



## Full wwPDB EM Validation Report ⓘ

Jun 29, 2025 – 09:07 am BST

PDB ID : 7Z31 / pdb\_00007z31  
EMDB ID : EMD-14470  
Title : Structure of yeast RNA Polymerase III-Ty1 integrase complex at 2.7 Å (focus subunit C11, no C11 C-terminal Zn-ribbon in the funnel pore).  
Authors : Nguyen, P.Q.; Huecas, S.; Plaza-Pegueroles, A.; Fernandez-Tornero, C.  
Deposited on : 2022-03-01  
Resolution : 2.76 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.dev118  
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) : 2.44

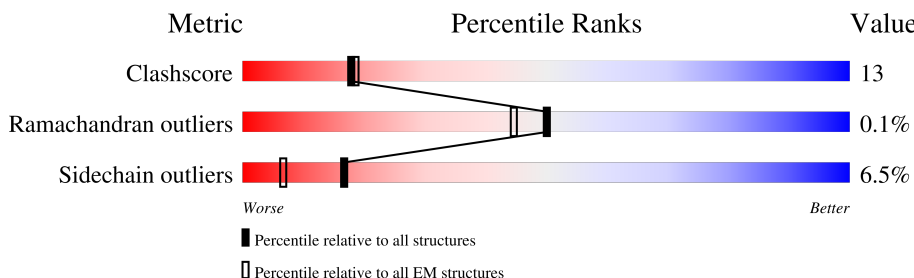
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.76 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1460	<div> <div>29%</div> <div>67%</div> <div>28%</div> <div>• •</div> </div>
2	B	1149	<div> <div>13%</div> <div>66%</div> <div>29%</div> <div>• •</div> </div>
3	C	335	<div> <div>5%</div> <div>77%</div> <div>21%</div> <div>•</div> </div>
4	D	161	<div> <div>85%</div> <div>50%</div> <div>36%</div> <div>• 10%</div> </div>
5	E	215	<div> <div>42%</div> <div>75%</div> <div>23%</div> <div>•</div> </div>
6	F	155	<div> <div>39%</div> <div>15%</div> <div>46%</div> </div>
7	G	212	<div> <div>60%</div> <div>53%</div> <div>34%</div> <div>• 10%</div> </div>
8	H	146	<div> <div>8%</div> <div>64%</div> <div>28%</div> <div>• 5%</div> </div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
9	I	110	
10	J	70	
11	K	142	
12	L	70	
13	M	282	
14	N	422	
15	O	654	
16	P	317	
17	Q	268	
18	W	635	
19	X	13	

## 2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 40156 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 III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1419	Total	C	N	O	S	0	0
			11123	7013	1962	2089	59		

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1102	Total	C	N	O	S	0	0
			8701	5507	1499	1635	60		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	335	Total	C	N	O	S	0	0
			2655	1681	454	511	9		

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	145	Total	C	N	O	S	0	0
			1140	723	191	220	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1759	1116	310	321	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			671	429	114	125	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	191	Total	C	N	O	S	0	0
			1544	1007	250	281	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	138	Total	C	N	O	S	0	0
			1103	694	186	218	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	47	Total	C	N	O	S	0	0
			365	233	57	69	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			549	350	95	98	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			792	496	130	161	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	50	Total	C	N	O	S	0	0
			381	235	76	66	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	183	Total	C	N	O	S	0	0
			1492	953	250	288	1		

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	151	Total	C	N	O	S	0	0
			1169	738	215	213	3		

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	568	Total	C	N	O	S	0	0
			4558	2897	784	858	19		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	136	Total	C	N	O	S	0	0
			1126	736	175	211	4		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0
			829	535	137	154	3		

- Molecule 18 is a protein called Integrase.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	17	Total	C	N	O	S	0	0
			141	86	27	27	1		

- Molecule 19 is a protein called Unknown RNA polymerase III chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	X	10	Total	C	N	O	0	0
			50	30	10	10		

- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
20	A	2	Total	Zn	0
			2	2	
20	B	1	Total	Zn	0
			1	1	
20	I	1	Total	Zn	0
			1	1	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
20	J	1	Total	Zn	0
			1	1	
20	L	1	Total	Zn	0
			1	1	

- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

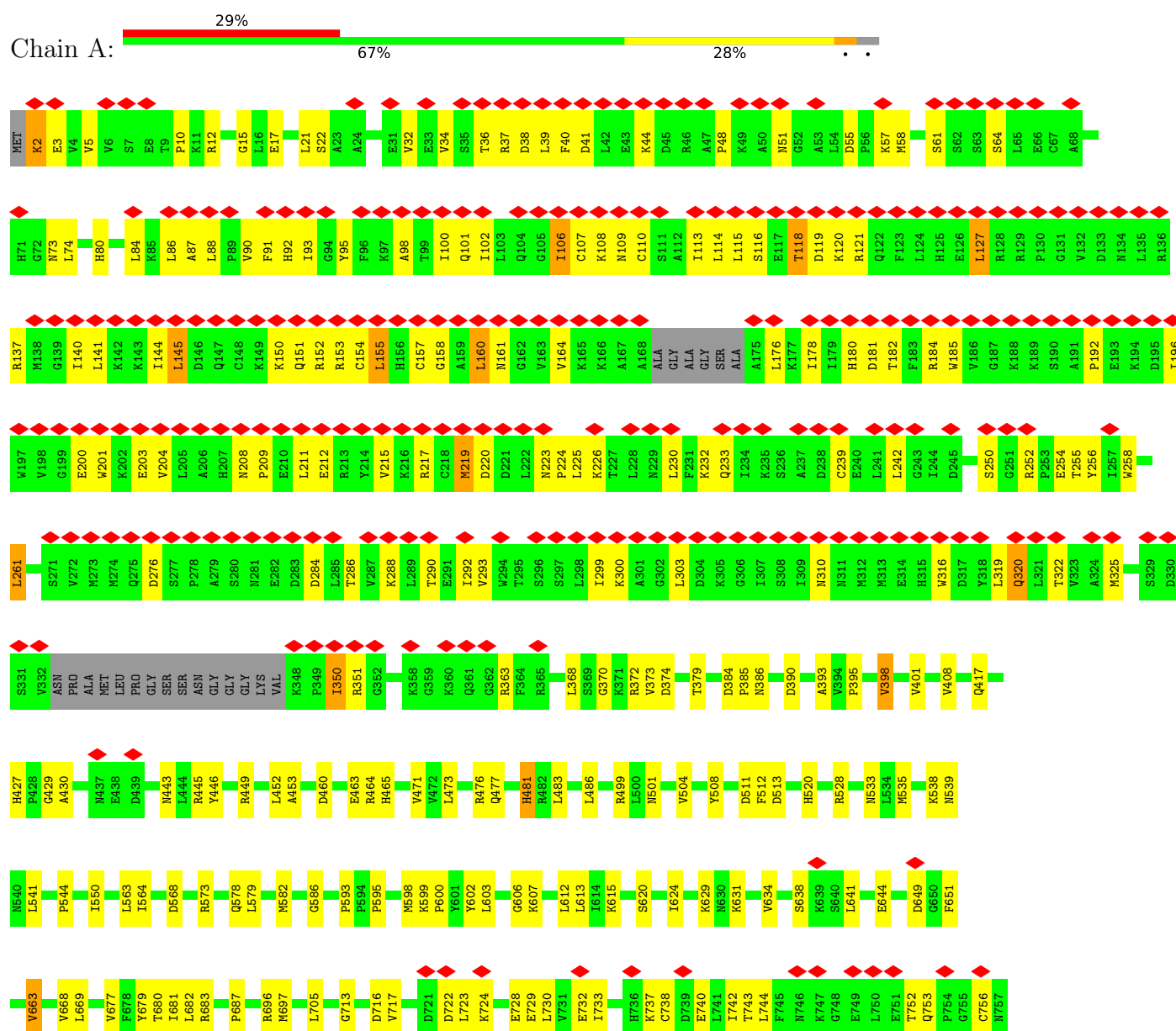
- Molecule 22 is water.

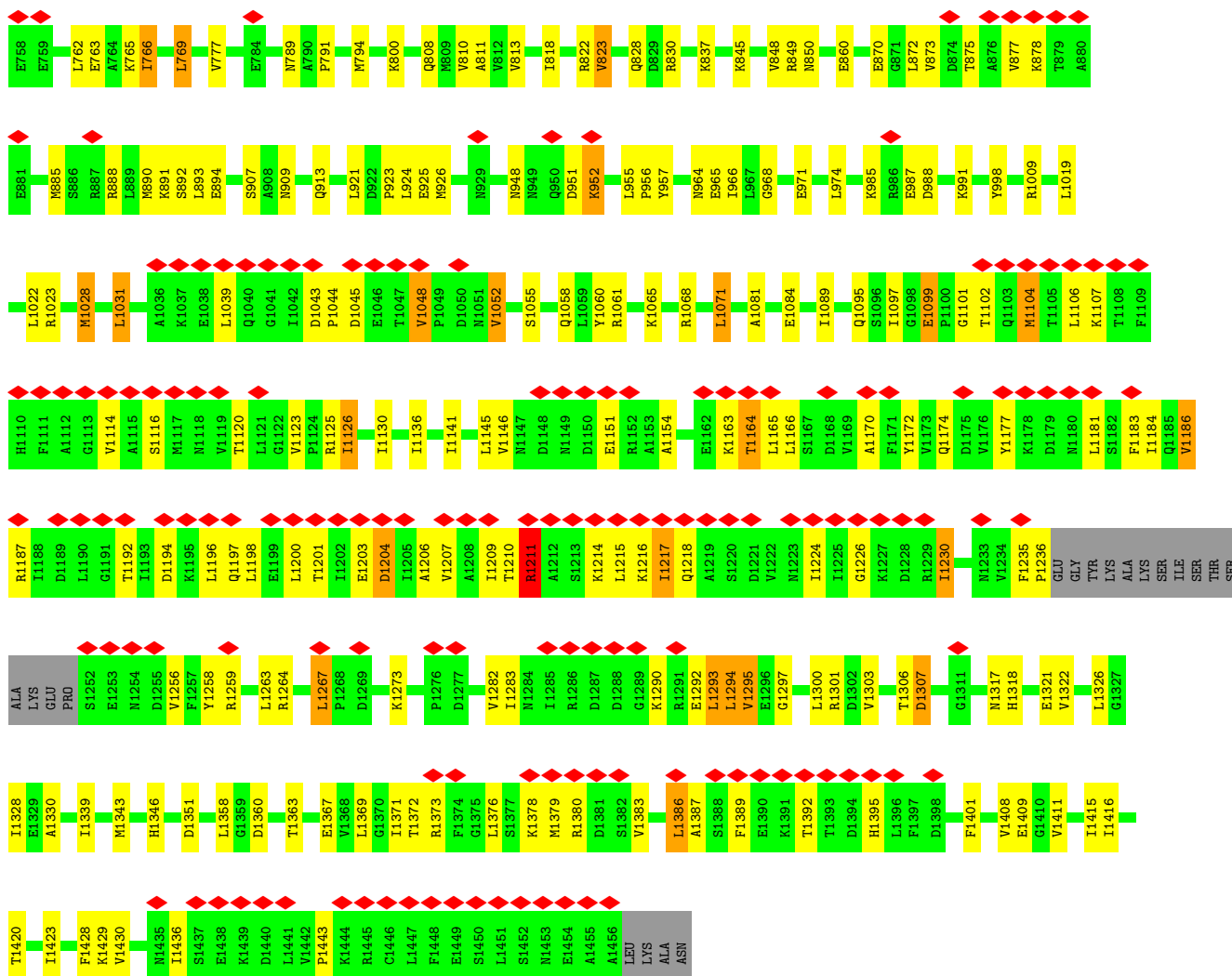
Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	O	0
			1	1	

### 3 Residue-property plots

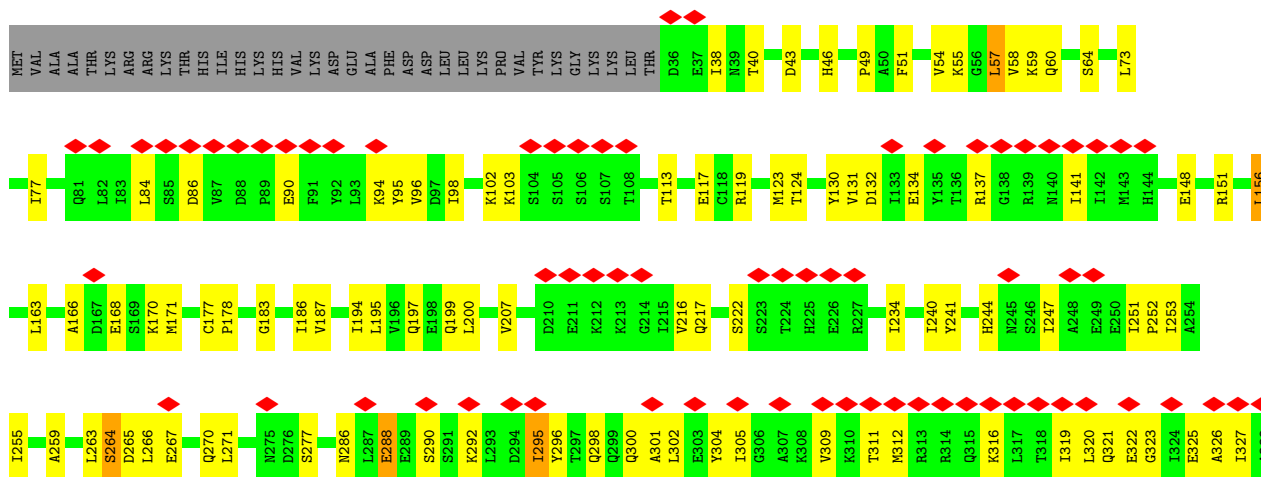
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

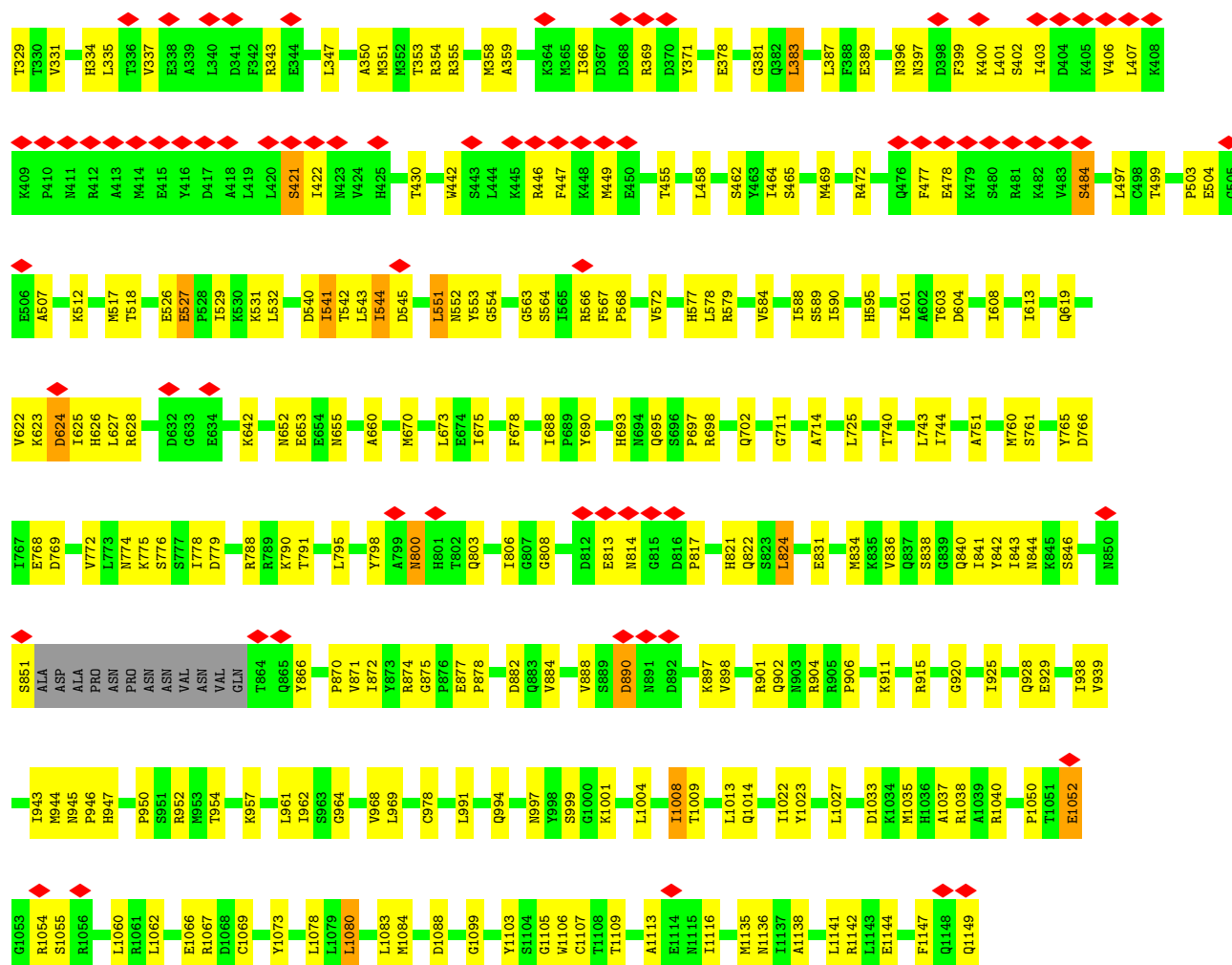
- Molecule 1: DNA-directed RNA polymerase III subunit RPC1



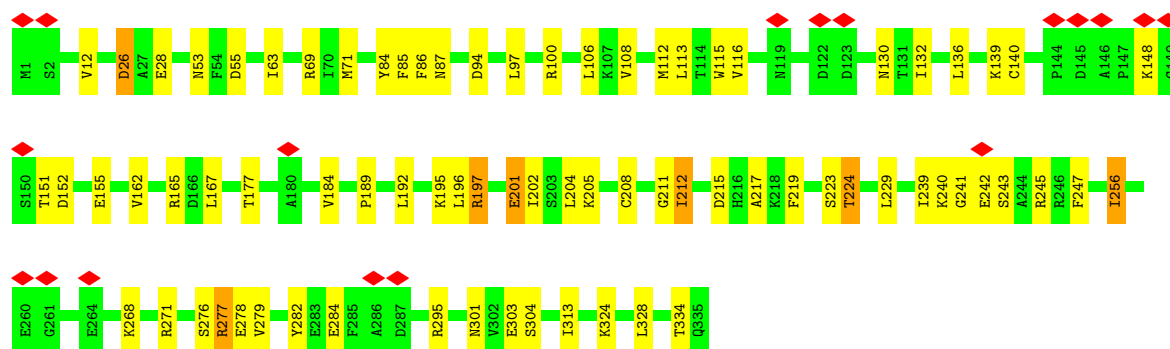
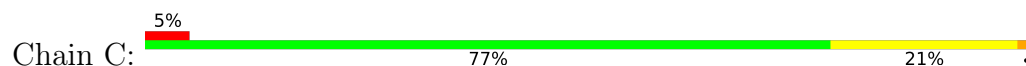


• Molecule 2: DNA-directed RNA polymerase III subunit RPC2

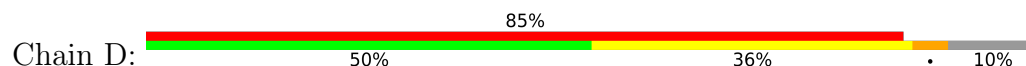


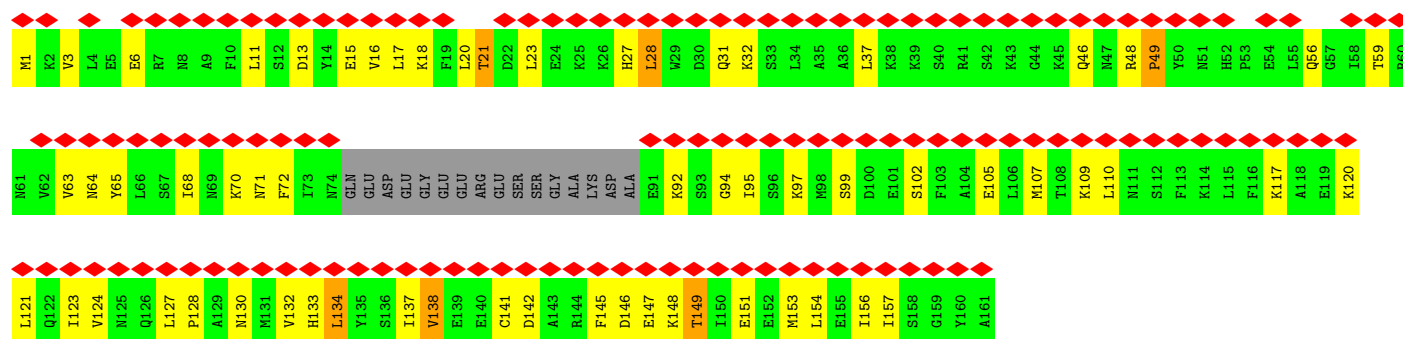


• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

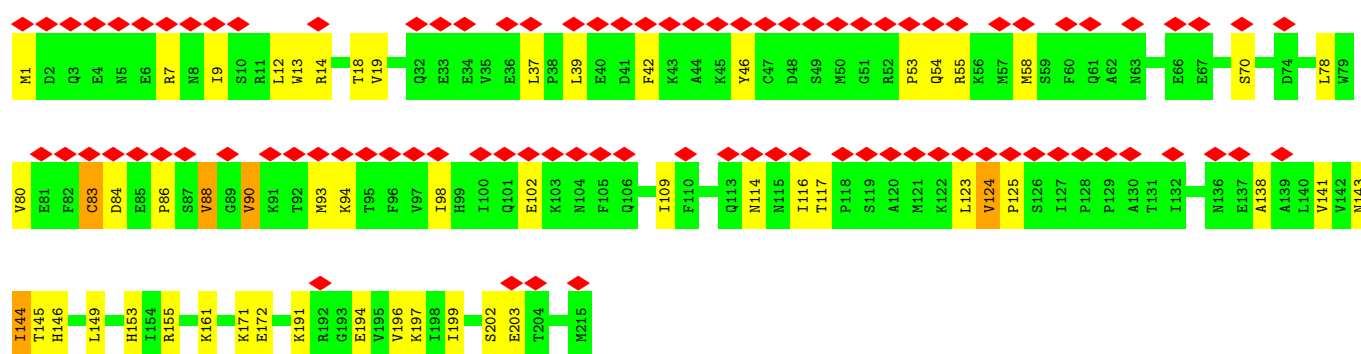
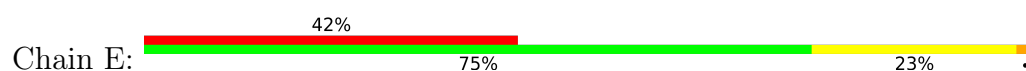


• Molecule 4: DNA-directed RNA polymerase III subunit RPC9

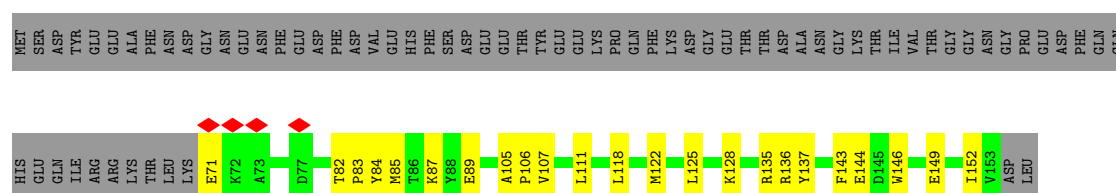




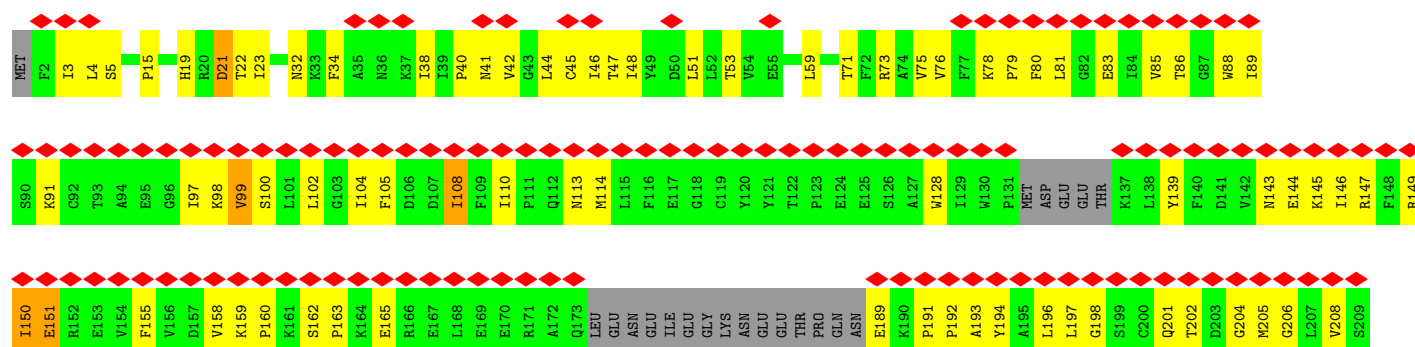
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



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

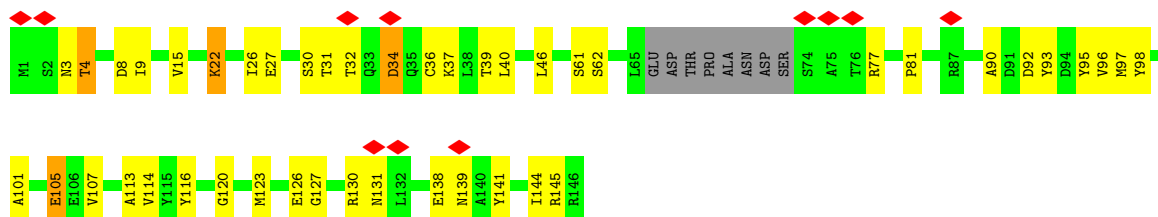


• Molecule 7: DNA-directed RNA polymerase III subunit RPC8

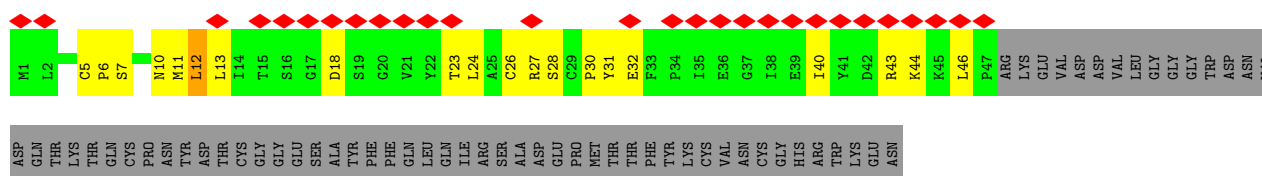




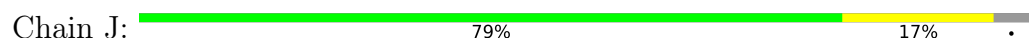
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



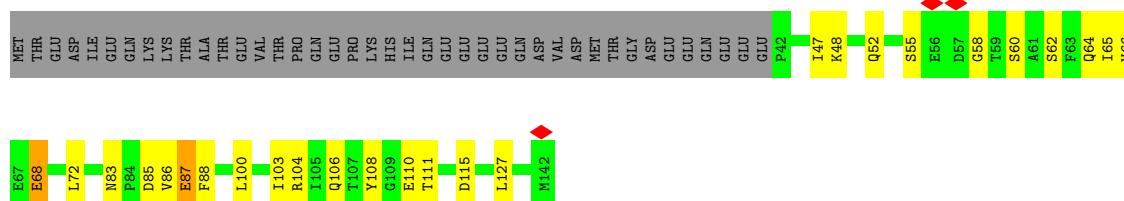
- Molecule 9: DNA-directed RNA polymerase III subunit RPC10



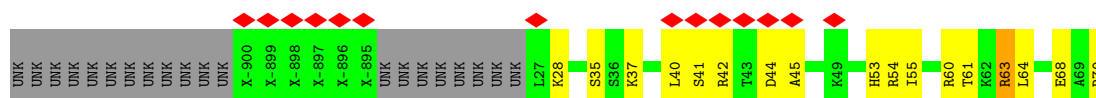
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



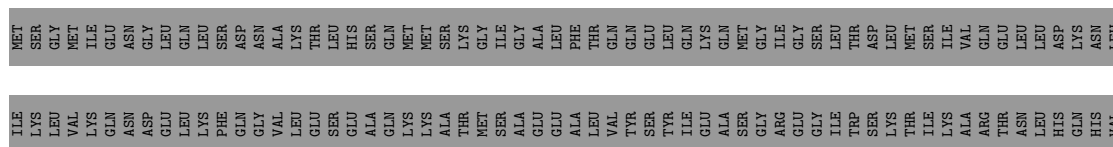
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

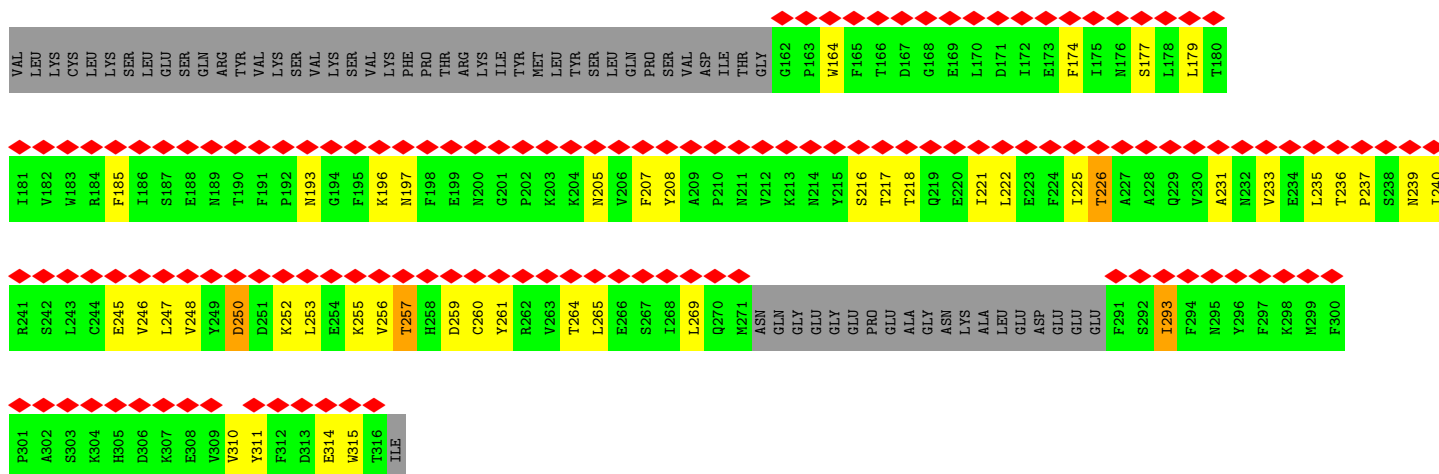


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

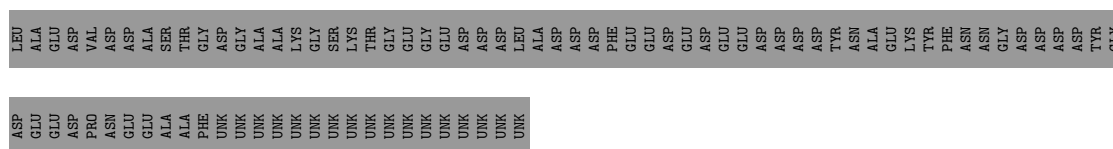
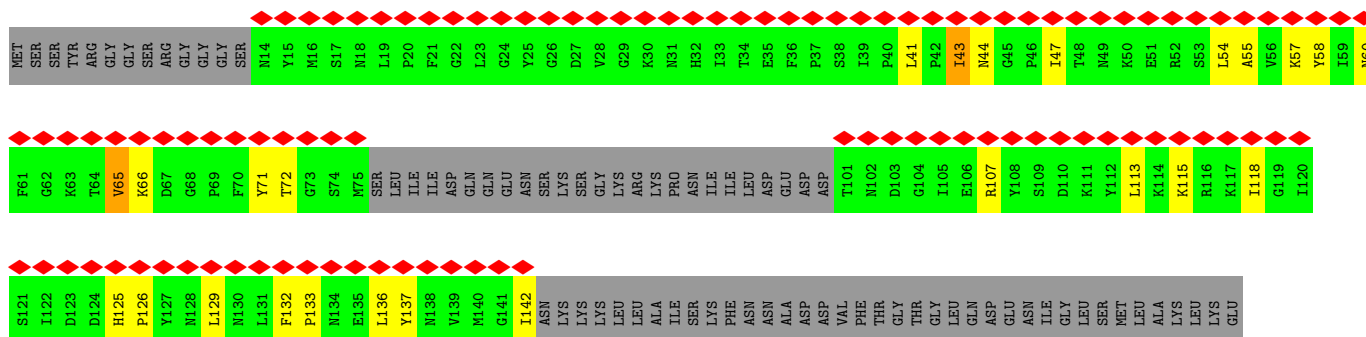
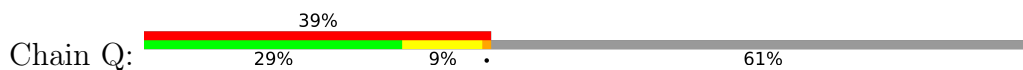




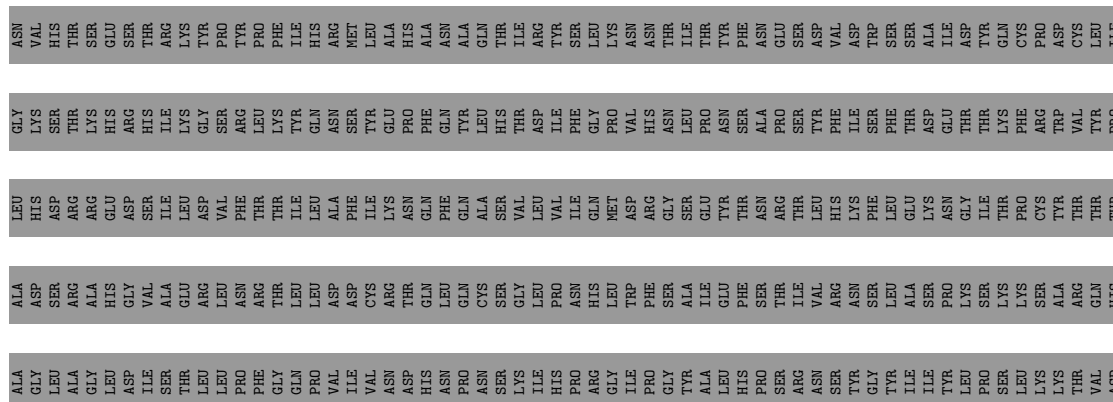




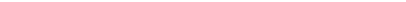
• Molecule 17: DNA-directed RNA polymerase III subunit RPC7



• Molecule 18: Integrase



GLU	ASP	ASN	GLU	THR	GLU	ILE	LYS	VE09	S610	R611	D612	T613	W614	N615	T616	K617	N618	R620	S621	L622	E623	P624	P625	ARG	SER	LYS	LYS	ARG	ILE	HIS	LEU	ILE	ALA
-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Chain X:  77% 77% 23%

X1001	UNK	X1008
X1002	UNK	X1009
X1003	UNK	X1010
X1004		X1011
		X1012
		X1013

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	273119	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	42.45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.162	Depositor
Minimum map value	-0.085	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0255	Depositor
Map size (Å)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.28	0/11322	0.42	0/15295
2	B	0.29	0/8853	0.40	0/11940
3	C	0.36	0/2711	0.47	0/3676
4	D	0.16	0/1158	0.42	0/1550
5	E	0.20	0/1795	0.40	0/2416
6	F	0.27	0/683	0.34	0/923
7	G	0.19	0/1583	0.39	0/2146
8	H	0.31	0/1121	0.42	0/1517
9	I	0.20	0/373	0.41	0/504
10	J	0.30	0/558	0.34	0/750
11	K	0.48	0/803	0.61	0/1083
12	L	0.26	0/353	0.36	0/468
13	M	0.18	0/1524	0.38	0/2061
14	N	0.25	0/1152	0.46	0/1546
15	O	0.19	0/4627	0.40	0/6243
16	P	0.14	0/1157	0.34	0/1571
17	Q	0.17	0/850	0.43	1/1148 (0.1%)
18	W	0.14	0/144	0.32	0/195
All	All	0.27	0/40767	0.41	1/55032 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	43	ILE	N-CA-C	-5.30	107.19	111.91

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1211	ARG	Sidechain

## 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	11123	0	11245	310	0
2	B	8701	0	8822	250	0
3	C	2655	0	2628	55	0
4	D	1140	0	1112	44	0
5	E	1759	0	1788	28	0
6	F	671	0	692	14	0
7	G	1544	0	1540	64	0
8	H	1103	0	1079	35	0
9	I	365	0	360	17	0
10	J	549	0	559	10	0
11	K	792	0	790	18	0
12	L	381	0	383	15	0
13	M	1492	0	1456	45	0
14	N	1169	0	1208	45	0
15	O	4558	0	4735	197	0
16	P	1126	0	1079	34	0
17	Q	829	0	819	22	0
18	W	141	0	137	0	0
19	X	50	0	16	0	0
20	A	2	0	0	0	0
20	B	1	0	0	0	0
20	I	1	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
21	A	1	0	0	0	0
22	A	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	40156	0	40448	1053	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 (1053) 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)
15:O:203:ILE:HD11	15:O:208:TYR:CE2	1.97	0.99
1:A:890:MET:O	1:A:894:GLU:HB2	1.70	0.90
15:O:203:ILE:HD11	15:O:208:TYR:HE2	1.33	0.88
1:A:1214:LYS:HA	1:A:1218:GLN:HA	1.53	0.88
2:B:1105:GLY:HA2	2:B:1116:ILE:HG21	1.57	0.85
3:C:53:ASN:HD22	3:C:301:ASN:HD22	1.23	0.85
4:D:127:LEU:HB3	4:D:133:HIS:HB3	1.62	0.82
1:A:892:SER:HB2	1:A:1371:ILE:HG23	1.62	0.81
2:B:791:THR:HG21	2:B:842:TYR:HE2	1.43	0.81
9:I:28:SER:HA	13:M:186:ILE:HD11	1.62	0.79
2:B:776:SER:HA	2:B:779:ASP:HB2	1.63	0.79
15:O:193:GLN:HG2	15:O:197:MET:HE2	1.66	0.78
4:D:65:TYR:HB2	7:G:102:LEU:HD21	1.66	0.77
11:K:83:ASN:HD22	11:K:86:VAL:HG23	1.47	0.77
1:A:233:GLN:HG2	15:O:579:GLN:HE22	1.49	0.77
15:O:578:ARG:HH12	15:O:648:TRP:HB2	1.49	0.77
2:B:774:ASN:ND2	2:B:775:LYS:O	2.19	0.75
1:A:1443:PRO:HB3	7:G:73:ARG:HH12	1.52	0.74
15:O:495:VAL:HG21	15:O:647:LEU:HD21	1.67	0.74
2:B:302:LEU:HB3	2:B:325:GLU:HG2	1.68	0.74
2:B:588:ILE:HG12	2:B:603:THR:HG22	1.69	0.74
1:A:393:ALA:HB3	1:A:499:ARG:HB2	1.68	0.74
15:O:326:ILE:HG12	15:O:653:MET:HG2	1.70	0.73
2:B:769:ASP:OD1	2:B:952:ARG:NH2	2.21	0.73
1:A:1322:VAL:HG13	1:A:1326:LEU:HD12	1.71	0.72
1:A:176:LEU:HB3	1:A:320:GLN:HE22	1.54	0.72
4:D:123:ILE:HG22	4:D:137:ILE:HD13	1.70	0.72
7:G:89:ILE:HG22	7:G:99:VAL:HA	1.71	0.71
15:O:523:ASN:ND2	15:O:530:GLU:OE2	2.23	0.71
1:A:160:LEU:HD21	1:A:185:TRP:HB2	1.72	0.71
1:A:217:ARG:HE	15:O:552:PRO:HG2	1.56	0.71
2:B:77:ILE:HG13	2:B:98:ILE:HB	1.73	0.71
15:O:370:LEU:HD11	15:O:453:ILE:HD12	1.73	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:GLN:NE2	1:A:453:ALA:O	2.24	0.70
1:A:818:ILE:HD13	1:A:823:VAL:HG12	1.73	0.70
1:A:219:MET:O	15:O:549:GLN:NE2	2.22	0.70
14:N:286:ASP:HB3	14:N:384:LYS:HB2	1.74	0.70
4:D:70:LYS:HG3	4:D:94:GLY:HA3	1.74	0.69
15:O:580:ASN:OD1	15:O:584:ASN:ND2	2.25	0.69
15:O:295:GLN:HE22	15:O:487:LEU:HD11	1.55	0.69
15:O:338:ASP:OD1	15:O:339:LEU:N	2.25	0.69
2:B:371:TYR:OH	2:B:655:ASN:ND2	2.25	0.69
1:A:395:PRO:HB2	1:A:398:VAL:HG13	1.75	0.69
2:B:795:LEU:HD21	2:B:806:ILE:HD11	1.74	0.69
15:O:73:ARG:NH2	15:O:121:TYR:OH	2.26	0.69
1:A:1373:ARG:H	1:A:1373:ARG:HE	1.41	0.68
2:B:532:LEU:HD21	2:B:578:LEU:HD13	1.75	0.68
12:L:68:GLU:HG2	12:L:70:ARG:HG3	1.75	0.68
11:K:60:SER:OG	11:K:104:ARG:NH2	2.27	0.68
15:O:166:LEU:HB3	15:O:169:LEU:HD21	1.75	0.68
1:A:12:ARG:NH1	2:B:1144:GLU:OE2	2.28	0.68
2:B:695:GLN:HG2	2:B:697:PRO:HD2	1.76	0.68
13:M:245:LEU:HD11	14:N:406:ALA:HB2	1.74	0.67
15:O:203:ILE:HD11	15:O:208:TYR:CZ	2.29	0.67
15:O:493:GLU:HG2	15:O:509:ARG:HD3	1.76	0.67
2:B:690:TYR:HB3	2:B:693:HIS:HD2	1.59	0.67
15:O:549:GLN:HE21	15:O:567:ARG:HH22	1.41	0.67
1:A:153:ARG:HE	15:O:339:LEU:HG	1.59	0.67
1:A:137:ARG:HH11	1:A:141:LEU:HD11	1.60	0.67
15:O:203:ILE:CD1	15:O:208:TYR:HE2	2.06	0.67
15:O:506:ARG:HD3	16:P:250:ASP:HB2	1.76	0.67
5:E:18:THR:HG23	5:E:143:ASN:HB3	1.77	0.67
14:N:382:ILE:HG13	14:N:418:VAL:HG22	1.77	0.66
1:A:1186:VAL:HG13	1:A:1230:ILE:HG23	1.77	0.66
5:E:9:ILE:HG22	5:E:39:LEU:HD11	1.77	0.66
15:O:252:ILE:HA	15:O:255:LYS:HE2	1.76	0.66
15:O:643:ARG:HG2	17:Q:43:ILE:HG23	1.78	0.66
2:B:882:ASP:HB3	2:B:901:ARG:HH11	1.60	0.66
15:O:303:ARG:HG3	16:P:264:THR:HB	1.77	0.65
1:A:1307:ASP:OD1	1:A:1307:ASP:N	2.29	0.65
2:B:168:GLU:HA	2:B:171:MET:HB2	1.79	0.65
15:O:376:LEU:HD12	15:O:448:HIS:HD2	1.60	0.65
1:A:386:ASN:ND2	2:B:765:TYR:OH	2.30	0.65
1:A:541:LEU:HD12	1:A:682:LEU:HD13	1.79	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:223:LEU:HD13	14:N:389:THR:HG21	1.78	0.65
1:A:1048:VAL:HG13	1:A:1052:VAL:HG23	1.79	0.64
15:O:509:ARG:HH12	15:O:513:ASP:HB2	1.61	0.64
1:A:473:LEU:HB2	1:A:520:HIS:HB2	1.79	0.64
2:B:252:PRO:HB2	2:B:255:ILE:HD13	1.79	0.64
1:A:1214:LYS:HA	1:A:1218:GLN:CA	2.26	0.64
7:G:79:PRO:HA	7:G:83:GLU:HG3	1.79	0.64
1:A:250:SER:HA	1:A:255:THR:HG21	1.79	0.64
1:A:538:LYS:HB3	1:A:687:PRO:HB2	1.80	0.64
8:H:34:ASP:OD1	8:H:34:ASP:N	2.29	0.64
14:N:364:ARG:HE	14:N:366:HIS:CE1	2.14	0.64
2:B:312:MET:HE1	2:B:319:ILE:HG22	1.79	0.64
6:F:82:THR:O	6:F:136:ARG:NH1	2.28	0.64
15:O:550:GLU:HG2	15:O:559:ALA:HB2	1.80	0.64
1:A:108:LYS:O	15:O:572:HIS:NE2	2.31	0.64
7:G:110:ILE:HG22	7:G:198:GLY:H	1.62	0.64
10:J:7:CYS:HA	10:J:49:MET:HG3	1.80	0.64
13:M:167:GLN:NE2	13:M:169:TYR:OH	2.31	0.64
15:O:581:LEU:HG	15:O:644:LEU:HD11	1.79	0.64
1:A:200:GLU:HB3	15:O:516:LEU:HD23	1.80	0.64
2:B:38:ILE:HD13	2:B:628:ARG:HG3	1.78	0.63
1:A:102:ILE:HG23	1:A:242:LEU:HD13	1.80	0.63
7:G:45:CYS:HA	7:G:76:VAL:HG12	1.79	0.63
17:Q:115:LYS:HD3	17:Q:118:ILE:HD11	1.80	0.62
1:A:668:VAL:HG22	1:A:677:VAL:HG23	1.81	0.62
7:G:102:LEU:HD23	7:G:102:LEU:H	1.64	0.62
17:Q:132:PHE:HB2	17:Q:137:TYR:HE1	1.65	0.62
7:G:91:LYS:HB3	7:G:98:LYS:HE2	1.82	0.62
5:E:53:PRO:HG2	5:E:55:ARG:HH12	1.63	0.62
7:G:46:ILE:HG22	7:G:47:THR:HG22	1.82	0.62
2:B:969:LEU:HB3	2:B:994:GLN:HG3	1.82	0.61
15:O:145:ARG:HG3	15:O:146:VAL:HG22	1.80	0.61
3:C:84:TYR:HB3	12:L:64:LEU:HD11	1.81	0.61
1:A:624:ILE:HD12	1:A:680:THR:HG22	1.82	0.61
3:C:100:ARG:NH2	3:C:192:LEU:O	2.33	0.61
2:B:788:ARG:NH2	2:B:882:ASP:OD2	2.33	0.61
1:A:813:VAL:O	1:A:848:VAL:HB	2.00	0.61
2:B:194:ILE:HG12	2:B:455:THR:HG22	1.81	0.61
11:K:87:GLU:HB3	11:K:108:TYR:CZ	2.36	0.61
2:B:551:LEU:HD13	14:N:216:LYS:HG2	1.81	0.61
2:B:915:ARG:HD2	2:B:1023:TYR:HD2	1.66	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:226:LYS:HG3	14:N:292:ARG:HH22	1.66	0.60
1:A:176:LEU:O	1:A:320:GLN:NE2	2.33	0.60
2:B:255:ILE:HG21	2:B:304:TYR:HD2	1.66	0.60
16:P:255:LYS:NZ	16:P:259:ASP:OD1	2.34	0.60
1:A:1224:ILE:HG22	1:A:1226:GLY:H	1.65	0.60
15:O:648:TRP:HZ3	15:O:652:GLN:HE21	1.48	0.60
15:O:359:LEU:HD23	15:O:477:TYR:HB2	1.83	0.60
2:B:40:THR:HB	2:B:624:ASP:HB3	1.84	0.60
2:B:622:VAL:O	2:B:626:HIS:ND1	2.28	0.60
7:G:46:ILE:HB	7:G:75:VAL:HG23	1.83	0.60
1:A:15:GLY:HA2	1:A:1408:VAL:HG23	1.82	0.60
15:O:636:ASN:O	15:O:640:ARG:HG2	2.01	0.60
2:B:102:LYS:NZ	2:B:103:LYS:O	2.35	0.60
1:A:150:LYS:O	1:A:152:ARG:NH1	2.34	0.60
1:A:1369:LEU:HD13	1:A:1378:LYS:HB3	1.84	0.60
15:O:259:LEU:HD23	15:O:261:GLN:HG2	1.83	0.60
15:O:450:ALA:HA	15:O:453:ILE:HG22	1.83	0.60
4:D:138:VAL:HG13	4:D:141:CYS:HB2	1.83	0.59
15:O:203:ILE:HD11	15:O:208:TYR:OH	2.02	0.59
4:D:109:LYS:HZ1	4:D:110:LEU:HA	1.67	0.59
1:A:1145:LEU:HD11	1:A:1293:LEU:HD23	1.84	0.59
2:B:277:SER:N	14:N:207:VAL:O	2.33	0.59
5:E:88:VAL:HG22	5:E:116:ILE:HG13	1.83	0.59
15:O:215:TRP:O	15:O:219:TYR:HB2	2.02	0.59
15:O:580:ASN:O	15:O:584:ASN:ND2	2.33	0.59
16:P:174:PHE:O	16:P:177:SER:OG	2.20	0.59
2:B:156:LEU:HD12	2:B:163:LEU:HD12	1.84	0.59
2:B:497:LEU:HD13	2:B:512:LYS:HD2	1.83	0.59
8:H:15:VAL:HG13	8:H:26:ILE:HG22	1.83	0.59
1:A:578:GLN:HG3	1:A:582:MET:HE2	1.85	0.59
15:O:492:TYR:CZ	15:O:573:SER:HB3	2.38	0.59
1:A:284:ASP:OD2	1:A:351:ARG:N	2.33	0.59
4:D:71:ASN:HD22	7:G:86:THR:HG21	1.68	0.59
1:A:964:ASN:HD21	1:A:1009:ARG:HE	1.49	0.59
14:N:219:ILE:HA	14:N:222:ALA:HB3	1.83	0.58
15:O:65:ILE:HA	15:O:68:LEU:HD12	1.85	0.58
15:O:492:TYR:HE1	15:O:577:MET:HG2	1.68	0.58
1:A:728:GLU:HG2	1:A:849:ARG:HH22	1.68	0.58
15:O:80:VAL:HG13	15:O:86:MET:HG2	1.85	0.58
1:A:449:ARG:HA	1:A:452:LEU:HD12	1.83	0.58
4:D:92:LYS:HD3	4:D:97:LYS:HD2	1.84	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:111:ARG:HB2	13:M:120:GLU:HB3	1.84	0.58
15:O:158:GLU:O	15:O:162:ASN:ND2	2.33	0.58
2:B:267:GLU:HA	2:B:270:GLN:HB2	1.85	0.58
15:O:289:LYS:NZ	15:O:324:PRO:O	2.36	0.58
1:A:40:PHE:HE1	1:A:48:PRO:HD3	1.67	0.58
2:B:403:ILE:O	2:B:407:LEU:HG	2.03	0.58
4:D:99:SER:H	4:D:102:SER:HB3	1.68	0.58
1:A:1172:TYR:HE1	1:A:1174:GLN:HB2	1.68	0.58
2:B:137:ARG:HB3	2:B:141:ILE:HB	1.86	0.58
2:B:207:VAL:HG12	2:B:366:ILE:HG22	1.86	0.58
3:C:63:ILE:HG21	11:K:127:LEU:HD21	1.85	0.58
13:M:124:PRO:HA	13:M:145:VAL:HA	1.85	0.58
15:O:510:CYS:SG	15:O:525:THR:OG1	2.57	0.58
1:A:427:HIS:O	1:A:465:HIS:ND1	2.24	0.58
2:B:846:SER:HB3	2:B:866:TYR:HB3	1.86	0.58
15:O:511:ILE:HA	15:O:517:VAL:HG21	1.86	0.58
15:O:625:ASN:HA	15:O:628:LYS:HG2	1.85	0.58
1:A:1429:LYS:HB2	6:F:135:ARG:HB3	1.85	0.57
4:D:147:GLU:HG2	4:D:148:LYS:H	1.69	0.57
15:O:45:ASP:OD1	15:O:45:ASP:N	2.35	0.57
16:P:225:ILE:HG21	16:P:235:LEU:HD12	1.86	0.57
2:B:579:ARG:NH1	2:B:653:GLU:OE2	2.34	0.57
4:D:31:GLN:HG2	4:D:32:LYS:HG3	1.86	0.57
1:A:1141:ILE:HB	1:A:1295:VAL:HG22	1.87	0.57
13:M:133:LYS:H	13:M:133:LYS:HD2	1.68	0.57
15:O:68:LEU:HD23	15:O:74:LEU:HD21	1.86	0.57
15:O:518:SER:OG	15:O:520:LYS:NZ	2.38	0.57
1:A:1386:LEU:HB3	1:A:1395:HIS:CD2	2.40	0.57
2:B:458:LEU:HD12	2:B:469:MET:HG2	1.86	0.57
3:C:116:VAL:HG22	3:C:130:ASN:HB3	1.86	0.57
1:A:390:ASP:OD2	1:A:538:LYS:NZ	2.33	0.57
2:B:326:ALA:HB3	13:M:231:LEU:HD23	1.85	0.57
2:B:347:LEU:HD13	2:B:541:ILE:HG13	1.87	0.57
3:C:155:GLU:N	3:C:155:GLU:OE1	2.38	0.57
1:A:923:PRO:HA	1:A:926:MET:HG2	1.87	0.57
2:B:389:GLU:OE2	2:B:446:ARG:NH1	2.29	0.57
14:N:388:THR:HB	14:N:390:PHE:CE1	2.40	0.57
5:E:138:ALA:HA	5:E:141:VAL:HG23	1.87	0.57
15:O:362:ASN:OD1	15:O:362:ASN:N	2.34	0.57
1:A:1125:ARG:NH2	1:A:1317:ASN:O	2.38	0.56
2:B:265:ASP:HB3	9:I:10:ASN:HA	1.87	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:808:GLY:HA3	2:B:844:ASN:HD22	1.70	0.56
15:O:343:LYS:HZ1	15:O:346:GLN:HB2	1.69	0.56
16:P:236:THR:HG23	16:P:239:ASN:H	1.70	0.56
1:A:368:LEU:HD22	1:A:1416:ILE:HG23	1.87	0.56
1:A:828:GLN:HE21	2:B:595:HIS:HD2	1.54	0.56
2:B:566:ARG:NH2	14:N:286:ASP:OD2	2.39	0.56
7:G:147:ARG:NH2	7:G:204:GLY:O	2.37	0.56
15:O:160:VAL:HA	15:O:163:VAL:HG12	1.88	0.56
1:A:127:LEU:HG	1:A:140:ILE:HG21	1.87	0.56
15:O:203:ILE:HD12	15:O:281:THR:HG21	1.87	0.56
1:A:84:LEU:N	1:A:261:LEU:O	2.39	0.56
2:B:1035:MET:O	2:B:1054:ARG:NH1	2.38	0.56
3:C:87:ASN:ND2	3:C:201:GLU:HG2	2.20	0.56
5:E:13:TRP:NE1	5:E:37:LEU:O	2.38	0.56
1:A:288:LYS:NZ	1:A:322:THR:O	2.37	0.56
1:A:722:ASP:OD1	1:A:723:LEU:N	2.39	0.56
2:B:38:ILE:H	2:B:628:ARG:HH12	1.54	0.56
2:B:166:ALA:HB1	2:B:170:LYS:HB3	1.87	0.56
15:O:565:LEU:H	15:O:565:LEU:HD23	1.71	0.56
13:M:75:PRO:HG2	13:M:167:GLN:HG2	1.87	0.56
15:O:456:HIS:HA	15:O:459:ILE:HG22	1.88	0.56
4:D:3:VAL:HG21	7:G:42:VAL:HG21	1.88	0.56
1:A:116:SER:HB2	1:A:119:ASP:HB2	1.88	0.56
1:A:1263:LEU:O	1:A:1267:LEU:HB2	2.05	0.56
7:G:89:ILE:HG23	7:G:146:ILE:HD13	1.88	0.56
14:N:365:VAL:HG22	14:N:371:LEU:HG	1.87	0.56
6:F:128:LYS:NZ	6:F:149:GLU:O	2.39	0.56
10:J:66:LEU:HA	12:L:35:SER:HB2	1.88	0.56
15:O:144:MET:O	15:O:147:ASN:ND2	2.39	0.56
1:A:1420:THR:HA	2:B:1080:LEU:HD21	1.87	0.55
1:A:1235:PHE:CG	1:A:1236:PRO:HD2	2.40	0.55
1:A:1387:ALA:HB1	1:A:1392:THR:HG23	1.87	0.55
2:B:813:GLU:OE2	2:B:814:ASN:ND2	2.40	0.55
3:C:113:LEU:HD11	3:C:132:ILE:HG12	1.88	0.55
4:D:17:LEU:O	4:D:21:THR:OG1	2.24	0.55
15:O:603:LEU:O	15:O:607:ASN:ND2	2.39	0.55
1:A:310:ASN:HA	15:O:564:PHE:HE1	1.72	0.55
1:A:1415:ILE:HD13	2:B:1067:ARG:HD2	1.88	0.55
2:B:207:VAL:HG21	2:B:355:ARG:HB3	1.87	0.55
15:O:641:LEU:O	15:O:645:LEU:HG	2.06	0.55
2:B:589:SER:HB2	2:B:653:GLU:HG3	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:808:GLY:HA3	2:B:844:ASN:ND2	2.22	0.55
13:M:87:VAL:HB	13:M:176:VAL:HG13	1.88	0.55
1:A:325:MET:SD	1:A:325:MET:N	2.79	0.55
13:M:227:LEU:O	13:M:232:LEU:HB2	2.07	0.55
14:N:310:PRO:HG3	14:N:380:MET:HE1	1.88	0.55
1:A:837:LYS:NZ	2:B:655:ASN:O	2.26	0.55
2:B:928:GLN:HG3	2:B:939:VAL:HG21	1.88	0.55
3:C:139:LYS:HD3	3:C:201:GLU:HB2	1.89	0.55
15:O:306:SER:HA	15:O:309:ALA:HB3	1.88	0.55
15:O:631:ASN:O	15:O:634:GLU:HG2	2.07	0.55
2:B:103:LYS:HG3	2:B:130:TYR:CE2	2.42	0.55
2:B:1001:LYS:O	3:C:277:ARG:NH2	2.32	0.55
8:H:127:GLY:HA3	8:H:130:ARG:HE	1.71	0.55
15:O:605:LYS:HD2	15:O:611:VAL:HG21	1.89	0.55
1:A:1378:LYS:HG3	1:A:1379:MET:H	1.72	0.55
1:A:607:LYS:HD2	8:H:120:GLY:HA3	1.88	0.55
2:B:322:GLU:O	2:B:325:GLU:HG3	2.06	0.55
2:B:834:MET:SD	12:L:63:ARG:HD2	2.47	0.55
11:K:88:PHE:HB3	11:K:106:GLN:HB2	1.89	0.55
1:A:239:CYS:SG	1:A:252:ARG:NH2	2.80	0.55
2:B:321:GLN:HG2	2:B:323:GLY:H	1.72	0.55
3:C:140:CYS:HB2	3:C:196:LEU:HG	1.88	0.55
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.41	0.55
2:B:791:THR:HG21	2:B:842:TYR:CE2	2.34	0.54
15:O:302:THR:HG22	16:P:265:LEU:HD22	1.89	0.54
1:A:762:LEU:O	1:A:766:ILE:HG23	2.07	0.54
2:B:77:ILE:HG23	2:B:95:TYR:HB3	1.89	0.54
1:A:483:LEU:HD13	1:A:550:ILE:HG21	1.90	0.54
8:H:31:THR:O	8:H:32:THR:OG1	2.22	0.54
1:A:777:VAL:HG12	1:A:811:ALA:HB1	1.90	0.54
2:B:1014:GLN:HA	3:C:12:VAL:HB	1.89	0.54
7:G:80:PHE:CG	7:G:81:LEU:N	2.75	0.54
13:M:164:LYS:HD3	13:M:256:LYS:HE2	1.89	0.54
1:A:41:ASP:HB2	1:A:44:LYS:HG2	1.88	0.54
1:A:891:LYS:HG2	1:A:1389:PHE:CD1	2.42	0.54
15:O:581:LEU:HD23	15:O:648:TRP:HB3	1.90	0.54
13:M:95:ARG:HA	14:N:391:LEU:HD23	1.88	0.54
15:O:79:LEU:HD22	15:O:83:ILE:HD11	1.90	0.54
1:A:1379:MET:SD	1:A:1380:ARG:NH1	2.80	0.54
1:A:110:CYS:HB3	1:A:157:CYS:SG	2.47	0.54
3:C:55:ASP:OD2	3:C:271:ARG:NH1	2.32	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:71:ILE:N	14:N:365:VAL:O	2.40	0.54
1:A:579:LEU:HA	1:A:582:MET:HE3	1.90	0.54
7:G:151:GLU:OE1	7:G:151:GLU:N	2.41	0.54
10:J:29:GLU:H	10:J:29:GLU:CD	2.16	0.54
1:A:116:SER:HA	1:A:155:LEU:HD22	1.89	0.53
1:A:885:MET:HE3	1:A:1130:ILE:HD13	1.90	0.53
1:A:1204:ASP:OD1	1:A:1204:ASP:N	2.42	0.53
1:A:1373:ARG:H	1:A:1373:ARG:NE	2.06	0.53
2:B:383:LEU:O	2:B:442:TRP:HZ3	1.91	0.53
3:C:224:THR:O	3:C:303:GLU:HG2	2.08	0.53
7:G:41:ASN:HA	7:G:155:PHE:CG	2.43	0.53
7:G:89:ILE:HD13	7:G:97:ILE:HD11	1.88	0.53
1:A:1192:THR:HG23	1:A:1196:LEU:HD13	1.89	0.53
2:B:553:TYR:CD1	2:B:568:PRO:HG3	2.43	0.53
3:C:303:GLU:OE2	10:J:43:ARG:NH1	2.37	0.53
13:M:136:ALA:HB1	13:M:143:VAL:HG21	1.90	0.53
14:N:384:LYS:NZ	14:N:387:GLU:OE2	2.40	0.53
1:A:223:ASN:OD1	1:A:226:LYS:N	2.25	0.53
1:A:286:THR:O	1:A:290:THR:HG23	2.09	0.53
15:O:380:LEU:HD13	15:O:452:LEU:HD23	1.91	0.53
16:P:245:GLU:O	16:P:248:VAL:HG12	2.09	0.53
17:Q:57:LYS:HA	17:Q:60:ASN:HD22	1.73	0.53
1:A:1172:TYR:HE1	1:A:1174:GLN:HE21	1.54	0.53
2:B:296:TYR:HA	2:B:300:GLN:NE2	2.24	0.53
1:A:51:ASN:N	1:A:55:ASP:OD2	2.40	0.53
2:B:295:ILE:HG12	9:I:27:ARG:HB3	1.90	0.53
2:B:772:VAL:HB	2:B:943:ILE:HB	1.90	0.53
8:H:95:TYR:HE2	8:H:97:MET:HE3	1.73	0.53
9:I:7:SER:O	13:M:92:ASN:ND2	2.42	0.53
15:O:263:LEU:HD12	15:O:272:ARG:HD3	1.91	0.53
1:A:599:LYS:HG3	1:A:600:PRO:HA	1.90	0.53
14:N:287:HIS:HE1	14:N:382:ILE:O	1.91	0.53
15:O:141:ILE:HD11	15:O:157:ALA:HB2	1.90	0.53
3:C:192:LEU:HG	10:J:2:ILE:HD11	1.90	0.53
1:A:153:ARG:NH1	1:A:158:GLY:O	2.38	0.53
2:B:477:PHE:CG	2:B:478:GLU:N	2.76	0.53
2:B:776:SER:HB2	3:C:217:ALA:HB2	1.91	0.53
7:G:89:ILE:HD11	7:G:143:ASN:H	1.74	0.53
8:H:27:GLU:OE2	8:H:39:THR:OG1	2.25	0.53
15:O:140:ILE:HG13	15:O:160:VAL:HG21	1.90	0.53
1:A:1101:GLY:HA2	1:A:1104:MET:SD	2.50	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1264:ARG:NH2	9:I:44:LYS:HG2	2.24	0.52
2:B:831:GLU:HB3	12:L:61:THR:HB	1.90	0.52
9:I:12:LEU:HD23	9:I:24:LEU:HD13	1.91	0.52
1:A:32:VAL:HG21	1:A:57:LYS:HD3	1.89	0.52
1:A:200:GLU:HG2	15:O:515:LYS:HB3	1.89	0.52
1:A:1303:VAL:O	1:A:1306:THR:HG22	2.09	0.52
2:B:84:LEU:O	2:B:400:LYS:NZ	2.37	0.52
12:L:41:SER:OG	12:L:42:ARG:N	2.41	0.52
15:O:203:ILE:HA	15:O:207:HIS:CE1	2.45	0.52
2:B:259:ALA:HB1	2:B:302:LEU:HD23	1.91	0.52
2:B:911:LYS:HG2	2:B:1027:LEU:HD12	1.91	0.52
13:M:252:PHE:CZ	13:M:256:LYS:HD2	2.45	0.52
1:A:586:GLY:O	11:K:62:SER:OG	2.20	0.52
4:D:28:LEU:O	4:D:56:GLN:NE2	2.28	0.52
6:F:105:ALA:HB2	7:G:15:PRO:HB3	1.91	0.52
7:G:105:PHE:HE2	7:G:196:LEU:HG	1.74	0.52
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.92	0.52
15:O:460:LEU:O	15:O:463:SER:OG	2.27	0.52
17:Q:57:LYS:HA	17:Q:60:ASN:ND2	2.24	0.52
4:D:127:LEU:N	4:D:128:PRO:HD3	2.25	0.52
7:G:4:LEU:HD22	7:G:73:ARG:HB3	1.91	0.52
15:O:642:SER:HA	15:O:645:LEU:HD12	1.91	0.52
1:A:92:HIS:HA	1:A:258:TRP:CD1	2.45	0.52
1:A:310:ASN:HD22	1:A:310:ASN:C	2.18	0.52
1:A:729:GLU:O	1:A:733:ILE:HG23	2.10	0.52
1:A:182:THR:OG1	1:A:220:ASP:HB2	2.09	0.52
1:A:1151:GLU:OE2	1:A:1197:GLN:NE2	2.42	0.52
1:A:1209:ILE:HD12	1:A:1230:ILE:HD13	1.92	0.52
4:D:130:ASN:HD22	4:D:133:HIS:CD2	2.28	0.52
8:H:95:TYR:CE2	8:H:97:MET:HE3	2.45	0.52
15:O:343:LYS:NZ	15:O:346:GLN:HB2	2.25	0.52
14:N:208:ARG:HE	14:N:210:GLU:HG2	1.75	0.51
2:B:247:ILE:HG21	2:B:251:ILE:HD11	1.92	0.51
3:C:136:LEU:HB2	3:C:167:LEU:HD23	1.91	0.51
3:C:196:LEU:N	3:C:196:LEU:HD23	2.25	0.51
7:G:147:ARG:HB3	7:G:206:GLY:H	1.75	0.51
15:O:80:VAL:HG23	15:O:91:VAL:HG11	1.93	0.51
16:P:179:LEU:HD21	16:P:246:VAL:HG12	1.93	0.51
16:P:265:LEU:HD12	16:P:269:LEU:HD23	1.92	0.51
1:A:115:LEU:HD13	1:A:120:LYS:HB2	1.92	0.51
1:A:766:ILE:HD11	1:A:822:ARG:CZ	2.41	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:VAL:HG11	2:B:484:SER:HB3	1.93	0.51
2:B:98:ILE:HG13	2:B:131:VAL:HG12	1.93	0.51
5:E:143:ASN:HD21	5:E:146:HIS:CD2	2.29	0.51
15:O:307:VAL:HG21	16:P:205:ASN:O	2.11	0.51
15:O:602:LEU:HB3	15:O:627:LEU:HD21	1.91	0.51
16:P:256:VAL:HG22	16:P:257:THR:H	1.75	0.51
1:A:872:LEU:O	1:A:875:THR:HG22	2.11	0.51
7:G:88:TRP:CE2	7:G:145:LYS:HD2	2.46	0.51
17:Q:54:LEU:HA	17:Q:57:LYS:HG2	1.92	0.51
7:G:81:LEU:HD23	17:Q:107:ARG:HH11	1.76	0.51
7:G:110:ILE:HG22	7:G:198:GLY:N	2.26	0.51
15:O:589:LEU:HA	15:O:592:LYS:HG2	1.93	0.51
1:A:36:THR:OG1	1:A:38:ASP:OD1	2.24	0.51
1:A:1163:LYS:HG3	1:A:1164:THR:HG22	1.93	0.51
7:G:144:GLU:HG3	7:G:145:LYS:H	1.75	0.51
2:B:938:ILE:HG12	10:J:43:ARG:HD2	1.93	0.51
2:B:964:GLY:O	2:B:968:VAL:HG22	2.10	0.51
13:M:75:PRO:HB2	13:M:77:LYS:HZ2	1.74	0.51
15:O:43:ASN:HB3	15:O:45:ASP:OD1	2.11	0.51
1:A:385:PRO:HD2	2:B:765:TYR:CZ	2.46	0.51
1:A:533:ASN:O	1:A:539:ASN:ND2	2.44	0.51
2:B:540:ASP:HB3	2:B:543:LEU:HD23	1.93	0.51
3:C:328:LEU:HD11	11:K:65:ILE:HD13	1.93	0.51
4:D:147:GLU:N	4:D:147:GLU:OE1	2.44	0.51
9:I:26:CYS:HB3	9:I:31:TYR:HB3	1.93	0.51
14:N:207:VAL:HG11	14:N:215:VAL:HG11	1.92	0.51
1:A:91:PHE:CE1	1:A:224:PRO:HA	2.46	0.51
1:A:1177:TYR:HB2	9:I:40:ILE:HG13	1.93	0.51
1:A:1443:PRO:HB3	7:G:73:ARG:HH22	1.75	0.51
2:B:383:LEU:HB3	2:B:442:TRP:CH2	2.46	0.51
15:O:527:LEU:HD13	16:P:246:VAL:HG21	1.93	0.51
1:A:1428:PHE:CZ	6:F:89:GLU:HA	2.46	0.50
2:B:517:MET:HE1	2:B:675:ILE:HB	1.93	0.50
7:G:53:THR:HB	7:G:71:THR:HB	1.92	0.50
15:O:537:LEU:O	15:O:541:ILE:HG12	2.11	0.50
15:O:640:ARG:CD	17:Q:44:ASN:HA	2.41	0.50
1:A:713:GLY:N	1:A:716:ASP:OD2	2.44	0.50
1:A:1172:TYR:CE2	1:A:1187:ARG:HB3	2.46	0.50
2:B:240:ILE:HG21	2:B:353:THR:HG23	1.94	0.50
2:B:961:LEU:HD12	2:B:1022:ILE:HD11	1.92	0.50
15:O:124:GLU:O	15:O:127:ILE:HG12	2.11	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLU:OE2	15:O:514:ASN:ND2	2.42	0.50
2:B:222:SER:HB3	2:B:334:HIS:HB3	1.93	0.50
2:B:267:GLU:O	2:B:271:LEU:N	2.43	0.50
15:O:94:THR:HA	17:Q:72:THR:HG21	1.93	0.50
15:O:133:SER:O	15:O:137:ILE:HG23	2.11	0.50
1:A:5:VAL:HG11	7:G:34:PHE:CE1	2.46	0.50
1:A:1411:VAL:HG11	1:A:1423:ILE:HD12	1.93	0.50
16:P:311:TYR:HB2	16:P:314:GLU:HB2	1.93	0.50
1:A:88:LEU:HG	1:A:316:TRP:CE2	2.46	0.50
1:A:885:MET:HE1	1:A:1126:ILE:HG22	1.93	0.50
1:A:964:ASN:ND2	1:A:1009:ARG:HE	2.08	0.50
1:A:1328:ILE:HD11	1:A:1363:THR:HB	1.93	0.50
2:B:347:LEU:O	2:B:351:MET:HG2	2.11	0.50
2:B:800:ASN:ND2	2:B:851:SER:O	2.45	0.50
2:B:890:ASP:OD1	2:B:890:ASP:N	2.43	0.50
3:C:165:ARG:HB3	3:C:189:PRO:HB2	1.94	0.50
3:C:223:SER:HB2	10:J:12:LYS:HA	1.91	0.50
1:A:93:ILE:H	1:A:93:ILE:HD12	1.77	0.50
3:C:229:LEU:HD13	3:C:295:ARG:HA	1.94	0.50
14:N:380:MET:HE2	14:N:418:VAL:HG12	1.93	0.50
15:O:60:ARG:NH2	15:O:90:SER:O	2.45	0.50
15:O:251:LYS:O	15:O:255:LYS:HG3	2.12	0.50
15:O:587:ASN:O	15:O:591:LYS:HG2	2.12	0.50
13:M:158:GLN:HG3	13:M:173:ILE:HD12	1.94	0.50
15:O:102:ARG:O	15:O:126:GLY:HA3	2.10	0.50
16:P:247:LEU:O	16:P:252:LYS:HB2	2.11	0.50
1:A:830:ARG:HD3	1:A:837:LYS:HA	1.94	0.50
2:B:567:PHE:HD1	14:N:279:GLU:HG2	1.76	0.50
5:E:191:LYS:N	5:E:194:GLU:OE2	2.36	0.50
7:G:47:THR:OG1	7:G:48:ILE:N	2.45	0.50
9:I:6:PRO:HG3	14:N:200:PHE:O	2.12	0.50
13:M:196:GLU:OE1	13:M:196:GLU:N	2.45	0.50
1:A:34:VAL:HG12	1:A:293:VAL:HG21	1.94	0.50
15:O:215:TRP:CD2	15:O:335:LEU:HD22	2.47	0.50
2:B:216:VAL:HG11	2:B:359:ALA:HB3	1.94	0.49
3:C:86:PHE:HE2	3:C:205:LYS:HG3	1.77	0.49
3:C:87:ASN:HD22	3:C:201:GLU:HG2	1.76	0.49
4:D:15:GLU:HA	4:D:18:LYS:HG2	1.93	0.49
8:H:92:ASP:N	8:H:92:ASP:OD1	2.44	0.49
3:C:328:LEU:HD12	11:K:72:LEU:HD21	1.94	0.49
15:O:505:MET:HG2	16:P:250:ASP:HA	1.95	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1084:GLU:OE1	6:F:87:LYS:NZ	2.33	0.49
2:B:775:LYS:O	2:B:776:SER:OG	2.23	0.49
8:H:61:SER:HB3	8:H:139:ASN:HB3	1.93	0.49
1:A:22:SER:HB3	1:A:250:SER:HB3	1.94	0.49
1:A:535:MET:HG2	2:B:1073:TYR:CG	2.46	0.49
1:A:1259:ARG:O	1:A:1263:LEU:HB2	2.13	0.49
2:B:698:ARG:CZ	2:B:952:ARG:HD3	2.41	0.49
2:B:1103:TYR:CE2	7:G:163:PRO:HG2	2.48	0.49
7:G:38:ILE:HG22	7:G:44:LEU:HA	1.94	0.49
7:G:89:ILE:HA	7:G:100:SER:HB3	1.95	0.49
7:G:23:ILE:HG23	7:G:51:LEU:HD12	1.94	0.49
15:O:73:ARG:HH12	15:O:107:LEU:HD11	1.78	0.49
15:O:156:VAL:HA	15:O:159:ILE:HG22	1.95	0.49
1:A:481:HIS:CD2	1:A:481:HIS:H	2.30	0.49
1:A:988:ASP:HB2	1:A:991:LYS:HB2	1.94	0.49
1:A:1326:LEU:HD23	5:E:144:ILE:HG22	1.95	0.49
7:G:42:VAL:O	7:G:78:LYS:HD3	2.12	0.49
15:O:332:GLN:HB3	15:O:337:GLN:HE22	1.76	0.49
16:P:185:PHE:HZ	16:P:221:ILE:HG23	1.78	0.49
1:A:578:GLN:O	1:A:582:MET:HG3	2.12	0.49
1:A:730:LEU:O	1:A:733:ILE:HG12	2.11	0.49
1:A:948:ASN:O	1:A:1061:ARG:NH2	2.46	0.49
2:B:590:ILE:HG13	2:B:601:ILE:HG12	1.93	0.49
1:A:477:GLN:NE2	2:B:1066:GLU:OE2	2.34	0.49
1:A:1206:ALA:O	1:A:1210:THR:HG23	2.12	0.49
2:B:541:ILE:HD12	2:B:544:ILE:HD11	1.94	0.49
5:E:93:MET:HE3	5:E:123:LEU:HD12	1.94	0.49
7:G:191:PRO:HG2	7:G:192:PRO:HD3	1.94	0.49
9:I:5:CYS:HB2	9:I:26:CYS:SG	2.52	0.49
9:I:23:THR:OG1	9:I:32:GLU:HG3	2.12	0.49
4:D:134:LEU:HA	4:D:137:ILE:HD12	1.94	0.49
4:D:142:ASP:HA	4:D:146:ASP:HB2	1.93	0.49
2:B:877:GLU:HB3	2:B:902:GLN:OE1	2.13	0.49
2:B:929:GLU:HB2	3:C:69:ARG:HG2	1.95	0.49
7:G:3:ILE:HG12	7:G:78:LYS:HB2	1.95	0.49
1:A:164:VAL:HG23	1:A:180:HIS:HB2	1.95	0.48
1:A:913:GLN:NE2	1:A:1360:ASP:OD2	2.46	0.48
2:B:327:ILE:HG23	13:M:231:LEU:HD21	1.95	0.48
1:A:154:CYS:N	1:A:158:GLY:HA2	2.28	0.48
1:A:288:LYS:O	1:A:292:ILE:HG13	2.14	0.48
1:A:923:PRO:HB3	1:A:1351:ASP:CG	2.38	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:HD11	1:A:185:TRP:H	1.78	0.48
1:A:1217:ILE:HG22	1:A:1218:GLN:N	2.28	0.48
2:B:343:ARG:HG2	2:B:542:THR:HG22	1.95	0.48
8:H:4:THR:O	8:H:4:THR:OG1	2.30	0.48
8:H:77:ARG:HA	8:H:77:ARG:HD2	1.72	0.48
1:A:192:PRO:O	1:A:196:ILE:HG12	2.13	0.48
1:A:473:LEU:HD11	2:B:1078:LEU:HD21	1.96	0.48
1:A:1443:PRO:HB3	7:G:73:ARG:NH1	2.25	0.48
3:C:26:ASP:O	3:C:28:GLU:N	2.44	0.48
13:M:190:ASN:O	13:M:194:LYS:HG2	2.14	0.48
15:O:120:TYR:CE2	17:Q:133:PRO:HG2	2.49	0.48
16:P:216:SER:OG	16:P:217:THR:N	2.45	0.48
2:B:1004:LEU:HB2	2:B:1013:LEU:HD12	1.95	0.48
8:H:114:VAL:HG21	8:H:130:ARG:HH12	1.79	0.48
2:B:624:ASP:HA	2:B:627:LEU:HB2	1.96	0.48
15:O:311:VAL:HG22	15:O:374:LEU:HD21	1.94	0.48
15:O:649:GLU:CD	15:O:649:GLU:H	2.22	0.48
1:A:1145:LEU:HD12	1:A:1292:GLU:HA	1.95	0.48
1:A:956:PRO:HG3	1:A:1019:LEU:HG	1.95	0.48
2:B:624:ASP:OD1	2:B:628:ARG:NH2	2.47	0.48
2:B:776:SER:CB	3:C:217:ALA:HB2	2.43	0.48
8:H:3:ASN:ND2	8:H:62:SER:OG	2.47	0.48
14:N:-105:UNK:O	14:N:-103:UNK:N	2.46	0.48
14:N:287:HIS:CD2	14:N:371:LEU:H	2.31	0.48
15:O:527:LEU:HD23	16:P:164:TRP:CD1	2.48	0.48
1:A:225:LEU:HD21	15:O:542:ARG:HA	1.95	0.48
1:A:430:ALA:HA	1:A:464:ARG:HA	1.96	0.48
3:C:282:TYR:C	3:C:284:GLU:H	2.21	0.48
4:D:147:GLU:CD	4:D:147:GLU:H	2.22	0.48
9:I:6:PRO:HB2	14:N:199:LEU:HD12	1.96	0.48
1:A:155:LEU:HG	15:O:336:LEU:HB2	1.96	0.48
1:A:728:GLU:O	1:A:732:GLU:HG2	2.14	0.48
2:B:462:SER:H	2:B:465:SER:HB3	1.78	0.48
2:B:577:HIS:NE2	14:N:422:ILE:HG21	2.29	0.48
2:B:660:ALA:HB2	2:B:670:MET:SD	2.53	0.48
3:C:115:TRP:HH2	3:C:212:ILE:HG12	1.79	0.48
1:A:108:LYS:HD2	1:A:180:HIS:ND1	2.29	0.47
1:A:753:GLN:HB2	1:A:756:CYS:HB2	1.95	0.47
1:A:1104:MET:HB2	1:A:1123:VAL:HG23	1.96	0.47
2:B:884:VAL:HG22	2:B:898:VAL:HG22	1.94	0.47
11:K:85:ASP:CG	11:K:110:GLU:HB3	2.38	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:44:PRO:HB3	15:O:583:TRP:HB2	1.96	0.47
15:O:492:TYR:CE1	15:O:577:MET:HG2	2.47	0.47
1:A:140:ILE:O	1:A:144:ILE:HG22	2.14	0.47
1:A:738:CYS:O	1:A:742:ILE:HG12	2.13	0.47
2:B:264:SER:C	2:B:266:LEU:H	2.22	0.47
14:N:226:LYS:HD3	14:N:293:LYS:HD2	1.96	0.47
1:A:463:GLU:OE1	2:B:1040:ARG:NH2	2.41	0.47
2:B:295:ILE:HB	9:I:27:ARG:HD2	1.96	0.47
2:B:904:ARG:HH22	2:B:1033:ASP:CG	2.22	0.47
3:C:197:ARG:HA	3:C:197:ARG:HD3	1.56	0.47
3:C:215:ASP:OD2	12:L:70:ARG:NH2	2.39	0.47
15:O:127:ILE:HA	15:O:130:LEU:HD13	1.97	0.47
1:A:1023:ARG:HH22	1:A:1045:ASP:CG	2.21	0.47
13:M:258:THR:O	13:M:262:GLU:HG2	2.15	0.47
1:A:988:ASP:N	1:A:988:ASP:OD1	2.48	0.47
2:B:117:GLU:HG3	12:L:55:ILE:HD11	1.96	0.47
8:H:105:GLU:HG2	8:H:113:ALA:HB3	1.97	0.47
15:O:316:LEU:HA	15:O:319:THR:HG22	1.96	0.47
15:O:361:PHE:O	15:O:475:VAL:HG13	2.15	0.47
15:O:530:GLU:O	15:O:533:ILE:HG13	2.15	0.47
1:A:573:ARG:HH21	11:K:87:GLU:HB2	1.80	0.47
2:B:387:LEU:HB2	2:B:442:TRP:CZ3	2.50	0.47
3:C:136:LEU:HB3	3:C:204:LEU:HG	1.95	0.47
3:C:278:GLU:OE2	3:C:282:TYR:OH	2.23	0.47
5:E:90:VAL:O	5:E:94:LYS:HG2	2.14	0.47
15:O:27:THR:HB	15:O:30:ASP:H	1.80	0.47
1:A:109:ASN:HA	15:O:572:HIS:HE2	1.80	0.47
1:A:957:TYR:HD2	1:A:1031:LEU:HB3	1.80	0.47
2:B:554:GLY:HA2	2:B:564:SER:HA	1.96	0.47
3:C:256:ILE:HA	3:C:268:LYS:H	1.79	0.47
11:K:87:GLU:HG3	11:K:106:GLN:O	2.14	0.47
13:M:76:LEU:HD23	13:M:168:VAL:HB	1.97	0.47
15:O:531:LYS:HA	15:O:534:ARG:HE	1.80	0.47
15:O:610:ASP:OD1	15:O:610:ASP:N	2.47	0.47
16:P:222:LEU:O	16:P:226:THR:OG1	2.30	0.47
17:Q:133:PRO:HD2	17:Q:136:LEU:HD12	1.96	0.47
1:A:325:MET:HB3	1:A:350:ILE:HG21	1.96	0.47
1:A:595:PRO:HG2	1:A:598:MET:HG2	1.97	0.47
1:A:985:LYS:C	1:A:987:GLU:H	2.22	0.47
2:B:94:LYS:HB3	2:B:134:GLU:HB2	1.96	0.47
2:B:766:ASP:HB3	2:B:772:VAL:HG23	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:872:ILE:HB	2:B:874:ARG:NH1	2.29	0.47
4:D:120:LYS:O	4:D:124:VAL:HG13	2.15	0.47
5:E:84:ASP:N	5:E:84:ASP:OD1	2.47	0.47
14:N:200:PHE:CD2	14:N:201:PRO:HD2	2.49	0.47
1:A:95:TYR:HB3	1:A:98:ALA:HB3	1.96	0.47
1:A:638:SER:HB3	1:A:641:LEU:HG	1.97	0.47
2:B:86:ASP:OD1	2:B:86:ASP:N	2.48	0.47
2:B:130:TYR:CE1	2:B:148:GLU:HB2	2.50	0.47
2:B:197:GLN:HB2	2:B:378:GLU:HG2	1.96	0.47
3:C:85:PHE:HE1	3:C:97:LEU:HD23	1.79	0.47
4:D:65:TYR:O	4:D:68:ILE:HG12	2.15	0.47
14:N:226:LYS:HG3	14:N:292:ARG:NH2	2.29	0.47
2:B:838:SER:HB2	2:B:875:GLY:O	2.14	0.47
3:C:192:LEU:HD21	3:C:195:LYS:HE2	1.96	0.47
15:O:174:TYR:O	15:O:178:VAL:HG23	2.15	0.47
15:O:345:PHE:O	15:O:348:GLU:HG3	2.15	0.47
1:A:1258:TYR:CZ	2:B:292:LYS:HA	2.50	0.46
11:K:87:GLU:HB3	11:K:108:TYR:CE1	2.50	0.46
14:N:396:ALA:HB2	14:N:409:LEU:HD11	1.97	0.46
15:O:626:GLN:O	15:O:629:MET:HG3	2.15	0.46
17:Q:125:HIS:ND1	17:Q:126:PRO:O	2.43	0.46
1:A:599:LYS:NZ	8:H:90:ALA:O	2.35	0.46
13:M:148:LEU:HB3	13:M:179:LEU:HB3	1.98	0.46
1:A:800:LYS:HG2	2:B:947:HIS:O	2.15	0.46
1:A:974:LEU:HD13	1:A:998:TYR:HB3	1.96	0.46
2:B:760:MET:C	2:B:946:PRO:HD3	2.40	0.46
6:F:118:LEU:HG	6:F:122:MET:HE3	1.97	0.46
14:N:354:ARG:HG3	14:N:356:LEU:HB2	1.97	0.46
15:O:105:LYS:HG3	15:O:123:ASN:HB2	1.96	0.46
1:A:372:ARG:HG3	2:B:1052:GLU:OE1	2.16	0.46
1:A:384:ASP:HB2	1:A:499:ARG:HB3	1.96	0.46
1:A:598:MET:SD	8:H:141:TYR:HE2	2.38	0.46
2:B:690:TYR:HB3	2:B:693:HIS:CD2	2.45	0.46
11:K:64:GLN:CD	11:K:100:LEU:HD11	2.40	0.46
15:O:60:ARG:HB2	17:Q:72:THR:O	2.15	0.46
15:O:267:PRO:HB2	15:O:270:SER:OG	2.16	0.46
1:A:92:HIS:HA	1:A:258:TRP:HD1	1.80	0.46
2:B:113:THR:HG21	2:B:123:MET:HE1	1.97	0.46
2:B:195:LEU:HD22	2:B:472:ARG:HB3	1.98	0.46
2:B:527:GLU:O	2:B:531:LYS:HE3	2.16	0.46
7:G:79:PRO:HB2	7:G:150:ILE:HG12	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:163:VAL:HB	14:N:297:MET:O	2.16	0.46
1:A:114:LEU:HD11	1:A:161:ASN:HD22	1.80	0.46
1:A:154:CYS:H	1:A:158:GLY:HA2	1.81	0.46
1:A:373:VAL:HG22	2:B:1060:LEU:O	2.16	0.46
1:A:705:LEU:HD23	1:A:705:LEU:HA	1.73	0.46
1:A:1339:ILE:HD13	1:A:1358:LEU:HD23	1.97	0.46
2:B:240:ILE:N	2:B:286:ASN:OD1	2.49	0.46
4:D:64:ASN:O	4:D:68:ILE:HG23	2.16	0.46
15:O:554:THR:OG1	15:O:561:ARG:NH1	2.48	0.46
17:Q:129:LEU:HD23	17:Q:129:LEU:H	1.81	0.46
1:A:256:TYR:CE2	1:A:1401:PHE:HA	2.50	0.46
1:A:463:GLU:CD	2:B:1040:ARG:HH22	2.22	0.46
1:A:1436:ILE:HD12	7:G:23:ILE:HG13	1.97	0.46
2:B:251:ILE:HD13	2:B:305:ILE:HD13	1.97	0.46
2:B:347:LEU:CD1	2:B:541:ILE:HG13	2.45	0.46
2:B:449:MET:HE3	2:B:449:MET:HB3	1.89	0.46
15:O:647:LEU:HG	16:P:293:ILE:HD13	1.98	0.46
1:A:153:ARG:HD2	1:A:158:GLY:HA3	1.98	0.46
1:A:822:ARG:HB3	1:A:845:LYS:HG2	1.98	0.46
2:B:64:SER:HB3	2:B:381:GLY:H	1.80	0.46
2:B:775:LYS:HB2	2:B:925:ILE:HG22	1.97	0.46
7:G:162:SER:HB3	7:G:165:GLU:OE1	2.16	0.46
1:A:1330:ALA:HB1	5:E:149:LEU:HB3	1.97	0.46
13:M:105:PRO:HB2	13:M:123:ILE:HD12	1.98	0.46
15:O:73:ARG:HG3	15:O:119:TYR:HB3	1.98	0.46
15:O:487:LEU:O	15:O:490:SER:OG	2.27	0.46
15:O:529:LYS:O	15:O:533:ILE:HG23	2.16	0.45
2:B:197:GLN:HB2	2:B:378:GLU:CG	2.46	0.45
5:E:144:ILE:HD12	5:E:145:THR:HG23	1.99	0.45
13:M:102:ALA:O	14:N:411:ARG:NH2	2.43	0.45
15:O:640:ARG:HD2	17:Q:44:ASN:HA	1.97	0.45
1:A:808:GLN:HG2	1:A:813:VAL:HA	1.98	0.45
2:B:54:VAL:HG23	2:B:55:LYS:HG3	1.97	0.45
3:C:201:GLU:HG3	3:C:202:ILE:N	2.28	0.45
5:E:197:LYS:HE2	5:E:199:ILE:HD11	1.98	0.45
13:M:163:VAL:HA	13:M:167:GLN:O	2.17	0.45
1:A:299:ILE:O	1:A:303:LEU:HG	2.17	0.45
1:A:697:MET:HE3	1:A:697:MET:HB3	1.72	0.45
1:A:737:LYS:O	1:A:740:GLU:HG3	2.16	0.45
1:A:1099:GLU:O	1:A:1102:THR:OG1	2.30	0.45
2:B:545:ASP:HB3	14:N:390:PHE:CE2	2.51	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:841:ILE:HG12	2:B:872:ILE:HD13	1.98	0.45
14:N:313:LEU:HB3	14:N:314:PRO:HD2	1.97	0.45
15:O:163:VAL:HA	15:O:169:LEU:CD2	2.46	0.45
15:O:254:ASN:HA	15:O:257:ASN:ND2	2.31	0.45
16:P:253:LEU:HD13	16:P:261:TYR:CG	2.51	0.45
1:A:118:THR:HA	1:A:121:ARG:HD3	1.99	0.45
1:A:145:LEU:HD13	1:A:145:LEU:HA	1.83	0.45
1:A:878:LYS:HB2	1:A:878:LYS:HE2	1.74	0.45
1:A:1097:ILE:HA	1:A:1343:MET:HE1	1.98	0.45
1:A:1104:MET:HG2	1:A:1346:HIS:ND1	2.32	0.45
2:B:302:LEU:HD22	2:B:325:GLU:OE1	2.17	0.45
2:B:997:ASN:OD1	2:B:999:SER:OG	2.29	0.45
3:C:94:ASP:OD2	12:L:60:ARG:NH2	2.50	0.45
6:F:106:PRO:HG3	7:G:19:HIS:HB3	1.98	0.45
15:O:214:LEU:O	15:O:218:LEU:HG	2.16	0.45
1:A:256:TYR:HE2	1:A:1401:PHE:HA	1.81	0.45
1:A:512:PHE:HB2	2:B:768:GLU:O	2.16	0.45
2:B:944:MET:HE3	2:B:957:LYS:HZ3	1.81	0.45
15:O:234:ASP:HA	15:O:237:LYS:HE3	1.98	0.45
15:O:263:LEU:HD23	15:O:263:LEU:H	1.81	0.45
1:A:789:ASN:ND2	1:A:791:PRO:HD2	2.31	0.45
2:B:124:THR:HG23	2:B:187:VAL:HG12	1.99	0.45
2:B:740:THR:O	2:B:744:ILE:HG12	2.17	0.45
7:G:102:LEU:H	7:G:102:LEU:CD2	2.30	0.45
8:H:30:SER:HB2	8:H:36:CYS:HB3	1.99	0.45
15:O:588:LEU:HD11	16:P:310:VAL:HG22	1.98	0.45
1:A:476:ARG:HD3	1:A:508:TYR:O	2.17	0.45
1:A:850:ASN:ND2	1:A:860:GLU:OE1	2.50	0.45
1:A:894:GLU:OE2	2:B:1067:ARG:NH2	2.50	0.45
1:A:1058:GLN:HE22	8:H:131:ASN:HA	1.82	0.45
2:B:168:GLU:HG2	2:B:178:PRO:HB3	1.99	0.45
7:G:88:TRP:CZ2	7:G:145:LYS:HD2	2.51	0.45
13:M:114:PRO:HD2	13:M:243:ILE:HG13	1.98	0.45
14:N:287:HIS:HD2	14:N:370:LYS:HB2	1.82	0.45
15:O:590:PHE:CZ	15:O:594:LYS:HE2	2.51	0.45
15:O:596:LYS:HG2	15:O:603:LEU:HD12	1.97	0.45
1:A:211:LEU:O	1:A:215:VAL:HG13	2.16	0.45
1:A:925:GLU:HB2	1:A:1081:ALA:HA	1.99	0.45
2:B:240:ILE:HG22	2:B:253:ILE:HB	1.99	0.45
14:N:363:ILE:HG12	14:N:373:VAL:HG22	1.98	0.45
15:O:233:SER:OG	15:O:234:ASP:N	2.48	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:GLU:OE1	2:B:1142:ARG:NE	2.50	0.45
1:A:100:ILE:HD11	1:A:178:ILE:HG12	1.99	0.45
1:A:486:LEU:HB2	1:A:508:TYR:OH	2.17	0.45
1:A:1258:TYR:OH	2:B:292:LYS:HA	2.16	0.45
2:B:915:ARG:HD2	2:B:1023:TYR:CD2	2.48	0.45
11:K:88:PHE:CE1	11:K:104:ARG:HG2	2.52	0.45
15:O:337:GLN:H	15:O:337:GLN:HG2	1.63	0.45
15:O:648:TRP:HZ3	15:O:652:GLN:NE2	2.13	0.45
1:A:10:PRO:HG2	2:B:1147:PHE:HE2	1.82	0.44
1:A:181:ASP:HB3	1:A:184:ARG:HB2	1.99	0.44
1:A:184:ARG:HG2	1:A:185:TRP:CD2	2.52	0.44
2:B:295:ILE:HD12	2:B:295:ILE:HA	1.78	0.44
2:B:678:PHE:HB2	2:B:978:CYS:HB3	1.99	0.44
7:G:105:PHE:CE2	7:G:196:LEU:HG	2.49	0.44
15:O:622:SER:O	15:O:626:GLN:NE2	2.49	0.44
1:A:87:ALA:HB2	1:A:300:LYS:NZ	2.31	0.44
1:A:564:ILE:O	1:A:606:GLY:HA3	2.16	0.44
1:A:1200:LEU:HB2	1:A:1204:ASP:HB2	1.98	0.44
2:B:397:ASN:O	2:B:401:LEU:HG	2.17	0.44
8:H:40:LEU:HD21	8:H:144:ILE:HD11	2.00	0.44
12:L:44:ASP:OD1	12:L:45:ALA:N	2.47	0.44
15:O:204:SER:OG	15:O:206:LEU:HD23	2.18	0.44
15:O:492:TYR:OH	15:O:573:SER:HB3	2.17	0.44
1:A:408:VAL:HG23	1:A:460:ASP:O	2.16	0.44
1:A:1058:GLN:NE2	8:H:131:ASN:HA	2.32	0.44
2:B:96:VAL:HG13	2:B:132:ASP:HB2	2.00	0.44
15:O:38:GLU:OE1	15:O:38:GLU:N	2.31	0.44
1:A:907:SER:HB2	1:A:1409:GLU:HB3	1.99	0.44
4:D:11:LEU:HD21	7:G:4:LEU:HG	1.98	0.44
7:G:21:ASP:OD1	7:G:21:ASP:N	2.43	0.44
7:G:99:VAL:HB	7:G:108:ILE:HD11	2.00	0.44
11:K:55:SER:OG	11:K:58:GLY:O	2.35	0.44
15:O:338:ASP:HB3	15:O:342:ALA:HA	1.98	0.44
1:A:966:ILE:HD12	1:A:1071:LEU:HD23	1.99	0.44
1:A:1318:HIS:O	1:A:1322:VAL:HG23	2.17	0.44
2:B:296:TYR:CD1	2:B:300:GLN:HB3	2.53	0.44
2:B:1142:ARG:HA	2:B:1142:ARG:HD3	1.71	0.44
7:G:149:ARG:HG2	7:G:150:ILE:H	1.83	0.44
16:P:217:THR:OG1	16:P:218:THR:N	2.51	0.44
2:B:60:GLN:H	2:B:60:GLN:CD	2.25	0.44
2:B:177:CYS:HB2	2:B:714:ALA:HB1	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:31:VAL:HG12	15:O:32:MET:HG3	1.99	0.44
2:B:688:ILE:HG12	2:B:702:GLN:HG2	1.98	0.44
3:C:71:MET:HG2	3:C:313:ILE:HG22	1.98	0.44
3:C:334:THR:OG1	11:K:48:LYS:NZ	2.50	0.44
9:I:30:PRO:HB3	13:M:136:ALA:HB2	1.99	0.44
14:N:361:GLY:HA3	14:N:374:LYS:O	2.16	0.44
1:A:106:ILE:HA	1:A:113:ILE:HA	1.99	0.44
1:A:292:ILE:HG23	1:A:319:LEU:HD11	1.99	0.44
1:A:613:LEU:O	1:A:696:ARG:NH1	2.51	0.44
1:A:1200:LEU:HD13	1:A:1273:LYS:HB2	2.00	0.44
4:D:154:LEU:HD12	4:D:157:ILE:HD11	2.00	0.44
12:L:37:LYS:HA	12:L:37:LYS:HD3	1.89	0.44
15:O:253:ILE:O	15:O:256:PRO:HD2	2.18	0.44
15:O:267:PRO:HD2	15:O:271:LEU:O	2.18	0.44
15:O:609:ASP:OD1	15:O:609:ASP:N	2.49	0.44
1:A:40:PHE:CE1	1:A:48:PRO:HD3	2.49	0.44
1:A:563:LEU:HD12	1:A:705:LEU:HD21	2.00	0.44
1:A:952:LYS:HE3	1:A:952:LYS:HB3	1.74	0.44
2:B:870:PRO:HG2	2:B:872:ILE:HD11	1.99	0.44
5:E:12:LEU:HD22	5:E:55:ARG:CZ	2.48	0.44
5:E:13:TRP:HB2	5:E:42:PHE:CD2	2.53	0.44
15:O:634:GLU:HA	15:O:637:VAL:HG12	1.99	0.44
1:A:511:ASP:OD1	1:A:511:ASP:N	2.51	0.43
2:B:57:LEU:HD13	2:B:57:LEU:HA	1.77	0.43
2:B:316:LYS:HD2	2:B:316:LYS:HA	1.74	0.43
2:B:821:HIS:CE1	2:B:841:ILE:HD12	2.53	0.43
5:E:124:VAL:HG12	5:E:125:PRO:HD3	2.00	0.43
13:M:75:PRO:HB3	14:N:359:LYS:HE3	1.99	0.43
1:A:73:ASN:OD1	1:A:73:ASN:N	2.48	0.43
1:A:513:ASP:HA	2:B:920:GLY:HA2	2.00	0.43
2:B:843:ILE:HB	2:B:871:VAL:HB	2.00	0.43
7:G:202:THR:HB	7:G:205:MET:HE2	1.99	0.43
15:O:164:ILE:HG22	15:O:282:ILE:HG21	2.00	0.43
1:A:101:GLN:HE21	1:A:145:LEU:HG	1.82	0.43
1:A:379:THR:HB	2:B:1035:MET:HA	2.00	0.43
1:A:794:MET:SD	2:B:950:PRO:HG3	2.58	0.43
1:A:1114:VAL:HG12	1:A:1116:SER:HB3	2.00	0.43
2:B:271:LEU:HB3	2:B:350:ALA:HB1	2.00	0.43
2:B:877:GLU:HG3	2:B:878:PRO:HD2	2.00	0.43
2:B:1008:ILE:HG13	2:B:1009:THR:N	2.34	0.43
4:D:27:HIS:CD2	4:D:28:LEU:HG	2.54	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:128:TRP:HB2	7:G:139:TYR:HB3	2.00	0.43
13:M:174:GLU:CD	13:M:175:ARG:HG3	2.43	0.43
14:N:391:LEU:HD22	14:N:411:ARG:HH21	1.83	0.43
1:A:106:ILE:HG22	1:A:113:ILE:HA	2.00	0.43
1:A:593:PRO:HD3	1:A:612:LEU:HD21	1.99	0.43
1:A:679:TYR:O	1:A:683:ARG:HG2	2.18	0.43
2:B:234:ILE:HG12	2:B:241:TYR:HB2	2.00	0.43
3:C:196:LEU:HD23	3:C:196:LEU:H	1.83	0.43
4:D:15:GLU:HA	4:D:18:LYS:HE2	2.00	0.43
4:D:56:GLN:HA	4:D:59:THR:HG22	2.00	0.43
13:M:140:TRP:HB3	13:M:185:TYR:HB2	2.01	0.43
15:O:107:LEU:HD11	15:O:119:TYR:HB2	2.00	0.43
15:O:328:ASP:C	15:O:330:LEU:H	2.25	0.43
1:A:766:ILE:HD11	1:A:822:ARG:NH2	2.34	0.43
1:A:968:GLY:HA2	1:A:971:GLU:HB2	2.01	0.43
2:B:137:ARG:CB	2:B:141:ILE:HB	2.48	0.43
2:B:806:ILE:HG22	2:B:806:ILE:O	2.19	0.43
7:G:5:SER:O	7:G:73:ARG:HA	2.18	0.43
10:J:43:ARG:O	10:J:47:ARG:HG3	2.18	0.43
13:M:111:ARG:HH12	13:M:113:LYS:NZ	2.16	0.43
15:O:222:HIS:CD2	15:O:244:ASN:HB3	2.54	0.43
15:O:232:LEU:HD13	15:O:237:LYS:HB3	2.00	0.43
1:A:443:ASN:OD1	1:A:445:ARG:HG3	2.18	0.43
1:A:501:ASN:O	1:A:504:VAL:HG22	2.17	0.43
2:B:55:LYS:HB3	2:B:59:LYS:HD3	1.99	0.43
9:I:13:LEU:HD22	9:I:27:ARG:NH2	2.33	0.43
1:A:1300:LEU:N	1:A:1321:GLU:OE2	2.51	0.43
14:N:303:ARG:HH12	14:N:411:ARG:HD3	1.83	0.43
1:A:885:MET:HE2	1:A:885:MET:HB3	1.77	0.43
1:A:1166:LEU:HD23	1:A:1267:LEU:O	2.18	0.43
2:B:817:PRO:HG2	2:B:822:GLN:NE2	2.34	0.43
5:E:153:HIS:HB3	5:E:196:VAL:HG21	2.01	0.43
7:G:38:ILE:HD11	7:G:193:ALA:HB3	1.99	0.43
11:K:68:GLU:HG3	11:K:72:LEU:HB3	2.00	0.43
13:M:153:VAL:O	13:M:175:ARG:HA	2.18	0.43
13:M:161:ALA:HB2	13:M:170:LEU:HD13	2.00	0.43
15:O:111:ALA:H	15:O:116:LYS:HB3	1.84	0.43
15:O:604:LYS:HA	15:O:607:ASN:HD21	1.83	0.43
1:A:91:PHE:O	1:A:258:TRP:HD1	2.02	0.43
1:A:602:TYR:CE2	8:H:81:PRO:HB3	2.54	0.43
1:A:766:ILE:HA	1:A:769:LEU:HB2	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1181:LEU:HD23	1:A:1183:PHE:CZ	2.54	0.43
2:B:678:PHE:CD1	2:B:678:PHE:C	2.96	0.43
10:J:45:CYS:O	10:J:49:MET:HG2	2.19	0.43
15:O:542:ARG:NH2	15:O:543:TYR:OH	2.52	0.43
16:P:253:LEU:HD13	16:P:261:TYR:HB3	2.00	0.43
1:A:37:ARG:H	1:A:37:ARG:HD3	1.84	0.43
2:B:151:ARG:HB2	2:B:430:THR:HG23	2.01	0.43
2:B:311:THR:OG1	2:B:312:MET:N	2.52	0.43
2:B:518:THR:HB	2:B:608:ILE:HD11	2.00	0.43
2:B:1067:ARG:HG3	2:B:1083:LEU:HD11	2.01	0.43
13:M:147:THR:HB	13:M:182:PHE:HB3	2.00	0.43
16:P:237:PRO:HA	16:P:240:ILE:HG12	2.01	0.43
1:A:629:LYS:HE3	1:A:629:LYS:HB2	1.91	0.42
2:B:579:ARG:HA	2:B:584:VAL:HG23	2.01	0.42
1:A:232:LYS:HD2	16:P:315:TRP:CZ2	2.54	0.42
1:A:615:LYS:NZ	1:A:620:SER:O	2.52	0.42
1:A:624:ILE:HD11	1:A:681:ILE:HA	2.01	0.42
1:A:1065:LYS:HB3	1:A:1065:LYS:HE2	1.75	0.42
2:B:301:ALA:O	2:B:305:ILE:HG12	2.19	0.42
4:D:134:LEU:HA	4:D:137:ILE:HB	1.99	0.42
5:E:161:LYS:NZ	5:E:172:GLU:OE1	2.40	0.42
8:H:90:ALA:CB	8:H:96:VAL:HG21	2.49	0.42
13:M:114:PRO:C	13:M:116:SER:H	2.27	0.42
15:O:581:LEU:HD21	15:O:647:LEU:HD22	2.01	0.42
16:P:193:ASN:O	16:P:196:LYS:HG2	2.19	0.42
1:A:114:LEU:HD11	1:A:161:ASN:ND2	2.34	0.42
1:A:374:ASP:OD1	2:B:1038:ARG:NE	2.45	0.42
1:A:818:ILE:CD1	1:A:823:VAL:HG12	2.47	0.42
2:B:888:VAL:HG21	12:L:54:ARG:HH21	1.84	0.42
2:B:1106:TRP:HE3	2:B:1113:ALA:HB2	1.83	0.42
4:D:72:PHE:HB3	4:D:128:PRO:HD2	2.02	0.42
4:D:109:LYS:HE2	4:D:156:ILE:HG21	2.02	0.42
8:H:37:LYS:HB2	8:H:126:GLU:HB3	2.00	0.42
13:M:78:ILE:HD11	13:M:159:TYR:CE1	2.55	0.42
15:O:499:THR:HG22	17:Q:41:LEU:HD11	2.00	0.42
1:A:716:ASP:OD2	2:B:1001:LYS:NZ	2.52	0.42
1:A:1055:SER:HB3	8:H:131:ASN:HD22	1.84	0.42
2:B:119:ARG:HG3	2:B:186:ILE:HD13	2.01	0.42
2:B:572:VAL:HA	2:B:590:ILE:HD13	2.01	0.42
4:D:134:LEU:HD13	4:D:153:MET:SD	2.59	0.42
7:G:78:LYS:HD2	7:G:194:TYR:OH	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:301:PRO:HD2	14:N:302:GLU:CD	2.44	0.42
1:A:398:VAL:HB	2:B:1037:ALA:HB2	2.01	0.42
2:B:73:LEU:HA	2:B:73:LEU:HD23	1.70	0.42
2:B:399:PHE:HE1	2:B:421:SER:HB2	1.85	0.42
2:B:652:ASN:O	2:B:655:ASN:HB2	2.19	0.42
3:C:247:PHE:CE1	3:C:279:VAL:HG21	2.55	0.42
5:E:86:PRO:O	5:E:114:ASN:HB3	2.19	0.42
15:O:105:LYS:HB2	15:O:121:TYR:HB2	2.01	0.42
1:A:201:TRP:HA	1:A:204:VAL:HG12	2.02	0.42
1:A:370:GLY:HA2	2:B:1062:LEU:O	2.19	0.42
1:A:1095:GLN:HE22	2:B:1069:CYS:HA	1.83	0.42
2:B:84:LEU:HD23	2:B:84:LEU:HA	1.91	0.42
2:B:769:ASP:O	2:B:920:GLY:HA3	2.19	0.42
5:E:54:GLN:H	5:E:54:GLN:HG2	1.69	0.42
5:E:155:ARG:HD2	5:E:194:GLU:OE1	2.20	0.42
5:E:202:SER:OG	5:E:203:GLU:N	2.52	0.42
13:M:276:ASP:N	13:M:276:ASP:OD1	2.52	0.42
15:O:170:THR:HG23	15:O:173:ASP:HB2	2.02	0.42
15:O:619:LEU:HB3	15:O:624:LEU:HB2	2.01	0.42
2:B:200:LEU:HD21	2:B:369:ARG:HH11	1.85	0.42
2:B:1088:ASP:OD1	2:B:1088:ASP:N	2.52	0.42
3:C:162:VAL:HG23	3:C:196:LEU:HD22	2.01	0.42
4:D:109:LYS:NZ	4:D:110:LEU:HD23	2.34	0.42
8:H:36:CYS:HA	8:H:126:GLU:O	2.20	0.42
15:O:47:PHE:CG	15:O:586:ALA:HB1	2.54	0.42
1:A:705:LEU:HD13	2:B:761:SER:CB	2.50	0.42
2:B:95:TYR:HE2	2:B:396:ASN:HD21	1.67	0.42
2:B:613:ILE:HB	2:B:673:LEU:HB3	2.01	0.42
2:B:711:GLY:HA3	2:B:751:ALA:HA	2.00	0.42
2:B:1107:CYS:C	2:B:1109:THR:H	2.28	0.42
6:F:107:VAL:HG21	6:F:111:LEU:HD21	2.02	0.42
12:L:28:LYS:HA	12:L:28:LYS:HD3	1.77	0.42
13:M:93:ARG:CZ	13:M:105:PRO:HB3	2.49	0.42
15:O:100:GLN:C	15:O:102:ARG:H	2.28	0.42
15:O:165:SER:OG	17:Q:65:VAL:HG12	2.19	0.42
15:O:467:PHE:O	15:O:479:PRO:HD2	2.19	0.42
15:O:518:SER:HB3	15:O:521:ILE:HD13	2.02	0.42
15:O:522:ILE:HG13	15:O:523:ASN:N	2.35	0.42
1:A:603:LEU:HD12	8:H:46:LEU:HD11	2.00	0.42
1:A:1318:HIS:ND1	1:A:1321:GLU:HB2	2.35	0.42
2:B:402:SER:O	2:B:406:VAL:HG23	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:90:SER:O	15:O:93:THR:HG22	2.20	0.42
15:O:273:ILE:HG13	15:O:274:VAL:O	2.19	0.42
15:O:590:PHE:CE2	15:O:594:LYS:HE2	2.55	0.42
16:P:193:ASN:HB2	16:P:197:ASN:ND2	2.34	0.42
1:A:2:LYS:HB2	1:A:3:GLU:H	1.50	0.42
2:B:244:HIS:HB3	2:B:247:ILE:HG12	2.02	0.42
2:B:529:ILE:HG12	2:B:588:ILE:HD13	2.01	0.42
2:B:541:ILE:HD13	2:B:563:GLY:HA2	2.02	0.42
2:B:824:LEU:HD12	2:B:824:LEU:HA	1.85	0.42
7:G:104:ILE:HG22	7:G:105:PHE:HD1	1.85	0.42
7:G:147:ARG:HG2	7:G:205:MET:HG2	2.02	0.42
8:H:8:ASP:OD1	8:H:9:ILE:N	2.52	0.42
10:J:17:LYS:HD2	10:J:39:LEU:HB3	2.01	0.42
14:N:293:LYS:HB3	14:N:305:MET:HE1	2.01	0.42
15:O:509:ARG:HD2	15:O:509:ARG:HA	1.77	0.42
1:A:233:GLN:CG	15:O:579:GLN:HE22	2.26	0.41
1:A:427:HIS:O	1:A:429:GLY:N	2.53	0.41
1:A:1207:VAL:O	1:A:1211:ARG:HG2	2.19	0.41
2:B:623:LYS:HG3	2:B:625:ILE:HG22	2.02	0.41
2:B:778:ILE:HG23	2:B:906:PRO:HG2	2.00	0.41
2:B:798:TYR:CG	2:B:851:SER:HB2	2.55	0.41
3:C:242:GLU:HA	3:C:245:ARG:HD3	2.02	0.41
13:M:88:PHE:O	14:N:392:GLN:HA	2.19	0.41
15:O:166:LEU:HB3	15:O:169:LEU:CD2	2.47	0.41
15:O:506:ARG:HH12	16:P:246:VAL:HG13	1.84	0.41
15:O:520:LYS:HA	15:O:523:ASN:OD1	2.20	0.41
1:A:644:GLU:HA	1:A:651:PHE:HB3	2.02	0.41
1:A:891:LYS:HG2	1:A:1389:PHE:HB2	2.02	0.41
1:A:1170:ALA:HB3	9:I:46:LEU:HD12	2.01	0.41
2:B:447:PHE:HB3	2:B:449:MET:HE1	2.01	0.41
3:C:223:SER:OG	3:C:303:GLU:HG3	2.20	0.41
6:F:137:TYR:CD1	6:F:143:PHE:HB3	2.54	0.41
8:H:62:SER:OG	8:H:62:SER:O	2.38	0.41
8:H:98:TYR:OH	8:H:138:GLU:HG3	2.20	0.41
12:L:63:ARG:H	12:L:63:ARG:HG2	1.63	0.41
15:O:200:LEU:HG	15:O:280:LEU:HB3	2.02	0.41
1:A:742:ILE:HD13	1:A:762:LEU:HD21	2.01	0.41
2:B:49:PRO:HG3	2:B:743:LEU:HD21	2.02	0.41
2:B:51:PHE:CD2	2:B:517:MET:HG3	2.56	0.41
2:B:354:ARG:O	2:B:358:MET:HG3	2.20	0.41
2:B:604:ASP:OD1	2:B:604:ASP:N	2.48	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:101:LEU:HD12	15:O:130:LEU:HD11	2.02	0.41
1:A:888:ARG:NH1	1:A:1372:THR:HG22	2.34	0.41
1:A:1043:ASP:OD1	1:A:1044:PRO:HD2	2.21	0.41
2:B:1083:LEU:HA	2:B:1083:LEU:HD23	1.82	0.41
11:K:110:GLU:HG2	11:K:111:THR:HG23	2.01	0.41
13:M:95:ARG:HG2	13:M:96:LEU:HD23	2.02	0.41
15:O:91:VAL:O	15:O:94:THR:HG22	2.20	0.41
1:A:1089:ILE:HD12	1:A:1089:ILE:HA	1.95	0.41
1:A:1136:ILE:HG12	1:A:1318:HIS:CD2	2.56	0.41
2:B:1149:GLN:HG2	6:F:71:GLU:HG3	2.02	0.41
4:D:17:LEU:HD11	4:D:63:VAL:HG23	2.02	0.41
7:G:159:LYS:N	7:G:160:PRO:HD3	2.35	0.41
1:A:613:LEU:HD11	1:A:697:MET:HA	2.02	0.41
2:B:51:PHE:CE1	2:B:55:LYS:HD2	2.56	0.41
2:B:58:VAL:HG11	2:B:183:GLY:HA3	2.02	0.41
2:B:288:GLU:HB2	9:I:11:MET:HE1	2.02	0.41
2:B:962:ILE:HG23	2:B:991:LEU:HD11	2.02	0.41
3:C:132:ILE:HB	3:C:208:CYS:HB2	2.02	0.41
3:C:211:GLY:HA3	3:C:219:PHE:CD1	2.56	0.41
3:C:328:LEU:HD23	3:C:328:LEU:HA	1.87	0.41
4:D:6:GLU:OE1	7:G:42:VAL:HG22	2.19	0.41
14:N:297:MET:SD	14:N:303:ARG:HB2	2.60	0.41
15:O:121:TYR:CE1	15:O:210:PRO:HG3	2.54	0.41
15:O:245:ALA:HA	15:O:248:ASP:OD2	2.21	0.41
17:Q:113:LEU:HD12	17:Q:113:LEU:HA	1.88	0.41
1:A:208:ASN:HA	1:A:209:PRO:HD3	1.92	0.41
1:A:595:PRO:HD2	1:A:598:MET:HE2	2.02	0.41
1:A:765:LYS:HD3	1:A:765:LYS:HA	1.94	0.41
2:B:698:ARG:HG3	2:B:954:THR:HG22	2.02	0.41
4:D:48:ARG:O	4:D:49:PRO:C	2.64	0.41
15:O:139:GLU:OE1	15:O:143:GLN:HB2	2.21	0.41
1:A:230:LEU:HA	1:A:233:GLN:HG3	2.02	0.41
1:A:668:VAL:O	1:A:669:LEU:HD23	2.21	0.41
1:A:1022:LEU:HD22	1:A:1060:TYR:HD2	1.86	0.41
1:A:1028:MET:H	1:A:1028:MET:HG2	1.58	0.41
2:B:541:ILE:HD12	2:B:541:ILE:HA	1.75	0.41
3:C:240:LYS:O	3:C:243:SER:OG	2.36	0.41
3:C:324:LYS:HE2	3:C:324:LYS:HB3	1.74	0.41
4:D:147:GLU:HG2	4:D:148:LYS:N	2.35	0.41
6:F:136:ARG:HD2	6:F:146:TRP:CD1	2.55	0.41
15:O:111:ALA:N	15:O:116:LYS:HB3	2.35	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:650:VAL:HA	15:O:653:MET:SD	2.60	0.41
16:P:231:ALA:O	16:P:233:VAL:HG23	2.21	0.41
1:A:58:MET:HA	1:A:80:HIS:HB2	2.03	0.41
1:A:471:VAL:HB	1:A:528:ARG:HG3	2.02	0.41
1:A:921:LEU:HD13	1:A:926:MET:HE1	2.03	0.41
1:A:965:GLU:CD	1:A:1068:ARG:HH22	2.29	0.41
1:A:1217:ILE:O	1:A:1218:GLN:HB3	2.20	0.41
1:A:1282:VAL:HB	1:A:1294:LEU:HD12	2.03	0.41
1:A:1430:VAL:HG12	7:G:59:LEU:HD13	2.02	0.41
2:B:296:TYR:HA	2:B:300:GLN:HE21	1.86	0.41
2:B:760:MET:HE3	2:B:760:MET:HB2	1.94	0.41
2:B:836:VAL:HG23	2:B:840:GLN:HB2	2.03	0.41
3:C:276:SER:O	3:C:277:ARG:HG2	2.21	0.41
4:D:117:LYS:HD3	17:Q:107:ARG:HA	2.02	0.41
6:F:85:MET:HE1	6:F:125:LEU:HD11	2.03	0.41
8:H:116:TYR:CD1	8:H:123:MET:HE2	2.56	0.41
13:M:188:ASP:O	13:M:191:VAL:HG12	2.21	0.41
15:O:120:TYR:HE2	17:Q:133:PRO:HG2	1.85	0.41
15:O:238:ARG:HA	15:O:238:ARG:NE	2.35	0.41
15:O:599:ASN:HB3	15:O:602:LEU:HD12	2.03	0.41
15:O:613:GLY:N	15:O:615:GLU:OE2	2.52	0.41
16:P:293:ILE:H	16:P:293:ILE:HG13	1.49	0.41
1:A:368:LEU:HB3	1:A:1416:ILE:HG12	2.04	0.41
1:A:568:ASP:CG	8:H:22:LYS:HG3	2.46	0.41
1:A:1267:LEU:HA	1:A:1267:LEU:HD22	1.80	0.41
2:B:790:LYS:HD2	2:B:897:LYS:HD3	2.03	0.41
2:B:945:ASN:ND2	2:B:947:HIS:HB2	2.36	0.41
2:B:1080:LEU:HD13	2:B:1080:LEU:HA	1.84	0.41
4:D:1:MET:HE1	7:G:40:PRO:HD2	2.02	0.41
7:G:89:ILE:CD1	7:G:143:ASN:H	2.33	0.41
15:O:51:GLU:HG2	15:O:590:PHE:N	2.35	0.41
15:O:584:ASN:O	15:O:588:LEU:HD22	2.21	0.41
15:O:635:LEU:HG	17:Q:55:ALA:CB	2.51	0.41
1:A:544:PRO:HA	1:A:924:LEU:HD13	2.03	0.40
1:A:717:VAL:HA	1:A:810:VAL:HG22	2.02	0.40
1:A:763:GLU:OE1	1:A:822:ARG:HD3	2.21	0.40
6:F:83:PRO:HG2	6:F:84:TYR:CE1	2.56	0.40
15:O:178:VAL:HG13	15:O:183:MET:HE3	2.03	0.40
15:O:195:CYS:SG	15:O:200:LEU:HB3	2.61	0.40
15:O:325:LYS:HE3	15:O:328:ASP:O	2.21	0.40
16:P:239:ASN:HD22	16:P:239:ASN:HA	1.66	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:256:VAL:HG12	16:P:260:CYS:HB2	2.03	0.40
1:A:252:ARG:HB3	1:A:254:GLU:CD	2.47	0.40
1:A:649:ASP:HB3	1:A:663:VAL:HG22	2.03	0.40
1:A:1165:LEU:HG	1:A:1198:LEU:HD21	2.03	0.40
2:B:790:LYS:HE2	2:B:790:LYS:HB3	1.93	0.40
2:B:1038:ARG:CZ	2:B:1050:PRO:HB3	2.50	0.40
2:B:1099:GLY:HA3	2:B:1141:LEU:N	2.35	0.40
4:D:145:PHE:HD2	4:D:149:THR:HG23	1.86	0.40
7:G:113:ASN:OD1	7:G:114:MET:N	2.54	0.40
8:H:90:ALA:HB2	8:H:96:VAL:HG21	2.01	0.40
13:M:122:ASP:OD1	13:M:147:THR:HG23	2.21	0.40
15:O:188:SER:HB2	15:O:273:ILE:HD13	2.03	0.40
15:O:257:ASN:OD1	15:O:258:GLU:N	2.54	0.40
15:O:275:LYS:HG3	15:O:278:VAL:HG21	2.04	0.40
1:A:10:PRO:HG2	2:B:1147:PHE:CE2	2.57	0.40
1:A:1295:VAL:HG23	1:A:1297:GLY:H	1.86	0.40
2:B:46:HIS:HA	2:B:49:PRO:HD2	2.03	0.40
3:C:241:GLY:O	3:C:245:ARG:HD2	2.21	0.40
4:D:70:LYS:HG3	4:D:94:GLY:CA	2.47	0.40
5:E:78:LEU:HD11	5:E:109:ILE:HD11	2.04	0.40
5:E:98:ILE:O	5:E:102:GLU:HG2	2.21	0.40
12:L:53:HIS:CE1	12:L:55:ILE:HB	2.56	0.40
15:O:168:SER:HA	15:O:281:THR:HG22	2.02	0.40
1:A:21:LEU:HG	2:B:1138:ALA:HB2	2.02	0.40
3:C:132:ILE:HG21	3:C:184:VAL:HG11	2.02	0.40
4:D:65:TYR:HB2	7:G:102:LEU:CD2	2.42	0.40
5:E:46:TYR:CG	5:E:58:MET:HG2	2.56	0.40
5:E:55:ARG:HD3	5:E:83:CYS:O	2.20	0.40
15:O:93:THR:HA	15:O:96:VAL:HG12	2.02	0.40
17:Q:66:LYS:HE3	17:Q:71:TYR:HE1	1.87	0.40
1:A:180:HIS:CE1	1:A:182:THR:HA	2.57	0.40
1:A:1154:ALA:HB1	1:A:1283:ILE:HD13	2.03	0.40
2:B:503:PRO:HG2	2:B:507:ALA:O	2.21	0.40
2:B:642:LYS:HB2	2:B:642:LYS:HE2	1.89	0.40
2:B:1106:TRP:CE3	2:B:1113:ALA:HB2	2.57	0.40
4:D:13:ASP:HA	4:D:16:VAL:HG12	2.03	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	1411/1460 (97%)	1316 (93%)	95 (7%)	0	100	100
2	B	1098/1149 (96%)	1030 (94%)	68 (6%)	0	100	100
3	C	333/335 (99%)	314 (94%)	19 (6%)	0	100	100
4	D	141/161 (88%)	122 (86%)	16 (11%)	3 (2%)	5	10
5	E	213/215 (99%)	203 (95%)	10 (5%)	0	100	100
6	F	81/155 (52%)	78 (96%)	3 (4%)	0	100	100
7	G	185/212 (87%)	160 (86%)	25 (14%)	0	100	100
8	H	134/146 (92%)	118 (88%)	16 (12%)	0	100	100
9	I	45/110 (41%)	41 (91%)	4 (9%)	0	100	100
10	J	65/70 (93%)	62 (95%)	3 (5%)	0	100	100
11	K	99/142 (70%)	92 (93%)	7 (7%)	0	100	100
12	L	42/70 (60%)	37 (88%)	5 (12%)	0	100	100
13	M	179/282 (64%)	165 (92%)	14 (8%)	0	100	100
14	N	139/422 (33%)	130 (94%)	9 (6%)	0	100	100
15	O	564/654 (86%)	531 (94%)	33 (6%)	0	100	100
16	P	132/317 (42%)	122 (92%)	10 (8%)	0	100	100
17	Q	100/268 (37%)	87 (87%)	13 (13%)	0	100	100
18	W	15/635 (2%)	14 (93%)	1 (7%)	0	100	100
All	All	4976/6803 (73%)	4622 (93%)	351 (7%)	3 (0%)	50	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	37	LEU
4	D	46	GLN
4	D	49	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1230/1257 (98%)	1150 (94%)	80 (6%)	14	26
2	B	965/1006 (96%)	920 (95%)	45 (5%)	22	40
3	C	296/296 (100%)	280 (95%)	16 (5%)	18	34
4	D	123/145 (85%)	110 (89%)	13 (11%)	5	9
5	E	197/197 (100%)	184 (93%)	13 (7%)	14	25
6	F	73/137 (53%)	71 (97%)	2 (3%)	40	61
7	G	170/190 (90%)	157 (92%)	13 (8%)	11	19
8	H	121/128 (94%)	116 (96%)	5 (4%)	26	46
9	I	43/98 (44%)	40 (93%)	3 (7%)	12	23
10	J	62/65 (95%)	61 (98%)	1 (2%)	58	75
11	K	91/130 (70%)	84 (92%)	7 (8%)	10	19
12	L	39/39 (100%)	37 (95%)	2 (5%)	20	36
13	M	159/249 (64%)	147 (92%)	12 (8%)	11	20
14	N	125/200 (62%)	110 (88%)	15 (12%)	4	6
15	O	521/593 (88%)	471 (90%)	50 (10%)	7	12
16	P	126/285 (44%)	120 (95%)	6 (5%)	21	39
17	Q	92/212 (43%)	88 (96%)	4 (4%)	25	44
18	W	17/586 (3%)	15 (88%)	2 (12%)	4	7
All	All	4450/5813 (77%)	4161 (94%)	289 (6%)	17	26

All (289) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	39	LEU
1	A	61	SER
1	A	64	SER
1	A	74	LEU
1	A	86	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	90	VAL
1	A	106	ILE
1	A	107	CYS
1	A	118	THR
1	A	127	LEU
1	A	145	LEU
1	A	151	GLN
1	A	155	LEU
1	A	160	LEU
1	A	212	GLU
1	A	219	MET
1	A	261	LEU
1	A	276	ASP
1	A	320	GLN
1	A	350	ILE
1	A	363	ARG
1	A	398	VAL
1	A	401	VAL
1	A	446	TYR
1	A	481	HIS
1	A	631	LYS
1	A	634	VAL
1	A	663	VAL
1	A	724	LYS
1	A	743	THR
1	A	744	LEU
1	A	752	THR
1	A	766	ILE
1	A	769	LEU
1	A	823	VAL
1	A	870	GLU
1	A	877	VAL
1	A	893	LEU
1	A	909	ASN
1	A	951	ASP
1	A	952	LYS
1	A	955	LEU
1	A	1028	MET
1	A	1031	LEU
1	A	1039	LEU
1	A	1048	VAL
1	A	1052	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1071	LEU
1	A	1099	GLU
1	A	1104	MET
1	A	1106	LEU
1	A	1107	LYS
1	A	1120	THR
1	A	1126	ILE
1	A	1146	VAL
1	A	1164	THR
1	A	1184	ILE
1	A	1186	VAL
1	A	1194	ASP
1	A	1201	THR
1	A	1203	GLU
1	A	1204	ASP
1	A	1211	ARG
1	A	1215	LEU
1	A	1216	LYS
1	A	1217	ILE
1	A	1230	ILE
1	A	1256	VAL
1	A	1267	LEU
1	A	1290	LYS
1	A	1293	LEU
1	A	1294	LEU
1	A	1295	VAL
1	A	1301	ARG
1	A	1307	ASP
1	A	1367	GLU
1	A	1376	LEU
1	A	1383	VAL
1	A	1386	LEU
2	B	43	ASP
2	B	57	LEU
2	B	90	GLU
2	B	156	LEU
2	B	199	GLN
2	B	217	GLN
2	B	263	LEU
2	B	264	SER
2	B	288	GLU
2	B	290	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	295	ILE
2	B	298	GLN
2	B	309	VAL
2	B	320	LEU
2	B	329	THR
2	B	331	VAL
2	B	335	LEU
2	B	337	VAL
2	B	383	LEU
2	B	421	SER
2	B	422	ILE
2	B	464	ILE
2	B	484	SER
2	B	499	THR
2	B	504	GLU
2	B	526	GLU
2	B	527	GLU
2	B	541	ILE
2	B	544	ILE
2	B	551	LEU
2	B	552	ASN
2	B	619	GLN
2	B	624	ASP
2	B	725	LEU
2	B	800	ASN
2	B	803	GLN
2	B	824	LEU
2	B	890	ASP
2	B	1008	ILE
2	B	1052	GLU
2	B	1055	SER
2	B	1080	LEU
2	B	1084	MET
2	B	1135	MET
2	B	1136	ASN
3	C	26	ASP
3	C	106	LEU
3	C	108	VAL
3	C	112	MET
3	C	148	LYS
3	C	151	THR
3	C	152	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	C	177	THR
3	C	197	ARG
3	C	201	GLU
3	C	212	ILE
3	C	224	THR
3	C	239	ILE
3	C	256	ILE
3	C	277	ARG
3	C	304	SER
4	D	20	LEU
4	D	21	THR
4	D	23	LEU
4	D	28	LEU
4	D	95	ILE
4	D	105	GLU
4	D	107	MET
4	D	121	LEU
4	D	132	VAL
4	D	134	LEU
4	D	138	VAL
4	D	149	THR
4	D	151	GLU
5	E	1	MET
5	E	7	ARG
5	E	14	ARG
5	E	19	VAL
5	E	70	SER
5	E	80	VAL
5	E	83	CYS
5	E	88	VAL
5	E	90	VAL
5	E	117	THR
5	E	124	VAL
5	E	144	ILE
5	E	171	LYS
6	F	144	GLU
6	F	152	ILE
7	G	21	ASP
7	G	22	THR
7	G	32	ASN
7	G	85	VAL
7	G	99	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	G	108	ILE
7	G	150	ILE
7	G	151	GLU
7	G	158	VAL
7	G	189	GLU
7	G	197	LEU
7	G	201	GLN
7	G	208	VAL
8	H	4	THR
8	H	22	LYS
8	H	34	ASP
8	H	105	GLU
8	H	107	VAL
9	I	12	LEU
9	I	18	ASP
9	I	43	ARG
10	J	30	LEU
11	K	47	ILE
11	K	52	GLN
11	K	66	VAL
11	K	68	GLU
11	K	87	GLU
11	K	103	ILE
11	K	115	ASP
12	L	40	LEU
12	L	63	ARG
13	M	96	LEU
13	M	97	VAL
13	M	123	ILE
13	M	168	VAL
13	M	171	VAL
13	M	191	VAL
13	M	235	LYS
13	M	245	LEU
13	M	268	LEU
13	M	271	LEU
13	M	274	GLN
13	M	276	ASP
14	N	200	PHE
14	N	205	VAL
14	N	281	GLU
14	N	288	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
14	N	294	LEU
14	N	298	ASN
14	N	302	GLU
14	N	311	THR
14	N	313	LEU
14	N	356	LEU
14	N	380	MET
14	N	382	ILE
14	N	390	PHE
14	N	395	ILE
14	N	409	LEU
15	O	27	THR
15	O	80	VAL
15	O	83	ILE
15	O	88	VAL
15	O	91	VAL
15	O	94	THR
15	O	97	SER
15	O	98	LEU
15	O	100	GLN
15	O	116	LYS
15	O	137	ILE
15	O	140	ILE
15	O	146	VAL
15	O	166	LEU
15	O	170	THR
15	O	180	SER
15	O	185	TYR
15	O	206	LEU
15	O	214	LEU
15	O	217	PHE
15	O	222	HIS
15	O	261	GLN
15	O	270	SER
15	O	275	LYS
15	O	284	LEU
15	O	322	LYS
15	O	323	SER
15	O	331	THR
15	O	335	LEU
15	O	362	ASN
15	O	364	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
15	O	377	ARG
15	O	452	LEU
15	O	477	TYR
15	O	478	VAL
15	O	482	LYS
15	O	488	LYS
15	O	511	ILE
15	O	554	THR
15	O	558	SER
15	O	561	ARG
15	O	578	ARG
15	O	588	LEU
15	O	589	LEU
15	O	601	THR
15	O	619	LEU
15	O	620	LEU
15	O	635	LEU
15	O	641	LEU
15	O	653	MET
16	P	207	PHE
16	P	208	TYR
16	P	226	THR
16	P	250	ASP
16	P	257	THR
16	P	293	ILE
17	Q	47	ILE
17	Q	58	TYR
17	Q	65	VAL
17	Q	142	ILE
18	W	613	THR
18	W	617	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	101	GLN
1	A	125	HIS
1	A	134	ASN
1	A	151	GLN
1	A	208	ASN
1	A	275	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	310	ASN
1	A	675	HIS
1	A	753	GLN
1	A	760	GLN
1	A	789	ASN
1	A	805	ASN
1	A	808	GLN
1	A	828	GLN
1	A	834	HIS
1	A	931	GLN
1	A	950	GLN
1	A	964	ASN
1	A	1006	HIS
1	A	1174	GLN
1	A	1233	ASN
1	A	1254	ASN
1	A	1284	ASN
1	A	1317	ASN
1	A	1385	GLN
1	A	1395	HIS
1	A	1453	ASN
2	B	39	ASN
2	B	80	ASN
2	B	81	GLN
2	B	197	GLN
2	B	244	HIS
2	B	275	ASN
2	B	280	GLN
2	B	299	GLN
2	B	300	GLN
2	B	374	ASN
2	B	382	GLN
2	B	423	ASN
2	B	513	ASN
2	B	652	ASN
2	B	693	HIS
2	B	695	GLN
2	B	774	ASN
2	B	837	GLN
2	B	928	GLN
2	B	936	GLN
2	B	945	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	1025	GLN
3	C	3	ASN
3	C	29	ASN
3	C	53	ASN
3	C	87	ASN
3	C	159	ASN
3	C	172	GLN
3	C	200	GLN
3	C	232	GLN
3	C	234	ASN
3	C	248	GLN
4	D	61	ASN
4	D	71	ASN
4	D	130	ASN
5	E	99	HIS
5	E	104	ASN
7	G	29	GLN
7	G	31	ASN
7	G	32	ASN
7	G	58	GLN
7	G	69	ASN
7	G	201	GLN
8	H	3	ASN
8	H	35	GLN
8	H	64	ASN
8	H	133	ASN
8	H	137	GLN
10	J	53	HIS
11	K	64	GLN
11	K	102	ASN
12	L	53	HIS
12	L	66	GLN
13	M	158	GLN
13	M	167	GLN
13	M	178	GLN
13	M	234	HIS
13	M	274	GLN
13	M	280	ASN
14	N	287	HIS
15	O	43	ASN
15	O	56	HIS
15	O	100	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
15	O	143	GLN
15	O	161	GLN
15	O	216	GLN
15	O	254	ASN
15	O	295	GLN
15	O	448	HIS
15	O	579	GLN
15	O	599	ASN
15	O	607	ASN
15	O	626	GLN
15	O	652	GLN
16	P	176	ASN
16	P	193	ASN
16	P	205	ASN
16	P	239	ASN
17	Q	102	ASN
18	W	615	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

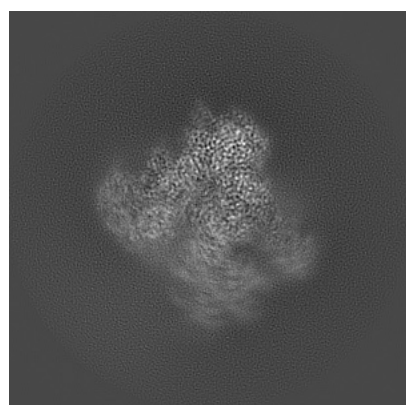
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14470. These allow visual inspection of the internal detail of the map and identification of artifacts.

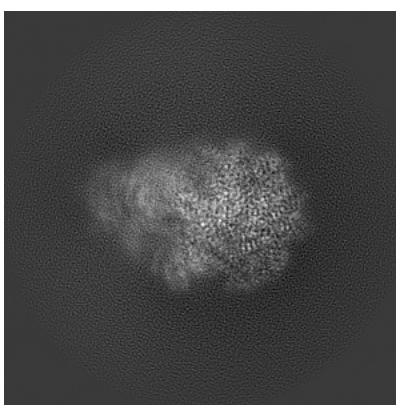
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

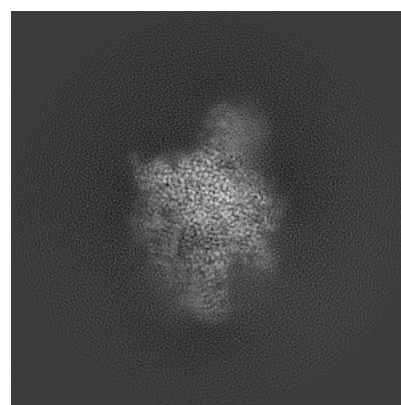
#### 6.1.1 Primary map



X



Y

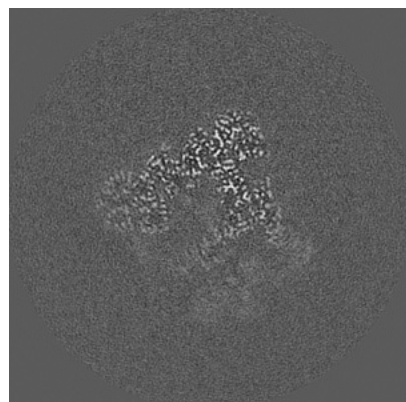


Z

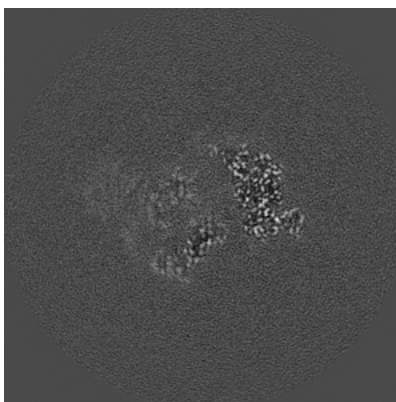
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

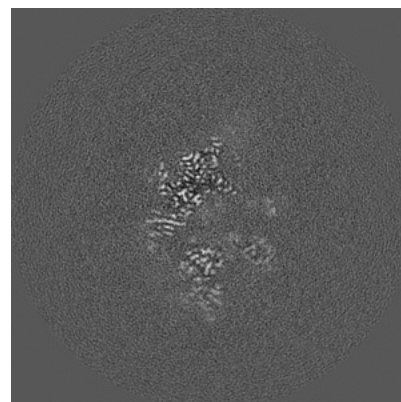
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

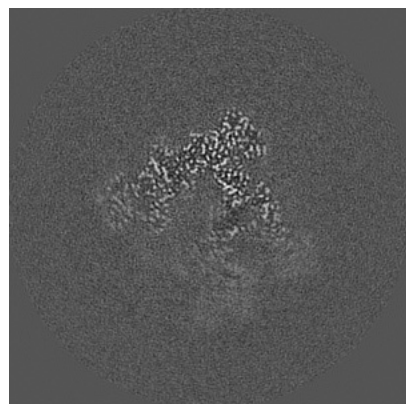


Z Index: 150

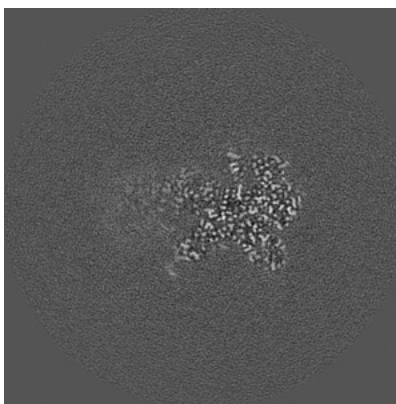
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

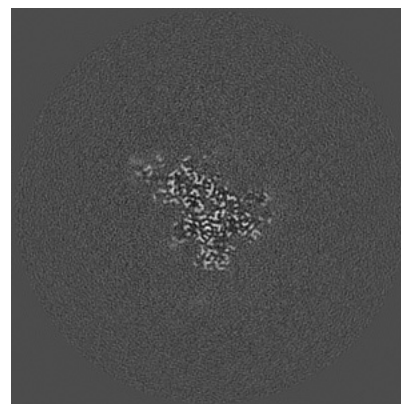
### 6.3.1 Primary map



X Index: 154



Y Index: 163

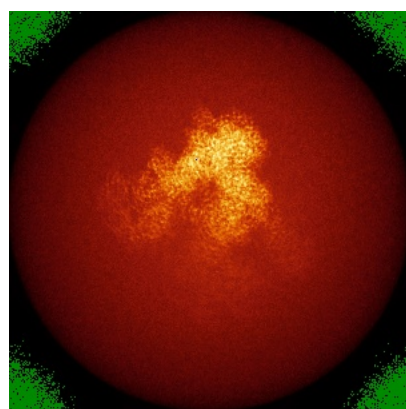


Z Index: 184

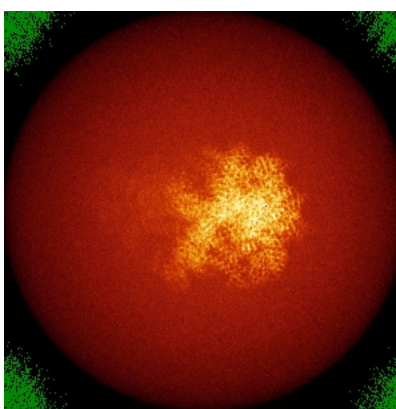
The images above show the largest variance slices of the map in three orthogonal directions.

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

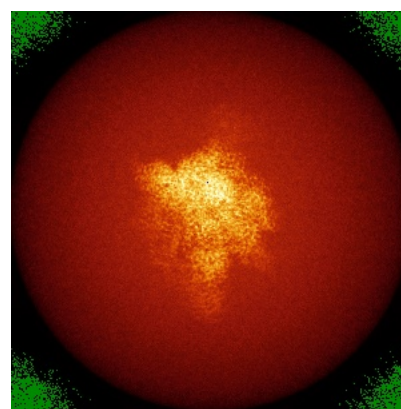
### 6.4.1 Primary map



X



Y



Z

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 0.0255. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

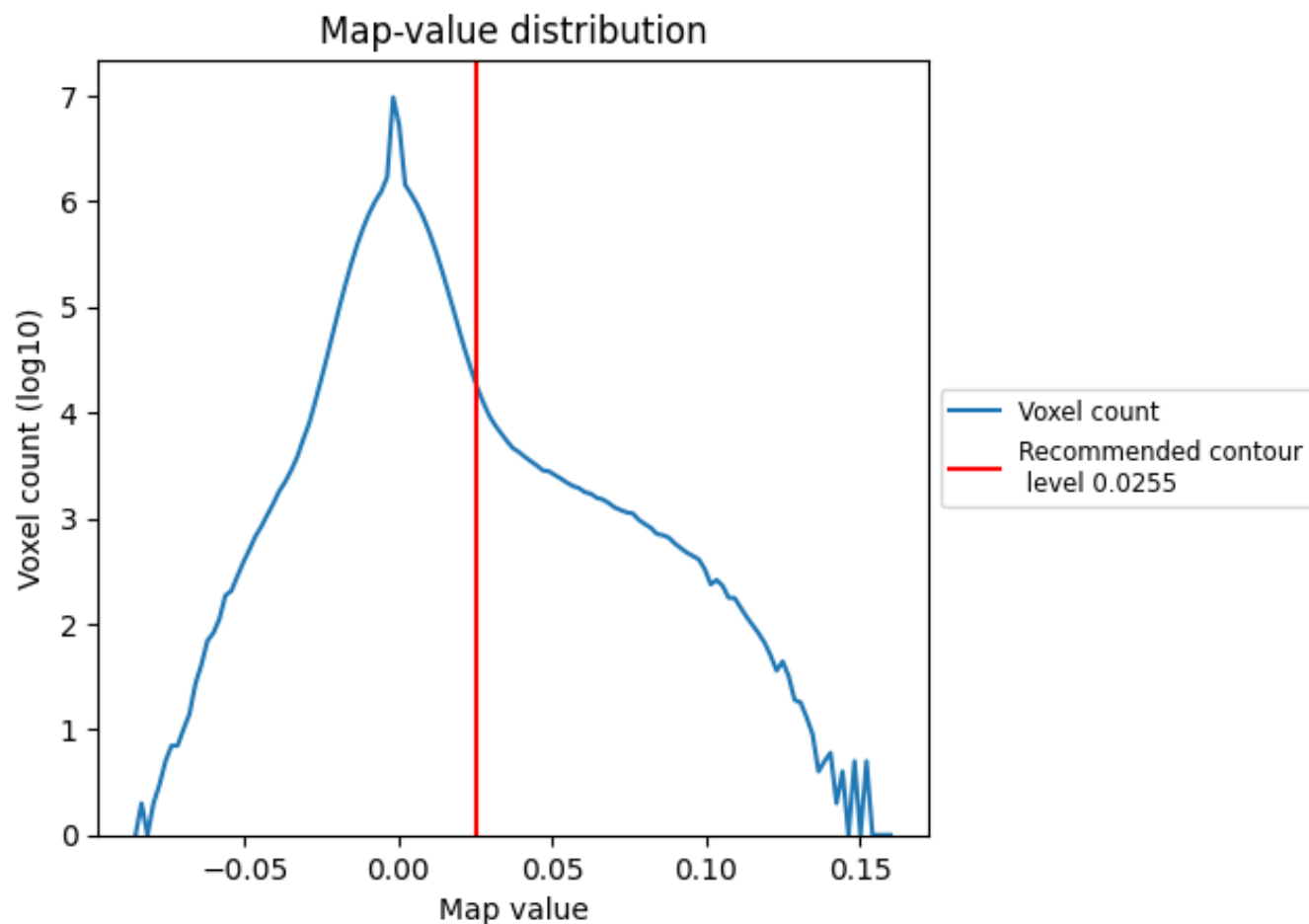
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

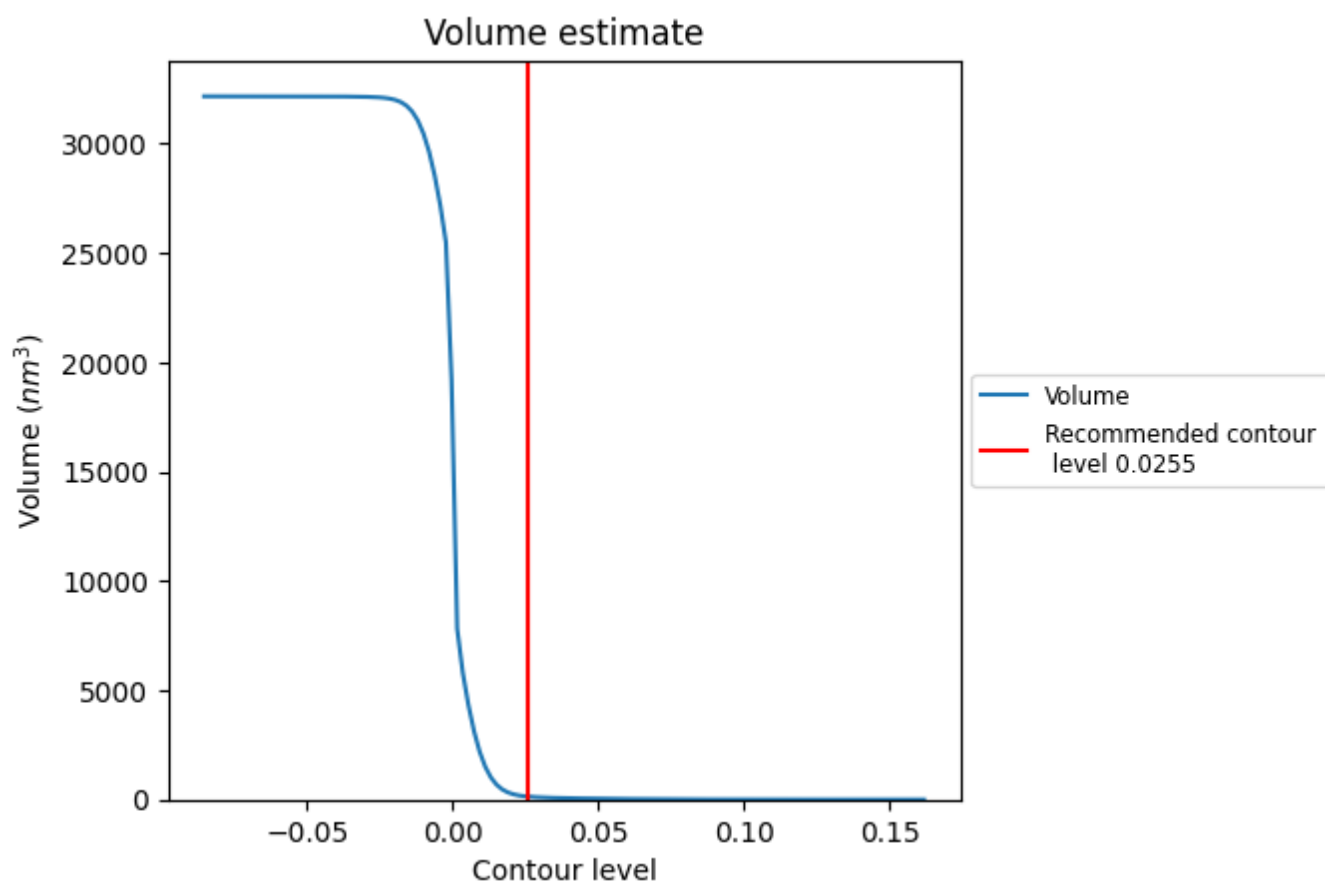
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

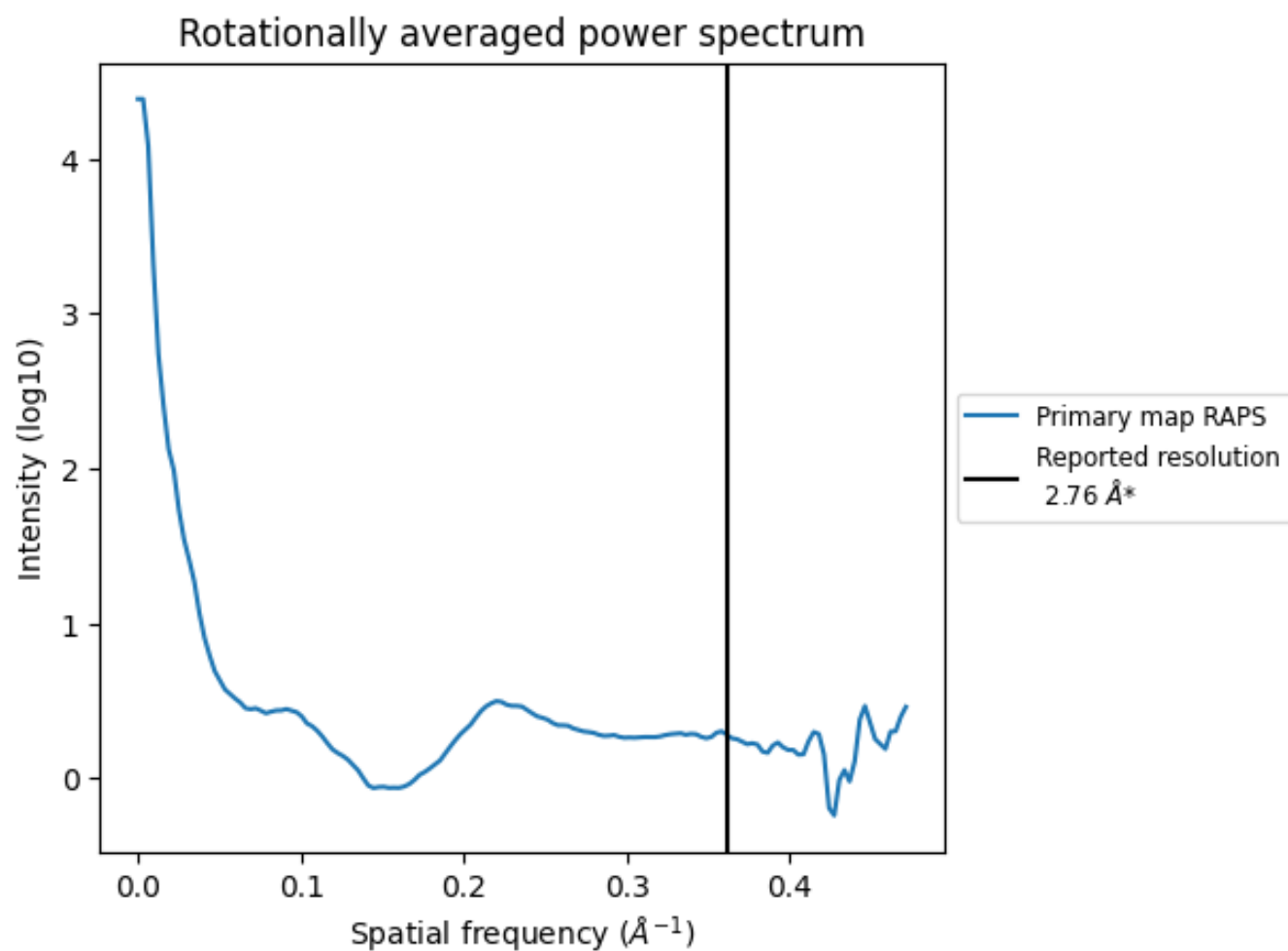
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 141 nm<sup>3</sup>; this corresponds to an approximate mass of 127 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 ⓘ

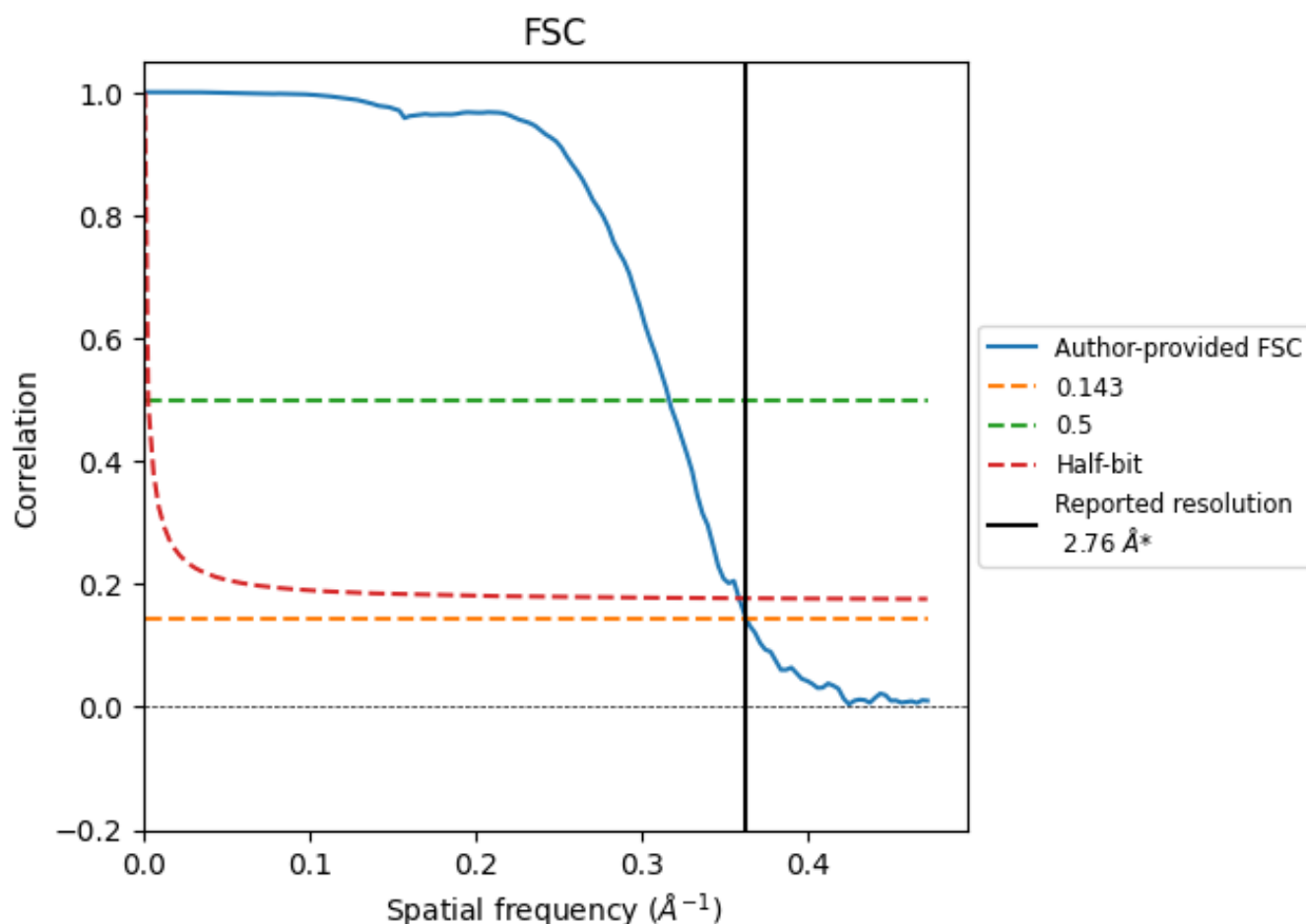


\*Reported resolution corresponds to spatial frequency of 0.362 Å<sup>-1</sup>

## 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 0.362 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

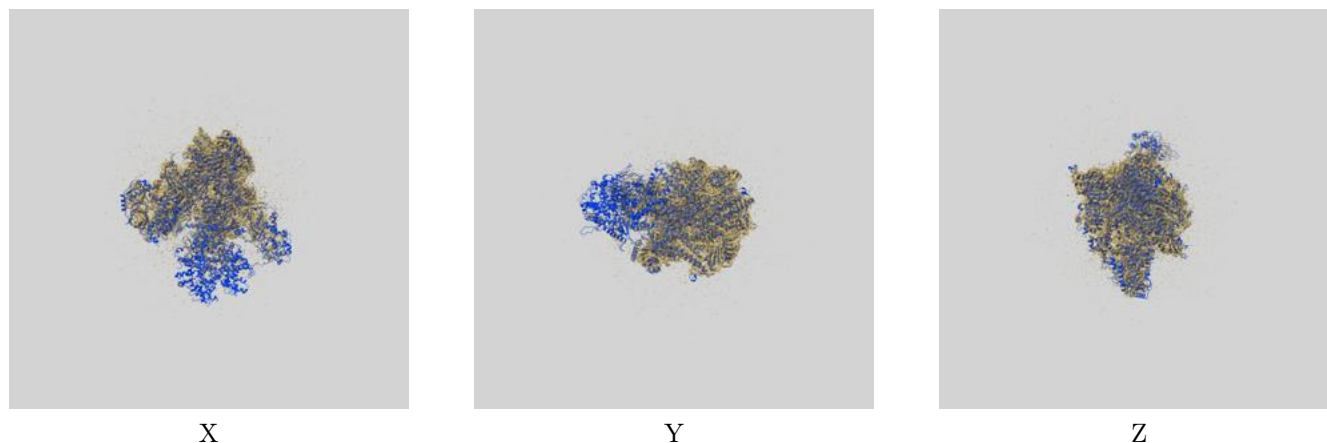
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	2.76	-
Author-provided FSC curve	2.75	3.16	2.79
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.5 CUT-OFF 3.16 differs from the reported value 2.76 by more than 10 %

## 9 Map-model fit [i](#)

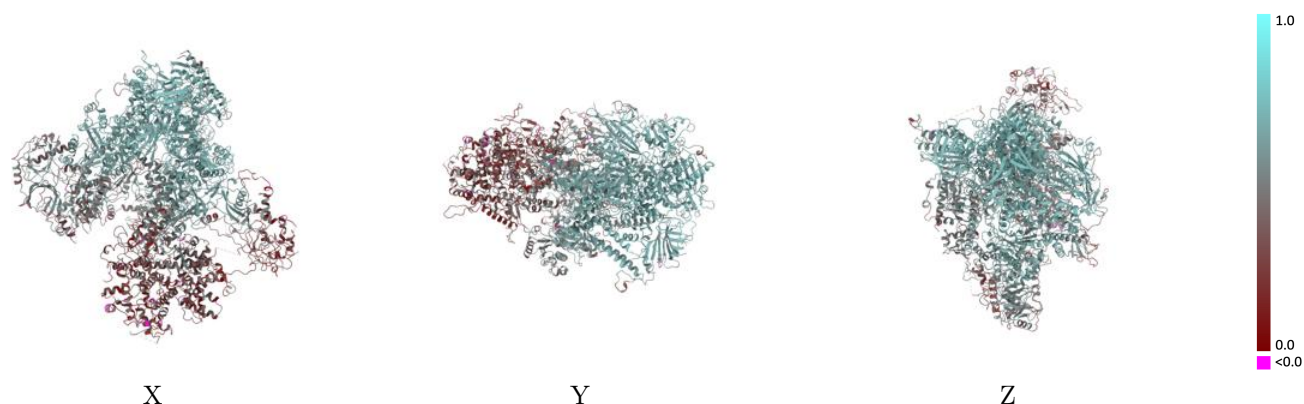
This section contains information regarding the fit between EMDB map EMD-14470 and PDB model 7Z31. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlay [i](#)



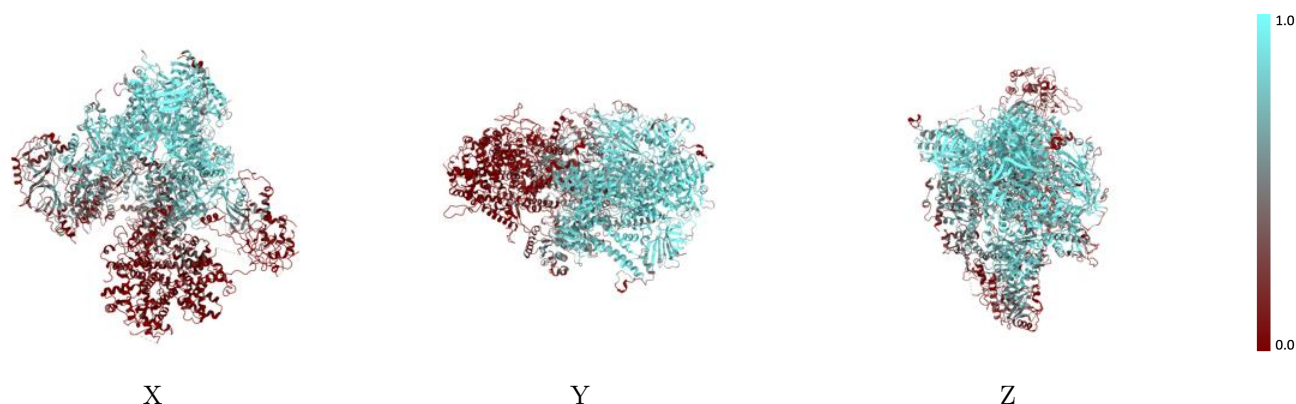
The images above show the 3D surface view of the map at the recommended contour level 0.0255 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



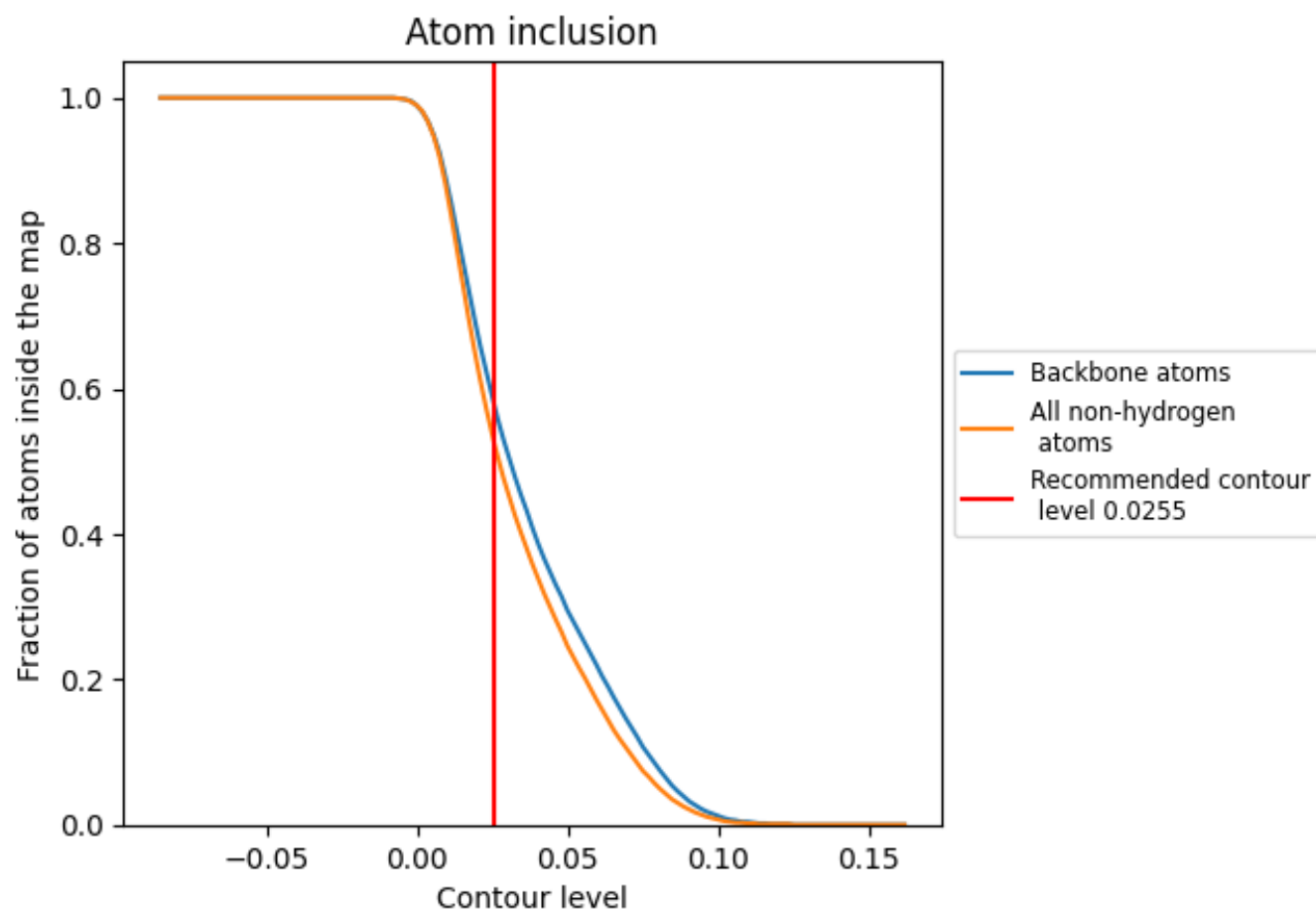
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0255).









































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 52% 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 (0.0255) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5250	 0.5190
A	 0.6220	 0.5570
B	 0.7490	 0.6080
C	 0.8440	 0.6420
D	 0.0950	 0.3100
E	 0.5030	 0.5200
F	 0.8450	 0.6480
G	 0.2910	 0.4220
H	 0.7980	 0.6130
I	 0.3870	 0.4920
J	 0.9040	 0.6660
K	 0.8580	 0.6460
L	 0.6450	 0.5830
M	 0.2970	 0.4650
N	 0.2530	 0.4420
O	 0.0530	 0.3300
P	 0.0280	 0.2650
Q	 0.0260	 0.2700
W	 0.0960	 0.4330
X	 0.1000	 0.5310

