



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:38 AM UTC

PDB ID : 5FJ8 / pdb_00005fj8
EMDB ID : EMD-3178
Title : Cryo-EM structure of yeast RNA polymerase III elongation complex at 3.9 Å
Authors : Hoffmann, N.A.; Jakobi, A.J.; Moreno-Morcillo, M.; Glatt, S.; Kosinski, J.; Hagen, W.J.; Sachse, C.; Muller, C.W.
Deposited on : 2015-10-06
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

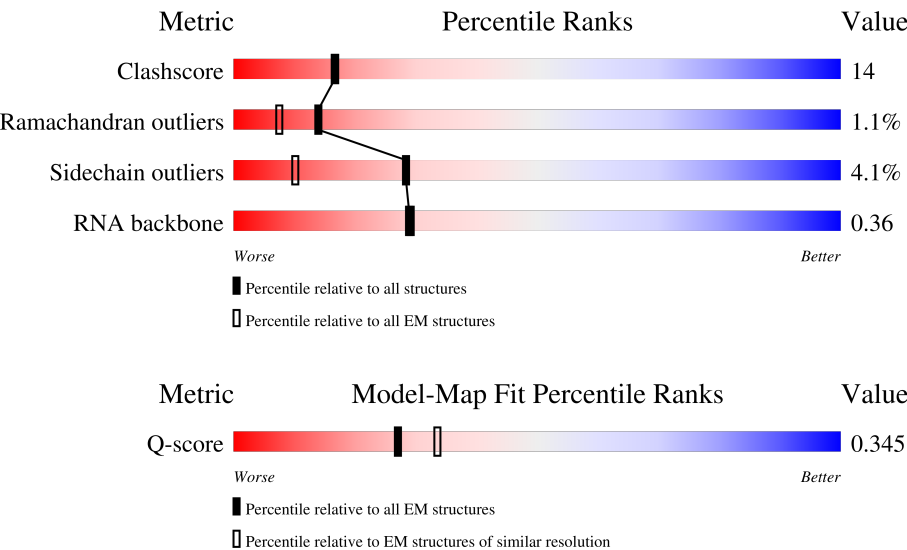
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	1460	
2	B	1149	
3	C	335	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	161	
5	E	215	
6	F	155	
7	G	212	
8	H	146	
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	104	
18	R	23	
19	S	15	
20	T	9	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 39284 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	1422	Total	C	N	O	S	0	0
			11130	7013	1966	2092	59		

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0
			8788	5558	1516	1654	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	119	Total	C	N	O	S	0	0
			977	628	156	187	6		

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

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 RPABC 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	140	Total	C	N	O	S	0	0
			1120	703	188	224	5		

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	42	Total	C	N	O	S	0	0
			321	204	47	64	6		

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

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 RPABC 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	164	Total	C	N	O	S	0	0
			1338	857	227	253	1		

- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	110	Total	C	N	O	S	0	0
			845	536	152	154	3		

- Molecule 15 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	539	Total	C	N	O	S	0	0
			4329	2756	741	813	19		

- Molecule 16 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	89	Total	C	N	O	S	0	0
			738	474	115	146	3		

- Molecule 17 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC7.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	63	Total	C	N	O	0	0
			390	243	73	74		

- Molecule 18 is a DNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	23	Total	C	N	O	P	0	0
			470	224	85	138	23		

- Molecule 19 is a DNA chain called NON-TEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	15	Total	C	N	O	P	0	0
			309	148	56	90	15		

- Molecule 20 is a RNA chain called TEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	9	Total	C	N	O	P	0	0
			195	87	39	60	9		

- Molecule 21 is ZINC ION (CCD ID: ZN) (formula: Zn).

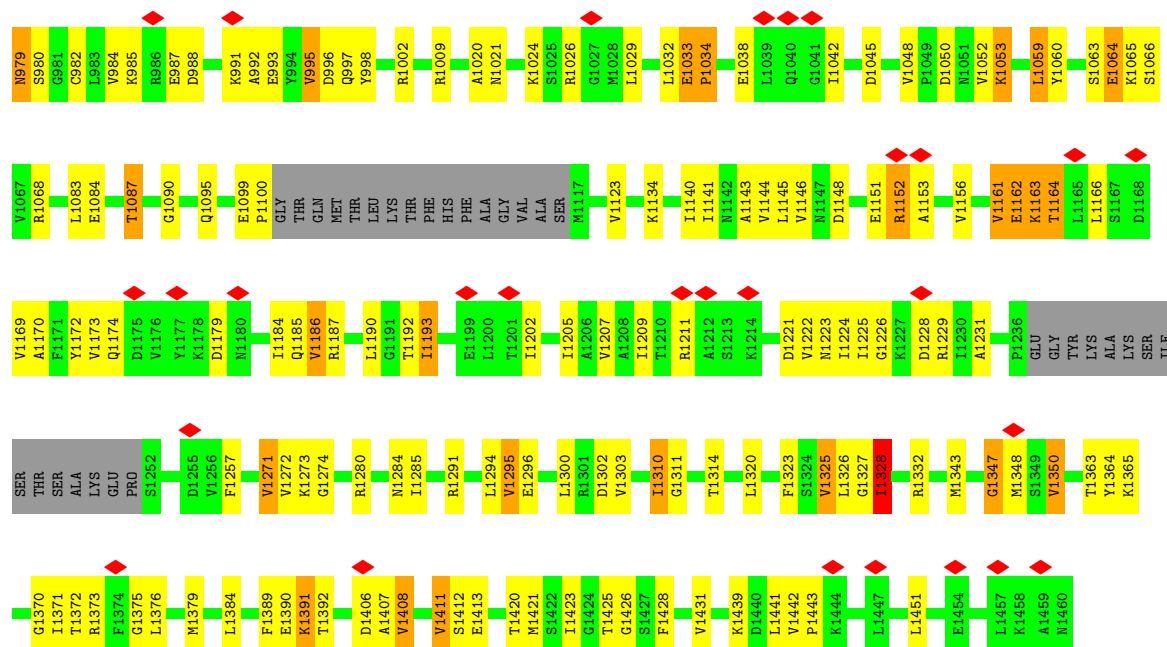
Mol	Chain	Residues	Atoms		AltConf
21	A	2	Total	Zn	0
			2	2	
21	B	1	Total	Zn	0
			1	1	
21	I	1	Total	Zn	0
			1	1	
21	J	1	Total	Zn	0
			1	1	
21	L	1	Total	Zn	0
			1	1	

3 Residue-property plots

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

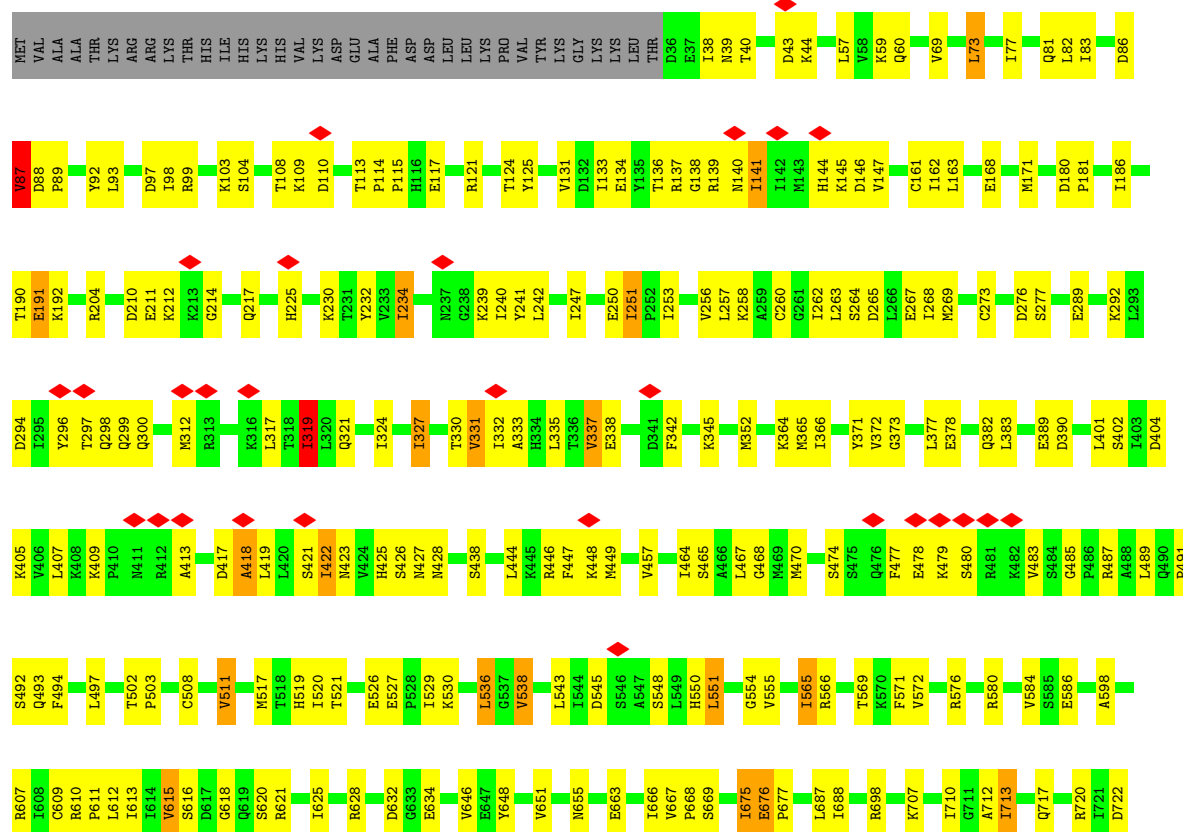
• Molecule 1: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC1

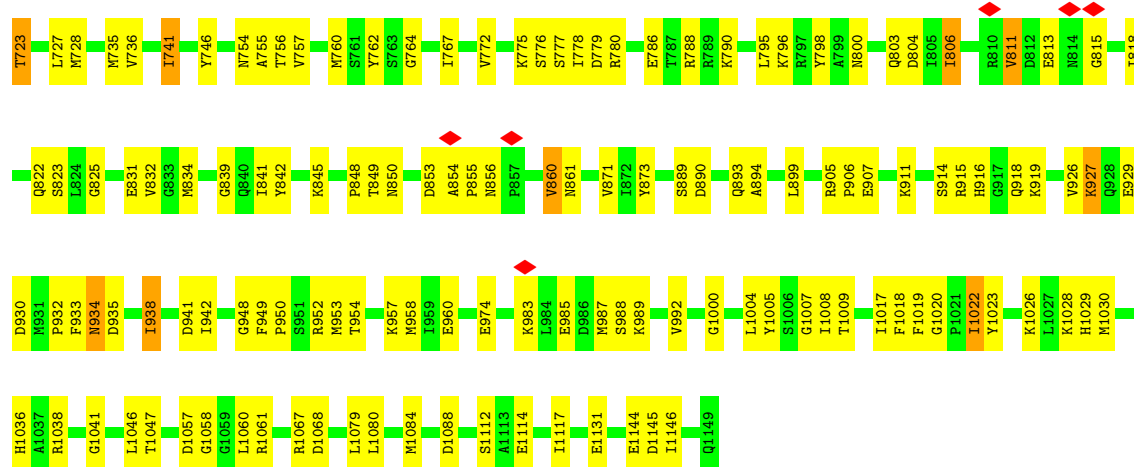




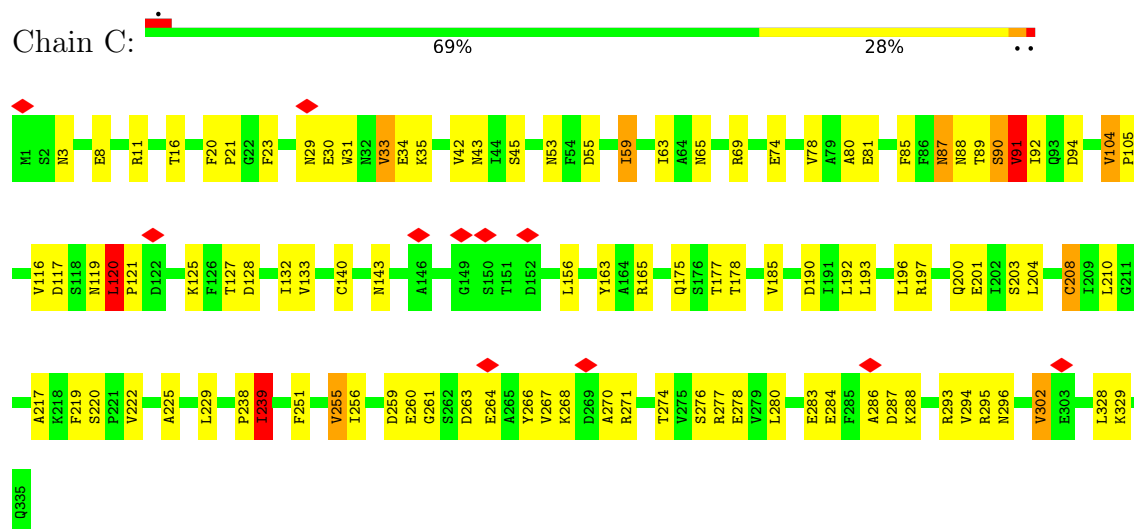
• Molecule 2: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC2

Chain B:

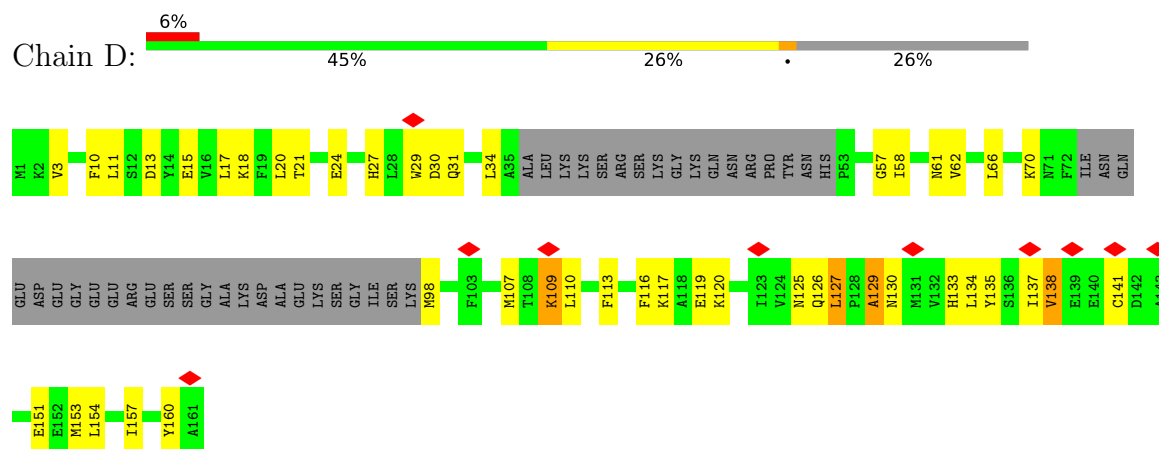




• Molecule 3: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1

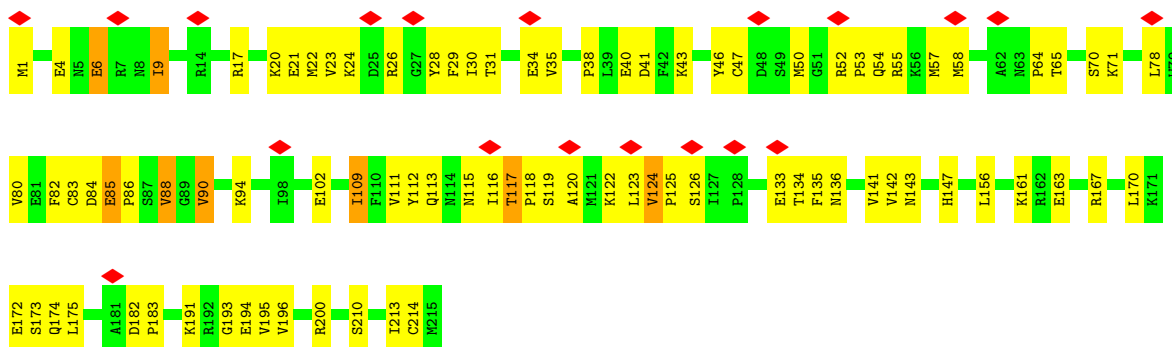


• Molecule 4: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC9



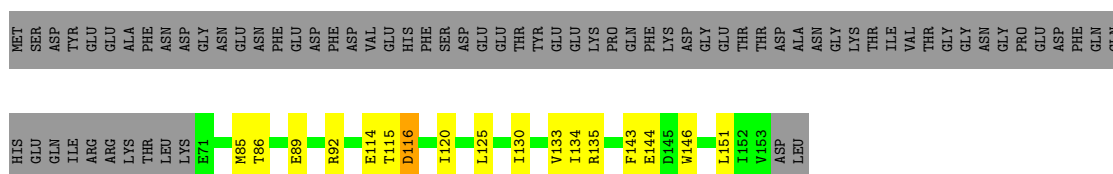
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1





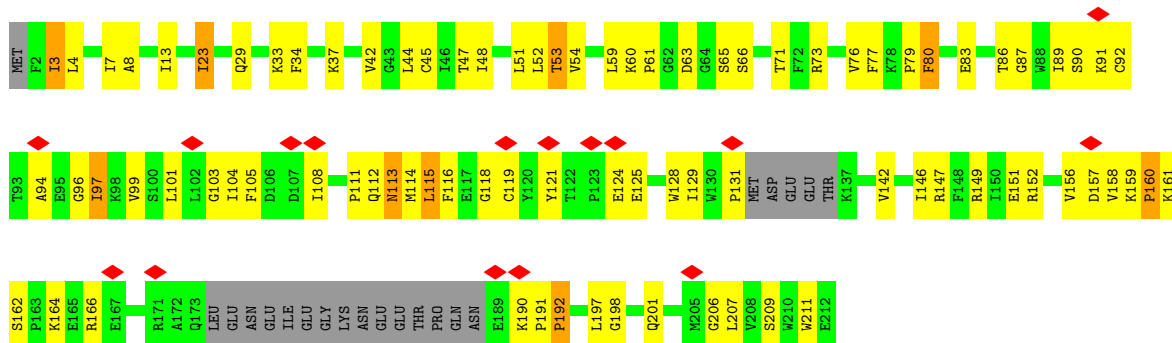
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2

Chain F: 43% 10% 46%



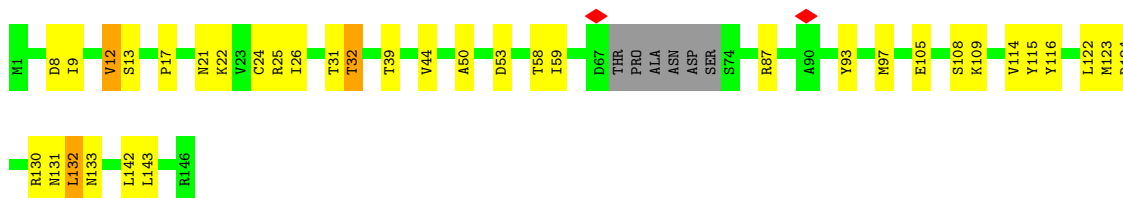
- Molecule 7: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC8

Chain G: 8% 50% 36% 10%



- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

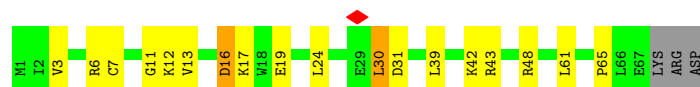
Chain H: 71% 23% 6%



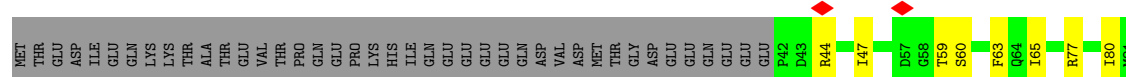
- Molecule 9: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC10

Chain I: 5% 28% 8% 62%

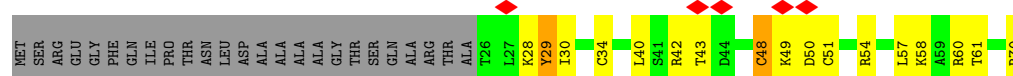
- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



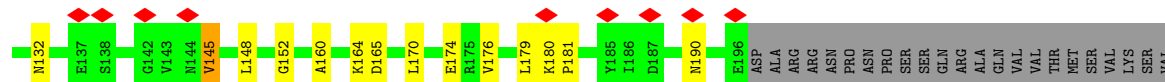
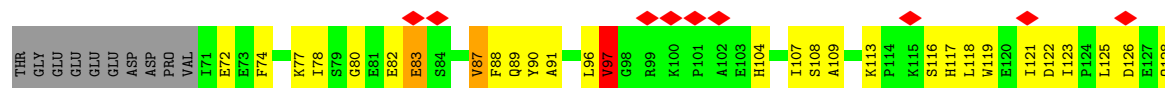
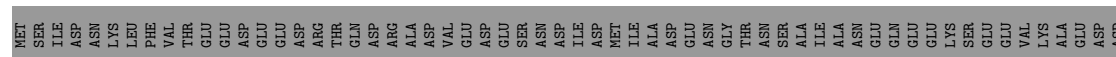
- Molecule 11: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2



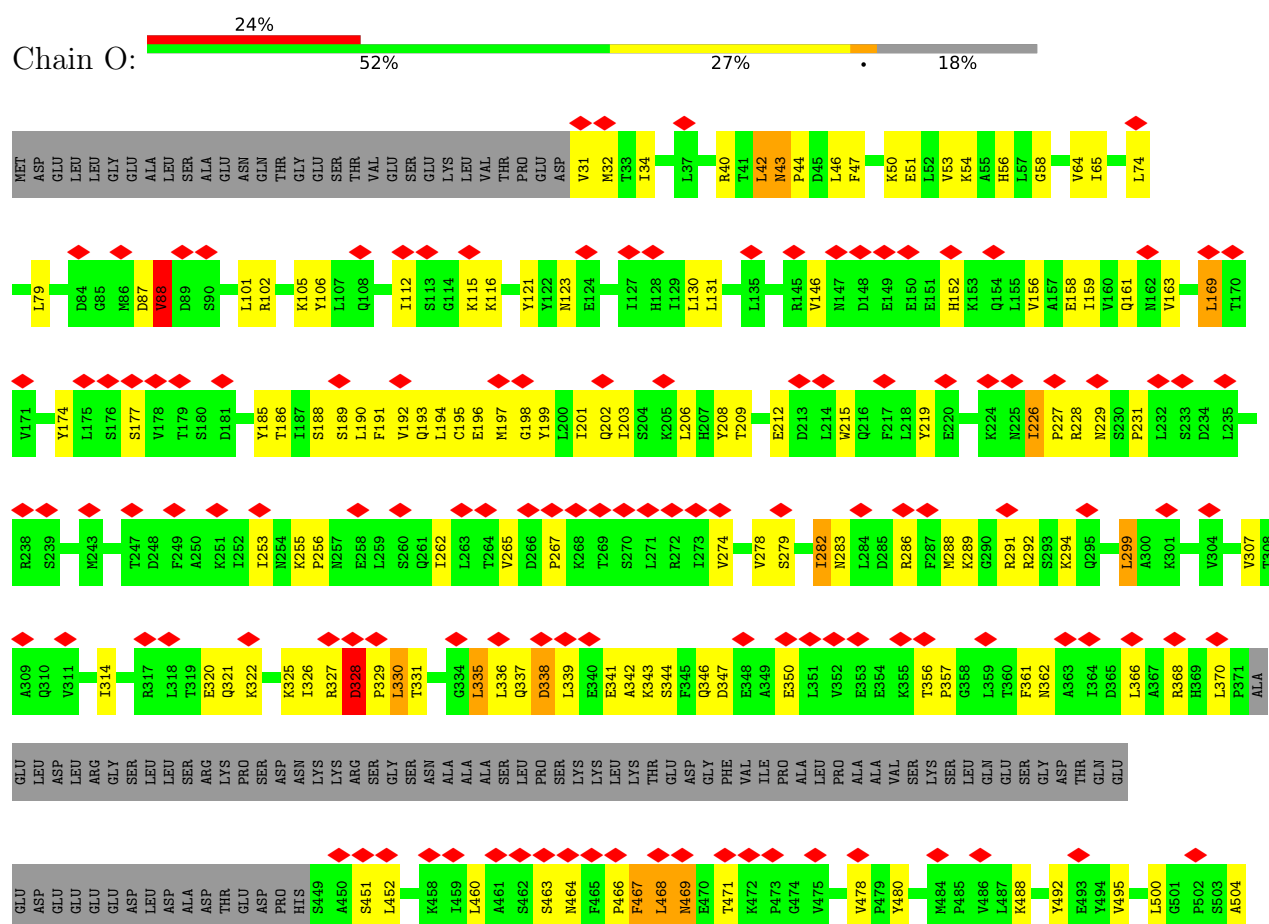
- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

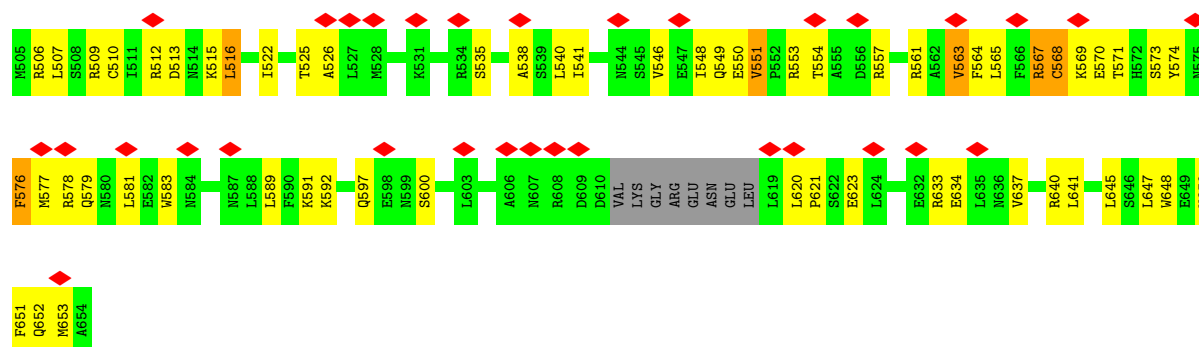


- Molecule 13: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC5

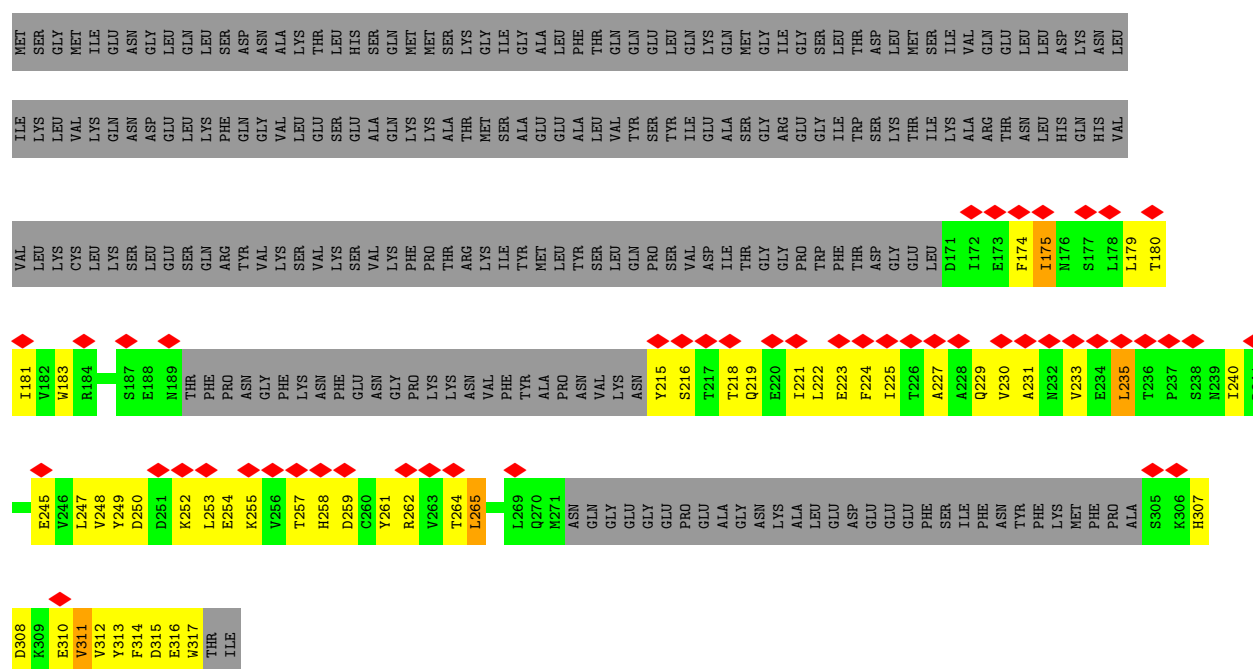


- Molecule 14: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC4

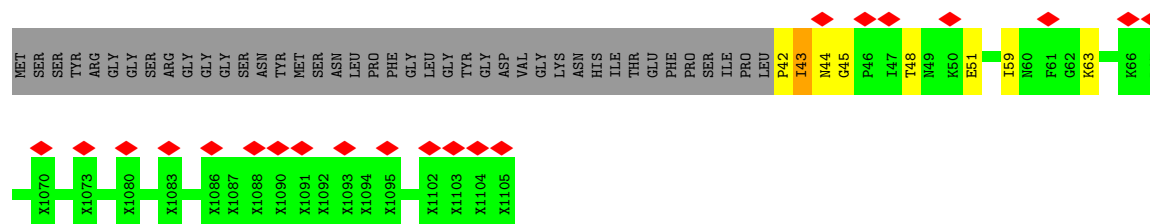




• Molecule 16: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC6



• Molecule 17: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC7

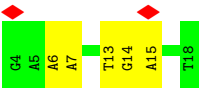


• Molecule 18: RNA

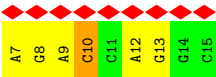




• Molecule 19: NON-TEMPLATE DNA



• Molecule 20: TEMPLATE DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	49543	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	4200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.536	Depositor
Minimum map value	-0.327	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.06	Depositor
Map size ($\text{\AA}$)	320.86398, 320.86398, 320.86398	wwPDB
Map dimensions	296, 296, 296	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.084, 1.084, 1.084	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

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	0.32	0/11328	0.86	32/15303 (0.2%)
2	B	0.30	0/8943	0.82	25/12068 (0.2%)
3	C	0.32	0/2711	0.83	6/3676 (0.2%)
4	D	0.31	0/991	0.86	1/1328 (0.1%)
5	E	0.31	0/1795	0.79	2/2416 (0.1%)
6	F	0.30	0/683	0.78	2/923 (0.2%)
7	G	0.33	0/1583	0.84	0/2146
8	H	0.28	0/1138	0.76	1/1540 (0.1%)
9	I	0.43	0/328	0.96	2/445 (0.4%)
10	J	0.27	0/558	0.73	0/750
11	K	0.29	0/803	0.79	1/1083 (0.1%)
12	L	0.30	0/360	0.78	1/478 (0.2%)
13	M	0.32	0/1369	0.88	5/1851 (0.3%)
14	N	0.39	0/855	0.94	0/1149
15	O	0.32	0/4394	0.86	12/5928 (0.2%)
16	P	0.41	0/750	0.89	2/1017 (0.2%)
17	Q	0.42	0/219	0.82	0/294
18	R	0.15	0/526	0.30	0/809
19	S	0.18	0/346	0.37	0/532
20	T	0.09	0/218	0.25	0/338
All	All	0.31	0/39898	0.83	92/54074 (0.2%)

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	3
2	B	0	2
11	K	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
14	N	0	2
All	All	0	8

There are no bond length outliers.

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	33	PHE	CA-C-N	8.62	128.84	119.87
9	I	33	PHE	C-N-CA	8.62	128.84	119.87
1	A	858	PRO	CA-C-N	-8.21	109.58	119.84
1	A	858	PRO	C-N-CA	-8.21	109.58	119.84
2	B	856	ASN	CA-C-N	7.14	127.19	119.90
2	B	856	ASN	C-N-CA	7.14	127.19	119.90
1	A	955	LEU	CA-C-N	7.11	126.60	118.85
1	A	955	LEU	C-N-CA	7.11	126.60	118.85
15	O	568	CYS	N-CA-C	6.75	117.99	108.00
2	B	319	ILE	N-CA-C	-6.74	106.16	112.83
1	A	1163	LYS	CB-CA-C	-6.72	106.94	116.34
15	O	328	ASP	CA-C-N	-6.67	111.50	119.84
15	O	328	ASP	C-N-CA	-6.67	111.50	119.84
2	B	634	GLU	N-CA-C	6.56	116.52	107.73
16	P	310	GLU	CB-CA-C	-6.55	108.31	117.23
16	P	235	LEU	N-CA-C	6.51	119.70	111.69
1	A	1034	PRO	CA-C-N	6.43	126.45	119.89
1	A	1034	PRO	C-N-CA	6.43	126.45	119.89
1	A	1123	VAL	CA-C-N	-6.41	113.08	119.56
1	A	1123	VAL	C-N-CA	-6.41	113.08	119.56
15	O	467	PHE	N-CA-C	6.29	116.31	108.19
1	A	1163	LYS	N-CA-C	6.23	117.22	108.00
1	A	1033	GLU	CA-C-N	-6.18	114.01	120.38
1	A	1033	GLU	C-N-CA	-6.18	114.01	120.38
13	M	104	HIS	CA-C-N	6.05	126.02	120.21
13	M	104	HIS	C-N-CA	6.05	126.02	120.21
4	D	129	ALA	N-CA-C	5.93	119.82	112.58
15	O	568	CYS	CB-CA-C	-5.89	108.09	116.34
2	B	780	ARG	N-CA-C	-5.88	105.86	113.16
15	O	451	SER	CB-CA-C	-5.87	109.82	116.63
3	C	120	LEU	CA-C-N	5.86	125.87	119.89
3	C	120	LEU	C-N-CA	5.86	125.87	119.89
15	O	199	TYR	CB-CA-C	-5.84	109.29	117.23
1	A	756	CYS	CB-CA-C	-5.83	109.86	116.63
13	M	174	GLU	CB-CA-C	-5.82	109.88	116.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	815	GLY	N-CA-C	-5.81	105.15	113.86
1	A	1050	ASP	CB-CA-C	-5.76	109.39	117.23
2	B	825	GLY	CA-C-N	5.75	125.43	119.05
2	B	825	GLY	C-N-CA	5.75	125.43	119.05
2	B	276	ASP	N-CA-C	5.72	115.83	108.34
1	A	1370	GLY	N-CA-C	5.69	118.30	110.56
2	B	409	LYS	CA-C-N	5.64	125.11	119.24
2	B	409	LYS	C-N-CA	5.64	125.11	119.24
15	O	43	ASN	N-CA-C	5.63	118.79	109.79
2	B	168	GLU	CB-CA-C	-5.57	109.65	117.23
1	A	263	ALA	CA-C-N	5.51	123.62	119.66
1	A	263	ALA	C-N-CA	5.51	123.62	119.66
13	M	165	ASP	CB-CA-C	-5.50	110.25	116.63
15	O	42	LEU	N-CA-C	5.50	120.10	113.17
1	A	1347	GLY	N-CA-C	5.50	118.60	110.63
15	O	567	ARG	N-CA-C	5.49	117.20	108.79
11	K	59	THR	CB-CA-C	-5.48	109.78	117.23
12	L	29	TYR	CB-CA-C	-5.47	109.28	115.79
2	B	934	ASN	N-CA-C	5.44	116.06	108.00
1	A	952	LYS	CB-CA-C	-5.42	108.75	116.34
3	C	90	SER	N-CA-C	5.42	117.58	107.99
1	A	448	ASP	CB-CA-C	-5.42	109.86	117.23
2	B	214	GLY	N-CA-C	5.42	117.31	110.38
5	E	85	GLU	CA-C-N	-5.41	113.45	119.19
5	E	85	GLU	C-N-CA	-5.41	113.45	119.19
2	B	418	ALA	N-CA-C	-5.39	106.48	113.16
1	A	1152	ARG	CB-CA-C	-5.38	109.92	117.23
2	B	548	SER	N-CA-C	5.37	117.39	108.20
2	B	1041	GLY	CA-C-N	5.37	125.38	119.90
2	B	1041	GLY	C-N-CA	5.37	125.38	119.90
1	A	555	GLN	CB-CA-C	-5.36	109.95	117.23
3	C	220	SER	CA-C-N	5.35	124.68	118.85
3	C	220	SER	C-N-CA	5.35	124.68	118.85
1	A	247	THR	N-CA-C	-5.32	106.46	113.17
13	M	226	ARG	CB-CA-C	-5.31	110.00	117.23
1	A	1179	ASP	CB-CA-C	-5.28	110.06	117.23
3	C	185	VAL	N-CA-C	5.22	113.47	109.19
1	A	979	ASN	CB-CA-C	-5.21	110.14	117.23
1	A	1162	GLU	N-CA-C	5.21	117.90	109.40
2	B	764	GLY	N-CA-C	-5.18	107.38	114.64
1	A	274	MET	CB-CA-C	-5.18	110.62	116.63
6	F	116	ASP	CA-C-N	5.18	124.68	119.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	116	ASP	C-N-CA	5.18	124.68	119.19
1	A	686	GLY	CA-C-N	5.17	124.67	119.19
1	A	686	GLY	C-N-CA	5.17	124.67	119.19
2	B	277	SER	CB-CA-C	-5.17	109.11	116.34
2	B	676	GLU	CA-C-N	5.16	124.82	119.56
2	B	676	GLU	C-N-CA	5.16	124.82	119.56
2	B	822	GLN	CB-CA-C	-5.15	110.65	116.63
1	A	248	VAL	N-CA-C	5.14	119.99	108.88
1	A	649	ASP	CB-CA-C	-5.14	110.24	117.23
8	H	32	THR	CB-CA-C	-5.12	110.26	117.23
1	A	952	LYS	N-CA-C	5.07	115.50	108.00
15	O	471	THR	N-CA-C	5.01	117.03	109.41
2	B	527	GLU	CA-C-N	-5.01	115.15	121.91
2	B	527	GLU	C-N-CA	-5.01	115.15	121.91
15	O	362	ASN	N-CA-C	5.01	117.30	110.24

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	38	ASP	Peptide
1	A	599	LYS	Peptide
1	A	601	TYR	Peptide
2	B	319	ILE	Peptide
2	B	839	GLY	Peptide
11	K	44	ARG	Peptide
14	N	300	LYS	Peptide
14	N	405	SER	Peptide

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	11130	0	11258	322	0
2	B	8788	0	8902	262	0
3	C	2655	0	2628	73	0
4	D	977	0	983	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1759	0	1788	55	0
6	F	671	0	692	13	0
7	G	1544	0	1540	65	0
8	H	1120	0	1089	25	0
9	I	321	0	304	12	0
10	J	549	0	560	13	0
11	K	792	0	790	22	0
12	L	358	0	381	21	0
13	M	1338	0	1307	41	0
14	N	845	0	891	39	0
15	O	4329	0	4497	172	0
16	P	738	0	719	43	0
17	Q	390	0	269	5	0
18	R	470	0	260	10	0
19	S	309	0	171	4	0
20	T	195	0	100	2	0
21	A	2	0	0	0	0
21	B	1	0	0	0	0
21	I	1	0	0	0	0
21	J	1	0	0	0	0
21	L	1	0	0	0	0
All	All	39284	0	39129	1091	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 14.

All (1091) 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:829:ASP:OD2	1:A:838:ASN:ND2	2.03	0.91
1:A:615:LYS:NZ	1:A:620:SER:O	2.05	0.88
4:D:126:GLN:HG3	4:D:127:LEU:HG	1.56	0.88
1:A:1163:LYS:HZ1	1:A:1280:ARG:HA	1.40	0.87
3:C:16:THR:O	3:C:295:ARG:NH1	2.07	0.87
2:B:192:LYS:NZ	2:B:438:SER:O	2.08	0.85
2:B:373:GLY:HA2	2:B:607:ARG:HH22	1.42	0.85
1:A:360:LYS:NZ	18:R:16:DG:OP1	2.10	0.84
1:A:69:THR:HA	7:G:164:LYS:HZ3	1.41	0.84
15:O:488:LYS:NZ	15:O:650:VAL:O	2.10	0.83
1:A:232:LYS:NZ	16:P:316:GLU:OE1	2.11	0.83
16:P:248:VAL:O	16:P:255:LYS:NZ	2.13	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLU:HB2	1:A:48:PRO:HD2	1.62	0.81
1:A:476:ARG:NH1	1:A:509:ASN:O	2.13	0.81
1:A:413:ARG:NH1	1:A:456:LEU:O	2.15	0.80
15:O:460:LEU:HD11	15:O:468:LEU:HD23	1.62	0.80
2:B:1026:LYS:NZ	2:B:1030:MET:SD	2.55	0.79
5:E:124:VAL:HG13	5:E:125:PRO:HD3	1.64	0.79
1:A:358:LYS:HG3	1:A:1392:THR:HG21	1.65	0.78
5:E:85:GLU:HG3	5:E:86:PRO:HD3	1.65	0.77
7:G:207:LEU:HD23	7:G:209:SER:H	1.50	0.76
12:L:48:CYS:SG	12:L:51:CYS:HB2	2.18	0.76
7:G:146:ILE:HG23	7:G:206:GLY:HA2	1.68	0.75
2:B:294:ASP:HB3	2:B:300:GLN:HG3	1.67	0.75
2:B:121:ARG:HH12	12:L:54:ARG:HH21	1.33	0.74
14:N:363:ILE:HG12	14:N:373:VAL:HG13	1.68	0.74
13:M:87:VAL:HA	14:N:396:ALA:HA	1.70	0.74
1:A:550:ILE:HG23	1:A:551:ILE:HG23	1.70	0.73
7:G:115:LEU:HD23	7:G:116:PHE:H	1.52	0.73
1:A:996:ASP:OD2	1:A:1002:ARG:NH2	2.22	0.73
4:D:119:GLU:HG3	4:D:138:VAL:HB	1.71	0.72
2:B:796:LYS:NZ	2:B:798:TYR:OH	2.23	0.72
11:K:65:ILE:HB	11:K:101:LEU:HB3	1.72	0.72
7:G:89:ILE:HA	7:G:99:VAL:HA	1.72	0.71
1:A:132:VAL:HG11	1:A:137:ARG:NH1	2.06	0.71
2:B:139:ARG:HE	2:B:141:ILE:HD11	1.53	0.71
2:B:258:LYS:HB3	2:B:297:THR:HA	1.70	0.71
1:A:49:LYS:HD2	1:A:54:LEU:HB3	1.72	0.70
13:M:113:LYS:HD3	13:M:241:ALA:HB2	1.73	0.70
4:D:110:LEU:HB3	4:D:120:LYS:NZ	2.06	0.70
10:J:12:LYS:HE3	10:J:43:ARG:NH2	2.07	0.70
15:O:322:LYS:HB3	15:O:361:PHE:HE1	1.57	0.70
7:G:96:GLY:HA3	7:G:111:PRO:HA	1.73	0.70
2:B:121:ARG:NH1	12:L:54:ARG:HH21	1.89	0.69
4:D:126:GLN:NE2	7:G:86:THR:OG1	2.22	0.69
2:B:234:ILE:HB	2:B:240:ILE:HG22	1.72	0.69
11:K:47:ILE:HG12	11:K:65:ILE:HG12	1.74	0.69
1:A:153:ARG:HA	1:A:160:LEU:HD22	1.75	0.68
1:A:482:ARG:HH12	1:A:924:LEU:HD11	1.59	0.68
2:B:755:ALA:HA	10:J:48:ARG:HH12	1.58	0.68
11:K:88:PHE:HB3	11:K:106:GLN:HB3	1.75	0.68
1:A:436:ARG:HD3	1:A:459:GLY:HA3	1.75	0.68
4:D:127:LEU:HB2	4:D:133:HIS:HB3	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:ARG:HH12	12:L:54:ARG:NH2	1.92	0.68
1:A:272:VAL:HG23	1:A:281:ASN:HB3	1.76	0.68
1:A:1020:ALA:HB2	1:A:1032:LEU:HD11	1.75	0.68
2:B:419:LEU:O	2:B:423:ASN:ND2	2.25	0.68
2:B:778:ILE:HD11	2:B:906:PRO:HG2	1.76	0.68
16:P:252:LYS:HZ2	16:P:253:LEU:HB2	1.59	0.68
13:M:247:TRP:HD1	14:N:406:ALA:HB1	1.58	0.67
15:O:488:LYS:HZ1	15:O:651:PHE:HA	1.59	0.67
16:P:223:GLU:O	16:P:227:ALA:N	2.23	0.67
15:O:516:LEU:HB2	15:O:565:LEU:HD23	1.75	0.67
5:E:161:LYS:NZ	5:E:193:GLY:O	2.27	0.67
15:O:549:GLN:HG3	15:O:565:LEU:HB2	1.76	0.67
8:H:24:CYS:SG	8:H:25:ARG:N	2.67	0.67
13:M:148:LEU:HG	13:M:181:PRO:HB3	1.77	0.67
1:A:1431:VAL:HG21	6:F:135:ARG:NH1	2.10	0.67
13:M:247:TRP:HE1	14:N:408:LEU:HB2	1.59	0.67
1:A:995:VAL:HG23	1:A:996:ASP:H	1.60	0.66
15:O:488:LYS:NZ	15:O:651:PHE:HA	2.10	0.66
2:B:755:ALA:HA	10:J:48:ARG:NH1	2.10	0.66
15:O:327:ARG:NH1	15:O:330:LEU:HD22	2.10	0.66
1:A:1162:GLU:HB2	1:A:1163:LYS:HD3	1.76	0.66
1:A:1163:LYS:HZ1	1:A:1280:ARG:CA	2.08	0.66
2:B:698:ARG:HH21	2:B:952:ARG:HG2	1.61	0.65
15:O:507:LEU:HD13	15:O:540:LEU:HD22	1.78	0.65
17:Q:43:ILE:HG23	17:Q:44:ASN:H	1.61	0.65
1:A:1045:ASP:HB2	1:A:1053:LYS:HE2	1.78	0.65
19:S:6:DA:H2"	19:S:7:DA:OP2	1.96	0.65
3:C:270:ALA:HB3	3:C:271:ARG:HH11	1.61	0.65
1:A:121:ARG:NH2	15:O:212:GLU:OE1	2.29	0.65
2:B:543:LEU:HD21	13:M:176:VAL:HG21	1.79	0.65
9:I:14:ILE:HD13	9:I:24:LEU:HB3	1.78	0.65
7:G:161:LYS:HE3	7:G:166:ARG:HA	1.78	0.65
15:O:185:TYR:HA	15:O:188:SER:HB2	1.78	0.65
1:A:378:ARG:HE	1:A:516:GLU:HB3	1.61	0.65
1:A:179:ILE:HD12	15:O:557:ARG:HE	1.62	0.65
7:G:104:ILE:HG23	7:G:105:PHE:H	1.62	0.65
1:A:310:ASN:HD21	15:O:561:ARG:H	1.44	0.64
2:B:760:MET:HE3	2:B:762:TYR:HB2	1.78	0.64
2:B:914:SER:OG	2:B:957:LYS:NZ	2.20	0.64
2:B:1067:ARG:NH1	2:B:1079:LEU:HD22	2.12	0.64
1:A:200:GLU:HB3	15:O:516:LEU:HD21	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:ASP:O	2:B:268:ILE:N	2.27	0.64
2:B:389:GLU:OE2	2:B:446:ARG:NH2	2.30	0.64
8:H:58:THR:HB	8:H:143:LEU:HB3	1.78	0.64
1:A:360:LYS:HB2	1:A:365:ARG:HH21	1.63	0.64
1:A:905:ARG:HH22	5:E:170:LEU:HD21	1.63	0.64
1:A:3:GLU:OE2	7:G:37:LYS:HE3	1.98	0.64
2:B:253:ILE:HD12	2:B:256:VAL:HB	1.79	0.64
3:C:270:ALA:HB3	3:C:271:ARG:NH1	2.13	0.64
8:H:132:LEU:HD12	8:H:133:ASN:H	1.62	0.64
2:B:247:ILE:HG21	2:B:251:ILE:HD11	1.79	0.63
1:A:1164:THR:HB	1:A:1271:VAL:HA	1.80	0.63
15:O:633:ARG:NH2	16:P:308:ASP:O	2.31	0.63
1:A:1372:THR:O	1:A:1376:LEU:N	2.31	0.63
1:A:160:LEU:HD21	15:O:339:LEU:HG	1.79	0.63
2:B:373:GLY:HA2	2:B:607:ARG:NH2	2.11	0.63
16:P:218:THR:HB	16:P:221:ILE:HB	1.81	0.63
4:D:130:ASN:O	4:D:133:HIS:ND1	2.32	0.63
20:T:9:A:H5'	20:T:10:C:OP2	1.98	0.63
1:A:220:ASP:OD1	1:A:220:ASP:N	2.32	0.63
15:O:106:TYR:HB3	15:O:208:TYR:HE2	1.63	0.62
1:A:1084:GLU:HB2	6:F:86:THR:HG23	1.82	0.62
3:C:222:VAL:HG11	3:C:225:ALA:HB2	1.81	0.62
1:A:956:PRO:HG2	1:A:957:TYR:HD1	1.65	0.62
2:B:483:VAL:HG12	2:B:485:GLY:H	1.63	0.62
10:J:17:LYS:HB3	10:J:39:LEU:HD21	1.81	0.62
1:A:252:ARG:O	1:A:254:GLU:N	2.32	0.62
5:E:90:VAL:HG12	5:E:94:LYS:HG2	1.82	0.62
16:P:174:PHE:O	16:P:175:ILE:HG12	2.00	0.62
1:A:38:ASP:HB3	1:A:39:LEU:HD12	1.82	0.62
1:A:1161:VAL:HG11	1:A:1303:VAL:HG23	1.82	0.62
2:B:426:SER:O	2:B:427:ASN:ND2	2.33	0.61
2:B:81:GLN:HG2	2:B:82:LEU:HG	1.83	0.61
3:C:29:ASN:HB2	3:C:35:LYS:NZ	2.15	0.61
9:I:32:GLU:HG2	13:M:132:ASN:HB2	1.82	0.61
16:P:179:LEU:O	16:P:183:TRP:NE1	2.33	0.61
1:A:347:VAL:HB	1:A:350:ILE:HD11	1.82	0.61
2:B:230:LYS:HB2	2:B:333:ALA:HB1	1.82	0.61
3:C:81:GLU:OE2	12:L:70:ARG:NH2	2.33	0.61
2:B:698:ARG:HE	2:B:952:ARG:HB3	1.65	0.61
5:E:112:TYR:HB2	5:E:136:ASN:HA	1.82	0.61
1:A:378:ARG:NH1	18:R:18:DC:H4'	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:97:MET:HB2	8:H:142:LEU:HB3	1.82	0.61
13:M:77:LYS:HE3	13:M:262:GLU:HB3	1.83	0.61
1:A:476:ARG:HG2	1:A:478:PRO:HD2	1.83	0.61
4:D:11:LEU:HD22	7:G:4:LEU:HD13	1.82	0.61
14:N:305:MET:HG2	14:N:414:GLY:H	1.65	0.61
1:A:486:LEU:HD23	1:A:537:VAL:HG22	1.83	0.61
2:B:775:LYS:HA	2:B:778:ILE:HG22	1.82	0.61
15:O:341:GLU:HG2	15:O:344:SER:HB2	1.81	0.61
15:O:578:ARG:HG2	15:O:648:TRP:HZ3	1.66	0.61
3:C:31:TRP:H	11:K:82:LYS:HE2	1.66	0.61
16:P:252:LYS:NZ	16:P:253:LEU:HB2	2.16	0.61
1:A:393:ALA:HA	1:A:491:LYS:HB2	1.83	0.60
1:A:573:ARG:HH21	11:K:87:GLU:HB3	1.65	0.60
15:O:198:GLY:HA3	15:O:286:ARG:HG2	1.83	0.60
9:I:35:ILE:HD12	9:I:36:GLU:H	1.66	0.60
14:N:398:SER:HB3	14:N:407:GLU:HB3	1.83	0.60
15:O:105:LYS:HB3	15:O:121:TYR:HB2	1.83	0.60
1:A:15:GLY:H	1:A:1408:VAL:HG12	1.66	0.60
4:D:110:LEU:HB3	4:D:120:LYS:HZ1	1.66	0.60
12:L:29:TYR:HE2	12:L:40:LEU:HB2	1.65	0.60
12:L:42:ARG:HG3	12:L:43:THR:HG23	1.84	0.60
1:A:582:MET:HE3	1:A:703:ARG:HB2	1.84	0.60
2:B:493:GLN:HG3	2:B:497:LEU:HB2	1.84	0.60
1:A:712:ILE:HG23	1:A:790:ALA:HB3	1.82	0.60
2:B:1112:SER:HB2	2:B:1114:GLU:HG2	1.82	0.60
6:F:92:ARG:HH12	7:G:61:PRO:HB3	1.67	0.60
15:O:31:VAL:HG12	15:O:32:MET:HG3	1.83	0.60
1:A:1169:VAL:HG13	1:A:1192:THR:HB	1.83	0.60
5:E:117:THR:HG23	5:E:119:SER:H	1.66	0.60
7:G:101:LEU:HD22	7:G:104:ILE:HG22	1.84	0.60
15:O:190:LEU:HG	15:O:193:GLN:HB3	1.82	0.60
15:O:538:ALA:HA	15:O:541:ILE:HG22	1.84	0.60
1:A:645:MET:HE1	8:H:124:ARG:HB2	1.83	0.59
4:D:127:LEU:HD11	4:D:137:ILE:HD13	1.84	0.59
1:A:15:GLY:HA2	1:A:1407:ALA:HA	1.84	0.59
1:A:69:THR:HG22	7:G:164:LYS:HZ3	1.67	0.59
1:A:712:ILE:HD12	2:B:949:PHE:HD2	1.66	0.59
2:B:832:VAL:HG12	12:L:60:ARG:HG3	1.84	0.59
9:I:12:LEU:HB3	9:I:24:LEU:HD13	1.84	0.59
1:A:1420:THR:HG22	2:B:1080:LEU:HD21	1.84	0.59
16:P:221:ILE:HA	16:P:224:PHE:HB2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1144:VAL:HG23	1:A:1310:ILE:HG23	1.84	0.59
15:O:286:ARG:NH1	15:O:320:GLU:O	2.35	0.59
15:O:469:ASN:H	15:O:478:VAL:HG22	1.67	0.59
1:A:1141:ILE:N	1:A:1295:VAL:O	2.31	0.59
2:B:137:ARG:HH11	2:B:139:ARG:HB2	1.67	0.59
4:D:129:ALA:HB2	4:D:157:ILE:HG23	1.85	0.59
1:A:221:ASP:H	15:O:550:GLU:HG3	1.67	0.59
1:A:828:GLN:HB3	2:B:655:ASN:HD21	1.68	0.59
1:A:1364:TYR:OH	1:A:1379:MET:SD	2.61	0.59
2:B:1007:GLY:O	3:C:69:ARG:NH1	2.35	0.59
15:O:328:ASP:OD1	15:O:328:ASP:N	2.36	0.59
16:P:223:GLU:HB3	16:P:240:ILE:HD13	1.85	0.59
13:M:108:SER:OG	13:M:109:ALA:N	2.36	0.59
2:B:299:GLN:HG3	2:B:300:GLN:H	1.68	0.59
4:D:24:GLU:OE2	4:D:30:ASP:HB2	2.03	0.59
2:B:1038:ARG:HH11	2:B:1057:ASP:CG	2.11	0.58
2:B:948:GLY:HA2	2:B:952:ARG:NH1	2.17	0.58
1:A:538:LYS:HB3	1:A:687:PRO:HB2	1.85	0.58
1:A:329:SER:HB3	1:A:355:GLN:HE22	1.68	0.58
1:A:666:LYS:HA	1:A:670:GLY:HA3	1.83	0.58
3:C:165:ARG:NH2	3:C:190:ASP:OD1	2.37	0.58
2:B:297:THR:HG23	2:B:298:GLN:HG2	1.84	0.58
1:A:1099:GLU:HA	1:A:1100:PRO:C	2.28	0.58
7:G:190:LYS:C	7:G:192:PRO:HD3	2.28	0.58
1:A:360:LYS:HA	1:A:365:ARG:HE	1.69	0.58
1:A:1257:PHE:HB2	9:I:14:ILE:HB	1.85	0.58
2:B:775:LYS:HB3	2:B:927:LYS:HA	1.83	0.58
5:E:21:GLU:HB3	5:E:35:VAL:HG21	1.86	0.58
8:H:87:ARG:HH11	8:H:87:ARG:HB2	1.69	0.58
15:O:158:GLU:OE1	15:O:161:GLN:NE2	2.37	0.58
15:O:633:ARG:HE	16:P:307:HIS:HB2	1.66	0.58
18:R:18:DC:H2''	18:R:19:DT:H5'	1.85	0.58
2:B:616:SER:HB2	2:B:621:ARG:HH21	1.68	0.57
7:G:112:GLN:HG2	7:G:115:LEU:HD13	1.86	0.57
15:O:163:VAL:HG22	15:O:169:LEU:HD22	1.85	0.57
1:A:541:LEU:HG	1:A:551:ILE:HD11	1.84	0.57
2:B:860:VAL:HG13	2:B:861:ASN:H	1.69	0.57
15:O:347:ASP:HA	15:O:350:GLU:HB2	1.86	0.57
15:O:620:LEU:HD12	15:O:621:PRO:HD2	1.86	0.57
1:A:225:LEU:O	1:A:229:ASN:ND2	2.37	0.57
2:B:832:VAL:HB	12:L:60:ARG:HA	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1008:ILE:HG13	2:B:1009:THR:H	1.69	0.57
5:E:83:CYS:SG	5:E:84:ASP:N	2.78	0.57
1:A:574:ALA:O	11:K:77:ARG:NH2	2.38	0.57
12:L:50:ASP:OD1	12:L:51:CYS:N	2.36	0.57
1:A:991:LYS:HG3	1:A:993:GLU:HG2	1.87	0.57
2:B:57:LEU:HD22	2:B:467:LEU:HD11	1.86	0.57
11:K:107:THR:OG1	11:K:108:TYR:N	2.36	0.57
5:E:200:ARG:NH1	5:E:210:SER:OG	2.38	0.57
12:L:49:LYS:N	12:L:51:CYS:SG	2.78	0.57
1:A:69:THR:HG22	7:G:164:LYS:NZ	2.20	0.57
1:A:402:LEU:HD23	1:A:466:LEU:HD22	1.87	0.57
3:C:140:CYS:HB2	3:C:196:LEU:HD13	1.86	0.57
1:A:42:LEU:HD12	1:A:42:LEU:H	1.70	0.57
1:A:213:ARG:O	1:A:213:ARG:NH1	2.38	0.57
12:L:28:LYS:HG3	12:L:29:TYR:HD2	1.69	0.57
15:O:159:ILE:HD12	15:O:174:TYR:HE1	1.68	0.57
15:O:288:MET:SD	15:O:291:ARG:NH1	2.78	0.57
1:A:22:SER:O	1:A:24:ALA:N	2.36	0.56
6:F:125:LEU:HA	6:F:130:ILE:HD11	1.86	0.56
15:O:228:ARG:HH12	15:O:231:PRO:HD3	1.69	0.56
15:O:540:LEU:HD21	15:O:546:VAL:HG11	1.85	0.56
2:B:161:CYS:SG	2:B:162:ILE:N	2.78	0.56
7:G:157:ASP:OD1	7:G:157:ASP:N	2.37	0.56
13:M:113:LYS:NZ	13:M:237:ALA:HB1	2.20	0.56
2:B:926:VAL:HG11	2:B:930:ASP:HB2	1.87	0.56
2:B:87:VAL:HG11	2:B:407:LEU:HB3	1.87	0.56
7:G:91:LYS:HG2	7:G:92:CYS:H	1.71	0.56
14:N:392:GLN:HB3	14:N:394:VAL:HG23	1.87	0.56
15:O:338:ASP:OD1	15:O:339:LEU:N	2.39	0.56
1:A:112:ALA:HA	1:A:234:ILE:HD11	1.88	0.56
15:O:292:ARG:HE	15:O:326:ILE:HD11	1.71	0.56
15:O:640:ARG:NH1	17:Q:42:PRO:O	2.36	0.56
1:A:39:LEU:O	1:A:41:ASP:N	2.38	0.56
7:G:114:MET:O	7:G:201:GLN:HB3	2.06	0.56
15:O:652:GLN:HE21	15:O:653:MET:HE3	1.71	0.56
1:A:62:SER:HB3	1:A:65:LEU:HG	1.88	0.56
2:B:1004:LEU:HD12	2:B:1017:ILE:HD12	1.88	0.56
2:B:1036:HIS:CE1	2:B:1058:GLY:HA3	2.41	0.56
1:A:473:LEU:HA	1:A:487:SER:HA	1.88	0.56
2:B:554:GLY:H	2:B:598:ALA:HA	1.70	0.56
1:A:34:VAL:HG23	1:A:35:SER:H	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1332:ARG:HB2	1:A:1363:THR:HG21	1.88	0.56
2:B:934:ASN:OD1	2:B:935:ASP:N	2.38	0.56
2:B:521:THR:OG1	2:B:609:CYS:SG	2.64	0.55
1:A:235:LYS:HZ1	15:O:44:PRO:HG2	1.71	0.55
1:A:412:ASN:HB3	1:A:416:LEU:HD13	1.86	0.55
1:A:1373:ARG:HD3	1:A:1390:GLU:OE2	2.06	0.55
2:B:242:LEU:HD11	2:B:253:ILE:HD13	1.87	0.55
10:J:12:LYS:HE3	10:J:43:ARG:HH22	1.71	0.55
15:O:509:ARG:HG2	16:P:249:TYR:HB2	1.88	0.55
2:B:480:SER:HB3	2:B:483:VAL:HB	1.88	0.55
11:K:65:ILE:HD12	11:K:101:LEU:HD23	1.88	0.55
15:O:343:LYS:O	15:O:347:ASP:N	2.34	0.55
15:O:338:ASP:HB3	15:O:342:ALA:N	2.22	0.55
1:A:1443:PRO:HG3	7:G:52:LEU:HD11	1.89	0.55
5:E:141:VAL:HG23	5:E:142:VAL:H	1.71	0.55
13:M:89:GLN:HB3	14:N:394:VAL:HG22	1.89	0.55
15:O:191:PHE:HD2	15:O:274:VAL:HG21	1.71	0.55
15:O:549:GLN:HE21	15:O:565:LEU:HD22	1.72	0.55
1:A:317:ASP:OD1	1:A:320:GLN:NE2	2.39	0.55
2:B:974:GLU:OE2	2:B:987:MET:HE1	2.07	0.55
3:C:80:ALA:HA	3:C:208:CYS:HA	1.87	0.55
7:G:13:ILE:HG13	7:G:66:SER:HB3	1.87	0.55
7:G:87:GLY:O	7:G:146:ILE:N	2.30	0.55
1:A:165:LYS:NZ	19:S:13:DT:OP2	2.40	0.55
5:E:28:TYR:HA	5:E:64:PRO:HA	1.89	0.55
5:E:88:VAL:HG21	5:E:117:THR:H	1.72	0.55
4:D:17:LEU:O	4:D:21:THR:OG1	2.21	0.55
7:G:3:ILE:HG13	7:G:76:VAL:HG23	1.88	0.55
14:N:297:MET:SD	14:N:303:ARG:NH1	2.80	0.55
2:B:59:LYS:HE2	2:B:519:HIS:HA	1.87	0.55
3:C:8:GLU:HB3	3:C:11:ARG:HG2	1.89	0.55
13:M:227:LEU:HD11	13:M:231:LEU:HD22	1.88	0.55
16:P:219:GLN:HB3	16:P:259:ASP:CG	2.32	0.55
2:B:569:THR:OG1	14:N:275:GLU:OE2	2.24	0.54
4:D:125:ASN:OD1	4:D:126:GLN:N	2.40	0.54
1:A:11:LYS:HG3	2:B:1117:ILE:HD13	1.90	0.54
1:A:481:HIS:HB3	1:A:1099:GLU:OE2	2.07	0.54
1:A:799:SER:OG	1:A:800:LYS:N	2.38	0.54
5:E:38:PRO:HB2	5:E:40:GLU:HG2	1.89	0.54
7:G:156:VAL:HG11	7:G:190:LYS:HZ3	1.73	0.54
1:A:69:THR:HA	7:G:164:LYS:NZ	2.19	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ARG:HB3	1:A:253:PRO:HD2	1.88	0.54
4:D:15:GLU:HA	4:D:18:LYS:HB3	1.89	0.54
5:E:88:VAL:HG23	5:E:117:THR:HG22	1.90	0.54
15:O:652:GLN:HG3	15:O:653:MET:HG3	1.90	0.54
1:A:100:ILE:HG13	1:A:166:LYS:HD3	1.88	0.54
4:D:17:LEU:HB2	4:D:66:LEU:HD23	1.89	0.54
15:O:185:TYR:O	15:O:189:SER:N	2.40	0.54
15:O:286:ARG:NH2	15:O:321:GLN:O	2.41	0.54
1:A:413:ARG:NH1	1:A:456:LEU:HB3	2.23	0.54
2:B:727:LEU:HD11	2:B:788:ARG:HE	1.72	0.54
3:C:197:ARG:NH1	10:J:61:LEU:HD13	2.23	0.54
2:B:263:LEU:HD12	2:B:297:THR:HG22	1.89	0.54
2:B:1022:ILE:HG22	2:B:1023:TYR:H	1.73	0.54
5:E:31:THR:HG22	5:E:34:GLU:HG2	1.88	0.54
7:G:45:CYS:HA	7:G:76:VAL:HA	1.88	0.54
15:O:343:LYS:HA	15:O:346:GLN:HB3	1.89	0.54
15:O:466:PRO:HG2	15:O:467:PHE:CD2	2.43	0.54
16:P:247:LEU:HB3	16:P:252:LYS:HD3	1.88	0.54
5:E:20:LYS:HB3	5:E:35:VAL:HG23	1.90	0.54
2:B:337:VAL:HG23	2:B:338:GLU:H	1.73	0.54
2:B:757:VAL:HG23	2:B:942:ILE:HB	1.90	0.54
2:B:115:PRO:HG3	2:B:163:LEU:HD11	1.88	0.53
5:E:156:LEU:HD11	5:E:195:VAL:HB	1.89	0.53
15:O:102:ARG:O	15:O:123:ASN:ND2	2.37	0.53
3:C:33:VAL:O	3:C:34:GLU:HG3	2.08	0.53
9:I:33:PHE:CD1	9:I:34:PRO:HD2	2.44	0.53
11:K:80:ILE:HG22	11:K:86:VAL:HG11	1.89	0.53
16:P:248:VAL:HG23	16:P:255:LYS:HE2	1.90	0.53
1:A:1163:LYS:NZ	1:A:1280:ARG:HA	2.19	0.53
2:B:914:SER:HB3	2:B:918:GLN:HB2	1.90	0.53
4:D:20:LEU:HD12	4:D:62:VAL:HG11	1.90	0.53
13:M:117:HIS:HB2	13:M:119:TRP:CD1	2.44	0.53
3:C:163:TYR:HD2	3:C:165:ARG:NH1	2.07	0.53
7:G:89:ILE:HD12	7:G:97:ILE:HB	1.91	0.53
10:J:30:LEU:HD22	10:J:31:ASP:H	1.73	0.53
14:N:366:HIS:HB3	14:N:370:LYS:HB2	1.91	0.53
1:A:1059:LEU:HD21	8:H:105:GLU:HA	1.91	0.53
2:B:1061:ARG:HG2	18:R:17:DC:H5"	1.90	0.53
12:L:30:ILE:N	12:L:57:LEU:O	2.42	0.53
15:O:322:LYS:HB3	15:O:361:PHE:CE1	2.42	0.53
1:A:235:LYS:HD2	1:A:252:ARG:HH11	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:541:ILE:HD11	15:O:548:ILE:HG12	1.91	0.53
1:A:1420:THR:HA	2:B:1080:LEU:HD11	1.91	0.53
2:B:618:GLY:HA2	2:B:668:PRO:HB3	1.90	0.53
5:E:112:TYR:HE2	5:E:134:THR:HB	1.74	0.53
8:H:50:ALA:N	8:H:53:ASP:OD2	2.42	0.53
13:M:80:GLY:HA3	13:M:261:LYS:HE2	1.90	0.53
6:F:115:THR:HG22	6:F:116:ASP:H	1.73	0.53
1:A:1223:ASN:HB3	1:A:1231:ALA:HB3	1.91	0.52
2:B:536:LEU:HD22	2:B:571:PHE:CD1	2.44	0.52
3:C:256:ILE:HG22	3:C:267:VAL:HA	1.90	0.52
5:E:88:VAL:HB	5:E:120:ALA:HB2	1.91	0.52
14:N:308:GLN:HB2	14:N:417:VAL:HG12	1.90	0.52
15:O:464:ASN:O	15:O:467:PHE:N	2.43	0.52
1:A:200:GLU:HG2	15:O:515:LYS:HD2	1.90	0.52
2:B:667:VAL:O	2:B:669:SER:N	2.41	0.52
8:H:114:VAL:HG21	8:H:130:ARG:HH11	1.74	0.52
15:O:289:LYS:HZ2	15:O:325:LYS:HG2	1.74	0.52
15:O:551:VAL:HG23	15:O:563:VAL:HG23	1.92	0.52
15:O:564:PHE:C	15:O:565:LEU:HD12	2.34	0.52
7:G:113:ASN:OD1	7:G:113:ASN:N	2.39	0.52
11:K:47:ILE:HG23	11:K:63:PHE:HB3	1.92	0.52
1:A:244:ILE:HG21	1:A:253:PRO:HD3	1.90	0.52
1:A:1207:VAL:O	1:A:1211:ARG:HG2	2.08	0.52
1:A:1311:GLY:O	5:E:147:HIS:NE2	2.42	0.52
2:B:332:ILE:HG13	2:B:333:ALA:H	1.74	0.52
14:N:290:ILE:HG13	14:N:293:LYS:HE2	1.90	0.52
1:A:247:THR:HG23	1:A:249:PRO:HD3	1.92	0.52
14:N:304:PHE:O	14:N:413:ASP:N	2.35	0.52
1:A:1384:LEU:HD12	1:A:1413:GLU:OE2	2.10	0.52
2:B:299:GLN:OE1	13:M:190:ASN:ND2	2.43	0.52
2:B:1067:ARG:HH12	2:B:1079:LEU:HD22	1.75	0.52
3:C:229:LEU:O	3:C:293:ARG:NH2	2.38	0.52
11:K:85:ASP:O	11:K:107:THR:OG1	2.19	0.52
14:N:363:ILE:HG23	14:N:373:VAL:HG22	1.92	0.52
15:O:467:PHE:HE1	15:O:468:LEU:HD22	1.74	0.52
16:P:254:GLU:HB2	16:P:262:ARG:HB2	1.92	0.52
1:A:535:MET:O	1:A:540:ASN:ND2	2.42	0.52
1:A:652:VAL:HG21	1:A:668:VAL:HG21	1.91	0.52
1:A:1145:LEU:HD23	1:A:1146:VAL:HG23	1.92	0.52
2:B:163:LEU:HD22	2:B:171:MET:HE1	1.91	0.52
2:B:536:LEU:HD22	2:B:571:PHE:HD1	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:96:LEU:O	13:M:97:VAL:HG12	2.09	0.52
15:O:337:GLN:O	15:O:338:ASP:HB2	2.09	0.52
1:A:614:ILE:HD13	1:A:624:ILE:HD12	1.92	0.52
2:B:712:ALA:O	2:B:717:GLN:NE2	2.43	0.52
11:K:112:THR:HG22	11:K:113:ALA:H	1.75	0.52
15:O:40:ARG:O	16:P:317:TRP:NE1	2.43	0.52
5:E:109:ILE:HG22	5:E:133:GLU:HB3	1.92	0.52
1:A:182:THR:HG22	1:A:185:TRP:HE1	1.75	0.51
1:A:304:ASP:O	15:O:535:SER:OG	2.15	0.51
4:D:57:GLY:O	4:D:61:ASN:ND2	2.43	0.51
1:A:67:CYS:SG	1:A:69:THR:OG1	2.68	0.51
1:A:221:ASP:N	15:O:550:GLU:HG3	2.25	0.51
1:A:1221:ASP:OD1	1:A:1222:VAL:N	2.43	0.51
2:B:137:ARG:NH2	2:B:413:ALA:O	2.36	0.51
2:B:526:GLU:O	2:B:529:ILE:HG22	2.10	0.51
5:E:50:MET:HG2	5:E:52:ARG:NH1	2.25	0.51
15:O:289:LYS:HD3	15:O:325:LYS:HB3	1.92	0.51
1:A:578:GLN:O	1:A:582:MET:N	2.43	0.51
1:A:653:ILE:HG23	1:A:660:LEU:HB2	1.91	0.51
1:A:1343:MET:HE3	1:A:1350:VAL:HG21	1.92	0.51
2:B:296:TYR:O	2:B:300:GLN:NE2	2.35	0.51
7:G:89:ILE:HG12	7:G:90:SER:N	2.24	0.51
14:N:305:MET:HE3	14:N:414:GLY:HA3	1.93	0.51
3:C:120:LEU:HD13	3:C:125:LYS:HA	1.92	0.51
15:O:188:SER:HA	15:O:191:PHE:HB2	1.92	0.51
16:P:311:VAL:O	16:P:313:TYR:N	2.44	0.51
1:A:305:LYS:HG3	1:A:306:GLY:H	1.76	0.51
1:A:383:PRO:HB3	1:A:502:GLU:HG2	1.92	0.51
1:A:714:ILE:HD13	2:B:958:MET:HE3	1.92	0.51
1:A:1323:PHE:HA	1:A:1327:GLY:HA2	1.93	0.51
1:A:12:ARG:HG3	2:B:1146:ILE:HG12	1.92	0.51
1:A:155:LEU:HG	15:O:336:LEU:HD23	1.92	0.51
1:A:235:LYS:HZ2	15:O:44:PRO:HD2	1.75	0.51
1:A:363:ARG:NH1	2:B:1131:GLU:OE2	2.43	0.51
2:B:137:ARG:HG2	2:B:138:GLY:H	1.75	0.51
2:B:853:ASP:HB2	2:B:855:PRO:HD3	1.93	0.51
8:H:21:ASN:OD1	8:H:22:LYS:N	2.42	0.51
13:M:78:ILE:HG22	13:M:170:LEU:HD22	1.93	0.51
1:A:127:LEU:HD11	1:A:140:ILE:HG21	1.93	0.51
1:A:200:GLU:HA	15:O:515:LYS:HE3	1.92	0.51
1:A:1425:THR:C	6:F:92:ARG:HH21	2.19	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:94:ASP:N	3:C:94:ASP:OD1	2.42	0.51
4:D:3:VAL:HG13	7:G:7:ILE:HG22	1.93	0.51
1:A:60:VAL:HG23	1:A:74:LEU:HD23	1.93	0.51
1:A:629:LYS:HB3	1:A:633:PHE:HE2	1.76	0.51
3:C:201:GLU:OE2	3:C:203:SER:HB2	2.10	0.51
13:M:117:HIS:CE1	13:M:152:GLY:HA3	2.45	0.51
15:O:265:VAL:HG12	15:O:267:PRO:HD3	1.93	0.51
2:B:44:LYS:NZ	2:B:663:GLU:HB2	2.26	0.51
2:B:59:LYS:NZ	2:B:520:ILE:HG13	2.25	0.51
2:B:140:ASN:O	2:B:140:ASN:ND2	2.45	0.50
2:B:262:ILE:HD11	13:M:180:LYS:NZ	2.26	0.50
5:E:20:LYS:O	5:E:23:VAL:HG12	2.11	0.50
9:I:15:THR:HG23	9:I:23:THR:HG23	1.92	0.50
12:L:29:TYR:HA	12:L:58:LYS:HA	1.93	0.50
14:N:303:ARG:HD3	14:N:411:ARG:HD3	1.93	0.50
2:B:390:ASP:OD2	2:B:444:LEU:HG	2.12	0.50
2:B:723:THR:HA	2:B:790:LYS:HG2	1.94	0.50
2:B:985:GLU:O	2:B:988:SER:OG	2.28	0.50
2:B:989:LYS:HA	2:B:992:VAL:HG12	1.92	0.50
3:C:255:VAL:HG22	3:C:256:ILE:H	1.76	0.50
1:A:5:VAL:HG22	7:G:37:LYS:HB3	1.93	0.50
2:B:59:LYS:HZ3	2:B:520:ILE:HG13	1.76	0.50
2:B:103:LYS:NZ	2:B:146:ASP:HB2	2.25	0.50
15:O:201:ILE:HG22	15:O:202:GLN:H	1.76	0.50
1:A:90:VAL:HG13	1:A:258:TRP:HB2	1.93	0.50
2:B:823:SER:OG	2:B:831:GLU:OE2	2.26	0.50
16:P:223:GLU:HG2	16:P:240:ILE:HA	1.94	0.50
1:A:1048:VAL:HG11	1:A:1053:LYS:HB2	1.93	0.50
2:B:83:ILE:HG13	2:B:93:LEU:HB3	1.93	0.50
5:E:123:LEU:HD11	5:E:126:SER:HB3	1.93	0.50
7:G:124:GLU:O	7:G:125:GLU:HB3	2.12	0.50
12:L:28:LYS:HG3	12:L:29:TYR:CD2	2.47	0.50
15:O:299:LEU:HD22	15:O:467:PHE:HE2	1.76	0.50
1:A:226:LYS:HE2	15:O:548:ILE:HG13	1.93	0.50
5:E:173:SER:OG	5:E:174:GLN:N	2.44	0.50
12:L:48:CYS:CB	12:L:51:CYS:HB2	2.38	0.50
1:A:524:THR:HG23	1:A:527:ALA:H	1.76	0.50
1:A:1273:LYS:HG2	1:A:1274:GLY:H	1.76	0.50
2:B:487:ARG:HH21	2:B:508:CYS:HB3	1.77	0.50
5:E:170:LEU:HB3	5:E:174:GLN:NE2	2.27	0.50
15:O:314:ILE:HG21	15:O:370:LEU:HD21	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ASN:ND2	15:O:561:ARG:HD3	2.27	0.50
1:A:1205:ILE:O	1:A:1209:ILE:N	2.44	0.50
15:O:463:SER:HB3	16:P:262:ARG:HH12	1.77	0.50
1:A:332:VAL:C	1:A:334:PRO:HD3	2.37	0.49
1:A:723:LEU:HD21	1:A:811:ALA:HA	1.93	0.49
1:A:1143:ALA:HA	1:A:1314:THR:HG22	1.93	0.49
2:B:831:GLU:OE1	2:B:831:GLU:N	2.38	0.49
2:B:1067:ARG:HH22	2:B:1079:LEU:HB3	1.77	0.49
7:G:44:LEU:O	7:G:77:PHE:N	2.44	0.49
12:L:29:TYR:CE2	12:L:40:LEU:HB2	2.45	0.49
13:M:72:GLU:O	14:N:364:ARG:HG2	2.12	0.49
1:A:896:LEU:HB3	1:A:1090:GLY:HA3	1.94	0.49
2:B:113:THR:OG1	2:B:117:GLU:OE1	2.24	0.49
2:B:258:LYS:O	2:B:297:THR:OG1	2.16	0.49
2:B:247:ILE:HG12	2:B:251:ILE:HD11	1.94	0.49
3:C:90:SER:HB2	3:C:200:GLN:HB3	1.94	0.49
5:E:115:ASN:OD1	5:E:116:ILE:N	2.45	0.49
5:E:213:ILE:HG12	5:E:214:CYS:H	1.77	0.49
6:F:134:ILE:N	6:F:146:TRP:O	2.46	0.49
1:A:1372:THR:HG23	1:A:1375:GLY:H	1.77	0.49
1:A:984:VAL:HG21	1:A:988:ASP:HB3	1.94	0.49
3:C:45:SER:HB2	3:C:53:ASN:HB3	1.92	0.49
1:A:127:LEU:HD22	1:A:240:GLU:OE2	2.12	0.49
7:G:121:TYR:HB2	7:G:128:TRP:CZ3	2.47	0.49
15:O:574:TYR:HB3	15:O:578:ARG:HH12	1.77	0.49
2:B:404:ASP:HA	2:B:407:LEU:HB2	1.93	0.49
15:O:549:GLN:CD	15:O:567:ARG:HE	2.20	0.49
1:A:356:ARG:NH2	2:B:1046:LEU:HD21	2.28	0.49
15:O:327:ARG:HH12	15:O:330:LEU:HD22	1.78	0.49
15:O:500:LEU:HD23	15:O:504:ALA:HB2	1.93	0.49
16:P:215:TYR:CZ	16:P:262:ARG:HD3	2.48	0.49
1:A:39:LEU:C	1:A:41:ASP:H	2.21	0.49
1:A:842:PRO:O	1:A:843:GLN:HB3	2.13	0.49
2:B:211:GLU:HG3	2:B:212:LYS:HD2	1.93	0.49
2:B:417:ASP:O	2:B:421:SER:HB2	2.12	0.49
2:B:615:VAL:HG12	2:B:620:SER:HA	1.94	0.49
14:N:292:ARG:O	14:N:296:LYS:N	2.46	0.49
15:O:50:LYS:HA	15:O:53:VAL:HG12	1.93	0.49
15:O:326:ILE:HG23	15:O:653:MET:HE1	1.94	0.49
1:A:22:SER:C	1:A:24:ALA:H	2.21	0.49
1:A:204:VAL:HG12	1:A:212:GLU:OE2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:GLN:HG2	2:B:232:TYR:CD1	2.48	0.49
3:C:239:ILE:HG22	3:C:288:LYS:HE2	1.95	0.49
3:C:280:LEU:HA	3:C:286:ALA:HB2	1.95	0.49
15:O:174:TYR:O	15:O:177:SER:OG	2.28	0.49
15:O:195:CYS:SG	15:O:196:GLU:N	2.86	0.49
1:A:303:LEU:HG	15:O:538:ALA:HB1	1.95	0.48
1:A:599:LYS:HG3	1:A:600:PRO:HD3	1.94	0.48
2:B:210:ASP:OD1	2:B:211:GLU:N	2.45	0.48
2:B:756:THR:HG23	2:B:941:ASP:H	1.78	0.48
2:B:849:THR:HG23	2:B:850:ASN:H	1.78	0.48
3:C:29:ASN:HB2	3:C:35:LYS:HZ1	1.76	0.48
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.93	0.48
2:B:934:ASN:HA	2:B:1005:TYR:CD2	2.48	0.48
15:O:581:LEU:HD13	15:O:648:TRP:CD2	2.48	0.48
16:P:247:LEU:CB	16:P:252:LYS:HD3	2.44	0.48
1:A:481:HIS:CD2	1:A:483:LEU:HB2	2.49	0.48
2:B:625:ILE:HD12	2:B:628:ARG:HE	1.79	0.48
7:G:162:SER:O	7:G:166:ARG:N	2.41	0.48
15:O:291:ARG:HA	15:O:294:LYS:HD3	1.94	0.48
1:A:742:ILE:HD11	1:A:840:LYS:HE2	1.96	0.48
1:A:955:LEU:HD13	1:A:959:ILE:HG12	1.94	0.48
3:C:329:LYS:NZ	11:K:122:LYS:HB2	2.29	0.48
4:D:61:ASN:HB3	7:G:103:GLY:O	2.13	0.48
8:H:8:ASP:OD1	8:H:9:ILE:N	2.43	0.48
8:H:39:THR:N	8:H:124:ARG:O	2.41	0.48
8:H:105:GLU:HG2	8:H:115:TYR:HE1	1.79	0.48
16:P:221:ILE:O	16:P:225:ILE:N	2.43	0.48
1:A:232:LYS:NZ	16:P:316:GLU:HB3	2.28	0.48
1:A:862:LEU:HD21	2:B:491:PRO:HA	1.95	0.48
1:A:1187:ARG:HG2	1:A:1229:ARG:HG3	1.95	0.48
2:B:720:ARG:NH2	2:B:722:ASP:OD2	2.37	0.48
15:O:215:TRP:O	15:O:219:TYR:HB2	2.14	0.48
1:A:1347:GLY:O	1:A:1348:MET:HG2	2.13	0.48
2:B:239:LYS:NZ	2:B:241:TYR:CZ	2.81	0.48
4:D:110:LEU:HB3	4:D:120:LYS:HZ2	1.78	0.48
15:O:583:TRP:HE1	16:P:315:ASP:HB3	1.79	0.48
1:A:980:SER:HB3	5:E:163:GLU:HG2	1.95	0.48
1:A:1225:ILE:HG23	1:A:1226:GLY:H	1.79	0.48
2:B:464:ILE:O	2:B:468:GLY:N	2.45	0.48
9:I:23:THR:OG1	9:I:24:LEU:N	2.47	0.48
9:I:33:PHE:CG	9:I:34:PRO:HD2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:159:ILE:HD12	15:O:174:TYR:CE1	2.48	0.48
2:B:86:ASP:O	2:B:87:VAL:HG23	2.14	0.48
2:B:727:LEU:HB2	2:B:786:GLU:HB2	1.95	0.48
2:B:775:LYS:HE3	2:B:927:LYS:HA	1.94	0.48
3:C:255:VAL:HG13	3:C:256:ILE:H	1.79	0.48
7:G:23:ILE:HG22	7:G:51:LEU:HD23	1.96	0.48
3:C:197:ARG:HH11	10:J:61:LEU:HD13	1.78	0.48
1:A:599:LYS:H	1:A:602:TYR:HE1	1.61	0.48
1:A:1140:ILE:HG22	1:A:1296:GLU:HG3	1.95	0.48
1:A:1325:VAL:HG23	1:A:1326:LEU:H	1.79	0.48
2:B:371:TYR:HB2	2:B:492:SER:OG	2.13	0.48
5:E:173:SER:C	5:E:175:LEU:H	2.22	0.48
1:A:674:LYS:HZ3	1:A:928:GLY:HA2	1.78	0.47
1:A:1441:LEU:HD21	7:G:54:VAL:HG12	1.96	0.47
2:B:776:SER:HA	2:B:779:ASP:HB3	1.95	0.47
10:J:16:ASP:OD1	10:J:16:ASP:N	2.47	0.47
15:O:203:ILE:HG13	15:O:203:ILE:O	2.14	0.47
15:O:299:LEU:HD22	15:O:467:PHE:CE2	2.49	0.47
15:O:467:PHE:HD1	15:O:468:LEU:HB2	1.79	0.47
15:O:553:ARG:NH1	15:O:554:THR:HB	2.29	0.47
16:P:264:THR:HG23	16:P:265:LEU:H	1.78	0.47
17:Q:48:THR:HG22	17:Q:51:GLU:H	1.79	0.47
1:A:1020:ALA:HA	1:A:1032:LEU:HD21	1.96	0.47
2:B:422:ILE:HA	2:B:425:HIS:HB3	1.96	0.47
2:B:811:VAL:HG12	2:B:813:GLU:H	1.79	0.47
3:C:3:ASN:HD21	3:C:296:ASN:HB2	1.79	0.47
10:J:7:CYS:SG	10:J:11:GLY:N	2.79	0.47
1:A:1411:VAL:HG13	1:A:1412:SER:H	1.78	0.47
2:B:519:HIS:O	2:B:609:CYS:N	2.45	0.47
7:G:104:ILE:HG13	7:G:105:PHE:CD2	2.48	0.47
15:O:328:ASP:OD1	15:O:329:PRO:HD3	2.13	0.47
1:A:766:ILE:HG21	1:A:822:ARG:NH1	2.30	0.47
3:C:43:ASN:HB2	3:C:55:ASP:HB3	1.96	0.47
3:C:105:PRO:HG3	10:J:6:ARG:HH21	1.79	0.47
15:O:255:LYS:HB3	15:O:256:PRO:HD3	1.97	0.47
1:A:1134:LYS:HA	1:A:1320:LEU:HD23	1.95	0.47
2:B:88:ASP:CG	2:B:89:PRO:HD2	2.39	0.47
2:B:181:PRO:HB2	2:B:470:MET:HE1	1.97	0.47
14:N:375:ILE:HG22	14:N:376:GLY:H	1.80	0.47
15:O:54:LYS:HA	15:O:58:GLY:HA2	1.96	0.47
1:A:39:LEU:C	1:A:41:ASP:N	2.72	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:117:THR:OG1	5:E:118:PRO:HD2	2.15	0.47
1:A:387:LEU:HD21	1:A:393:ALA:HB2	1.95	0.47
1:A:408:VAL:HG23	1:A:412:ASN:HB2	1.96	0.47
1:A:444:LEU:HD21	1:A:449:ARG:HG2	1.96	0.47
1:A:1095:GLN:NE2	2:B:1068:ASP:OD2	2.44	0.47
1:A:1284:ASN:OD1	1:A:1285:ILE:N	2.47	0.47
1:A:1408:VAL:HG23	1:A:1413:GLU:HG3	1.95	0.47
2:B:331:VAL:HG23	2:B:335:LEU:HD22	1.97	0.47
2:B:698:ARG:NH2	2:B:952:ARG:HG2	2.28	0.47
2:B:992:VAL:HG23	3:C:278:GLU:HG2	1.97	0.47
5:E:70:SER:OG	5:E:71:LYS:N	2.47	0.47
5:E:86:PRO:HA	5:E:113:GLN:HB3	1.97	0.47
8:H:87:ARG:HB2	8:H:87:ARG:NH1	2.29	0.47
1:A:308:SER:N	1:A:311:ASN:HD21	2.12	0.47
1:A:674:LYS:NZ	1:A:928:GLY:HA2	2.29	0.47
1:A:1064:GLU:HB3	1:A:1065:LYS:H	1.43	0.47
7:G:118:GLY:HA3	7:G:131:PRO:HD3	1.96	0.47
7:G:151:GLU:HB3	7:G:198:GLY:HA2	1.97	0.47
1:A:21:LEU:HD22	1:A:25:ASP:OD2	2.14	0.47
2:B:225:HIS:HA	2:B:446:ARG:HH11	1.80	0.47
7:G:80:PHE:CE2	7:G:83:GLU:HB2	2.50	0.47
9:I:34:PRO:O	9:I:35:ILE:HG13	2.15	0.47
14:N:316:PHE:HE1	14:N:360:VAL:HA	1.80	0.47
1:A:333:ASN:OD1	1:A:333:ASN:N	2.48	0.47
1:A:1390:GLU:OE2	18:R:13:DT:H4'	2.15	0.47
2:B:741:ILE:HB	2:B:746:TYR:HB3	1.97	0.47
5:E:55:ARG:HD2	5:E:82:PHE:HE2	1.80	0.47
15:O:506:ARG:HH12	15:O:526:ALA:HB1	1.79	0.47
2:B:204:ARG:HB2	2:B:204:ARG:NH1	2.30	0.46
5:E:143:ASN:OD1	5:E:143:ASN:N	2.48	0.46
15:O:325:LYS:HD3	15:O:480:TYR:CD1	2.50	0.46
1:A:311:ASN:OD1	1:A:312:MET:N	2.43	0.46
1:A:395:PRO:HG2	1:A:398:VAL:HG22	1.97	0.46
1:A:890:MET:O	1:A:894:GLU:N	2.48	0.46
2:B:613:ILE:HG12	2:B:646:VAL:HG12	1.97	0.46
15:O:492:TYR:HH	15:O:573:SER:HG	1.63	0.46
1:A:133:ASP:OD1	1:A:134:ASN:N	2.48	0.46
1:A:183:PHE:CD2	1:A:184:ARG:HG3	2.51	0.46
2:B:108:THR:OG1	2:B:109:LYS:N	2.47	0.46
2:B:299:GLN:HB2	13:M:190:ASN:HD22	1.81	0.46
3:C:30:GLU:HG3	11:K:84:PRO:HD3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:98:MET:SD	4:D:160:TYR:OH	2.72	0.46
5:E:1:MET:HB3	5:E:4:GLU:HG2	1.97	0.46
14:N:296:LYS:HA	14:N:296:LYS:HD3	1.76	0.46
15:O:51:GLU:OE2	15:O:589:LEU:HB3	2.15	0.46
2:B:269:MET:O	2:B:273:CYS:HB3	2.14	0.46
2:B:543:LEU:HG	13:M:176:VAL:HG11	1.97	0.46
15:O:467:PHE:CD1	15:O:468:LEU:HB2	2.50	0.46
15:O:549:GLN:HB2	15:O:565:LEU:O	2.14	0.46
1:A:386:ASN:ND2	11:K:94:PRO:O	2.48	0.46
2:B:854:ALA:N	2:B:855:PRO:HD3	2.31	0.46
3:C:127:THR:HG22	3:C:128:ASP:H	1.81	0.46
4:D:130:ASN:HB3	4:D:133:HIS:CE1	2.51	0.46
4:D:135:TYR:HA	4:D:141:CYS:SG	2.55	0.46
16:P:257:THR:OG1	16:P:258:HIS:N	2.48	0.46
1:A:1033:GLU:HG2	1:A:1034:PRO:HD2	1.96	0.46
2:B:378:GLU:OE2	2:B:382:GLN:HB2	2.15	0.46
16:P:255:LYS:HE3	16:P:261:TYR:CE1	2.50	0.46
1:A:444:LEU:HD11	1:A:449:ARG:H	1.81	0.46
2:B:98:ILE:HG13	2:B:131:VAL:HG12	1.97	0.46
2:B:916:HIS:CD2	2:B:957:LYS:HB2	2.51	0.46
19:S:14:DG:H2"	19:S:15:DA:C8	2.50	0.46
1:A:179:ILE:HD12	15:O:557:ARG:NE	2.29	0.46
5:E:6:GLU:HA	5:E:9:ILE:HG12	1.98	0.46
15:O:192:VAL:HG12	15:O:274:VAL:H	1.80	0.46
1:A:869:ARG:HH21	2:B:489:LEU:HD12	1.81	0.46
1:A:978:ASP:N	1:A:982:CYS:O	2.45	0.46
1:A:1153:ALA:HA	1:A:1156:VAL:HB	1.96	0.46
2:B:121:ARG:CZ	12:L:54:ARG:HH21	2.29	0.46
2:B:831:GLU:OE2	2:B:834:MET:HB3	2.17	0.46
3:C:74:GLU:HA	3:C:212:ILE:HD11	1.97	0.46
3:C:175:GLN:O	3:C:178:THR:HG23	2.16	0.46
3:C:251:PHE:CD2	3:C:255:VAL:HG21	2.51	0.46
4:D:10:PHE:HD2	4:D:117:LYS:HE3	1.81	0.46
13:M:255:PHE:O	13:M:259:ILE:HG12	2.15	0.46
15:O:282:ILE:HG22	15:O:283:ASN:H	1.80	0.46
1:A:542:LEU:HD21	1:A:679:TYR:HE1	1.80	0.45
1:A:1059:LEU:HD22	1:A:1060:TYR:CE1	2.51	0.45
1:A:1451:LEU:HG	4:D:107:MET:HB3	1.98	0.45
2:B:572:VAL:HG12	2:B:576:ARG:HH12	1.80	0.45
2:B:1088:ASP:OD1	2:B:1088:ASP:N	2.49	0.45
3:C:81:GLU:OE2	3:C:219:PHE:HZ	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:122:ASP:HB3	13:M:145:VAL:HG21	1.98	0.45
13:M:126:ASP:HB3	13:M:128:GLN:HG2	1.97	0.45
16:P:216:SER:HB3	16:P:222:LEU:HD11	1.97	0.45
2:B:92:TYR:CZ	2:B:136:THR:HG21	2.51	0.45
2:B:312:MET:HB3	2:B:317:LEU:HG	1.98	0.45
2:B:795:LEU:HB2	2:B:894:ALA:HB3	1.99	0.45
5:E:29:PHE:HB2	5:E:65:THR:HB	1.97	0.45
15:O:620:LEU:HD23	15:O:623:GLU:HB2	1.98	0.45
3:C:229:LEU:HB3	3:C:293:ARG:CZ	2.47	0.45
15:O:515:LYS:O	15:O:516:LEU:HD12	2.16	0.45
1:A:51:ASN:O	1:A:55:ASP:HB2	2.15	0.45
1:A:132:VAL:HG11	1:A:137:ARG:HH11	1.81	0.45
2:B:625:ILE:HD11	2:B:628:ARG:HH21	1.81	0.45
3:C:116:VAL:HG22	3:C:117:ASP:H	1.81	0.45
4:D:109:LYS:NZ	4:D:109:LYS:HB3	2.32	0.45
4:D:110:LEU:O	4:D:120:LYS:NZ	2.50	0.45
15:O:191:PHE:O	15:O:194:LEU:HB2	2.17	0.45
1:A:163:VAL:HG22	1:A:164:VAL:H	1.81	0.45
3:C:255:VAL:HG13	3:C:256:ILE:N	2.32	0.45
1:A:235:LYS:NZ	1:A:254:GLU:OE2	2.49	0.45
1:A:1391:LYS:NZ	18:R:12:DT:H4'	2.32	0.45
5:E:172:GLU:HG2	5:E:173:SER:H	1.82	0.45
7:G:52:LEU:O	7:G:53:THR:HG22	2.17	0.45
15:O:87:ASP:O	15:O:88:VAL:HG12	2.16	0.45
15:O:289:LYS:NZ	15:O:325:LYS:HG2	2.32	0.45
1:A:235:LYS:HD3	1:A:235:LYS:HA	1.83	0.45
1:A:372:ARG:HG3	2:B:1060:LEU:O	2.17	0.45
1:A:671:ASP:CG	1:A:672:GLY:H	2.20	0.45
1:A:1151:GLU:HG3	1:A:1152:ARG:H	1.81	0.45
2:B:1000:GLY:HA3	2:B:1018:PHE:HD1	1.81	0.45
4:D:116:PHE:O	4:D:120:LYS:HB2	2.16	0.45
1:A:11:LYS:NZ	2:B:1145:ASP:HB3	2.32	0.45
1:A:742:ILE:HG12	1:A:840:LYS:HB3	1.99	0.45
1:A:1173:VAL:HG22	1:A:1186:VAL:HG12	1.98	0.45
1:A:1323:PHE:HD1	1:A:1328:ILE:H	1.63	0.45
2:B:93:LEU:HD12	2:B:134:GLU:O	2.17	0.45
2:B:804:ASP:OD1	2:B:804:ASP:N	2.49	0.45
6:F:143:PHE:O	6:F:144:GLU:HB2	2.16	0.45
7:G:119:CYS:HA	7:G:129:ILE:O	2.17	0.45
7:G:159:LYS:N	7:G:160:PRO:HD3	2.32	0.45
1:A:62:SER:H	1:A:65:LEU:HD12	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ASN:HD21	15:O:561:ARG:N	2.10	0.45
2:B:465:SER:OG	2:B:707:LYS:O	2.33	0.45
2:B:517:MET:HE2	2:B:611:PRO:HG2	1.99	0.45
2:B:889:SER:OG	2:B:893:GLN:HG2	2.17	0.45
4:D:20:LEU:HD21	7:G:47:THR:HG21	1.99	0.45
15:O:569:LYS:HD3	15:O:569:LYS:HA	1.81	0.45
1:A:913:GLN:NE2	1:A:915:THR:O	2.50	0.45
2:B:77:ILE:HD13	2:B:98:ILE:HB	1.98	0.45
2:B:103:LYS:HG2	2:B:104:SER:H	1.82	0.45
3:C:222:VAL:HG13	3:C:302:VAL:HG23	1.99	0.45
3:C:256:ILE:HA	3:C:268:LYS:H	1.81	0.45
13:M:121:ILE:O	13:M:148:LEU:N	2.44	0.45
15:O:550:GLU:HG2	15:O:550:GLU:O	2.17	0.45
16:P:245:GLU:HA	16:P:248:VAL:HB	1.99	0.45
1:A:997:GLN:HB2	1:A:998:TYR:HD1	1.82	0.44
1:A:1190:LEU:HA	1:A:1193:ILE:HD12	1.99	0.44
1:A:1300:LEU:O	1:A:1303:VAL:HG12	2.16	0.44
2:B:217:GLN:NE2	2:B:352:MET:HG2	2.32	0.44
2:B:983:LYS:HG3	2:B:985:GLU:H	1.82	0.44
4:D:27:HIS:C	4:D:29:TRP:H	2.25	0.44
1:A:179:ILE:HA	1:A:221:ASP:HA	1.99	0.44
1:A:409:THR:O	1:A:411:TYR:N	2.51	0.44
1:A:706:GLY:HA2	2:B:762:TYR:HA	1.99	0.44
2:B:289:GLU:HA	2:B:292:LYS:HG2	1.98	0.44
2:B:447:PHE:HB3	2:B:449:MET:HG2	1.98	0.44
3:C:255:VAL:HG22	3:C:256:ILE:N	2.31	0.44
5:E:47:CYS:HA	5:E:53:PRO:HA	1.98	0.44
7:G:97:ILE:HG22	7:G:128:TRP:NE1	2.32	0.44
15:O:163:VAL:HA	15:O:169:LEU:HD13	1.99	0.44
15:O:553:ARG:HH11	15:O:554:THR:HB	1.83	0.44
2:B:240:ILE:HG13	2:B:253:ILE:HG21	2.00	0.44
2:B:425:HIS:O	2:B:428:ASN:ND2	2.50	0.44
16:P:252:LYS:HG2	16:P:253:LEU:HG	1.99	0.44
1:A:1163:LYS:HB3	1:A:1164:THR:H	1.41	0.44
3:C:85:PHE:CE1	3:C:204:LEU:HD22	2.53	0.44
7:G:104:ILE:HG23	7:G:105:PHE:N	2.32	0.44
12:L:60:ARG:HG2	12:L:61:THR:H	1.82	0.44
15:O:253:ILE:HD13	15:O:330:LEU:HD21	1.99	0.44
16:P:315:ASP:O	16:P:317:TRP:HD1	1.99	0.44
1:A:321:LEU:HD22	1:A:336:MET:HG3	2.00	0.44
1:A:378:ARG:HH12	18:R:18:DC:H4'	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:MET:HE1	2:B:950:PRO:HA	1.99	0.44
2:B:97:ASP:OD2	2:B:99:ARG:NH1	2.39	0.44
2:B:241:TYR:CD2	2:B:250:GLU:HB2	2.53	0.44
5:E:54:GLN:HG3	5:E:57:MET:HE2	2.00	0.44
7:G:44:LEU:HD23	7:G:104:ILE:HD11	1.99	0.44
1:A:365:ARG:HH11	1:A:887:ARG:NH2	2.15	0.44
1:A:630:ASN:ND2	1:A:650:GLY:O	2.51	0.44
1:A:817:ILE:HG13	1:A:821:ASN:O	2.18	0.44
2:B:241:TYR:CG	2:B:250:GLU:HB2	2.52	0.44
2:B:804:ASP:HB3	2:B:848:PRO:HD3	1.98	0.44
2:B:842:TYR:HE1	2:B:873:TYR:HB2	1.82	0.44
13:M:88:PHE:HD2	14:N:397:LEU:HD13	1.82	0.44
15:O:634:GLU:O	15:O:637:VAL:HG12	2.17	0.44
1:A:371:LYS:HZ1	2:B:1088:ASP:CG	2.25	0.44
2:B:69:VAL:HA	2:B:73:LEU:HD23	1.99	0.44
2:B:550:HIS:NE2	2:B:551:LEU:HD23	2.33	0.44
2:B:717:GLN:OE1	2:B:727:LEU:HD22	2.17	0.44
2:B:932:PRO:HB3	2:B:1004:LEU:HB3	1.99	0.44
3:C:284:GLU:HA	3:C:287:ASP:OD2	2.18	0.44
15:O:495:VAL:HG11	15:O:577:MET:HE3	1.99	0.44
15:O:576:PHE:O	15:O:579:GLN:HG2	2.18	0.44
1:A:182:THR:HG22	1:A:185:TRP:NE1	2.33	0.44
2:B:39:ASN:OD1	2:B:40:THR:N	2.47	0.44
2:B:60:GLN:CD	2:B:60:GLN:H	2.26	0.44
2:B:190:THR:OG1	2:B:191:GLU:N	2.51	0.44
2:B:1008:ILE:O	3:C:65:ASN:ND2	2.51	0.44
14:N:399:ILE:HD13	14:N:406:ALA:H	1.83	0.44
1:A:1202:ILE:HD12	1:A:1228:ASP:HA	1.98	0.44
2:B:337:VAL:HG23	2:B:345:LYS:HZ3	1.83	0.44
2:B:444:LEU:O	2:B:448:LYS:HA	2.18	0.44
2:B:803:GLN:HG2	2:B:804:ASP:H	1.82	0.44
3:C:283:GLU:O	3:C:286:ALA:N	2.51	0.44
7:G:60:LYS:NZ	7:G:63:ASP:HB2	2.32	0.44
15:O:549:GLN:CG	15:O:565:LEU:HB2	2.46	0.44
1:A:93:ILE:HG23	1:A:94:GLY:H	1.83	0.43
1:A:252:ARG:HH12	15:O:46:LEU:HD22	1.83	0.43
1:A:431:ASN:OD1	1:A:465:HIS:NE2	2.51	0.43
1:A:541:LEU:HD22	1:A:682:LEU:HD22	1.98	0.43
2:B:418:ALA:O	2:B:422:ILE:HG12	2.18	0.43
2:B:1028:LYS:HG2	2:B:1029:HIS:H	1.83	0.43
3:C:92:ILE:H	3:C:92:ILE:HG13	1.59	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:123:ILE:C	13:M:145:VAL:HG23	2.42	0.43
14:N:373:VAL:HG12	14:N:374:LYS:H	1.83	0.43
15:O:74:LEU:HD21	15:O:79:LEU:HG	2.00	0.43
15:O:641:LEU:O	15:O:645:LEU:HB2	2.17	0.43
1:A:46:ARG:HG3	1:A:48:PRO:HD3	1.99	0.43
1:A:862:LEU:HD22	2:B:494:PHE:HB2	1.99	0.43
1:A:985:LYS:O	1:A:987:GLU:N	2.51	0.43
2:B:938:ILE:H	2:B:938:ILE:HG13	1.63	0.43
8:H:12:VAL:HG12	8:H:13:SER:H	1.82	0.43
15:O:115:LYS:HB3	15:O:116:LYS:H	1.58	0.43
15:O:197:MET:HG3	15:O:198:GLY:H	1.83	0.43
16:P:252:LYS:HZ2	16:P:253:LEU:CB	2.28	0.43
16:P:254:GLU:HG3	16:P:264:THR:HG22	2.01	0.43
18:R:15:DC:H2"	18:R:16:DG:OP2	2.18	0.43
1:A:113:ILE:HG12	1:A:115:LEU:H	1.82	0.43
1:A:424:PRO:HG3	1:A:444:LEU:O	2.18	0.43
1:A:988:ASP:O	1:A:992:ALA:N	2.46	0.43
2:B:934:ASN:HB3	2:B:1004:LEU:HA	2.01	0.43
3:C:33:VAL:HG12	3:C:34:GLU:H	1.84	0.43
3:C:177:THR:HG23	3:C:178:THR:H	1.83	0.43
5:E:24:LYS:HB2	5:E:30:ILE:HD11	2.00	0.43
13:M:228:THR:HG22	13:M:229:GLY:H	1.82	0.43
14:N:366:HIS:N	14:N:370:LYS:O	2.51	0.43
14:N:390:PHE:CD1	14:N:390:PHE:C	2.95	0.43
15:O:159:ILE:O	15:O:163:VAL:HG23	2.18	0.43
15:O:329:PRO:C	15:O:331:THR:H	2.25	0.43
1:A:143:LYS:HA	1:A:146:ASP:OD2	2.18	0.43
1:A:387:LEU:O	1:A:501:ASN:ND2	2.51	0.43
1:A:979:ASN:O	5:E:167:ARG:NH2	2.51	0.43
2:B:477:PHE:C	2:B:479:LYS:H	2.27	0.43
2:B:775:LYS:C	2:B:777:SER:H	2.27	0.43
3:C:132:ILE:O	3:C:208:CYS:HB2	2.18	0.43
3:C:328:LEU:HG	11:K:121:LEU:HD21	2.01	0.43
4:D:70:LYS:HG3	4:D:98:MET:SD	2.59	0.43
18:R:3:DG:H2"	18:R:4:DT:OP2	2.18	0.43
1:A:409:THR:C	1:A:411:TYR:H	2.26	0.43
1:A:627:ASP:OD1	1:A:627:ASP:N	2.51	0.43
1:A:666:LYS:HG2	1:A:797:CYS:O	2.19	0.43
1:A:862:LEU:O	1:A:866:ILE:HG12	2.19	0.43
1:A:995:VAL:O	1:A:996:ASP:HB3	2.19	0.43
2:B:87:VAL:HG12	2:B:407:LEU:HD22	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:698:ARG:HH21	2:B:952:ARG:CG	2.29	0.43
2:B:929:GLU:HB3	3:C:69:ARG:HG2	2.00	0.43
3:C:59:ILE:HB	3:C:63:ILE:HD11	2.01	0.43
15:O:226:ILE:HG23	15:O:229:ASN:H	1.83	0.43
15:O:262:ILE:HG12	15:O:278:VAL:HG21	2.00	0.43
1:A:310:ASN:HD22	15:O:561:ARG:HD3	1.83	0.43
1:A:379:THR:HG22	1:A:380:VAL:H	1.84	0.43
1:A:757:ASN:OD1	1:A:757:ASN:N	2.52	0.43
2:B:59:LYS:HZ2	2:B:60:GLN:NE2	2.17	0.43
7:G:7:ILE:O	7:G:71:THR:OG1	2.27	0.43
7:G:89:ILE:HG23	7:G:142:VAL:HA	2.00	0.43
13:M:90:TYR:HB3	13:M:179:LEU:HB3	2.01	0.43
15:O:356:THR:HB	15:O:357:PRO:HD3	2.01	0.43
15:O:597:GLN:HA	15:O:600:SER:HB2	2.01	0.43
1:A:378:ARG:HH21	1:A:516:GLU:HB2	1.83	0.43
1:A:661:SER:HB2	8:H:122:LEU:HD11	1.99	0.43
1:A:1426:GLY:HA2	6:F:92:ARG:NH2	2.34	0.43
1:A:1439:LYS:HE2	1:A:1439:LYS:HA	2.00	0.43
5:E:43:LYS:O	5:E:47:CYS:HB2	2.19	0.43
7:G:47:THR:OG1	7:G:48:ILE:N	2.51	0.43
11:K:83:ASN:HA	11:K:84:PRO:HD3	1.87	0.43
15:O:516:LEU:HB3	15:O:567:ARG:HD3	1.99	0.43
1:A:493:ARG:HB3	1:A:494:PRO:HD2	2.01	0.43
1:A:1038:GLU:HB3	1:A:1042:ILE:HD11	2.01	0.43
1:A:1365:LYS:HE3	1:A:1379:MET:HB2	1.99	0.43
1:A:1442:VAL:HA	1:A:1443:PRO:HD3	1.76	0.43
2:B:327:ILE:O	2:B:330:THR:OG1	2.35	0.43
5:E:40:GLU:HG3	5:E:41:ASP:H	1.82	0.43
7:G:147:ARG:NH2	7:G:211:TRP:HH2	2.17	0.43
15:O:370:LEU:HD13	15:O:370:LEU:HA	1.91	0.43
16:P:314:PHE:C	16:P:316:GLU:H	2.27	0.43
17:Q:59:ILE:HG22	17:Q:63:LYS:HE3	2.01	0.43
1:A:376:SER:HB2	2:B:1060:LEU:HD12	2.01	0.43
2:B:676:GLU:HA	2:B:677:PRO:HD2	1.91	0.43
2:B:736:VAL:HG21	2:B:960:GLU:HG3	2.01	0.43
14:N:290:ILE:HD13	14:N:384:LYS:HE3	2.00	0.43
15:O:53:VAL:HA	15:O:56:HIS:HB3	2.00	0.43
1:A:220:ASP:HA	15:O:550:GLU:OE2	2.19	0.43
1:A:1084:GLU:O	1:A:1087:THR:OG1	2.34	0.43
2:B:687:LEU:O	2:B:915:ARG:NH2	2.52	0.43
3:C:104:VAL:HA	3:C:105:PRO:HD3	1.90	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:85:MET:HE2	6:F:151:LEU:HD22	2.00	0.43
8:H:132:LEU:HD12	8:H:133:ASN:N	2.32	0.43
11:K:97:SER:OG	11:K:98:GLU:N	2.52	0.43
16:P:255:LYS:HD2	16:P:255:LYS:N	2.34	0.43
1:A:545:LYS:HG3	1:A:546:SER:H	1.83	0.42
1:A:635:PRO:HA	1:A:636:PRO:HD3	1.88	0.42
1:A:1174:GLN:HB3	1:A:1185:GLN:HB3	2.01	0.42
2:B:401:LEU:HA	2:B:404:ASP:OD2	2.19	0.42
2:B:933:PHE:O	2:B:934:ASN:ND2	2.52	0.42
13:M:109:ALA:HB3	13:M:122:ASP:HB2	2.01	0.42
15:O:510:CYS:HA	15:O:513:ASP:OD2	2.19	0.42
1:A:196:ILE:O	1:A:200:GLU:HG3	2.20	0.42
1:A:393:ALA:HB3	1:A:499:ARG:HG3	2.00	0.42
15:O:550:GLU:CD	15:O:550:GLU:H	2.27	0.42
1:A:165:LYS:HZ2	1:A:184:ARG:HH22	1.67	0.42
1:A:185:TRP:HE3	1:A:194:LYS:HE2	1.85	0.42
1:A:247:THR:C	1:A:249:PRO:HD3	2.44	0.42
1:A:308:SER:OG	1:A:309:ILE:N	2.52	0.42
1:A:774:ARG:HH22	1:A:804:LEU:HD11	1.83	0.42
2:B:38:ILE:HD11	2:B:43:ASP:OD2	2.19	0.42
2:B:44:LYS:HZ1	2:B:663:GLU:HB2	1.83	0.42
2:B:260:CYS:O	2:B:342:PHE:HB3	2.19	0.42
2:B:610:ARG:HA	2:B:611:PRO:HD3	1.77	0.42
2:B:905:ARG:O	2:B:907:GLU:N	2.50	0.42
14:N:395:ILE:HD12	14:N:396:ALA:H	1.84	0.42
1:A:667:SER:HA	1:A:671:ASP:O	2.19	0.42
1:A:1302:ASP:OD1	1:A:1303:VAL:N	2.53	0.42
2:B:364:LYS:HG3	2:B:365:MET:H	1.84	0.42
8:H:58:THR:O	8:H:143:LEU:N	2.48	0.42
13:M:91:ALA:HA	14:N:391:LEU:HD21	2.01	0.42
15:O:192:VAL:HG12	15:O:274:VAL:HG13	2.02	0.42
15:O:467:PHE:CE1	15:O:468:LEU:HD22	2.53	0.42
1:A:270:PRO:HD3	2:B:1046:LEU:HD13	2.01	0.42
1:A:468:ASP:OD1	1:A:469:GLY:N	2.52	0.42
1:A:712:ILE:HG22	1:A:713:GLY:H	1.84	0.42
1:A:1166:LEU:O	1:A:1170:ALA:HB2	2.20	0.42
2:B:372:VAL:O	2:B:607:ARG:NH1	2.51	0.42
2:B:675:ILE:HG13	2:B:676:GLU:H	1.84	0.42
2:B:914:SER:C	2:B:916:HIS:H	2.28	0.42
3:C:20:PHE:CE2	3:C:23:PHE:HB3	2.54	0.42
3:C:192:LEU:HD11	10:J:19:GLU:HG2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:113:PHE:CE2	4:D:153:MET:HG2	2.55	0.42
13:M:113:LYS:HG3	13:M:116:SER:O	2.19	0.42
13:M:164:LYS:NZ	14:N:300:LYS:HG2	2.35	0.42
15:O:105:LYS:HD2	15:O:209:THR:N	2.35	0.42
1:A:952:LYS:HB3	1:A:953:GLY:H	1.53	0.42
2:B:110:ASP:OD1	2:B:110:ASP:N	2.53	0.42
5:E:195:VAL:HG22	5:E:213:ILE:HG13	2.01	0.42
7:G:29:GLN:O	7:G:33:LYS:HG2	2.20	0.42
14:N:293:LYS:HA	14:N:296:LYS:HB2	2.02	0.42
15:O:156:VAL:HA	15:O:159:ILE:HG12	2.02	0.42
19:S:6:DA:OP2	19:S:6:DA:C8	2.73	0.42
2:B:806:ILE:H	2:B:806:ILE:HG13	1.62	0.42
2:B:911:LYS:HD3	2:B:919:LYS:NZ	2.35	0.42
5:E:82:PHE:CE1	5:E:111:VAL:HB	2.55	0.42
10:J:42:LYS:HG3	10:J:43:ARG:H	1.85	0.42
15:O:512:ARG:HH22	15:O:568:CYS:HA	1.84	0.42
16:P:229:GLN:C	16:P:231:ALA:H	2.26	0.42
1:A:967:LEU:HD11	1:A:1009:ARG:HD3	2.02	0.42
2:B:121:ARG:NH2	12:L:54:ARG:HH21	2.17	0.42
2:B:321:GLN:O	2:B:324:ILE:HG22	2.19	0.42
2:B:474:SER:HA	2:B:511:VAL:HG12	2.01	0.42
3:C:120:LEU:HA	3:C:121:PRO:HD2	1.88	0.42
3:C:259:ASP:HB2	3:C:266:TYR:HE1	1.85	0.42
3:C:260:GLU:HG2	3:C:261:GLY:H	1.84	0.42
5:E:112:TYR:N	5:E:135:PHE:O	2.45	0.42
5:E:182:ASP:HA	5:E:183:PRO:HD2	1.85	0.42
7:G:59:LEU:HD13	7:G:65:SER:O	2.19	0.42
15:O:203:ILE:HG12	15:O:279:SER:HB2	2.02	0.42
1:A:360:LYS:HA	1:A:360:LYS:HD2	1.83	0.42
1:A:1148:ASP:OD1	1:A:1291:ARG:NH1	2.52	0.42
1:A:1406:ASP:CG	1:A:1407:ALA:H	2.28	0.42
2:B:502:THR:HA	2:B:503:PRO:HD3	1.83	0.42
7:G:149:ARG:O	7:G:198:GLY:HA3	2.19	0.42
15:O:46:LEU:HB3	15:O:47:PHE:H	1.64	0.42
2:B:586:GLU:HG3	2:B:648:TYR:HD2	1.85	0.42
2:B:779:ASP:OD2	3:C:217:ALA:N	2.32	0.42
7:G:4:LEU:HD23	7:G:73:ARG:HH21	1.85	0.42
7:G:8:ALA:HA	7:G:71:THR:HA	2.01	0.42
7:G:89:ILE:HG12	7:G:90:SER:H	1.85	0.42
15:O:570:GLU:HG2	15:O:571:THR:N	2.35	0.42
17:Q:44:ASN:CG	17:Q:45:GLY:H	2.28	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:TYR:O	1:A:99:THR:N	2.52	0.41
1:A:643:ASN:HB2	1:A:651:PHE:CE2	2.55	0.41
1:A:955:LEU:HA	1:A:956:PRO:HD2	1.89	0.41
4:D:138:VAL:HG13	4:D:141:CYS:HB2	2.01	0.41
8:H:131:ASN:OD1	8:H:131:ASN:N	2.53	0.41
15:O:53:VAL:HG21	15:O:65:ILE:HD12	2.01	0.41
2:B:319:ILE:HD12	2:B:319:ILE:HA	1.92	0.41
2:B:529:ILE:HG23	2:B:530:LYS:N	2.35	0.41
3:C:263:ASP:OD1	3:C:264:GLU:N	2.52	0.41
2:B:477:PHE:HB3	2:B:478:GLU:H	1.47	0.41
2:B:800:ASN:ND2	2:B:853:ASP:O	2.51	0.41
3:C:87:ASN:O	3:C:88:ASN:HB2	2.20	0.41
5:E:191:LYS:HB2	5:E:194:GLU:OE2	2.20	0.41
6:F:114:GLU:OE2	6:F:120:ILE:HG22	2.20	0.41
8:H:93:TYR:CD2	8:H:143:LEU:HG	2.55	0.41
15:O:193:GLN:NE2	15:O:196:GLU:OE1	2.53	0.41
1:A:571:TYR:O	1:A:604:TRP:N	2.49	0.41
1:A:676:SER:O	1:A:680:THR:OG1	2.32	0.41
1:A:1065:LYS:HA	1:A:1068:ARG:HB2	2.02	0.41
2:B:124:THR:OG1	2:B:125:TYR:N	2.53	0.41
2:B:915:ARG:HD2	2:B:1023:TYR:HD2	1.85	0.41
2:B:1080:LEU:O	2:B:1084:MET:HB3	2.20	0.41
3:C:91:VAL:HB	3:C:92:ILE:H	1.63	0.41
9:I:35:ILE:CD1	9:I:36:GLU:H	2.32	0.41
13:M:82:GLU:O	13:M:83:GLU:HG2	2.20	0.41
13:M:83:GLU:HB2	14:N:400:ALA:HB2	2.01	0.41
15:O:43:ASN:HB3	15:O:47:PHE:HB2	2.03	0.41
15:O:169:LEU:O	15:O:279:SER:HB3	2.21	0.41
15:O:335:LEU:HD12	15:O:336:LEU:O	2.20	0.41
15:O:591:LYS:HB2	16:P:308:ASP:OD2	2.21	0.41
1:A:220:ASP:HA	15:O:550:GLU:CG	2.50	0.41
1:A:326:TYR:CD2	1:A:327:ILE:HG23	2.56	0.41
2:B:134:GLU:HG2	2:B:144:HIS:ND1	2.35	0.41
7:G:152:ARG:HB3	7:G:197:LEU:HG	2.02	0.41
11:K:60:SER:HB3	11:K:104:ARG:NH2	2.35	0.41
14:N:395:ILE:HD13	14:N:410:GLY:C	2.46	0.41
15:O:592:LYS:HG3	15:O:637:VAL:HG11	2.03	0.41
1:A:827:PHE:HB3	2:B:655:ASN:OD1	2.20	0.41
2:B:145:LYS:HD2	2:B:419:LEU:HD21	2.02	0.41
2:B:757:VAL:O	2:B:1019:PHE:HB2	2.19	0.41
3:C:42:VAL:HG13	11:K:138:LYS:HD3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:238:PRO:O	3:C:239:ILE:HG13	2.20	0.41
1:A:371:LYS:HE3	1:A:371:LYS:HB3	1.95	0.41
1:A:995:VAL:HB	1:A:997:GLN:H	1.86	0.41
1:A:1172:TYR:HE1	1:A:1174:GLN:HB2	1.85	0.41
13:M:246:THR:O	14:N:405:SER:HB2	2.21	0.41
15:O:468:LEU:HA	15:O:468:LEU:HD12	1.85	0.41
1:A:132:VAL:HG13	1:A:136:ARG:HB2	2.01	0.41
1:A:1026:ARG:NH2	1:A:1052:VAL:HG13	2.36	0.41
2:B:576:ARG:HG2	2:B:580:ARG:HD3	2.03	0.41
5:E:46:TYR:CZ	5:E:58:MET:HA	2.56	0.41
8:H:108:SER:OG	8:H:109:LYS:N	2.53	0.41
15:O:101:LEU:HD21	15:O:130:LEU:HD11	2.03	0.41
15:O:208:TYR:O	15:O:209:THR:OG1	2.37	0.41
1:A:132:VAL:HG11	1:A:137:ARG:HH12	1.80	0.41
1:A:297:SER:HA	1:A:300:LYS:HB3	2.02	0.41
1:A:1428:PHE:CZ	6:F:89:GLU:HA	2.56	0.41
2:B:139:ARG:HB3	2:B:141:ILE:HD11	2.02	0.41
2:B:265:ASP:O	2:B:267:GLU:N	2.54	0.41
2:B:269:MET:HE1	9:I:2:LEU:HD21	2.03	0.41
2:B:710:ILE:HG13	2:B:728:MET:HE3	2.03	0.41
2:B:795:LEU:HD23	2:B:845:LYS:HZ3	1.86	0.41
2:B:796:LYS:HZ3	2:B:798:TYR:HE1	1.65	0.41
2:B:841:ILE:H	2:B:841:ILE:HG12	1.67	0.41
2:B:890:ASP:N	2:B:890:ASP:OD1	2.54	0.41
4:D:13:ASP:OD2	4:D:66:LEU:HG	2.21	0.41
5:E:17:ARG:HD3	5:E:35:VAL:HG22	2.03	0.41
7:G:94:ALA:HB2	7:G:121:TYR:CD2	2.56	0.41
13:M:74:PHE:CE2	14:N:364:ARG:NH1	2.89	0.41
13:M:113:LYS:HE3	13:M:118:LEU:HD23	2.02	0.41
14:N:389:THR:O	14:N:390:PHE:CD2	2.74	0.41
14:N:404:SER:OG	14:N:405:SER:N	2.54	0.41
15:O:357:PRO:HA	15:O:361:PHE:CD2	2.55	0.41
15:O:516:LEU:O	15:O:565:LEU:HD23	2.21	0.41
15:O:579:GLN:HB2	16:P:317:TRP:C	2.46	0.41
15:O:591:LYS:HE2	16:P:308:ASP:OD2	2.20	0.41
16:P:252:LYS:HE3	16:P:252:LYS:HB3	1.94	0.41
20:T:12:A:H2'	20:T:13:G:O4'	2.21	0.41
1:A:115:LEU:HG	1:A:116:SER:H	1.86	0.41
1:A:1145:LEU:O	1:A:1310:ILE:HG22	2.21	0.41
1:A:1163:LYS:HZ1	1:A:1280:ARG:N	2.18	0.41
2:B:538:VAL:HG12	2:B:565:ILE:HD12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:934:ASN:ND2	2:B:1004:LEU:HD22	2.36	0.41
3:C:21:PRO:HD2	11:K:82:LYS:HA	2.02	0.41
7:G:34:PHE:O	7:G:37:LYS:HD3	2.21	0.41
7:G:115:LEU:HD23	7:G:116:PHE:HD1	1.85	0.41
13:M:160:ALA:HA	14:N:306:VAL:HA	2.03	0.41
15:O:366:LEU:HD23	15:O:452:LEU:HD13	2.03	0.41
1:A:382:SER:HA	1:A:383:PRO:HD3	1.83	0.40
1:A:653:ILE:HG12	1:A:660:LEU:HD22	2.03	0.40
1:A:1021:ASN:HA	1:A:1024:LYS:HG2	2.03	0.40
1:A:1411:VAL:HG23	1:A:1421:MET:HE2	2.02	0.40
2:B:180:ASP:HA	2:B:181:PRO:HD3	1.89	0.40
2:B:402:SER:HA	2:B:405:LYS:HZ3	1.85	0.40
2:B:735:MET:HB2	2:B:754:ASN:HD21	1.85	0.40
3:C:284:GLU:CD	3:C:288:LYS:HZ1	2.29	0.40
8:H:17:PRO:HB3	8:H:24:CYS:HB2	2.03	0.40
13:M:122:ASP:HB3	13:M:145:VAL:CG2	2.51	0.40
15:O:647:LEU:O	15:O:650:VAL:HG12	2.21	0.40
1:A:96:PHE:CZ	1:A:166:LYS:HD2	2.56	0.40
1:A:238:ASP:OD1	1:A:238:ASP:N	2.53	0.40
1:A:645:MET:HE1	8:H:124:ARG:HD2	2.02	0.40
2:B:757:VAL:HG12	2:B:1020:GLY:O	2.21	0.40
3:C:276:SER:O	3:C:277:ARG:HG2	2.21	0.40
4:D:151:GLU:HA	4:D:154:LEU:HD13	2.03	0.40
5:E:22:MET:HE3	5:E:26:ARG:HH21	1.86	0.40
8:H:31:THR:OG1	8:H:32:THR:N	2.54	0.40
15:O:492:TYR:OH	15:O:573:SER:OG	2.32	0.40
1:A:620:SER:HA	1:A:621:PRO:HD3	1.85	0.40
1:A:905:ARG:NH2	5:E:170:LEU:HD21	2.32	0.40
1:A:1083:LEU:HD23	1:A:1083:LEU:HA	1.91	0.40
1:A:1184:ILE:O	1:A:1231:ALA:HA	2.21	0.40
3:C:31:TRP:CE2	11:K:123:ASP:HB3	2.57	0.40
4:D:31:GLN:HA	4:D:34:LEU:HD12	2.02	0.40
15:O:550:GLU:N	15:O:550:GLU:OE1	2.54	0.40
18:R:2:DA:H2''	18:R:3:DG:H5'	2.03	0.40
1:A:14:LYS:NZ	2:B:1144:GLU:OE1	2.41	0.40
1:A:252:ARG:HH22	15:O:46:LEU:CD2	2.34	0.40
1:A:284:ASP:O	1:A:288:LYS:HG2	2.22	0.40
1:A:953:GLY:HA2	1:A:1063:SER:HB2	2.02	0.40
1:A:1391:LYS:HA	1:A:1391:LYS:HD2	1.58	0.40
2:B:257:LEU:HD12	2:B:257:LEU:HA	1.95	0.40
3:C:143:ASN:HB3	3:C:156:LEU:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:34:ILE:HD12	15:O:34:ILE:HA	1.98	0.40
15:O:522:ILE:HD13	15:O:522:ILE:HA	1.92	0.40
15:O:568:CYS:HB3	15:O:569:LYS:H	1.48	0.40
1:A:809:MET:HE2	2:B:953:MET:HA	2.04	0.40
1:A:946:THR:HG21	1:A:1066:SER:HA	2.04	0.40
2:B:113:THR:HA	2:B:114:PRO:HD3	1.88	0.40
2:B:121:ARG:NH1	12:L:54:ARG:NH2	2.57	0.40
2:B:565:ILE:HG12	2:B:566:ARG:N	2.36	0.40
2:B:688:ILE:HD12	2:B:688:ILE:H	1.87	0.40
4:D:58:ILE:H	4:D:58:ILE:HG13	1.74	0.40
6:F:115:THR:HG22	6:F:116:ASP:N	2.35	0.40
15:O:581:LEU:HD13	15:O:648:TRP:CE2	2.57	0.40
16:P:180:THR:HG23	16:P:181:ILE:H	1.86	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	1414/1460 (97%)	1166 (82%)	234 (16%)	14 (1%)	12	45
2	B	1112/1149 (97%)	943 (85%)	160 (14%)	9 (1%)	16	50
3	C	333/335 (99%)	284 (85%)	44 (13%)	5 (2%)	8	37
4	D	113/161 (70%)	83 (74%)	30 (26%)	0	100	100
5	E	213/215 (99%)	172 (81%)	39 (18%)	2 (1%)	14	47
6	F	81/155 (52%)	73 (90%)	8 (10%)	0	100	100
7	G	185/212 (87%)	155 (84%)	24 (13%)	6 (3%)	3	25
8	H	136/146 (93%)	115 (85%)	21 (15%)	0	100	100
9	I	40/110 (36%)	33 (82%)	6 (15%)	1 (2%)	4	29
10	J	65/70 (93%)	53 (82%)	11 (17%)	1 (2%)	8	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	99/142 (70%)	84 (85%)	15 (15%)	0	100	100
12	L	43/70 (61%)	34 (79%)	9 (21%)	0	100	100
13	M	160/282 (57%)	138 (86%)	20 (12%)	2 (1%)	9	40
14	N	106/422 (25%)	82 (77%)	23 (22%)	1 (1%)	14	47
15	O	533/654 (82%)	437 (82%)	89 (17%)	7 (1%)	9	40
16	P	83/317 (26%)	54 (65%)	24 (29%)	5 (6%)	1	15
17	Q	26/104 (25%)	23 (88%)	2 (8%)	1 (4%)	2	21
All	All	4742/6004 (79%)	3929 (83%)	759 (16%)	54 (1%)	14	43

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	587	ILE
1	A	1371	ILE
13	M	97	VAL
13	M	107	ILE
15	O	88	VAL
15	O	146	VAL
16	P	175	ILE
16	P	311	VAL
16	P	312	VAL
1	A	40	PHE
1	A	602	TYR
1	A	632	VAL
2	B	87	VAL
3	C	239	ILE
14	N	411	ARG
15	O	469	ASN
16	P	230	VAL
1	A	39	LEU
1	A	307	ILE
1	A	975	VAL
1	A	995	VAL
2	B	811	VAL
2	B	927	LYS
9	I	35	ILE
1	A	23	ALA
1	A	601	TYR
1	A	1328	ILE
2	B	632	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	651	VAL
2	B	713	ILE
2	B	767	ILE
3	C	91	VAL
3	C	119	ASN
3	C	255	VAL
7	G	191	PRO
15	O	338	ASP
15	O	368	ARG
17	Q	43	ILE
1	A	599	LYS
1	A	1389	PHE
2	B	264	SER
3	C	87	ASN
7	G	79	PRO
7	G	80	PHE
10	J	65	PRO
5	E	122	LYS
15	O	330	LEU
16	P	233	VAL
5	E	88	VAL
7	G	158	VAL
7	G	160	PRO
7	G	192	PRO
2	B	584	VAL
15	O	227	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	1231/1257 (98%)	1186 (96%)	45 (4%)	30	53
2	B	975/1006 (97%)	934 (96%)	41 (4%)	26	50
3	C	296/296 (100%)	281 (95%)	15 (5%)	21	46
4	D	110/145 (76%)	106 (96%)	4 (4%)	31	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	197/197 (100%)	187 (95%)	10 (5%)	21	46
6	F	73/137 (53%)	72 (99%)	1 (1%)	59	71
7	G	170/190 (90%)	162 (95%)	8 (5%)	23	48
8	H	123/128 (96%)	118 (96%)	5 (4%)	27	51
9	I	38/98 (39%)	37 (97%)	1 (3%)	40	60
10	J	62/65 (95%)	57 (92%)	5 (8%)	11	35
11	K	91/130 (70%)	91 (100%)	0	100	100
12	L	40/57 (70%)	38 (95%)	2 (5%)	22	47
13	M	142/249 (57%)	135 (95%)	7 (5%)	22	47
14	N	92/360 (26%)	88 (96%)	4 (4%)	26	49
15	O	495/593 (84%)	474 (96%)	21 (4%)	26	50
16	P	86/285 (30%)	83 (96%)	3 (4%)	32	54
17	Q	24/56 (43%)	24 (100%)	0	100	100
All	All	4245/5249 (81%)	4073 (96%)	172 (4%)	28	51

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	55	ASP
1	A	104	GLN
1	A	124	LEU
1	A	160	LEU
1	A	164	VAL
1	A	220	ASP
1	A	222	LEU
1	A	247	THR
1	A	289	LEU
1	A	327	ILE
1	A	379	THR
1	A	381	ILE
1	A	408	VAL
1	A	506	THR
1	A	542	LEU
1	A	712	ILE
1	A	747	LYS
1	A	813	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	817	ILE
1	A	848	VAL
1	A	904	VAL
1	A	955	LEU
1	A	1029	LEU
1	A	1053	LYS
1	A	1059	LEU
1	A	1064	GLU
1	A	1087	THR
1	A	1161	VAL
1	A	1164	THR
1	A	1186	VAL
1	A	1193	ILE
1	A	1224	ILE
1	A	1271	VAL
1	A	1272	VAL
1	A	1294	LEU
1	A	1295	VAL
1	A	1310	ILE
1	A	1325	VAL
1	A	1328	ILE
1	A	1350	VAL
1	A	1391	LYS
1	A	1408	VAL
1	A	1411	VAL
1	A	1423	ILE
2	B	73	LEU
2	B	87	VAL
2	B	133	ILE
2	B	141	ILE
2	B	147	VAL
2	B	186	ILE
2	B	191	GLU
2	B	234	ILE
2	B	251	ILE
2	B	327	ILE
2	B	331	VAL
2	B	337	VAL
2	B	366	ILE
2	B	377	LEU
2	B	383	LEU
2	B	422	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	457	VAL
2	B	511	VAL
2	B	536	LEU
2	B	538	VAL
2	B	545	ASP
2	B	551	LEU
2	B	555	VAL
2	B	565	ILE
2	B	612	LEU
2	B	615	VAL
2	B	666	ILE
2	B	675	ILE
2	B	713	ILE
2	B	723	THR
2	B	741	ILE
2	B	772	VAL
2	B	806	ILE
2	B	818	ILE
2	B	860	VAL
2	B	871	VAL
2	B	899	LEU
2	B	938	ILE
2	B	954	THR
2	B	1022	ILE
2	B	1047	THR
3	C	33	VAL
3	C	59	ILE
3	C	78	VAL
3	C	89	THR
3	C	91	VAL
3	C	104	VAL
3	C	120	LEU
3	C	133	VAL
3	C	193	LEU
3	C	208	CYS
3	C	210	LEU
3	C	239	ILE
3	C	274	THR
3	C	294	VAL
3	C	302	VAL
4	D	109	LYS
4	D	127	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	134	LEU
4	D	138	VAL
5	E	6	GLU
5	E	9	ILE
5	E	78	LEU
5	E	80	VAL
5	E	90	VAL
5	E	102	GLU
5	E	109	ILE
5	E	117	THR
5	E	124	VAL
5	E	196	VAL
6	F	133	VAL
7	G	3	ILE
7	G	23	ILE
7	G	42	VAL
7	G	53	THR
7	G	97	ILE
7	G	108	ILE
7	G	113	ASN
7	G	115	LEU
8	H	12	VAL
8	H	26	ILE
8	H	44	VAL
8	H	59	ILE
8	H	132	LEU
9	I	35	ILE
10	J	3	VAL
10	J	13	VAL
10	J	16	ASP
10	J	24	LEU
10	J	30	LEU
12	L	34	CYS
12	L	48	CYS
13	M	83	GLU
13	M	87	VAL
13	M	97	VAL
13	M	125	LEU
13	M	145	VAL
13	M	228	THR
13	M	242	ASN
14	N	313	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	N	373	VAL
14	N	412	VAL
14	N	416	ILE
15	O	42	LEU
15	O	64	VAL
15	O	88	VAL
15	O	112	ILE
15	O	131	LEU
15	O	152	HIS
15	O	169	LEU
15	O	186	THR
15	O	206	LEU
15	O	226	ILE
15	O	282	ILE
15	O	299	LEU
15	O	307	VAL
15	O	328	ASP
15	O	335	LEU
15	O	468	LEU
15	O	516	LEU
15	O	525	THR
15	O	551	VAL
15	O	563	VAL
15	O	576	PHE
16	P	235	LEU
16	P	250	ASP
16	P	265	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	HIS
1	A	310	ASN
1	A	355	GLN
1	A	412	ASN
1	A	422	ASN
1	A	566	HIS
1	A	675	HIS
1	A	934	ASN
1	A	1233	ASN
1	A	1317	ASN
1	A	1385	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	60	GLN
2	B	626	HIS
2	B	655	ASN
2	B	702	GLN
2	B	865	GLN
4	D	27	HIS
4	D	122	GLN
5	E	5	ASN
5	E	54	GLN
5	E	113	GLN
6	F	104	ASN
8	H	133	ASN
13	M	117	HIS
13	M	190	ASN
15	O	244	ASN
15	O	298	ASN
15	O	337	GLN
15	O	346	GLN
15	O	549	GLN
15	O	652	GLN
16	P	176	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	T	9/9 (100%)	2 (22%)	1 (11%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	T	8	G
20	T	10	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	T	7	A

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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
17	Q	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Q	1088:UNK	C	1090:UNK	N	14.86
1	Q	69:PRO	C	1070:UNK	N	8.26

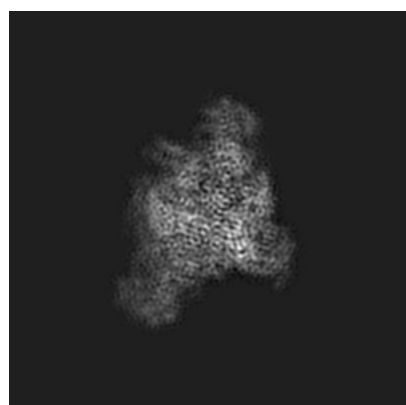
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3178. These allow visual inspection of the internal detail of the map and identification of artifacts.

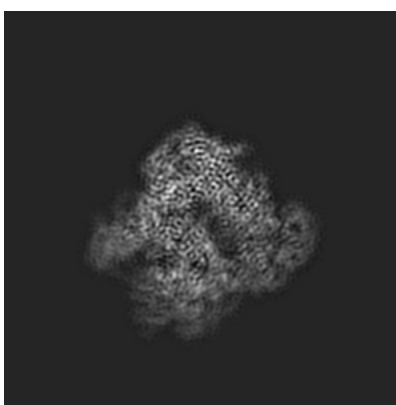
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

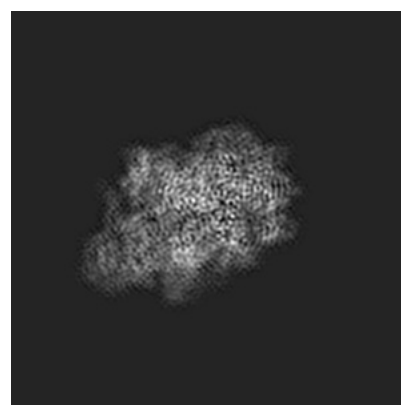
6.1.1 Primary map



X



Y

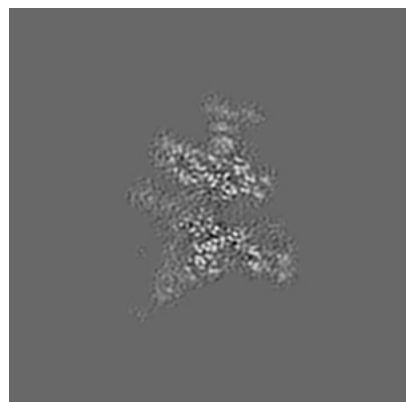


Z

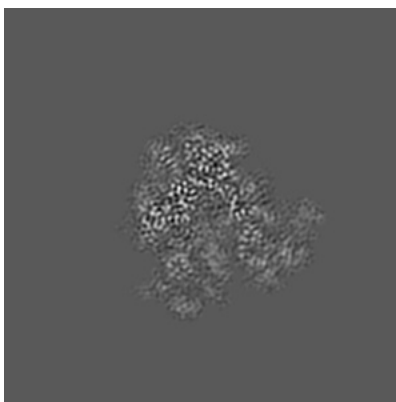
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

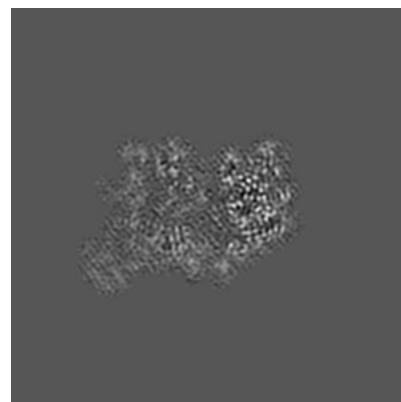
6.2.1 Primary map



X Index: 148



Y Index: 148

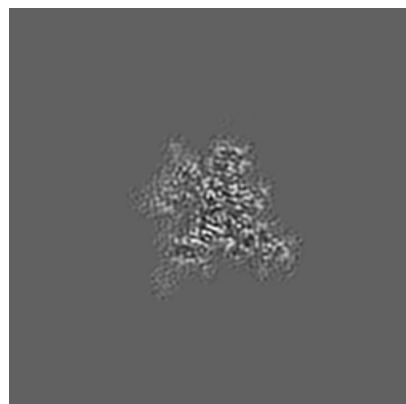


Z Index: 148

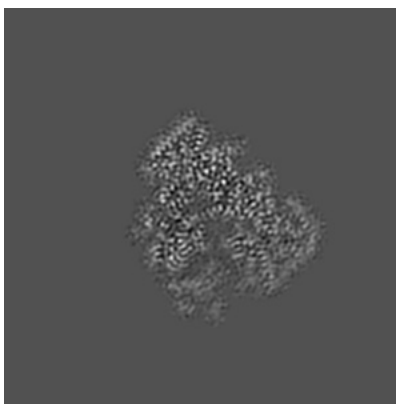
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

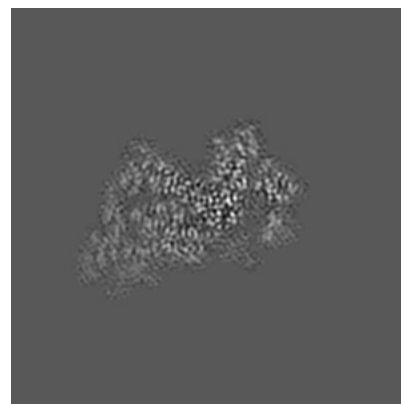
6.3.1 Primary map



X Index: 161



Y Index: 161

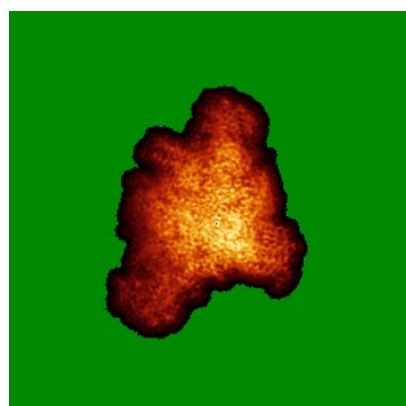


Z Index: 132

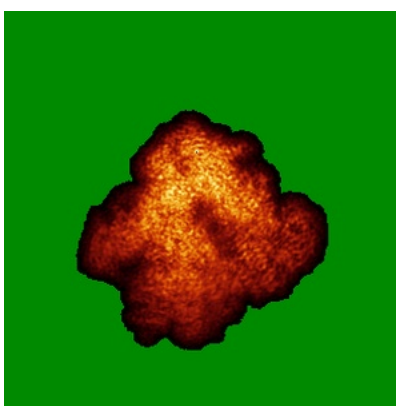
The images above show the largest variance slices of the map in three orthogonal directions.

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

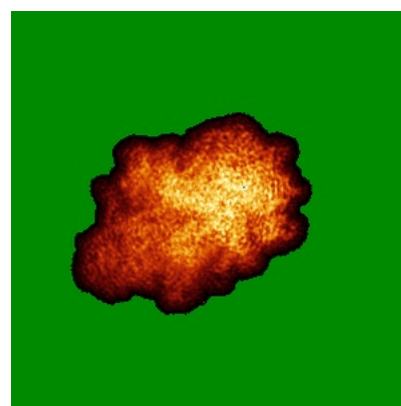
6.4.1 Primary map



X



Y

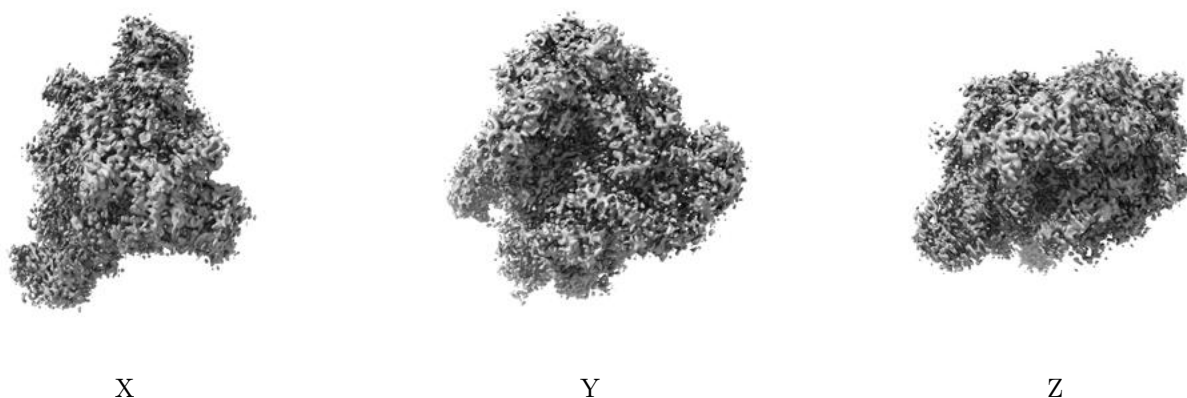


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

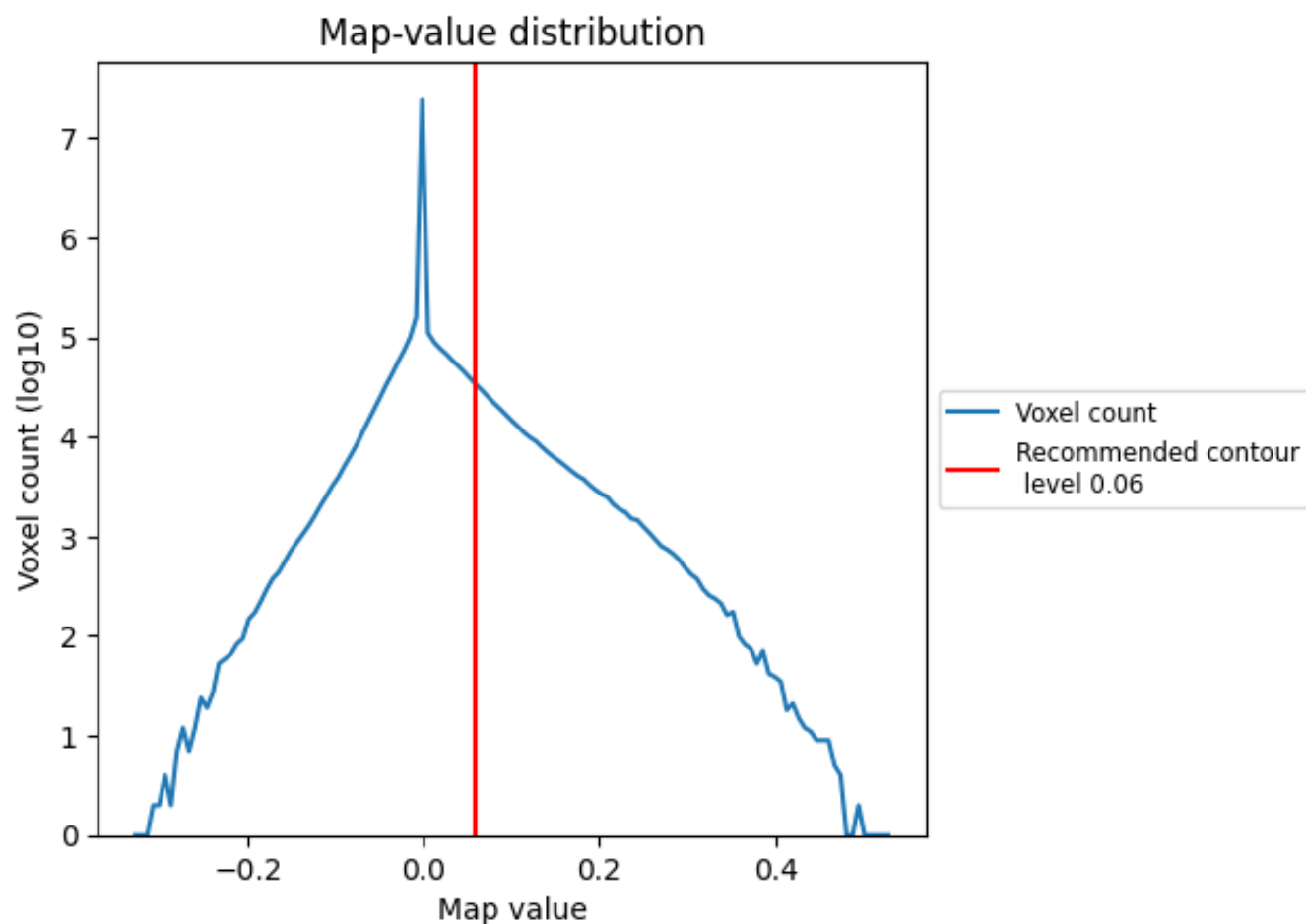
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

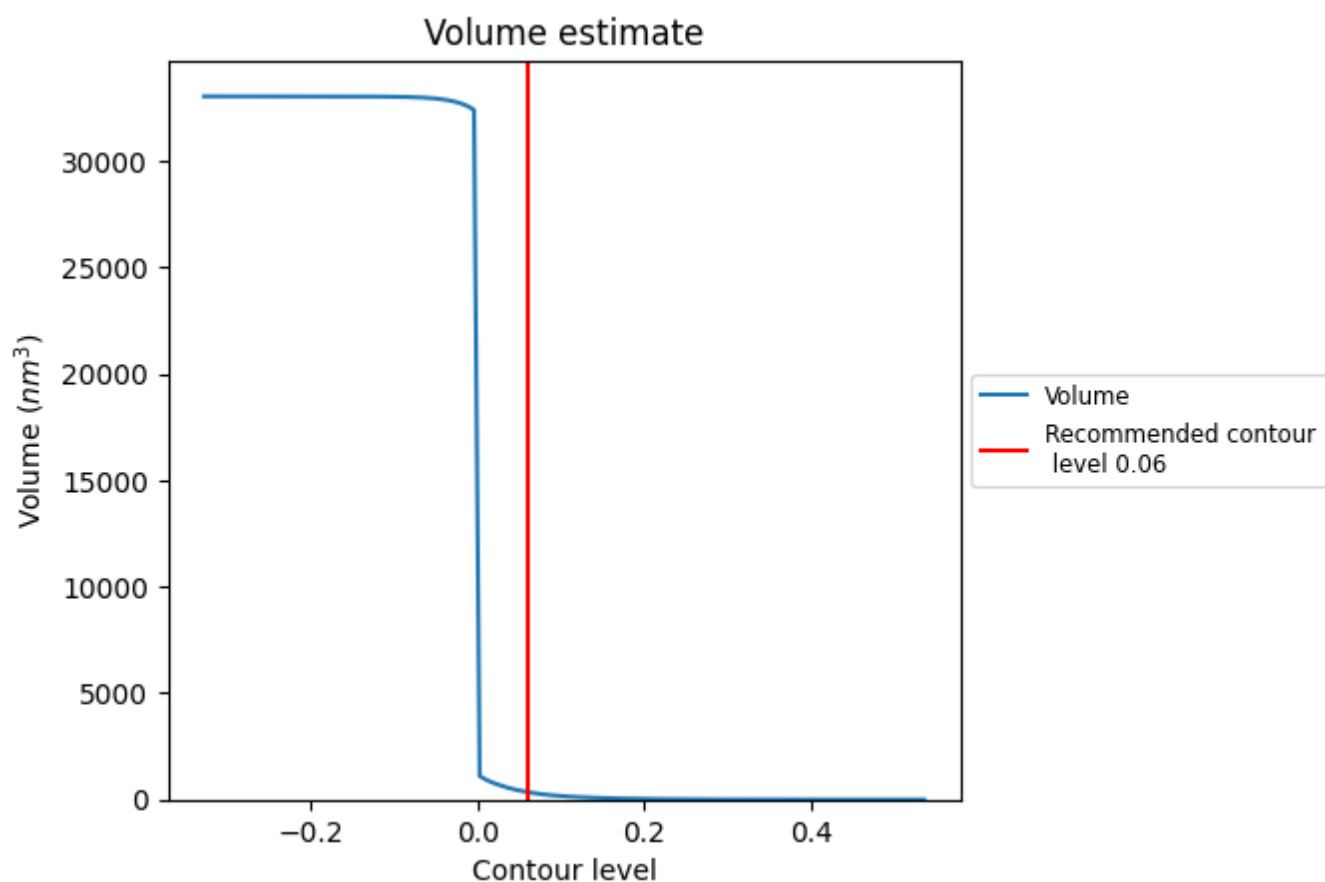
This section contains the results of statistical analysis of the map.

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.

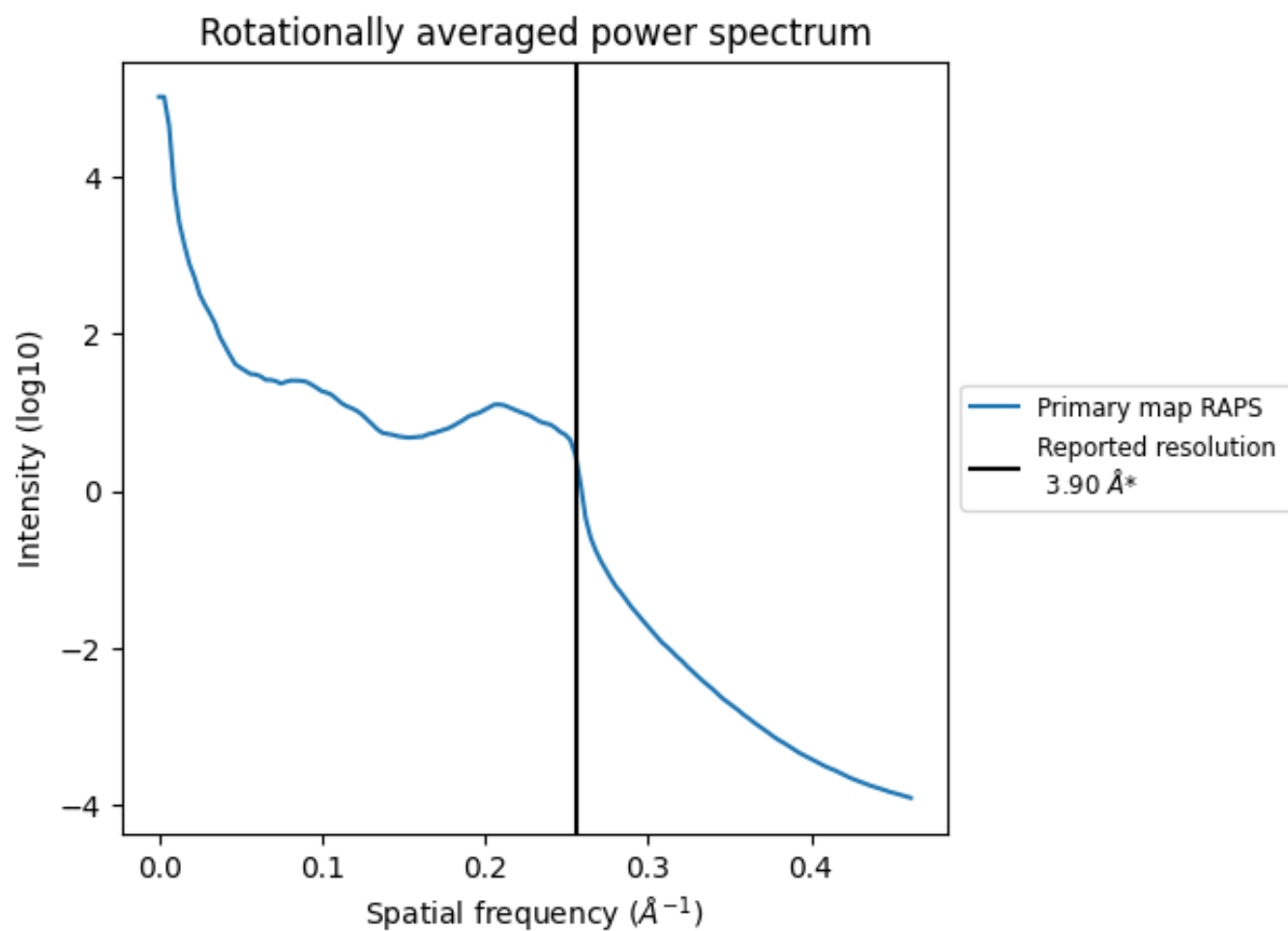
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 352 nm^3 ; this corresponds to an approximate mass of 318 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 ⓘ

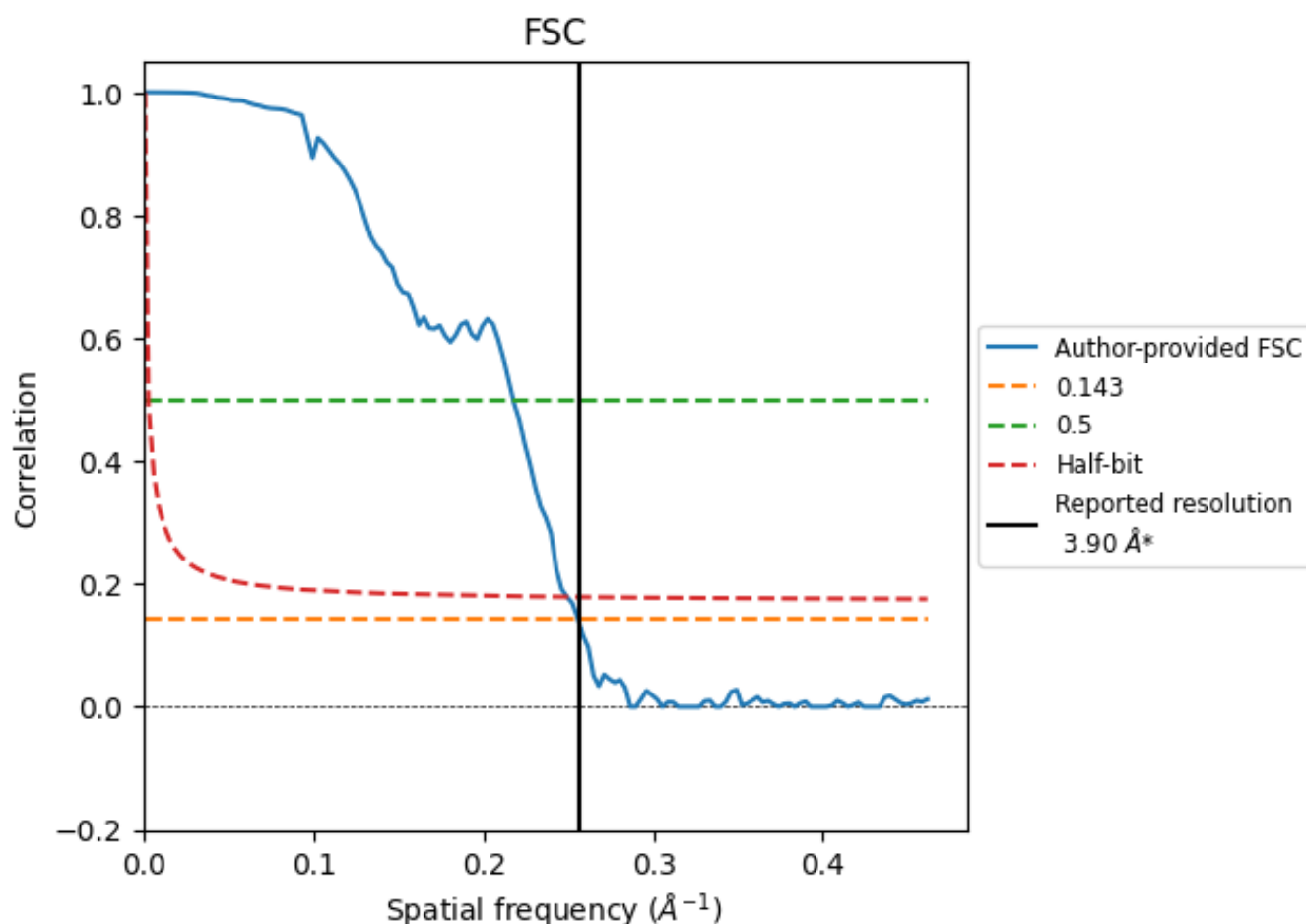


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

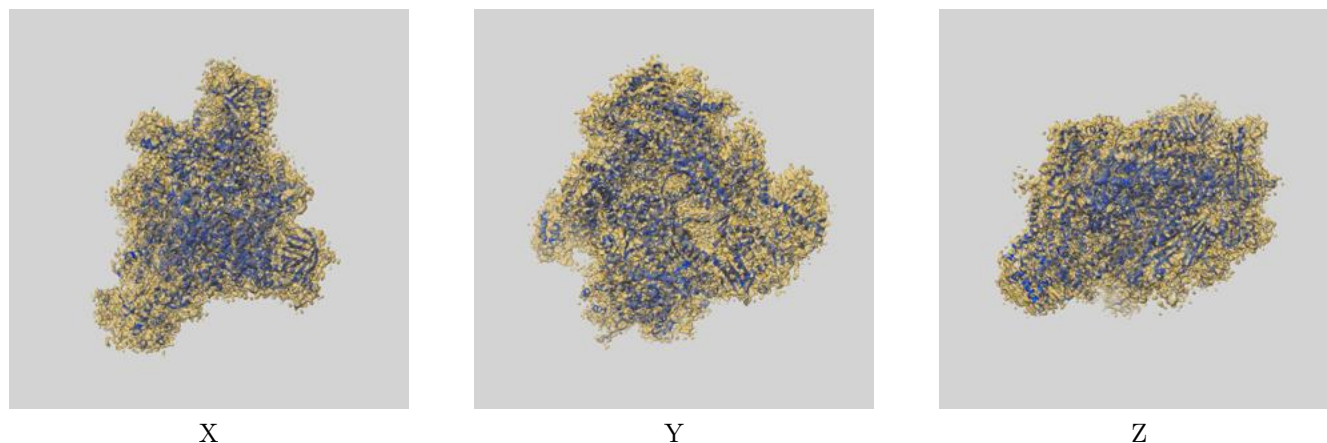
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	3.91	4.60	4.01
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3178 and PDB model 5FJ8. 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 0.06 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](#)

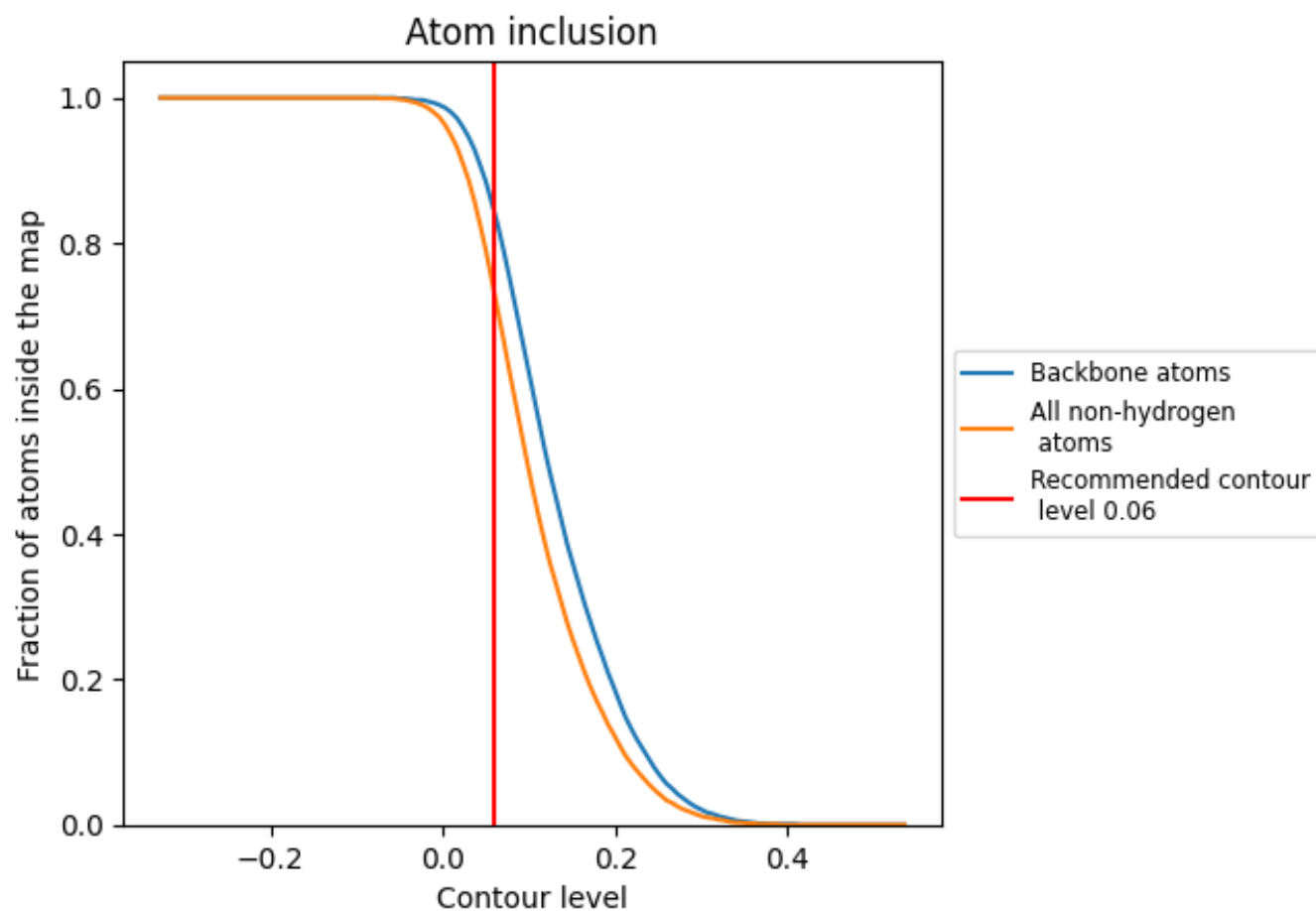


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7300	 0.3450
A	 0.7720	 0.3750
B	 0.8050	 0.3940
C	 0.8330	 0.3950
D	 0.7090	 0.2710
E	 0.7440	 0.3350
F	 0.8520	 0.4190
G	 0.6950	 0.3020
H	 0.8260	 0.3960
I	 0.6660	 0.2970
J	 0.8430	 0.4180
K	 0.8260	 0.4020
L	 0.7280	 0.3370
M	 0.6250	 0.2580
N	 0.6930	 0.2990
O	 0.5380	 0.2430
P	 0.3620	 0.1680
Q	 0.5760	 0.1970
R	 0.4300	 0.2000
S	 0.5400	 0.1870
T	 0.2310	 0.1480

