



Full wwPDB EM Validation Report ⓘ

Feb 24, 2025 – 12:21 PM EST

PDB ID : 9EI4
EMDB ID : EMD-48076
Title : Cryo-EM structure of Human RNA polymerase II Elongation Complex bound to the RECQL5 helicase in the presence of ADP
Authors : Florez Ariza, A.; Lue, N.; Nogales, E.
Deposited on : 2024-11-25
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

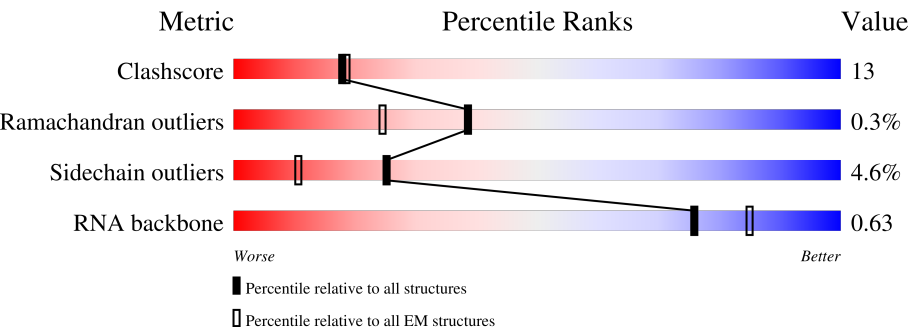
EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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.





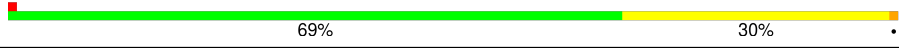



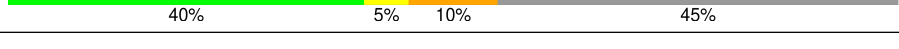
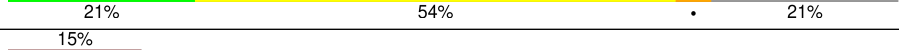
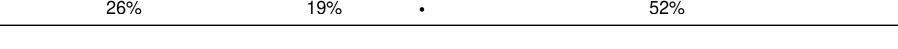
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1970	<div><div></div><div>49%22%28%</div></div>
2	B	1174	<div><div></div><div>68%27%</div></div>
3	C	275	<div><div></div><div>59%32%7%</div></div>
4	D	142	<div><div>39%</div><div>65%23%10%</div></div>
5	E	210	<div><div></div><div>71%26%</div></div>
6	F	127	<div><div></div><div>49%15%35%</div></div>
7	G	172	<div><div></div><div>45%75%23%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	N	43	
14	P	20	
15	T	28	
16	U	991	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 35854 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1428	Total	C	N	O	S	0	0
			11317	7123	2025	2097	72		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1134	Total	C	N	O	S	0	0
			9062	5732	1595	1671	64		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	257	Total	C	N	O	S	0	0
			2060	1296	351	407	6		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	128	Total	C	N	O	S	0	0
			1005	632	172	197	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1711	1084	300	319	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	44	PHE	SER	conflict	UNP P19388

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	S	0	0
			658	419	113	121	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1334	867	216	243	8		

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

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

- 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
			533	345	90	92	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 13 is a DNA chain called Non-template DNA, nucleic acid scaffold.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	17	Total	C	N	O	P	0	0
			355	169	68	101	17		

- Molecule 14 is a RNA chain called RNA, nucleic acid scaffold.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	11	Total	C	N	O	P	0	0
			239	107	49	72	11		

- Molecule 15 is a DNA chain called Template DNA, nucleic acid scaffold.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	22	Total	C	N	O	P	0	0
			447	214	77	134	22		

- Molecule 16 is a protein called ATP-dependent DNA helicase Q5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	472	Total	C	N	O	S	1	0
			3692	2330	665	672	25		

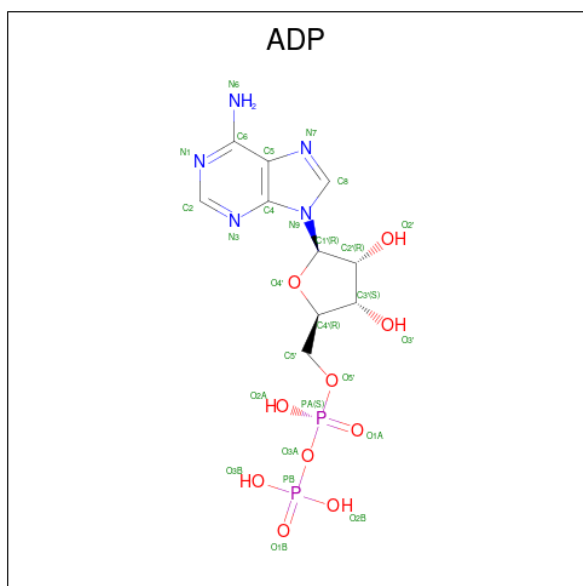
- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

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

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

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

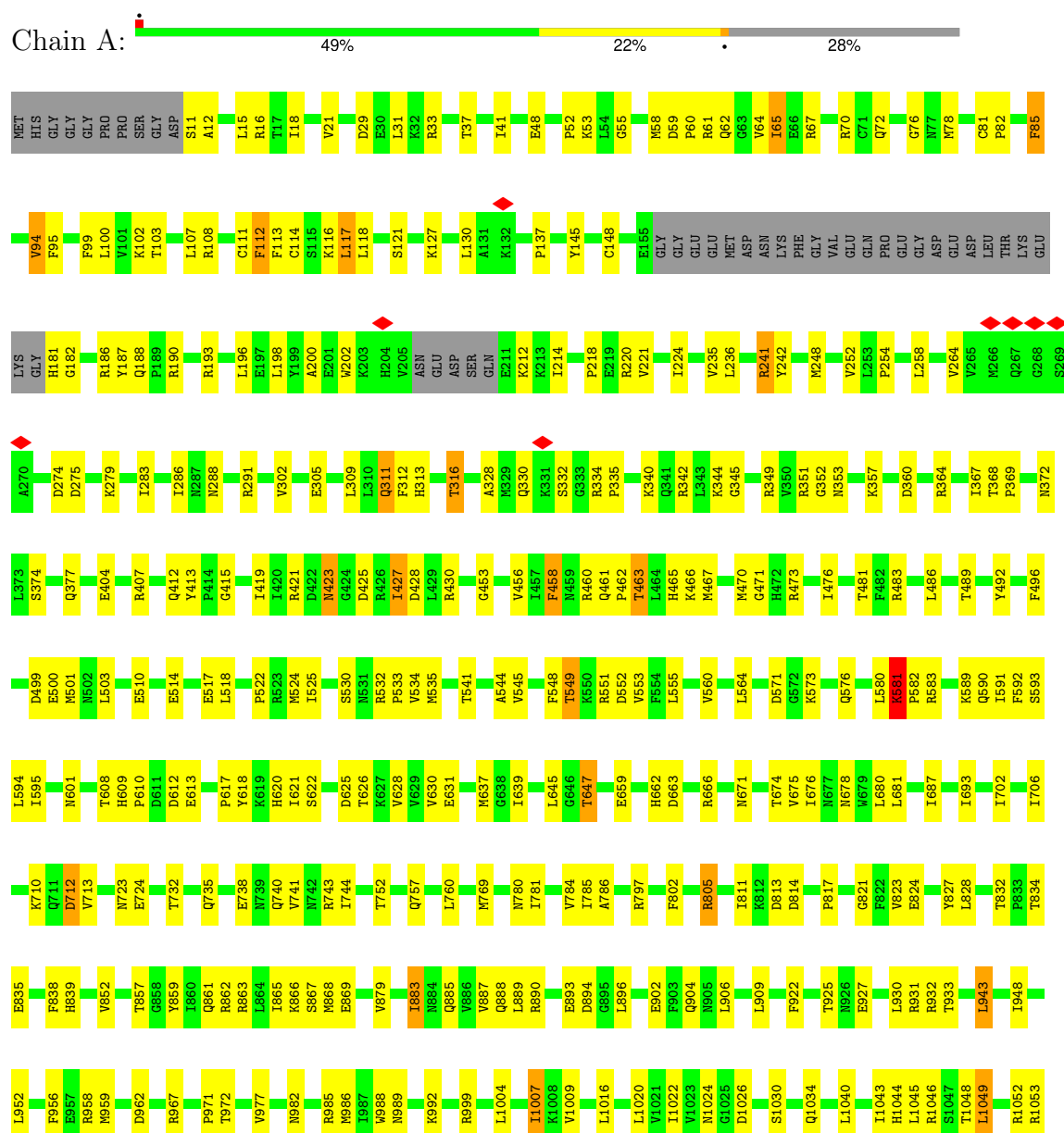


Mol	Chain	Residues	Atoms					AltConf
19	U	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots

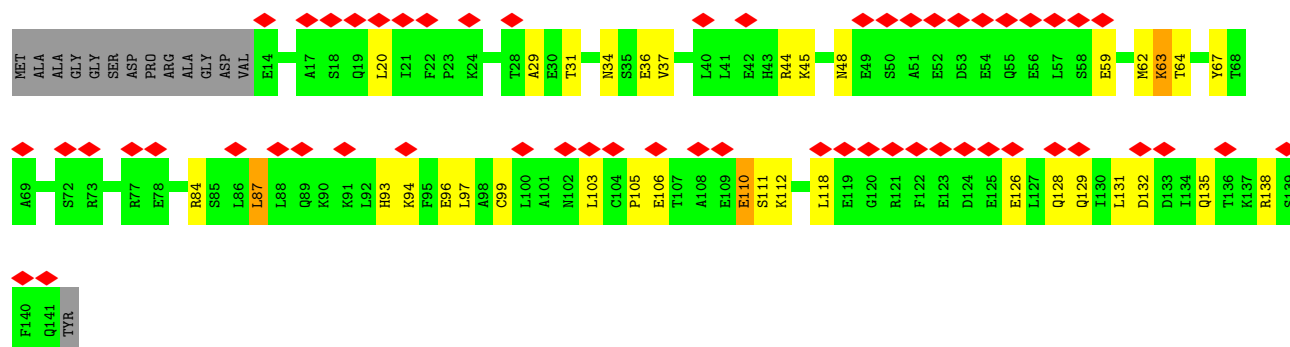
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

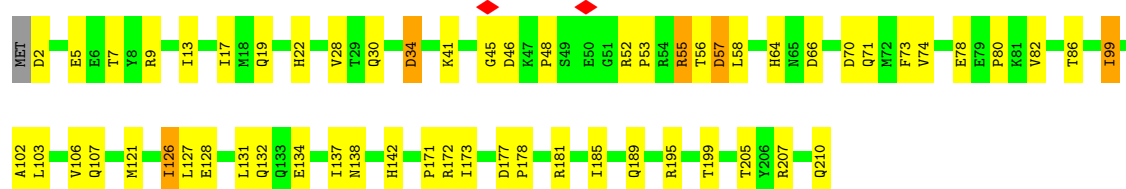




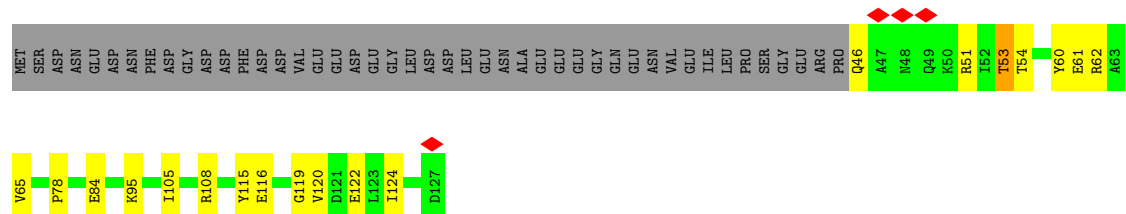
ME1	TYR	ASP	ALA	ASP	GLU	ASP	MET	GLN	TYR	ASP	GLU	ASP	ASP	E16	I17	I18	P19	D20	L21	I22	Y23	K37	Q42	Q43	F50	S54	V59	I65	D66	L67	Q68	ALA	ALA	GLN	HIS	ALA	SER	GLY	GLU	VAL	GLU	GLU	P81	P82	R83	L86	L93
S94	R95	R101				G103	P110	M111	E112	A113	R114	M117	L118	T119	L124	V132	I135	K134	E135	G136	E137	E138	H144	I149	I154	M155	L156	L162	L163	E176	C177	Y184	I187	M188	G189	S190	E191	X192	V193	I194	I195	A196	G197	E198	K199	M200	A216



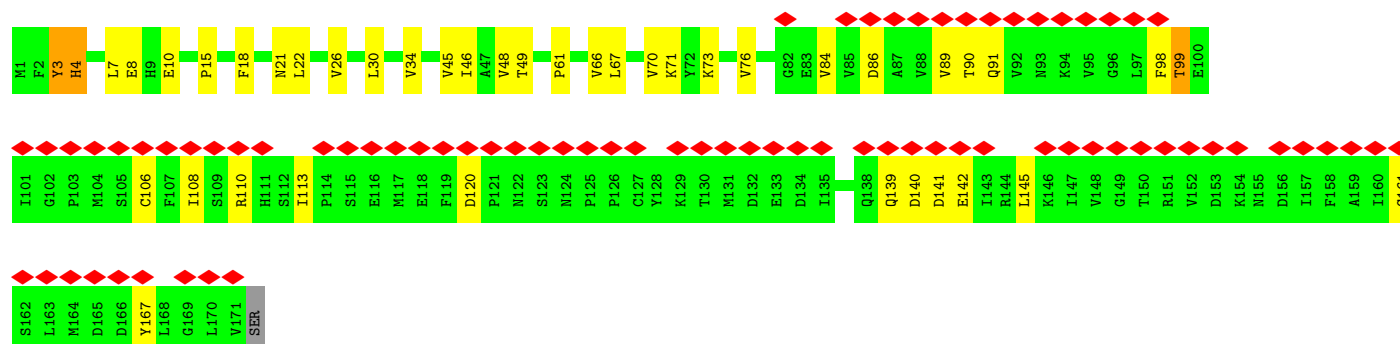
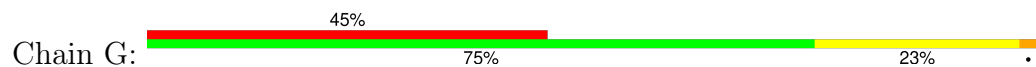
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



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



- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



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

Y93	Y96	Y97	Y98	T104	S105	T106	E107	L112	Y115	Y118	L122	M123	G127	D128	A129	M130	N131	L132	F135	R140	V141	L144	A148	L149	PHE														
A2	L5	E7	D8	F10	P17	K20	D23	R24	R27	L28	H29	S32	E33	R37	L40	L41	D42	L45	V50	R57	I60	L64	D71	D72	G73	E74	Y75	N76	D79	D80	R81	P82	S83	R84	A85	F88	E89	Y90	V91

-
- Figure 1: Schematic representation of the 120 amino acid residues of the protein. The residues are arranged in two rows. The top row contains residues MET, GLU, PRO, ASP, GLY, THR, TYR, PRO, GLU, GLY, PHE, V12, C17, Q18, Y25, P26, K27, E28, D29, R33, I34, L35, L36, R40, Q45, Q46, E47, A48, D49, I53, Y54, V55, N56, T59, H60, E61, E64, L65, T66, V72, L78, P79, R80, T81, C86, H91, and F96. The bottom row contains residues H100, R103, A104, E105, D108, R109, L110, C114, T115, A116, and E125. Residues are color-coded: MET (grey), GLU (light blue), PRO (light blue), ASP (light blue), GLY (light blue), THR (light blue), TYR (light blue), PRO (light blue), GLU (light blue), GLY (light blue), PHE (light blue), V12 (green), C17 (yellow), Q18 (yellow), Y25 (yellow), P26 (yellow), K27 (orange), E28 (green), D29 (yellow), R33 (green), I34 (green), L35 (green), L36 (orange), R40 (yellow), Q45 (yellow), Q46 (yellow), E47 (yellow), A48 (green), D49 (yellow), I53 (yellow), Y54 (yellow), V55 (green), N56 (yellow), T59 (yellow), H60 (yellow), E61 (yellow), E64 (yellow), L65 (green), T66 (yellow), V72 (orange), L78 (yellow), P79 (yellow), R80 (green), T81 (yellow), C86 (yellow), H91 (yellow), and F96 (yellow). Residues H100, R103, A104, E105, D108, R109, L110, C114, T115, A116, and E125 are shown in a separate row below the main sequence. Residues H100, R103, A104, E105, D108, R109, L110, C114, T115, A116, and E125 are color-coded: H100 (green), R103 (orange), A104 (yellow), E105 (yellow), D108 (green), R109 (yellow), L110 (yellow), C114 (yellow), T115 (yellow), A116 (yellow), and E125 (green). Red diamonds are placed above residues H100, E105, and D108.

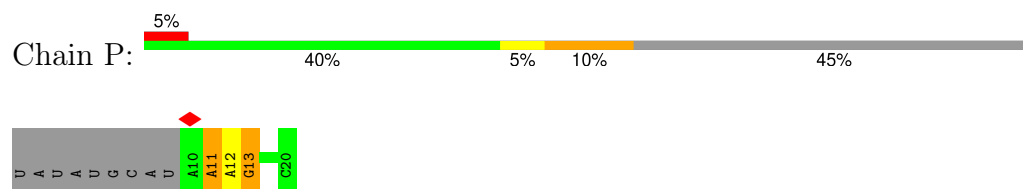
- | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| M1 | I2 | I3 | P4 | V5 | R6 | G7 | F8 | T9 | C10 | G11 | K12 | L25 | E28 | E31 | D36 | R42 | R46 | R47 | A51 | H52 | V53 | P64 | L65 | E66 | K67 |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- | | ILE | GLU |
|------|-----|-----|
| M1 | | |
| P5 | | |
| A6 | | |
| F7 | | |
| E8 | | |
| L11 | | |
| L12 | | |
| F13 | | |
| E16 | | |
| I19 | | |
| K23 | | |
| D24 | | |
| S48 | | |
| Q49 | | |
| L50 | | |
| D53 | | |
| P54 | | |
| Q55 | | |
| V56 | | |
| L57 | | |
| F58 | | |
| Y61 | | |
| P64 | | |
| H65 | | |
| P66 | | |
| L67 | | |
| K70 | | |
| T73 | | |
| Q76 | | |
| T77 | | |
| F87 | | |
| I91 | | |
| T92 | | |
| D93 | | |
| L94 | | |
| I95 | | |
| L100 | | |
| R104 | | |
| F105 | | |
| R106 | | |
| I109 | | |
| G115 | | |

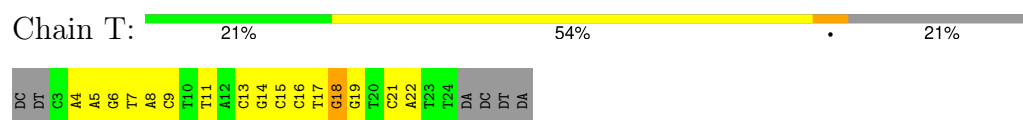
- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | ASP | THR | GLN | LYS | ASP | VAL | PRO | PRO | LYS | GLN | GLN | PRO | M15 | I16 | Y17 | I18 | I19 | G20 | H23 | N26 | E27 | I28 | I34 | R35 | G40 | Y41 | R42 | T43 | M44 | Y45 | K46 | T49 | D56 | A57 | R58 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|----|----|----|----|----|----|----|----|----|----|----|----|----|-----|-----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|--|-----|-----|-----|----|----|----|----|----|----|----|----|----|----|----|----|
| DT | DA | DG | DT | DA | DA | DA | DC | DT | DA | DG | DG | DA | DA | T15 | G16 | | G20 | T21 | A22 | C23 | T24 | T25 | G26 | A27 | G28 | DC | | T31 | A32 | G33 | DA | DC | DC | DA | DG | DC | DA | DA | DG | DC | DT | DC |
|----|----|----|----|----|----|----|----|----|----|----|----|----|----|-----|-----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|--|-----|-----|-----|----|----|----|----|----|----|----|----|----|----|----|----|

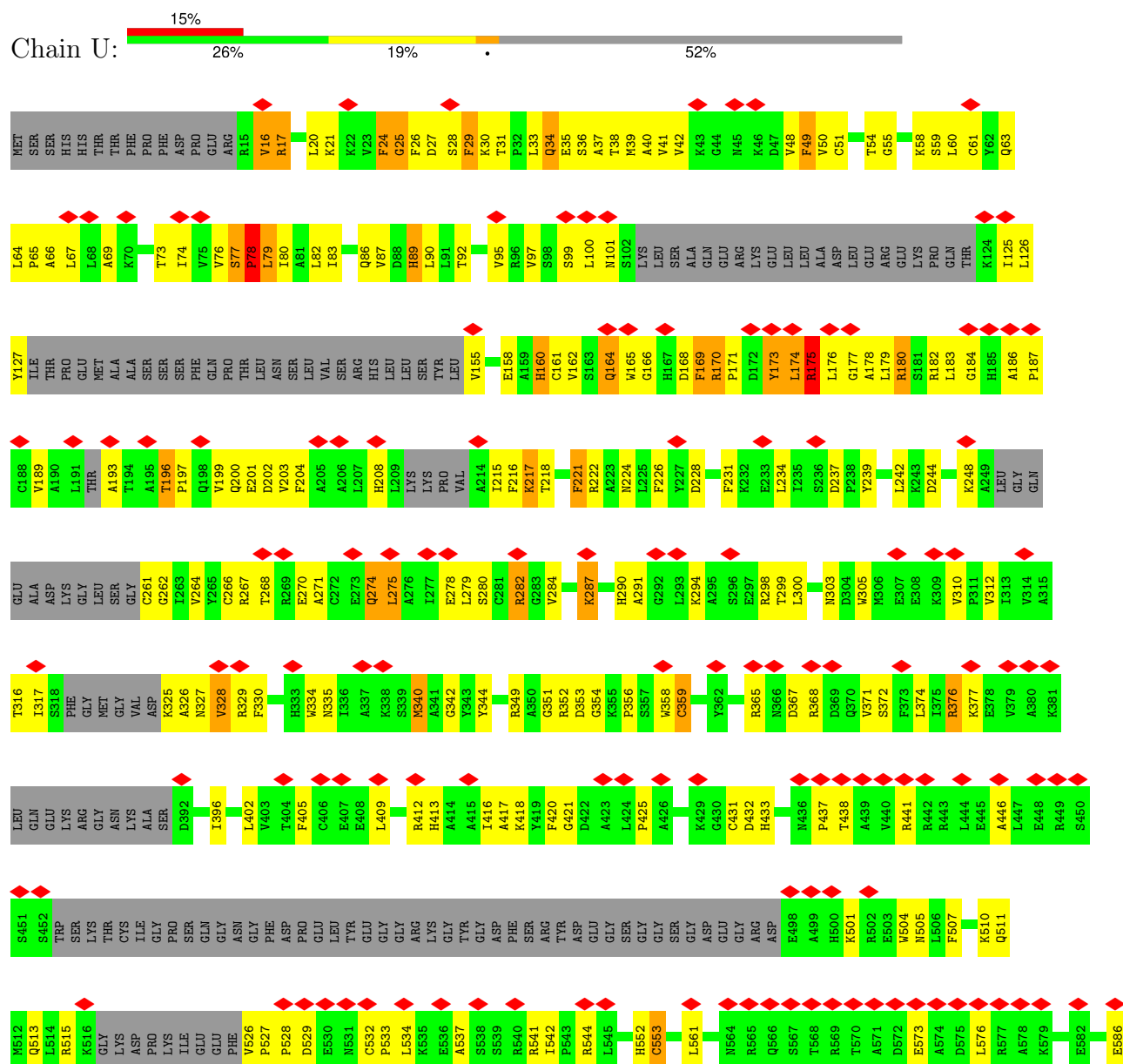
- Molecule 14: RNA, nucleic acid scaffold



- Molecule 15: Template DNA, nucleic acid scaffold



- Molecule 16: ATP-dependent DNA helicase Q5



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17442	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.220	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	335.36, 335.36, 335.36	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.40	0/11525	0.53	0/15558
2	B	0.44	0/9243	0.53	0/12475
3	C	0.45	0/2103	0.53	0/2858
4	D	0.24	0/1019	0.49	0/1374
5	E	0.38	0/1742	0.51	0/2353
6	F	0.43	0/668	0.51	0/903
7	G	0.31	0/1365	0.48	0/1853
8	H	0.43	0/1207	0.54	0/1628
9	I	0.39	0/948	0.51	0/1284
10	J	0.47	0/542	0.51	0/730
11	K	0.41	0/939	0.48	0/1271
12	L	0.46	0/377	0.62	0/500
13	N	0.78	0/398	1.02	0/611
14	P	0.87	0/268	0.97	0/416
15	T	0.96	0/499	1.08	2/767 (0.3%)
16	U	0.26	0/3756	0.49	0/5066
All	All	0.42	0/36599	0.55	2/49647 (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
10	J	0	1
16	U	0	5
All	All	0	7

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	18	DG	O4'-C4'-C3'	-6.75	101.80	104.50
15	T	18	DG	C4'-C3'-C2'	-5.29	98.34	103.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	583	ARG	Sidechain
10	J	28	GLU	Peptide
16	U	25	GLY	Peptide
16	U	76	VAL	Mainchain
16	U	77[A]	SER	Mainchain
16	U	77[B]	SER	Mainchain

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	11317	0	11453	309	0
2	B	9062	0	9107	233	0
3	C	2060	0	2011	75	0
4	D	1005	0	964	24	0
5	E	1711	0	1729	40	0
6	F	658	0	686	16	0
7	G	1334	0	1333	23	0
8	H	1186	0	1147	45	0
9	I	927	0	859	22	0
10	J	533	0	553	22	0
11	K	920	0	942	23	0
12	L	372	0	378	15	0
13	N	355	0	194	12	0
14	P	239	0	121	2	0
15	T	447	0	250	19	0
16	U	3692	0	3686	169	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
19	U	27	0	11	5	0
All	All	35854	0	35424	931	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 (931) 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:11:SER:N	2:B:1135:TYR:HH	1.55	1.05
1:A:1210:TRP:HD1	1:A:1281:ASP:HB2	1.35	0.88
16:U:31:THR:O	16:U:34:GLN:N	2.07	0.87
1:A:1128:ILE:HG23	1:A:1414:ILE:HB	1.57	0.86
1:A:1130:ILE:HG12	1:A:1413:ALA:HB2	1.64	0.80
2:B:827:GLU:HG2	2:B:871:VAL:HG22	1.63	0.79
15:T:4:DA:H2'	15:T:5:DA:C8	2.19	0.78
16:U:164:GLN:H	16:U:164:GLN:HE21	1.29	0.77
2:B:869:LYS:NZ	2:B:892:CYS:SG	2.57	0.77
1:A:560:VAL:HG22	1:A:591:ILE:HD11	1.66	0.76
1:A:1406:THR:O	5:E:207:ARG:NH2	2.19	0.75
3:C:240:ARG:NH1	3:C:242:GLU:OE2	2.20	0.75
1:A:811:ILE:HD12	9:I:79:PRO:HB3	1.66	0.74
1:A:769:MET:HE1	2:B:970:HIS:HA	1.69	0.74
2:B:384:ASP:HB3	2:B:387:HIS:HB2	1.68	0.74
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.68	0.74
3:C:70:LEU:HB3	10:J:6:ARG:HG3	1.70	0.73
3:C:59:LEU:HD12	3:C:151:VAL:HG12	1.68	0.73
16:U:501:LYS:O	16:U:505:ASN:ND2	2.22	0.73
16:U:50:VAL:HA	16:U:216:PHE:HB2	1.70	0.73
2:B:513:GLU:OE2	2:B:730:LYS:NZ	2.23	0.72
10:J:5:VAL:HG22	10:J:6:ARG:HG2	1.71	0.72
1:A:904:GLN:OE1	1:A:1044:HIS:NE2	2.22	0.72
1:A:349:ARG:NH1	2:B:1071:ASN:OD1	2.24	0.71
1:A:517:GLU:OE1	6:F:62:ARG:NH1	2.23	0.71
2:B:403:LEU:HD23	2:B:444:LEU:HD23	1.73	0.71
4:D:105:PRO:O	4:D:135:GLN:NE2	2.24	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:78:PRO:HG2	16:U:161:CYS:HB2	1.71	0.71
2:B:194:LEU:HD11	2:B:448:LEU:HD22	1.71	0.70
1:A:1210:TRP:CD1	1:A:1281:ASP:HB2	2.23	0.70
5:E:172:ARG:HD3	5:E:210:GLN:HG2	1.73	0.70
2:B:200:MET:HE1	2:B:222:ARG:HH11	1.57	0.70
5:E:103:LEU:HD23	5:E:128:GLU:HB2	1.75	0.69
8:H:84:ARG:NH1	8:H:85:ALA:O	2.25	0.69
3:C:205:LYS:NZ	3:C:216:SER:O	2.26	0.69
16:U:39:MET:HA	16:U:42:VAL:HB	1.73	0.69
2:B:789:ASN:HB3	2:B:795:ILE:HG13	1.75	0.69
1:A:687:ILE:HG22	2:B:782:ILE:HG21	1.75	0.69
5:E:13:ILE:HD11	5:E:132:GLN:HG3	1.72	0.69
2:B:1038:THR:HG22	3:C:196:VAL:HG22	1.76	0.68
13:N:22:DA:H2'	13:N:23:DC:C6	2.29	0.68
16:U:196:THR:O	16:U:200:GLN:N	2.20	0.68
1:A:1241:ASP:HB2	16:U:544:ARG:HH21	1.59	0.68
2:B:245:GLN:HE21	2:B:248:LYS:HB3	1.58	0.68
13:N:25:DT:H2'	13:N:26:DG:C8	2.28	0.68
1:A:551:ARG:NH1	8:H:42:ASP:OD2	2.27	0.68
1:A:811:ILE:HG22	2:B:674:MET:HE3	1.75	0.68
1:A:1355:VAL:HG23	1:A:1356:ARG:HG3	1.75	0.68
1:A:1301:ILE:HG23	1:A:1345:ARG:HH11	1.59	0.67
16:U:261:CYS:SG	16:U:262:GLY:N	2.67	0.67
2:B:236:TRP:HB2	2:B:259:THR:HB	1.76	0.67
16:U:228:ASP:HA	16:U:432:ASP:HB3	1.75	0.67
3:C:10:ARG:NH1	3:C:24:GLU:OE2	2.28	0.67
1:A:114:CYS:SG	1:A:116:LYS:NZ	2.65	0.67
1:A:94:VAL:HG13	1:A:311:GLN:HG2	1.76	0.66
4:D:112:LYS:NZ	4:D:118:LEU:O	2.28	0.66
1:A:760:LEU:HD11	1:A:781:ILE:HG21	1.76	0.66
2:B:300:MET:HG2	2:B:373:LEU:HD22	1.78	0.66
2:B:471:ASN:ND2	2:B:477:SER:OG	2.29	0.66
3:C:190:ASN:O	3:C:193:ARG:NH1	2.28	0.66
1:A:52:PRO:HB2	1:A:60:PRO:HD3	1.78	0.66
1:A:364:ARG:NH1	1:A:500:GLU:OE1	2.29	0.66
1:A:967:ARG:NH2	1:A:1326:GLY:O	2.28	0.66
1:A:1004:LEU:HD13	1:A:1062:GLY:HA2	1.76	0.66
12:L:26:ASN:ND2	12:L:44:MET:SD	2.67	0.66
1:A:865:ILE:HD11	1:A:1093:GLN:HG3	1.76	0.66
1:A:111:CYS:SG	1:A:188:GLN:NE2	2.68	0.65
2:B:803:ARG:NH1	10:J:8:PHE:O	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:89:VAL:HA	7:G:99:THR:HA	1.78	0.65
1:A:330:GLN:NE2	1:A:332:SER:OG	2.29	0.65
2:B:411:LEU:HD11	2:B:435:ILE:HG23	1.79	0.65
16:U:79:LEU:HB2	16:U:82:LEU:HB3	1.77	0.65
1:A:780:ASN:ND2	2:B:976:MET:SD	2.63	0.65
1:A:971:PRO:O	1:A:972:THR:OG1	2.15	0.65
1:A:732:THR:OG1	1:A:735:GLN:OE1	2.15	0.65
2:B:502:HIS:ND1	2:B:504:THR:OG1	2.27	0.65
8:H:128:ASP:N	8:H:128:ASP:OD1	2.29	0.65
7:G:10:GLU:HB3	7:G:67:LEU:HD11	1.79	0.64
16:U:278:GLU:OE1	16:U:282:ARG:NH2	2.30	0.64
2:B:796:MET:HE3	2:B:929:PRO:HB2	1.79	0.64
1:A:1210:TRP:HH2	9:I:35:LEU:HD13	1.61	0.64
2:B:240:LEU:HD22	2:B:255:ARG:HH21	1.63	0.64
2:B:1132:THR:HB	2:B:1134:THR:HG22	1.80	0.64
2:B:65:ILE:HB	2:B:86:LEU:HB2	1.81	0.63
5:E:55:ARG:NH1	5:E:107:GLN:OE1	2.31	0.63
16:U:287:LYS:HB2	16:U:310:VAL:HG21	1.79	0.63
1:A:890:ARG:NH2	1:A:1022:ILE:O	2.31	0.63
1:A:894:ASP:OD2	5:E:199:THR:OG1	2.17	0.63
1:A:706:ILE:HG21	1:A:824:GLU:HG3	1.81	0.63
1:A:1474:LEU:HB2	6:F:105:ILE:HG13	1.81	0.63
2:B:245:GLN:HE22	2:B:249:LYS:HG3	1.63	0.63
9:I:61:GLU:OE1	9:I:61:GLU:N	2.30	0.63
1:A:82:PRO:O	2:B:1156:LYS:NZ	2.30	0.62
16:U:271:ALA:HB3	16:U:316:THR:HG22	1.81	0.62
2:B:759:VAL:HG12	2:B:999:ALA:HB2	1.82	0.62
10:J:3:ILE:HD12	10:J:4:PRO:HD2	1.80	0.62
1:A:1244:ASN:HB2	1:A:1262:MET:HG2	1.81	0.62
1:A:1087:VAL:HG12	1:A:1400:LEU:HD22	1.79	0.62
2:B:777:ASN:O	10:J:47:ARG:NH1	2.32	0.62
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.81	0.62
16:U:180:ARG:HH12	16:U:184:GLY:HA2	1.65	0.62
16:U:290:HIS:O	16:U:298:ARG:NH1	2.29	0.62
2:B:113:ALA:HA	2:B:118:LEU:HB2	1.80	0.62
16:U:35:GLU:O	16:U:38:THR:OG1	2.15	0.62
1:A:532:ARG:NH1	1:A:647:THR:O	2.32	0.62
1:A:927:GLU:OE2	1:A:931:ARG:NH1	2.32	0.62
15:T:21:DC:H2"	15:T:22:DA:C8	2.35	0.62
1:A:1212:LEU:HB3	1:A:1259:ILE:HG23	1.82	0.61
2:B:808:SER:OG	2:B:1050:ARG:NH1	2.32	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:13:PHE:N	11:K:16:GLU:OE2	2.33	0.61
16:U:270:GLU:O	16:U:274:GLN:NE2	2.33	0.61
1:A:419:ILE:HB	1:A:427:ILE:HG23	1.82	0.61
1:A:933:THR:HG22	1:A:1059:ARG:HH12	1.66	0.61
16:U:30:LYS:NZ	19:U:1000:ADP:O4'	2.31	0.61
2:B:486:ASN:OD1	2:B:491:ARG:NH2	2.34	0.61
7:G:90:THR:O	7:G:139:GLN:NE2	2.33	0.61
16:U:416:ILE:O	16:U:420:PHE:N	2.28	0.61
4:D:36:GLU:OE2	4:D:84:ARG:NH1	2.33	0.61
2:B:276:LEU:HD21	2:B:343:LEU:HD12	1.82	0.61
2:B:929:PRO:O	2:B:948:GLN:NE2	2.32	0.61
10:J:25:LEU:HD21	10:J:31:GLU:HA	1.82	0.61
1:A:552:ASP:OD1	8:H:24:ARG:NE	2.34	0.61
12:L:18:ILE:HG13	12:L:45:TYR:HB2	1.83	0.61
1:A:1166:LEU:O	1:A:1170:THR:OG1	2.19	0.61
6:F:51:ARG:NH1	6:F:122:GLU:OE1	2.32	0.61
1:A:1048:THR:HA	1:A:1053:ARG:HH21	1.66	0.60
1:A:1200:PRO:HD3	16:U:552:HIS:HD2	1.66	0.60
16:U:586:GLU:OE1	16:U:589:ARG:NH2	2.33	0.60
1:A:879:VAL:HG11	1:A:1400:LEU:HD11	1.83	0.60
2:B:1115:GLN:HG2	2:B:1150:ARG:HG2	1.83	0.60
7:G:21:ASN:O	7:G:21:ASN:ND2	2.34	0.60
2:B:817:GLN:OE1	2:B:912:ASN:ND2	2.33	0.60
1:A:545:VAL:HG23	1:A:676:ILE:HG13	1.82	0.60
5:E:80:PRO:HA	5:E:107:GLN:HB2	1.82	0.60
16:U:221:PHE:HZ	16:U:417:ALA:HB2	1.66	0.60
1:A:927:GLU:H	1:A:930:LEU:HD13	1.65	0.60
1:A:1171:ALA:N	1:A:1215:GLU:O	2.31	0.60
2:B:352:GLY:O	2:B:361:LYS:NZ	2.27	0.60
2:B:907:VAL:HG13	2:B:921:ILE:HG12	1.83	0.60
1:A:1372:GLU:OE2	5:E:207:ARG:NH1	2.35	0.60
2:B:1142:ASN:HD21	2:B:1145:GLN:HB2	1.66	0.60
1:A:1358:THR:HG22	5:E:142:HIS:HE1	1.65	0.60
8:H:64:LEU:HD13	8:H:84:ARG:HD3	1.83	0.60
8:H:81:ARG:HG3	8:H:82:PRO:HD3	1.84	0.60
1:A:1214:VAL:HG23	1:A:1257:LEU:HB3	1.83	0.60
2:B:855:ALA:HB3	12:L:49:THR:HB	1.83	0.60
16:U:329:ARG:NH2	16:U:356:PRO:O	2.35	0.60
1:A:510:GLU:OE1	2:B:1101:GLN:NE2	2.34	0.59
5:E:70:ASP:OD1	5:E:71:GLN:N	2.34	0.59
1:A:740:GLN:OE1	1:A:743:ARG:NH1	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:SER:O	1:A:127:LYS:NZ	2.35	0.59
2:B:480:SER:OG	2:B:525:ASN:ND2	2.36	0.59
2:B:1028:LEU:HD11	2:B:1043:ILE:HD11	1.85	0.59
3:C:32:ASN:OD1	3:C:35:ARG:NH1	2.36	0.59
5:E:30:GLN:NE2	5:E:34:ASP:OD2	2.35	0.59
1:A:48:GLU:HB3	1:A:53:LYS:HD3	1.84	0.59
1:A:1173:THR:OG1	1:A:1289:GLU:OE2	2.17	0.59
2:B:934:LYS:HZ1	2:B:942:LYS:HB2	1.68	0.59
1:A:909:LEU:O	1:A:967:ARG:NH1	2.35	0.59
2:B:773:PRO:HG2	10:J:53:VAL:HG11	1.83	0.59
1:A:1213:ARG:NH1	1:A:1215:GLU:OE2	2.35	0.59
8:H:32:SER:OG	8:H:33:GLU:N	2.36	0.59
7:G:3:TYR:HD1	7:G:4:HIS:H	1.50	0.59
13:N:21:DT:H2"	13:N:22:DA:H8	1.68	0.59
16:U:405:PHE:O	16:U:412:ARG:NH1	2.36	0.59
3:C:172:GLU:OE2	12:L:58:ARG:NH2	2.36	0.58
3:C:236:CYS:HG	3:C:238:SER:HG	1.50	0.58
16:U:593:VAL:HG22	16:U:596:LEU:HB2	1.85	0.58
1:A:1179:PRO:O	9:I:33:ARG:NH2	2.36	0.58
2:B:240:LEU:O	2:B:249:LYS:NZ	2.36	0.58
16:U:409:LEU:HD22	16:U:441:ARG:HG2	1.85	0.58
1:A:592:PHE:HA	1:A:595:ILE:HD12	1.84	0.58
16:U:49:PHE:O	16:U:216:PHE:N	2.27	0.58
1:A:681:LEU:HD21	2:B:786:THR:HG22	1.86	0.58
2:B:984:CYS:SG	2:B:1046:THR:OG1	2.46	0.58
16:U:326:ALA:HA	16:U:352:ARG:H	1.68	0.58
7:G:18:PHE:HA	7:G:22:LEU:HD13	1.86	0.58
16:U:299:THR:O	16:U:303:ASN:ND2	2.35	0.58
3:C:263:LEU:HD22	11:K:87:PHE:HD2	1.68	0.58
10:J:65:LEU:O	12:L:23:HIS:ND1	2.36	0.58
2:B:480:SER:HG	2:B:525:ASN:ND2	2.02	0.58
9:I:36:LEU:HD12	9:I:45:GLN:HB3	1.86	0.58
16:U:180:ARG:NH2	16:U:183:LEU:O	2.36	0.57
1:A:31:LEU:HD23	1:A:252:VAL:HG13	1.84	0.57
1:A:486:LEU:O	1:A:489:THR:HB	2.04	0.57
1:A:659:GLU:OE2	1:A:985:ARG:NH1	2.37	0.57
1:A:813:ASP:OD2	9:I:100:HIS:NE2	2.32	0.57
16:U:33:LEU:O	16:U:37:ALA:N	2.37	0.57
16:U:312:VAL:HG22	16:U:330:PHE:HZ	1.69	0.57
1:A:1279:MET:O	16:U:515:ARG:NH2	2.37	0.57
1:A:95:PHE:HE1	1:A:221:VAL:HG11	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:33:DG:H2'	16:U:170:ARG:HD3	1.86	0.57
1:A:351:ARG:HD2	1:A:862:ARG:HH22	1.69	0.57
8:H:23:ASP:OD1	8:H:23:ASP:N	2.36	0.57
10:J:66:GLU:HA	12:L:23:HIS:HB3	1.85	0.57
1:A:710:LYS:HG2	1:A:817:PRO:HG3	1.87	0.57
2:B:404:PHE:HA	2:B:407:MET:HE2	1.86	0.57
2:B:801:VAL:HG13	2:B:929:PRO:HG2	1.87	0.56
11:K:7:PHE:HB2	11:K:11:LEU:HD12	1.87	0.56
1:A:95:PHE:CE1	1:A:221:VAL:HG11	2.40	0.56
1:A:671:ASN:O	1:A:675:VAL:HG12	2.05	0.56
8:H:104:THR:O	8:H:106:THR:N	2.37	0.56
1:A:551:ARG:HH12	8:H:27:ARG:NH2	2.03	0.56
2:B:552:ASN:N	2:B:552:ASN:OD1	2.38	0.56
3:C:4:ALA:HB2	11:K:93:ASP:HB3	1.87	0.56
3:C:51:GLN:OE1	3:C:162:ARG:NH2	2.38	0.56
16:U:164:GLN:HA	16:U:169:PHE:HB2	1.87	0.56
2:B:17:ILE:HG13	2:B:19:PRO:HD3	1.87	0.56
2:B:249:LYS:HE3	2:B:254:GLN:H	1.71	0.56
2:B:285:LEU:HD21	2:B:305:LEU:HD11	1.87	0.56
1:A:869:GLU:OE1	2:B:1091:ARG:NH2	2.38	0.56
6:F:46:GLN:N	6:F:115:TYR:O	2.38	0.56
16:U:325:LYS:HB3	16:U:328:VAL:HG22	1.88	0.56
2:B:909:VAL:HG21	12:L:17:TYR:CE2	2.40	0.56
16:U:90:LEU:HB3	16:U:95:VAL:HB	1.88	0.56
16:U:203:VAL:O	16:U:208:HIS:N	2.38	0.56
2:B:285:LEU:HD11	2:B:301:VAL:HG11	1.88	0.56
16:U:300:LEU:HA	16:U:303:ASN:HD21	1.71	0.56
2:B:393:LEU:HD13	2:B:485:LEU:HD22	1.87	0.56
2:B:776:ILE:HD11	10:J:8:PHE:HE2	1.71	0.56
16:U:67:LEU:HD22	16:U:125:ILE:HD11	1.88	0.56
3:C:260:GLN:HB2	11:K:91:ILE:HG21	1.87	0.55
1:A:1415:THR:HG23	1:A:1417:HIS:H	1.72	0.55
2:B:50:PHE:HA	2:B:54:SER:HB3	1.88	0.55
2:B:177:CYS:SG	2:B:738:THR:OG1	2.53	0.55
2:B:474:THR:OG1	2:B:732:ALA:O	2.24	0.55
2:B:854:ILE:HD12	2:B:904:VAL:HG21	1.86	0.55
6:F:84:GLU:OE1	6:F:95:LYS:NZ	2.35	0.55
4:D:99:CYS:O	4:D:103:LEU:HB2	2.06	0.55
5:E:134:GLU:OE1	5:E:181:ARG:NH2	2.36	0.55
7:G:106:CYS:SG	7:G:161:GLY:N	2.79	0.55
16:U:31:THR:H	16:U:34:GLN:HB2	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:LEU:HD23	1:A:1045:LEU:HD21	1.89	0.55
2:B:66:ASP:OD1	2:B:83:ARG:NH2	2.38	0.55
2:B:866:ILE:HG22	2:B:921:ILE:HD12	1.89	0.55
1:A:412:GLN:OE1	1:A:412:GLN:N	2.37	0.55
1:A:1485:GLU:HB3	6:F:78:PRO:HB3	1.89	0.55
16:U:325:LYS:HG3	16:U:327:ASN:HD21	1.72	0.55
2:B:956:PHE:CE2	3:C:184:PHE:HB3	2.42	0.55
2:B:1129:ASN:HB3	2:B:1134:THR:HG23	1.89	0.55
10:J:9:THR:OG1	10:J:47:ARG:NH2	2.40	0.55
16:U:374:LEU:HA	16:U:377:LYS:HE3	1.89	0.55
3:C:52:ILE:HD13	3:C:64:ILE:HD11	1.87	0.55
16:U:534:LEU:HB2	16:U:537:ALA:HB2	1.88	0.55
5:E:5:GLU:OE2	5:E:9:ARG:NH1	2.40	0.55
16:U:201:GLU:HA	16:U:204:PHE:HB2	1.87	0.55
2:B:561:ILE:HG13	2:B:576:ILE:HG21	1.89	0.54
2:B:758:LEU:HD21	10:J:51:ALA:HB2	1.90	0.54
16:U:77[A]:SER:HA	16:U:158:GLU:HG3	1.88	0.54
16:U:174:LEU:HB3	16:U:178:ALA:HB2	1.90	0.54
8:H:32:SER:HB3	8:H:37:MET:H	1.73	0.54
13:N:26:DG:HI'	13:N:27:DA:H5'	1.87	0.54
16:U:165:TRP:HD1	16:U:199:VAL:HG13	1.71	0.54
16:U:34:GLN:O	16:U:37:ALA:HB3	2.08	0.54
16:U:51:CYS:HG	16:U:193:ALA:N	2.05	0.54
16:U:291:ALA:O	16:U:298:ARG:NH2	2.40	0.54
1:A:274:ASP:OD2	1:A:342:ARG:NH2	2.40	0.54
1:A:1192:TRP:HZ3	1:A:1246:ILE:HG22	1.72	0.54
16:U:193:ALA:HB1	16:U:344:TYR:HE2	1.72	0.54
16:U:77[A]:SER:O	16:U:78:PRO:C	2.46	0.54
1:A:220:ARG:O	1:A:224:ILE:HG13	2.08	0.54
1:A:573:LYS:HD2	8:H:74:GLU:HG3	1.90	0.54
2:B:1021:HIS:NE2	3:C:202:GLU:OE1	2.41	0.54
4:D:44:ARG:O	4:D:48:ASN:ND2	2.41	0.54
1:A:932:ARG:NH1	8:H:107:GLU:O	2.41	0.54
16:U:529:ASP:OD1	16:U:529:ASP:N	2.41	0.54
3:C:179:THR:HG22	3:C:244:ILE:HD13	1.89	0.54
6:F:105:ILE:HG22	6:F:119:GLY:HA2	1.88	0.54
9:I:59:THR:O	9:I:60:HIS:ND1	2.41	0.54
16:U:196:THR:HA	16:U:420:PHE:HA	1.89	0.54
1:A:601:ASN:HA	1:A:630:VAL:O	2.08	0.53
1:A:866:LYS:HG2	1:A:1432:PHE:HB2	1.90	0.53
1:A:549:THR:HG22	1:A:589:LYS:HG2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:848:LEU:HD23	2:B:854:ILE:HG23	1.90	0.53
16:U:267:ARG:NH1	16:U:268:THR:OG1	2.41	0.53
3:C:55:ASN:ND2	3:C:61:ASP:OD1	2.33	0.53
8:H:5:LEU:HB2	8:H:60:ILE:HG22	1.90	0.53
1:A:1429:LYS:HB2	1:A:1438:VAL:HG11	1.90	0.53
1:A:1471:PHE:O	6:F:64:ARG:NH1	2.42	0.53
3:C:9:VAL:HG21	11:K:105:PHE:CD2	2.44	0.53
3:C:9:VAL:HG21	11:K:105:PHE:HD2	1.73	0.53
9:I:64:GLU:OE2	9:I:103:ARG:NH1	2.41	0.53
15:T:13:DC:H2'	15:T:14:DG:C8	2.44	0.53
16:U:31:THR:O	16:U:33:LEU:N	2.41	0.53
16:U:325:LYS:O	16:U:327:ASN:ND2	2.41	0.53
1:A:589:LYS:HZ1	1:A:625:ASP:CG	2.12	0.53
3:C:7:PRO:HA	3:C:24:GLU:O	2.09	0.53
16:U:197:PRO:O	16:U:201:GLU:HB2	2.09	0.53
1:A:576:GLN:O	1:A:590:GLN:NE2	2.41	0.53
16:U:160:HIS:HB2	16:U:166:GLY:HA3	1.90	0.53
1:A:328:ALA:O	1:A:335:PRO:HA	2.08	0.53
2:B:114:ARG:NH2	2:B:176:GLU:OE2	2.38	0.53
2:B:1085:ARG:NE	15:T:15:DC:OP1	2.42	0.53
2:B:986:GLN:HA	2:B:989:VAL:HG12	1.90	0.52
11:K:56:VAL:HG22	11:K:77:THR:HG22	1.90	0.52
2:B:313:GLU:HB3	2:B:316:VAL:HG12	1.91	0.52
2:B:785:TYR:CE2	2:B:955:PRO:HD3	2.45	0.52
10:J:10:CYS:SG	10:J:11:GLY:N	2.82	0.52
2:B:332:LYS:HD3	2:B:335:ARG:HH12	1.74	0.52
5:E:45:GLY:HA3	5:E:52:ARG:HB2	1.91	0.52
16:U:54:THR:HB	16:U:352:ARG:NH2	2.24	0.52
16:U:573:GLU:HA	16:U:576:LEU:HB2	1.90	0.52
1:A:1016:LEU:HD11	1:A:1073:GLU:HB2	1.90	0.52
1:A:1366:PHE:HB2	1:A:1374:VAL:HG21	1.91	0.52
2:B:223:SER:HB3	2:B:349:PRO:HD2	1.92	0.52
15:T:4:DA:C6	15:T:5:DA:C6	2.98	0.52
16:U:24:PHE:HZ	16:U:64:LEU:HD12	1.75	0.52
2:B:549:SER:HG	2:B:577:HIS:HE2	1.57	0.52
2:B:794:VAL:O	2:B:946:GLY:N	2.39	0.52
3:C:47:ILE:HG13	3:C:73:LEU:HD11	1.91	0.52
7:G:120:ASP:N	7:G:120:ASP:OD1	2.41	0.52
14:P:11:A:H2'	14:P:12:A:C8	2.44	0.52
1:A:367:ILE:HD13	1:A:501:MET:HE3	1.91	0.52
2:B:483:ARG:HB3	2:B:526:LEU:HD12	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:27:ARG:HH11	8:H:40:ILE:HG22	1.74	0.52
16:U:221:PHE:CZ	16:U:417:ALA:HB2	2.44	0.52
16:U:325:LYS:HG3	16:U:327:ASN:ND2	2.24	0.52
16:U:340:MET:HG2	16:U:402:LEU:HG	1.92	0.52
1:A:1056:GLU:O	1:A:1059:ARG:NH2	2.42	0.52
1:A:1301:ILE:HG23	1:A:1345:ARG:HD3	1.91	0.52
1:A:1394:ASN:OD1	1:A:1396:ARG:NH1	2.42	0.52
2:B:694:THR:O	2:B:695:HIS:ND1	2.43	0.52
2:B:907:VAL:HB	12:L:46:LYS:HG3	1.92	0.52
9:I:36:LEU:HD22	9:I:47:GLU:HA	1.92	0.52
16:U:155:VAL:HG13	16:U:189:VAL:HB	1.92	0.52
3:C:178:PRO:HG2	3:C:179:THR:HG23	1.90	0.52
1:A:545:VAL:HG11	1:A:645:LEU:HD12	1.92	0.52
1:A:1263:ASN:CB	16:U:515:ARG:HB3	2.40	0.52
16:U:561:LEU:HD13	16:U:576:LEU:HD22	1.91	0.52
1:A:423:ASN:OD1	1:A:423:ASN:N	2.40	0.51
1:A:823:VAL:HG13	1:A:835:GLU:HB3	1.92	0.51
1:A:958:ARG:HH11	1:A:1046:ARG:HD3	1.75	0.51
1:A:1318:LYS:HD2	1:A:1330:ALA:HB1	1.92	0.51
2:B:738:THR:HG23	2:B:772:LEU:HD21	1.93	0.51
2:B:778:SER:HB3	2:B:805:PHE:HZ	1.75	0.51
1:A:1475:LEU:HD22	7:G:66:VAL:HG21	1.93	0.51
2:B:986:GLN:HE21	2:B:997:GLY:HA3	1.76	0.51
4:D:126:GLU:O	4:D:129:GLN:HG3	2.10	0.51
15:T:7:DT:H2'	15:T:8:DA:C8	2.45	0.51
1:A:218:PRO:HA	1:A:221:VAL:HG12	1.92	0.51
1:A:1286:ARG:CZ	1:A:1286:ARG:HA	2.41	0.51
2:B:852:GLY:O	2:B:868:GLY:N	2.37	0.51
5:E:55:ARG:HA	5:E:58:LEU:HD12	1.92	0.51
2:B:663:GLU:OE1	2:B:695:HIS:NE2	2.38	0.51
12:L:35:ARG:NH2	12:L:40:GLY:HA2	2.24	0.51
1:A:466:LYS:HA	2:B:1093:CYS:SG	2.50	0.51
1:A:625:ASP:O	1:A:639:ILE:HG12	2.11	0.51
1:A:832:THR:OG1	1:A:835:GLU:OE1	2.26	0.51
1:A:1143:LEU:HD21	1:A:1336:LEU:HG	1.92	0.51
3:C:47:ILE:O	3:C:175:LYS:NZ	2.28	0.51
1:A:784:VAL:HA	1:A:827:TYR:HB2	1.92	0.51
2:B:254:GLN:HB3	2:B:303:PRO:HG2	1.92	0.51
2:B:311:ILE:HG23	2:B:316:VAL:HG13	1.93	0.51
2:B:331:THR:HG22	2:B:334:LYS:HE2	1.93	0.51
16:U:20:LEU:HA	16:U:27:ASP:HB2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:205:LYS:HD2	3:C:211:LEU:HD11	1.91	0.51
1:A:67:ARG:HA	1:A:78:MET:SD	2.51	0.51
16:U:89:HIS:O	16:U:92:THR:OG1	2.28	0.51
1:A:861:GLN:HG2	1:A:1096:GLY:HA3	1.93	0.51
2:B:42:GLN:HG2	2:B:43:GLN:N	2.26	0.51
2:B:588:ARG:O	2:B:592:ARG:HD3	2.11	0.51
15:T:4:DA:H2'	15:T:5:DA:H8	1.73	0.51
15:T:18:DG:H2'	15:T:19:DG:C8	2.46	0.51
16:U:59:SER:O	16:U:63:GLN:HB2	2.11	0.51
1:A:889:LEU:O	1:A:890:ARG:HD2	2.11	0.51
1:A:1295:ASP:HB3	16:U:501:LYS:HE2	1.92	0.51
16:U:553:CYS:SG	16:U:597:TYR:OH	2.61	0.51
1:A:76:GLY:HA2	1:A:81:CYS:HB2	1.92	0.50
1:A:1200:PRO:HD3	16:U:552:HIS:CD2	2.45	0.50
4:D:34:ASN:HA	4:D:37:VAL:HG12	1.94	0.50
8:H:60:ILE:HG23	8:H:141:VAL:HG13	1.93	0.50
16:U:41:VAL:HG11	16:U:65:PRO:HG3	1.92	0.50
16:U:63:GLN:HE21	16:U:86:GLN:HE21	1.57	0.50
1:A:1288:ILE:HD13	16:U:504:TRP:HZ2	1.77	0.50
1:A:1416:ARG:O	1:A:1420:ASN:HB2	2.12	0.50
2:B:1115:GLN:HB3	2:B:1148:LEU:HD21	1.92	0.50
1:A:15:LEU:HD11	2:B:1150:ARG:HG3	1.92	0.50
1:A:857:THR:HG21	1:A:1100:THR:HA	1.92	0.50
2:B:675:LEU:HD22	2:B:697:GLU:HG3	1.93	0.50
4:D:64:THR:HG21	7:G:46:ILE:HG23	1.93	0.50
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.94	0.50
16:U:180:ARG:O	16:U:180:ARG:NH1	2.44	0.50
2:B:451:GLY:HA2	2:B:467:SER:OG	2.11	0.50
2:B:712:PRO:HG2	2:B:939:HIS:CE1	2.46	0.50
5:E:102:ALA:HB3	5:E:127:LEU:HG	1.92	0.50
1:A:286:ILE:HD13	1:A:309:LEU:HD23	1.93	0.50
1:A:458:PHE:HB3	1:A:492:TYR:OH	2.11	0.50
1:A:1184:THR:OG1	1:A:1190:GLN:NE2	2.45	0.50
2:B:854:ILE:HD11	2:B:866:ILE:HG23	1.92	0.50
16:U:24:PHE:HD1	16:U:25:GLY:H	1.59	0.50
16:U:73:THR:HG22	16:U:155:VAL:HG23	1.92	0.50
1:A:33:ARG:HB3	2:B:1139:GLY:HA2	1.92	0.50
2:B:285:LEU:O	2:B:289:ILE:N	2.44	0.50
6:F:61:GLU:OE2	6:F:108:ARG:NE	2.42	0.50
3:C:70:LEU:HD23	10:J:6:ARG:HB2	1.94	0.50
13:N:27:DA:H2''	13:N:28:DG:C8	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:883:ILE:HD11	1:A:1424:THR:HG22	1.93	0.50
1:A:1157:ILE:HD13	1:A:1160:ARG:HH21	1.76	0.50
3:C:154:ARG:HH11	10:J:64:PRO:HD3	1.75	0.50
16:U:26:PHE:CE1	19:U:1000:ADP:H2'	2.47	0.50
16:U:237:ASP:OD1	16:U:237:ASP:N	2.45	0.50
1:A:702:ILE:HD13	1:A:786:ALA:HA	1.94	0.49
2:B:561:ILE:HD11	2:B:573:TRP:CZ2	2.47	0.49
3:C:48:ASP:HB3	3:C:166:LYS:HE2	1.93	0.49
8:H:17:PRO:HG3	8:H:29:HIS:CE1	2.46	0.49
16:U:221:PHE:CE2	16:U:425:PRO:HB3	2.46	0.49
16:U:224:ASN:HD22	16:U:351:GLY:HA3	1.77	0.49
16:U:267:ARG:HG2	16:U:268:THR:H	1.77	0.49
1:A:555:LEU:HD12	1:A:591:ILE:HD12	1.93	0.49
1:A:1177:TYR:HB2	1:A:1210:TRP:CZ3	2.47	0.49
1:A:674:THR:O	1:A:678:ASN:ND2	2.42	0.49
3:C:61:ASP:OD1	3:C:61:ASP:N	2.45	0.49
3:C:173:HIS:HD2	3:C:175:LYS:HG2	1.78	0.49
15:T:17:DT:H2'	15:T:18:DG:C8	2.48	0.49
16:U:261:CYS:N	16:U:327:ASN:OD1	2.45	0.49
1:A:107:LEU:HD21	1:A:221:VAL:HG23	1.94	0.49
2:B:386:ASP:CG	13:N:16:DG:H22	2.15	0.49
2:B:556:ILE:HG12	2:B:576:ILE:HD11	1.93	0.49
3:C:60:HIS:CD2	3:C:63:PHE:H	2.30	0.49
3:C:263:LEU:HB2	11:K:19:ILE:HD13	1.94	0.49
16:U:74:ILE:HG13	16:U:179:LEU:HB3	1.94	0.49
2:B:395:LEU:HD23	2:B:532:ILE:HG21	1.94	0.49
5:E:48:PRO:HA	5:E:53:PRO:HG2	1.94	0.49
7:G:141:ASP:OD1	7:G:142:GLU:N	2.45	0.49
1:A:130:LEU:HD21	1:A:235:VAL:HG23	1.94	0.49
2:B:1067:ILE:HD12	2:B:1072:ARG:HG3	1.94	0.49
3:C:56:SER:HB2	3:C:158:GLU:H	1.78	0.49
4:D:20:LEU:HD11	4:D:93:HIS:CD2	2.48	0.49
1:A:456:VAL:HG21	1:A:503:LEU:HD11	1.94	0.49
1:A:581:LYS:O	1:A:582:PRO:C	2.51	0.49
1:A:834:THR:HG23	2:B:677:MET:HE3	1.95	0.49
1:A:264:VAL:HG22	2:B:1069:ILE:HD13	1.95	0.49
1:A:1208:SER:OG	1:A:1281:ASP:OD2	2.27	0.49
2:B:384:ASP:OD2	2:B:502:HIS:NE2	2.40	0.49
2:B:979:GLY:O	2:B:983:GLU:HB2	2.12	0.49
8:H:76:ASN:N	8:H:76:ASN:OD1	2.44	0.49
16:U:174:LEU:HD12	16:U:177:GLY:HA3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:PHE:O	1:A:316:THR:OG1	2.25	0.49
1:A:713:VAL:HG23	1:A:741:VAL:HG22	1.93	0.49
8:H:41:LEU:HD13	8:H:123:MET:HB2	1.95	0.49
1:A:821:GLY:HA2	1:A:838:PHE:CD2	2.48	0.48
2:B:542:LEU:HD22	2:B:574:VAL:HG21	1.95	0.48
2:B:591:ARG:NH2	2:B:663:GLU:OE2	2.46	0.48
3:C:122:SER:OG	3:C:123:ASN:N	2.46	0.48
1:A:345:GLY:HA2	1:A:351:ARG:HD3	1.94	0.48
2:B:529:MET:HB3	2:B:624:PRO:HD2	1.95	0.48
16:U:16:VAL:HB	16:U:42:VAL:HG11	1.95	0.48
16:U:36:SER:O	16:U:40:ALA:N	2.30	0.48
1:A:100:LEU:HD23	1:A:193:ARG:HE	1.79	0.48
1:A:1358:THR:HG22	5:E:142:HIS:CE1	2.47	0.48
2:B:587:LEU:HD22	2:B:597:ILE:HD11	1.94	0.48
3:C:94:CYS:N	3:C:97:CYS:SG	2.81	0.48
7:G:30:LEU:O	7:G:34:VAL:HG12	2.13	0.48
16:U:267:ARG:H	16:U:335:ASN:HB2	1.77	0.48
1:A:37:THR:HA	1:A:61:ARG:HH21	1.77	0.48
2:B:802:ASP:CG	3:C:174:ALA:H	2.17	0.48
16:U:28:SER:HB3	19:U:1000:ADP:N1	2.29	0.48
1:A:85:PHE:CE1	1:A:254:PRO:HB2	2.49	0.48
1:A:590:GLN:O	1:A:593:SER:OG	2.26	0.48
2:B:796:MET:O	2:B:948:GLN:HA	2.14	0.48
2:B:924:ARG:NH1	3:C:62:GLU:OE1	2.46	0.48
3:C:76:ASP:HA	3:C:239:LEU:HD23	1.96	0.48
9:I:91:HIS:CE1	9:I:116:ALA:HB2	2.48	0.48
16:U:80:ILE:HG12	16:U:101:ASN:HB2	1.95	0.48
1:A:738:GLU:OE2	1:A:797:ARG:NE	2.26	0.48
16:U:432:ASP:OD1	16:U:433:HIS:N	2.47	0.48
1:A:421:ARG:HB2	1:A:425:ASP:OD1	2.14	0.48
4:D:29:ALA:O	4:D:94:LYS:NZ	2.36	0.48
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.94	0.48
12:L:56:ASP:OD1	12:L:56:ASP:N	2.44	0.48
13:N:21:DT:H2"	13:N:22:DA:C8	2.49	0.48
16:U:87:VAL:HG22	16:U:97:VAL:HG22	1.95	0.48
1:A:279:LYS:HE2	1:A:316:THR:HB	1.96	0.48
1:A:784:VAL:HG13	1:A:785:ILE:HG13	1.96	0.48
1:A:1210:TRP:CH2	9:I:53:ILE:HD11	2.48	0.48
4:D:59:GLU:O	4:D:63:LYS:HB2	2.14	0.48
9:I:25:TYR:HB2	9:I:40:ARG:HH11	1.79	0.48
1:A:601:ASN:ND2	1:A:989:ASN:OD1	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1318:LYS:HG2	1:A:1331:LEU:O	2.14	0.47
3:C:18:ASN:ND2	3:C:232:ASN:OD1	2.47	0.47
8:H:93:TYR:HE2	8:H:140:ARG:HH21	1.62	0.47
1:A:580:LEU:O	1:A:581:LYS:C	2.51	0.47
1:A:805:ARG:NH1	2:B:671:GLU:O	2.47	0.47
2:B:473:LEU:HD21	2:B:1052:LYS:HB3	1.95	0.47
2:B:776:ILE:HG22	2:B:806:PHE:CE1	2.49	0.47
4:D:67:TYR:OH	7:G:86:ASP:O	2.33	0.47
8:H:57:ARG:HG3	8:H:148:LEU:HD11	1.95	0.47
1:A:428:ASP:OD1	1:A:430:ARG:HG3	2.14	0.47
1:A:868:MET:HE3	1:A:1400:LEU:HD23	1.96	0.47
2:B:59:VAL:HG13	2:B:408:PHE:CZ	2.49	0.47
3:C:67:ARG:NH2	3:C:149:LEU:O	2.34	0.47
15:T:21:DC:H2"	15:T:22:DA:H8	1.77	0.47
16:U:36:SER:HA	16:U:39:MET:HB2	1.96	0.47
1:A:628:VAL:HA	1:A:637:MET:O	2.13	0.47
2:B:513:GLU:OE2	2:B:525:ASN:ND2	2.48	0.47
2:B:941:GLN:HE22	2:B:975:ARG:HD2	1.78	0.47
7:G:34:VAL:HG22	7:G:45:VAL:HG11	1.96	0.47
8:H:20:LYS:HE2	8:H:23:ASP:HA	1.96	0.47
16:U:155:VAL:HG22	16:U:189:VAL:HG23	1.97	0.47
1:A:514:GLU:O	1:A:518:LEU:HB2	2.14	0.47
1:A:802:PHE:HB2	1:A:805:ARG:O	2.14	0.47
1:A:977:VAL:HG21	1:A:1040:LEU:HD21	1.96	0.47
2:B:149:ILE:HA	2:B:437:THR:HG22	1.97	0.47
2:B:237:VAL:HG12	2:B:372:LEU:HD22	1.96	0.47
2:B:869:LYS:N	2:B:893:SER:OG	2.43	0.47
16:U:226:PHE:N	16:U:358:TRP:O	2.48	0.47
1:A:16:ARG:HG2	2:B:1173:SER:HB2	1.97	0.47
1:A:453:GLY:HA2	1:A:473:ARG:HG2	1.97	0.47
1:A:551:ARG:NH2	1:A:622:SER:O	2.48	0.47
2:B:470:LEU:HD21	2:B:478:THR:HG23	1.96	0.47
6:F:53:THR:OG1	6:F:116:GLU:OE1	2.32	0.47
7:G:15:PRO:HA	7:G:18:PHE:CZ	2.49	0.47
8:H:7:GLU:OE2	8:H:57:ARG:NH1	2.35	0.47
8:H:112:LEU:HB3	8:H:132:LEU:HD23	1.95	0.47
1:A:274:ASP:OD1	1:A:275:ASP:N	2.45	0.47
1:A:612:ASP:OD1	1:A:612:ASP:N	2.46	0.47
1:A:712:ASP:HB3	1:A:744:ILE:HD13	1.96	0.47
1:A:1106:THR:HB	1:A:1119:LEU:H	1.79	0.47
1:A:1347:LEU:HB3	5:E:137:ILE:HD13	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:GLU:OE1	2:B:472:ARG:NE	2.48	0.47
2:B:752:TYR:HE1	3:C:60:HIS:HE1	1.63	0.47
3:C:234:GLU:OE2	10:J:12:LYS:NZ	2.42	0.47
15:T:18:DG:H2'	15:T:19:DG:H8	1.79	0.47
16:U:165:TRP:CD1	16:U:199:VAL:HG22	2.50	0.47
16:U:261:CYS:SG	16:U:325:LYS:HG2	2.55	0.47
2:B:992:ASN:O	10:J:46:ARG:NH1	2.48	0.47
16:U:158:GLU:OE1	16:U:160:HIS:NE2	2.48	0.47
8:H:60:ILE:HG21	8:H:135:PHE:CE2	2.50	0.47
1:A:1234:LYS:HG2	1:A:1298:LEU:HA	1.97	0.47
1:A:1433:GLU:HB3	15:T:11:DT:H5''	1.97	0.47
2:B:117:ASN:HA	2:B:189:GLY:HA3	1.97	0.47
2:B:118:LEU:HD23	2:B:913:GLN:HG2	1.95	0.47
1:A:59:ASP:HB3	1:A:62:GLN:HB2	1.97	0.46
1:A:814:ASP:OD2	2:B:689:TYR:OH	2.25	0.46
1:A:893:GLU:OE2	5:E:195:ARG:NH1	2.48	0.46
1:A:1175:ILE:HD12	1:A:1286:ARG:HE	1.80	0.46
1:A:1370:GLY:HA2	5:E:178:PRO:HD2	1.97	0.46
2:B:866:ILE:HG22	2:B:867:ILE:HG13	1.97	0.46
2:B:1022:LEU:HD21	3:C:202:GLU:HB2	1.97	0.46
4:D:20:LEU:HD21	4:D:93:HIS:CG	2.49	0.46
8:H:88:PHE:CG	8:H:144:LEU:HB3	2.51	0.46
1:A:368:THR:O	1:A:483:ARG:HA	2.15	0.46
1:A:413:TYR:O	1:A:415:GLY:N	2.48	0.46
2:B:149:ILE:HG22	2:B:435:ILE:HG21	1.96	0.46
3:C:105:VAL:HG21	3:C:115:VAL:HG22	1.97	0.46
5:E:56:THR:C	5:E:58:LEU:H	2.18	0.46
8:H:84:ARG:HD2	8:H:85:ALA:N	2.30	0.46
8:H:90:TYR:HE2	8:H:92:MET:HE3	1.80	0.46
16:U:83:ILE:HG23	16:U:127:TYR:HB3	1.96	0.46
1:A:181:HIS:CG	1:A:182:GLY:H	2.33	0.46
1:A:196:LEU:HB3	1:A:311:GLN:OE1	2.15	0.46
1:A:460:ARG:HD3	1:A:492:TYR:O	2.16	0.46
7:G:22:LEU:O	7:G:26:VAL:HG23	2.16	0.46
16:U:87:VAL:HG21	16:U:99:SER:HB3	1.98	0.46
1:A:360:ASP:OD1	2:B:1062:ARG:NE	2.41	0.46
1:A:1243:LEU:HD12	1:A:1261:ILE:HA	1.97	0.46
2:B:407:MET:HE2	2:B:407:MET:HB2	1.77	0.46
2:B:473:LEU:HD22	2:B:1052:LYS:HD2	1.98	0.46
2:B:838:GLN:N	2:B:889:LYS:O	2.43	0.46
5:E:22:HIS:HB2	5:E:28:VAL:HG21	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:180:ARG:NH2	16:U:186:ALA:O	2.49	0.46
16:U:196:THR:HG23	16:U:199:VAL:HB	1.96	0.46
3:C:40:ALA:O	3:C:170:GLY:N	2.47	0.46
5:E:55:ARG:NE	5:E:107:GLN:HE22	2.13	0.46
8:H:79:ASP:O	8:H:82:PRO:HD2	2.15	0.46
2:B:264:LYS:NZ	2:B:325:GLY:O	2.35	0.46
2:B:584:MET:HG3	2:B:605:ARG:HB2	1.97	0.46
3:C:37:VAL:HG21	3:C:252:LEU:HD12	1.96	0.46
9:I:49:ASP:OD1	9:I:49:ASP:N	2.49	0.46
1:A:58:MET:HG2	1:A:65:ILE:HD13	1.97	0.46
1:A:374:SER:HB3	1:A:377:GLN:HG3	1.97	0.46
1:A:631:GLU:HG2	1:A:988:TRP:CZ2	2.51	0.46
1:A:1157:ILE:HD13	1:A:1160:ARG:HE	1.81	0.46
3:C:27:ASP:OD1	3:C:28:LEU:N	2.46	0.46
5:E:82:VAL:HG23	5:E:106:VAL:HG13	1.98	0.46
1:A:241:ARG:HD3	1:A:242:TYR:CZ	2.51	0.46
2:B:748:ALA:HB3	2:B:811:TYR:HB2	1.98	0.46
3:C:84:TYR:HB3	3:C:86:ARG:HG2	1.98	0.46
10:J:42:ARG:O	10:J:46:ARG:HG3	2.15	0.46
1:A:113:PHE:CE1	1:A:186:ARG:HD3	2.51	0.46
1:A:467:MET:HG2	1:A:534:VAL:HG11	1.98	0.46
1:A:713:VAL:HG11	1:A:817:PRO:HD3	1.97	0.46
16:U:224:ASN:ND2	16:U:351:GLY:HA3	2.31	0.46
16:U:279:LEU:HD22	16:U:284:VAL:HB	1.98	0.46
16:U:325:LYS:NZ	16:U:327:ASN:HD21	2.14	0.46
16:U:358:TRP:O	16:U:359:CYS:HB3	2.16	0.46
16:U:511:GLN:O	16:U:515:ARG:NH1	2.48	0.46
1:A:353:ASN:O	1:A:357:LYS:HE2	2.15	0.45
1:A:1139:LEU:HD12	1:A:1358:THR:O	2.16	0.45
3:C:78:ILE:HA	3:C:81:LYS:HG2	1.98	0.45
1:A:352:GLY:O	1:A:353:ASN:ND2	2.49	0.45
1:A:865:ILE:HG21	2:B:1092:ASP:CG	2.37	0.45
16:U:274:GLN:OE1	16:U:275:LEU:N	2.49	0.45
16:U:284:VAL:HG12	16:U:312:VAL:HG21	1.97	0.45
2:B:810:PHE:HB2	2:B:927:ARG:HD2	1.98	0.45
5:E:19:GLN:OE1	5:E:138:ASN:ND2	2.37	0.45
16:U:413:HIS:O	16:U:416:ILE:HG22	2.15	0.45
1:A:118:LEU:HB2	1:A:148:CYS:SG	2.56	0.45
1:A:220:ARG:HD2	1:A:220:ARG:HA	1.84	0.45
1:A:1371:ILE:O	1:A:1374:VAL:HG12	2.16	0.45
8:H:105:SER:OG	8:H:106:THR:N	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:372:SER:C	16:U:513:GLN:HE22	2.19	0.45
1:A:12:ALA:HB3	2:B:1135:TYR:HE2	1.82	0.45
1:A:190:ARG:HH22	13:N:25:DT:H5''	1.81	0.45
1:A:631:GLU:HG2	1:A:988:TRP:HZ2	1.81	0.45
1:A:1307:VAL:HG13	1:A:1338:THR:HG22	1.98	0.45
15:T:13:DC:H2'	15:T:14:DG:H8	1.80	0.45
1:A:200:ALA:HB3	1:A:214:ILE:HG23	1.97	0.45
1:A:544:ALA:HB2	1:A:680:LEU:HD13	1.98	0.45
1:A:956:PHE:HA	1:A:959:MET:HE2	1.98	0.45
1:A:1177:TYR:OH	1:A:1179:PRO:HB3	2.16	0.45
2:B:412:LEU:HA	2:B:415:VAL:HG12	1.99	0.45
3:C:101:PHE:CE2	3:C:122:SER:HB2	2.51	0.45
16:U:173:TYR:HB2	16:U:175:ARG:HH21	1.80	0.45
1:A:525:ILE:O	1:A:534:VAL:HG22	2.17	0.45
2:B:955:PRO:O	2:B:963:PRO:HD2	2.17	0.45
3:C:154:ARG:NH1	10:J:64:PRO:HD3	2.31	0.45
5:E:71:GLN:HB2	5:E:99:ILE:HG22	1.99	0.45
10:J:10:CYS:SG	10:J:42:ARG:NH1	2.89	0.45
16:U:376:ARG:HD3	16:U:376:ARG:HA	1.84	0.45
1:A:316:THR:HG21	1:A:328:ALA:HB2	1.99	0.45
1:A:1009:VAL:HA	1:A:1065:PHE:CZ	2.52	0.45
2:B:528:LEU:HD23	2:B:528:LEU:HA	1.82	0.45
1:A:302:VAL:HA	1:A:305:GLU:HG2	1.98	0.45
1:A:1191:GLU:HA	1:A:1194:ASN:HD21	1.82	0.45
1:A:1243:LEU:HD21	1:A:1259:ILE:HD11	1.99	0.45
2:B:124:LEU:HD22	2:B:149:ILE:HD11	1.99	0.45
2:B:871:VAL:HG23	2:B:892:CYS:SG	2.56	0.45
2:B:956:PHE:HB3	2:B:962:THR:HG22	1.97	0.45
3:C:30:VAL:O	3:C:34:ILE:HG13	2.17	0.45
14:P:12:A:O2'	14:P:13:G:H8	2.00	0.45
1:A:58:MET:HA	1:A:258:LEU:HD21	1.98	0.45
2:B:332:LYS:O	2:B:336:ILE:HG12	2.17	0.44
3:C:44:ILE:HG22	3:C:176:TRP:HD1	1.81	0.44
5:E:2:ASP:N	5:E:2:ASP:OD1	2.51	0.44
1:A:1231:ILE:O	1:A:1235:ILE:HG12	2.16	0.44
2:B:346:GLU:O	2:B:349:PRO:HD3	2.17	0.44
4:D:93:HIS:N	4:D:96:GLU:OE2	2.50	0.44
5:E:66:ASP:OD1	5:E:66:ASP:N	2.49	0.44
11:K:5:PRO:HD2	11:K:8:GLU:HG3	1.99	0.44
3:C:40:ALA:O	3:C:169:PHE:HB2	2.18	0.44
3:C:214:ASP:OD1	3:C:215:GLU:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:86:CYS:HB2	9:I:114:CYS:SG	2.58	0.44
16:U:226:PHE:HB3	16:U:358:TRP:HA	1.98	0.44
16:U:528:PRO:HB3	16:U:532:CYS:HB2	1.99	0.44
1:A:1020:LEU:O	1:A:1034:GLN:NE2	2.51	0.44
4:D:87:LEU:HB3	4:D:97:LEU:HD11	2.00	0.44
1:A:885:GLN:NE2	1:A:1423:ASP:OD1	2.50	0.44
2:B:291:ASP:OD1	2:B:291:ASP:N	2.51	0.44
3:C:253:LYS:NZ	11:K:95:ILE:O	2.50	0.44
12:L:19:CYS:SG	12:L:20:GLY:N	2.89	0.44
1:A:1228:MET:HB3	1:A:1247:PHE:CD2	2.53	0.44
2:B:388:TYR:HB3	2:B:667:THR:HG21	1.99	0.44
3:C:2:PRO:HA	11:K:53:ASP:HA	2.00	0.44
4:D:45:LYS:HA	4:D:48:ASN:HD21	1.82	0.44
10:J:36:ASP:OD1	10:J:46:ARG:NH2	2.51	0.44
2:B:256:ILE:HD12	2:B:256:ILE:H	1.82	0.44
2:B:265:GLN:N	2:B:265:GLN:OE1	2.50	0.44
2:B:799:SER:O	2:B:802:ASP:HB3	2.17	0.44
2:B:1162:LEU:HD22	2:B:1167:ILE:HD12	1.98	0.44
8:H:37:MET:SD	8:H:127:GLY:HA3	2.58	0.44
16:U:244:ASP:O	16:U:248:LYS:HG2	2.17	0.44
2:B:114:ARG:HH22	2:B:176:GLU:CD	2.20	0.44
5:E:171:PRO:HB2	5:E:207:ARG:HG2	2.00	0.44
6:F:64:ARG:HH21	7:G:61:PRO:HG3	1.82	0.44
16:U:41:VAL:HG13	16:U:187:PRO:HB3	1.98	0.44
16:U:100:LEU:HD22	16:U:126:LEU:HD21	2.00	0.44
1:A:117:LEU:HD21	1:A:236:LEU:HD21	1.99	0.43
1:A:617:PRO:HG2	1:A:618:TYR:CD2	2.53	0.43
2:B:1022:LEU:HD23	2:B:1022:LEU:H	1.82	0.43
8:H:10:PHE:CE2	8:H:32:SER:HB2	2.53	0.43
16:U:30:LYS:HB2	19:U:1000:ADP:N6	2.33	0.43
16:U:417:ALA:O	16:U:421:GLY:N	2.51	0.43
9:I:81:THR:HG23	9:I:96:PHE:CE1	2.53	0.43
16:U:316:THR:OG1	16:U:317:ILE:N	2.51	0.43
1:A:288:ASN:OD1	1:A:291:ARG:NH1	2.27	0.43
1:A:413:TYR:OH	1:A:476:ILE:HG13	2.19	0.43
1:A:571:ASP:N	1:A:571:ASP:OD1	2.48	0.43
1:A:723:ASN:HD21	9:I:109:ARG:HB3	1.83	0.43
1:A:867:SER:HB2	1:A:1414:ILE:HG23	2.00	0.43
1:A:922:PHE:HA	1:A:1052:ARG:HD3	2.00	0.43
2:B:199:LYS:NZ	2:B:394:ASP:OD1	2.47	0.43
2:B:844:ILE:H	2:B:844:ILE:HG13	1.60	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:24:GLU:HG2	3:C:228:ARG:HG3	2.00	0.43
4:D:106:GLU:HA	4:D:135:GLN:HE22	1.83	0.43
11:K:106:ARG:HA	11:K:109:ILE:HG22	2.00	0.43
16:U:79:LEU:HD12	16:U:79:LEU:H	1.82	0.43
16:U:433:HIS:CE1	16:U:437:PRO:HB3	2.53	0.43
1:A:102:LYS:HB2	1:A:102:LYS:HE2	1.83	0.43
2:B:119:THR:HG23	2:B:187:ILE:HD13	1.99	0.43
2:B:216:ALA:HB2	2:B:241:ALA:HA	1.99	0.43
2:B:251:ALA:HB3	2:B:254:GLN:NE2	2.33	0.43
16:U:165:TRP:O	16:U:342:GLY:N	2.51	0.43
3:C:173:HIS:CD2	3:C:175:LYS:HG2	2.54	0.43
8:H:118:TYR:OH	8:H:123:MET:SD	2.66	0.43
16:U:49:PHE:HB3	16:U:215:ILE:HA	2.00	0.43
16:U:90:LEU:HD13	16:U:95:VAL:HG11	2.00	0.43
1:A:610:PRO:HG2	1:A:613:GLU:HG3	2.00	0.43
8:H:27:ARG:HH11	8:H:40:ILE:CG2	2.32	0.43
8:H:93:TYR:OH	8:H:140:ARG:NE	2.37	0.43
16:U:38:THR:O	16:U:42:VAL:N	2.41	0.43
16:U:294:LYS:H	16:U:294:LYS:HD2	1.84	0.43
1:A:99:PHE:HB3	1:A:248:MET:HE3	2.01	0.43
1:A:859:TYR:OH	1:A:1433:GLU:OE2	2.34	0.43
1:A:1045:LEU:O	1:A:1049:LEU:HB2	2.18	0.43
2:B:19:PRO:C	2:B:21:LEU:H	2.21	0.43
2:B:95:LYS:HE3	2:B:162:LEU:HD23	2.00	0.43
2:B:721:ARG:HA	2:B:721:ARG:HD3	1.71	0.43
2:B:1136:GLU:OE1	2:B:1138:ARG:HG2	2.19	0.43
12:L:28:ILE:HD13	12:L:34:ILE:HD13	1.99	0.43
16:U:221:PHE:HB2	16:U:222:ARG:H	1.62	0.43
1:A:1189:ASP:OD1	1:A:1192:TRP:NE1	2.52	0.43
5:E:17:ILE:HD13	5:E:17:ILE:HA	1.75	0.43
12:L:35:ARG:HD3	12:L:42:ARG:NH1	2.34	0.43
15:T:17:DT:H2'	15:T:18:DG:H8	1.84	0.43
1:A:1155:LYS:HA	1:A:1158:LEU:HD23	2.01	0.43
2:B:796:MET:HB3	2:B:796:MET:HE2	1.88	0.43
2:B:1111:SER:O	2:B:1113:PRO:HD3	2.19	0.43
1:A:72:GLN:N	1:A:72:GLN:OE1	2.52	0.43
1:A:522:PRO:HB2	1:A:662:HIS:HB2	1.99	0.43
1:A:740:GLN:CD	1:A:743:ARG:HH12	2.20	0.43
2:B:154:ILE:HD13	2:B:154:ILE:HA	1.90	0.43
3:C:37:VAL:O	3:C:42:VAL:HG23	2.19	0.43
3:C:128:ILE:O	3:C:130:VAL:N	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:74:VAL:HG13	5:E:103:LEU:HB2	2.01	0.43
1:A:564:LEU:HD21	1:A:594:LEU:HD12	2.00	0.42
1:A:1361:ASP:N	1:A:1361:ASP:OD1	2.48	0.42
1:A:1401:LEU:O	1:A:1404:THR:HG22	2.19	0.42
2:B:245:GLN:NE2	2:B:255:ARG:HD3	2.33	0.42
15:T:5:DA:C6	15:T:6:DG:C5	3.07	0.42
1:A:902:GLU:CD	1:A:982:ASN:HB2	2.40	0.42
2:B:911:LEU:HD12	12:L:42:ARG:HD2	2.02	0.42
8:H:82:PRO:O	8:H:83:SER:OG	2.35	0.42
9:I:17:CYS:SG	9:I:18:GLN:N	2.92	0.42
16:U:261:CYS:SG	16:U:305:TRP:NE1	2.92	0.42
1:A:202:TRP:N	1:A:212:LYS:O	2.52	0.42
1:A:461:GLN:O	1:A:463:THR:N	2.52	0.42
1:A:462:PRO:HD3	15:T:14:DG:H21	1.85	0.42
2:B:110:PRO:HG2	2:B:163:LEU:HD11	2.00	0.42
4:D:63:LYS:HB3	4:D:63:LYS:HE3	1.52	0.42
7:G:49:THR:N	7:G:73:LYS:O	2.52	0.42
9:I:26:PRO:HG3	9:I:53:ILE:HG23	2.01	0.42
1:A:100:LEU:O	1:A:103:THR:OG1	2.30	0.42
1:A:496:PHE:HD2	2:B:791:GLU:HB2	1.85	0.42
2:B:715:ASP:OD1	2:B:715:ASP:N	2.37	0.42
8:H:8:ASP:OD2	8:H:32:SER:OG	2.23	0.42
1:A:580:LEU:HD13	8:H:91:VAL:HG22	2.00	0.42
1:A:1301:ILE:HG12	1:A:1345:ARG:NH1	2.34	0.42
2:B:260:LEU:HD22	2:B:347:MET:HG3	2.01	0.42
7:G:8:GLU:OE1	7:G:71:LYS:HG2	2.20	0.42
16:U:27:ASP:OD1	16:U:60:LEU:HD11	2.19	0.42
1:A:18:ILE:HD11	2:B:1149:VAL:HG21	2.01	0.42
1:A:533:PRO:HG2	1:A:647:THR:HA	2.02	0.42
1:A:1435:THR:OG1	1:A:1436:VAL:N	2.50	0.42
6:F:65:VAL:HG21	6:F:120:VAL:HG21	2.02	0.42
7:G:91:GLN:HB3	7:G:98:PHE:HD2	1.84	0.42
16:U:367:ASP:O	16:U:371:VAL:HG23	2.19	0.42
1:A:95:PHE:CZ	1:A:198:LEU:HD22	2.54	0.42
1:A:340:LYS:HG3	1:A:1436:VAL:HG21	2.00	0.42
1:A:962:ASP:HB3	1:A:1043:ILE:HG12	2.00	0.42
4:D:129:GLN:HA	4:D:132:ASP:OD2	2.20	0.42
8:H:37:MET:HE2	8:H:37:MET:HB2	1.73	0.42
8:H:45:ILE:HD13	8:H:45:ILE:HA	1.78	0.42
9:I:27:LYS:HE2	9:I:27:LYS:HB3	1.94	0.42
11:K:23:LYS:NZ	11:K:24:ASP:O	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:64:PRO:HD2	11:K:70:LYS:O	2.19	0.42
11:K:65:HIS:HE1	11:K:67:LEU:HD12	1.85	0.42
15:T:15:DC:H2'	15:T:16:DC:H6	1.84	0.42
1:A:108:ARG:HD2	1:A:145:TYR:HE1	1.85	0.42
1:A:112:PHE:HD1	1:A:113:PHE:N	2.18	0.42
1:A:372:ASN:HB2	11:K:65:HIS:HD2	1.85	0.42
1:A:1024:ASN:O	1:A:1030:SER:OG	2.22	0.42
2:B:545:LEU:HB3	2:B:550:MET:SD	2.60	0.42
11:K:11:LEU:HD23	11:K:11:LEU:HA	1.93	0.42
1:A:1443:ALA:HB2	2:B:1167:ILE:HG23	2.02	0.42
4:D:128:GLN:O	4:D:131:LEU:HG	2.20	0.42
16:U:79:LEU:HB2	16:U:82:LEU:CB	2.49	0.42
16:U:541:ARG:HG3	16:U:542:ILE:HG13	2.02	0.42
1:A:344:LYS:HD2	1:A:344:LYS:HA	1.86	0.42
1:A:609:HIS:HA	1:A:626:THR:HG21	2.01	0.42
2:B:33:TYR:CZ	2:B:37:LYS:HD2	2.55	0.42
2:B:144:HIS:ND1	2:B:431:LEU:HB2	2.34	0.42
2:B:567:ILE:O	2:B:574:VAL:HG12	2.20	0.42
2:B:752:TYR:HH	3:C:60:HIS:CE1	2.34	0.42
3:C:106:ARG:NH1	3:C:108:ASN:OD1	2.53	0.42
16:U:58:LYS:HA	16:U:61:CYS:SG	2.60	0.42
16:U:231:PHE:HB2	16:U:234:LEU:HD13	2.01	0.42
1:A:1218:ARG:NE	1:A:1255:LEU:HD11	2.36	0.41
2:B:198:GLU:HB2	2:B:488:PRO:HD3	2.02	0.41
2:B:854:ILE:O	2:B:907:VAL:HG21	2.20	0.41
5:E:126:ILE:H	5:E:126:ILE:HG12	1.53	0.41
16:U:161:CYS:SG	16:U:162:VAL:N	2.93	0.41
16:U:196:THR:O	16:U:199:VAL:N	2.53	0.41
16:U:239:TYR:O	16:U:242:LEU:HG	2.20	0.41
16:U:602:LEU:HA	16:U:605:VAL:HG12	2.02	0.41
1:A:802:PHE:CZ	2:B:504:THR:HA	2.54	0.41
1:A:1471:PHE:CE2	6:F:64:ARG:HD3	2.55	0.41
2:B:348:LEU:O	2:B:361:LYS:HE3	2.20	0.41
2:B:836:THR:O	2:B:888:THR:OG1	2.38	0.41
2:B:910:THR:OG1	2:B:911:LEU:N	2.53	0.41
3:C:2:PRO:HB3	11:K:54:PRO:HD2	2.03	0.41
3:C:52:ILE:HD12	3:C:61:ASP:HB3	2.02	0.41
4:D:87:LEU:HD12	4:D:87:LEU:HA	1.87	0.41
11:K:100:LEU:O	11:K:104:ARG:HD2	2.20	0.41
16:U:66:ALA:HA	16:U:73:THR:OG1	2.20	0.41
1:A:589:LYS:NZ	1:A:625:ASP:OD1	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1068:LEU:O	1:A:1072:ILE:HG12	2.20	0.41
1:A:1436:VAL:HG13	2:B:1165:MET:HE1	2.01	0.41
2:B:319:ASN:OD1	2:B:335:ARG:NH1	2.54	0.41
2:B:717:ASN:ND2	2:B:977:THR:HG23	2.35	0.41
2:B:783:ALA:HB2	2:B:1041:ILE:CG2	2.50	0.41
3:C:27:ASP:OD2	11:K:48:SER:OG	2.38	0.41
5:E:56:THR:OG1	5:E:78:GLU:OE2	2.37	0.41
6:F:61:GLU:CD	6:F:108:ARG:HH21	2.23	0.41
8:H:98:ARG:HG2	8:H:115:TYR:CD1	2.55	0.41
13:N:20:DG:C8	13:N:21:DT:H72	2.55	0.41
1:A:29:ASP:CG	1:A:33:ARG:HE	2.22	0.41
1:A:283:ILE:HG12	1:A:313:HIS:HB3	2.01	0.41
1:A:992:LYS:HD3	1:A:992:LYS:HA	1.85	0.41
1:A:1451:MET:SD	1:A:1456:GLU:HB3	2.60	0.41
1:A:1468:THR:H	6:F:60:TYR:HB3	1.85	0.41
2:B:386:ASP:OD1	13:N:16:DG:N2	2.51	0.41
2:B:819:SER:H	2:B:827:GLU:HB2	1.86	0.41
16:U:30:LYS:HB3	16:U:34:GLN:HG3	2.02	0.41
16:U:174:LEU:O	16:U:176:LEU:N	2.53	0.41
16:U:221:PHE:HE2	16:U:425:PRO:HB3	1.85	0.41
1:A:334:ARG:HA	2:B:460:HIS:CE1	2.55	0.41
1:A:456:VAL:O	1:A:471:GLY:HA2	2.20	0.41
1:A:859:TYR:O	1:A:863:ARG:HG3	2.20	0.41
2:B:156:LEU:HG	2:B:184:TYR:CE2	2.55	0.41
2:B:380:ARG:HD3	2:B:609:GLU:CD	2.41	0.41
2:B:539:SER:N	2:B:540:PRO:HD2	2.35	0.41
2:B:776:ILE:HG22	2:B:806:PHE:CZ	2.56	0.41
7:G:108:ILE:HD11	7:G:145:LEU:HD22	2.03	0.41
1:A:368:THR:HG23	1:A:369:PRO:HD2	2.03	0.41
1:A:548:PHE:O	1:A:553:VAL:HG11	2.20	0.41
2:B:626:LEU:HD23	2:B:662:VAL:HG22	2.03	0.41
2:B:1032:PHE:O	3:C:32:ASN:ND2	2.54	0.41
10:J:8:PHE:HB2	10:J:47:ARG:HH22	1.86	0.41
12:L:35:ARG:CZ	12:L:40:GLY:HA2	2.51	0.41
16:U:77[A]:SER:O	16:U:83:ILE:HG13	2.21	0.41
16:U:416:ILE:HD12	16:U:416:ILE:HA	1.94	0.41
1:A:99:PHE:O	1:A:103:THR:HG23	2.20	0.41
1:A:404:GLU:OE2	1:A:407:ARG:NH2	2.32	0.41
1:A:943:LEU:HD23	1:A:943:LEU:HA	1.70	0.41
1:A:1178:ASP:HB3	1:A:1260:ARG:HH21	1.86	0.41
1:A:1403:ASP:O	1:A:1407:CYS:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:409:LYS:HE2	2:B:409:LYS:HB2	1.79	0.41
3:C:34:ILE:HG22	3:C:38:PHE:CZ	2.56	0.41
3:C:77:ASP:OD2	3:C:126:ARG:NH1	2.43	0.41
4:D:110:GLU:OE1	4:D:111:SER:N	2.53	0.41
16:U:55:GLY:N	19:U:1000:ADP:O3B	2.47	0.41
16:U:326:ALA:HA	16:U:352:ARG:N	2.33	0.41
16:U:438:THR:HG22	16:U:441:ARG:HH21	1.86	0.41
1:A:41:ILE:HG23	1:A:55:GLY:O	2.20	0.41
1:A:551:ARG:NH2	8:H:122:LEU:HD12	2.36	0.41
1:A:620:HIS:HB2	8:H:115:TYR:CE2	2.55	0.41
1:A:986:MET:HE1	1:A:1075:LYS:HG3	2.03	0.41
1:A:1282:ASP:OD1	1:A:1283:VAL:N	2.53	0.41
2:B:16:GLU:O	2:B:636:LYS:HD2	2.21	0.41
2:B:200:MET:HB2	13:N:15:DT:O2	2.20	0.41
2:B:987:GLY:C	2:B:1045:PRO:HG2	2.41	0.41
4:D:135:GLN:HA	4:D:138:ARG:HG2	2.02	0.41
6:F:64:ARG:NH2	7:G:61:PRO:HG3	2.36	0.41
15:T:9:DC:OP2	15:T:9:DC:H2'	2.21	0.41
1:A:470:MET:HG2	1:A:524:MET:HE3	2.02	0.41
1:A:530:SER:O	1:A:532:ARG:HG3	2.20	0.41
1:A:887:VAL:HG12	1:A:888:GLN:HG3	2.02	0.41
1:A:1141:VAL:HA	1:A:1357:THR:HG23	2.02	0.41
2:B:251:ALA:HB3	2:B:254:GLN:HE22	1.86	0.41
3:C:159:LEU:HD11	3:C:161:LEU:HD23	2.03	0.41
5:E:7:THR:OG1	5:E:48:PRO:HD3	2.21	0.41
5:E:56:THR:HG22	5:E:57:ASP:H	1.86	0.41
8:H:91:VAL:HB	8:H:144:LEU:HD12	2.03	0.41
9:I:54:TYR:CE2	9:I:56:ASN:HB2	2.56	0.41
9:I:72:VAL:HG22	9:I:78:LEU:HD11	2.01	0.41
15:T:5:DA:H2'	15:T:6:DG:O4'	2.20	0.41
16:U:78:PRO:O	16:U:79:LEU:C	2.59	0.41
16:U:234:LEU:HD21	16:U:446:ALA:HB3	2.03	0.41
16:U:349:ARG:C	16:U:352:ARG:HH12	2.25	0.41
1:A:369:PRO:HD3	1:A:496:PHE:CG	2.55	0.41
1:A:752:THR:HB	1:A:786:ALA:HB1	2.03	0.41
1:A:948:ILE:HD12	1:A:1007:ILE:HG13	2.02	0.41
2:B:491:ARG:HA	2:B:491:ARG:HD3	1.91	0.41
2:B:869:LYS:HG2	2:B:892:CYS:SG	2.61	0.41
5:E:185:ILE:CG2	5:E:189:GLN:HB2	2.51	0.41
9:I:29:ASP:O	9:I:33:ARG:N	2.49	0.41
16:U:179:LEU:O	16:U:183:LEU:HG	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:GLU:OE2	2:B:1058:LYS:HB3	2.21	0.40
1:A:663:ASP:OD1	1:A:666:ARG:NH2	2.52	0.40
1:A:693:ILE:HG12	1:A:828:LEU:HD21	2.02	0.40
1:A:1130:ILE:HG21	1:A:1411:LEU:HG	2.02	0.40
5:E:7:THR:HG21	5:E:41:LYS:HG2	2.02	0.40
8:H:130:ASN:OD1	8:H:131:ASN:N	2.54	0.40
16:U:65:PRO:O	16:U:69:ALA:N	2.54	0.40
16:U:266:CYS:HB3	16:U:334:TRP:HB3	2.03	0.40
16:U:526:VAL:HA	16:U:527:PRO:HD3	1.94	0.40
1:A:279:LYS:HD2	1:A:279:LYS:HA	1.92	0.40
1:A:757:GLN:NE2	1:A:781:ILE:HD12	2.36	0.40
2:B:28:ILE:HD13	2:B:28:ILE:HA	1.96	0.40
2:B:196:ALA:HA	2:B:394:ASP:O	2.21	0.40
7:G:110:ARG:NH2	7:G:113:ILE:HG13	2.36	0.40
16:U:17:ARG:HD3	16:U:29:PHE:CE1	2.56	0.40
16:U:217:LYS:NZ	16:U:221:PHE:HA	2.35	0.40
1:A:21:VAL:HA	2:B:1170:ARG:O	2.21	0.40
1:A:710:LYS:O	1:A:713:VAL:HG12	2.20	0.40
2:B:643:LEU:O	2:B:646:ARG:HB2	2.22	0.40
2:B:643:LEU:HD11	2:B:656:LEU:HD22	2.03	0.40
2:B:728:MET:SD	2:B:942:LYS:HE3	2.60	0.40
2:B:738:THR:H	2:B:738:THR:HG1	1.66	0.40
2:B:1151:MET:HE2	2:B:1155:CYS:HB3	2.02	0.40
3:C:189:ASP:OD1	3:C:189:ASP:N	2.41	0.40
4:D:31:THR:HB	4:D:94:LYS:HB2	2.03	0.40
16:U:365:ARG:HE	16:U:368:ARG:NH2	2.20	0.40
16:U:507:PHE:O	16:U:510:LYS:HG2	2.21	0.40
16:U:532:CYS:HA	16:U:533:PRO:HD3	1.91	0.40
1:A:137:PRO:HB2	1:A:1445:HIS:HB3	2.03	0.40
1:A:187:TYR:OH	16:U:280:SER:HB3	2.21	0.40
1:A:534:VAL:HG23	1:A:535:MET:HG3	2.02	0.40
1:A:678:ASN:HA	1:A:681:LEU:HD12	2.03	0.40
2:B:712:PRO:O	2:B:939:HIS:HE1	2.05	0.40
2:B:737:ILE:HD12	2:B:737:ILE:HA	2.00	0.40
2:B:911:LEU:HA	2:B:916:TYR:O	2.22	0.40
2:B:1088:GLU:HA	2:B:1091:ARG:HG2	2.03	0.40
11:K:61:TYR:HB2	11:K:73:ILE:HG12	2.04	0.40
16:U:175:ARG:O	16:U:179:LEU:N	2.41	0.40
16:U:353:ASP:OD1	16:U:354:GLY:N	2.54	0.40
1:A:33:ARG:HH11	2:B:1139:GLY:HA2	1.85	0.40
2:B:802:ASP:OD1	3:C:173:HIS:CD2	2.75	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:55:ARG:CZ	5:E:107:GLN:HE22	2.34	0.40
5:E:131:LEU:HD23	5:E:131:LEU:HA	1.92	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	1418/1970 (72%)	1323 (93%)	94 (7%)	1 (0%)	48	78
2	B	1128/1174 (96%)	1052 (93%)	73 (6%)	3 (0%)	37	67
3	C	253/275 (92%)	238 (94%)	15 (6%)	0	100	100
4	D	126/142 (89%)	118 (94%)	8 (6%)	0	100	100
5	E	207/210 (99%)	193 (93%)	13 (6%)	1 (0%)	25	57
6	F	80/127 (63%)	78 (98%)	2 (2%)	0	100	100
7	G	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
8	H	146/150 (97%)	134 (92%)	11 (8%)	1 (1%)	19	51
9	I	112/125 (90%)	104 (93%)	7 (6%)	1 (1%)	14	47
10	J	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
11	K	113/117 (97%)	107 (95%)	6 (5%)	0	100	100
12	L	42/58 (72%)	36 (86%)	6 (14%)	0	100	100
16	U	453/991 (46%)	397 (88%)	50 (11%)	6 (1%)	10	40
All	All	4312/5578 (77%)	4002 (93%)	297 (7%)	13 (0%)	38	67

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	581	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	46	ASP
8	H	105	SER
16	U	78	PRO
16	U	328	VAL
2	B	550	MET
16	U	79	LEU
16	U	171	PRO
16	U	175	ARG
2	B	355	ASP
16	U	359	CYS
9	I	116	ALA
2	B	230	ARG

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	1258/1748 (72%)	1206 (96%)	52 (4%)	26	52
2	B	993/1028 (97%)	962 (97%)	31 (3%)	35	57
3	C	234/252 (93%)	224 (96%)	10 (4%)	25	50
4	D	106/126 (84%)	102 (96%)	4 (4%)	28	53
5	E	189/192 (98%)	177 (94%)	12 (6%)	15	42
6	F	71/111 (64%)	68 (96%)	3 (4%)	25	51
7	G	147/153 (96%)	137 (93%)	10 (7%)	13	40
8	H	129/131 (98%)	121 (94%)	8 (6%)	15	42
9	I	103/112 (92%)	96 (93%)	7 (7%)	13	40
10	J	56/56 (100%)	55 (98%)	1 (2%)	54	71
11	K	104/106 (98%)	102 (98%)	2 (2%)	52	70
12	L	41/55 (74%)	41 (100%)	0	100	100
16	U	391/820 (48%)	354 (90%)	37 (10%)	7	29
All	All	3822/4890 (78%)	3645 (95%)	177 (5%)	25	49

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	VAL
1	A	65	ILE
1	A	70	ARG
1	A	85	PHE
1	A	94	VAL
1	A	112	PHE
1	A	117	LEU
1	A	241	ARG
1	A	311	GLN
1	A	316	THR
1	A	423	ASN
1	A	427	ILE
1	A	458	PHE
1	A	463	THR
1	A	465	HIS
1	A	481	THR
1	A	499	ASP
1	A	541	THR
1	A	549	THR
1	A	581	LYS
1	A	608	THR
1	A	621	ILE
1	A	647	THR
1	A	712	ASP
1	A	724	GLU
1	A	805	ARG
1	A	839	HIS
1	A	852	VAL
1	A	883	ILE
1	A	896	LEU
1	A	906	LEU
1	A	925	THR
1	A	943	LEU
1	A	952	LEU
1	A	999	ARG
1	A	1007	ILE
1	A	1026	ASP
1	A	1049	LEU
1	A	1158	LEU
1	A	1170	THR
1	A	1178	ASP
1	A	1186	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1198	GLU
1	A	1223	ASP
1	A	1259	ILE
1	A	1314	THR
1	A	1329	LYS
1	A	1364	GLU
1	A	1374	VAL
1	A	1400	LEU
1	A	1408	ARG
1	A	1423	ASP
2	B	67	LEU
2	B	93	LEU
2	B	111	ASN
2	B	132	VAL
2	B	193	VAL
2	B	225	LEU
2	B	234	THR
2	B	254	GLN
2	B	257	VAL
2	B	300	MET
2	B	422	PHE
2	B	442	ASP
2	B	472	ARG
2	B	489	ILE
2	B	552	ASN
2	B	592	ARG
2	B	668	LEU
2	B	725	GLN
2	B	728	MET
2	B	746	THR
2	B	805	PHE
2	B	809	VAL
2	B	863	ASP
2	B	891	ASP
2	B	909	VAL
2	B	957	THR
2	B	1022	LEU
2	B	1048	TYR
2	B	1059	ILE
2	B	1134	THR
2	B	1140	CYS
3	C	5	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	30	VAL
3	C	35	ARG
3	C	44	ILE
3	C	63	PHE
3	C	66	HIS
3	C	94	CYS
3	C	105	VAL
3	C	169	PHE
3	C	240	ARG
4	D	62	MET
4	D	63	LYS
4	D	87	LEU
4	D	110	GLU
5	E	34	ASP
5	E	55	ARG
5	E	57	ASP
5	E	64	HIS
5	E	73	PHE
5	E	86	THR
5	E	99	ILE
5	E	121	MET
5	E	126	ILE
5	E	173	ILE
5	E	177	ASP
5	E	205	THR
6	F	53	THR
6	F	54	THR
6	F	124	ILE
7	G	3	TYR
7	G	4	HIS
7	G	7	LEU
7	G	48	VAL
7	G	70	VAL
7	G	76	VAL
7	G	84	VAL
7	G	99	THR
7	G	140	ASP
7	G	167	TYR
8	H	23	ASP
8	H	50	VAL
8	H	72	ASP
8	H	81	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	91	VAL
8	H	96	VAL
8	H	128	ASP
8	H	144	LEU
9	I	27	LYS
9	I	36	LEU
9	I	66	THR
9	I	72	VAL
9	I	103	ARG
9	I	105	GLU
9	I	110	LEU
10	J	47	ARG
11	K	50	LEU
11	K	109	ILE
16	U	16	VAL
16	U	17	ARG
16	U	21	LYS
16	U	24	PHE
16	U	29	PHE
16	U	34	GLN
16	U	48	VAL
16	U	49	PHE
16	U	78	PRO
16	U	89	HIS
16	U	160	HIS
16	U	164	GLN
16	U	168	ASP
16	U	169	PHE
16	U	170	ARG
16	U	173	TYR
16	U	174	LEU
16	U	175	ARG
16	U	180	ARG
16	U	182	ARG
16	U	196	THR
16	U	202	ASP
16	U	217	LYS
16	U	218	THR
16	U	221	PHE
16	U	264	VAL
16	U	274	GLN
16	U	275	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	U	282	ARG
16	U	287	LYS
16	U	340	MET
16	U	376	ARG
16	U	396	ILE
16	U	418	LYS
16	U	431	CYS
16	U	553	CYS
16	U	588	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	GLN
1	A	372	ASN
1	A	472	HIS
1	A	601	ASN
1	A	989	ASN
1	A	1190	GLN
1	A	1194	ASN
2	B	245	GLN
2	B	254	GLN
2	B	468	GLN
2	B	525	ASN
2	B	717	ASN
2	B	939	HIS
2	B	948	GLN
2	B	980	HIS
2	B	1068	GLN
3	C	173	HIS
4	D	135	GLN
5	E	132	GLN
11	K	113	GLN
16	U	84	GLN
16	U	86	GLN
16	U	164	GLN
16	U	198	GLN
16	U	230	GLN
16	U	303	ASN
16	U	327	ASN
16	U	333	HIS
16	U	513	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	U	564	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	10/20 (50%)	2 (20%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	11	A
14	P	13	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
19	ADP	U	1000	-	24,29,29	3.29	8 (33%)	29,45,45	2.16	3 (10%)

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
19	ADP	U	1000	-	-	8/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	U	1000	ADP	C3'-C4'	-8.66	1.31	1.53
19	U	1000	ADP	O4'-C4'	7.64	1.62	1.45
19	U	1000	ADP	O4'-C1'	-7.50	1.31	1.40
19	U	1000	ADP	PA-O3A	5.25	1.65	1.59
19	U	1000	ADP	C6-N6	3.19	1.45	1.34
19	U	1000	ADP	O3'-C3'	2.80	1.49	1.43
19	U	1000	ADP	O2'-C2'	-2.73	1.36	1.43
19	U	1000	ADP	C2-N3	2.14	1.35	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	U	1000	ADP	C1'-N9-C4	8.42	141.43	126.64
19	U	1000	ADP	N3-C2-N1	-6.52	119.82	128.67
19	U	1000	ADP	C4'-O4'-C1'	-2.16	107.94	109.92

There are no chirality outliers.

All (8) torsion outliers are listed below:

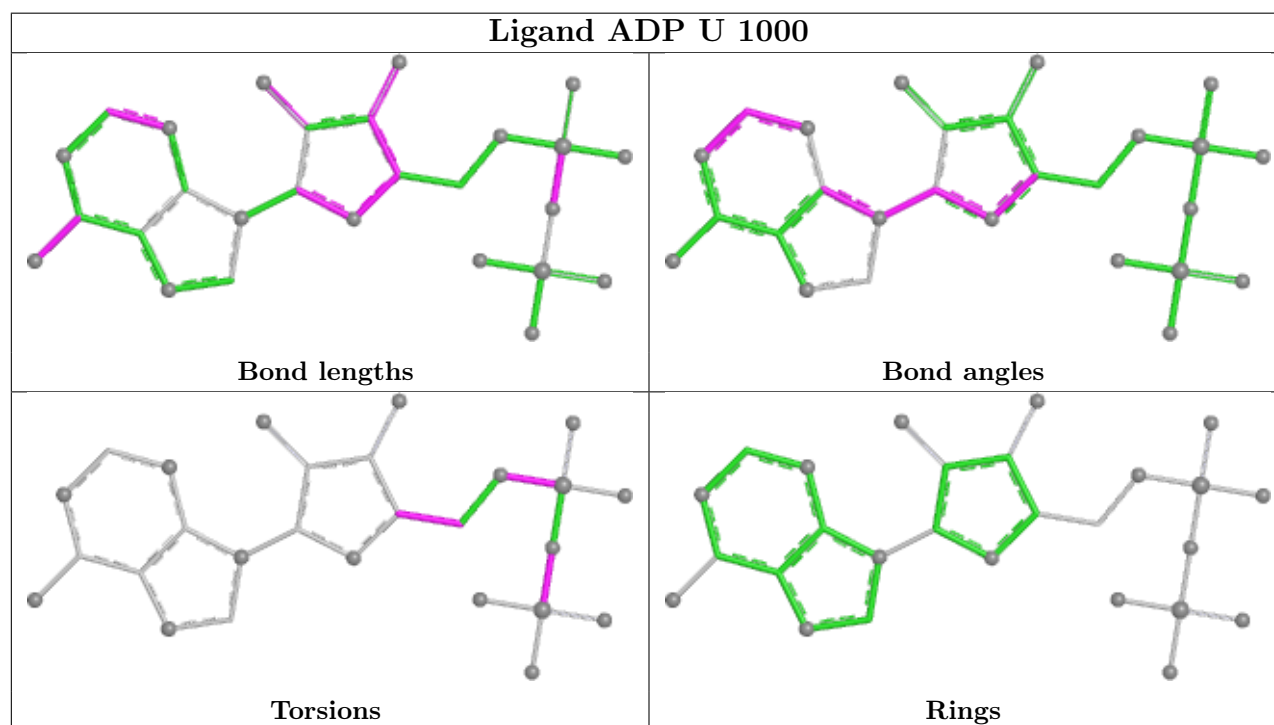
Mol	Chain	Res	Type	Atoms
19	U	1000	ADP	PA-O3A-PB-O2B
19	U	1000	ADP	PA-O3A-PB-O3B
19	U	1000	ADP	C5'-O5'-PA-O1A
19	U	1000	ADP	C5'-O5'-PA-O2A
19	U	1000	ADP	O4'-C4'-C5'-O5'
19	U	1000	ADP	C3'-C4'-C5'-O5'
19	U	1000	ADP	C5'-O5'-PA-O3A
19	U	1000	ADP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	U	1000	ADP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

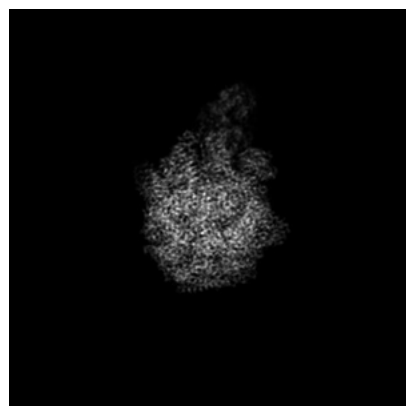
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48076. These allow visual inspection of the internal detail of the map and identification of artifacts.

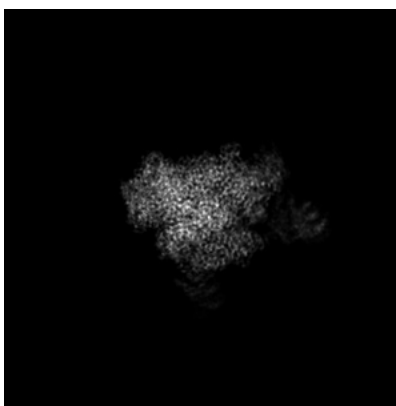
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

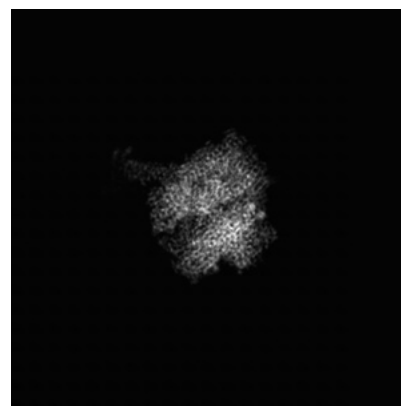
6.1.1 Primary map



X

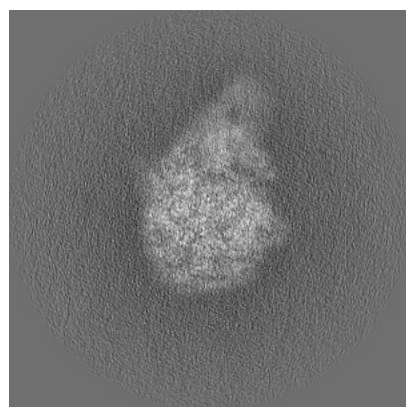


Y

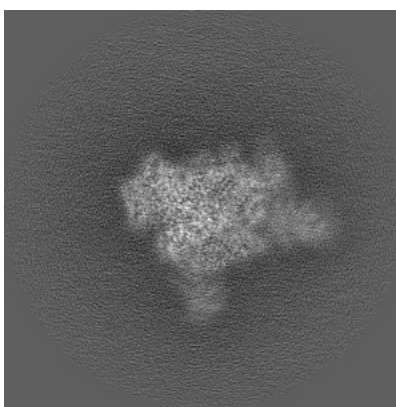


Z

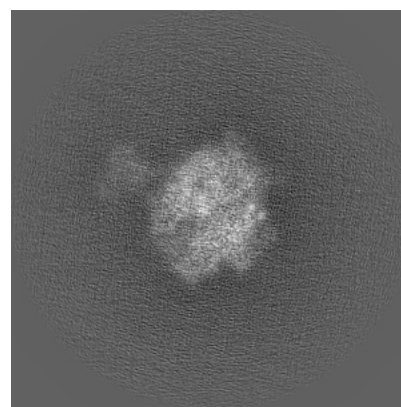
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160

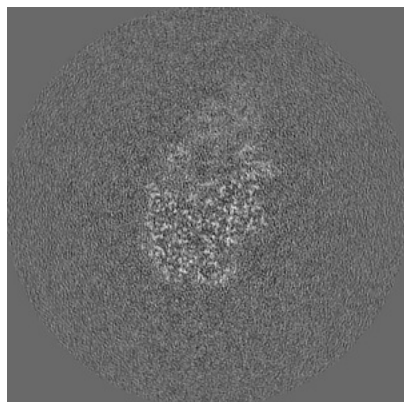


Y Index: 160

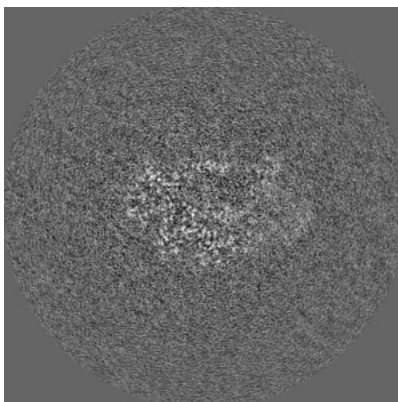


Z Index: 160

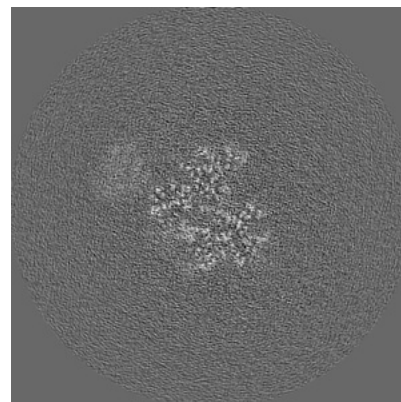
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

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: 165

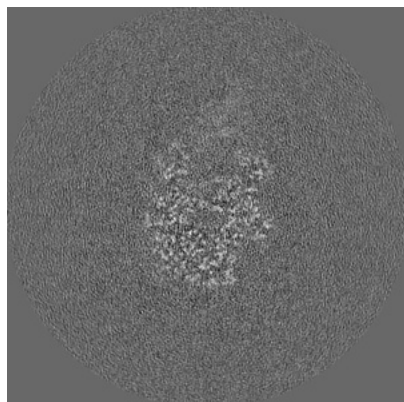


Y Index: 134

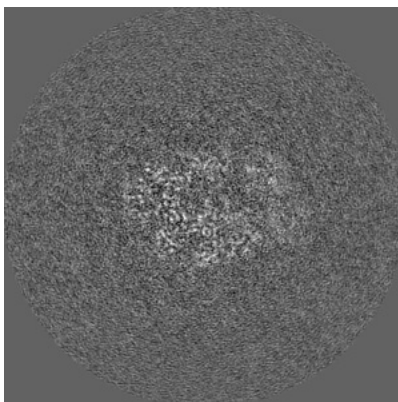


Z Index: 157

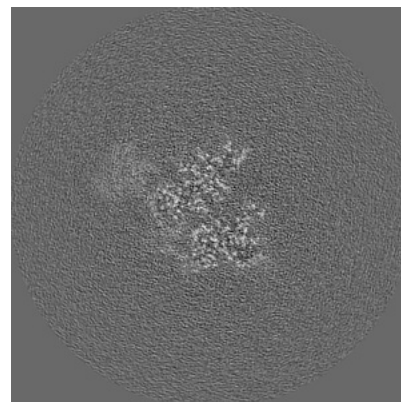
6.3.2 Raw map



X Index: 165



Y Index: 159

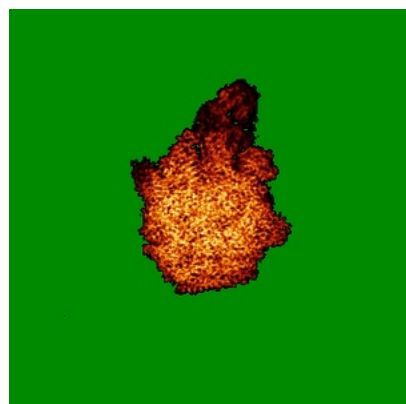


Z Index: 156

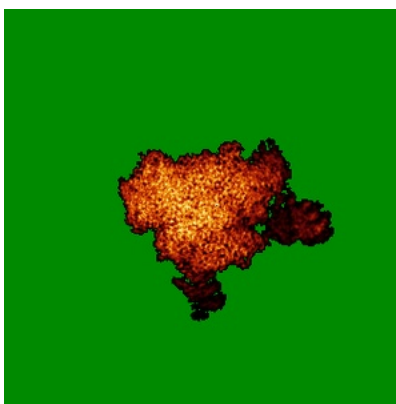
The images above show the largest variance slices of the map in three orthogonal directions.

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

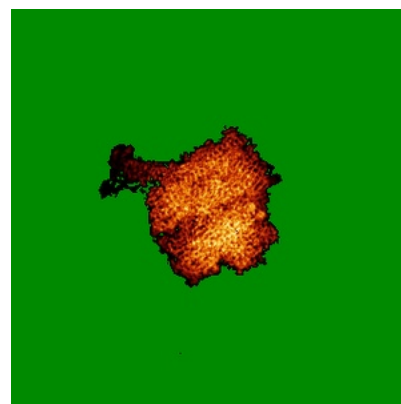
6.4.1 Primary map



X

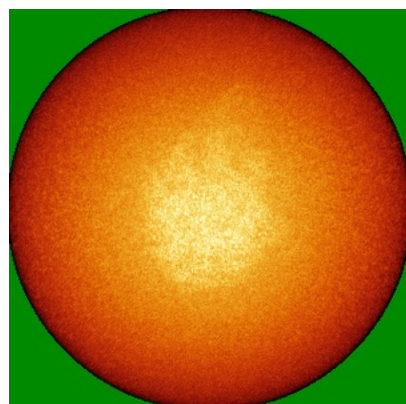


Y

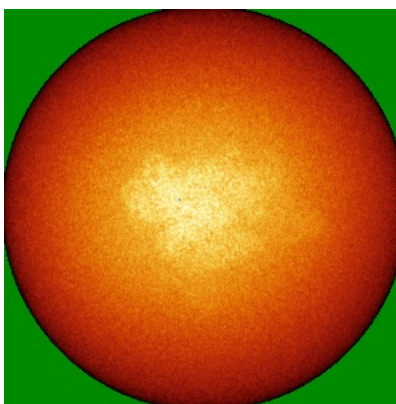


Z

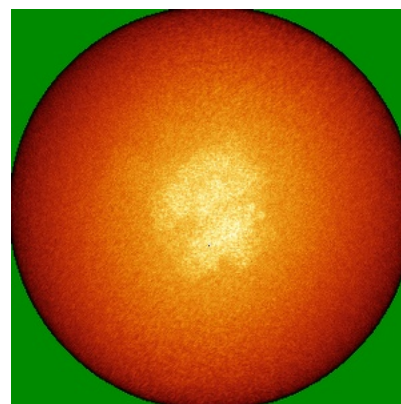
6.4.2 Raw map



X



Y

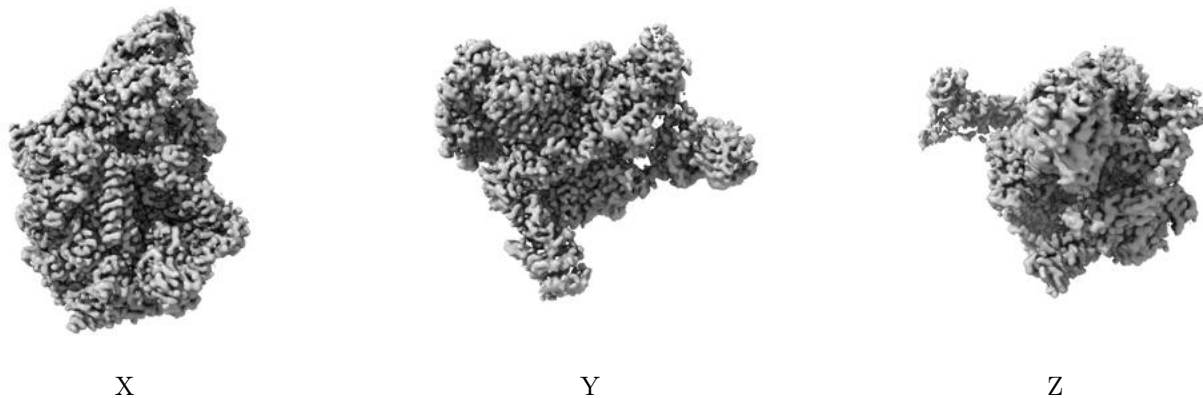


Z

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

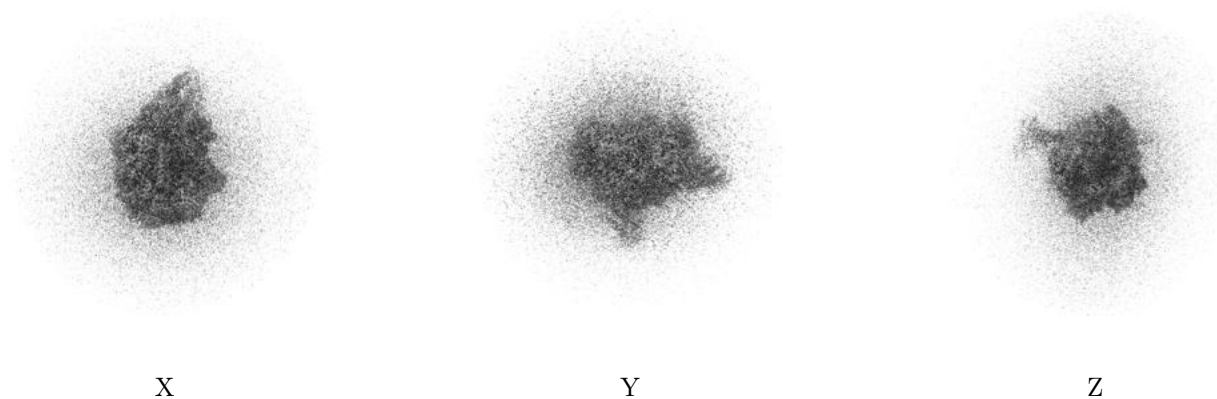
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

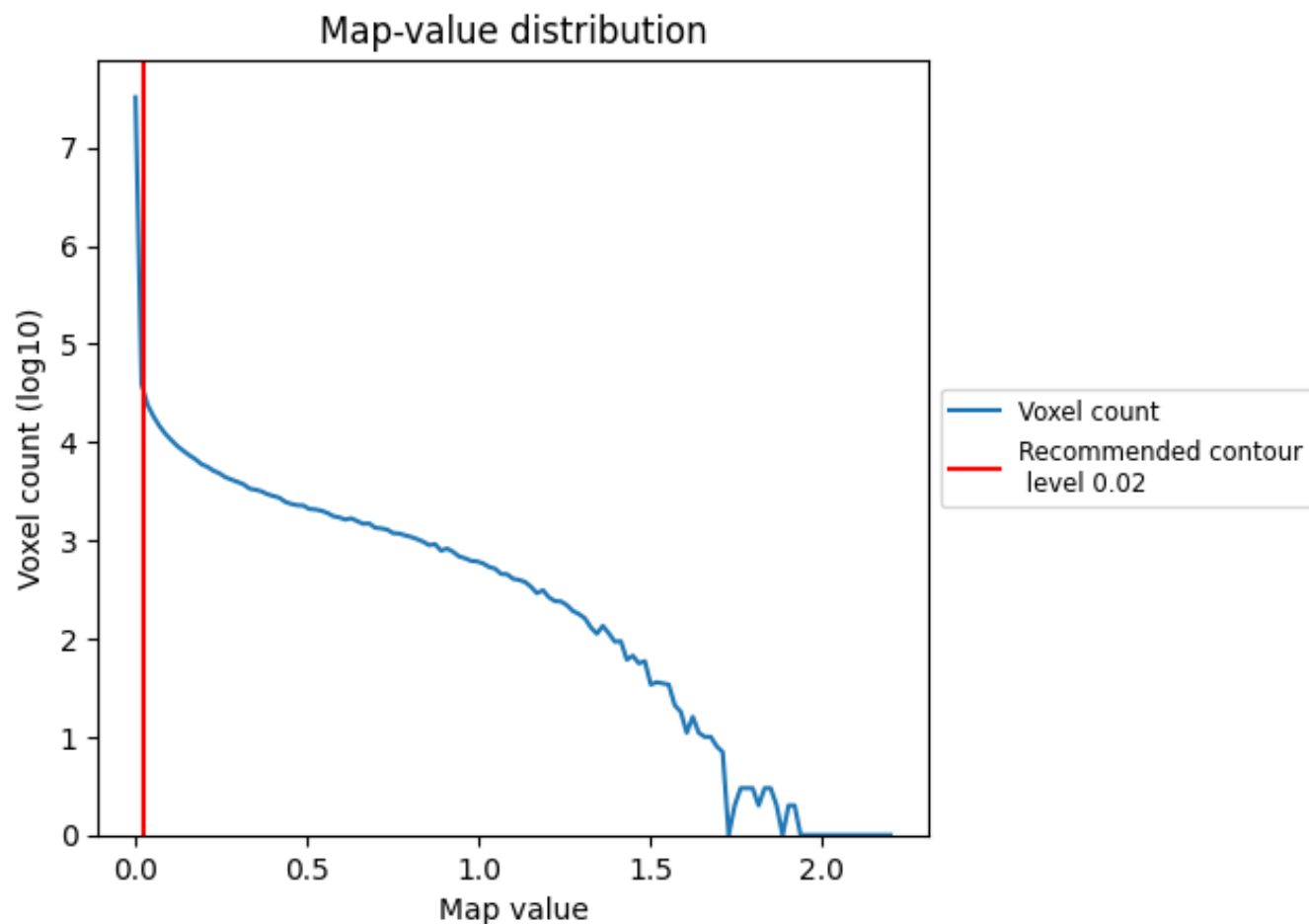
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

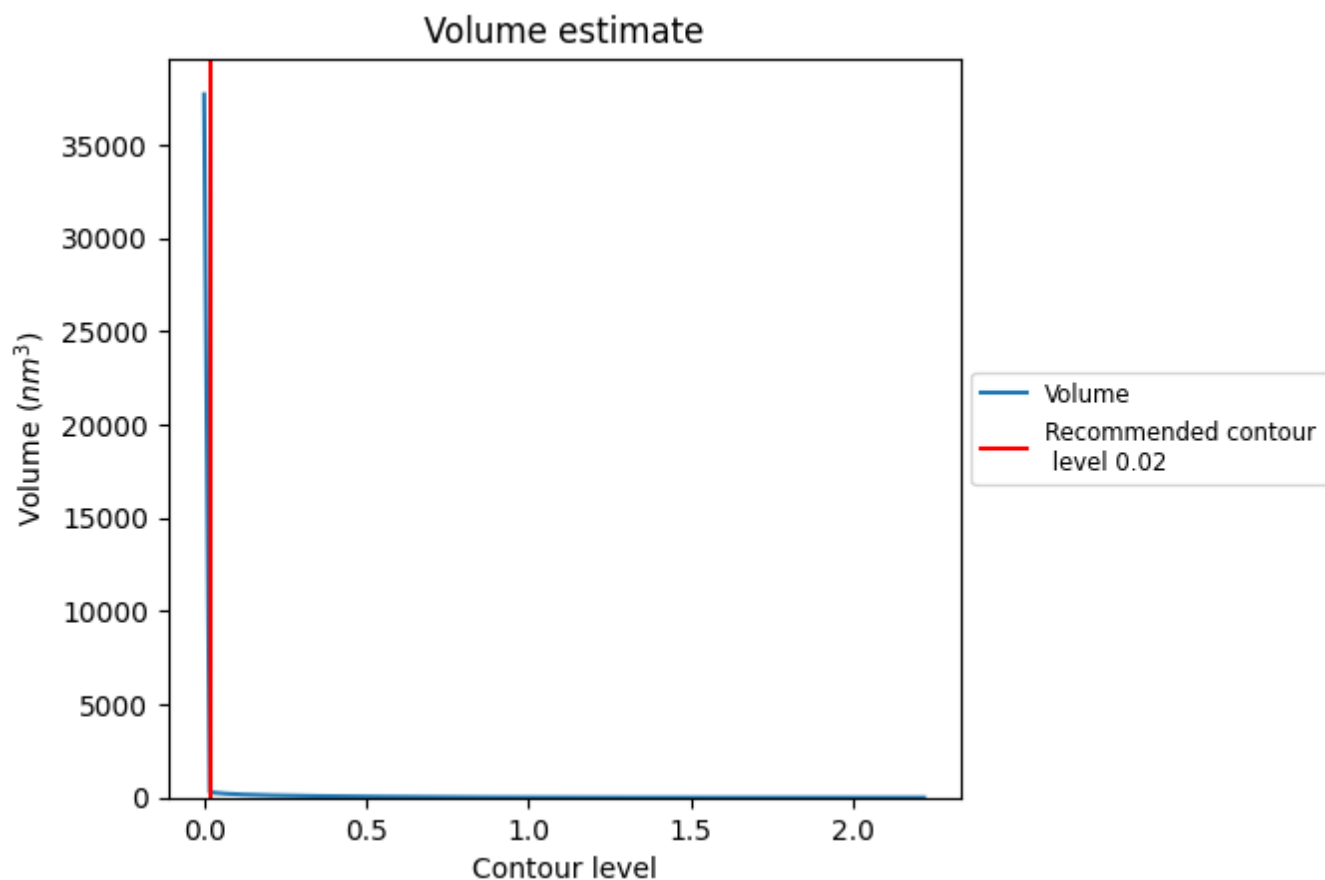
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

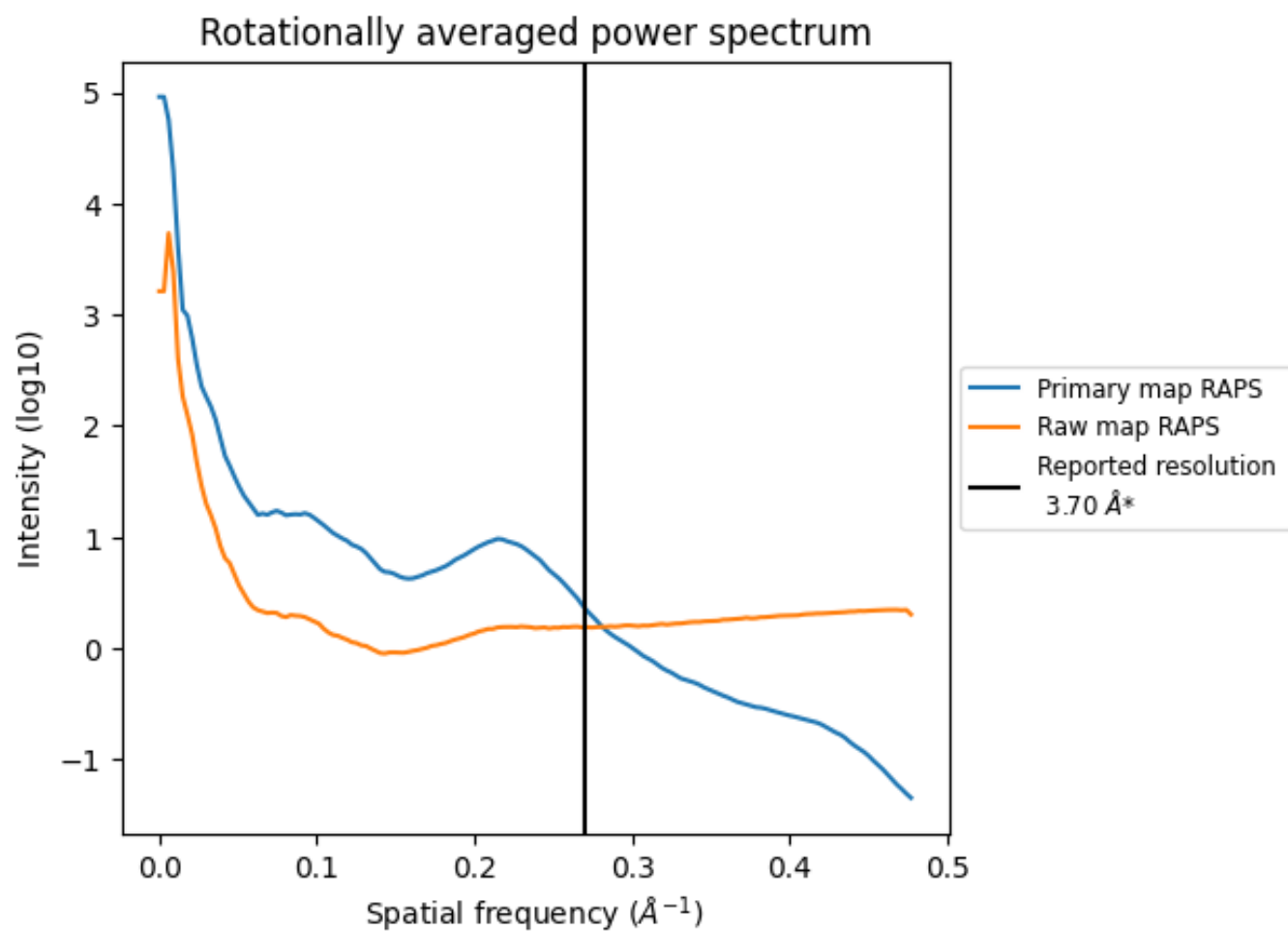
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 287 nm^3 ; this corresponds to an approximate mass of 260 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 ⓘ

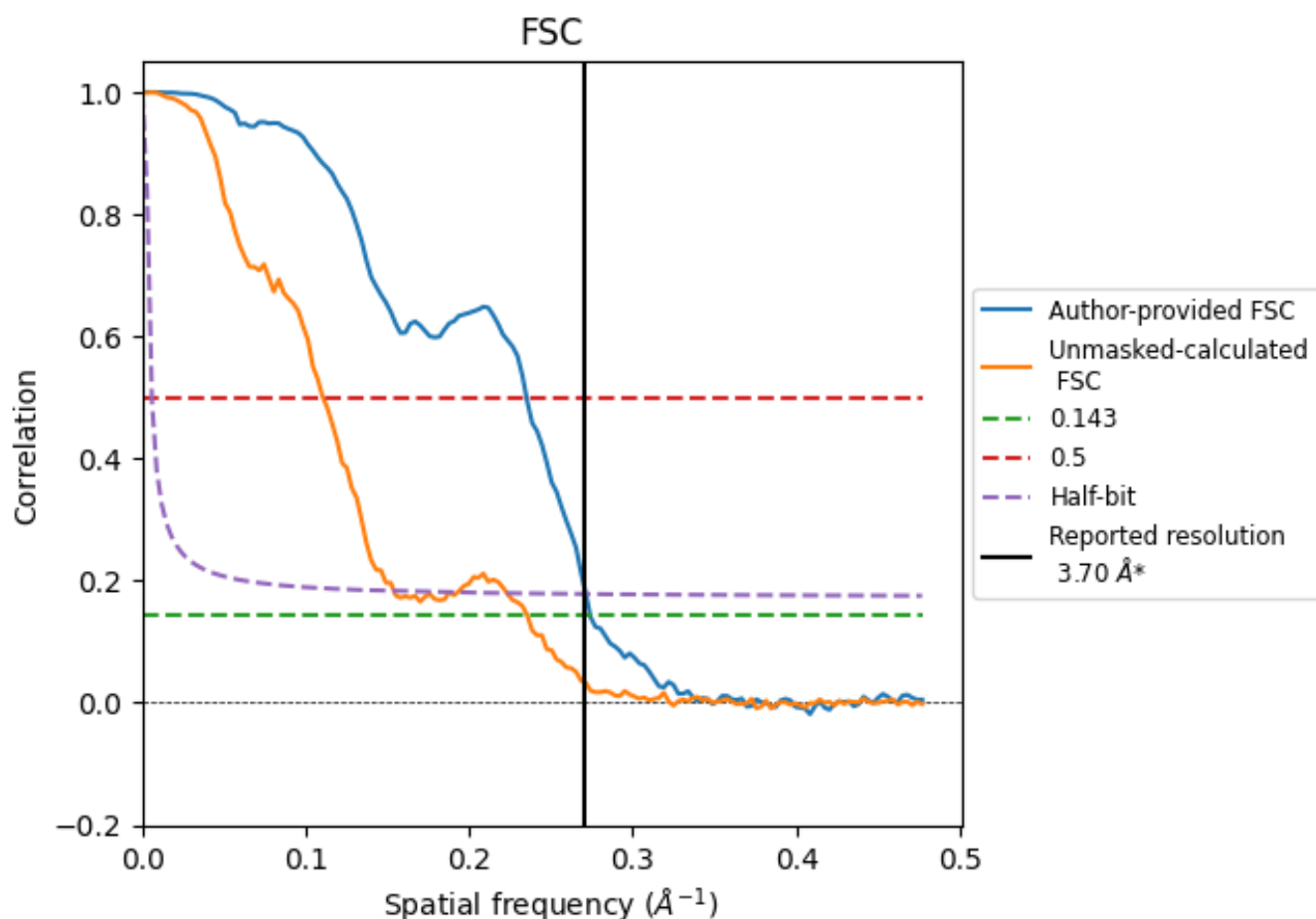


*Reported resolution corresponds to spatial frequency of 0.270 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

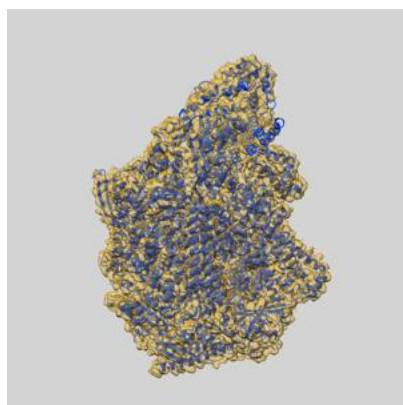
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.65	4.25	3.68
Unmasked-calculated*	4.24	9.04	6.49

*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 4.24 differs from the reported value 3.7 by more than 10 %

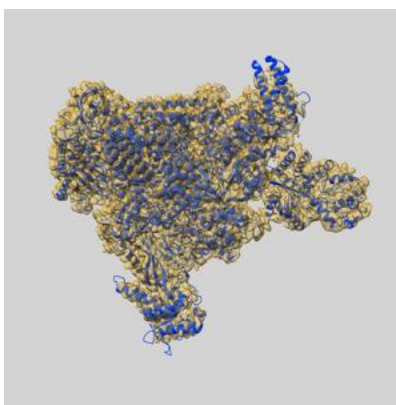
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48076 and PDB model 9EI4. Per-residue inclusion information can be found in section 3 on page 8.

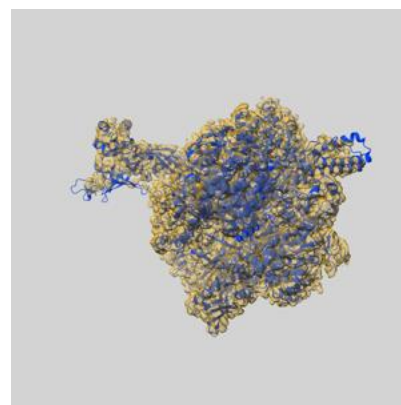
9.1 Map-model overlay [i](#)



X



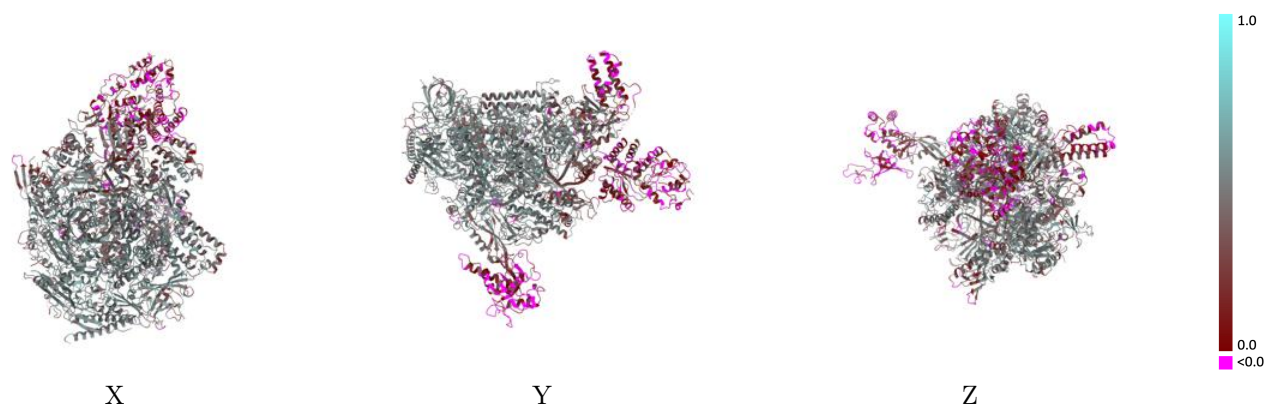
Y



Z

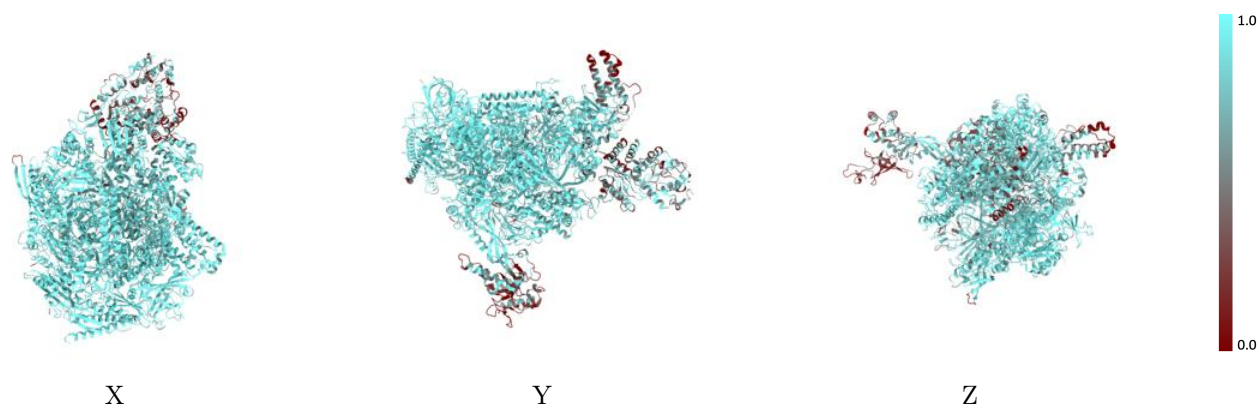
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



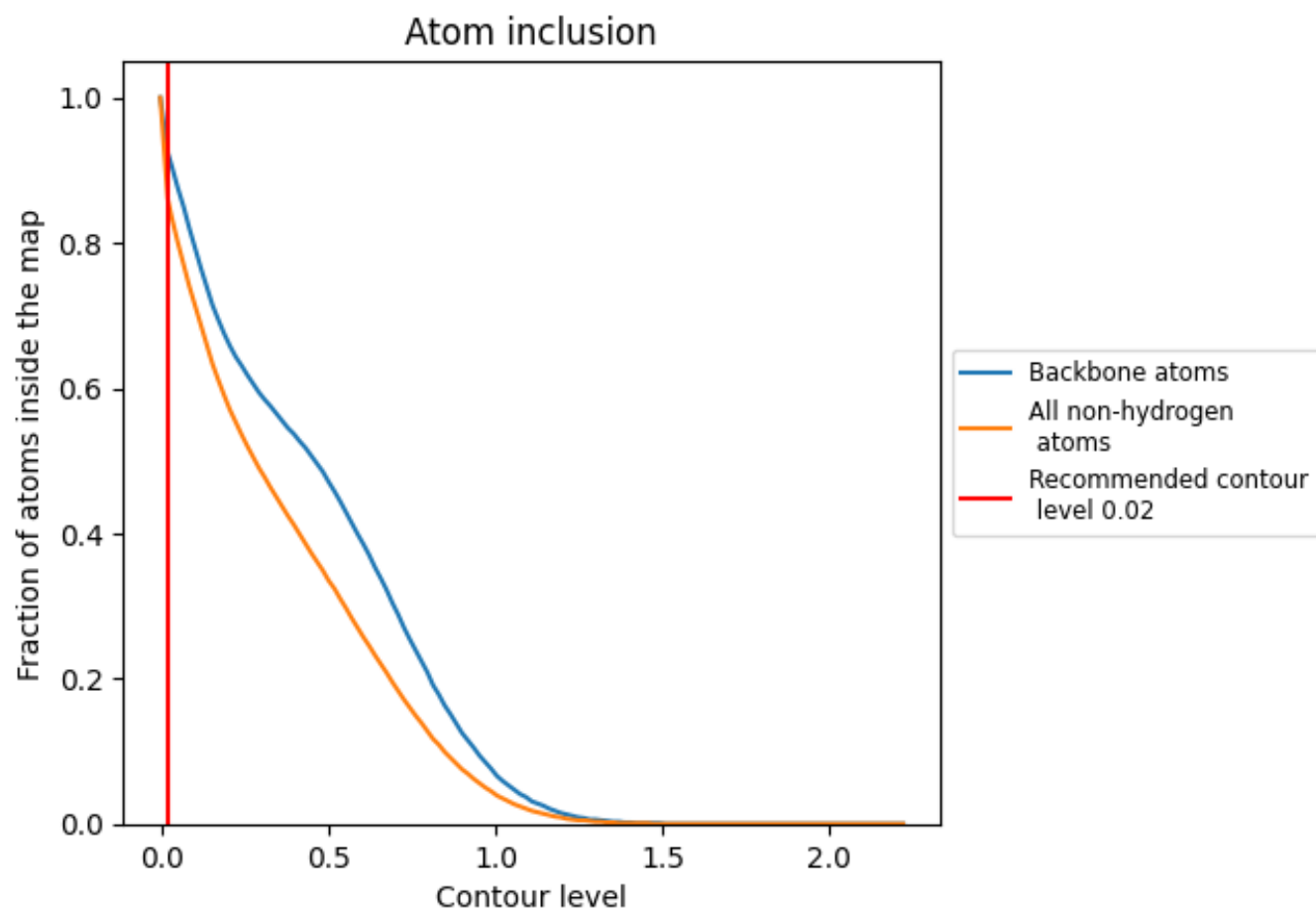
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8610	 0.4100
A	 0.9330	 0.4750
B	 0.9270	 0.4780
C	 0.9440	 0.4990
D	 0.5160	 0.0720
E	 0.9040	 0.4380
F	 0.9140	 0.4850
G	 0.5060	 0.1790
H	 0.9210	 0.4630
I	 0.8880	 0.4140
J	 0.9440	 0.5060
K	 0.9570	 0.4990
L	 0.8880	 0.4300
N	 0.8390	 0.2690
P	 0.8830	 0.3870
T	 0.9150	 0.3960
U	 0.5620	 0.1050

