



Full wwPDB EM Validation Report ⓘ

Jul 9, 2025 – 01:49 pm BST

PDB ID : 9HWG / pdb_00009hwg
EMDB ID : EMD-52449
Title : Structure of the transcribing Pol II-TCR-RECQL5 complex
Authors : Zhang, L.; Zhang, S.
Deposited on : 2025-01-03
Resolution : 3.50 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

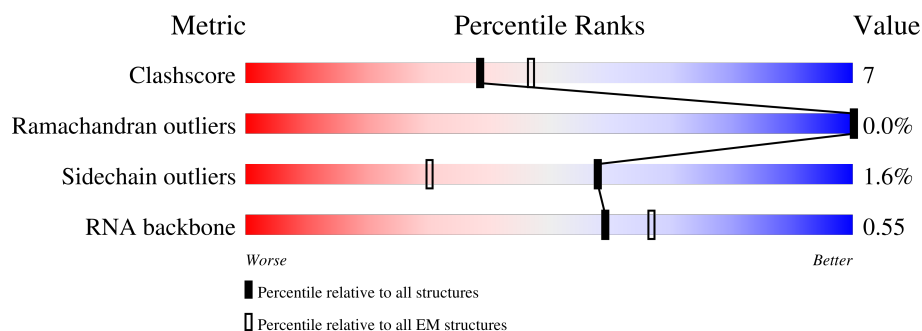
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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





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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1970	
2	B	1174	
3	C	275	
4	D	142	
5	E	210	
6	F	127	
7	G	172	

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Mol	Chain	Length	Quality of chain
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	N	47	
14	O	991	
15	P	45	
16	T	47	
17	a	396	
18	b	1493	
19	c	709	
20	d	1140	
21	e	83	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 51212 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 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1422	Total	C	N	O	S	0	0
			11263	7082	2018	2093	70		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1131	Total	C	N	O	S	0	0
			9052	5727	1592	1669	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	N	O	S	0	0
			2089	1309	359	415	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	126	Total	C	N	O	S	0	0
			1030	642	175	209	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	N	O	S	0	0
			1720	1089	300	323	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	S	0	0
			657	418	113	121	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	117	Total	C	N	O	S	0	0
			949	587	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	N	O	S	0	0
			533	345	90	92	6		

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

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

- Molecule 12 is a protein called RNA polymerase II, I and III subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 13 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	35	Total	C	N	O	P	0	0
			727	344	142	206	35		

- Molecule 14 is a protein called ATP-dependent DNA helicase Q5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	120	Total	C	N	O	S	0	0
			974	602	187	182	3		

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	10	Total	C	N	O	P	0	0
			220	98	45	67	10		

- Molecule 16 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	43	Total	C	N	O	P	0	0
			864	414	144	263	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	363	Total	C	N	O	S	0	0
			2835	1766	505	545	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	b	519	Total	C	N	O	S	0	0
			4248	2740	742	745	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	c	148	Total	C	N	O	S	0	0
			1215	771	217	223	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	d	1094	Total	C	N	O	S	0	0
			8474	5388	1419	1621	46		

- Molecule 21 is a protein called Transcription elongation factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	e	64	Total	C	N	O	S	0	0
			505	312	81	105	7		

- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

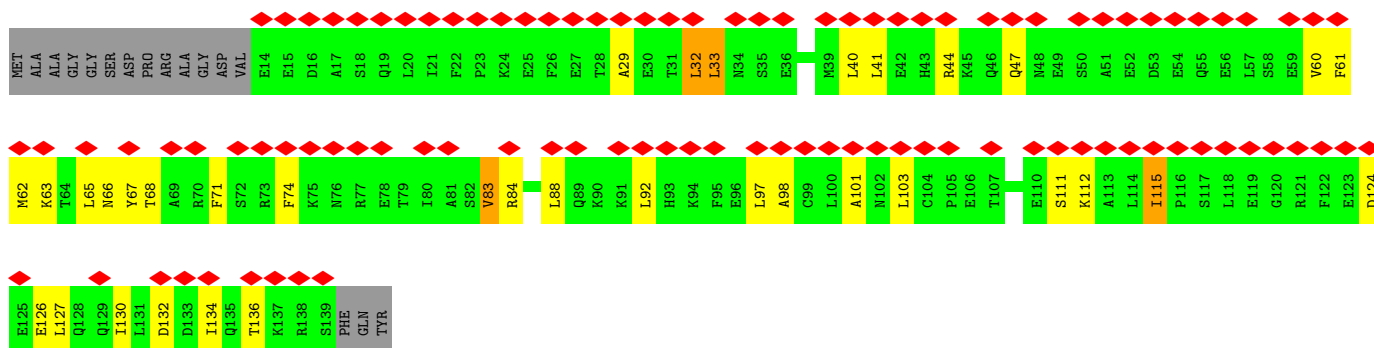
- Molecule 2: DNA-directed RNA polymerase subunit beta

[illegible]

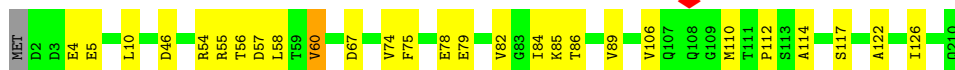
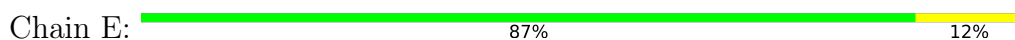
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Figure 1: Schematic representation of the protein structure of the 1000-residue protein. The protein is shown as a horizontal bar with various residues labeled. Residues are color-coded: green for residues 1-100, yellow for residues 101-200, and grey for residues 201-300. Red diamonds indicate specific residues: N134, E144, Q145, and E213. The residues are labeled as follows: MET, P2, V9, R10, I11, S53, I44, D48, D61, S75, D76, E91, E92, Q111, N134, ARG, ASP, ASN, ASP, PRO, SER, ASP, TYR, VAL, E144, Q145, L149, K152, E158, L159, R160, K166, K175, A180, A183, N190, R193, H194, T195, E213.

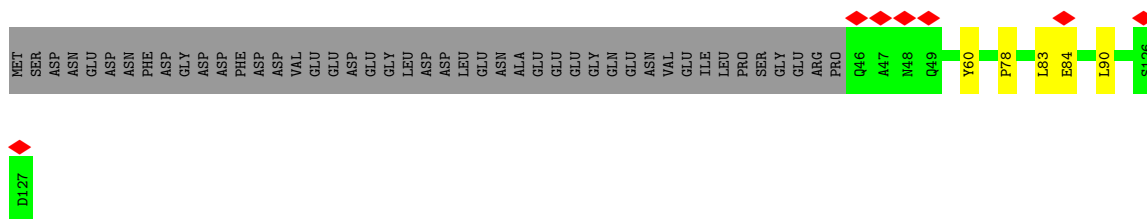
- Molecule 4: RNA polymerase II subunit D



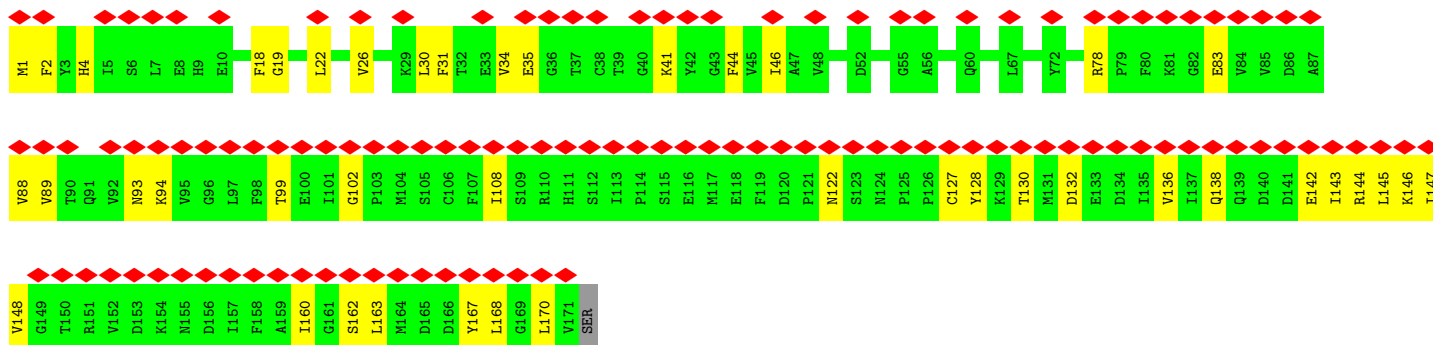
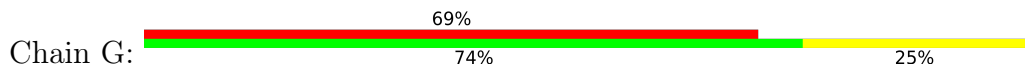
• Molecule 5: DNA-directed RNA polymerase II subunit E



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



• Molecule 7: DNA-directed RNA polymerase subunit

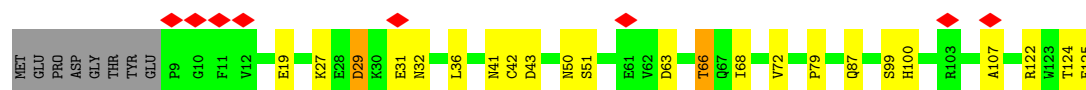
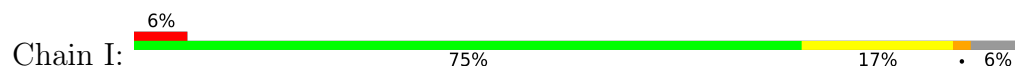


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

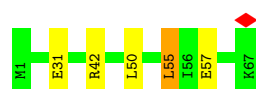




- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



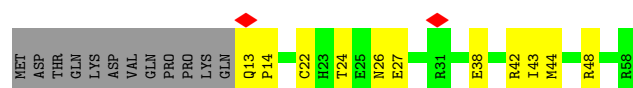
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



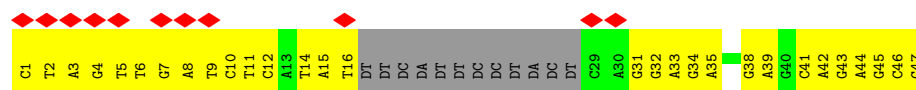
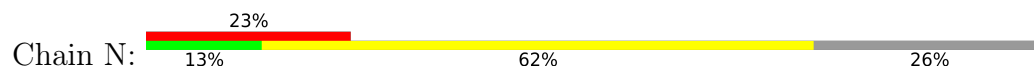
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a



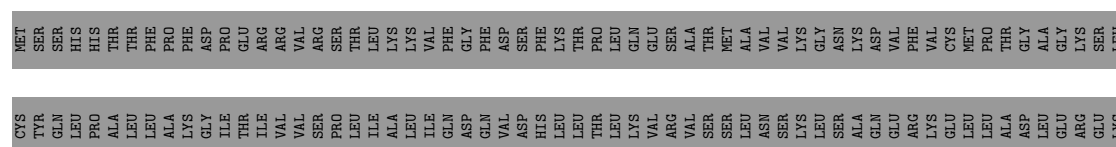
- Molecule 12: RNA polymerase II, I and III subunit K



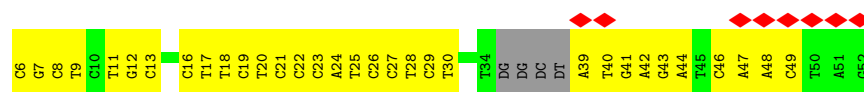
- Molecule 13: Non-template DNA



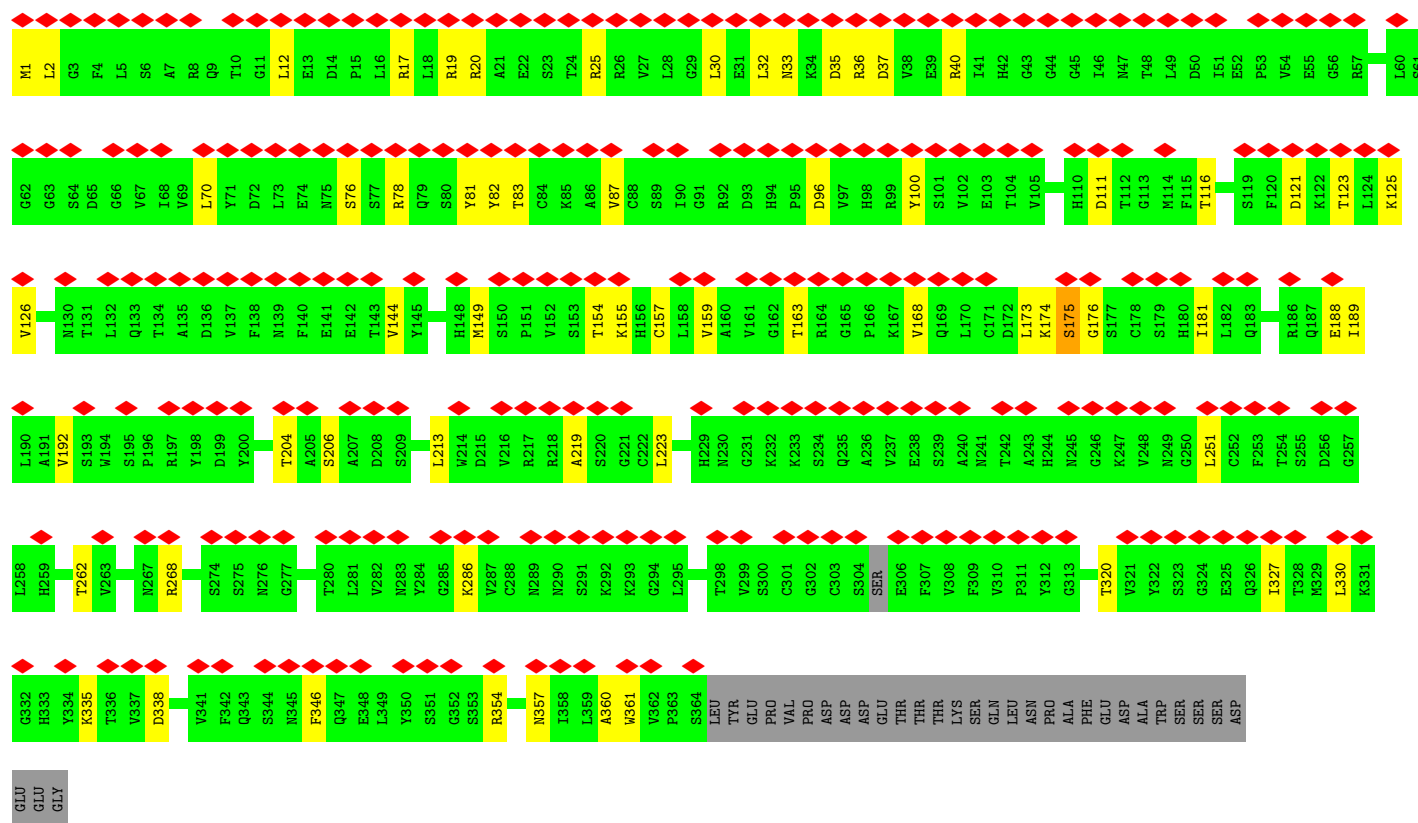
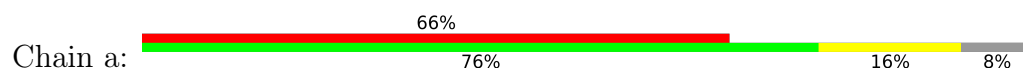
- Molecule 14: ATP-dependent DNA helicase Q5





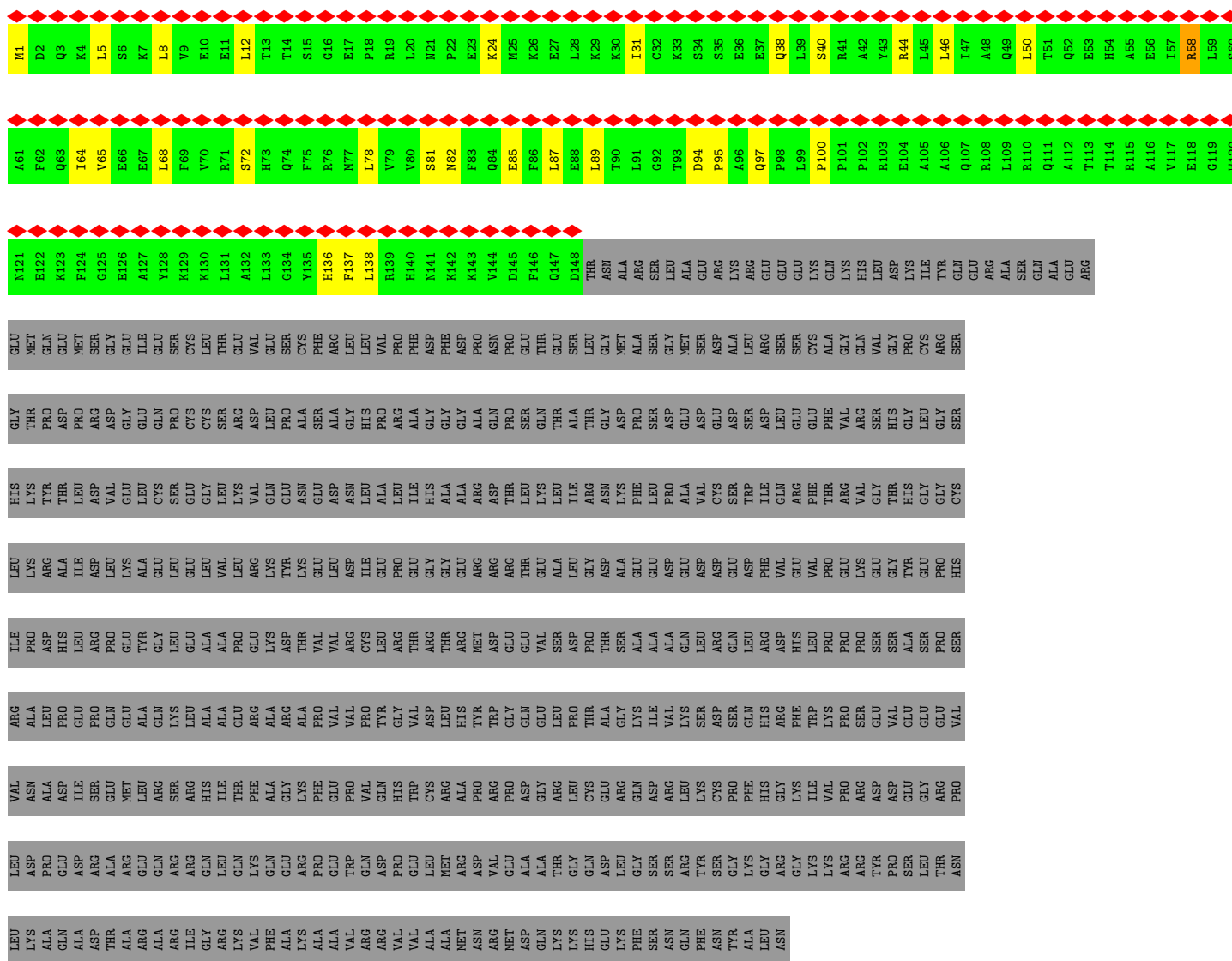


• Molecule 17: DNA excision repair protein ERCC-8

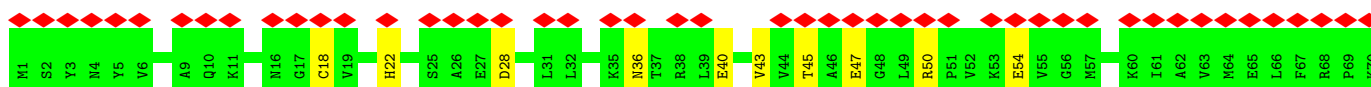
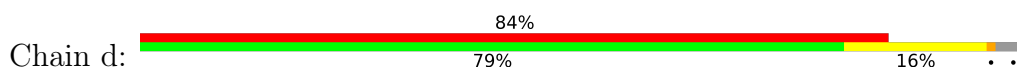




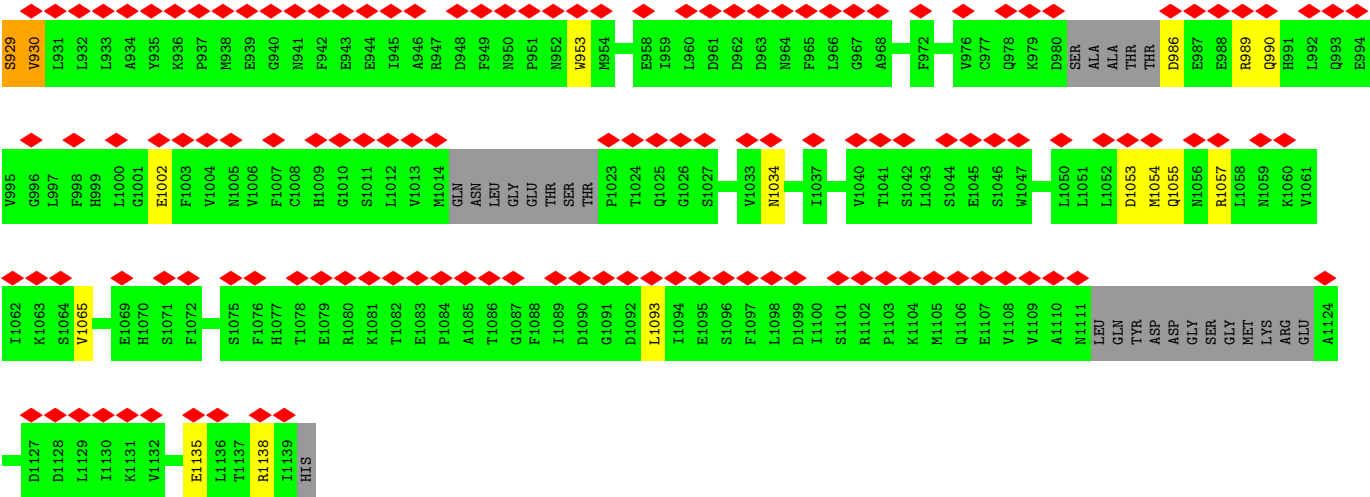
- Molecule 19: UV-stimulated scaffold protein A



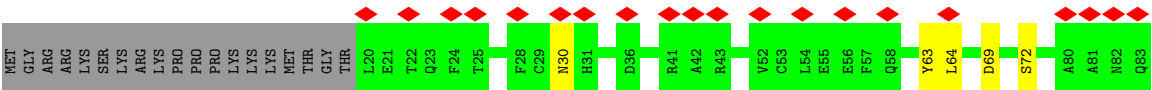
- Molecule 20: DNA damage-binding protein 1



G71	E72	S73	L76	L77	F78	F79	L80	T81	A82	K83	Y84	N85	A86	C87	I88	L89	E90	Y91	K92	Q93	S94	G95	E96	S97	I98	D99	I100	I101	I102	G106	N107	N108	Q109	D110	R111	I112	G113	R114	P115	S116	E117	T118	G119	I120	I121	G122	I123	I124	D125	P126	E127	C128	R129	M130	I131	G132	L133		
R134	L135	Y136	D137	G138	L139	F140	K141	V142	I143	P144	L145	D146	R147	A148	N149	K150	E151	L152	K153	A154	F155	N156	I157	R158	L159	E160	E161	L162	H163	V164	I165	D166	V167	K168	F169	L170	Y171	G172	C173	Q174	A175	P176	T177	I178	C179	F180	V181	Y182	Q183	D184	P185	Q186	G187	R188	H189	V190	I191	T192	Y193
E194	V195	S196	L197	R198	E199	K200	E201	F202	N203	K204	G205	P206	W207	K208	Q209	E210	L211	N212	E213	A214	E215	A216	S217	M218	V219	I220	A221	V222	P223	E224	P225	F226	G227	G228	A229	I230	I231	I232	G233	Q234	E235	S236	I237	T238	Y239	H240	N241	G242	D243	K244	Y245	L246	A247	I248	A249	P250	E251	I252	I253
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GLY	G748	T749	T750	A751	R752	R753	P754	S755	A756	S757	T758	Q759	A760	L761	S762	S763	S764	V765	S766	S767	S768	K769	L770	F771	S772	SER	THR	ALA	PRO	HIS	GLU	THR	SER	PHE	GLY	E784	E785	V786	E787	H788	H789	N790	L791	T794	D795	T796	S854	D855	G856	K857	L858	Q859	H803	A804	H805	Q806	F807	L808	
Q809	M810	E811	Y812	A813	L814	S815	L816	L817	S818	C819	K820	L821	G822	K823	D824	P825	N826	T827	Y828	F829	L830	Y891	E892	W893	A834	T895	E896	K897	P838	L899	R900	A841	E842	P843	K844	Q845	G846	N907	I848	V849	N850	F851	Y852	S853	L914	K915	T916	K917	G918	D919	T860	V861	A862	E863	K864	E865	L866	K867	G868
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A869	V870	Y871	S872	M873	A874	E875	F876	M877	G878	K879	L880	L881	A882	S883	I884	N885	S886	T887	V888	R889	L890	Y891	E892	W893	A834	T895	E896	K897	P838	L899	R900	A841	E842	P843	K844	Q845	G846	N907	I848	V849	N850	F851	Y852	S853	L914	K915	T916	K917	G918	D919	T860	V861	A862	E863	K864	E865	L866	K867	G868
A869	V870	Y871	S872	M873	A874	E875	F876	M877	G878	K879	L880	L881	A882	S883	I884	N885	S886	T887	V888	R889	L890	Y891	E892	W893	A834	T895	E896	K897	P838	L899	R900	A841	E842	P843	K844	Q845	G846	N907	I848	V849	N850	F851	Y852	S853	L914	K915	T916	K917	G918	D919	T860	V861	A862	E863	K864	E865	L866	K867	G868
A869	V870	Y871	S872	M873	A874	E875	F876	M877	G878	K879	L880	L881	A882	S883	I884	N885	S886	T887	V888	R889	L890	Y891	E892	W893	A834	T895	E896	K897	P838	L899	R900	A841	E842	P843	K844	Q845	G846	N907	I848	V849	N850	F851	Y852	S853	L914	K915	T916	K917	G918	D919	T860	V861	A862	E863	K864	E865	L866	K867	G868
A869	V870	Y871	S872	M873	A874	E875	F876	M877	G878	K879	L880	L881	A882	S883	I884	N885	S886	T887	V888	R889	L890	Y891	E892	W893	A834	T895	E896	K897	P838	L899	R900	A841	E842	P843	K844	Q845	G846	N907	I848	V849	N850	F851	Y852	S853	L914	K915	T916	K917	G918	D919	T860	V861	A862	E863	K864	E865	L866	K867	G868
A869	V870	Y871	S872	M873	A874	E875	F876	M877	G878	K879	L880	L881	A882	S883	I884	N885	S886	T887	V888	R889	L890	Y891	E892	W893	A834	T895	E896	K897	P838	L899	R900	A841	E842	P843	K844	Q845	G846	N907	I848	V849	N850	F851	Y852	S853	L914	K915	T916	K917	G918	D919	T860	V861	A862	E863	K864	E865	L866	K867	G868
A869	V870	Y871	S872	M873	A874	E875	F876	M877	G878	K879	L880	L881	A882	S883	I884	N885	S886	T887	V888	R889	L890	Y891	E892	W893	A834	T895	E896	K897	P838	L899	R900	A841	E842	P843	K844	Q845	G846	N907	I848	V849	N850	F851	Y852	S853	L914	K915	T916	K917	G918	D919	T860	V861	A862	E863	K864	E865	L866	K867	G868
A869	V870	Y871	S872	M873	A874	E875	F876	M877	G878	K879	L880	L881	A882	S883	I884	N885	S886	T887	V888	R889	L890	Y891	E892	W893	A834	T895	E896	K897	P838	L899	R900	A841	E842	P843	K844	Q845	G846	N907	I848	V849	N850	F851	Y852	S853	L914	K915	T916	K917	G918	D919	T860	V861	A862	E863	K864	E865	L866	K867	G868
A869	V870	Y871	S872	M873	A874	E875	F876	M877	G878	K879	L880	L881	A882	S883	I884	N885	S886	T887	V888	R889	L890	Y891	E892	W893	A834	T895	E896	K897	P838	L899	R900	A841	E842	P843	K844	Q845	G846	N907	I848	V849	N850	F851	Y852	S853	L914	K915	T916	K917	G918	D919	T860	V861	A862	E863	K864	E865	L866	K867	G868
A869	V870	Y871	S872	M873	A874	E875	F876	M877	G878	K879	L880	L881	A882	S883	I884	N885	S886	T887	V888	R889	L890	Y891	E892	W893	A834	T895	E896	K897	P838	L899	R900	A841	E842	P843	K844	Q845	G846	N907	I848	V849	N850	F851	Y852	S853	L914	K915	T916	K917	G918	D919	T860	V861	A862	E863	K864	E865	L866	K867	G868
A869	V870	Y871	S872	M873	A874	E875	F876	M877	G878	K879	L880	L881	A882	S883	I884	N885	S886	T887	V888	R889	L890	Y891	E892	W893	A834	T895	E896	K897	P838	L899	R900	A841	E842	P843	K844	Q845	G846	N907	I848	V849	N850	F851	Y852	S853	L914	K915	T916	K917	G918	D919	T860	V861	A862	E863	K864	E865	L866	K867	G868
A869	V870	Y871	S872	M873	A874	E875	F876	M877	G878	K879	L880	L881	A882	S883	I884	N885	S886	T887	V888	R889	L890	Y891	E892	W893	A834	T895	E896	K897	P838	L899	R900	A841	E842	P843	K844	Q845	G846	N907	I848	V849	N850	F851	Y852	S853	L914	K915	T916	K917	G918	D919	T860	V861	A862	E863	K864	E865	L866	K867	G868
A869	V870	Y871	S872	M873	A874	E875	F876	M877	G878	K879	L880	L881	A882	S883	I884	N885	S886	T887	V888	R889	L890	Y89																																					



● Molecule 21: Transcription elongation factor 1 homolog



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19458	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	36.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.912	Depositor
Minimum map value	-0.416	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	391.48798, 391.48798, 391.48798	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8156, 0.8156, 0.8156	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.13	0/11468	0.30	0/15484
2	B	0.17	0/9233	0.38	1/12463 (0.0%)
3	C	0.13	0/2132	0.30	0/2896
4	D	0.39	0/1043	0.81	3/1400 (0.2%)
5	E	0.12	0/1751	0.30	0/2366
6	F	0.12	0/667	0.27	0/901
7	G	0.13	0/1382	0.30	0/1874
8	H	0.11	0/1207	0.26	0/1628
9	I	0.12	0/972	0.31	0/1316
10	J	0.14	0/542	0.30	0/730
11	K	0.14	0/939	0.29	0/1271
12	L	0.14	0/394	0.32	0/524
13	N	0.20	0/817	0.32	0/1258
14	O	0.48	1/989 (0.1%)	0.74	2/1326 (0.2%)
15	P	0.37	0/247	0.35	0/384
16	T	0.29	0/962	0.43	0/1476
17	a	0.25	0/2893	0.49	0/3917
18	b	0.23	0/4351	0.49	0/5876
19	c	0.60	1/1238 (0.1%)	0.64	2/1664 (0.1%)
20	d	0.88	2/8628 (0.0%)	0.83	10/11702 (0.1%)
21	e	0.33	0/515	0.63	0/700
All	All	0.41	4/52370 (0.0%)	0.50	18/71156 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
20	d	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	c	100	PRO	C-N	18.09	1.54	1.33
14	O	519	ASP	C-N	8.89	1.54	1.33
20	d	623	LEU	CG-CD2	-5.74	1.33	1.52
20	d	596	PHE	C-N	5.40	1.40	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	O	519	ASP	CA-C-N	8.75	130.78	119.84
14	O	519	ASP	C-N-CA	8.75	130.78	119.84
19	c	100	PRO	CA-C-N	8.63	129.27	120.38
19	c	100	PRO	C-N-CA	8.63	129.27	120.38
20	d	705	ASP	N-CA-C	6.07	117.69	111.14
20	d	596	PHE	CA-C-O	-6.05	108.97	120.96
4	D	32	LEU	CA-C-N	5.86	131.78	122.59
4	D	32	LEU	C-N-CA	5.86	131.78	122.59
4	D	32	LEU	O-C-N	-5.76	114.79	122.74
20	d	707	ILE	N-CA-C	5.72	121.23	109.34
20	d	930	VAL	N-CA-CB	5.64	120.55	111.23
20	d	394	ILE	CB-CG1-CD1	-5.56	102.12	113.80
20	d	597	GLU	N-CA-CB	-5.48	107.93	114.17
20	d	929	SER	N-CA-C	5.42	122.35	110.80
20	d	708	GLN	CB-CA-C	-5.33	101.59	110.81
20	d	563	ASP	N-CA-C	-5.13	104.28	110.44
2	B	340	LYS	N-CA-C	-5.08	105.82	111.36
20	d	1054	MET	N-CA-CB	5.07	117.57	110.12

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	538	VAL	Peptide
20	d	596	PHE	Mainchain
20	d	884	ILE	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	11263	0	11389	120	0
2	B	9052	0	9087	63	0
3	C	2089	0	2031	18	0
4	D	1030	0	1016	25	0
5	E	1720	0	1737	19	0
6	F	657	0	684	3	0
7	G	1351	0	1358	35	0
8	H	1186	0	1147	7	0
9	I	949	0	881	17	0
10	J	533	0	553	5	0
11	K	920	0	942	8	0
12	L	388	0	393	8	0
13	N	727	0	394	77	0
14	O	974	0	984	38	0
15	P	220	0	110	0	0
16	T	864	0	488	67	0
17	a	2835	0	2760	74	0
18	b	4248	0	4288	114	0
19	c	1215	0	1235	19	0
20	d	8474	0	8390	150	0
21	e	505	0	463	12	0
22	A	2	0	0	0	0
22	B	1	0	0	0	0
22	C	1	0	0	0	0
22	I	2	0	0	0	0
22	J	1	0	0	0	0
22	L	1	0	0	0	0
22	O	1	0	0	0	0
22	e	1	0	0	0	0
23	A	1	0	0	0	0
23	b	1	0	0	0	0
All	All	51212	0	50330	715	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 (715) 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)
17:a:157:CYS:SG	17:a:173:LEU:HD12	1.42	1.55
1:A:1279:MET:N	14:O:511:GLN:HE22	1.16	1.42
13:N:16:DT:O2	18:b:795:ILE:CD1	1.78	1.32
13:N:16:DT:P	18:b:975:ARG:HE	1.59	1.23
2:B:821:LYS:O	18:b:783:LYS:HE2	1.42	1.20
17:a:111:ASP:OD2	18:b:1386:SER:OG	1.56	1.20
1:A:1279:MET:N	14:O:511:GLN:NE2	1.91	1.18
17:a:78:ARG:NE	20:d:990:GLN:OE1	1.76	1.17
13:N:16:DT:O2	18:b:795:ILE:HD11	1.49	1.10
17:a:157:CYS:SG	17:a:173:LEU:CD1	2.38	1.10
13:N:16:DT:H4'	18:b:1002:TYR:HB3	1.21	1.09
19:c:12:LEU:HD22	19:c:64:ILE:HD11	1.34	1.04
17:a:25:ARG:NH2	20:d:842:GLU:OE2	1.89	1.03
16:T:11:DT:H2''	16:T:12:DG:H5'	1.42	1.02
13:N:16:DT:OP1	18:b:975:ARG:NH2	1.93	1.01
13:N:14:DT:H4'	18:b:936:TRP:HB2	1.43	1.00
13:N:16:DT:H4'	18:b:1002:TYR:CB	1.92	1.00
2:B:320:PHE:HE2	21:e:64:LEU:HB3	1.23	0.99
17:a:100:TYR:CZ	21:e:30:ASN:HB2	2.00	0.97
1:A:1284:PHE:CE2	14:O:512:MET:CE	2.49	0.95
13:N:15:DA:N1	18:b:796:PHE:CZ	2.34	0.94
2:B:821:LYS:O	18:b:783:LYS:CE	2.16	0.94
1:A:1284:PHE:CE2	14:O:512:MET:HE3	2.03	0.94
16:T:42:DA:OP1	18:b:865:ARG:HB3	1.67	0.93
16:T:12:DG:H1'	16:T:13:DC:H5''	1.47	0.93
17:a:100:TYR:CE1	21:e:30:ASN:HB2	2.04	0.92
13:N:16:DT:O2	18:b:795:ILE:HD12	1.64	0.92
13:N:16:DT:P	18:b:975:ARG:NE	2.43	0.91
13:N:1:DC:H2''	13:N:2:DT:H5'	1.51	0.90
1:A:1287:CYS:HB3	14:O:504:TRP:CZ3	2.09	0.88
13:N:16:DT:OP1	18:b:975:ARG:NE	2.07	0.87
20:d:408:LYS:HA	20:d:678:TYR:CZ	2.10	0.86
1:A:346:LYS:NZ	16:T:25:DT:OP2	2.08	0.86
20:d:394:ILE:HD11	20:d:669:SER:OG	1.75	0.86
1:A:1284:PHE:HE2	14:O:512:MET:CE	1.89	0.86
17:a:154:THR:HG22	18:b:1383:PRO:HB3	1.58	0.85
1:A:358:ARG:NH1	16:T:27:DC:OP1	2.09	0.84
5:E:4:GLU:N	5:E:4:GLU:OE1	2.10	0.84
1:A:1284:PHE:CZ	14:O:512:MET:HE3	2.13	0.83
16:T:42:DA:OP1	18:b:865:ARG:CB	2.25	0.83
2:B:320:PHE:CE2	21:e:64:LEU:HB3	2.13	0.82
3:C:152:LYS:NZ	10:J:57:GLU:OE1	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:ASP:OD1	2:B:646:ARG:NH1	2.13	0.81
16:T:42:DA:OP1	18:b:865:ARG:N	2.14	0.81
2:B:311:ILE:CD1	21:e:64:LEU:HD12	2.11	0.81
16:T:42:DA:P	18:b:865:ARG:HB3	2.19	0.81
14:O:506:LEU:O	14:O:506:LEU:HD12	1.81	0.80
17:a:12:LEU:HD11	20:d:382:PHE:HZ	1.43	0.80
1:A:911:PRO:O	1:A:963:ARG:NH2	2.15	0.80
4:D:32:LEU:HD21	7:G:4:HIS:HB2	1.63	0.79
13:N:16:DT:OP1	18:b:975:ARG:CZ	2.30	0.79
1:A:1281:ASP:OD1	14:O:515:ARG:NE	2.16	0.79
9:I:87:GLN:OE1	9:I:87:GLN:N	2.16	0.79
1:A:1287:CYS:HB3	14:O:504:TRP:CH2	2.19	0.78
5:E:84:ILE:HD11	13:N:45:DG:H5''	1.64	0.78
20:d:275:ASP:OD2	20:d:279:ARG:NH1	2.16	0.78
1:A:1284:PHE:HE2	14:O:512:MET:HE1	1.49	0.78
17:a:168:VAL:HG22	17:a:189:ILE:HD13	1.64	0.78
13:N:16:DT:C4'	18:b:1002:TYR:HB3	2.10	0.77
9:I:68:ILE:O	9:I:122:ARG:NH1	2.18	0.77
20:d:186:GLN:N	20:d:186:GLN:OE1	2.18	0.77
17:a:154:THR:CG2	18:b:1383:PRO:HB3	2.14	0.77
13:N:16:DT:OP2	18:b:975:ARG:NE	2.16	0.76
17:a:154:THR:CB	18:b:1383:PRO:HB3	2.15	0.76
20:d:408:LYS:HA	20:d:678:TYR:CE1	2.20	0.76
18:b:945:ARG:NH1	18:b:946:GLU:OE2	2.19	0.76
16:T:16:DC:H2'	16:T:17:DT:H71	1.67	0.75
20:d:408:LYS:O	20:d:678:TYR:CE2	2.39	0.75
18:b:713:MET:SD	18:b:723:GLN:NE2	2.60	0.75
17:a:219:ALA:HB2	18:b:693:PHE:CD1	2.22	0.75
3:C:158:GLU:OE2	3:C:160:ARG:NH1	2.19	0.74
3:C:61:ASP:OD2	12:L:48:ARG:NH2	2.19	0.74
17:a:155:LYS:O	17:a:174:LYS:NZ	2.20	0.74
20:d:394:ILE:HG12	20:d:670:ASN:O	1.87	0.74
2:B:830:GLU:OE1	2:B:870:THR:OG1	2.04	0.74
5:E:56:THR:HG23	5:E:78:GLU:OE2	1.87	0.73
17:a:78:ARG:HE	20:d:990:GLN:CD	1.93	0.73
20:d:706:GLU:HB3	20:d:708:GLN:NE2	2.03	0.73
1:A:154:CYS:SG	1:A:188:GLN:NE2	2.61	0.73
2:B:887:TYR:O	2:B:888:THR:HG22	1.87	0.73
14:O:541:ARG:NH2	14:O:591:ALA:O	2.21	0.73
3:C:266:GLU:OE2	11:K:17:LYS:NZ	2.22	0.73
20:d:36:ASN:ND2	20:d:1002:GLU:OE2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:d:706:GLU:OE2	20:d:708:GLN:NE2	2.20	0.72
19:c:5:LEU:HD21	19:c:31:ILE:HG21	1.70	0.72
16:T:43:DG:OP2	18:b:865:ARG:NH2	2.17	0.72
2:B:686:GLU:N	2:B:686:GLU:OE1	2.22	0.72
7:G:30:LEU:O	7:G:34:VAL:HG22	1.88	0.72
14:O:565:ARG:O	14:O:569:ARG:N	2.23	0.72
1:A:1193:VAL:O	1:A:1197:TYR:N	2.22	0.72
2:B:327:LYS:HG3	2:B:327:LYS:O	1.90	0.71
20:d:102:THR:OG1	20:d:1065:VAL:O	2.08	0.71
13:N:4:DG:H2''	13:N:5:DT:H71	1.71	0.71
17:a:33:ASN:HD22	17:a:360:ALA:HB3	1.56	0.71
13:N:8:DA:H2''	13:N:9:DT:H5'	1.72	0.71
20:d:456:GLN:O	20:d:472:THR:OG1	2.03	0.71
20:d:18:CYS:SG	20:d:315:THR:OG1	2.42	0.70
17:a:121:ASP:OD1	17:a:123:THR:OG1	2.06	0.70
1:A:1166:LEU:O	1:A:1170:THR:HG23	1.91	0.70
17:a:149:MET:HG2	17:a:159:VAL:HG22	1.74	0.69
16:T:12:DG:H4'	16:T:13:DC:OP1	1.91	0.69
16:T:42:DA:H2''	18:b:865:ARG:NH2	2.07	0.69
1:A:1249:ASP:OD2	14:O:602:LEU:CD2	2.41	0.69
16:T:11:DT:C2'	16:T:12:DG:H5'	2.21	0.68
2:B:649:ASN:O	2:B:650:ASN:ND2	2.27	0.68
20:d:394:ILE:CD1	20:d:707:ILE:HA	2.23	0.68
20:d:415:SER:O	20:d:481:GLN:NE2	2.26	0.68
17:a:2:LEU:HD11	20:d:843:PRO:HG2	1.74	0.68
1:A:1291:ASN:ND2	14:O:504:TRP:CD1	2.62	0.68
1:A:388:MET:HE1	1:A:503:LEU:HD22	1.76	0.68
2:B:307:GLU:O	21:e:63:TYR:OH	2.07	0.68
17:a:100:TYR:OH	21:e:30:ASN:CG	2.38	0.67
20:d:47:GLU:OE1	20:d:47:GLU:N	2.28	0.67
1:A:91:ALA:HB3	1:A:290:LEU:HD23	1.77	0.67
8:H:136:GLU:O	8:H:139:SER:OG	2.10	0.67
20:d:477:ARG:HB3	20:d:486:LEU:HD11	1.77	0.67
1:A:1229:GLU:N	1:A:1229:GLU:OE1	2.27	0.67
17:a:100:TYR:CZ	21:e:30:ASN:CB	2.77	0.67
2:B:623:ARG:NH2	2:B:697:GLU:OE2	2.28	0.67
5:E:79:GLU:OE2	5:E:86:THR:HG21	1.95	0.67
1:A:1284:PHE:CE2	14:O:512:MET:HE1	2.26	0.66
13:N:14:DT:H4'	18:b:936:TRP:CB	2.21	0.66
17:a:30:LEU:HD23	17:a:330:LEU:HD11	1.78	0.66
16:T:43:DG:OP2	18:b:887:GLY:HA3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:a:78:ARG:CD	20:d:990:GLN:OE1	2.43	0.66
20:d:1002:GLU:OE1	20:d:1034:ASN:ND2	2.29	0.66
7:G:146:LYS:N	7:G:162:SER:O	2.29	0.65
4:D:60:VAL:HG11	7:G:44:PHE:CZ	2.30	0.65
16:T:47:DA:H4'	16:T:48:DA:OP1	1.95	0.65
13:N:4:DG:C2'	13:N:5:DT:H71	2.26	0.65
1:A:1287:CYS:HB3	14:O:504:TRP:HZ3	1.61	0.65
4:D:33:LEU:HD11	4:D:101:ALA:HB3	1.79	0.65
13:N:11:DT:H1'	13:N:12:DC:H5'	1.78	0.65
20:d:381:ALA:O	20:d:385:GLY:N	2.30	0.65
20:d:567:ARG:HE	20:d:579:LYS:CB	2.10	0.65
17:a:181:ILE:HD11	18:b:699:THR:HG23	1.77	0.65
1:A:1143:LEU:HD22	1:A:1157:ILE:HD12	1.79	0.65
18:b:575:THR:HA	18:b:578:MET:HE2	1.78	0.64
1:A:413:TYR:O	1:A:449:HIS:ND1	2.30	0.64
14:O:512:MET:C	14:O:516:LYS:HE2	2.23	0.64
20:d:546:LEU:HB3	20:d:600:HIS:CE1	2.33	0.64
7:G:130:THR:HG23	7:G:132:ASP:H	1.62	0.64
4:D:132:ASP:O	4:D:136:THR:HG23	1.98	0.64
4:D:66:ASN:OD1	4:D:67:TYR:N	2.31	0.64
2:B:311:ILE:HD11	21:e:64:LEU:HD12	1.80	0.63
17:a:96:ASP:O	17:a:125:LYS:NZ	2.29	0.63
7:G:1:MET:SD	7:G:2:PHE:N	2.70	0.63
16:T:42:DA:P	18:b:865:ARG:CB	2.86	0.63
19:c:50:LEU:HB3	19:c:89:LEU:HD13	1.79	0.63
16:T:42:DA:C2'	18:b:865:ARG:NH2	2.61	0.63
1:A:1279:MET:N	14:O:511:GLN:CD	2.57	0.63
2:B:835:GLU:O	2:B:886:ARG:N	2.32	0.62
13:N:16:DT:H4'	18:b:1002:TYR:CA	2.29	0.62
18:b:534:MET:O	18:b:747:LYS:NZ	2.22	0.62
8:H:8:ASP:OD2	8:H:32:SER:OG	2.11	0.62
13:N:43:DG:H2''	13:N:44:DA:C8	2.35	0.62
17:a:33:ASN:ND2	17:a:360:ALA:HB3	2.13	0.62
1:A:1279:MET:O	14:O:515:ARG:NH2	2.33	0.62
13:N:14:DT:C4	18:b:796:PHE:CE1	2.88	0.62
17:a:1:MET:HB2	20:d:841:ALA:O	2.00	0.62
16:T:19:DC:H2''	16:T:20:DT:H71	1.81	0.62
16:T:42:DA:OP1	18:b:865:ARG:CA	2.48	0.62
17:a:154:THR:O	18:b:1383:PRO:HA	1.99	0.62
2:B:311:ILE:HD13	21:e:64:LEU:HD12	1.80	0.61
3:C:44:ILE:HD12	3:C:238:SER:OG	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:a:37:ASP:HB2	17:a:83:THR:HG22	1.80	0.61
14:O:506:LEU:HD12	14:O:506:LEU:C	2.25	0.61
17:a:2:LEU:HD12	20:d:836:VAL:CG2	2.30	0.61
13:N:38:DG:H1'	13:N:39:DA:H5'	1.81	0.61
17:a:154:THR:HB	18:b:1383:PRO:HB3	1.82	0.61
18:b:633:ASP:OD1	18:b:634:ASP:N	2.33	0.61
20:d:658:VAL:HG11	20:d:707:ILE:HG21	1.83	0.61
13:N:1:DC:C2'	13:N:2:DT:H5'	2.28	0.61
13:N:16:DT:H5''	18:b:1002:TYR:HA	1.81	0.61
2:B:994:GLY:HA2	10:J:50:LEU:HD11	1.81	0.60
17:a:192:VAL:HG12	17:a:204:THR:HG22	1.83	0.60
1:A:144:VAL:O	1:A:148:CYS:SG	2.59	0.60
9:I:50:ASN:O	9:I:51:SER:OG	2.15	0.60
7:G:163:LEU:O	7:G:163:LEU:HD12	2.01	0.60
2:B:15:ASP:OD1	2:B:15:ASP:N	2.34	0.60
16:T:12:DG:C1'	16:T:13:DC:H5''	2.27	0.60
20:d:706:GLU:HB3	20:d:708:GLN:HE22	1.65	0.60
17:a:19:ARG:HG3	20:d:953:TRP:CZ2	2.37	0.59
20:d:130:MET:HE3	20:d:176:PRO:HG2	1.83	0.59
4:D:103:LEU:O	7:G:144:ARG:NH2	2.35	0.59
2:B:1037:ILE:O	3:C:195:THR:HG22	2.02	0.59
20:d:396:ILE:HG21	20:d:673:LEU:HD23	1.84	0.59
20:d:407:ILE:HD13	20:d:694:ALA:HB1	1.83	0.59
17:a:144:VAL:HA	17:a:163:THR:HG22	1.85	0.59
13:N:16:DT:OP2	18:b:975:ARG:CD	2.51	0.59
16:T:39:DA:H2'	16:T:40:DT:C6	2.38	0.59
13:N:5:DT:H1'	13:N:6:DT:H5'	1.85	0.59
1:A:205:VAL:HG13	1:A:207:GLU:O	2.03	0.59
20:d:1135:GLU:HA	20:d:1138:ARG:HH11	1.67	0.59
20:d:708:GLN:O	20:d:709:LYS:HB2	2.01	0.58
18:b:517:TRP:CZ2	18:b:521:LEU:HD11	2.37	0.58
7:G:41:LYS:O	7:G:78:ARG:NH1	2.37	0.58
13:N:16:DT:OP2	18:b:975:ARG:HD2	2.04	0.58
19:c:82:ASN:ND2	19:c:85:GLU:OE2	2.36	0.58
2:B:489:ILE:HD13	2:B:498:PRO:HB2	1.86	0.58
1:A:187:TYR:N	1:A:206:ASN:OD1	2.36	0.58
1:A:289:GLN:NE2	1:A:306:ASP:OD2	2.33	0.58
13:N:5:DT:C2'	13:N:6:DT:H71	2.32	0.58
1:A:1236:ASN:ND2	14:O:593:VAL:HG11	2.18	0.58
1:A:374:SER:OG	1:A:376:ASP:OD1	2.16	0.57
14:O:524:GLU:OE1	14:O:525:PHE:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:c:94:ASP:OD1	19:c:95:PRO:HD2	2.04	0.57
9:I:50:ASN:OD1	9:I:51:SER:N	2.37	0.57
16:T:47:DA:H2''	16:T:48:DA:H5''	1.86	0.57
20:d:40:GLU:HG2	20:d:54:GLU:HG3	1.86	0.57
13:N:14:DT:H2''	18:b:936:TRP:CD1	2.39	0.57
14:O:584:GLU:OE1	14:O:597:TYR:OH	2.18	0.57
16:T:16:DC:C2'	16:T:17:DT:H71	2.35	0.57
9:I:63:ASP:O	9:I:66:THR:OG1	2.22	0.57
17:a:35:ASP:O	17:a:81:TYR:HA	2.04	0.57
13:N:15:DA:O5'	18:b:936:TRP:CE3	2.57	0.57
17:a:76:SER:O	20:d:990:GLN:NE2	2.37	0.57
4:D:33:LEU:HD11	4:D:98:ALA:HA	1.87	0.57
1:A:92:LYS:HG3	1:A:290:LEU:HD21	1.86	0.57
16:T:8:DC:H2''	16:T:9:DT:O5'	2.05	0.57
20:d:213:GLU:OE1	20:d:234:GLN:N	2.38	0.57
20:d:1053:ASP:OD2	20:d:1057:ARG:NH2	2.36	0.57
1:A:582:PRO:HD2	8:H:47:ILE:HD12	1.87	0.56
2:B:18:THR:O	2:B:22:TRP:N	2.38	0.56
13:N:14:DT:O3'	18:b:936:TRP:HB3	2.04	0.56
1:A:668:PHE:CE1	1:A:672:ILE:HD11	2.39	0.56
1:A:1218:ARG:NH2	1:A:1250:ASP:O	2.38	0.56
13:N:5:DT:H2''	13:N:6:DT:H71	1.87	0.56
13:N:14:DT:O3'	18:b:936:TRP:CB	2.53	0.56
13:N:15:DA:C2	18:b:796:PHE:CZ	2.93	0.56
20:d:432:GLN:OE1	20:d:432:GLN:N	2.37	0.56
1:A:1284:PHE:HZ	14:O:508:TYR:CD2	2.22	0.56
16:T:29:DC:H2'	16:T:30:DT:C6	2.40	0.56
5:E:112:PRO:HG3	16:T:13:DC:OP1	2.06	0.56
13:N:42:DA:H2''	13:N:43:DG:C5'	2.36	0.56
13:N:14:DT:O3'	18:b:936:TRP:CG	2.58	0.56
17:a:116:THR:HG22	17:a:126:VAL:HG22	1.88	0.56
13:N:10:DC:C2'	13:N:11:DT:H71	2.36	0.56
17:a:1:MET:HE2	20:d:910:MET:HE1	1.87	0.56
20:d:99:ASP:OD1	20:d:100:ILE:N	2.38	0.56
7:G:108:ILE:HD11	7:G:145:LEU:HD22	1.88	0.56
12:L:26:ASN:OD1	12:L:44:MET:HE1	2.05	0.56
7:G:93:ASN:OD1	7:G:94:LYS:N	2.39	0.55
19:c:5:LEU:HD21	19:c:31:ILE:CG2	2.35	0.55
17:a:335:LYS:HE3	19:c:137:PHE:HE1	1.71	0.55
18:b:910:PHE:CE2	18:b:912:LEU:HD21	2.42	0.55
2:B:414:GLU:HG3	2:B:439:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:535:LYS:NZ	14:O:582:GLU:OE1	2.38	0.55
16:T:11:DT:H4'	16:T:11:DT:OP1	2.05	0.55
3:C:9:VAL:HG11	11:K:105:PHE:HD1	1.72	0.55
5:E:84:ILE:HG13	13:N:45:DG:OP1	2.06	0.55
17:a:2:LEU:HD12	20:d:836:VAL:HG22	1.89	0.55
18:b:768:LEU:HD11	18:b:967:THR:HG22	1.89	0.55
18:b:643:VAL:HG12	18:b:643:VAL:O	2.06	0.55
17:a:25:ARG:HH22	20:d:842:GLU:CD	2.13	0.55
17:a:100:TYR:HH	21:e:30:ASN:CG	2.15	0.55
10:J:55:LEU:HD13	10:J:55:LEU:O	2.07	0.55
13:N:31:DG:H5'	13:N:31:DG:H8	1.72	0.55
1:A:937:ASP:OD1	1:A:937:ASP:N	2.40	0.54
18:b:647:GLU:N	18:b:673:LEU:O	2.39	0.54
20:d:288:GLU:HB2	20:d:298:LYS:HB2	1.89	0.54
1:A:1263:ASN:O	14:O:515:ARG:O	2.26	0.54
13:N:38:DG:H1'	13:N:39:DA:C5'	2.38	0.54
12:L:22:CYS:SG	12:L:24:THR:OG1	2.62	0.54
20:d:704:ILE:HD12	20:d:707:ILE:CG2	2.38	0.54
4:D:40:LEU:HD12	4:D:41:LEU:N	2.23	0.54
7:G:83:GLU:O	7:G:147:ILE:HD12	2.08	0.54
17:a:20:ARG:HH12	20:d:114:ARG:HG3	1.73	0.54
1:A:760:LEU:HD11	1:A:781:ILE:HG21	1.90	0.54
18:b:973:TYR:CZ	18:b:977:ILE:HD11	2.43	0.54
20:d:516:LEU:O	20:d:531:HIS:ND1	2.41	0.53
20:d:538:VAL:O	20:d:561:TRP:NE1	2.41	0.53
1:A:1236:ASN:CG	14:O:593:VAL:HG21	2.33	0.53
2:B:347:MET:O	2:B:361:LYS:NZ	2.39	0.53
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.90	0.53
8:H:72:ASP:OD1	8:H:74:GLU:N	2.38	0.53
13:N:10:DC:H1'	13:N:11:DT:H5''	1.89	0.53
16:T:16:DC:H2''	16:T:17:DT:O5'	2.08	0.53
17:a:37:ASP:O	17:a:83:THR:HA	2.08	0.53
18:b:510:TYR:OH	18:b:536:LEU:O	2.12	0.53
13:N:10:DC:H5'	13:N:10:DC:C6	2.44	0.53
16:T:18:DT:H6	16:T:18:DT:H5'	1.74	0.53
19:c:40:SER:OG	19:c:44:ARG:NH1	2.41	0.53
18:b:717:SER:OG	18:b:995:PHE:O	2.22	0.53
20:d:243:ASP:OD1	20:d:244:LYS:N	2.41	0.53
4:D:29:ALA:HB1	7:G:4:HIS:O	2.08	0.53
13:N:3:DA:H2''	13:N:4:DG:C8	2.43	0.53
16:T:25:DT:H2'	16:T:26:DC:C6	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:b:776:TYR:CZ	18:b:802:LEU:HD22	2.43	0.53
4:D:88:LEU:HD23	4:D:88:LEU:O	2.08	0.53
20:d:542:ASP:OD2	20:d:592:LEU:HD12	2.09	0.53
3:C:76:ASP:HA	3:C:239:LEU:HD23	1.91	0.52
5:E:85:LYS:O	5:E:89:VAL:HG23	2.10	0.52
13:N:11:DT:H2''	13:N:12:DC:H5'	1.91	0.52
7:G:127:CYS:SG	7:G:128:TYR:N	2.81	0.52
20:d:503:CYS:SG	20:d:504:ASN:N	2.83	0.52
2:B:567:ILE:HD11	2:B:577:HIS:HB2	1.90	0.52
1:A:811:ILE:HD12	9:I:79:PRO:HB3	1.91	0.52
1:A:1313:GLN:OE1	1:A:1332:GLN:NE2	2.43	0.52
13:N:34:DG:H2''	13:N:35:DA:C8	2.45	0.52
2:B:687:VAL:HG23	2:B:687:VAL:O	2.09	0.52
13:N:10:DC:H5'	13:N:10:DC:H6	1.74	0.52
13:N:43:DG:H2''	13:N:44:DA:H8	1.72	0.52
17:a:37:ASP:CB	17:a:83:THR:HG22	2.39	0.52
18:b:529:ILE:HG13	18:b:692:ILE:HD13	1.92	0.52
10:J:31:GLU:CD	10:J:31:GLU:H	2.18	0.52
1:A:1417:HIS:O	1:A:1421:ARG:HG2	2.09	0.52
4:D:111:SER:O	4:D:115:ILE:HD12	2.09	0.52
13:N:8:DA:C2'	13:N:9:DT:H5'	2.38	0.52
17:a:181:ILE:CD1	18:b:699:THR:HG23	2.39	0.52
7:G:1:MET:N	7:G:78:ARG:O	2.42	0.52
8:H:80:ASP:OD1	8:H:80:ASP:N	2.41	0.52
14:O:522:ILE:HG23	14:O:522:ILE:O	2.09	0.51
16:T:17:DT:C2'	16:T:18:DT:H71	2.40	0.51
2:B:908:MET:SD	2:B:910:THR:HG23	2.50	0.51
13:N:11:DT:C2'	13:N:12:DC:H5'	2.41	0.51
13:N:10:DC:H2'	13:N:11:DT:H71	1.91	0.51
20:d:542:ASP:OD1	20:d:543:ILE:N	2.44	0.51
1:A:1422:GLN:O	1:A:1429:LYS:NZ	2.38	0.51
13:N:46:DC:H2''	13:N:47:DG:N7	2.24	0.51
1:A:140:ARG:O	1:A:144:VAL:HG23	2.11	0.51
2:B:19:PRO:HA	2:B:22:TRP:HB3	1.93	0.51
18:b:840:LYS:NZ	18:b:969:GLU:OE2	2.42	0.51
1:A:463:THR:OG1	2:B:1090:GLU:OE2	2.28	0.51
1:A:769:MET:HE3	2:B:973:PRO:CG	2.41	0.51
18:b:912:LEU:HD22	18:b:917:GLY:CA	2.41	0.51
20:d:394:ILE:CD1	20:d:669:SER:OG	2.55	0.51
7:G:127:CYS:SG	7:G:138:GLN:NE2	2.83	0.51
18:b:603:TYR:O	18:b:604:THR:OG1	2.20	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:a:40:ARG:NE	17:a:357:ASN:OD1	2.41	0.51
19:c:46:LEU:HD13	19:c:65:VAL:CG2	2.40	0.51
7:G:22:LEU:O	7:G:26:VAL:HG23	2.11	0.50
13:N:31:DG:H5'	13:N:31:DG:C8	2.46	0.50
13:N:46:DC:H2''	13:N:47:DG:C8	2.46	0.50
16:T:18:DT:H5'	16:T:18:DT:C6	2.47	0.50
17:a:35:ASP:O	17:a:81:TYR:CD1	2.64	0.50
18:b:922:ASN:OD1	18:b:950:ARG:NE	2.38	0.50
20:d:706:GLU:CD	20:d:708:GLN:HE22	2.18	0.50
1:A:1194:ASN:OD1	1:A:1195:VAL:N	2.44	0.50
16:T:41:DG:H5''	18:b:866:GLN:OE1	2.10	0.50
16:T:43:DG:P	18:b:887:GLY:HA3	2.51	0.50
1:A:854:THR:HG23	1:A:855:ALA:N	2.26	0.50
13:N:15:DA:H1'	13:N:16:DT:C2	2.47	0.50
18:b:868:LEU:HD22	18:b:913:THR:HG23	1.94	0.50
1:A:513:ALA:HB2	6:F:90:LEU:HD21	1.93	0.50
1:A:1139:LEU:HD11	1:A:1342:SER:H	1.77	0.50
1:A:1302:GLU:CD	1:A:1302:GLU:H	2.20	0.50
18:b:896:PRO:O	18:b:899:THR:OG1	2.22	0.50
1:A:18:ILE:HD12	2:B:1171:MET:HB3	1.94	0.50
1:A:440:LEU:O	1:A:440:LEU:HD12	2.11	0.50
14:O:515:ARG:HG3	14:O:515:ARG:HH11	1.77	0.50
17:a:219:ALA:HB2	18:b:693:PHE:CE1	2.45	0.50
19:c:1:MET:O	19:c:5:LEU:HD23	2.12	0.50
18:b:924:THR:O	18:b:953:GLN:NE2	2.45	0.50
1:A:152:ASN:O	1:A:152:ASN:ND2	2.42	0.50
2:B:629:GLU:O	2:B:630:LYS:C	2.54	0.50
20:d:454:ASP:OD1	20:d:454:ASP:N	2.40	0.50
9:I:27:LYS:O	9:I:36:LEU:N	2.38	0.49
14:O:597:TYR:O	14:O:601:VAL:HG23	2.12	0.49
16:T:47:DA:H2''	16:T:48:DA:C5'	2.42	0.49
1:A:97:VAL:HG21	1:A:322:LEU:HD11	1.94	0.49
3:C:48:ASP:OD1	3:C:175:LYS:NZ	2.36	0.49
20:d:929:SER:O	20:d:930:VAL:HG13	2.12	0.49
13:N:32:DG:H2''	13:N:33:DA:OP2	2.13	0.49
17:a:335:LYS:HE3	19:c:137:PHE:CE1	2.47	0.49
20:d:603:LEU:N	20:d:603:LEU:CD2	2.76	0.49
9:I:99:SER:O	9:I:100:HIS:ND1	2.45	0.49
18:b:766:CYS:N	18:b:963:LEU:O	2.43	0.49
1:A:42:LYS:O	1:A:288:ASN:ND2	2.38	0.49
7:G:144:ARG:O	7:G:168:LEU:HD12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:541:ARG:NH2	14:O:588:PHE:O	2.46	0.49
18:b:754:LEU:HD21	18:b:951:ILE:HG12	1.94	0.49
18:b:921:VAL:O	18:b:947:ARG:NH1	2.43	0.49
1:A:269:SER:OG	2:B:825:GLN:OE1	2.12	0.49
7:G:18:PHE:O	7:G:22:LEU:HD22	2.13	0.49
16:T:39:DA:H2''	16:T:40:DT:O5'	2.12	0.49
18:b:938:PRO:O	18:b:942:THR:HG23	2.13	0.49
1:A:413:TYR:O	1:A:415:GLY:N	2.42	0.49
1:A:959:MET:HE1	1:A:1050:CYS:HB3	1.95	0.49
7:G:143:ILE:HG21	7:G:145:LEU:HD21	1.94	0.49
20:d:546:LEU:HD21	20:d:594:THR:HA	1.94	0.49
20:d:690:SER:HA	20:d:703:THR:HG22	1.95	0.49
2:B:1077:GLY:HA2	16:T:28:DT:OP1	2.13	0.48
20:d:467:GLN:NE2	20:d:479:VAL:O	2.46	0.48
18:b:614:VAL:HG11	18:b:621:LEU:HB2	1.95	0.48
5:E:67:ASP:OD1	5:E:67:ASP:O	2.31	0.48
16:T:19:DC:C2'	16:T:20:DT:H71	2.43	0.48
13:N:33:DA:OP2	13:N:33:DA:H2'	2.13	0.48
1:A:706:ILE:HD11	1:A:787:VAL:CG1	2.43	0.48
4:D:62:MET:SD	4:D:65:LEU:HD23	2.53	0.48
4:D:112:LYS:NZ	4:D:124:ASP:OD2	2.45	0.48
13:N:11:DT:C1'	13:N:12:DC:H5'	2.43	0.48
2:B:554:GLU:OE1	2:B:554:GLU:N	2.43	0.48
20:d:408:LYS:CA	20:d:678:TYR:CZ	2.90	0.48
20:d:719:GLU:OE2	20:d:737:SER:OG	2.25	0.48
1:A:927:GLU:OE1	1:A:931:ARG:NH1	2.47	0.48
16:T:29:DC:H2''	16:T:30:DT:H5'	1.96	0.48
18:b:635:ILE:O	18:b:640:TRP:NE1	2.40	0.48
1:A:609:HIS:HA	1:A:626:THR:HG21	1.96	0.48
1:A:1085:GLU:OE1	6:F:60:TYR:OH	2.30	0.48
5:E:46:ASP:O	5:E:46:ASP:OD2	2.31	0.48
13:N:42:DA:H2''	13:N:43:DG:O5'	2.14	0.48
17:a:30:LEU:HD11	17:a:361:TRP:HB2	1.96	0.48
20:d:546:LEU:HD21	20:d:594:THR:CA	2.43	0.48
1:A:693:ILE:HD13	1:A:828:LEU:HD21	1.95	0.47
13:N:7:DG:H2''	13:N:8:DA:H5'	1.96	0.47
2:B:728:MET:SD	2:B:942:LYS:HB3	2.54	0.47
3:C:91:GLU:O	3:C:92:GLU:C	2.57	0.47
13:N:3:DA:H2''	13:N:4:DG:H8	1.79	0.47
16:T:43:DG:OP2	18:b:887:GLY:CA	2.61	0.47
18:b:534:MET:SD	18:b:534:MET:N	2.86	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:d:558:ILE:HG13	20:d:569:LEU:HD11	1.97	0.47
1:A:606:HIS:HB3	1:A:626:THR:HG22	1.95	0.47
16:T:8:DC:H2'	16:T:9:DT:H72	1.95	0.47
17:a:1:MET:CB	20:d:841:ALA:O	2.62	0.47
17:a:12:LEU:HD11	20:d:382:PHE:CZ	2.35	0.47
1:A:186:ARG:NH2	1:A:210:GLN:OE1	2.48	0.47
1:A:1249:ASP:OD2	14:O:602:LEU:HD21	2.14	0.47
5:E:84:ILE:CD1	13:N:45:DG:H5''	2.41	0.47
18:b:973:TYR:CE2	18:b:977:ILE:HD11	2.50	0.47
20:d:706:GLU:HB3	20:d:708:GLN:CD	2.39	0.47
1:A:1156:ASP:C	1:A:1156:ASP:OD1	2.58	0.47
4:D:47:GLN:C	4:D:47:GLN:OE1	2.58	0.47
5:E:10:LEU:HD13	5:E:58:LEU:HD11	1.96	0.47
5:E:114:ALA:O	5:E:117:SER:OG	2.28	0.47
16:T:17:DT:H1'	16:T:18:DT:H5''	1.95	0.47
18:b:857:ARG:NH1	18:b:901:TYR:O	2.44	0.47
20:d:404:LEU:O	20:d:697:SER:O	2.33	0.47
1:A:1166:LEU:HD22	1:A:1296:MET:HE2	1.97	0.47
16:T:24:DA:H2'	16:T:25:DT:C6	2.49	0.47
20:d:668:PHE:N	20:d:668:PHE:CD2	2.82	0.47
1:A:413:TYR:CD1	1:A:413:TYR:C	2.92	0.47
2:B:274:ARG:NH2	2:B:281:ASP:OD2	2.47	0.47
2:B:910:THR:HG22	12:L:43:ILE:HA	1.96	0.47
16:T:21:DC:H2'	16:T:22:DC:C6	2.50	0.47
1:A:734:ARG:HH21	9:I:107:ALA:HB3	1.80	0.47
4:D:111:SER:OG	4:D:127:LEU:HD21	2.14	0.47
18:b:537:GLY:O	18:b:541:GLN:NE2	2.41	0.46
19:c:46:LEU:HD13	19:c:65:VAL:HG22	1.97	0.46
16:T:6:DC:H1'	16:T:7:DG:C8	2.50	0.46
16:T:7:DG:H2''	16:T:8:DC:OP2	2.15	0.46
20:d:45:THR:OG1	20:d:47:GLU:O	2.33	0.46
1:A:1281:ASP:CG	14:O:515:ARG:HE	2.22	0.46
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.97	0.46
18:b:651:ILE:HG22	18:b:651:ILE:O	2.15	0.46
20:d:612:PHE:HE2	20:d:628:LYS:HD2	1.81	0.46
13:N:7:DG:H2''	13:N:8:DA:C5'	2.46	0.46
20:d:150:LYS:O	20:d:150:LYS:HG3	2.15	0.46
20:d:394:ILE:HD13	20:d:394:ILE:HA	1.50	0.46
1:A:67:ARG:O	1:A:68:THR:OG1	2.29	0.46
1:A:668:PHE:CZ	1:A:672:ILE:HD11	2.51	0.46
1:A:1324:GLU:OE2	1:A:1324:GLU:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:28:DT:H2'	16:T:29:DC:C6	2.51	0.46
18:b:659:THR:HG22	18:b:663:LYS:HD2	1.97	0.46
19:c:78:LEU:O	19:c:81:SER:OG	2.29	0.46
4:D:88:LEU:HD23	4:D:88:LEU:C	2.41	0.46
7:G:142:GLU:O	7:G:170:LEU:HD13	2.16	0.46
17:a:17:ARG:NH1	20:d:117:GLU:O	2.46	0.46
20:d:616:LEU:HD21	20:d:623:LEU:CD2	2.45	0.46
9:I:31:GLU:OE2	9:I:31:GLU:N	2.45	0.46
16:T:48:DA:H2''	16:T:49:DC:O4'	2.16	0.46
20:d:679:MET:SD	20:d:680:CYS:N	2.89	0.46
20:d:119:GLY:O	20:d:134:ARG:NH2	2.45	0.46
20:d:421:THR:OG1	20:d:683:ASN:O	2.28	0.46
20:d:875:GLU:OE2	20:d:878:GLY:N	2.38	0.46
7:G:31:PHE:O	7:G:35:GLU:HB2	2.15	0.46
7:G:136:VAL:HG23	7:G:136:VAL:O	2.15	0.46
16:T:16:DC:H1'	16:T:17:DT:H5'	1.97	0.46
1:A:621:ILE:HG23	1:A:621:ILE:O	2.16	0.45
13:N:8:DA:H1'	13:N:9:DT:H5'	1.98	0.45
13:N:11:DT:H6	13:N:11:DT:H5'	1.82	0.45
13:N:16:DT:OP1	18:b:1004:LEU:HD13	2.15	0.45
18:b:542:ILE:HG13	18:b:673:LEU:HD11	1.98	0.45
19:c:50:LEU:O	19:c:58:ARG:CZ	2.64	0.45
20:d:438:LEU:HA	20:d:443:VAL:HA	1.98	0.45
20:d:832:GLY:HA3	20:d:873:MET:HE3	1.98	0.45
1:A:1284:PHE:CZ	14:O:508:TYR:CD2	3.04	0.45
17:a:175:SER:OG	18:b:736:ASP:OD2	2.33	0.45
17:a:338:ASP:OD2	17:a:354:ARG:NH1	2.47	0.45
1:A:346:LYS:HD2	16:T:25:DT:OP1	2.15	0.45
1:A:1011:GLU:O	1:A:1015:GLU:HG2	2.15	0.45
1:A:1282:ASP:OD2	1:A:1283:VAL:N	2.48	0.45
2:B:337:LYS:HA	2:B:337:LYS:HE2	1.99	0.45
2:B:467:SER:O	2:B:467:SER:OG	2.33	0.45
9:I:29:ASP:OD2	9:I:29:ASP:N	2.48	0.45
20:d:426:VAL:C	20:d:427:LEU:HD12	2.42	0.45
3:C:190:ASN:O	3:C:193:ARG:NH1	2.39	0.45
18:b:840:LYS:NZ	18:b:932:TYR:O	2.46	0.45
20:d:341:ASN:O	20:d:343:GLN:NE2	2.49	0.45
20:d:396:ILE:HG13	20:d:397:HIS:N	2.32	0.45
5:E:5:GLU:OE1	5:E:5:GLU:HA	2.17	0.45
18:b:607:LYS:O	18:b:610:LEU:N	2.50	0.45
20:d:231:ILE:HD13	20:d:240:HIS:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1416:ARG:O	1:A:1420:ASN:HB2	2.17	0.45
2:B:900:GLU:C	2:B:901:THR:HG22	2.41	0.45
20:d:427:LEU:HD13	20:d:436:LEU:HD23	1.99	0.45
1:A:713:VAL:HG11	1:A:817:PRO:HD3	1.98	0.45
4:D:92:LEU:HB2	4:D:97:LEU:HD21	1.98	0.45
4:D:63:LYS:HE2	7:G:102:GLY:O	2.17	0.45
20:d:673:LEU:HD11	20:d:676:VAL:CG2	2.46	0.45
20:d:698:THR:OG1	20:d:699:LEU:N	2.50	0.45
1:A:66:GLU:OE2	1:A:66:GLU:C	2.60	0.45
17:a:25:ARG:NH2	20:d:842:GLU:CD	2.70	0.45
1:A:732:THR:OG1	1:A:733:LEU:N	2.50	0.45
17:a:346:PHE:CE1	20:d:928:ARG:NH1	2.86	0.45
18:b:540:ILE:HD12	18:b:588:TRP:CE2	2.51	0.45
20:d:413:LEU:HD13	20:d:426:VAL:HG23	1.98	0.45
20:d:599:SER:OG	20:d:600:HIS:N	2.48	0.45
2:B:333:GLU:CD	2:B:333:GLU:C	2.85	0.44
17:a:154:THR:HB	18:b:1383:PRO:CB	2.46	0.44
20:d:405:PRO:O	20:d:429:PHE:CD2	2.70	0.44
20:d:480:SER:O	20:d:484:LYS:O	2.35	0.44
20:d:515:ALA:HA	20:d:533:GLU:HA	1.99	0.44
7:G:18:PHE:O	7:G:22:LEU:HB3	2.17	0.44
16:T:8:DC:C6	16:T:9:DT:H72	2.52	0.44
16:T:40:DT:H4'	18:b:800:ILE:HG21	1.99	0.44
18:b:532:ASP:OD2	18:b:745:ARG:NH2	2.49	0.44
1:A:346:LYS:CD	16:T:25:DT:OP1	2.66	0.44
2:B:794:VAL:HG12	2:B:967:ILE:HG22	1.98	0.44
4:D:61:PHE:CZ	7:G:35:GLU:HG3	2.53	0.44
16:T:28:DT:H2'	16:T:29:DC:H6	1.82	0.44
17:a:40:ARG:HD2	19:c:136:HIS:NE2	2.32	0.44
20:d:407:ILE:CD1	20:d:694:ALA:HB1	2.47	0.44
12:L:27:GLU:OE2	12:L:27:GLU:HA	2.17	0.44
13:N:10:DC:H2''	13:N:11:DT:H5'	2.00	0.44
16:T:17:DT:H2''	16:T:18:DT:H5'	2.00	0.44
20:d:720:SER:O	20:d:720:SER:OG	2.32	0.44
16:T:25:DT:H2'	16:T:26:DC:H6	1.82	0.44
17:a:36:ARG:HD3	17:a:82:TYR:OH	2.18	0.44
2:B:1081:ASP:CG	2:B:1081:ASP:O	2.60	0.44
2:B:1085:ARG:NE	16:T:26:DC:OP1	2.39	0.44
17:a:219:ALA:HB2	18:b:693:PHE:HD1	1.80	0.44
17:a:346:PHE:CZ	20:d:928:ARG:NH1	2.85	0.44
18:b:539:THR:HG22	18:b:543:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:b:582:VAL:HG21	18:b:596:ILE:HD11	1.99	0.44
18:b:754:LEU:HD21	18:b:951:ILE:CG1	2.48	0.44
20:d:367:LEU:O	20:d:368:GLU:HB2	2.17	0.44
20:d:1055:GLN:HG3	20:d:1093:LEU:HD23	1.99	0.44
5:E:122:ALA:O	5:E:126:ILE:HD13	2.18	0.44
13:N:14:DT:H72	18:b:800:ILE:HD11	2.00	0.44
16:T:22:DC:H2'	16:T:23:DC:C6	2.53	0.44
20:d:658:VAL:HG11	20:d:707:ILE:CG2	2.46	0.44
5:E:60:VAL:HG22	5:E:74:VAL:HB	2.00	0.44
20:d:408:LYS:C	20:d:678:TYR:CE2	2.96	0.44
18:b:667:THR:O	18:b:670:ARG:NE	2.51	0.43
20:d:256:SER:OG	20:d:275:ASP:OD2	2.36	0.43
20:d:603:LEU:HD13	20:d:613:TYR:HB3	2.00	0.43
20:d:884:ILE:HG22	20:d:885:ASN:H	1.83	0.43
2:B:837:CYS:SG	2:B:891:ASP:N	2.91	0.43
4:D:71:PHE:CZ	7:G:88:VAL:HG22	2.53	0.43
7:G:122:ASN:N	7:G:122:ASN:OD1	2.50	0.43
18:b:1001:LEU:HD23	18:b:1001:LEU:H	1.83	0.43
20:d:396:ILE:CG2	20:d:673:LEU:HD23	2.47	0.43
3:C:149:LEU:HD21	3:C:152:LYS:HE3	2.00	0.43
18:b:859:LEU:HD11	18:b:912:LEU:CD1	2.48	0.43
19:c:8:LEU:HD11	19:c:24:LYS:HB2	2.00	0.43
20:d:538:VAL:HG11	20:d:541:LEU:HD11	1.99	0.43
20:d:986:ASP:OD1	20:d:986:ASP:N	2.50	0.43
13:N:33:DA:H2''	13:N:34:DG:C8	2.54	0.43
14:O:512:MET:O	14:O:516:LYS:HG3	2.18	0.43
20:d:468:LEU:HD22	20:d:479:VAL:HB	2.00	0.43
20:d:637:VAL:HG12	20:d:652:CYS:HB2	2.01	0.43
1:A:1236:ASN:ND2	14:O:593:VAL:HG21	2.34	0.43
2:B:448:LEU:O	2:B:467:SER:OG	2.35	0.43
20:d:650:PHE:CE2	20:d:671:VAL:HG21	2.54	0.43
2:B:957:THR:HG22	2:B:1028:LEU:CD2	2.48	0.43
3:C:44:ILE:HD11	3:C:239:LEU:CD1	2.49	0.43
3:C:180:ALA:O	10:J:42:ARG:NH2	2.52	0.43
1:A:1153:ARG:O	1:A:1157:ILE:HG13	2.18	0.43
9:I:41:ASN:OD1	9:I:42:CYS:N	2.52	0.43
13:N:41:DC:H2''	13:N:42:DA:OP2	2.18	0.43
18:b:648:GLY:HA3	18:b:672:ILE:HG23	2.00	0.43
20:d:405:PRO:O	20:d:429:PHE:HD2	2.02	0.43
2:B:199:LYS:NZ	2:B:394:ASP:OD2	2.50	0.43
2:B:628:VAL:HG12	2:B:629:GLU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:44:DA:H4'	18:b:626:SER:OG	2.19	0.43
19:c:87:LEU:HD22	19:c:138:LEU:HD11	2.01	0.43
1:A:986:MET:HE2	1:A:1075:LYS:HG3	2.01	0.43
1:A:1147:SER:HA	1:A:1153:ARG:HB2	2.01	0.43
16:T:24:DA:H2'	16:T:25:DT:H6	1.82	0.43
17:a:19:ARG:HA	20:d:953:TRP:CH2	2.54	0.43
17:a:168:VAL:CG2	17:a:189:ILE:HD13	2.43	0.43
19:c:31:ILE:HG22	19:c:38:GLN:OE1	2.18	0.43
19:c:68:LEU:O	19:c:72:SER:N	2.50	0.43
20:d:478:LEU:HD11	20:d:521:ILE:HG23	1.99	0.43
20:d:659:ILE:C	20:d:659:ILE:HD12	2.44	0.43
8:H:91:VAL:HG22	8:H:144:LEU:HD13	2.01	0.42
17:a:70:LEU:O	17:a:87:VAL:N	2.52	0.42
17:a:268:ARG:NH1	17:a:286:LYS:HG2	2.33	0.42
20:d:22:HIS:ND1	20:d:28:ASP:O	2.46	0.42
20:d:130:MET:HE3	20:d:176:PRO:CG	2.48	0.42
1:A:145:TYR:HA	1:A:148:CYS:SG	2.59	0.42
1:A:693:ILE:HG22	1:A:694:ALA:N	2.34	0.42
1:A:910:LYS:N	1:A:911:PRO:HD2	2.33	0.42
2:B:327:LYS:HE2	2:B:327:LYS:HB2	1.87	0.42
11:K:64:PRO:HG3	11:K:72:ILE:HD12	2.01	0.42
18:b:831:GLN:O	18:b:837:ARG:NH2	2.52	0.42
20:d:570:LYS:O	20:d:574:PHE:N	2.47	0.42
4:D:32:LEU:HD21	7:G:4:HIS:N	2.34	0.42
16:T:17:DT:H2''	16:T:18:DT:H71	2.01	0.42
18:b:808:HIS:O	18:b:810:ASP:N	2.52	0.42
18:b:1004:LEU:H	18:b:1004:LEU:HD23	1.85	0.42
20:d:393:GLY:HA3	20:d:672:ASN:OD1	2.20	0.42
1:A:1086:MET:SD	1:A:1466:ALA:HB1	2.60	0.42
5:E:54:ARG:N	5:E:57:ASP:OD1	2.47	0.42
8:H:97:TYR:CZ	8:H:115:TYR:HB3	2.55	0.42
20:d:130:MET:HE2	20:d:197:LEU:HD21	2.01	0.42
20:d:518:TYR:HB2	20:d:574:PHE:CZ	2.54	0.42
20:d:616:LEU:CD1	20:d:623:LEU:HD23	2.50	0.42
20:d:659:ILE:HD12	20:d:660:TYR:N	2.35	0.42
1:A:693:ILE:HD13	1:A:828:LEU:CD2	2.50	0.42
2:B:207:VAL:HG11	2:B:375:ALA:CB	2.49	0.42
2:B:1085:ARG:HG2	16:T:26:DC:H5''	2.02	0.42
20:d:706:GLU:O	20:d:707:ILE:CG1	2.68	0.42
3:C:33:SER:OG	11:K:45:ILE:HG23	2.19	0.42
1:A:121:SER:HA	1:A:126:ILE:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1146:GLN:OE1	1:A:1149:ARG:NH1	2.53	0.42
16:T:43:DG:OP2	18:b:887:GLY:N	2.53	0.42
18:b:912:LEU:HD22	18:b:917:GLY:HA3	2.01	0.42
20:d:539:ALA:N	20:d:559:GLY:O	2.51	0.42
1:A:381:PRO:HG2	1:A:384:ILE:HD12	2.01	0.42
2:B:19:PRO:O	2:B:22:TRP:N	2.52	0.42
2:B:491:ARG:HG3	2:B:518:HIS:CE1	2.55	0.42
4:D:126:GLU:O	4:D:130:ILE:HD13	2.20	0.42
13:N:34:DG:H2"	13:N:35:DA:H8	1.85	0.42
17:a:100:TYR:CZ	21:e:30:ASN:CG	2.97	0.42
20:d:43:VAL:HB	20:d:50:ARG:HG3	2.01	0.42
20:d:394:ILE:HD12	20:d:394:ILE:HG23	1.34	0.42
4:D:61:PHE:CE2	7:G:46:ILE:O	2.72	0.42
4:D:74:PHE:CE2	4:D:83:VAL:HG11	2.55	0.42
6:F:78:PRO:HG2	7:G:19:GLY:HA2	2.02	0.42
7:G:89:VAL:HA	7:G:99:THR:HG22	2.02	0.42
16:T:40:DT:H2"	16:T:41:DG:C8	2.55	0.42
17:a:154:THR:HG22	18:b:1383:PRO:CB	2.38	0.42
9:I:99:SER:C	9:I:100:HIS:ND1	2.78	0.42
20:d:660:TYR:CG	20:d:707:ILE:HD12	2.54	0.42
20:d:989:ARG:HG2	20:d:989:ARG:O	2.19	0.42
1:A:490:THR:HB	1:A:491:PRO:HD3	2.02	0.41
1:A:521:VAL:HG13	1:A:535:MET:HE1	2.01	0.41
9:I:99:SER:C	9:I:100:HIS:HD1	2.27	0.41
16:T:20:DT:H2"	16:T:21:DC:C6	2.55	0.41
17:a:320:THR:OG1	17:a:327:ILE:HD11	2.19	0.41
18:b:912:LEU:HD22	18:b:917:GLY:HA2	2.00	0.41
20:d:556:CYS:SG	20:d:571:LEU:HD13	2.59	0.41
1:A:1231:ILE:O	1:A:1235:ILE:HG13	2.20	0.41
1:A:1282:ASP:OD2	1:A:1283:VAL:HG13	2.20	0.41
2:B:489:ILE:HD13	2:B:498:PRO:CB	2.49	0.41
16:T:46:DC:H2"	16:T:47:DA:OP2	2.20	0.41
17:a:149:MET:CG	17:a:159:VAL:HG22	2.47	0.41
3:C:11:ILE:HG12	11:K:108:ALA:HB1	2.02	0.41
13:N:38:DG:H2"	13:N:39:DA:OP2	2.20	0.41
14:O:568:THR:O	14:O:568:THR:HG22	2.20	0.41
18:b:682:LEU:HD12	18:b:708:SER:HA	2.02	0.41
20:d:469:ILE:HD11	20:d:476:VAL:HG22	2.03	0.41
20:d:478:LEU:CD1	20:d:521:ILE:HG23	2.50	0.41
1:A:425:ASP:OD1	1:A:425:ASP:N	2.47	0.41
16:T:41:DG:H2"	16:T:42:DA:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:d:252:ILE:HD12	20:d:252:ILE:H	1.85	0.41
20:d:564:ILE:HD12	20:d:564:ILE:H	1.84	0.41
20:d:673:LEU:HD12	20:d:673:LEU:C	2.45	0.41
20:d:1053:ASP:O	20:d:1057:ARG:HG3	2.21	0.41
1:A:234:PHE:CD1	1:A:234:PHE:C	2.98	0.41
2:B:338:TYR:CD2	2:B:338:TYR:C	2.99	0.41
2:B:910:THR:HG22	12:L:42:ARG:O	2.21	0.41
3:C:44:ILE:HD13	3:C:44:ILE:HA	1.92	0.41
1:A:592:PHE:HA	1:A:595:ILE:HD12	2.03	0.41
1:A:628:VAL:HA	1:A:638:GLY:HA3	2.03	0.41
2:B:1075:MET:HE3	2:B:1075:MET:HB3	1.99	0.41
1:A:119:VAL:HB	1:A:126:ILE:HD11	2.02	0.41
2:B:279:VAL:HG23	2:B:280:SER:N	2.36	0.41
2:B:457:LYS:N	2:B:457:LYS:HD2	2.36	0.41
17:a:251:LEU:CD2	17:a:262:THR:HG22	2.51	0.41
20:d:631:LEU:O	20:d:631:LEU:HD12	2.21	0.41
1:A:394:VAL:O	1:A:442:THR:O	2.39	0.41
1:A:733:LEU:HD13	1:A:733:LEU:O	2.21	0.41
1:A:1247:PHE:CD1	1:A:1247:PHE:N	2.89	0.41
20:d:616:LEU:CD2	20:d:623:LEU:HD23	2.51	0.41
20:d:654:ASP:OD1	20:d:655:ARG:N	2.54	0.41
1:A:128:ASP:OD1	1:A:129:ILE:N	2.54	0.41
1:A:458:PHE:CE1	1:A:484:LEU:HD21	2.56	0.41
7:G:108:ILE:CD1	7:G:145:LEU:HD22	2.50	0.41
11:K:37:LYS:N	11:K:69:HIS:O	2.51	0.41
13:N:42:DA:OP2	13:N:42:DA:H3'	2.20	0.41
2:B:320:PHE:O	2:B:324:ARG:HG2	2.21	0.41
7:G:148:VAL:HB	7:G:160:ILE:HG23	2.02	0.41
20:d:455:GLN:HB3	20:d:472:THR:OG1	2.20	0.41
20:d:813:ALA:HA	20:d:833:THR:HG22	2.03	0.41
9:I:32:ASN:HD22	9:I:32:ASN:C	2.24	0.40
9:I:87:GLN:N	9:I:87:GLN:CD	2.77	0.40
18:b:693:PHE:CD2	18:b:696:LYS:HB2	2.55	0.40
1:A:83:GLY:HA3	1:A:257:PRO:HB2	2.03	0.40
1:A:1235:ILE:HG12	1:A:1296:MET:HE1	2.02	0.40
4:D:44:ARG:HH11	4:D:44:ARG:HG2	1.86	0.40
13:N:8:DA:H5'	13:N:8:DA:H8	1.86	0.40
17:a:213:LEU:O	17:a:223:LEU:N	2.45	0.40
5:E:82:VAL:HG21	5:E:106:VAL:HG12	2.03	0.40
5:E:110:MET:CG	5:E:114:ALA:HB3	2.51	0.40
20:d:190:VAL:O	20:d:209:GLN:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:d:312:GLU:N	20:d:325:GLY:O	2.50	0.40
2:B:910:THR:HG21	12:L:43:ILE:HG12	2.03	0.40
12:L:13:GLN:N	12:L:14:PRO:HD2	2.37	0.40
20:d:80:LEU:HD23	20:d:120:ILE:HG21	2.03	0.40
20:d:881:LEU:HD21	20:d:921:ILE:HG21	2.03	0.40
1:A:432:HIS:N	1:A:433:PRO:HD3	2.36	0.40
1:A:469:MET:HG3	2:B:1093:CYS:SG	2.62	0.40
1:A:478:PRO:O	11:K:2:ASN:HB3	2.22	0.40
5:E:55:ARG:HA	5:E:58:LEU:HD12	2.03	0.40
7:G:167:TYR:O	7:G:168:LEU:HD22	2.22	0.40
9:I:124:THR:HG22	9:I:125:GLU:N	2.37	0.40
11:K:110:LYS:O	11:K:114:GLU:HG2	2.21	0.40
13:N:33:DA:H2''	13:N:34:DG:OP2	2.21	0.40
17:a:188:GLU:C	17:a:206:SER:HG	2.29	0.40
18:b:928:ARG:HD3	18:b:958:THR:HG22	2.02	0.40
20:d:394:ILE:HD12	20:d:707:ILE:HA	1.98	0.40
20:d:410:LEU:HD11	20:d:694:ALA:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1414/1970 (72%)	1379 (98%)	35 (2%)	0	100	100
2	B	1123/1174 (96%)	1085 (97%)	38 (3%)	0	100	100
3	C	256/275 (93%)	251 (98%)	5 (2%)	0	100	100
4	D	124/142 (87%)	118 (95%)	6 (5%)	0	100	100
5	E	207/210 (99%)	204 (99%)	3 (1%)	0	100	100
6	F	80/127 (63%)	79 (99%)	1 (1%)	0	100	100
7	G	169/172 (98%)	156 (92%)	13 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	146/150 (97%)	145 (99%)	1 (1%)	0	100	100
9	I	115/125 (92%)	114 (99%)	1 (1%)	0	100	100
10	J	65/67 (97%)	65 (100%)	0	0	100	100
11	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
12	L	44/58 (76%)	40 (91%)	4 (9%)	0	100	100
14	O	118/991 (12%)	114 (97%)	4 (3%)	0	100	100
17	a	359/396 (91%)	340 (95%)	18 (5%)	1 (0%)	37	68
18	b	511/1493 (34%)	485 (95%)	26 (5%)	0	100	100
19	c	146/709 (21%)	142 (97%)	4 (3%)	0	100	100
20	d	1080/1140 (95%)	1008 (93%)	72 (7%)	0	100	100
21	e	62/83 (75%)	61 (98%)	1 (2%)	0	100	100
All	All	6132/9399 (65%)	5896 (96%)	235 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	a	176	GLY

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	1252/1749 (72%)	1228 (98%)	24 (2%)	52	73
2	B	992/1027 (97%)	968 (98%)	24 (2%)	44	68
3	C	237/252 (94%)	234 (99%)	3 (1%)	65	81
4	D	116/126 (92%)	110 (95%)	6 (5%)	19	47
5	E	191/192 (100%)	189 (99%)	2 (1%)	73	84
6	F	71/111 (64%)	69 (97%)	2 (3%)	38	65
7	G	152/153 (99%)	152 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	129/131 (98%)	123 (95%)	6 (5%)	22	51
9	I	105/112 (94%)	100 (95%)	5 (5%)	21	50
10	J	56/56 (100%)	55 (98%)	1 (2%)	54	74
11	K	104/106 (98%)	103 (99%)	1 (1%)	73	84
12	L	43/55 (78%)	42 (98%)	1 (2%)	45	69
14	O	104/820 (13%)	101 (97%)	3 (3%)	37	64
17	a	318/348 (91%)	316 (99%)	2 (1%)	84	91
18	b	465/1297 (36%)	464 (100%)	1 (0%)	92	97
19	c	132/608 (22%)	130 (98%)	2 (2%)	60	77
20	d	936/999 (94%)	931 (100%)	5 (0%)	86	93
21	e	59/76 (78%)	57 (97%)	2 (3%)	32	60
All	All	5462/8218 (66%)	5372 (98%)	90 (2%)	58	76

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	VAL
1	A	112	PHE
1	A	128	ASP
1	A	209	SER
1	A	440	LEU
1	A	488	VAL
1	A	545	VAL
1	A	576	GLN
1	A	757	GLN
1	A	769	MET
1	A	805	ARG
1	A	845	GLU
1	A	865	ILE
1	A	900	SER
1	A	1020	LEU
1	A	1021	VAL
1	A	1050	CYS
1	A	1059	ARG
1	A	1085	GLU
1	A	1101	GLN
1	A	1186	VAL
1	A	1255	LEU

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Mol	Chain	Res	Type
1	A	1351	ASP
1	A	1423	ASP
2	B	65	ILE
2	B	233	SER
2	B	259	THR
2	B	267	VAL
2	B	309	PHE
2	B	327	LYS
2	B	330	VAL
2	B	331	THR
2	B	332	LYS
2	B	335	ARG
2	B	336	ILE
2	B	340	LYS
2	B	361	LYS
2	B	412	LEU
2	B	447	SER
2	B	489	ILE
2	B	589	LYS
2	B	675	LEU
2	B	719	SER
2	B	778	SER
2	B	837	CYS
2	B	846	ASP
2	B	1131	ARG
2	B	1142	ASN
3	C	75	SER
3	C	111	GLN
3	C	166	LYS
4	D	33	LEU
4	D	68	THR
4	D	83	VAL
4	D	84	ARG
4	D	115	ILE
4	D	134	ILE
5	E	60	VAL
5	E	75	PHE
6	F	83	LEU
6	F	84	GLU
8	H	32	SER
8	H	69	THR
8	H	71	ASP

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Mol	Chain	Res	Type
8	H	74	GLU
8	H	95	LYS
8	H	136	GLU
9	I	19	GLU
9	I	29	ASP
9	I	43	ASP
9	I	66	THR
9	I	72	VAL
10	J	55	LEU
11	K	13	PHE
12	L	38	GLU
14	O	498	GLU
14	O	502	ARG
14	O	506	LEU
17	a	32	LEU
17	a	175	SER
18	b	1399	LEU
19	c	58	ARG
19	c	97	GLN
20	d	407	ILE
20	d	596	PHE
20	d	603	LEU
20	d	659	ILE
20	d	666	LEU
21	e	69	ASP
21	e	72	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	HIS
1	A	278	HIS
1	A	330	GLN
1	A	662	HIS
1	A	673	GLN
1	A	700	GLN
1	A	790	GLN
1	A	792	ASN
1	A	861	GLN
1	A	926	ASN
1	A	1093	GLN
1	A	1182	GLN

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Mol	Chain	Res	Type
1	A	1236	ASN
1	A	1244	ASN
1	A	1291	ASN
1	A	1332	GLN
1	A	1417	HIS
1	A	1422	GLN
2	B	144	HIS
2	B	319	ASN
2	B	631	GLN
2	B	650	ASN
2	B	741	HIS
3	C	83	GLN
3	C	217	GLN
4	D	19	GLN
5	E	133	GLN
11	K	89	ASN
14	O	500	HIS
14	O	505	ASN
14	O	585	HIS
17	a	133	GLN
17	a	267	ASN
18	b	777	GLN
20	d	4	ASN
20	d	261	HIS
20	d	399	HIS
20	d	467	GLN
20	d	617	ASN
20	d	670	ASN
20	d	711	HIS
20	d	731	GLN
20	d	904	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	9/45 (20%)	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 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

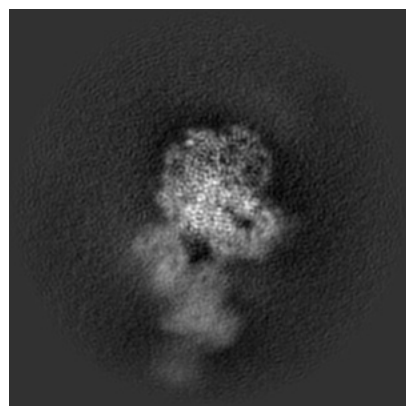
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52449. These allow visual inspection of the internal detail of the map and identification of artifacts.

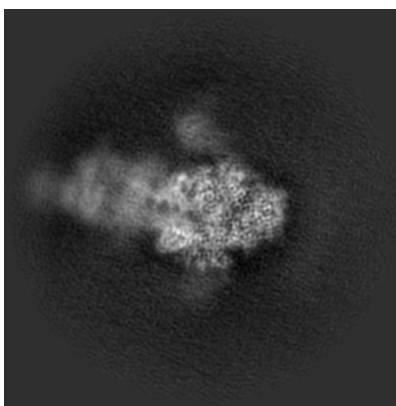
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

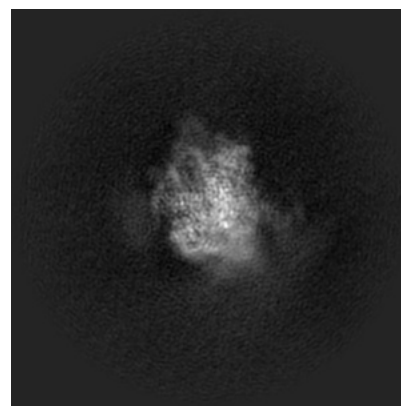
6.1.1 Primary map



X

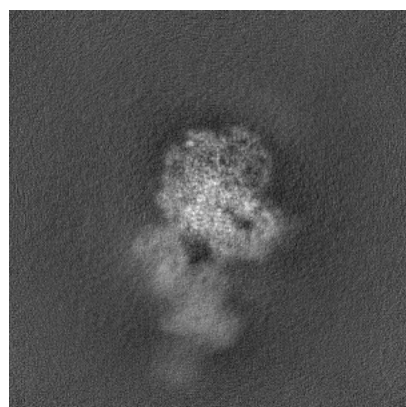


Y

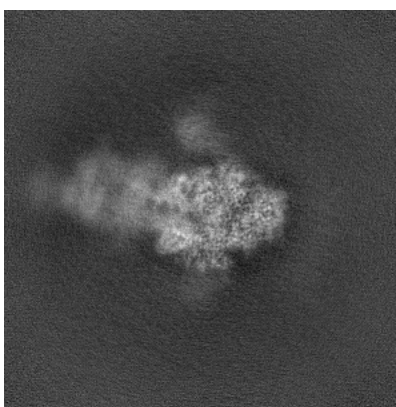


Z

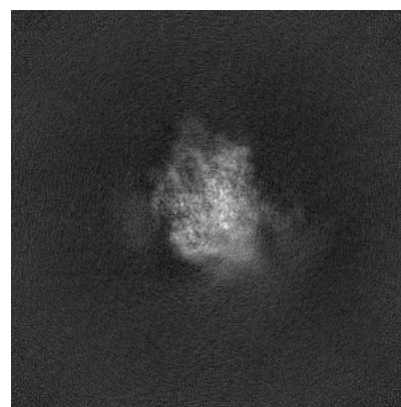
6.1.2 Raw map



X



Y

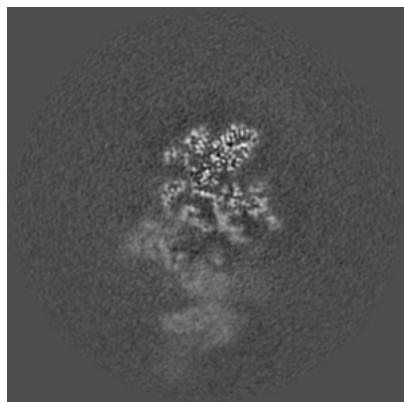


Z

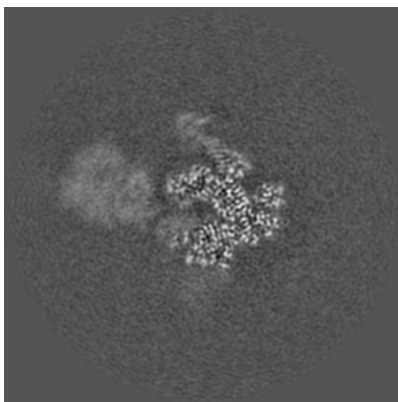
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

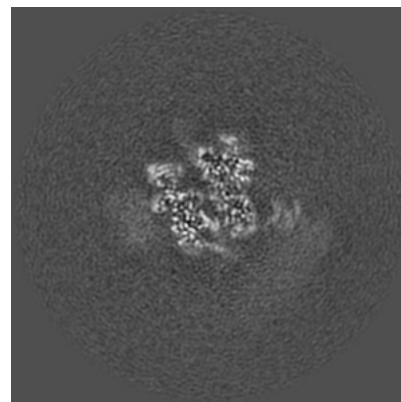
6.2.1 Primary map



X Index: 240

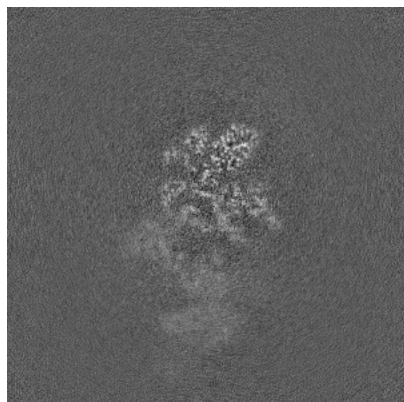


Y Index: 240

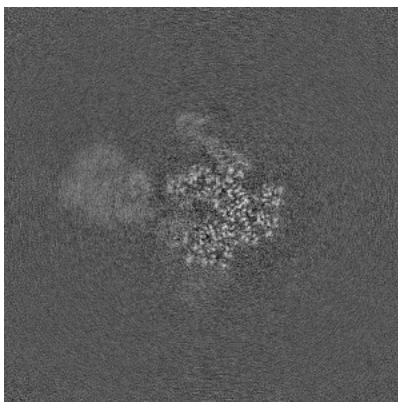


Z Index: 240

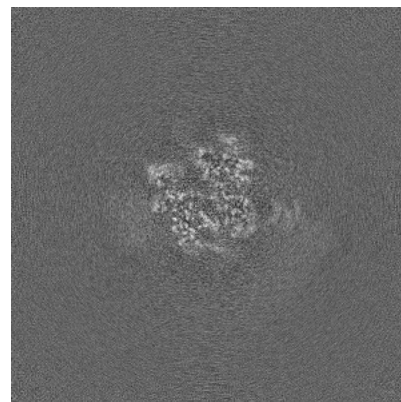
6.2.2 Raw map



X Index: 240



Y Index: 240

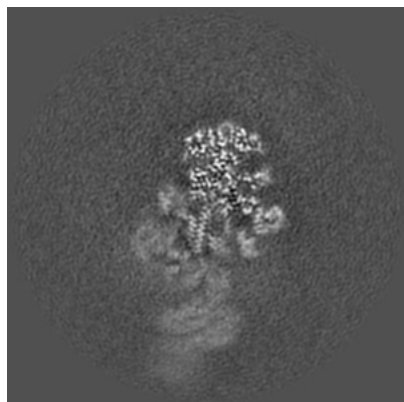


Z Index: 240

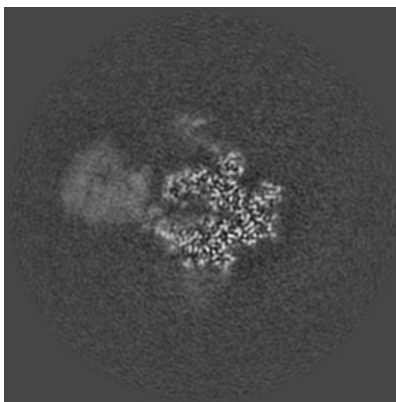
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

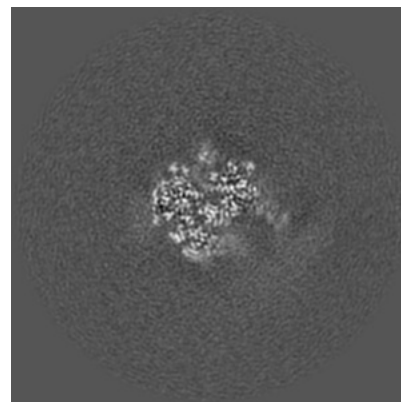
6.3.1 Primary map



X Index: 252

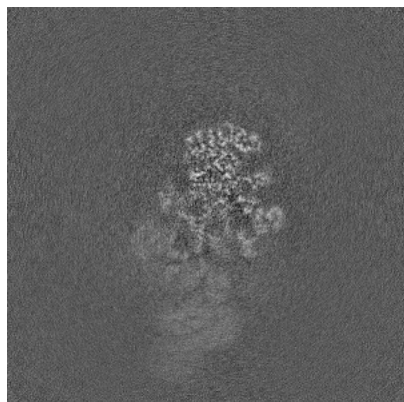


Y Index: 246

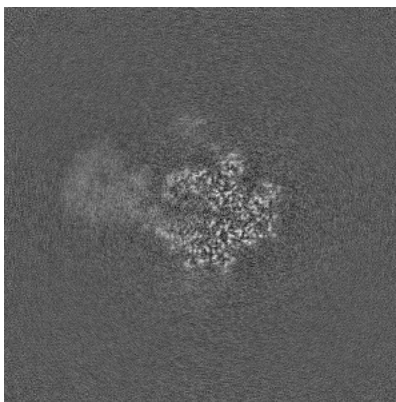


Z Index: 257

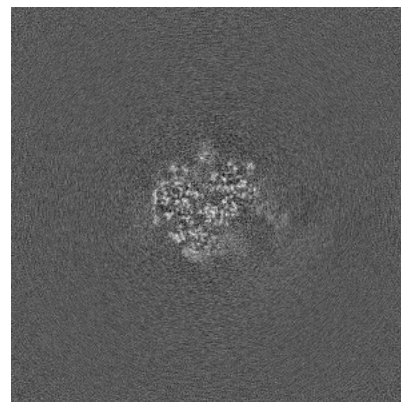
6.3.2 Raw map



X Index: 251



Y Index: 247

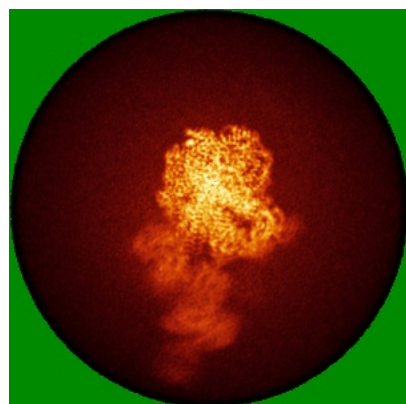


Z Index: 257

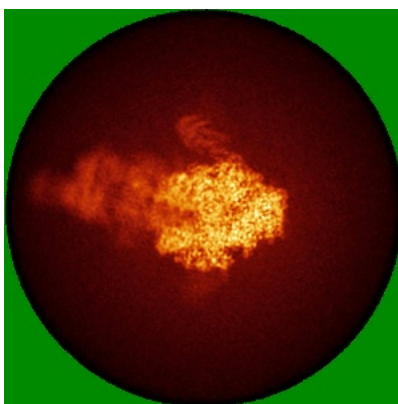
The images above show the largest variance slices of the map in three orthogonal directions.

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

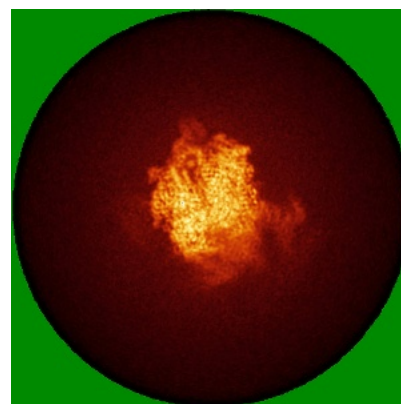
6.4.1 Primary map



X

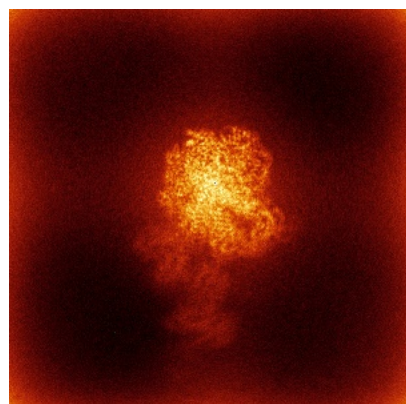


Y

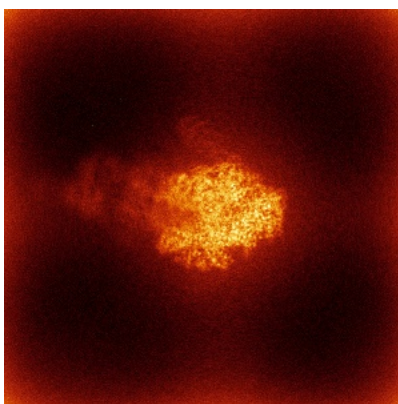


Z

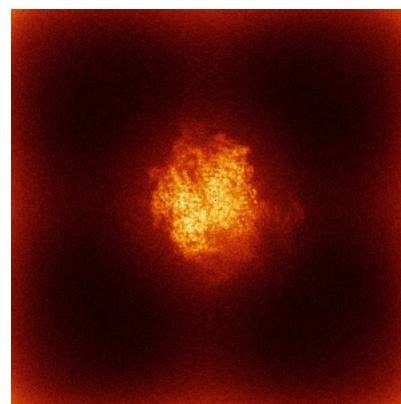
6.4.2 Raw map



X



Y

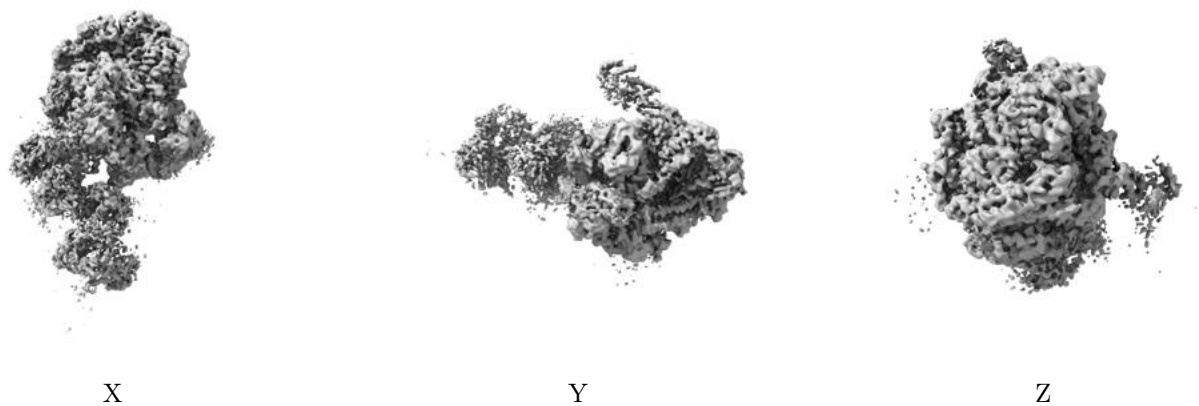


Z

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

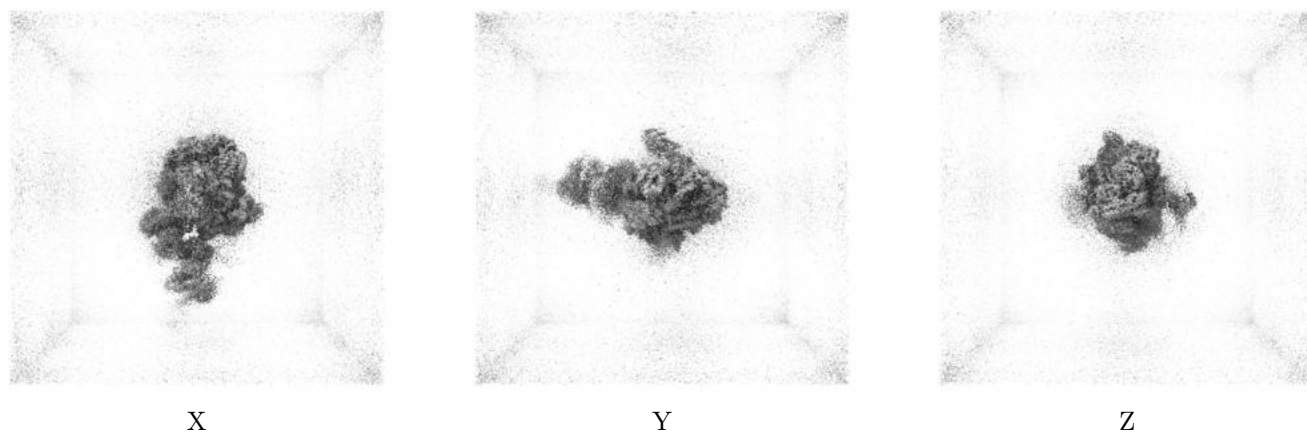
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

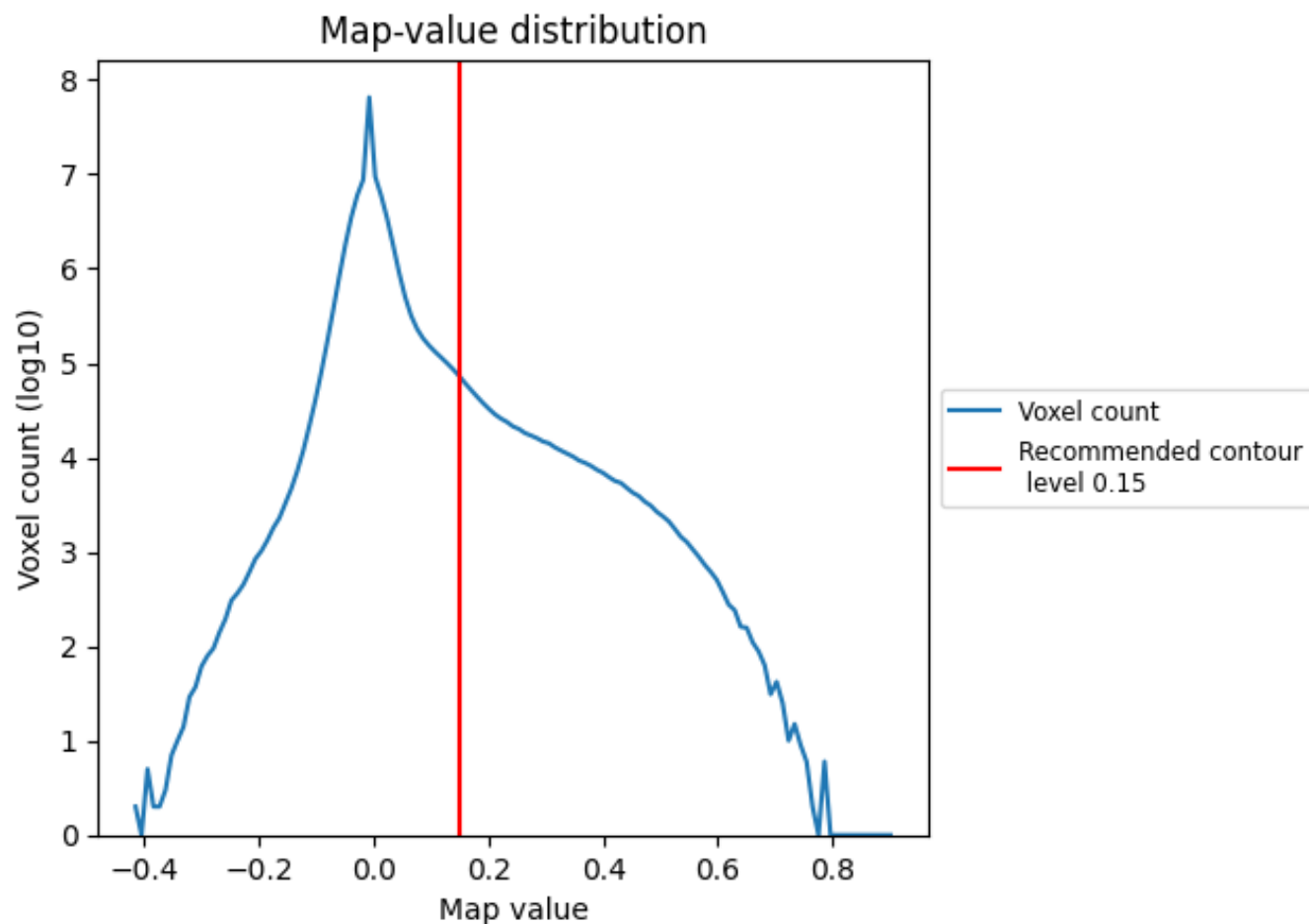
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

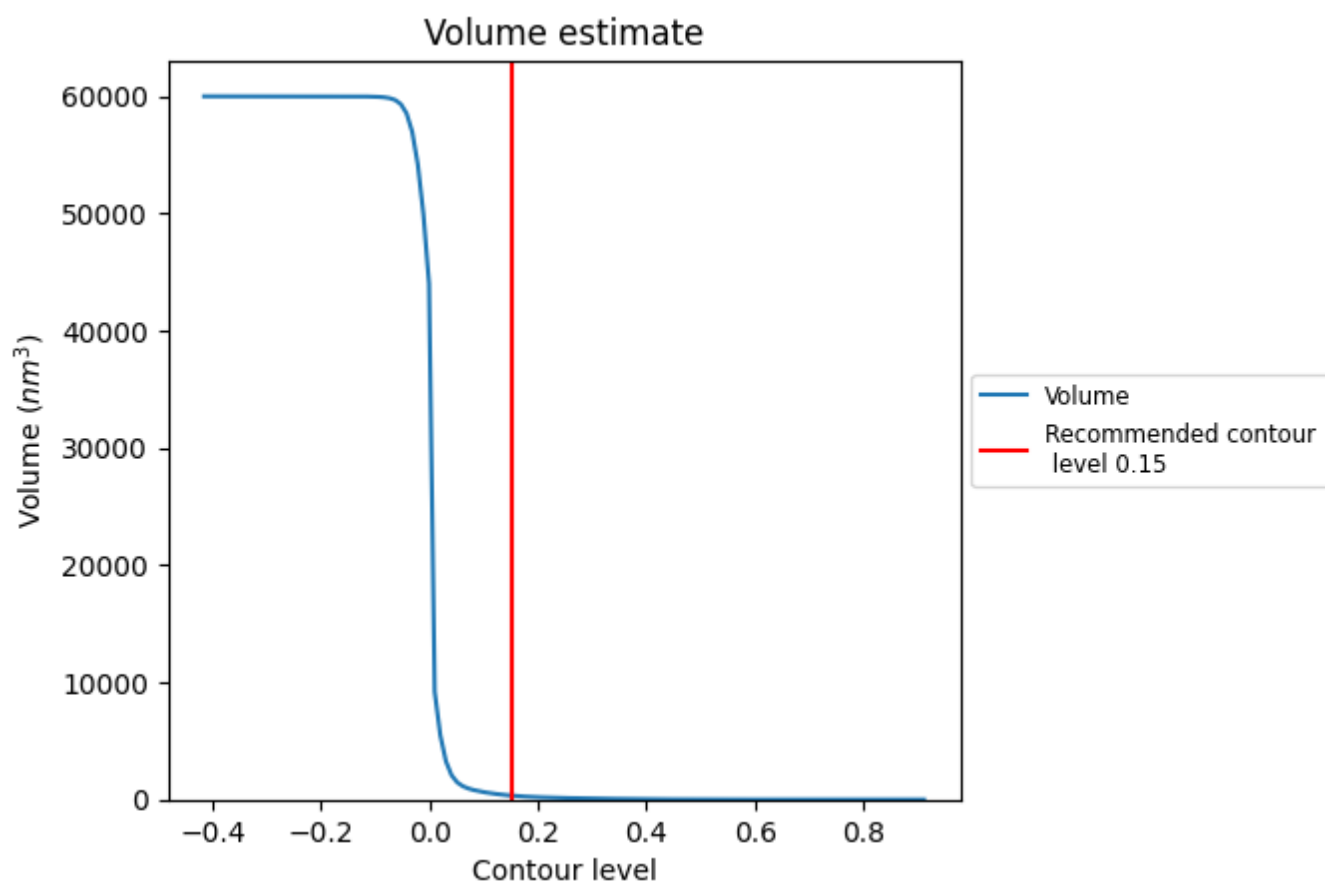
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

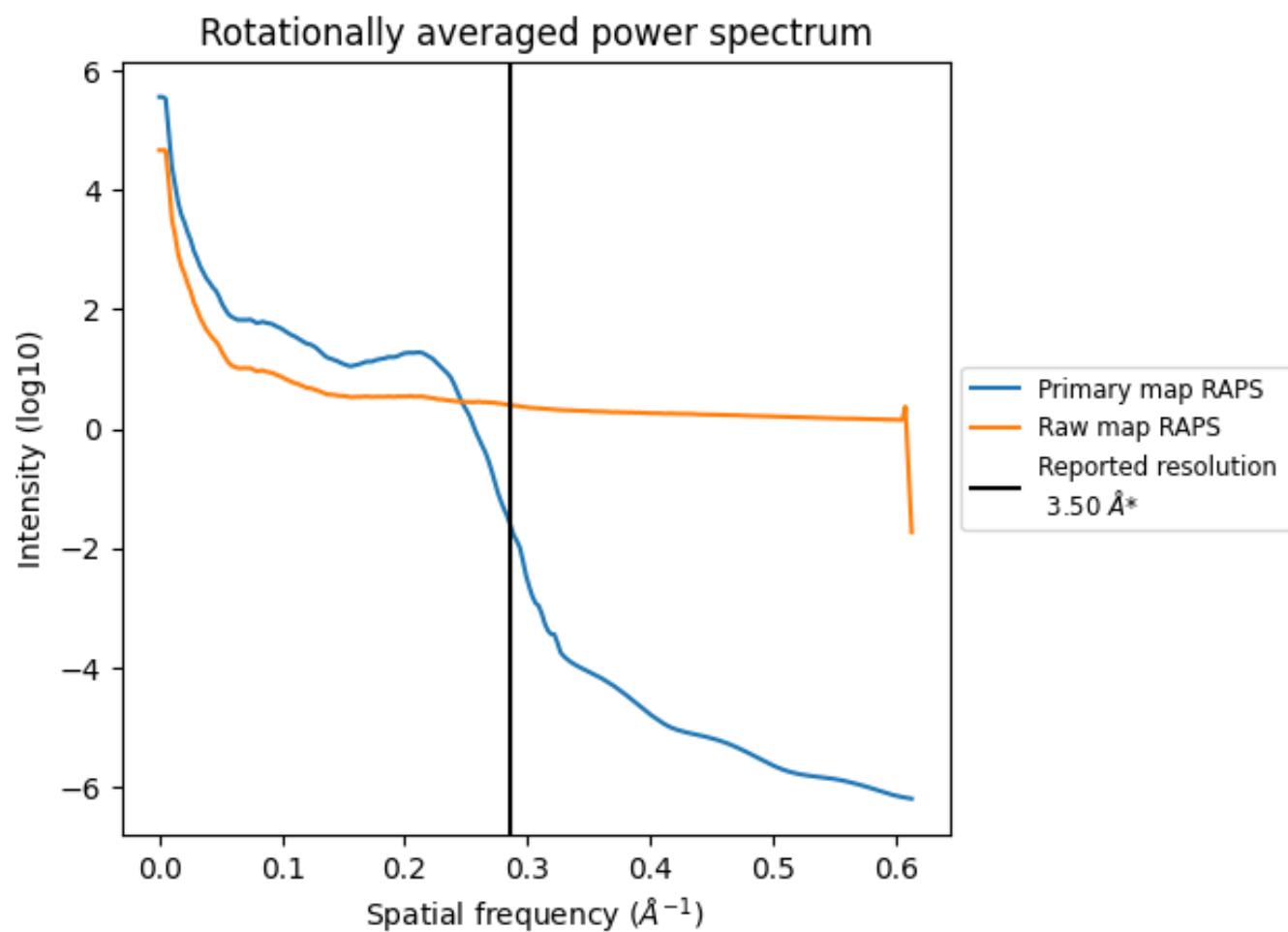
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 342 nm³; this corresponds to an approximate mass of 309 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 ⓘ

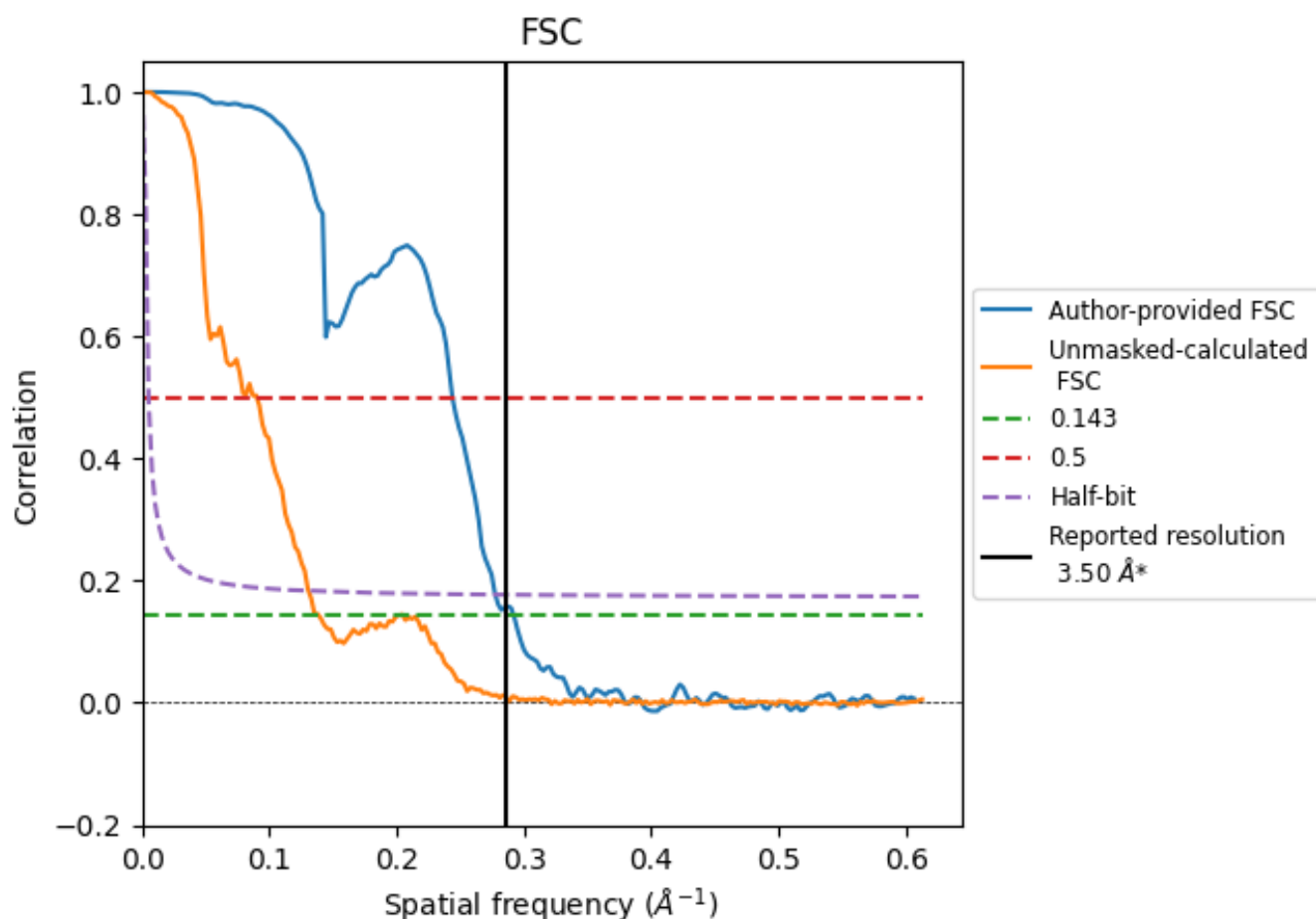


*Reported resolution corresponds to spatial frequency of 0.286 \AA^{-1}

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

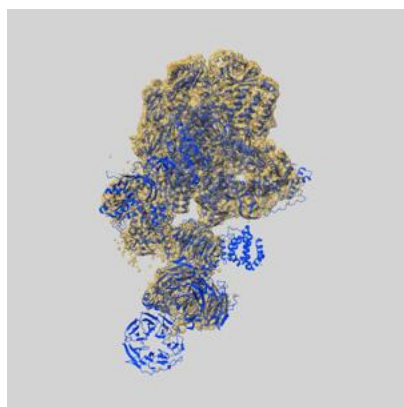
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.43	4.10	3.60
Unmasked-calculated*	7.21	11.12	7.65

*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 7.21 differs from the reported value 3.5 by more than 10 %

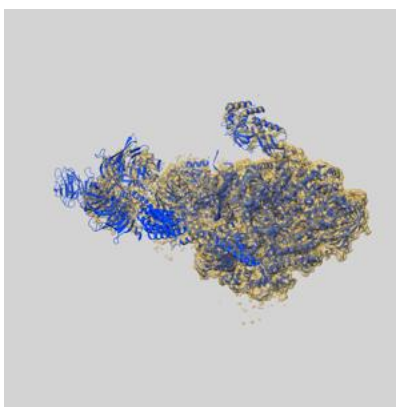
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52449 and PDB model 9HWG. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

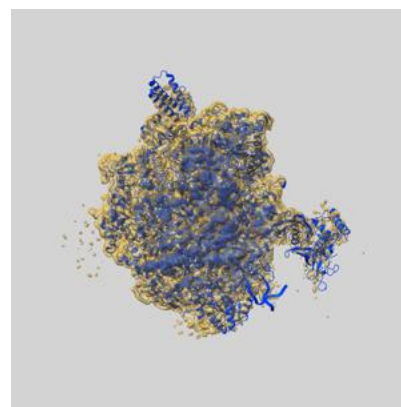
9.1 Map-model overlay [i](#)



X



Y



Z

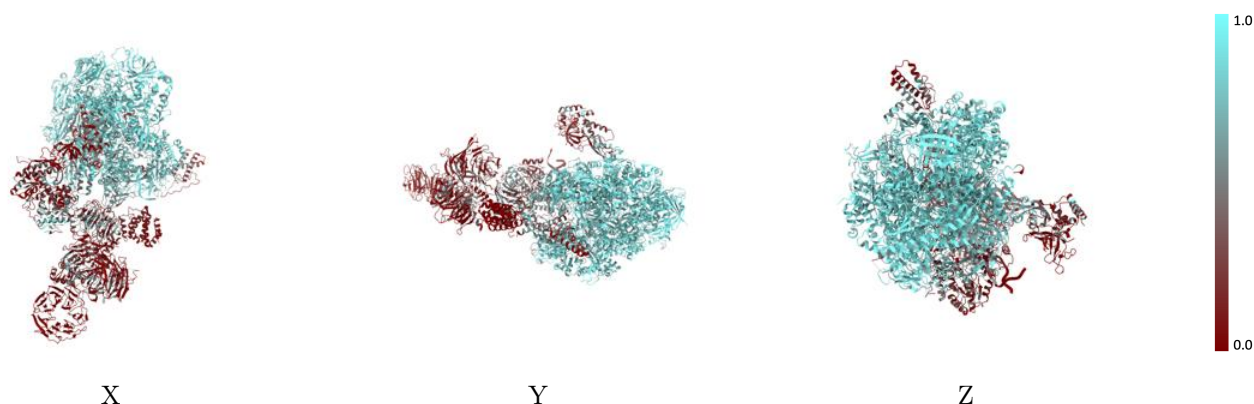
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



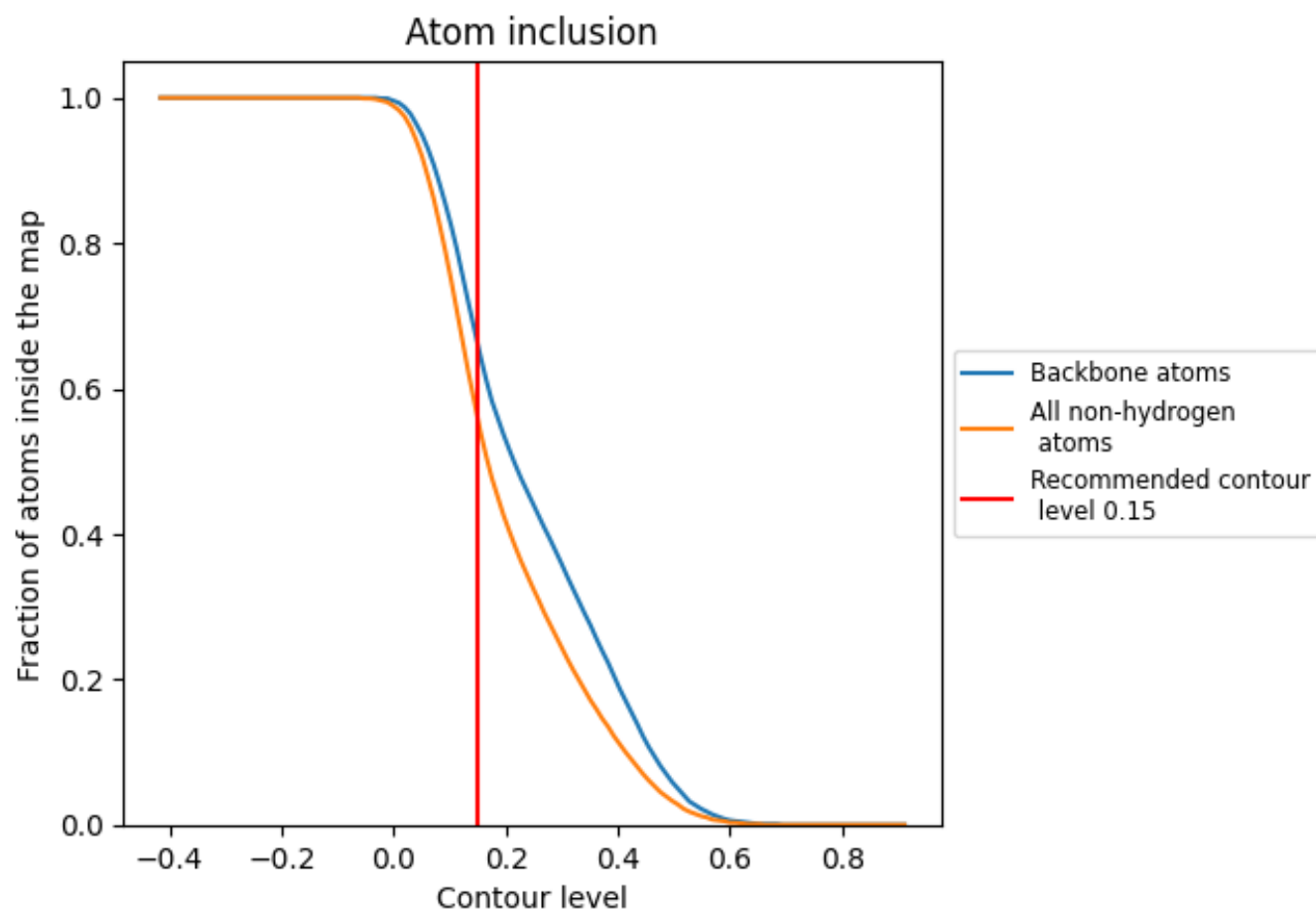
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 56% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5600	 0.2540
A	 0.7960	 0.3870
B	 0.7950	 0.3950
C	 0.8550	 0.4100
D	 0.2160	 0.1160
E	 0.8270	 0.3620
F	 0.7950	 0.3670
G	 0.2530	 0.1550
H	 0.8380	 0.4100
I	 0.7710	 0.3270
J	 0.8430	 0.4060
K	 0.8510	 0.4090
L	 0.7930	 0.3610
N	 0.5450	 0.1600
O	 0.2790	 0.0940
P	 0.9590	 0.4190
T	 0.7260	 0.2420
a	 0.2730	 0.0900
b	 0.3090	 0.0510
c	 0.0030	 0.0150
d	 0.1310	 0.0440
e	 0.5250	 0.2190

