS:HB2	1:A:118:LEU:HB3	1.78	0.65
16:M:300:TYR:CE2	16:M:314:ASP:HB3	2.31	0.65
1:A:692:SER:HB3	1:A:828:LEU:HD21	1.79	0.65
2:B:841:ARG:NE	12:P:34:G:H4'	2.11	0.65
2:B:809:VAL:HA	2:B:926:VAL:HA	1.79	0.65
2:B:509:VAL:HG11	2:B:524:LYS:HD3	1.79	0.65
2:B:725:GLN:NE2	2:B:937:SER:O	2.30	0.65
2:B:790:GLN:O	2:B:968:ASN:ND2	2.27	0.65
2:B:939:HIS:NE2	2:B:983:GLU:OE1	2.26	0.65
4:E:24:ARG:HH11	4:E:72:MET:HE3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:PRO:HB2	1:A:60:PRO:HD3	1.77	0.65
2:B:37:LYS:HD2	2:B:41:ARG:HG2	1.79	0.65
15:G:18:PHE:HA	15:G:22:LEU:HD13	1.79	0.64
2:B:483:ARG:HH12	2:B:528:LEU:HA	1.61	0.64
4:E:61:LEU:HD11	4:E:71:GLN:HB3	1.79	0.64
1:A:1087:VAL:HG12	1:A:1400:LEU:HD22	1.80	0.64
12:P:35:A:N3	12:P:35:A:H5'	2.13	0.64
2:B:285:LEU:HD21	2:B:305:LEU:HD11	1.78	0.64
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.78	0.64
4:E:24:ARG:NH2	4:E:182:TYR:O	2.29	0.64
1:A:70:ARG:NH1	1:A:75:ALA:O	2.30	0.64
1:A:421:ARG:HH22	16:M:496:ARG:HG2	1.62	0.64
1:A:763:TYR:OH	6:H:23:ASP:OD2	2.14	0.64
1:A:1476:ASP:HB2	5:F:105:ILE:HG23	1.80	0.64
15:G:17:TYR:HE2	16:M:481:LEU:HA	1.62	0.64
15:G:117:MET:HB3	15:G:128:TYR:HD1	1.63	0.64
16:M:277:ASP:H	16:M:280:ASN:HB2	1.63	0.63
1:A:704:ASN:O	1:A:708:LYS:HG2	1.98	0.63
1:A:922:PHE:HA	1:A:1052:ARG:HD3	1.80	0.63
2:B:192:LYS:HE3	2:B:449:ALA:HA	1.79	0.63
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.80	0.63
2:B:298:MET:HB3	7:I:14:ILE:HD12	1.80	0.63
15:G:144:ARG:NH2	15:G:170:LEU:O	2.32	0.63
1:A:406:VAL:HG13	1:A:429:LEU:HD21	1.80	0.63
10:L:27:GLU:H	10:L:37:ARG:HH22	1.47	0.62
1:A:36:VAL:HG21	1:A:73:THR:HG21	1.81	0.62
4:E:72:MET:SD	4:E:101:ARG:HG3	2.39	0.62
15:G:145:LEU:HD21	15:G:161:GLY:HA3	1.81	0.62
15:G:146:LYS:NZ	15:G:147:ILE:O	2.33	0.62
16:M:467:VAL:HB	16:M:537:ASN:HD21	1.64	0.62
1:A:87:HIS:NE2	1:A:89:GLU:OE2	2.31	0.62
2:B:952:GLU:HB2	3:C:36:ARG:HG3	1.82	0.62
10:L:29:LYS:HE3	10:L:29:LYS:HA	1.82	0.62
1:A:470:MET:HE3	1:A:521:VAL:HG23	1.82	0.62
2:B:88:PHE:HB3	2:B:128:ILE:HG23	1.81	0.61
16:M:277:ASP:HB2	16:M:551:ASN:HD21	1.63	0.61
2:B:242:ARG:HA	2:B:242:ARG:HH11	1.65	0.61
1:A:289:GLN:NE2	1:A:293:ASN:OD1	2.33	0.61
12:P:34:G:OP2	12:P:34:G:C8	2.54	0.61
1:A:556:GLU:OE1	1:A:583:ARG:NH1	2.34	0.61
3:C:32:ASN:OD1	3:C:35:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:629:GLU:HG2	2:B:634:LEU:HD21	1.82	0.61
2:B:816:GLU:OE2	2:B:869:LYS:NZ	2.25	0.61
14:D:100:LEU:HD11	14:D:118:LEU:HD11	1.83	0.61
2:B:48:ASP:OD1	2:B:158:SER:OG	2.19	0.61
1:A:689:ILE:HG21	2:B:985:LEU:HD22	1.82	0.60
3:C:9:VAL:HG22	3:C:23:ILE:HG12	1.84	0.60
5:F:78:PRO:HG2	15:G:19:GLY:HA2	1.83	0.60
10:L:27:GLU:OE2	10:L:29:LYS:NZ	2.33	0.60
1:A:623:PRO:HA	6:H:27:ARG:HH21	1.66	0.60
1:A:930:LEU:HD23	1:A:939:VAL:HG22	1.83	0.60
8:J:18:TRP:NE1	8:J:54:ASP:OD1	2.34	0.60
16:M:543:MET:O	16:M:547:ASN:ND2	2.34	0.60
2:B:604:ILE:HG12	2:B:668:LEU:HB3	1.84	0.60
1:A:801:GLY:HA3	2:B:503:ASN:HB2	1.83	0.60
2:B:506:TRP:NE1	2:B:697:GLU:OE2	2.29	0.60
16:M:238:VAL:HG11	16:M:408:PHE:HD2	1.67	0.60
1:A:561:MET:HE2	9:K:58:PHE:HA	1.83	0.60
1:A:54:LEU:O	1:A:61:ARG:NH2	2.34	0.60
1:A:727:PRO:HA	1:A:736:THR:HG21	1.83	0.60
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.84	0.60
5:F:82:GLU:O	5:F:95:LYS:NZ	2.35	0.60
14:D:67:TYR:HA	14:D:70:ARG:HH12	1.66	0.60
16:M:328:PRO:HD2	16:M:392:ARG:HG2	1.82	0.60
1:A:540:ASP:OD2	2:B:790:GLN:HG2	2.02	0.60
15:G:110:ARG:HH22	15:G:118:GLU:HA	1.66	0.60
7:I:88:LYS:HE2	7:I:121:HIS:HB2	1.83	0.60
2:B:223:SER:HG	2:B:350:HIS:HD1	1.46	0.59
2:B:456:GLN:NE2	13:T:34:DT:OP2	2.36	0.59
4:E:111:THR:HG23	4:E:114:ALA:H	1.67	0.59
6:H:106:THR:OG1	6:H:107:GLU:OE1	2.20	0.59
14:D:36:GLU:HA	14:D:39:MET:HG2	1.84	0.59
14:D:41:LEU:HD22	14:D:61:PHE:HE1	1.67	0.59
1:A:1130:ILE:HD13	1:A:1411:LEU:HD22	1.85	0.59
1:A:22:GLN:HB3	2:B:1172:MET:HE1	1.83	0.59
2:B:242:ARG:HA	2:B:242:ARG:NH1	2.17	0.59
1:A:26:LEU:HD13	1:A:31:LEU:HD21	1.85	0.59
1:A:912:SER:HB3	1:A:915:ALA:H	1.67	0.59
2:B:626:LEU:HD23	2:B:662:VAL:HG12	1.84	0.59
2:B:905:ASP:HB2	2:B:924:ARG:HG3	1.85	0.59
3:C:67:ARG:NH2	3:C:149:LEU:O	2.32	0.59
14:D:38:HIS:ND1	14:D:68:THR:HG23	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:817:GLN:HB3	2:B:918:PHE:HD1	1.68	0.59
14:D:31:THR:O	14:D:84:ARG:NH2	2.30	0.59
1:A:927:GLU:O	1:A:931:ARG:HG2	2.03	0.59
2:B:289:ILE:HG12	2:B:297:MET:HB3	1.83	0.59
2:B:581:GLU:O	2:B:582:GLN:HG3	2.03	0.59
5:F:51:ARG:NH2	5:F:122:GLU:OE2	2.32	0.59
14:D:34:ASN:H	14:D:102:ASN:HD21	1.49	0.59
1:A:552:ASP:HB2	6:H:24:ARG:HB2	1.85	0.58
3:C:2:PRO:HB3	9:K:54:PRO:HD2	1.85	0.58
3:C:44:ILE:HG21	3:C:178:PRO:HB3	1.84	0.58
1:A:790:GLN:HA	1:A:822:PHE:HA	1.85	0.58
2:B:117:ASN:HA	2:B:189:GLY:HA3	1.84	0.58
1:A:610:PRO:HG2	1:A:613:GLU:HB2	1.85	0.58
1:A:1189:ASP:HA	1:A:1192:TRP:HD1	1.66	0.58
14:D:105:PRO:O	14:D:135:GLN:NE2	2.37	0.58
1:A:369:PRO:HB3	1:A:486:LEU:HD21	1.85	0.58
1:A:514:GLU:OE1	2:B:1101:GLN:HB3	2.03	0.58
2:B:332:LYS:O	2:B:336:ILE:HG12	2.03	0.58
15:G:163:LEU:HA	15:G:168:LEU:HD23	1.85	0.58
1:A:1147:SER:HA	1:A:1153:ARG:HB2	1.86	0.58
16:M:322:VAL:HG11	16:M:325:LEU:HD23	1.84	0.58
1:A:140:ARG:NH1	1:A:234:PHE:O	2.37	0.57
5:F:57:MET:HE3	5:F:62:ARG:HA	1.86	0.57
1:A:757:GLN:HA	1:A:760:LEU:HD12	1.84	0.57
2:B:677:MET:H	2:B:682:LEU:HD22	1.68	0.57
2:B:369:VAL:O	2:B:373:LEU:HG	2.04	0.57
2:B:903:ILE:O	2:B:924:ARG:N	2.37	0.57
4:E:47:LYS:H	4:E:53:PRO:HG3	1.70	0.57
2:B:310:VAL:HG23	2:B:311:ILE:HD12	1.86	0.57
2:B:870:THR:HA	2:B:891:ASP:HA	1.87	0.57
1:A:410:ASN:HD22	1:A:430:ARG:HB3	1.70	0.57
2:B:954:MET:SD	2:B:955:PRO:HD2	2.44	0.57
16:M:520:GLU:HG2	16:M:521:ASN:N	2.17	0.57
1:A:349:ARG:O	1:A:353:ASN:HB2	2.04	0.57
1:A:532:ARG:NH1	1:A:647:THR:O	2.36	0.57
8:J:54:ASP:OD2	8:J:56:ILE:HG22	2.04	0.57
2:B:861:SER:HA	2:B:901:THR:HA	1.87	0.57
1:A:1375:ARG:NE	1:A:1403:ASP:OD1	2.37	0.57
2:B:191:GLU:OE2	2:B:743:ARG:NH2	2.38	0.57
5:F:105:ILE:HG22	5:F:119:GLY:HA2	1.86	0.57
6:H:66:GLU:HA	6:H:84:ARG:HH21	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1151:MET:CE	2:B:1171:MET:HE1	2.35	0.57
14:D:36:GLU:HB2	14:D:39:MET:HE2	1.87	0.56
1:A:972:THR:HG22	1:A:1320:ILE:HG13	1.87	0.56
14:D:70:ARG:HB3	14:D:70:ARG:NH1	2.20	0.56
16:M:421:SER:HA	16:M:424:LEU:HD12	1.86	0.56
1:A:111:CYS:HA	1:A:118:LEU:HD23	1.87	0.56
1:A:1130:ILE:HG21	1:A:1411:LEU:HD13	1.85	0.56
1:A:104:MET:HG2	1:A:198:LEU:HD21	1.88	0.56
1:A:668:PHE:CZ	1:A:672:ILE:HD11	2.40	0.56
1:A:760:LEU:HD22	1:A:764:ASN:ND2	2.20	0.56
1:A:1416:ARG:NH2	13:T:21:DT:O2	2.39	0.56
4:E:97:GLU:HB2	4:E:99:ILE:HG12	1.88	0.56
9:K:85:GLU:HA	9:K:88:THR:HG22	1.86	0.56
16:M:301:MET:N	16:M:313:ILE:O	2.21	0.56
3:C:234:GLU:OE2	8:J:42:ARG:NH2	2.37	0.56
1:A:66:GLU:N	1:A:66:GLU:OE1	2.39	0.56
6:H:85:ALA:HB1	6:H:91:VAL:HG21	1.87	0.56
15:G:44:PHE:CZ	15:G:104:MET:HB2	2.41	0.56
2:B:193:VAL:HG21	2:B:470:LEU:HD13	1.87	0.56
2:B:837:CYS:HB2	2:B:840:MET:HE3	1.87	0.56
1:A:922:PHE:HD1	1:A:1052:ARG:HA	1.71	0.56
2:B:1038:THR:HA	3:C:195:THR:HA	1.86	0.56
2:B:956:PHE:HB3	2:B:962:THR:HG22	1.87	0.56
2:B:1115:GLN:HB3	2:B:1148:LEU:HD11	1.88	0.56
15:G:44:PHE:CE2	15:G:104:MET:HB2	2.41	0.56
16:M:246:THR:O	16:M:250:LEU:HD23	2.06	0.56
2:B:721:ARG:HD2	2:B:975:ARG:HB3	1.89	0.55
3:C:103:LEU:HD23	3:C:161:LEU:HD21	1.88	0.55
1:A:375:ILE:HG12	1:A:666:ARG:HG3	1.87	0.55
1:A:465:HIS:CD2	1:A:467:MET:HB2	2.40	0.55
12:P:33:A:OP2	12:P:33:A:H3'	2.06	0.55
2:B:470:LEU:HD11	2:B:478:THR:HG23	1.89	0.55
10:L:26:ASN:ND2	10:L:44:MET:HE1	2.20	0.55
15:G:30:LEU:O	15:G:34:VAL:HG22	2.06	0.55
1:A:661:GLY:H	1:A:664:ILE:HD12	1.71	0.55
3:C:56:SER:OG	3:C:158:GLU:N	2.31	0.55
6:H:90:TYR:CE1	6:H:92:MET:HG3	2.41	0.55
8:J:40:LEU:HD22	8:J:45:CYS:HB3	1.87	0.55
16:M:504:THR:HB	16:M:507:LEU:HG	1.89	0.55
1:A:1429:LYS:HG3	1:A:1438:VAL:HG11	1.89	0.55
1:A:1474:LEU:HB2	5:F:105:ILE:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:46:LYS:O	10:L:47:LYS:HG2	2.07	0.55
1:A:1123:ARG:NH2	1:A:1360:ASN:OD1	2.39	0.55
2:B:780:VAL:HG12	2:B:965:ILE:HB	1.88	0.55
14:D:38:HIS:HE1	14:D:69:ALA:HB2	1.72	0.55
16:M:246:THR:HG21	16:M:249:LYS:HD2	1.89	0.55
1:A:977:VAL:HG21	1:A:1040:LEU:HD21	1.89	0.55
2:B:286:GLU:HB3	2:B:558:PRO:HG2	1.88	0.55
2:B:841:ARG:HE	12:P:34:G:H4'	1.72	0.55
12:P:31:G:N3	12:P:31:G:C2'	2.70	0.55
1:A:546:ARG:HD3	1:A:772:SER:HB3	1.89	0.55
2:B:302:LYS:HG3	2:B:303:PRO:HD3	1.87	0.55
2:B:628:VAL:HG22	2:B:633:LEU:HD23	1.89	0.55
4:E:74:VAL:HG12	4:E:103:LEU:HB2	1.88	0.55
3:C:47:ILE:HD11	3:C:68:LEU:HB3	1.89	0.55
4:E:67:ASP:OD1	4:E:69:THR:OG1	2.22	0.55
6:H:10:PHE:CE1	6:H:32:SER:HB2	2.42	0.55
15:G:46:ILE:HD11	15:G:77:PHE:HB2	1.88	0.55
16:M:385:GLU:O	16:M:389:ILE:HG22	2.07	0.55
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.88	0.55
15:G:40:GLY:HA2	15:G:157:ILE:HD11	1.89	0.55
15:G:91:GLN:HB3	15:G:98:PHE:HB2	1.88	0.54
1:A:520:MET:HB3	1:A:522:PRO:HD2	1.89	0.54
1:A:935:GLN:O	1:A:939:VAL:HG23	2.07	0.54
1:A:1117:VAL:HG23	1:A:1119:LEU:HG	1.89	0.54
2:B:1040:GLN:NE2	3:C:196:VAL:O	2.40	0.54
1:A:358:ARG:NH1	13:T:27:DT:OP1	2.41	0.54
2:B:801:VAL:HG13	2:B:929:PRO:HD2	1.88	0.54
1:A:1054:MET:HE1	1:A:1060:LEU:HD12	1.88	0.54
4:E:149:VAL:O	4:E:192:LYS:N	2.39	0.54
15:G:119:PHE:HB3	15:G:121:PRO:HD2	1.89	0.54
1:A:456:VAL:HG21	1:A:503:LEU:HD11	1.88	0.54
1:A:441:GLN:NE2	1:A:444:TYR:OH	2.41	0.54
8:J:6:ARG:HG2	8:J:13:ILE:HD13	1.90	0.54
1:A:1374:VAL:HG11	1:A:1411:LEU:HD21	1.89	0.54
1:A:30:GLU:O	1:A:34:MET:HG2	2.08	0.53
2:B:86:LEU:HA	2:B:130:LYS:HA	1.91	0.53
1:A:865:ILE:HG21	2:B:1092:ASP:CG	2.33	0.53
1:A:1344:MET:HE2	4:E:134:GLU:HA	1.88	0.53
16:M:425:LEU:HB2	16:M:555:LYS:HE3	1.90	0.53
1:A:931:ARG:HH22	1:A:936:GLU:HG3	1.73	0.53
15:G:97:LEU:HB3	15:G:108:ILE:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LEU:HD11	1:A:235:VAL:HG13	1.91	0.53
1:A:228:ILE:HG23	1:A:232:GLU:HG2	1.90	0.53
3:C:175:LYS:HZ3	10:L:57:ALA:HB3	1.74	0.53
4:E:64:HIS:ND1	4:E:66:ASP:OD1	2.41	0.53
14:D:32:LEU:HD11	15:G:4:HIS:HB2	1.91	0.53
15:G:118:GLU:N	15:G:129:LYS:O	2.40	0.53
1:A:77:ASN:OD1	1:A:78:MET:N	2.35	0.53
1:A:489:THR:HG23	1:A:494:ALA:HB3	1.89	0.53
2:B:584:MET:HE1	2:B:603:MET:HB3	1.90	0.53
3:C:175:LYS:NZ	10:L:57:ALA:HB3	2.24	0.53
7:I:54:TYR:CE2	7:I:56:ASN:HB2	2.43	0.53
1:A:90:LEU:HA	1:A:287:ASN:HD21	1.74	0.53
1:A:107:LEU:HD21	1:A:221:VAL:HG13	1.91	0.53
1:A:190:ARG:NH2	11:N:34:DC:OP1	2.42	0.53
1:A:1166:LEU:HD13	1:A:1292:MET:HE1	1.91	0.53
15:G:145:LEU:HD23	15:G:146:LYS:N	2.24	0.53
1:A:350:VAL:HG11	1:A:1435:THR:HG21	1.91	0.53
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.90	0.53
1:A:1105:ASN:HB3	1:A:1107:PHE:CE2	2.44	0.53
2:B:410:ASN:HA	2:B:413:LYS:HG2	1.90	0.52
2:B:545:LEU:HB3	2:B:550:MET:SD	2.49	0.52
16:M:312:MET:HE2	16:M:346:MET:HE3	1.91	0.52
1:A:461:GLN:OE1	1:A:502:ASN:ND2	2.42	0.52
1:A:491:PRO:HG3	1:A:534:VAL:HG12	1.90	0.52
1:A:455:ILE:HD13	1:A:516:GLN:HB2	1.91	0.52
4:E:24:ARG:HH12	4:E:103:LEU:HD11	1.74	0.52
11:N:31:DC:H2"	11:N:32:DA:C8	2.44	0.52
2:B:854:ILE:HD11	2:B:866:ILE:HA	1.91	0.52
1:A:45:GLU:OE1	1:A:53:LYS:NZ	2.43	0.52
1:A:1030:SER:OG	4:E:162:ARG:NE	2.36	0.52
2:B:152:ILE:HG13	2:B:444:LEU:HD13	1.90	0.52
9:K:45:ILE:HB	9:K:94:LEU:HD21	1.90	0.52
12:P:32:G:H5"	12:P:32:G:N3	2.23	0.52
1:A:448:ARG:NH2	1:A:454:ASP:OD1	2.37	0.52
1:A:466:LYS:HA	2:B:1093:CYS:SG	2.50	0.52
1:A:533:PRO:O	1:A:647:THR:OG1	2.25	0.52
1:A:1005:HIS:HB3	1:A:1008:LYS:HG2	1.91	0.52
9:K:82:SER:HB3	9:K:85:GLU:HG2	1.92	0.52
11:N:9:DA:H2"	11:N:10:DG:C8	2.45	0.52
12:P:27:A:N6	16:M:254:GLN:HE21	1.93	0.52
1:A:29:ASP:OD1	1:A:30:GLU:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:ARG:NH1	1:A:815:TYR:OH	2.43	0.52
1:A:1027:ASP:OD1	1:A:1027:ASP:N	2.42	0.52
2:B:399:LEU:HB3	2:B:453:TRP:CZ2	2.45	0.52
3:C:15:THR:HG22	3:C:17:GLU:H	1.74	0.52
4:E:91:CYS:O	4:E:94:MET:HB2	2.10	0.52
6:H:3:GLY:O	6:H:84:ARG:NH1	2.42	0.52
1:A:496:PHE:HD2	2:B:791:GLU:HB3	1.75	0.52
2:B:223:SER:OG	2:B:350:HIS:ND1	2.31	0.52
2:B:283:ASP:OD1	2:B:284:ILE:N	2.42	0.52
16:M:257:CYS:SG	16:M:303:LEU:HD22	2.50	0.52
2:B:427:LYS:HG3	2:B:428:ASP:H	1.75	0.52
2:B:783:ALA:HB2	2:B:1041:ILE:HG23	1.92	0.52
2:B:789:ASN:HA	2:B:793:SER:HB2	1.91	0.52
2:B:859:ARG:HE	2:B:903:ILE:HD11	1.74	0.52
16:M:239:LYS:O	16:M:407:PRO:HB3	2.10	0.52
1:A:460:ARG:HB2	1:A:501:MET:HE2	1.92	0.51
1:A:861:GLN:NE2	1:A:1096:GLY:O	2.42	0.51
1:A:1344:MET:HE1	4:E:137:ILE:HG12	1.91	0.51
2:B:180:ASP:OD2	2:B:184:TYR:OH	2.25	0.51
1:A:496:PHE:CD2	2:B:791:GLU:HB3	2.45	0.51
16:M:366:LYS:HE3	16:M:369:SER:HA	1.93	0.51
1:A:330:GLN:HG2	1:A:331:LYS:H	1.75	0.51
2:B:505:LEU:HD22	2:B:509:VAL:HB	1.93	0.51
2:B:549:SER:OG	2:B:577:HIS:NE2	2.25	0.51
15:G:123:SER:OG	15:G:125:PRO:O	2.22	0.51
5:F:73:ILE:HD12	5:F:79:VAL:HG12	1.91	0.51
11:N:34:DC:H2''	11:N:35:DA:H8	1.76	0.51
1:A:502:ASN:HB2	2:B:1084:LEU:HG	1.92	0.51
4:E:117:SER:HB2	4:E:121:MET:HE1	1.93	0.51
6:H:25:VAL:HG21	6:H:121:LEU:HD22	1.92	0.51
1:A:554:PHE:HB3	1:A:585:LEU:HD23	1.92	0.51
1:A:790:GLN:HB2	1:A:822:PHE:HD1	1.75	0.51
16:M:233:LEU:HD22	16:M:346:MET:HB3	1.92	0.51
1:A:460:ARG:NH2	12:P:46:U:O2'	2.43	0.51
16:M:440:LEU:HB2	16:M:459:TRP:HB3	1.92	0.51
1:A:910:LYS:HB3	1:A:1328:PHE:CE2	2.46	0.51
2:B:483:ARG:NH2	2:B:527:ALA:O	2.44	0.51
2:B:549:SER:HG	2:B:577:HIS:CD2	2.27	0.51
1:A:188:GLN:HE22	1:A:190:ARG:HA	1.77	0.50
1:A:367:ILE:HD13	1:A:501:MET:HE3	1.92	0.50
1:A:1189:ASP:HA	1:A:1192:TRP:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:46:ILE:HG21	9:K:73:ILE:HD13	1.93	0.50
16:M:471:LEU:HD13	16:M:489:LEU:HD23	1.94	0.50
16:M:506:GLU:HA	16:M:509:GLN:HE22	1.76	0.50
1:A:18:ILE:HD12	2:B:1171:MET:HB2	1.92	0.50
1:A:364:ARG:HD2	2:B:1084:LEU:HD11	1.92	0.50
1:A:1139:LEU:HB3	1:A:1141:VAL:HG23	1.94	0.50
4:E:152:THR:O	4:E:156:VAL:HG23	2.11	0.50
14:D:105:PRO:HB2	14:D:131:LEU:HD21	1.93	0.50
2:B:726:SER:O	2:B:730:LYS:NZ	2.45	0.50
2:B:956:PHE:CE2	3:C:184:PHE:HB3	2.46	0.50
10:L:41:TYR:CE2	10:L:43:ILE:HB	2.47	0.50
1:A:375:ILE:HD13	1:A:669:TYR:HD2	1.76	0.50
1:A:828:LEU:HD22	2:B:978:ILE:HG21	1.91	0.50
2:B:67:LEU:HB3	2:B:420:GLN:OE1	2.12	0.50
2:B:584:MET:SD	2:B:605:ARG:HB2	2.51	0.50
12:P:26:U:H3	16:M:272:GLN:HG3	1.76	0.50
14:D:103:LEU:HD13	14:D:114:LEU:HD13	1.94	0.50
16:M:359:TYR:CE2	16:M:361:ILE:HG12	2.46	0.50
1:A:275:ASP:HB3	1:A:336:LEU:HD22	1.92	0.50
1:A:811:ILE:HD11	7:I:78:LEU:C	2.37	0.50
2:B:35:ASP:OD2	2:B:646:ARG:NH2	2.44	0.50
3:C:9:VAL:HG11	9:K:105:PHE:HD1	1.75	0.50
16:M:258:HIS:HD1	16:M:263:TRP:HD1	1.60	0.50
2:B:1076:GLU:OE2	2:B:1080:ARG:NH2	2.44	0.50
13:T:35:DG:H5'	13:T:35:DG:C8	2.47	0.50
2:B:601:VAL:HG22	2:B:616:THR:HG23	1.92	0.50
3:C:134:ASN:OD1	3:C:145:GLN:NE2	2.44	0.50
9:K:35:ILE:HB	9:K:71:ILE:HG22	1.94	0.50
14:D:67:TYR:CE1	15:G:101:ILE:HD12	2.47	0.50
16:M:515:ILE:HG22	16:M:529:GLN:HG2	1.94	0.50
4:E:104:ILE:HD11	4:E:127:LEU:HD12	1.94	0.50
5:F:80:MET:HG3	5:F:103:PRO:HD3	1.94	0.50
6:H:75:TYR:CZ	6:H:77:PRO:HG3	2.47	0.50
15:G:35:GLU:OE2	15:G:47:ALA:HA	2.12	0.50
1:A:274:ASP:OD1	1:A:275:ASP:N	2.45	0.49
1:A:1052:ARG:O	1:A:1056:GLU:HG2	2.11	0.49
2:B:931:ILE:HA	2:B:945:CYS:HB3	1.94	0.49
6:H:111:ARG:HA	6:H:128:ASP:HA	1.94	0.49
14:D:34:ASN:O	14:D:68:THR:OG1	2.29	0.49
1:A:189:PRO:HB3	1:A:202:TRP:CE2	2.46	0.49
14:D:38:HIS:CE1	14:D:69:ALA:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:256:LYS:HZ2	16:M:303:LEU:HD11	1.76	0.49
16:M:376:ASP:O	16:M:380:ARG:HG3	2.11	0.49
16:M:475:ARG:HA	16:M:485:ASN:HA	1.94	0.49
2:B:98:HIS:N	2:B:106:SER:O	2.39	0.49
3:C:221:ASP:OD1	3:C:221:ASP:N	2.46	0.49
1:A:435:PRO:HA	1:A:438:LEU:HD23	1.94	0.49
1:A:732:THR:HG22	1:A:733:LEU:H	1.77	0.49
1:A:932:ARG:HH12	6:H:103:GLU:HB2	1.77	0.49
2:B:260:LEU:HD11	2:B:347:MET:HB2	1.93	0.49
2:B:589:LYS:O	2:B:593:GLN:HG3	2.11	0.49
16:M:322:VAL:CG1	16:M:325:LEU:HD23	2.42	0.49
2:B:1112:ASP:OD1	2:B:1112:ASP:N	2.45	0.49
16:M:241:VAL:HG13	16:M:322:VAL:HG22	1.95	0.49
1:A:185:GLY:H	1:A:187:TYR:HE1	1.60	0.49
1:A:461:GLN:NE2	2:B:1090:GLU:OE2	2.45	0.49
2:B:177:CYS:HB3	2:B:180:ASP:HB2	1.94	0.49
4:E:117:SER:O	4:E:120:ASP:N	2.46	0.49
6:H:7:GLU:OE1	6:H:59:VAL:HG22	2.12	0.49
10:L:34:ILE:O	10:L:35:ARG:HD2	2.12	0.49
16:M:300:TYR:HB3	16:M:312:MET:CE	2.43	0.49
1:A:556:GLU:CD	1:A:583:ARG:HH12	2.19	0.49
1:A:983:LEU:HD12	1:A:1044:HIS:ND1	2.27	0.49
1:A:1443:ALA:HB2	2:B:1167:ILE:HG23	1.94	0.49
8:J:35:LEU:HD11	8:J:50:LEU:HD12	1.95	0.49
10:L:37:ARG:HG3	10:L:38:GLU:OE1	2.12	0.49
14:D:112:LYS:HZ3	14:D:112:LYS:HB2	1.78	0.49
16:M:466:SER:N	16:M:517:CYS:O	2.46	0.49
1:A:810:PHE:CZ	1:A:834:THR:HG21	2.48	0.49
2:B:1119:CYS:SG	2:B:1142:ASN:ND2	2.86	0.49
6:H:6:PHE:HB3	6:H:60:ILE:HB	1.94	0.49
6:H:130:ASN:OD1	6:H:131:ASN:N	2.45	0.49
1:A:24:GLY:O	2:B:1168:ALA:N	2.37	0.49
1:A:316:THR:HA	1:A:319:ASP:O	2.12	0.49
2:B:54:SER:HA	2:B:57:ARG:HG2	1.94	0.49
2:B:220:GLU:HB3	2:B:236:TRP:CD1	2.48	0.48
2:B:513:GLU:OE2	2:B:525:ASN:ND2	2.46	0.48
6:H:71:ASP:N	6:H:71:ASP:OD1	2.46	0.48
9:K:39:ASP:N	9:K:39:ASP:OD2	2.45	0.48
12:P:37:G:C8	12:P:37:G:C5'	2.95	0.48
16:M:386:ARG:O	16:M:390:SER:OG	2.31	0.48
1:A:1027:ASP:O	1:A:1031:ARG:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:367:TYR:OH	2:B:611:GLU:OE2	2.27	0.48
2:B:956:PHE:HE2	3:C:184:PHE:HB3	1.78	0.48
14:D:105:PRO:HG3	14:D:114:LEU:HD12	1.95	0.48
16:M:363:ASP:OD1	16:M:364:ILE:N	2.46	0.48
1:A:117:LEU:HG	1:A:119:VAL:HG12	1.95	0.48
1:A:465:HIS:HD2	1:A:467:MET:HB2	1.78	0.48
1:A:1475:LEU:HG	15:G:59:ILE:HD11	1.96	0.48
2:B:587:LEU:HD13	2:B:603:MET:HG2	1.94	0.48
14:D:94:LYS:HA	14:D:97:LEU:HD13	1.95	0.48
1:A:421:ARG:NH2	16:M:496:ARG:HG2	2.28	0.48
1:A:962:ASP:OD2	1:A:1046:ARG:NH2	2.32	0.48
2:B:738:THR:OG1	8:J:62:TYR:OH	2.30	0.48
1:A:96:HIS:HB2	1:A:250:VAL:HG23	1.94	0.48
1:A:253:LEU:HD12	1:A:254:PRO:HD2	1.95	0.48
1:A:479:TRP:HB2	1:A:483:ARG:HH21	1.79	0.48
1:A:1004:LEU:HD13	1:A:1062:GLY:HA2	1.94	0.48
2:B:751:LEU:HD12	2:B:808:SER:HB3	1.95	0.48
4:E:36:THR:OG1	4:E:39:GLU:OE1	2.21	0.48
16:M:477:GLY:HA3	16:M:483:PRO:HA	1.96	0.48
1:A:77:ASN:H	1:A:80:GLU:HB3	1.79	0.48
1:A:561:MET:HG2	9:K:58:PHE:CD1	2.49	0.48
2:B:276:LEU:HD21	2:B:358:GLU:O	2.13	0.48
2:B:829:PHE:HD2	2:B:917:LYS:HD2	1.79	0.48
7:I:83:ASP:OD1	7:I:84:HIS:N	2.47	0.48
1:A:340:LYS:HE3	1:A:1436:VAL:HG21	1.95	0.48
2:B:260:LEU:HD23	2:B:263:ILE:HG13	1.96	0.48
2:B:1078:ARG:N	13:T:28:DG:OP1	2.46	0.48
3:C:259:LEU:HD11	9:K:35:ILE:HD12	1.95	0.48
1:A:109:CYS:HA	1:A:148:CYS:SG	2.54	0.48
1:A:379:GLY:HA3	1:A:477:LEU:HD12	1.96	0.48
1:A:871:VAL:HB	1:A:1088:GLY:HA3	1.96	0.48
2:B:1029:TYR:HD2	3:C:184:PHE:HD2	1.62	0.48
2:B:1071:ASN:HD22	2:B:1071:ASN:C	2.22	0.48
6:H:128:ASP:OD1	6:H:131:ASN:ND2	2.46	0.48
9:K:10:PHE:HA	9:K:37:LYS:HB3	1.96	0.48
1:A:281:ALA:O	1:A:285:LYS:HG3	2.14	0.48
16:M:291:VAL:HG21	16:M:421:SER:HB3	1.95	0.48
1:A:739:ASN:HB3	1:A:743:ARG:HH21	1.78	0.48
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.94	0.48
2:B:1163:MET:HA	2:B:1167:ILE:O	2.13	0.48
14:D:34:ASN:ND2	14:D:71:PHE:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:D:41:LEU:HD22	14:D:61:PHE:CE1	2.47	0.48
1:A:407:ARG:HG2	1:A:407:ARG:HH11	1.78	0.47
1:A:57:LEU:HD21	1:A:284:VAL:HG21	1.96	0.47
1:A:488:VAL:O	1:A:491:PRO:HD2	2.14	0.47
1:A:651:SER:O	1:A:655:ILE:HG12	2.13	0.47
1:A:653:VAL:HG21	1:A:669:TYR:CE1	2.50	0.47
1:A:1289:GLU:O	1:A:1292:MET:HG3	2.14	0.47
1:A:1473:LEU:HD12	5:F:104:ILE:HG21	1.96	0.47
2:B:109:MET:HE2	2:B:109:MET:HA	1.97	0.47
2:B:757:PRO:HA	2:B:777:ASN:HD21	1.78	0.47
14:D:37:VAL:O	14:D:41:LEU:HG	2.13	0.47
16:M:360:LEU:HB3	16:M:413:LYS:HB2	1.96	0.47
1:A:812:LYS:HE2	7:I:77:THR:OG1	2.14	0.47
1:A:1040:LEU:HB2	4:E:201:GLY:N	2.28	0.47
2:B:42:GLN:HG2	2:B:43:GLN:N	2.29	0.47
2:B:50:PHE:HB2	2:B:397:GLY:HA2	1.96	0.47
2:B:264:LYS:HE3	2:B:326:ALA:HB2	1.97	0.47
4:E:194:ILE:HG13	4:E:204:ILE:HD12	1.97	0.47
11:N:34:DC:H2"	11:N:35:DA:C8	2.50	0.47
1:A:1118:THR:O	1:A:1123:ARG:HB2	2.13	0.47
1:A:1281:ASP:OD1	1:A:1282:ASP:N	2.47	0.47
2:B:46:SER:HB3	2:B:397:GLY:H	1.79	0.47
3:C:259:LEU:HD22	9:K:42:LEU:HD21	1.97	0.47
8:J:65:LEU:HD11	10:L:45:TYR:CG	2.49	0.47
16:M:388:ILE:O	16:M:392:ARG:HG3	2.14	0.47
16:M:510:TYR:CE2	16:M:515:ILE:HG21	2.49	0.47
1:A:1083:PRO:HD2	5:F:58:THR:HG21	1.96	0.47
2:B:508:MET:HA	2:B:530:ALA:HB2	1.94	0.47
3:C:59:LEU:HD12	3:C:151:VAL:HG23	1.96	0.47
1:A:199:TYR:HB3	1:A:215:LEU:HA	1.97	0.47
1:A:1177:TYR:CD2	7:I:35:LEU:HD13	2.49	0.47
1:A:1221:MET:HE1	1:A:1226:LEU:HB2	1.97	0.47
6:H:64:LEU:O	6:H:84:ARG:N	2.33	0.47
1:A:1221:MET:HE2	1:A:1221:MET:HA	1.95	0.47
1:A:1368:VAL:HG12	1:A:1369:LEU:HD12	1.97	0.47
1:A:1439:LEU:HD13	2:B:1162:LEU:HD21	1.97	0.47
2:B:1029:TYR:HE2	3:C:185:GLU:HA	1.80	0.47
4:E:94:MET:HE3	4:E:99:ILE:HG13	1.96	0.47
16:M:367:PHE:CE1	16:M:387:GLU:HG2	2.50	0.47
1:A:551:ARG:HG2	6:H:25:VAL:HG11	1.97	0.47
1:A:852:VAL:O	2:B:494:LYS:NZ	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1139:LEU:HD13	1:A:1359:SER:HA	1.97	0.47
7:I:113:VAL:HG22	7:I:122:ARG:HG2	1.97	0.47
1:A:528:PRO:HG2	1:A:1090:LEU:HD11	1.97	0.47
2:B:216:ALA:N	2:B:241:ALA:HB2	2.30	0.47
3:C:240:ARG:HB2	3:C:243:THR:HG22	1.95	0.47
4:E:101:ARG:HB3	4:E:126:ILE:HG13	1.97	0.47
12:P:35:A:H5''	12:P:36:G:H2'	1.97	0.47
14:D:32:LEU:CD1	15:G:4:HIS:HB2	2.45	0.47
15:G:52:ASP:N	15:G:71:LYS:O	2.47	0.47
16:M:393:HIS:HA	16:M:396:MET:HE3	1.96	0.47
1:A:539:GLN:HE22	1:A:775:LYS:HE2	1.80	0.47
2:B:617:ASP:N	2:B:617:ASP:OD1	2.47	0.47
16:M:276:MET:HA	16:M:280:ASN:HD22	1.79	0.47
1:A:434:LYS:HZ1	16:M:494:TYR:HD2	1.61	0.46
1:A:579:ILE:HG13	6:H:92:MET:HG2	1.97	0.46
2:B:126:VAL:O	2:B:147:THR:N	2.46	0.46
2:B:126:VAL:HG12	2:B:149:ILE:HD11	1.97	0.46
16:M:303:LEU:HD13	16:M:341:LEU:HD13	1.97	0.46
2:B:16:GLU:HG2	2:B:17:ILE:H	1.79	0.46
3:C:105:VAL:HG11	3:C:115:VAL:HG22	1.97	0.46
4:E:29:THR:HG23	4:E:32:GLU:H	1.78	0.46
14:D:60:VAL:HG13	15:G:103:PRO:HB3	1.96	0.46
1:A:62:GLN:HE22	1:A:255:VAL:HG13	1.81	0.46
2:B:908:MET:HE2	2:B:920:LYS:HB2	1.98	0.46
4:E:54:ARG:O	4:E:58:LEU:HD23	2.15	0.46
1:A:85:PHE:CE1	1:A:257:PRO:HD3	2.50	0.46
2:B:611:GLU:OE1	2:B:613:ARG:NH1	2.48	0.46
3:C:47:ILE:HG23	3:C:73:LEU:HD11	1.96	0.46
15:G:52:ASP:H	15:G:72:TYR:HA	1.80	0.46
1:A:375:ILE:HG21	1:A:669:TYR:HD2	1.80	0.46
1:A:599:HIS:ND1	1:A:632:ASN:OD1	2.48	0.46
1:A:1290:SER:O	1:A:1293:LEU:HG	2.16	0.46
2:B:477:SER:HB2	2:B:730:LYS:HA	1.97	0.46
2:B:807:ARG:NH1	10:L:58:ARG:O	2.49	0.46
2:B:1119:CYS:HB2	2:B:1137:CYS:SG	2.55	0.46
15:G:43:GLY:HA3	15:G:78:ARG:HB2	1.97	0.46
1:A:506:PRO:HB2	1:A:511:THR:HG23	1.98	0.46
1:A:552:ASP:HB3	6:H:25:VAL:HG12	1.98	0.46
1:A:1040:LEU:HB2	4:E:201:GLY:H	1.80	0.46
2:B:34:PHE:HZ	2:B:528:LEU:HB3	1.79	0.46
2:B:719:SER:OG	2:B:720:PRO:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:VAL:HA	1:A:354:LEU:HD12	1.97	0.46
1:A:859:TYR:OH	1:A:1433:GLU:OE2	2.24	0.46
2:B:759:VAL:HG11	2:B:983:GLU:HG3	1.98	0.46
2:B:1123:GLY:HA3	2:B:1171:MET:H	1.80	0.46
3:C:260:GLN:HB2	9:K:91:ILE:HG21	1.96	0.46
12:P:36:G:H1'	12:P:37:G:OP2	2.16	0.46
1:A:530:SER:O	1:A:532:ARG:HG3	2.16	0.46
1:A:937:ASP:HA	1:A:940:LYS:NZ	2.30	0.46
1:A:1467:GLY:H	1:A:1470:CYS:HB2	1.81	0.46
4:E:106:VAL:HG22	4:E:130:PHE:O	2.16	0.46
16:M:494:TYR:CZ	16:M:496:ARG:HB2	2.51	0.46
1:A:855:ALA:HB3	2:B:494:LYS:NZ	2.31	0.46
1:A:863:ARG:HG3	1:A:1432:PHE:CZ	2.51	0.46
2:B:460:HIS:CE1	2:B:461:GLN:HG3	2.51	0.46
2:B:780:VAL:HG11	2:B:1048:TYR:CE2	2.50	0.46
4:E:93:ARG:HA	4:E:96:GLU:HG3	1.98	0.46
5:F:83:LEU:HD12	5:F:85:GLY:H	1.81	0.46
7:I:86:CYS:HB2	7:I:114:CYS:SG	2.55	0.46
16:M:441:ILE:HG23	16:M:443:GLN:HE22	1.80	0.46
16:M:513:LYS:HE3	16:M:529:GLN:NE2	2.30	0.46
16:M:528:ARG:NH1	16:M:530:ARG:HG2	2.31	0.46
1:A:606:HIS:CE1	1:A:641:CYS:HB3	2.51	0.46
1:A:655:ILE:HG23	1:A:985:ARG:HD2	1.98	0.46
1:A:813:ASP:OD1	7:I:100:HIS:NE2	2.48	0.46
2:B:341:GLU:HG3	2:B:345:LYS:NZ	2.32	0.46
2:B:934:LYS:HG2	2:B:1051:LEU:HD12	1.98	0.46
3:C:42:VAL:HB	3:C:178:PRO:HG3	1.98	0.46
6:H:100:GLU:O	6:H:113:SER:N	2.45	0.46
14:D:62:MET:HE2	14:D:62:MET:HA	1.98	0.46
1:A:317:MET:HE2	1:A:318:VAL:HG13	1.98	0.45
1:A:1022:ILE:N	1:A:1034:GLN:OE1	2.33	0.45
2:B:516:GLU:HG2	2:B:724:TYR:CE1	2.51	0.45
2:B:794:VAL:CG2	2:B:965:ILE:HG23	2.45	0.45
1:A:917:GLU:OE2	1:A:921:ARG:NH1	2.47	0.45
3:C:189:ASP:O	3:C:191:ALA:N	2.48	0.45
12:P:35:A:N3	12:P:35:A:C5'	2.79	0.45
14:D:73:ARG:O	14:D:138:ARG:NH1	2.50	0.45
16:M:328:PRO:HG3	16:M:395:LYS:HD3	1.99	0.45
16:M:510:TYR:CD2	16:M:515:ILE:HG21	2.50	0.45
1:A:892:GLY:O	1:A:893:GLU:HG2	2.16	0.45
1:A:906:LEU:HD23	1:A:1044:HIS:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:88:PHE:HA	6:H:146:LYS:HD3	1.98	0.45
1:A:74:CYS:SG	1:A:84:HIS:CE1	3.00	0.45
1:A:464:LEU:HD22	1:A:861:GLN:HE22	1.82	0.45
1:A:479:TRP:HB2	2:B:931:ILE:HD11	1.98	0.45
1:A:687:ILE:HD11	1:A:766:PHE:CE1	2.52	0.45
2:B:785:TYR:CZ	2:B:955:PRO:HD3	2.51	0.45
15:G:44:PHE:CE1	15:G:157:ILE:HB	2.52	0.45
15:G:165:ASP:OD1	15:G:166:ASP:N	2.48	0.45
1:A:290:LEU:HD13	1:A:306:ASP:HB3	1.97	0.45
1:A:927:GLU:OE2	1:A:931:ARG:HD3	2.16	0.45
1:A:996:ILE:HG13	1:A:1060:LEU:HD23	1.98	0.45
1:A:1163:HIS:NE2	1:A:1302:GLU:OE1	2.49	0.45
1:A:1434:GLU:O	1:A:1435:THR:OG1	2.28	0.45
3:C:76:ASP:HA	3:C:239:LEU:HD23	1.98	0.45
11:N:37:DG:H2''	11:N:38:DG:C8	2.52	0.45
12:P:34:G:P	12:P:34:G:H3'	2.56	0.45
2:B:573:TRP:HZ2	2:B:576:ILE:HD11	1.81	0.45
16:M:521:ASN:CG	16:M:522:ASN:H	2.24	0.45
16:M:532:ASP:OD2	16:M:532:ASP:N	2.48	0.45
1:A:343:LEU:HD23	2:B:1161:GLU:OE2	2.17	0.45
1:A:469:MET:HE2	1:A:469:MET:HB3	1.92	0.45
1:A:1153:ARG:HG3	1:A:1153:ARG:HH11	1.82	0.45
4:E:18:MET:SD	4:E:60:VAL:HG11	2.57	0.45
16:M:389:ILE:O	16:M:393:HIS:ND1	2.25	0.45
1:A:809:HIS:CD2	2:B:677:MET:HE1	2.52	0.45
1:A:901:VAL:HG12	1:A:980:PRO:HA	1.99	0.45
1:A:1172:ASN:OD1	1:A:1215:GLU:HB3	2.17	0.45
1:A:1401:LEU:HD11	1:A:1414:ILE:HD11	1.97	0.45
2:B:529:MET:HG3	2:B:702:MET:HB3	1.99	0.45
2:B:796:MET:HB2	2:B:948:GLN:HG2	1.99	0.45
6:H:59:VAL:O	6:H:144:LEU:HB2	2.16	0.45
1:A:115:SER:OG	1:A:227:ARG:NE	2.24	0.45
1:A:597:PRO:HD3	1:A:668:PHE:CD1	2.52	0.45
1:A:1146:GLN:NE2	1:A:1150:ASP:OD2	2.49	0.45
1:A:1343:LEU:HD22	1:A:1359:SER:OG	2.17	0.45
4:E:171:PRO:HB2	4:E:207:ARG:HD3	1.97	0.45
7:I:80:ARG:HG2	7:I:95:VAL:HG22	1.99	0.45
8:J:10:CYS:SG	8:J:42:ARG:NH2	2.90	0.45
2:B:276:LEU:HD22	2:B:362:ALA:HB2	1.98	0.45
2:B:368:MET:HE2	2:B:368:MET:HB3	1.84	0.45
4:E:84:ILE:HA	4:E:87:ILE:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:173:ILE:O	4:E:209:VAL:HA	2.17	0.45
9:K:89:ASN:HA	9:K:92:THR:HG22	1.98	0.45
16:M:256:LYS:NZ	16:M:303:LEU:HD21	2.32	0.45
16:M:324:ASN:ND2	16:M:405:GLN:O	2.49	0.45
1:A:137:PRO:HB2	1:A:1445:HIS:HB3	1.98	0.44
1:A:567:LEU:HD21	1:A:595:ILE:HG12	1.99	0.44
1:A:848:ILE:HA	2:B:520:VAL:HG21	2.00	0.44
2:B:425:ARG:HD3	2:B:427:LYS:HE3	1.98	0.44
16:M:275:SER:O	16:M:280:ASN:ND2	2.50	0.44
16:M:300:TYR:HD2	16:M:312:MET:HE3	1.81	0.44
16:M:460:LYS:HD2	16:M:461:PRO:HD2	2.00	0.44
1:A:571:ASP:OD1	1:A:571:ASP:N	2.50	0.44
4:E:91:CYS:SG	4:E:95:GLN:NE2	2.85	0.44
6:H:37:MET:HE2	6:H:125:LEU:HD11	1.99	0.44
7:I:12:VAL:HG21	7:I:53:ILE:O	2.17	0.44
15:G:8:GLU:OE2	15:G:71:LYS:HG2	2.17	0.44
15:G:17:TYR:HB3	15:G:25:THR:HG21	1.99	0.44
16:M:359:TYR:HE2	16:M:361:ILE:HG12	1.81	0.44
1:A:291:ARG:O	1:A:295:GLN:OE1	2.36	0.44
1:A:783:GLN:HA	1:A:787:VAL:O	2.17	0.44
2:B:670:GLU:HA	2:B:673:VAL:HG12	1.99	0.44
2:B:989:VAL:HG22	2:B:1015:LEU:HB2	2.00	0.44
5:F:86:GLU:CD	5:F:86:GLU:H	2.24	0.44
6:H:63:THR:HG21	6:H:68:GLY:HA2	2.00	0.44
9:K:61:TYR:CD2	9:K:71:ILE:HD11	2.52	0.44
16:M:347:ILE:O	16:M:347:ILE:HG13	2.17	0.44
1:A:108:ARG:NH2	1:A:191:ILE:O	2.50	0.44
1:A:481:THR:HG21	2:B:932:GLY:HA3	1.99	0.44
1:A:495:ASP:N	1:A:499:ASP:OD2	2.43	0.44
1:A:795:GLY:CA	1:A:1107:PHE:HB3	2.48	0.44
1:A:1436:VAL:HG23	1:A:1437:ASP:H	1.81	0.44
2:B:1123:GLY:HA3	2:B:1171:MET:N	2.33	0.44
2:B:1143:LYS:HZ3	2:B:1143:LYS:HB2	1.83	0.44
3:C:19:VAL:HG12	3:C:21:PHE:HD1	1.82	0.44
3:C:147:ASP:N	3:C:147:ASP:OD1	2.50	0.44
1:A:803:LYS:O	1:A:812:LYS:NZ	2.49	0.44
1:A:1323:THR:OG1	1:A:1325:ASP:OD1	2.29	0.44
1:A:1479:LYS:HE2	5:F:121:ASP:OD2	2.17	0.44
3:C:123:ASN:OD1	3:C:124:SER:N	2.51	0.44
11:N:42:DT:H2"	11:N:43:DG:C8	2.52	0.44
16:M:326:GLU:OE2	16:M:336:HIS:NE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:GLN:HB3	6:H:93:TYR:CE2	2.53	0.44
1:A:739:ASN:HB3	1:A:743:ARG:NH2	2.33	0.44
1:A:922:PHE:HB2	1:A:1052:ARG:HB2	1.98	0.44
1:A:1316:ASN:OD1	1:A:1317:LYS:N	2.51	0.44
2:B:1062:ARG:NH2	2:B:1066:PRO:O	2.48	0.44
6:H:95:LYS:C	6:H:116:VAL:HG23	2.42	0.44
7:I:11:PHE:HA	7:I:55:VAL:HG11	1.99	0.44
1:A:402:LEU:HD22	1:A:446:VAL:HG11	2.00	0.44
1:A:480:SER:HB3	9:K:2:ASN:HD22	1.82	0.44
1:A:775:LYS:HG2	2:B:970:HIS:O	2.18	0.44
1:A:991:GLN:HA	1:A:996:ILE:HG12	1.99	0.44
1:A:1247:PHE:HA	1:A:1257:LEU:HA	2.00	0.44
6:H:5:LEU:N	6:H:60:ILE:O	2.51	0.44
8:J:10:CYS:HB2	8:J:44:CYS:SG	2.57	0.44
13:T:24:DG:H2'	13:T:25:DA:C8	2.53	0.44
14:D:48:ASN:O	14:D:48:ASN:ND2	2.49	0.44
1:A:67:ARG:NH1	12:P:35:A:O2'	2.51	0.44
15:G:117:MET:HA	15:G:117:MET:HE2	2.00	0.44
15:G:147:ILE:HA	15:G:161:GLY:HA2	2.00	0.44
1:A:539:GLN:NE2	1:A:775:LYS:HE2	2.33	0.44
1:A:545:VAL:HG23	1:A:676:ILE:HG21	1.99	0.44
1:A:837:PHE:HB2	2:B:506:TRP:HZ3	1.83	0.44
1:A:1112:VAL:HG21	1:A:1115:LYS:HB2	2.00	0.44
2:B:212:ASP:OD1	2:B:212:ASP:N	2.46	0.44
2:B:293:GLU:O	2:B:295:PRO:HD3	2.18	0.44
14:D:108:ALA:HB1	14:D:127:LEU:HD23	2.00	0.44
1:A:809:HIS:HE2	2:B:506:TRP:NE1	2.15	0.43
2:B:82:PRO:HB2	2:B:133:ILE:O	2.18	0.43
2:B:344:GLN:O	2:B:361:LYS:NZ	2.51	0.43
2:B:566:LYS:HA	2:B:576:ILE:HD13	2.00	0.43
2:B:1151:MET:HG2	2:B:1152:PRO:O	2.18	0.43
6:H:39:LEU:HD13	6:H:125:LEU:HD13	1.99	0.43
6:H:88:PHE:CD2	6:H:144:LEU:HB3	2.53	0.43
14:D:112:LYS:HD2	14:D:119:GLU:HA	1.99	0.43
1:A:910:LYS:HB3	1:A:1328:PHE:HE2	1.82	0.43
2:B:1075:MET:HG3	2:B:1076:GLU:H	1.81	0.43
16:M:256:LYS:HD3	16:M:260:PHE:CZ	2.53	0.43
1:A:1458:ILE:HD13	2:B:1091:ARG:HD3	2.00	0.43
2:B:387:HIS:CD2	2:B:504:THR:HG21	2.54	0.43
2:B:564:ALA:HB2	2:B:578:LYS:HD3	2.00	0.43
15:G:90:THR:CG2	15:G:100:GLU:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:246:THR:CG2	16:M:249:LYS:HD2	2.48	0.43
1:A:480:SER:HB3	9:K:2:ASN:HB2	2.00	0.43
1:A:723:ASN:HD21	7:I:109:ARG:HB2	1.82	0.43
1:A:1243:LEU:HB2	1:A:1260:ARG:O	2.18	0.43
2:B:50:PHE:HD2	2:B:51:ILE:HG23	1.83	0.43
2:B:563:ASP:O	2:B:610:ARG:NH1	2.51	0.43
3:C:10:ARG:HH22	3:C:228:ARG:HH22	1.66	0.43
4:E:44:PHE:O	4:E:52:ARG:HG2	2.17	0.43
7:I:74:GLN:OE1	7:I:74:GLN:N	2.50	0.43
15:G:117:MET:SD	15:G:128:TYR:HB3	2.58	0.43
2:B:295:PRO:O	2:B:299:GLU:HG2	2.18	0.43
2:B:962:THR:O	8:J:9:THR:HG23	2.17	0.43
3:C:51:GLN:OE1	10:L:52:LEU:HD22	2.18	0.43
16:M:393:HIS:O	16:M:397:LYS:HG3	2.18	0.43
1:A:459:ASN:HB3	1:A:469:MET:HG2	1.99	0.43
1:A:477:LEU:HD13	1:A:483:ARG:HD2	2.01	0.43
1:A:1020:LEU:HD21	1:A:1073:GLU:HA	2.00	0.43
1:A:1321:ILE:HD13	1:A:1331:LEU:HD11	2.01	0.43
2:B:167:THR:HG23	2:B:170:ASP:H	1.83	0.43
2:B:731:GLN:NE2	12:P:44:A:O3'	2.52	0.43
2:B:1101:GLN:HE22	2:B:1104:ARG:NH2	2.16	0.43
7:I:87:GLN:HE22	7:I:123:TRP:CB	2.31	0.43
1:A:1128:ILE:HG23	1:A:1414:ILE:HB	2.00	0.43
2:B:1125:MET:HE1	2:B:1156:LYS:HD2	2.01	0.43
1:A:937:ASP:HA	1:A:940:LYS:HZ1	1.83	0.43
4:E:8:TYR:CZ	4:E:12:LYS:HD2	2.54	0.43
6:H:15:ILE:HG13	6:H:16:ASP:H	1.84	0.43
1:A:16:ARG:HG3	1:A:16:ARG:HH11	1.83	0.43
1:A:352:GLY:HA2	2:B:1085:ARG:HH22	1.84	0.43
2:B:311:ILE:HG21	2:B:317:ALA:HB2	2.00	0.43
6:H:7:GLU:OE1	6:H:7:GLU:HA	2.18	0.43
9:K:57:LEU:N	9:K:76:GLN:O	2.51	0.43
16:M:390:SER:OG	16:M:391:PRO:HD3	2.18	0.43
1:A:1362:ILE:HG22	1:A:1411:LEU:HD11	2.01	0.43
1:A:1377:ALA:O	1:A:1381:GLU:HG2	2.18	0.43
2:B:56:GLN:OE1	2:B:91:ILE:HG22	2.19	0.43
2:B:359:THR:HG21	2:B:554:GLU:HG3	2.00	0.43
3:C:251:GLY:O	3:C:254:LYS:HG3	2.19	0.43
6:H:25:VAL:HA	6:H:44:ASN:HA	1.99	0.43
14:D:96:GLU:HA	14:D:99:CYS:SG	2.59	0.43
16:M:422:ARG:HH11	16:M:562:ILE:HG21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:553:VAL:HA	16:M:557:MET:SD	2.59	0.43
16:M:558:LEU:O	16:M:562:ILE:HD12	2.19	0.43
1:A:436:SER:HB3	16:M:539:TYR:HE1	1.84	0.42
1:A:1430:CYS:C	1:A:1435:THR:HG22	2.44	0.42
2:B:949:TYR:HB3	2:B:953:ASP:HB2	2.00	0.42
2:B:952:GLU:HG2	2:B:953:ASP:N	2.34	0.42
3:C:8:THR:HG22	9:K:104:ARG:NH1	2.34	0.42
6:H:97:TYR:CZ	6:H:115:TYR:HB3	2.54	0.42
7:I:64:GLU:O	7:I:68:ILE:HG12	2.18	0.42
7:I:87:GLN:HE22	7:I:123:TRP:CG	2.37	0.42
8:J:35:LEU:HD22	8:J:40:LEU:HD12	2.00	0.42
9:K:65:HIS:HE1	9:K:67:LEU:HD12	1.83	0.42
16:M:345:GLU:O	16:M:359:TYR:HA	2.19	0.42
1:A:120:ASP:O	1:A:123:ASN:N	2.52	0.42
1:A:286:ILE:HD11	1:A:309:LEU:HB3	2.01	0.42
1:A:663:ASP:OD2	1:A:663:ASP:N	2.52	0.42
1:A:1040:LEU:HD23	4:E:199:THR:O	2.19	0.42
2:B:529:MET:SD	2:B:702:MET:HG3	2.59	0.42
3:C:30:VAL:O	3:C:34:ILE:HG12	2.19	0.42
5:F:71:LEU:HG	5:F:75:MET:HE3	2.00	0.42
6:H:11:ASP:OD1	6:H:55:LYS:HG3	2.19	0.42
16:M:300:TYR:CD1	16:M:346:MET:HG2	2.55	0.42
1:A:22:GLN:HE22	1:A:1446:GLY:C	2.28	0.42
1:A:58:MET:HE3	1:A:58:MET:HB2	1.89	0.42
1:A:593:SER:HB3	1:A:634:GLU:HG3	2.01	0.42
2:B:280:SER:OG	2:B:281:ASP:N	2.52	0.42
4:E:24:ARG:NH1	4:E:103:LEU:HD11	2.32	0.42
4:E:59:THR:HB	4:E:74:VAL:O	2.19	0.42
6:H:87:GLN:HG2	6:H:88:PHE:CD1	2.54	0.42
16:M:299:ARG:HA	16:M:299:ARG:HD3	1.64	0.42
1:A:22:GLN:NE2	1:A:23:PHE:O	2.46	0.42
1:A:212:LYS:HB3	1:A:214:ILE:HG23	2.00	0.42
1:A:276:LEU:O	1:A:280:LEU:HG	2.19	0.42
1:A:350:VAL:HG13	1:A:351:ARG:N	2.33	0.42
1:A:1155:LYS:HD2	1:A:1158:LEU:HD23	2.00	0.42
2:B:123:PRO:HA	2:B:151:LYS:HA	2.01	0.42
2:B:279:VAL:HG13	2:B:312:GLN:O	2.19	0.42
3:C:38:PHE:CE1	3:C:245:VAL:HA	2.54	0.42
9:K:17:LYS:HB3	9:K:17:LYS:HE3	1.84	0.42
1:A:527:THR:HG23	1:A:530:SER:H	1.84	0.42
1:A:833:PRO:HG3	2:B:1002:PHE:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1036:ASN:OD1	4:E:202:ARG:NH1	2.50	0.42
1:A:1180:ASN:O	1:A:1183:SER:OG	2.26	0.42
2:B:127:ASP:OD1	2:B:127:ASP:N	2.50	0.42
16:M:470:ARG:NH1	16:M:472:LYS:HE3	2.34	0.42
2:B:224:CYS:SG	2:B:232:THR:HG22	2.60	0.42
2:B:255:ARG:HD2	2:B:307:GLU:HG3	2.01	0.42
2:B:270:ILE:HD12	2:B:270:ILE:H	1.85	0.42
2:B:735:VAL:HG23	2:B:754:PRO:HG2	2.01	0.42
2:B:759:VAL:HG22	2:B:999:ALA:HB2	2.01	0.42
3:C:184:PHE:CD1	3:C:231:TYR:HE1	2.37	0.42
12:P:26:U:O2	12:P:26:U:O4'	2.37	0.42
15:G:94:LYS:N	15:G:94:LYS:HD3	2.34	0.42
16:M:422:ARG:HD2	16:M:562:ILE:HB	2.01	0.42
16:M:461:PRO:HA	16:M:462:PRO:HD3	1.92	0.42
1:A:565:MET:HE3	1:A:565:MET:HB3	1.86	0.42
1:A:671:ASN:O	1:A:675:VAL:HG12	2.20	0.42
1:A:1434:GLU:HB3	1:A:1435:THR:H	1.66	0.42
2:B:225:LEU:HG	2:B:226:GLU:H	1.84	0.42
2:B:1029:TYR:HA	2:B:1036:LYS:HA	2.02	0.42
6:H:39:LEU:HD11	6:H:123:MET:SD	2.59	0.42
6:H:60:ILE:HG21	6:H:135:PHE:HZ	1.84	0.42
10:L:47:LYS:HA	10:L:47:LYS:HD2	1.84	0.42
15:G:97:LEU:HB3	15:G:108:ILE:CG2	2.50	0.42
16:M:376:ASP:HB3	16:M:379:VAL:HG23	2.02	0.42
1:A:27:SER:HB2	1:A:30:GLU:HB2	2.01	0.42
1:A:31:LEU:HD22	1:A:254:PRO:HB3	2.02	0.42
1:A:621:ILE:HA	6:H:122:LEU:HD13	2.00	0.42
1:A:1042:ASN:HB3	1:A:1046:ARG:NH1	2.35	0.42
2:B:237:VAL:HG12	2:B:372:LEU:HD22	2.01	0.42
2:B:1118:VAL:HG21	2:B:1171:MET:HG3	2.02	0.42
3:C:61:ASP:OD2	10:L:48:ARG:NH2	2.53	0.42
4:E:14:ARG:O	4:E:18:MET:HG2	2.19	0.42
4:E:44:PHE:C	4:E:53:PRO:HB3	2.45	0.42
4:E:149:VAL:HB	4:E:192:LYS:HB2	2.02	0.42
14:D:37:VAL:HG21	15:G:2:PHE:CD2	2.47	0.42
1:A:106:VAL:HG13	1:A:236:LEU:HD21	2.02	0.42
1:A:693:ILE:HD11	2:B:1008:VAL:HG11	2.02	0.42
2:B:404:PHE:HA	2:B:407:MET:HE3	2.02	0.42
2:B:1028:LEU:HG	2:B:1041:ILE:HB	2.02	0.42
2:B:1151:MET:HE1	2:B:1171:MET:HE1	2.01	0.42
3:C:21:PHE:CZ	3:C:231:TYR:HD2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:66:ASP:OD1	4:E:66:ASP:N	2.51	0.42
5:F:69:ARG:O	5:F:73:ILE:HG12	2.19	0.42
16:M:311:PHE:HB3	16:M:319:VAL:CG1	2.50	0.42
1:A:856:GLU:HG2	2:B:494:LYS:HD2	2.02	0.42
3:C:103:LEU:HB2	3:C:120:LEU:HD23	2.01	0.42
14:D:92:LEU:HA	14:D:121:ARG:HH21	1.84	0.42
16:M:312:MET:HE2	16:M:346:MET:CE	2.50	0.42
1:A:353:ASN:O	1:A:357:LYS:HE2	2.20	0.41
1:A:375:ILE:HD13	1:A:669:TYR:CD2	2.54	0.41
1:A:522:PRO:O	1:A:662:HIS:HB2	2.20	0.41
2:B:1060:HIS:HB3	2:B:1078:ARG:HG3	2.02	0.41
2:B:1094:GLN:HB2	2:B:1103:LEU:HD13	2.02	0.41
3:C:22:ILE:HG12	3:C:230:TYR:CD1	2.55	0.41
16:M:258:HIS:ND1	16:M:263:TRP:HD1	2.18	0.41
1:A:509:LEU:HD11	5:F:89:PRO:HG2	2.02	0.41
1:A:1167:ARG:HG3	1:A:1293:LEU:O	2.20	0.41
1:A:1473:LEU:HD11	5:F:65:VAL:HG22	2.01	0.41
2:B:18:THR:HG23	2:B:18:THR:O	2.20	0.41
2:B:47:PHE:O	2:B:51:ILE:HG12	2.20	0.41
2:B:193:VAL:HG23	2:B:470:LEU:HB2	2.02	0.41
2:B:384:ASP:O	2:B:390:ASN:ND2	2.51	0.41
4:E:130:PHE:CD1	4:E:135:LEU:HD21	2.55	0.41
6:H:16:ASP:HA	6:H:17:PRO:HD3	1.85	0.41
7:I:82:GLU:HB3	7:I:92:LYS:HE3	2.02	0.41
12:P:35:A:P	12:P:35:A:C3'	3.04	0.41
15:G:150:THR:HA	15:G:159:ALA:HA	2.02	0.41
1:A:732:THR:HG22	1:A:733:LEU:N	2.35	0.41
1:A:821:GLY:HA2	1:A:838:PHE:CD2	2.55	0.41
1:A:957:GLU:O	1:A:961:GLU:HG2	2.20	0.41
1:A:1427:LEU:HA	1:A:1430:CYS:SG	2.60	0.41
2:B:199:LYS:NZ	2:B:394:ASP:OD1	2.38	0.41
2:B:615:TYR:HB3	2:B:620:ARG:HD3	2.03	0.41
6:H:12:VAL:HA	6:H:30:CYS:HB3	2.02	0.41
14:D:48:ASN:C	14:D:48:ASN:HD22	2.25	0.41
14:D:91:LYS:C	14:D:92:LEU:HD12	2.45	0.41
15:G:118:GLU:HG2	15:G:129:LYS:O	2.19	0.41
1:A:392:GLU:CD	1:A:448:ARG:HE	2.23	0.41
1:A:421:ARG:HA	1:A:444:TYR:CD1	2.56	0.41
1:A:481:THR:HG22	2:B:1055:VAL:HG21	2.02	0.41
1:A:548:PHE:HE1	1:A:555:LEU:HD11	1.85	0.41
1:A:713:VAL:HG11	1:A:817:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:878:THR:HG21	1:A:880:ARG:HE	1.85	0.41
2:B:124:LEU:HD23	2:B:150:GLY:O	2.21	0.41
2:B:235:ILE:HD12	2:B:347:MET:HG3	2.03	0.41
2:B:577:HIS:ND1	2:B:583:LEU:HD13	2.36	0.41
4:E:47:LYS:H	4:E:53:PRO:CG	2.34	0.41
4:E:61:LEU:HD22	4:E:73:PHE:CZ	2.56	0.41
6:H:116:VAL:HG11	6:H:123:MET:HE2	2.03	0.41
7:I:71:ASP:OD2	7:I:71:ASP:N	2.51	0.41
15:G:162:SER:HB2	15:G:164:MET:HE1	2.01	0.41
1:A:29:ASP:O	1:A:33:ARG:HG3	2.20	0.41
1:A:416:ALA:HA	1:A:448:ARG:HA	2.02	0.41
1:A:1088:GLY:HA2	1:A:1400:LEU:HD21	2.03	0.41
1:A:1474:LEU:HD11	5:F:107:ARG:CZ	2.50	0.41
3:C:38:PHE:HE1	3:C:245:VAL:HA	1.85	0.41
7:I:78:LEU:HD22	7:I:97:PHE:HB3	2.01	0.41
16:M:361:ILE:H	16:M:412:ASN:HA	1.84	0.41
16:M:539:TYR:CE1	16:M:543:MET:HE3	2.55	0.41
1:A:88:ILE:HB	1:A:253:LEU:HB3	2.03	0.41
1:A:273:GLN:HB2	1:A:278:HIS:NE2	2.35	0.41
1:A:545:VAL:HG11	1:A:645:LEU:HD12	2.02	0.41
2:B:225:LEU:HD23	2:B:228:SER:HB2	2.01	0.41
2:B:756:LYS:O	8:J:51:ALA:HB1	2.21	0.41
3:C:27:ASP:HB2	3:C:30:VAL:HG23	2.01	0.41
4:E:87:ILE:HA	4:E:90:TYR:HD1	1.85	0.41
16:M:380:ARG:O	16:M:384:ILE:HG13	2.20	0.41
1:A:191:ILE:HA	1:A:200:ALA:HA	2.03	0.41
1:A:532:ARG:HG2	1:A:649:ALA:HB2	2.02	0.41
1:A:831:LEU:HG	2:B:715:ASP:O	2.20	0.41
1:A:1370:GLY:O	1:A:1374:VAL:HG23	2.21	0.41
2:B:23:GLN:O	2:B:27:TRP:HD1	2.04	0.41
2:B:796:MET:HE3	2:B:796:MET:HB3	1.89	0.41
2:B:817:GLN:HB3	2:B:918:PHE:CD1	2.51	0.41
2:B:896:LEU:HD23	2:B:897:ARG:O	2.21	0.41
2:B:935:PHE:HE1	2:B:1050:ARG:HG3	1.85	0.41
4:E:172:ARG:HA	4:E:208:LEU:H	1.85	0.41
7:I:50:ASN:OD1	7:I:51:SER:N	2.54	0.41
9:K:7:PHE:CD1	9:K:11:LEU:HD12	2.55	0.41
1:A:321:GLU:O	1:A:321:GLU:HG2	2.20	0.41
3:C:59:LEU:HD13	3:C:63:PHE:CE2	2.56	0.41
15:G:125:PRO:HB2	15:G:138:GLN:CD	2.46	0.41
1:A:102:LYS:O	1:A:106:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:VAL:HG23	1:A:1087:VAL:HG21	2.03	0.41
1:A:893:GLU:HB2	4:E:203:TYR:CD1	2.55	0.41
1:A:894:ASP:OD2	1:A:896:LEU:HB2	2.21	0.41
1:A:930:LEU:HD22	1:A:939:VAL:HG13	2.03	0.41
1:A:1163:HIS:NE2	1:A:1297:THR:HG22	2.36	0.41
1:A:1177:TYR:OH	1:A:1282:ASP:OD2	2.37	0.41
2:B:98:HIS:O	2:B:99:TRP:CG	2.74	0.41
2:B:236:TRP:HB2	2:B:259:THR:HG22	2.03	0.41
2:B:313:GLU:HG3	2:B:316:VAL:HG22	2.03	0.41
2:B:419:ALA:O	2:B:423:ILE:HG12	2.20	0.41
2:B:733:MET:CE	2:B:1050:ARG:HG2	2.51	0.41
2:B:859:ARG:NE	2:B:903:ILE:HD11	2.36	0.41
3:C:78:ILE:HG22	3:C:82:LEU:HG	2.03	0.41
5:F:51:ARG:HH22	5:F:122:GLU:CD	2.28	0.41
15:G:138:GLN:N	15:G:141:ASP:OD2	2.51	0.41
16:M:247:GLN:N	16:M:248:PRO:HD2	2.36	0.41
16:M:519:PHE:HB2	16:M:524:TRP:CD1	2.56	0.41
16:M:555:LYS:HE3	16:M:555:LYS:HB2	1.87	0.41
1:A:461:GLN:HG2	13:T:26:DG:H1'	2.03	0.41
2:B:709:SER:HB2	2:B:767:LEU:HD11	2.03	0.41
2:B:721:ARG:HG3	2:B:977:THR:HG22	2.02	0.41
2:B:778:SER:HB3	2:B:805:PHE:HZ	1.86	0.41
2:B:927:ARG:HH12	2:B:1057:ASP:CG	2.29	0.41
3:C:44:ILE:CG2	3:C:178:PRO:HB3	2.51	0.41
9:K:98:LEU:O	9:K:102:GLU:HG3	2.20	0.41
1:A:533:PRO:HD3	1:A:654:HIS:CG	2.56	0.40
1:A:784:VAL:O	1:A:828:LEU:HD23	2.20	0.40
2:B:472:ARG:HG3	2:B:736:TYR:CD2	2.56	0.40
2:B:787:GLY:O	2:B:790:GLN:HG3	2.21	0.40
3:C:49:TRP:CE3	3:C:164:TYR:HD2	2.40	0.40
4:E:70:ASP:OD1	4:E:70:ASP:N	2.54	0.40
6:H:29:HIS:ND1	6:H:40:ILE:HG12	2.35	0.40
6:H:56:PHE:HE2	6:H:58:LEU:HD11	1.86	0.40
9:K:7:PHE:HB2	9:K:11:LEU:HD12	2.03	0.40
16:M:454:ASP:OD2	16:M:455:ASP:N	2.54	0.40
1:A:636:ILE:HD11	6:H:95:LYS:NZ	2.36	0.40
1:A:790:GLN:HE21	1:A:790:GLN:HB3	1.72	0.40
1:A:1428:MET:HB2	1:A:1456:GLU:OE2	2.21	0.40
2:B:623:ARG:HH12	2:B:697:GLU:CD	2.29	0.40
2:B:1119:CYS:HA	2:B:1146:ILE:HD12	2.04	0.40
3:C:78:ILE:HA	3:C:81:LYS:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:240:ARG:O	3:C:244:ILE:HG13	2.21	0.40
4:E:151:MET:HE3	4:E:192:LYS:HD2	2.03	0.40
11:N:32:DA:H2'	11:N:33:DG:H8	1.87	0.40
1:A:35:SER:HB2	1:A:86:GLY:HA2	2.04	0.40
1:A:265:VAL:HA	1:A:271:ARG:HG2	2.03	0.40
1:A:548:PHE:CE1	1:A:555:LEU:HD11	2.56	0.40
1:A:601:ASN:ND2	1:A:989:ASN:OD1	2.54	0.40
1:A:1307:VAL:HG22	1:A:1338:THR:HG22	2.03	0.40
1:A:1424:THR:HG21	1:A:1428:MET:HE2	2.03	0.40
2:B:1056:ASP:O	2:B:1078:ARG:NH2	2.54	0.40
15:G:130:THR:OG1	15:G:134:ASP:OD1	2.32	0.40
16:M:325:LEU:HD13	16:M:392:ARG:HH22	1.86	0.40
1:A:117:LEU:O	1:A:118:LEU:HG	2.22	0.40
1:A:224:ILE:HA	1:A:227:ARG:HG2	2.04	0.40
1:A:496:PHE:HB2	2:B:791:GLU:O	2.21	0.40
1:A:775:LYS:HD2	2:B:974:SER:HB3	2.03	0.40
1:A:940:LYS:HZ3	1:A:940:LYS:HB2	1.86	0.40
1:A:1211:LEU:HD23	1:A:1211:LEU:H	1.86	0.40
2:B:117:ASN:ND2	2:B:188:ASN:O	2.33	0.40
2:B:782:ILE:HG12	2:B:967:ILE:HD11	2.03	0.40
2:B:1032:PHE:O	3:C:32:ASN:ND2	2.55	0.40
4:E:80:PRO:HB3	4:E:108:GLN:HG3	2.02	0.40
7:I:88:LYS:CE	7:I:121:HIS:HB2	2.52	0.40
14:D:111:SER:HB2	14:D:131:LEU:HD21	2.04	0.40
15:G:51:ILE:HA	15:G:72:TYR:HA	2.03	0.40
16:M:300:TYR:CD2	16:M:312:MET:HE3	2.55	0.40
16:M:475:ARG:HD3	16:M:483:PRO:HB3	2.03	0.40
1:A:855:ALA:HB3	2:B:494:LYS:HZ2	1.85	0.40
2:B:627:ILE:HD11	2:B:663:GLU:HG3	2.04	0.40
6:H:60:ILE:HG21	6:H:135:PHE:CZ	2.56	0.40
9:K:13:PHE:HB2	9:K:16:GLU:HG3	2.03	0.40
13:T:27:DT:H2'	13:T:28:DG:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1398/1970 (71%)	1315 (94%)	82 (6%)	1 (0%)	48	79
2	B	1122/1174 (96%)	1062 (95%)	60 (5%)	0	100	100
3	C	259/275 (94%)	246 (95%)	13 (5%)	0	100	100
4	E	207/210 (99%)	198 (96%)	8 (4%)	1 (0%)	24	59
5	F	80/127 (63%)	79 (99%)	1 (1%)	0	100	100
6	H	146/150 (97%)	137 (94%)	9 (6%)	0	100	100
7	I	115/125 (92%)	104 (90%)	11 (10%)	0	100	100
8	J	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
9	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
10	L	44/58 (76%)	37 (84%)	7 (16%)	0	100	100
14	D	124/142 (87%)	120 (97%)	4 (3%)	0	100	100
15	G	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
16	M	327/597 (55%)	317 (97%)	10 (3%)	0	100	100
All	All	4169/5184 (80%)	3951 (95%)	216 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	57	ASP
1	A	911	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1241/1749 (71%)	1241 (100%)	0	100	100
2	B	992/1027 (97%)	991 (100%)	1 (0%)	88	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	240/252 (95%)	240 (100%)	0	100	100
4	E	191/192 (100%)	191 (100%)	0	100	100
5	F	71/111 (64%)	71 (100%)	0	100	100
6	H	129/131 (98%)	129 (100%)	0	100	100
7	I	105/112 (94%)	105 (100%)	0	100	100
8	J	56/56 (100%)	56 (100%)	0	100	100
9	K	104/106 (98%)	104 (100%)	0	100	100
10	L	43/55 (78%)	43 (100%)	0	100	100
14	D	109/126 (86%)	109 (100%)	0	100	100
15	G	146/153 (95%)	146 (100%)	0	100	100
16	M	294/534 (55%)	294 (100%)	0	100	100
All	All	3721/4604 (81%)	3720 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1071	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	GLN
1	A	289	GLN
1	A	504	HIS
1	A	529	GLN
1	A	539	GLN
1	A	731	ASN
1	A	904	GLN
1	A	935	GLN
1	A	995	HIS
1	A	1044	HIS
2	B	90	GLN
2	B	197	GLN
2	B	315	ASN
2	B	460	HIS
2	B	525	ASN
2	B	593	GLN

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Mol	Chain	Res	Type
2	B	725	GLN
2	B	797	ASN
2	B	930	GLN
2	B	980	HIS
3	C	145	GLN
7	I	46	GLN
7	I	98	GLN
7	I	118	HIS
7	I	121	HIS
9	K	29	ASN
9	K	55	GLN
14	D	48	ASN
14	D	102	ASN
15	G	111	HIS
16	M	254	GLN
16	M	280	ASN
16	M	382	GLN
16	M	443	GLN
16	M	537	ASN
16	M	547	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	P	21/22 (95%)	13 (61%)	3 (14%)

All (13) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	P	27	A
12	P	28	A
12	P	29	C
12	P	30	C
12	P	31	G
12	P	32	G
12	P	33	A
12	P	34	G
12	P	35	A
12	P	36	G
12	P	37	G
12	P	38	G

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Mol	Chain	Res	Type
12	P	39	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	P	36	G
12	P	37	G
12	P	38	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	N	1
16	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	14:DC	O3'	26:DG	P	30.85
1	M	465:ASN	C	466:SER	N	4.87

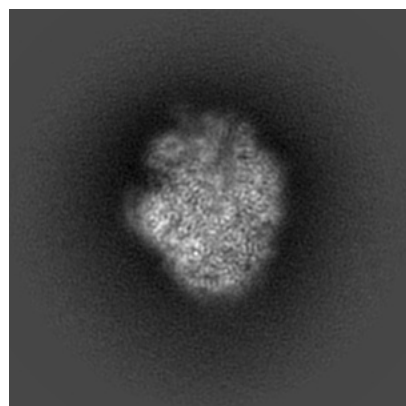
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17404. These allow visual inspection of the internal detail of the map and identification of artifacts.

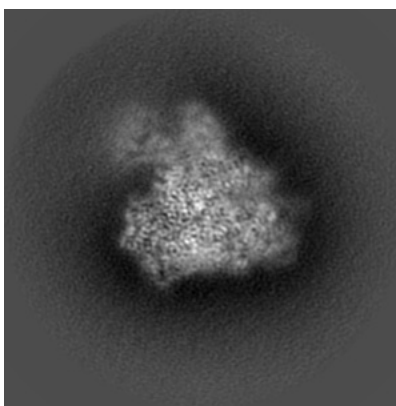
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

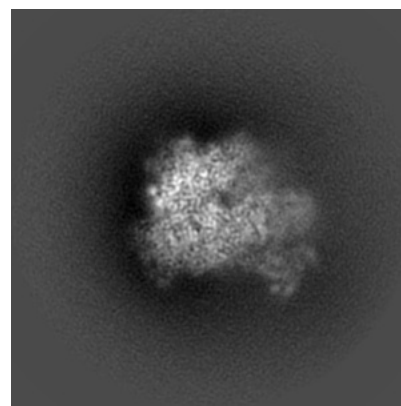
6.1.1 Primary map



X

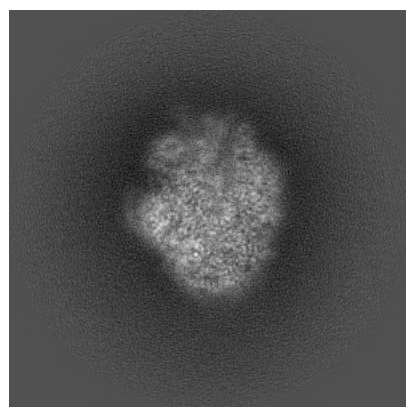


Y

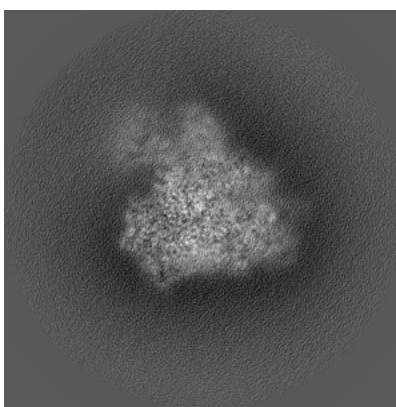


Z

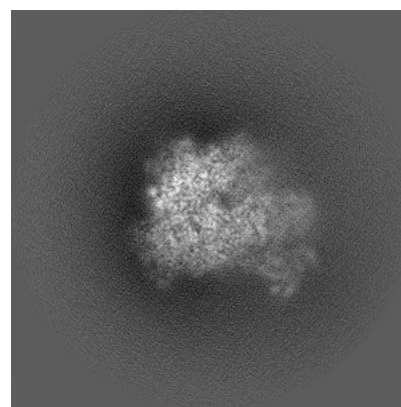
6.1.2 Raw map



X



Y

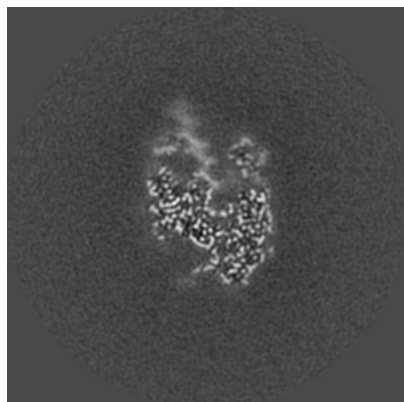


Z

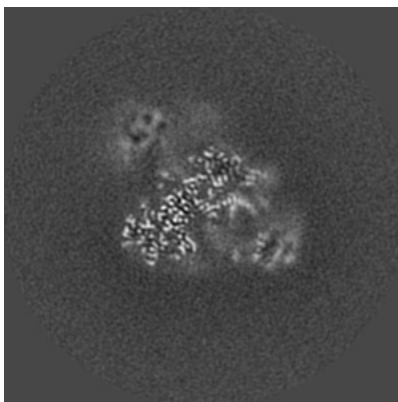
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

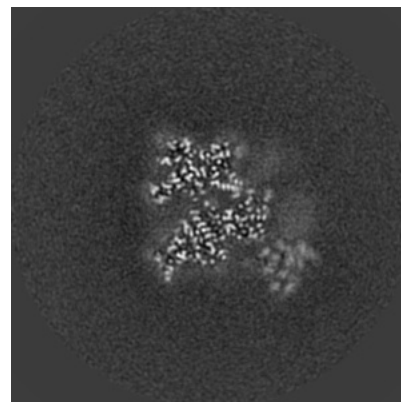
6.2.1 Primary map



X Index: 150

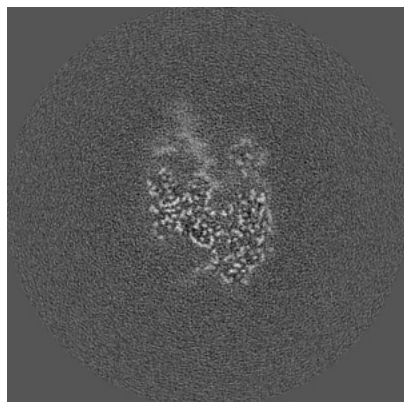


Y Index: 150

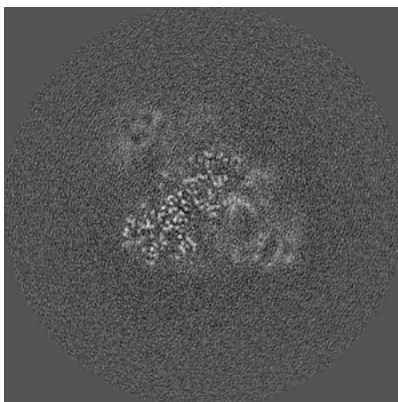


Z Index: 150

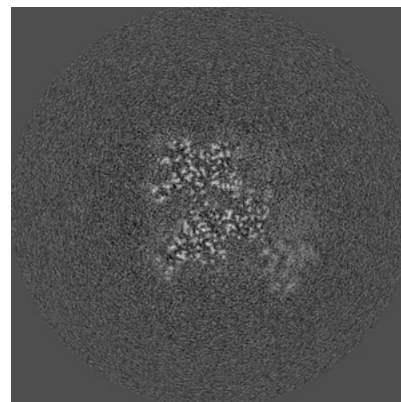
6.2.2 Raw map



X Index: 150



Y Index: 150

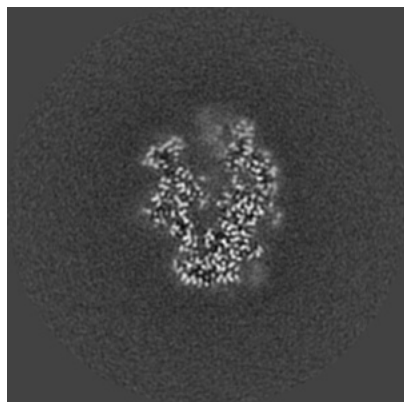


Z Index: 150

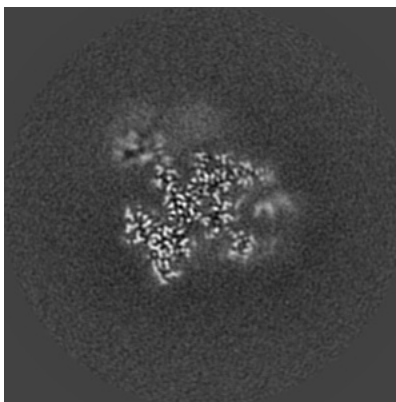
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

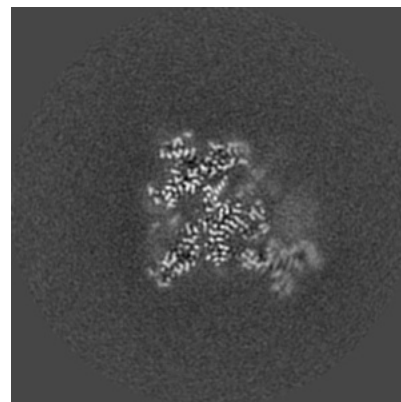
6.3.1 Primary map



X Index: 134

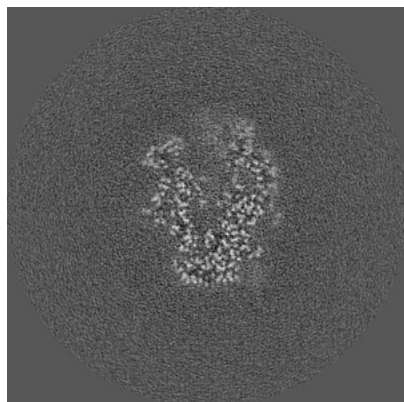


Y Index: 140

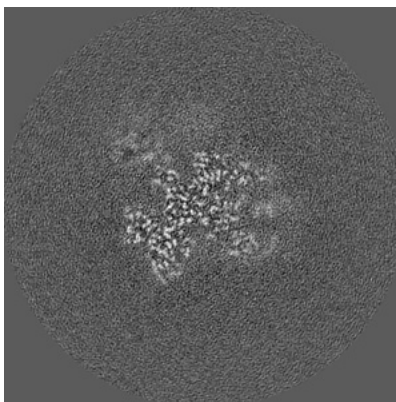


Z Index: 143

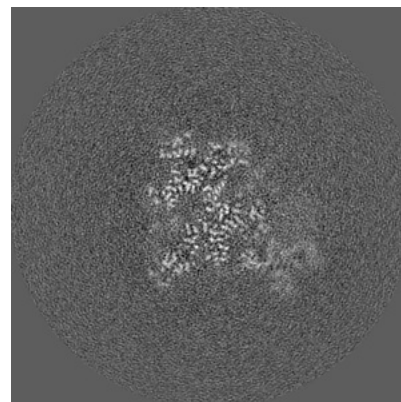
6.3.2 Raw map



X Index: 134



Y Index: 141

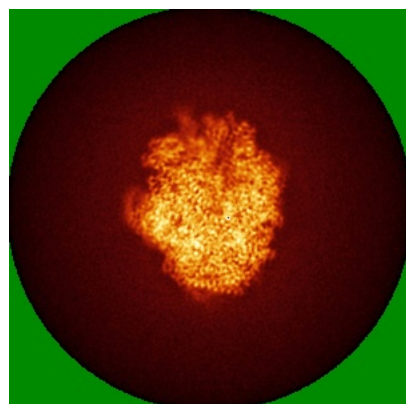


Z Index: 143

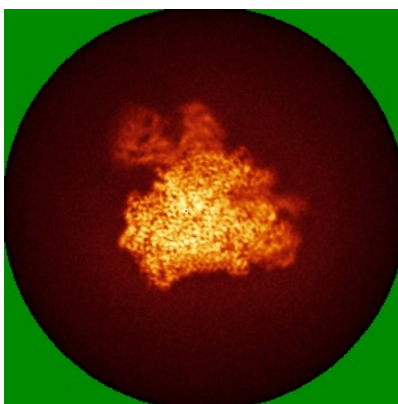
The images above show the largest variance slices of the map in three orthogonal directions.

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

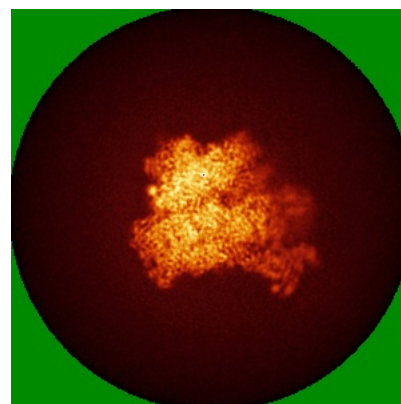
6.4.1 Primary map



X

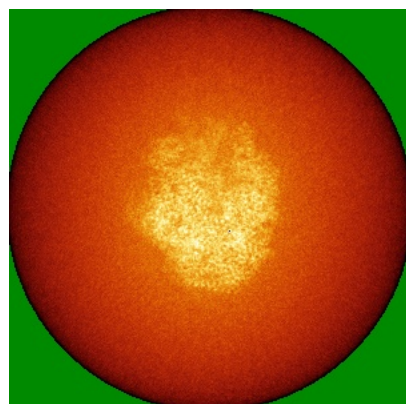


Y

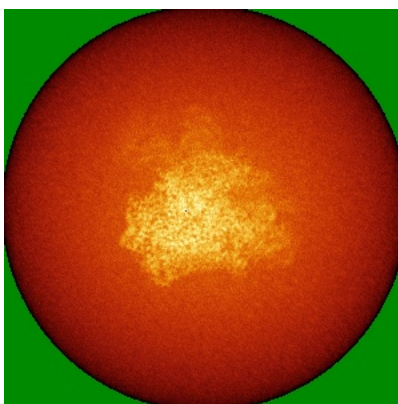


Z

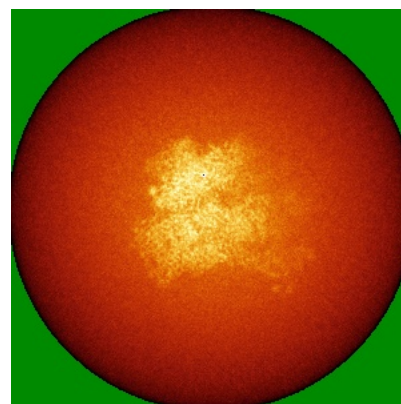
6.4.2 Raw map



X



Y

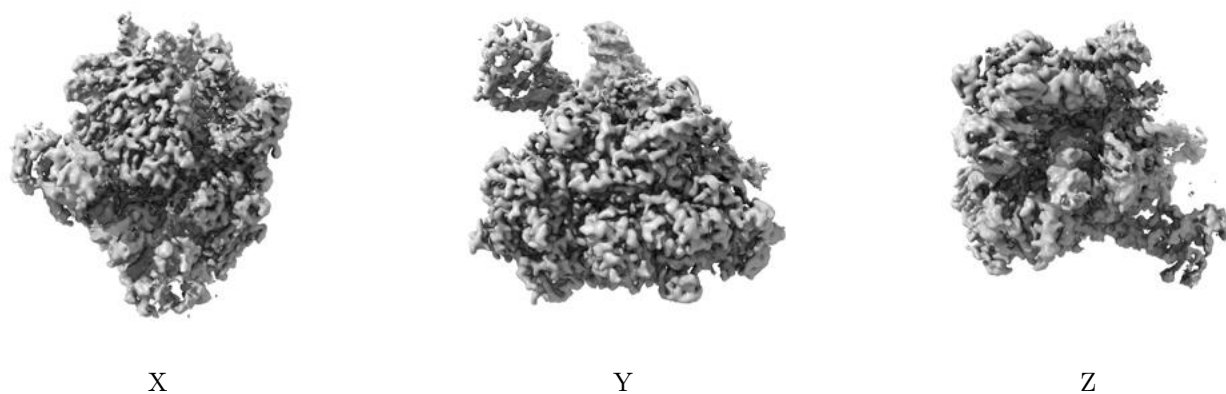


Z

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

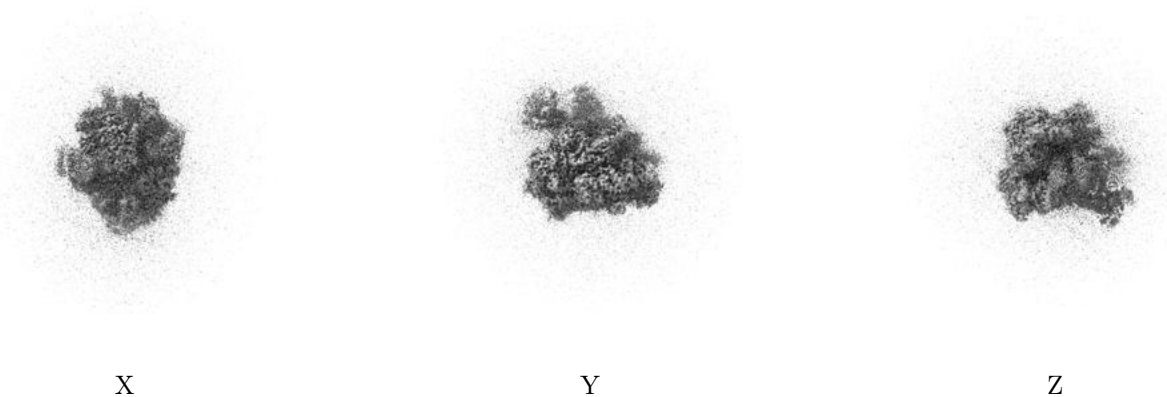
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00683. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

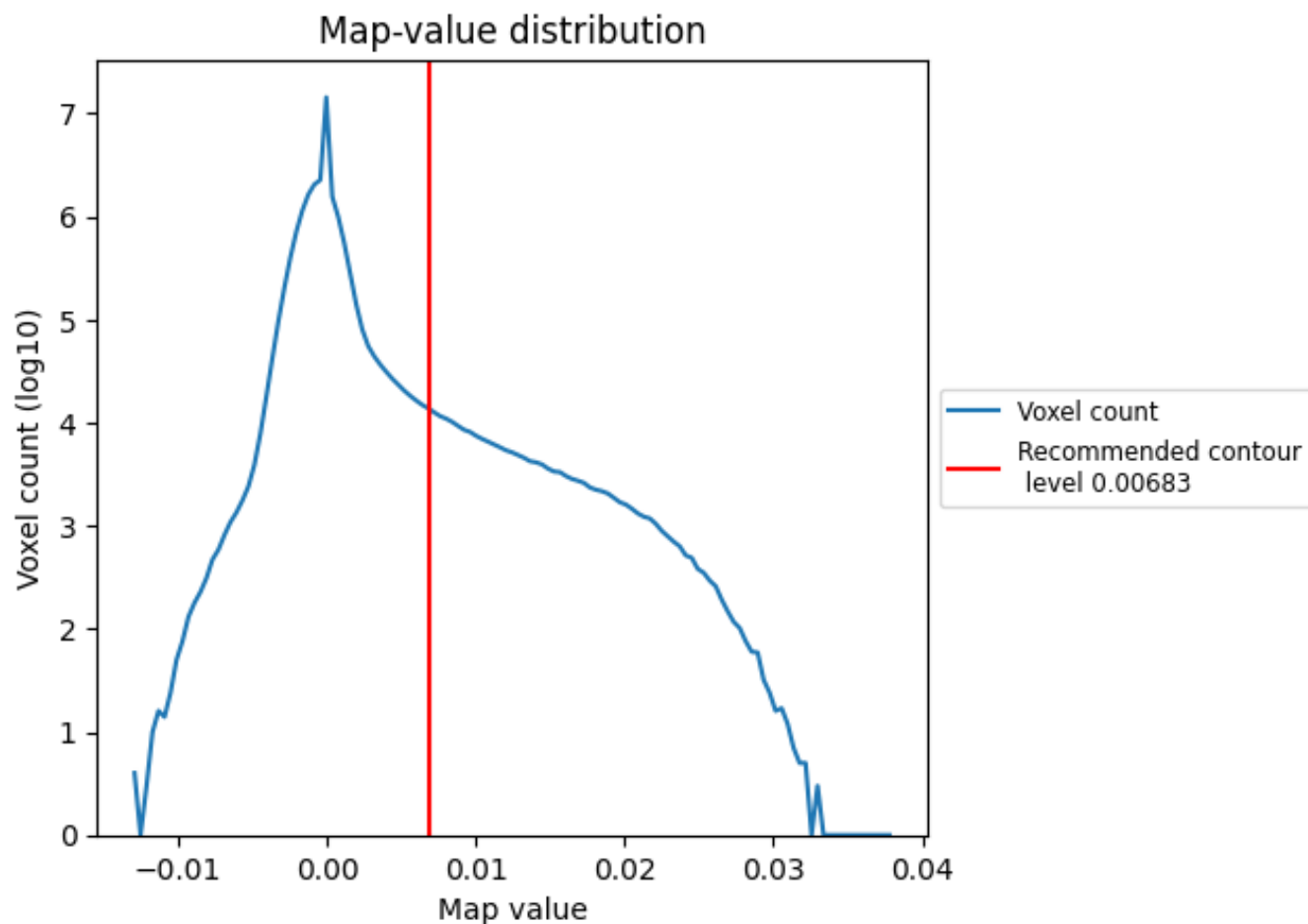
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

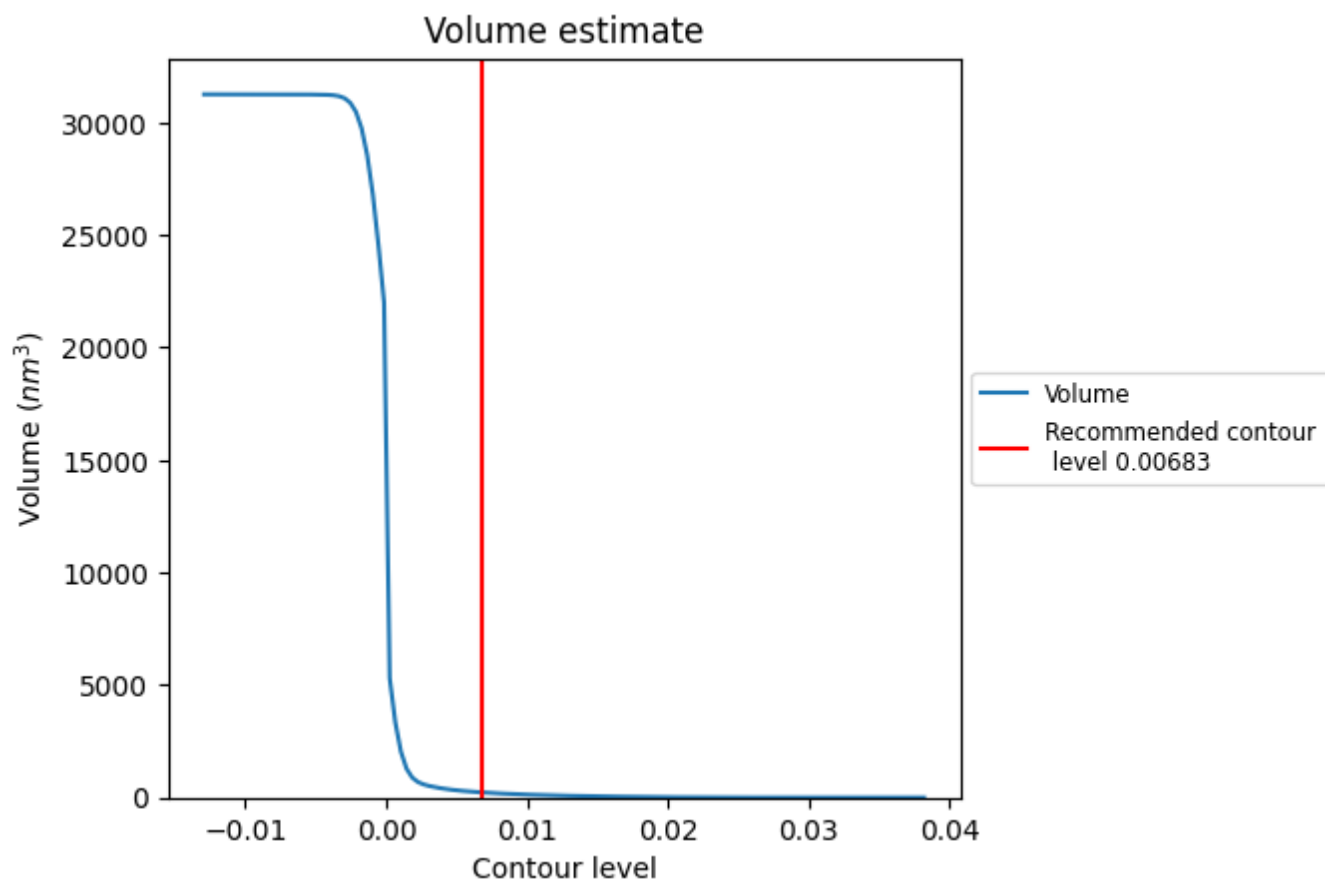
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

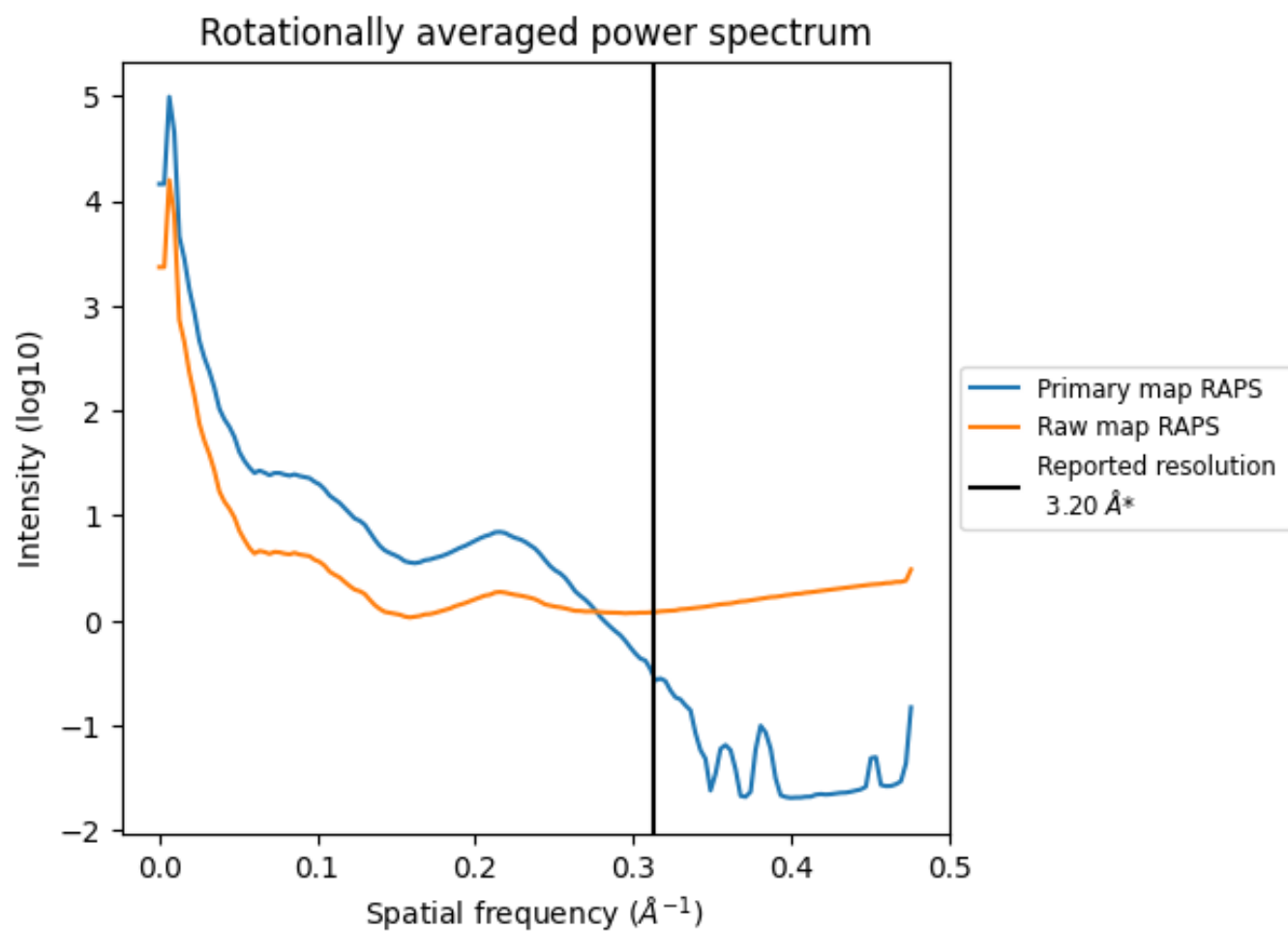
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 228 nm³; this corresponds to an approximate mass of 206 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

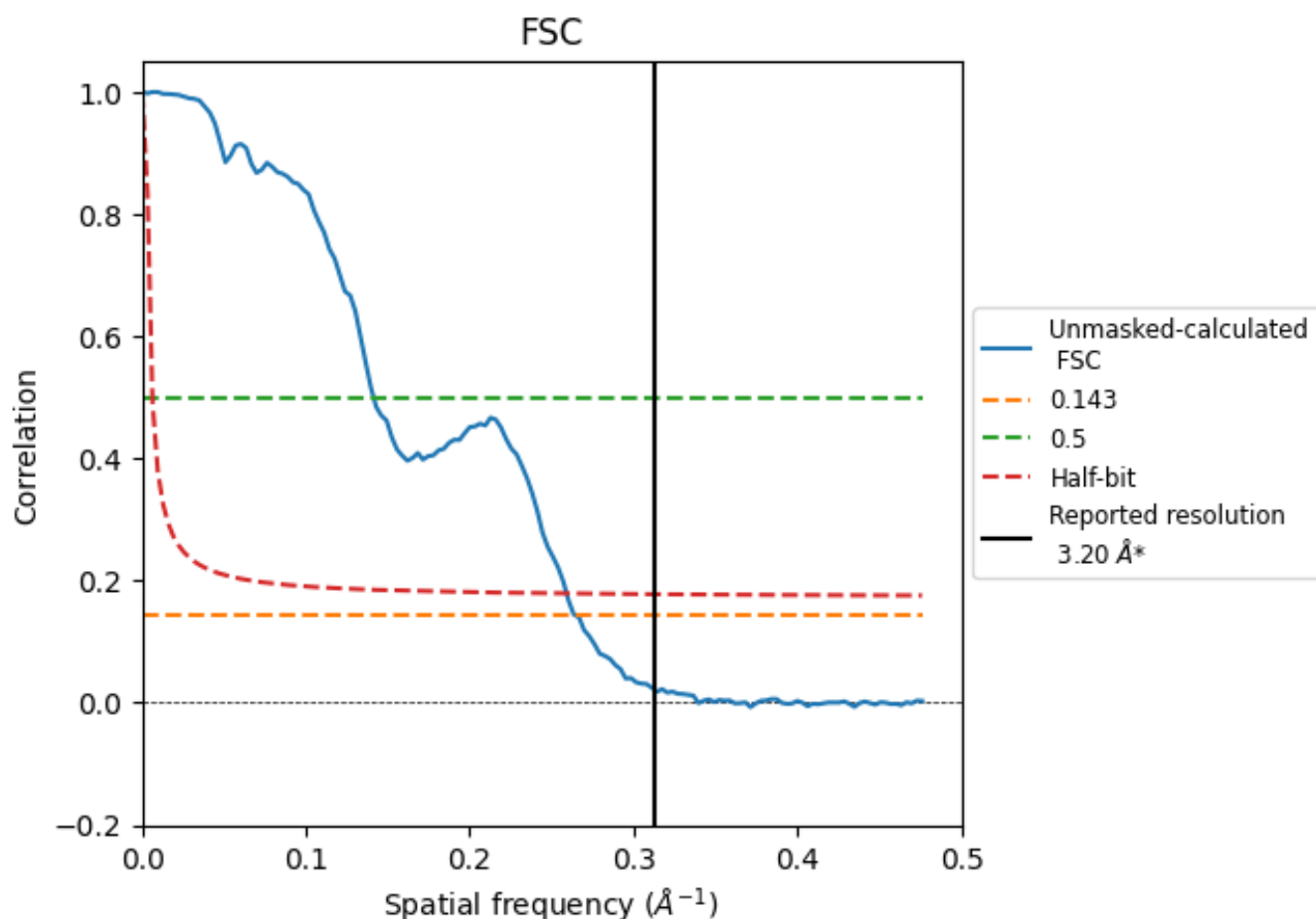


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.312 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

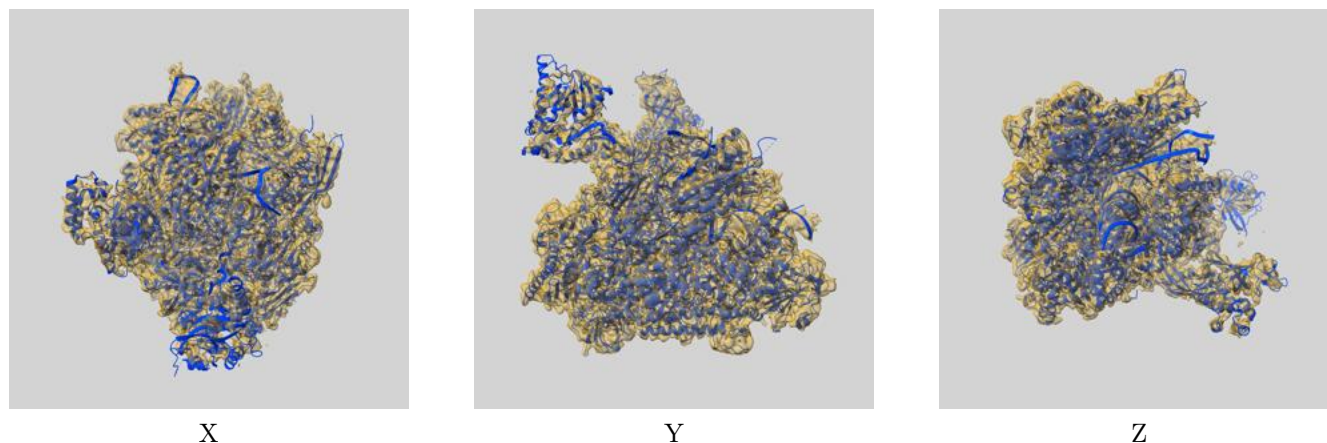
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.78	7.08	3.86

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.78 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

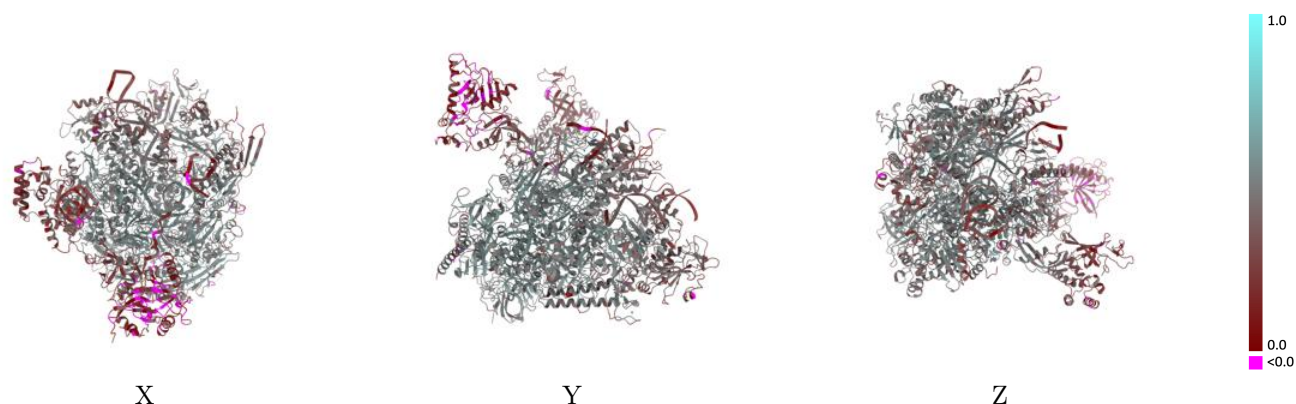
This section contains information regarding the fit between EMDB map EMD-17404 and PDB model 8P4B. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



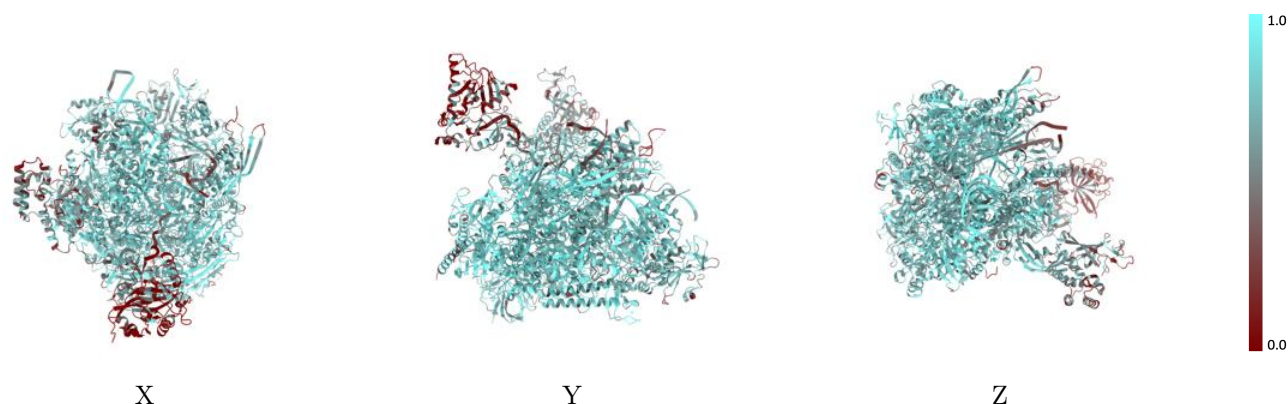
The images above show the 3D surface view of the map at the recommended contour level 0.00683 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



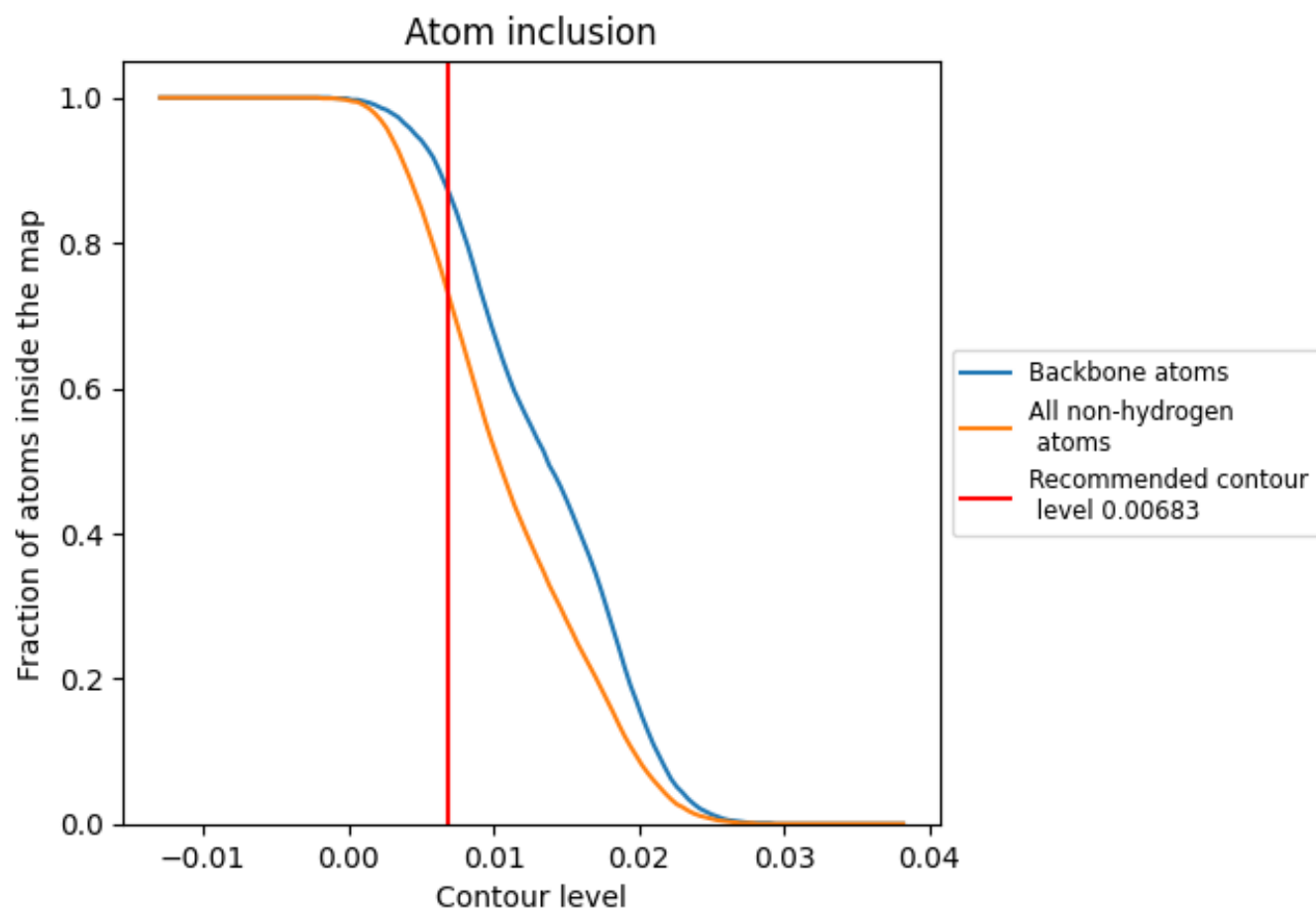
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00683).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 73% 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 (0.00683) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7340	 0.4340
A	 0.7900	 0.4700
B	 0.7960	 0.4790
C	 0.8160	 0.4940
D	 0.4470	 0.2820
E	 0.7800	 0.4430
F	 0.8060	 0.4980
G	 0.6090	 0.3300
H	 0.7830	 0.4800
I	 0.7170	 0.4050
J	 0.8410	 0.5120
K	 0.8420	 0.5090
L	 0.7290	 0.4550
M	 0.2980	 0.1650
N	 0.7380	 0.2780
P	 0.5410	 0.3590
T	 0.7930	 0.3800

