



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 02:00 PM UTC

PDB ID : 9G26 / pdb_00009g26
EMDB ID : EMD-50965
Title : Yeast RNA polymerase I elongation complex stalled by an apurinic site, closed state
Authors : Santos-Aledo, A.; Plaza-Pegueroles, A.; Ruiz, F.M.; Fernandez-Tornero, C.
Deposited on : 2024-07-10
Resolution : 3.40 Å(reported)
Based on initial model : 6hko

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
Mogul : 2022.3.0, CSD as543be (2022)
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

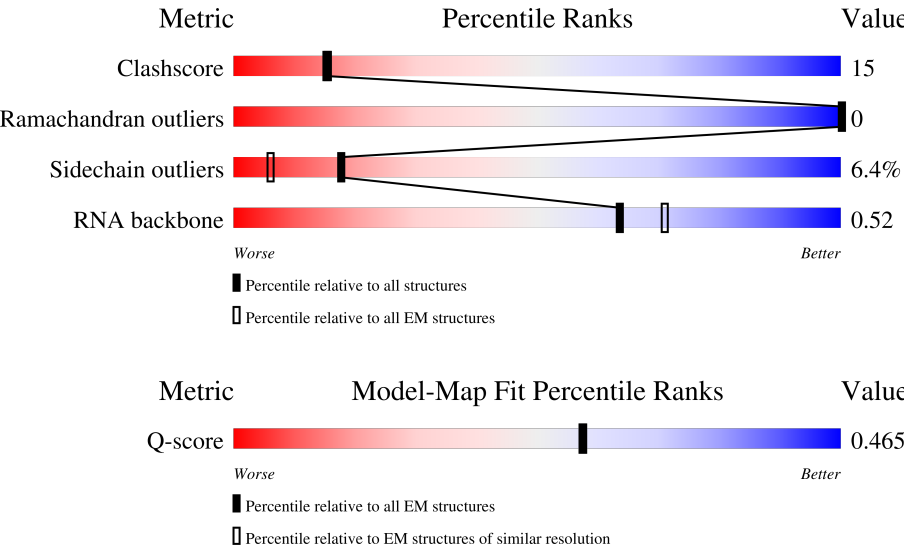
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	1664	17% 54% 31% 12%
2	B	1203	13% 61% 33% •
3	C	335	13% 65% 23% • 9%

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Mol	Chain	Length	Quality of chain
4	D	137	
5	E	215	
6	F	155	
7	G	326	
8	H	146	
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	
15	R	12	
16	S	38	
17	T	38	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 33973 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 I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1462	Total	C	N	O	S	0	0
			11549	7290	2012	2185	62		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1164	Total	C	N	O	S	0	0
			9254	5852	1626	1725	51		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	304	Total	C	N	O	S	0	0
			2415	1535	414	458	8		

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	59	Total	C	N	O	0	0
			467	293	80	94		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1751	1111	309	320	11		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	101	Total	C	N	O	S	0	0
			827	524	145	155	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	148	Total	C	N	O	S	0	0
			1164	756	196	208	4		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	131	Total	C	N	O	S	0	0
			1052	664	176	208	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	65	Total	C	N	O	S	0	0
			479	300	79	96	4		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	97	Total	C	N	O	S	0	0
			758	476	123	155	4		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	108	Total	C	N	O		0	0
			856	543	142	171			

- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	139	Total	C	N	O	S	0	0
			1105	705	181	215	4		

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	9	Total	C	N	O	P	0	0
			197	88	40	60	9		

- Molecule 16 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	25	Total	C	N	O	P	0	0
			506	242	85	154	25		

- Molecule 17 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	33	Total	C	N	O	P	0	0
			665	317	117	198	33		

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

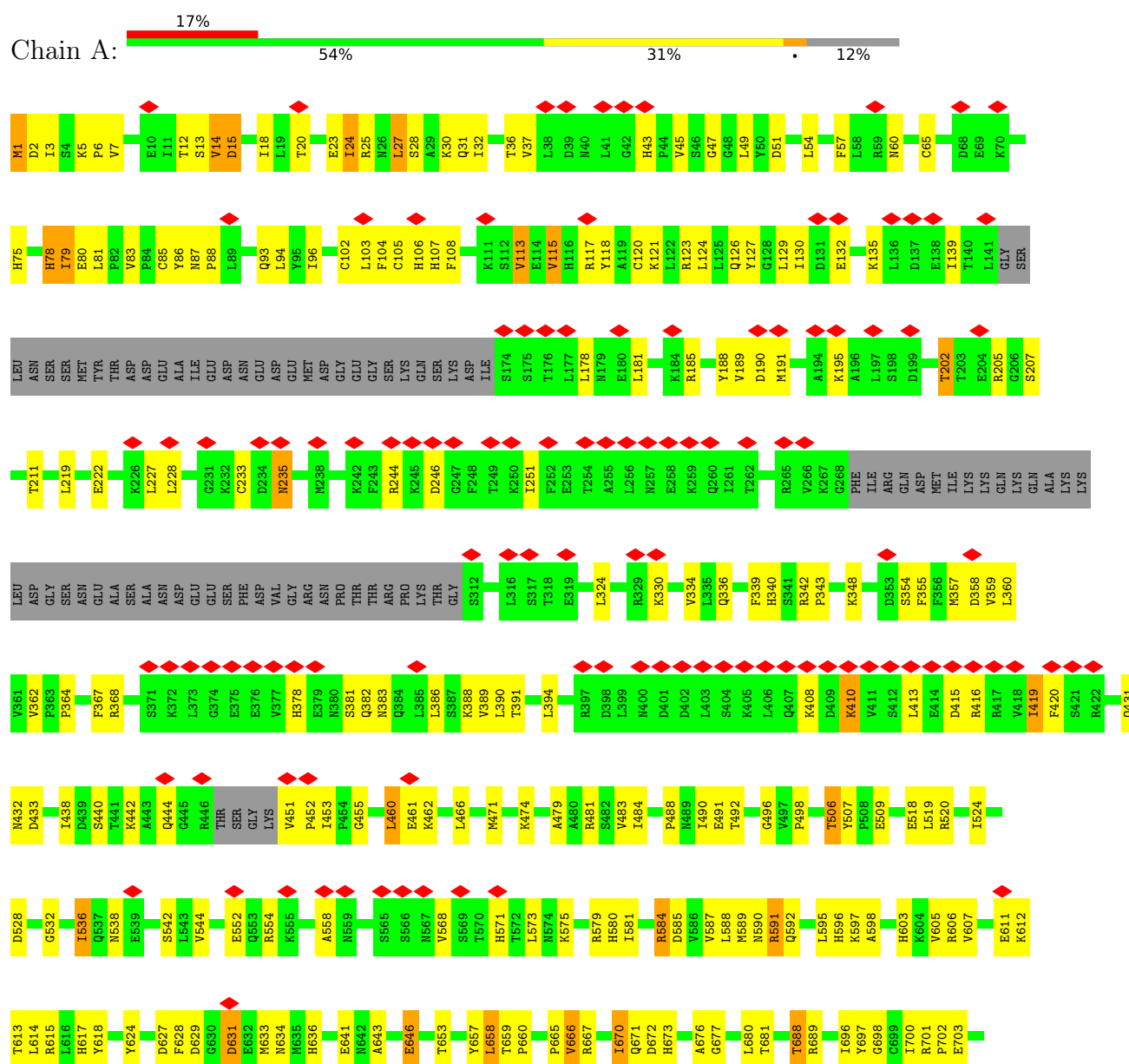
- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

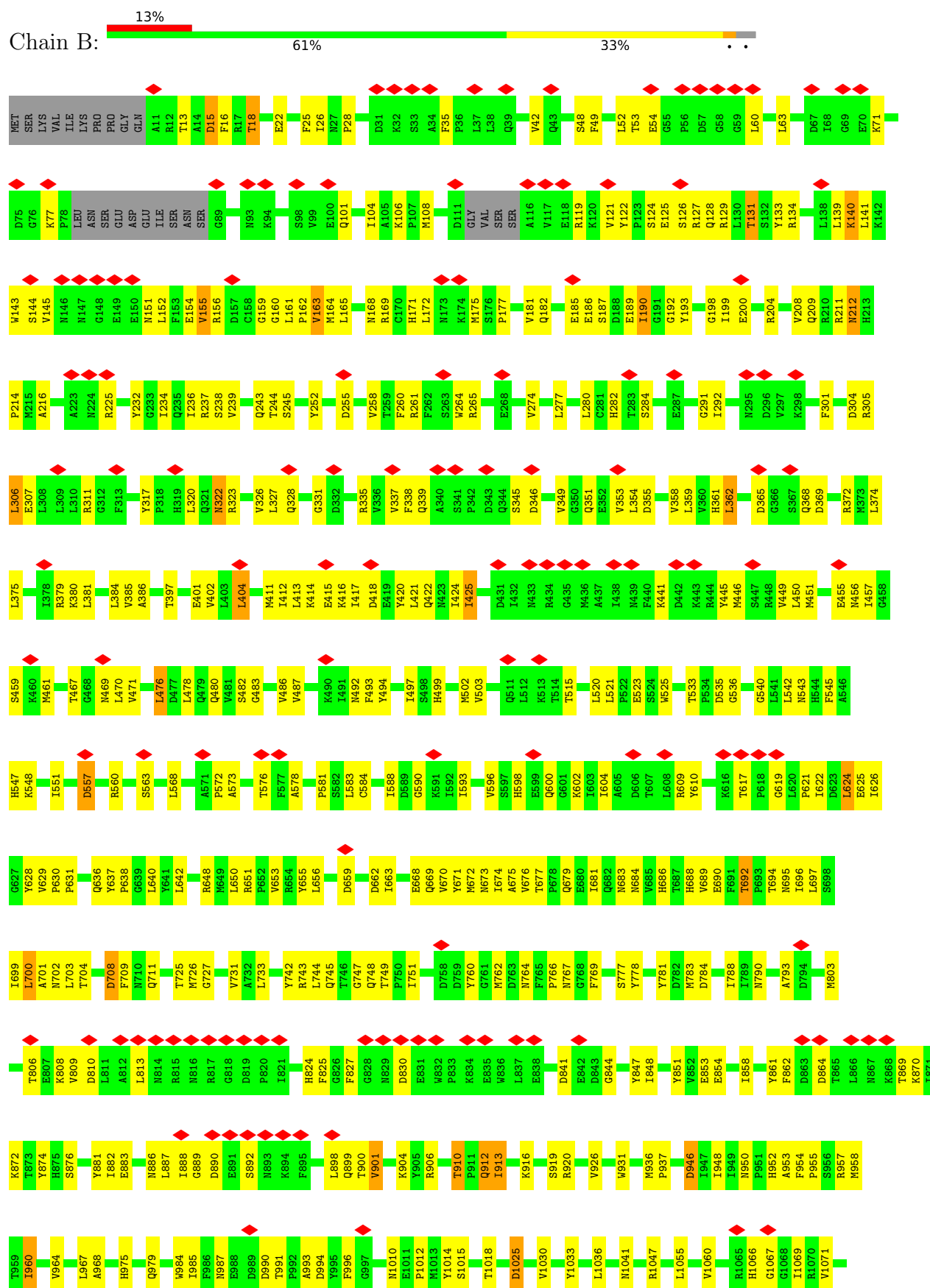
3 Residue-property plots

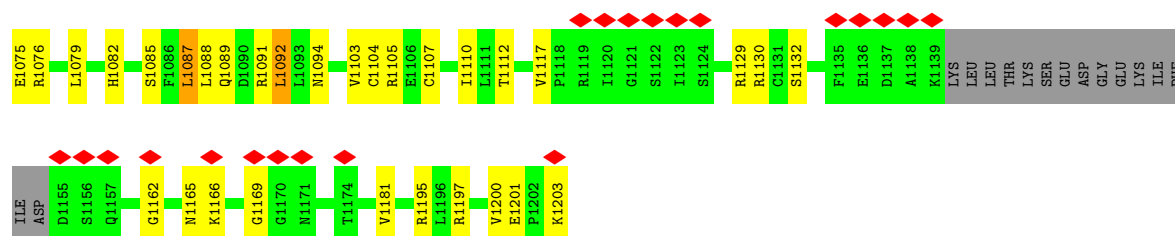
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 I subunit RPA190

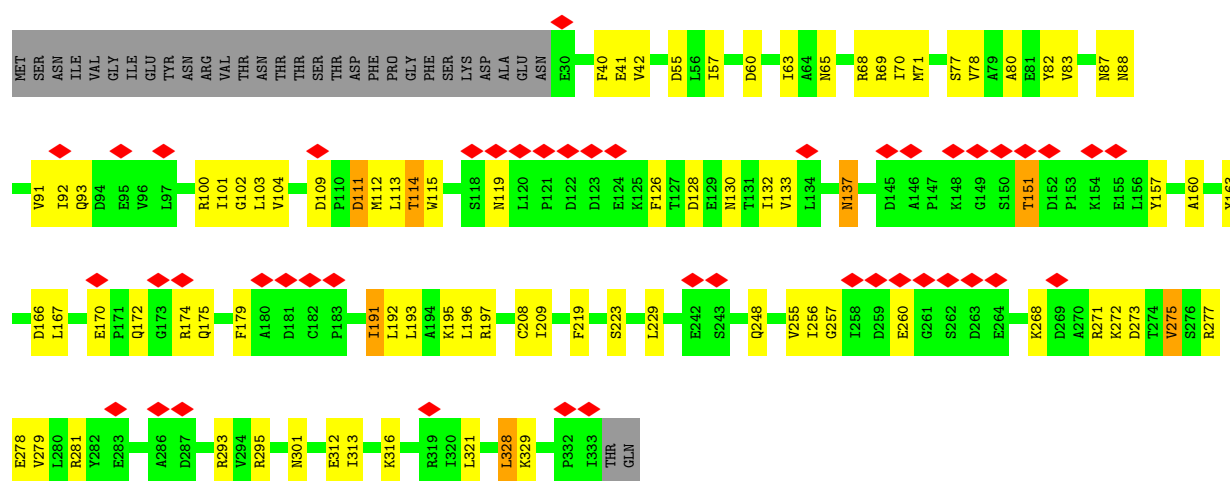




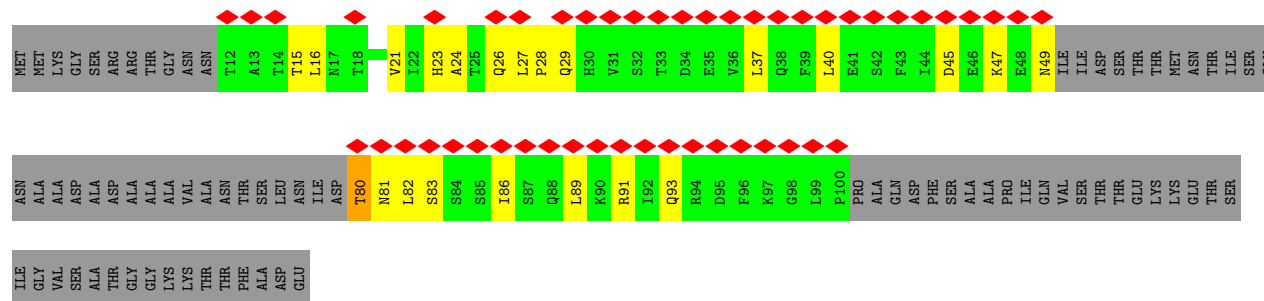




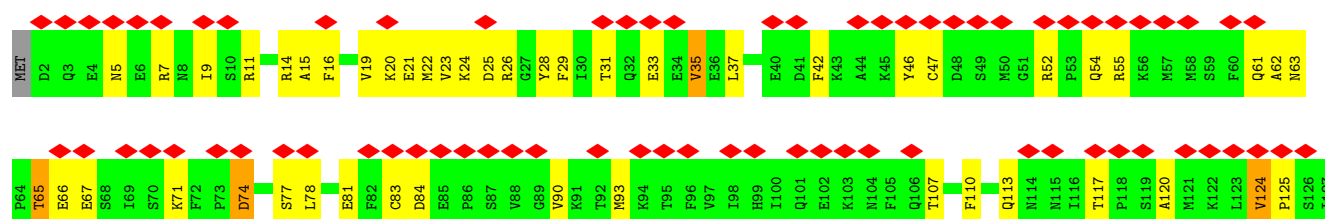
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



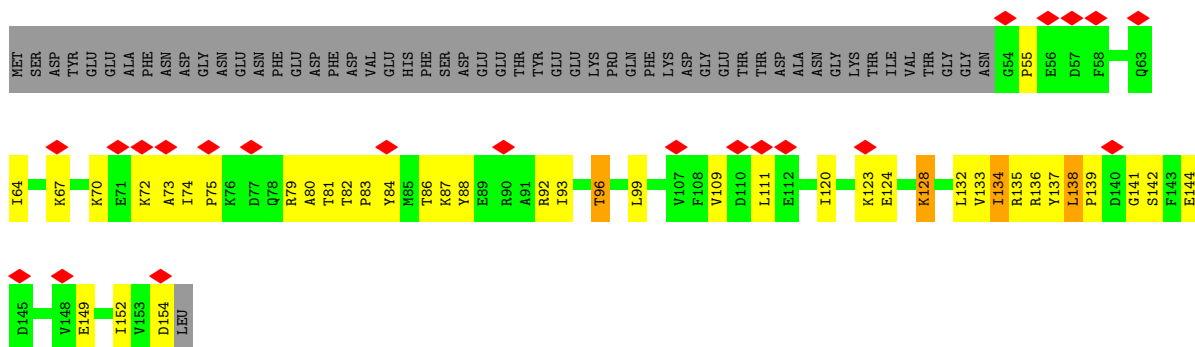
• Molecule 4: DNA-directed RNA polymerase I subunit RPA14



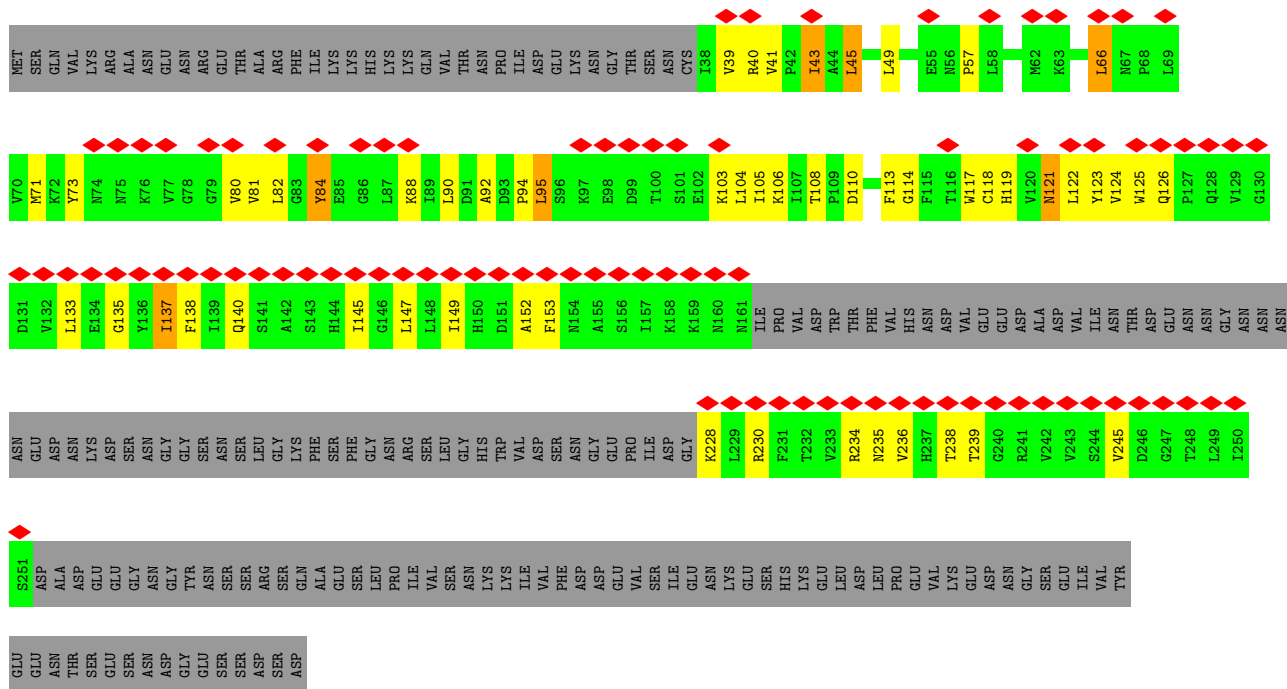
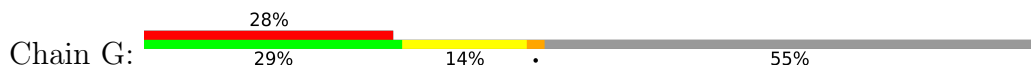
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

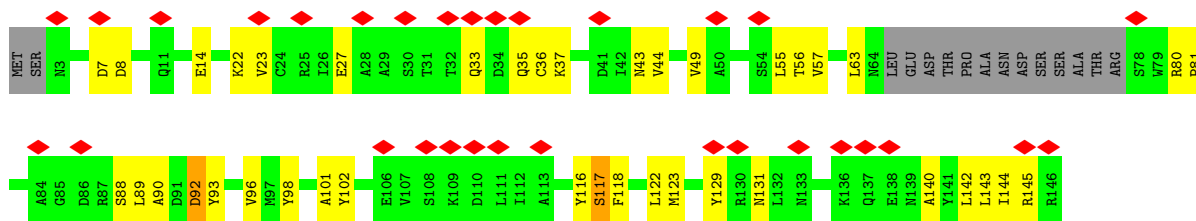


- Molecule 7: DNA-directed RNA polymerase I subunit RPA43

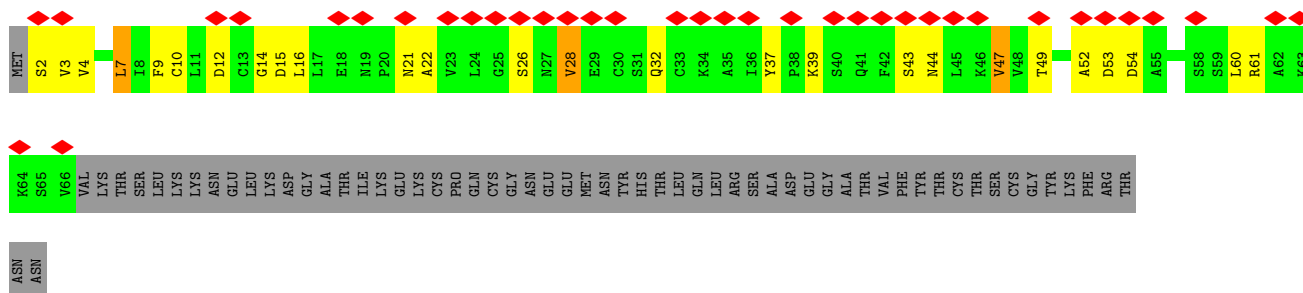
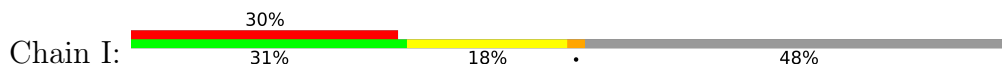


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3





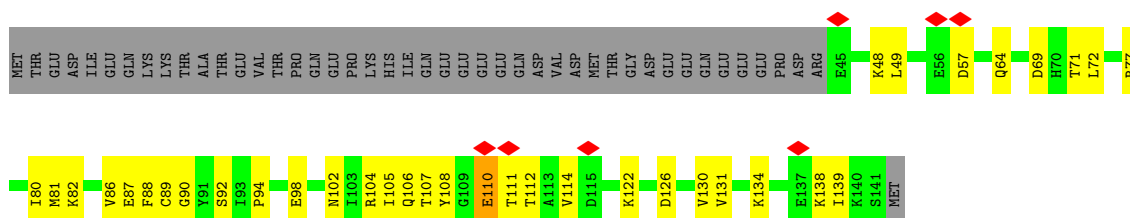
• Molecule 9: DNA-directed RNA polymerase I subunit RPA12



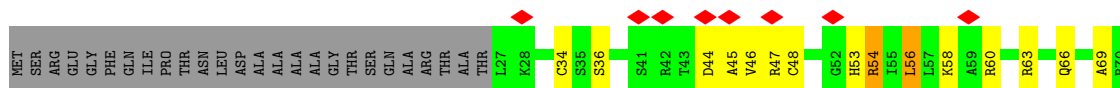
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

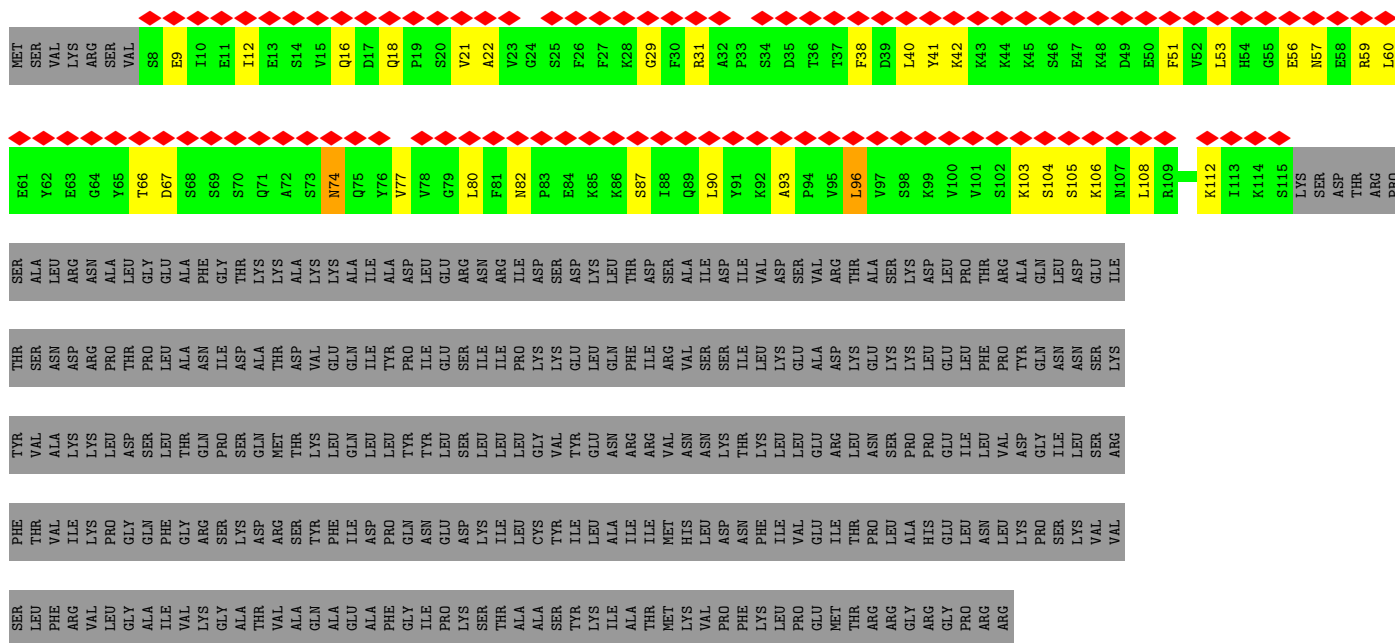


• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

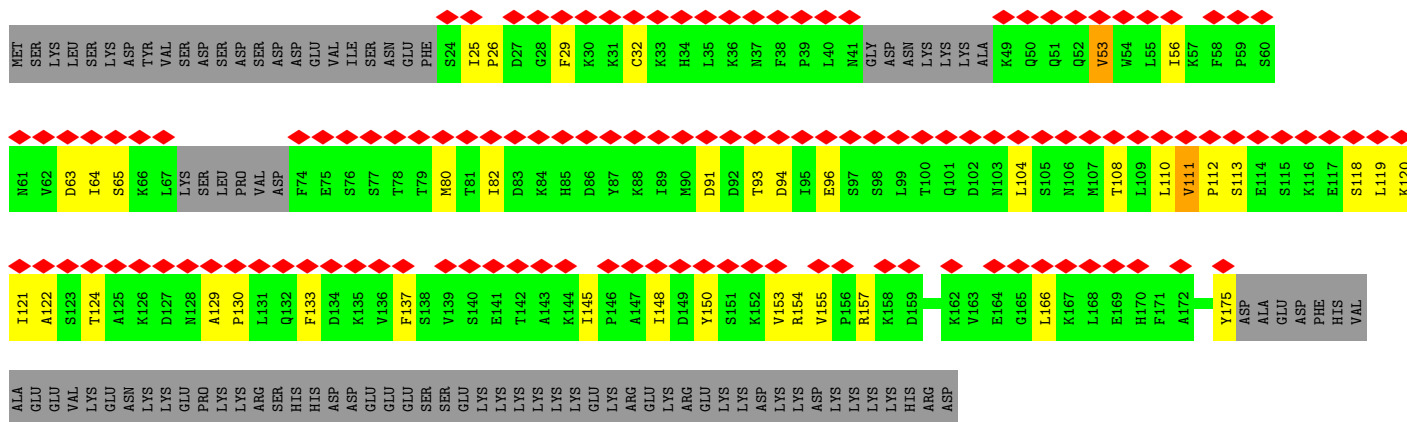


• Molecule 13: DNA-directed RNA polymerase I subunit RPA49

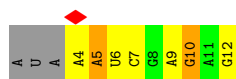
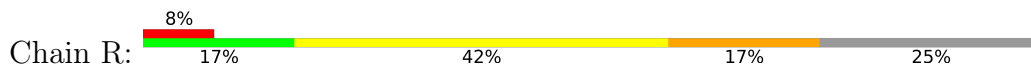




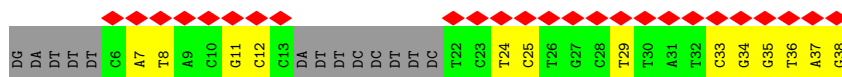
- Molecule 14: DNA-directed RNA polymerase I subunit RPA34



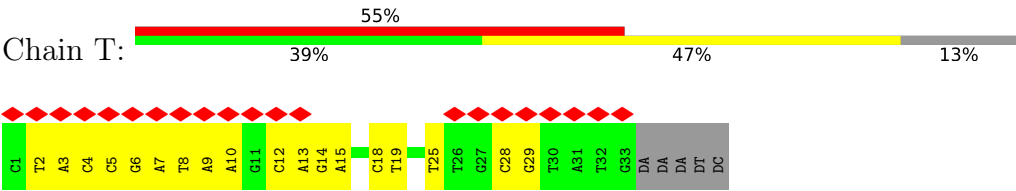
- Molecule 15: RNA



- Molecule 16: Non-template DNA



● Molecule 17: Template DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	125239	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.134	Depositor
Minimum map value	-0.082	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0237	Depositor
Map size ($\text{\AA}$)	301.536, 301.536, 301.536	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.047, 1.047, 1.047	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 3DR

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	0.21	0/11758	0.33	0/15878
2	B	0.22	0/9459	0.33	0/12785
3	C	0.22	0/2467	0.31	0/3344
4	D	0.11	0/473	0.25	0/641
5	E	0.17	0/1787	0.31	0/2406
6	F	0.20	0/842	0.35	0/1135
7	G	0.15	0/1190	0.32	0/1618
8	H	0.18	0/1070	0.30	0/1449
9	I	0.15	0/485	0.33	0/657
10	J	0.25	0/578	0.34	0/775
11	K	0.23	0/768	0.28	0/1037
12	L	0.17	0/354	0.33	0/468
13	M	0.12	0/872	0.30	0/1170
14	N	0.12	0/1125	0.32	0/1515
15	R	0.22	0/221	0.31	0/343
16	S	0.20	0/563	0.40	0/863
17	T	0.24	0/731	0.41	0/1123
All	All	0.20	0/34743	0.33	0/47207

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11549	0	11632	416	0
2	B	9254	0	9146	321	0
3	C	2415	0	2403	64	0
4	D	467	0	468	14	0
5	E	1751	0	1776	68	0
6	F	827	0	843	33	0
7	G	1164	0	1194	40	0
8	H	1052	0	1021	27	0
9	I	479	0	480	21	0
10	J	569	0	585	19	0
11	K	758	0	756	29	0
12	L	352	0	375	13	0
13	M	856	0	855	25	0
14	N	1105	0	1121	31	0
15	R	197	0	98	9	0
16	S	506	0	285	9	0
17	T	665	0	370	13	0
18	A	1	0	0	0	0
19	A	2	0	0	0	0
19	B	1	0	0	0	0
19	I	1	0	0	0	0
19	J	1	0	0	0	0
19	L	1	0	0	0	0
All	All	33973	0	33408	991	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 (991) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:CYS:SG	1:A:235:ASN:ND2	2.39	0.95
1:A:671:GLN:HB2	2:B:952:HIS:HD2	1.42	0.82
1:A:755:ILE:HD12	1:A:780:ILE:HD11	1.62	0.81
1:A:631:ASP:OD2	15:R:12:G:O2'	2.00	0.80
12:L:48:CYS:HB3	12:L:53:HIS:H	1.47	0.79
1:A:942:GLN:HG3	2:B:958:MET:HE1	1.65	0.78
1:A:1226:VAL:HA	1:A:1589:MET:HE1	1.65	0.77
1:A:631:ASP:CG	15:R:12:G:O2'	2.27	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:PHE:HE1	8:H:98:TYR:HB2	1.51	0.76
1:A:1473:LYS:NZ	1:A:1475:GLU:OE2	2.19	0.75
2:B:1105:ARG:HD3	2:B:1203:LYS:HA	1.68	0.74
2:B:71:LYS:HE2	2:B:422:GLN:HA	1.69	0.74
1:A:520:ARG:HG3	1:A:558:ALA:HB1	1.69	0.74
1:A:481:ARG:NH1	1:A:634:ASN:OD1	2.19	0.74
5:E:29:PHE:HB3	5:E:65:THR:HB	1.70	0.74
1:A:785:GLN:HB3	1:A:793:ILE:HG22	1.69	0.73
1:A:641:GLU:HB2	6:F:99:LEU:HG	1.68	0.73
3:C:128:ASP:O	3:C:175:GLN:NE2	2.22	0.73
1:A:753:ASN:ND2	1:A:780:ILE:O	2.22	0.73
2:B:790:ASN:HB2	2:B:946:ASP:HA	1.71	0.72
1:A:1124:LEU:HB3	1:A:1129:PRO:HG3	1.72	0.71
2:B:25:PHE:HB3	10:J:58:GLU:HB2	1.72	0.71
2:B:216:ALA:HB1	2:B:384:LEU:HD22	1.72	0.71
1:A:1660:VAL:HG22	7:G:103:LYS:H	1.56	0.71
1:A:700:ILE:O	1:A:706:HIS:ND1	2.24	0.71
1:A:1024:THR:O	1:A:1028:GLU:HB3	1.91	0.71
2:B:182:GLN:O	10:J:69:ARG:NH1	2.22	0.71
3:C:100:ARG:NH2	10:J:3:VAL:O	2.16	0.70
5:E:24:LYS:HE3	5:E:35:VAL:HG21	1.72	0.70
1:A:1587:ASP:OD2	5:E:200:ARG:NH1	2.25	0.70
5:E:200:ARG:N	5:E:208:TYR:O	2.20	0.70
1:A:1628:ASP:N	1:A:1628:ASP:OD1	2.23	0.70
1:A:1181:PRO:HD2	6:F:86:THR:HG21	1.72	0.69
1:A:1241:PRO:HB2	1:A:1537:ASP:HB3	1.73	0.69
2:B:129:ARG:NH2	2:B:889:GLY:O	2.25	0.69
15:R:4:A:H2'	15:R:5:A:C8	2.27	0.69
2:B:128:GLN:OE1	2:B:886:ASN:ND2	2.26	0.69
5:E:67:GLU:O	5:E:71:LYS:NZ	2.25	0.69
1:A:105:CYS:SG	1:A:235:ASN:ND2	2.62	0.69
2:B:480:GLN:NE2	2:B:482:SER:O	2.26	0.69
2:B:1079:LEU:HD11	2:B:1087:LEU:HD23	1.74	0.69
1:A:1462:PHE:HD1	1:A:1470:CYS:HB2	1.59	0.68
1:A:581:ILE:HD11	1:A:605:VAL:HG11	1.76	0.68
5:E:28:TYR:CZ	5:E:78:LEU:HB2	2.28	0.68
1:A:1559:ARG:NH2	1:A:1560:ASN:OD1	2.27	0.68
1:A:734:THR:O	1:A:738:ASN:ND2	2.26	0.68
1:A:1094:ALA:HB2	1:A:1132:TYR:HB3	1.74	0.68
1:A:120:CYS:HB3	1:A:189:VAL:HG21	1.76	0.67
1:A:1439:MET:SD	1:A:1439:MET:N	2.65	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:GLY:N	1:A:615:ARG:O	2.24	0.67
2:B:53:THR:OG1	2:B:169:ARG:NH1	2.27	0.67
5:E:26:ARG:NE	5:E:187:TYR:O	2.21	0.67
1:A:596:HIS:HD2	1:A:1195:GLU:HG3	1.60	0.67
2:B:568:LEU:HB3	2:B:604:ILE:HD12	1.75	0.67
1:A:389:VAL:HG22	1:A:433:ASP:HB3	1.76	0.67
1:A:1221:ARG:NH1	1:A:1224:GLU:OE2	2.28	0.67
3:C:113:LEU:HB2	3:C:130:ASN:HA	1.76	0.67
2:B:204:ARG:HD2	2:B:486:VAL:HB	1.77	0.66
3:C:103:LEU:HD22	10:J:6:ARG:HD2	1.76	0.66
4:D:47:LYS:NZ	7:G:84:TYR:OH	2.28	0.66
1:A:132:GLU:HG3	1:A:135:LYS:HE2	1.78	0.66
1:A:25:ARG:NH2	1:A:358:ASP:OD2	2.29	0.66
1:A:886:ASN:O	1:A:955:ARG:NH2	2.29	0.66
2:B:320:LEU:HB3	2:B:326:VAL:HG12	1.77	0.66
2:B:809:VAL:HB	2:B:901:VAL:HG23	1.77	0.66
1:A:1063:MET:SD	1:A:1173:LYS:NZ	2.64	0.66
1:A:1053:ASP:HB3	5:E:205:SER:HB3	1.78	0.66
2:B:291:GLY:HA3	2:B:375:LEU:HD13	1.78	0.65
5:E:83:CYS:O	5:E:113:GLN:NE2	2.29	0.65
2:B:368:GLN:O	2:B:372:ARG:NH1	2.29	0.65
2:B:733:LEU:O	2:B:904:LYS:NZ	2.29	0.65
1:A:1102:LEU:HG	1:A:1106:LYS:HE2	1.79	0.65
2:B:317:TYR:HB3	2:B:320:LEU:HD13	1.77	0.65
1:A:1094:ALA:O	1:A:1098:SER:OG	2.13	0.65
1:A:496:GLY:HA3	1:A:615:ARG:HB2	1.78	0.65
1:A:857:ALA:HB2	1:A:899:LYS:HD2	1.78	0.65
13:M:29:GLY:HA2	14:N:104:LEU:HD11	1.79	0.65
2:B:232:TYR:HD2	2:B:385:VAL:HG22	1.60	0.65
4:D:45:ASP:HA	4:D:49:ASN:HB2	1.78	0.65
1:A:1298:ASP:HA	1:A:1468:LYS:HE3	1.77	0.65
1:A:1299:ASN:H	1:A:1468:LYS:HZ1	1.43	0.65
2:B:609:ARG:NH1	2:B:668:GLU:OE2	2.23	0.65
2:B:725:THR:HG21	2:B:767:ASN:HB3	1.79	0.64
13:M:41:TYR:HB3	14:N:29:PHE:HB3	1.79	0.64
1:A:23:GLU:OE1	2:B:1130:ARG:NH1	2.31	0.64
1:A:87:ASN:HA	1:A:357:MET:HE2	1.79	0.64
1:A:782:ASP:OD1	1:A:783:LYS:N	2.30	0.64
2:B:209:GLN:HB3	2:B:237:ARG:HD3	1.79	0.64
8:H:63:LEU:HB3	8:H:88:SER:HB2	1.79	0.64
13:M:21:VAL:HG23	13:M:93:ALA:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:SER:OG	3:C:219:PHE:O	2.14	0.64
2:B:626:ILE:HG22	2:B:642:LEU:HD22	1.80	0.64
1:A:671:GLN:HB2	2:B:952:HIS:CD2	2.31	0.64
1:A:781:LEU:HB3	1:A:786:TYR:HE1	1.63	0.64
1:A:735:VAL:HG21	1:A:816:LEU:HD22	1.80	0.64
6:F:70:LYS:HA	7:G:94:PRO:HB3	1.80	0.64
1:A:86:TYR:N	1:A:431:GLN:OE1	2.28	0.64
2:B:467:THR:HG22	17:T:25:DT:H4'	1.80	0.64
14:N:108:THR:HG22	14:N:130:PRO:HB3	1.80	0.63
17:T:28:DC:H2'	17:T:29:DG:C8	2.32	0.63
2:B:708:ASP:OD1	2:B:708:ASP:N	2.30	0.63
1:A:57:PHE:O	1:A:60:ASN:ND2	2.23	0.63
1:A:462:LYS:NZ	17:T:15:DA:OP2	2.30	0.63
1:A:536:ILE:HG23	1:A:544:VAL:HB	1.79	0.63
3:C:55:ASP:OD1	3:C:271:ARG:NH1	2.31	0.63
1:A:507:TYR:OH	1:A:641:GLU:OE2	2.16	0.63
1:A:956:ARG:HH21	1:A:979:GLY:HA3	1.63	0.63
2:B:264:TRP:CD1	2:B:265:ARG:HG2	2.33	0.63
2:B:674:ILE:HG12	2:B:688:HIS:HB2	1.81	0.63
4:D:40:LEU:HB3	4:D:93:GLN:HG3	1.80	0.63
2:B:560:ARG:O	2:B:563:SER:OG	2.15	0.63
3:C:170:GLU:OE2	3:C:172:GLN:NE2	2.31	0.63
5:E:93:MET:HG3	5:E:120:ALA:HB1	1.80	0.63
1:A:886:ASN:OD1	1:A:955:ARG:NH2	2.31	0.62
1:A:1587:ASP:OD1	5:E:212:ARG:NH2	2.31	0.62
11:K:80:ILE:HG21	11:K:105:ILE:HD12	1.81	0.62
1:A:1039:ARG:NH1	1:A:1043:GLY:O	2.32	0.62
1:A:1194:GLY:O	1:A:1197:SER:OG	2.10	0.62
1:A:1314:GLN:OE1	1:A:1318:SER:OG	2.17	0.62
3:C:157:TYR:HB2	3:C:160:ALA:HB2	1.79	0.62
1:A:573:LEU:HD11	4:D:16:LEU:HD22	1.81	0.62
1:A:413:LEU:HA	1:A:416:ARG:HB3	1.82	0.62
1:A:483:VAL:O	1:A:613:THR:OG1	2.17	0.62
13:M:57:ASN:HD21	13:M:60:LEU:HB2	1.64	0.62
1:A:18:ILE:HG21	1:A:354:SER:HB2	1.81	0.62
2:B:557:ASP:OD1	2:B:557:ASP:N	2.33	0.62
2:B:533:THR:HG21	2:B:540:GLY:H	1.65	0.62
3:C:132:ILE:HB	3:C:208:CYS:HB2	1.82	0.62
1:A:874:GLU:OE2	1:A:878:ARG:NH1	2.32	0.61
8:H:92:ASP:N	8:H:92:ASP:OD1	2.33	0.61
1:A:1039:ARG:HH22	5:E:170:LEU:HD11	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:THR:OG1	1:A:689:ARG:N	2.31	0.61
1:A:834:ARG:NH2	2:B:994:ASP:OD1	2.33	0.61
5:E:21:GLU:OE1	5:E:146:HIS:NE2	2.33	0.61
2:B:327:LEU:HD21	2:B:351:GLN:HB2	1.82	0.61
1:A:20:THR:N	1:A:23:GLU:OE2	2.33	0.61
1:A:1533:GLU:OE1	5:E:14:ARG:NH1	2.34	0.61
2:B:345:SER:HB2	13:M:112:LYS:HE2	1.81	0.61
2:B:244:THR:HA	2:B:411:MET:HE2	1.81	0.61
2:B:760:TYR:HB2	2:B:762:MET:HE2	1.83	0.61
2:B:1104:CYS:HB3	2:B:1107:CYS:HB3	1.83	0.61
1:A:1288:ARG:NH1	1:A:1480:THR:O	2.33	0.61
1:A:126:GLN:NE2	1:A:340:HIS:O	2.33	0.61
1:A:1221:ARG:NH2	1:A:1565:GLU:OE1	2.34	0.60
2:B:26:ILE:O	10:J:62:ARG:NH1	2.34	0.60
3:C:328:LEU:HD12	11:K:72:LEU:HD21	1.82	0.60
1:A:15:ASP:N	1:A:15:ASP:OD1	2.34	0.60
6:F:124:GLU:O	6:F:128:LYS:N	2.33	0.60
1:A:1235:THR:O	1:A:1544:ASN:ND2	2.34	0.60
4:D:26:GLN:NE2	4:D:29:GLN:OE1	2.34	0.60
3:C:102:GLY:HA3	12:L:69:ALA:HB1	1.82	0.60
2:B:154:GLU:OE2	2:B:156:ARG:NH2	2.35	0.60
3:C:42:VAL:O	11:K:138:LYS:NZ	2.35	0.60
16:S:29:DT:H71	17:T:10:DA:H2	1.65	0.60
1:A:1055:ILE:O	1:A:1580:ARG:NH1	2.34	0.60
1:A:1118:VAL:HG21	5:E:154:ILE:HD13	1.82	0.60
3:C:293:ARG:O	3:C:295:ARG:NH1	2.34	0.60
1:A:603:HIS:NE2	1:A:624:TYR:OH	2.30	0.60
2:B:968:ALA:HB1	2:B:979:GLN:HG2	1.84	0.60
1:A:830:MET:HE2	2:B:993:ALA:HB2	1.84	0.59
2:B:890:ASP:OD2	2:B:892:SER:OG	2.20	0.59
3:C:78:VAL:HG21	3:C:113:LEU:HD21	1.84	0.59
1:A:1139:ASN:OD1	5:E:206:GLY:N	2.35	0.59
8:H:23:VAL:HA	8:H:43:ASN:HA	1.84	0.59
1:A:1128:ASN:OD1	1:A:1128:ASN:N	2.35	0.59
2:B:841:ASP:OD2	12:L:58:LYS:NZ	2.30	0.59
2:B:898:LEU:O	2:B:899:GLN:NE2	2.33	0.59
8:H:116:TYR:O	8:H:123:MET:N	2.26	0.59
2:B:683:ASN:OD1	14:N:154:ARG:NH2	2.36	0.59
1:A:597:LYS:O	2:B:1082:HIS:NE2	2.36	0.59
2:B:781:TYR:HB2	2:B:788:ILE:HD11	1.84	0.59
10:J:41:LEU:HD22	10:J:46:CYS:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:888:ILE:HB	2:B:900:THR:HB	1.84	0.59
1:A:1238:MET:HA	1:A:1543:SER:HA	1.84	0.59
2:B:1088:LEU:HD12	2:B:1092:LEU:HD23	1.84	0.59
2:B:71:LYS:HD3	2:B:421:LEU:HB3	1.85	0.58
2:B:525:TRP:NE1	2:B:690:GLU:OE2	2.32	0.58
3:C:65:ASN:OD1	3:C:68:ARG:NH2	2.30	0.58
1:A:1051:GLY:HA3	1:A:1580:ARG:HG2	1.86	0.58
1:A:1124:LEU:HD23	1:A:1129:PRO:HB3	1.84	0.58
1:A:1225:ILE:O	1:A:1595:TYR:OH	2.21	0.58
2:B:1012:PRO:HG2	3:C:275:VAL:HG23	1.85	0.58
1:A:1436:ASN:HD21	1:A:1439:MET:HA	1.68	0.58
7:G:149:ILE:N	7:G:153:PHE:O	2.36	0.58
2:B:351:GLN:NE2	2:B:355:ASP:OD2	2.34	0.58
2:B:745:GLN:NE2	10:J:1:MET:SD	2.73	0.58
2:B:910:THR:O	2:B:912:GLN:NE2	2.37	0.58
1:A:88:PRO:O	1:A:442:LYS:NZ	2.35	0.58
1:A:847:LEU:HD21	1:A:946:LEU:HD22	1.84	0.58
2:B:1103:VAL:HB	2:B:1110:ILE:HD13	1.86	0.58
1:A:491:GLU:OE2	1:A:811:SER:OG	2.16	0.58
1:A:1276:THR:HG23	1:A:1288:ARG:HG2	1.85	0.58
5:E:22:MET:O	5:E:26:ARG:HG2	2.03	0.58
1:A:536:ILE:HD11	1:A:575:LYS:HB3	1.85	0.58
2:B:49:PHE:HZ	2:B:163:VAL:HG12	1.68	0.58
8:H:56:THR:HG21	8:H:145:ARG:HH21	1.68	0.58
1:A:1298:ASP:OD1	1:A:1298:ASP:N	2.36	0.58
2:B:1107:CYS:SG	2:B:1130:ARG:NE	2.76	0.58
5:E:61:GLN:O	5:E:63:ASN:ND2	2.36	0.57
1:A:718:THR:OG1	1:A:730:GLN:OE1	2.21	0.57
2:B:369:ASP:OD1	2:B:372:ARG:NH2	2.29	0.57
7:G:140:GLN:HA	7:G:145:ILE:HG23	1.86	0.57
2:B:134:ARG:HA	2:B:162:PRO:HA	1.87	0.57
15:R:4:A:H2'	15:R:5:A:H8	1.68	0.57
1:A:631:ASP:OD1	15:R:12:G:O2'	2.22	0.57
1:A:760:TRP:HZ2	1:A:780:ILE:HD13	1.69	0.57
1:A:1240:LEU:HB3	1:A:1536:ILE:HD12	1.87	0.57
1:A:1447:GLN:HE22	1:A:1459:LYS:HA	1.68	0.57
2:B:412:ILE:HG23	2:B:461:MET:HE1	1.86	0.57
1:A:93:GLN:HG3	1:A:1627:LEU:HD13	1.87	0.57
1:A:106:HIS:O	1:A:107:HIS:ND1	2.38	0.57
1:A:132:GLU:HA	1:A:135:LYS:HG2	1.87	0.57
1:A:697:TYR:HE1	1:A:702:PRO:HD2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:10:CYS:SG	10:J:11:GLY:N	2.78	0.57
1:A:1657:LEU:HG	7:G:104:LEU:HD13	1.85	0.57
1:A:1127:TYR:HB3	1:A:1132:TYR:HD2	1.70	0.57
1:A:1447:GLN:O	1:A:1451:ILE:HG12	2.05	0.57
2:B:214:PRO:O	2:B:380:LYS:NZ	2.33	0.57
3:C:195:LYS:NZ	10:J:58:GLU:OE2	2.32	0.56
2:B:337:VAL:HG23	2:B:338:PHE:HD1	1.70	0.56
11:K:86:VAL:HA	11:K:107:THR:HA	1.87	0.56
1:A:362:VAL:HG12	1:A:386:LEU:HD13	1.86	0.56
1:A:781:LEU:HB3	1:A:786:TYR:CE1	2.41	0.56
1:A:884:ARG:HH12	1:A:961:VAL:HG23	1.70	0.56
1:A:925:MET:HE1	2:B:955:PRO:HA	1.88	0.56
1:A:1242:ILE:HD12	1:A:1519:LEU:HD11	1.86	0.56
1:A:1463:ASP:OD1	1:A:1466:SER:N	2.30	0.56
1:A:1557:ALA:HB2	5:E:150:VAL:HG22	1.88	0.56
2:B:15:ASP:OD1	2:B:15:ASP:N	2.37	0.56
2:B:280:LEU:HA	2:B:354:LEU:HD21	1.87	0.56
7:G:125:TRP:CD1	7:G:126:GLN:H	2.24	0.56
17:T:7:DA:H2'	17:T:8:DT:H71	1.88	0.56
2:B:129:ARG:HA	2:B:888:ILE:HD12	1.88	0.56
1:A:498:PRO:HB3	1:A:612:LYS:HA	1.88	0.56
1:A:862:THR:HB	1:A:878:ARG:HD3	1.87	0.56
2:B:124:SER:N	2:B:185:GLU:OE2	2.38	0.56
2:B:125:GLU:O	2:B:126:SER:OG	2.23	0.56
2:B:858:ILE:HD11	2:B:874:TYR:HA	1.87	0.56
1:A:771:PHE:HZ	1:A:781:LEU:HD21	1.70	0.56
11:K:104:ARG:NH2	11:K:106:GLN:OE1	2.35	0.56
1:A:65:CYS:HB3	1:A:75:HIS:CE1	2.41	0.56
1:A:811:SER:OG	1:A:815:ARG:NH1	2.32	0.56
2:B:825:PHE:HA	2:B:861:TYR:HB3	1.87	0.56
4:D:83:SER:HA	4:D:86:ILE:HG12	1.87	0.56
1:A:244:ARG:NH1	1:A:246:ASP:OD1	2.39	0.56
1:A:1306:TYR:HE2	9:I:60:LEU:HD22	1.70	0.56
2:B:415:GLU:HG3	2:B:476:LEU:HD21	1.86	0.56
5:E:81:GLU:HB3	5:E:110:PHE:HD1	1.71	0.56
13:M:57:ASN:ND2	13:M:60:LEU:HB2	2.21	0.56
2:B:535:ASP:OD1	2:B:536:GLY:N	2.38	0.56
12:L:48:CYS:N	12:L:53:HIS:O	2.39	0.56
3:C:133:VAL:HG21	3:C:172:GLN:HE21	1.70	0.55
4:D:80:THR:OG1	4:D:81:ASN:N	2.38	0.55
2:B:337:VAL:O	2:B:339:GLN:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:114:THR:HG23	3:C:130:ASN:HB3	1.88	0.55
5:E:143:ASN:OD1	5:E:145:THR:OG1	2.25	0.55
1:A:628:PHE:HD2	2:B:784:ASP:HB2	1.71	0.55
1:A:1657:LEU:HB2	6:F:133:VAL:HB	1.88	0.55
2:B:335:ARG:NH2	2:B:346:ASP:OD1	2.30	0.55
6:F:109:VAL:HG21	6:F:123:LYS:HG2	1.88	0.55
1:A:1176:ARG:HH21	6:F:154:ASP:HA	1.71	0.55
11:K:110:GLU:HG2	11:K:111:THR:HG23	1.88	0.55
2:B:547:HIS:CE1	2:B:548:LYS:HG2	2.42	0.55
2:B:1015:SER:OG	2:B:1018:THR:OG1	2.21	0.55
1:A:339:PHE:O	1:A:340:HIS:ND1	2.40	0.55
1:A:672:ASP:CG	2:B:950:ASN:HD21	2.15	0.55
7:G:228:LYS:HB3	7:G:230:ARG:HH12	1.71	0.55
9:I:26:SER:H	9:I:39:LYS:HD3	1.71	0.55
1:A:410:LYS:HZ1	1:A:413:LEU:HD12	1.72	0.55
2:B:145:VAL:HG21	2:B:441:LYS:HG2	1.89	0.55
1:A:1530:TRP:HZ3	5:E:139:ALA:HA	1.72	0.55
1:A:1557:ALA:O	1:A:1561:THR:OG1	2.25	0.55
2:B:967:LEU:HD23	2:B:996:PHE:HB2	1.89	0.55
1:A:590:ASN:OD1	1:A:592:GLN:NE2	2.40	0.54
2:B:134:ARG:NE	2:B:160:GLY:O	2.36	0.54
2:B:681:ILE:HD11	2:B:689:VAL:HG21	1.89	0.54
3:C:114:THR:OG1	3:C:115:TRP:N	2.32	0.54
1:A:32:ILE:HG22	1:A:390:LEU:HD22	1.89	0.54
1:A:1654:PHE:HZ	6:F:92:ARG:HB3	1.72	0.54
1:A:618:TYR:CE1	2:B:783:MET:HB2	2.43	0.54
2:B:48:SER:HB3	2:B:404:LEU:HB3	1.89	0.54
2:B:252:TYR:HA	2:B:258:VAL:HG12	1.90	0.54
2:B:883:GLU:OE1	2:B:906:ARG:NH1	2.37	0.54
2:B:1010:ASN:HB3	2:B:1025:ASP:HB2	1.88	0.54
1:A:720:PHE:CE1	8:H:98:TYR:HB2	2.37	0.54
2:B:545:PHE:CE2	2:B:551:ILE:HD11	2.42	0.54
13:M:59:ARG:HA	13:M:103:LYS:HB2	1.89	0.54
1:A:627:ASP:OD1	1:A:627:ASP:N	2.41	0.54
1:A:1560:ASN:ND2	5:E:149:LEU:O	2.41	0.54
2:B:129:ARG:HG2	2:B:888:ILE:HG23	1.89	0.54
2:B:547:HIS:HE1	2:B:695:ASN:HA	1.72	0.54
6:F:135:ARG:NH2	7:G:92:ALA:O	2.37	0.54
2:B:808:LYS:HE3	2:B:810:ASP:HB2	1.88	0.54
1:A:1:MET:N	2:B:1094:ASN:O	2.39	0.54
1:A:1478:ALA:HB1	9:I:21:ASN:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:93:ILE:HD11	6:F:134:ILE:HG22	1.89	0.53
2:B:625:GLU:OE1	2:B:648:ARG:NH1	2.41	0.53
2:B:651:ARG:NH2	2:B:669:GLN:OE1	2.41	0.53
3:C:191:ILE:HD11	10:J:5:VAL:HG22	1.90	0.53
12:L:47:ARG:HA	12:L:54:ARG:HA	1.90	0.53
13:M:31:ARG:HE	14:N:129:ALA:HB2	1.74	0.53
1:A:121:LYS:HB3	1:A:219:LEU:HD21	1.90	0.53
1:A:117:ARG:HB2	1:A:185:ARG:NH1	2.24	0.53
14:N:148:ILE:HD12	14:N:148:ILE:H	1.74	0.53
15:R:6:U:H2'	15:R:7:C:C6	2.44	0.53
2:B:307:GLU:OE2	2:B:311:ARG:NE	2.35	0.53
2:B:480:GLN:NE2	2:B:483:GLY:O	2.41	0.53
2:B:672:MET:HE3	2:B:674:ILE:HD11	1.90	0.53
2:B:694:THR:OG1	2:B:702:ASN:OD1	2.25	0.53
11:K:81:MET:HE2	11:K:81:MET:HA	1.91	0.53
1:A:12:THR:HB	2:B:1201:GLU:HG2	1.91	0.53
1:A:850:SER:HA	1:A:853:THR:HB	1.89	0.53
2:B:26:ILE:HG21	3:C:151:THR:HG23	1.90	0.53
13:M:105:SER:HA	13:M:108:LEU:HD23	1.90	0.53
2:B:277:LEU:HD21	2:B:374:LEU:HB3	1.91	0.53
5:E:180:ARG:NH1	5:E:192:ARG:HG3	2.24	0.53
1:A:588:LEU:HD21	2:B:1087:LEU:HD21	1.91	0.53
14:N:113:SER:HB2	14:N:120:LYS:HD3	1.90	0.53
1:A:113:VAL:HG11	1:A:178:LEU:HD22	1.90	0.53
1:A:634:ASN:HB3	2:B:1069:ILE:HD12	1.90	0.53
1:A:1613:MET:HB3	1:A:1618:THR:HG23	1.89	0.53
3:C:248:GLN:NE2	3:C:256:ILE:O	2.42	0.53
15:R:5:A:H2'	15:R:6:U:C6	2.44	0.53
1:A:460:LEU:HA	1:A:466:LEU:H	1.74	0.52
1:A:942:GLN:HB2	1:A:947:LEU:HD23	1.91	0.52
1:A:1218:GLY:H	1:A:1569:VAL:HG23	1.73	0.52
2:B:985:ILE:O	14:N:157:ARG:NH1	2.40	0.52
1:A:509:GLU:HG3	1:A:579:ARG:HE	1.74	0.52
1:A:1237:GLN:H	1:A:1544:ASN:HB3	1.73	0.52
1:A:1589:MET:HB3	1:A:1598:PHE:HE1	1.72	0.52
1:A:653:THR:OG1	1:A:667:ARG:NH1	2.43	0.52
14:N:63:ASP:OD2	14:N:65:SER:OG	2.24	0.52
1:A:611:GLU:HB2	2:B:913:ILE:HG23	1.91	0.52
2:B:252:TYR:HB2	2:B:381:LEU:HD21	1.91	0.52
2:B:727:GLY:HA2	2:B:744:LEU:HB2	1.91	0.52
3:C:41:GLU:HA	11:K:134:LYS:HE2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:848:ILE:O	12:L:60:ARG:NH1	2.42	0.52
9:I:53:ASP:OD1	9:I:61:ARG:NH1	2.42	0.52
1:A:872:ASP:OD2	1:A:875:LEU:N	2.40	0.52
1:A:1330:VAL:HG11	1:A:1455:ARG:HH22	1.74	0.52
1:A:1053:ASP:OD1	1:A:1053:ASP:N	2.40	0.52
2:B:854:GLU:OE2	2:B:876:SER:N	2.39	0.52
5:E:161:LYS:HD2	5:E:195:VAL:HG22	1.91	0.52
1:A:124:LEU:HG	1:A:189:VAL:HG13	1.92	0.52
1:A:1183:GLU:OE2	6:F:88:TYR:OH	2.17	0.52
16:S:33:DC:H2"	16:S:34:DG:C8	2.45	0.52
1:A:966:LEU:HB2	1:A:969:PHE:HD2	1.74	0.52
1:A:1541:ILE:O	5:E:147:HIS:NE2	2.39	0.52
6:F:111:LEU:HD22	6:F:120:ILE:HD13	1.92	0.52
1:A:1038:ILE:HD11	1:A:1047:GLN:HB2	1.90	0.52
1:A:1600:ARG:NH1	1:A:1616:GLU:OE2	2.41	0.52
2:B:679:GLN:HG2	14:N:157:ARG:HB2	1.92	0.52
1:A:1103:LYS:O	1:A:1107:LYS:HG2	2.10	0.51
1:A:1256:LYS:O	1:A:1499:ARG:NH2	2.43	0.51
2:B:239:VAL:HG22	2:B:245:SER:HB2	1.92	0.51
8:H:80:ARG:HG2	8:H:81:PRO:HD2	1.91	0.51
1:A:518:GLU:OE2	1:A:584:ARG:NH2	2.43	0.51
1:A:595:LEU:HD13	1:A:1198:THR:HG21	1.91	0.51
2:B:936:MET:HE3	2:B:937:PRO:HD2	1.92	0.51
1:A:37:VAL:HG12	1:A:49:LEU:HB2	1.91	0.51
2:B:16:PHE:HZ	2:B:751:ILE:HG12	1.75	0.51
10:J:14:VAL:HA	10:J:17:LYS:HD2	1.93	0.51
1:A:1296:PHE:HZ	1:A:1317:ILE:HD11	1.76	0.51
2:B:543:ASN:OD1	2:B:543:ASN:N	2.44	0.51
7:G:121:ASN:OD1	7:G:121:ASN:N	2.42	0.51
1:A:79:ILE:HG23	1:A:360:LEU:HB2	1.91	0.51
1:A:388:LYS:O	1:A:391:THR:OG1	2.24	0.51
2:B:709:PHE:HB3	2:B:960:ILE:HB	1.93	0.51
1:A:1580:ARG:HE	5:E:204:THR:HG21	1.75	0.51
2:B:600:GLN:O	2:B:604:ILE:HG12	2.11	0.51
3:C:312:GLU:HG2	3:C:316:LYS:HZ2	1.74	0.51
3:C:128:ASP:OD1	3:C:174:ARG:NH1	2.44	0.51
17:T:18:DC:H2'	17:T:19:DT:C6	2.45	0.51
1:A:826:PHE:HB3	2:B:777:SER:HB3	1.93	0.51
1:A:1217:LEU:HD13	1:A:1572:ARG:HD2	1.92	0.51
2:B:143:TRP:HB3	2:B:152:LEU:HB2	1.93	0.51
2:B:212:ASN:HB3	2:B:590:GLY:HA3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:38:PHE:O	14:N:118:SER:OG	2.25	0.51
14:N:111:VAL:HG22	14:N:112:PRO:HD2	1.92	0.51
2:B:42:VAL:HG21	2:B:190:ILE:HD12	1.93	0.51
1:A:1243:TRP:NE1	1:A:1533:GLU:O	2.34	0.51
3:C:192:LEU:HD21	3:C:195:LYS:HE3	1.91	0.51
6:F:64:ILE:HA	6:F:67:LYS:HE3	1.92	0.51
1:A:1057:ILE:HD11	1:A:1580:ARG:HD2	1.92	0.50
1:A:1130:ALA:HB1	6:F:82:THR:HG23	1.92	0.50
1:A:1221:ARG:HE	1:A:1225:ILE:HD11	1.76	0.50
1:A:1275:THR:O	1:A:1289:SER:N	2.45	0.50
2:B:502:MET:HE3	2:B:542:LEU:HD21	1.93	0.50
2:B:703:LEU:HD11	2:B:762:MET:SD	2.51	0.50
2:B:919:SER:OG	2:B:920:ARG:N	2.44	0.50
5:E:137:GLU:HA	5:E:140:LEU:HB2	1.91	0.50
7:G:135:GLY:HA3	7:G:149:ILE:HG23	1.93	0.50
1:A:708:THR:HB	1:A:742:PRO:HD3	1.94	0.50
1:A:752:LYS:HE2	1:A:768:GLU:HB3	1.94	0.50
1:A:1007:ILE:HG21	2:B:515:THR:HG23	1.91	0.50
2:B:655:TYR:O	2:B:659:ASP:HA	2.10	0.50
1:A:1258:ILE:HD11	1:A:1532:GLN:HE22	1.76	0.50
1:A:1478:ALA:O	9:I:21:ASN:ND2	2.45	0.50
3:C:69:ARG:HB2	11:K:71:THR:HG23	1.94	0.50
17:T:2:DT:H2"	17:T:3:DA:C8	2.46	0.50
1:A:568:VAL:O	1:A:571:HIS:ND1	2.41	0.50
1:A:701:ARG:NH1	11:K:94:PRO:HA	2.27	0.50
2:B:121:VAL:HG12	2:B:133:TYR:CE1	2.46	0.50
2:B:1132:SER:HA	2:B:1169:GLY:HA3	1.92	0.50
6:F:73:ALA:HB2	7:G:94:PRO:HG2	1.92	0.50
1:A:882:ILE:HG12	1:A:888:LYS:HB3	1.94	0.50
1:A:1053:ASP:HB2	1:A:1055:ILE:HG13	1.94	0.50
5:E:154:ILE:HG13	5:E:197:LYS:HB3	1.94	0.50
1:A:135:LYS:HE3	1:A:188:TYR:HE1	1.77	0.50
1:A:697:TYR:HB2	11:K:88:PHE:CZ	2.46	0.50
1:A:1040:ASP:OD1	1:A:1041:ALA:N	2.43	0.50
2:B:572:PRO:O	2:B:576:THR:OG1	2.22	0.50
2:B:697:LEU:HD12	2:B:701:ALA:HB1	1.94	0.50
2:B:946:ASP:OD1	2:B:946:ASP:N	2.30	0.50
5:E:155:ARG:NH1	5:E:194:GLU:OE1	2.45	0.50
1:A:368:ARG:HD3	1:A:382:GLN:HG2	1.94	0.50
1:A:1553:TYR:CZ	5:E:147:HIS:HD2	2.29	0.50
2:B:679:GLN:OE1	2:B:679:GLN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:19:VAL:HA	5:E:22:MET:HE2	1.94	0.50
2:B:168:ASN:OD1	2:B:169:ARG:N	2.45	0.49
11:K:89:CYS:SG	11:K:90:GLY:N	2.83	0.49
1:A:956:ARG:NH2	1:A:979:GLY:HA3	2.26	0.49
8:H:117:SER:HA	8:H:122:LEU:HA	1.94	0.49
11:K:87:GLU:HB2	11:K:108:TYR:CZ	2.47	0.49
1:A:1032:VAL:HG21	1:A:1179:ILE:HD12	1.94	0.49
2:B:292:ILE:HD12	2:B:306:LEU:HD21	1.94	0.49
2:B:469:ASN:OD1	2:B:470:LEU:N	2.45	0.49
3:C:196:LEU:O	3:C:197:ARG:NH1	2.42	0.49
3:C:278:GLU:OE2	3:C:281:ARG:NH1	2.45	0.49
14:N:94:ASP:O	14:N:96:GLU:N	2.42	0.49
2:B:492:ASN:ND2	2:B:494:TYR:HB2	2.26	0.49
2:B:1010:ASN:HB3	2:B:1025:ASP:CB	2.43	0.49
3:C:132:ILE:HD11	3:C:179:PHE:HE2	1.76	0.49
6:F:92:ARG:O	6:F:96:THR:OG1	2.27	0.49
1:A:1589:MET:HE2	1:A:1595:TYR:HE1	1.76	0.49
2:B:525:TRP:HB3	2:B:669:GLN:HE22	1.78	0.49
1:A:27:LEU:HD11	2:B:1112:THR:HG22	1.94	0.49
1:A:702:PRO:HD3	1:A:712:ILE:HD11	1.95	0.49
1:A:746:GLY:HA3	1:A:774:GLY:N	2.27	0.49
2:B:887:LEU:HB2	12:L:56:LEU:HB2	1.95	0.49
4:D:89:LEU:HD13	7:G:82:LEU:HD21	1.95	0.49
1:A:992:PRO:HG3	2:B:984:TRP:CD2	2.47	0.49
2:B:862:PHE:HA	2:B:869:THR:HA	1.94	0.49
2:B:140:LYS:HB3	2:B:155:VAL:HG12	1.95	0.49
2:B:670:VAL:HG23	2:B:671:TYR:CD1	2.47	0.49
3:C:70:ILE:HD13	3:C:321:LEU:HB2	1.94	0.49
9:I:10:CYS:HB3	9:I:15:ASP:H	1.78	0.49
2:B:1025:ASP:OD1	2:B:1025:ASP:N	2.45	0.48
16:S:7:DA:H2'	16:S:8:DT:H71	1.94	0.48
2:B:106:LYS:HE2	2:B:171:HIS:HD2	1.78	0.48
2:B:890:ASP:O	12:L:47:ARG:NH2	2.46	0.48
17:T:12:DC:H2''	17:T:13:DA:C8	2.48	0.48
1:A:115:VAL:HG13	1:A:334:VAL:HG21	1.95	0.48
1:A:677:GLY:O	1:A:681:THR:OG1	2.31	0.48
1:A:961:VAL:HG21	2:B:636:GLN:HB2	1.94	0.48
2:B:292:ILE:O	2:B:379:ARG:NH1	2.36	0.48
2:B:1105:ARG:HG3	2:B:1200:VAL:HG21	1.95	0.48
7:G:40:ARG:HG2	7:G:123:TYR:HD1	1.79	0.48
11:K:69:ASP:N	11:K:69:ASP:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:PRO:HG3	1:A:618:TYR:HE2	1.78	0.48
1:A:657:TYR:CE1	1:A:665:PRO:HB3	2.48	0.48
1:A:1025:LYS:HG2	1:A:1615:TYR:CD1	2.49	0.48
1:A:1122:PRO:HD3	5:E:207:ARG:NH1	2.29	0.48
1:A:1312:GLU:O	1:A:1316:VAL:HG23	2.14	0.48
2:B:662:ASP:OD1	2:B:663:ILE:N	2.46	0.48
2:B:824:HIS:NE2	2:B:864:ASP:OD2	2.46	0.48
2:B:1010:ASN:ND2	2:B:1025:ASP:O	2.45	0.48
16:S:37:DA:H2''	16:S:38:DG:C8	2.49	0.48
1:A:13:SER:OG	1:A:14:VAL:N	2.47	0.48
1:A:31:GLN:HG2	1:A:78:HIS:CE1	2.48	0.48
1:A:840:ASN:O	1:A:844:THR:OG1	2.28	0.48
2:B:359:LEU:HD21	2:B:374:LEU:HD13	1.95	0.48
2:B:987:ASN:ND2	14:N:157:ARG:HH21	2.10	0.48
2:B:1195:ARG:HH22	2:B:1197:ARG:HH11	1.61	0.48
7:G:138:PHE:HB2	7:G:147:LEU:HA	1.95	0.48
1:A:1533:GLU:HB2	5:E:14:ARG:HH12	1.78	0.48
3:C:80:ALA:HA	3:C:208:CYS:HA	1.95	0.48
6:F:93:ILE:HG13	6:F:132:LEU:HD22	1.95	0.48
1:A:592:GLN:NE2	2:B:1075:GLU:OE2	2.42	0.48
3:C:163:TYR:N	3:C:166:ASP:OD2	2.46	0.48
1:A:103:LEU:HD12	1:A:106:HIS:CD2	2.49	0.48
1:A:506:THR:OG1	1:A:507:TYR:N	2.47	0.48
1:A:1131:LYS:HG2	6:F:83:PRO:HD3	1.95	0.48
2:B:521:LEU:HB3	2:B:523:GLU:OE1	2.14	0.48
2:B:916:LYS:HG2	2:B:926:VAL:HG12	1.94	0.48
1:A:211:THR:OG1	5:E:173:SER:HB2	2.13	0.48
2:B:238:SER:HB3	2:B:361:HIS:H	1.79	0.48
3:C:229:LEU:HB2	3:C:293:ARG:HD3	1.95	0.48
5:E:78:LEU:HD12	5:E:107:THR:HB	1.95	0.48
16:S:24:DT:H2''	16:S:25:DC:H5''	1.95	0.48
1:A:1450:ILE:HG23	1:A:1454:HIS:CE1	2.49	0.47
2:B:493:PHE:O	2:B:497:ILE:HG22	2.14	0.47
5:E:31:THR:HG22	5:E:33:GLU:H	1.79	0.47
2:B:881:TYR:O	2:B:906:ARG:N	2.41	0.47
2:B:987:ASN:OD1	2:B:990:ASP:N	2.46	0.47
15:R:6:U:H2'	15:R:7:C:H6	1.79	0.47
1:A:47:GLY:N	1:A:51:ASP:OD2	2.39	0.47
1:A:579:ARG:HH22	1:A:585:ASP:CG	2.22	0.47
2:B:991:THR:HG22	2:B:993:ALA:H	1.78	0.47
1:A:846:ILE:HB	1:A:907:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:684:ASN:OD1	14:N:150:TYR:OH	2.30	0.47
5:E:20:LYS:HB3	5:E:35:VAL:HG22	1.96	0.47
1:A:730:GLN:O	1:A:734:THR:HG22	2.15	0.47
2:B:673:ASN:HB2	2:B:686:HIS:HA	1.96	0.47
3:C:87:ASN:OD1	3:C:88:ASN:N	2.47	0.47
11:K:112:THR:HG22	11:K:114:VAL:H	1.79	0.47
1:A:102:CYS:SG	1:A:104:PHE:HB2	2.55	0.47
1:A:643:ALA:HB1	2:B:1087:LEU:HD12	1.97	0.47
1:A:32:ILE:HD11	1:A:54:LEU:HD11	1.97	0.47
1:A:410:LYS:NZ	1:A:413:LEU:HD12	2.29	0.47
1:A:589:MET:HE3	1:A:633:MET:HE2	1.96	0.47
1:A:657:TYR:HD1	1:A:658:LEU:HG	1.80	0.47
1:A:980:GLY:HA2	1:A:997:PHE:CD2	2.50	0.47
1:A:1000:MET:HG2	2:B:520:LEU:HB3	1.97	0.47
1:A:1305:GLU:HG3	9:I:60:LEU:HD13	1.95	0.47
2:B:851:TYR:CE1	2:B:853:GLU:HG3	2.49	0.47
2:B:861:TYR:HE2	2:B:872:LYS:HE2	1.80	0.47
5:E:25:ASP:OD2	5:E:152:LYS:NZ	2.31	0.47
8:H:93:TYR:HA	8:H:145:ARG:HB2	1.95	0.47
13:M:38:PHE:HB2	14:N:119:LEU:HB2	1.95	0.47
1:A:20:THR:O	1:A:23:GLU:HG2	2.14	0.47
1:A:1128:ASN:HD21	6:F:80:ALA:HB1	1.79	0.47
2:B:492:ASN:OD1	2:B:493:PHE:N	2.48	0.47
2:B:630:PRO:HD2	2:B:671:TYR:CE2	2.49	0.47
1:A:1539:ASP:O	5:E:147:HIS:ND1	2.47	0.47
1:A:1542:THR:HG23	5:E:149:LEU:HD22	1.97	0.47
2:B:404:LEU:HD13	2:B:404:LEU:HA	1.79	0.47
1:A:532:GLY:O	1:A:580:HIS:N	2.45	0.47
1:A:697:TYR:HB2	11:K:88:PHE:CE1	2.50	0.47
1:A:1485:MET:H	1:A:1488:ILE:HD11	1.80	0.47
2:B:181:VAL:HG22	2:B:187:SER:HA	1.97	0.47
2:B:747:GLY:HA3	2:B:766:PRO:HB2	1.96	0.47
13:M:74:ASN:OD1	13:M:74:ASN:N	2.48	0.47
1:A:118:TYR:OH	1:A:222:GLU:OE1	2.26	0.46
1:A:591:ARG:HG2	1:A:633:MET:HB3	1.97	0.46
2:B:129:ARG:HG2	2:B:888:ILE:HD12	1.97	0.46
8:H:90:ALA:HA	8:H:143:LEU:HD23	1.98	0.46
2:B:71:LYS:HE3	2:B:71:LYS:HB3	1.72	0.46
4:D:24:ALA:HA	7:G:43:ILE:HG22	1.96	0.46
4:D:91:ARG:HD2	7:G:152:ALA:HB2	1.98	0.46
6:F:72:LYS:HD2	6:F:141:GLY:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:82:THR:O	6:F:136:ARG:NH1	2.38	0.46
12:L:54:ARG:H	12:L:54:ARG:HE	1.61	0.46
1:A:123:ARG:NH1	1:A:190:ASP:OD1	2.47	0.46
1:A:636:HIS:HB3	2:B:1091:ARG:HD2	1.97	0.46
1:A:986:PHE:HB3	2:B:960:ILE:HG13	1.96	0.46
1:A:1222:LEU:O	1:A:1226:VAL:HG12	2.16	0.46
2:B:703:LEU:HD21	2:B:762:MET:HE1	1.98	0.46
3:C:109:ASP:H	3:C:112:MET:HE2	1.81	0.46
12:L:34:CYS:SG	12:L:36:SER:OG	2.56	0.46
1:A:1657:LEU:HD12	7:G:104:LEU:HB3	1.97	0.46
5:E:15:ALA:O	5:E:19:VAL:HG23	2.15	0.46
1:A:2:ASP:HB3	1:A:5:LYS:HG2	1.98	0.46
1:A:618:TYR:CD1	1:A:670:ILE:HD11	2.50	0.46
1:A:1049:MET:N	5:E:208:TYR:OH	2.48	0.46
7:G:41:VAL:HG12	7:G:43:ILE:HG23	1.97	0.46
7:G:73:TYR:CD1	7:G:238:THR:HG21	2.50	0.46
13:M:82:ASN:ND2	13:M:87:SER:O	2.49	0.46
1:A:1289:SER:HA	1:A:1475:GLU:HG3	1.96	0.46
2:B:578:ALA:HB1	2:B:583:LEU:HD12	1.97	0.46
3:C:272:LYS:HD2	14:N:175:TYR:CD2	2.50	0.46
11:K:57:ASP:OD1	11:K:57:ASP:N	2.46	0.46
13:M:22:ALA:HB3	14:N:110:LEU:HD12	1.97	0.46
1:A:31:GLN:HG2	1:A:78:HIS:HE1	1.81	0.46
1:A:96:ILE:HG23	1:A:228:LEU:HD11	1.98	0.46
1:A:191:MET:HE3	1:A:195:LYS:HB2	1.98	0.46
2:B:621:PRO:HG2	2:B:624:LEU:HB2	1.97	0.46
2:B:669:GLN:HA	2:B:672:MET:HE2	1.97	0.46
2:B:1025:ASP:OD2	3:C:277:ARG:NH1	2.48	0.46
2:B:182:GLN:HA	2:B:182:GLN:HE21	1.81	0.46
6:F:75:PRO:HA	7:G:95:LEU:HD13	1.97	0.46
1:A:135:LYS:HE3	1:A:188:TYR:CE1	2.51	0.46
1:A:202:THR:HG23	1:A:207:SER:HB2	1.97	0.46
1:A:673:HIS:CD2	2:B:783:MET:HE1	2.51	0.46
1:A:938:VAL:O	1:A:942:GLN:HG2	2.16	0.46
1:A:1010:ALA:O	1:A:1013:THR:OG1	2.34	0.46
1:A:1068:PHE:O	1:A:1072:ASN:ND2	2.32	0.46
2:B:301:PHE:CE1	2:B:386:ALA:HB2	2.50	0.46
2:B:1165:ASN:OD1	2:B:1166:LYS:N	2.48	0.46
5:E:16:PHE:CD2	5:E:42:PHE:HE2	2.34	0.46
5:E:52:ARG:O	5:E:55:ARG:HG3	2.15	0.46
7:G:95:LEU:H	7:G:95:LEU:HG	1.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:111:VAL:HG11	14:N:122:ALA:HB2	1.98	0.46
1:A:440:SER:OG	1:A:455:GLY:N	2.49	0.46
2:B:1047:ARG:HD2	2:B:1067:GLY:O	2.16	0.46
1:A:1101:THR:HG23	1:A:1120:TYR:HB3	1.99	0.45
1:A:1121:ASP:OD1	1:A:1121:ASP:N	2.48	0.45
2:B:18:THR:O	2:B:22:GLU:HG2	2.16	0.45
2:B:260:PHE:CZ	2:B:358:VAL:HG12	2.51	0.45
2:B:629:VAL:HB	2:B:638:PRO:HA	1.98	0.45
2:B:1055:LEU:HD23	2:B:1055:LEU:H	1.81	0.45
3:C:101:ILE:O	3:C:104:VAL:HG22	2.16	0.45
14:N:91:ASP:OD1	14:N:91:ASP:N	2.46	0.45
1:A:94:LEU:HD12	1:A:355:PHE:HB3	1.99	0.45
1:A:415:ASP:O	1:A:419:ILE:HG23	2.16	0.45
1:A:826:PHE:CE2	2:B:952:HIS:HE1	2.34	0.45
1:A:1057:ILE:O	1:A:1060:GLU:HG3	2.15	0.45
1:A:1258:ILE:HD11	1:A:1532:GLN:NE2	2.32	0.45
1:A:1277:GLY:HA3	9:I:43:SER:O	2.16	0.45
2:B:119:ARG:NH1	2:B:125:GLU:OE1	2.46	0.45
2:B:861:TYR:CE1	2:B:870:LYS:HB3	2.51	0.45
3:C:257:GLY:HA3	3:C:268:LYS:HE3	1.98	0.45
9:I:52:ALA:C	9:I:54:ASP:H	2.24	0.45
11:K:104:ARG:O	11:K:105:ILE:HD13	2.16	0.45
12:L:54:ARG:H	12:L:54:ARG:NE	2.13	0.45
1:A:27:LEU:O	2:B:1129:ARG:NH2	2.45	0.45
1:A:1482:LYS:HD2	2:B:307:GLU:HG2	1.99	0.45
1:A:1573:TYR:HB2	1:A:1575:ILE:HG13	1.98	0.45
2:B:692:THR:HB	2:B:694:THR:HG22	1.98	0.45
5:E:66:GLU:CD	5:E:66:GLU:H	2.24	0.45
8:H:116:TYR:CE1	8:H:140:ALA:HB3	2.52	0.45
10:J:7:CYS:HA	10:J:49:MET:SD	2.57	0.45
1:A:88:PRO:HD2	1:A:438:ILE:HD12	1.99	0.45
1:A:378:HIS:O	1:A:378:HIS:ND1	2.49	0.45
1:A:628:PHE:CD2	2:B:784:ASP:HB2	2.49	0.45
1:A:657:TYR:HA	1:A:667:ARG:HD3	1.98	0.45
1:A:703:GLU:OE2	11:K:102:ASN:ND2	2.50	0.45
2:B:420:TYR:O	2:B:424:ILE:HG23	2.16	0.45
3:C:172:GLN:H	3:C:175:GLN:HB2	1.82	0.45
1:A:107:HIS:CE1	1:A:330:LYS:HB3	2.51	0.45
1:A:498:PRO:HG3	1:A:613:THR:O	2.16	0.45
2:B:164:MET:HE3	2:B:192:GLY:HA2	1.97	0.45
5:E:169:ARG:HD2	6:F:138:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:22:LYS:O	8:H:44:VAL:HG22	2.17	0.45
13:M:38:PHE:HB3	13:M:53:LEU:HD11	1.98	0.45
1:A:1657:LEU:HD13	7:G:106:LYS:HA	1.99	0.45
2:B:172:LEU:HD22	2:B:175:MET:HE2	1.98	0.45
2:B:748:GLN:HB2	2:B:769:PHE:HA	1.97	0.45
2:B:1047:ARG:NH1	2:B:1066:HIS:O	2.50	0.45
3:C:329:LYS:HZ1	11:K:122:LYS:N	2.14	0.45
5:E:156:LEU:HG	5:E:160:GLU:HG3	1.99	0.45
14:N:91:ASP:HA	14:N:137:PHE:HA	1.99	0.45
14:N:118:SER:OG	14:N:119:LEU:N	2.50	0.45
1:A:479:ALA:HB1	2:B:1069:ILE:HD11	1.97	0.45
1:A:1018:TYR:HA	1:A:1021:ARG:HG2	1.99	0.45
1:A:1497:ILE:HD12	1:A:1500:GLN:HB3	1.98	0.45
2:B:143:TRP:CE2	2:B:446:MET:HG2	2.52	0.45
2:B:122:TYR:O	2:B:125:GLU:HB3	2.16	0.45
2:B:726:MET:HG3	2:B:742:TYR:HB3	1.99	0.45
1:A:31:GLN:HA	1:A:78:HIS:O	2.17	0.45
1:A:524:ILE:O	1:A:554:ARG:NH2	2.50	0.45
1:A:1033:SER:OG	1:A:1037:SER:O	2.33	0.45
1:A:1538:VAL:HG11	5:E:142:VAL:HG21	1.98	0.45
1:A:108:PHE:HB3	1:A:227:LEU:HD11	1.98	0.45
1:A:799:GLU:OE1	1:A:1061:SER:OG	2.22	0.45
2:B:338:PHE:CE2	2:B:353:VAL:HG22	2.52	0.45
2:B:968:ALA:HB2	2:B:996:PHE:CE2	2.52	0.45
4:D:27:LEU:HD23	6:F:55:PRO:HG2	1.98	0.45
10:J:14:VAL:HB	10:J:50:ILE:HD11	1.97	0.45
13:M:42:LYS:NZ	14:N:32:CYS:HB3	2.32	0.45
1:A:24:ILE:O	1:A:28:SER:N	2.38	0.44
2:B:323:ARG:HA	2:B:326:VAL:HG22	1.99	0.44
3:C:71:MET:HG3	3:C:313:ILE:HG22	1.98	0.44
1:A:358:ASP:OD1	1:A:359:VAL:N	2.50	0.44
1:A:589:MET:HE3	1:A:589:MET:HB3	1.90	0.44
1:A:900:VAL:HG21	1:A:949:GLN:HE21	1.82	0.44
2:B:236:ILE:HG12	2:B:237:ARG:O	2.18	0.44
2:B:404:LEU:HD11	2:B:551:ILE:HG21	1.99	0.44
2:B:711:GLN:HG3	2:B:958:MET:HB2	1.99	0.44
2:B:912:GLN:NE2	2:B:1041:ASN:HD21	2.14	0.44
3:C:260:GLU:OE1	3:C:260:GLU:N	2.45	0.44
5:E:62:ALA:HB3	5:E:78:LEU:HB3	2.00	0.44
7:G:228:LYS:HB3	7:G:230:ARG:NH1	2.32	0.44
11:K:48:LYS:HD2	11:K:48:LYS:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:HIS:CE1	2:B:322:ASN:HB2	2.52	0.44
3:C:41:GLU:HG2	3:C:57:ILE:HB	1.99	0.44
7:G:49:LEU:N	7:G:114:GLY:O	2.42	0.44
9:I:12:ASP:HB3	13:M:60:LEU:HD11	1.99	0.44
13:M:9:GLU:OE1	13:M:9:GLU:N	2.51	0.44
13:M:103:LYS:HD2	13:M:106:LYS:HD3	1.99	0.44
1:A:754:LYS:HG3	1:A:784:SER:OG	2.17	0.44
1:A:797:LEU:HD13	1:A:809:VAL:HG21	2.00	0.44
2:B:71:LYS:HE3	2:B:425:ILE:HD12	2.00	0.44
2:B:581:PRO:HG3	2:B:637:TYR:CE1	2.51	0.44
10:J:4:PRO:HG2	10:J:49:MET:HE1	2.00	0.44
10:J:36:LEU:HD11	10:J:51:LEU:HB2	1.99	0.44
1:A:127:TYR:HD2	1:A:202:THR:HG21	1.82	0.44
1:A:1038:ILE:HD12	1:A:1584:LEU:HD13	1.99	0.44
1:A:1196:PRO:HB3	1:A:1575:ILE:HG21	2.00	0.44
1:A:1314:GLN:NE2	1:A:1462:PHE:HB3	2.33	0.44
2:B:953:ALA:O	2:B:957:ARG:HB2	2.18	0.44
3:C:229:LEU:HB2	3:C:293:ARG:HH11	1.82	0.44
5:E:63:ASN:OD1	5:E:77:SER:OG	2.22	0.44
1:A:496:GLY:O	1:A:614:LEU:HA	2.18	0.44
2:B:106:LYS:O	2:B:108:MET:HG2	2.18	0.44
2:B:1092:LEU:HD13	2:B:1092:LEU:HA	1.77	0.44
3:C:82:TYR:CD2	3:C:126:PHE:HZ	2.36	0.44
9:I:2:SER:HB2	9:I:9:PHE:O	2.18	0.44
15:R:9:A:H2'	15:R:10:G:O4'	2.18	0.44
1:A:597:LYS:HE2	1:A:660:PRO:HG3	1.99	0.44
1:A:1450:ILE:HD12	1:A:1454:HIS:HE1	1.82	0.44
2:B:49:PHE:CZ	2:B:163:VAL:HG12	2.51	0.44
2:B:499:HIS:O	2:B:502:MET:HG2	2.17	0.44
3:C:41:GLU:HG3	3:C:57:ILE:HD13	2.00	0.44
7:G:236:VAL:HG22	7:G:238:THR:HG23	2.00	0.44
1:A:966:LEU:HB2	1:A:969:PHE:CD2	2.53	0.44
1:A:1274:GLU:HB3	9:I:47:VAL:HG13	2.00	0.44
2:B:362:LEU:HD12	2:B:362:LEU:HA	1.74	0.44
2:B:830:ASP:OD2	2:B:869:THR:N	2.48	0.44
5:E:19:VAL:O	5:E:23:VAL:HG23	2.18	0.44
14:N:80:MET:HE2	14:N:80:MET:HB2	1.70	0.44
1:A:911:CYS:O	1:A:915:GLY:N	2.51	0.44
2:B:494:TYR:HB3	2:B:700:LEU:HD11	1.98	0.44
2:B:790:ASN:HB3	2:B:793:ALA:HB3	1.99	0.44
4:D:28:PRO:HB2	7:G:39:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:11:DG:H2''	16:S:12:DC:C4	2.52	0.44
1:A:509:GLU:HB3	1:A:519:LEU:HD11	1.99	0.43
1:A:676:ALA:HB2	1:A:821:ILE:HD13	2.00	0.43
2:B:28:PRO:HG2	2:B:181:VAL:HG21	2.00	0.43
2:B:697:LEU:HB3	2:B:701:ALA:HB3	1.99	0.43
1:A:697:TYR:CE1	1:A:702:PRO:HD2	2.50	0.43
2:B:306:LEU:HD23	2:B:306:LEU:HA	1.75	0.43
5:E:21:GLU:CD	5:E:146:HIS:HE2	2.26	0.43
6:F:138:LEU:HB3	6:F:139:PRO:HD2	1.99	0.43
9:I:4:VAL:O	9:I:7:LEU:HD12	2.18	0.43
1:A:14:VAL:HG13	1:A:1632:GLU:HB3	2.01	0.43
1:A:368:ARG:NH1	1:A:383:ASN:OD1	2.47	0.43
2:B:766:PRO:HG2	10:J:54:VAL:HG21	2.00	0.43
9:I:7:LEU:HB2	9:I:16:LEU:HD11	2.00	0.43
1:A:925:MET:HA	1:A:928:MET:HE2	2.00	0.43
1:A:1504:ILE:HD11	1:A:1529:MET:HE1	2.00	0.43
1:A:1619:CYS:SG	1:A:1620:GLN:N	2.92	0.43
3:C:255:VAL:HG11	3:C:273:ASP:HB2	2.00	0.43
13:M:16:GLN:OE1	13:M:18:GLN:N	2.51	0.43
17:T:4:DC:C4	17:T:5:DC:C4	3.06	0.43
1:A:336:GLN:NE2	1:A:348:LYS:O	2.52	0.43
1:A:855:ARG:HH12	1:A:867:ASP:HA	1.84	0.43
1:A:861:VAL:HG11	1:A:892:LEU:HB2	1.99	0.43
1:A:966:LEU:HD23	1:A:966:LEU:HA	1.85	0.43
2:B:144:SER:HA	2:B:151:ASN:HA	2.01	0.43
2:B:1014:TYR:OH	3:C:293:ARG:NH1	2.52	0.43
3:C:167:LEU:HD11	3:C:193:LEU:HD11	2.00	0.43
11:K:82:LYS:HA	11:K:82:LYS:HD3	1.63	0.43
13:M:40:LEU:HD22	13:M:51:PHE:HD2	1.83	0.43
16:S:35:DG:H2''	16:S:36:DT:H5'	1.99	0.43
1:A:677:GLY:HA2	1:A:817:PHE:CE1	2.53	0.43
1:A:1080:TYR:HB2	1:A:1169:LEU:HD11	2.00	0.43
2:B:193:TYR:CD2	2:B:200:GLU:HB3	2.53	0.43
2:B:1079:LEU:HD12	2:B:1079:LEU:HA	1.83	0.43
5:E:200:ARG:HB2	5:E:208:TYR:HB3	2.01	0.43
7:G:88:LYS:HE3	7:G:119:HIS:HB2	2.00	0.43
1:A:129:LEU:HD23	1:A:132:GLU:HG2	2.00	0.43
1:A:1578:SER:HB3	1:A:1581:HIS:CD2	2.54	0.43
1:A:1609:SER:O	1:A:1613:MET:HG3	2.18	0.43
2:B:323:ARG:NH2	2:B:351:GLN:OE1	2.52	0.43
2:B:602:LYS:HE3	2:B:628:TYR:HE2	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:137:ASN:OD1	3:C:137:ASN:N	2.51	0.43
7:G:45:LEU:HD12	7:G:118:CYS:HB2	2.01	0.43
8:H:56:THR:HG21	8:H:145:ARG:NH2	2.31	0.43
9:I:10:CYS:N	9:I:15:ASP:O	2.42	0.43
1:A:85:CYS:HB3	1:A:431:GLN:NE2	2.33	0.43
1:A:490:ILE:O	1:A:617:HIS:HD2	2.02	0.43
1:A:942:GLN:HB2	1:A:947:LEU:HA	2.00	0.43
1:A:1197:SER:HA	1:A:1200:MET:HG2	2.01	0.43
2:B:165:LEU:HD22	2:B:193:TYR:CZ	2.54	0.43
2:B:301:PHE:O	2:B:305:ARG:HG2	2.19	0.43
2:B:374:LEU:HD12	2:B:374:LEU:HA	1.88	0.43
7:G:81:VAL:HA	7:G:124:VAL:HG13	2.00	0.43
8:H:92:ASP:O	8:H:145:ARG:HD3	2.18	0.43
8:H:102:TYR:HE2	8:H:117:SER:HB2	1.84	0.43
1:A:368:ARG:HD2	1:A:383:ASN:OD1	2.19	0.43
1:A:1314:GLN:HB2	1:A:1462:PHE:CD2	2.53	0.43
2:B:953:ALA:O	2:B:957:ARG:HD3	2.18	0.43
3:C:119:ASN:OD1	3:C:119:ASN:N	2.52	0.43
14:N:26:PRO:HB2	14:N:29:PHE:CD1	2.54	0.43
17:T:14:DG:H2"	17:T:15:DA:C8	2.54	0.43
1:A:130:ILE:HB	5:E:215:MET:HE2	2.00	0.43
1:A:596:HIS:CE1	1:A:598:ALA:HB3	2.54	0.43
1:A:659:THR:HG23	1:A:666:VAL:HB	2.00	0.43
1:A:24:ILE:H	1:A:24:ILE:HG12	1.60	0.42
1:A:606:ARG:NH2	11:K:98:GLU:OE2	2.52	0.42
1:A:1121:ASP:HA	5:E:207:ARG:HH12	1.83	0.42
1:A:1326:GLU:HG3	1:A:1456:PHE:CZ	2.54	0.42
1:A:1482:LYS:HE2	2:B:304:ASP:HA	2.01	0.42
2:B:49:PHE:O	2:B:52:LEU:HG	2.19	0.42
2:B:125:GLU:C	2:B:127:ARG:H	2.27	0.42
5:E:124:VAL:HG13	5:E:125:PRO:HD3	2.01	0.42
5:E:128:PRO:O	5:E:130:ALA:N	2.52	0.42
8:H:33:GLN:HB2	8:H:36:CYS:HB2	2.01	0.42
1:A:357:MET:HE3	1:A:357:MET:HB2	1.84	0.42
1:A:646:GLU:OE2	1:A:1651:THR:HG21	2.18	0.42
1:A:822:THR:HG22	2:B:778:TYR:O	2.18	0.42
1:A:1180:ASN:HD22	6:F:87:LYS:H	1.67	0.42
1:A:1274:GLU:OE2	1:A:1290:TYR:OH	2.33	0.42
1:A:1495:LYS:HD3	1:A:1495:LYS:HA	1.90	0.42
2:B:131:THR:O	2:B:198:GLY:N	2.51	0.42
1:A:30:LYS:HG3	1:A:31:GLN:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ILE:HG13	1:A:362:VAL:HG11	2.01	0.42
1:A:769:VAL:HA	1:A:778:CYS:O	2.19	0.42
1:A:842:TRP:O	1:A:846:ILE:HG12	2.20	0.42
1:A:1503:HIS:HB2	1:A:1525:ASN:HB2	2.01	0.42
1:A:1609:SER:HA	1:A:1612:LYS:HE2	2.02	0.42
7:G:105:ILE:HD13	7:G:105:ILE:HA	1.85	0.42
8:H:57:VAL:HG13	8:H:142:LEU:HD11	2.00	0.42
2:B:35:PHE:HE2	2:B:764:ASN:HD21	1.66	0.42
2:B:60:LEU:HA	2:B:63:LEU:HD12	2.00	0.42
2:B:573:ALA:N	2:B:593:ILE:O	2.53	0.42
8:H:98:TYR:C	8:H:118:PHE:HD2	2.28	0.42
1:A:432:ASN:OD1	1:A:444:GLN:HG2	2.19	0.42
1:A:461:GLU:HG3	1:A:462:LYS:HG3	2.02	0.42
1:A:1042:ASP:N	1:A:1042:ASP:OD1	2.49	0.42
1:A:1046:VAL:HG12	1:A:1047:GLN:HG3	2.01	0.42
2:B:727:GLY:O	2:B:743:ARG:HA	2.18	0.42
2:B:847:TYR:CG	12:L:63:ARG:HD2	2.53	0.42
3:C:60:ASP:OD1	3:C:60:ASP:N	2.48	0.42
6:F:137:TYR:HA	6:F:142:SER:O	2.20	0.42
8:H:37:LYS:HE3	8:H:37:LYS:HB3	1.93	0.42
8:H:101:ALA:HB2	8:H:116:TYR:CZ	2.54	0.42
12:L:44:ASP:OD1	12:L:45:ALA:N	2.52	0.42
1:A:698:GLY:HA2	11:K:92:SER:HB3	2.01	0.42
1:A:827:THR:OG1	1:A:828:CYS:N	2.52	0.42
1:A:1085:LEU:HD22	6:F:152:ILE:HD12	2.00	0.42
5:E:54:GLN:N	5:E:84:ASP:HB3	2.35	0.42
1:A:1112:PRO:HB2	1:A:1114:TYR:CE1	2.55	0.42
1:A:1238:MET:SD	1:A:1524:VAL:HA	2.59	0.42
2:B:225:ARG:HH12	2:B:261:ARG:CZ	2.33	0.42
2:B:284:SER:HB2	9:I:14:GLY:O	2.20	0.42
2:B:584:CYS:N	2:B:596:VAL:O	2.47	0.42
2:B:861:TYR:CE2	2:B:872:LYS:HE2	2.55	0.42
3:C:69:ARG:HH21	11:K:71:THR:H	1.67	0.42
5:E:74:ASP:OD1	5:E:74:ASP:N	2.52	0.42
1:A:394:LEU:HD23	1:A:394:LEU:HA	1.79	0.42
1:A:589:MET:HE1	1:A:614:LEU:HD13	2.01	0.42
1:A:1032:VAL:HG22	1:A:1038:ILE:HG22	2.02	0.42
1:A:1647:ASN:HD22	1:A:1649:VAL:H	1.66	0.42
2:B:177:PRO:O	2:B:181:VAL:HG23	2.20	0.42
3:C:65:ASN:O	3:C:69:ARG:HG3	2.18	0.42
6:F:82:THR:HG22	6:F:84:TYR:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:53:VAL:O	14:N:133:PHE:HB3	2.20	0.42
1:A:342:ARG:HH21	1:A:1631:ARG:HB2	1.85	0.42
1:A:381:SER:HB3	1:A:453:ILE:HG23	2.00	0.42
1:A:471:MET:O	1:A:474:LYS:NZ	2.53	0.42
1:A:696:ILE:HD11	1:A:731:ILE:HG23	2.02	0.42
1:A:835:LEU:O	1:A:917:MET:HB3	2.20	0.42
1:A:887:ASN:O	1:A:891:ILE:HG12	2.19	0.42
1:A:1562:ILE:O	1:A:1566:ILE:HG22	2.20	0.42
2:B:354:LEU:O	2:B:358:VAL:HG22	2.20	0.42
2:B:369:ASP:HA	2:B:372:ARG:NH2	2.35	0.42
2:B:413:LEU:HB2	2:B:461:MET:HE2	2.00	0.42
16:S:34:DG:H2"	16:S:35:DG:C8	2.54	0.42
1:A:1050:TYR:OH	1:A:1581:HIS:ND1	2.53	0.42
1:A:1137:SER:OG	1:A:1138:GLU:N	2.53	0.42
2:B:609:ARG:HD2	2:B:655:TYR:CE1	2.55	0.42
2:B:830:ASP:OD1	2:B:830:ASP:N	2.52	0.42
1:A:364:PRO:HD2	1:A:367:PHE:HD2	1.85	0.41
1:A:1076:LEU:O	1:A:1079:LYS:HG2	2.21	0.41
1:A:1260:LYS:HG3	1:A:1500:GLN:HB2	2.02	0.41
1:A:1592:GLN:HB3	5:E:177:ARG:HH21	1.84	0.41
2:B:239:VAL:HA	2:B:245:SER:HA	2.02	0.41
2:B:345:SER:O	2:B:349:VAL:HG12	2.20	0.41
17:T:9:DA:H2"	17:T:10:DA:C8	2.55	0.41
1:A:552:GLU:OE1	1:A:552:GLU:N	2.52	0.41
1:A:589:MET:HB3	1:A:633:MET:HE2	2.02	0.41
2:B:533:THR:CG2	2:B:540:GLY:H	2.30	0.41
2:B:704:THR:HG23	2:B:920:ARG:O	2.20	0.41
8:H:49:VAL:HG11	8:H:55:LEU:HD11	2.02	0.41
9:I:32:GLN:O	13:M:104:SER:OG	2.38	0.41
13:M:53:LEU:HB2	13:M:96:LEU:HD22	2.03	0.41
1:A:896:THR:O	1:A:900:VAL:HG22	2.20	0.41
1:A:1162:ASN:OD1	1:A:1162:ASN:N	2.53	0.41
1:A:1314:GLN:HE22	1:A:1462:PHE:HB3	1.86	0.41
1:A:1317:ILE:HG21	1:A:1470:CYS:SG	2.60	0.41
1:A:1651:THR:OG1	2:B:1085:SER:HB3	2.19	0.41
2:B:412:ILE:HD12	2:B:470:LEU:HD12	2.01	0.41
2:B:547:HIS:CE1	2:B:695:ASN:HA	2.52	0.41
2:B:598:HIS:HB3	2:B:631:PRO:HD3	2.02	0.41
2:B:610:TYR:CG	14:N:145:ILE:HG22	2.55	0.41
2:B:650:LEU:HB3	2:B:663:ILE:HG23	2.02	0.41
6:F:79:ARG:HB3	6:F:144:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:122:LEU:HB3	7:G:124:VAL:HG23	2.02	0.41
17:T:12:DC:H2"	17:T:13:DA:H8	1.85	0.41
1:A:627:ASP:OD2	1:A:629:ASP:CG	2.45	0.41
2:B:414:LYS:O	2:B:417:ILE:HG12	2.21	0.41
2:B:975:HIS:ND1	14:N:166:LEU:HG	2.35	0.41
3:C:111:ASP:N	3:C:111:ASP:OD1	2.50	0.41
5:E:169:ARG:NH1	6:F:74:ILE:HD11	2.35	0.41
9:I:28:VAL:HG13	9:I:37:TYR:HB2	2.01	0.41
1:A:519:LEU:HD23	1:A:519:LEU:HA	1.71	0.41
1:A:920:PHE:CD1	1:A:921:PRO:HA	2.56	0.41
1:A:1042:ASP:OD1	1:A:1044:THR:HG22	2.20	0.41
1:A:1193:VAL:HG21	1:A:1585:ILE:HD12	2.03	0.41
2:B:141:LEU:HD11	2:B:450:LEU:HD11	2.01	0.41
2:B:171:HIS:O	2:B:172:LEU:HD23	2.20	0.41
2:B:186:GLU:OE2	2:B:731:VAL:N	2.51	0.41
13:M:57:ASN:OD1	13:M:60:LEU:N	2.51	0.41
1:A:818:THR:O	1:A:822:THR:HG23	2.20	0.41
1:A:1102:LEU:O	1:A:1106:LYS:HG3	2.21	0.41
2:B:628:TYR:HB2	2:B:640:LEU:HD13	2.03	0.41
2:B:656:LEU:HD23	2:B:656:LEU:HA	1.85	0.41
2:B:675:ALA:HB3	2:B:689:VAL:HG22	2.01	0.41
3:C:40:PHE:CE2	11:K:131:VAL:HA	2.56	0.41
5:E:37:LEU:HD23	5:E:37:LEU:HA	1.86	0.41
7:G:66:LEU:HD13	7:G:66:LEU:HA	1.88	0.41
8:H:93:TYR:HB3	8:H:144:ILE:O	2.20	0.41
1:A:730:GLN:HE21	1:A:730:GLN:HB3	1.58	0.41
1:A:1222:LEU:HD11	1:A:1570:PHE:CE1	2.55	0.41
2:B:52:LEU:O	2:B:60:LEU:N	2.46	0.41
2:B:159:GLY:HA3	2:B:456:ASN:OD1	2.19	0.41
2:B:581:PRO:HG3	2:B:637:TYR:HE1	1.86	0.41
2:B:673:ASN:OD1	2:B:673:ASN:N	2.54	0.41
2:B:912:GLN:CD	2:B:1041:ASN:HD21	2.29	0.41
13:M:12:ILE:HG12	13:M:90:LEU:HD12	2.02	0.41
17:T:5:DC:H2"	17:T:6:DG:C8	2.56	0.41
1:A:498:PRO:HD3	1:A:614:LEU:HD23	2.02	0.41
1:A:1169:LEU:HA	1:A:1169:LEU:HD12	1.88	0.41
1:A:1465:GLU:OE1	1:A:1465:GLU:N	2.50	0.41
2:B:77:LYS:HD3	2:B:77:LYS:HA	1.73	0.41
2:B:122:TYR:O	2:B:125:GLU:N	2.49	0.41
2:B:172:LEU:HA	2:B:175:MET:HG3	2.02	0.41
2:B:282:HIS:HE1	2:B:322:ASN:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:331:GLY:HA3	2:B:349:VAL:HG13	2.02	0.41
2:B:696:ILE:HG13	2:B:697:LEU:HD22	2.03	0.41
2:B:851:TYR:OH	2:B:853:GLU:OE2	2.22	0.41
2:B:916:LYS:HE2	2:B:1036:LEU:HD12	2.03	0.41
2:B:931:TRP:HB3	2:B:936:MET:SD	2.61	0.41
3:C:63:ILE:HD13	3:C:63:ILE:HA	1.94	0.41
3:C:92:ILE:HD11	10:J:57:ILE:HD12	2.03	0.41
8:H:80:ARG:HG3	11:K:108:TYR:CE1	2.56	0.41
8:H:102:TYR:CE2	8:H:117:SER:HB2	2.56	0.41
1:A:6:PRO:HG3	7:G:113:PHE:CG	2.56	0.41
1:A:124:LEU:HD22	1:A:129:LEU:HD22	2.02	0.41
1:A:451:VAL:N	1:A:452:PRO:HD2	2.36	0.41
1:A:538:ASN:N	1:A:542:SER:O	2.38	0.41
1:A:596:HIS:CD2	1:A:1195:GLU:HG3	2.48	0.41
1:A:606:ARG:NH1	1:A:607:VAL:O	2.54	0.41
2:B:523:GLU:OE1	2:B:523:GLU:N	2.49	0.41
2:B:684:ASN:N	14:N:150:TYR:OH	2.53	0.41
2:B:813:LEU:HD23	2:B:813:LEU:H	1.86	0.41
3:C:229:LEU:O	3:C:293:ARG:NH1	2.53	0.41
5:E:7:ARG:O	5:E:11:ARG:HG3	2.20	0.41
5:E:169:ARG:HH12	6:F:74:ILE:HD11	1.86	0.41
7:G:108:THR:HG22	7:G:110:ASP:H	1.86	0.41
8:H:14:GLU:HB3	8:H:27:GLU:HB3	2.02	0.41
11:K:126:ASP:O	11:K:130:VAL:HG13	2.20	0.41
14:N:93:THR:O	14:N:93:THR:OG1	2.35	0.41
1:A:80:GLU:HA	1:A:359:VAL:HG22	2.03	0.41
1:A:753:ASN:OD1	1:A:753:ASN:N	2.54	0.41
1:A:1510:PRO:HG3	1:A:1520:VAL:HG12	2.03	0.41
2:B:25:PHE:CE2	10:J:56:LEU:HA	2.56	0.41
2:B:187:SER:N	10:J:63:TYR:OH	2.54	0.41
5:E:178:ILE:N	5:E:213:ILE:O	2.38	0.41
11:K:139:ILE:HD13	11:K:139:ILE:HA	1.87	0.41
1:A:484:ILE:HD11	1:A:631:ASP:HB3	2.03	0.40
2:B:307:GLU:OE1	9:I:7:LEU:HD23	2.21	0.40
2:B:1117:VAL:HG21	2:B:1162:GLY:HA2	2.03	0.40
5:E:47:CYS:HB2	5:E:55:ARG:NH1	2.36	0.40
6:F:82:THR:HG22	6:F:84:TYR:N	2.35	0.40
7:G:137:ILE:HA	7:G:147:LEU:HB2	2.03	0.40
8:H:7:ASP:OD1	8:H:8:ASP:N	2.54	0.40
9:I:21:ASN:OD1	9:I:22:ALA:N	2.53	0.40
1:A:181:LEU:HA	1:A:181:LEU:HD12	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ARG:O	1:A:343:PRO:HD2	2.21	0.40
1:A:680:LEU:O	1:A:728:GLY:HA3	2.21	0.40
1:A:1066:PHE:CD1	1:A:1170:MET:HE2	2.57	0.40
1:A:1183:GLU:O	1:A:1185:VAL:N	2.54	0.40
2:B:211:ARG:NH2	2:B:243:GLN:OE1	2.47	0.40
2:B:451:MET:HE3	2:B:451:MET:HB3	1.87	0.40
2:B:455:GLU:O	2:B:457:ILE:N	2.52	0.40
2:B:617:THR:HG22	2:B:619:GLY:H	1.85	0.40
3:C:82:TYR:HD2	3:C:126:PHE:HZ	1.69	0.40
4:D:40:LEU:HD22	4:D:93:GLN:HA	2.04	0.40
7:G:234:ARG:HH21	7:G:235:ASN:HB3	1.86	0.40
16:S:35:DG:C5	16:S:36:DT:C4	3.09	0.40
1:A:744:MET:HG2	1:A:801:TYR:CE2	2.56	0.40
1:A:1031:HIS:ND1	1:A:1031:HIS:O	2.55	0.40
1:A:1288:ARG:NH2	1:A:1481:GLU:O	2.47	0.40
1:A:1647:ASN:O	1:A:1652:GLY:HA3	2.21	0.40
2:B:52:LEU:C	2:B:60:LEU:H	2.28	0.40
2:B:445:TYR:O	2:B:449:VAL:HG12	2.21	0.40
2:B:456:ASN:HB3	2:B:459:SER:OG	2.21	0.40
2:B:743:ARG:NH1	3:C:93:GLN:HE22	2.19	0.40
7:G:90:LEU:HD23	7:G:117:TRP:HB2	2.03	0.40
9:I:44:ASN:N	9:I:44:ASN:OD1	2.53	0.40
14:N:25:ILE:HA	14:N:26:PRO:HD3	1.94	0.40
1:A:613:THR:O	1:A:615:ARG:NH2	2.38	0.40
1:A:1458:THR:OG1	1:A:1475:GLU:OE1	2.29	0.40
1:A:1654:PHE:HD2	1:A:1655:ASP:O	2.04	0.40
1:A:1660:VAL:HB	7:G:57:PRO:HG3	2.03	0.40
2:B:101:GLN:HB3	2:B:140:LYS:HG2	2.03	0.40
2:B:208:VAL:N	2:B:401:GLU:O	2.52	0.40
4:D:21:VAL:HG22	4:D:23:HIS:H	1.86	0.40
5:E:5:ASN:O	5:E:9:ILE:HG13	2.22	0.40
7:G:43:ILE:HG12	7:G:122:LEU:HG	2.04	0.40
1:A:460:LEU:HA	1:A:466:LEU:N	2.35	0.40
1:A:1243:TRP:O	1:A:1246:VAL:HG22	2.21	0.40
2:B:418:ASP:O	2:B:422:GLN:HG2	2.22	0.40
2:B:593:ILE:HD13	2:B:593:ILE:HA	1.85	0.40
2:B:827:PHE:HE1	2:B:844:GLY:HA2	1.87	0.40
2:B:936:MET:HE1	2:B:948:ILE:HG13	2.02	0.40
2:B:954:PHE:N	2:B:955:PRO:HD2	2.36	0.40
2:B:960:ILE:O	2:B:964:VAL:HG12	2.21	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	1446/1664 (87%)	1364 (94%)	82 (6%)	0	100	100
2	B	1156/1203 (96%)	1064 (92%)	92 (8%)	0	100	100
3	C	302/335 (90%)	284 (94%)	18 (6%)	0	100	100
4	D	55/137 (40%)	52 (94%)	3 (6%)	0	100	100
5	E	212/215 (99%)	195 (92%)	17 (8%)	0	100	100
6	F	99/155 (64%)	91 (92%)	8 (8%)	0	100	100
7	G	144/326 (44%)	130 (90%)	14 (10%)	0	100	100
8	H	127/146 (87%)	120 (94%)	7 (6%)	0	100	100
9	I	63/125 (50%)	60 (95%)	3 (5%)	0	100	100
10	J	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
11	K	95/142 (67%)	92 (97%)	3 (3%)	0	100	100
12	L	42/70 (60%)	39 (93%)	3 (7%)	0	100	100
13	M	106/415 (26%)	99 (93%)	7 (7%)	0	100	100
14	N	133/233 (57%)	117 (88%)	16 (12%)	0	100	100
All	All	4047/5236 (77%)	3773 (93%)	274 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	1291/1465 (88%)	1206 (93%)	85 (7%)	15	41
2	B	1017/1053 (97%)	953 (94%)	64 (6%)	16	42
3	C	268/296 (90%)	255 (95%)	13 (5%)	22	49
4	D	56/116 (48%)	52 (93%)	4 (7%)	13	39
5	E	196/197 (100%)	184 (94%)	12 (6%)	17	43
6	F	90/137 (66%)	84 (93%)	6 (7%)	15	41
7	G	131/291 (45%)	119 (91%)	12 (9%)	8	29
8	H	115/128 (90%)	108 (94%)	7 (6%)	17	43
9	I	57/110 (52%)	52 (91%)	5 (9%)	9	31
10	J	64/65 (98%)	62 (97%)	2 (3%)	35	59
11	K	87/130 (67%)	83 (95%)	4 (5%)	24	50
12	L	39/57 (68%)	35 (90%)	4 (10%)	7	24
13	M	98/371 (26%)	91 (93%)	7 (7%)	13	39
14	N	130/220 (59%)	121 (93%)	9 (7%)	14	40
All	All	3639/4636 (78%)	3405 (94%)	234 (6%)	18	42

All (234) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	ILE
1	A	7	VAL
1	A	14	VAL
1	A	15	ASP
1	A	24	ILE
1	A	27	LEU
1	A	36	THR
1	A	43	HIS
1	A	45	VAL
1	A	78	HIS
1	A	79	ILE
1	A	81	LEU
1	A	83	VAL
1	A	113	VAL
1	A	115	VAL
1	A	139	ILE
1	A	202	THR
1	A	235	ASN

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Mol	Chain	Res	Type
1	A	251	ILE
1	A	324	LEU
1	A	408	LYS
1	A	410	LYS
1	A	419	ILE
1	A	420	PHE
1	A	460	LEU
1	A	492	THR
1	A	506	THR
1	A	528	ASP
1	A	536	ILE
1	A	584	ARG
1	A	587	VAL
1	A	591	ARG
1	A	631	ASP
1	A	646	GLU
1	A	658	LEU
1	A	666	VAL
1	A	670	ILE
1	A	688	THR
1	A	715	LEU
1	A	723	TYR
1	A	753	ASN
1	A	805	VAL
1	A	812	VAL
1	A	853	THR
1	A	912	VAL
1	A	940	VAL
1	A	943	ILE
1	A	947	LEU
1	A	957	VAL
1	A	1022	CYS
1	A	1028	GLU
1	A	1030	VAL
1	A	1031	HIS
1	A	1035	ASP
1	A	1118	VAL
1	A	1124	LEU
1	A	1128	ASN
1	A	1185	VAL
1	A	1187	ILE
1	A	1223	ARG

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Mol	Chain	Res	Type
1	A	1233	ILE
1	A	1239	THR
1	A	1258	ILE
1	A	1261	VAL
1	A	1270	VAL
1	A	1298	ASP
1	A	1326	GLU
1	A	1336	GLN
1	A	1439	MET
1	A	1442	VAL
1	A	1443	GLN
1	A	1446	ARG
1	A	1479	ASP
1	A	1480	THR
1	A	1484	LEU
1	A	1488	ILE
1	A	1524	VAL
1	A	1535	PHE
1	A	1561	THR
1	A	1567	ASN
1	A	1628	ASP
1	A	1629	ASN
1	A	1632	GLU
1	A	1660	VAL
2	B	13	THR
2	B	15	ASP
2	B	18	THR
2	B	54	GLU
2	B	104	ILE
2	B	131	THR
2	B	139	LEU
2	B	140	LYS
2	B	155	VAL
2	B	161	LEU
2	B	163	VAL
2	B	189	GLU
2	B	190	ILE
2	B	199	ILE
2	B	212	ASN
2	B	234	ILE
2	B	255	ASP
2	B	274	VAL

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Mol	Chain	Res	Type
2	B	306	LEU
2	B	322	ASN
2	B	328	GLN
2	B	362	LEU
2	B	365	ASP
2	B	397	THR
2	B	402	VAL
2	B	404	LEU
2	B	416	LYS
2	B	425	ILE
2	B	471	VAL
2	B	476	LEU
2	B	478	LEU
2	B	487	VAL
2	B	503	VAL
2	B	557	ASP
2	B	588	ILE
2	B	622	ILE
2	B	624	LEU
2	B	653	VAL
2	B	676	VAL
2	B	677	THR
2	B	692	THR
2	B	699	ILE
2	B	700	LEU
2	B	708	ASP
2	B	749	THR
2	B	803	MET
2	B	806	THR
2	B	882	ILE
2	B	901	VAL
2	B	910	THR
2	B	912	GLN
2	B	913	ILE
2	B	946	ASP
2	B	960	ILE
2	B	1025	ASP
2	B	1030	VAL
2	B	1033	TYR
2	B	1060	VAL
2	B	1071	VAL
2	B	1076	ARG

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Mol	Chain	Res	Type
2	B	1087	LEU
2	B	1089	GLN
2	B	1092	LEU
2	B	1181	VAL
3	C	83	VAL
3	C	91	VAL
3	C	111	ASP
3	C	114	THR
3	C	137	ASN
3	C	151	THR
3	C	191	ILE
3	C	209	ILE
3	C	223	SER
3	C	275	VAL
3	C	279	VAL
3	C	301	ASN
3	C	328	LEU
4	D	15	THR
4	D	37	LEU
4	D	80	THR
4	D	82	LEU
5	E	35	VAL
5	E	46	TYR
5	E	65	THR
5	E	74	ASP
5	E	90	VAL
5	E	117	THR
5	E	124	VAL
5	E	132	ILE
5	E	140	LEU
5	E	156	LEU
5	E	196	VAL
5	E	204	THR
6	F	81	THR
6	F	96	THR
6	F	128	LYS
6	F	134	ILE
6	F	138	LEU
6	F	149	GLU
7	G	43	ILE
7	G	45	LEU
7	G	66	LEU

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Mol	Chain	Res	Type
7	G	71	MET
7	G	80	VAL
7	G	84	TYR
7	G	95	LEU
7	G	121	ASN
7	G	133	LEU
7	G	137	ILE
7	G	239	THR
7	G	245	VAL
8	H	35	GLN
8	H	89	LEU
8	H	92	ASP
8	H	96	VAL
8	H	117	SER
8	H	129	TYR
8	H	131	ASN
9	I	3	VAL
9	I	7	LEU
9	I	28	VAL
9	I	47	VAL
9	I	49	THR
10	J	25	LEU
10	J	49	MET
11	K	49	LEU
11	K	64	GLN
11	K	77	ARG
11	K	110	GLU
12	L	46	VAL
12	L	54	ARG
12	L	56	LEU
12	L	66	GLN
13	M	56	GLU
13	M	66	THR
13	M	67	ASP
13	M	74	ASN
13	M	77	VAL
13	M	80	LEU
13	M	96	LEU
14	N	53	VAL
14	N	56	ILE
14	N	64	ILE
14	N	82	ILE

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Mol	Chain	Res	Type
14	N	111	VAL
14	N	121	ILE
14	N	124	THR
14	N	153	VAL
14	N	155	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	76	GLN
1	A	93	GLN
1	A	384	GLN
1	A	425	ASN
1	A	444	GLN
1	A	596	HIS
1	A	636	HIS
1	A	950	GLN
1	A	1065	GLN
1	A	1081	ASN
1	A	1141	GLN
1	A	1151	ASN
1	A	1180	ASN
1	A	1244	ASN
1	A	1250	GLN
1	A	1300	ASN
1	A	1315	ASN
1	A	1454	HIS
1	A	1503	HIS
1	A	1509	HIS
2	B	128	GLN
2	B	182	GLN
2	B	282	HIS
2	B	427	GLN
2	B	462	GLN
2	B	547	HIS
2	B	739	ASN
2	B	748	GLN
2	B	829	ASN
2	B	886	ASN
2	B	950	ASN
2	B	952	HIS

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Mol	Chain	Res	Type
2	B	1041	ASN
2	B	1157	GLN
3	C	172	GLN
3	C	296	ASN
4	D	30	HIS
5	E	61	GLN
5	E	115	ASN
5	E	179	GLN
7	G	64	GLN
7	G	74	ASN
8	H	3	ASN
8	H	11	GLN
8	H	83	GLN
10	J	23	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	R	8/12 (66%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	R	5	A
15	R	10	G

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	3DR	T	17	17	8,11,12	0.48	0	7,14,17	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	3DR	T	17	17	-	1/3/15/16	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	T	17	3DR	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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.

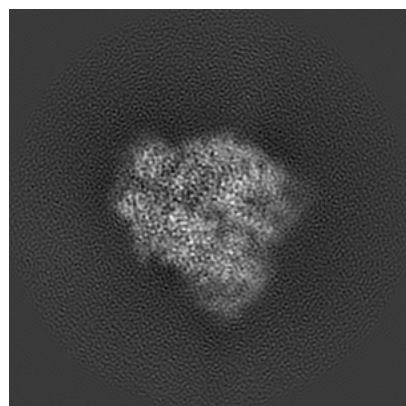
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50965. These allow visual inspection of the internal detail of the map and identification of artifacts.

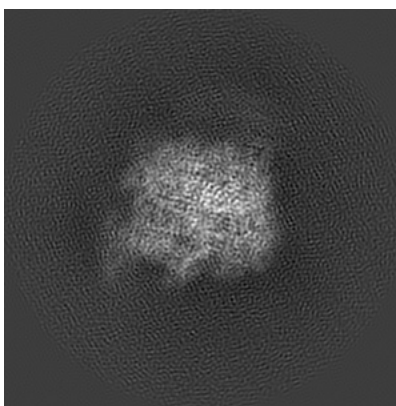
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

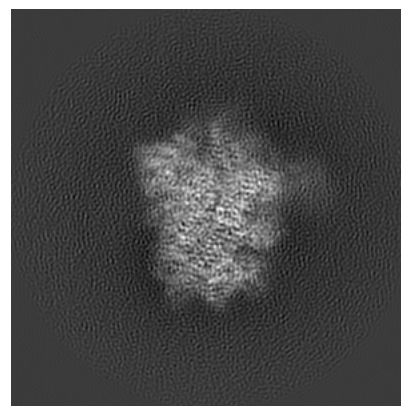
6.1.1 Primary map



X

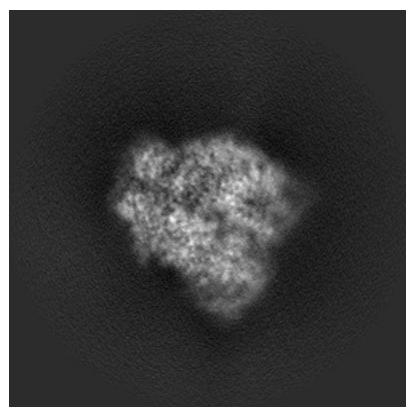


Y

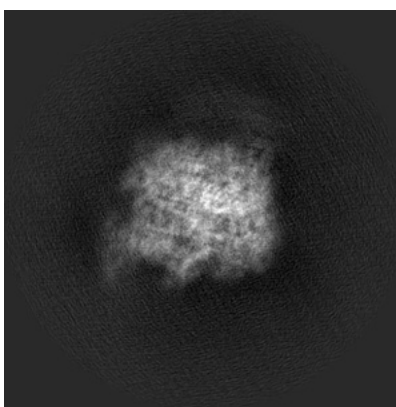


Z

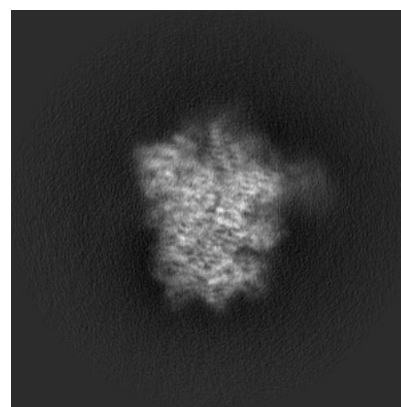
6.1.2 Raw map



X



Y

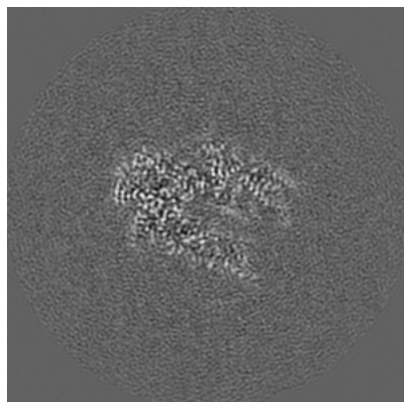


Z

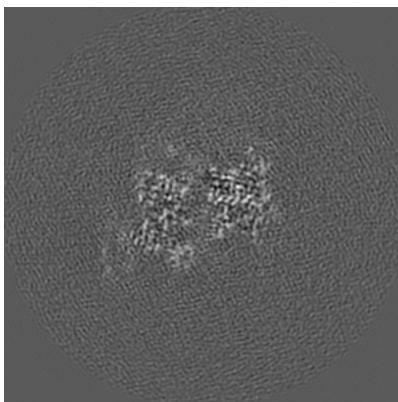
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

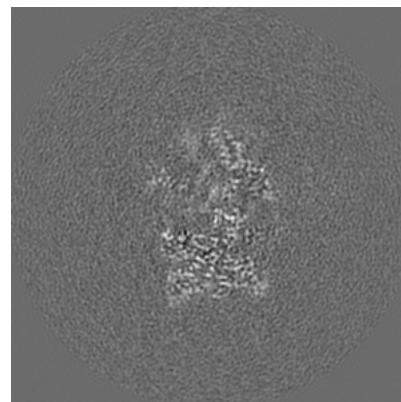
6.2.1 Primary map



X Index: 144

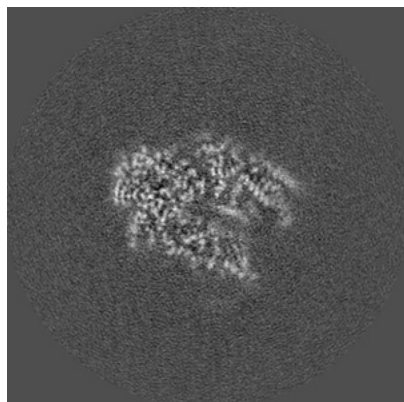


Y Index: 144

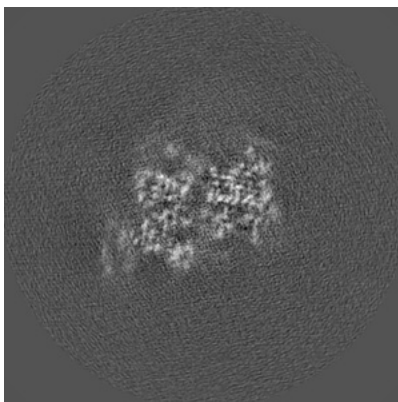


Z Index: 144

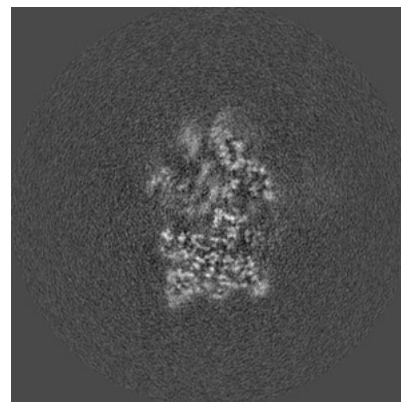
6.2.2 Raw map



X Index: 144



Y Index: 144

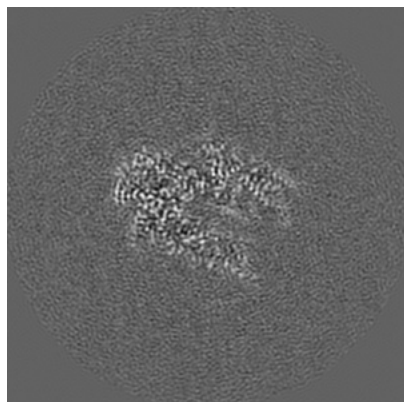


Z Index: 144

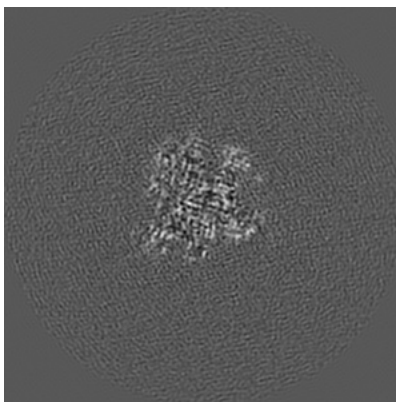
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

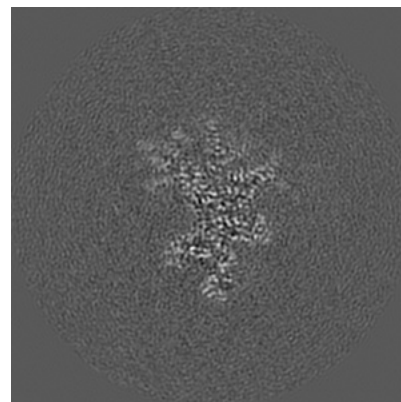
6.3.1 Primary map



X Index: 144

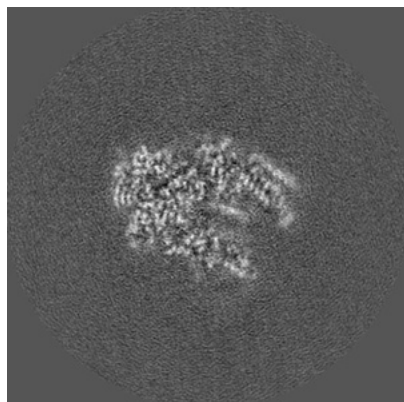


Y Index: 123

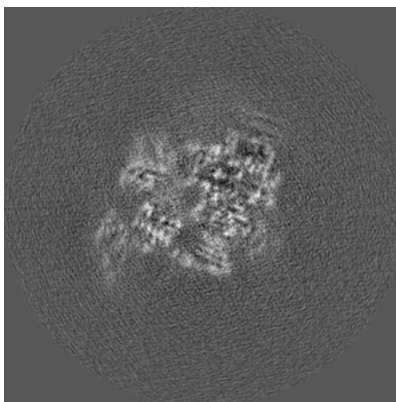


Z Index: 162

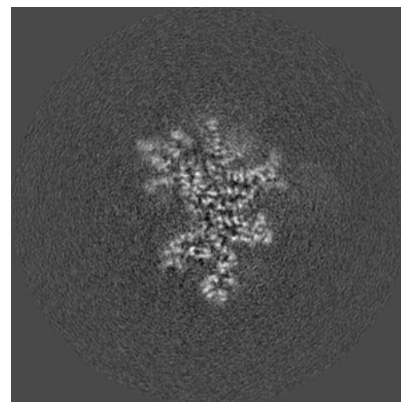
6.3.2 Raw map



X Index: 145



Y Index: 158

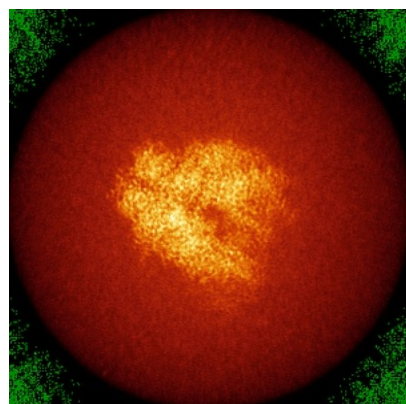


Z Index: 162

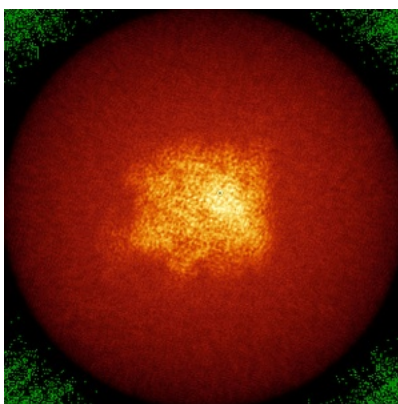
The images above show the largest variance slices of the map in three orthogonal directions.

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

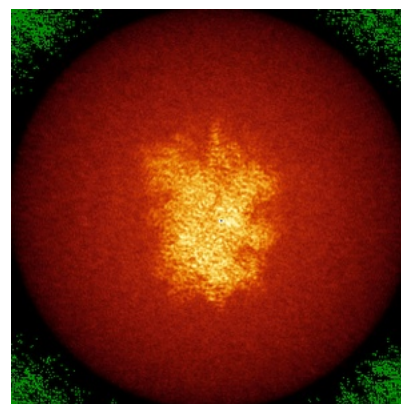
6.4.1 Primary map



X

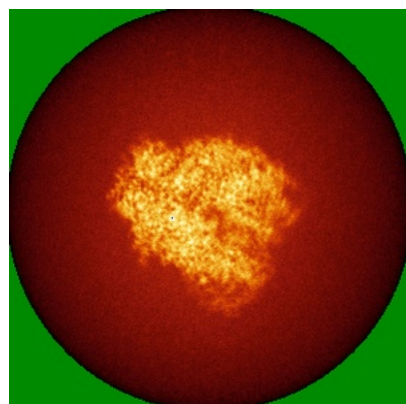


Y

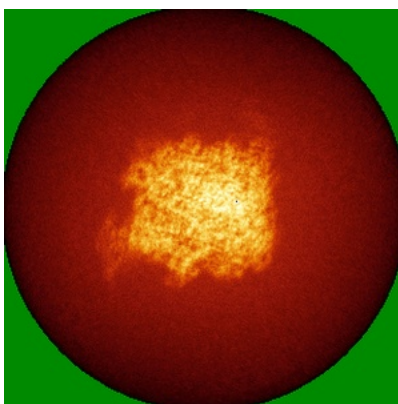


Z

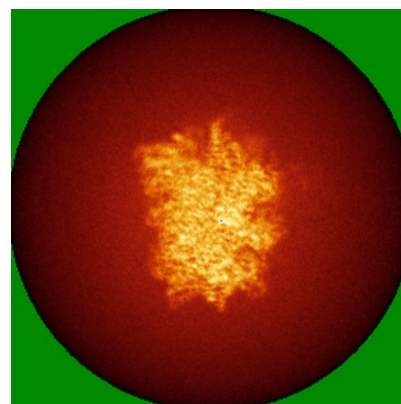
6.4.2 Raw map



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](#)

This section was not generated.

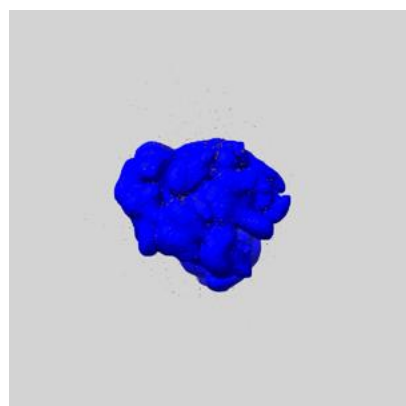
6.6 Mask visualisation [i](#)

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

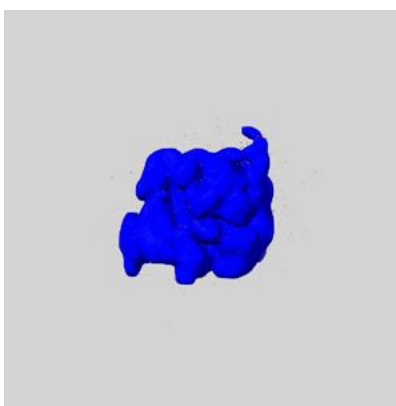
A mask typically either:

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

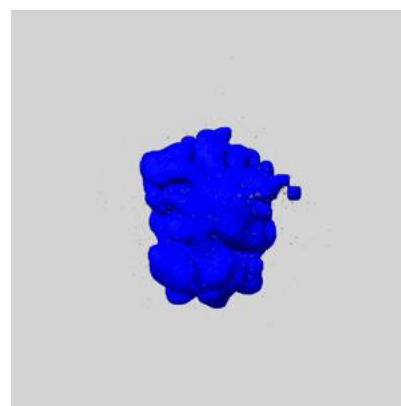
6.6.1 emd_50965_msk_1.map [i](#)



X



Y

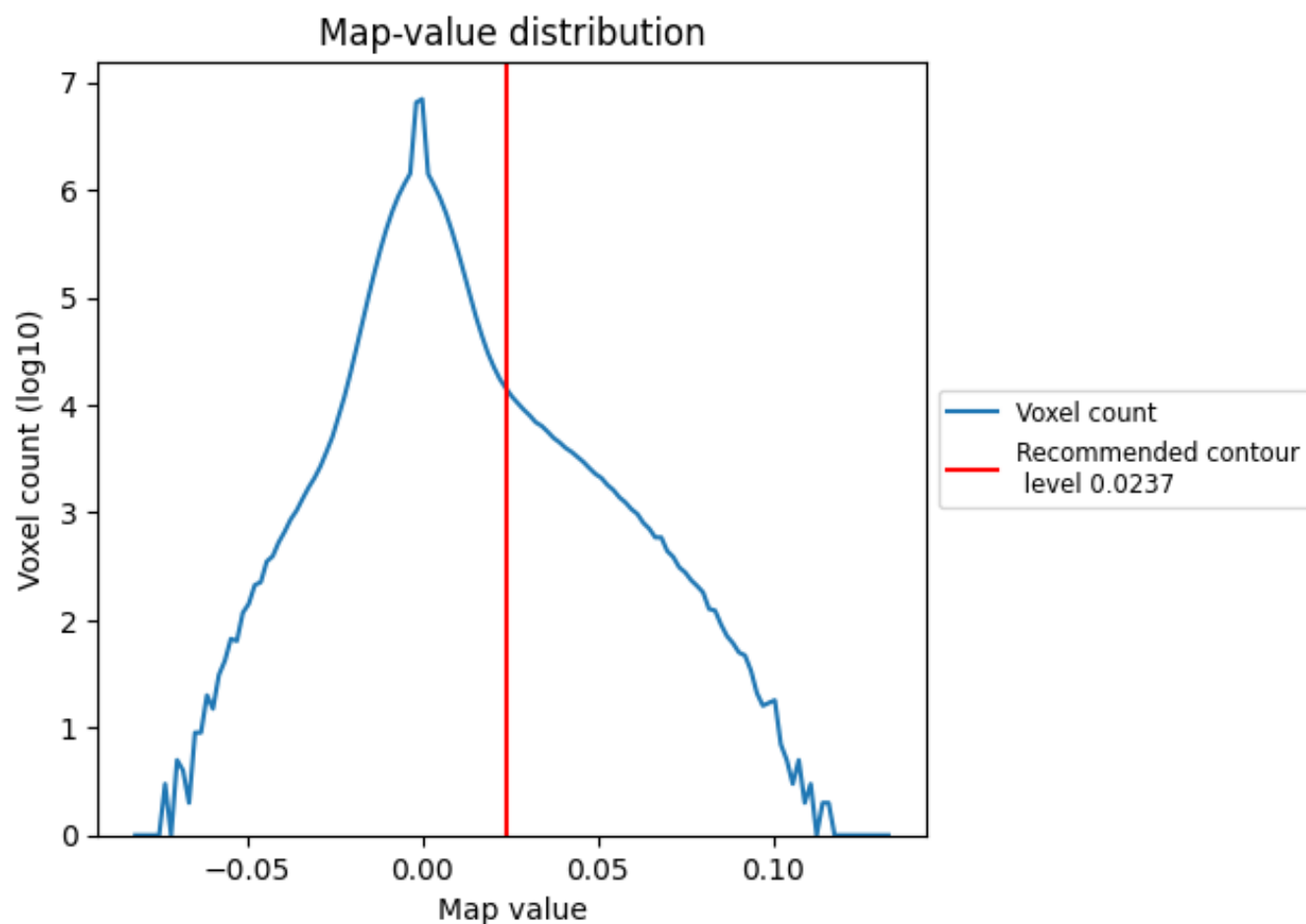


Z

7 Map analysis [i](#)

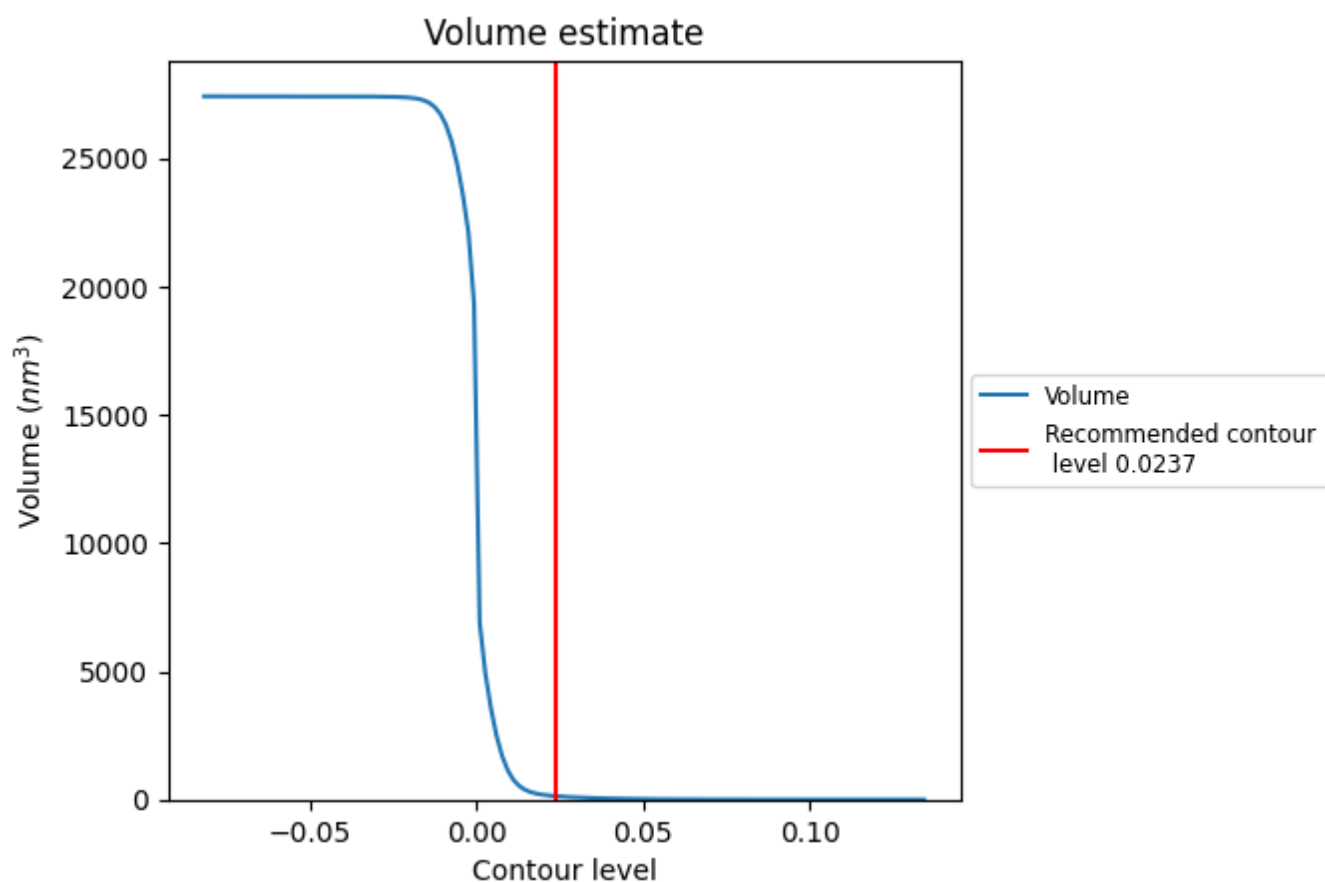
This section contains the results of statistical analysis of the map.

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.

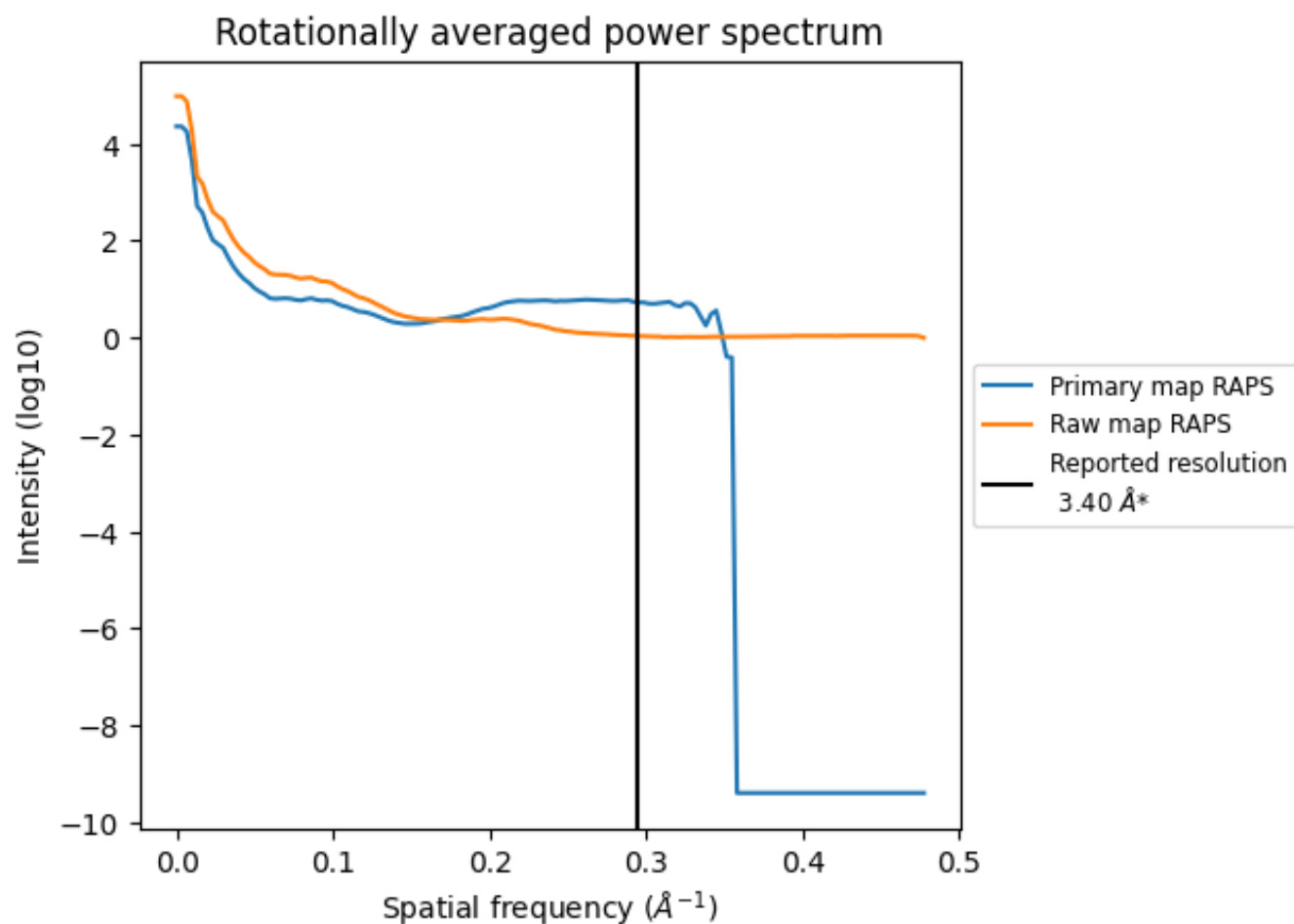
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 135 nm³; this corresponds to an approximate mass of 122 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 ⓘ

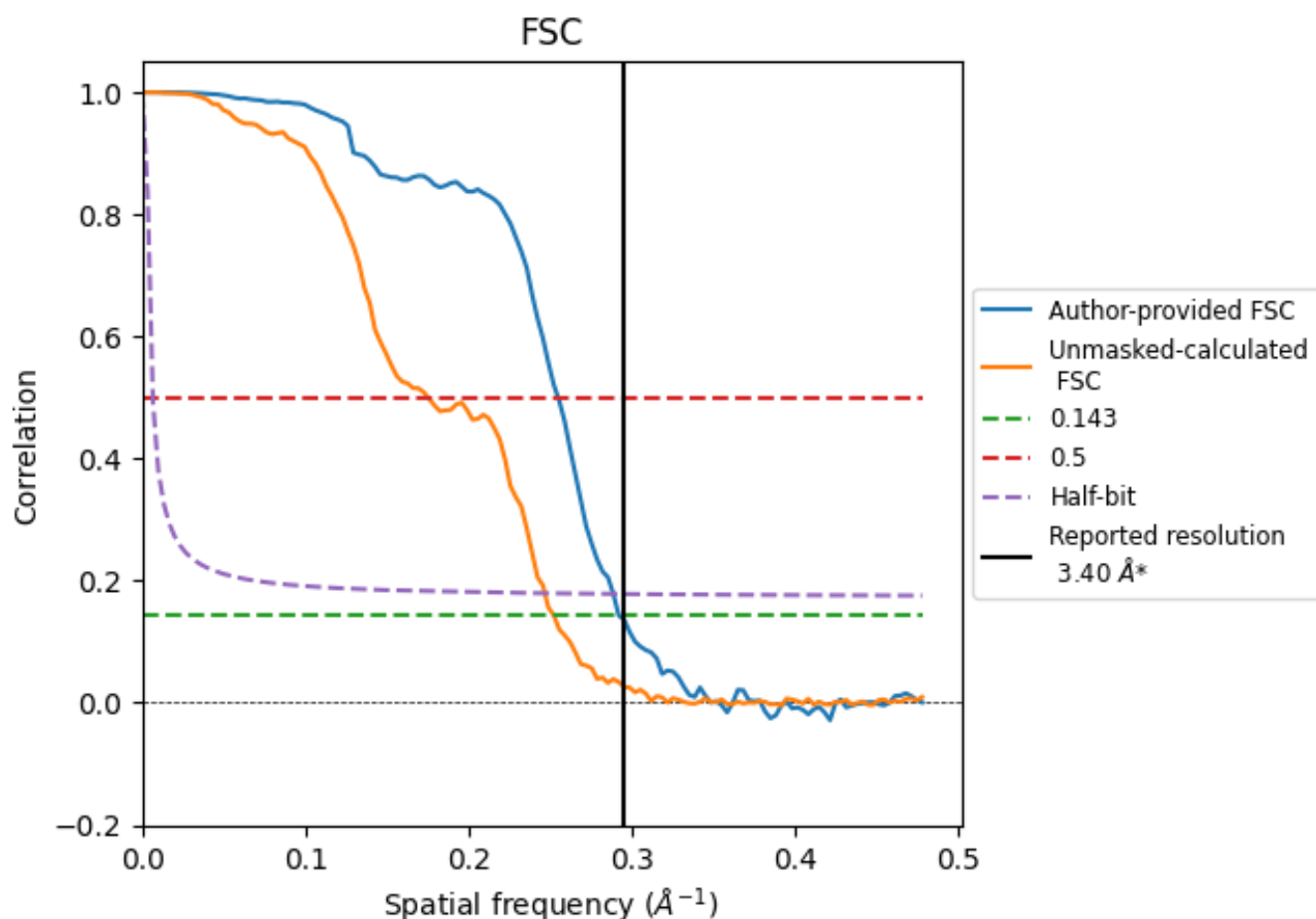


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 $0.294 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

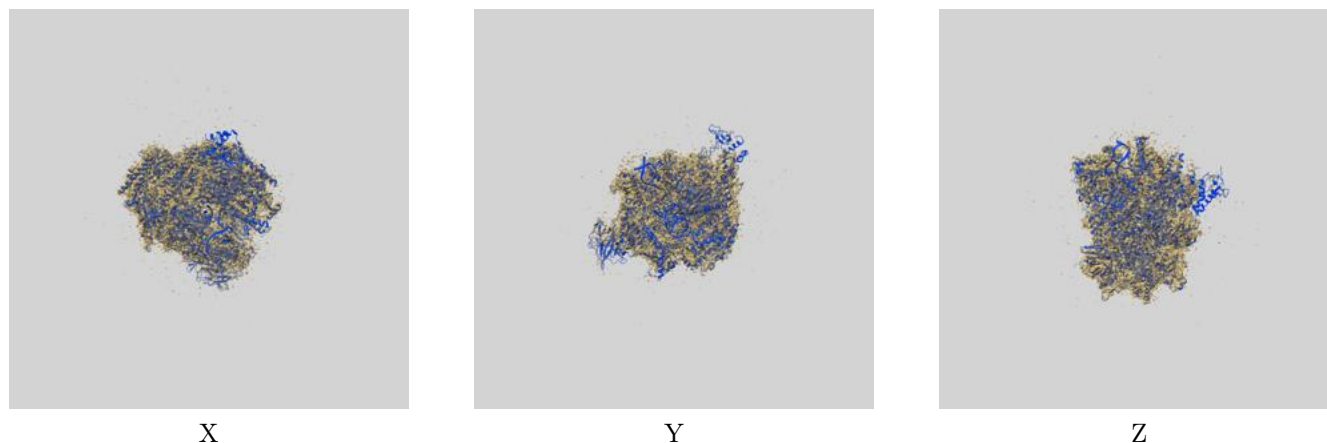
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.43	3.93	3.47
Unmasked-calculated*	3.97	5.71	4.06

*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 3.97 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

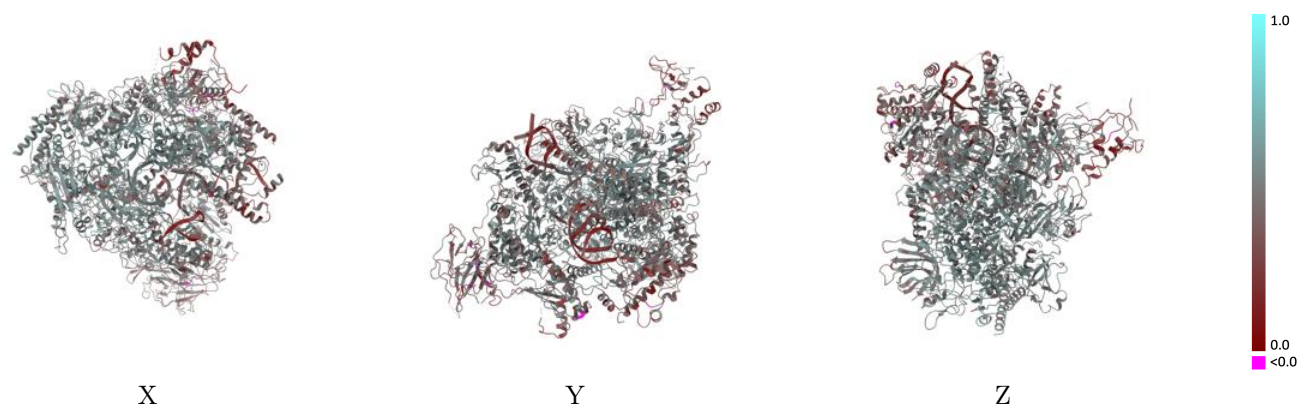
This section contains information regarding the fit between EMDB map EMD-50965 and PDB model 9G26. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



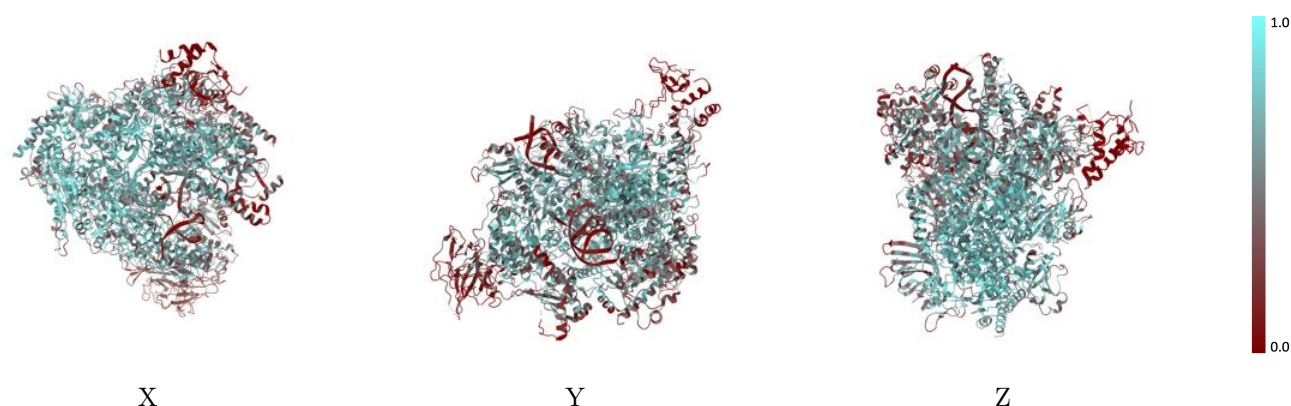
The images above show the 3D surface view of the map at the recommended contour level 0.0237 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



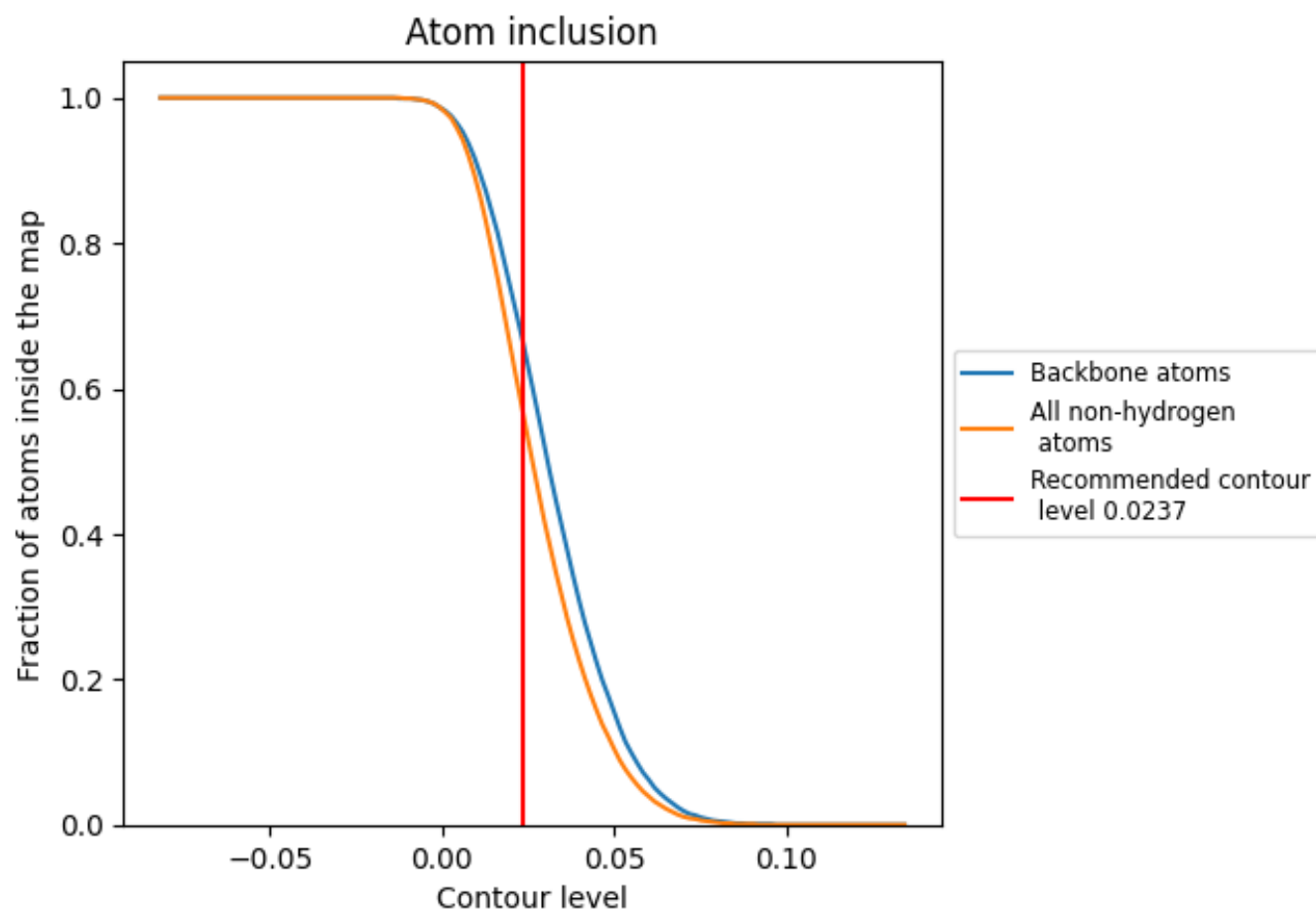
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0237).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 56% 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 (0.0237) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5630	 0.4650
A	 0.6070	 0.4800
B	 0.6700	 0.5010
C	 0.6580	 0.5070
D	 0.1450	 0.3180
E	 0.4480	 0.3900
F	 0.6160	 0.4770
G	 0.3050	 0.3880
H	 0.5560	 0.4750
I	 0.3980	 0.4190
J	 0.7230	 0.5230
K	 0.7150	 0.5050
L	 0.6210	 0.4900
M	 0.1410	 0.3670
N	 0.1260	 0.3710
R	 0.7110	 0.4660
S	 0.1220	 0.2320
T	 0.3430	 0.3190

