Full wwPDB EM Validation Report

Jun 8, 2025 – 04:19 pm BST

PDB ID	:	9G1X / pdb_00009g1x
EMDB ID	:	EMD-50956
Title	:	Yeast RNA polymerase I elongation complex stalled by an apurinic site, 11-subunit
Authors	:	Santos-Aledo, A.; Plaza-Pegueroles, A.; Ruiz, F.M.; Fernandez-Tornero, C.
Deposited on	:	2024-07-10
Resolution	:	3.50 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 (i) 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 (i)) were used in the production of this report:

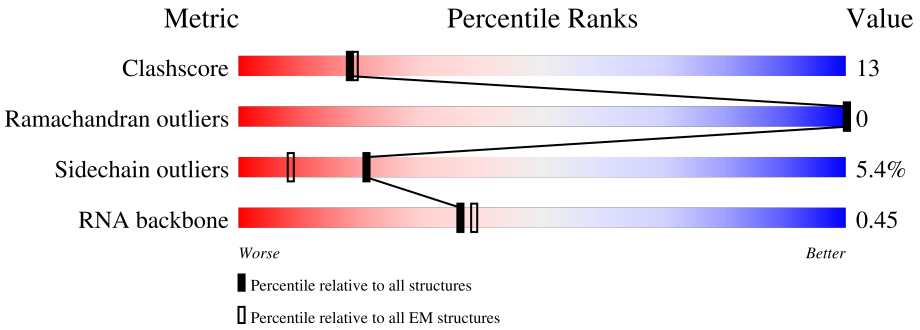
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.50 Å.

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



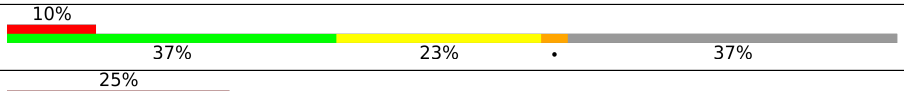
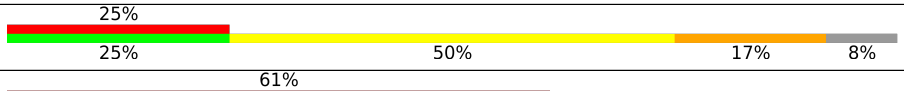
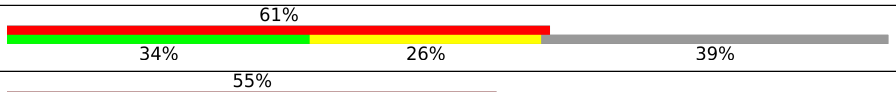
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	1664	17% 50% 22% • 26%
2	B	1203	19% 60% 30% • 7%
3	C	335	18% 65% 23% • 9%
4	D	137	• 9% • 87%
5	E	215	52% 63% 30% • 5%
6	F	155	7% 41% 23% • 35%
7	G	326	12% 20% 7% • 72%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	H	146	
9	J	70	
10	K	142	
11	L	70	
12	R	12	
13	S	38	
14	T	38	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 28341 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
			Total	C	N	O	S		
1	A	1226	9634	6091	1676	1815	52	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1113	8839	5590	1549	1649	51	0	0

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	18	133	84	23	26	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	205	1681	1072	295	304	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	100	823	522	144	154	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	91	Total	C	N	O	S	0	0
			722	475	115	127	5		

- 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 polymerases I, II, and III subunit RPABC5.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	98	Total	C	N	O	S	0	0
			766	481	124	156	5		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 12 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	11	Total	C	N	O	P	0	0
			239	107	47	74	11		

- Molecule 13 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	23	Total	C	N	O	P	0	0
			468	224	79	142	23		

- Molecule 14 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	32	Total	C	N	O	P	0	0
			643	307	112	192	32		

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

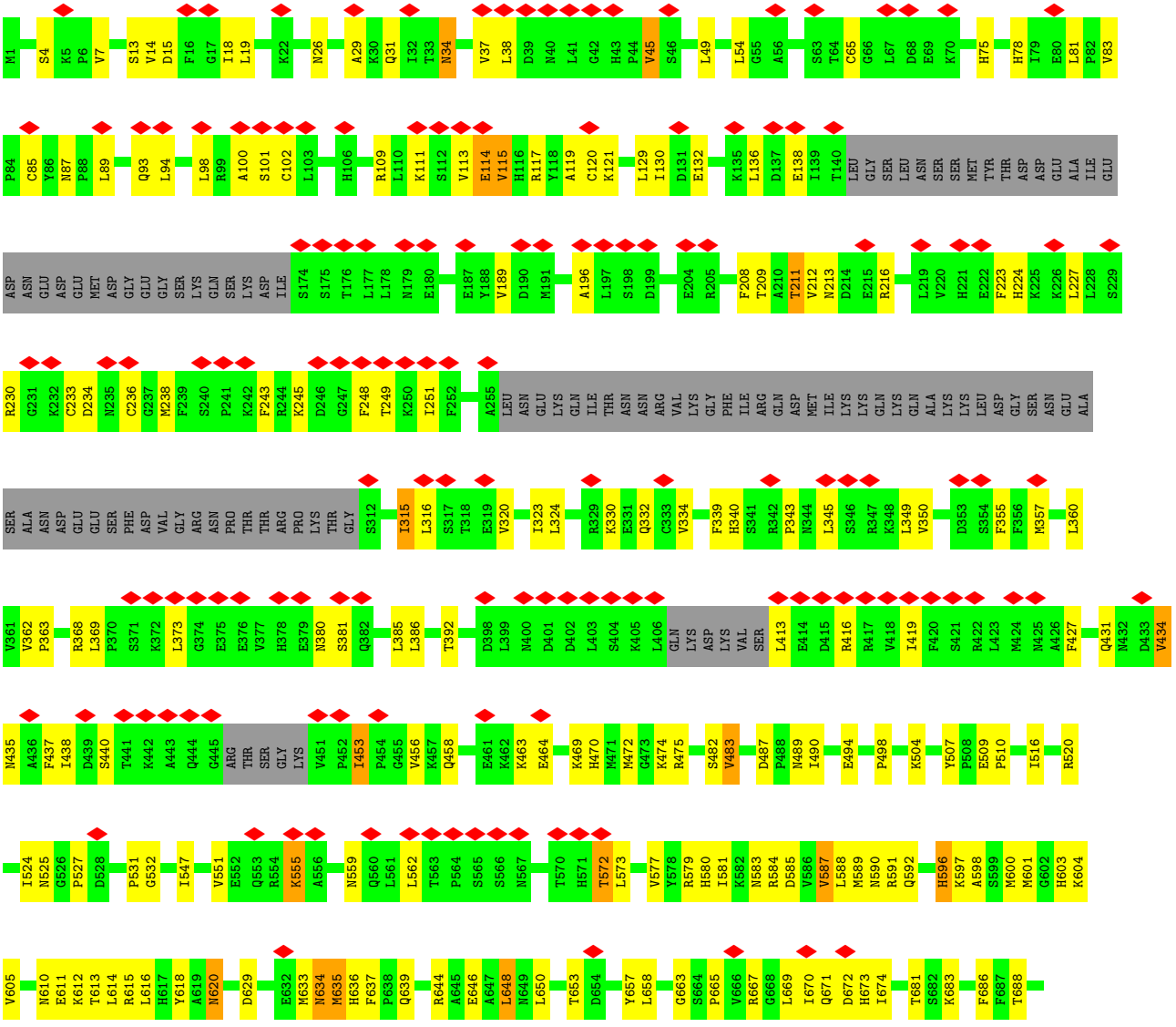
Mol	Chain	Residues	Atoms		AltConf
15	A	2	Total	Zn	0
			2	2	
15	B	1	Total	Zn	0
			1	1	
15	J	1	Total	Zn	0
			1	1	
15	L	1	Total	Zn	0
			1	1	

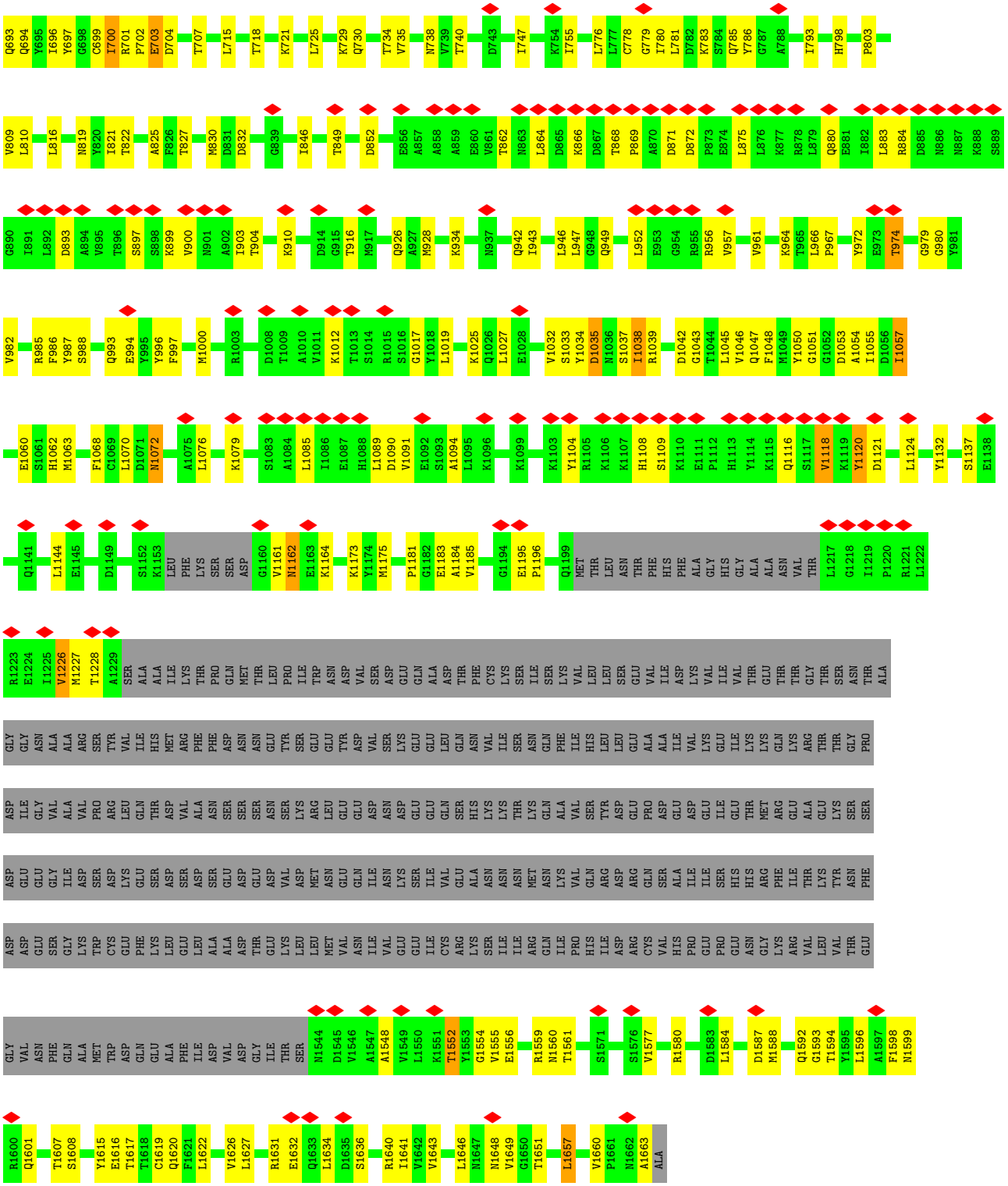
3 Residue-property plots (i)

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

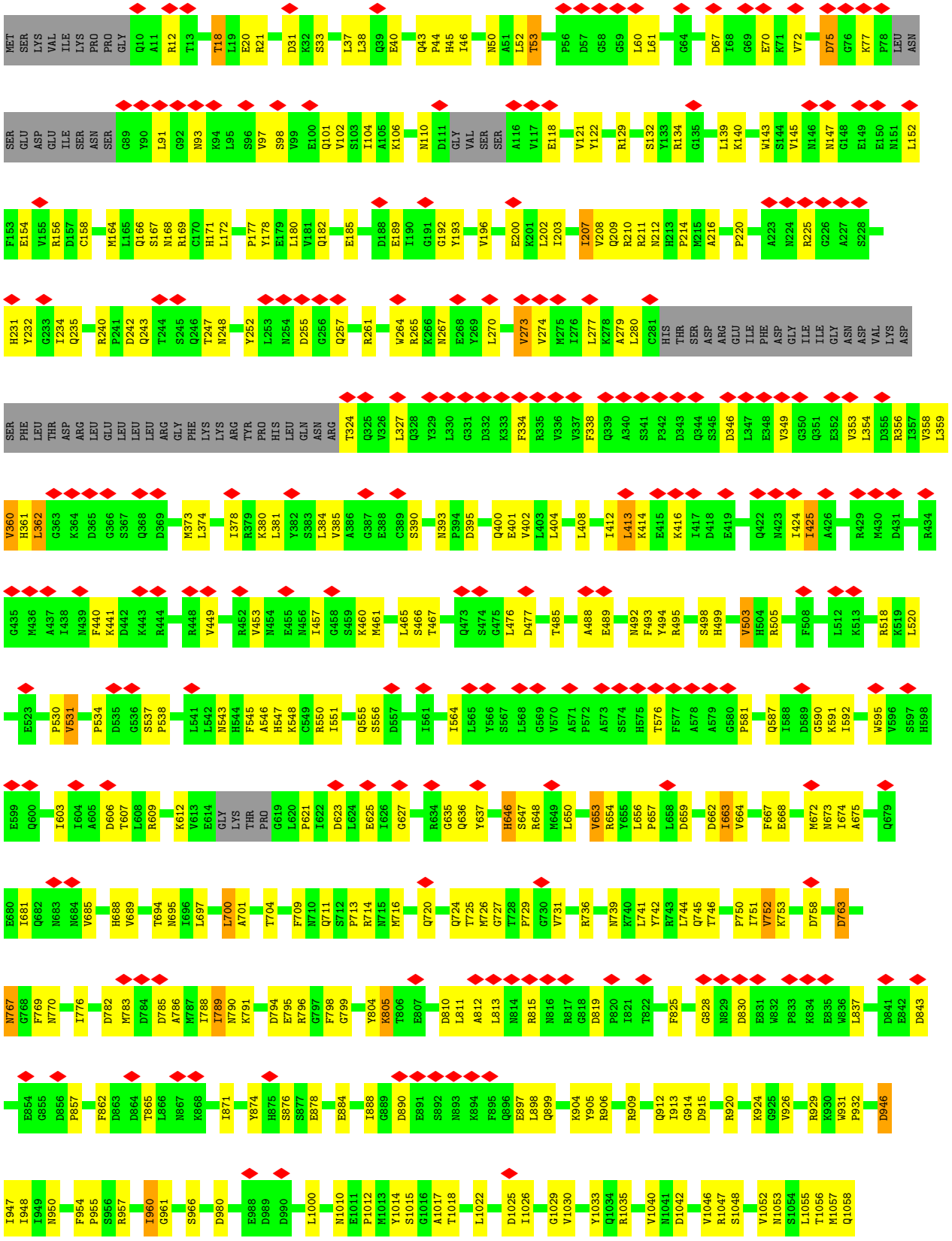
- Molecule 1: DNA-directed RNA polymerase I subunit RPA190

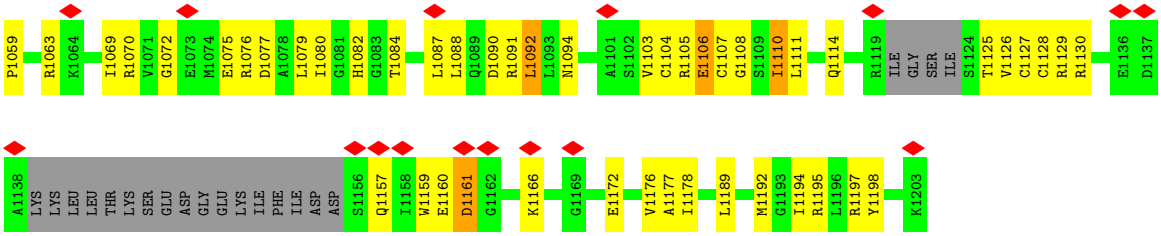
Chain A:





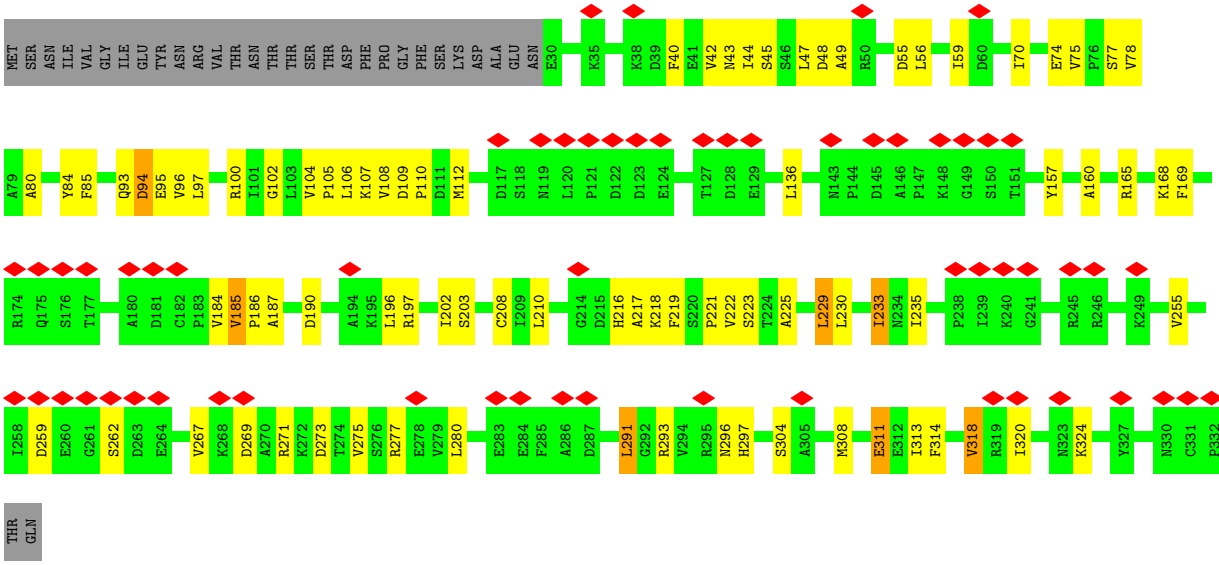
• Molecule 2: DNA-directed RNA polymerase I subunit RPA135





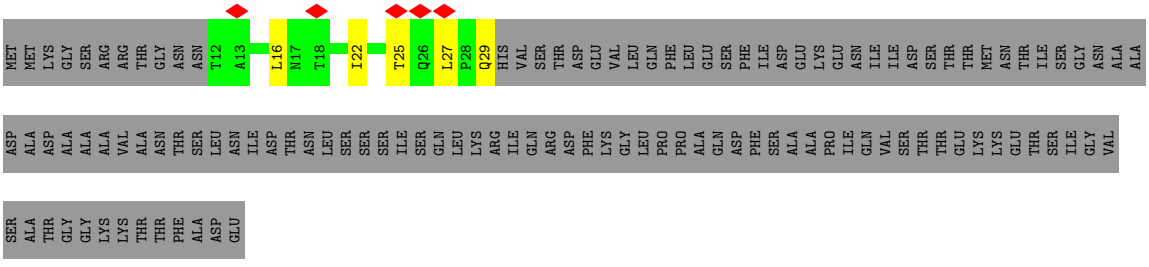
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C:



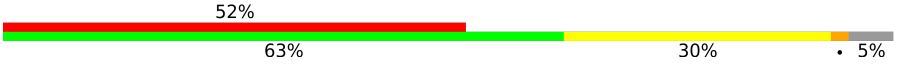
• Molecule 4: DNA-directed RNA polymerase I subunit RPA14

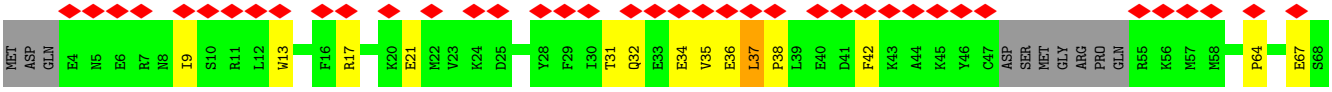
Chain D:

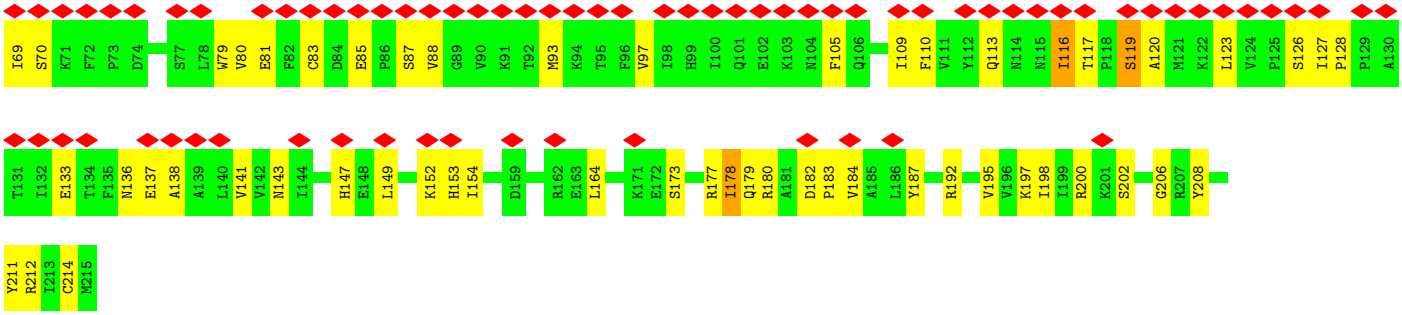


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

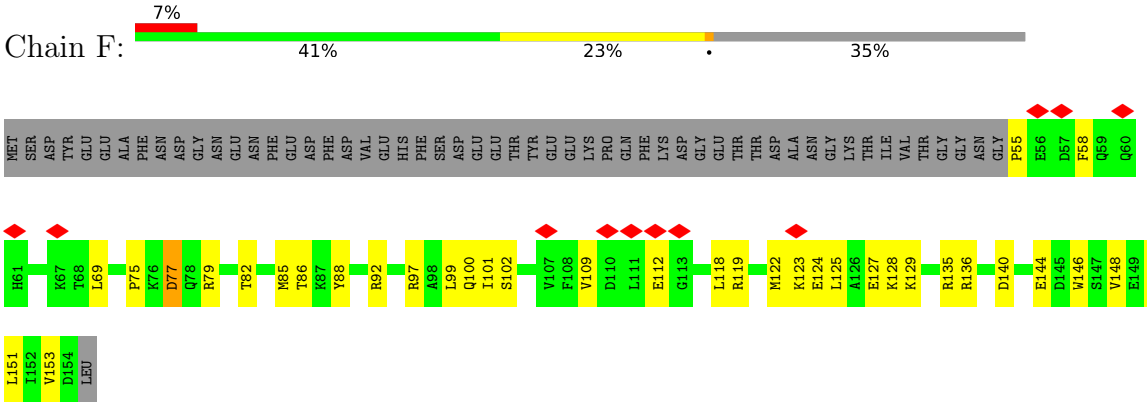
Chain E:



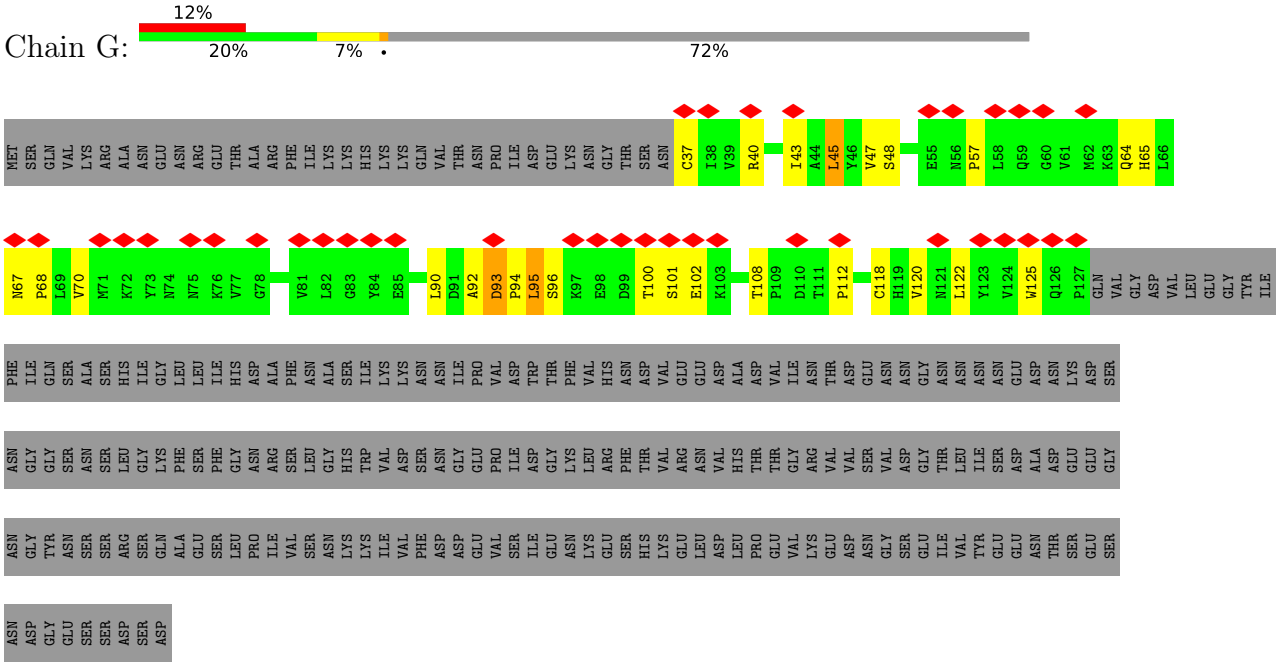




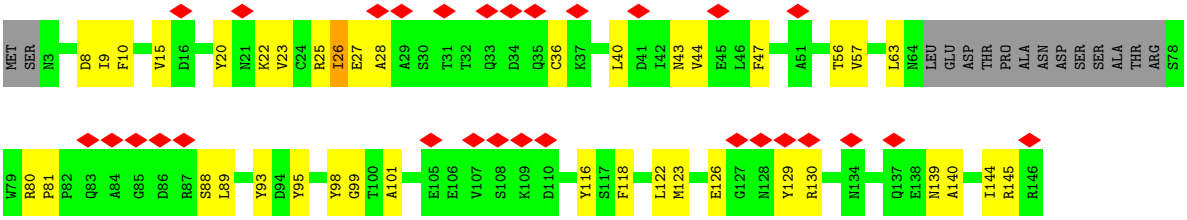
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



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

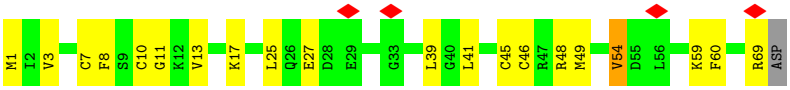


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



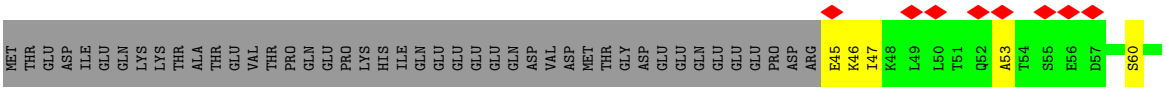
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC5

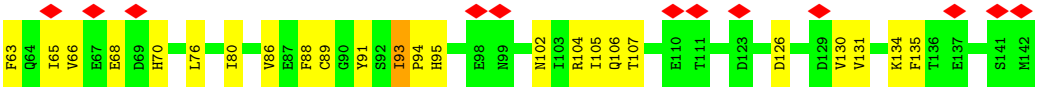
Chain J:



• Molecule 10: DNA-directed RNA polymerases I and III subunit RPAC2

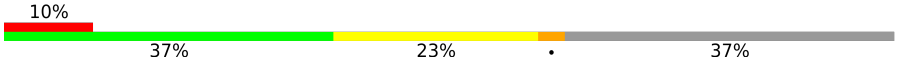
Chain K:

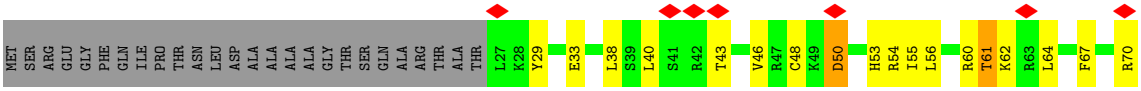




• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC4

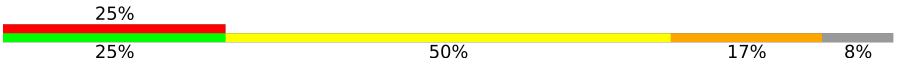
Chain L:

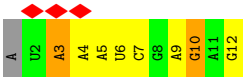




• Molecule 12: RNA

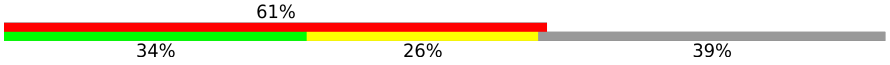
Chain R:

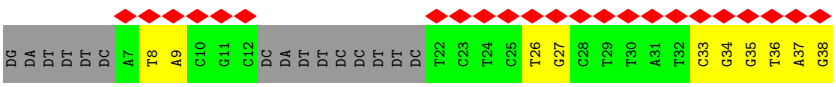




• Molecule 13: Non-template DNA

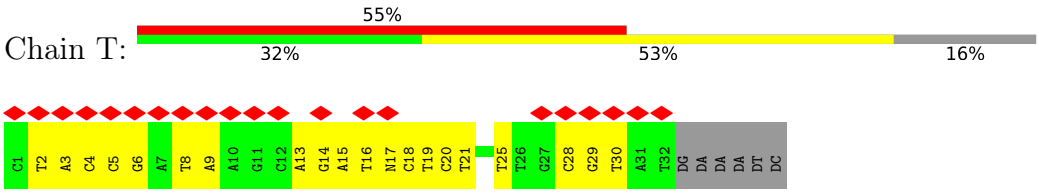
Chain S:





• Molecule 14: Template DNA

Chain T:


55%
32%
53%
16%
C1
T2
A3
C4
C5
G6
A7
T8
A9
A10
G11
C12
A13
G14
A15
T16
N17
C18
T19
C20
T21
T25
T26
G27
C28
G29
T30
A31
T32
DG
DA
DA
DA
DT
DC

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95419	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 ($e^-/Å^2$)	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	0.127	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0277	Depositor
Map size (Å)	301.536, 301.536, 301.536	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.047, 1.047, 1.047	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3DR, 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	0.22	0/9813	0.35	0/13254
2	B	0.23	0/9033	0.36	0/12209
3	C	0.22	0/2467	0.32	0/3344
4	D	0.18	0/135	0.32	0/188
5	E	0.17	0/1715	0.29	0/2308
6	F	0.22	0/838	0.33	0/1129
7	G	0.21	0/742	0.34	0/1013
8	H	0.21	0/1070	0.34	0/1449
9	J	0.25	0/578	0.28	0/775
10	K	0.22	0/776	0.33	0/1047
11	L	0.23	0/354	0.36	0/468
12	R	0.21	0/268	0.28	0/416
13	S	0.20	0/521	0.41	0/799
14	T	0.26	0/706	0.44	0/1084
All	All	0.22	0/29016	0.35	0/39483

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

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	9634	0	9717	285	0
2	B	8839	0	8719	269	0
3	C	2415	0	2403	64	0
4	D	133	0	138	4	0
5	E	1681	0	1714	47	0
6	F	823	0	841	33	0
7	G	722	0	740	24	0
8	H	1052	0	1021	23	0
9	J	569	0	585	14	0
10	K	766	0	765	29	0
11	L	352	0	374	14	0
12	R	239	0	120	7	0
13	S	468	0	263	8	0
14	T	643	0	359	17	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
All	All	28341	0	27759	724	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 13.

All (724) 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:1634:LEU:HD13	1:A:1643:VAL:HG21	1.61	0.81
2:B:623:ASP:HB3	2:B:648:ARG:HH22	1.43	0.81
2:B:424:ILE:HG22	2:B:453:VAL:HG21	1.64	0.79
1:A:579:ARG:NH1	1:A:585:ASP:OD2	2.15	0.79
1:A:620:ASN:OD1	1:A:620:ASN:N	2.16	0.78
5:E:79:TRP:NE1	5:E:81:GLU:OE1	2.17	0.77
1:A:216:ARG:NH2	1:A:340:HIS:O	2.18	0.76
2:B:796:ARG:NH2	9:J:8:PHE:O	2.17	0.76
2:B:395:ASP:HA	2:B:505:ARG:HH12	1.50	0.75
1:A:464:GLU:HA	1:A:469:LYS:HD2	1.70	0.74
1:A:1035:ASP:N	1:A:1035:ASP:OD1	2.20	0.74
2:B:731:VAL:HG11	9:J:59:LYS:HD2	1.70	0.73
1:A:115:VAL:HG13	1:A:334:VAL:HG11	1.71	0.73
1:A:729:LYS:HG3	1:A:776:LEU:HG	1.70	0.72
1:A:1184:ALA:HB2	1:A:1649:VAL:HG11	1.70	0.71
1:A:694:GLN:NE2	10:K:91:TYR:O	2.21	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:LYS:O	2:B:1082:HIS:NE2	2.23	0.71
2:B:857:PRO:HB3	2:B:871:ILE:HD13	1.72	0.70
3:C:74:GLU:OE2	3:C:324:LYS:NZ	2.23	0.70
12:R:4:A:H2'	12:R:5:A:H8	1.56	0.70
2:B:672:MET:HE3	2:B:674:ILE:HD11	1.74	0.70
1:A:83:VAL:HG11	1:A:427:PHE:HE1	1.55	0.69
1:A:98:LEU:HA	1:A:324:LEU:HD21	1.73	0.69
2:B:745:GLN:OE1	3:C:93:GLN:NE2	2.25	0.69
2:B:1104:CYS:HB3	2:B:1107:CYS:SG	2.32	0.69
5:E:31:THR:HG22	5:E:34:GLU:HG3	1.73	0.69
2:B:609:ARG:NH1	2:B:668:GLU:OE2	2.26	0.69
3:C:94:ASP:N	3:C:94:ASP:OD1	2.26	0.69
1:A:880:GLN:HE21	1:A:884:ARG:HH12	1.39	0.68
12:R:4:A:H2'	12:R:5:A:C8	2.28	0.68
3:C:80:ALA:HB3	3:C:102:GLY:HA2	1.76	0.68
6:F:79:ARG:NH2	6:F:150:GLU:OE1	2.26	0.68
2:B:210:ARG:NH2	2:B:625:GLU:OE1	2.27	0.68
1:A:581:ILE:HD11	1:A:605:VAL:HG11	1.76	0.67
1:A:982:VAL:HG13	1:A:994:GLU:HB3	1.75	0.67
1:A:1050:TYR:HB3	1:A:1054:ALA:HA	1.77	0.67
2:B:1080:ILE:HG13	2:B:1088:LEU:HD22	1.76	0.67
1:A:943:ILE:HG23	2:B:960:ILE:HD11	1.77	0.67
2:B:1105:ARG:N	2:B:1172:GLU:O	2.21	0.67
5:E:97:VAL:HG13	5:E:127:ILE:HD13	1.76	0.67
7:G:48:SER:O	7:G:64:GLN:NE2	2.27	0.67
13:S:26:DT:H2'	13:S:27:DG:C8	2.29	0.67
1:A:489:ASN:ND2	10:K:94:PRO:O	2.27	0.67
1:A:1640:ARG:NE	1:A:1646:LEU:O	2.25	0.67
3:C:255:VAL:HG11	3:C:273:ASP:HB2	1.75	0.67
2:B:75:ASP:OD1	2:B:75:ASP:N	2.28	0.66
2:B:203:ILE:HD11	2:B:408:LEU:HD23	1.77	0.66
2:B:1015:SER:HB3	2:B:1022:LEU:HD21	1.77	0.66
1:A:509:GLU:OE2	1:A:584:ARG:NH2	2.27	0.66
2:B:211:ARG:NH1	2:B:243:GLN:OE1	2.27	0.66
2:B:129:ARG:HG2	11:L:55:ILE:HD11	1.76	0.66
5:E:200:ARG:NH1	5:E:208:TYR:OH	2.28	0.66
3:C:235:ILE:HD11	3:C:267:VAL:HG13	1.77	0.66
2:B:101:GLN:HB3	2:B:140:LYS:HG2	1.76	0.66
2:B:726:MET:HG3	2:B:742:TYR:HB3	1.77	0.66
2:B:1047:ARG:NE	2:B:1048:SER:O	2.21	0.66
3:C:48:ASP:OD1	3:C:49:ALA:N	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:SER:HB3	1:A:458:GLN:HG3	1.78	0.65
3:C:222:VAL:HG11	3:C:225:ALA:HB2	1.78	0.65
10:K:63:PHE:O	10:K:102:ASN:HA	1.96	0.65
1:A:470:HIS:O	2:B:1058:GLN:NE2	2.29	0.65
2:B:212:ASN:HB3	2:B:590:GLY:HA3	1.77	0.65
9:J:17:LYS:NZ	9:J:39:LEU:O	2.25	0.65
1:A:525:ASN:ND2	1:A:531:PRO:O	2.29	0.65
1:A:1554:GLY:HA2	5:E:183:PRO:HD2	1.79	0.65
2:B:795:GLU:O	3:C:216:HIS:NE2	2.26	0.65
3:C:216:HIS:HE1	11:L:70:ARG:HA	1.61	0.65
1:A:648:LEU:HD13	6:F:118:LEU:HD23	1.78	0.65
2:B:1012:PRO:HG2	3:C:275:VAL:HB	1.79	0.65
1:A:634:ASN:HD22	2:B:1069:ILE:HG21	1.62	0.65
1:A:827:THR:HG22	2:B:776:ILE:HA	1.79	0.65
1:A:846:ILE:HD11	1:A:910:LYS:HD3	1.79	0.65
1:A:1039:ARG:HA	1:A:1046:VAL:HG23	1.79	0.64
1:A:1616:GLU:HG3	1:A:1617:THR:HG23	1.79	0.64
1:A:363:PRO:O	1:A:368:ARG:NH1	2.30	0.64
2:B:518:ARG:NH2	2:B:537:SER:O	2.30	0.64
1:A:1038:ILE:HD12	1:A:1584:LEU:HD13	1.78	0.64
3:C:185:VAL:HG22	3:C:186:PRO:HD2	1.80	0.64
1:A:29:ALA:HA	2:B:1129:ARG:HH22	1.63	0.63
2:B:878:GLU:OE2	2:B:909:ARG:NH2	2.24	0.63
3:C:109:ASP:HB2	3:C:112:MET:HE3	1.79	0.63
3:C:222:VAL:HG22	3:C:313:ILE:HD13	1.79	0.63
1:A:646:GLU:HG2	1:A:650:LEU:HD12	1.78	0.63
2:B:1106:GLU:O	2:B:1197:ARG:NH2	2.32	0.63
1:A:1227:MET:O	1:A:1599:ASN:ND2	2.32	0.62
1:A:1608:SER:OG	1:A:1632:GLU:OE1	2.16	0.62
2:B:75:ASP:OD2	2:B:77:LYS:NZ	2.31	0.62
2:B:404:LEU:HD11	2:B:551:ILE:HG12	1.81	0.62
6:F:77:ASP:N	6:F:77:ASP:OD1	2.32	0.62
5:E:17:ARG:NE	5:E:21:GLU:OE2	2.26	0.62
5:E:143:ASN:ND2	5:E:187:TYR:OH	2.32	0.62
1:A:211:THR:OG1	5:E:177:ARG:NH1	2.32	0.62
1:A:869:PRO:HG2	1:A:872:ASP:HB2	1.82	0.62
2:B:587:GLN:HG2	2:B:592:ILE:HA	1.80	0.62
1:A:634:ASN:OD1	1:A:634:ASN:N	2.32	0.62
3:C:229:LEU:HB3	3:C:293:ARG:HB3	1.82	0.62
3:C:78:VAL:HG12	3:C:106:LEU:HD12	1.81	0.62
7:G:43:ILE:HD13	7:G:122:LEU:HD11	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:SER:O	1:A:109:ARG:NH1	2.32	0.62
1:A:1162:ASN:OD1	1:A:1162:ASN:N	2.33	0.62
2:B:785:ASP:OD1	2:B:957:ARG:NH1	2.33	0.62
2:B:662:ASP:OD1	2:B:663:ILE:N	2.32	0.61
5:E:85:GLU:HG2	5:E:87:SER:H	1.65	0.61
1:A:1068:PHE:O	1:A:1072:ASN:ND2	2.32	0.61
1:A:785:GLN:HB3	1:A:793:ILE:HG22	1.82	0.61
1:A:509:GLU:HG3	1:A:579:ARG:HE	1.65	0.61
3:C:157:TYR:HB2	3:C:160:ALA:HB2	1.81	0.61
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.81	0.61
1:A:1017:GLY:HA3	14:T:17:3DR:H1'1	1.83	0.60
1:A:572:THR:HG22	1:A:573:LEU:HD23	1.83	0.60
8:H:8:ASP:OD1	8:H:9:ILE:N	2.34	0.60
1:A:683:LYS:HB2	8:H:20:TYR:CE1	2.36	0.60
1:A:734:THR:O	1:A:738:ASN:ND2	2.28	0.60
1:A:703:GLU:HA	10:K:53:ALA:HB2	1.83	0.60
1:A:1051:GLY:HA3	1:A:1580:ARG:HG2	1.83	0.60
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.83	0.60
6:F:119:ARG:NH1	6:F:122:MET:SD	2.74	0.60
1:A:1559:ARG:NH1	1:A:1560:ASN:OD1	2.35	0.60
1:A:1560:ASN:ND2	5:E:149:LEU:O	2.34	0.60
4:D:29:GLN:OE1	7:G:40:ARG:NH1	2.35	0.60
6:F:99:LEU:HB3	7:G:112:PRO:HB3	1.84	0.60
2:B:416:LYS:HG3	2:B:461:MET:HE3	1.83	0.60
1:A:98:LEU:HD13	1:A:320:VAL:HG13	1.84	0.60
2:B:225:ARG:HH21	2:B:261:ARG:CZ	2.15	0.60
13:S:36:DT:H2"	13:S:37:DA:C8	2.36	0.60
6:F:135:ARG:NH2	7:G:92:ALA:O	2.32	0.60
1:A:438:ILE:HA	1:A:456:VAL:HG12	1.84	0.59
5:E:152:LYS:HE3	5:E:154:ILE:HD11	1.84	0.59
8:H:63:LEU:HB3	8:H:88:SER:HB2	1.84	0.59
1:A:483:VAL:O	1:A:613:THR:OG1	2.19	0.59
1:A:1055:ILE:HD13	1:A:1063:MET:HE1	1.84	0.59
8:H:36:CYS:HA	8:H:126:GLU:O	2.03	0.59
1:A:704:ASP:OD1	1:A:704:ASP:N	2.35	0.59
1:A:1651:THR:HG23	6:F:92:ARG:HB2	1.83	0.59
3:C:84:TYR:HD2	11:L:64:LEU:HD11	1.67	0.59
2:B:751:ILE:HD12	2:B:1030:VAL:HG11	1.83	0.59
1:A:1640:ARG:NH1	1:A:1648:ASN:OD1	2.36	0.59
11:L:38:LEU:HD13	11:L:48:CYS:HA	1.84	0.59
1:A:87:ASN:ND2	1:A:357:MET:SD	2.75	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1010:ASN:HB3	2:B:1025:ASP:HB3	1.85	0.59
2:B:1128:CYS:SG	2:B:1129:ARG:N	2.76	0.59
3:C:136:LEU:O	3:C:203:SER:HA	2.02	0.59
2:B:790:ASN:HB2	2:B:946:ASP:HA	1.85	0.59
2:B:247:THR:O	2:B:248:ASN:ND2	2.36	0.59
2:B:362:LEU:HD11	2:B:591:LYS:HB3	1.84	0.59
2:B:556:SER:HB3	2:B:621:PRO:HG3	1.84	0.59
6:F:109:VAL:HG21	6:F:124:GLU:HA	1.85	0.59
1:A:38:LEU:HA	1:A:45:VAL:HG12	1.85	0.58
14:T:8:DT:H2"	14:T:9:DA:C8	2.38	0.58
1:A:7:VAL:HG21	2:B:1177:ALA:HB2	1.85	0.58
1:A:1660:VAL:HB	7:G:57:PRO:HG3	1.85	0.58
2:B:674:ILE:HG12	2:B:688:HIS:HB2	1.85	0.58
1:A:588:LEU:HD21	2:B:1079:LEU:HD21	1.85	0.58
2:B:581:PRO:HG3	2:B:637:TYR:CE2	2.39	0.58
1:A:653:THR:HB	1:A:667:ARG:HH22	1.67	0.58
9:J:10:CYS:SG	9:J:11:GLY:N	2.77	0.58
13:S:8:DT:H2"	13:S:9:DA:N7	2.19	0.58
1:A:956:ARG:HH21	1:A:979:GLY:HA3	1.69	0.58
2:B:720:GLN:OE1	2:B:724:GLN:NE2	2.24	0.58
2:B:166:GLN:NE2	2:B:189:GLU:OE1	2.36	0.58
1:A:85:CYS:HB2	1:A:431:GLN:OE1	2.04	0.57
1:A:120:CYS:HB2	1:A:189:VAL:HG21	1.86	0.57
1:A:700:ILE:HD11	1:A:735:VAL:HG22	1.85	0.57
2:B:209:GLN:NE2	2:B:235:GLN:OE1	2.36	0.57
2:B:264:TRP:HE1	2:B:338:PHE:HA	1.68	0.57
2:B:1014:TYR:OH	3:C:293:ARG:NH2	2.35	0.57
1:A:592:GLN:HE22	1:A:634:ASN:ND2	2.03	0.57
2:B:745:GLN:HE22	9:J:1:MET:HE2	1.68	0.57
2:B:763:ASP:OD1	2:B:763:ASP:N	2.30	0.57
1:A:697:TYR:HE1	1:A:702:PRO:HD2	1.69	0.57
8:H:25:ARG:NH2	8:H:27:GLU:OE2	2.34	0.57
9:J:7:CYS:HA	9:J:49:MET:HE2	1.87	0.57
9:J:69:ARG:NH2	11:L:33:GLU:O	2.37	0.57
5:E:109:ILE:HG22	5:E:133:GLU:HB2	1.85	0.57
2:B:897:GLU:HG2	2:B:898:LEU:HD23	1.85	0.57
2:B:909:ARG:O	2:B:1035:ARG:NH1	2.33	0.57
14:T:8:DT:H2"	14:T:9:DA:H8	1.70	0.57
2:B:492:ASN:ND2	2:B:725:THR:O	2.34	0.57
13:S:34:DG:H2'	13:S:35:DG:C8	2.40	0.57
1:A:591:ARG:HB2	1:A:633:MET:HE3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:89:CYS:HA	10:K:104:ARG:O	2.04	0.57
2:B:890:ASP:O	11:L:54:ARG:NH1	2.38	0.57
1:A:718:THR:OG1	1:A:730:GLN:OE1	2.17	0.56
1:A:494:GLU:HA	1:A:604:LYS:O	2.04	0.56
2:B:50:ASN:OD1	2:B:167:SER:OG	2.17	0.56
2:B:216:ALA:HB1	2:B:384:LEU:HD22	1.87	0.56
6:F:148:VAL:HA	6:F:151:LEU:HD12	1.88	0.56
7:G:45:LEU:HD13	7:G:47:VAL:HG13	1.87	0.56
1:A:323:ILE:HG22	1:A:324:LEU:HD23	1.88	0.56
5:E:116:ILE:HG23	5:E:120:ALA:HB3	1.87	0.56
6:F:99:LEU:HD13	7:G:112:PRO:HD3	1.88	0.56
2:B:154:GLU:HG3	2:B:156:ARG:HG2	1.87	0.56
2:B:240:ARG:HG2	2:B:360:VAL:HB	1.87	0.56
1:A:527:PRO:HG3	1:A:547:ILE:HA	1.87	0.56
1:A:1556:GLU:OE2	5:E:212:ARG:NE	2.25	0.56
5:E:64:PRO:HB2	5:E:69:ILE:HG12	1.88	0.55
5:E:138:ALA:HA	5:E:141:VAL:HG23	1.87	0.55
2:B:788:ILE:HB	2:B:948:ILE:HB	1.87	0.55
1:A:456:VAL:HG13	2:B:1192:MET:HE2	1.88	0.55
1:A:596:HIS:NE2	1:A:598:ALA:HB3	2.22	0.55
2:B:220:PRO:HA	2:B:231:HIS:HB3	1.87	0.55
2:B:1079:LEU:O	2:B:1084:THR:OG1	2.24	0.55
8:H:23:VAL:HA	8:H:43:ASN:HA	1.87	0.55
3:C:43:ASN:ND2	3:C:55:ASP:OD2	2.40	0.55
1:A:129:LEU:HD21	1:A:196:ALA:HB2	1.89	0.55
2:B:40:GLU:OE1	2:B:550:ARG:NH1	2.30	0.55
2:B:547:HIS:CE1	2:B:548:LYS:HG2	2.42	0.55
1:A:243:PHE:HB3	1:A:251:ILE:HD11	1.89	0.55
8:H:10:PHE:HB3	8:H:28:ALA:HB1	1.89	0.55
1:A:31:GLN:HB3	1:A:78:HIS:CE1	2.42	0.54
2:B:1047:ARG:NH1	2:B:1059:PRO:HB3	2.22	0.54
2:B:264:TRP:CD1	2:B:265:ARG:HG2	2.42	0.54
2:B:467:THR:HG22	14:T:25:DT:H4'	1.88	0.54
6:F:85:MET:HE1	6:F:125:LEU:HD11	1.89	0.54
6:F:97:ARG:O	6:F:101:ILE:HG12	2.07	0.54
1:A:1047:GLN:HE21	1:A:1587:ASP:HB2	1.72	0.54
8:H:57:VAL:HG22	8:H:144:ILE:HD12	1.90	0.54
2:B:67:ASP:O	2:B:356:ARG:NH2	2.29	0.54
2:B:465:LEU:HA	2:B:485:THR:HG21	1.89	0.54
5:E:83:CYS:O	5:E:113:GLN:NE2	2.39	0.54
7:G:96:SER:HB2	7:G:100:THR:HG21	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLN:NE2	1:A:1627:LEU:HD13	2.23	0.54
1:A:730:GLN:O	1:A:734:THR:HG22	2.08	0.53
2:B:555:GLN:HB2	2:B:646:HIS:HE1	1.73	0.53
2:B:650:LEU:HB3	2:B:663:ILE:HG23	1.89	0.53
2:B:769:PHE:CE2	2:B:799:GLY:HA2	2.43	0.53
2:B:242:ASP:OD2	2:B:414:LYS:NZ	2.31	0.53
2:B:770:ASN:O	9:J:48:ARG:NH1	2.40	0.53
6:F:112:GLU:HB2	6:F:123:LYS:HZ3	1.73	0.53
1:A:1053:ASP:OD1	1:A:1580:ARG:NH1	2.42	0.53
2:B:673:ASN:ND2	2:B:685:VAL:O	2.41	0.53
1:A:15:ASP:HB3	1:A:1631:ARG:HB2	1.89	0.53
2:B:38:LEU:HD11	2:B:493:PHE:HZ	1.74	0.53
7:G:37:CYS:HG	7:G:125:TRP:CD1	2.26	0.53
1:A:985:ARG:HG3	1:A:988:SER:H	1.72	0.53
2:B:33:SER:HA	2:B:177:PRO:HG3	1.89	0.53
3:C:255:VAL:HG12	3:C:269:ASP:O	2.09	0.53
3:C:70:ILE:HG23	3:C:74:GLU:HB2	1.90	0.53
8:H:47:PHE:CD1	8:H:95:TYR:HB2	2.43	0.53
1:A:603:HIS:HE1	1:A:620:ASN:HD22	1.57	0.53
1:A:697:TYR:CZ	10:K:104:ARG:HB2	2.44	0.53
1:A:781:LEU:HB3	1:A:786:TYR:HE1	1.74	0.53
2:B:393:ASN:HD21	2:B:395:ASP:HB2	1.73	0.53
2:B:725:THR:OG1	2:B:767:ASN:OD1	2.17	0.53
1:A:875:LEU:HD21	1:A:974:THR:HG21	1.91	0.53
8:H:93:TYR:CD1	8:H:145:ARG:HB2	2.44	0.53
2:B:416:LYS:HD2	2:B:460:LYS:HD3	1.92	0.52
2:B:711:GLN:HG2	2:B:713:PRO:HD2	1.91	0.52
5:E:88:VAL:HG11	5:E:110:PHE:HE2	1.74	0.52
5:E:178:ILE:HG23	5:E:214:CYS:HA	1.91	0.52
2:B:726:MET:O	2:B:744:LEU:HB2	2.09	0.52
2:B:1042:ASP:O	2:B:1063:ARG:NE	2.43	0.52
1:A:4:SER:HB2	1:A:573:LEU:HD13	1.91	0.52
2:B:274:VAL:HA	2:B:277:LEU:HD12	1.91	0.52
1:A:637:PHE:O	1:A:639:GLN:NE2	2.39	0.52
2:B:1015:SER:HG	2:B:1018:THR:HG1	1.56	0.52
1:A:251:ILE:HG23	1:A:315:ILE:HG23	1.91	0.52
1:A:721:LYS:NZ	8:H:93:TYR:O	2.40	0.52
1:A:1641:ILE:HD11	2:B:1088:LEU:HD21	1.92	0.52
3:C:105:PRO:HG3	9:J:13:VAL:HG21	1.90	0.52
1:A:524:ILE:HG12	1:A:555:LYS:HG2	1.92	0.52
1:A:1042:ASP:OD1	1:A:1043:GLY:N	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:VAL:HG21	2:B:441:LYS:HD3	1.92	0.52
3:C:94:ASP:OD2	11:L:60:ARG:NH2	2.25	0.52
2:B:45:HIS:HB3	2:B:164:MET:HE1	1.92	0.52
3:C:233:ILE:HB	3:C:267:VAL:HG11	1.91	0.52
2:B:1161:ASP:OD1	2:B:1161:ASP:N	2.42	0.51
2:B:214:PRO:O	2:B:380:LYS:NZ	2.35	0.51
14:T:14:DG:H2"	14:T:15:DA:C8	2.46	0.51
1:A:1094:ALA:HB2	1:A:1132:TYR:HB3	1.93	0.51
2:B:1076:ARG:HG3	2:B:1088:LEU:HD11	1.93	0.51
2:B:1127:CYS:HG	2:B:1159:TRP:CG	2.29	0.51
2:B:280:LEU:HD11	2:B:358:VAL:HG11	1.92	0.51
5:E:147:HIS:HE1	5:E:149:LEU:HG	1.75	0.51
1:A:1619:CYS:SG	1:A:1620:GLN:N	2.83	0.51
2:B:21:ARG:NH2	9:J:54:VAL:HA	2.26	0.51
1:A:385:LEU:HD13	1:A:437:PHE:HA	1.92	0.51
2:B:273:VAL:HG21	2:B:378:ILE:HD11	1.92	0.51
2:B:361:HIS:NE2	2:B:590:GLY:O	2.33	0.51
6:F:128:LYS:NZ	6:F:151:LEU:O	2.34	0.51
1:A:825:ALA:HB2	2:B:1022:LEU:HD13	1.92	0.51
1:A:1626:VAL:HG21	2:B:1194:ILE:HD12	1.92	0.51
2:B:898:LEU:O	2:B:899:GLN:NE2	2.30	0.51
1:A:13:SER:HB2	1:A:1632:GLU:O	2.10	0.50
2:B:914:GLY:HA2	2:B:926:VAL:HB	1.92	0.50
1:A:332:GLN:OE1	1:A:350:VAL:N	2.44	0.50
1:A:1181:PRO:HD2	6:F:86:THR:HG21	1.93	0.50
2:B:93:ASN:HB2	2:B:440:PHE:HD2	1.77	0.50
1:A:475:ARG:NH1	14:T:20:DC:OP1	2.37	0.50
1:A:827:THR:HG21	2:B:1026:ILE:HG23	1.93	0.50
1:A:1548:ALA:O	1:A:1552:THR:OG1	2.29	0.50
3:C:216:HIS:CD2	3:C:218:LYS:H	2.30	0.50
2:B:18:THR:C	2:B:20:GLU:H	2.18	0.50
2:B:581:PRO:HG3	2:B:637:TYR:CZ	2.46	0.50
5:E:119:SER:HB2	13:S:37:DA:OP1	2.11	0.50
2:B:1072:GLY:N	2:B:1075:GLU:OE1	2.32	0.50
3:C:230:LEU:HD22	3:C:297:HIS:CE1	2.47	0.50
1:A:681:THR:O	1:A:780:ILE:HG22	2.12	0.50
2:B:675:ALA:HB3	2:B:689:VAL:HG12	1.93	0.50
1:A:986:PHE:C	2:B:960:ILE:HD12	2.36	0.50
5:E:147:HIS:CE1	5:E:149:LEU:HG	2.47	0.50
14:T:18:DC:H2'	14:T:19:DT:C6	2.47	0.50
1:A:686:PHE:HB3	1:A:725:LEU:HD13	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1663:ALA:HB2	7:G:101:SER:HA	1.93	0.49
1:A:1657:LEU:HD11	6:F:135:ARG:HB2	1.94	0.49
2:B:180:LEU:HD22	2:B:185:GLU:HG2	1.92	0.49
2:B:656:LEU:HB3	2:B:657:PRO:HD3	1.94	0.49
2:B:1176:VAL:HG12	2:B:1178:ILE:HG23	1.95	0.49
5:E:80:VAL:HG22	5:E:109:ILE:HD11	1.94	0.49
7:G:93:ASP:N	7:G:93:ASP:OD1	2.45	0.49
2:B:753:LYS:NZ	2:B:758:ASP:OD2	2.34	0.49
2:B:828:GLY:HA3	2:B:862:PHE:CD1	2.47	0.49
2:B:1108:GLY:HA3	2:B:1197:ARG:HG3	1.95	0.49
7:G:37:CYS:SG	7:G:125:TRP:NE1	2.86	0.49
8:H:56:THR:HB	8:H:145:ARG:HB3	1.94	0.49
1:A:1121:ASP:OD1	5:E:197:LYS:NZ	2.46	0.49
1:A:629:ASP:HB2	2:B:924:LYS:HG3	1.95	0.49
2:B:636:GLN:HG2	2:B:637:TYR:N	2.28	0.49
5:E:32:GLN:HA	5:E:35:VAL:HB	1.94	0.49
1:A:1109:SER:HA	1:A:1116:GLN:NE2	2.28	0.49
10:K:60:SER:HB3	10:K:106:GLN:HG2	1.94	0.49
1:A:111:LYS:N	1:A:234:ASP:OD2	2.46	0.48
2:B:727:GLY:O	2:B:744:LEU:N	2.41	0.48
1:A:100:ALA:HB1	1:A:227:LEU:HG	1.96	0.48
1:A:862:THR:HG23	1:A:864:LEU:HG	1.94	0.48
1:A:993:GLN:OE1	1:A:993:GLN:N	2.36	0.48
1:A:15:ASP:N	1:A:15:ASP:OD1	2.44	0.48
1:A:233:CYS:SG	1:A:234:ASP:N	2.86	0.48
2:B:402:VAL:O	2:B:647:SER:HB2	2.12	0.48
2:B:1025:ASP:OD2	3:C:277:ARG:NH1	2.46	0.48
1:A:129:LEU:HD23	1:A:132:GLU:HG3	1.96	0.48
1:A:120:CYS:SG	1:A:136:LEU:HD21	2.54	0.48
1:A:985:ARG:HE	1:A:987:TYR:HD2	1.62	0.48
2:B:623:ASP:HB3	2:B:648:ARG:NH2	2.20	0.48
12:R:6:U:H2'	12:R:7:C:C6	2.49	0.48
2:B:102:VAL:HG22	2:B:139:LEU:HG	1.95	0.48
2:B:657:PRO:C	2:B:659:ASP:H	2.21	0.48
3:C:42:VAL:HG11	10:K:135:PHE:HD1	1.78	0.48
1:A:1062:HIS:O	1:A:1173:LYS:NZ	2.32	0.48
1:A:1085:LEU:O	1:A:1089:LEU:HD12	2.14	0.48
1:A:1555:VAL:HG21	1:A:1593:GLY:HA2	1.94	0.48
2:B:946:ASP:OD1	2:B:946:ASP:N	2.35	0.48
2:B:954:PHE:N	2:B:955:PRO:HD2	2.29	0.48
2:B:636:GLN:HG2	2:B:637:TYR:H	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:45:SER:HB2	3:C:271:ARG:NH2	2.29	0.48
8:H:8:ASP:HB3	8:H:10:PHE:CE1	2.48	0.48
11:L:50:ASP:OD1	11:L:50:ASP:N	2.47	0.48
1:A:996:TYR:HE1	2:B:530:PRO:HB3	1.79	0.48
2:B:346:ASP:HA	2:B:349:VAL:HG12	1.96	0.48
2:B:874:TYR:CZ	2:B:876:SER:HB3	2.49	0.48
2:B:547:HIS:CE1	2:B:695:ASN:HA	2.49	0.47
1:A:470:HIS:ND1	2:B:1056:THR:HG21	2.29	0.47
2:B:402:VAL:HG21	2:B:545:PHE:HZ	1.79	0.47
1:A:980:GLY:HA2	1:A:997:PHE:CD2	2.49	0.47
2:B:208:VAL:HG22	2:B:209:GLN:H	1.78	0.47
1:A:674:ILE:HD13	1:A:783:LYS:HB2	1.96	0.47
6:F:75:PRO:HA	7:G:95:LEU:HD13	1.96	0.47
6:F:112:GLU:HB2	6:F:123:LYS:NZ	2.29	0.47
1:A:587:VAL:HG12	1:A:589:MET:HG2	1.96	0.47
1:A:657:TYR:CE2	1:A:665:PRO:HB3	2.49	0.47
1:A:798:HIS:CE1	1:A:803:PRO:HB3	2.50	0.47
1:A:381:SER:HB2	1:A:453:ILE:HD13	1.96	0.47
1:A:846:ILE:O	1:A:849:THR:OG1	2.15	0.47
1:A:899:LYS:O	1:A:903:ILE:HG12	2.14	0.47
2:B:110:ASN:HB2	2:B:118:GLU:HG2	1.96	0.47
2:B:232:TYR:CE2	2:B:385:VAL:HA	2.49	0.47
3:C:216:HIS:CE1	11:L:70:ARG:HA	2.45	0.47
1:A:952:LEU:HD23	1:A:957:VAL:HA	1.96	0.47
2:B:158:CYS:HB3	2:B:457:ILE:HB	1.96	0.47
2:B:349:VAL:O	2:B:353:VAL:HG23	2.14	0.47
3:C:216:HIS:HD2	3:C:218:LYS:H	1.63	0.47
5:E:164:LEU:HD23	5:E:195:VAL:HG11	1.97	0.47
1:A:1032:VAL:HG23	1:A:1185:VAL:HG21	1.97	0.47
2:B:697:LEU:HB3	2:B:701:ALA:HB3	1.96	0.47
10:K:45:GLU:OE1	10:K:45:GLU:N	2.47	0.47
1:A:65:CYS:HB3	1:A:75:HIS:CE1	2.50	0.47
10:K:76:LEU:O	10:K:80:ILE:HG22	2.15	0.47
1:A:1070:LEU:HD11	1:A:1161:VAL:HG11	1.97	0.47
6:F:82:THR:O	6:F:136:ARG:NH1	2.42	0.47
7:G:47:VAL:HB	7:G:65:HIS:CD2	2.50	0.47
1:A:699:CYS:SG	1:A:816:LEU:HB2	2.55	0.46
2:B:412:ILE:HG12	2:B:461:MET:HE1	1.96	0.46
2:B:1070:ARG:NH1	14:T:19:DT:OP1	2.49	0.46
3:C:110:PRO:HB3	3:C:210:LEU:HD11	1.96	0.46
1:A:520:ARG:NH1	1:A:559:ASN:HA	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:PRO:HB3	1:A:707:THR:HG22	1.97	0.46
1:A:866:LYS:HE3	1:A:866:LYS:HB2	1.70	0.46
2:B:390:SER:N	2:B:635:GLY:O	2.47	0.46
2:B:489:GLU:HG3	2:B:495:ARG:HH21	1.81	0.46
3:C:75:VAL:HB	3:C:221:PRO:HG3	1.96	0.46
4:D:25:THR:HA	6:F:58:PHE:CE2	2.50	0.46
1:A:474:LYS:HD2	2:B:1092:LEU:O	2.16	0.46
1:A:1034:TYR:CE1	6:F:136:ARG:HD3	2.50	0.46
2:B:255:ASP:HB3	2:B:257:GLN:HG2	1.97	0.46
3:C:165:ARG:NH1	3:C:190:ASP:OD1	2.49	0.46
7:G:45:LEU:CD1	7:G:118:CYS:HB2	2.45	0.46
1:A:416:ARG:HA	1:A:419:ILE:HG22	1.96	0.46
2:B:196:VAL:HG11	2:B:466:SER:HB3	1.98	0.46
10:K:47:ILE:HG13	10:K:65:ILE:HG12	1.97	0.46
1:A:589:MET:HE3	1:A:633:MET:HE2	1.98	0.46
1:A:697:TYR:HB2	10:K:88:PHE:CZ	2.50	0.46
1:A:1037:SER:HB2	1:A:1045:LEU:HD11	1.97	0.46
2:B:178:TYR:O	2:B:182:GLN:HG2	2.14	0.46
2:B:709:PHE:O	2:B:961:GLY:N	2.49	0.46
3:C:280:LEU:HD12	3:C:280:LEU:H	1.81	0.46
1:A:964:LYS:NZ	1:A:967:PRO:HA	2.31	0.46
2:B:1053:ASN:O	2:B:1057:MET:N	2.40	0.46
3:C:45:SER:HB2	3:C:271:ARG:HH21	1.79	0.46
5:E:178:ILE:HG22	5:E:212:ARG:HB3	1.97	0.46
5:E:178:ILE:HG13	5:E:182:ASP:OD2	2.15	0.46
6:F:127:GLU:HB2	6:F:129:LYS:HG2	1.98	0.46
1:A:498:PRO:HB3	1:A:612:LYS:HA	1.98	0.46
1:A:996:TYR:CZ	2:B:520:LEU:HD21	2.51	0.46
2:B:488:ALA:HA	2:B:499:HIS:CD2	2.51	0.46
2:B:811:LEU:HD23	2:B:825:PHE:CZ	2.51	0.46
2:B:929:ARG:HD3	2:B:931:TRP:CZ3	2.51	0.46
14:T:13:DA:H2"	14:T:14:DG:C8	2.51	0.46
1:A:572:THR:HG21	4:D:16:LEU:HD21	1.98	0.45
1:A:589:MET:SD	1:A:635:MET:HB2	2.55	0.45
2:B:884:GLU:HG2	2:B:904:LYS:HB3	1.98	0.45
2:B:1014:TYR:HH	3:C:293:ARG:HH22	1.63	0.45
1:A:942:GLN:HG2	1:A:947:LEU:HA	1.99	0.45
1:A:964:LYS:NZ	2:B:672:MET:O	2.49	0.45
2:B:1103:VAL:HG22	2:B:1110:ILE:HG23	1.98	0.45
3:C:42:VAL:HG23	10:K:134:LYS:HB3	1.99	0.45
11:L:61:THR:OG1	11:L:62:LYS:N	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:324:THR:HA	2:B:327:LEU:HD13	1.98	0.45
1:A:236:CYS:O	1:A:238:MET:N	2.48	0.45
3:C:107:LYS:HE3	3:C:187:ALA:HA	1.98	0.45
3:C:196:LEU:HD21	3:C:202:ILE:HG13	1.97	0.45
1:A:339:PHE:O	1:A:340:HIS:ND1	2.50	0.45
1:A:996:TYR:CE1	2:B:530:PRO:HB3	2.51	0.45
2:B:267:ASN:OD1	2:B:267:ASN:N	2.49	0.45
3:C:40:PHE:HE2	10:K:131:VAL:HA	1.81	0.45
8:H:80:ARG:HG3	8:H:81:PRO:HD2	1.98	0.45
1:A:673:HIS:NE2	2:B:783:MET:HE1	2.31	0.45
2:B:21:ARG:HD2	2:B:763:ASP:HB2	1.99	0.45
2:B:830:ASP:OD1	2:B:830:ASP:N	2.50	0.45
7:G:65:HIS:C	7:G:68:PRO:HD2	2.42	0.45
10:K:89:CYS:SG	10:K:105:ILE:HG12	2.56	0.45
1:A:900:VAL:HG21	1:A:949:GLN:OE1	2.17	0.45
10:K:126:ASP:O	10:K:130:VAL:HG13	2.16	0.45
14:T:29:DG:H4'	14:T:30:DT:OP1	2.17	0.45
1:A:102:CYS:HB2	1:A:233:CYS:HB2	1.98	0.45
1:A:611:GLU:OE1	1:A:615:ARG:NH1	2.50	0.45
2:B:52:LEU:HA	2:B:60:LEU:HB2	1.97	0.45
3:C:216:HIS:HD2	3:C:217:ALA:N	2.15	0.45
1:A:636:HIS:HB3	2:B:1091:ARG:HD2	1.99	0.45
2:B:609:ARG:HA	2:B:612:LYS:HG2	1.98	0.45
1:A:798:HIS:HE1	1:A:803:PRO:HB3	1.82	0.45
1:A:1076:LEU:O	1:A:1079:LYS:HG2	2.16	0.45
1:A:1651:THR:HG22	6:F:92:ARG:HD2	1.98	0.45
2:B:794:ASP:HA	2:B:798:PHE:H	1.81	0.45
2:B:811:LEU:HD13	2:B:811:LEU:HA	1.84	0.45
1:A:94:LEU:HD12	1:A:324:LEU:HD12	1.99	0.44
1:A:653:THR:HB	1:A:667:ARG:NH2	2.32	0.44
2:B:211:ARG:HH12	2:B:243:GLN:CD	2.24	0.44
2:B:416:LYS:NZ	2:B:460:LYS:HB3	2.32	0.44
2:B:656:LEU:HD21	2:B:681:ILE:HD13	1.99	0.44
2:B:750:PRO:HB2	2:B:752:VAL:O	2.17	0.44
3:C:100:ARG:NH2	9:J:3:VAL:O	2.46	0.44
14:T:28:DC:H2"	14:T:29:DG:H2'	1.98	0.44
1:A:610:ASN:ND2	1:A:611:GLU:OE2	2.50	0.44
1:A:1053:ASP:HA	1:A:1124:LEU:HD13	1.99	0.44
2:B:753:LYS:O	2:B:980:ASP:HA	2.18	0.44
2:B:1017:ALA:HB1	10:K:70:HIS:CD2	2.53	0.44
5:E:79:TRP:HB2	5:E:105:PHE:CE2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:38:LEU:HD21	11:L:56:LEU:HD22	2.00	0.44
1:A:94:LEU:HD13	1:A:355:PHE:HB3	1.99	0.44
1:A:516:ILE:HG21	1:A:562:LEU:HB2	1.99	0.44
1:A:592:GLN:HE22	1:A:634:ASN:HD21	1.64	0.44
2:B:334:PHE:HB3	2:B:338:PHE:CD1	2.52	0.44
2:B:505:ARG:HD2	2:B:505:ARG:HA	1.70	0.44
6:F:109:VAL:HG11	6:F:123:LYS:HB3	1.98	0.44
1:A:1057:ILE:H	1:A:1057:ILE:HG13	1.50	0.44
2:B:819:ASP:OD1	2:B:819:ASP:N	2.50	0.44
1:A:1000:MET:HG2	2:B:520:LEU:HD22	1.99	0.44
1:A:1183:GLU:HG2	6:F:88:TYR:OH	2.18	0.44
2:B:43:GLN:N	2:B:44:PRO:HD2	2.33	0.44
1:A:672:ASP:HB2	2:B:783:MET:HE2	1.99	0.44
2:B:143:TRP:CH2	2:B:449:VAL:HG11	2.53	0.44
2:B:704:THR:OG1	2:B:920:ARG:O	2.30	0.44
1:A:942:GLN:HB3	1:A:947:LEU:HD12	2.00	0.44
1:A:1118:VAL:C	1:A:1120:TYR:H	2.25	0.44
2:B:810:ASP:OD1	2:B:812:ALA:N	2.51	0.44
3:C:197:ARG:HA	3:C:197:ARG:HD3	1.79	0.44
3:C:314:PHE:O	3:C:318:VAL:HG13	2.18	0.44
5:E:36:GLU:O	5:E:38:PRO:HD3	2.18	0.44
8:H:15:VAL:HG22	8:H:26:ILE:HG23	2.00	0.44
1:A:83:VAL:HG11	1:A:427:PHE:CE1	2.44	0.44
1:A:504:LYS:HA	1:A:504:LYS:HD3	1.65	0.44
7:G:64:GLN:O	7:G:68:PRO:HG2	2.18	0.44
8:H:95:TYR:HB3	8:H:144:ILE:HB	2.00	0.44
9:J:41:LEU:HD22	9:J:46:CYS:HB3	2.00	0.44
2:B:40:GLU:HA	2:B:43:GLN:HG2	2.00	0.44
2:B:53:THR:HG21	2:B:169:ARG:HD2	2.00	0.44
2:B:627:GLY:HA3	2:B:667:PHE:CD1	2.53	0.44
2:B:731:VAL:HG12	9:J:60:PHE:CE1	2.52	0.44
2:B:1114:GLN:OE1	2:B:1129:ARG:HD3	2.18	0.44
1:A:223:PHE:O	1:A:227:LEU:HB2	2.18	0.43
1:A:245:LYS:HE3	1:A:245:LYS:HB3	1.82	0.43
1:A:248:PHE:O	1:A:249:THR:OG1	2.27	0.43
1:A:928:MET:SD	2:B:955:PRO:HG3	2.58	0.43
1:A:1033:SER:OG	1:A:1034:TYR:N	2.51	0.43
2:B:909:ARG:HD3	2:B:909:ARG:HA	1.87	0.43
3:C:59:ILE:H	3:C:296:ASN:HB3	1.82	0.43
1:A:671:GLN:HE21	1:A:934:LYS:HD3	1.83	0.43
2:B:106:LYS:NZ	2:B:168:ASN:O	2.37	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:TRP:CD1	2:B:152:LEU:HD12	2.53	0.43
2:B:425:ILE:HD13	2:B:425:ILE:HA	1.74	0.43
2:B:700:LEU:HD13	2:B:700:LEU:HA	1.87	0.43
2:B:1189:LEU:HD23	2:B:1189:LEU:HA	1.79	0.43
2:B:216:ALA:HA	2:B:234:ILE:HD13	2.00	0.43
2:B:280:LEU:HD23	2:B:354:LEU:HD13	2.01	0.43
2:B:548:LYS:HD3	2:B:548:LYS:HA	1.72	0.43
5:E:180:ARG:HD2	5:E:192:ARG:HG3	1.99	0.43
6:F:99:LEU:O	6:F:102:SER:OG	2.28	0.43
14:T:2:DT:H2"	14:T:3:DA:C8	2.53	0.43
1:A:93:GLN:HE21	1:A:1627:LEU:HD13	1.82	0.43
1:A:618:TYR:CD1	1:A:670:ILE:HD11	2.54	0.43
1:A:810:LEU:HD23	1:A:810:LEU:HA	1.84	0.43
1:A:904:THR:HG23	1:A:946:LEU:HD11	1.99	0.43
1:A:957:VAL:HG11	1:A:997:PHE:CE1	2.54	0.43
2:B:38:LEU:HA	2:B:38:LEU:HD12	1.75	0.43
2:B:393:ASN:ND2	2:B:395:ASP:HB2	2.33	0.43
1:A:230:ARG:NH2	14:T:4:DC:O5'	2.43	0.43
1:A:755:ILE:HD12	1:A:780:ILE:HD11	2.01	0.43
1:A:1104:TYR:O	1:A:1108:HIS:ND1	2.31	0.43
2:B:46:ILE:HD11	2:B:192:GLY:H	1.84	0.43
2:B:122:TYR:CE1	2:B:171:HIS:HB3	2.53	0.43
2:B:207:ILE:HD11	2:B:400:GLN:HB3	2.00	0.43
2:B:1055:LEU:HD23	2:B:1055:LEU:H	1.84	0.43
8:H:116:TYR:HE2	8:H:140:ALA:HB3	1.84	0.43
1:A:89:LEU:HD11	2:B:1192:MET:HB3	2.00	0.43
1:A:588:LEU:HD11	1:A:600:MET:HG2	2.01	0.43
1:A:832:ASP:OD1	1:A:832:ASP:N	2.51	0.43
1:A:373:LEU:HB2	12:R:3:A:N7	2.34	0.43
1:A:1039:ARG:CZ	1:A:1045:LEU:HD13	2.49	0.43
2:B:214:PRO:HD3	2:B:373:MET:HE1	2.01	0.43
2:B:782:ASP:HA	2:B:786:ALA:HB3	2.00	0.43
2:B:843:ASP:OD2	11:L:29:TYR:OH	2.23	0.43
3:C:43:ASN:OD1	3:C:44:ILE:N	2.52	0.43
1:A:100:ALA:H	1:A:109:ARG:HH22	1.67	0.43
1:A:510:PRO:HG2	6:F:102:SER:HB2	2.01	0.43
1:A:964:LYS:HZ1	1:A:967:PRO:HA	1.84	0.43
3:C:259:ASP:HB3	3:C:262:SER:O	2.19	0.43
6:F:69:LEU:HG	7:G:94:PRO:HG3	2.00	0.43
1:A:360:LEU:HD11	1:A:434:VAL:HG22	2.01	0.43
1:A:360:LEU:HD23	1:A:360:LEU:HA	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:GLN:NE2	1:A:435:ASN:OD1	2.52	0.43
1:A:588:LEU:HD12	1:A:601:MET:O	2.19	0.43
1:A:916:THR:HG21	1:A:926:GLN:NE2	2.34	0.43
1:A:1027:LEU:HD23	1:A:1588:MET:HG2	2.01	0.43
2:B:338:PHE:CE2	2:B:353:VAL:HG22	2.53	0.43
2:B:546:ALA:HB1	2:B:695:ASN:O	2.19	0.43
2:B:745:GLN:HG3	2:B:746:THR:HG23	2.01	0.43
2:B:804:TYR:CE1	2:B:906:ARG:HB3	2.54	0.43
2:B:1125:THR:OG1	2:B:1126:VAL:N	2.52	0.43
6:F:119:ARG:HA	6:F:119:ARG:HD3	1.72	0.43
7:G:90:LEU:HD23	7:G:90:LEU:HA	1.89	0.43
1:A:119:ALA:HB2	1:A:334:VAL:HG13	2.01	0.42
1:A:520:ARG:HH12	1:A:559:ASN:HA	1.84	0.42
2:B:97:VAL:HG11	2:B:425:ILE:HD11	2.01	0.42
2:B:912:GLN:N	2:B:915:ASP:OD2	2.50	0.42
11:L:55:ILE:O	11:L:56:LEU:HD23	2.19	0.42
1:A:475:ARG:HH12	14:T:20:DC:P	2.39	0.42
1:A:1228:THR:HB	13:S:26:DT:H5'	2.01	0.42
1:A:1636:SER:O	1:A:1640:ARG:HG3	2.19	0.42
1:A:1660:VAL:O	7:G:102:GLU:HA	2.19	0.42
2:B:207:ILE:HG12	2:B:400:GLN:NE2	2.34	0.42
2:B:1090:ASP:HA	2:B:1094:ASN:HB2	2.01	0.42
14:T:15:DA:H2'	14:T:16:DT:C6	2.54	0.42
1:A:693:GLN:OE1	10:K:88:PHE:HA	2.18	0.42
2:B:531:VAL:O	2:B:716:MET:HG2	2.19	0.42
2:B:739:ASN:O	2:B:805:LYS:HG3	2.19	0.42
6:F:146:TRP:HB3	6:F:151:LEU:HD21	2.01	0.42
2:B:739:ASN:O	2:B:805:LYS:HA	2.19	0.42
5:E:67:GLU:O	5:E:70:SER:OG	2.29	0.42
1:A:114:GLU:OE2	1:A:117:ARG:NH2	2.52	0.42
1:A:373:LEU:HD22	12:R:3:A:N7	2.34	0.42
1:A:819:ASN:HA	1:A:822:THR:HG22	2.00	0.42
1:A:956:ARG:HH21	1:A:979:GLY:CA	2.32	0.42
2:B:132:SER:HB2	2:B:134:ARG:HH11	1.84	0.42
2:B:782:ASP:OD1	2:B:782:ASP:N	2.51	0.42
5:E:93:MET:HG2	5:E:120:ALA:O	2.19	0.42
13:S:37:DA:H2"	13:S:38:DG:C8	2.54	0.42
1:A:1592:GLN:HG3	1:A:1596:LEU:HD11	2.01	0.42
2:B:714:ARG:HA	2:B:714:ARG:HD3	1.81	0.42
2:B:1000:LEU:HD23	2:B:1000:LEU:HA	1.86	0.42
1:A:697:TYR:CE1	10:K:104:ARG:HB2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:942:GLN:HA	1:A:946:LEU:O	2.20	0.42
2:B:252:TYR:CG	2:B:385:VAL:HG11	2.54	0.42
2:B:837:LEU:HD13	2:B:837:LEU:HA	1.92	0.42
5:E:202:SER:N	5:E:206:GLY:O	2.44	0.42
12:R:6:U:H2'	12:R:7:C:H6	1.84	0.42
1:A:697:TYR:OH	1:A:703:GLU:OE2	2.21	0.42
1:A:781:LEU:HB3	1:A:786:TYR:CE1	2.53	0.42
2:B:791:LYS:HB3	2:B:932:PRO:HA	2.01	0.42
3:C:42:VAL:HG11	10:K:135:PHE:CD1	2.53	0.42
3:C:216:HIS:CD2	3:C:217:ALA:N	2.87	0.42
8:H:99:GLY:HA3	8:H:118:PHE:CD1	2.55	0.42
12:R:9:A:H2'	12:R:10:G:O4'	2.20	0.42
1:A:463:LYS:O	1:A:464:GLU:HB2	2.20	0.42
1:A:475:ARG:O	2:B:1059:PRO:HD2	2.19	0.42
1:A:721:LYS:HE2	1:A:721:LYS:HB3	1.88	0.42
1:A:1175:MET:HE2	1:A:1175:MET:HB3	1.79	0.42
2:B:12:ARG:HB3	2:B:980:ASP:OD1	2.20	0.42
2:B:129:ARG:HD2	2:B:888:ILE:HG23	2.01	0.42
2:B:147:ASN:O	2:B:147:ASN:ND2	2.53	0.42
2:B:359:LEU:HD13	2:B:373:MET:HG2	2.02	0.42
5:E:136:ASN:CG	5:E:137:GLU:H	2.28	0.42
5:E:179:GLN:HB2	5:E:182:ASP:OD1	2.19	0.42
9:J:45:CYS:SG	9:J:46:CYS:N	2.92	0.42
1:A:208:PHE:CZ	1:A:213:ASN:HB2	2.55	0.42
1:A:362:VAL:HG12	1:A:386:LEU:HD13	2.02	0.42
1:A:482:SER:HB3	1:A:614:LEU:HG	2.02	0.42
1:A:658:LEU:HD22	1:A:663:GLY:O	2.20	0.42
1:A:701:ARG:HB3	1:A:703:GLU:OE2	2.19	0.42
2:B:489:GLU:HG3	2:B:495:ARG:NH2	2.34	0.42
5:E:153:HIS:CE1	5:E:184:VAL:HG11	2.55	0.42
8:H:22:LYS:O	8:H:44:VAL:HG22	2.20	0.42
10:K:66:VAL:O	10:K:68:GLU:HG2	2.20	0.42
1:A:893:ASP:O	1:A:897:SER:OG	2.32	0.41
8:H:129:TYR:CE1	8:H:130:ARG:HG3	2.55	0.41
1:A:487:ASP:CG	10:K:95:HIS:HE2	2.28	0.41
1:A:1090:ASP:OD1	1:A:1091:VAL:N	2.53	0.41
1:A:26:ASN:ND2	2:B:1130:ARG:O	2.53	0.41
2:B:729:PRO:HG2	2:B:741:LEU:HG	2.00	0.41
3:C:85:PHE:CE2	3:C:97:LEU:HD23	2.54	0.41
3:C:95:GLU:HG2	3:C:96:VAL:N	2.34	0.41
5:E:13:TRP:HB2	5:E:42:PHE:CD2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:33:DC:H2"	13:S:34:DG:H8	1.85	0.41
14:T:5:DC:H2"	14:T:6:DG:H8	1.85	0.41
1:A:644:ARG:O	1:A:648:LEU:HB2	2.20	0.41
1:A:866:LYS:H	1:A:866:LYS:HG3	1.68	0.41
2:B:653:VAL:HG12	2:B:654:ARG:H	1.86	0.41
6:F:97:ARG:NH1	6:F:100:GLN:OE1	2.54	0.41
8:H:101:ALA:HB2	8:H:116:TYR:CZ	2.56	0.41
10:K:93:ILE:H	10:K:93:ILE:HG13	1.53	0.41
1:A:19:LEU:HD13	2:B:1195:ARG:HD2	2.02	0.41
1:A:1025:LYS:HG2	1:A:1615:TYR:CD1	2.56	0.41
1:A:1601:GLN:N	1:A:1601:GLN:OE1	2.54	0.41
2:B:211:ARG:HG2	2:B:401:GLU:OE2	2.20	0.41
2:B:279:ALA:HB1	2:B:354:LEU:HD11	2.02	0.41
2:B:494:TYR:HB3	2:B:700:LEU:HD21	2.02	0.41
3:C:280:LEU:HD11	3:C:291:LEU:HD13	2.02	0.41
10:K:46:LYS:HD3	10:K:66:VAL:HG22	2.03	0.41
1:A:100:ALA:H	1:A:109:ARG:NH2	2.18	0.41
1:A:330:LYS:HA	1:A:330:LYS:HD3	1.74	0.41
1:A:489:ASN:HB2	10:K:95:HIS:CD2	2.55	0.41
2:B:1108:GLY:O	2:B:1197:ARG:HA	2.21	0.41
3:C:40:PHE:CE2	10:K:131:VAL:HG12	2.55	0.41
3:C:80:ALA:HA	3:C:208:CYS:HB3	2.03	0.41
1:A:830:MET:HE3	1:A:987:TYR:CE1	2.55	0.41
1:A:1048:PHE:CZ	5:E:211:TYR:HB2	2.56	0.41
2:B:61:LEU:HD21	2:B:413:LEU:HD13	2.01	0.41
2:B:70:GLU:HG2	2:B:98:SER:HB3	2.01	0.41
2:B:576:THR:HG21	2:B:595:TRP:HD1	1.85	0.41
2:B:966:SER:OG	2:B:1029:GLY:HA3	2.20	0.41
3:C:304:SER:OG	3:C:308:MET:O	2.28	0.41
4:D:27:LEU:HD23	6:F:55:PRO:HG2	2.02	0.41
2:B:338:PHE:CZ	2:B:353:VAL:HG22	2.56	0.41
2:B:503:VAL:HG23	2:B:543:ASN:HB2	2.03	0.41
3:C:169:PHE:CG	3:C:184:VAL:HB	2.56	0.41
8:H:98:TYR:CE1	8:H:139:ASN:HB3	2.55	0.41
1:A:490:ILE:HD13	1:A:490:ILE:HA	1.89	0.41
1:A:532:GLY:O	1:A:580:HIS:ND1	2.54	0.41
1:A:1045:LEU:HD12	1:A:1045:LEU:HA	1.86	0.41
2:B:44:PRO:HB3	2:B:551:ILE:HG21	2.03	0.41
2:B:534:PRO:HG2	2:B:538:PRO:HB2	2.03	0.41
2:B:915:ASP:OD1	2:B:1040:VAL:HG23	2.21	0.41
2:B:1087:LEU:HD12	2:B:1087:LEU:HA	1.94	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:LEU:HD21	3:C:311:GLU:OE1	2.20	0.41
5:E:34:GLU:HA	5:E:37:LEU:HD13	2.01	0.41
7:G:67:ASN:O	7:G:70:VAL:HG22	2.21	0.41
1:A:419:ILE:HD12	1:A:419:ILE:HA	1.90	0.41
1:A:778:CYS:SG	1:A:779:GLY:N	2.93	0.41
1:A:1195:GLU:HB3	1:A:1196:PRO:HD3	2.01	0.41
1:A:1556:GLU:HG3	5:E:198:ILE:HD13	2.02	0.41
2:B:815:ARG:HB2	2:B:819:ASP:OD1	2.21	0.41
3:C:77:SER:HB3	3:C:219:PHE:O	2.21	0.41
3:C:94:ASP:HB2	11:L:67:PHE:CE2	2.55	0.41
1:A:34:ASN:OD1	1:A:34:ASN:N	2.43	0.40
1:A:117:ARG:HD2	1:A:121:LYS:HD2	2.03	0.40
1:A:702:PRO:HB3	1:A:707:THR:CG2	2.51	0.40
1:A:883:LEU:HD22	1:A:972:TYR:HE1	1.85	0.40
1:A:1226:VAL:HG13	1:A:1598:PHE:CD2	2.56	0.40
2:B:374:LEU:HD23	2:B:374:LEU:HA	1.93	0.40
2:B:603:ILE:O	2:B:607:THR:OG1	2.25	0.40
5:E:123:LEU:HA	5:E:126:SER:HB3	2.03	0.40
7:G:37:CYS:HG	7:G:125:TRP:NE1	2.19	0.40
1:A:672:ASP:CG	2:B:950:ASN:HD21	2.29	0.40
1:A:1038:ILE:H	1:A:1038:ILE:HG12	1.71	0.40
2:B:1110:ILE:HD11	2:B:1198:TYR:CD1	2.57	0.40
3:C:40:PHE:CE2	10:K:131:VAL:HA	2.56	0.40
5:E:79:TRP:HB2	5:E:105:PHE:CD2	2.56	0.40
1:A:138:GLU:HB3	5:E:128:PRO:HG3	2.02	0.40
1:A:669:LEU:H	1:A:669:LEU:HG	1.69	0.40
1:A:697:TYR:HB2	10:K:88:PHE:CE1	2.56	0.40
1:A:1038:ILE:HD11	1:A:1047:GLN:OE1	2.21	0.40
2:B:193:TYR:CD2	2:B:200:GLU:HB3	2.57	0.40
2:B:380:LYS:HG3	2:B:637:TYR:CD2	2.57	0.40
2:B:612:LYS:HB2	2:B:612:LYS:HE2	1.85	0.40
2:B:789:ILE:HG12	2:B:947:ILE:HD13	2.04	0.40
6:F:79:ARG:HB2	6:F:144:GLU:OE1	2.21	0.40
10:K:86:VAL:HA	10:K:107:THR:HA	2.03	0.40
1:A:81:LEU:HD23	1:A:81:LEU:HA	1.82	0.40
1:A:211:THR:HG21	5:E:173:SER:HB3	2.03	0.40
1:A:223:PHE:HD2	1:A:224:HIS:CD2	2.39	0.40
1:A:343:PRO:O	1:A:345:LEU:N	2.54	0.40
1:A:369:LEU:C	1:A:380:ASN:HD21	2.28	0.40
1:A:507:TYR:HB2	1:A:637:PHE:CE2	2.57	0.40
1:A:1012:LYS:HD3	1:A:1012:LYS:HA	1.90	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:381:LEU:O	2:B:385:VAL:HG22	2.20	0.40
2:B:1160:GLU:HG3	2:B:1166:LYS:HG2	2.02	0.40
1:A:37:VAL:HG22	1:A:49:LEU:HD12	2.04	0.40
1:A:472:MET:O	2:B:1092:LEU:HD11	2.22	0.40
1:A:498:PRO:HB3	1:A:611:GLU:O	2.21	0.40
1:A:507:TYR:CD1	1:A:509:GLU:HG2	2.57	0.40
1:A:1032:VAL:HG12	1:A:1181:PRO:HA	2.03	0.40
2:B:1063:ARG:HB2	14:T:21:DT:OP1	2.20	0.40
3:C:168:LYS:HE2	3:C:168:LYS:HB3	1.78	0.40
5:E:200:ARG:HD2	5:E:208:TYR:CE1	2.57	0.40
7:G:102:GLU:N	7:G:102:GLU:OE1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1210/1664 (73%)	1124 (93%)	86 (7%)	0	100	100
2	B	1099/1203 (91%)	1023 (93%)	76 (7%)	0	100	100
3	C	302/335 (90%)	289 (96%)	13 (4%)	0	100	100
4	D	16/137 (12%)	16 (100%)	0	0	100	100
5	E	201/215 (94%)	194 (96%)	7 (4%)	0	100	100
6	F	98/155 (63%)	93 (95%)	5 (5%)	0	100	100
7	G	89/326 (27%)	81 (91%)	8 (9%)	0	100	100
8	H	127/146 (87%)	118 (93%)	9 (7%)	0	100	100
9	J	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
10	K	96/142 (68%)	93 (97%)	3 (3%)	0	100	100
11	L	42/70 (60%)	39 (93%)	3 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3347/4463 (75%)	3135 (94%)	212 (6%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1073/1465 (73%)	1005 (94%)	68 (6%)	15 42
2	B	971/1053 (92%)	918 (94%)	53 (6%)	18 46
3	C	268/296 (90%)	256 (96%)	12 (4%)	23 53
4	D	16/116 (14%)	15 (94%)	1 (6%)	15 42
5	E	188/197 (95%)	182 (97%)	6 (3%)	34 62
6	F	90/137 (66%)	87 (97%)	3 (3%)	33 61
7	G	82/291 (28%)	77 (94%)	5 (6%)	15 43
8	H	115/128 (90%)	112 (97%)	3 (3%)	41 66
9	J	64/65 (98%)	61 (95%)	3 (5%)	22 51
10	K	88/130 (68%)	87 (99%)	1 (1%)	70 83
11	L	39/57 (68%)	33 (85%)	6 (15%)	2 14
All	All	2994/3935 (76%)	2833 (95%)	161 (5%)	21 46

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	18	ILE
1	A	34	ASN
1	A	45	VAL
1	A	54	LEU
1	A	113	VAL
1	A	114	GLU
1	A	115	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	130	ILE
1	A	209	THR
1	A	211	THR
1	A	212	VAL
1	A	315	ILE
1	A	316	LEU
1	A	349	LEU
1	A	392	THR
1	A	413	LEU
1	A	434	VAL
1	A	453	ILE
1	A	483	VAL
1	A	551	VAL
1	A	555	LYS
1	A	572	THR
1	A	577	VAL
1	A	583	ASN
1	A	587	VAL
1	A	590	ASN
1	A	596	HIS
1	A	616	LEU
1	A	620	ASN
1	A	634	ASN
1	A	635	MET
1	A	648	LEU
1	A	688	THR
1	A	696	ILE
1	A	700	ILE
1	A	703	GLU
1	A	715	LEU
1	A	740	THR
1	A	747	ILE
1	A	809	VAL
1	A	821	ILE
1	A	852	ASP
1	A	868	THR
1	A	871	ASP
1	A	961	VAL
1	A	966	LEU
1	A	974	THR
1	A	1019	LEU
1	A	1035	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1038	ILE
1	A	1057	ILE
1	A	1060	GLU
1	A	1072	ASN
1	A	1118	VAL
1	A	1120	TYR
1	A	1137	SER
1	A	1144	LEU
1	A	1162	ASN
1	A	1164	LYS
1	A	1226	VAL
1	A	1552	THR
1	A	1561	THR
1	A	1577	VAL
1	A	1594	THR
1	A	1607	THR
1	A	1622	LEU
1	A	1657	LEU
2	B	18	THR
2	B	31	ASP
2	B	37	LEU
2	B	53	THR
2	B	72	VAL
2	B	75	ASP
2	B	91	LEU
2	B	104	ILE
2	B	121	VAL
2	B	172	LEU
2	B	202	LEU
2	B	207	ILE
2	B	270	LEU
2	B	273	VAL
2	B	360	VAL
2	B	362	LEU
2	B	413	LEU
2	B	425	ILE
2	B	476	LEU
2	B	477	ASP
2	B	498	SER
2	B	503	VAL
2	B	531	VAL
2	B	564	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	606	ASP
2	B	646	HIS
2	B	653	VAL
2	B	663	ILE
2	B	664	VAL
2	B	694	THR
2	B	700	LEU
2	B	736	ARG
2	B	752	VAL
2	B	763	ASP
2	B	767	ASN
2	B	789	ILE
2	B	805	LYS
2	B	813	LEU
2	B	865	THR
2	B	905	TYR
2	B	913	ILE
2	B	946	ASP
2	B	960	ILE
2	B	1033	TYR
2	B	1046	VAL
2	B	1052	VAL
2	B	1077	ASP
2	B	1092	LEU
2	B	1106	GLU
2	B	1110	ILE
2	B	1111	LEU
2	B	1157	GLN
2	B	1161	ASP
3	C	56	LEU
3	C	94	ASP
3	C	104	VAL
3	C	108	VAL
3	C	185	VAL
3	C	223	SER
3	C	229	LEU
3	C	233	ILE
3	C	291	LEU
3	C	311	GLU
3	C	318	VAL
3	C	320	ILE
4	D	22	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	9	ILE
5	E	37	LEU
5	E	116	ILE
5	E	117	THR
5	E	119	SER
5	E	178	ILE
6	F	77	ASP
6	F	140	ASP
6	F	153	VAL
7	G	45	LEU
7	G	93	ASP
7	G	95	LEU
7	G	108	THR
7	G	120	VAL
8	H	26	ILE
8	H	89	LEU
8	H	122	LEU
9	J	25	LEU
9	J	27	GLU
9	J	54	VAL
10	K	93	ILE
11	L	40	LEU
11	L	43	THR
11	L	46	VAL
11	L	50	ASP
11	L	53	HIS
11	L	61	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	380	ASN
1	A	431	GLN
1	A	559	ASN
1	A	634	ASN
1	A	730	GLN
1	A	880	GLN
1	A	1047	GLN
2	B	27	ASN
2	B	128	GLN
2	B	231	HIS
2	B	368	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	423	ASN
2	B	469	ASN
2	B	547	HIS
2	B	598	HIS
2	B	646	HIS
2	B	669	GLN
2	B	673	ASN
2	B	867	ASN
2	B	886	ASN
2	B	1010	ASN
2	B	1094	ASN
2	B	1157	GLN
4	D	17	ASN
5	E	61	GLN
5	E	63	ASN
5	E	136	ASN
5	E	179	GLN
6	F	59	GLN
6	F	63	GLN
7	G	59	GLN
7	G	121	ASN
7	G	126	GLN
10	K	118	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	R	10/12 (83%)	3 (30%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	R	3	A
12	R	10	G
12	R	12	G

There are no RNA pucker outliers to report.

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

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	$\#\|Z\| > 2$
14	3DR	T	17	14	8,11,12	0.50	0	9,14,17	0.77	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
14	3DR	T	17	14	-	0/3/15/16	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	17	3DR	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

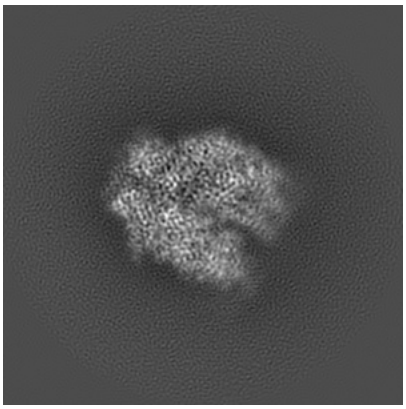
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50956. These allow visual inspection of the internal detail of the map and identification of artifacts.

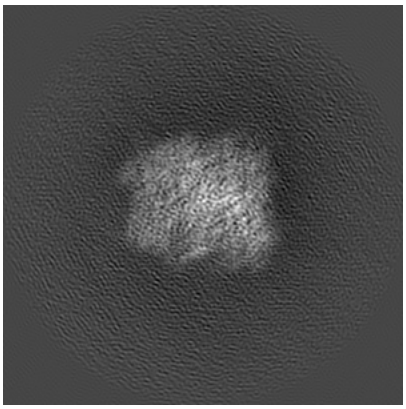
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

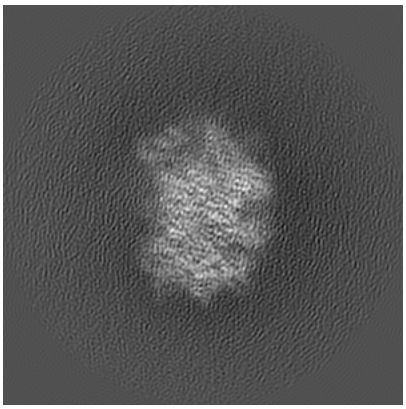
6.1.1 Primary map



X

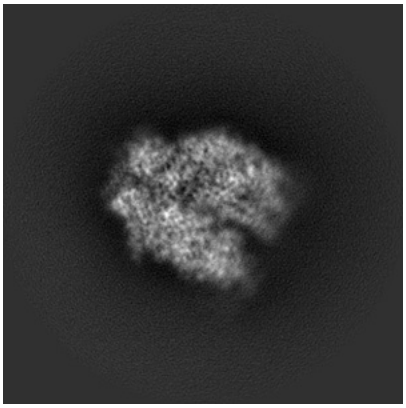


Y

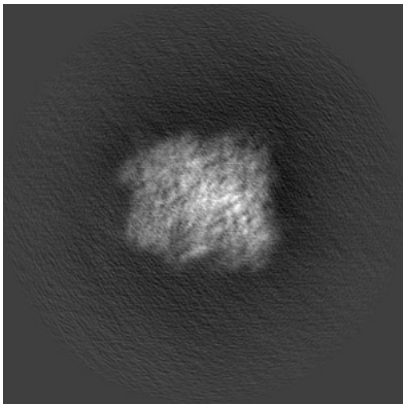


Z

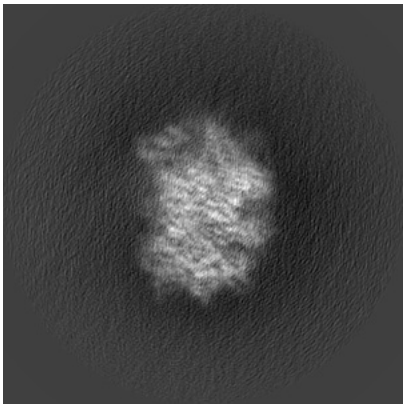
6.1.2 Raw map



X



Y

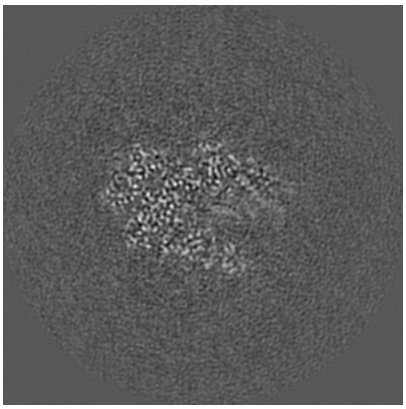


Z

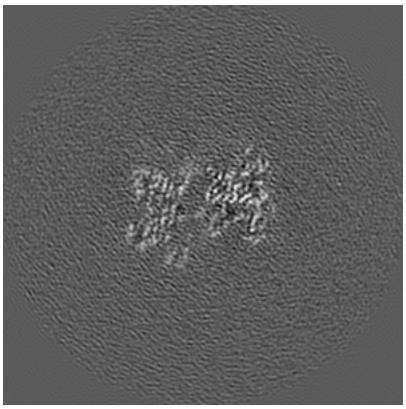
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

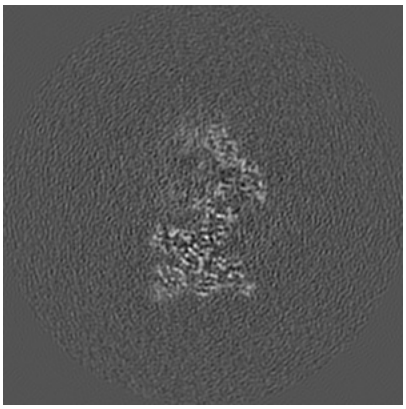
6.2.1 Primary map



X Index: 144

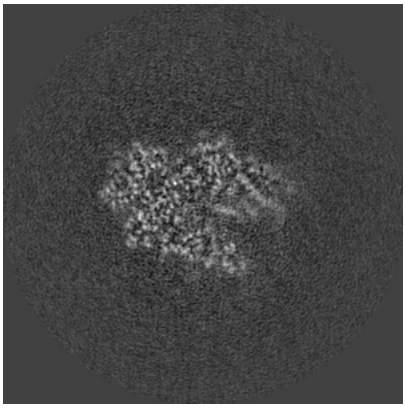


Y Index: 144



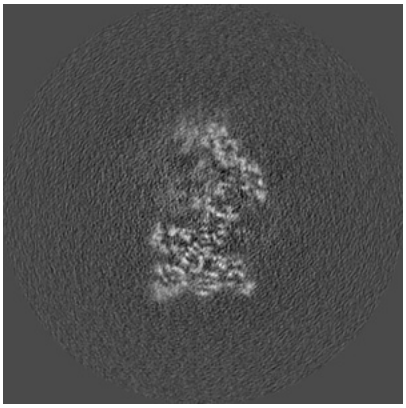
Z Index: 144

6.2.2 Raw map



X Index: 144

Y Index: 144

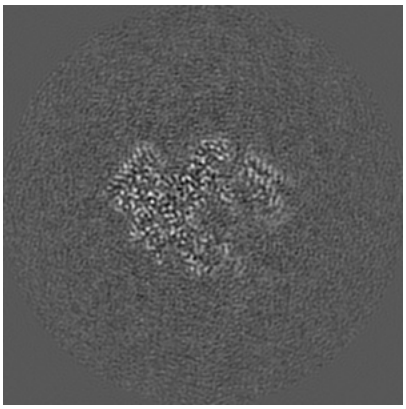


Z Index: 144

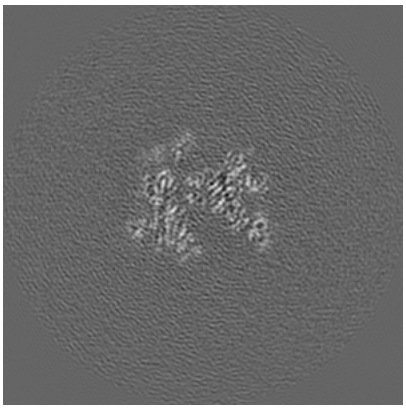
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

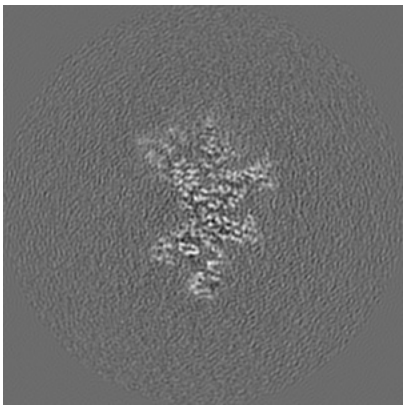
6.3.1 Primary map



X Index: 150

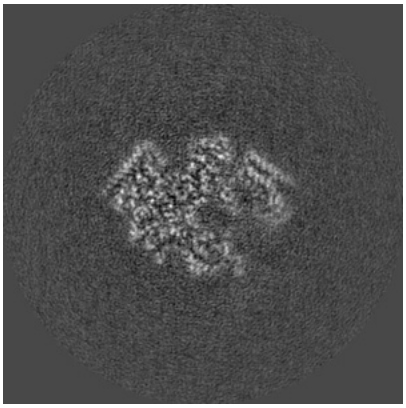


Y Index: 132

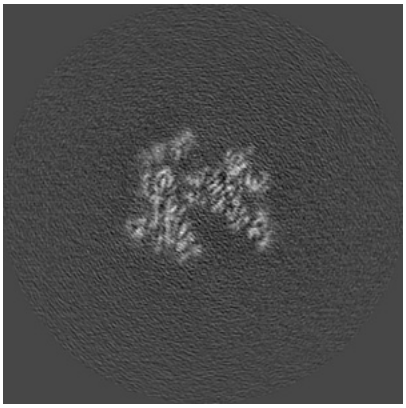


Z Index: 161

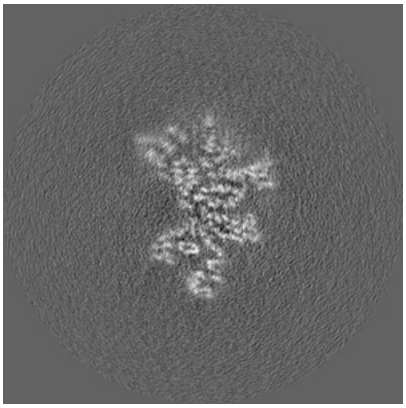
6.3.2 Raw map



X Index: 150



Y Index: 132

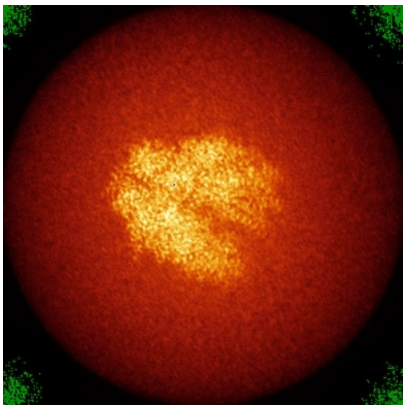


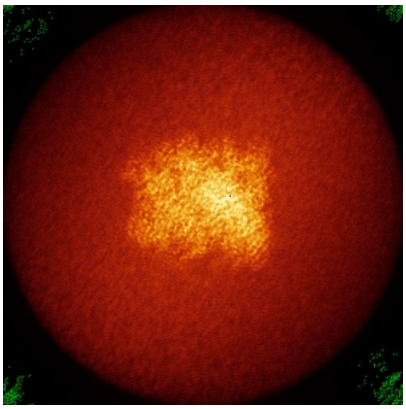
Z Index: 161

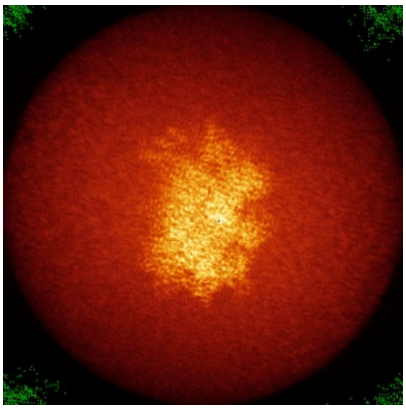
The images above show the largest variance slices of the map in three orthogonal directions.

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

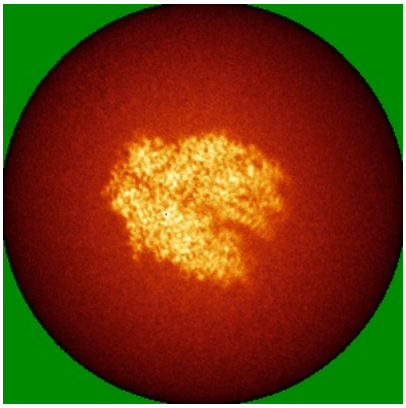
6.4.1 Primary map

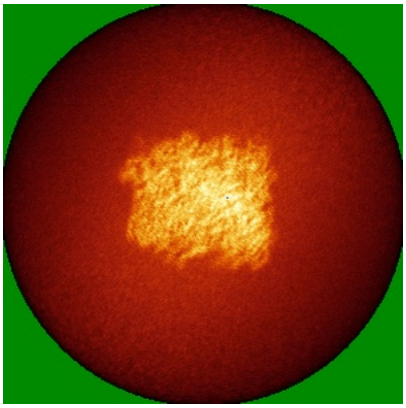

X

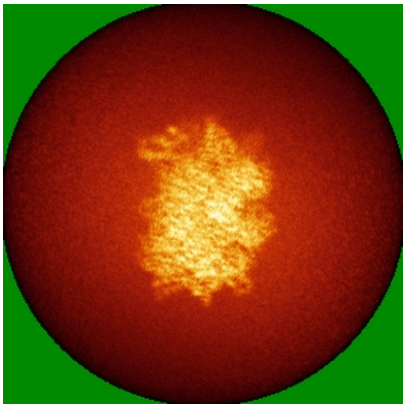

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0277. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

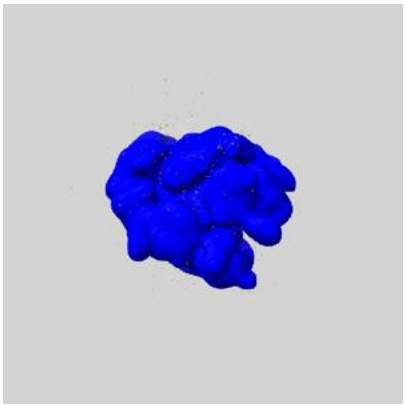
6.6 Mask visualisation

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

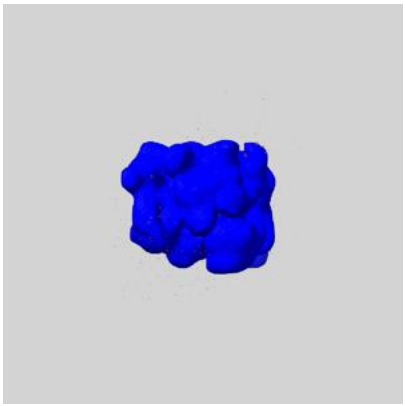
A mask typically either:

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

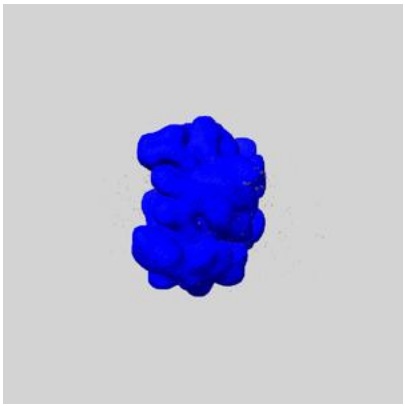
6.6.1 emd_50956_msk_1.map



X



Y

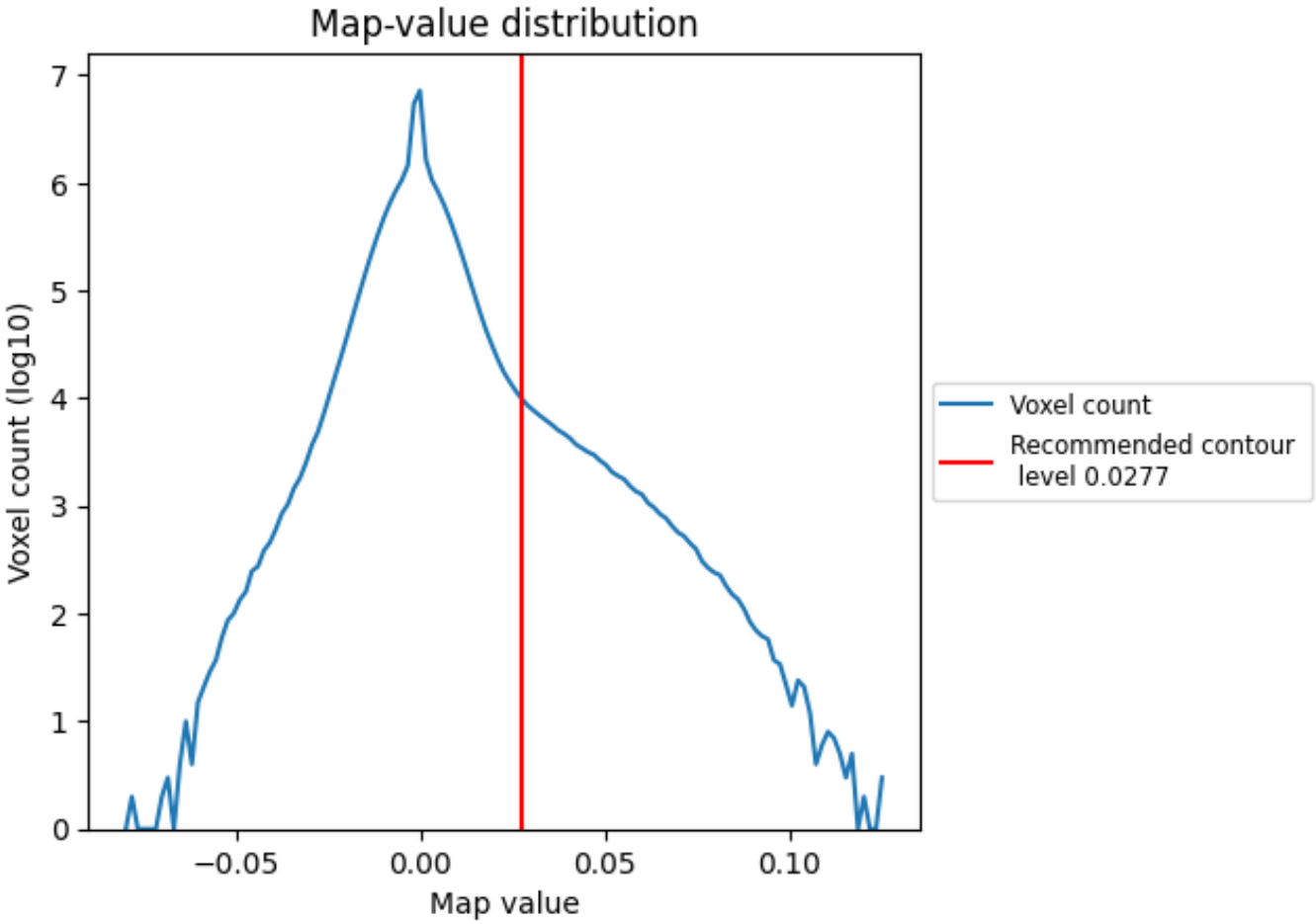


Z

7 Map analysis

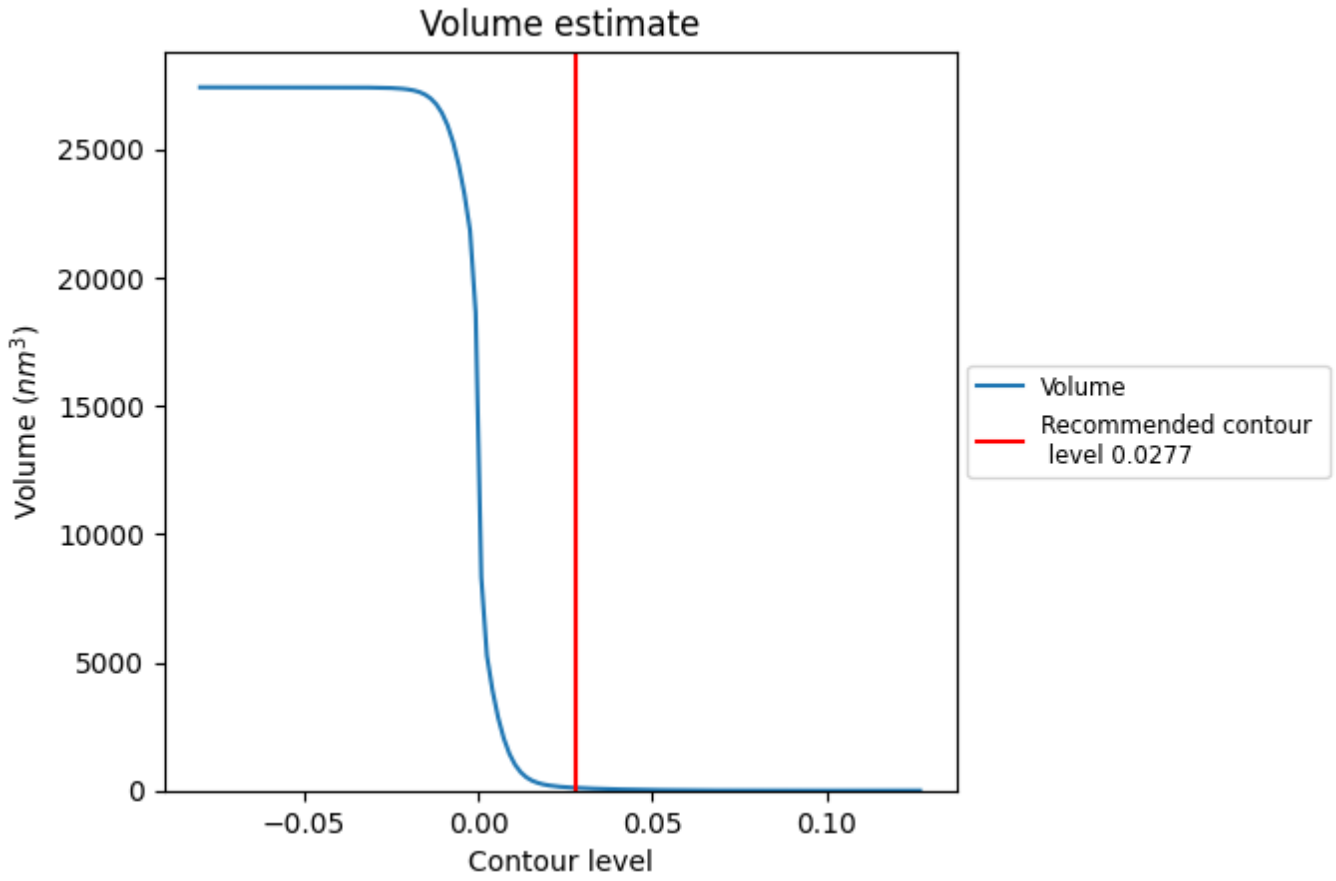
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

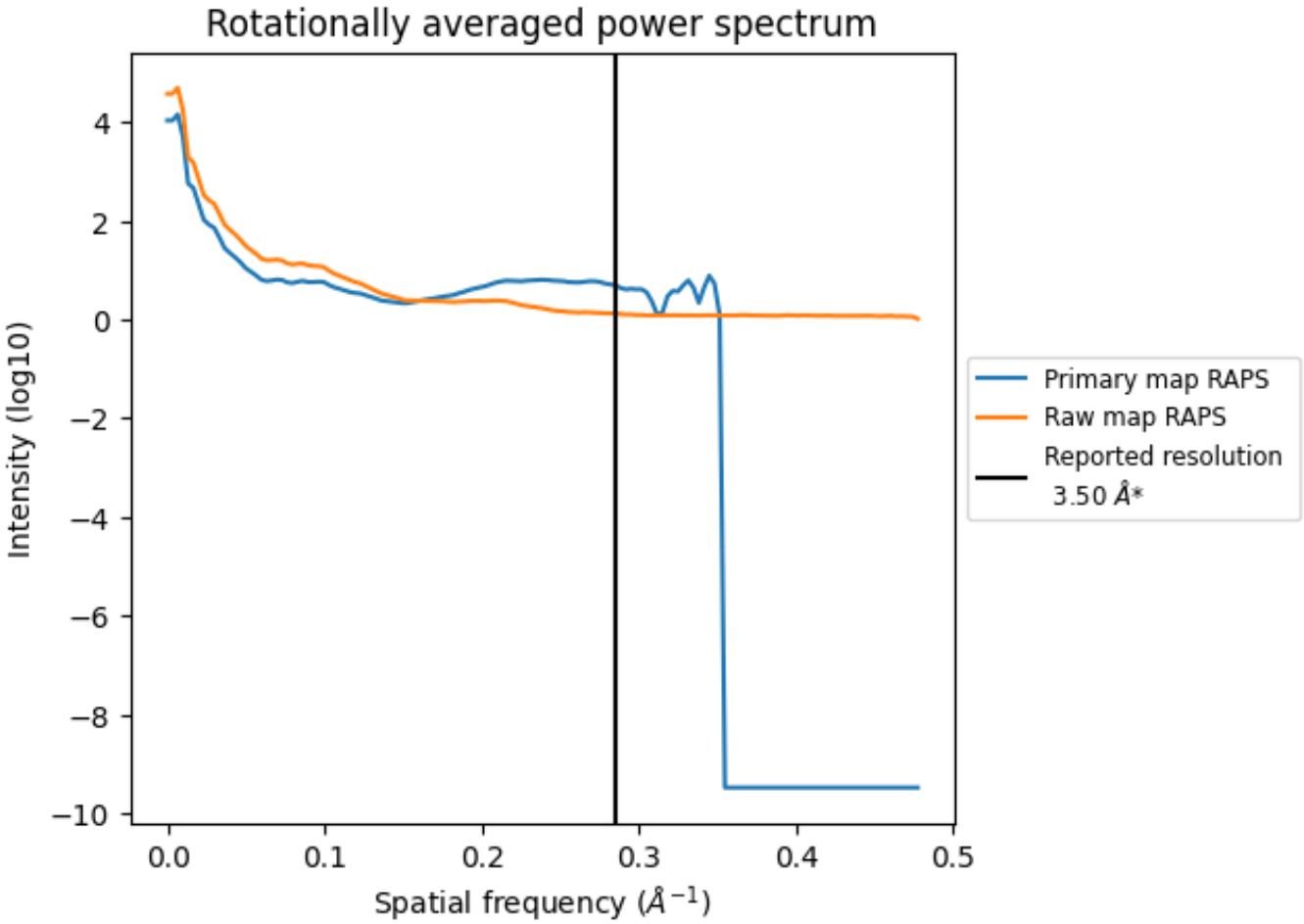
7.2 Volume estimate



The volume at the recommended contour level is 109 nm^3; this corresponds to an approximate mass of 98 kDa.

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

7.3 Rotationally averaged power spectrum (i)

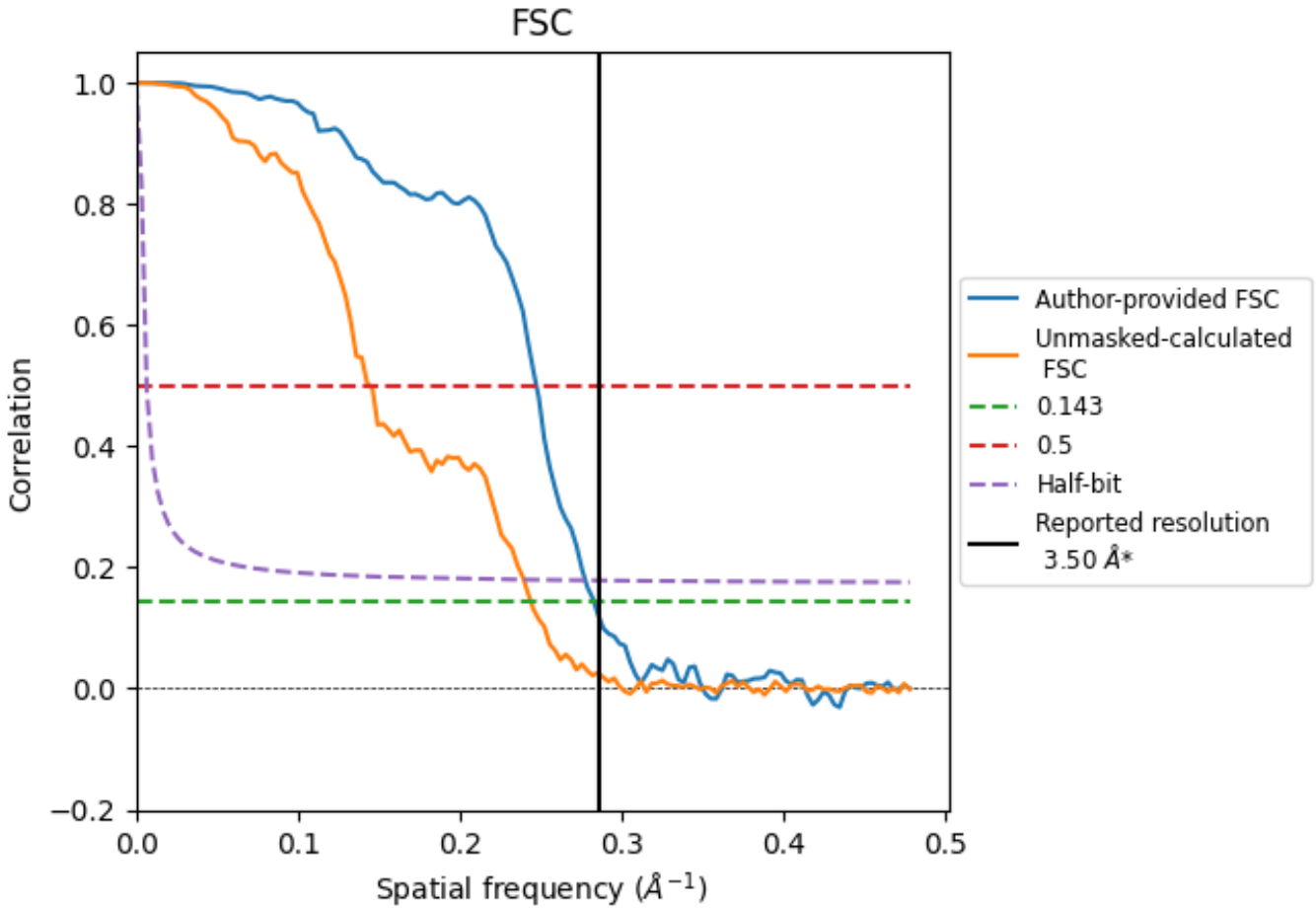


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

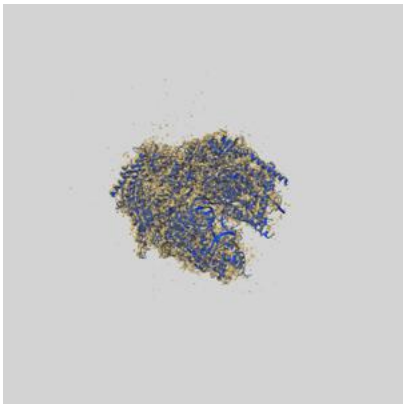
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.54	4.05	3.60
Unmasked-calculated*	4.10	6.93	4.18

*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 4.10 differs from the reported value 3.5 by more than 10 %

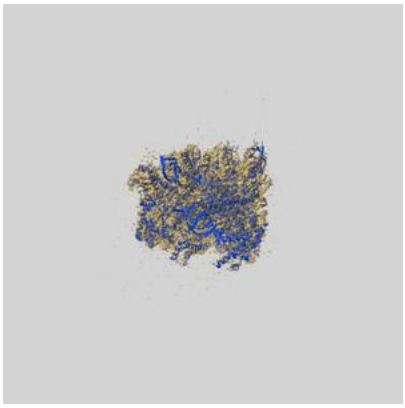
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50956 and PDB model 9G1X. Per-residue inclusion information can be found in section 3 on page 7.

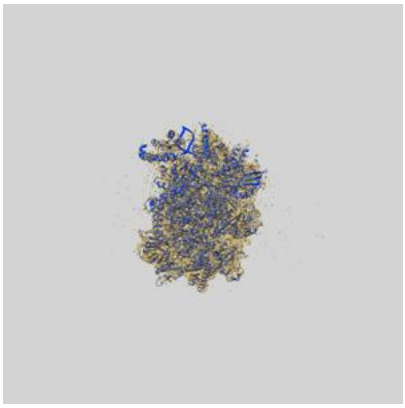
9.1 Map-model overlay



X



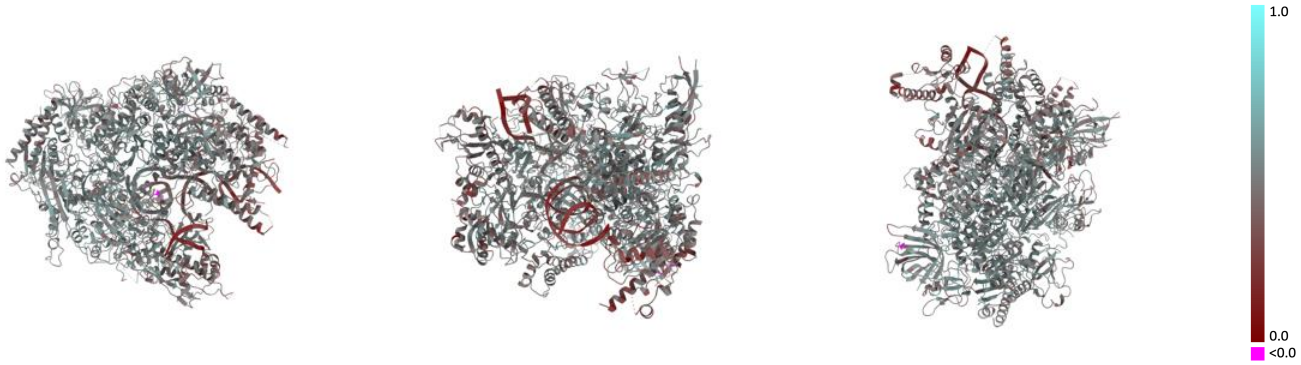
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0277 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

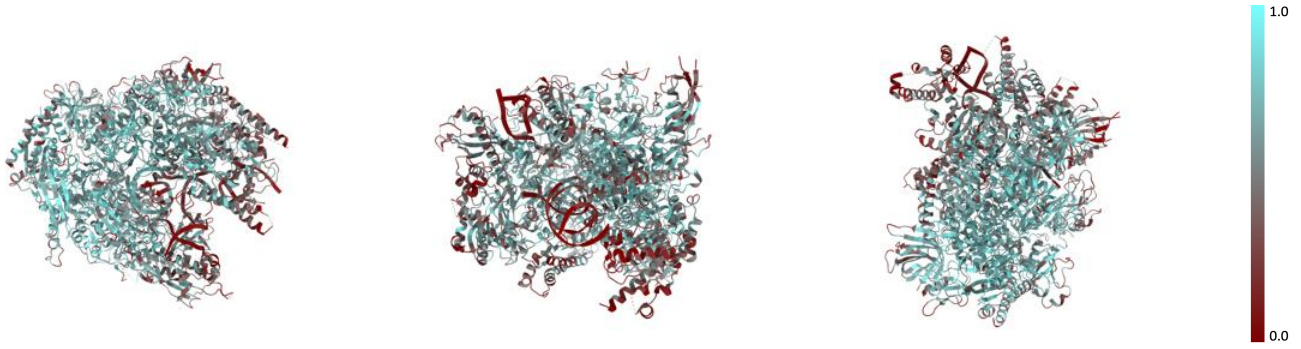
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

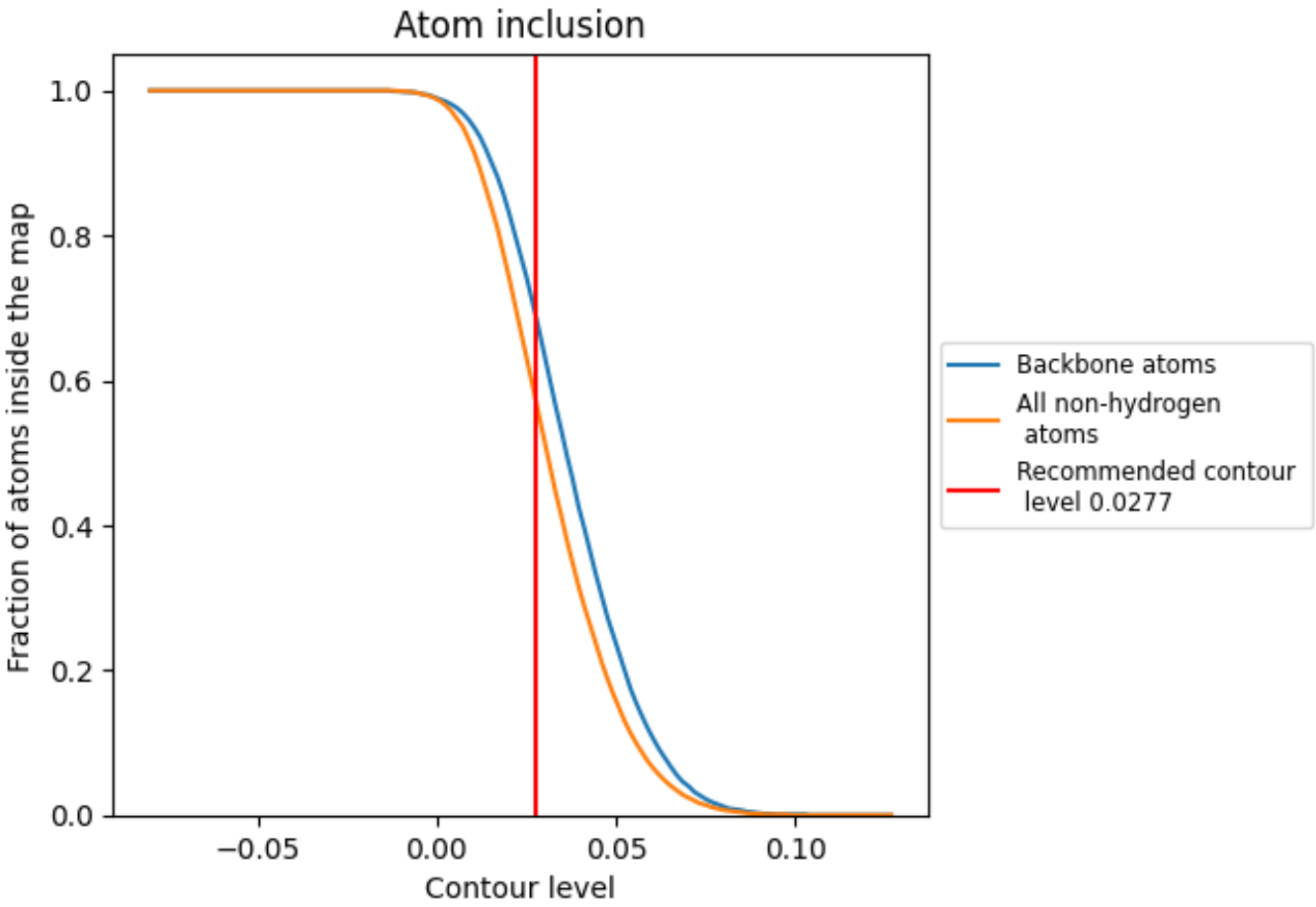
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0277).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 57% 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 (0.0277) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5710	0.4790
A	0.5910	0.4870
B	0.6060	0.4950
C	0.6180	0.4990
D	0.5490	0.4960
E	0.3670	0.4090
F	0.6520	0.5000
G	0.4540	0.4760
H	0.5980	0.4990
J	0.7160	0.5300
K	0.6180	0.4850
L	0.6090	0.5090
R	0.6030	0.4670
S	0.0880	0.2130
T	0.3020	0.2960