



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 09:41 PM UTC

PDB ID : 4V1M / pdb_00004v1m
EMDB ID : EMD-2784
Title : Architecture of the RNA polymerase II-Mediator core transcription initiation complex
Authors : Plaschka, C.; Lariviere, L.; Wenzek, L.; Hemann, M.; Tegunov, D.; Petrotchenko, E.V.; Borchers, C.H.; Baumeister, W.; Herzog, F.; Villa, E.; Cramer, P.
Deposited on : 2014-09-29
Resolution : 6.60 Å(reported)
Based on initial model : 4A3D

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:

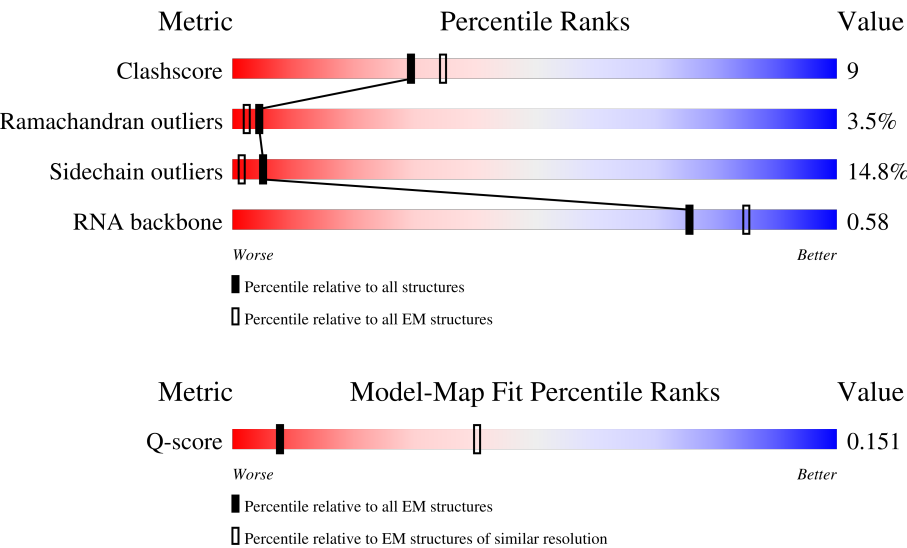
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 6.60 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.



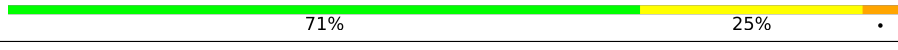
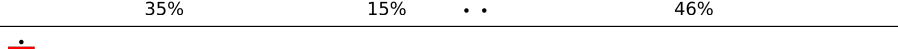
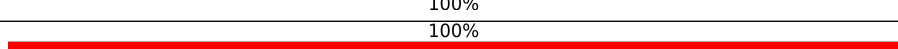
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	531 (6.10 - 7.10)

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	1733	53%22%5%18%
2	B	1224	60%28%6%6%

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Mol	Chain	Length	Quality of chain
3	C	318	
4	E	215	
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	N	10	
12	P	6	
13	T	20	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 29447 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1422	Total	C	N	O	S	0	0
			11174	7037	1954	2121	62		

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1156	Total	C	N	O	S	0	0
			9143	5784	1606	1697	56		

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	266	Total	C	N	O	S	0	0
			2095	1317	348	417	13		

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	84	Total	C	N	O	S	0	0
			679	434	115	127	3		

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	133	Total	C	N	O	S	0	0
			1068	673	180	211	4		

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	119	Total	C	N	O	S	0	0
			971	596	179	186	10		

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	115	Total	C	N	O	S	0	1
			920	590	157	171	2		

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	46	Total	C	N	O	S	0	0
			363	224	72	63	4		

- Molecule 11 is a DNA chain called 5'-D(*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	10	Total	C	N	O	P	0	0
			207	99	39	59	10		

- Molecule 12 is a RNA chain called 5'-D(*CP*CP*AP*GP*GP*AP)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	6	Total	C	N	O	P	0	0
			130	58	26	40	6		

- Molecule 13 is a DNA chain called 5'-D(*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*TP*TP*TP*CP*CP*BRUP*GP*GP*TP*C)-3'.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	T	20	Total	Br	C	N	O	P	0	0
			404	1	194	63	126	20		

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

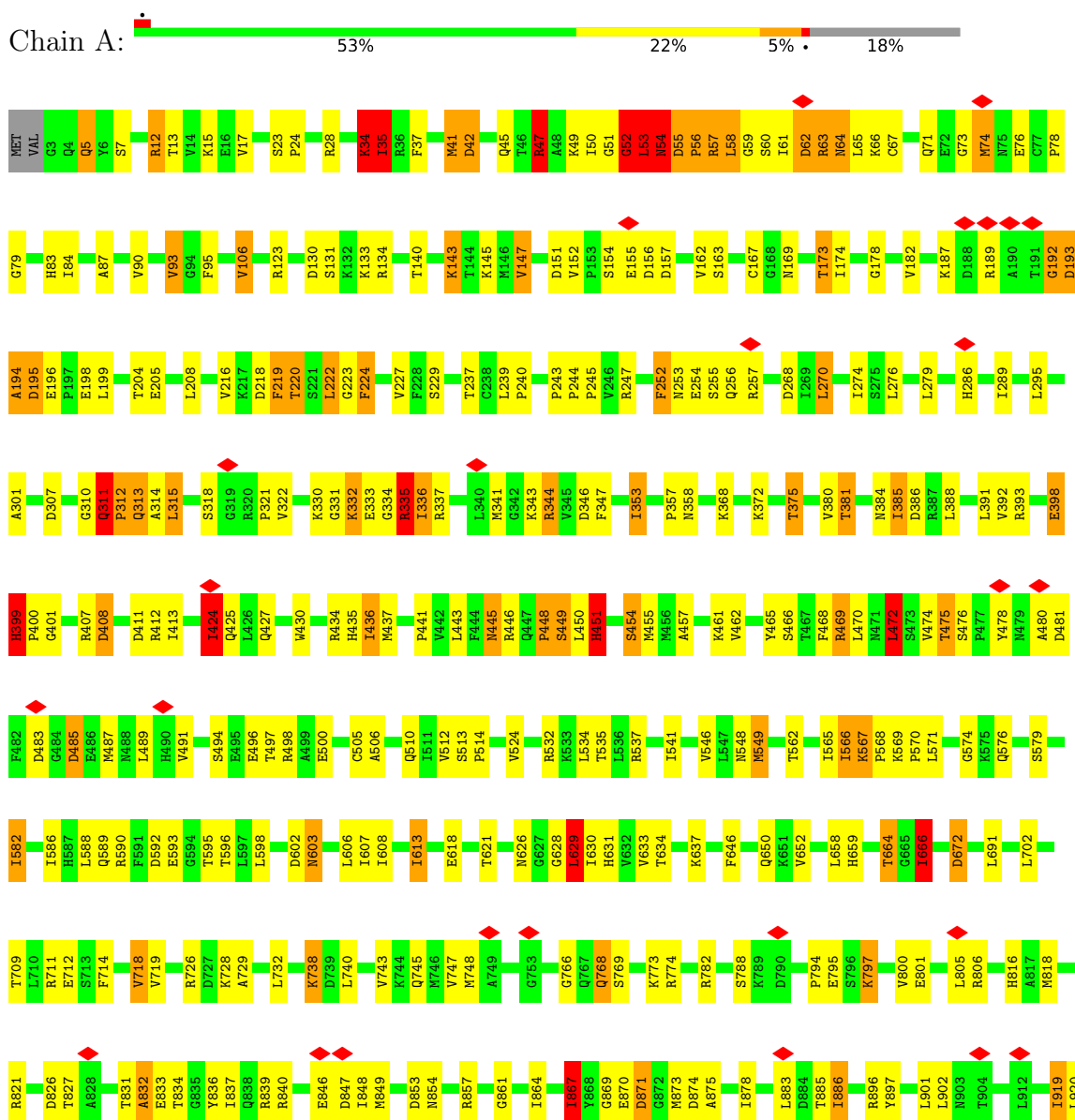
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

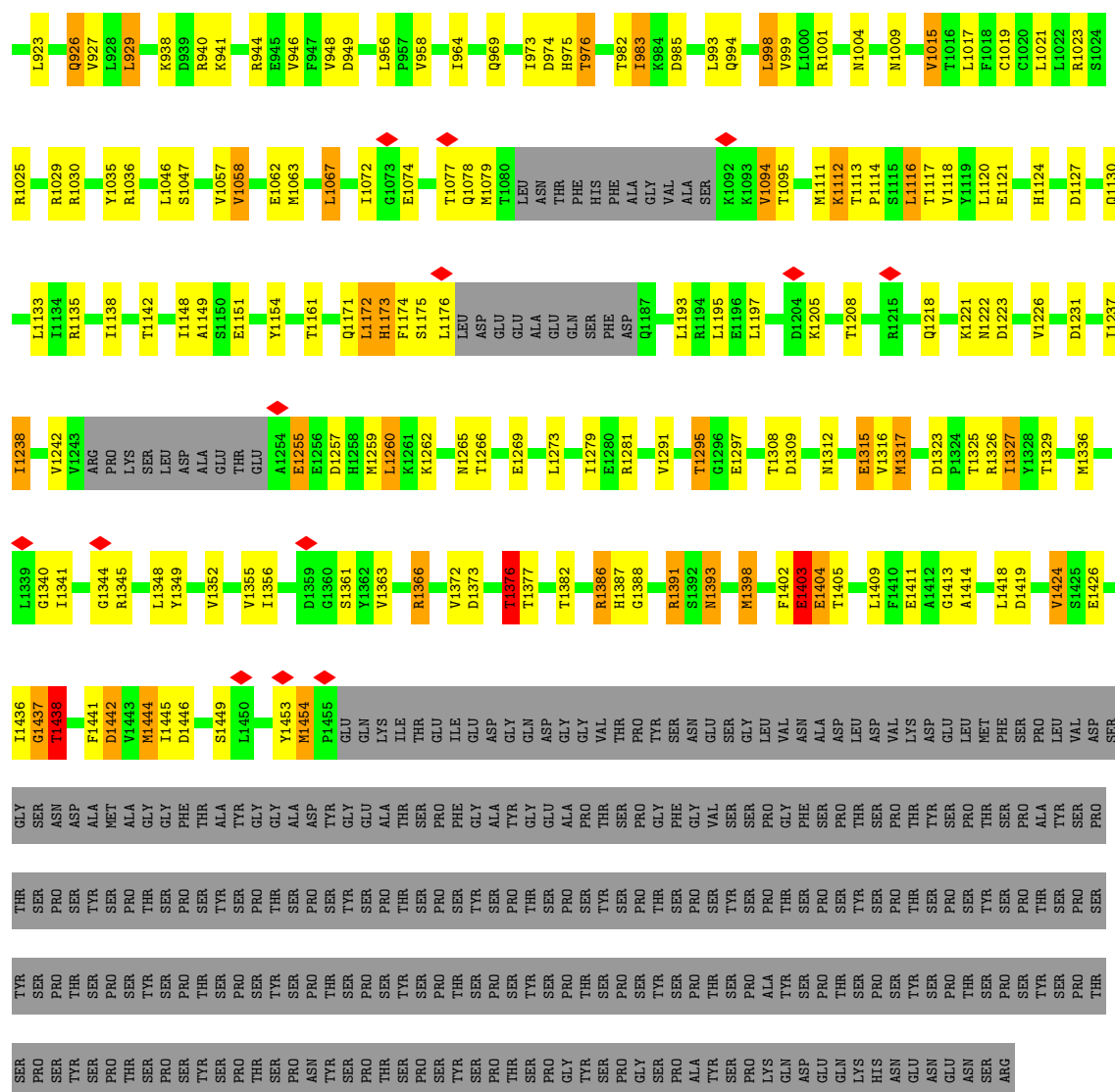
Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	Mg	0
			1	1	

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.

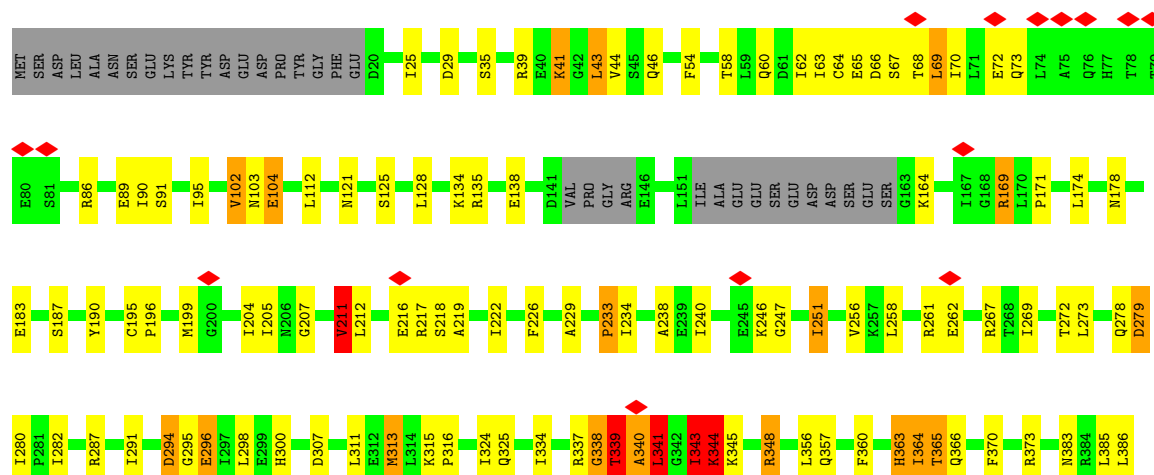
• Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1

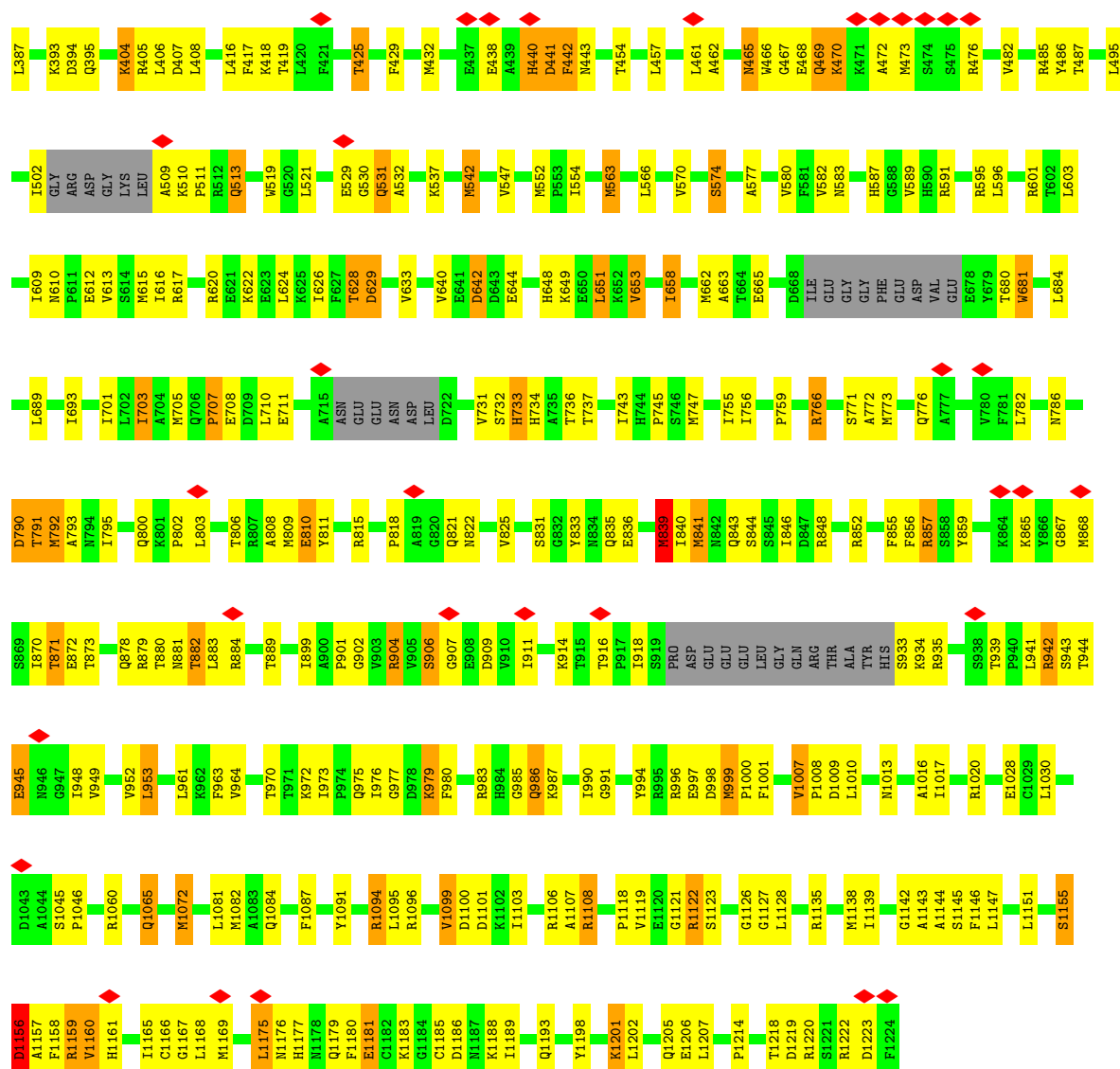




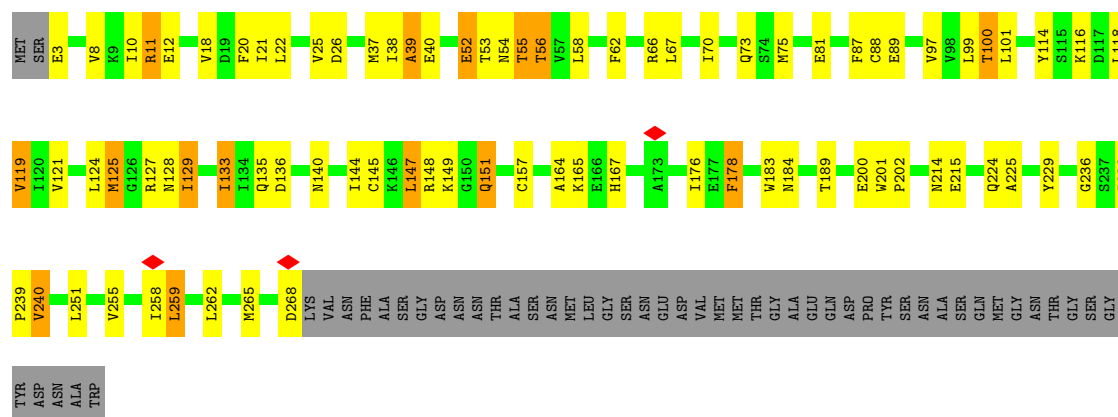
• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

Chain B: 60% 28% 6% 6%



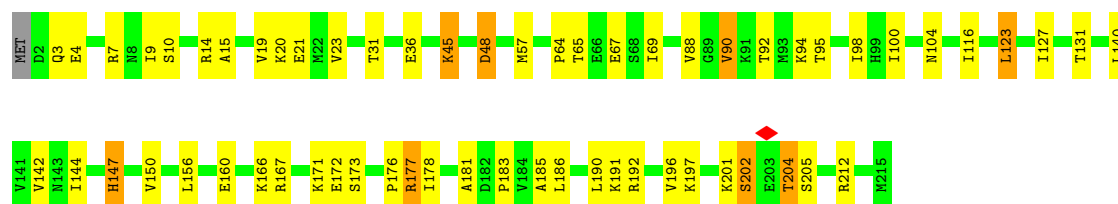


• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3



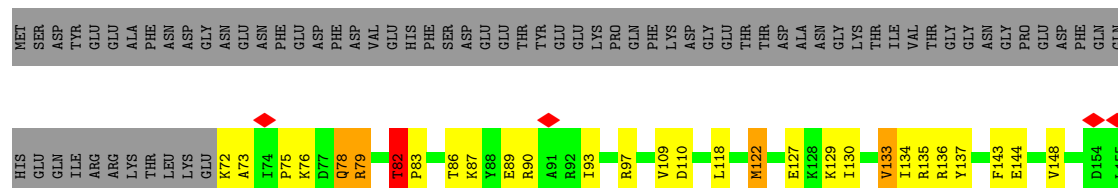
• Molecule 4: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

Chain E: 



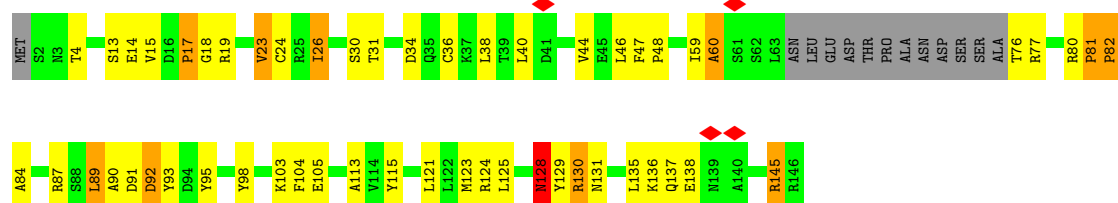
- Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain F: 



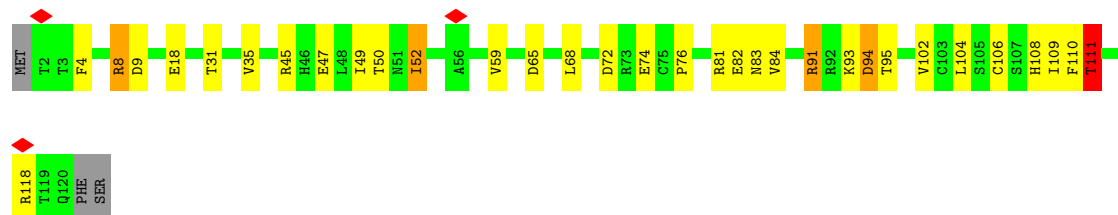
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H: 



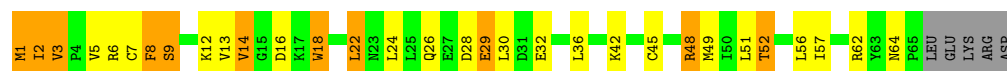
- Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

Chain I: 



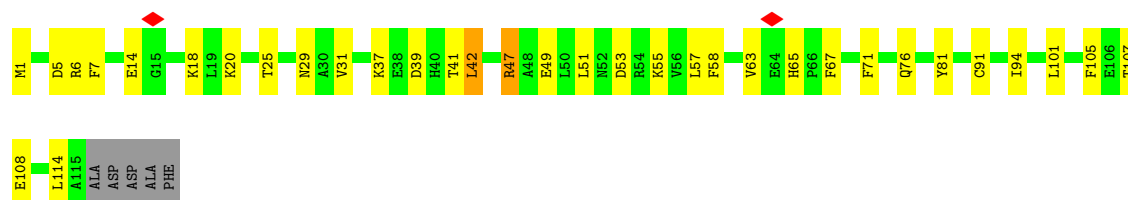
- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J: 

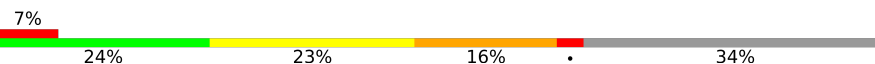


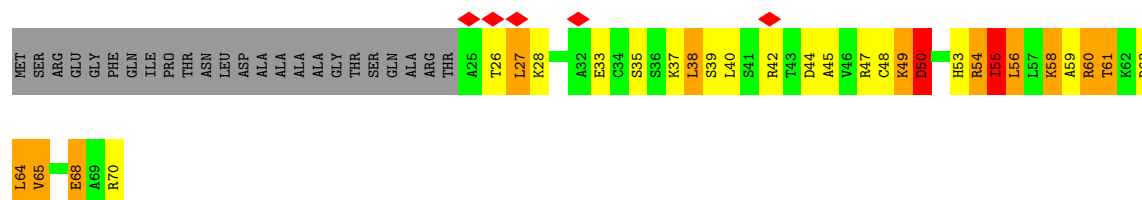
- Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K: 

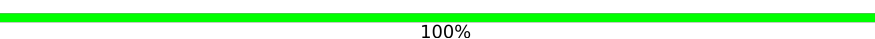


- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L: 



- Molecule 11: 5'-D(*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP)-3'

Chain N: 

There are no outlier residues recorded for this chain.

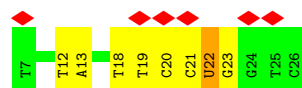
- Molecule 12: 5'-D(*CP*CP*AP*GP*GP*AP)-3'

Chain P: 



- Molecule 13: 5'-D(*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*TP*TP*TP*CP *CP*BRUP*GP*GP*TP*C)-3'

Chain T: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14777	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	37169	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.101	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.019	Depositor
Map size ($\text{\AA}$)	378.0, 378.0, 378.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.35, 1.35, 1.35	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, MG, BRU

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	0.92	13/11374 (0.1%)	1.56	134/15383 (0.9%)
2	B	0.82	5/9318 (0.1%)	1.39	75/12565 (0.6%)
3	C	0.84	0/2133	1.42	15/2891 (0.5%)
4	E	0.83	0/1788	1.41	13/2406 (0.5%)
5	F	1.00	1/691 (0.1%)	1.41	5/933 (0.5%)
6	H	0.85	0/1086	1.43	13/1470 (0.9%)
7	I	0.82	0/989	1.37	8/1331 (0.6%)
8	J	0.90	0/541	1.60	8/727 (1.1%)
9	K	0.77	0/938	1.35	1/1267 (0.1%)
10	L	0.93	0/365	1.51	5/485 (1.0%)
11	N	0.47	0/232	0.67	0/356
12	P	0.82	0/145	0.71	0/224
13	T	0.55	0/426	0.65	0/652
All	All	0.86	19/30026 (0.1%)	1.45	277/40690 (0.7%)

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	2
2	B	0	2
All	All	0	4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	867	ILE	CG1-CD1	8.15	1.83	1.51
1	A	549	MET	SD-CE	-7.57	1.60	1.79
2	B	465	ASN	C-N	-7.49	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1454	MET	CA-C	6.89	1.61	1.52
1	A	54	ASN	CA-C	6.48	1.61	1.52
5	F	122	MET	SD-CE	6.22	1.95	1.79
1	A	57	ARG	CA-C	6.15	1.61	1.52
1	A	1398	MET	SD-CE	5.97	1.94	1.79
2	B	839	MET	SD-CE	-5.70	1.65	1.79
1	A	52	GLY	C-N	5.51	1.42	1.33
1	A	437	MET	SD-CE	5.49	1.93	1.79
1	A	57	ARG	C-N	5.37	1.41	1.33
2	B	1017	ILE	CA-C	5.35	1.58	1.52
2	B	881	ASN	C-N	5.34	1.40	1.33
1	A	56	PRO	C-N	5.14	1.40	1.33
1	A	1057	VAL	C-N	5.10	1.39	1.33
1	A	332	LYS	CA-C	-5.06	1.46	1.52
2	B	1169	MET	SD-CE	-5.05	1.67	1.79
1	A	53	LEU	N-CA	5.02	1.52	1.45

All (277) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	465	ASN	O-C-N	18.98	147.44	122.38
2	B	465	ASN	CA-C-N	-12.52	97.63	121.54
2	B	465	ASN	C-N-CA	-12.52	97.63	121.54
2	B	218	SER	CA-C-N	-11.77	104.00	120.71
2	B	218	SER	C-N-CA	-11.77	104.00	120.71
1	A	34	LYS	CA-C-N	10.01	139.72	121.70
1	A	34	LYS	C-N-CA	10.01	139.72	121.70
6	H	92	ASP	N-CA-C	-9.77	101.59	112.72
2	B	296	GLU	N-CA-C	-9.71	99.75	111.69
2	B	218	SER	O-C-N	9.70	134.39	123.04
3	C	39	ALA	N-CA-C	9.52	125.69	112.45
8	J	5	VAL	N-CA-C	-9.44	97.40	109.58
2	B	628	THR	CA-C-N	9.38	135.29	121.31
2	B	628	THR	C-N-CA	9.38	135.29	121.31
6	H	81	PRO	N-CA-C	8.70	121.32	110.70
1	A	54	ASN	CA-CB-CG	8.51	121.11	112.60
2	B	1122	ARG	CA-C-N	8.44	131.93	120.54
2	B	1122	ARG	C-N-CA	8.44	131.93	120.54
1	A	42	ASP	CA-CB-CG	8.23	120.83	112.60
6	H	129	TYR	N-CA-C	8.15	119.80	111.07
1	A	1403	GLU	CA-C-N	-7.99	109.86	122.65
1	A	1403	GLU	C-N-CA	-7.99	109.86	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	PRO	CA-C-N	7.95	136.72	121.54
1	A	56	PRO	C-N-CA	7.95	136.72	121.54
1	A	194	ALA	CA-C-N	7.86	135.84	121.70
1	A	194	ALA	C-N-CA	7.86	135.84	121.70
1	A	143	LYS	CA-C-N	7.67	130.56	120.28
1	A	143	LYS	C-N-CA	7.67	130.56	120.28
1	A	35	ILE	N-CA-CB	7.65	124.50	111.50
1	A	485	ASP	CA-CB-CG	7.55	120.15	112.60
2	B	340	ALA	CA-C-N	7.52	135.91	121.54
2	B	340	ALA	C-N-CA	7.52	135.91	121.54
2	B	629	ASP	CA-CB-CG	7.48	120.08	112.60
1	A	399	HIS	N-CA-CB	7.47	123.67	110.37
1	A	998	LEU	N-CA-C	7.33	120.61	108.96
1	A	311	GLN	N-CA-C	7.32	125.99	109.81
1	A	1404	GLU	N-CA-C	7.32	121.92	112.92
2	B	736	THR	N-CA-C	-7.31	104.22	113.72
2	B	1169	MET	CA-C-N	7.31	131.05	120.38
2	B	1169	MET	C-N-CA	7.31	131.05	120.38
5	F	87	LYS	CA-C-N	7.20	129.93	120.28
5	F	87	LYS	C-N-CA	7.20	129.93	120.28
1	A	5	GLN	N-CA-C	7.20	120.03	110.53
6	H	128	ASN	CA-C-N	7.18	129.77	120.44
6	H	128	ASN	C-N-CA	7.18	129.77	120.44
3	C	62	PHE	CA-C-N	7.16	129.58	120.56
3	C	62	PHE	C-N-CA	7.16	129.58	120.56
8	J	9	SER	N-CA-C	7.15	118.72	111.07
1	A	1419	ASP	CA-C-N	7.08	129.77	120.28
1	A	1419	ASP	C-N-CA	7.08	129.77	120.28
3	C	183	TRP	N-CA-C	-6.99	97.84	109.24
1	A	53	LEU	N-CA-CB	6.82	120.97	110.60
1	A	64	ASN	N-CA-C	-6.69	101.89	110.53
8	J	18	TRP	N-CA-C	6.64	118.40	111.03
2	B	1181	GLU	N-CA-C	6.60	124.87	110.80
1	A	1403	GLU	N-CA-C	6.57	124.79	110.80
3	C	40	GLU	N-CA-C	6.55	121.43	113.17
2	B	294	ASP	CA-CB-CG	6.55	119.15	112.60
1	A	897	TYR	N-CA-C	6.52	121.36	113.41
2	B	790	ASP	CA-CB-CG	6.51	119.11	112.60
2	B	339	THR	CA-C-N	6.51	133.98	121.54
2	B	339	THR	C-N-CA	6.51	133.98	121.54
1	A	219	PHE	CA-CB-CG	6.48	120.28	113.80
1	A	223	GLY	CA-C-N	6.47	133.90	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	GLY	C-N-CA	6.47	133.90	121.54
1	A	472	LEU	N-CA-C	6.47	119.15	111.71
2	B	1156	ASP	N-CA-C	6.43	124.50	110.80
2	B	1219	ASP	CA-CB-CG	6.43	119.03	112.60
3	C	178	PHE	CA-CB-CG	6.42	120.22	113.80
3	C	89	GLU	N-CA-C	-6.37	96.69	108.02
2	B	1177	HIS	N-CA-C	-6.35	105.57	113.38
3	C	135	GLN	CA-C-N	6.35	131.47	121.56
3	C	135	GLN	C-N-CA	6.35	131.47	121.56
3	C	200	GLU	N-CA-C	6.33	118.26	111.36
2	B	818	PRO	N-CA-C	6.33	120.08	111.22
1	A	341	MET	CA-C-N	6.29	126.46	121.61
1	A	341	MET	C-N-CA	6.29	126.46	121.61
1	A	408	ASP	CA-C-N	6.23	130.66	120.63
1	A	408	ASP	C-N-CA	6.23	130.66	120.63
2	B	1180	PHE	CA-CB-CG	-6.23	107.57	113.80
1	A	411	ASP	CA-C-N	6.22	130.39	121.50
1	A	411	ASP	C-N-CA	6.22	130.39	121.50
1	A	169	ASN	N-CA-C	6.21	119.04	110.35
1	A	334	GLY	CA-C-N	6.19	133.36	121.54
1	A	334	GLY	C-N-CA	6.19	133.36	121.54
1	A	123	ARG	CA-C-N	6.16	128.82	120.44
1	A	123	ARG	C-N-CA	6.16	128.82	120.44
2	B	363	HIS	N-CA-C	-6.14	102.58	110.19
1	A	398	GLU	CA-C-O	-6.13	114.88	121.56
1	A	60	SER	N-CA-C	6.08	118.65	109.23
7	I	8	ARG	N-CA-C	-6.07	100.11	109.76
9	K	53	ASP	CA-CB-CG	6.04	118.64	112.60
2	B	906	SER	N-CA-C	6.03	122.34	114.75
6	H	131	ASN	N-CA-C	-6.02	104.80	111.36
1	A	1112	LYS	N-CA-C	6.01	119.08	111.69
2	B	642	ASP	N-CA-C	-6.00	105.06	112.38
1	A	1376	THR	CB-CA-C	6.00	120.92	111.39
1	A	244	PRO	N-CA-C	5.99	118.01	110.70
2	B	338	GLY	CA-C-N	5.99	132.49	121.70
2	B	338	GLY	C-N-CA	5.99	132.49	121.70
8	J	14	VAL	N-CA-C	-5.98	107.30	113.10
7	I	94	ASP	CA-C-N	5.98	132.96	121.54
7	I	94	ASP	C-N-CA	5.98	132.96	121.54
2	B	707	PRO	CA-C-N	5.95	128.58	120.54
2	B	707	PRO	C-N-CA	5.95	128.58	120.54
1	A	78	PRO	N-CA-C	-5.95	101.93	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	123	LEU	CA-C-N	5.93	125.07	120.33
4	E	123	LEU	C-N-CA	5.93	125.07	120.33
2	B	791	THR	N-CA-C	-5.91	100.91	109.59
1	A	853	ASP	CA-CB-CG	5.86	118.45	112.60
2	B	211	VAL	CB-CA-C	-5.85	102.41	110.96
1	A	718	VAL	CA-C-N	5.84	128.77	120.53
1	A	718	VAL	C-N-CA	5.84	128.77	120.53
4	E	171	LYS	N-CA-C	-5.84	100.77	110.17
1	A	794	PRO	CA-C-N	5.84	128.69	120.28
1	A	794	PRO	C-N-CA	5.84	128.69	120.28
1	A	424	ILE	CA-C-N	-5.80	115.30	122.84
1	A	424	ILE	C-N-CA	-5.80	115.30	122.84
1	A	800	VAL	CA-C-N	5.79	128.04	120.28
1	A	800	VAL	C-N-CA	5.79	128.04	120.28
1	A	462	VAL	N-CA-CB	5.78	117.42	110.31
1	A	871	ASP	CA-CB-CG	5.78	118.38	112.60
10	L	44	ASP	CA-C-N	5.78	132.58	121.54
10	L	44	ASP	C-N-CA	5.78	132.58	121.54
4	E	95	THR	CA-C-N	5.76	128.00	120.28
4	E	95	THR	C-N-CA	5.76	128.00	120.28
7	I	52	ILE	N-CA-CB	5.76	118.23	111.66
2	B	43	LEU	N-CA-C	5.75	119.92	113.02
1	A	728	LYS	CA-C-N	5.73	128.24	120.38
1	A	728	LYS	C-N-CA	5.73	128.24	120.38
1	A	833	GLU	CA-C-N	5.73	127.96	120.28
1	A	833	GLU	C-N-CA	5.73	127.96	120.28
7	I	93	LYS	CA-C-N	5.73	129.42	120.82
7	I	93	LYS	C-N-CA	5.73	129.42	120.82
2	B	703	ILE	N-CA-C	5.73	117.25	108.71
8	J	14	VAL	CB-CA-C	5.73	117.23	110.93
1	A	938	LYS	CA-C-N	5.71	128.25	120.54
1	A	938	LYS	C-N-CA	5.71	128.25	120.54
1	A	832	ALA	CA-C-N	5.71	127.86	120.44
1	A	832	ALA	C-N-CA	5.71	127.86	120.44
2	B	825	VAL	N-CA-C	5.71	116.07	107.80
10	L	49	LYS	CA-C-N	5.69	132.41	121.54
10	L	49	LYS	C-N-CA	5.69	132.41	121.54
1	A	537	ARG	CA-C-N	5.68	128.67	120.38
1	A	537	ARG	C-N-CA	5.68	128.67	120.38
1	A	23	SER	N-CA-C	-5.63	102.95	109.93
2	B	732	SER	N-CA-C	5.63	116.80	108.86
1	A	34	LYS	N-CA-C	-5.62	98.02	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	LEU	N-CA-C	-5.58	103.55	110.41
2	B	1155	SER	CA-C-N	5.58	132.19	121.54
2	B	1155	SER	C-N-CA	5.58	132.19	121.54
2	B	343	ILE	CA-C-N	5.57	132.18	121.54
2	B	343	ILE	C-N-CA	5.57	132.18	121.54
1	A	602	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	629	LEU	N-CA-C	-5.56	105.22	111.28
2	B	1013	ASN	N-CA-C	5.55	117.66	109.50
1	A	1344	GLY	CA-C-N	5.55	127.65	120.44
1	A	1344	GLY	C-N-CA	5.55	127.65	120.44
1	A	1138	ILE	N-CA-C	5.54	116.39	111.90
2	B	1017	ILE	N-CA-C	5.54	120.85	108.88
1	A	54	ASN	CA-C-N	5.53	135.30	121.80
1	A	54	ASN	C-N-CA	5.53	135.30	121.80
1	A	496	GLU	CA-C-N	5.53	127.68	120.28
1	A	496	GLU	C-N-CA	5.53	127.68	120.28
1	A	229	SER	N-CA-C	5.52	117.71	107.60
1	A	1072	ILE	N-CA-C	-5.52	107.43	111.90
2	B	755	ILE	N-CA-C	-5.52	107.42	113.43
1	A	218	ASP	CA-CB-CG	5.51	118.11	112.60
2	B	41	LYS	N-CA-C	5.51	117.36	111.36
1	A	1269	GLU	N-CA-C	5.50	118.45	111.69
1	A	1231	ASP	CA-C-N	5.49	128.09	120.63
1	A	1231	ASP	C-N-CA	5.49	128.09	120.63
2	B	733	HIS	CA-C-N	5.47	127.88	120.38
2	B	733	HIS	C-N-CA	5.47	127.88	120.38
1	A	57	ARG	CA-C-N	5.47	131.99	121.54
1	A	57	ARG	C-N-CA	5.47	131.99	121.54
1	A	173	THR	CB-CA-C	5.47	120.50	111.31
2	B	1009	ASP	N-CA-C	-5.47	105.74	112.90
1	A	1001	ARG	N-CA-C	5.46	120.59	113.88
2	B	945	GLU	N-CA-C	5.44	117.55	110.53
1	A	1413	GLY	CA-C-N	5.43	127.82	120.38
1	A	1413	GLY	C-N-CA	5.43	127.82	120.38
2	B	1185	CYS	N-CA-C	-5.43	106.78	113.41
2	B	1180	PHE	N-CA-C	5.42	119.56	112.13
4	E	172	GLU	CA-C-N	5.40	127.83	120.54
4	E	172	GLU	C-N-CA	5.40	127.83	120.54
5	F	82	THR	CB-CA-C	-5.40	100.99	109.52
1	A	399	HIS	CA-CB-CG	-5.38	108.42	113.80
1	A	1295	THR	CB-CA-C	5.38	121.14	110.17
6	H	137	GLN	CA-C-N	5.37	128.01	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	137	GLN	C-N-CA	5.37	128.01	120.28
1	A	510	GLN	N-CA-C	5.37	119.45	113.01
1	A	1161	THR	N-CA-C	5.36	118.22	109.59
1	A	224	PHE	CA-CB-CG	-5.36	108.44	113.80
8	J	8	PHE	CA-CB-CG	5.36	119.16	113.80
10	L	40	LEU	N-CA-C	5.35	117.60	110.53
1	A	874	ASP	CA-CB-CG	5.35	117.95	112.60
2	B	1186	ASP	CA-CB-CG	5.34	117.94	112.60
2	B	1099	VAL	N-CA-CB	5.33	116.42	110.51
8	J	16	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	592	ASP	CA-CB-CG	5.33	117.92	112.60
3	C	87	PHE	N-CA-C	5.32	119.76	113.16
6	H	128	ASN	CA-CB-CG	5.31	117.91	112.60
1	A	1403	GLU	CB-CG-CD	5.29	121.60	112.60
1	A	664	THR	CB-CA-C	5.29	118.83	109.89
1	A	1205	LYS	N-CA-C	-5.29	98.21	107.73
2	B	1065	GLN	CB-CA-C	5.28	118.95	110.29
1	A	1117	THR	CB-CA-C	5.27	120.08	111.23
1	A	310	GLY	CA-C-N	5.26	134.64	121.80
1	A	310	GLY	C-N-CA	5.26	134.64	121.80
2	B	628	THR	N-CA-C	-5.26	106.86	113.28
6	H	83	GLN	CA-C-N	5.26	130.77	120.99
6	H	83	GLN	C-N-CA	5.26	130.77	120.99
1	A	17	VAL	N-CA-CB	5.25	118.52	111.90
1	A	331	GLY	CA-C-N	5.24	131.55	121.54
1	A	331	GLY	C-N-CA	5.24	131.55	121.54
2	B	881	ASN	CA-C-N	5.24	127.25	120.44
2	B	881	ASN	C-N-CA	5.24	127.25	120.44
4	E	21	GLU	CA-C-N	5.24	127.30	120.28
4	E	21	GLU	C-N-CA	5.24	127.30	120.28
1	A	1266	THR	N-CA-C	-5.23	105.47	111.07
1	A	73	GLY	CA-C-N	5.22	131.51	121.54
1	A	73	GLY	C-N-CA	5.22	131.51	121.54
1	A	451	HIS	N-CA-CB	-5.22	101.81	111.52
4	E	147	HIS	CA-C-N	5.21	129.48	121.19
4	E	147	HIS	C-N-CA	5.21	129.48	121.19
4	E	177	ARG	N-CA-C	5.21	117.46	109.07
1	A	535	THR	N-CA-C	5.21	118.49	112.97
2	B	222	ILE	CA-C-N	5.20	128.98	121.18
2	B	222	ILE	C-N-CA	5.20	128.98	121.18
1	A	24	PRO	CA-C-N	5.19	127.50	120.38
1	A	24	PRO	C-N-CA	5.19	127.50	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	233	PRO	CA-C-N	5.19	128.82	121.66
2	B	233	PRO	C-N-CA	5.19	128.82	121.66
1	A	47	ARG	CA-C-N	5.18	131.44	121.54
1	A	47	ARG	C-N-CA	5.18	131.44	121.54
1	A	666	ILE	N-CA-CB	5.17	119.49	110.65
1	A	969	GLN	N-CA-CB	5.17	117.81	110.16
7	I	110	PHE	CA-CB-CG	5.16	118.96	113.80
3	C	225	ALA	N-CA-C	5.16	116.67	108.67
5	F	122	MET	CA-C-N	5.14	127.12	120.44
5	F	122	MET	C-N-CA	5.14	127.12	120.44
2	B	810	GLU	CA-C-N	5.14	129.41	120.68
2	B	810	GLU	C-N-CA	5.14	129.41	120.68
1	A	193	ASP	CA-C-N	5.13	130.93	121.70
1	A	193	ASP	C-N-CA	5.13	130.93	121.70
1	A	1079	MET	N-CA-C	5.13	116.88	108.52
1	A	1315	GLU	N-CA-C	5.11	116.66	111.14
2	B	366	GLN	N-CA-C	-5.11	105.94	113.61
3	C	262	LEU	CA-C-N	5.11	127.13	120.28
3	C	262	LEU	C-N-CA	5.11	127.13	120.28
8	J	64	ASN	N-CA-C	5.10	121.08	109.81
2	B	681	TRP	N-CA-C	-5.09	105.82	111.36
1	A	408	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	106	VAL	N-CA-CB	-5.08	106.55	112.34
2	B	472	ALA	CA-C-N	5.07	131.22	121.54
2	B	472	ALA	C-N-CA	5.07	131.22	121.54
6	H	145	ARG	CA-C-N	5.07	130.83	121.70
6	H	145	ARG	C-N-CA	5.07	130.83	121.70
1	A	478	TYR	CA-C-N	5.07	129.75	122.35
1	A	478	TYR	C-N-CA	5.07	129.75	122.35
1	A	1127	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	192	GLY	CA-C-N	5.07	131.22	121.54
1	A	192	GLY	C-N-CA	5.07	131.22	121.54
1	A	268	ASP	CA-CB-CG	5.04	117.64	112.60
2	B	296	GLU	CA-C-N	5.04	126.90	120.56
2	B	296	GLU	C-N-CA	5.04	126.90	120.56
1	A	147	VAL	N-CA-C	5.03	115.17	108.27
1	A	466	SER	N-CA-C	5.03	120.31	113.37
4	E	48	ASP	CA-CB-CG	5.03	117.63	112.60
2	B	222	ILE	N-CA-C	5.03	115.09	107.75
2	B	998	ASP	CA-CB-CG	5.01	117.61	112.60
1	A	818	MET	CA-C-N	5.01	125.54	119.98
1	A	818	MET	C-N-CA	5.01	125.54	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	136	ASP	CA-CB-CG	5.01	117.61	112.60
2	B	663	ALA	N-CA-C	-5.00	105.30	111.40
7	I	111	THR	CB-CA-C	5.00	119.26	110.36

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	LYS	Mainchain,Peptide
2	B	404	LYS	Mainchain
2	B	43	LEU	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11174	0	11233	215	0
2	B	9143	0	9122	209	0
3	C	2095	0	2051	45	0
4	E	1752	0	1776	27	0
5	F	679	0	701	17	0
6	H	1068	0	1040	26	0
7	I	971	0	927	15	0
8	J	532	0	542	17	0
9	K	920	0	929	20	0
10	L	363	0	386	20	0
11	N	207	0	114	0	0
12	P	130	0	66	1	0
13	T	404	0	227	6	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	29447	0	29114	537	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 9.

All (537) 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:867:ILE:CG1	1:A:867:ILE:CD1	1.83	1.51
2:B:104:GLU:OE2	10:L:54:ARG:HD3	1.50	1.10
1:A:53:LEU:HD23	1:A:54:ASN:H	1.03	1.10
2:B:121:ASN:ND2	2:B:963:PHE:CZ	2.25	1.04
2:B:104:GLU:OE2	10:L:54:ARG:CD	2.10	1.00
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.27	0.98
1:A:1444:MET:HE1	5:F:135:ARG:HB2	1.46	0.95
2:B:121:ASN:ND2	2:B:963:PHE:HZ	1.62	0.92
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.52	0.91
1:A:53:LEU:HD23	1:A:54:ASN:N	1.87	0.90
5:F:76:LYS:HA	5:F:79:ARG:HD3	1.56	0.88
3:C:148:ARG:H	3:C:151:GLN:HG3	1.43	0.82
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.59	0.82
3:C:148:ARG:HD3	3:C:149:LYS:HG2	1.61	0.82
2:B:416:LEU:HD23	2:B:457:LEU:HD23	1.60	0.82
1:A:53:LEU:CD2	1:A:54:ASN:H	1.91	0.81
2:B:465:ASN:O	2:B:467:GLY:N	2.13	0.81
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.64	0.78
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.66	0.78
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.67	0.77
2:B:405:ARG:NE	2:B:629:ASP:OD2	2.17	0.77
3:C:147:LEU:HB3	3:C:151:GLN:HB2	1.66	0.77
1:A:1116:LEU:HD12	1:A:1329:THR:HB	1.67	0.75
6:H:38:LEU:HD11	6:H:123:MET:HE2	1.70	0.74
1:A:497:THR:HG22	2:B:1146:PHE:HD1	1.52	0.73
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.71	0.72
5:F:75:PRO:HG2	5:F:78:GLN:HB2	1.72	0.72
6:H:84:ALA:HA	6:H:87:ARG:HB2	1.71	0.72
2:B:1198:TYR:CE2	2:B:1201:LYS:HE3	2.25	0.71
2:B:104:GLU:OE2	10:L:54:ARG:NE	2.24	0.71
2:B:246:LYS:HG2	2:B:418:LYS:CE	2.21	0.71
3:C:66:ARG:NH2	8:J:3:VAL:O	2.23	0.71
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.74	0.70
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.72	0.70
2:B:104:GLU:CD	10:L:54:ARG:NE	2.49	0.70
2:B:104:GLU:OE1	10:L:47:ARG:NH2	2.25	0.69
2:B:405:ARG:NH2	2:B:629:ASP:OD2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:185:ALA:HA	4:E:190:LEU:HD12	1.74	0.69
1:A:61:ILE:HG22	1:A:62:ASP:H	1.57	0.69
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.74	0.69
2:B:246:LYS:HG2	2:B:418:LYS:HE2	1.75	0.69
3:C:259:LEU:HD22	9:K:91:CYS:HB3	1.75	0.68
1:A:140:THR:HA	1:A:143:LYS:HE2	1.75	0.68
1:A:347:PHE:HE1	1:A:375:THR:HG22	1.60	0.67
4:E:4:GLU:HB3	4:E:7:ARG:HE	1.59	0.67
1:A:34:LYS:HB3	1:A:83:HIS:CE1	2.30	0.67
2:B:121:ASN:HD21	2:B:963:PHE:HZ	1.37	0.67
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.76	0.66
1:A:870:GLU:HB2	4:E:204:THR:HG21	1.75	0.66
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.76	0.66
2:B:429:PHE:HA	2:B:432:MET:HE2	1.77	0.66
1:A:1442:ASP:HB2	5:F:137:TYR:HE1	1.61	0.66
10:L:61:THR:CG2	10:L:63:ARG:HG2	2.26	0.66
2:B:563:MET:HE1	2:B:587:HIS:HB2	1.76	0.65
2:B:296:GLU:O	2:B:300:HIS:HD2	1.80	0.65
1:A:388:LEU:O	1:A:392:VAL:HG23	1.96	0.65
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.79	0.65
6:H:82:PRO:C	6:H:84:ALA:H	2.05	0.65
1:A:37:PHE:CD2	1:A:52:GLY:HA3	2.32	0.64
2:B:68:THR:HG22	2:B:91:SER:HA	1.80	0.64
2:B:806:THR:HG22	2:B:808:ALA:H	1.63	0.64
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	1.79	0.64
2:B:104:GLU:CD	10:L:54:ARG:HE	2.06	0.64
10:L:28:LYS:HB2	10:L:39:SER:HA	1.80	0.64
3:C:56:THR:HG21	3:C:145:CYS:SG	2.37	0.64
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.80	0.64
1:A:1402:PHE:CE1	1:A:1403:GLU:HG2	2.33	0.63
3:C:10:ILE:HD12	9:K:108:GLU:HB3	1.81	0.63
2:B:918:ILE:HD13	2:B:935:ARG:HH22	1.65	0.62
2:B:841:MET:HB3	2:B:846:ILE:HD11	1.81	0.62
9:K:49:GLU:HG3	9:K:94:ILE:HG13	1.81	0.62
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.81	0.62
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.82	0.62
1:A:946:VAL:HG22	4:E:201:LYS:HD2	1.82	0.62
1:A:343:LYS:HD3	2:B:1156:ASP:HB2	1.82	0.61
2:B:465:ASN:C	2:B:467:GLY:N	2.58	0.61
3:C:11:ARG:HH21	3:C:229:TYR:HD2	1.48	0.61
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:PRO:O	1:A:449:SER:HB2	2.01	0.61
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.41	0.61
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.83	0.61
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.82	0.61
4:E:4:GLU:HB3	4:E:7:ARG:NE	2.16	0.61
2:B:486:TYR:HB3	2:B:1096:ARG:CZ	2.31	0.61
4:E:202:SER:HB3	4:E:205:SER:H	1.66	0.61
2:B:205:ILE:HD11	2:B:461:LEU:HD13	1.82	0.61
2:B:405:ARG:HE	2:B:629:ASP:CG	2.09	0.61
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.83	0.60
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.34	0.60
1:A:1387:HIS:O	1:A:1391:ARG:HG2	2.02	0.60
2:B:246:LYS:HG3	2:B:418:LYS:HZ1	1.67	0.60
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.82	0.60
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.36	0.60
3:C:184:ASN:HD21	3:C:189:THR:H	1.50	0.60
2:B:216:GLU:OE2	2:B:404:LYS:HD2	2.02	0.60
1:A:483:ASP:HB2	2:B:987:LYS:HE3	1.84	0.59
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.84	0.59
1:A:629:LEU:O	1:A:633:VAL:HG23	2.02	0.59
1:A:857:ARG:HD3	1:A:861:GLY:O	2.03	0.59
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	2.02	0.59
10:L:61:THR:HG21	10:L:63:ARG:HG2	1.84	0.59
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.85	0.59
1:A:566:ILE:HD11	6:H:98:TYR:HB2	1.85	0.59
2:B:976:ILE:O	2:B:990:ILE:HB	2.02	0.58
1:A:315:LEU:HA	1:A:321:PRO:HA	1.86	0.58
6:H:47:PHE:HB3	6:H:95:TYR:CD2	2.38	0.58
1:A:588:LEU:HD23	1:A:607:ILE:HD12	1.86	0.58
2:B:405:ARG:CZ	2:B:629:ASP:OD2	2.52	0.58
10:L:47:ARG:HH21	10:L:54:ARG:HH21	1.50	0.58
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.85	0.58
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.85	0.58
4:E:147:HIS:HB3	4:E:150:VAL:HG23	1.84	0.58
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.36	0.58
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.84	0.58
2:B:363:HIS:O	2:B:364:ILE:HB	2.02	0.57
2:B:792:MET:HA	2:B:856:PHE:O	2.04	0.57
2:B:810:GLU:HA	2:B:815:ARG:HH12	1.69	0.57
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.70	0.57
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:847:ASP:HB3	1:A:1398:MET:HE1	1.88	0.56
2:B:211:VAL:HG13	2:B:495:LEU:HD23	1.86	0.56
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.87	0.56
2:B:542:MET:HE1	2:B:743:ILE:HD12	1.87	0.56
2:B:313:MET:HE2	2:B:386:LEU:HD22	1.87	0.56
5:F:79:ARG:HG2	5:F:144:GLU:HB3	1.88	0.56
2:B:406:LEU:HD12	2:B:633:VAL:HG22	1.87	0.56
6:H:89:LEU:C	6:H:91:ASP:H	2.14	0.56
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.88	0.56
5:F:118:LEU:O	5:F:122:MET:HG3	2.06	0.56
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.88	0.55
5:F:89:GLU:O	5:F:93:ILE:HD12	2.06	0.55
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.39	0.55
8:J:48:ARG:HE	8:J:49:MET:CE	2.19	0.55
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.87	0.55
2:B:246:LYS:CG	2:B:418:LYS:NZ	2.70	0.55
2:B:792:MET:HE2	2:B:857:ARG:NH2	2.21	0.55
2:B:246:LYS:HG2	2:B:418:LYS:NZ	2.21	0.55
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.88	0.55
1:A:1015:VAL:HG13	1:A:1019:CYS:SG	2.47	0.55
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.87	0.55
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.40	0.55
1:A:35:ILE:HA	1:A:52:GLY:O	2.07	0.54
9:K:57:LEU:HB2	9:K:76:GLN:HG2	1.88	0.54
1:A:344:ARG:HB3	2:B:1118:PRO:HB2	1.89	0.54
1:A:497:THR:HG23	2:B:1146:PHE:HA	1.89	0.54
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.88	0.54
2:B:219:ALA:HB2	2:B:405:ARG:HG2	1.88	0.54
2:B:343:ILE:O	2:B:344:LYS:HB2	2.07	0.54
2:B:216:GLU:OE2	2:B:404:LYS:CD	2.56	0.54
8:J:24:LEU:O	8:J:30:LEU:HB2	2.08	0.54
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.89	0.54
2:B:486:TYR:HB3	2:B:1096:ARG:NH2	2.22	0.54
5:F:109:VAL:HG23	5:F:127:GLU:OE1	2.07	0.54
2:B:1100:ASP:OD2	9:K:1:MET:HB3	2.07	0.54
3:C:37:MET:HE3	3:C:176:ILE:HD13	1.90	0.54
8:J:1:MET:HB2	8:J:56:LEU:HB2	1.89	0.54
1:A:832:ALA:HB1	13:T:18:DT:H2''	1.89	0.54
4:E:94:LYS:HE2	4:E:98:ILE:HD11	1.90	0.54
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.90	0.54
2:B:280:ILE:HD13	2:B:334:ILE:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.90	0.54
1:A:1116:LEU:H	1:A:1308:THR:HB	1.73	0.54
2:B:54:PHE:HA	2:B:58:THR:HB	1.88	0.54
1:A:608:ILE:HD12	1:A:613:ILE:HD13	1.89	0.53
1:A:982:THR:HB	1:A:985:ASP:H	1.73	0.53
1:A:1004:ASN:CG	4:E:167:ARG:HD2	2.33	0.53
3:C:52:GLU:HA	10:L:64:LEU:HD22	1.91	0.53
2:B:815:ARG:HG3	2:B:815:ARG:HH11	1.72	0.53
2:B:338:GLY:CA	2:B:339:THR:HB	2.38	0.53
4:E:19:VAL:O	4:E:23:VAL:HG23	2.08	0.53
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.42	0.53
3:C:73:GLN:O	3:C:129:ILE:HA	2.08	0.53
3:C:164:ALA:HA	3:C:167:HIS:O	2.09	0.53
5:F:134:ILE:HG22	5:F:136:ARG:HG3	1.91	0.53
1:A:1172:LEU:C	1:A:1174:PHE:H	2.16	0.53
2:B:295:GLY:HA2	2:B:298:LEU:HB2	1.91	0.53
2:B:510:LYS:HB2	2:B:513:GLN:OE1	2.08	0.53
8:J:48:ARG:HE	8:J:49:MET:HE2	1.74	0.53
2:B:174:LEU:HD11	2:B:204:ILE:HG13	1.91	0.52
1:A:646:PHE:O	1:A:650:GLN:HG2	2.10	0.52
1:A:1376:THR:HG23	4:E:212:ARG:HH22	1.72	0.52
2:B:291:ILE:HD12	2:B:291:ILE:H	1.74	0.52
1:A:63:ARG:HA	1:A:74:MET:HG3	1.91	0.52
2:B:438:GLU:HG3	2:B:440:HIS:HB2	1.91	0.52
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.91	0.52
2:B:90:ILE:HD11	2:B:134:LYS:HE2	1.91	0.52
2:B:873:THR:O	2:B:914:LYS:HA	2.10	0.52
9:K:55:LYS:HB3	9:K:81:TYR:CD2	2.45	0.52
1:A:1149:ALA:HB2	7:I:47:GLU:HA	1.92	0.52
9:K:5:ASP:HB3	9:K:7:PHE:CE2	2.45	0.52
1:A:658:LEU:HD23	1:A:659:HIS:NE2	2.23	0.52
4:E:156:LEU:HD11	4:E:197:LYS:HB2	1.90	0.52
2:B:246:LYS:CG	2:B:418:LYS:HZ1	2.22	0.51
1:A:472:LEU:O	1:A:475:THR:HB	2.10	0.51
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.92	0.51
1:A:940:ARG:HB3	1:A:941:LYS:HE2	1.92	0.51
1:A:1095:THR:HG23	1:A:1113:THR:HG23	1.92	0.51
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.93	0.51
1:A:497:THR:CG2	2:B:1146:PHE:HD1	2.23	0.51
2:B:373:ARG:HG2	2:B:566:LEU:HD23	1.92	0.51
1:A:254:GLU:HB3	2:B:935:ARG:HH21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.93	0.51
1:A:55:ASP:H	1:A:56:PRO:HD3	1.75	0.51
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.44	0.51
2:B:70:ILE:HG22	2:B:89:GLU:HG2	1.93	0.51
9:K:49:GLU:HG3	9:K:94:ILE:CG1	2.40	0.51
1:A:494:SER:HB3	1:A:497:THR:OG1	2.10	0.51
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.11	0.51
1:A:79:GLY:HA3	1:A:243:PRO:HB2	1.92	0.50
1:A:95:PHE:CE1	1:A:1414:ALA:HB2	2.45	0.50
2:B:882:THR:C	2:B:884:ARG:H	2.19	0.50
4:E:64:PRO:HB2	4:E:69:ILE:HD11	1.93	0.50
2:B:806:THR:HB	2:B:809:MET:HG3	1.94	0.50
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.94	0.50
4:E:15:ALA:O	4:E:19:VAL:HG23	2.10	0.50
5:F:73:ALA:HB2	5:F:143:PHE:CZ	2.46	0.50
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.93	0.50
1:A:52:GLY:N	1:A:56:PRO:HB3	2.26	0.50
1:A:1095:THR:HG21	1:A:1112:LYS:HB2	1.93	0.50
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.77	0.50
2:B:1122:ARG:HB3	13:T:23:DG:OP1	2.12	0.50
1:A:1444:MET:HB2	5:F:133:VAL:HG12	1.92	0.50
2:B:530:GLY:O	2:B:532:ALA:N	2.44	0.50
2:B:773:MET:CE	2:B:985:GLY:HA2	2.40	0.50
2:B:852:ARG:HH22	10:L:70:ARG:C	2.19	0.50
2:B:1072:MET:HB3	2:B:1081:LEU:HD12	1.94	0.50
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.93	0.50
3:C:114:TYR:HB2	3:C:116:LYS:HG2	1.93	0.50
2:B:574:SER:HB3	2:B:591:ARG:HE	1.77	0.50
2:B:904:ARG:HG3	2:B:948:ILE:HG13	1.93	0.50
2:B:1201:LYS:HD3	2:B:1205:GLN:OE1	2.11	0.50
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.93	0.50
2:B:60:GLN:OE1	2:B:95:ILE:HG22	2.12	0.50
1:A:1193:LEU:HB2	1:A:1260:LEU:CD2	2.42	0.49
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.94	0.49
2:B:902:GLY:O	10:L:65:VAL:HG11	2.11	0.49
2:B:916:THR:O	2:B:935:ARG:HG2	2.12	0.49
1:A:315:LEU:H	1:A:315:LEU:HD12	1.76	0.49
1:A:919:ILE:HG12	1:A:983:ILE:HD13	1.94	0.49
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.94	0.49
1:A:714:PHE:O	1:A:718:VAL:HG23	2.12	0.49
1:A:1402:PHE:CD1	1:A:1403:GLU:HG2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:SER:HA	2:B:811:TYR:HE1	1.77	0.49
1:A:252:PHE:HD1	1:A:256:GLN:HB3	1.78	0.49
2:B:693:ILE:HG21	2:B:701:ILE:HD13	1.95	0.49
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	1.94	0.49
1:A:216:VAL:O	1:A:220:THR:HB	2.12	0.49
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.12	0.49
1:A:448:PRO:HG3	13:T:19:DT:O2	2.13	0.49
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.95	0.49
6:H:80:ARG:HG2	9:K:57:LEU:HD22	1.95	0.49
7:I:65:ASP:HB3	7:I:68:LEU:HD12	1.94	0.49
1:A:497:THR:HG22	2:B:1146:PHE:CD1	2.41	0.49
6:H:17:PRO:HB3	6:H:24:CYS:SG	2.52	0.49
10:L:27:LEU:HD13	10:L:37:LYS:HG2	1.95	0.49
1:A:58:LEU:HB3	1:A:59:GLY:H	1.45	0.48
2:B:62:ILE:HG21	2:B:417:PHE:HD2	1.78	0.48
2:B:338:GLY:HA2	2:B:339:THR:HB	1.94	0.48
2:B:441:ASP:O	2:B:443:ASN:N	2.46	0.48
2:B:486:TYR:HB3	2:B:1096:ARG:NE	2.29	0.48
2:B:640:VAL:HG22	2:B:651:LEU:HG	1.95	0.48
2:B:933:SER:O	2:B:935:ARG:N	2.45	0.48
1:A:37:PHE:HD2	1:A:52:GLY:HA3	1.77	0.48
1:A:55:ASP:N	1:A:56:PRO:HD3	2.28	0.48
6:H:23:VAL:HG11	6:H:121:LEU:HD22	1.95	0.48
10:L:68:GLU:HB2	10:L:70:ARG:HD2	1.96	0.48
1:A:66:LYS:HB3	1:A:71:GLN:O	2.13	0.48
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.95	0.48
2:B:187:SER:HB3	8:J:62:ARG:HH22	1.77	0.48
2:B:345:LYS:HA	2:B:348:ARG:HD2	1.96	0.48
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.96	0.48
1:A:870:GLU:HB2	4:E:204:THR:CG2	2.40	0.48
1:A:1116:LEU:HG	1:A:1327:ILE:HD11	1.95	0.48
1:A:55:ASP:HA	1:A:58:LEU:HB2	1.96	0.48
2:B:705:MET:H	2:B:710:LEU:HD12	1.78	0.48
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.96	0.48
1:A:1436:ILE:O	1:A:1437:GLY:C	2.56	0.48
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.96	0.48
2:B:212:LEU:HD23	2:B:212:LEU:HA	1.73	0.48
2:B:840:ILE:HG21	2:B:994:TYR:HD2	1.79	0.48
6:H:115:TYR:CE1	6:H:124:ARG:HG3	2.49	0.48
1:A:64:ASN:O	1:A:65:LEU:HB3	2.12	0.47
1:A:738:LYS:HA	6:H:19:ARG:HH12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:LEU:HD21	1:A:983:ILE:HG21	1.96	0.47
2:B:542:MET:HG3	2:B:747:MET:HB3	1.95	0.47
1:A:12:ARG:HB3	2:B:1218:THR:HB	1.96	0.47
1:A:568:PRO:HG2	6:H:46:LEU:HD12	1.95	0.47
3:C:165:LYS:O	9:K:6:ARG:NH1	2.46	0.47
2:B:1166:CYS:O	2:B:1168:LEU:N	2.42	0.47
8:J:9:SER:HB2	8:J:45:CYS:HB2	1.95	0.47
1:A:448:PRO:O	1:A:449:SER:CB	2.63	0.47
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.96	0.47
1:A:956:LEU:HD21	1:A:1017:LEU:HG	1.96	0.47
1:A:253:ASN:HB3	2:B:935:ARG:NE	2.29	0.47
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.95	0.47
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.95	0.47
3:C:58:LEU:HD21	8:J:57:ILE:HD12	1.97	0.47
1:A:475:THR:HG21	2:B:836:GLU:OE2	2.14	0.47
1:A:709:THR:HG22	1:A:711:ARG:H	1.80	0.47
7:I:106:CYS:SG	7:I:108:HIS:HB3	2.55	0.47
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.97	0.47
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.95	0.47
9:K:63:VAL:HG12	9:K:71:PHE:HB3	1.96	0.47
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.80	0.47
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.50	0.47
6:H:40:LEU:HD13	6:H:123:MET:HG3	1.95	0.47
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.95	0.46
1:A:399:HIS:O	1:A:401:GLY:N	2.48	0.46
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.15	0.46
7:I:102:VAL:HG22	7:I:109:ILE:HG12	1.98	0.46
2:B:882:THR:HG21	2:B:935:ARG:HA	1.97	0.46
4:E:176:PRO:O	4:E:212:ARG:HA	2.14	0.46
3:C:100:THR:HG22	3:C:119:VAL:HG22	1.97	0.46
1:A:745:GLN:HA	1:A:748:MET:HE3	1.98	0.46
1:A:1074:GLU:O	1:A:1077:THR:HB	2.16	0.46
1:A:565:ILE:O	1:A:570:PRO:HA	2.16	0.46
4:E:65:THR:O	4:E:69:ILE:HD12	2.16	0.46
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.45	0.46
2:B:64:CYS:HA	2:B:67:SER:HB3	1.98	0.46
2:B:803:LEU:HG	8:J:52:THR:HG21	1.98	0.46
3:C:8:VAL:HG11	9:K:105:PHE:HD1	1.81	0.46
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.97	0.46
1:A:579:SER:HA	1:A:582:ILE:HG13	1.97	0.46
1:A:923:LEU:O	1:A:927:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1386:ARG:HB3	1:A:1403:GLU:HG3	1.97	0.46
2:B:365:THR:HG21	2:B:370:PHE:CG	2.51	0.46
2:B:756:ILE:O	2:B:759:PRO:HD3	2.15	0.46
2:B:211:VAL:CG1	2:B:495:LEU:HD23	2.45	0.46
2:B:406:LEU:HD12	2:B:633:VAL:CG2	2.46	0.46
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.97	0.46
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.98	0.46
7:I:83:ASN:HA	7:I:104:LEU:HG	1.98	0.46
1:A:7:SER:HG	2:B:1161:HIS:HE2	1.63	0.45
1:A:514:PRO:HG2	1:A:1067:LEU:HD11	1.99	0.45
1:A:743:VAL:O	1:A:747:VAL:HG23	2.16	0.45
1:A:883:LEU:HD23	1:A:1021:LEU:HB2	1.97	0.45
2:B:291:ILE:HD12	2:B:291:ILE:N	2.30	0.45
1:A:311:GLN:O	1:A:312:PRO:C	2.59	0.45
2:B:86:ARG:HG2	2:B:138:GLU:HG3	1.98	0.45
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.81	0.45
4:E:90:VAL:HG23	4:E:123:LEU:HD11	1.98	0.45
6:H:30:SER:HB3	6:H:36:CYS:HB3	1.98	0.45
1:A:270:LEU:HD12	1:A:274:ILE:HD11	1.98	0.45
3:C:18:VAL:HG12	3:C:20:PHE:HD1	1.81	0.45
6:H:93:TYR:HA	6:H:145:ARG:HB3	1.99	0.45
2:B:468:GLU:HG2	2:B:469:GLN:HB2	1.99	0.45
2:B:901:PRO:O	10:L:60:ARG:HA	2.17	0.45
7:I:50:THR:HG22	7:I:52:ILE:H	1.81	0.45
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.99	0.45
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.98	0.45
3:C:55:THR:HB	3:C:151:GLN:HA	1.99	0.45
1:A:151:ASP:HA	1:A:163:SER:HA	1.99	0.45
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.52	0.45
9:K:65:HIS:HE1	9:K:67:PHE:CG	2.35	0.45
4:E:88:VAL:HB	4:E:116:ILE:HG12	1.97	0.45
5:F:89:GLU:C	5:F:93:ILE:HD12	2.42	0.45
12:P:8:G:H2'	12:P:9:G:H8	1.81	0.45
1:A:187:LYS:HE3	1:A:198:GLU:HB2	1.99	0.45
1:A:254:GLU:H	2:B:935:ARG:HH21	1.64	0.45
1:A:534:LEU:O	1:A:574:GLY:HA3	2.17	0.45
8:J:1:MET:HE3	8:J:1:MET:HB3	1.87	0.45
1:A:1444:MET:HB2	1:A:1444:MET:HE2	1.62	0.45
2:B:662:MET:HA	2:B:665:GLU:HB2	1.97	0.45
1:A:35:ILE:HG13	1:A:56:PRO:HG2	1.99	0.44
1:A:548:ASN:HD21	9:K:47:ARG:HH21	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HA	1:A:568:PRO:C	2.41	0.44
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.99	0.44
13:T:12:DT:H2'	13:T:13:DA:C8	2.52	0.44
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.99	0.44
2:B:394:ASP:OD2	7:I:91:ARG:HD2	2.17	0.44
1:A:974:ASP:C	1:A:976:THR:H	2.25	0.44
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.99	0.44
2:B:102:VAL:HG23	2:B:112:LEU:HD22	2.00	0.44
7:I:72:ASP:O	7:I:81:ARG:HG2	2.16	0.44
1:A:589:GLN:HG2	1:A:606:LEU:HD13	1.99	0.44
1:A:1154:TYR:CE1	7:I:18:GLU:HG3	2.53	0.44
8:J:28:ASP:C	8:J:30:LEU:H	2.24	0.44
1:A:1148:ILE:HA	7:I:49:ILE:HD12	2.00	0.44
1:A:1151:GLU:HG2	7:I:45:ARG:HG3	1.99	0.44
1:A:1393:ASN:ND2	1:A:1393:ASN:H	2.15	0.44
1:A:869:GLY:O	4:E:204:THR:HG21	2.18	0.44
1:A:41:MET:HB3	1:A:49:LYS:HA	2.00	0.44
1:A:449:SER:HA	1:A:454:SER:HB3	1.99	0.44
3:C:133:ILE:HG21	3:C:236:GLY:HA3	2.00	0.44
1:A:875:ALA:HB2	1:A:1366:ARG:CD	2.48	0.44
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.18	0.44
2:B:617:ARG:HG3	2:B:624:LEU:HD12	2.00	0.44
1:A:130:ASP:HB3	1:A:133:LYS:HB2	2.00	0.44
1:A:446:ARG:HB2	1:A:487:MET:SD	2.57	0.44
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	2.00	0.44
6:H:4:THR:HA	6:H:60:ALA:HB2	2.00	0.44
1:A:62:ASP:HB2	1:A:65:LEU:HD22	1.99	0.43
2:B:509:ALA:C	2:B:511:PRO:HD3	2.43	0.43
2:B:563:MET:HE3	2:B:580:VAL:HB	1.99	0.43
2:B:521:LEU:HD22	2:B:633:VAL:HG12	2.01	0.43
1:A:53:LEU:O	1:A:54:ASN:C	2.60	0.43
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.53	0.43
2:B:69:LEU:HD22	2:B:425:THR:HG23	2.00	0.43
13:T:19:DT:H2'	13:T:20:DC:C6	2.54	0.43
1:A:774:ARG:HH21	1:A:797:LYS:HB2	1.83	0.43
2:B:89:GLU:HB2	2:B:135:ARG:HB2	1.99	0.43
13:T:21:DC:H2'	13:T:22:BRU:H6	2.01	0.43
1:A:1356:ILE:HG21	1:A:1363:VAL:HG23	1.99	0.43
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.84	0.43
1:A:347:PHE:H	2:B:1107:ALA:HA	1.82	0.43
2:B:766:ARG:NH2	2:B:1020:ARG:HD3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:ARG:HE	3:C:21:ILE:HD11	1.83	0.43
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.53	0.43
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.83	0.43
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.65	0.43
2:B:383:ASN:O	2:B:387:LEU:HB2	2.19	0.43
2:B:1158:PHE:HE2	2:B:1160:VAL:HG13	1.83	0.43
1:A:413:ILE:HD13	1:A:424:ILE:HD11	2.01	0.43
2:B:171:PRO:HG2	2:B:461:LEU:HD12	2.01	0.43
6:H:105:GLU:HB3	6:H:113:ALA:HB3	2.00	0.43
8:J:36:LEU:HD11	8:J:51:LEU:HB2	2.00	0.43
1:A:239:LEU:HD12	1:A:240:PRO:HD2	2.01	0.43
1:A:873:MET:HB3	1:A:878:ILE:HD11	2.01	0.43
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	2.01	0.43
1:A:1438:THR:HB	2:B:1142:GLY:O	2.19	0.43
5:F:82:THR:HG22	5:F:83:PRO:HD2	2.01	0.43
5:F:130:ILE:HB	5:F:148:VAL:HG21	1.99	0.43
10:L:49:LYS:O	10:L:50:ASP:HB2	2.19	0.43
2:B:199:MET:SD	2:B:199:MET:N	2.90	0.43
1:A:344:ARG:HG2	2:B:1127:GLY:O	2.18	0.42
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.20	0.42
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.84	0.42
1:A:1323:ASP:CG	1:A:1326:ARG:HG3	2.44	0.42
2:B:125:SER:HA	2:B:171:PRO:HA	2.00	0.42
6:H:15:VAL:HG22	6:H:26:ILE:HG13	2.00	0.42
1:A:399:HIS:HB3	1:A:400:PRO:HD3	2.02	0.42
1:A:449:SER:HA	1:A:454:SER:CB	2.49	0.42
1:A:481:ASP:OD1	1:A:485:ASP:OD1	2.37	0.42
1:A:709:THR:HB	1:A:712:GLU:H	1.83	0.42
2:B:65:GLU:HG3	2:B:66:ASP:H	1.85	0.42
2:B:169:ARG:HB2	2:B:454:THR:HG23	2.01	0.42
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.19	0.42
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.49	0.42
1:A:358:ASN:HB2	9:K:65:HIS:HD2	1.83	0.42
1:A:562:THR:O	1:A:576:GLN:NE2	2.53	0.42
2:B:980:PHE:CD1	2:B:1094:ARG:HA	2.54	0.42
3:C:184:ASN:ND2	3:C:189:THR:O	2.52	0.42
1:A:873:MET:C	1:A:1058:VAL:HG22	2.44	0.42
2:B:857:ARG:NH1	2:B:945:GLU:OE2	2.52	0.42
1:A:1025:ARG:O	1:A:1035:TYR:HE2	2.01	0.42
2:B:273:LEU:HD12	2:B:280:ILE:HD12	2.01	0.42
3:C:148:ARG:HG3	3:C:151:GLN:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:149:LYS:C	3:C:151:GLN:H	2.28	0.42
4:E:10:SER:O	4:E:14:ARG:HG3	2.19	0.42
6:H:38:LEU:HD13	6:H:125:LEU:HD13	2.02	0.42
7:I:76:PRO:HD2	7:I:108:HIS:HD2	1.84	0.42
8:J:22:LEU:O	8:J:26:GLN:HG2	2.20	0.42
8:J:48:ARG:HH21	8:J:49:MET:HE1	1.85	0.42
3:C:99:LEU:HB3	3:C:118:LEU:HD22	2.02	0.42
1:A:1036:ARG:HH11	1:A:1036:ARG:HG2	1.85	0.42
2:B:952:VAL:HB	10:L:58:LYS:HB2	2.01	0.42
4:E:181:ALA:HA	4:E:186:LEU:HD21	2.01	0.42
1:A:469:ARG:NH2	2:B:991:GLY:O	2.52	0.42
1:A:871:ASP:CG	1:A:1366:ARG:HH22	2.28	0.42
2:B:848:ARG:HD2	8:J:8:PHE:O	2.20	0.42
1:A:194:ALA:HA	1:A:195:ASP:C	2.45	0.41
1:A:336:ILE:H	1:A:336:ILE:HG12	1.68	0.41
1:A:1094:VAL:HG22	1:A:1113:THR:HB	2.02	0.41
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.01	0.41
2:B:311:LEU:HB3	7:I:4:PHE:HE2	1.85	0.41
2:B:642:ASP:HA	2:B:649:LYS:HA	2.02	0.41
2:B:1143:ALA:HB1	2:B:1146:PHE:HB3	2.01	0.41
6:H:38:LEU:CD1	6:H:123:MET:HE2	2.46	0.41
6:H:125:LEU:HG	6:H:130:ARG:HH22	1.85	0.41
2:B:190:TYR:CE2	2:B:196:PRO:HG3	2.55	0.41
2:B:195:CYS:HB3	2:B:782:LEU:HD22	2.01	0.41
3:C:125:MET:HE3	3:C:125:MET:HA	2.02	0.41
1:A:313:GLN:O	1:A:314:ALA:C	2.63	0.41
1:A:381:THR:HG22	1:A:384:ASN:CG	2.46	0.41
2:B:681:TRP:HA	2:B:684:LEU:HD12	2.03	0.41
2:B:986:GLN:OE1	2:B:1016:ALA:HB1	2.20	0.41
2:B:865:LYS:HB2	2:B:961:LEU:HD21	2.00	0.41
10:L:38:LEU:HD21	10:L:48:CYS:HA	2.02	0.41
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.02	0.41
1:A:729:ALA:HA	1:A:732:LEU:HD12	2.01	0.41
2:B:226:PHE:HA	2:B:395:GLN:CG	2.49	0.41
2:B:953:LEU:HD11	10:L:55:ILE:HG22	2.03	0.41
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	2.03	0.41
2:B:341:LEU:HD11	2:B:343:ILE:HB	2.02	0.41
3:C:251:LEU:O	3:C:255:VAL:HG23	2.19	0.41
1:A:541:ILE:HG21	1:A:549:MET:CE	2.49	0.41
2:B:792:MET:HG2	2:B:855:PHE:CZ	2.55	0.41
3:C:148:ARG:N	3:C:151:GLN:HG3	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:PHE:O	1:A:53:LEU:HB2	2.21	0.41
2:B:279:ASP:OD1	2:B:279:ASP:N	2.53	0.41
2:B:841:MET:HG2	2:B:1010:LEU:HD12	2.01	0.41
6:H:82:PRO:O	6:H:84:ALA:N	2.52	0.41
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.86	0.41
2:B:39:ARG:HE	2:B:665:GLU:HG2	1.86	0.41
2:B:792:MET:H	2:B:857:ARG:HA	1.86	0.41
2:B:899:ILE:HG21	2:B:949:VAL:HG21	2.03	0.41
4:E:156:LEU:HD23	4:E:160:GLU:HB3	2.03	0.41
9:K:39:ASP:OD1	9:K:41:THR:HB	2.21	0.41
1:A:1317:MET:HE2	4:E:142:VAL:HG11	2.02	0.41
2:B:315:LYS:N	2:B:316:PRO:HD2	2.36	0.41
2:B:1082:MET:HA	3:C:189:THR:HA	2.03	0.41
3:C:258:ILE:HG13	9:K:42:LEU:HD21	2.03	0.41
5:F:97:ARG:HD2	5:F:97:ARG:HA	1.82	0.41
1:A:93:VAL:HG22	1:A:301:ALA:HA	2.03	0.40
1:A:93:VAL:HG13	1:A:301:ALA:HB1	2.03	0.40
1:A:441:PRO:HD2	1:A:498:ARG:CZ	2.52	0.40
1:A:1418:LEU:HD23	2:B:1222:ARG:HD3	2.03	0.40
2:B:509:ALA:O	2:B:511:PRO:HD3	2.20	0.40
2:B:563:MET:CE	2:B:580:VAL:HB	2.51	0.40
3:C:75:MET:HE1	3:C:239:PRO:HG3	2.03	0.40
3:C:255:VAL:HG21	9:K:94:ILE:HG21	2.03	0.40
6:H:82:PRO:HB2	6:H:83:GLN:H	1.65	0.40
7:I:111:THR:HG21	7:I:118:ARG:HD2	2.03	0.40
1:A:133:LYS:HE3	1:A:1391:ARG:HH12	1.85	0.40
1:A:586:ILE:HD11	1:A:637:LYS:HG2	2.03	0.40
1:A:626:ASN:O	1:A:631:HIS:ND1	2.53	0.40
1:A:1221:LYS:HB3	1:A:1222:ASN:H	1.72	0.40
2:B:577:ALA:HB1	2:B:589:VAL:HB	2.03	0.40
2:B:622:LYS:HE3	7:I:59:VAL:HG22	2.02	0.40
2:B:979:LYS:HD3	2:B:1095:LEU:HD13	2.04	0.40
2:B:1119:VAL:HG23	2:B:1126:GLY:HA2	2.03	0.40
8:J:32:GLU:CD	8:J:32:GLU:H	2.29	0.40
1:A:497:THR:CG2	2:B:1146:PHE:CD1	3.02	0.40
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	2.04	0.40
2:B:469:GLN:HB3	2:B:470:LYS:H	1.72	0.40
2:B:610:ASN:HB3	2:B:613:VAL:HG23	2.04	0.40
3:C:99:LEU:HD12	3:C:118:LEU:HB3	2.02	0.40
3:C:201:TRP:HA	3:C:202:PRO:HD3	1.97	0.40
4:E:167:ARG:HA	4:E:167:ARG:HD3	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:89:LEU:C	6:H:91:ASP:N	2.79	0.40
6:H:104:PHE:CE1	6:H:136:LYS:HG3	2.57	0.40
1:A:87:ALA:HB3	1:A:276:LEU:HD23	2.04	0.40
1:A:886:ILE:HD13	1:A:944:ARG:HG2	2.04	0.40
1:A:1356:ILE:HG23	1:A:1361:SER:HB2	2.03	0.40
2:B:65:GLU:OE1	2:B:247:GLY:HA2	2.20	0.40
2:B:871:THR:HG22	2:B:872:GLU:H	1.86	0.40
9:K:65:HIS:CE1	9:K:67:PHE:CG	3.10	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	1414/1733 (82%)	1236 (87%)	126 (9%)	52 (4%)	2	19
2	B	1138/1224 (93%)	1008 (89%)	86 (8%)	44 (4%)	2	18
3	C	264/318 (83%)	242 (92%)	20 (8%)	2 (1%)	16	54
4	E	212/215 (99%)	195 (92%)	13 (6%)	4 (2%)	6	32
5	F	82/155 (53%)	76 (93%)	6 (7%)	0	100	100
6	H	129/146 (88%)	106 (82%)	14 (11%)	9 (7%)	1	11
7	I	117/122 (96%)	98 (84%)	16 (14%)	3 (3%)	4	25
8	J	63/70 (90%)	51 (81%)	9 (14%)	3 (5%)	2	16
9	K	113/120 (94%)	109 (96%)	4 (4%)	0	100	100
10	L	44/70 (63%)	27 (61%)	9 (20%)	8 (18%)	0	2
All	All	3576/4173 (86%)	3148 (88%)	303 (8%)	125 (4%)	4	20

All (125) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	58	LEU
1	A	76	GLU
1	A	189	ARG
1	A	195	ASP
1	A	257	ARG
1	A	318	SER
1	A	399	HIS
1	A	449	SER
1	A	628	GLY
1	A	1377	THR
1	A	1403	GLU
1	A	1405	THR
2	B	229	ALA
2	B	307	ASP
2	B	344	LYS
2	B	442	PHE
2	B	466	TRP
2	B	473	MET
2	B	531	GLN
2	B	772	ALA
2	B	867	GLY
2	B	943	SER
2	B	1046	PRO
2	B	1181	GLU
7	I	9	ASP
7	I	95	THR
10	L	50	ASP
10	L	53	HIS
1	A	47	ARG
1	A	54	ASN
1	A	167	CYS
1	A	178	GLY
1	A	193	ASP
1	A	224	PHE
1	A	286	HIS
1	A	332	LYS
1	A	672	ASP
1	A	1175	SER
1	A	1281	ARG
2	B	262	GLU
2	B	282	ILE
2	B	339	THR

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Mol	Chain	Res	Type
2	B	341	LEU
2	B	707	PRO
2	B	731	VAL
2	B	792	MET
2	B	879	ARG
2	B	1175	LEU
2	B	1176	ASN
4	E	36	GLU
6	H	17	PRO
6	H	81	PRO
6	H	82	PRO
6	H	83	GLN
6	H	90	ALA
8	J	6	ARG
10	L	45	ALA
10	L	56	LEU
1	A	335	ARG
1	A	975	HIS
1	A	1173	HIS
2	B	340	ALA
2	B	343	ILE
2	B	711	GLU
2	B	1156	ASP
2	B	1157	ALA
2	B	1167	GLY
4	E	45	LYS
4	E	48	ASP
6	H	18	GLY
10	L	59	ALA
1	A	42	ASP
1	A	52	GLY
1	A	74	MET
1	A	465	TYR
1	A	569	LYS
1	A	846	GLU
1	A	958	VAL
1	A	1255	GLU
1	A	1437	GLY
1	A	1438	THR
2	B	441	ASP
2	B	648	HIS
2	B	883	LEU

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Mol	Chain	Res	Type
2	B	942	ARG
2	B	1108	ARG
2	B	1155	SER
3	C	88	CYS
7	I	91	ARG
8	J	29	GLU
10	L	26	THR
10	L	55	ILE
10	L	64	LEU
1	A	156	ASP
1	A	311	GLN
1	A	336	ILE
1	A	567	LYS
1	A	1171	GLN
1	A	1366	ARG
2	B	251	ILE
2	B	462	ALA
2	B	469	GLN
2	B	880	THR
2	B	907	GLY
2	B	1223	ASP
6	H	60	ALA
6	H	128	ASN
8	J	2	ILE
1	A	35	ILE
1	A	55	ASP
1	A	155	GLU
1	A	885	THR
3	C	214	ASN
1	A	196	GLU
1	A	1388	GLY
4	E	90	VAL
2	B	44	VAL
2	B	364	ILE
1	A	192	GLY
1	A	312	PRO
2	B	1121	GLY
1	A	448	PRO
2	B	1214	PRO
6	H	59	ILE

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	1240/1520 (82%)	1040 (84%)	200 (16%)	2	11
2	B	986/1061 (93%)	845 (86%)	141 (14%)	3	13
3	C	234/274 (85%)	204 (87%)	30 (13%)	4	15
4	E	196/197 (100%)	173 (88%)	23 (12%)	5	18
5	F	74/137 (54%)	65 (88%)	9 (12%)	5	17
6	H	117/128 (91%)	101 (86%)	16 (14%)	3	14
7	I	113/116 (97%)	105 (93%)	8 (7%)	13	35
8	J	60/65 (92%)	48 (80%)	12 (20%)	1	7
9	K	99/102 (97%)	86 (87%)	13 (13%)	4	15
10	L	40/57 (70%)	26 (65%)	14 (35%)	0	1
All	All	3159/3657 (86%)	2693 (85%)	466 (15%)	5	13

All (466) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	13	THR
1	A	15	LYS
1	A	28	ARG
1	A	34	LYS
1	A	41	MET
1	A	45	GLN
1	A	47	ARG
1	A	50	ILE
1	A	53	LEU
1	A	54	ASN
1	A	62	ASP
1	A	63	ARG
1	A	67	CYS
1	A	84	ILE
1	A	90	VAL

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Mol	Chain	Res	Type
1	A	93	VAL
1	A	106	VAL
1	A	131	SER
1	A	134	ARG
1	A	145	LYS
1	A	147	VAL
1	A	152	VAL
1	A	157	ASP
1	A	173	THR
1	A	174	ILE
1	A	182	VAL
1	A	199	LEU
1	A	204	THR
1	A	205	GLU
1	A	208	LEU
1	A	219	PHE
1	A	220	THR
1	A	222	LEU
1	A	227	VAL
1	A	237	THR
1	A	252	PHE
1	A	255	SER
1	A	270	LEU
1	A	279	LEU
1	A	289	ILE
1	A	295	LEU
1	A	307	ASP
1	A	313	GLN
1	A	315	LEU
1	A	322	VAL
1	A	330	LYS
1	A	333	GLU
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	353	ILE
1	A	375	THR
1	A	381	THR
1	A	385	ILE
1	A	386	ASP
1	A	393	ARG
1	A	398	GLU

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Mol	Chain	Res	Type
1	A	408	ASP
1	A	412	ARG
1	A	424	ILE
1	A	425	GLN
1	A	427	GLN
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	454	SER
1	A	461	LYS
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	489	LEU
1	A	500	GLU
1	A	505	CYS
1	A	512	VAL
1	A	513	SER
1	A	524	VAL
1	A	532	ARG
1	A	566	ILE
1	A	571	LEU
1	A	582	ILE
1	A	593	GLU
1	A	596	THR
1	A	603	ASN
1	A	613	ILE
1	A	618	GLU
1	A	629	LEU
1	A	630	ILE
1	A	634	THR
1	A	652	VAL
1	A	664	THR
1	A	666	ILE
1	A	672	ASP
1	A	691	LEU

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Mol	Chain	Res	Type
1	A	702	LEU
1	A	719	VAL
1	A	738	LYS
1	A	740	LEU
1	A	768	GLN
1	A	769	SER
1	A	773	LYS
1	A	782	ARG
1	A	788	SER
1	A	795	GLU
1	A	797	LYS
1	A	801	GLU
1	A	805	LEU
1	A	806	ARG
1	A	821	ARG
1	A	826	ASP
1	A	827	THR
1	A	831	THR
1	A	834	THR
1	A	837	ILE
1	A	839	ARG
1	A	848	ILE
1	A	849	MET
1	A	854	ASN
1	A	864	ILE
1	A	867	ILE
1	A	886	ILE
1	A	896	ARG
1	A	919	ILE
1	A	920	LEU
1	A	926	GLN
1	A	929	LEU
1	A	948	VAL
1	A	949	ASP
1	A	964	ILE
1	A	973	ILE
1	A	976	THR
1	A	983	ILE
1	A	998	LEU
1	A	999	VAL
1	A	1009	ASN
1	A	1015	VAL

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Mol	Chain	Res	Type
1	A	1029	ARG
1	A	1030	ARG
1	A	1047	SER
1	A	1058	VAL
1	A	1062	GLU
1	A	1067	LEU
1	A	1078	GLN
1	A	1094	VAL
1	A	1116	LEU
1	A	1118	VAL
1	A	1120	LEU
1	A	1121	GLU
1	A	1124	HIS
1	A	1135	ARG
1	A	1142	THR
1	A	1172	LEU
1	A	1173	HIS
1	A	1176	LEU
1	A	1195	LEU
1	A	1208	THR
1	A	1218	GLN
1	A	1223	ASP
1	A	1226	VAL
1	A	1237	ILE
1	A	1238	ILE
1	A	1242	VAL
1	A	1255	GLU
1	A	1257	ASP
1	A	1260	LEU
1	A	1265	ASN
1	A	1273	LEU
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1309	ASP
1	A	1315	GLU
1	A	1317	MET
1	A	1325	THR
1	A	1327	ILE
1	A	1336	MET
1	A	1341	ILE
1	A	1355	VAL

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Mol	Chain	Res	Type
1	A	1376	THR
1	A	1382	THR
1	A	1386	ARG
1	A	1391	ARG
1	A	1393	ASN
1	A	1403	GLU
1	A	1404	GLU
1	A	1411	GLU
1	A	1424	VAL
1	A	1426	GLU
1	A	1438	THR
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1453	TYR
1	A	1454	MET
2	B	25	ILE
2	B	41	LYS
2	B	46	GLN
2	B	63	ILE
2	B	69	LEU
2	B	72	GLU
2	B	73	GLN
2	B	102	VAL
2	B	103	ASN
2	B	104	GLU
2	B	128	LEU
2	B	164	LYS
2	B	169	ARG
2	B	178	ASN
2	B	183	GLU
2	B	211	VAL
2	B	240	ILE
2	B	251	ILE
2	B	261	ARG
2	B	267	ARG
2	B	272	THR
2	B	278	GLN
2	B	279	ASP
2	B	287	ARG
2	B	294	ASP
2	B	313	MET

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Mol	Chain	Res	Type
2	B	324	ILE
2	B	325	GLN
2	B	337	ARG
2	B	341	LEU
2	B	343	ILE
2	B	344	LYS
2	B	348	ARG
2	B	357	GLN
2	B	365	THR
2	B	393	LYS
2	B	408	LEU
2	B	419	THR
2	B	425	THR
2	B	440	HIS
2	B	442	PHE
2	B	470	LYS
2	B	476	ARG
2	B	482	VAL
2	B	485	ARG
2	B	487	THR
2	B	502	ILE
2	B	513	GLN
2	B	529	GLU
2	B	531	GLN
2	B	537	LYS
2	B	542	MET
2	B	547	VAL
2	B	552	MET
2	B	554	ILE
2	B	563	MET
2	B	570	VAL
2	B	574	SER
2	B	595	ARG
2	B	596	LEU
2	B	601	ARG
2	B	603	LEU
2	B	609	ILE
2	B	612	GLU
2	B	615	MET
2	B	616	ILE
2	B	620	ARG
2	B	644	GLU

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Mol	Chain	Res	Type
2	B	651	LEU
2	B	653	VAL
2	B	658	ILE
2	B	680	THR
2	B	708	GLU
2	B	734	HIS
2	B	737	THR
2	B	766	ARG
2	B	771	SER
2	B	776	GLN
2	B	786	ASN
2	B	790	ASP
2	B	791	THR
2	B	795	ILE
2	B	831	SER
2	B	835	GLN
2	B	839	MET
2	B	841	MET
2	B	844	SER
2	B	857	ARG
2	B	868	MET
2	B	870	ILE
2	B	871	THR
2	B	878	GLN
2	B	882	THR
2	B	889	THR
2	B	904	ARG
2	B	906	SER
2	B	909	ASP
2	B	911	ILE
2	B	934	LYS
2	B	939	THR
2	B	942	ARG
2	B	944	THR
2	B	953	LEU
2	B	964	VAL
2	B	970	THR
2	B	972	LYS
2	B	973	ILE
2	B	975	GLN
2	B	979	LYS
2	B	986	GLN

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Mol	Chain	Res	Type
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1028	GLU
2	B	1045	SER
2	B	1060	ARG
2	B	1065	GLN
2	B	1072	MET
2	B	1084	GLN
2	B	1094	ARG
2	B	1101	ASP
2	B	1106	ARG
2	B	1123	SER
2	B	1128	LEU
2	B	1138	MET
2	B	1145	SER
2	B	1147	LEU
2	B	1151	LEU
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1165	ILE
2	B	1175	LEU
2	B	1179	GLN
2	B	1183	LYS
2	B	1188	LYS
2	B	1189	ILE
2	B	1193	GLN
2	B	1201	LYS
2	B	1202	LEU
2	B	1220	ARG
3	C	3	GLU
3	C	11	ARG
3	C	12	GLU
3	C	22	LEU
3	C	25	VAL
3	C	26	ASP
3	C	52	GLU
3	C	53	THR
3	C	54	ASN
3	C	55	THR
3	C	56	THR

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Mol	Chain	Res	Type
3	C	81	GLU
3	C	100	THR
3	C	101	LEU
3	C	119	VAL
3	C	121	VAL
3	C	124	LEU
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	147	LEU
3	C	151	GLN
3	C	215	GLU
3	C	224	GLN
3	C	238	ILE
3	C	240	VAL
3	C	259	LEU
3	C	265	MET
3	C	268	ASP
4	E	3	GLN
4	E	9	ILE
4	E	20	LYS
4	E	31	THR
4	E	45	LYS
4	E	57	MET
4	E	67	GLU
4	E	92	THR
4	E	100	ILE
4	E	104	ASN
4	E	127	ILE
4	E	131	THR
4	E	140	LEU
4	E	144	ILE
4	E	166	LYS
4	E	173	SER
4	E	177	ARG
4	E	178	ILE
4	E	191	LYS
4	E	192	ARG
4	E	196	VAL
4	E	202	SER
4	E	204	THR

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Mol	Chain	Res	Type
5	F	72	LYS
5	F	78	GLN
5	F	79	ARG
5	F	82	THR
5	F	86	THR
5	F	90	ARG
5	F	110	ASP
5	F	129	LYS
5	F	133	VAL
6	H	13	SER
6	H	14	GLU
6	H	23	VAL
6	H	26	ILE
6	H	31	THR
6	H	34	ASP
6	H	76	THR
6	H	77	ARG
6	H	83	GLN
6	H	89	LEU
6	H	92	ASP
6	H	103	LYS
6	H	128	ASN
6	H	130	ARG
6	H	135	LEU
6	H	138	GLU
7	I	8	ARG
7	I	31	THR
7	I	35	VAL
7	I	74	GLU
7	I	82	GLU
7	I	84	VAL
7	I	94	ASP
7	I	111	THR
8	J	1	MET
8	J	2	ILE
8	J	3	VAL
8	J	7	CYS
8	J	12	LYS
8	J	13	VAL
8	J	14	VAL
8	J	22	LEU
8	J	29	GLU

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Mol	Chain	Res	Type
8	J	42	LYS
8	J	48	ARG
8	J	52	THR
9	K	14	GLU
9	K	18	LYS
9	K	20	LYS
9	K	25	THR
9	K	29	ASN
9	K	31	VAL
9	K	37	LYS
9	K	42	LEU
9	K	47	ARG
9	K	51	LEU
9	K	101	LEU
9	K	107	THR
9	K	114	LEU
10	L	27	LEU
10	L	33	GLU
10	L	35	SER
10	L	38	LEU
10	L	42	ARG
10	L	50	ASP
10	L	54	ARG
10	L	55	ILE
10	L	56	LEU
10	L	58	LYS
10	L	60	ARG
10	L	61	THR
10	L	65	VAL
10	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	282	ASN
1	A	390	GLN
1	A	394	ASN
1	A	399	HIS
1	A	425	GLN
1	A	451	HIS
1	A	517	ASN

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Mol	Chain	Res	Type
1	A	545	GLN
1	A	548	ASN
1	A	603	ASN
1	A	760	GLN
1	A	811	GLN
1	A	838	GLN
1	A	965	GLN
1	A	966	ASN
1	A	969	GLN
1	A	994	GLN
1	A	1106	ASN
1	A	1128	GLN
1	A	1140	HIS
1	A	1173	HIS
1	A	1232	ASN
1	A	1270	ASN
1	A	1393	ASN
1	A	1427	ASN
2	B	110	HIS
2	B	278	GLN
2	B	300	HIS
2	B	350	GLN
2	B	357	GLN
2	B	415	GLN
2	B	449	ASN
2	B	538	ASN
2	B	686	ASN
2	B	786	ASN
2	B	842	ASN
2	B	1117	GLN
2	B	1176	ASN
2	B	1177	HIS
3	C	112	ASN
3	C	131	HIS
3	C	135	GLN
3	C	184	ASN
3	C	203	GLN
3	C	214	ASN
3	C	231	ASN
4	E	3	GLN
4	E	54	GLN
4	E	115	ASN

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Mol	Chain	Res	Type
4	E	146	HIS
4	E	179	GLN
6	H	35	GLN
6	H	52	GLN
6	H	83	GLN
6	H	131	ASN
7	I	83	ASN
7	I	89	GLN
7	I	108	HIS
8	J	26	GLN
8	J	64	ASN
9	K	44	ASN
9	K	76	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	P	5/6 (83%)	1 (20%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	P	8	G

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BRU	T	22	12,13	18,21,22	1.01	1 (5%)	25,30,33	1.66	6 (24%)

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
13	BRU	T	22	12,13	-	0/7/21/22	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	22	BRU	C4-N3	-2.28	1.34	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	22	BRU	O4'-C1'-N1	4.20	115.31	107.86
13	T	22	BRU	BR-C5-C4	2.88	121.33	118.02
13	T	22	BRU	N3-C2-N1	2.74	118.46	114.89
13	T	22	BRU	BR-C5-C6	-2.61	117.00	120.64
13	T	22	BRU	C2'-C1'-N1	-2.22	108.25	113.81
13	T	22	BRU	O2-C2-N3	-2.12	117.58	121.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	T	22	BRU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	934:LYS	C	935:ARG	N	5.39
1	B	351:TYR	C	352:ALA	N	3.28

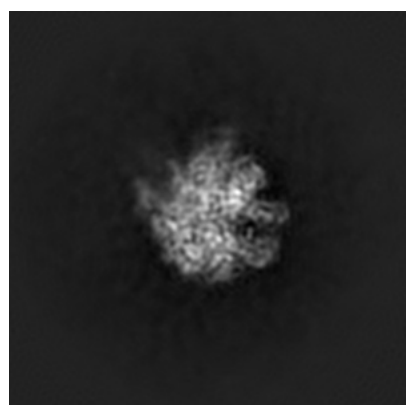
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2784. These allow visual inspection of the internal detail of the map and identification of artifacts.

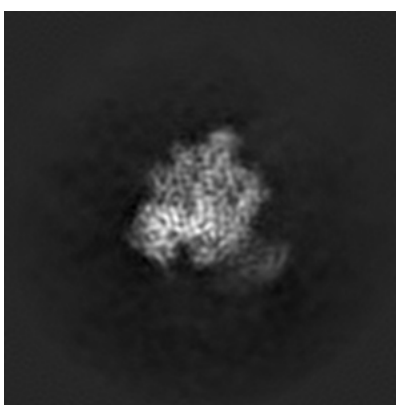
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

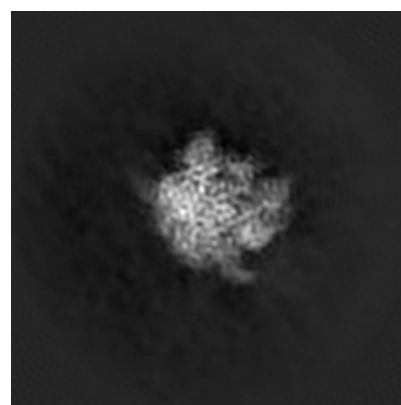
6.1.1 Primary map



X



Y

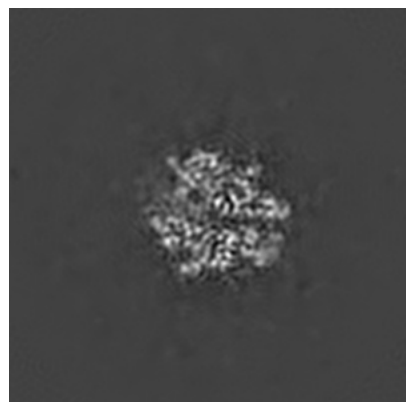


Z

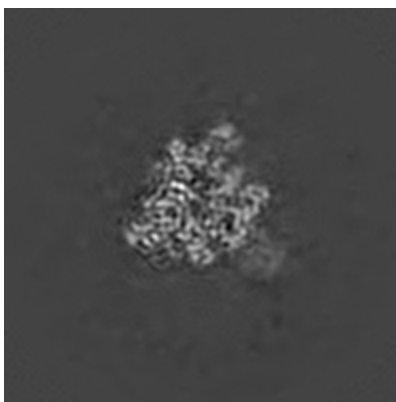
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

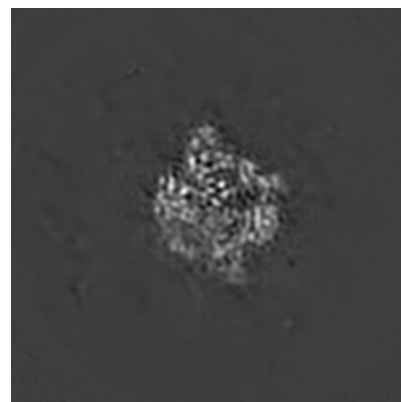
6.2.1 Primary map



X Index: 140



Y Index: 140

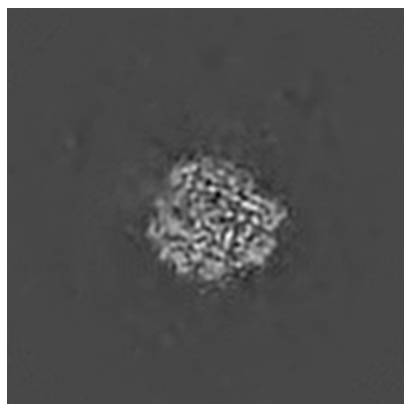


Z Index: 140

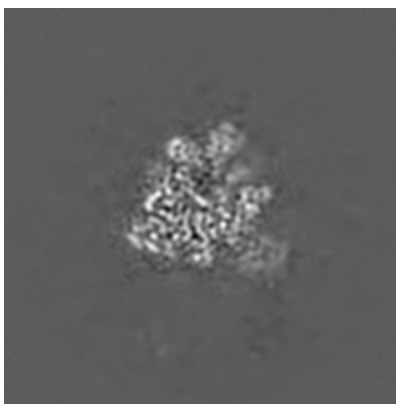
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

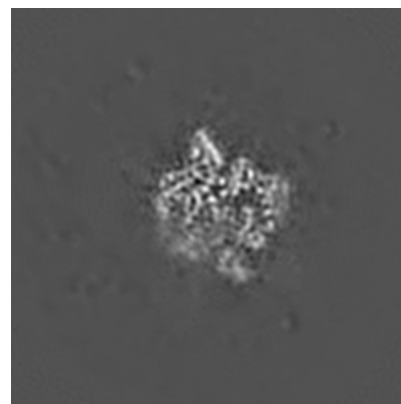
6.3.1 Primary map



X Index: 127



Y Index: 143

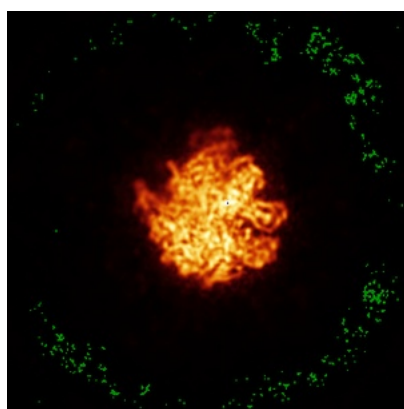


Z Index: 144

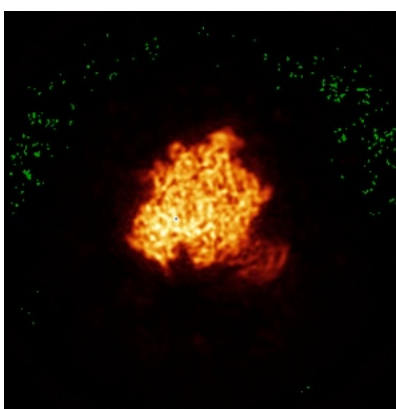
The images above show the largest variance slices of the map in three orthogonal directions.

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

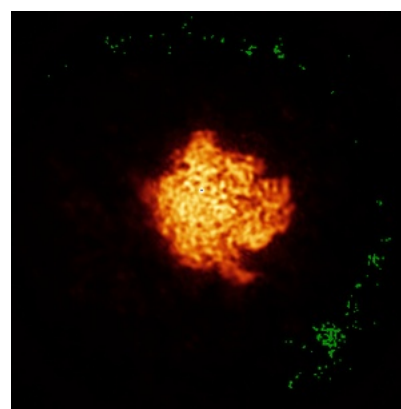
6.4.1 Primary map



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

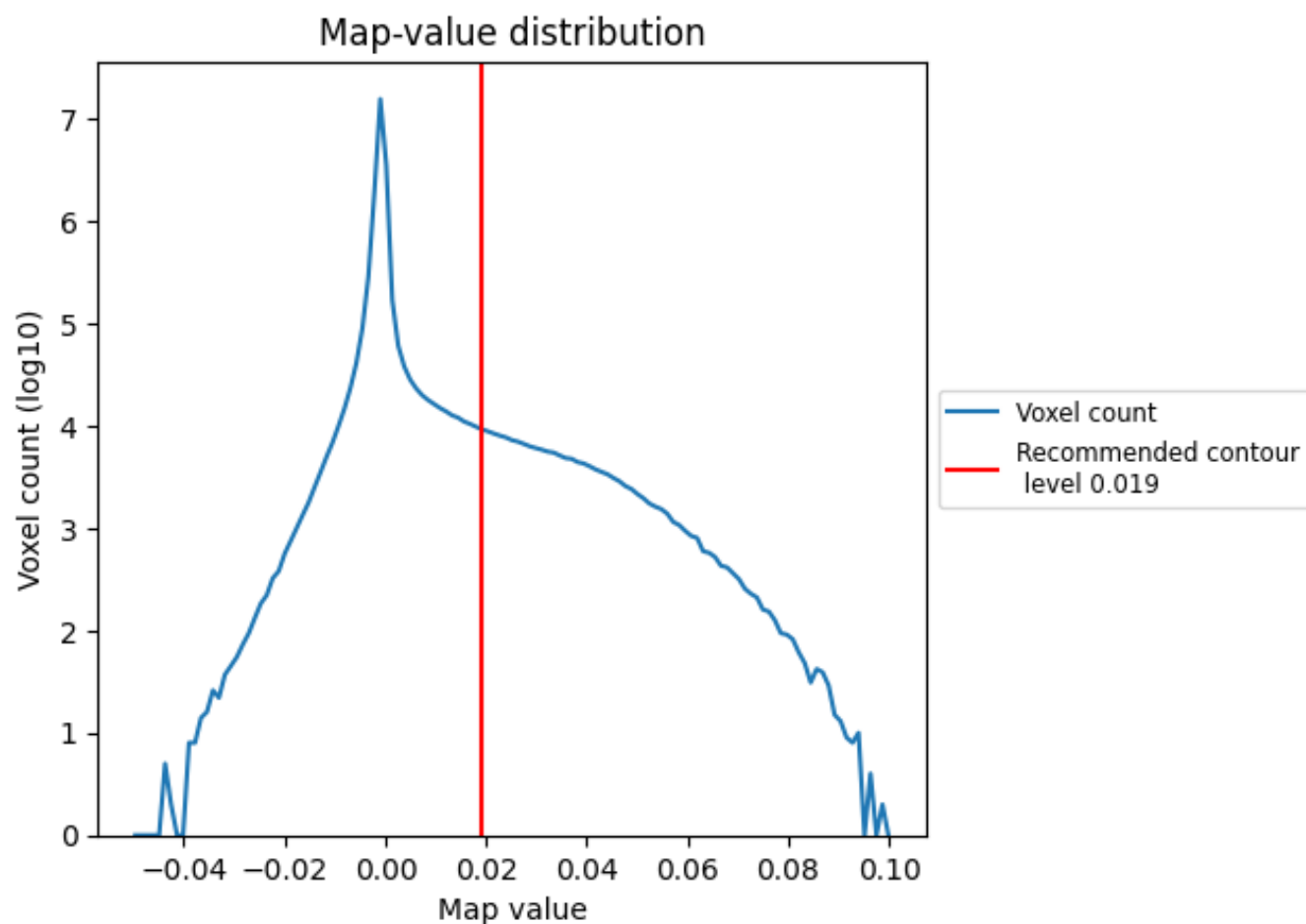
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

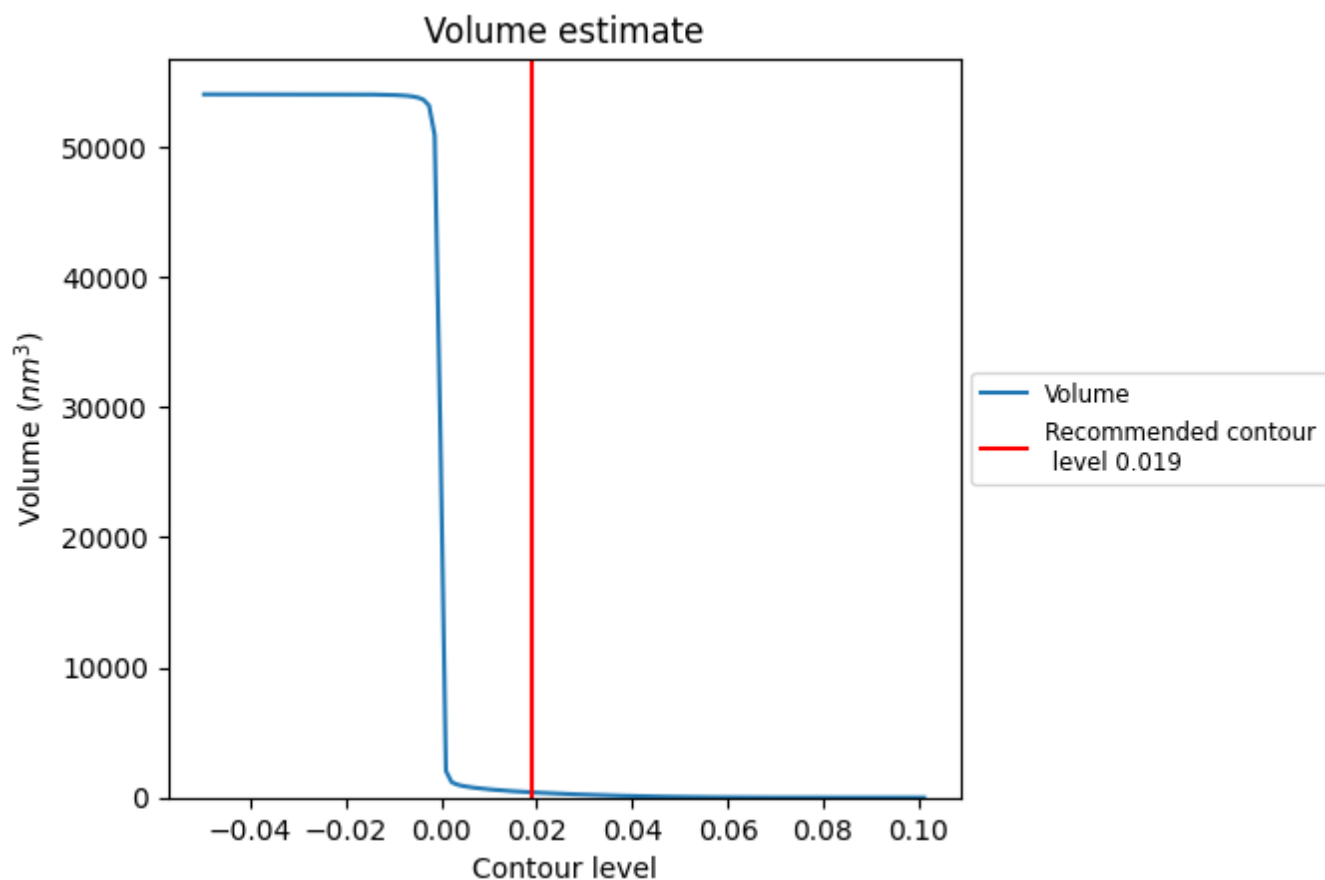
This section contains the results of statistical analysis of the map.

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.

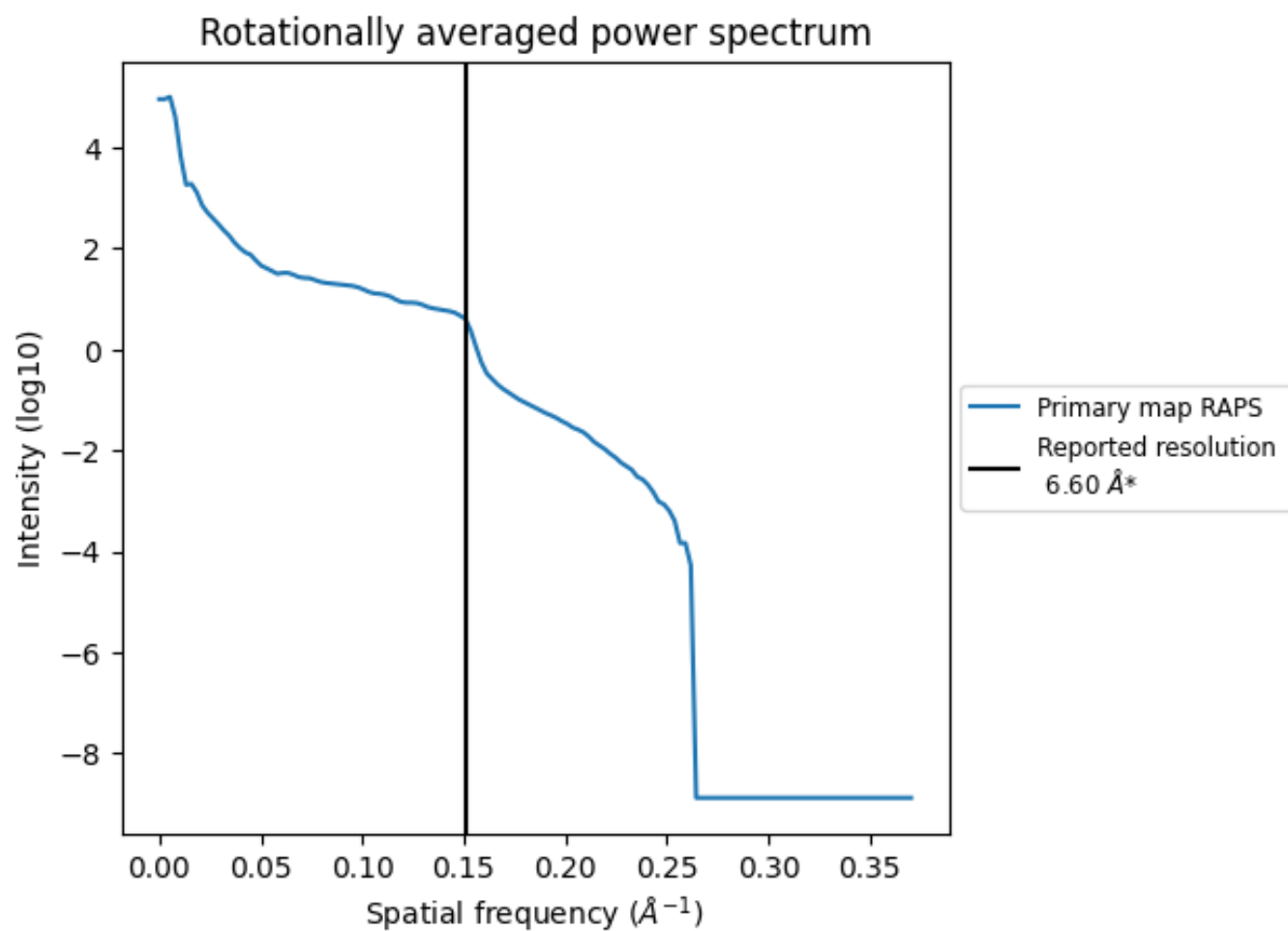
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 400 nm³; this corresponds to an approximate mass of 361 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 0.152 Å⁻¹

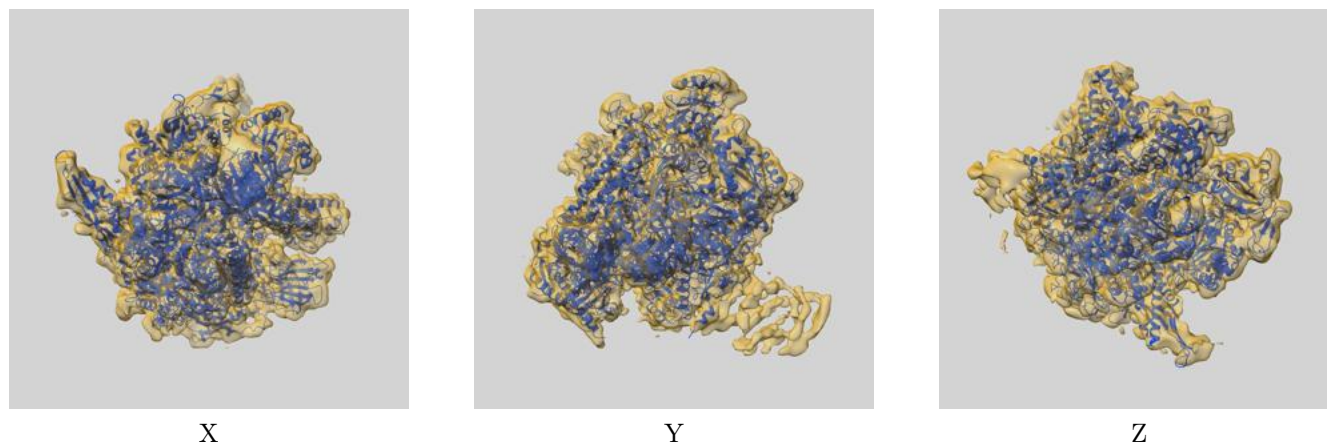
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

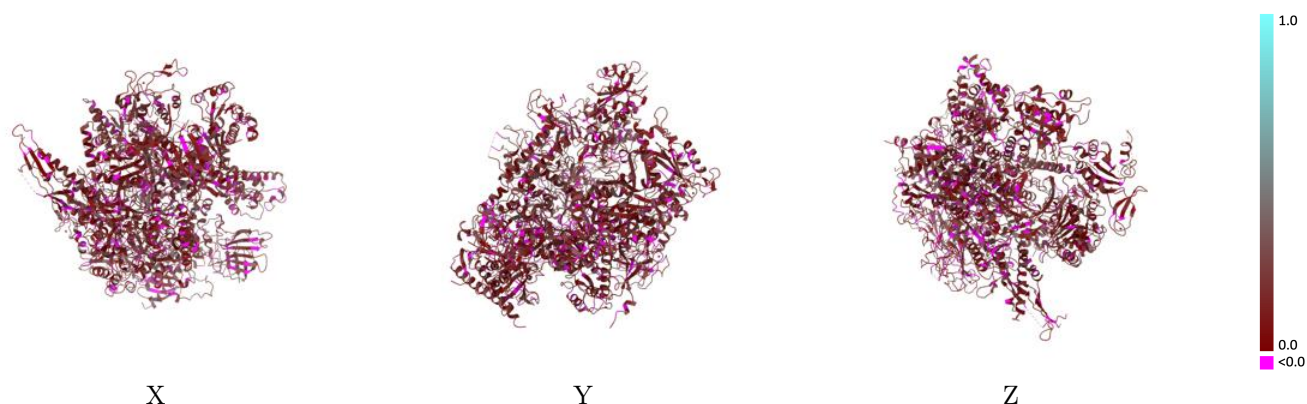
This section contains information regarding the fit between EMDB map EMD-2784 and PDB model 4V1M. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



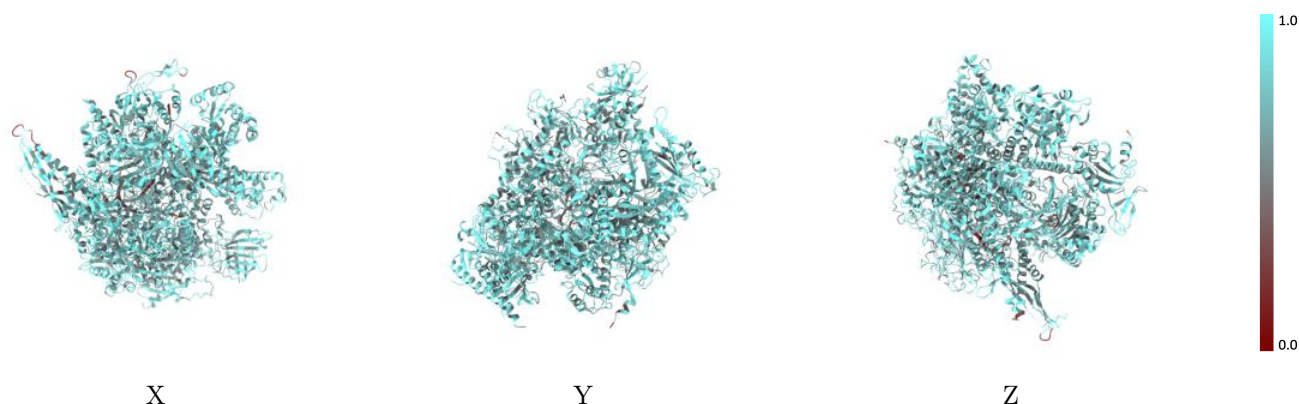
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



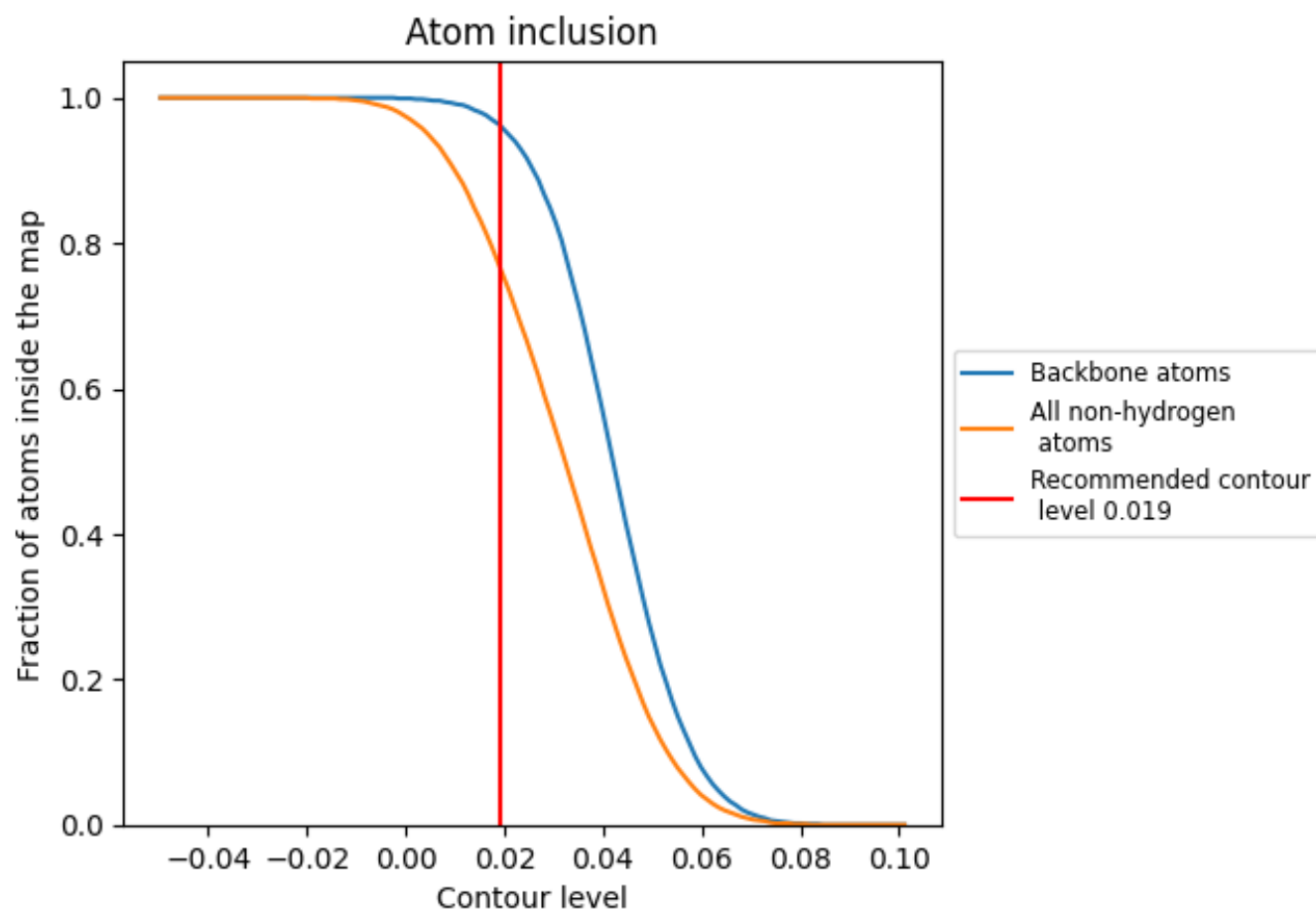
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.019).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 77% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7690	0.1510
A	0.7660	0.1530
B	0.7610	0.1480
C	0.8280	0.1650
E	0.7990	0.1630
F	0.7680	0.1520
H	0.8170	0.1620
I	0.7950	0.1420
J	0.7560	0.1280
K	0.7880	0.1550
L	0.7610	0.1120
N	0.7780	0.1840
P	0.2540	-0.0070
T	0.5870	0.1150

1.0

0.0

<0.0