



Full wwPDB EM Validation Report ⓘ

Aug 27, 2026 – 06:26 am BST

PDB ID : 8B3D / pdb_00008b3d
EMDB ID : EMD-15825
Title : Structure of the Pol II-TCR-ELOF1 complex.
Authors : Kokic, G.; Cramer, P.
Deposited on : 2022-09-16
Resolution : 2.60 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:

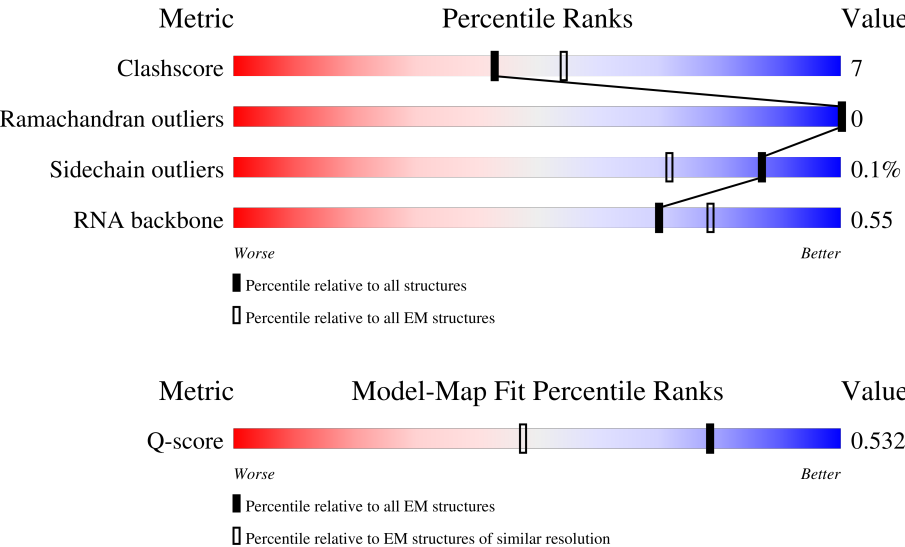
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 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	8728 (2.10 - 3.10)

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	
2	B	1167	
3	C	275	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	142	
5	E	210	
6	F	127	
7	G	254	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	83	
14	N	52	
15	P	10	
16	T	52	
17	a	396	
18	b	1493	
19	c	709	
20	d	1140	

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 95808 atoms, of which 46954 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 subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1409	Total	C	H	N	O	S	0	0
			22460	7022	11299	1998	2070	71		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	THR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	TYR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	THR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	1130	Total	C	H	N	O	S	0	0
			18131	5725	9083	1591	1668	64		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	260	Total	C	H	N	O	S	0	0
			4120	1309	2031	359	415	6		

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	128	Total	C	H	N	O	S	0	0
			1985	636	972	172	201	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	209	Total	C	H	N	O	S	0	0
			3457	1089	1737	300	323	8		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	82	Total	C	H	N	O	S	0	0
			1341	418	684	113	121	5		

- Molecule 7 is a protein called RPB7.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	171	Total	C	H	N	O	S	0	0
			2665	867	1331	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	H	N	O	S	0	0
			2333	750	1147	194	237	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	117	Total	C	H	N	O	S	0	0
			1827	587	878	169	182	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	H	N	O	S	0	0
			1086	345	553	90	92	6		

- Molecule 11 is a protein called RNA_pol_L_2 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	115	Total	C	H	N	O	S	0	0
			1862	593	942	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	46	Total	C	H	N	O	S	0	0
			781	241	393	75	66	6		

- Molecule 13 is a protein called Transcription elongation factor 1 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	64	Total	C	H	N	O	S	0	0
			968	312	463	81	105	7		

- Molecule 14 is a DNA chain called NTS.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	40	Total	C	H	N	O	P	0	0
			913	393	84	162	234	40		

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	P	10	Total	C	H	N	O	P	0	0
			330	98	110	45	67	10		

- Molecule 16 is a DNA chain called TS.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	T	52	Total	C	H	N	O	P	0	0
			1078	476	87	160	303	52		

- Molecule 17 is a protein called DNA excision repair protein ERCC-8.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	a	365	Total	C	H	N	O	S	0	0
			5624	1775	2775	507	548	19		

- Molecule 18 is a protein called DNA excision repair protein ERCC-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	b	520	Total	C	H	N	O	S	0	0
			8561	2746	4302	746	746	21		

- Molecule 19 is a protein called UV-stimulated scaffold protein A.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	c	264	Total	C	H	N	O	S	0	0
			3910	1237	1911	390	363	9		

- Molecule 20 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	d	781	Total	C	H	N	O	S	0	0
			12321	3916	6160	1038	1173	34		

- 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	C	1	Total	Zn	0
			1	1	
21	I	2	Total	Zn	0
			2	2	
21	J	1	Total	Zn	0
			1	1	
21	L	1	Total	Zn	0
			1	1	
21	M	1	Total	Zn	0
			1	1	
21	c	1	Total	Zn	0
			1	1	

- Molecule 22 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	Mg	0
			1	1	
22	b	1	Total	Mg	0
			1	1	

- # ADP

Mol	Chain	Residues	Atoms						AltConf
23	b	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

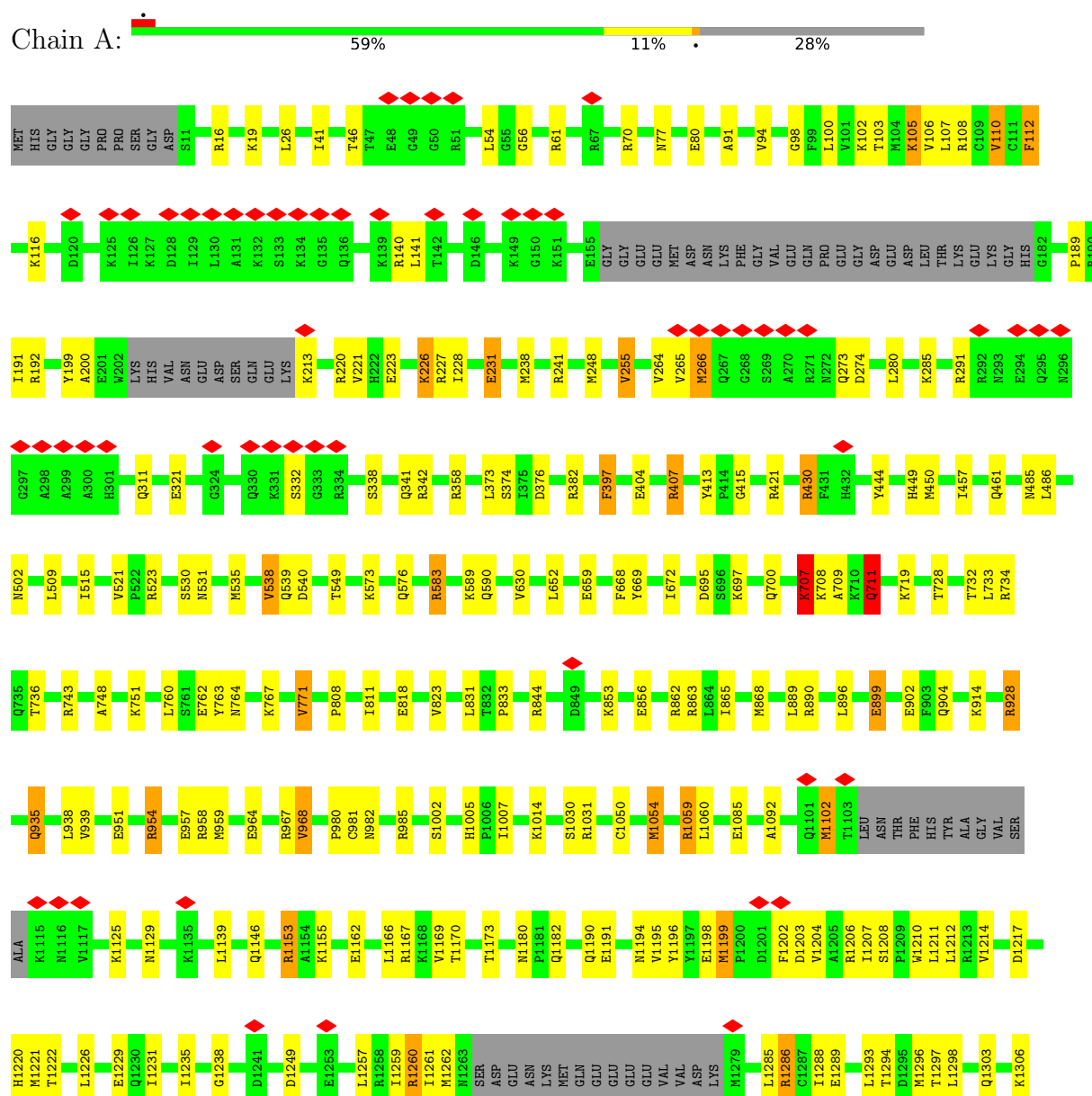
- BEF
- F3
- F⁻
- BE Be⁺² F⁻ F1
- F⁻
- F2

Mol	Chain	Residues	Atoms			AltConf
24	b	1	Total 4	Be 1	F 3	0

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 subunit



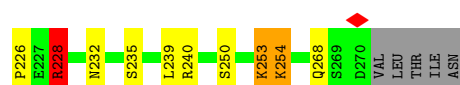
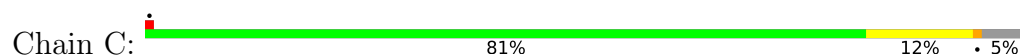


5% 82% 14% ..

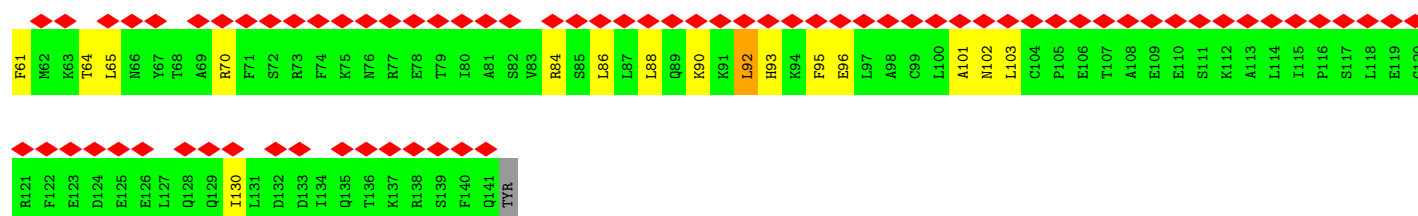
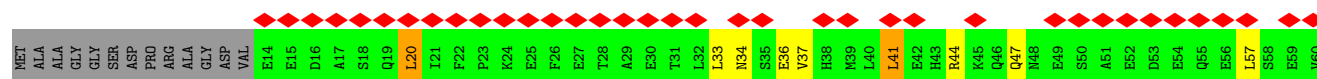
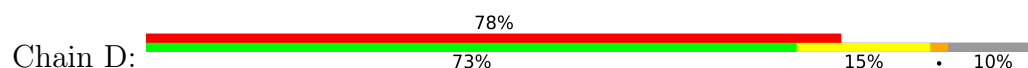




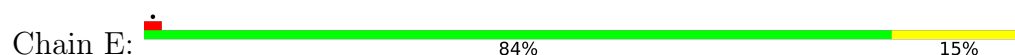
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



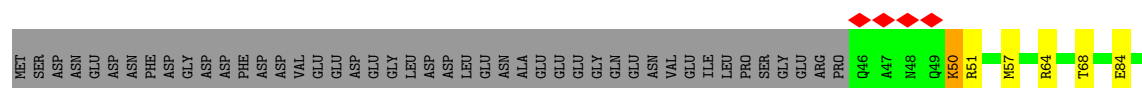
• Molecule 4: RNA polymerase II subunit D



• Molecule 5: DNA-directed RNA polymerase II subunit E

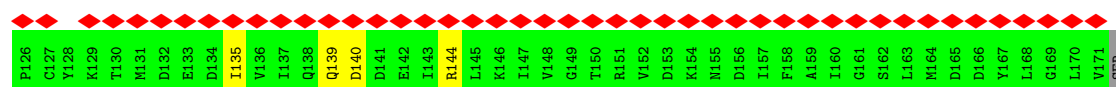
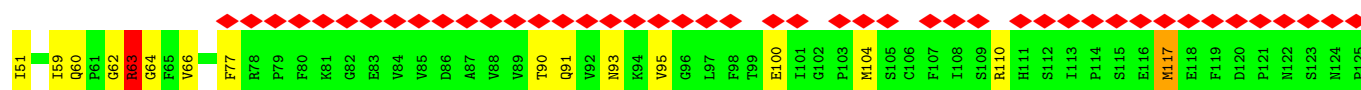
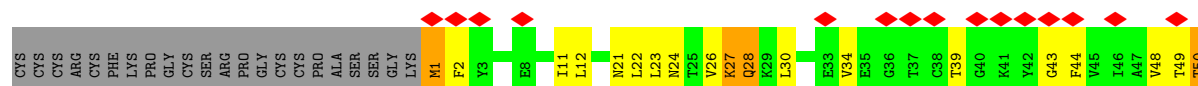
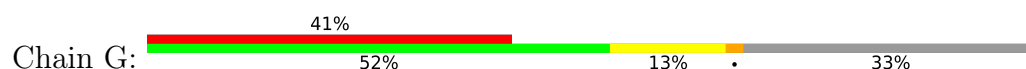


• Molecule 6: DNA-directed RNA polymerase II subunit F

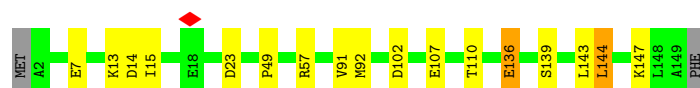
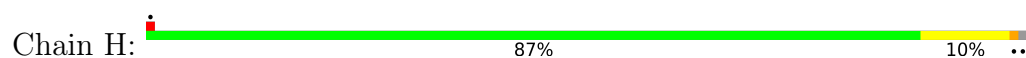




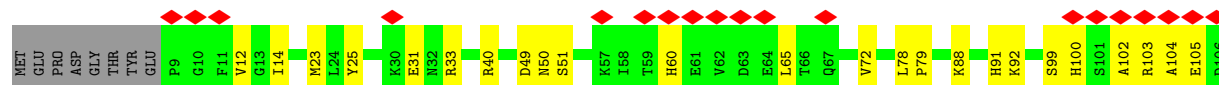
- Molecule 7: RPB7



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



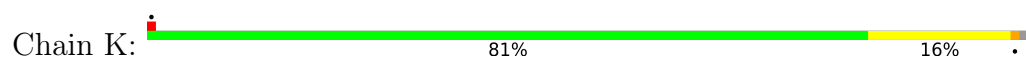
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

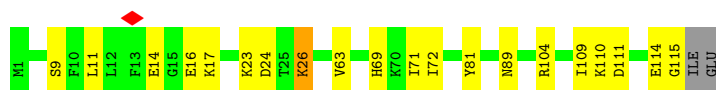


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 11: RNA_pol_L_2 domain-containing protein

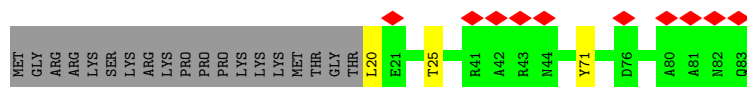
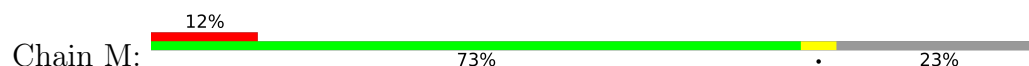




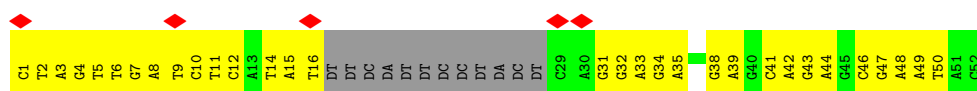
- Molecule 12: RNA polymerase II subunit K



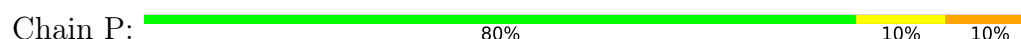
- Molecule 13: Transcription elongation factor 1 homolog



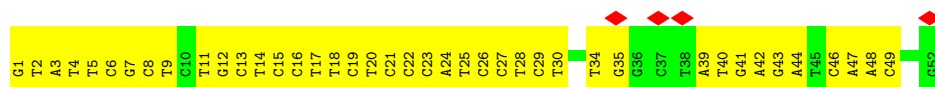
- Molecule 14: NTS



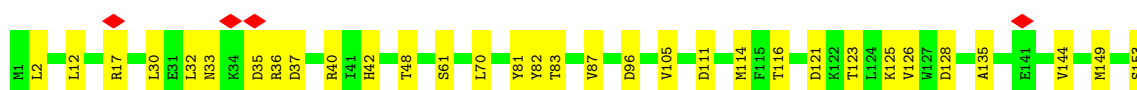
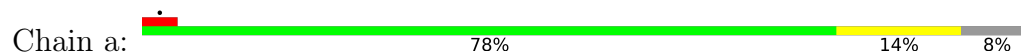
- Molecule 15: RNA



- Molecule 16: TS

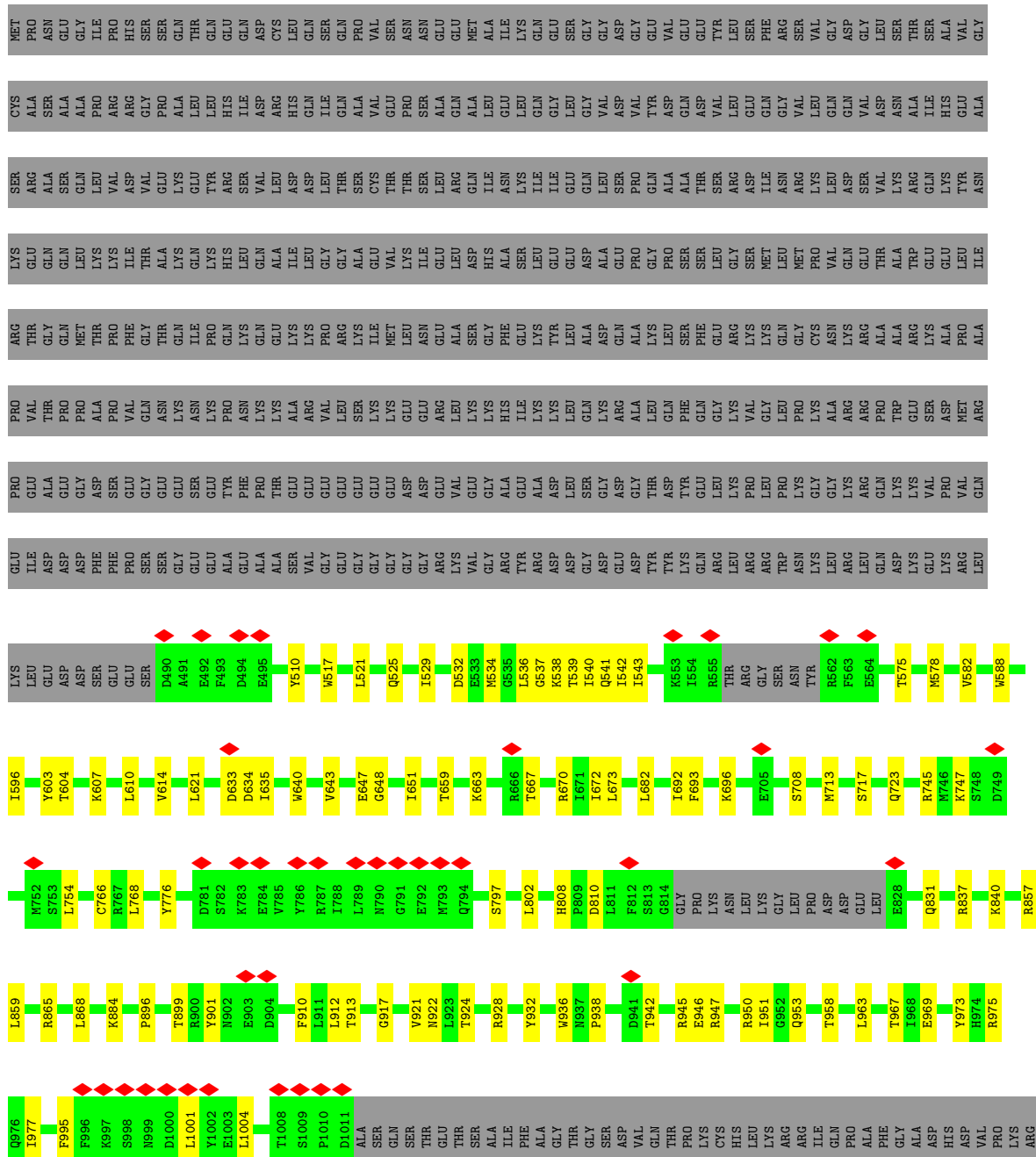


- Molecule 17: DNA excision repair protein ERCC-8



- Molecule 18: DNA excision repair protein ERCC-6

Chain b: 28% 7% 65%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	544306	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	144	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.182	Depositor
Minimum map value	-0.120	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.00912	Depositor
Map size ($\text{\AA}$)	440.99997, 440.99997, 440.99997	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	9/11364 (0.1%)	1.08	130/15342 (0.8%)
2	B	0.49	5/9229 (0.1%)	0.87	66/12458 (0.5%)
3	C	0.53	1/2132 (0.0%)	1.02	22/2896 (0.8%)
4	D	0.55	2/1027 (0.2%)	1.15	17/1384 (1.2%)
5	E	0.61	1/1751 (0.1%)	1.19	29/2366 (1.2%)
6	F	0.41	0/667	0.96	5/901 (0.6%)
7	G	0.54	1/1365 (0.1%)	1.27	19/1853 (1.0%)
8	H	0.40	0/1207	0.69	5/1628 (0.3%)
9	I	0.50	0/972	1.12	13/1316 (1.0%)
10	J	0.38	0/542	1.00	3/730 (0.4%)
11	K	0.57	2/939 (0.2%)	1.13	15/1271 (1.2%)
12	L	0.79	2/394 (0.5%)	1.57	13/524 (2.5%)
13	M	0.17	0/515	0.33	0/700
14	N	0.19	0/932	0.32	0/1435
15	P	0.37	0/247	0.35	0/384
16	T	0.28	0/1102	0.42	0/1682
17	a	0.21	0/2908	0.45	0/3939
18	b	0.19	0/4362	0.42	0/5890
19	c	0.24	0/2034	0.49	0/2715
20	d	0.19	0/6268	0.43	1/8466 (0.0%)
All	All	0.43	23/49957 (0.0%)	0.86	338/67880 (0.5%)

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	9
2	B	0	6
3	C	0	5

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	1
6	F	0	1
7	G	0	2
9	I	0	2
12	L	0	1
17	a	0	1
All	All	0	28

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1	MET	CB-CG	-8.21	1.27	1.52
11	K	26	LYS	CG-CD	-5.97	1.34	1.52
11	K	26	LYS	CD-CE	-5.93	1.34	1.52
3	C	111	GLN	CG-CD	-5.79	1.37	1.52
12	L	35	ARG	CZ-NH1	-5.76	1.24	1.32
5	E	187	ARG	CB-CG	-5.75	1.35	1.52
1	A	407	ARG	CD-NE	-5.75	1.38	1.46
1	A	1014	LYS	CE-NZ	-5.73	1.32	1.49
1	A	1153	ARG	CZ-NH2	-5.67	1.26	1.33
1	A	407	ARG	NE-CZ	-5.62	1.26	1.33
1	A	771	VAL	CB-CG1	-5.51	1.34	1.52
2	B	301	VAL	CB-CG2	-5.47	1.34	1.52
1	A	928	ARG	CB-CG	-5.40	1.36	1.52
2	B	271	ILE	CG1-CD1	-5.39	1.30	1.51
4	D	41	LEU	CG-CD2	5.19	1.69	1.52
1	A	1405	MET	SD-CE	-5.18	1.66	1.79
2	B	393	LEU	CG-CD2	-5.17	1.35	1.52
12	L	51	ARG	CZ-NH2	-5.09	1.26	1.33
4	D	65	LEU	CG-CD2	5.09	1.69	1.52
1	A	1286	ARG	CD-NE	-5.09	1.39	1.46
2	B	53	MET	SD-CE	-5.04	1.67	1.79
2	B	1150	ARG	CZ-NH1	-5.03	1.25	1.32
1	A	227	ARG	CZ-NH1	-5.02	1.25	1.32

All (338) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1286	ARG	CG-CD-NE	22.17	160.77	112.00
1	A	958	ARG	CG-CD-NE	21.44	159.16	112.00
7	G	28	GLN	CA-CB-CG	18.44	150.98	114.10
1	A	711	GLN	CA-CB-CG	18.21	150.52	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	LYS	CA-CB-CG	17.35	148.80	114.10
3	C	240	ARG	CG-CD-NE	16.74	148.82	112.00
1	A	266	MET	CA-CB-CG	15.33	144.77	114.10
10	J	41	LYS	CA-CB-CG	15.13	144.36	114.10
1	A	1031	ARG	CG-CD-NE	14.93	144.84	112.00
1	A	708	LYS	CB-CG-CD	14.87	145.50	111.30
11	K	26	LYS	CB-CG-CD	14.84	145.43	111.30
7	G	63	ARG	CG-CD-NE	14.11	143.05	112.00
7	G	117	MET	CB-CG-SD	13.84	154.22	112.70
1	A	105	LYS	CB-CG-CD	13.75	142.92	111.30
1	A	707	LYS	CG-CD-CE	13.69	142.79	111.30
1	A	70	ARG	CG-CD-NE	13.39	141.47	112.00
1	A	1031	ARG	CB-CG-CD	13.21	141.67	111.30
1	A	958	ARG	CA-CB-CG	13.09	140.28	114.10
3	C	111	GLN	CA-CB-CG	13.09	140.27	114.10
4	D	41	LEU	CB-CG-CD1	13.04	149.81	110.70
7	G	28	GLN	N-CA-CB	13.04	129.28	110.12
1	A	407	ARG	CA-CB-CG	13.02	140.14	114.10
2	B	169	ARG	CG-CD-NE	12.86	140.28	112.00
1	A	241	ARG	CA-CB-CG	12.84	139.78	114.10
1	A	928	ARG	CG-CD-NE	-12.50	84.50	112.00
6	F	50	LYS	CA-CB-CG	12.46	139.02	114.10
3	C	225	LYS	CA-CB-CG	12.40	138.90	114.10
1	A	266	MET	CB-CG-SD	12.11	149.02	112.70
1	A	407	ARG	CG-CD-NE	12.07	138.55	112.00
4	D	41	LEU	CD1-CG-CD2	-11.95	84.52	110.80
5	E	166	ARG	CB-CG-CD	11.91	138.70	111.30
1	A	1153	ARG	CG-CD-NE	11.90	138.19	112.00
2	B	95	LYS	CG-CD-CE	11.81	138.47	111.30
3	C	254	LYS	N-CA-C	-11.81	99.00	113.41
10	J	41	LYS	CB-CG-CD	11.58	137.94	111.30
1	A	914	LYS	CB-CG-CD	11.31	137.32	111.30
1	A	958	ARG	N-CA-CB	11.25	129.07	110.39
12	L	37	ARG	CA-CB-CG	11.01	136.12	114.10
1	A	938	LEU	CD1-CG-CD2	-10.98	86.64	110.80
11	K	23	LYS	CA-CB-CG	10.92	135.94	114.10
2	B	87	LYS	CG-CD-CE	10.83	136.22	111.30
10	J	41	LYS	CB-CA-C	-10.79	94.22	110.95
3	C	240	ARG	CB-CG-CD	10.76	136.04	111.30
1	A	1478	GLU	N-CA-CB	-10.75	96.05	110.88
4	D	65	LEU	CB-CG-CD2	-10.73	78.51	110.70
1	A	407	ARG	CB-CG-CD	-10.70	86.69	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1479	LYS	N-CA-C	10.69	122.93	111.28
2	B	1138	ARG	CG-CD-NE	10.59	135.30	112.00
6	F	50	LYS	CB-CG-CD	10.41	135.24	111.30
9	I	88	LYS	CB-CG-CD	10.29	134.98	111.30
2	B	296	GLU	CA-CB-CG	10.23	134.55	114.10
1	A	241	ARG	CG-CD-NE	10.21	134.47	112.00
4	D	41	LEU	CB-CG-CD2	-10.06	80.52	110.70
7	G	28	GLN	CB-CA-C	-9.99	94.21	110.79
1	A	928	ARG	CB-CG-CD	9.94	134.15	111.30
9	I	40	ARG	CB-CG-CD	9.89	134.04	111.30
7	G	12	LEU	CD1-CG-CD2	-9.85	89.12	110.80
5	E	132	GLN	CA-CB-CG	9.84	133.77	114.10
5	E	12	LYS	CA-CB-CG	9.50	133.10	114.10
11	K	17	LYS	CG-CD-CE	9.47	133.08	111.30
9	I	33	ARG	CB-CG-CD	9.47	133.08	111.30
1	A	1478	GLU	CB-CA-C	9.43	125.22	109.38
2	B	169	ARG	CB-CG-CD	9.36	132.83	111.30
5	E	88	LYS	CA-CB-CG	9.33	132.76	114.10
1	A	1479	LYS	CA-CB-CG	9.31	132.73	114.10
1	A	743	ARG	CG-CD-NE	-9.12	91.93	112.00
2	B	159	THR	OG1-CB-CG2	-9.04	91.22	109.30
2	B	1010	LYS	CG-CD-CE	9.04	132.09	111.30
1	A	266	MET	N-CA-CB	-8.99	97.57	111.05
1	A	928	ARG	CA-CB-CG	8.91	131.92	114.10
1	A	573	LYS	CG-CD-CE	8.90	131.76	111.30
4	D	44	ARG	CB-CG-CD	8.87	131.71	111.30
3	C	109	GLU	CA-CB-CG	8.83	131.77	114.10
2	B	301	VAL	CB-CA-C	-8.78	97.85	112.16
7	G	63	ARG	CB-CG-CD	8.70	131.30	111.30
5	E	12	LYS	N-CA-CB	8.69	122.90	110.12
1	A	583	ARG	CB-CG-CD	8.52	130.90	111.30
1	A	1341	VAL	CG1-CB-CG2	-8.47	92.16	110.80
2	B	548	TRP	N-CA-C	-8.47	92.76	110.80
2	B	173	GLU	CA-CB-CG	8.45	130.99	114.10
2	B	24	GLU	CA-CB-CG	8.41	130.93	114.10
1	A	266	MET	CB-CA-C	8.40	126.04	110.24
1	A	241	ARG	CB-CG-CD	-8.36	92.07	111.30
5	E	103	LEU	CD1-CG-CD2	-8.34	92.44	110.80
1	A	1459	MET	CB-CG-SD	-8.31	87.76	112.70
2	B	109	MET	CB-CG-SD	8.28	137.53	112.70
1	A	19	LYS	CG-CD-CE	8.27	130.33	111.30
12	L	37	ARG	CG-CD-NE	-8.26	93.82	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	914	LYS	CA-CB-CG	8.25	130.60	114.10
11	K	110	LYS	CG-CD-CE	8.22	130.20	111.30
1	A	711	GLN	N-CA-CB	-8.16	97.74	110.30
9	I	40	ARG	CG-CD-NE	-8.14	94.09	112.00
1	A	1376	LYS	CG-CD-CE	8.11	129.96	111.30
3	C	111	GLN	CB-CA-C	8.06	124.28	109.70
12	L	37	ARG	CB-CG-CD	8.06	129.83	111.30
1	A	1059	ARG	CB-CG-CD	8.05	129.81	111.30
2	B	380	ARG	CB-CG-CD	8.05	129.81	111.30
1	A	1085	GLU	CA-CB-CG	8.01	130.12	114.10
12	L	25	GLU	N-CA-C	-8.01	97.95	109.96
4	D	65	LEU	CD1-CG-CD2	-7.92	93.38	110.80
2	B	780	VAL	CG1-CB-CG2	-7.90	93.43	110.80
3	C	253	LYS	CA-C-N	-7.88	107.98	122.09
3	C	253	LYS	C-N-CA	-7.88	107.98	122.09
8	H	144	LEU	CD1-CG-CD2	-7.86	93.51	110.80
1	A	1155	LYS	CA-CB-CG	7.83	129.76	114.10
4	D	65	LEU	CB-CG-CD1	7.78	134.03	110.70
1	A	1478	GLU	CA-CB-CG	7.77	129.65	114.10
1	A	583	ARG	N-CA-C	7.76	122.03	110.32
3	C	111	GLN	CB-CG-CD	7.75	125.77	112.60
3	C	228	ARG	CD-NE-CZ	7.72	135.21	124.40
1	A	255	VAL	CG1-CB-CG2	-7.70	93.85	110.80
1	A	226	LYS	CG-CD-CE	7.66	128.93	111.30
2	B	995	GLU	CA-CB-CG	7.58	129.26	114.10
5	E	47	LYS	CD-CE-NZ	7.55	136.05	111.90
2	B	95	LYS	CB-CG-CD	-7.55	93.94	111.30
4	D	20	LEU	CD1-CG-CD2	-7.53	94.23	110.80
7	G	48	VAL	CG1-CB-CG2	-7.53	94.23	110.80
2	B	917	LYS	CG-CD-CE	7.43	128.39	111.30
5	E	101	ARG	CD-NE-CZ	7.41	134.78	124.40
1	A	407	ARG	CB-CA-C	-7.40	98.97	110.81
3	C	254	LYS	CB-CG-CD	7.38	128.26	111.30
5	E	153	LYS	CD-CE-NZ	7.36	135.45	111.90
4	D	92	LEU	CA-CB-CG	7.31	141.87	116.30
1	A	1405	MET	N-CA-CB	-7.25	98.58	110.40
9	I	92	LYS	N-CA-C	-7.25	104.05	113.12
1	A	223	GLU	N-CA-C	-7.15	104.37	113.23
3	C	111	GLN	N-CA-CB	-7.14	98.44	110.80
1	A	1286	ARG	CD-NE-CZ	-7.14	114.40	124.40
5	E	5	GLU	CA-CB-CG	7.10	128.30	114.10
1	A	430	ARG	CB-CG-CD	-7.06	95.06	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	12	LYS	CG-CD-CE	7.06	127.54	111.30
12	L	29	LYS	CG-CD-CE	7.06	127.53	111.30
5	E	39	GLU	N-CA-CB	7.05	121.20	110.28
3	C	268	GLN	CA-CB-CG	7.01	128.12	114.10
7	G	12	LEU	CA-CB-CG	7.01	140.83	116.30
3	C	240	ARG	CD-NE-CZ	-6.97	114.64	124.40
3	C	109	GLU	N-CA-CB	6.93	119.88	110.38
12	L	29	LYS	CB-CG-CD	6.90	127.16	111.30
1	A	914	LYS	CG-CD-CE	-6.88	95.47	111.30
4	D	88	LEU	CB-CG-CD1	-6.88	90.07	110.70
5	E	96	GLU	CA-CB-CG	6.86	127.82	114.10
1	A	938	LEU	CB-CG-CD1	6.84	131.23	110.70
2	B	770	ARG	CG-CD-NE	6.84	127.05	112.00
5	E	85	LYS	N-CA-C	-6.83	103.62	112.23
1	A	407	ARG	CD-NE-CZ	6.82	133.95	124.40
2	B	296	GLU	N-CA-CB	-6.79	100.03	110.42
1	A	771	VAL	CG1-CB-CG2	-6.78	95.88	110.80
5	E	101	ARG	CB-CG-CD	6.77	126.87	111.30
1	A	105	LYS	N-CA-CB	-6.76	100.21	110.01
2	B	301	VAL	CA-CB-CG2	6.72	121.83	110.40
1	A	108	ARG	CD-NE-CZ	6.70	133.78	124.40
1	A	711	GLN	CB-CG-CD	6.68	123.95	112.60
1	A	573	LYS	CB-CG-CD	6.68	126.66	111.30
9	I	33	ARG	CA-CB-CG	-6.68	100.75	114.10
1	A	1199	MET	CB-CG-SD	6.67	132.71	112.70
5	E	85	LYS	CA-CB-CG	6.67	127.44	114.10
8	H	144	LEU	CB-CG-CD1	6.66	130.68	110.70
1	A	743	ARG	CB-CA-C	6.65	123.89	109.99
2	B	555	GLU	CA-CB-CG	6.63	127.35	114.10
1	A	762	GLU	CA-CB-CG	6.62	127.33	114.10
2	B	53	MET	CA-CB-CG	6.62	127.33	114.10
2	B	917	LYS	CD-CE-NZ	6.61	133.04	111.90
11	K	26	LYS	CD-CE-NZ	-6.58	90.84	111.90
1	A	241	ARG	N-CA-CB	6.56	121.09	110.40
5	E	4	GLU	CB-CG-CD	6.53	123.70	112.60
1	A	1031	ARG	N-CA-C	6.52	119.38	111.82
1	A	914	LYS	CD-CE-NZ	6.51	132.73	111.90
1	A	1155	LYS	CD-CE-NZ	6.50	132.72	111.90
12	L	51	ARG	CG-CD-NE	6.50	126.29	112.00
9	I	40	ARG	CA-CB-CG	6.49	127.08	114.10
1	A	711	GLN	CB-CA-C	6.48	123.60	110.38
5	E	12	LYS	CB-CA-C	-6.47	100.05	110.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	57	ARG	NE-CZ-NH2	6.47	125.02	119.20
7	G	12	LEU	CB-CG-CD1	6.47	130.10	110.70
1	A	1404	THR	CA-C-N	6.45	132.42	121.14
1	A	1404	THR	C-N-CA	6.45	132.42	121.14
9	I	88	LYS	CA-CB-CG	6.43	126.97	114.10
2	B	255	ARG	NE-CZ-NH2	6.40	124.96	119.20
2	B	255	ARG	CG-CD-NE	6.40	126.08	112.00
1	A	110	VAL	CA-CB-CG2	6.38	121.25	110.40
4	D	92	LEU	CD1-CG-CD2	-6.38	96.77	110.80
11	K	114	GLU	CA-CB-CG	6.35	126.80	114.10
1	A	1260	ARG	NE-CZ-NH2	6.32	124.89	119.20
3	C	254	LYS	CA-CB-CG	-6.31	101.48	114.10
9	I	31	GLU	CA-CB-CG	6.21	126.53	114.10
1	A	110	VAL	N-CA-C	-6.21	100.14	108.96
7	G	27	LYS	CA-C-N	-6.20	111.97	120.28
7	G	27	LYS	C-N-CA	-6.20	111.97	120.28
1	A	226	LYS	CB-CG-CD	6.18	125.51	111.30
9	I	92	LYS	CA-CB-CG	6.17	126.43	114.10
1	A	938	LEU	CB-CG-CD2	-6.16	92.21	110.70
1	A	1153	ARG	CB-CG-CD	-6.15	97.16	111.30
2	B	173	GLU	CB-CA-C	6.14	122.16	109.95
1	A	899	GLU	CA-CB-CG	6.12	126.35	114.10
2	B	548	TRP	CB-CG-CD2	-6.12	118.23	126.80
1	A	105	LYS	CG-CD-CE	6.12	125.37	111.30
1	A	719	LYS	CG-CD-CE	6.11	125.35	111.30
1	A	116	LYS	CB-CG-CD	6.10	125.32	111.30
3	C	111	GLN	CG-CD-NE2	-6.08	107.27	116.40
1	A	707	LYS	CD-CE-NZ	-6.07	92.47	111.90
1	A	818	GLU	CA-CB-CG	6.07	126.24	114.10
1	A	708	LYS	CG-CD-CE	-6.04	97.42	111.30
2	B	301	VAL	CA-CB-CG1	6.03	120.65	110.40
7	G	1	MET	CG-SD-CE	-6.03	87.64	100.90
5	E	39	GLU	CA-CB-CG	6.03	126.16	114.10
1	A	1260	ARG	CA-CB-CG	6.02	126.14	114.10
6	F	50	LYS	CG-CD-CE	-5.99	97.53	111.30
11	K	110	LYS	CB-CG-CD	-5.99	97.53	111.30
1	A	708	LYS	CD-CE-NZ	5.98	131.05	111.90
1	A	700	GLN	CA-CB-CG	5.97	126.03	114.10
2	B	613	ARG	NE-CZ-NH2	5.97	124.57	119.20
1	A	856	GLU	CA-CB-CG	5.96	126.02	114.10
3	C	108	ASN	CB-CA-C	-5.95	99.74	109.56
1	A	1286	ARG	CB-CG-CD	5.94	124.97	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	266	GLU	CA-CB-CG	5.93	125.97	114.10
1	A	382	ARG	NE-CZ-NH2	5.93	124.54	119.20
1	A	116	LYS	CD-CE-NZ	-5.92	92.95	111.90
7	G	12	LEU	CB-CG-CD2	-5.92	92.93	110.70
4	D	41	LEU	CA-CB-CG	-5.92	95.60	116.30
4	D	47	GLN	CB-CG-CD	-5.91	102.56	112.60
1	A	1102	MET	CB-CG-SD	5.87	130.30	112.70
2	B	1163	MET	CA-CB-CG	5.86	125.81	114.10
2	B	53	MET	CG-SD-CE	5.86	113.78	100.90
2	B	325	GLY	N-CA-C	5.85	127.05	113.18
1	A	958	ARG	CA-C-N	-5.83	111.88	120.28
1	A	958	ARG	C-N-CA	-5.83	111.88	120.28
1	A	743	ARG	CD-NE-CZ	5.82	132.55	124.40
3	C	228	ARG	CG-CD-NE	5.78	124.71	112.00
2	B	613	ARG	CG-CD-NE	5.77	124.70	112.00
2	B	840	MET	CB-CG-SD	5.77	130.00	112.70
8	H	136	GLU	N-CA-CB	5.75	120.06	110.85
1	A	957	GLU	CA-C-N	-5.75	111.12	120.72
1	A	957	GLU	C-N-CA	-5.75	111.12	120.72
1	A	1459	MET	CA-C-N	-5.74	113.13	122.65
1	A	1459	MET	C-N-CA	-5.74	113.13	122.65
11	K	110	LYS	N-CA-C	-5.73	104.94	111.07
7	G	28	GLN	CA-C-N	-5.72	112.04	120.28
7	G	28	GLN	C-N-CA	-5.72	112.04	120.28
5	E	103	LEU	CB-CG-CD2	-5.71	93.58	110.70
9	I	49	ASP	CA-C-N	5.70	130.11	120.88
9	I	49	ASP	C-N-CA	5.70	130.11	120.88
2	B	632	LYS	CD-CE-NZ	5.69	130.12	111.90
1	A	751	LYS	CD-CE-NZ	5.69	130.10	111.90
1	A	573	LYS	CD-CE-NZ	-5.68	93.71	111.90
6	F	100	ARG	CG-CD-NE	5.68	124.50	112.00
2	B	520	VAL	CA-CB-CG1	5.67	120.04	110.40
1	A	1479	LYS	CG-CD-CE	5.67	124.33	111.30
2	B	380	ARG	CG-CD-NE	5.67	124.47	112.00
1	A	110	VAL	CA-CB-CG1	5.66	120.02	110.40
1	A	1054	MET	CB-CG-SD	5.66	129.67	112.70
5	E	101	ARG	CG-CD-NE	5.65	124.43	112.00
1	A	719	LYS	CB-CG-CD	-5.65	98.31	111.30
2	B	301	VAL	N-CA-C	-5.64	103.88	111.44
11	K	72	ILE	CB-CG1-CD1	5.64	125.65	113.80
2	B	520	VAL	N-CA-C	-5.64	101.45	108.89
1	A	968	VAL	N-CA-C	-5.63	103.89	111.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	173	GLU	N-CA-CB	-5.63	100.95	110.41
2	B	326	ALA	N-CA-C	5.62	117.09	111.07
4	D	47	GLN	CA-CB-CG	5.62	125.33	114.10
8	H	144	LEU	CB-CG-CD2	-5.60	93.89	110.70
5	E	88	LYS	N-CA-CB	-5.60	101.87	110.16
1	A	1478	GLU	CA-C-N	5.59	127.78	120.28
1	A	1478	GLU	C-N-CA	5.59	127.78	120.28
3	C	240	ARG	N-CA-C	5.58	117.60	109.84
2	B	654	GLN	N-CA-C	-5.58	105.98	112.89
1	A	407	ARG	NE-CZ-NH2	-5.57	114.19	119.20
4	D	44	ARG	CA-CB-CG	5.57	125.23	114.10
1	A	818	GLU	CB-CA-C	-5.56	102.16	110.88
5	E	166	ARG	CA-CB-CG	-5.53	103.03	114.10
1	A	1303	GLN	CA-CB-CG	5.53	125.16	114.10
2	B	770	ARG	NE-CZ-NH2	5.52	124.17	119.20
6	F	95	LYS	CD-CE-NZ	5.52	129.57	111.90
9	I	122	ARG	CG-CD-NE	5.52	124.14	112.00
2	B	578	LYS	CD-CE-NZ	5.51	129.54	111.90
1	A	285	LYS	CG-CD-CE	5.50	123.95	111.30
7	G	117	MET	N-CA-C	5.50	118.20	110.23
7	G	50	THR	CA-CB-CG2	5.50	119.84	110.50
4	D	47	GLN	N-CA-CB	-5.47	102.48	110.53
2	B	52	GLN	CA-C-N	5.47	130.90	122.42
2	B	52	GLN	C-N-CA	5.47	130.90	122.42
1	A	1125	LYS	CB-CG-CD	5.47	123.88	111.30
5	E	5	GLU	CB-CA-C	-5.44	101.71	110.74
1	A	708	LYS	N-CA-CB	5.40	118.90	109.72
5	E	101	ARG	NE-CZ-NH2	-5.40	114.34	119.20
2	B	632	LYS	CB-CG-CD	5.40	123.71	111.30
8	H	13	LYS	CB-CG-CD	5.39	123.69	111.30
2	B	995	GLU	CB-CA-C	-5.38	100.35	111.22
7	G	1	MET	CB-CA-C	-5.35	99.93	110.10
11	K	14	GLU	N-CA-CB	5.34	117.90	109.83
2	B	613	ARG	CB-CG-CD	5.33	123.55	111.30
1	A	231	GLU	CA-CB-CG	5.32	124.75	114.10
1	A	266	MET	CG-SD-CE	-5.32	89.19	100.90
1	A	397	PHE	N-CA-CB	-5.32	102.08	110.06
11	K	26	LYS	CA-CB-CG	5.32	124.73	114.10
4	D	88	LEU	N-CA-C	-5.31	105.07	112.45
1	A	954	ARG	CG-CD-NE	-5.30	100.34	112.00
1	A	743	ARG	CA-CB-CG	5.30	124.70	114.10
1	A	914	LYS	N-CA-C	-5.30	106.50	113.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1145	GLN	CA-CB-CG	5.29	124.68	114.10
2	B	1138	ARG	CB-CG-CD	5.29	123.46	111.30
12	L	25	GLU	CB-CA-C	-5.27	101.46	109.89
11	K	114	GLU	CB-CG-CD	-5.26	103.66	112.60
20	d	1052	LEU	N-CA-C	-5.25	105.45	111.07
2	B	591	ARG	CB-CG-CD	5.24	123.35	111.30
11	K	17	LYS	CD-CE-NZ	5.24	128.66	111.90
2	B	358	GLU	CA-CB-CG	5.23	124.56	114.10
1	A	227	ARG	CB-CG-CD	5.22	123.31	111.30
2	B	24	GLU	CB-CA-C	5.21	117.82	109.07
2	B	555	GLU	N-CA-CB	-5.20	102.33	110.44
2	B	548	TRP	CB-CG-CD1	5.20	134.70	126.90
1	A	1102	MET	CG-SD-CE	5.19	112.32	100.90
5	E	132	GLN	CB-CG-CD	5.19	121.42	112.60
1	A	968	VAL	CA-CB-CG2	5.18	119.20	110.40
5	E	158	GLU	CA-CB-CG	5.17	124.44	114.10
2	B	1134	THR	OG1-CB-CG2	5.17	119.64	109.30
1	A	16	ARG	N-CA-C	5.16	117.03	109.24
5	E	103	LEU	CB-CG-CD1	5.14	126.13	110.70
1	A	1180	ASN	N-CA-C	-5.14	101.62	109.64
12	L	51	ARG	NH1-CZ-NH2	-5.14	112.62	119.30
1	A	914	LYS	N-CA-CB	-5.13	102.56	110.42
12	L	25	GLU	CA-CB-CG	5.13	124.37	114.10
5	E	10	LEU	N-CA-C	-5.12	105.77	112.23
1	A	116	LYS	CA-CB-CG	-5.11	103.88	114.10
1	A	697	LYS	CD-CE-NZ	5.10	128.22	111.90
11	K	16	GLU	CA-C-N	-5.08	113.49	122.74
11	K	16	GLU	C-N-CA	-5.08	113.49	122.74
1	A	404	GLU	N-CA-CB	5.08	117.37	110.01
2	B	654	GLN	CA-CB-CG	5.07	124.25	114.10
12	L	25	GLU	CB-CG-CD	5.07	121.22	112.60
3	C	199	LYS	CG-CD-CE	5.07	122.96	111.30
2	B	1121	LEU	CB-CG-CD2	5.06	125.89	110.70
12	L	38	GLU	CB-CG-CD	-5.05	104.01	112.60
12	L	42	ARG	NE-CZ-NH2	5.05	123.75	119.20
2	B	388	TYR	N-CA-CB	5.04	118.88	110.41
1	A	1180	ASN	CB-CA-C	-5.02	103.55	109.47
2	B	108	MET	CA-C-N	-5.01	111.97	123.15
2	B	108	MET	C-N-CA	-5.01	111.97	123.15
2	B	393	LEU	CB-CG-CD2	5.01	125.73	110.70

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	PHE	Sidechain
1	A	1478	GLU	Peptide
1	A	397	PHE	Sidechain
1	A	407	ARG	Sidechain
1	A	430	ARG	Sidechain
1	A	538	VAL	Peptide
1	A	707	LYS	Peptide
1	A	711	GLN	Sidechain
1	A	935	GLN	Peptide
2	B	1135	TYR	Sidechain
2	B	1138	ARG	Sidechain
2	B	169	ARG	Sidechain
2	B	388	TYR	Sidechain
2	B	547	GLU	Peptide
2	B	995	GLU	Peptide
3	C	110	ASP	Peptide
3	C	111	GLN	Sidechain,Peptide
3	C	228	ARG	Sidechain
3	C	253	LYS	Peptide
5	E	131	LEU	Peptide
6	F	50	LYS	Peptide
7	G	28	GLN	Sidechain
7	G	63	ARG	Sidechain
9	I	122	ARG	Sidechain
9	I	91	HIS	Peptide
12	L	37	ARG	Peptide
17	a	174	LYS	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	11161	11299	11297	153	0
2	B	9048	9083	9084	103	0
3	C	2089	2031	2031	21	0
4	D	1013	972	972	19	0
5	E	1720	1737	1737	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	657	684	684	9	0
7	G	1334	1331	1333	26	0
8	H	1186	1147	1147	9	0
9	I	949	878	879	21	0
10	J	533	553	553	4	0
11	K	920	942	942	9	0
12	L	388	393	393	4	0
13	M	505	463	463	2	0
14	N	829	84	450	63	0
15	P	220	110	109	2	0
16	T	991	87	553	71	0
17	a	2849	2775	2777	39	0
18	b	4259	4302	4302	71	0
19	c	1999	1911	1916	32	0
20	d	6161	6160	6159	50	0
21	A	2	0	0	0	0
21	B	1	0	0	0	0
21	C	1	0	0	0	0
21	I	2	0	0	0	0
21	J	1	0	0	0	0
21	L	1	0	0	0	0
21	M	1	0	0	0	0
21	c	1	0	0	0	0
22	A	1	0	0	0	0
22	b	1	0	0	0	0
23	b	27	12	12	2	0
24	b	4	0	0	1	0
All	All	48854	46954	47793	634	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 7.

All (634) 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)
14:N:41:DC:C5'	19:c:679:LYS:HE3	1.71	1.21
14:N:41:DC:H5''	19:c:679:LYS:CE	1.82	1.09
19:c:12:LEU:HD22	19:c:64:ILE:HD11	1.34	1.09
14:N:41:DC:H5''	19:c:679:LYS:HE3	1.34	1.00
16:T:11:DT:H2''	16:T:12:DG:H5'	1.42	0.99
16:T:12:DG:H1'	16:T:13:DC:H5''	1.47	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:1:DC:H2''	14:N:2:DT:H5'	1.51	0.91
2:B:733:MET:HE1	2:B:1054:MET:HE2	1.52	0.91
1:A:1378:LEU:HD21	1:A:1405:MET:HE2	1.55	0.87
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.57	0.86
1:A:338:SER:OG	1:A:341:GLN:OE1	1.92	0.86
1:A:1257:LEU:HD12	1:A:1259:ILE:HD11	1.60	0.83
2:B:549:SER:OG	2:B:577:HIS:NE2	2.12	0.83
14:N:41:DC:C4'	19:c:679:LYS:HE3	2.11	0.80
17:a:168:VAL:HG22	17:a:189:ILE:HD13	1.64	0.79
16:T:1:DG:H4'	16:T:2:DT:H5'	1.64	0.77
2:B:565:THR:OG1	2:B:610:ARG:O	2.01	0.77
2:B:1104:ARG:NH1	2:B:1109:GLU:OE2	2.17	0.77
17:a:17:ARG:NH1	20:d:117:GLU:O	2.18	0.76
20:d:36:ASN:ND2	20:d:1002:GLU:OE2	2.19	0.76
16:T:16:DC:H2'	16:T:17:DT:H71	1.67	0.76
2:B:924:ARG:NH1	3:C:62:GLU:OE1	2.19	0.75
2:B:393:LEU:HD23	2:B:485:LEU:HD22	1.67	0.75
1:A:538:VAL:HG12	1:A:539:GLN:H	1.52	0.75
18:b:945:ARG:NH1	18:b:946:GLU:OE2	2.19	0.74
14:N:41:DC:C5'	19:c:679:LYS:CE	2.49	0.74
18:b:713:MET:SD	18:b:723:GLN:NE2	2.60	0.74
17:a:121:ASP:OD1	17:a:123:THR:OG1	2.06	0.74
1:A:1257:LEU:CD1	1:A:1259:ILE:HD11	2.17	0.74
2:B:274:ARG:NH1	2:B:311:ILE:O	2.21	0.73
14:N:41:DC:H4'	19:c:679:LYS:HE3	1.68	0.73
4:D:20:LEU:HD11	4:D:93:HIS:HD2	1.53	0.73
3:C:225:LYS:HB2	3:C:226:PRO:CD	2.17	0.73
3:C:225:LYS:HB2	3:C:226:PRO:HD2	1.71	0.73
5:E:112:PRO:HB3	16:T:12:DG:H5''	1.71	0.72
20:d:102:THR:OG1	20:d:1065:VAL:O	2.07	0.72
1:A:1238:GLY:O	19:c:675:LYS:NZ	2.22	0.72
1:A:576:GLN:O	1:A:590:GLN:NE2	2.23	0.72
14:N:4:DG:H2''	14:N:5:DT:H71	1.72	0.72
19:c:5:LEU:HD21	19:c:31:ILE:HG21	1.70	0.71
8:H:91:VAL:HG13	8:H:144:LEU:HD12	1.73	0.71
2:B:847:LYS:NZ	2:B:864:ASP:OD2	2.18	0.71
1:A:332:SER:HB3	16:T:34:DT:H5''	1.72	0.71
2:B:239:MET:SD	2:B:254:GLN:HB3	2.31	0.71
2:B:957:THR:OG1	2:B:959:GLU:O	2.08	0.70
1:A:865:ILE:HD13	1:A:1092:ALA:HB3	1.73	0.70
1:A:238:MET:HE1	1:A:248:MET:SD	2.31	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:15:DC:H4'	19:c:683:ARG:NH1	2.06	0.70
2:B:816:GLU:OE2	2:B:894:THR:OG1	2.09	0.70
5:E:134:GLU:OE1	5:E:181:ARG:NH2	2.25	0.70
16:T:12:DG:H4'	16:T:13:DC:OP1	1.91	0.69
20:d:47:GLU:OE1	20:d:47:GLU:N	2.25	0.69
1:A:1173:THR:HG22	1:A:1214:VAL:HG12	1.73	0.69
1:A:1235:ILE:HG12	1:A:1296:MET:HE1	1.74	0.69
2:B:207:VAL:HG11	2:B:375:ALA:CB	2.22	0.69
1:A:321:GLU:OE1	1:A:341:GLN:NE2	2.26	0.69
14:N:8:DA:H2''	14:N:9:DT:H5'	1.72	0.69
17:a:33:ASN:HD22	17:a:360:ALA:HB3	1.56	0.69
16:T:14:DT:H1'	16:T:15:DC:H5'	1.75	0.68
17:a:149:MET:HG2	17:a:159:VAL:HG22	1.74	0.68
14:N:47:DG:H2'	14:N:48:DA:C8	2.28	0.68
9:I:50:ASN:O	9:I:51:SER:OG	2.10	0.68
4:D:20:LEU:HD11	4:D:93:HIS:CD2	2.29	0.67
12:L:22:CYS:SG	12:L:24:THR:OG1	2.45	0.67
17:a:135:ALA:O	18:b:1397:ASN:ND2	2.27	0.67
16:T:44:DA:OP1	18:b:575:THR:OG1	2.14	0.66
1:A:374:SER:OG	1:A:376:ASP:OD1	2.12	0.66
16:T:11:DT:C2'	16:T:12:DG:H5'	2.21	0.66
1:A:413:TYR:O	1:A:415:GLY:N	2.28	0.66
1:A:862:ARG:NH1	2:B:1088:GLU:OE2	2.28	0.66
1:A:1182:GLN:O	1:A:1190:GLN:NE2	2.28	0.66
17:a:30:LEU:HD23	17:a:330:LEU:HD11	1.78	0.66
14:N:11:DT:H1'	14:N:12:DC:H5'	1.78	0.66
1:A:808:PRO:HG2	2:B:675:LEU:HD12	1.77	0.65
16:T:47:DA:H4'	16:T:48:DA:OP1	1.95	0.65
1:A:549:THR:O	1:A:589:LYS:NZ	2.29	0.65
1:A:358:ARG:NH1	16:T:27:DC:OP1	2.30	0.65
1:A:659:GLU:OE2	1:A:985:ARG:NH1	2.30	0.65
2:B:473:LEU:HD22	2:B:731:GLN:HA	1.77	0.65
9:I:109:ARG:HE	9:I:124:THR:HG21	1.59	0.65
18:b:575:THR:HA	18:b:578:MET:HE2	1.78	0.65
20:d:381:ALA:O	20:d:385:GLY:N	2.29	0.65
2:B:613:ARG:NH1	2:B:615:TYR:OH	2.30	0.65
1:A:255:VAL:HG22	1:A:280:LEU:HD13	1.78	0.65
1:A:413:TYR:OH	1:A:450:MET:O	2.13	0.65
14:N:4:DG:C2'	14:N:5:DT:H71	2.26	0.65
2:B:1007:ASN:OD1	2:B:1010:LYS:HD3	1.96	0.65
2:B:993:LYS:NZ	2:B:995:GLU:OE2	2.21	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:298:MET:HE3	9:I:14:ILE:HG22	1.79	0.64
1:A:862:ARG:NH2	1:A:1432:PHE:O	2.31	0.64
4:D:90:LYS:HE2	4:D:130:ILE:HD12	1.78	0.64
1:A:767:LYS:O	1:A:771:VAL:HG22	1.98	0.64
17:a:37:ASP:HB2	17:a:83:THR:HG22	1.80	0.63
17:a:33:ASN:ND2	17:a:360:ALA:HB3	2.14	0.63
16:T:19:DC:H2''	16:T:20:DT:H71	1.81	0.62
19:c:50:LEU:HB3	19:c:89:LEU:HD13	1.79	0.62
3:C:106:ARG:HE	3:C:158:GLU:HG3	1.63	0.62
1:A:461:GLN:NE2	2:B:1090:GLU:OE2	2.32	0.62
1:A:964:GLU:O	1:A:968:VAL:HG23	1.99	0.62
16:T:12:DG:C1'	16:T:13:DC:H5''	2.27	0.62
4:D:37:VAL:CG1	4:D:41:LEU:HD12	2.29	0.62
14:N:43:DG:H2''	14:N:44:DA:C8	2.35	0.62
17:a:96:ASP:O	17:a:125:LYS:NZ	2.29	0.62
18:b:633:ASP:OD1	18:b:634:ASP:N	2.33	0.62
14:N:38:DG:H1'	14:N:39:DA:H5'	1.81	0.62
1:A:1169:VAL:HG23	1:A:1220:HIS:HB3	1.79	0.62
2:B:1120:ASN:OD1	2:B:1147:SER:OG	2.18	0.62
1:A:77:ASN:OD1	1:A:80:GLU:HG2	2.00	0.62
1:A:192:ARG:HG3	1:A:199:TYR:HB2	1.81	0.62
2:B:252:ILE:O	2:B:252:ILE:HG22	1.99	0.62
5:E:112:PRO:CB	16:T:12:DG:H5''	2.29	0.61
16:T:4:DT:OP2	16:T:4:DT:H3'	2.00	0.61
16:T:1:DG:C4'	16:T:2:DT:H5'	2.30	0.61
18:b:534:MET:O	18:b:747:LYS:NZ	2.22	0.61
1:A:1311:LEU:HD12	1:A:1332:GLN:HG3	1.80	0.61
20:d:196:SER:OG	20:d:203:ASN:OD1	2.18	0.61
17:a:192:VAL:HG12	17:a:204:THR:HG22	1.83	0.61
3:C:59:LEU:HD13	3:C:63:PHE:CD1	2.36	0.60
6:F:100:ARG:NH2	6:F:121:ASP:O	2.34	0.60
14:N:41:DC:H5'	19:c:679:LYS:HE3	1.78	0.60
3:C:180:ALA:O	10:J:42:ARG:NH2	2.35	0.60
1:A:760:LEU:HD22	1:A:764:ASN:ND2	2.17	0.60
2:B:794:VAL:HG12	2:B:967:ILE:HG22	1.84	0.60
20:d:917:LYS:NZ	20:d:962:ASP:OD1	2.25	0.60
5:E:91:CYS:SG	5:E:121:MET:HE1	2.41	0.60
16:T:14:DT:H2''	16:T:15:DC:H5'	1.84	0.60
1:A:26:LEU:HD11	2:B:1163:MET:HG2	1.84	0.60
1:A:1190:GLN:O	1:A:1194:ASN:ND2	2.34	0.60
1:A:373:LEU:O	1:A:485:ASN:ND2	2.34	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1191:GLU:O	1:A:1195:VAL:HG23	2.01	0.59
2:B:254:GLN:OE1	2:B:254:GLN:HA	2.02	0.59
8:H:92:MET:HE2	8:H:143:LEU:HD22	1.84	0.59
11:K:63:VAL:HG22	11:K:71:ILE:HG22	1.83	0.59
1:A:865:ILE:HD13	1:A:1092:ALA:CB	2.31	0.59
2:B:214:LYS:C	2:B:241:ALA:HB2	2.27	0.59
2:B:324:ARG:HG3	13:M:20:LEU:HD11	1.84	0.59
14:N:5:DT:C2'	14:N:6:DT:H71	2.32	0.59
2:B:210:LYS:NZ	2:B:212:ASP:O	2.35	0.59
2:B:1127:ILE:CD1	2:B:1138:ARG:HD2	2.33	0.59
4:D:37:VAL:HG13	4:D:41:LEU:HD12	1.85	0.59
5:E:78:GLU:OE1	5:E:78:GLU:N	2.35	0.59
14:N:14:DT:H4'	18:b:936:TRP:HB2	1.83	0.59
17:a:128:ASP:OD2	18:b:1394:ARG:NH2	2.36	0.59
2:B:359:THR:HG21	2:B:554:GLU:HA	1.85	0.59
18:b:517:TRP:CZ2	18:b:521:LEU:HD11	2.37	0.59
1:A:457:ILE:HD11	1:A:515:ILE:HD12	1.84	0.58
17:a:144:VAL:HA	17:a:163:THR:HG22	1.85	0.58
1:A:112:PHE:O	1:A:220:ARG:NH1	2.36	0.58
16:T:1:DG:H1'	16:T:2:DT:C6	2.38	0.58
16:T:39:DA:H2'	16:T:40:DT:C6	2.38	0.58
1:A:413:TYR:O	1:A:449:HIS:ND1	2.36	0.58
20:d:929:SER:O	20:d:930:VAL:HG13	2.04	0.58
5:E:26:TYR:CE2	5:E:72:MET:HE2	2.37	0.58
16:T:14:DT:C2'	16:T:15:DC:H5'	2.32	0.58
20:d:1043:LEU:HD13	20:d:1051:LEU:HD12	1.84	0.58
14:N:1:DC:C2'	14:N:2:DT:H5'	2.28	0.58
14:N:49:DA:H2''	14:N:50:DT:H71	1.86	0.58
2:B:1127:ILE:HD12	2:B:1138:ARG:HD2	1.84	0.58
7:G:100:GLU:N	7:G:100:GLU:OE1	2.37	0.58
20:d:118:THR:OG1	20:d:134:ARG:NH2	2.37	0.58
5:E:120:ASP:OD1	5:E:121:MET:N	2.37	0.57
1:A:1211:LEU:HA	1:A:1260:ARG:HB3	1.85	0.57
2:B:565:THR:HG21	2:B:580:PRO:HB3	1.86	0.57
5:E:56:THR:OG1	5:E:78:GLU:OE2	2.19	0.57
16:T:47:DA:H2''	16:T:48:DA:H5''	1.86	0.57
19:c:82:ASN:ND2	19:c:85:GLU:OE2	2.36	0.57
4:D:103:LEU:O	7:G:144:ARG:NH2	2.37	0.57
1:A:853:LYS:NZ	1:A:1102:MET:O	2.35	0.57
2:B:255:ARG:HD2	2:B:307:GLU:OE1	2.03	0.57
20:d:166:ASP:OD1	20:d:167:VAL:N	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:PHE:CE1	1:A:672:ILE:HD11	2.39	0.57
17:a:35:ASP:O	17:a:81:TYR:HA	2.03	0.57
20:d:816:LEU:HD13	20:d:831:VAL:HG22	1.86	0.57
4:D:33:LEU:HD22	4:D:101:ALA:HB3	1.86	0.57
9:I:100:HIS:ND1	9:I:100:HIS:O	2.36	0.57
14:N:5:DT:H1'	14:N:6:DT:H5'	1.85	0.57
1:A:1198:GLU:OE1	1:A:1198:GLU:N	2.35	0.56
16:T:29:DC:H2'	16:T:30:DT:C6	2.40	0.56
14:N:41:DC:H5''	19:c:679:LYS:NZ	2.19	0.56
2:B:270:ILE:HG23	2:B:284:ILE:HD13	1.87	0.56
18:b:538:LYS:N	23:b:1501:ADP:O2B	2.39	0.56
1:A:191:ILE:HD13	1:A:200:ALA:HB2	1.87	0.56
1:A:521:VAL:HG13	1:A:535:MET:HE1	1.87	0.56
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.87	0.56
16:T:8:DC:H2''	16:T:9:DT:O5'	2.05	0.56
18:b:603:TYR:O	18:b:604:THR:OG1	2.20	0.56
2:B:207:VAL:HG11	2:B:375:ALA:HB3	1.87	0.56
16:T:11:DT:H4'	16:T:11:DT:OP1	2.05	0.56
16:T:5:DT:H2''	16:T:6:DC:O5'	2.06	0.56
1:A:1203:ASP:HB3	1:A:1206:ARG:HD3	1.88	0.56
11:K:111:ASP:O	11:K:115:GLY:N	2.33	0.56
14:N:42:DA:H2''	14:N:43:DG:C5'	2.36	0.56
20:d:282:MET:HE2	20:d:305:LEU:HD11	1.88	0.55
2:B:87:LYS:HD3	2:B:89:GLU:HB3	1.88	0.55
2:B:274:ARG:NH2	2:B:281:ASP:OD1	2.40	0.55
19:c:5:LEU:HD21	19:c:31:ILE:CG2	2.35	0.55
1:A:54:LEU:O	1:A:61:ARG:NH2	2.39	0.55
1:A:102:LYS:O	1:A:105:LYS:HB3	2.06	0.55
6:F:84:GLU:OE2	6:F:84:GLU:N	2.40	0.55
16:T:16:DC:C2'	16:T:17:DT:H71	2.35	0.55
18:b:643:VAL:HG12	18:b:643:VAL:O	2.06	0.55
1:A:1460:LEU:HD22	2:B:1155:CYS:SG	2.47	0.55
2:B:625:LEU:HD13	2:B:675:LEU:HD21	1.89	0.55
20:d:130:MET:HE1	20:d:195:VAL:HG11	1.88	0.55
14:N:5:DT:H2''	14:N:6:DT:H71	1.87	0.55
14:N:10:DC:C2'	14:N:11:DT:H71	2.36	0.55
2:B:927:ARG:NH1	2:B:1057:ASP:OD1	2.38	0.55
18:b:768:LEU:HD11	18:b:967:THR:HG22	1.89	0.55
16:T:42:DA:OP1	18:b:865:ARG:N	2.39	0.55
1:A:1204:VAL:O	1:A:1207:ILE:HG22	2.06	0.55
18:b:910:PHE:CE2	18:b:912:LEU:HD21	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:102:ASP:OD2	8:H:110:THR:OG1	2.24	0.55
14:N:10:DC:H1'	14:N:11:DT:H5''	1.89	0.55
1:A:763:TYR:OH	8:H:23:ASP:OD2	2.08	0.54
2:B:224:CYS:HB2	2:B:232:THR:HG22	1.87	0.54
1:A:951:GLU:OE2	1:A:954:ARG:NH2	2.40	0.54
1:A:1338:THR:OG1	1:A:1340:GLY:O	2.12	0.54
17:a:116:THR:HG22	17:a:126:VAL:HG22	1.88	0.54
20:d:232:ILE:HD13	20:d:237:ILE:HG23	1.89	0.54
1:A:1162:GLU:OE1	1:A:1306:LYS:HD2	2.07	0.54
3:C:190:ASN:O	3:C:193:ARG:NH1	2.39	0.54
14:N:31:DG:H5'	14:N:31:DG:H8	1.72	0.54
2:B:501:LEU:HD12	2:B:505:LEU:CD1	2.34	0.54
1:A:421:ARG:NH1	1:A:444:TYR:OH	2.40	0.54
11:K:24:ASP:OD1	11:K:26:LYS:HG2	2.07	0.54
13:M:25:THR:O	13:M:71:TYR:OH	2.15	0.54
18:b:973:TYR:CZ	18:b:977:ILE:HD11	2.43	0.54
7:G:95:VAL:O	7:G:110:ARG:N	2.39	0.54
18:b:647:GLU:N	18:b:673:LEU:O	2.39	0.54
14:N:38:DG:H1'	14:N:39:DA:C5'	2.38	0.54
1:A:1208:SER:CB	1:A:1261:ILE:HG23	2.37	0.54
16:T:25:DT:H2'	16:T:26:DC:C6	2.43	0.54
1:A:1357:THR:O	5:E:142:HIS:NE2	2.38	0.53
14:N:3:DA:H2''	14:N:4:DG:C8	2.43	0.53
2:B:214:LYS:O	2:B:241:ALA:HB2	2.07	0.53
18:b:776:TYR:CZ	18:b:802:LEU:HD22	2.43	0.53
19:c:40:SER:OG	19:c:44:ARG:NH1	2.41	0.53
1:A:540:ASP:OD1	2:B:784:SER:OG	2.15	0.53
1:A:1208:SER:HB3	1:A:1261:ILE:HG23	1.90	0.53
16:T:43:DG:OP1	18:b:913:THR:OG1	2.21	0.53
18:b:510:TYR:OH	18:b:536:LEU:O	2.12	0.53
20:d:308:THR:O	20:d:383:LYS:NZ	2.32	0.53
11:K:9:SER:HA	11:K:69:HIS:CG	2.44	0.53
17:a:37:ASP:CB	17:a:83:THR:HG22	2.39	0.53
7:G:39:THR:O	7:G:43:GLY:N	2.41	0.53
2:B:270:ILE:HD12	2:B:284:ILE:HG21	1.90	0.53
2:B:549:SER:OG	2:B:577:HIS:CE1	2.61	0.53
2:B:1078:ARG:HG3	16:T:28:DT:H5''	1.90	0.53
4:D:92:LEU:HD12	4:D:96:GLU:HB2	1.89	0.53
14:N:10:DC:H5'	14:N:10:DC:C6	2.44	0.53
16:T:14:DT:C1'	16:T:15:DC:H5'	2.39	0.53
17:a:2:LEU:HD12	20:d:836:VAL:CG2	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:a:37:ASP:O	17:a:83:THR:HA	2.08	0.53
16:T:18:DT:H6	16:T:18:DT:H5'	1.74	0.53
2:B:360:LYS:HE3	2:B:554:GLU:OE2	2.08	0.52
20:d:1055:GLN:HG3	20:d:1093:LEU:HD23	1.91	0.52
16:T:16:DC:H2''	16:T:17:DT:O5'	2.08	0.52
7:G:60:GLN:HB3	7:G:63:ARG:HD3	1.91	0.52
14:N:43:DG:H2''	14:N:44:DA:H8	1.72	0.52
2:B:761:THR:H	2:B:764:MET:HE3	1.73	0.52
16:T:4:DT:H2''	16:T:5:DT:O5'	2.09	0.52
1:A:728:THR:H	1:A:736:THR:HG21	1.75	0.52
14:N:11:DT:H2''	14:N:12:DC:H5'	1.91	0.52
14:N:34:DG:H2''	14:N:35:DA:C8	2.45	0.52
2:B:812:ARG:NH2	2:B:900:GLU:OE2	2.40	0.52
1:A:1202:PHE:HB2	1:A:1262:MET:HE1	1.92	0.52
17:a:42:HIS:HE2	17:a:61:SER:HG	1.57	0.52
1:A:103:THR:HG22	1:A:248:MET:HE2	1.92	0.52
2:B:602:SER:OG	2:B:620:ARG:NH1	2.43	0.52
14:N:8:DA:C2'	14:N:9:DT:H5'	2.38	0.52
18:b:840:LYS:NZ	18:b:969:GLU:OE2	2.42	0.52
1:A:1222:THR:HG21	19:c:559:LYS:HB2	1.91	0.51
14:N:10:DC:H5'	14:N:10:DC:H6	1.74	0.51
18:b:635:ILE:O	18:b:640:TRP:NE1	2.40	0.51
14:N:11:DT:C2'	14:N:12:DC:H5'	2.40	0.51
14:N:46:DC:H2''	14:N:47:DG:N7	2.24	0.51
1:A:707:LYS:O	1:A:711:GLN:HB3	2.09	0.51
14:N:10:DC:H2'	14:N:11:DT:H71	1.91	0.51
18:b:717:SER:OG	18:b:995:PHE:O	2.22	0.51
19:c:46:LEU:HD13	19:c:65:VAL:CG2	2.40	0.51
7:G:91:GLN:NE2	7:G:93:ASN:OD1	2.44	0.51
20:d:915:LYS:NZ	20:d:958:GLU:OE1	2.42	0.51
1:A:734:ARG:CD	9:I:108:MET:SD	2.99	0.51
16:T:17:DT:C2'	16:T:18:DT:H71	2.40	0.51
17:a:35:ASP:O	17:a:81:TYR:CD1	2.64	0.51
18:b:529:ILE:HG13	18:b:692:ILE:HD13	1.92	0.51
7:G:90:THR:O	7:G:139:GLN:NE2	2.41	0.51
1:A:523:ARG:NH1	6:F:127:ASP:OD2	2.44	0.50
1:A:709:ALA:HB2	1:A:748:ALA:HB2	1.92	0.50
3:C:7:PRO:O	11:K:104:ARG:NH1	2.44	0.50
4:D:90:LYS:CE	4:D:130:ILE:HD12	2.41	0.50
17:a:40:ARG:NE	17:a:357:ASN:OD1	2.41	0.50
18:b:912:LEU:HD22	18:b:917:GLY:CA	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:959:GLU:O	2:B:961:ILE:N	2.41	0.50
7:G:62:GLY:C	7:G:63:ARG:HG2	2.36	0.50
14:N:46:DC:H2''	14:N:47:DG:C8	2.46	0.50
16:T:18:DT:H5'	16:T:18:DT:C6	2.47	0.50
18:b:922:ASN:OD1	18:b:950:ARG:NE	2.37	0.50
2:B:254:GLN:O	2:B:303:PRO:HB2	2.11	0.50
19:c:1:MET:O	19:c:5:LEU:HD23	2.12	0.50
2:B:381:GLU:OE1	2:B:381:GLU:N	2.39	0.50
14:N:31:DG:H5'	14:N:31:DG:C8	2.46	0.50
18:b:754:LEU:HD21	18:b:951:ILE:HG12	1.94	0.50
17:a:111:ASP:OD2	18:b:1386:SER:OG	2.24	0.50
1:A:91:ALA:HB2	1:A:291:ARG:HB2	1.93	0.50
17:a:218:ARG:NH1	18:b:525:GLN:OE1	2.45	0.50
1:A:1341:VAL:HG22	1:A:1364:GLU:OE2	2.12	0.50
1:A:486:LEU:HD13	2:B:790:GLN:CD	2.37	0.50
14:N:49:DA:C2'	14:N:50:DT:H71	2.41	0.50
16:T:40:DT:OP1	18:b:797:SER:OG	2.29	0.49
1:A:1211:LEU:HA	1:A:1260:ARG:CB	2.42	0.49
23:b:1501:ADP:O3B	24:b:1502:BEF:F1	2.20	0.49
16:T:47:DA:H2''	16:T:48:DA:C5'	2.42	0.49
17:a:219:ALA:HB2	18:b:693:PHE:HD1	1.76	0.49
1:A:904:GLN:NE2	1:A:981:CYS:O	2.44	0.49
18:b:868:LEU:HD22	18:b:913:THR:HG23	1.94	0.49
7:G:1:MET:O	7:G:77:PHE:HA	2.12	0.49
20:d:1054:MET:SD	20:d:1129:LEU:HD13	2.52	0.49
1:A:461:GLN:OE1	1:A:502:ASN:ND2	2.45	0.49
8:H:49:PRO:O	8:H:147:LYS:NZ	2.45	0.49
14:N:15:DA:H1'	14:N:16:DT:C2	2.47	0.49
14:N:32:DG:H2''	14:N:33:DA:OP2	2.13	0.49
1:A:1249:ASP:OD2	19:c:580:GLN:N	2.42	0.49
16:T:17:DT:H1'	16:T:18:DT:H5''	1.95	0.49
16:T:39:DA:H2''	16:T:40:DT:O5'	2.12	0.49
18:b:896:PRO:O	18:b:899:THR:OG1	2.22	0.49
18:b:921:VAL:O	18:b:947:ARG:NH1	2.43	0.49
1:A:1139:LEU:HD21	1:A:1341:VAL:HG23	1.95	0.49
5:E:55:ARG:NH2	5:E:132:GLN:OE1	2.46	0.49
18:b:766:CYS:N	18:b:963:LEU:O	2.43	0.49
18:b:924:THR:O	18:b:953:GLN:NE2	2.45	0.49
2:B:310:VAL:HG23	2:B:311:ILE:HG13	1.95	0.49
3:C:189:ASP:O	3:C:191:ALA:N	2.46	0.49
18:b:534:MET:SD	18:b:534:MET:N	2.86	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:b:1395:ALA:O	18:b:1399:LEU:HD23	2.12	0.49
14:N:16:DT:OP1	18:b:975:ARG:NE	2.46	0.48
7:G:22:LEU:HD12	7:G:23:LEU:HD22	1.96	0.48
1:A:928:ARG:NH1	8:H:107:GLU:OE1	2.46	0.48
1:A:1235:ILE:HG12	1:A:1296:MET:CE	2.42	0.48
17:a:213:LEU:O	17:a:223:LEU:N	2.45	0.48
18:b:614:VAL:HG11	18:b:621:LEU:HB2	1.95	0.48
18:b:938:PRO:O	18:b:942:THR:HG23	2.13	0.48
1:A:1146:GLN:HB3	1:A:1153:ARG:HE	1.78	0.48
1:A:1217:ASP:OD2	1:A:1220:HIS:ND1	2.46	0.48
1:A:1221:MET:SD	1:A:1231:ILE:HD11	2.53	0.48
2:B:302:LYS:HD3	9:I:23:MET:HE1	1.94	0.48
9:I:99:SER:HB3	9:I:104:ALA:HB1	1.94	0.48
9:I:72:VAL:HG22	9:I:78:LEU:HD11	1.95	0.48
14:N:7:DG:H2''	14:N:8:DA:H5'	1.96	0.48
18:b:537:GLY:O	18:b:541:GLN:NE2	2.41	0.48
1:A:1433:GLU:OE2	16:T:22:DC:H4'	2.13	0.48
3:C:85:SER:OG	3:C:166:LYS:HE3	2.13	0.48
7:G:117:MET:SD	7:G:135:ILE:HG13	2.54	0.48
16:T:29:DC:H2''	16:T:30:DT:H5'	1.96	0.48
20:d:963:ASP:OD1	20:d:963:ASP:N	2.45	0.48
2:B:735:VAL:HG21	10:J:55:LEU:HD13	1.95	0.48
3:C:59:LEU:HD13	3:C:63:PHE:CE1	2.49	0.48
14:N:33:DA:OP2	14:N:33:DA:H2'	2.13	0.48
1:A:733:LEU:HD13	9:I:107:ALA:HA	1.96	0.47
2:B:217:TYR:CE2	2:B:376:ALA:HA	2.49	0.47
16:T:24:DA:H2'	16:T:25:DT:C6	2.49	0.47
1:A:899:GLU:N	1:A:899:GLU:OE1	2.47	0.47
14:N:42:DA:H2''	14:N:43:DG:O5'	2.14	0.47
18:b:857:ARG:NH1	18:b:901:TYR:O	2.45	0.47
4:D:95:PHE:CE1	7:G:1:MET:HE3	2.50	0.47
16:T:19:DC:C2'	16:T:20:DT:H71	2.43	0.47
3:C:228:ARG:HB2	3:C:228:ARG:HH21	1.79	0.47
17:a:157:CYS:SG	17:a:173:LEU:HD12	2.55	0.47
1:A:107:LEU:HD21	1:A:221:VAL:HG13	1.97	0.47
17:a:30:LEU:HD11	17:a:361:TRP:HB2	1.96	0.47
2:B:942:LYS:NZ	15:P:10:A:OP1	2.41	0.47
7:G:49:THR:OG1	7:G:50:THR:N	2.47	0.47
14:N:11:DT:C1'	14:N:12:DC:H5'	2.43	0.47
16:T:6:DC:H1'	16:T:7:DG:C8	2.50	0.47
16:T:7:DG:H2''	16:T:8:DC:OP2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:14:DT:H6	16:T:14:DT:H5''	1.80	0.47
16:T:16:DC:H1'	16:T:17:DT:H5'	1.97	0.47
20:d:226:PHE:O	20:d:241:ASN:ND2	2.48	0.47
20:d:248:ILE:HD12	20:d:250:PRO:HG3	1.97	0.47
8:H:136:GLU:O	8:H:139:SER:OG	2.29	0.47
2:B:733:MET:CE	2:B:1054:MET:HE2	2.35	0.46
4:D:34:ASN:OD1	4:D:102:ASN:ND2	2.48	0.46
16:T:8:DC:H2'	16:T:9:DT:H72	1.95	0.46
1:A:935:GLN:O	1:A:939:VAL:HG23	2.16	0.46
2:B:209:ALA:N	2:B:382:LEU:HD13	2.31	0.46
4:D:37:VAL:HG12	4:D:41:LEU:HD12	1.96	0.46
5:E:127:LEU:HD23	5:E:127:LEU:H	1.81	0.46
18:b:973:TYR:CE2	18:b:977:ILE:HD11	2.50	0.46
19:c:46:LEU:HD13	19:c:65:VAL:HG22	1.97	0.46
1:A:1167:ARG:HH12	1:A:1294:THR:HG22	1.80	0.46
4:D:57:LEU:HD13	4:D:61:PHE:CE2	2.50	0.46
17:a:338:ASP:OD2	17:a:354:ARG:NH1	2.47	0.46
20:d:1002:GLU:OE1	20:d:1034:ASN:ND2	2.46	0.46
1:A:98:GLY:HA3	1:A:1440:MET:HE3	1.97	0.46
1:A:110:VAL:HG11	1:A:228:ILE:HD11	1.98	0.46
1:A:1005:HIS:ND1	1:A:1007:ILE:HG22	2.30	0.46
3:C:144:GLU:OE1	3:C:144:GLU:N	2.48	0.46
18:b:651:ILE:HG22	18:b:651:ILE:O	2.15	0.46
1:A:535:MET:O	1:A:669:TYR:OH	2.26	0.46
1:A:889:LEU:O	1:A:890:ARG:NH1	2.42	0.46
18:b:659:THR:HG22	18:b:663:LYS:HD2	1.97	0.46
16:T:21:DC:H2'	16:T:22:DC:C6	2.50	0.46
18:b:840:LYS:NZ	18:b:932:TYR:O	2.46	0.46
1:A:863:ARG:NH2	1:A:1129:ASN:OD1	2.48	0.46
16:T:28:DT:H2'	16:T:29:DC:C6	2.51	0.46
1:A:760:LEU:HD22	1:A:764:ASN:HD22	1.81	0.46
14:N:50:DT:H5''	14:N:50:DT:H6	1.79	0.46
20:d:821:LEU:HD11	20:d:830:ILE:HD11	1.98	0.46
2:B:777:ASN:O	10:J:47:ARG:NH1	2.44	0.45
3:C:70:LEU:O	10:J:6:ARG:NE	2.40	0.45
20:d:310:ILE:HG21	20:d:328:LEU:HD12	1.97	0.45
1:A:865:ILE:HG21	2:B:1092:ASP:CG	2.40	0.45
9:I:23:MET:HE2	9:I:25:TYR:CE1	2.51	0.45
14:N:7:DG:H2''	14:N:8:DA:C5'	2.46	0.45
16:T:2:DT:H2''	16:T:3:DA:OP2	2.15	0.45
1:A:46:THR:HG21	1:A:273:GLN:OE1	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1035:ARG:NH1	2:B:1036:LYS:O	2.47	0.45
7:G:44:PHE:CE1	7:G:104:MET:HB2	2.51	0.45
1:A:902:GLU:OE2	1:A:982:ASN:HB2	2.17	0.45
1:A:1166:LEU:O	1:A:1170:THR:OG1	2.16	0.45
4:D:86:LEU:O	4:D:90:LYS:NZ	2.49	0.45
1:A:100:LEU:O	1:A:103:THR:OG1	2.33	0.45
4:D:36:GLU:OE2	4:D:84:ARG:NH1	2.50	0.45
20:d:791:LEU:HD23	20:d:858:LEU:HD21	1.98	0.45
1:A:274:ASP:OD2	1:A:342:ARG:NH2	2.50	0.45
1:A:1259:ILE:O	1:A:1259:ILE:HG22	2.15	0.45
1:A:1285:LEU:HA	1:A:1288:ILE:HD12	1.99	0.45
18:b:539:THR:HG22	18:b:543:ILE:HD12	1.98	0.45
7:G:11:ILE:HD11	7:G:26:VAL:HG13	1.99	0.45
16:T:34:DT:H2''	16:T:35:DG:O3'	2.16	0.45
1:A:106:VAL:O	1:A:110:VAL:HG13	2.17	0.45
16:T:48:DA:H2''	16:T:49:DC:O4'	2.16	0.45
18:b:542:ILE:HG13	18:b:673:LEU:HD11	1.98	0.45
20:d:768:SER:HB3	20:d:808:LEU:HD11	1.98	0.45
2:B:95:LYS:HD2	2:B:162:LEU:HD23	1.99	0.45
1:A:967:ARG:NH2	1:A:1326:GLY:O	2.49	0.44
18:b:540:ILE:HD12	18:b:588:TRP:CE2	2.51	0.44
20:d:8:THR:HG23	20:d:1036:MET:HG3	1.99	0.44
20:d:807:PHE:CZ	20:d:831:VAL:HG11	2.52	0.44
2:B:432:GLU:OE1	2:B:432:GLU:N	2.48	0.44
16:T:28:DT:H2'	16:T:29:DC:H6	1.82	0.44
18:b:582:VAL:HG21	18:b:596:ILE:HD11	1.99	0.44
14:N:3:DA:H2''	14:N:4:DG:H8	1.79	0.44
16:T:15:DC:H2''	16:T:16:DC:C6	2.52	0.44
17:a:36:ARG:HD3	17:a:82:TYR:OH	2.18	0.44
19:c:8:LEU:HD11	19:c:24:LYS:HB2	2.00	0.44
20:d:881:LEU:HD21	20:d:921:ILE:HG21	1.98	0.44
1:A:1286:ARG:HH21	1:A:1286:ARG:HD3	1.43	0.44
2:B:628:VAL:HG12	2:B:629:GLU:O	2.16	0.44
14:N:8:DA:H1'	14:N:9:DT:H5'	1.98	0.44
14:N:11:DT:H6	14:N:11:DT:H5'	1.82	0.44
20:d:311:ALA:HB2	20:d:324:VAL:HG13	2.00	0.44
1:A:811:ILE:HD12	9:I:79:PRO:HB3	1.99	0.44
1:A:1294:THR:OG1	19:c:685:VAL:HG22	2.18	0.44
6:F:51:ARG:NH1	6:F:117:ASP:O	2.48	0.44
7:G:21:ASN:OD1	7:G:24:ASN:HB2	2.18	0.44
18:b:1001:LEU:HD23	18:b:1001:LEU:H	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:d:821:LEU:HD11	20:d:830:ILE:CD1	2.46	0.44
2:B:710:ILE:HD12	2:B:769:PHE:CD1	2.52	0.44
2:B:785:TYR:O	2:B:786:THR:OG1	2.33	0.44
18:b:532:ASP:OD2	18:b:745:ARG:NH2	2.49	0.44
2:B:35:ASP:OD2	2:B:646:ARG:NH2	2.51	0.44
2:B:887:TYR:O	2:B:888:THR:HG22	2.18	0.44
18:b:754:LEU:HD21	18:b:951:ILE:CG1	2.48	0.44
20:d:1026:GLY:O	20:d:1041:THR:HG22	2.17	0.44
16:T:24:DA:H2'	16:T:25:DT:H6	1.83	0.44
18:b:912:LEU:HD22	18:b:917:GLY:HA2	2.00	0.44
1:A:868:MET:HE2	1:A:1401:LEU:HD13	1.99	0.44
2:B:227:ASN:O	2:B:229:SER:N	2.50	0.44
2:B:1105:GLU:HA	2:B:1109:GLU:HG2	2.00	0.44
16:T:8:DC:C6	16:T:9:DT:H72	2.52	0.44
2:B:544:PHE:HB2	2:B:596:ILE:CD1	2.48	0.43
2:B:905:ASP:N	2:B:922:ARG:O	2.51	0.43
7:G:62:GLY:O	7:G:64:GLY:N	2.51	0.43
18:b:607:LYS:O	18:b:610:LEU:N	2.50	0.43
18:b:667:THR:O	18:b:670:ARG:NE	2.51	0.43
18:b:859:LEU:HD11	18:b:912:LEU:CD1	2.48	0.43
20:d:356:LEU:HD11	20:d:712:ILE:HD13	2.00	0.43
20:d:884:ILE:HG22	20:d:885:ASN:H	1.83	0.43
1:A:1207:ILE:HA	1:A:1262:MET:HG3	2.00	0.43
16:T:22:DC:H2'	16:T:23:DC:C6	2.53	0.43
19:c:31:ILE:HG22	19:c:38:GLN:OE1	2.18	0.43
2:B:67:LEU:HD11	2:B:416:ARG:HA	1.99	0.43
1:A:105:LYS:HD3	1:A:141:LEU:CD2	2.48	0.43
2:B:378:GLY:HA3	9:I:102:ALA:HB3	2.00	0.43
9:I:65:LEU:O	9:I:122:ARG:HD2	2.18	0.43
20:d:1109:VAL:HG12	20:d:1109:VAL:O	2.19	0.43
1:A:1030:SER:OG	5:E:162:ARG:NE	2.52	0.43
14:N:10:DC:H2''	14:N:11:DT:H5'	2.00	0.43
14:N:33:DA:H2''	14:N:34:DG:C8	2.54	0.43
17:a:114:MET:HE1	18:b:1389:LEU:HD23	2.01	0.43
18:b:648:GLY:HA3	18:b:672:ILE:HG23	2.00	0.43
1:A:509:LEU:CD2	6:F:90:LEU:HD12	2.48	0.43
1:A:1475:LEU:HB2	7:G:66:VAL:HG21	2.01	0.43
4:D:61:PHE:HA	4:D:64:THR:HG22	2.01	0.43
1:A:823:VAL:CG1	1:A:831:LEU:HD22	2.49	0.43
1:A:959:MET:HE1	1:A:1050:CYS:SG	2.58	0.43
20:d:310:ILE:O	20:d:326:SER:OG	2.29	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:764:MET:HE1	2:B:938:ARG:NH1	2.34	0.43
3:C:11:ILE:HD13	11:K:109:ILE:HD13	2.00	0.43
14:N:41:DC:H2''	14:N:42:DA:OP2	2.18	0.43
16:T:17:DT:H2''	16:T:18:DT:H5'	2.00	0.43
19:c:87:LEU:HD22	19:c:138:LEU:HD11	2.01	0.43
1:A:823:VAL:HG11	1:A:831:LEU:HD22	2.01	0.43
1:A:1196:TYR:O	1:A:1199:MET:SD	2.77	0.43
1:A:1229:GLU:OE2	19:c:582:ARG:N	2.52	0.43
2:B:285:LEU:HD21	2:B:301:VAL:HG11	2.01	0.43
3:C:86:ARG:HD3	11:K:11:LEU:HD11	2.00	0.43
12:L:27:GLU:OE1	12:L:29:LYS:HD2	2.18	0.43
14:N:47:DG:H2''	14:N:48:DA:H5'	2.00	0.43
16:T:25:DT:H2'	16:T:26:DC:H6	1.82	0.43
1:A:192:ARG:CG	1:A:199:TYR:HB2	2.49	0.43
2:B:406:GLY:O	2:B:410:ASN:ND2	2.48	0.43
20:d:362:MET:HB2	20:d:377:THR:HG22	2.01	0.43
1:A:1229:GLU:OE1	1:A:1229:GLU:N	2.43	0.42
2:B:333:GLU:CD	2:B:333:GLU:C	2.87	0.42
2:B:549:SER:OG	2:B:577:HIS:CD2	2.72	0.42
2:B:934:LYS:HD2	2:B:1051:LEU:HD12	2.00	0.42
3:C:250:SER:O	3:C:254:LYS:HB2	2.19	0.42
7:G:90:THR:HG23	7:G:100:GLU:OE1	2.19	0.42
1:A:41:ILE:HD12	1:A:56:GLY:O	2.19	0.42
18:b:808:HIS:O	18:b:810:ASP:N	2.52	0.42
1:A:1206:ARG:C	1:A:1262:MET:HG3	2.44	0.42
1:A:1210:TRP:O	1:A:1260:ARG:HB2	2.19	0.42
6:F:57:MET:HE1	6:F:120:VAL:HG13	2.00	0.42
1:A:833:PRO:HB2	2:B:677:MET:HE3	2.01	0.42
8:H:7:GLU:OE2	8:H:57:ARG:NH1	2.52	0.42
17:a:2:LEU:HD12	20:d:836:VAL:HG22	2.00	0.42
17:a:12:LEU:HD11	20:d:382:PHE:HE2	1.85	0.42
18:b:831:GLN:O	18:b:837:ARG:NH2	2.52	0.42
19:c:78:LEU:O	19:c:81:SER:OG	2.29	0.42
20:d:305:LEU:HD13	20:d:336:LEU:HD22	2.01	0.42
7:G:77:PHE:HE2	7:G:104:MET:HB3	1.84	0.42
11:K:24:ASP:CG	11:K:26:LYS:HG2	2.44	0.42
19:c:68:LEU:O	19:c:72:SER:N	2.50	0.42
20:d:1048:TYR:CD1	20:d:1048:TYR:C	2.97	0.42
11:K:81:TYR:OH	11:K:89:ASN:OD1	2.31	0.42
17:a:70:LEU:O	17:a:87:VAL:N	2.52	0.42
18:b:1389:LEU:HG	18:b:1393:MET:HE3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:d:196:SER:O	20:d:200:LYS:N	2.53	0.42
20:d:742:VAL:HG13	20:d:743:GLN:N	2.34	0.42
1:A:630:VAL:HG21	1:A:652:LEU:HD21	2.02	0.42
1:A:734:ARG:HD2	9:I:108:MET:SD	2.60	0.42
1:A:844:ARG:NH2	2:B:501:LEU:HD13	2.34	0.42
2:B:1068:GLN:NE2	2:B:1074:PRO:O	2.44	0.42
14:N:41:DC:H5''	19:c:679:LYS:HZ1	1.84	0.42
14:N:42:DA:OP2	14:N:42:DA:H3'	2.20	0.42
16:T:20:DT:H2''	16:T:21:DC:C6	2.55	0.42
1:A:189:PRO:HB2	1:A:200:ALA:HB1	2.01	0.41
2:B:274:ARG:HD3	2:B:279:VAL:HA	2.02	0.41
2:B:850:ASP:OD2	12:L:13:GLN:HA	2.19	0.41
1:A:668:PHE:CZ	1:A:672:ILE:HD11	2.55	0.41
1:A:1050:CYS:O	1:A:1054:MET:HG2	2.20	0.41
1:A:1166:LEU:HD23	1:A:1293:LEU:HD23	2.02	0.41
1:A:1297:THR:HG23	1:A:1297:THR:O	2.19	0.41
2:B:209:ALA:CB	2:B:382:LEU:HD11	2.50	0.41
2:B:371:ARG:NE	2:B:380:ARG:HH11	2.18	0.41
5:E:209:VAL:O	5:E:210:GLN:NE2	2.48	0.41
14:N:34:DG:H2''	14:N:35:DA:H8	1.84	0.41
16:T:41:DG:H2''	16:T:42:DA:C8	2.55	0.41
17:a:320:THR:OG1	17:a:327:ILE:HD11	2.20	0.41
18:b:682:LEU:HD12	18:b:708:SER:HA	2.02	0.41
20:d:1058:LEU:O	20:d:1062:ILE:N	2.49	0.41
1:A:1231:ILE:HG12	1:A:1298:LEU:HD13	2.02	0.41
16:T:4:DT:H2''	16:T:5:DT:C5'	2.50	0.41
16:T:40:DT:H2''	16:T:41:DG:C8	2.55	0.41
1:A:530:SER:O	1:A:531:ASN:OD1	2.38	0.41
1:A:1226:LEU:HD21	1:A:1298:LEU:HD13	2.01	0.41
4:D:37:VAL:HG21	7:G:2:PHE:CB	2.50	0.41
9:I:60:HIS:CD2	9:I:103:ARG:HH21	2.37	0.41
1:A:94:VAL:HG21	1:A:311:GLN:HA	2.01	0.41
1:A:140:ARG:HG3	1:A:140:ARG:HH11	1.85	0.41
1:A:695:ASP:OD1	1:A:695:ASP:N	2.53	0.41
2:B:421:LYS:HG3	2:B:422:PHE:HD1	1.86	0.41
16:T:46:DC:H2''	16:T:47:DA:OP2	2.20	0.41
17:a:153:SER:OG	17:a:156:HIS:O	2.31	0.41
18:b:859:LEU:HD12	18:b:910:PHE:HB3	2.03	0.41
1:A:141:LEU:HD23	1:A:141:LEU:O	2.21	0.41
2:B:363:TYR:HB3	2:B:553:LEU:HD21	2.02	0.41
2:B:516:GLU:HA	2:B:520:VAL:HG23	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1124:ILE:HD12	2:B:1163:MET:HE2	2.02	0.41
3:C:105:VAL:HG11	3:C:115:VAL:HG22	2.03	0.41
4:D:70:ARG:NH2	7:G:140:ASP:O	2.54	0.41
7:G:30:LEU:O	7:G:34:VAL:HG12	2.20	0.41
16:T:17:DT:H2''	16:T:18:DT:H71	2.01	0.41
1:A:265:VAL:HG22	1:A:266:MET:H	1.85	0.41
2:B:302:LYS:HE2	9:I:14:ILE:HD12	2.03	0.41
2:B:629:GLU:HG3	2:B:634:LEU:HD12	2.03	0.41
9:I:109:ARG:NE	9:I:124:THR:HG21	2.32	0.41
14:N:38:DG:H2''	14:N:39:DA:OP2	2.20	0.41
18:b:912:LEU:HD22	18:b:917:GLY:HA3	2.02	0.41
20:d:32:LEU:CD2	20:d:77:LEU:HD22	2.51	0.41
2:B:302:LYS:CG	9:I:23:MET:HE1	2.51	0.41
2:B:908:MET:SD	12:L:43:ILE:HG23	2.61	0.41
16:T:17:DT:H2'	16:T:18:DT:H71	2.03	0.41
17:a:48:THR:HG23	17:a:105:VAL:HG12	2.03	0.41
17:a:149:MET:CG	17:a:159:VAL:HG22	2.47	0.41
17:a:251:LEU:CD2	17:a:262:THR:HG22	2.51	0.41
1:A:226:LYS:O	1:A:226:LYS:HG2	2.21	0.41
1:A:509:LEU:HD22	6:F:90:LEU:HD12	2.03	0.41
1:A:734:ARG:HG3	9:I:105:GLU:OE2	2.21	0.41
1:A:1054:MET:CE	1:A:1060:LEU:HD12	2.51	0.41
14:N:33:DA:H2''	14:N:34:DG:OP2	2.21	0.41
14:N:47:DG:H2''	14:N:48:DA:C5'	2.51	0.41
17:a:168:VAL:HG21	17:a:204:THR:HG21	2.03	0.41
18:b:1004:LEU:H	18:b:1004:LEU:HD23	1.85	0.41
9:I:60:HIS:CB	9:I:103:ARG:HD3	2.51	0.41
14:N:41:DC:H4'	19:c:679:LYS:HG3	2.03	0.41
20:d:20:THR:HB	20:d:315:THR:HG21	2.03	0.41
1:A:264:VAL:HG21	15:P:1:A:O2'	2.22	0.40
1:A:1002:SER:HB2	1:A:1059:ARG:HG3	2.02	0.40
2:B:87:LYS:HG2	2:B:88:PHE:N	2.36	0.40
1:A:192:ARG:HH22	1:A:213:LYS:CE	2.35	0.40
1:A:231:GLU:OE2	1:A:231:GLU:N	2.43	0.40
1:A:583:ARG:NH1	3:C:222:PRO:O	2.54	0.40
4:D:95:PHE:CE1	7:G:1:MET:CE	3.05	0.40
18:b:693:PHE:CD2	18:b:696:LYS:HB2	2.55	0.40
1:A:1212:LEU:HD11	1:A:1289:GLU:HB2	2.03	0.40
1:A:1471:PHE:O	6:F:64:ARG:NH1	2.52	0.40
2:B:327:LYS:HD2	2:B:327:LYS:HA	1.86	0.40
6:F:68:THR:HG23	7:G:59:ILE:HG21	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:b:868:LEU:HD23	18:b:884:LYS:HE3	2.03	0.40
18:b:928:ARG:HD3	18:b:958:THR:HG22	2.02	0.40
20:d:739:ARG:NH2	20:d:806:GLN:OE1	2.54	0.40
1:A:732:THR:O	1:A:736:THR:HG23	2.20	0.40
7:G:27:LYS:HE3	7:G:51:ILE:HD11	2.04	0.40
2:B:95:LYS:HA	2:B:95:LYS:HD3	1.91	0.40
3:C:183:ALA:HB3	3:C:232:ASN:HB3	2.02	0.40
3:C:235:SER:OG	3:C:239:LEU:O	2.36	0.40
8:H:14:ASP:OD1	8:H:15:ILE:N	2.54	0.40
9:I:12:VAL:HG23	9:I:50:ASN:ND2	2.36	0.40
16:T:15:DC:H5''	19:c:683:ARG:CZ	2.51	0.40
19:c:39:LEU:HD13	19:c:74:GLN:HE21	1.87	0.40
20:d:719:GLU:OE2	20:d:737:SER:OG	2.30	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	1399/1970 (71%)	1348 (96%)	51 (4%)	0	100	100
2	B	1122/1167 (96%)	1072 (96%)	50 (4%)	0	100	100
3	C	256/275 (93%)	248 (97%)	8 (3%)	0	100	100
4	D	126/142 (89%)	117 (93%)	9 (7%)	0	100	100
5	E	207/210 (99%)	196 (95%)	11 (5%)	0	100	100
6	F	80/127 (63%)	75 (94%)	5 (6%)	0	100	100
7	G	169/254 (66%)	159 (94%)	10 (6%)	0	100	100
8	H	146/150 (97%)	141 (97%)	5 (3%)	0	100	100
9	I	115/125 (92%)	106 (92%)	9 (8%)	0	100	100
10	J	65/67 (97%)	64 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	113/117 (97%)	109 (96%)	4 (4%)	0	100	100
12	L	44/58 (76%)	40 (91%)	4 (9%)	0	100	100
13	M	62/83 (75%)	61 (98%)	1 (2%)	0	100	100
17	a	363/396 (92%)	343 (94%)	20 (6%)	0	100	100
18	b	512/1493 (34%)	486 (95%)	26 (5%)	0	100	100
19	c	258/709 (36%)	247 (96%)	11 (4%)	0	100	100
20	d	765/1140 (67%)	730 (95%)	35 (5%)	0	100	100
All	All	5802/8483 (68%)	5542 (96%)	260 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1241/1749 (71%)	1241 (100%)	0	100	100
2	B	992/1021 (97%)	989 (100%)	3 (0%)	86	94
3	C	237/252 (94%)	237 (100%)	0	100	100
4	D	108/126 (86%)	108 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	71/111 (64%)	71 (100%)	0	100	100
7	G	147/217 (68%)	147 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	105/112 (94%)	105 (100%)	0	100	100
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	43/55 (78%)	43 (100%)	0	100	100
13	M	59/76 (78%)	59 (100%)	0	100	100
17	a	320/348 (92%)	319 (100%)	1 (0%)	86	94

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	b	466/1297 (36%)	466 (100%)	0	100	100
19	c	196/608 (32%)	196 (100%)	0	100	100
20	d	685/999 (69%)	685 (100%)	0	100	100
All	All	5150/7456 (69%)	5146 (100%)	4 (0%)	87	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	301	VAL
2	B	331	THR
2	B	393	LEU
17	a	32	LEU

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

Mol	Chain	Res	Type
1	A	516	GLN
1	A	531	ASN
1	A	700	GLN
1	A	792	ASN
1	A	804	HIS
1	A	1077	ASN
1	A	1291	ASN
2	B	287	HIS
2	B	350	HIS
2	B	430	ASN
2	B	654	GLN
2	B	1053	HIS
2	B	1094	GLN
2	B	1115	GLN
4	D	19	GLN
4	D	38	HIS
4	D	43	HIS
4	D	47	GLN
7	G	4	HIS
12	L	23	HIS
17	a	110	HIS
17	a	133	GLN
17	a	267	ASN
18	b	706	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	b	773	HIS
18	b	777	GLN
18	b	1397	ASN
19	c	141	ASN
20	d	156	ASN
20	d	261	HIS
20	d	372	GLN
20	d	789	HIS
20	d	952	ASN
20	d	1056	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	9/10 (90%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	10	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 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	$\# Z > 2$
24	BEF	b	1502	-	0,3,3	-	-	-		
23	ADP	b	1501	22	27,29,29	1.33	4 (14%)	42,45,45	1.96	10 (23%)

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
23	ADP	b	1501	22	-	3/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	1501	ADP	C5-C4	4.26	1.47	1.39
23	b	1501	ADP	C5-C6	2.51	1.48	1.41
23	b	1501	ADP	C8-N7	2.40	1.36	1.31
23	b	1501	ADP	C5-N7	-2.23	1.34	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	1501	ADP	C5-C4-N3	-6.02	118.90	126.75
23	b	1501	ADP	N3-C4-N9	4.86	135.09	127.08
23	b	1501	ADP	C2-N3-C4	4.01	121.23	111.75
23	b	1501	ADP	N3-C2-N1	-3.68	122.84	128.60
23	b	1501	ADP	C4-C5-N7	-3.12	106.82	110.62
23	b	1501	ADP	C4-N9-C8	3.06	109.04	105.73
23	b	1501	ADP	PA-O3A-PB	-2.93	122.78	132.83
23	b	1501	ADP	C5-N7-C8	2.84	107.55	103.51
23	b	1501	ADP	N9-C8-N7	-2.44	110.58	113.91
23	b	1501	ADP	C6-C5-N7	2.25	136.22	132.02

There are no chirality outliers.

All (3) torsion outliers are listed below:

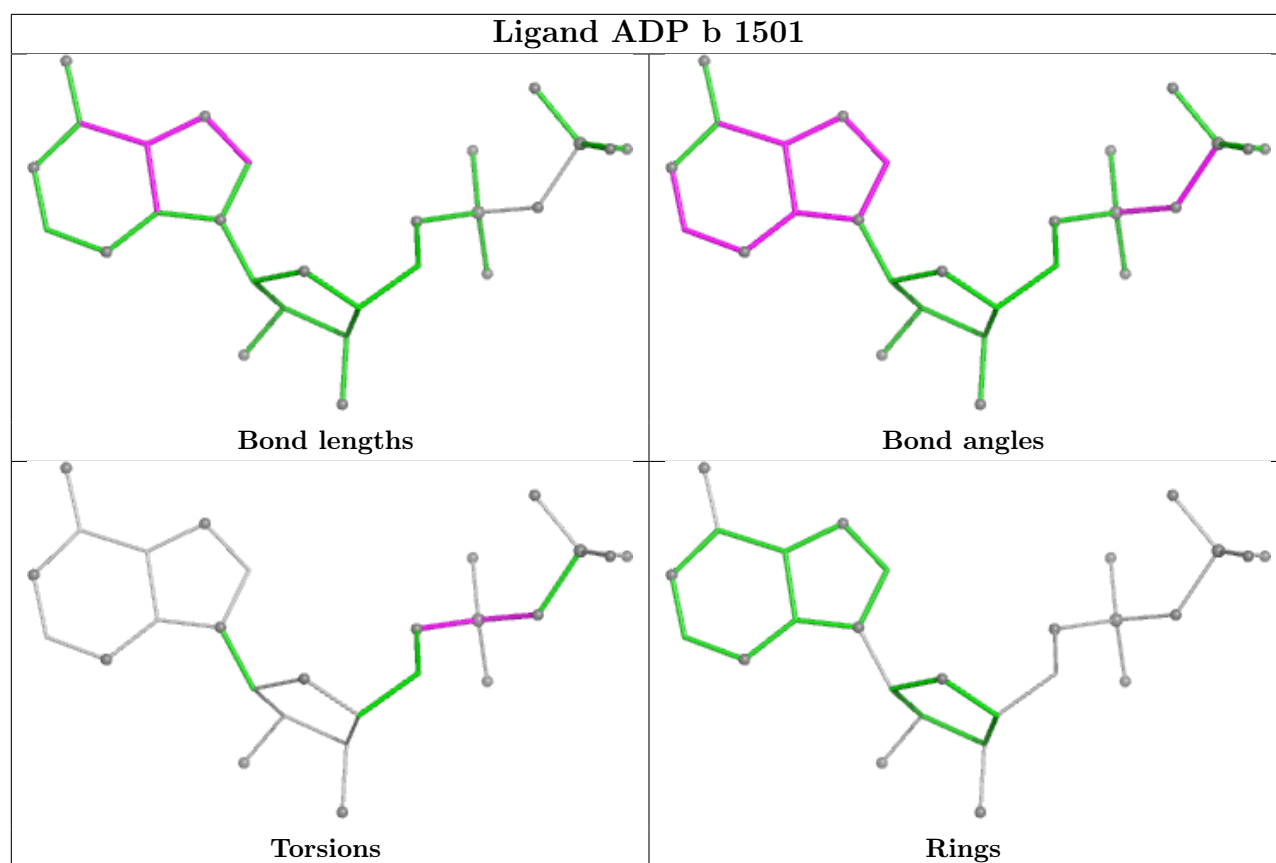
Mol	Chain	Res	Type	Atoms
23	b	1501	ADP	PB-O3A-PA-O2A
23	b	1501	ADP	PB-O3A-PA-O1A
23	b	1501	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	1502	BEF	1	0
23	b	1501	ADP	2	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.

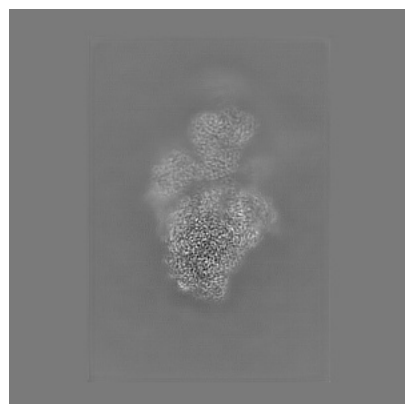
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15825. These allow visual inspection of the internal detail of the map and identification of artifacts.

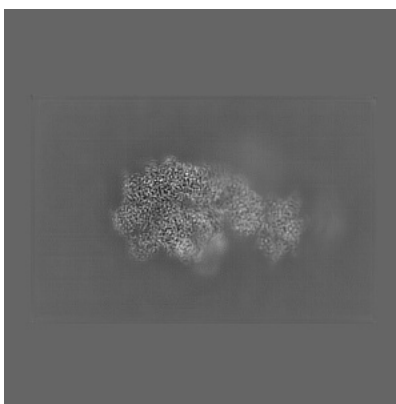
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

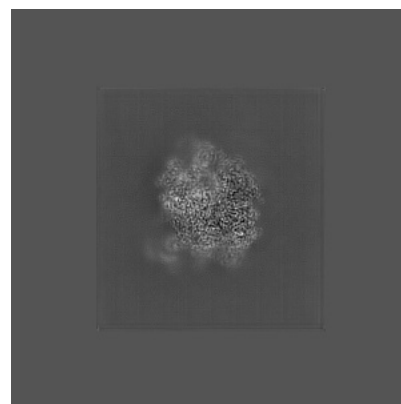
6.1.1 Primary map



X

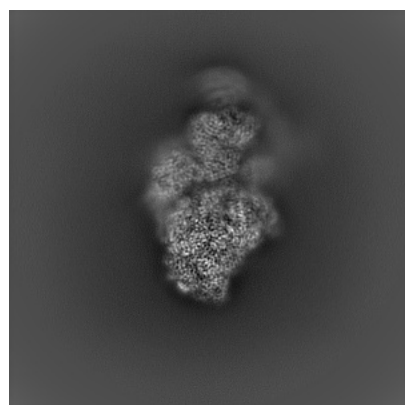


Y

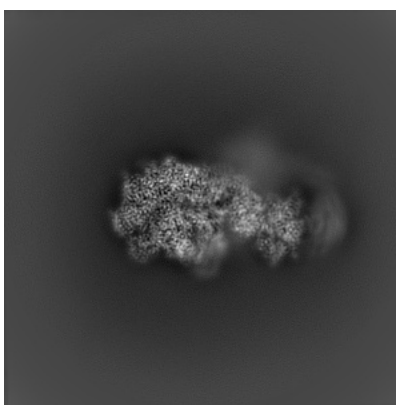


Z

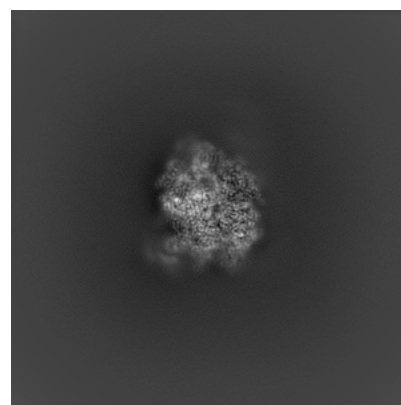
6.1.2 Raw map



X



Y

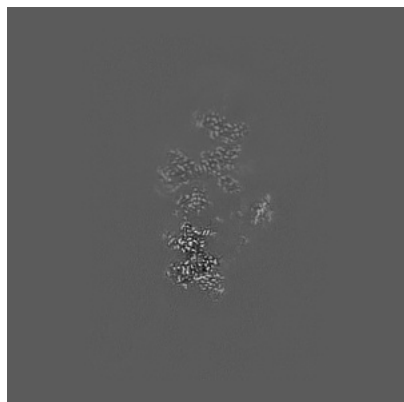


Z

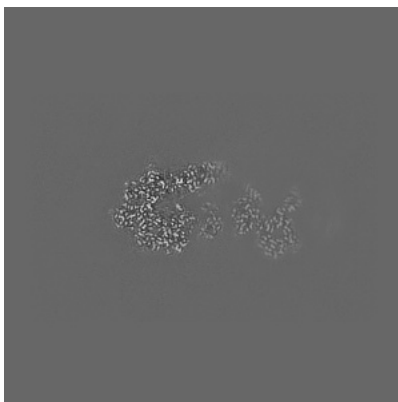
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

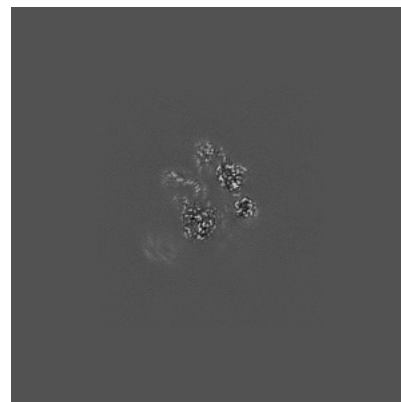
6.2.1 Primary map



X Index: 210

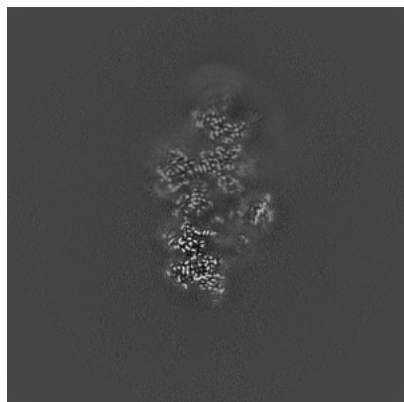


Y Index: 210

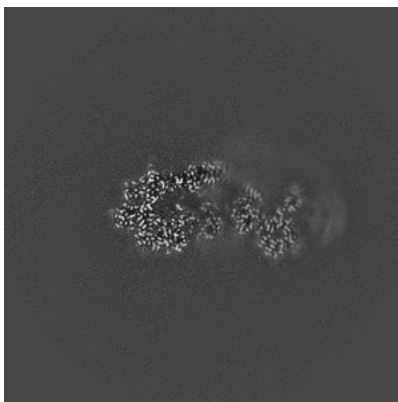


Z Index: 210

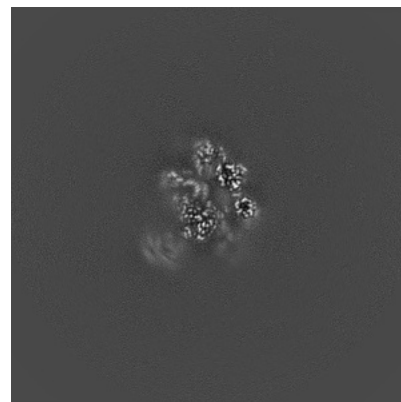
6.2.2 Raw map



X Index: 210



Y Index: 210

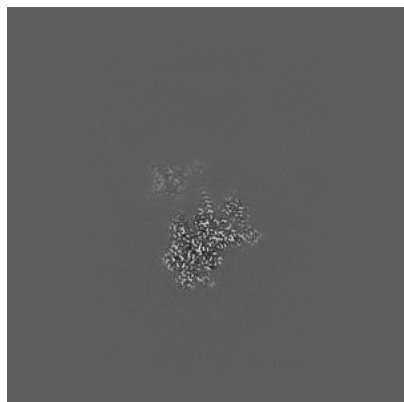


Z Index: 210

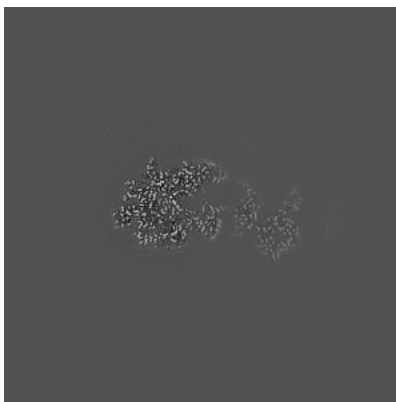
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

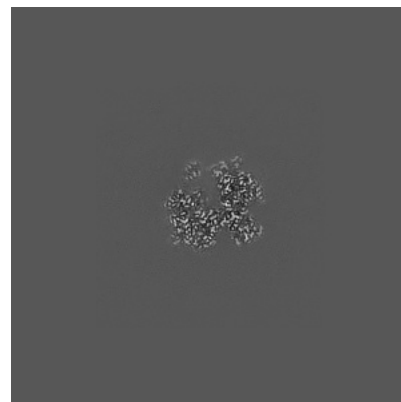
6.3.1 Primary map



X Index: 236

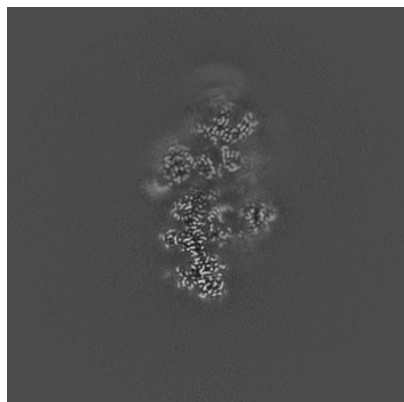


Y Index: 206

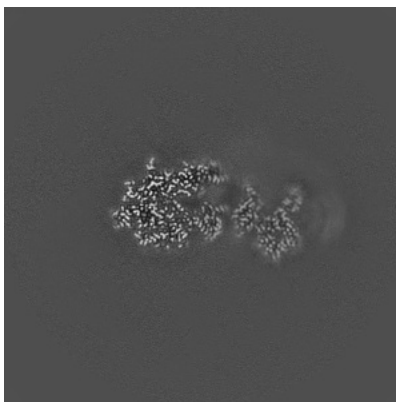


Z Index: 173

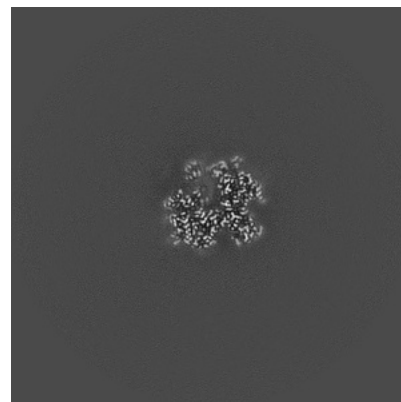
6.3.2 Raw map



X Index: 202



Y Index: 207

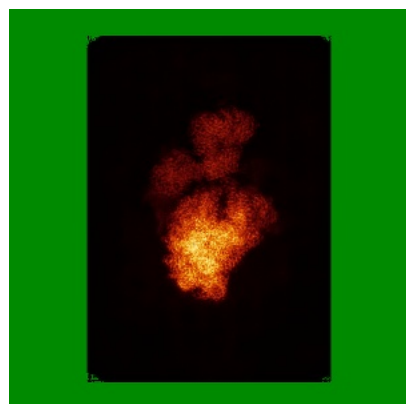


Z Index: 173

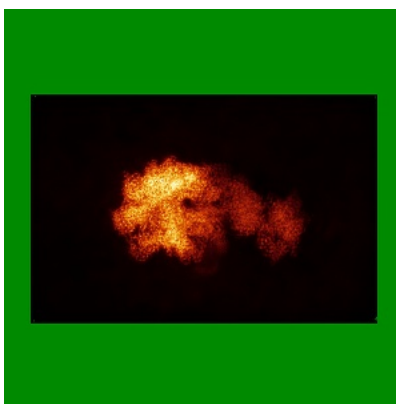
The images above show the largest variance slices of the map in three orthogonal directions.

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

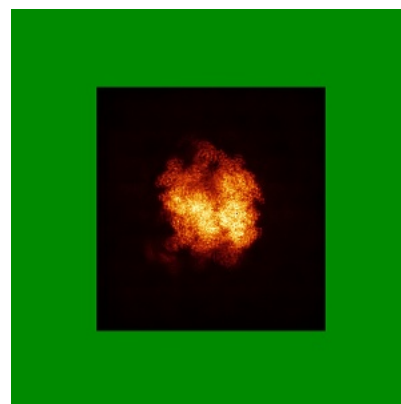
6.4.1 Primary map



X

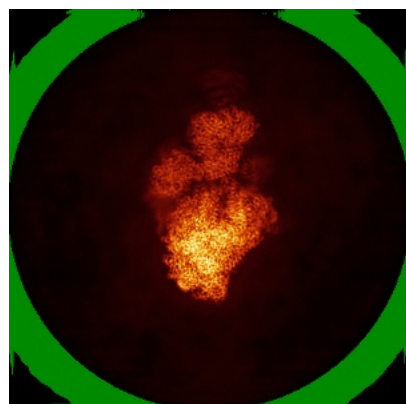


Y

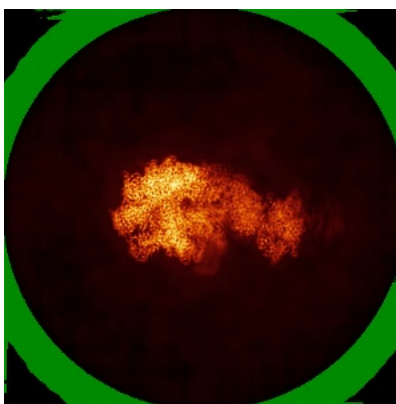


Z

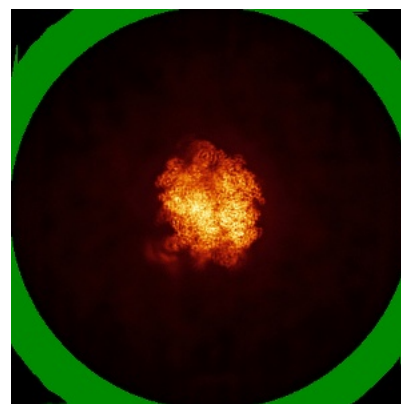
6.4.2 Raw map



X



Y



Z

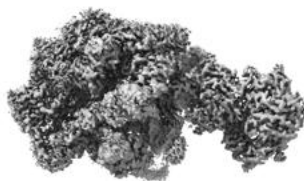
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

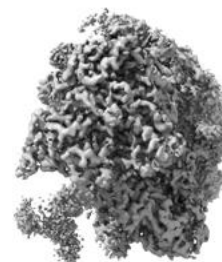
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00912. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

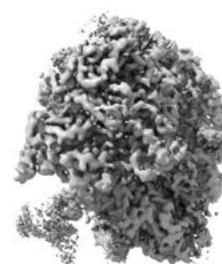
6.5.2 Raw map



X



Y



Z

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

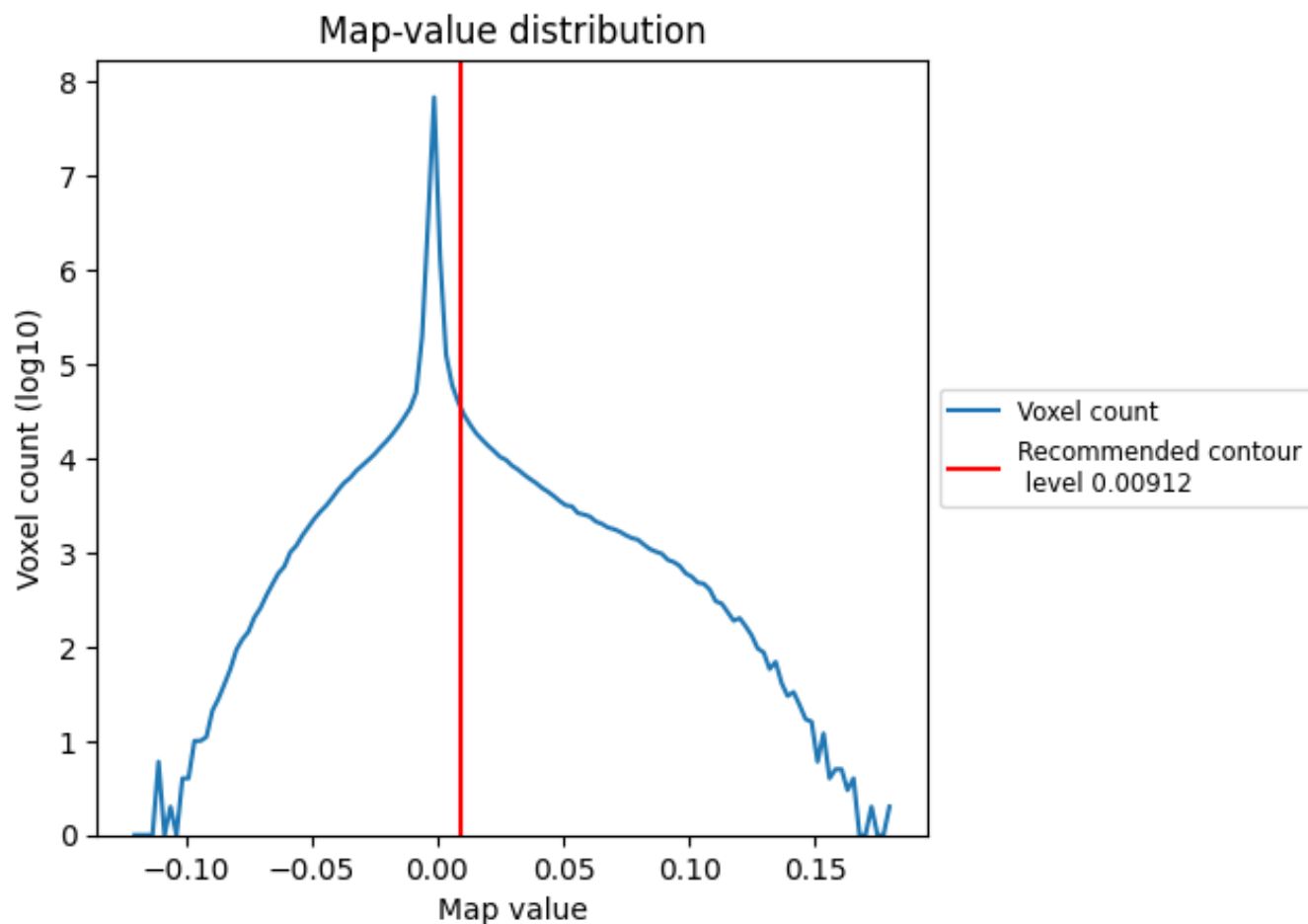
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

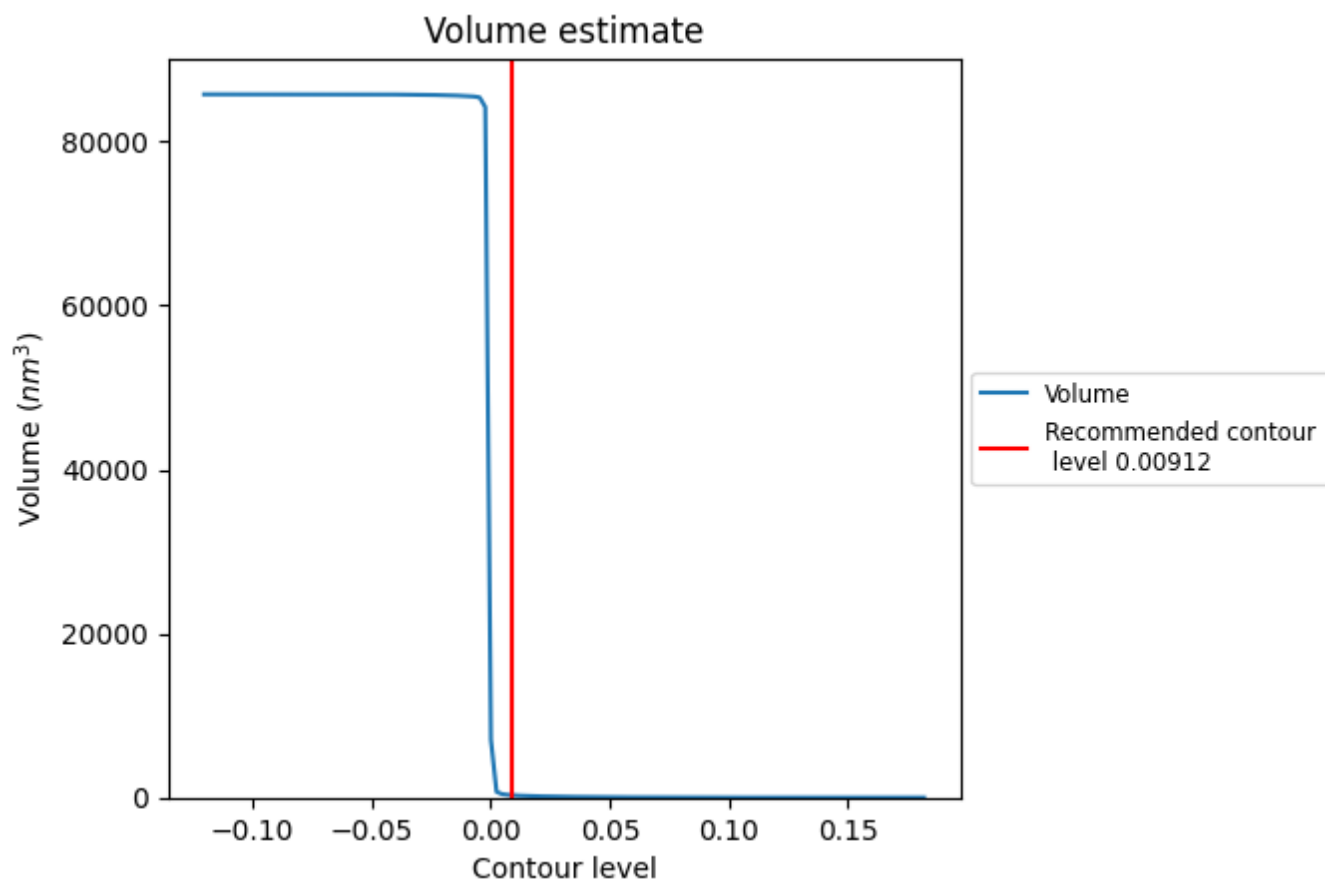
This section contains the results of statistical analysis of the map.

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.

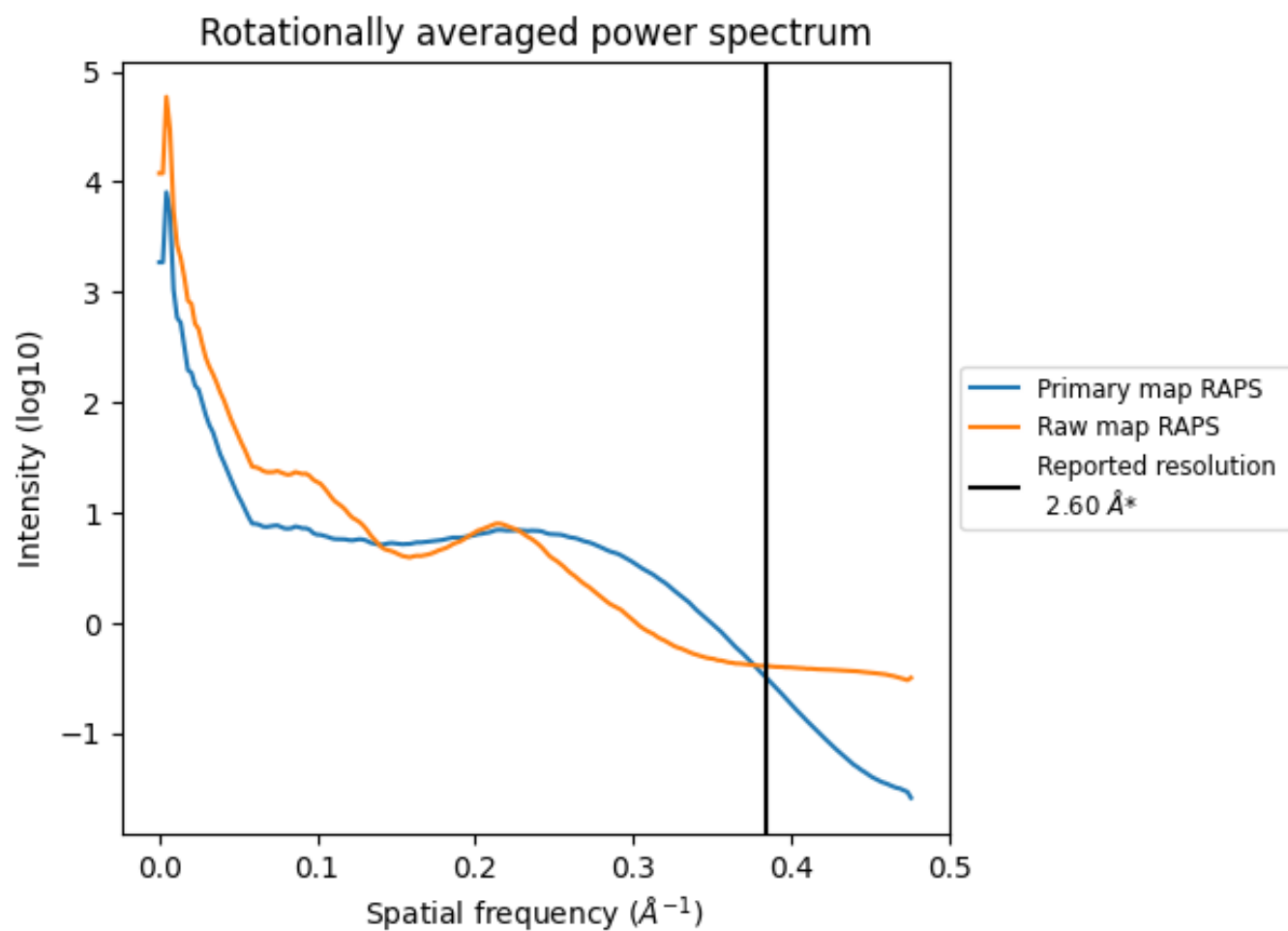
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 287 nm³; this corresponds to an approximate mass of 259 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 ⓘ

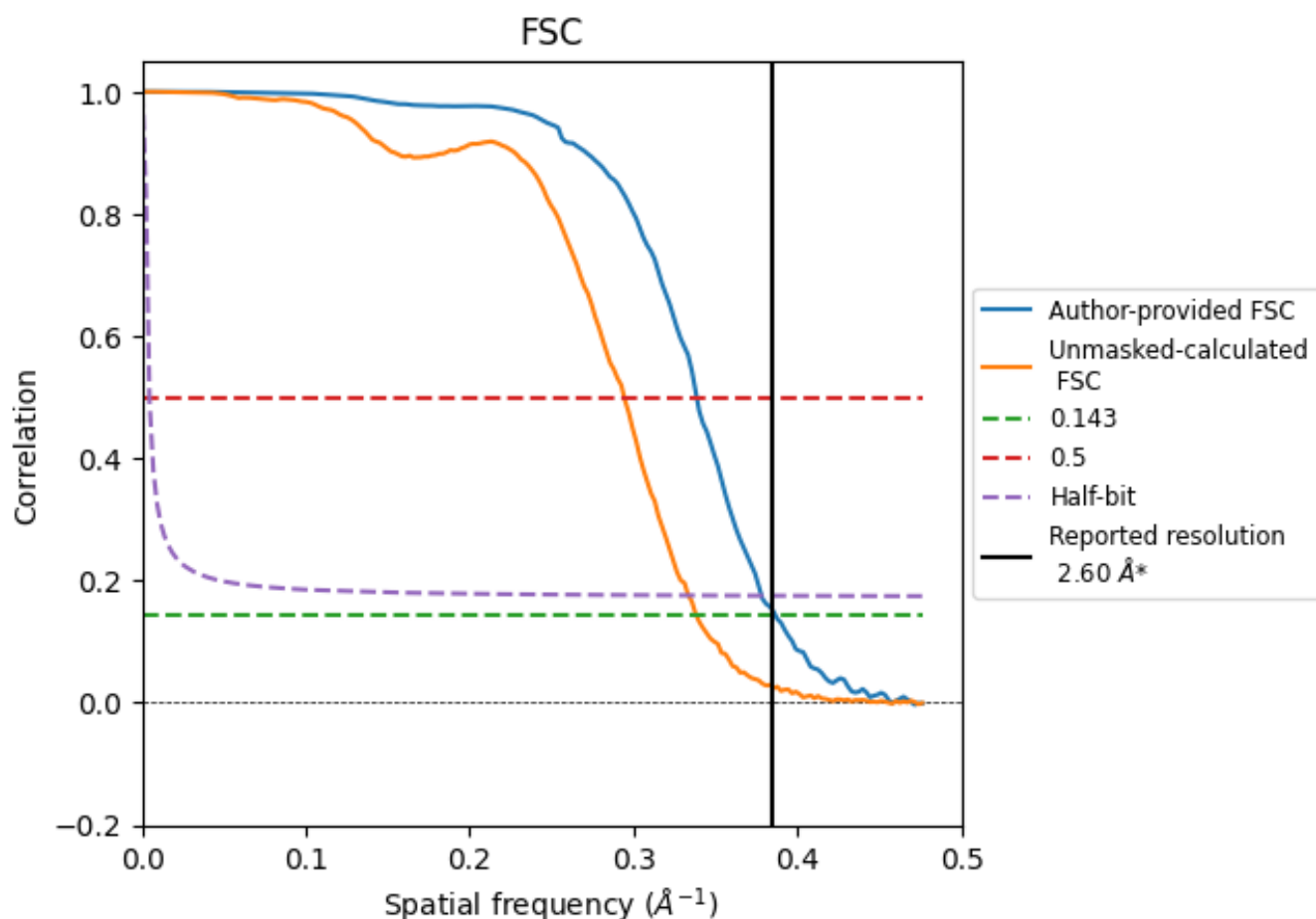


*Reported resolution corresponds to spatial frequency of 0.385 $\text{\AA}^{-1}$

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 0.385 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

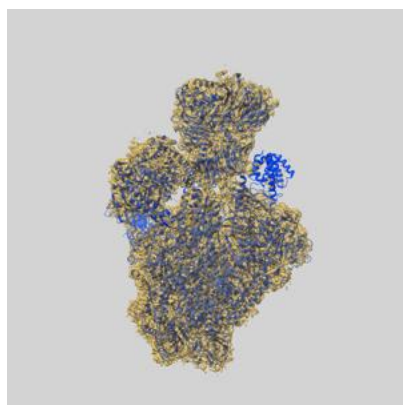
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.59	2.95	2.64
Unmasked-calculated*	2.96	3.40	3.00

*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 2.96 differs from the reported value 2.6 by more than 10 %

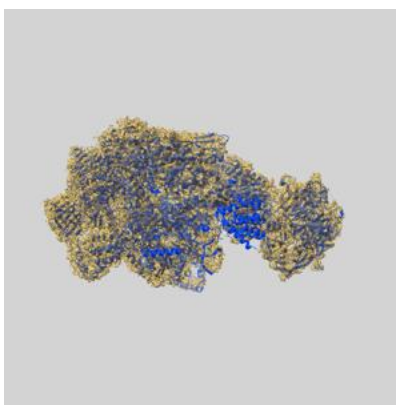
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15825 and PDB model 8B3D. Per-residue inclusion information can be found in section [3](#) on page [9](#).

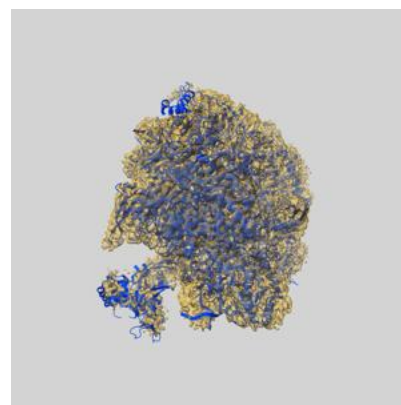
9.1 Map-model overlay [i](#)



X



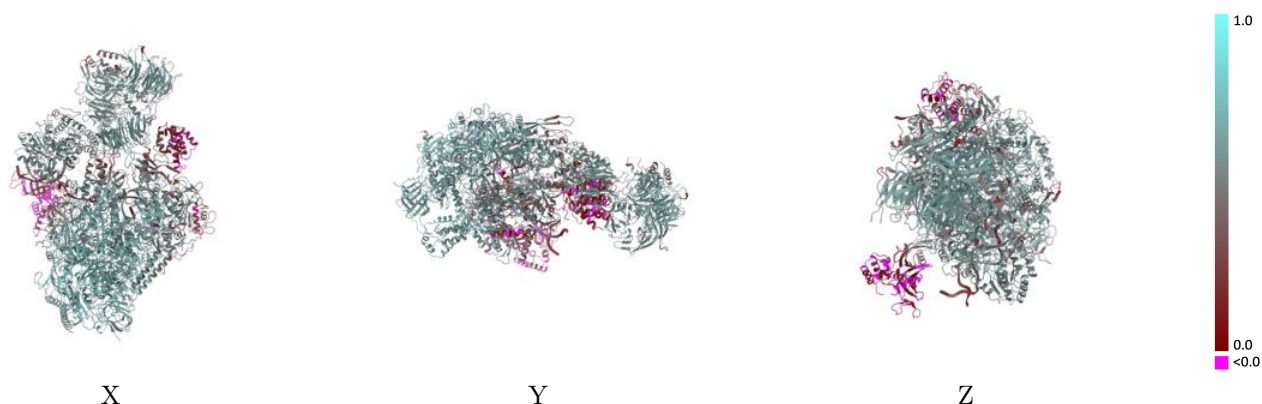
Y



Z

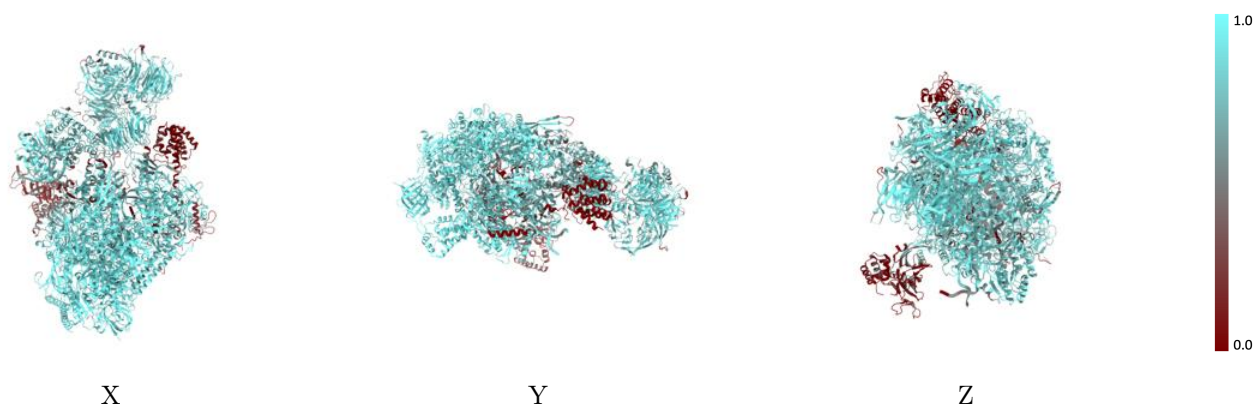
The images above show the 3D surface view of the map at the recommended contour level 0.00912 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



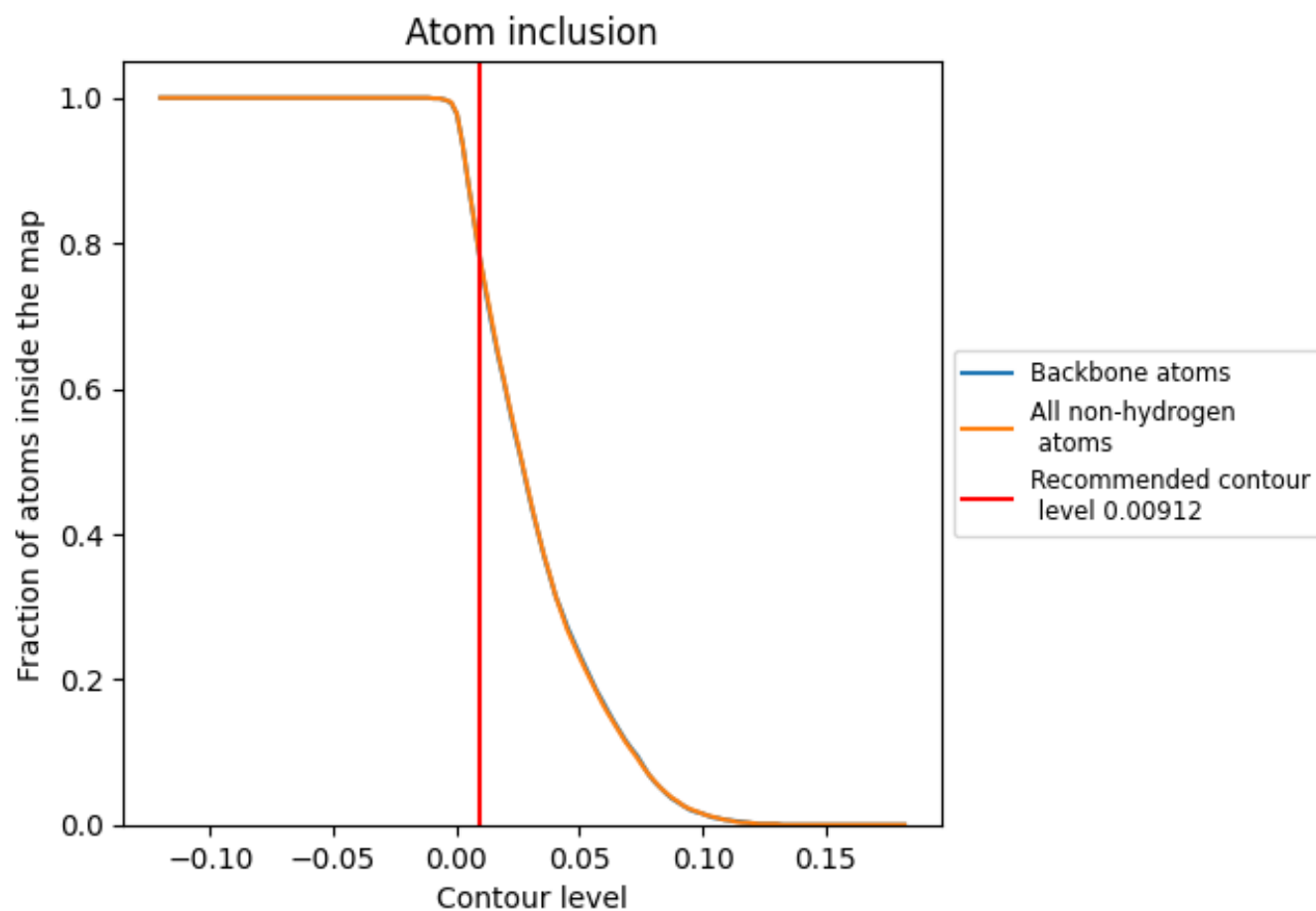
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00912).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 79% 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 (0.00912) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7880	 0.5320
A	 0.8690	 0.5780
B	 0.8870	 0.5940
C	 0.9310	 0.6250
D	 0.1550	 0.0350
E	 0.8810	 0.5270
F	 0.8920	 0.6000
G	 0.3650	 0.1960
H	 0.9350	 0.6150
I	 0.7550	 0.4910
J	 0.9410	 0.6430
K	 0.9320	 0.6250
L	 0.8390	 0.5290
M	 0.6490	 0.4530
N	 0.6920	 0.4340
P	 0.9550	 0.6520
T	 0.8170	 0.4740
a	 0.8470	 0.5770
b	 0.7660	 0.5240
c	 0.1030	 0.2010
d	 0.8110	 0.5550

