



Full wwPDB EM Validation Report ⓘ

Aug 3, 2026 – 06:37 pm BST

PDB ID : 9S5A / pdb_00009s5a
EMDB ID : EMD-54593
Title : Down class, Apo-state RyR1 in the native membrane solved by StA
Authors : Mikirtumov, V.
Deposited on : 2025-07-29
Resolution : 5.98 Å(reported)
Based on initial model : 7tzc

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

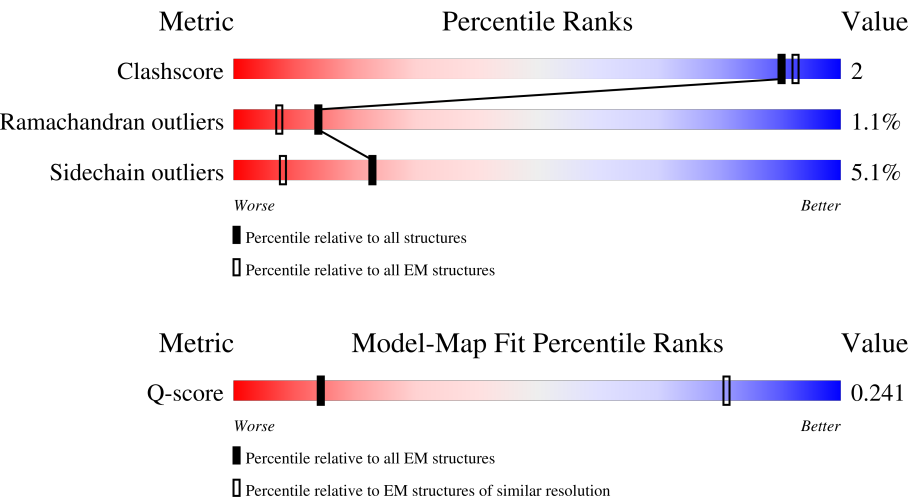
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 5.98 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	-
Q-score	-	25397	474 (5.48 - 6.48)

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	5037	10% 78% 9% 13%
1	B	5037	10% 77% 9% 13%
1	C	5037	10% 77% 9% 13%
1	D	5037	10% 77% 9% 13%

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Mol	Chain	Length	Quality of chain
2	E	108	12% 88% 10% ..
2	F	108	12% 90% 8% ..
2	G	108	14% 89% 9% ..
2	H	108	12% 88% 10% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 285956 atoms, of which 142276 are hydrogens and 0 are deuteriums.

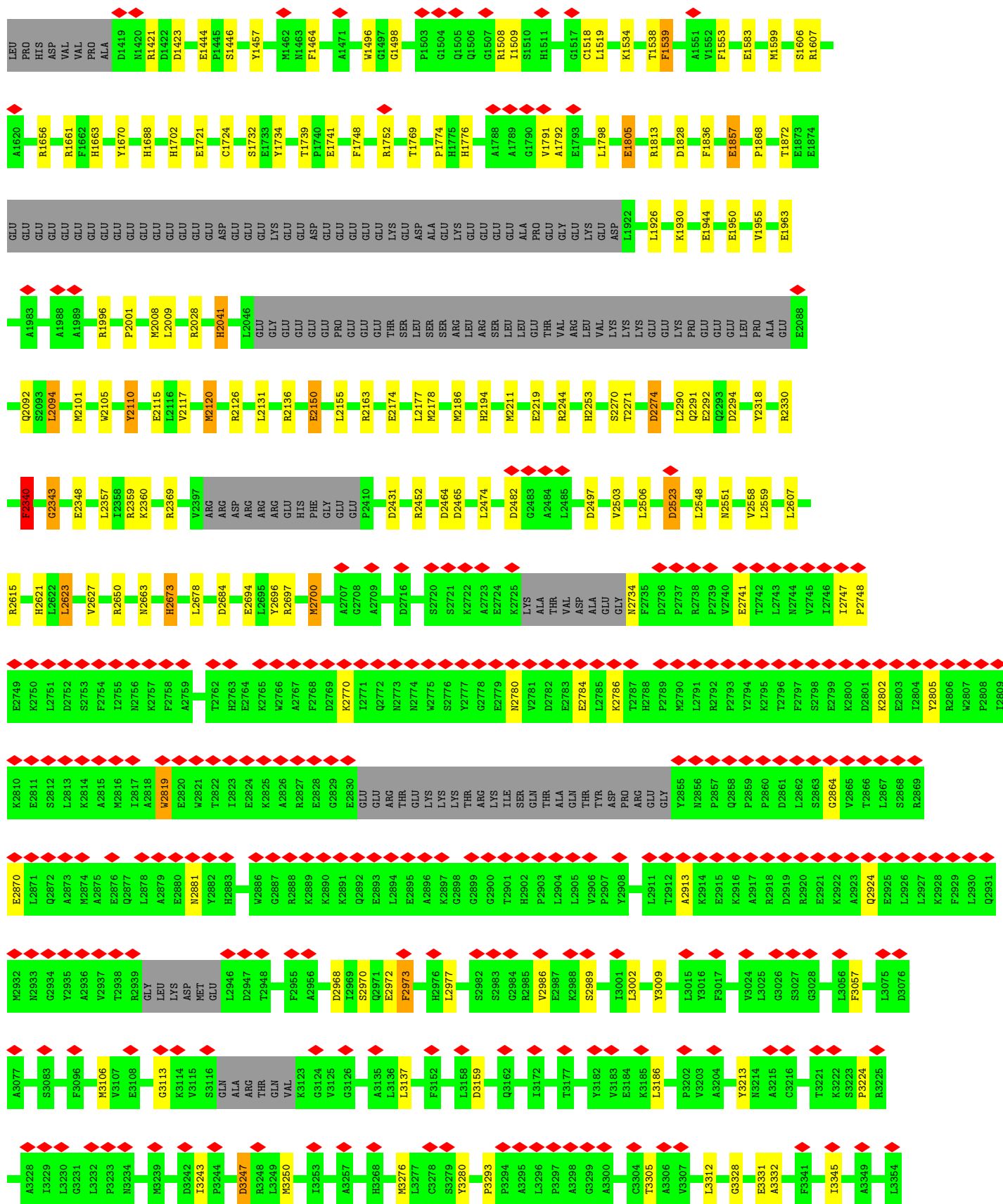
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

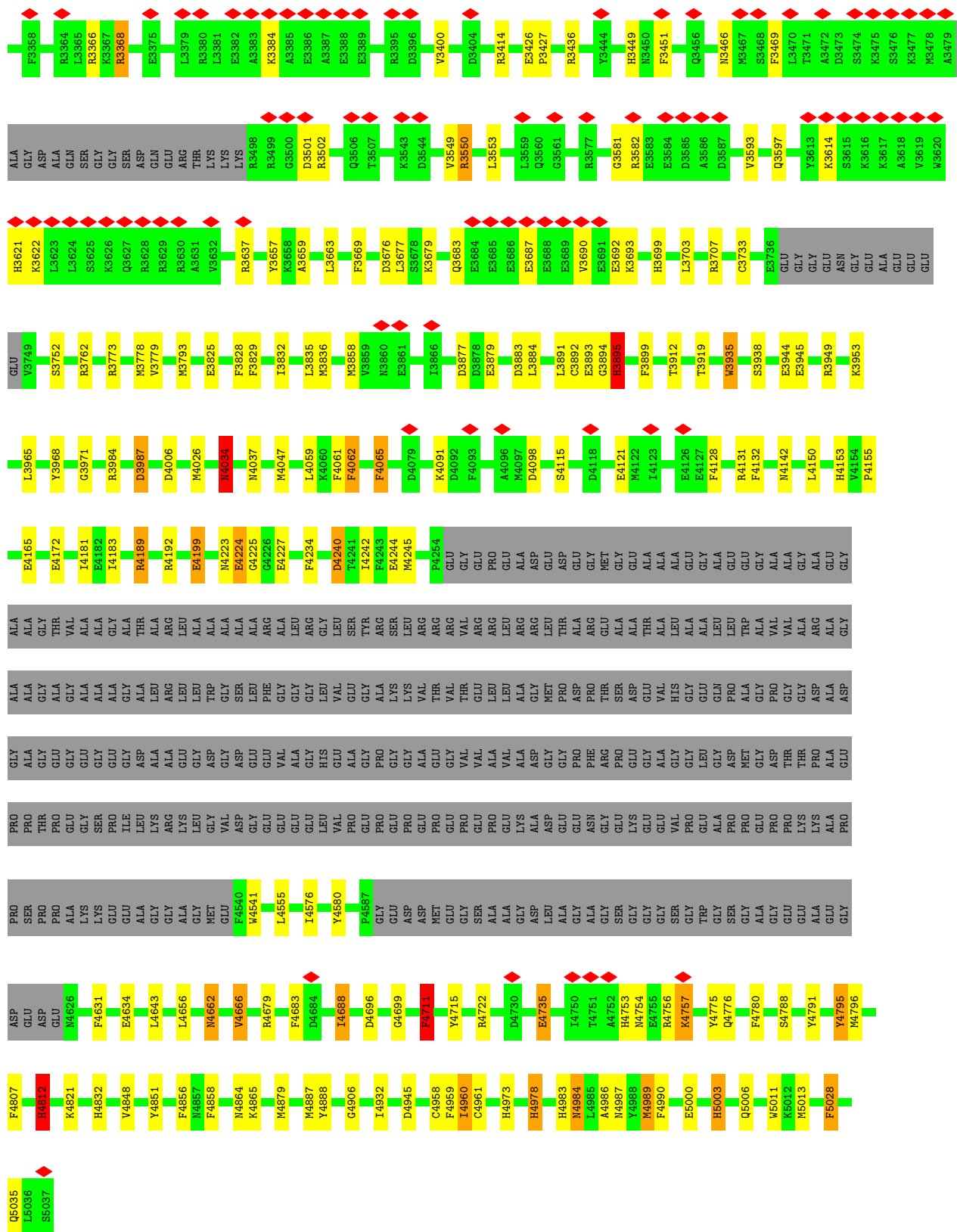
- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	4404	Total	C	H	N	O	S	0	0
			69828	22323	34740	6046	6482	237		
1	B	4404	Total	C	H	N	O	S	0	0
			69828	22323	34740	6046	6482	237		
1	C	4404	Total	C	H	N	O	S	0	0
			69828	22323	34740	6046	6482	237		
1	D	4404	Total	C	H	N	O	S	0	0
			69828	22323	34740	6046	6482	237		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

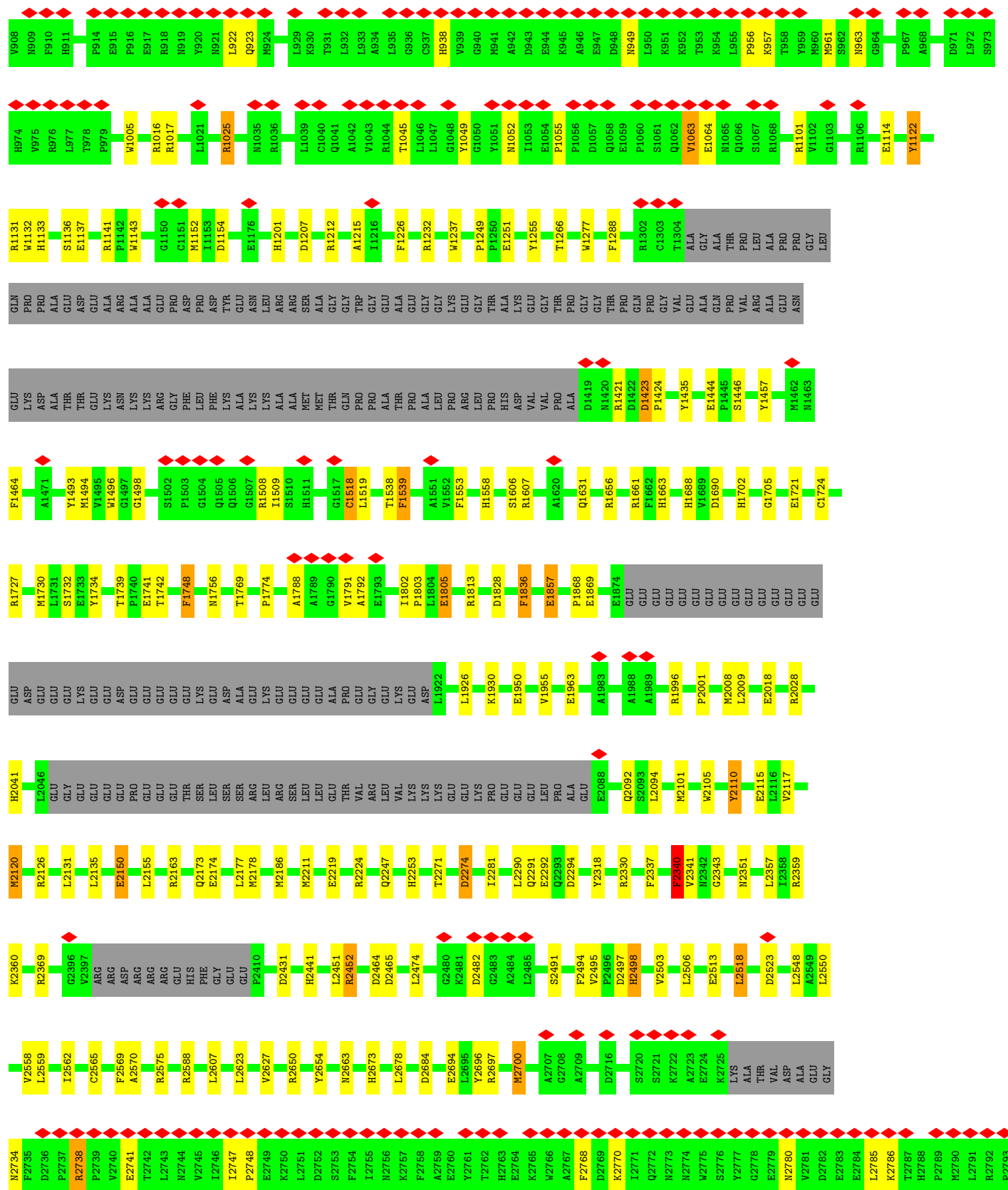
Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	F	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	G	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	H	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		



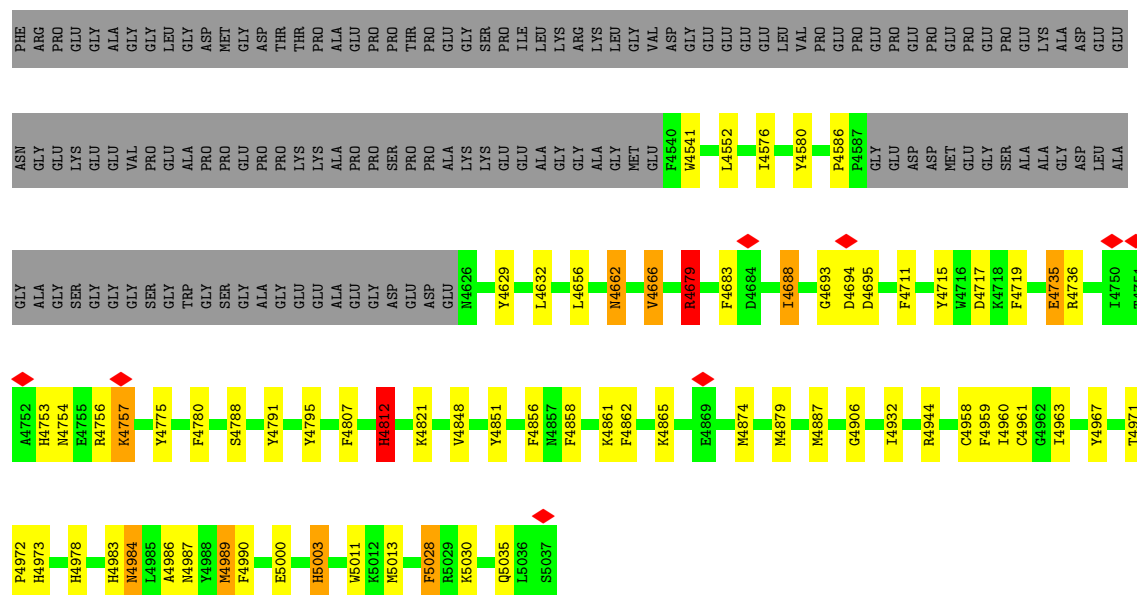




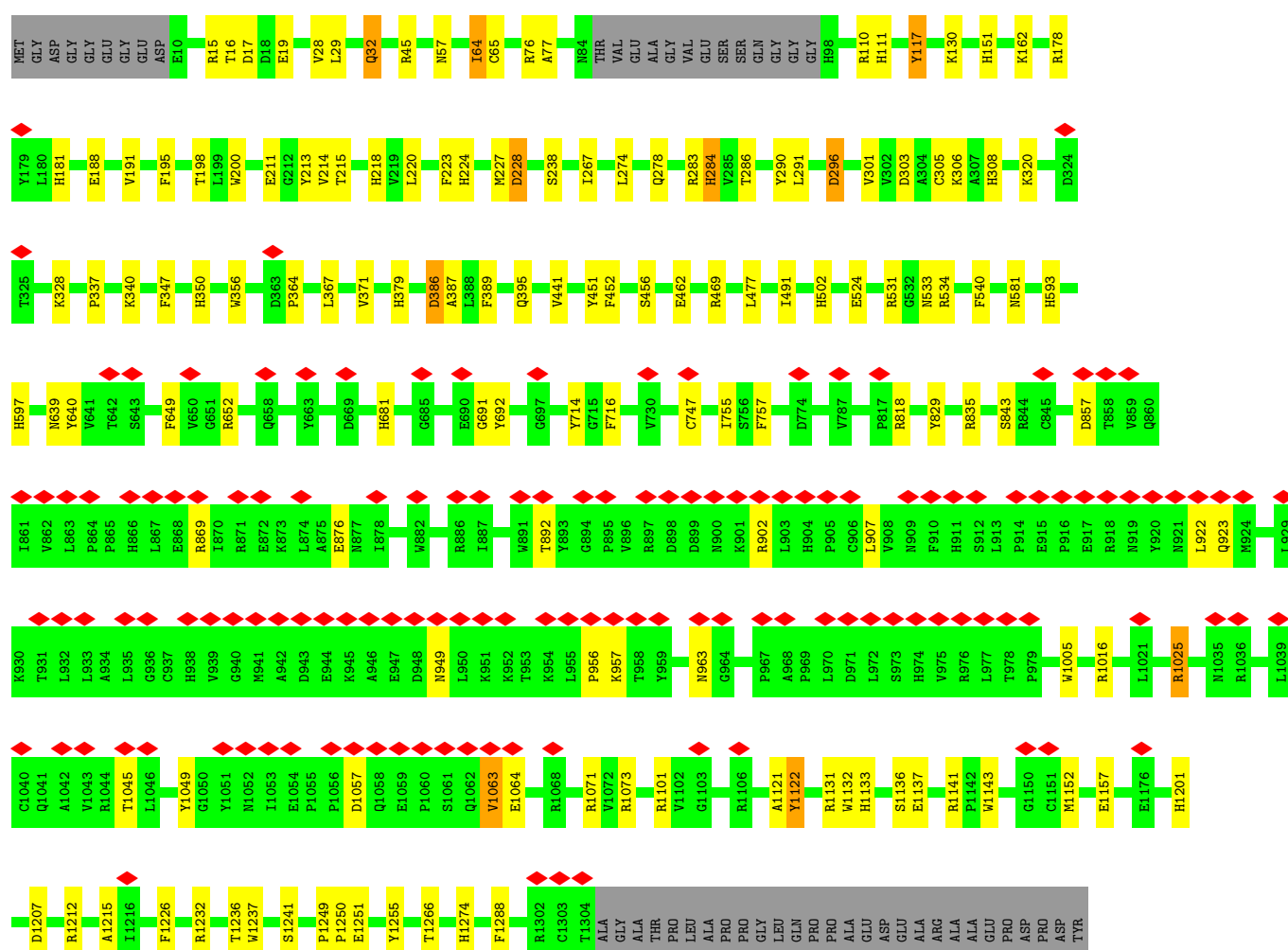
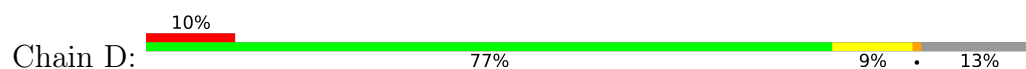


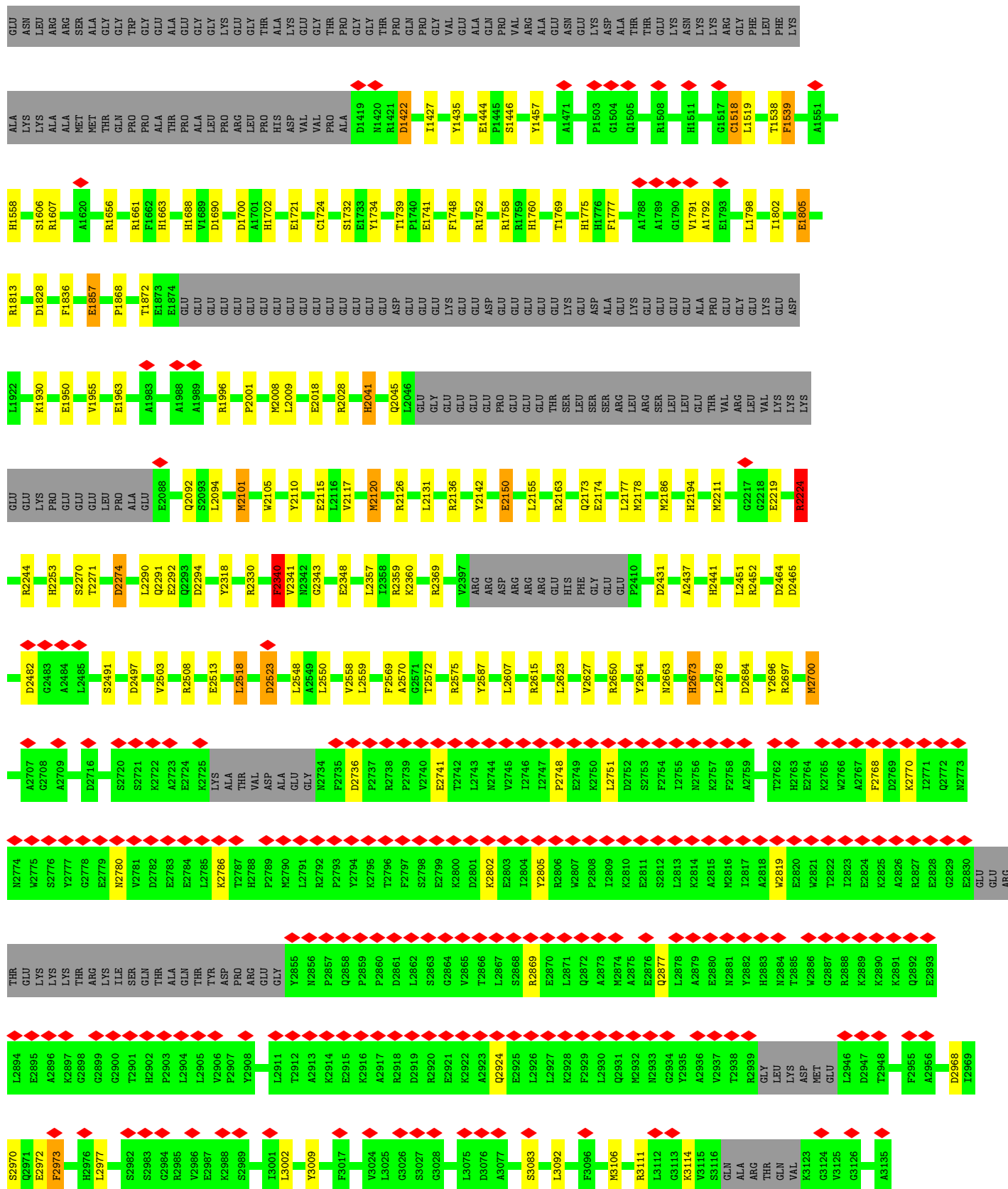






• Molecule 1: Ryanodine receptor 1

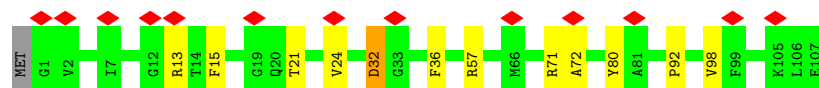
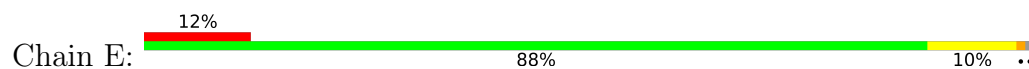




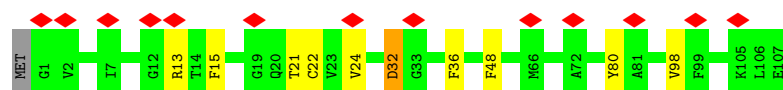
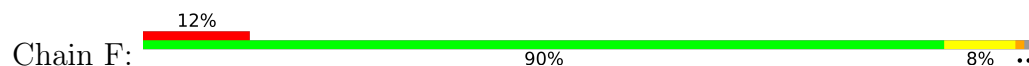




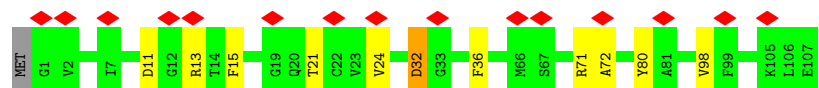
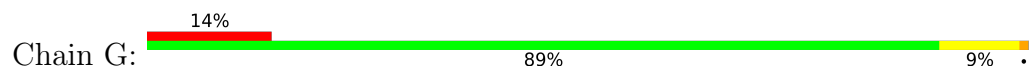
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



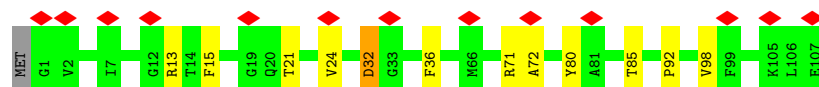
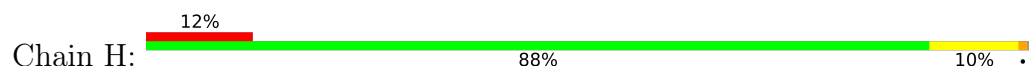
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



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4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of subtomograms used	4402	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 ($e^-/\text{\AA}^2$)	132	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	64000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.639	Depositor
Minimum map value	-0.367	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.0795	Depositor
Map size (Å)	496.74, 496.74, 496.74	wwPDB
Map dimensions	170, 170, 170	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.922, 2.922, 2.922	Depositor

5 Model quality

5.1 Standard geometry

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	0.78	0/35885	1.38	147/48603 (0.3%)
1	B	0.78	0/35885	1.38	147/48603 (0.3%)
1	C	0.78	0/35885	1.38	153/48603 (0.3%)
1	D	0.78	0/35885	1.39	142/48603 (0.3%)
2	E	0.79	1/851 (0.1%)	1.44	6/1146 (0.5%)
2	F	0.79	0/851	1.42	3/1146 (0.3%)
2	G	0.79	0/851	1.43	4/1146 (0.3%)
2	H	0.80	1/851 (0.1%)	1.44	4/1146 (0.3%)
All	All	0.78	2/146944 (0.0%)	1.38	606/198996 (0.3%)

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	45
1	B	0	44
1	C	0	38
1	D	0	39
2	E	0	1
2	G	0	1
2	H	0	1
All	All	0	169

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	92	PRO	CA-C	5.10	1.54	1.51
2	E	92	PRO	CA-C	5.06	1.54	1.51

All (606) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5028	PHE	CA-CB-CG	9.78	123.58	113.80
1	B	5028	PHE	CA-CB-CG	9.49	123.29	113.80
1	C	5028	PHE	CA-CB-CG	9.10	122.90	113.80
1	D	5028	PHE	CA-CB-CG	8.89	122.69	113.80
1	C	2340	PHE	CA-CB-CG	8.69	122.49	113.80
1	D	4240	ASP	CA-CB-CG	8.24	120.84	112.60
1	B	2340	PHE	CA-CB-CG	8.16	121.96	113.80
1	A	4240	ASP	CA-CB-CG	8.07	120.67	112.60
1	C	4240	ASP	CA-CB-CG	8.07	120.67	112.60
1	D	2340	PHE	CA-CB-CG	8.03	121.83	113.80
1	B	4240	ASP	CA-CB-CG	7.88	120.48	112.60
1	B	3293	PRO	N-CA-C	7.83	120.25	110.70
1	A	2340	PHE	CA-CB-CG	7.74	121.54	113.80
1	D	1422	ASP	CA-CB-CG	7.70	120.30	112.60
1	B	2523	ASP	CA-CB-CG	7.63	120.23	112.60
1	B	76	ARG	NE-CZ-NH2	7.63	126.07	119.20
1	B	3878	ASP	CA-CB-CG	7.37	119.97	112.60
1	D	3878	ASP	CA-CB-CG	7.33	119.92	112.60
1	A	3829	PHE	CA-CB-CG	-7.24	106.56	113.80
1	B	4065	PHE	CA-CB-CG	7.24	121.04	113.80
1	C	2684	ASP	CA-CB-CG	7.22	119.82	112.60
1	A	2523	ASP	CA-CB-CG	7.20	119.80	112.60
1	C	3293	PRO	N-CA-C	7.16	119.44	110.70
1	C	3829	PHE	CA-CB-CG	-7.15	106.65	113.80
1	A	1553	PHE	CA-CB-CG	7.12	120.92	113.80
1	B	3829	PHE	CA-CB-CG	-7.08	106.72	113.80
1	D	76	ARG	NE-CZ-NH2	7.07	125.57	119.20
1	D	3829	PHE	CA-CB-CG	-7.05	106.75	113.80
1	D	2523	ASP	CA-CB-CG	7.01	119.61	112.60
1	C	2968	ASP	CA-CB-CG	6.98	119.58	112.60
1	D	3987	ASP	CA-CB-CG	6.93	119.53	112.60
1	A	3293	PRO	N-CA-C	6.89	119.10	110.70
1	D	3934	TYR	N-CA-C	6.87	118.45	110.97
2	H	32	ASP	CA-CB-CG	6.86	119.46	112.60
1	A	3987	ASP	CA-CB-CG	6.85	119.45	112.60
1	A	3945	GLU	N-CA-C	6.84	118.74	111.28
1	A	1663	HIS	CA-CB-CG	-6.80	107.00	113.80
1	B	1663	HIS	CA-CB-CG	-6.79	107.00	113.80
1	B	3934	TYR	N-CA-C	6.79	118.34	111.07
1	A	2684	ASP	CA-CB-CG	6.76	119.36	112.60
2	F	32	ASP	CA-CB-CG	6.73	119.33	112.60
1	B	4098	ASP	CA-CB-CG	6.69	119.29	112.60
1	A	4858	PHE	CA-CB-CG	-6.68	107.12	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3301	PRO	N-CA-CB	6.65	106.91	103.19
1	C	1663	HIS	CA-CB-CG	-6.62	107.17	113.80
1	D	2684	ASP	CA-CB-CG	6.60	119.20	112.60
1	A	4683	PHE	CA-CB-CG	-6.60	107.20	113.80
1	A	1288	PHE	CA-CB-CG	6.57	120.37	113.80
1	A	3502	ARG	NE-CZ-NH2	6.57	125.11	119.20
2	G	32	ASP	CA-CB-CG	6.57	119.17	112.60
1	B	4858	PHE	CA-CB-CG	-6.55	107.25	113.80
1	D	4858	PHE	CA-CB-CG	-6.55	107.25	113.80
1	A	2968	ASP	CA-CB-CG	6.55	119.15	112.60
1	D	1813	ARG	NE-CZ-NH2	6.54	125.09	119.20
1	C	3945	GLU	N-CA-C	6.53	118.40	111.28
1	D	2968	ASP	CA-CB-CG	6.53	119.13	112.60
1	C	1813	ARG	NE-CZ-NH2	6.52	125.06	119.20
1	B	1288	PHE	CA-CB-CG	6.51	120.31	113.80
1	A	1813	ARG	NE-CZ-NH2	6.51	125.06	119.20
2	H	15	PHE	CA-CB-CG	6.51	120.31	113.80
1	D	3368	ARG	NE-CZ-NH2	6.50	125.05	119.20
1	A	76	ARG	NE-CZ-NH2	6.50	125.05	119.20
1	B	1813	ARG	NE-CZ-NH2	6.49	125.04	119.20
1	B	2968	ASP	CA-CB-CG	6.48	119.08	112.60
1	C	4098	ASP	CA-CB-CG	6.47	119.07	112.60
1	A	4065	PHE	CA-CB-CG	6.46	120.26	113.80
1	D	4131	ARG	NE-CZ-NH2	6.46	125.01	119.20
1	D	3293	PRO	N-CA-C	6.46	118.58	110.70
1	D	1288	PHE	CA-CB-CG	6.46	120.26	113.80
1	A	4945	ASP	N-CA-CB	-6.45	100.64	110.12
1	B	3883	ASP	CA-CB-CG	6.45	119.05	112.60
1	D	45	ARG	NE-CZ-NH2	6.45	125.00	119.20
1	D	3883	ASP	CA-CB-CG	6.45	119.05	112.60
1	C	3502	ARG	NE-CZ-NH2	6.43	124.98	119.20
1	B	533	ASN	CA-CB-CG	-6.38	106.22	112.60
1	D	1057	ASP	CA-CB-CG	6.37	118.97	112.60
1	A	4945	ASP	CA-CB-CG	6.35	118.95	112.60
2	F	15	PHE	CA-CB-CG	6.35	120.15	113.80
1	C	4858	PHE	CA-CB-CG	-6.35	107.45	113.80
1	C	1288	PHE	CA-CB-CG	6.34	120.14	113.80
1	C	3368	ARG	NE-CZ-NH2	6.34	124.91	119.20
1	A	533	ASN	CA-CB-CG	-6.34	106.26	112.60
1	D	1663	HIS	CA-CB-CG	-6.33	107.47	113.80
1	B	5028	PHE	N-CA-CB	-6.33	99.46	109.78
1	C	1553	PHE	CA-CB-CG	6.33	120.13	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	32	ASP	CA-CB-CG	6.33	118.92	112.60
1	A	4098	ASP	CA-CB-CG	6.30	118.90	112.60
1	C	5028	PHE	N-CA-CB	-6.30	99.84	110.49
1	D	3502	ARG	NE-CZ-NH2	6.29	124.86	119.20
1	C	4131	ARG	NE-CZ-NH2	6.29	124.86	119.20
1	B	178	ARG	NE-CZ-NH2	6.29	124.86	119.20
1	A	261	ARG	NE-CZ-NH2	6.28	124.85	119.20
1	C	533	ASN	CA-CB-CG	-6.28	106.32	112.60
1	A	3368	ARG	NE-CZ-NH2	6.27	124.85	119.20
1	B	4225	GLY	CA-C-N	6.27	126.44	121.61
1	B	4225	GLY	C-N-CA	6.27	126.44	121.61
1	D	2359	ARG	NE-CZ-NH2	6.27	124.84	119.20
1	D	4065	PHE	CA-CB-CG	6.27	120.07	113.80
1	C	3287	ARG	NE-CZ-NH2	6.27	124.84	119.20
1	D	3443	ILE	CB-CA-C	-6.24	103.71	112.14
1	B	3368	ARG	NE-CZ-NH2	6.23	124.81	119.20
1	C	4683	PHE	CA-CB-CG	-6.22	107.58	113.80
1	A	178	ARG	NE-CZ-NH2	6.21	124.79	119.20
1	D	228	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	2136	ARG	NE-CZ-NH2	6.20	124.78	119.20
1	A	1057	ASP	CA-CB-CG	6.19	118.79	112.60
1	D	3945	GLU	N-CA-C	6.17	118.01	111.28
1	C	76	ARG	NE-CZ-NH2	6.17	124.75	119.20
1	C	2523	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	4832	HIS	CA-CB-CG	-6.16	107.64	113.80
1	A	284	HIS	CA-CB-CG	-6.16	107.64	113.80
1	B	3945	GLU	N-CA-C	6.16	117.99	111.28
1	D	1828	ASP	CA-CB-CG	6.15	118.75	112.60
1	B	350	HIS	CA-CB-CG	-6.15	107.65	113.80
1	C	1836	PHE	CA-CB-CG	6.14	119.94	113.80
1	C	3883	ASP	CA-CB-CG	6.14	118.74	112.60
1	B	2684	ASP	CA-CB-CG	6.13	118.73	112.60
1	D	2274	ASP	CA-CB-CG	6.13	118.73	112.60
1	C	4225	GLY	CA-C-N	6.13	126.33	121.61
1	C	4225	GLY	C-N-CA	6.13	126.33	121.61
1	D	4945	ASP	N-CA-CB	-6.13	101.11	110.12
1	A	2741	GLU	CA-C-N	6.13	130.40	120.60
1	A	2741	GLU	C-N-CA	6.13	130.40	120.60
1	B	2136	ARG	NE-CZ-NH2	6.13	124.71	119.20
1	A	3883	ASP	CA-CB-CG	6.12	118.72	112.60
1	A	1828	ASP	CA-CB-CG	6.11	118.71	112.60
1	D	2973	PHE	CA-CB-CG	6.09	119.89	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	818	ARG	NE-CZ-NH2	6.08	124.67	119.20
1	A	2359	ARG	NE-CZ-NH2	6.08	124.67	119.20
1	D	4683	PHE	CA-CB-CG	-6.05	107.75	113.80
1	B	1131	ARG	NE-CZ-NH2	6.05	124.64	119.20
1	D	818	ARG	NE-CZ-NH2	6.05	124.64	119.20
1	C	2359	ARG	NE-CZ-NH2	6.03	124.63	119.20
1	B	2274	ASP	CA-CB-CG	6.03	118.63	112.60
1	B	4683	PHE	CA-CB-CG	-6.03	107.78	113.80
1	A	5028	PHE	N-CA-CB	-6.02	99.97	109.78
1	C	1017	ARG	NE-CZ-NH2	6.01	124.61	119.20
1	C	502	HIS	CA-CB-CG	6.01	119.81	113.80
1	A	818	ARG	NE-CZ-NH2	6.00	124.60	119.20
1	B	350	HIS	CB-CG-CD2	-6.00	123.40	131.20
1	A	399	GLN	N-CA-CB	-5.99	101.32	110.01
1	C	284	HIS	CA-CB-CG	-5.99	107.81	113.80
1	D	502	HIS	CA-CB-CG	5.97	119.77	113.80
1	A	2274	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	3935	TRP	N-CA-C	5.95	117.76	111.28
1	B	3301	PRO	N-CA-CB	5.94	106.52	103.19
1	D	533	ASN	CA-CB-CG	-5.93	106.67	112.60
1	D	2136	ARG	NE-CZ-NH2	5.93	124.54	119.20
1	C	1828	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	284	HIS	CB-CG-CD2	-5.91	123.51	131.20
1	B	227	MET	CA-C-N	5.90	128.47	120.44
1	B	227	MET	C-N-CA	5.90	128.47	120.44
1	A	1212	ARG	NE-CZ-NH2	5.90	124.51	119.20
1	B	2360	LYS	CA-C-N	5.89	125.59	119.82
1	B	2360	LYS	C-N-CA	5.89	125.59	119.82
1	A	4984	ASN	CA-CB-CG	-5.88	106.72	112.60
1	D	5028	PHE	N-CA-CB	-5.88	100.20	109.78
1	D	4098	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	2802	LYS	N-CA-C	5.87	120.59	112.90
1	C	228	ASP	CA-CB-CG	5.87	118.47	112.60
1	D	350	HIS	CB-CG-CD2	-5.87	123.57	131.20
1	A	45	ARG	NE-CZ-NH2	5.86	124.48	119.20
1	C	4807	PHE	CA-CB-CG	-5.86	107.94	113.80
1	D	2360	LYS	CA-C-N	5.86	125.56	119.82
1	D	2360	LYS	C-N-CA	5.86	125.56	119.82
1	C	2360	LYS	CA-C-N	5.85	125.55	119.82
1	C	2360	LYS	C-N-CA	5.85	125.55	119.82
1	B	2359	ARG	NE-CZ-NH2	5.84	124.45	119.20
1	A	1101	ARG	NE-CZ-NH2	5.83	124.45	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	ASP	CA-CB-CG	5.83	118.43	112.60
1	C	3436	ARG	NE-CZ-NH2	5.83	124.45	119.20
1	A	1836	PHE	CA-CB-CG	5.83	119.63	113.80
1	C	178	ARG	NE-CZ-NH2	5.83	124.44	119.20
1	B	3501	ASP	CA-CB-CG	5.83	118.43	112.60
1	D	540	PHE	CA-CB-CG	-5.83	107.97	113.80
1	B	2126	ARG	NE-CZ-NH2	5.82	124.44	119.20
1	B	4984	ASN	CA-CB-CG	-5.82	106.78	112.60
1	C	2163	ARG	NE-CZ-NH2	5.82	124.44	119.20
1	B	4807	PHE	CA-CB-CG	-5.82	107.98	113.80
1	C	284	HIS	CB-CG-CD2	-5.82	123.64	131.20
1	D	15	ARG	NE-CZ-NH2	5.81	124.43	119.20
1	C	4984	ASN	CA-CB-CG	-5.81	106.79	112.60
1	A	350	HIS	CB-CG-CD2	-5.81	123.65	131.20
1	C	1212	ARG	NE-CZ-NH2	5.81	124.43	119.20
1	B	3502	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	C	818	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	D	2163	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	C	45	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	B	17	ASP	CA-CB-CG	5.78	118.38	112.60
1	D	2741	GLU	CA-C-N	5.77	129.83	120.60
1	D	2741	GLU	C-N-CA	5.77	129.83	120.60
1	B	2747	ILE	N-CA-C	5.77	114.86	108.05
1	B	45	ARG	NE-CZ-NH2	5.76	124.39	119.20
1	B	4192	ARG	NE-CZ-NH2	5.76	124.39	119.20
1	D	3669	PHE	CA-C-N	5.76	128.00	120.28
1	D	3669	PHE	C-N-CA	5.76	128.00	120.28
1	C	2274	ASP	CA-CB-CG	5.75	118.36	112.60
1	C	3858	MET	N-CA-C	5.75	117.75	110.33
1	B	3858	MET	N-CA-C	5.75	117.48	110.41
1	C	1131	ARG	NE-CZ-NH2	5.75	124.37	119.20
1	D	284	HIS	CB-CG-CD2	-5.74	123.73	131.20
1	A	4192	ARG	NE-CZ-NH2	5.74	124.36	119.20
1	B	284	HIS	CA-CB-CG	-5.73	108.07	113.80
1	A	2973	PHE	CA-CB-CG	5.73	119.53	113.80
1	A	220	LEU	N-CA-C	5.72	116.95	108.60
1	A	2163	ARG	NE-CZ-NH2	5.72	124.35	119.20
2	G	24	VAL	N-CA-C	5.71	116.59	108.42
1	A	3984	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	B	2741	GLU	CA-C-N	5.71	130.25	120.72
1	B	2741	GLU	C-N-CA	5.71	130.25	120.72
1	B	2163	ARG	NE-CZ-NH2	5.70	124.33	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2869	ARG	NE-CZ-NH2	5.70	124.33	119.20
2	F	24	VAL	N-CA-C	5.70	116.57	108.42
1	A	2126	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	B	4662	ASN	CA-CB-CG	5.70	118.30	112.60
1	C	350	HIS	CB-CG-CD2	-5.70	123.79	131.20
1	B	2973	PHE	CA-CB-CG	5.70	119.50	113.80
1	C	2747	ILE	N-CA-C	5.70	114.10	107.89
1	A	1131	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	A	2360	LYS	CA-C-N	5.68	125.39	119.82
1	A	2360	LYS	C-N-CA	5.68	125.39	119.82
1	C	4065	PHE	CA-CB-CG	5.68	119.48	113.80
1	A	218	HIS	CB-CG-CD2	-5.68	123.81	131.20
1	B	1828	ASP	CA-CB-CG	5.68	118.28	112.60
1	D	1690	ASP	N-CA-C	5.68	117.24	109.18
1	B	228	ASP	CA-CB-CG	5.67	118.27	112.60
1	C	681	HIS	CB-CG-CD2	-5.67	123.83	131.20
1	C	2741	GLU	CA-C-N	5.67	129.67	120.60
1	C	2741	GLU	C-N-CA	5.67	129.67	120.60
1	D	4225	GLY	CA-C-N	5.66	126.84	121.46
1	D	4225	GLY	C-N-CA	5.66	126.84	121.46
1	B	502	HIS	CA-CB-CG	5.66	119.46	113.80
1	A	19	GLU	CB-CA-C	5.66	119.09	109.53
1	A	296	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	1017	ARG	NE-CZ-NH2	5.66	124.29	119.20
1	D	3858	MET	N-CA-C	5.66	118.00	110.53
1	D	178	ARG	NE-CZ-NH2	5.66	124.29	119.20
1	D	284	HIS	CA-CB-CG	-5.66	108.14	113.80
1	D	4192	ARG	NE-CZ-NH2	5.66	124.29	119.20
1	C	181	HIS	N-CA-C	5.65	118.77	109.72
1	A	4864	ASN	CA-CB-CG	-5.65	106.95	112.60
1	D	386	ASP	CA-CB-CG	5.65	118.25	112.60
1	D	3451	PHE	CA-CB-CG	5.65	119.45	113.80
1	C	4142	ASN	CA-CB-CG	-5.64	106.96	112.60
1	D	1131	ARG	NE-CZ-NH2	5.63	124.27	119.20
1	B	1553	PHE	CA-CB-CG	5.62	119.42	113.80
1	D	1836	PHE	CA-CB-CG	5.62	119.42	113.80
1	D	4989	MET	CB-CA-C	5.62	119.71	110.88
1	D	1955	VAL	N-CA-CB	-5.62	103.97	110.55
1	B	2001	PRO	CA-C-N	5.62	124.81	118.97
1	B	2001	PRO	C-N-CA	5.62	124.81	118.97
1	D	4812	HIS	CB-CG-CD2	-5.62	123.89	131.20
1	A	4812	HIS	CB-CG-CD2	-5.62	123.90	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4989	MET	CB-CA-C	5.62	119.70	110.88
1	B	111	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	C	4662	ASN	CA-CB-CG	5.61	118.21	112.60
1	D	681	HIS	CB-CG-CD2	-5.60	123.92	131.20
1	B	284	HIS	CB-CG-CD2	-5.60	123.92	131.20
1	A	4989	MET	CB-CA-C	5.60	119.67	110.88
1	D	4984	ASN	CA-CB-CG	-5.59	107.01	112.60
1	D	111	HIS	CB-CG-CD2	-5.59	123.94	131.20
1	C	2650	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	C	533	ASN	N-CA-C	5.58	117.50	108.41
1	C	4736	ARG	NE-CZ-NH2	5.57	124.22	119.20
1	D	4142	ASN	CA-CB-CG	-5.57	107.03	112.60
1	C	1101	ARG	NE-CZ-NH2	5.57	124.21	119.20
1	B	2884	ASN	CA-CB-CG	5.57	118.17	112.60
1	C	3426	GLU	CA-C-N	5.56	126.79	119.84
1	C	3426	GLU	C-N-CA	5.56	126.79	119.84
1	B	2028	ARG	NE-CZ-NH2	5.55	124.20	119.20
1	B	3426	GLU	CA-C-N	5.55	126.78	119.84
1	B	3426	GLU	C-N-CA	5.55	126.78	119.84
1	B	218	HIS	CB-CG-CD2	-5.55	123.99	131.20
1	B	1690	ASP	N-CA-C	5.55	117.06	109.18
1	C	151	HIS	CB-CG-CD2	-5.55	123.99	131.20
1	B	1423	ASP	CA-C-N	5.54	125.38	119.28
1	B	1423	ASP	C-N-CA	5.54	125.38	119.28
1	C	169	LEU	N-CA-C	5.54	118.59	109.85
1	C	3443	ILE	CB-CA-C	-5.54	104.67	112.14
2	H	24	VAL	N-CA-C	5.54	116.34	108.42
1	C	1423	ASP	N-CA-C	5.53	117.64	109.62
1	C	296	ASP	CA-CB-CG	5.53	118.13	112.60
1	D	949	ASN	CA-CB-CG	5.53	118.13	112.60
1	A	2673	HIS	CB-CG-CD2	-5.52	124.02	131.20
1	A	681	HIS	CB-CG-CD2	-5.52	124.03	131.20
1	C	220	LEU	N-CA-C	5.52	116.66	108.60
1	C	540	PHE	CA-CB-CG	-5.51	108.29	113.80
1	C	1055	PRO	N-CA-CB	5.51	106.28	103.19
1	C	4944	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	B	1274	HIS	CA-CB-CG	-5.50	108.30	113.80
1	C	4180	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	D	1656	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	B	4989	MET	CB-CA-C	5.49	119.50	110.88
1	A	4807	PHE	CA-CB-CG	-5.49	108.31	113.80
1	B	1836	PHE	CA-CB-CG	5.49	119.29	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	681	HIS	CB-CG-CD2	-5.49	124.07	131.20
1	D	3426	GLU	CA-C-N	5.47	126.68	119.84
1	D	3426	GLU	C-N-CA	5.47	126.68	119.84
1	D	181	HIS	N-CA-C	5.47	118.49	109.85
1	B	2551	ASN	CA-CB-CG	5.47	118.07	112.60
1	B	4784	PHE	CA-CB-CG	5.47	119.27	113.80
1	A	1232	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	A	111	HIS	CB-CG-CD2	-5.46	124.10	131.20
1	B	3451	PHE	CA-CB-CG	5.46	119.26	113.80
1	A	2028	ARG	NE-CZ-NH2	5.46	124.11	119.20
1	C	1690	ASP	N-CA-C	5.45	116.92	109.18
1	D	2802	LYS	N-CA-C	5.45	120.04	112.90
1	B	533	ASN	N-CA-C	5.45	117.29	108.41
1	A	1423	ASP	CA-C-N	5.45	125.27	119.28
1	A	1423	ASP	C-N-CA	5.45	125.27	119.28
1	C	3773	ARG	NE-CZ-NH2	5.45	124.10	119.20
1	B	4812	HIS	CB-CG-CD2	-5.44	124.12	131.20
1	D	220	LEU	N-CA-C	5.44	116.55	108.60
1	B	1223	PHE	CA-CB-CG	5.44	119.24	113.80
1	B	1955	VAL	N-CA-CB	-5.44	104.19	110.55
1	D	3906	GLN	OE1-CD-NE2	-5.44	117.16	122.60
1	C	263	GLU	CA-C-N	5.43	126.19	120.11
1	C	263	GLU	C-N-CA	5.43	126.19	120.11
1	B	4722	ARG	NE-CZ-NH2	5.43	124.08	119.20
1	D	296	ASP	CA-CB-CG	5.43	118.03	112.60
1	D	2224	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	C	117	TYR	N-CA-C	5.42	118.29	109.24
1	D	2001	PRO	CA-C-N	5.42	124.61	118.97
1	D	2001	PRO	C-N-CA	5.42	124.61	118.97
1	B	1212	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	B	1214	PHE	CA-CB-CG	5.42	119.22	113.80
1	A	117	TYR	N-CA-C	5.42	118.29	109.24
1	C	4812	HIS	CB-CG-CD2	-5.42	124.16	131.20
1	A	1423	ASP	N-CA-C	5.42	117.47	109.62
1	C	2126	ARG	NE-CZ-NH2	5.42	124.07	119.20
1	C	3054	VAL	N-CA-C	5.41	116.04	110.36
1	D	3436	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	B	540	PHE	CA-CB-CG	-5.41	108.39	113.80
1	D	3935	TRP	N-CA-C	5.41	117.93	111.71
2	E	24	VAL	N-CA-C	5.41	116.15	108.42
1	A	869	ARG	NE-CZ-NH2	5.41	124.06	119.20
1	B	2574	HIS	CB-CG-CD2	-5.41	124.17	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	HIS	N-CA-C	5.40	118.39	109.85
2	E	72	ALA	N-CA-C	5.40	116.19	108.74
1	C	2884	ASN	CA-CB-CG	5.40	118.00	112.60
1	C	2673	HIS	CB-CG-CD2	-5.39	124.19	131.20
1	A	4666	VAL	N-CA-CB	-5.39	106.91	110.52
1	B	869	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	D	593	HIS	CB-CG-CD2	-5.39	124.19	131.20
2	E	15	PHE	CA-CB-CG	5.39	119.19	113.80
1	B	1423	ASP	N-CA-C	5.39	117.43	109.62
1	C	240	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	3366	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	D	5003	HIS	CB-CG-CD2	-5.38	124.20	131.20
1	D	456	SER	N-CA-C	5.38	118.08	110.50
1	B	296	ASP	CA-CB-CG	5.37	117.97	112.60
1	D	117	TYR	N-CA-C	5.37	118.21	109.24
1	A	2041	HIS	CB-CG-CD2	-5.37	124.22	131.20
1	C	2001	PRO	CA-C-N	5.37	124.55	118.97
1	C	2001	PRO	C-N-CA	5.37	124.55	118.97
1	B	19	GLU	CB-CA-C	5.37	118.60	109.53
1	B	4142	ASN	CA-CB-CG	-5.36	107.24	112.60
1	C	938	HIS	CB-CG-CD2	-5.36	124.23	131.20
1	D	2650	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	D	4757	LYS	N-CA-C	5.36	116.45	109.64
1	B	4224	GLU	N-CA-C	5.36	118.95	111.56
1	D	218	HIS	CB-CG-CD2	-5.36	124.24	131.20
1	D	1141	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	C	4125	PHE	N-CA-C	5.36	117.87	111.71
1	A	379	HIS	CB-CG-CD2	-5.35	124.24	131.20
1	A	1955	VAL	N-CA-CB	-5.35	104.29	110.55
1	A	2001	PRO	CA-C-N	5.34	124.53	118.97
1	A	2001	PRO	C-N-CA	5.34	124.53	118.97
1	A	540	PHE	CA-CB-CG	-5.34	108.46	113.80
1	B	3436	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	C	2041	HIS	CB-CG-CD2	-5.34	124.26	131.20
1	D	19	GLU	CB-CA-C	5.34	118.56	109.53
1	A	4142	ASN	CA-CB-CG	-5.34	107.26	112.60
1	B	1499	ASP	CA-CB-CG	5.34	117.94	112.60
1	D	2786	LYS	N-CA-C	5.34	119.09	112.47
1	D	4945	ASP	CA-CB-CG	5.34	117.94	112.60
1	B	181	HIS	N-CA-C	5.33	118.26	109.72
1	A	1791	VAL	CA-C-N	5.33	131.73	121.54
1	A	1791	VAL	C-N-CA	5.33	131.73	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	218	HIS	CB-CG-CD2	-5.33	124.28	131.20
1	D	1212	ARG	NE-CZ-NH2	5.33	123.99	119.20
1	D	4807	PHE	CA-CB-CG	-5.33	108.47	113.80
1	D	3773	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	A	1702	HIS	CB-CG-CD2	-5.32	124.29	131.20
1	B	69	LEU	N-CA-CB	-5.32	103.39	110.57
1	B	4679	ARG	NE-CZ-NH2	5.32	123.98	119.20
1	D	16	THR	N-CA-C	5.32	116.78	110.19
1	D	869	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	C	2973	PHE	CA-CB-CG	5.30	119.10	113.80
1	B	871	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	A	4225	GLY	CA-C-N	5.29	126.49	121.46
1	A	4225	GLY	C-N-CA	5.29	126.49	121.46
1	D	379	HIS	CB-CG-CD2	-5.29	124.32	131.20
1	D	1758	ARG	NE-CZ-NH2	5.29	123.97	119.20
1	A	1656	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	B	3223	SER	CA-C-N	5.29	126.45	119.84
1	B	3223	SER	C-N-CA	5.29	126.45	119.84
1	D	2126	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	B	151	HIS	CB-CG-CD2	-5.29	124.33	131.20
1	A	3895	HIS	CB-CG-CD2	-5.28	124.33	131.20
1	D	3283	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	A	4131	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	B	1690	ASP	CA-CB-CG	-5.27	107.33	112.60
1	D	1702	HIS	CB-CG-CD2	-5.27	124.34	131.20
1	D	2673	HIS	CB-CG-CD2	-5.27	124.35	131.20
1	B	3773	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	C	1869	GLU	N-CA-C	5.27	117.77	111.71
1	C	4666	VAL	N-CA-CB	-5.26	106.99	110.52
2	G	72	ALA	N-CA-C	5.26	116.00	108.74
1	C	593	HIS	CB-CG-CD2	-5.26	124.36	131.20
1	D	2194	HIS	CB-CG-CD2	-5.26	124.36	131.20
1	A	3773	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	A	1688	HIS	CA-CB-CG	-5.25	108.55	113.80
1	D	4662	ASN	CA-CB-CG	5.25	117.85	112.60
1	A	3858	MET	N-CA-C	5.25	117.46	110.53
1	B	4963	ILE	CA-C-N	5.25	125.33	120.34
1	B	4963	ILE	C-N-CA	5.25	125.33	120.34
1	D	2575	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	A	4722	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	B	2802	LYS	N-CA-C	5.25	119.81	113.41
1	C	2869	ARG	NE-CZ-NH2	5.25	123.92	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4224	GLU	N-CA-C	5.25	118.80	111.56
1	C	2247	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	B	1749	PRO	N-CA-CB	5.24	106.12	103.19
1	B	379	HIS	CB-CG-CD2	-5.24	124.39	131.20
1	C	1955	VAL	N-CA-CB	-5.24	104.42	110.55
1	D	1791	VAL	CA-C-N	5.24	131.54	121.54
1	D	1791	VAL	C-N-CA	5.24	131.54	121.54
1	D	2615	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	A	1274	HIS	CA-CB-CG	-5.23	108.57	113.80
2	E	57	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	A	949	ASN	CA-CB-CG	5.22	117.82	112.60
1	A	3733	CYS	N-CA-C	5.22	118.77	112.93
1	C	2224	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	A	3692	GLU	CA-C-N	5.22	131.50	121.54
1	A	3692	GLU	C-N-CA	5.22	131.50	121.54
1	A	5003	HIS	CB-CG-CD2	-5.21	124.43	131.20
1	A	2650	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	A	4662	ASN	CA-CB-CG	5.21	117.81	112.60
1	D	524	GLU	N-CA-CB	-5.21	102.46	110.01
1	D	1558	HIS	CB-CG-CD2	-5.21	124.43	131.20
1	D	2173	GLN	CA-C-N	5.20	128.21	120.31
1	D	2173	GLN	C-N-CA	5.20	128.21	120.31
1	B	1688	HIS	CA-CB-CG	-5.20	108.60	113.80
1	C	1688	HIS	CA-CB-CG	-5.20	108.60	113.80
1	C	1423	ASP	CA-C-N	5.20	125.00	119.28
1	C	1423	ASP	C-N-CA	5.20	125.00	119.28
1	C	2441	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	A	263	GLU	CA-C-N	5.19	125.93	120.11
1	A	263	GLU	C-N-CA	5.19	125.93	120.11
1	A	2747	ILE	N-CA-C	5.19	114.18	108.05
1	D	1274	HIS	CA-CB-CG	-5.19	108.61	113.80
1	D	2041	HIS	CB-CG-CD2	-5.19	124.46	131.20
1	D	3895	HIS	CB-CG-CD2	-5.19	124.46	131.20
1	A	17	ASP	CA-CB-CG	5.18	117.78	112.60
1	C	3366	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	C	3733	CYS	N-CA-C	5.18	118.46	112.97
1	A	1139	PHE	CA-CB-CG	-5.18	108.62	113.80
1	C	1201	HIS	CB-CG-CD2	-5.18	124.47	131.20
1	D	2736	ASP	CA-CB-CG	5.18	117.78	112.60
1	C	379	HIS	CB-CG-CD2	-5.17	124.47	131.20
1	D	4224	GLU	N-CA-C	5.17	118.70	111.56
1	C	2785	LEU	CA-C-N	5.17	130.68	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2785	LEU	C-N-CA	5.17	130.68	122.61
2	H	72	ALA	N-CA-C	5.17	116.15	108.86
1	C	4149	ASN	CA-CB-CG	-5.17	107.43	112.60
1	B	2676	ARG	NE-CZ-NH2	5.16	123.85	119.20
1	C	869	ARG	NE-CZ-NH2	5.16	123.85	119.20
1	B	1656	ARG	CA-C-N	5.16	127.20	120.28
1	B	1656	ARG	C-N-CA	5.16	127.20	120.28
1	B	2244	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	B	3692	GLU	CA-C-N	5.15	131.38	121.54
1	B	3692	GLU	C-N-CA	5.15	131.38	121.54
1	A	3762	ARG	NE-CZ-NH2	5.15	123.84	119.20
1	B	1558	HIS	CB-CG-CD2	-5.15	124.50	131.20
1	C	1631	GLN	OE1-CD-NE2	-5.15	117.45	122.60
1	C	4973	HIS	CB-CG-CD2	-5.15	124.51	131.20
1	A	4224	GLU	N-CA-C	5.15	118.66	111.56
1	C	2738	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	D	1201	HIS	CB-CG-CD2	-5.14	124.52	131.20
1	C	2173	GLN	CA-C-N	5.14	128.12	120.31
1	C	2173	GLN	C-N-CA	5.14	128.12	120.31
1	B	1041	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	C	4192	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	C	2498	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	A	1656	ARG	CA-C-N	5.13	127.16	120.28
1	A	1656	ARG	C-N-CA	5.13	127.16	120.28
1	C	5003	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	D	1232	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	A	4973	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	B	4728	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	C	3895	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	B	3283	ARG	NE-CZ-NH2	5.13	123.81	119.20
1	A	3436	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	C	4963	ILE	CA-C-N	5.12	125.21	120.34
1	C	4963	ILE	C-N-CA	5.12	125.21	120.34
1	D	1688	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	B	2482	ASP	N-CA-C	5.12	119.37	113.38
1	B	4153	HIS	CA-CB-CG	-5.12	108.68	113.80
1	C	1656	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	C	1748	PHE	CA-CB-CG	5.12	118.92	113.80
1	D	4756	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	C	1558	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	B	1114	GLU	N-CA-C	5.12	117.72	110.50
1	B	2869	ARG	NE-CZ-NH2	5.12	123.81	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2244	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	D	151	HIS	CB-CG-CD2	-5.12	124.55	131.20
1	A	151	HIS	CB-CG-CD2	-5.11	124.55	131.20
1	A	2615	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	B	220	LEU	N-CA-C	5.11	116.06	108.60
1	B	4679	ARG	CD-NE-CZ	5.11	131.56	124.40
1	A	346	CYS	N-CA-C	5.11	116.75	109.14
1	A	3550	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	B	263	GLU	CA-C-N	5.11	125.83	120.11
1	B	263	GLU	C-N-CA	5.11	125.83	120.11
1	B	4973	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	C	18	ASP	CA-C-N	5.11	128.72	121.42
1	C	18	ASP	C-N-CA	5.11	128.72	121.42
1	A	531	ARG	NE-CZ-NH2	5.11	123.79	119.20
1	A	3582	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	C	2786	LYS	N-CA-C	5.10	118.80	112.47
1	D	3366	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	A	2864	GLY	CA-C-N	5.10	130.16	123.17
1	A	2864	GLY	C-N-CA	5.10	130.16	123.17
1	C	949	ASN	CA-CB-CG	5.10	117.70	112.60
1	A	266	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	A	3699	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	C	4756	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	B	593	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	C	3451	PHE	CA-CB-CG	5.09	118.89	113.80
1	D	3984	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	C	1702	HIS	CB-CG-CD2	-5.09	124.59	131.20
1	A	2194	HIS	CB-CG-CD2	-5.08	124.59	131.20
1	A	3426	GLU	CA-C-N	5.08	126.19	119.84
1	A	3426	GLU	C-N-CA	5.08	126.19	119.84
1	B	2194	HIS	CB-CG-CD2	-5.08	124.59	131.20
1	B	2224	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	B	2247	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	C	19	GLU	CB-CA-C	5.08	118.11	109.53
1	B	1688	HIS	CB-CG-CD2	-5.08	124.60	131.20
1	B	1773	PRO	N-CA-CB	5.08	105.86	103.22
1	D	4717	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	524	GLU	N-CA-CB	-5.08	102.65	110.01
1	D	2441	HIS	CB-CG-CD2	-5.08	124.60	131.20
1	B	1201	HIS	CB-CG-CD2	-5.08	124.60	131.20
1	C	835	ARG	NE-CZ-NH2	5.07	123.77	119.20
1	C	3950	ASN	CA-CB-CG	5.07	117.67	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2351	ASN	CA-CB-CG	5.07	117.67	112.60
1	C	1791	VAL	CA-C-N	5.07	131.22	121.54
1	C	1791	VAL	C-N-CA	5.07	131.22	121.54
1	D	531	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	B	261	ARG	NE-CZ-NH2	5.06	123.76	119.20
2	G	15	PHE	CA-CB-CG	5.06	118.86	113.80
1	A	3247	ASP	CA-CB-CG	5.06	117.66	112.60
1	B	4223	ASN	CA-CB-CG	-5.06	107.54	112.60
1	A	593	HIS	CB-CG-CD2	-5.06	124.62	131.20
1	C	261	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	D	1121	ALA	N-CA-C	5.06	116.76	109.07
1	C	4679	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	A	2244	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	C	4717	ASP	CA-CB-CG	5.05	117.65	112.60
1	B	3343	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	A	3451	PHE	CA-CB-CG	5.05	118.85	113.80
1	C	4189	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	D	835	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	D	1688	HIS	CA-CB-CG	-5.05	108.75	113.80
1	D	1690	ASP	CA-CB-CG	-5.05	107.55	112.60
1	B	957	LYS	N-CA-C	5.04	117.17	111.02
1	C	716	PHE	CA-CB-CG	-5.04	108.76	113.80
1	C	1141	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	C	2575	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	D	3628	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	B	5003	HIS	CB-CG-CD2	-5.04	124.65	131.20
1	B	2494	PHE	CA-CB-CG	-5.04	108.76	113.80
2	E	92	PRO	N-CA-CB	5.04	106.01	103.19
1	D	4944	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	A	1106	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	A	1201	HIS	CB-CG-CD2	-5.03	124.66	131.20
1	A	4776	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	C	1114	GLU	N-CA-C	5.03	117.59	110.50
1	B	3839	CYS	N-CA-C	5.03	117.59	110.10
1	A	2551	ASN	CA-CB-CG	5.03	117.63	112.60
1	A	2913	ALA	N-CA-C	5.03	116.76	111.28
1	D	4540	PHE	CA-C-N	5.03	126.97	120.44
1	D	4540	PHE	C-N-CA	5.03	126.97	120.44
1	C	69	LEU	N-CA-CB	-5.02	103.06	110.49
1	A	1688	HIS	CB-CG-CD2	-5.02	124.67	131.20
1	A	4223	ASN	CA-CB-CG	-5.02	107.58	112.60
1	A	1534	LYS	CA-C-N	5.02	128.33	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1534	LYS	C-N-CA	5.02	128.33	120.75
1	C	474	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	C	3223	SER	CA-C-N	5.02	126.11	119.84
1	C	3223	SER	C-N-CA	5.02	126.11	119.84
1	D	1760	HIS	CB-CG-CD2	-5.02	124.68	131.20
1	D	716	PHE	CA-CB-CG	-5.01	108.78	113.80
1	A	3621	HIS	CA-C-N	5.01	131.11	121.54
1	A	3621	HIS	C-N-CA	5.01	131.11	121.54
1	C	2452	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	A	1114	GLU	N-CA-C	5.01	117.56	110.50
1	A	4189	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	B	2673	HIS	CB-CG-CD2	-5.01	124.69	131.20
1	B	2772	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	C	3699	HIS	CB-CG-CD2	-5.01	124.69	131.20
1	C	1232	ARG	NE-CZ-NH2	5.00	123.70	119.20
1	A	716	PHE	CA-CB-CG	-5.00	108.80	113.80
1	B	4153	HIS	CB-CG-CD2	-5.00	124.70	131.20

There are no chirality outliers.

All (169) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ARG	Sidechain
1	A	1101	ARG	Sidechain
1	A	1122	TYR	Sidechain
1	A	117	TYR	Sidechain
1	A	1607	ARG	Sidechain
1	A	1670	TYR	Sidechain
1	A	1734	TYR	Sidechain
1	A	2318	TYR	Sidechain
1	A	2330	ARG	Sidechain
1	A	2340	PHE	Sidechain
1	A	242	ARG	Sidechain
1	A	2452	ARG	Sidechain
1	A	247	TYR	Sidechain
1	A	2696	TYR	Sidechain
1	A	2805	TYR	Sidechain
1	A	3009	TYR	Sidechain
1	A	3213	TYR	Sidechain
1	A	3280	TYR	Sidechain
1	A	3366	ARG	Sidechain
1	A	3414	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	347	PHE	Sidechain
1	A	3657	TYR	Sidechain
1	A	3707	ARG	Sidechain
1	A	3949	ARG	Sidechain
1	A	4062	PHE	Sidechain
1	A	4189	ARG	Sidechain
1	A	4631	PHE	Sidechain
1	A	469	ARG	Sidechain
1	A	4711	PHE	Sidechain
1	A	4715	TYR	Sidechain
1	A	4791	TYR	Sidechain
1	A	4795	TYR	Sidechain
1	A	4812	HIS	Sidechain
1	A	4851	TYR	Sidechain
1	A	4888	TYR	Sidechain
1	A	4959	PHE	Sidechain
1	A	4978	HIS	Sidechain
1	A	5028	PHE	Sidechain
1	A	534	ARG	Sidechain
1	A	640	TYR	Sidechain
1	A	712	TYR	Sidechain
1	A	714	TYR	Sidechain
1	A	757	PHE	Sidechain
1	A	829	TYR	Sidechain
1	A	893	TYR	Sidechain
1	B	1025	ARG	Sidechain
1	B	110	ARG	Sidechain
1	B	1101	ARG	Sidechain
1	B	1122	TYR	Sidechain
1	B	117	TYR	Sidechain
1	B	1607	ARG	Sidechain
1	B	1670	TYR	Sidechain
1	B	1734	TYR	Sidechain
1	B	2142	TYR	Sidechain
1	B	2318	TYR	Sidechain
1	B	2330	ARG	Sidechain
1	B	2340	PHE	Sidechain
1	B	242	ARG	Sidechain
1	B	2452	ARG	Sidechain
1	B	247	TYR	Sidechain
1	B	2615	ARG	Sidechain
1	B	2696	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	2697	ARG	Sidechain
1	B	3009	TYR	Sidechain
1	B	3213	TYR	Sidechain
1	B	3280	TYR	Sidechain
1	B	3366	ARG	Sidechain
1	B	3414	ARG	Sidechain
1	B	3657	TYR	Sidechain
1	B	3902	TYR	Sidechain
1	B	3949	ARG	Sidechain
1	B	4062	PHE	Sidechain
1	B	4153	HIS	Sidechain
1	B	4189	ARG	Sidechain
1	B	4631	PHE	Sidechain
1	B	469	ARG	Sidechain
1	B	4711	PHE	Sidechain
1	B	4715	TYR	Sidechain
1	B	4791	TYR	Sidechain
1	B	4795	TYR	Sidechain
1	B	4812	HIS	Sidechain
1	B	4851	TYR	Sidechain
1	B	4888	TYR	Sidechain
1	B	4959	PHE	Sidechain
1	B	534	ARG	Sidechain
1	B	640	TYR	Sidechain
1	B	714	TYR	Sidechain
1	B	757	PHE	Sidechain
1	B	829	TYR	Sidechain
1	C	1025	ARG	Sidechain
1	C	110	ARG	Sidechain
1	C	1122	TYR	Sidechain
1	C	117	TYR	Sidechain
1	C	1493	TYR	Sidechain
1	C	1607	ARG	Sidechain
1	C	1734	TYR	Sidechain
1	C	2028	ARG	Sidechain
1	C	2318	TYR	Sidechain
1	C	2330	ARG	Sidechain
1	C	2340	PHE	Sidechain
1	C	242	ARG	Sidechain
1	C	2452	ARG	Sidechain
1	C	247	TYR	Sidechain
1	C	2696	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	C	3009	TYR	Sidechain
1	C	3213	TYR	Sidechain
1	C	3366	ARG	Sidechain
1	C	3414	ARG	Sidechain
1	C	3657	TYR	Sidechain
1	C	3949	ARG	Sidechain
1	C	4062	PHE	Sidechain
1	C	4189	ARG	Sidechain
1	C	469	ARG	Sidechain
1	C	4711	PHE	Sidechain
1	C	4715	TYR	Sidechain
1	C	4791	TYR	Sidechain
1	C	4812	HIS	Sidechain
1	C	4851	TYR	Sidechain
1	C	4959	PHE	Sidechain
1	C	497	TYR	Sidechain
1	C	5028	PHE	Sidechain
1	C	534	ARG	Sidechain
1	C	640	TYR	Sidechain
1	C	714	TYR	Sidechain
1	C	757	PHE	Sidechain
1	C	829	TYR	Sidechain
1	C	893	TYR	Sidechain
1	D	1025	ARG	Sidechain
1	D	110	ARG	Sidechain
1	D	1101	ARG	Sidechain
1	D	1122	TYR	Sidechain
1	D	117	TYR	Sidechain
1	D	1607	ARG	Sidechain
1	D	1734	TYR	Sidechain
1	D	2028	ARG	Sidechain
1	D	2142	TYR	Sidechain
1	D	2318	TYR	Sidechain
1	D	2330	ARG	Sidechain
1	D	2340	PHE	Sidechain
1	D	2452	ARG	Sidechain
1	D	2587	TYR	Sidechain
1	D	2696	TYR	Sidechain
1	D	2805	TYR	Sidechain
1	D	3009	TYR	Sidechain
1	D	3213	TYR	Sidechain
1	D	3280	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	D	3366	ARG	Sidechain
1	D	3414	ARG	Sidechain
1	D	3657	TYR	Sidechain
1	D	3902	TYR	Sidechain
1	D	3949	ARG	Sidechain
1	D	4062	PHE	Sidechain
1	D	4189	ARG	Sidechain
1	D	4631	PHE	Sidechain
1	D	469	ARG	Sidechain
1	D	4715	TYR	Sidechain
1	D	4775	TYR	Sidechain
1	D	4791	TYR	Sidechain
1	D	4812	HIS	Sidechain
1	D	4851	TYR	Sidechain
1	D	4959	PHE	Sidechain
1	D	534	ARG	Sidechain
1	D	640	TYR	Sidechain
1	D	692	TYR	Sidechain
1	D	714	TYR	Sidechain
1	D	829	TYR	Sidechain
2	E	71	ARG	Sidechain
2	G	71	ARG	Sidechain
2	H	71	ARG	Sidechain

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	35088	34740	34717	106	0
1	B	35088	34740	34717	118	0
1	C	35088	34740	34717	130	0
1	D	35088	34740	34717	123	0
2	E	832	829	831	0	0
2	F	832	829	831	1	0
2	G	832	829	831	0	0
2	H	832	829	831	0	0
All	All	143680	142276	142192	471	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 2.

All (471) 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:C:4984:ASN:HD21	1:C:4986:ALA:HB3	1.65	0.61
1:D:3670:GLU:CD	1:D:3670:GLU:H	2.10	0.59
1:A:283:ARG:HD3	1:A:290:TYR:CZ	2.38	0.59
1:D:32:GLN:CD	1:D:32:GLN:H	2.12	0.58
1:A:4059:LEU:HA	1:A:4062:PHE:CZ	2.40	0.57
1:B:283:ARG:HD3	1:B:290:TYR:CZ	2.40	0.57
1:B:4059:LEU:HA	1:B:4062:PHE:CZ	2.39	0.57
1:C:4059:LEU:HA	1:C:4062:PHE:CZ	2.40	0.57
1:D:283:ARG:HD3	1:D:290:TYR:CZ	2.40	0.56
1:D:2101:MET:SD	1:D:2101:MET:C	2.88	0.56
1:A:32:GLN:H	1:A:32:GLN:CD	2.14	0.56
1:B:4199:GLU:H	1:B:4199:GLU:CD	2.14	0.56
1:A:4978:HIS:CE1	1:A:4983:HIS:CD2	2.94	0.56
1:C:4978:HIS:CE1	1:C:4983:HIS:CD2	2.94	0.56
1:D:4984:ASN:HD21	1:D:4986:ALA:HB3	1.71	0.56
1:C:32:GLN:CD	1:C:32:GLN:H	2.14	0.56
1:C:283:ARG:HD3	1:C:290:TYR:CZ	2.41	0.56
1:D:4059:LEU:HA	1:D:4062:PHE:CZ	2.41	0.56
1:B:32:GLN:CD	1:B:32:GLN:H	2.14	0.55
1:B:4978:HIS:CE1	1:B:4983:HIS:CD2	2.94	0.55
1:C:4199:GLU:CD	1:C:4199:GLU:H	2.14	0.55
1:D:4978:HIS:CE1	1:D:4983:HIS:CD2	2.94	0.55
1:A:4199:GLU:CD	1:A:4199:GLU:H	2.15	0.55
1:B:2101:MET:SD	1:B:2105:TRP:CD2	2.99	0.55
1:B:4984:ASN:HD21	1:B:4986:ALA:HB3	1.72	0.55
1:A:3368:ARG:HH12	1:A:3400:VAL:HG13	1.72	0.54
1:A:2292:GLU:H	1:A:2292:GLU:CD	2.15	0.54
1:B:2101:MET:SD	1:B:2101:MET:C	2.91	0.54
1:B:3466:ASN:HA	1:B:3469:PHE:CD2	2.43	0.54
1:A:4984:ASN:HD21	1:A:4986:ALA:HB3	1.73	0.53
1:C:4978:HIS:CE1	1:C:4983:HIS:CG	2.96	0.53
1:C:4065:PHE:CE1	1:C:4132:PHE:CD2	2.95	0.53
1:D:2101:MET:SD	1:D:2105:TRP:CD2	3.02	0.53
1:D:4199:GLU:H	1:D:4199:GLU:CD	2.17	0.53
1:C:2292:GLU:H	1:C:2292:GLU:CD	2.17	0.52
1:D:4753:HIS:CE1	1:D:4754:ASN:HD22	2.28	0.52
1:D:4978:HIS:CE1	1:D:4983:HIS:CG	2.97	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2292:GLU:CD	1:D:2292:GLU:H	2.18	0.52
1:B:2292:GLU:CD	1:B:2292:GLU:H	2.18	0.52
1:D:214:VAL:HG12	1:D:274:LEU:HD12	1.90	0.52
1:A:3466:ASN:HA	1:A:3469:PHE:CD2	2.44	0.52
1:D:3466:ASN:HA	1:D:3469:PHE:CD2	2.45	0.52
1:D:4065:PHE:CE1	1:D:4132:PHE:CD2	2.97	0.51
1:B:4978:HIS:CE1	1:B:4983:HIS:CG	2.99	0.51
1:C:3466:ASN:HA	1:C:3469:PHE:CD2	2.46	0.51
1:B:1249:PRO:HD2	1:B:1599:MET:HE1	1.92	0.51
1:C:4753:HIS:CE1	1:C:4754:ASN:HD22	2.29	0.51
1:D:4181:ILE:HD12	1:D:4181:ILE:C	2.36	0.51
1:B:2627:VAL:HA	1:B:2678:LEU:HD13	1.91	0.51
1:C:213:TYR:CZ	1:C:337:PRO:HB2	2.46	0.51
1:A:4753:HIS:CE1	1:A:4754:ASN:HD22	2.28	0.51
1:B:4181:ILE:C	1:B:4181:ILE:HD12	2.35	0.51
1:B:3670:GLU:CD	1:B:3670:GLU:H	2.18	0.51
1:C:121:LEU:HD23	1:C:122:THR:H	1.75	0.51
1:D:597:HIS:CG	1:D:1661:ARG:HH22	2.28	0.51
1:A:4115:SER:HA	1:A:4128:PHE:CE1	2.46	0.51
1:C:77:ALA:HA	1:D:3935:TRP:CZ3	2.46	0.51
1:B:3962:PHE:CE1	1:B:4026:MET:HE1	2.46	0.50
1:B:4753:HIS:CE1	1:B:4754:ASN:HD22	2.30	0.50
1:B:4987:ASN:HA	1:B:4990:PHE:CD2	2.45	0.50
1:A:4978:HIS:CE1	1:A:4983:HIS:CG	3.00	0.50
1:C:2474:LEU:HD21	1:C:2494:PHE:CD1	2.47	0.50
1:A:284:HIS:CE1	1:A:286:THR:H	2.30	0.50
1:A:3676:ASP:HA	1:A:3679:LYS:HE2	1.94	0.50
1:A:4181:ILE:C	1:A:4181:ILE:HD12	2.37	0.50
1:B:347:PHE:CE1	1:B:387:ALA:HB2	2.47	0.50
1:C:1805:GLU:H	1:C:1805:GLU:CD	2.20	0.50
1:C:4023:MET:HA	1:C:4026:MET:HE2	1.94	0.50
1:A:2627:VAL:HA	1:A:2678:LEU:HD13	1.94	0.50
1:C:1122:TYR:CE2	1:C:1133:HIS:CD2	3.00	0.50
1:C:2506:LEU:C	1:C:2506:LEU:HD23	2.37	0.50
1:B:3368:ARG:HH12	1:B:3400:VAL:HG13	1.76	0.49
1:A:3553:LEU:HB3	1:A:3593:VAL:HG12	1.94	0.49
1:D:4023:MET:HG2	1:D:4026:MET:HE3	1.95	0.49
1:A:4065:PHE:CE1	1:A:4132:PHE:CD2	3.00	0.49
1:D:213:TYR:CZ	1:D:337:PRO:HB2	2.47	0.49
1:D:4987:ASN:HA	1:D:4990:PHE:CD2	2.47	0.49
1:B:284:HIS:CE1	1:B:286:THR:H	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4023:MET:HG2	1:B:4026:MET:HE3	1.94	0.49
1:C:291:LEU:HA	1:C:301:VAL:HG12	1.94	0.49
1:B:3435:PHE:CE2	1:B:3521:GLY:HA3	2.48	0.49
1:A:291:LEU:HA	1:A:301:VAL:HG12	1.94	0.49
1:B:121:LEU:HD23	1:B:122:THR:H	1.77	0.49
1:A:4987:ASN:HA	1:A:4990:PHE:CD2	2.47	0.49
1:D:347:PHE:CE1	1:D:387:ALA:HB2	2.48	0.49
1:B:305:CYS:SG	1:B:306:LYS:HE2	2.53	0.49
1:A:2506:LEU:C	1:A:2506:LEU:HD23	2.38	0.48
1:B:4795:TYR:CE1	1:B:4812:HIS:CD2	3.01	0.48
1:B:1805:GLU:CD	1:B:1805:GLU:H	2.20	0.48
1:D:4065:PHE:CZ	1:D:4132:PHE:CG	3.02	0.48
1:A:1805:GLU:CD	1:A:1805:GLU:H	2.21	0.48
1:B:4199:GLU:CD	1:B:4199:GLU:N	2.71	0.48
1:C:4199:GLU:CD	1:C:4199:GLU:N	2.71	0.48
1:C:284:HIS:CE1	1:C:286:THR:H	2.31	0.48
1:A:4199:GLU:CD	1:A:4199:GLU:N	2.72	0.48
1:B:1122:TYR:CE2	1:B:1133:HIS:CD2	3.01	0.48
1:B:2101:MET:HE1	1:B:2105:TRP:NE1	2.29	0.48
1:B:213:TYR:CZ	1:B:337:PRO:HB2	2.48	0.48
1:B:1132:TRP:CE2	1:B:1136:SER:HB3	2.49	0.48
1:C:146:CYS:HG	1:C:147:TRP:CD1	2.32	0.48
1:C:4023:MET:HG2	1:C:4026:MET:HE3	1.95	0.48
1:C:4987:ASN:HA	1:C:4990:PHE:CD2	2.48	0.48
1:D:3670:GLU:CD	1:D:3670:GLU:N	2.71	0.48
1:A:1721:GLU:HA	1:A:1724:CYS:SG	2.54	0.48
1:D:2150:GLU:CD	1:D:2150:GLU:H	2.22	0.48
1:A:2348:GLU:CD	1:A:2348:GLU:H	2.22	0.47
1:B:4023:MET:HA	1:B:4026:MET:HE2	1.97	0.47
1:C:4065:PHE:CZ	1:C:4132:PHE:CG	3.02	0.47
1:D:284:HIS:CE1	1:D:286:THR:H	2.32	0.47
1:D:1132:TRP:CE2	1:D:1136:SER:HB3	2.49	0.47
1:A:77:ALA:HA	1:B:3935:TRP:CZ3	2.49	0.47
1:B:3893:GLU:CD	1:B:3894:GLY:H	2.22	0.47
1:C:1063:VAL:HG13	1:C:1064:GLU:H	1.79	0.47
1:D:2101:MET:SD	1:D:2105:TRP:CE3	3.07	0.47
1:B:2211:MET:SD	1:B:2211:MET:C	2.98	0.47
1:B:4065:PHE:CE1	1:B:4132:PHE:CD2	3.03	0.47
1:C:907:LEU:O	1:C:961:MET:HE3	2.13	0.47
1:C:1721:GLU:HA	1:C:1724:CYS:SG	2.54	0.47
1:D:2627:VAL:HA	1:D:2678:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2150:GLU:CD	1:A:2150:GLU:H	2.22	0.47
1:C:2110:TYR:CD1	1:C:2110:TYR:C	2.92	0.47
1:D:1435:TYR:CE1	1:D:1518:CYS:HB2	2.50	0.47
1:D:1805:GLU:CD	1:D:1805:GLU:H	2.22	0.47
1:B:3879:GLU:CD	1:B:3879:GLU:H	2.23	0.47
1:D:305:CYS:SG	1:D:306:LYS:HE2	2.55	0.47
1:D:213:TYR:CD2	1:D:340:LYS:HE3	2.50	0.47
1:D:2348:GLU:CD	1:D:2348:GLU:H	2.23	0.47
1:D:3962:PHE:CE1	1:D:4026:MET:HE1	2.49	0.47
1:A:4688:ILE:HD12	1:A:4688:ILE:N	2.30	0.46
1:B:3676:ASP:HA	1:B:3679:LYS:HE2	1.97	0.46
1:D:2117:VAL:HA	1:D:2120:MET:SD	2.55	0.46
1:D:4735:GLU:H	1:D:4735:GLU:CD	2.23	0.46
1:D:3368:ARG:HH12	1:D:3400:VAL:HG13	1.79	0.46
1:A:597:HIS:CG	1:A:1661:ARG:HH22	2.33	0.46
1:C:305:CYS:SG	1:C:306:LYS:HE2	2.54	0.46
1:C:1464:PHE:CD1	1:C:1464:PHE:C	2.93	0.46
1:D:1063:VAL:HG13	1:D:1064:GLU:H	1.79	0.46
1:D:4023:MET:HA	1:D:4026:MET:HE2	1.97	0.46
1:A:4848:VAL:HG11	1:A:4887:MET:SD	2.55	0.46
1:B:451:TYR:CD2	1:B:452:PHE:CE1	3.04	0.46
1:B:2574:HIS:H	1:B:2574:HIS:CD2	2.30	0.46
1:B:4065:PHE:CZ	1:B:4132:PHE:CG	3.03	0.46
1:C:1237:TRP:CE3	1:C:1606:SER:C	2.93	0.46
1:D:291:LEU:HA	1:D:301:VAL:HG12	1.96	0.46
1:D:2101:MET:HE1	1:D:2105:TRP:CE2	2.51	0.46
1:D:4199:GLU:CD	1:D:4199:GLU:N	2.73	0.46
1:A:4795:TYR:CE1	1:A:4812:HIS:CD2	3.03	0.46
1:B:4242:ILE:HA	1:B:4245:MET:SD	2.55	0.46
1:C:1435:TYR:CE1	1:C:1518:CYS:HB2	2.51	0.46
1:D:2101:MET:HE1	1:D:2105:TRP:CD1	2.50	0.46
1:A:1237:TRP:CE3	1:A:1606:SER:C	2.94	0.46
1:C:2627:VAL:HA	1:C:2678:LEU:HD13	1.98	0.46
1:C:3778:MET:SD	1:C:3778:MET:C	2.98	0.46
1:A:4242:ILE:HA	1:A:4245:MET:SD	2.56	0.46
1:B:4688:ILE:N	1:B:4688:ILE:HD12	2.31	0.46
1:C:1132:TRP:CE2	1:C:1136:SER:HB3	2.51	0.46
1:C:3879:GLU:CD	1:C:3879:GLU:H	2.24	0.46
1:D:32:GLN:H	1:D:32:GLN:NE2	2.13	0.46
1:D:1237:TRP:CE3	1:D:1606:SER:C	2.93	0.46
1:A:1132:TRP:CE2	1:A:1136:SER:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2117:VAL:HA	1:A:2120:MET:SD	2.56	0.46
1:C:2150:GLU:H	1:C:2150:GLU:CD	2.23	0.46
1:D:1721:GLU:HA	1:D:1724:CYS:SG	2.56	0.46
1:A:223:PHE:CD1	1:A:227:MET:HA	2.50	0.46
1:A:938:HIS:CE1	1:A:1052:ASN:HD21	2.34	0.46
1:B:2178:MET:SD	1:B:2178:MET:C	2.99	0.46
1:C:3553:LEU:HB3	1:C:3593:VAL:HG12	1.97	0.46
1:D:2115:GLU:CD	1:D:2115:GLU:H	2.24	0.46
1:D:4242:ILE:HA	1:D:4245:MET:SD	2.56	0.46
1:D:4688:ILE:HD12	1:D:4688:ILE:N	2.30	0.46
1:A:305:CYS:SG	1:A:306:LYS:HE2	2.56	0.45
1:B:1063:VAL:HG13	1:B:1064:GLU:H	1.81	0.45
1:A:4986:ALA:HB1	1:A:4990:PHE:CZ	2.51	0.45
1:B:32:GLN:H	1:B:32:GLN:NE2	2.14	0.45
1:B:3892:CYS:SG	1:B:3899:PHE:CG	3.09	0.45
1:C:3892:CYS:SG	1:C:3899:PHE:CG	3.10	0.45
1:B:291:LEU:HA	1:B:301:VAL:HG12	1.98	0.45
1:C:2495:VAL:H	1:C:2498:HIS:CD2	2.34	0.45
1:B:2224:ARG:H	1:B:2224:ARG:HD3	1.81	0.45
1:B:3832:ILE:HA	1:B:3835:LEU:HD12	1.99	0.45
1:B:3894:GLY:C	1:B:3895:HIS:CG	2.95	0.45
1:C:4735:GLU:CD	1:C:4735:GLU:H	2.24	0.45
1:D:451:TYR:CD2	1:D:452:PHE:CE1	3.05	0.45
1:B:1237:TRP:CE3	1:B:1606:SER:C	2.94	0.45
1:B:2115:GLU:CD	1:B:2115:GLU:H	2.24	0.45
1:B:2150:GLU:CD	1:B:2150:GLU:H	2.24	0.45
1:B:3670:GLU:CD	1:B:3670:GLU:N	2.74	0.45
1:B:4735:GLU:H	1:B:4735:GLU:CD	2.25	0.45
1:C:1045:THR:HG22	1:C:1049:TYR:CE2	2.52	0.45
1:D:3879:GLU:H	1:D:3879:GLU:CD	2.25	0.45
1:D:3892:CYS:SG	1:D:3899:PHE:CG	3.10	0.45
1:A:2131:LEU:HD23	1:A:2131:LEU:H	1.82	0.45
1:A:2178:MET:SD	1:A:2178:MET:C	3.00	0.45
1:B:2797:PHE:CD2	1:B:2802:LYS:HE2	2.52	0.45
1:D:2101:MET:HE1	1:D:2105:TRP:NE1	2.31	0.45
1:D:4986:ALA:HB1	1:D:4990:PHE:CZ	2.51	0.45
1:C:223:PHE:CD1	1:C:227:MET:HA	2.52	0.45
1:C:3676:ASP:HA	1:C:3679:LYS:HE2	1.98	0.45
1:C:4986:ALA:HB1	1:C:4990:PHE:CZ	2.52	0.45
1:C:2115:GLU:CD	1:C:2115:GLU:H	2.25	0.45
1:C:2117:VAL:HA	1:C:2120:MET:SD	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4072:VAL:HA	1:C:4077:PHE:CE1	2.51	0.45
1:C:4693:GLY:C	1:C:4695:ASP:H	2.25	0.45
1:D:2174:GLU:H	1:D:2174:GLU:CD	2.25	0.45
1:D:3334:TRP:CD1	1:D:3334:TRP:H	2.35	0.45
1:D:3778:MET:SD	1:D:3778:MET:C	3.00	0.45
1:A:1022:VAL:HG22	1:A:1023:PRO:HD2	1.99	0.44
1:A:2110:TYR:CD1	1:A:2110:TYR:C	2.94	0.44
1:A:3892:CYS:SG	1:A:3899:PHE:CG	3.10	0.44
1:B:64:ILE:C	1:B:65:CYS:SG	3.00	0.44
1:C:2174:GLU:CD	1:C:2174:GLU:H	2.25	0.44
1:C:3965:LEU:HA	1:C:3968:TYR:CD2	2.52	0.44
1:D:223:PHE:CD1	1:D:227:MET:HA	2.52	0.44
1:B:1721:GLU:HA	1:B:1724:CYS:SG	2.57	0.44
1:B:3965:LEU:HA	1:B:3968:TYR:CD2	2.52	0.44
1:B:4115:SER:HA	1:B:4128:PHE:CE1	2.53	0.44
1:C:2178:MET:SD	1:C:2178:MET:C	3.00	0.44
1:A:451:TYR:CD2	1:A:452:PHE:CE1	3.06	0.44
1:A:1249:PRO:HD2	1:A:1599:MET:HE1	1.98	0.44
1:A:5000:GLU:HA	1:A:5003:HIS:CG	2.53	0.44
1:B:1249:PRO:C	1:B:1251:GLU:H	2.26	0.44
1:B:1930:LYS:C	1:B:1931:LEU:HD22	2.42	0.44
1:C:4242:ILE:HA	1:C:4245:MET:SD	2.57	0.44
1:A:64:ILE:C	1:A:65:CYS:SG	3.00	0.44
1:A:3106:MET:C	1:A:3106:MET:SD	3.00	0.44
1:A:3778:MET:SD	1:A:3778:MET:C	3.00	0.44
1:A:3935:TRP:CZ3	1:D:77:ALA:HA	2.52	0.44
1:B:597:HIS:CG	1:B:1661:ARG:HH22	2.36	0.44
1:B:3778:MET:SD	1:B:3778:MET:C	3.00	0.44
1:C:3894:GLY:C	1:C:3895:HIS:CG	2.96	0.44
1:A:3935:TRP:HA	1:A:3938:SER:OG	2.17	0.44
1:C:3312:LEU:N	1:C:3312:LEU:HD12	2.32	0.44
1:D:2211:MET:C	1:D:2211:MET:SD	3.00	0.44
1:B:3553:LEU:HB3	1:B:3593:VAL:HG12	1.99	0.44
1:C:1705:GLY:HA3	1:C:1836:PHE:CD2	2.53	0.44
1:C:2340:PHE:CZ	1:C:2343:GLY:C	2.96	0.44
1:C:77:ALA:HA	1:D:3935:TRP:CE3	2.52	0.44
1:C:308:HIS:CD2	1:C:311:ALA:H	2.36	0.44
1:C:597:HIS:CG	1:C:1661:ARG:HH22	2.36	0.44
1:A:1249:PRO:C	1:A:1251:GLU:H	2.25	0.44
1:A:4065:PHE:CZ	1:A:4132:PHE:CG	3.06	0.44
1:D:1005:TRP:CE2	1:D:1016:ARG:HD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1857:GLU:CD	1:D:1857:GLU:H	2.26	0.44
1:D:3553:LEU:HB3	1:D:3593:VAL:HG12	1.99	0.44
1:B:1741:GLU:CD	1:B:1741:GLU:H	2.25	0.44
1:C:76:ARG:HH22	1:D:3933:PHE:C	2.26	0.44
1:C:451:TYR:CD2	1:C:452:PHE:CE1	3.05	0.44
1:C:3893:GLU:CD	1:C:3894:GLY:H	2.26	0.44
1:D:3659:ALA:HA	1:D:3663:LEU:HD12	1.99	0.44
1:A:32:GLN:H	1:A:32:GLN:NE2	2.15	0.43
1:C:64:ILE:C	1:C:65:CYS:SG	3.01	0.43
1:C:1857:GLU:H	1:C:1857:GLU:CD	2.25	0.43
1:D:1249:PRO:C	1:D:1251:GLU:H	2.26	0.43
1:A:213:TYR:CD2	1:A:340:LYS:HE3	2.53	0.43
1:B:3106:MET:SD	1:B:3106:MET:C	3.01	0.43
1:D:64:ILE:C	1:D:65:CYS:SG	3.00	0.43
1:D:4795:TYR:CE1	1:D:4812:HIS:CD2	3.06	0.43
1:A:2101:MET:SD	1:A:2105:TRP:CE2	3.11	0.43
1:A:2211:MET:SD	1:A:2211:MET:C	3.01	0.43
1:B:1775:HIS:HB2	1:B:1777:PHE:CZ	2.54	0.43
1:B:1857:GLU:CD	1:B:1857:GLU:H	2.26	0.43
1:B:5000:GLU:HA	1:B:5003:HIS:CG	2.54	0.43
1:C:32:GLN:H	1:C:32:GLN:NE2	2.16	0.43
1:C:2518:LEU:HD21	1:C:2569:PHE:CE1	2.53	0.43
1:C:5000:GLU:HA	1:C:5003:HIS:CG	2.53	0.43
1:A:1509:ILE:HD12	1:A:1509:ILE:H	1.83	0.43
1:B:1509:ILE:HD12	1:B:1509:ILE:H	1.84	0.43
1:C:4795:TYR:CE1	1:C:4812:HIS:CD2	3.06	0.43
1:D:3768:SER:HA	1:D:3771:HIS:CD2	2.54	0.43
1:D:4861:LYS:HE3	1:D:4862:PHE:CE1	2.53	0.43
1:A:77:ALA:HA	1:B:3935:TRP:CE3	2.52	0.43
1:C:1457:TYR:CD1	1:C:1457:TYR:C	2.97	0.43
1:C:3935:TRP:HA	1:C:3938:SER:OG	2.18	0.43
1:D:1741:GLU:CD	1:D:1741:GLU:H	2.27	0.43
1:D:3962:PHE:CD1	1:D:4026:MET:HE1	2.54	0.43
1:A:2115:GLU:H	1:A:2115:GLU:CD	2.26	0.43
1:A:3368:ARG:NH1	1:A:3400:VAL:HG13	2.34	0.43
1:B:213:TYR:CD2	1:B:340:LYS:HE3	2.53	0.43
1:B:3836:MET:SD	1:B:3919:THR:HA	2.58	0.43
1:A:3893:GLU:CD	1:A:3894:GLY:H	2.26	0.43
1:A:3894:GLY:C	1:A:3895:HIS:CG	2.96	0.43
1:B:1775:HIS:HB2	1:B:1777:PHE:CE2	2.53	0.43
1:B:4693:GLY:C	1:B:4695:ASP:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2562:ILE:HA	1:C:2565:CYS:HG	1.82	0.43
1:C:3962:PHE:CE1	1:C:4026:MET:HE1	2.53	0.43
1:C:4971:THR:HG23	1:C:4972:PRO:HD2	2.00	0.43
1:D:3935:TRP:HA	1:D:3938:SER:OG	2.19	0.43
1:A:497:TYR:HA	1:A:502:HIS:CE1	2.54	0.43
1:A:2131:LEU:H	1:A:2131:LEU:CD2	2.31	0.43
1:A:2174:GLU:CD	1:A:2174:GLU:H	2.26	0.43
1:A:2340:PHE:CZ	1:A:2343:GLY:HA2	2.54	0.43
1:B:5000:GLU:HA	1:B:5003:HIS:CD2	2.54	0.43
1:C:347:PHE:CE1	1:C:387:ALA:HB2	2.54	0.43
1:D:2155:LEU:HD23	1:D:2155:LEU:C	2.44	0.43
1:D:2178:MET:C	1:D:2178:MET:SD	3.02	0.43
1:D:3836:MET:SD	1:D:3919:THR:HA	2.59	0.43
1:A:4696:ASP:CG	1:A:4699:GLY:H	2.27	0.43
1:B:223:PHE:CD1	1:B:227:MET:HA	2.53	0.43
1:B:4711:PHE:CD1	1:B:4711:PHE:C	2.96	0.43
2:F:22:CYS:HB3	2:F:48:PHE:CZ	2.53	0.43
1:A:4711:PHE:CD1	1:A:4711:PHE:C	2.95	0.43
1:C:3106:MET:SD	1:C:3106:MET:C	3.01	0.43
1:D:1122:TYR:CE2	1:D:1133:HIS:CD2	3.07	0.43
1:A:2770:LYS:HE2	1:A:2770:LYS:N	2.34	0.42
1:B:3312:LEU:HD12	1:B:3312:LEU:N	2.34	0.42
1:C:3832:ILE:HA	1:C:3835:LEU:HD12	2.01	0.42
1:D:5000:GLU:HA	1:D:5003:HIS:CD2	2.54	0.42
1:A:1457:TYR:CD1	1:A:1457:TYR:C	2.96	0.42
1:B:220:LEU:HD12	1:B:220:LEU:C	2.44	0.42
1:B:4986:ALA:HB1	1:B:4990:PHE:CZ	2.53	0.42
1:A:1857:GLU:CD	1:A:1857:GLU:H	2.26	0.42
1:A:3250:MET:C	1:A:3250:MET:SD	3.03	0.42
1:C:4688:ILE:N	1:C:4688:ILE:HD12	2.34	0.42
1:D:3316:LEU:C	1:D:3316:LEU:HD23	2.45	0.42
1:D:3712:GLU:CD	1:D:3712:GLU:C	2.86	0.42
1:B:2174:GLU:H	1:B:2174:GLU:CD	2.26	0.42
1:C:4861:LYS:HE3	1:C:4862:PHE:CE1	2.54	0.42
1:D:2131:LEU:H	1:D:2131:LEU:CD2	2.32	0.42
1:D:3106:MET:SD	1:D:3106:MET:C	3.02	0.42
1:D:4711:PHE:CD1	1:D:4711:PHE:C	2.96	0.42
1:B:3659:ALA:HA	1:B:3663:LEU:HD12	2.02	0.42
1:D:5000:GLU:HA	1:D:5003:HIS:CG	2.54	0.42
1:A:2174:GLU:CD	1:A:2174:GLU:N	2.77	0.42
1:C:320:LYS:HA	1:C:356:TRP:CH2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1741:GLU:CD	1:C:1741:GLU:H	2.27	0.42
1:C:4072:VAL:HA	1:C:4077:PHE:CD1	2.54	0.42
1:C:4848:VAL:HG11	1:C:4887:MET:SD	2.59	0.42
1:C:4856:PHE:CZ	1:C:4879:MET:HE3	2.54	0.42
1:D:4173:TYR:CD1	1:D:4173:TYR:C	2.98	0.42
1:A:1741:GLU:H	1:A:1741:GLU:CD	2.28	0.42
1:D:2131:LEU:H	1:D:2131:LEU:HD23	1.84	0.42
1:D:3092:LEU:C	1:D:3092:LEU:HD23	2.44	0.42
1:D:4064:MET:HE2	1:D:4064:MET:HA	2.02	0.42
1:A:4735:GLU:CD	1:A:4735:GLU:H	2.28	0.42
1:B:2101:MET:HE1	1:B:2105:TRP:CE2	2.55	0.42
1:B:3092:LEU:C	1:B:3092:LEU:HD23	2.45	0.42
1:C:2697:ARG:HA	1:C:2700:MET:SD	2.60	0.42
1:C:3828:PHE:CD1	1:C:3828:PHE:C	2.98	0.42
1:C:3836:MET:SD	1:C:3919:THR:HA	2.59	0.42
1:C:4115:SER:HA	1:C:4128:PHE:CE1	2.55	0.42
1:C:4679:ARG:HH21	1:C:4679:ARG:HG3	1.85	0.42
1:C:4967:TYR:CZ	1:C:5030:LYS:HE2	2.55	0.42
1:A:2623:LEU:O	1:A:2627:VAL:HG23	2.20	0.42
1:C:3281:LEU:HB3	1:C:3312:LEU:HD11	2.01	0.42
1:D:4679:ARG:HH21	1:D:4679:ARG:HG3	1.85	0.42
1:A:1538:THR:C	1:A:1539:PHE:CG	2.97	0.42
1:A:4958:CYS:CB	1:A:4961:CYS:SG	3.08	0.42
1:B:2928:LYS:HE2	1:B:2932:MET:SD	2.60	0.42
1:C:240:ASP:CG	1:C:243:ARG:H	2.27	0.42
1:A:3836:MET:SD	1:A:3919:THR:HA	2.59	0.41
1:A:4757:LYS:H	1:A:4757:LYS:HD3	1.85	0.41
1:D:1457:TYR:CD1	1:D:1457:TYR:C	2.98	0.41
1:D:2150:GLU:CD	1:D:2150:GLU:N	2.78	0.41
1:D:3842:LEU:HA	1:D:3875:MET:SD	2.60	0.41
1:D:3894:GLY:C	1:D:3895:HIS:CG	2.97	0.41
1:A:2340:PHE:CZ	1:A:2343:GLY:C	2.99	0.41
1:A:2697:ARG:HA	1:A:2700:MET:SD	2.60	0.41
1:B:2770:LYS:N	1:B:2770:LYS:HE2	2.35	0.41
1:B:4034:ASN:HD21	1:B:4153:HIS:CD2	2.38	0.41
1:C:2131:LEU:HD23	1:C:2131:LEU:H	1.84	0.41
1:C:4023:MET:SD	1:C:4023:MET:C	3.03	0.41
1:D:1045:THR:HG22	1:D:1049:TYR:CE2	2.55	0.41
1:A:2155:LEU:C	1:A:2155:LEU:HD23	2.46	0.41
1:A:3832:ILE:HA	1:A:3835:LEU:HD12	2.02	0.41
1:B:1116:GLY:HA3	1:B:1132:TRP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4679:ARG:HH21	1:B:4679:ARG:HG3	1.84	0.41
1:B:4861:LYS:HE3	1:B:4862:PHE:CE1	2.55	0.41
1:C:1005:TRP:CE2	1:C:1016:ARG:HD2	2.56	0.41
1:C:2211:MET:SD	1:C:2211:MET:C	3.03	0.41
1:C:2970:SER:HA	1:C:2973:PHE:CZ	2.56	0.41
1:C:3927:GLN:HA	1:C:3930:ILE:HG22	2.02	0.41
1:D:195:PHE:CD1	1:D:195:PHE:N	2.88	0.41
1:D:1775:HIS:HB2	1:D:1777:PHE:CZ	2.55	0.41
1:A:3891:LEU:HB3	1:A:3899:PHE:CE2	2.56	0.41
1:B:1457:TYR:CD1	1:B:1457:TYR:C	2.97	0.41
1:C:2770:LYS:N	1:C:2770:LYS:HE2	2.36	0.41
1:D:1748:PHE:CZ	1:D:2041:HIS:CD2	3.08	0.41
1:D:2174:GLU:CD	1:D:2174:GLU:N	2.79	0.41
1:D:2970:SER:HA	1:D:2973:PHE:CZ	2.55	0.41
1:D:4856:PHE:CZ	1:D:4879:MET:HE3	2.56	0.41
1:A:2094:LEU:C	1:A:2094:LEU:HD23	2.46	0.41
1:B:77:ALA:HA	1:C:3935:TRP:CZ3	2.55	0.41
1:B:2340:PHE:CZ	1:B:2343:GLY:C	2.98	0.41
1:B:2518:LEU:HD21	1:B:2569:PHE:CE1	2.55	0.41
1:B:2697:ARG:HA	1:B:2700:MET:SD	2.60	0.41
1:B:4231:MET:SD	1:B:4231:MET:N	2.94	0.41
1:B:4958:CYS:SG	1:B:4960:ILE:HB	2.61	0.41
1:C:2174:GLU:CD	1:C:2174:GLU:N	2.79	0.41
1:C:2281:ILE:HD13	1:C:2337:PHE:CD1	2.56	0.41
1:D:2770:LYS:HE2	1:D:2770:LYS:N	2.36	0.41
1:A:320:LYS:HA	1:A:356:TRP:CH2	2.55	0.41
1:A:1496:TRP:CE2	1:A:1498:GLY:HA3	2.56	0.41
1:A:3659:ALA:HA	1:A:3663:LEU:HD12	2.02	0.41
1:B:98:HIS:N	1:B:99:ARG:HH11	2.18	0.41
1:B:2131:LEU:CD2	1:B:2131:LEU:H	2.33	0.41
1:B:2198:MET:HE2	1:B:2198:MET:N	2.36	0.41
1:B:3828:PHE:CD1	1:B:3828:PHE:C	2.98	0.41
1:B:4848:VAL:HG11	1:B:4887:MET:SD	2.60	0.41
1:C:3334:TRP:CZ3	1:C:3335:MET:HG2	2.55	0.41
1:C:5000:GLU:HA	1:C:5003:HIS:CD2	2.56	0.41
1:D:1775:HIS:HB2	1:D:1777:PHE:CE2	2.55	0.41
1:A:4856:PHE:CZ	1:A:4879:MET:HE3	2.56	0.41
1:B:4958:CYS:CB	1:B:4961:CYS:SG	3.08	0.41
1:B:4967:TYR:CZ	1:B:5030:LYS:HE2	2.56	0.41
1:C:1249:PRO:C	1:C:1251:GLU:H	2.28	0.41
1:D:198:THR:HB	1:D:200:TRP:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3893:GLU:CD	1:D:3894:GLY:H	2.28	0.41
1:A:1748:PHE:CZ	1:A:2041:HIS:CD2	3.09	0.41
1:A:3312:LEU:N	1:A:3312:LEU:HD12	2.36	0.41
1:A:4679:ARG:HG3	1:A:4679:ARG:HH21	1.86	0.41
1:B:3243:ILE:HA	1:B:3244:PRO:HD3	1.92	0.41
1:B:3891:LEU:HB3	1:B:3899:PHE:CE2	2.56	0.41
1:C:1538:THR:C	1:C:1539:PHE:CG	2.99	0.41
1:C:2131:LEU:H	1:C:2131:LEU:CD2	2.33	0.41
1:C:2494:PHE:CZ	1:C:2498:HIS:HB2	2.55	0.41
1:D:1538:THR:C	1:D:1539:PHE:CG	2.99	0.41
1:D:3435:PHE:CE2	1:D:3521:GLY:HA3	2.55	0.41
1:A:1464:PHE:CD1	1:A:1464:PHE:C	2.98	0.41
1:A:2150:GLU:CD	1:A:2150:GLU:N	2.79	0.41
1:A:3965:LEU:HA	1:A:3968:TYR:CD2	2.55	0.41
1:A:4034:ASN:HD21	1:A:4153:HIS:CE1	2.39	0.41
1:A:5000:GLU:HA	1:A:5003:HIS:CD2	2.56	0.41
1:B:1538:THR:C	1:B:1539:PHE:CG	2.98	0.41
1:B:4173:TYR:CD1	1:B:4173:TYR:C	2.99	0.41
1:C:1423:ASP:HA	1:C:1424:PRO:HD3	1.97	0.41
1:C:3316:LEU:C	1:C:3316:LEU:HD23	2.46	0.41
1:C:3962:PHE:CD1	1:C:4026:MET:HE1	2.56	0.41
1:D:320:LYS:HA	1:D:356:TRP:CZ2	2.55	0.41
1:D:2518:LEU:HD21	1:D:2569:PHE:CE1	2.56	0.41
1:D:3832:ILE:HA	1:D:3835:LEU:HD12	2.03	0.41
1:A:198:THR:HB	1:A:200:TRP:HE1	1.86	0.41
1:A:1122:TYR:CE2	1:A:1133:HIS:CD2	3.08	0.41
1:A:4958:CYS:SG	1:A:4960:ILE:HB	2.61	0.41
1:C:1496:TRP:CD1	1:C:1498:GLY:H	2.38	0.41
1:D:3828:PHE:CD1	1:D:3828:PHE:C	2.99	0.41
1:A:2970:SER:HA	1:A:2973:PHE:CZ	2.55	0.40
1:B:3842:LEU:HA	1:B:3875:MET:SD	2.61	0.40
1:C:1509:ILE:HD12	1:C:1509:ILE:H	1.85	0.40
1:C:1805:GLU:CD	1:C:1805:GLU:N	2.79	0.40
1:C:3250:MET:SD	1:C:3250:MET:C	3.05	0.40
1:D:2224:ARG:H	1:D:2224:ARG:HD3	1.85	0.40
1:D:2340:PHE:CZ	1:D:2343:GLY:C	2.98	0.40
1:D:2437:ALA:HB3	1:D:2508:ARG:HE	1.85	0.40
1:D:2697:ARG:HA	1:D:2700:MET:SD	2.60	0.40
1:A:1776:HIS:HB2	1:A:1798:LEU:HD22	2.04	0.40
1:B:1805:GLU:CD	1:B:1805:GLU:N	2.79	0.40
1:B:2044:ILE:HG23	1:B:2045:GLN:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1727:ARG:HA	1:C:1730:MET:SD	2.61	0.40
1:C:2101:MET:SD	1:C:2105:TRP:CE2	3.14	0.40
1:C:2150:GLU:CD	1:C:2150:GLU:N	2.80	0.40
1:D:367:LEU:HD12	1:D:367:LEU:C	2.46	0.40
1:C:308:HIS:CD2	1:C:308:HIS:C	3.00	0.40
1:C:1122:TYR:CD1	1:C:1122:TYR:N	2.89	0.40
1:C:2897:LYS:HE2	1:C:2897:LYS:HA	2.03	0.40
1:D:4023:MET:SD	1:D:4023:MET:C	3.05	0.40
1:A:3828:PHE:CD1	1:A:3828:PHE:C	2.98	0.40
1:B:2155:LEU:HD23	1:B:2155:LEU:C	2.47	0.40
1:B:2174:GLU:CD	1:B:2174:GLU:N	2.80	0.40
1:B:4065:PHE:CZ	1:B:4132:PHE:CD2	3.09	0.40
1:C:35:LEU:HD23	1:C:51:PRO:HA	2.03	0.40
1:C:4586:PRO:HD3	1:C:4629:TYR:CZ	2.56	0.40
1:C:4757:LYS:HD3	1:C:4757:LYS:H	1.86	0.40
1:D:308:HIS:CD2	1:D:308:HIS:C	3.00	0.40
1:D:3250:MET:C	1:D:3250:MET:SD	3.05	0.40
1:C:198:THR:HB	1:C:200:TRP:HE1	1.86	0.40
1:C:1496:TRP:CE2	1:C:1498:GLY:HA3	2.56	0.40
1:C:2155:LEU:C	1:C:2155:LEU:HD23	2.47	0.40
1:C:4958:CYS:CB	1:C:4961:CYS:SG	3.10	0.40
1:D:3312:LEU:HD12	1:D:3312:LEU:N	2.36	0.40
1:D:4947:GLN:HA	1:D:4950:VAL:HG12	2.03	0.40
1:D:4958:CYS:SG	1:D:4960:ILE:HB	2.62	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	4376/5037 (87%)	4057 (93%)	276 (6%)	43 (1%)	12 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	4376/5037 (87%)	4042 (92%)	283 (6%)	51 (1%)	10	43
1	C	4376/5037 (87%)	4030 (92%)	298 (7%)	48 (1%)	11	45
1	D	4376/5037 (87%)	4039 (92%)	290 (7%)	47 (1%)	11	45
2	E	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
2	F	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
2	G	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
2	H	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
All	All	17924/20580 (87%)	16563 (92%)	1172 (6%)	189 (1%)	14	45

All (189) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	HIS
1	A	3669	PHE
1	A	3687	GLU
1	A	3693	LYS
1	B	224	HIS
1	B	238	SER
1	B	3669	PHE
1	B	3687	GLU
1	B	3693	LYS
1	C	224	HIS
1	C	238	SER
1	C	3669	PHE
1	C	3687	GLU
1	C	3693	LYS
1	C	4075	GLU
1	D	238	SER
1	D	3687	GLU
1	D	3693	LYS
1	A	1792	ALA
1	A	1868	PRO
1	A	2663	ASN
1	A	4034	ASN
1	A	4155	PRO
1	B	1868	PRO
1	B	4034	ASN
1	B	4155	PRO
1	C	1792	ALA
1	C	1868	PRO

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Mol	Chain	Res	Type
1	C	2663	ASN
1	C	3877	ASP
1	C	4155	PRO
1	D	162	LYS
1	D	224	HIS
1	D	1792	ALA
1	D	1868	PRO
1	D	2570	ALA
1	D	3669	PHE
1	D	3877	ASP
1	A	364	PRO
1	A	691	GLY
1	A	843	SER
1	A	1508	ARG
1	A	1930	LYS
1	A	2092	GLN
1	A	2748	PRO
1	A	2786	LYS
1	A	2819	TRP
1	A	3159	ASP
1	A	3622	LYS
1	A	4906	GLY
1	A	4960	ILE
1	B	364	PRO
1	B	691	GLY
1	B	843	SER
1	B	1508	ARG
1	B	1792	ALA
1	B	1930	LYS
1	B	2662	ALA
1	B	2663	ASN
1	B	3113	GLY
1	B	3427	PRO
1	B	3614	LYS
1	B	3622	LYS
1	B	3877	ASP
1	B	4906	GLY
1	B	4960	ILE
1	C	124	SER
1	C	177	GLU
1	C	364	PRO
1	C	691	GLY

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Mol	Chain	Res	Type
1	C	1508	ARG
1	C	1930	LYS
1	C	2092	GLN
1	C	3427	PRO
1	C	3614	LYS
1	C	4694	ASP
1	C	4906	GLY
1	C	4960	ILE
1	D	364	PRO
1	D	691	GLY
1	D	1930	LYS
1	D	2092	GLN
1	D	2663	ASN
1	D	3427	PRO
1	D	3614	LYS
1	D	3622	LYS
1	D	4694	ASP
1	D	4906	GLY
1	A	956	PRO
1	A	3224	PRO
1	A	3427	PRO
1	A	3614	LYS
1	A	3877	ASP
1	A	4711	PHE
1	B	124	SER
1	B	956	PRO
1	B	2092	GLN
1	B	2819	TRP
1	B	3159	ASP
1	B	3224	PRO
1	C	195	PHE
1	C	1063	VAL
1	C	1215	ALA
1	C	2482	ASP
1	C	2570	ALA
1	C	2748	PRO
1	C	3114	LYS
1	C	3159	ASP
1	C	3224	PRO
1	C	3387	ALA
1	C	3622	LYS
1	D	843	SER

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Mol	Chain	Res	Type
1	D	1215	ALA
1	D	3114	LYS
1	D	3159	ASP
1	D	4155	PRO
1	D	4960	ILE
1	A	177	GLU
1	A	3113	GLY
1	A	3328	GLY
1	A	3501	ASP
1	A	3690	VAL
1	B	177	GLU
1	B	858	THR
1	B	902	ARG
1	B	1063	VAL
1	B	1241	SER
1	B	1756	ASN
1	B	1788	ALA
1	B	2748	PRO
1	B	3328	GLY
1	B	3690	VAL
1	B	4694	ASP
1	B	4711	PHE
1	C	122	THR
1	C	956	PRO
1	C	1756	ASN
1	C	1788	ALA
1	C	2819	TRP
1	D	857	ASP
1	D	902	ARG
1	D	956	PRO
1	D	1063	VAL
1	D	1241	SER
1	D	1700	ASP
1	D	2748	PRO
1	D	2819	TRP
1	D	3111	ARG
1	D	3332	ALA
1	A	64	ILE
1	A	2343	GLY
1	A	3332	ALA
1	B	64	ILE
1	B	146	CYS

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Mol	Chain	Res	Type
1	B	1250	PRO
1	B	3052	HIS
1	C	64	ILE
1	C	143	GLY
1	C	3328	GLY
1	C	3581	GLY
1	D	64	ILE
1	D	2572	THR
1	D	3328	GLY
1	D	3501	ASP
1	A	1250	PRO
1	A	1774	PRO
1	A	2989	SER
1	A	3581	GLY
1	D	1250	PRO
1	A	371	VAL
1	A	1063	VAL
1	C	3971	GLY
1	D	371	VAL
1	D	3581	GLY
1	B	3581	GLY
1	B	3971	GLY
1	C	371	VAL
1	D	4711	PHE
1	A	3971	GLY
1	B	371	VAL
1	B	1509	ILE
1	B	3029	GLY
1	B	3307	VAL
1	C	3690	VAL
1	D	3233	PRO
1	C	1774	PRO
1	C	1803	PRO
1	D	3231	GLY
1	D	3690	VAL

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	3827/4276 (90%)	3640 (95%)	187 (5%)	22	43
1	B	3827/4276 (90%)	3621 (95%)	206 (5%)	20	41
1	C	3827/4276 (90%)	3638 (95%)	189 (5%)	22	43
1	D	3827/4276 (90%)	3630 (95%)	197 (5%)	21	42
2	E	89/90 (99%)	83 (93%)	6 (7%)	15	36
2	F	89/90 (99%)	83 (93%)	6 (7%)	15	36
2	G	89/90 (99%)	82 (92%)	7 (8%)	11	32
2	H	89/90 (99%)	82 (92%)	7 (8%)	11	32
All	All	15664/17464 (90%)	14859 (95%)	805 (5%)	23	42

All (805) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	28	VAL
1	A	29	LEU
1	A	32	GLN
1	A	57	ASN
1	A	130	LYS
1	A	172	VAL
1	A	188	GLU
1	A	197	GLN
1	A	211	GLU
1	A	215	THR
1	A	220	LEU
1	A	228	ASP
1	A	229	GLU
1	A	247	TYR
1	A	267	ILE
1	A	278	GLN
1	A	296	ASP
1	A	303	ASP
1	A	308	HIS
1	A	328	LYS
1	A	389	PHE
1	A	395	GLN
1	A	476	SER
1	A	477	LEU

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Mol	Chain	Res	Type
1	A	491	ILE
1	A	581	ASN
1	A	639	ASN
1	A	649	PHE
1	A	652	ARG
1	A	747	CYS
1	A	755	ILE
1	A	757	PHE
1	A	922	LEU
1	A	923	GLN
1	A	957	LYS
1	A	963	ASN
1	A	1003	GLN
1	A	1022	VAL
1	A	1052	ASN
1	A	1071	ARG
1	A	1137	GLU
1	A	1143	TRP
1	A	1152	MET
1	A	1157	GLU
1	A	1207	ASP
1	A	1226	PHE
1	A	1236	THR
1	A	1255	TYR
1	A	1266	THR
1	A	1421	ARG
1	A	1444	GLU
1	A	1446	SER
1	A	1518	CYS
1	A	1519	LEU
1	A	1539	PHE
1	A	1583	GLU
1	A	1732	SER
1	A	1739	THR
1	A	1752	ARG
1	A	1769	THR
1	A	1805	GLU
1	A	1857	GLU
1	A	1872	THR
1	A	1926	LEU
1	A	1944	GLU
1	A	1950	GLU

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Mol	Chain	Res	Type
1	A	1963	GLU
1	A	1996	ARG
1	A	2008	MET
1	A	2009	LEU
1	A	2094	LEU
1	A	2110	TYR
1	A	2120	MET
1	A	2150	GLU
1	A	2177	LEU
1	A	2186	MET
1	A	2219	GLU
1	A	2253	HIS
1	A	2270	SER
1	A	2271	THR
1	A	2274	ASP
1	A	2290	LEU
1	A	2291	GLN
1	A	2294	ASP
1	A	2357	LEU
1	A	2369	ARG
1	A	2431	ASP
1	A	2464	ASP
1	A	2465	ASP
1	A	2474	LEU
1	A	2482	ASP
1	A	2497	ASP
1	A	2503	VAL
1	A	2523	ASP
1	A	2548	LEU
1	A	2558	VAL
1	A	2559	LEU
1	A	2607	LEU
1	A	2621	HIS
1	A	2623	LEU
1	A	2673	HIS
1	A	2694	GLU
1	A	2700	MET
1	A	2734	ASN
1	A	2780	ASN
1	A	2784	GLU
1	A	2819	TRP
1	A	2870	GLU

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Mol	Chain	Res	Type
1	A	2881	ASN
1	A	2924	GLN
1	A	2972	GLU
1	A	2977	LEU
1	A	2986	VAL
1	A	3002	LEU
1	A	3057	PHE
1	A	3137	LEU
1	A	3186	LEU
1	A	3243	ILE
1	A	3247	ASP
1	A	3276	MET
1	A	3305	THR
1	A	3331	GLU
1	A	3345	ILE
1	A	3384	LYS
1	A	3449	HIS
1	A	3549	VAL
1	A	3550	ARG
1	A	3597	GLN
1	A	3637	ARG
1	A	3677	LEU
1	A	3683	GLN
1	A	3703	LEU
1	A	3752	SER
1	A	3779	VAL
1	A	3793	MET
1	A	3825	GLU
1	A	3879	GLU
1	A	3884	LEU
1	A	3895	HIS
1	A	3912	THR
1	A	3944	GLU
1	A	3953	LYS
1	A	3987	ASP
1	A	4006	ASP
1	A	4026	MET
1	A	4034	ASN
1	A	4037	ASN
1	A	4047	MET
1	A	4061	PHE
1	A	4091	LYS

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Mol	Chain	Res	Type
1	A	4121	GLU
1	A	4150	LEU
1	A	4165	GLU
1	A	4172	GLU
1	A	4183	ILE
1	A	4199	GLU
1	A	4224	GLU
1	A	4227	GLU
1	A	4234	PHE
1	A	4240	ASP
1	A	4244	GLU
1	A	4541	TRP
1	A	4555	LEU
1	A	4576	ILE
1	A	4580	TYR
1	A	4634	GLU
1	A	4643	LEU
1	A	4656	LEU
1	A	4662	ASN
1	A	4666	VAL
1	A	4688	ILE
1	A	4735	GLU
1	A	4756	ARG
1	A	4757	LYS
1	A	4775	TYR
1	A	4780	PHE
1	A	4788	SER
1	A	4796	MET
1	A	4821	LYS
1	A	4865	LYS
1	A	4932	ILE
1	A	4989	MET
1	A	5006	GLN
1	A	5011	TRP
1	A	5013	MET
1	A	5035	GLN
1	B	17	ASP
1	B	28	VAL
1	B	29	LEU
1	B	32	GLN
1	B	57	ASN
1	B	69	LEU

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Mol	Chain	Res	Type
1	B	99	ARG
1	B	121	LEU
1	B	130	LYS
1	B	144	GLU
1	B	168	ASP
1	B	172	VAL
1	B	188	GLU
1	B	191	VAL
1	B	211	GLU
1	B	215	THR
1	B	228	ASP
1	B	229	GLU
1	B	233	ILE
1	B	247	TYR
1	B	267	ILE
1	B	278	GLN
1	B	296	ASP
1	B	303	ASP
1	B	328	LYS
1	B	389	PHE
1	B	395	GLN
1	B	441	VAL
1	B	462	GLU
1	B	476	SER
1	B	477	LEU
1	B	491	ILE
1	B	581	ASN
1	B	639	ASN
1	B	649	PHE
1	B	652	ARG
1	B	747	CYS
1	B	755	ILE
1	B	757	PHE
1	B	783	PHE
1	B	876	GLU
1	B	884	LEU
1	B	892	THR
1	B	922	LEU
1	B	923	GLN
1	B	950	LEU
1	B	953	THR
1	B	957	LYS

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Mol	Chain	Res	Type
1	B	963	ASN
1	B	1003	GLN
1	B	1025	ARG
1	B	1071	ARG
1	B	1125	ASN
1	B	1137	GLU
1	B	1152	MET
1	B	1154	ASP
1	B	1226	PHE
1	B	1255	TYR
1	B	1266	THR
1	B	1421	ARG
1	B	1444	GLU
1	B	1446	SER
1	B	1518	CYS
1	B	1519	LEU
1	B	1539	PHE
1	B	1732	SER
1	B	1739	THR
1	B	1769	THR
1	B	1798	LEU
1	B	1802	ILE
1	B	1805	GLU
1	B	1857	GLU
1	B	1926	LEU
1	B	1944	GLU
1	B	1950	GLU
1	B	1963	GLU
1	B	1996	ARG
1	B	2008	MET
1	B	2009	LEU
1	B	2045	GLN
1	B	2094	LEU
1	B	2101	MET
1	B	2110	TYR
1	B	2150	GLU
1	B	2177	LEU
1	B	2186	MET
1	B	2219	GLU
1	B	2224	ARG
1	B	2253	HIS
1	B	2270	SER

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Mol	Chain	Res	Type
1	B	2271	THR
1	B	2274	ASP
1	B	2290	LEU
1	B	2291	GLN
1	B	2294	ASP
1	B	2341	VAL
1	B	2357	LEU
1	B	2369	ARG
1	B	2431	ASP
1	B	2440	MET
1	B	2464	ASP
1	B	2465	ASP
1	B	2489	LYS
1	B	2497	ASP
1	B	2513	GLU
1	B	2523	ASP
1	B	2550	LEU
1	B	2559	LEU
1	B	2588	ARG
1	B	2607	LEU
1	B	2623	LEU
1	B	2700	MET
1	B	2724	GLU
1	B	2734	ASN
1	B	2738	ARG
1	B	2768	PHE
1	B	2773	ASN
1	B	2774	ASN
1	B	2802	LYS
1	B	2819	TRP
1	B	2827	ARG
1	B	2881	ASN
1	B	2892	GLN
1	B	2915	GLU
1	B	2924	GLN
1	B	2972	GLU
1	B	2977	LEU
1	B	2981	VAL
1	B	3002	LEU
1	B	3057	PHE
1	B	3083	SER
1	B	3137	LEU

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Mol	Chain	Res	Type
1	B	3186	LEU
1	B	3218	VAL
1	B	3247	ASP
1	B	3249	LEU
1	B	3276	MET
1	B	3305	THR
1	B	3307	VAL
1	B	3331	GLU
1	B	3549	VAL
1	B	3550	ARG
1	B	3597	GLN
1	B	3670	GLU
1	B	3677	LEU
1	B	3683	GLN
1	B	3703	LEU
1	B	3752	SER
1	B	3757	GLU
1	B	3779	VAL
1	B	3793	MET
1	B	3816	MET
1	B	3820	LEU
1	B	3842	LEU
1	B	3878	ASP
1	B	3879	GLU
1	B	3884	LEU
1	B	3895	HIS
1	B	3912	THR
1	B	3943	ILE
1	B	3944	GLU
1	B	3953	LYS
1	B	4006	ASP
1	B	4017	LEU
1	B	4023	MET
1	B	4034	ASN
1	B	4037	ASN
1	B	4047	MET
1	B	4061	PHE
1	B	4075	GLU
1	B	4091	LYS
1	B	4121	GLU
1	B	4150	LEU
1	B	4165	GLU

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Mol	Chain	Res	Type
1	B	4172	GLU
1	B	4199	GLU
1	B	4224	GLU
1	B	4227	GLU
1	B	4240	ASP
1	B	4244	GLU
1	B	4245	MET
1	B	4541	TRP
1	B	4576	ILE
1	B	4580	TYR
1	B	4634	GLU
1	B	4662	ASN
1	B	4666	VAL
1	B	4679	ARG
1	B	4688	ILE
1	B	4735	GLU
1	B	4757	LYS
1	B	4767	TRP
1	B	4768	LEU
1	B	4775	TYR
1	B	4780	PHE
1	B	4788	SER
1	B	4796	MET
1	B	4821	LYS
1	B	4865	LYS
1	B	4883	TYR
1	B	4932	ILE
1	B	4989	MET
1	B	5006	GLN
1	B	5011	TRP
1	B	5013	MET
1	B	5020	ASP
1	C	17	ASP
1	C	28	VAL
1	C	29	LEU
1	C	32	GLN
1	C	57	ASN
1	C	69	LEU
1	C	121	LEU
1	C	130	LYS
1	C	188	GLU
1	C	191	VAL

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Mol	Chain	Res	Type
1	C	196	MET
1	C	211	GLU
1	C	228	ASP
1	C	229	GLU
1	C	247	TYR
1	C	267	ILE
1	C	278	GLN
1	C	296	ASP
1	C	303	ASP
1	C	328	LYS
1	C	389	PHE
1	C	395	GLN
1	C	441	VAL
1	C	477	LEU
1	C	491	ILE
1	C	581	ASN
1	C	612	VAL
1	C	639	ASN
1	C	649	PHE
1	C	652	ARG
1	C	747	CYS
1	C	757	PHE
1	C	884	LEU
1	C	922	LEU
1	C	923	GLN
1	C	957	LYS
1	C	963	ASN
1	C	1025	ARG
1	C	1052	ASN
1	C	1137	GLU
1	C	1143	TRP
1	C	1152	MET
1	C	1154	ASP
1	C	1207	ASP
1	C	1226	PHE
1	C	1255	TYR
1	C	1266	THR
1	C	1277	TRP
1	C	1421	ARG
1	C	1444	GLU
1	C	1446	SER
1	C	1494	MET

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Mol	Chain	Res	Type
1	C	1518	CYS
1	C	1519	LEU
1	C	1539	PHE
1	C	1732	SER
1	C	1739	THR
1	C	1742	THR
1	C	1748	PHE
1	C	1769	THR
1	C	1802	ILE
1	C	1805	GLU
1	C	1857	GLU
1	C	1926	LEU
1	C	1950	GLU
1	C	1963	GLU
1	C	1996	ARG
1	C	2008	MET
1	C	2009	LEU
1	C	2018	GLU
1	C	2094	LEU
1	C	2110	TYR
1	C	2120	MET
1	C	2135	LEU
1	C	2150	GLU
1	C	2177	LEU
1	C	2186	MET
1	C	2219	GLU
1	C	2253	HIS
1	C	2271	THR
1	C	2274	ASP
1	C	2290	LEU
1	C	2291	GLN
1	C	2294	ASP
1	C	2341	VAL
1	C	2357	LEU
1	C	2369	ARG
1	C	2431	ASP
1	C	2451	LEU
1	C	2464	ASP
1	C	2465	ASP
1	C	2491	SER
1	C	2497	ASP
1	C	2503	VAL

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Mol	Chain	Res	Type
1	C	2513	GLU
1	C	2518	LEU
1	C	2548	LEU
1	C	2550	LEU
1	C	2558	VAL
1	C	2559	LEU
1	C	2588	ARG
1	C	2607	LEU
1	C	2623	LEU
1	C	2654	TYR
1	C	2694	GLU
1	C	2700	MET
1	C	2734	ASN
1	C	2738	ARG
1	C	2768	PHE
1	C	2780	ASN
1	C	2819	TRP
1	C	2827	ARG
1	C	2881	ASN
1	C	2892	GLN
1	C	2894	LEU
1	C	2915	GLU
1	C	2924	GLN
1	C	2972	GLU
1	C	2977	LEU
1	C	3002	LEU
1	C	3020	THR
1	C	3137	LEU
1	C	3186	LEU
1	C	3247	ASP
1	C	3249	LEU
1	C	3287	ARG
1	C	3331	GLU
1	C	3469	PHE
1	C	3549	VAL
1	C	3550	ARG
1	C	3597	GLN
1	C	3637	ARG
1	C	3677	LEU
1	C	3683	GLN
1	C	3703	LEU
1	C	3752	SER

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Mol	Chain	Res	Type
1	C	3779	VAL
1	C	3793	MET
1	C	3816	MET
1	C	3842	LEU
1	C	3878	ASP
1	C	3879	GLU
1	C	3884	LEU
1	C	3895	HIS
1	C	3912	THR
1	C	3933	PHE
1	C	3944	GLU
1	C	4040	ILE
1	C	4047	MET
1	C	4061	PHE
1	C	4089	SER
1	C	4092	ASP
1	C	4093	PHE
1	C	4094	GLN
1	C	4123	ILE
1	C	4150	LEU
1	C	4165	GLU
1	C	4172	GLU
1	C	4196	GLU
1	C	4199	GLU
1	C	4224	GLU
1	C	4227	GLU
1	C	4234	PHE
1	C	4240	ASP
1	C	4244	GLU
1	C	4541	TRP
1	C	4552	LEU
1	C	4576	ILE
1	C	4580	TYR
1	C	4632	LEU
1	C	4656	LEU
1	C	4662	ASN
1	C	4666	VAL
1	C	4679	ARG
1	C	4688	ILE
1	C	4719	PHE
1	C	4735	GLU
1	C	4757	LYS

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Mol	Chain	Res	Type
1	C	4775	TYR
1	C	4780	PHE
1	C	4788	SER
1	C	4821	LYS
1	C	4865	LYS
1	C	4874	MET
1	C	4932	ILE
1	C	4989	MET
1	C	5011	TRP
1	C	5013	MET
1	C	5035	GLN
1	D	17	ASP
1	D	28	VAL
1	D	29	LEU
1	D	32	GLN
1	D	57	ASN
1	D	130	LYS
1	D	188	GLU
1	D	191	VAL
1	D	211	GLU
1	D	215	THR
1	D	228	ASP
1	D	267	ILE
1	D	278	GLN
1	D	296	ASP
1	D	303	ASP
1	D	328	LYS
1	D	386	ASP
1	D	389	PHE
1	D	395	GLN
1	D	441	VAL
1	D	462	GLU
1	D	477	LEU
1	D	491	ILE
1	D	581	ASN
1	D	639	ASN
1	D	649	PHE
1	D	652	ARG
1	D	747	CYS
1	D	755	ILE
1	D	757	PHE
1	D	876	GLU

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Mol	Chain	Res	Type
1	D	892	THR
1	D	907	LEU
1	D	922	LEU
1	D	923	GLN
1	D	957	LYS
1	D	963	ASN
1	D	1025	ARG
1	D	1071	ARG
1	D	1073	ARG
1	D	1137	GLU
1	D	1143	TRP
1	D	1152	MET
1	D	1157	GLU
1	D	1207	ASP
1	D	1226	PHE
1	D	1236	THR
1	D	1255	TYR
1	D	1266	THR
1	D	1422	ASP
1	D	1427	ILE
1	D	1444	GLU
1	D	1446	SER
1	D	1518	CYS
1	D	1519	LEU
1	D	1539	PHE
1	D	1732	SER
1	D	1739	THR
1	D	1752	ARG
1	D	1769	THR
1	D	1798	LEU
1	D	1802	ILE
1	D	1805	GLU
1	D	1857	GLU
1	D	1872	THR
1	D	1950	GLU
1	D	1963	GLU
1	D	1996	ARG
1	D	2008	MET
1	D	2009	LEU
1	D	2018	GLU
1	D	2045	GLN
1	D	2094	LEU

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Mol	Chain	Res	Type
1	D	2101	MET
1	D	2110	TYR
1	D	2120	MET
1	D	2150	GLU
1	D	2177	LEU
1	D	2186	MET
1	D	2219	GLU
1	D	2224	ARG
1	D	2253	HIS
1	D	2270	SER
1	D	2271	THR
1	D	2274	ASP
1	D	2290	LEU
1	D	2291	GLN
1	D	2294	ASP
1	D	2341	VAL
1	D	2357	LEU
1	D	2369	ARG
1	D	2431	ASP
1	D	2451	LEU
1	D	2464	ASP
1	D	2465	ASP
1	D	2482	ASP
1	D	2491	SER
1	D	2497	ASP
1	D	2503	VAL
1	D	2513	GLU
1	D	2518	LEU
1	D	2523	ASP
1	D	2548	LEU
1	D	2550	LEU
1	D	2558	VAL
1	D	2559	LEU
1	D	2607	LEU
1	D	2623	LEU
1	D	2654	TYR
1	D	2673	HIS
1	D	2700	MET
1	D	2751	LEU
1	D	2768	PHE
1	D	2780	ASN
1	D	2877	GLN

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Mol	Chain	Res	Type
1	D	2924	GLN
1	D	2972	GLU
1	D	2977	LEU
1	D	3002	LEU
1	D	3083	SER
1	D	3137	LEU
1	D	3186	LEU
1	D	3247	ASP
1	D	3249	LEU
1	D	3264	THR
1	D	3276	MET
1	D	3384	LYS
1	D	3449	HIS
1	D	3549	VAL
1	D	3550	ARG
1	D	3597	GLN
1	D	3624	LEU
1	D	3668	SER
1	D	3670	GLU
1	D	3673	MET
1	D	3677	LEU
1	D	3683	GLN
1	D	3703	LEU
1	D	3712	GLU
1	D	3752	SER
1	D	3779	VAL
1	D	3789	GLU
1	D	3793	MET
1	D	3816	MET
1	D	3825	GLU
1	D	3842	LEU
1	D	3878	ASP
1	D	3879	GLU
1	D	3884	LEU
1	D	3895	HIS
1	D	3912	THR
1	D	3933	PHE
1	D	3943	ILE
1	D	3944	GLU
1	D	3953	LYS
1	D	3987	ASP
1	D	4026	MET

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Mol	Chain	Res	Type
1	D	4037	ASN
1	D	4047	MET
1	D	4061	PHE
1	D	4089	SER
1	D	4092	ASP
1	D	4093	PHE
1	D	4095	LYS
1	D	4100	GLN
1	D	4150	LEU
1	D	4165	GLU
1	D	4172	GLU
1	D	4199	GLU
1	D	4224	GLU
1	D	4227	GLU
1	D	4234	PHE
1	D	4240	ASP
1	D	4244	GLU
1	D	4541	TRP
1	D	4552	LEU
1	D	4555	LEU
1	D	4576	ILE
1	D	4580	TYR
1	D	4656	LEU
1	D	4662	ASN
1	D	4666	VAL
1	D	4688	ILE
1	D	4719	PHE
1	D	4735	GLU
1	D	4757	LYS
1	D	4780	PHE
1	D	4788	SER
1	D	4801	LEU
1	D	4821	LYS
1	D	4865	LYS
1	D	4874	MET
1	D	4989	MET
1	D	5006	GLN
1	D	5013	MET
1	D	5020	ASP
1	D	5035	GLN
2	E	13	ARG
2	E	21	THR

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Mol	Chain	Res	Type
2	E	32	ASP
2	E	36	PHE
2	E	80	TYR
2	E	98	VAL
2	F	13	ARG
2	F	21	THR
2	F	32	ASP
2	F	36	PHE
2	F	80	TYR
2	F	98	VAL
2	G	11	ASP
2	G	13	ARG
2	G	21	THR
2	G	32	ASP
2	G	36	PHE
2	G	80	TYR
2	G	98	VAL
2	H	13	ARG
2	H	21	THR
2	H	32	ASP
2	H	36	PHE
2	H	80	TYR
2	H	85	THR
2	H	98	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (195) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	32	GLN
1	A	113	HIS
1	A	203	ASN
1	A	380	GLN
1	A	446	GLN
1	A	636	ASN
1	A	735	GLN
1	A	765	GLN
1	A	812	HIS
1	A	921	ASN
1	A	938	HIS
1	A	1052	ASN
1	A	1084	GLN

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Mol	Chain	Res	Type
1	A	1281	ASN
1	A	1299	GLN
1	A	1459	GLN
1	A	1545	ASN
1	A	1560	ASN
1	A	1691	GLN
1	A	1949	GLN
1	A	2180	GLN
1	A	2184	ASN
1	A	2194	HIS
1	A	2196	ASN
1	A	2291	GLN
1	A	2351	ASN
1	A	2417	HIS
1	A	2475	GLN
1	A	2515	GLN
1	A	2931	GLN
1	A	3033	ASN
1	A	3268	HIS
1	A	3605	HIS
1	A	3683	GLN
1	A	3850	GLN
1	A	3851	ASN
1	A	3927	GLN
1	A	3946	GLN
1	A	3960	GLN
1	A	3982	HIS
1	A	4009	GLN
1	A	4034	ASN
1	A	4216	GLN
1	A	4547	GLN
1	A	4662	ASN
1	A	4753	HIS
1	A	4754	ASN
1	A	4812	HIS
1	A	5003	HIS
1	A	5031	GLN
1	B	23	GLN
1	B	32	GLN
1	B	197	GLN
1	B	203	ASN
1	B	380	GLN

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Mol	Chain	Res	Type
1	B	636	ASN
1	B	765	GLN
1	B	911	HIS
1	B	921	ASN
1	B	938	HIS
1	B	1052	ASN
1	B	1127	HIS
1	B	1254	HIS
1	B	1280	GLN
1	B	1281	ASN
1	B	1296	GLN
1	B	1459	GLN
1	B	1560	ASN
1	B	1861	GLN
1	B	1949	GLN
1	B	2180	GLN
1	B	2184	ASN
1	B	2194	HIS
1	B	2196	ASN
1	B	2291	GLN
1	B	2351	ASN
1	B	2414	ASN
1	B	2417	HIS
1	B	2475	GLN
1	B	2487	GLN
1	B	2931	GLN
1	B	3033	ASN
1	B	3523	ASN
1	B	3699	HIS
1	B	3850	GLN
1	B	3851	ASN
1	B	3867	ASN
1	B	3946	GLN
1	B	4009	GLN
1	B	4034	ASN
1	B	4054	ASN
1	B	4216	GLN
1	B	4547	GLN
1	B	4662	ASN
1	B	4753	HIS
1	B	4754	ASN
1	B	5035	GLN

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Mol	Chain	Res	Type
1	C	23	GLN
1	C	32	GLN
1	C	197	GLN
1	C	203	ASN
1	C	380	GLN
1	C	399	GLN
1	C	446	GLN
1	C	636	ASN
1	C	735	GLN
1	C	911	HIS
1	C	921	ASN
1	C	938	HIS
1	C	1052	ASN
1	C	1299	GLN
1	C	1545	ASN
1	C	1560	ASN
1	C	1949	GLN
1	C	2003	GLN
1	C	2161	GLN
1	C	2173	GLN
1	C	2180	GLN
1	C	2184	ASN
1	C	2196	ASN
1	C	2291	GLN
1	C	2351	ASN
1	C	2414	ASN
1	C	2417	HIS
1	C	2475	GLN
1	C	2515	GLN
1	C	2663	ASN
1	C	2883	HIS
1	C	2924	GLN
1	C	2931	GLN
1	C	3033	ASN
1	C	3109	ASN
1	C	3418	ASN
1	C	3430	ASN
1	C	3461	GLN
1	C	3523	ASN
1	C	3699	HIS
1	C	3850	GLN
1	C	3946	GLN

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Mol	Chain	Res	Type
1	C	4043	GLN
1	C	4054	ASN
1	C	4162	ASN
1	C	4547	GLN
1	C	4662	ASN
1	C	4753	HIS
1	C	4754	ASN
1	C	5003	HIS
1	D	23	GLN
1	D	32	GLN
1	D	98	HIS
1	D	197	GLN
1	D	203	ASN
1	D	380	GLN
1	D	446	GLN
1	D	636	ASN
1	D	735	GLN
1	D	765	GLN
1	D	1052	ASN
1	D	1084	GLN
1	D	1127	HIS
1	D	1254	HIS
1	D	1281	ASN
1	D	1459	GLN
1	D	1560	ASN
1	D	1949	GLN
1	D	2003	GLN
1	D	2180	GLN
1	D	2184	ASN
1	D	2196	ASN
1	D	2291	GLN
1	D	2351	ASN
1	D	2414	ASN
1	D	2417	HIS
1	D	2475	GLN
1	D	2515	GLN
1	D	2931	GLN
1	D	3033	ASN
1	D	3128	ASN
1	D	3268	HIS
1	D	3523	ASN
1	D	3556	ASN

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Mol	Chain	Res	Type
1	D	3734	HIS
1	D	3850	GLN
1	D	3946	GLN
1	D	4009	GLN
1	D	4142	ASN
1	D	4662	ASN
1	D	4753	HIS
1	D	4754	ASN
1	D	5003	HIS
2	E	94	HIS
2	F	65	GLN
2	F	94	HIS
2	G	65	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

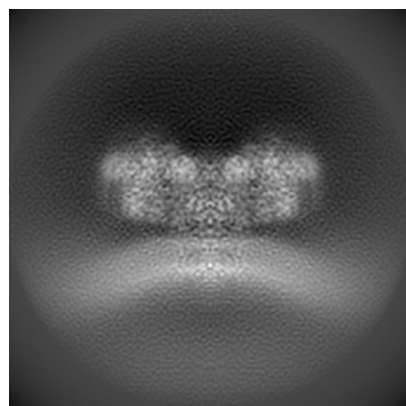
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54593. These allow visual inspection of the internal detail of the map and identification of artifacts.

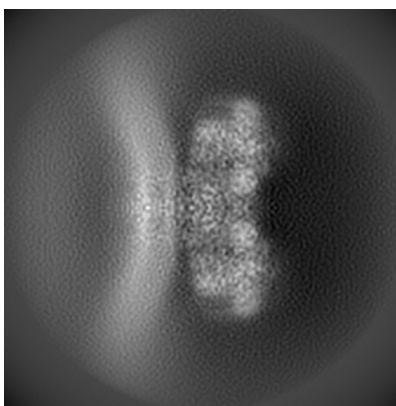
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

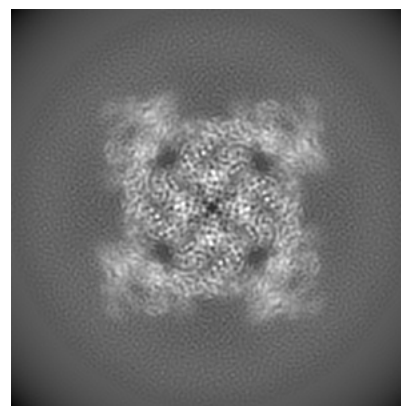
6.1.1 Primary map



X

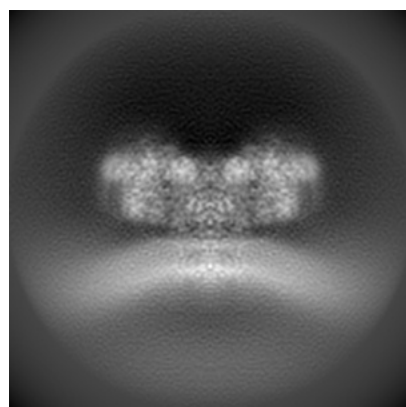


Y

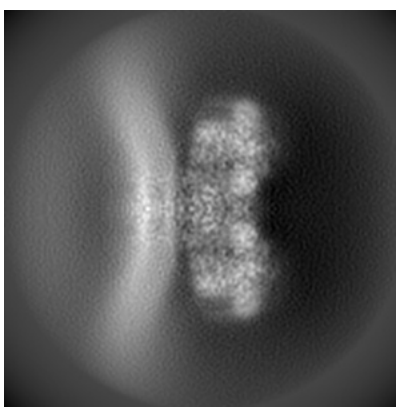


Z

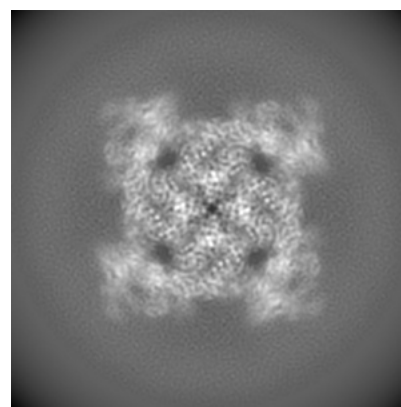
6.1.2 Raw map



X



Y

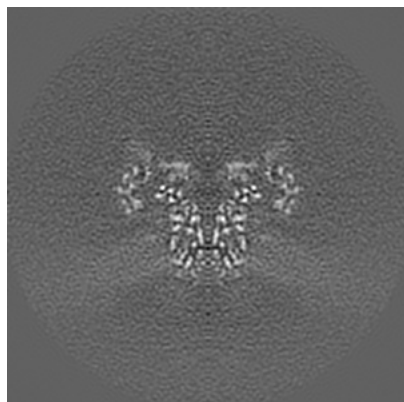


Z

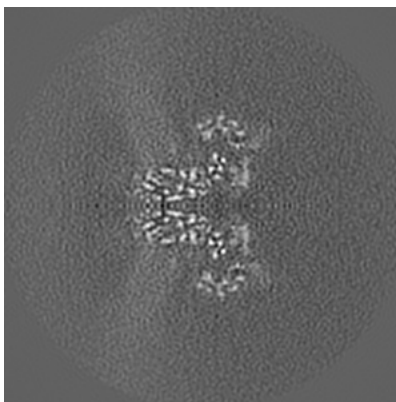
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

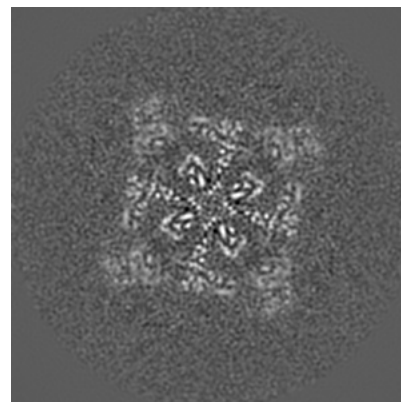
6.2.1 Primary map



X Index: 85

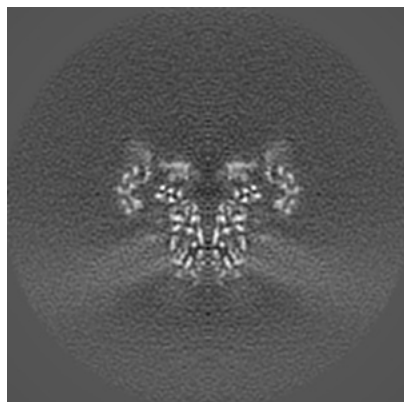


Y Index: 85

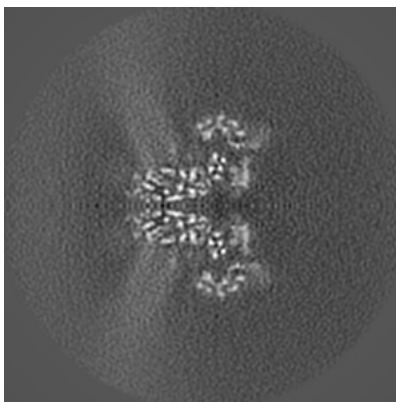


Z Index: 85

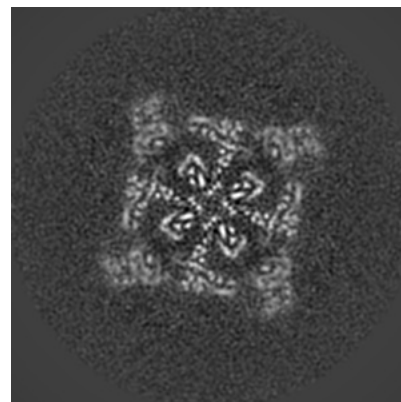
6.2.2 Raw map



X Index: 85



Y Index: 85

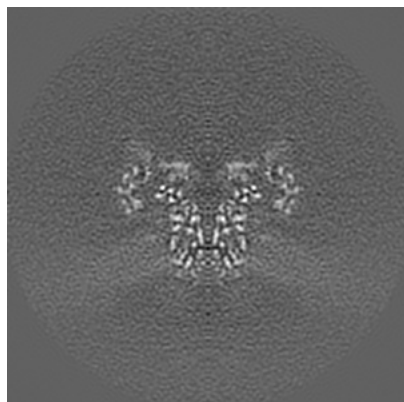


Z Index: 85

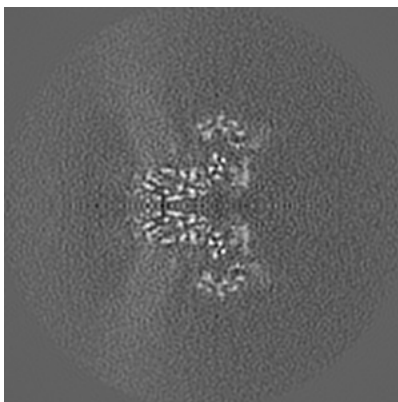
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

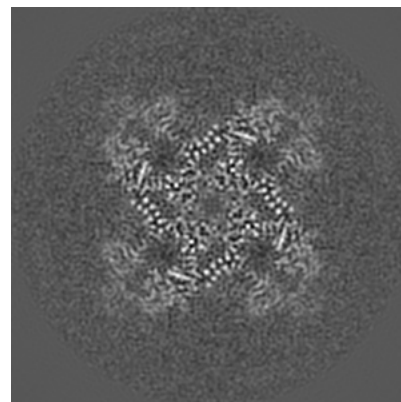
6.3.1 Primary map



X Index: 85

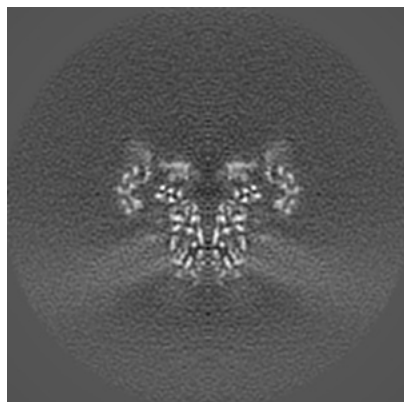


Y Index: 85

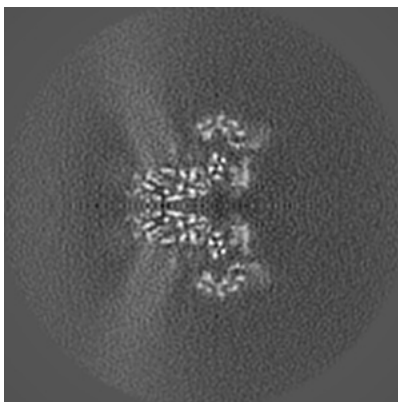


Z Index: 99

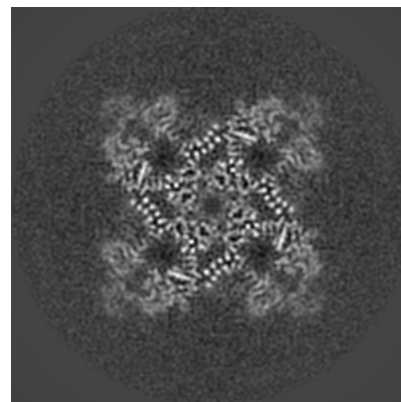
6.3.2 Raw map



X Index: 85



Y Index: 85

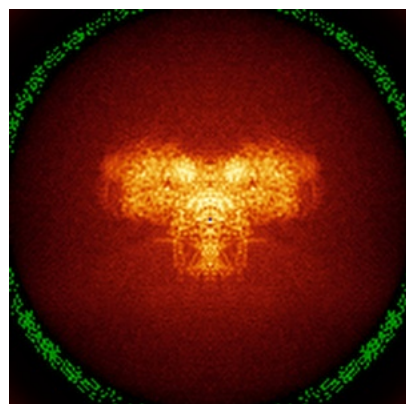


Z Index: 99

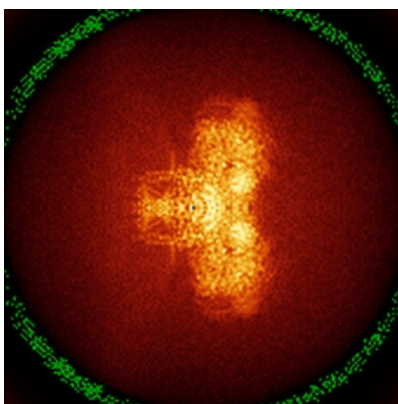
The images above show the largest variance slices of the map in three orthogonal directions.

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

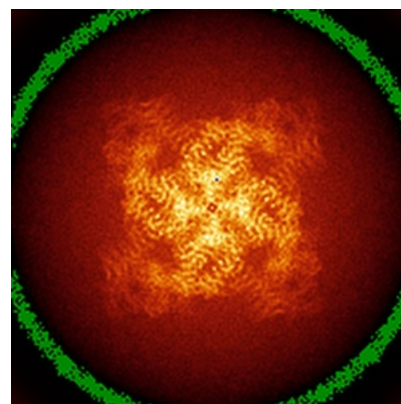
6.4.1 Primary map



X

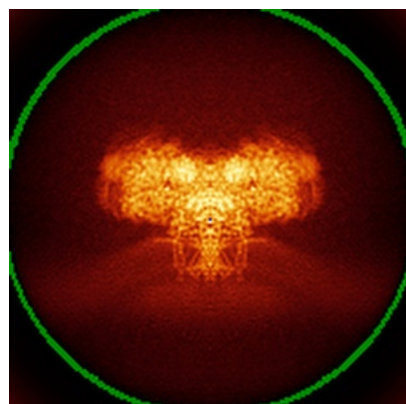


Y

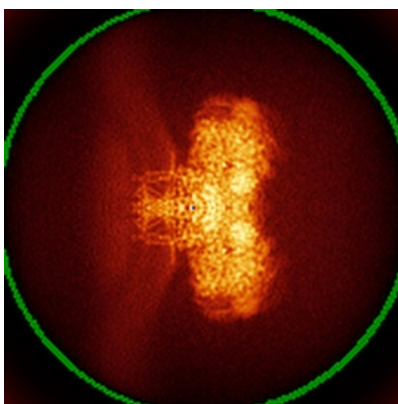


Z

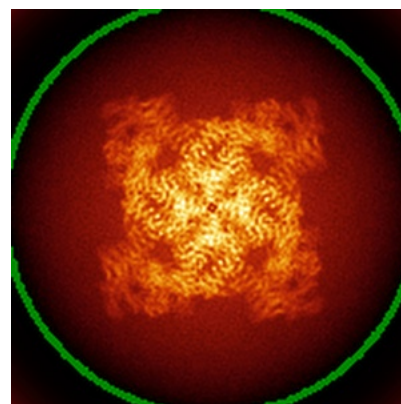
6.4.2 Raw map



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.

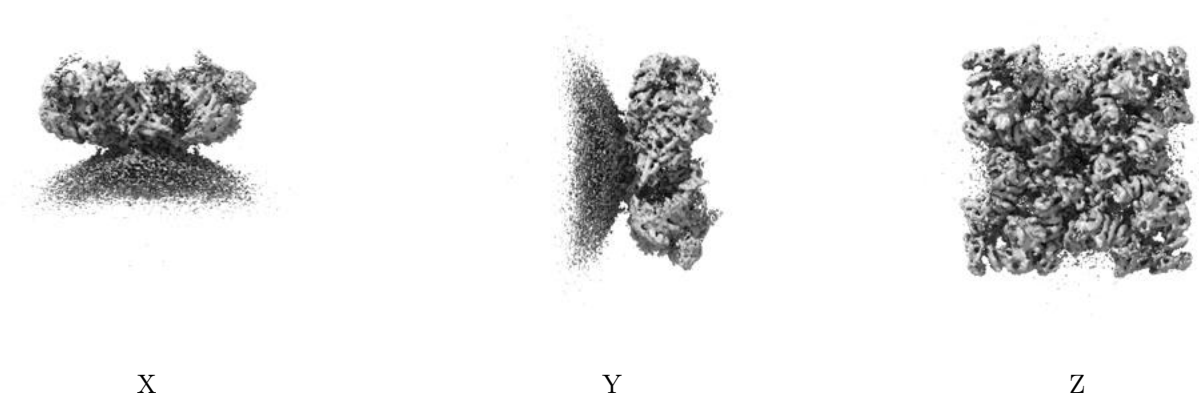
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0795. 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.

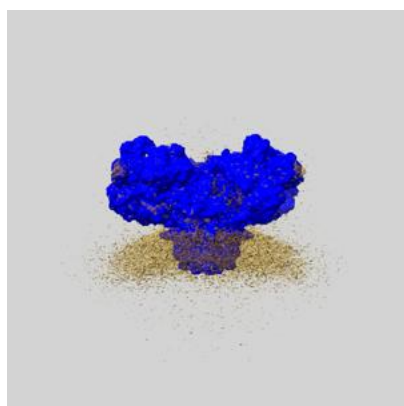
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

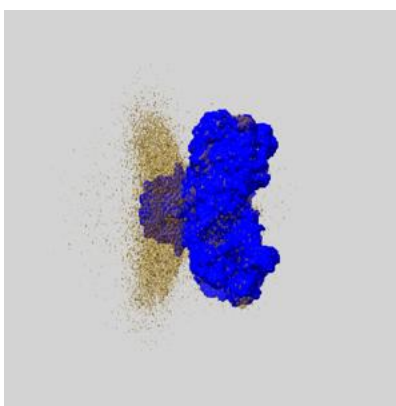
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

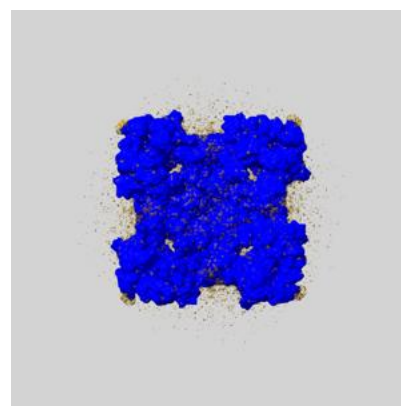
6.6.1 emd_54593_msk_1.map [i](#)



X



Y

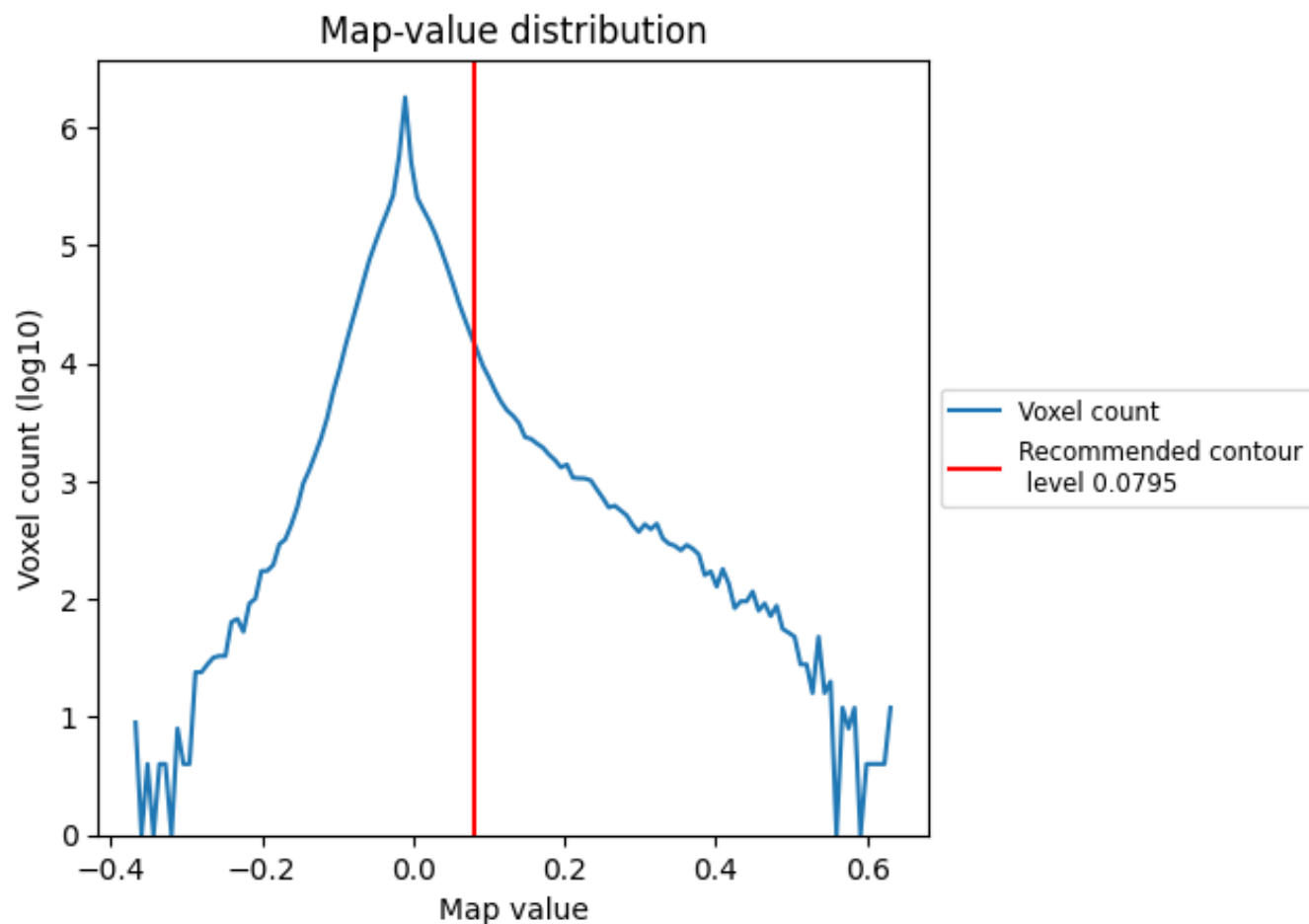


Z

7 Map analysis [i](#)

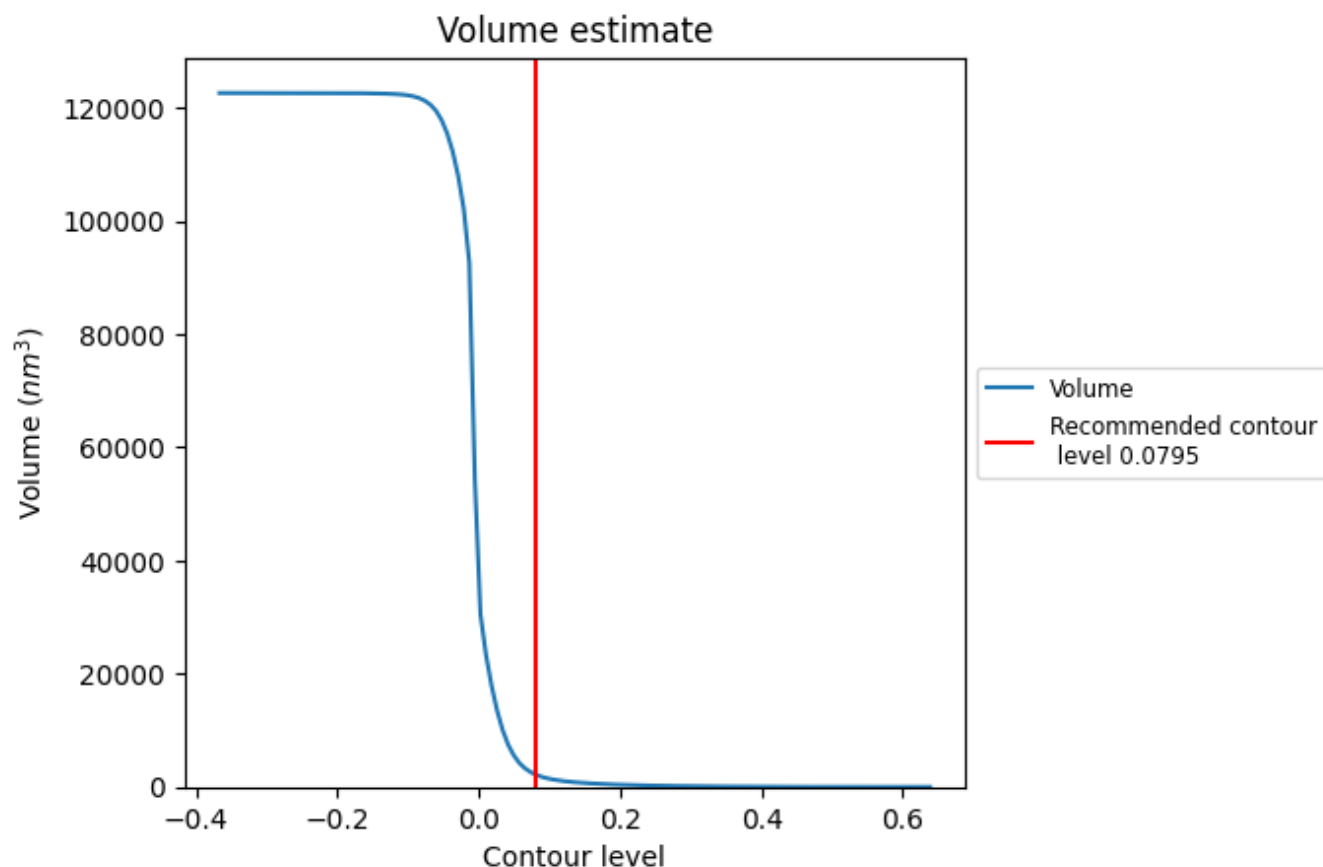
This section contains the results of statistical analysis of the map.

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.

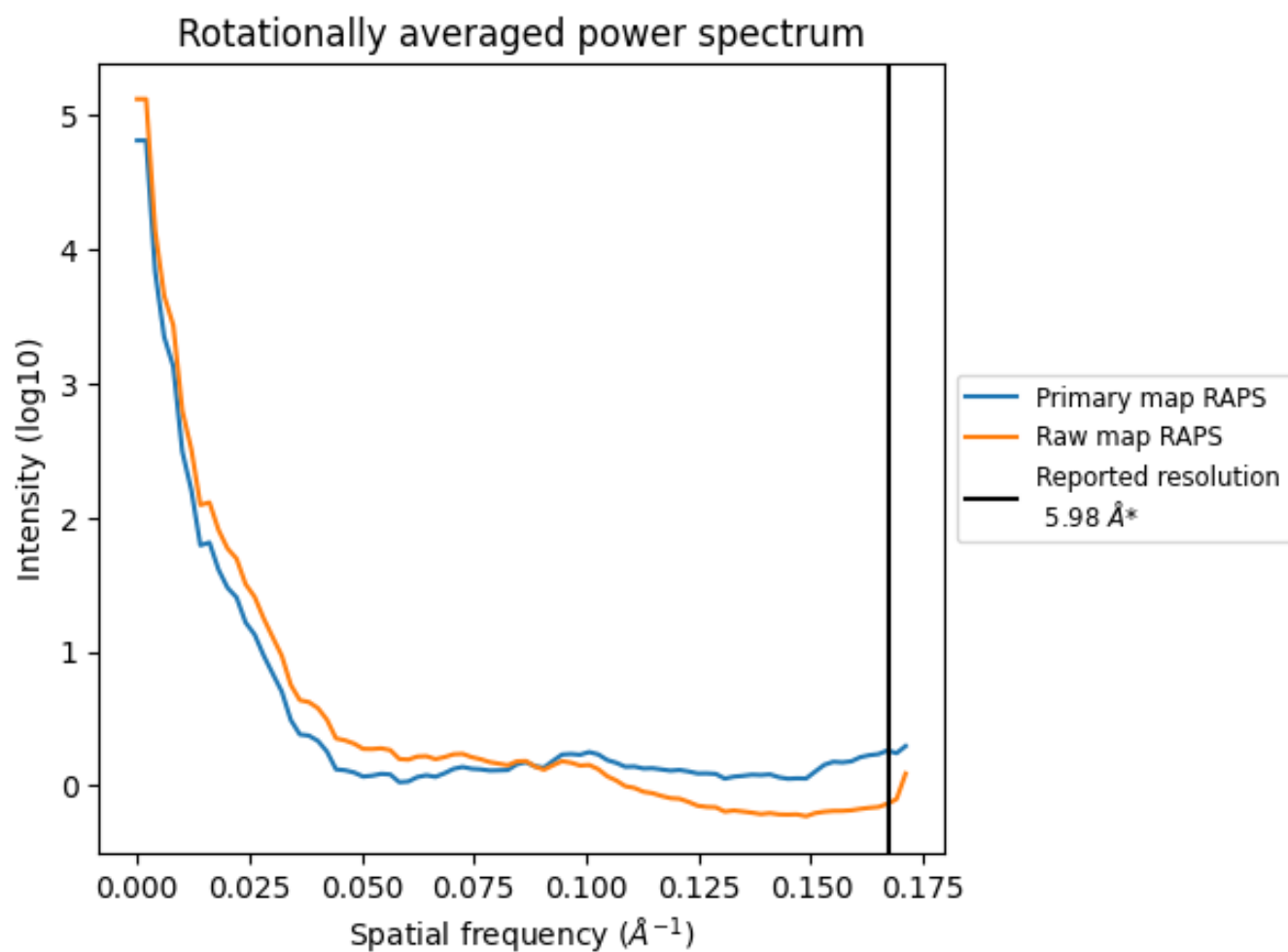
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2245 nm³; this corresponds to an approximate mass of 2028 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 ⓘ

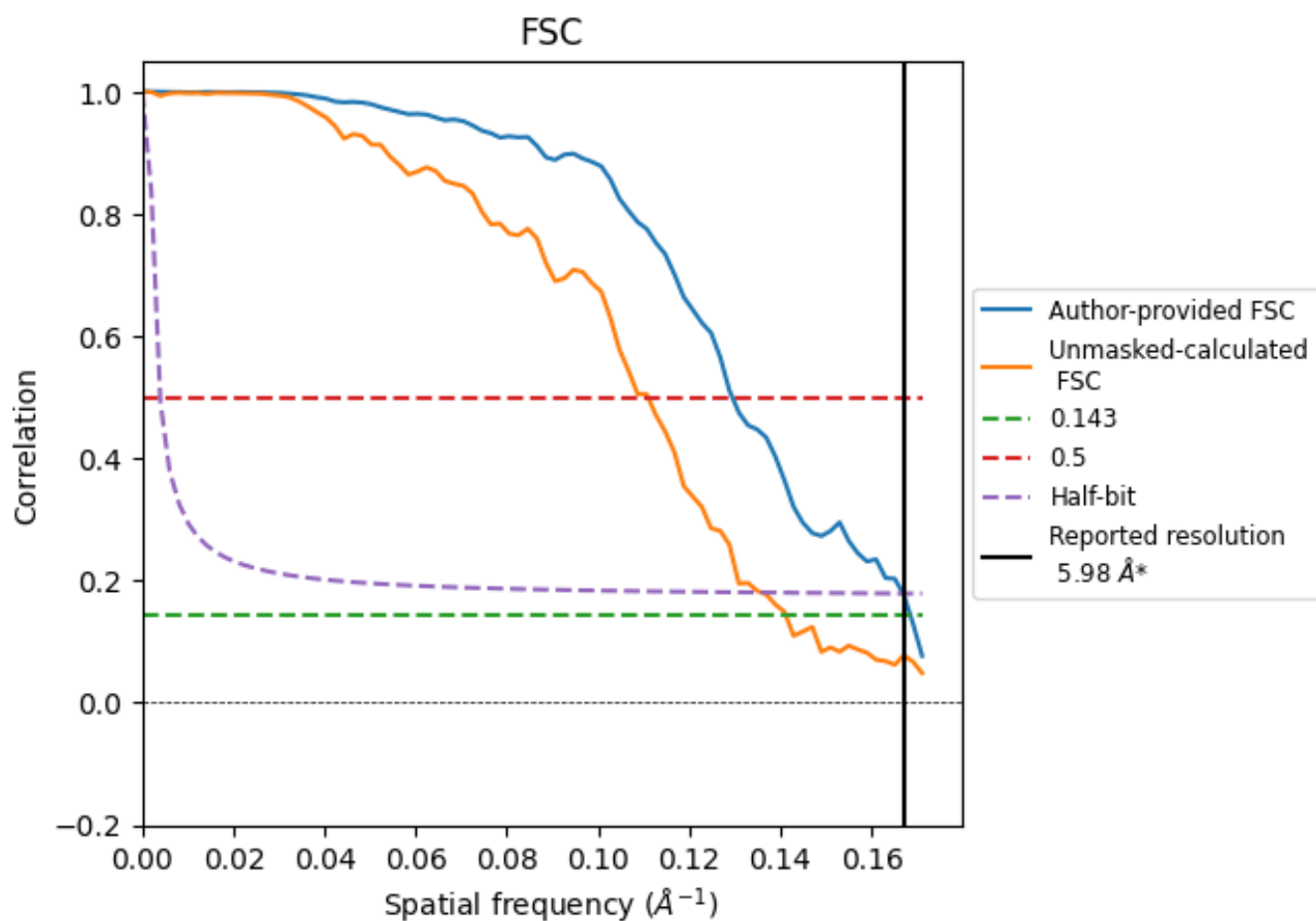


*Reported resolution corresponds to spatial frequency of 0.167 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.167 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

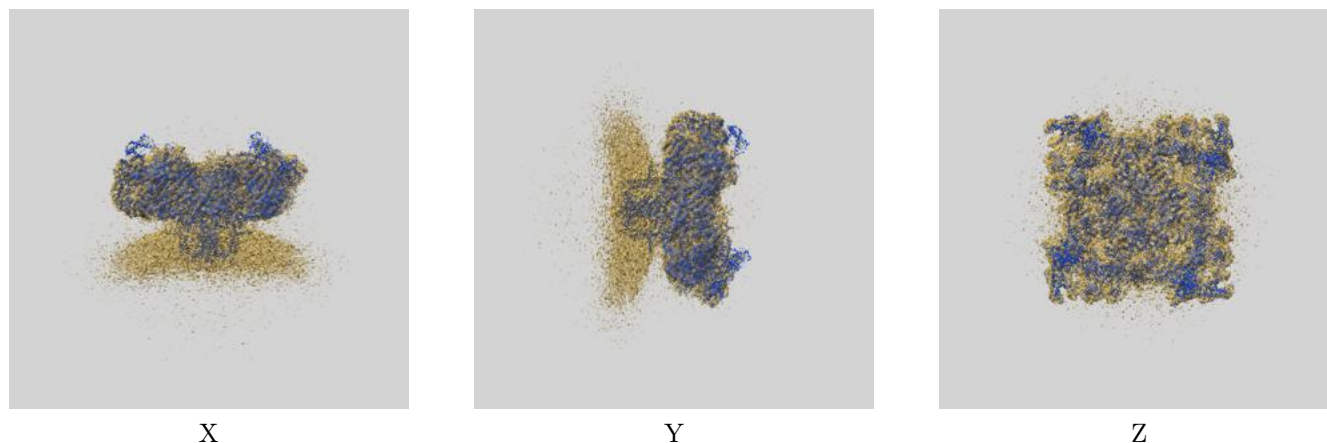
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.98	-	-
Author-provided FSC curve	5.93	7.72	5.99
Unmasked-calculated*	7.08	9.01	7.36

*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 7.08 differs from the reported value 5.98 by more than 10 %

9 Map-model fit [i](#)

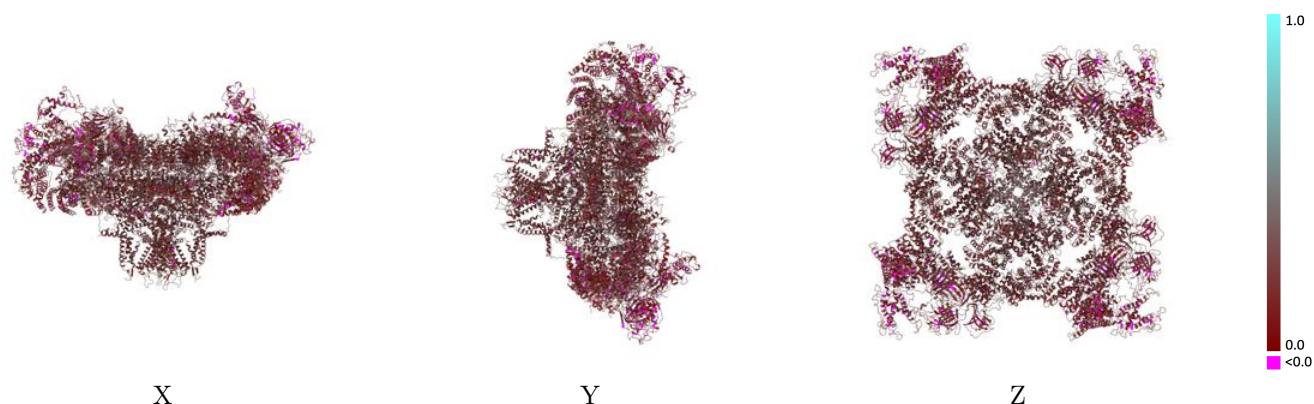
This section contains information regarding the fit between EMDB map EMD-54593 and PDB model 9S5A. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



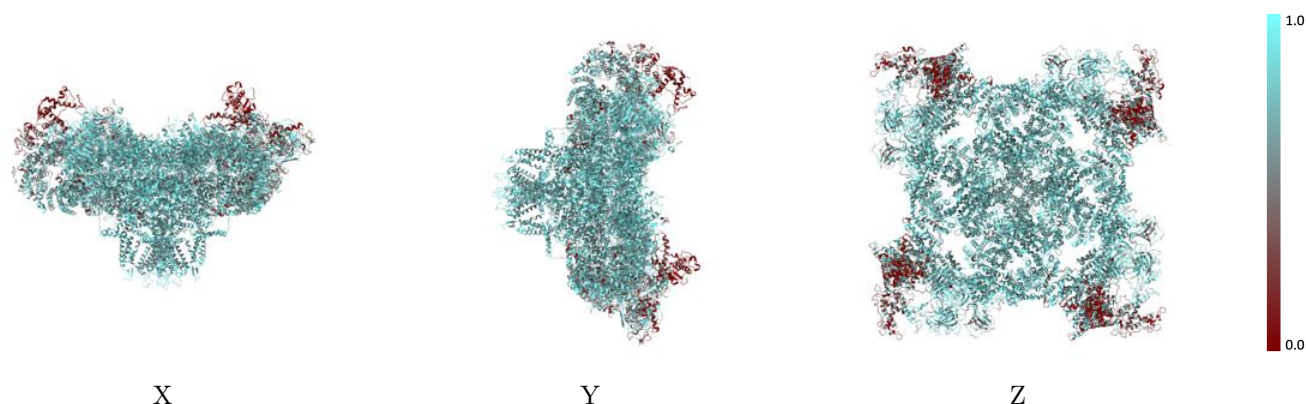
The images above show the 3D surface view of the map at the recommended contour level 0.0795 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



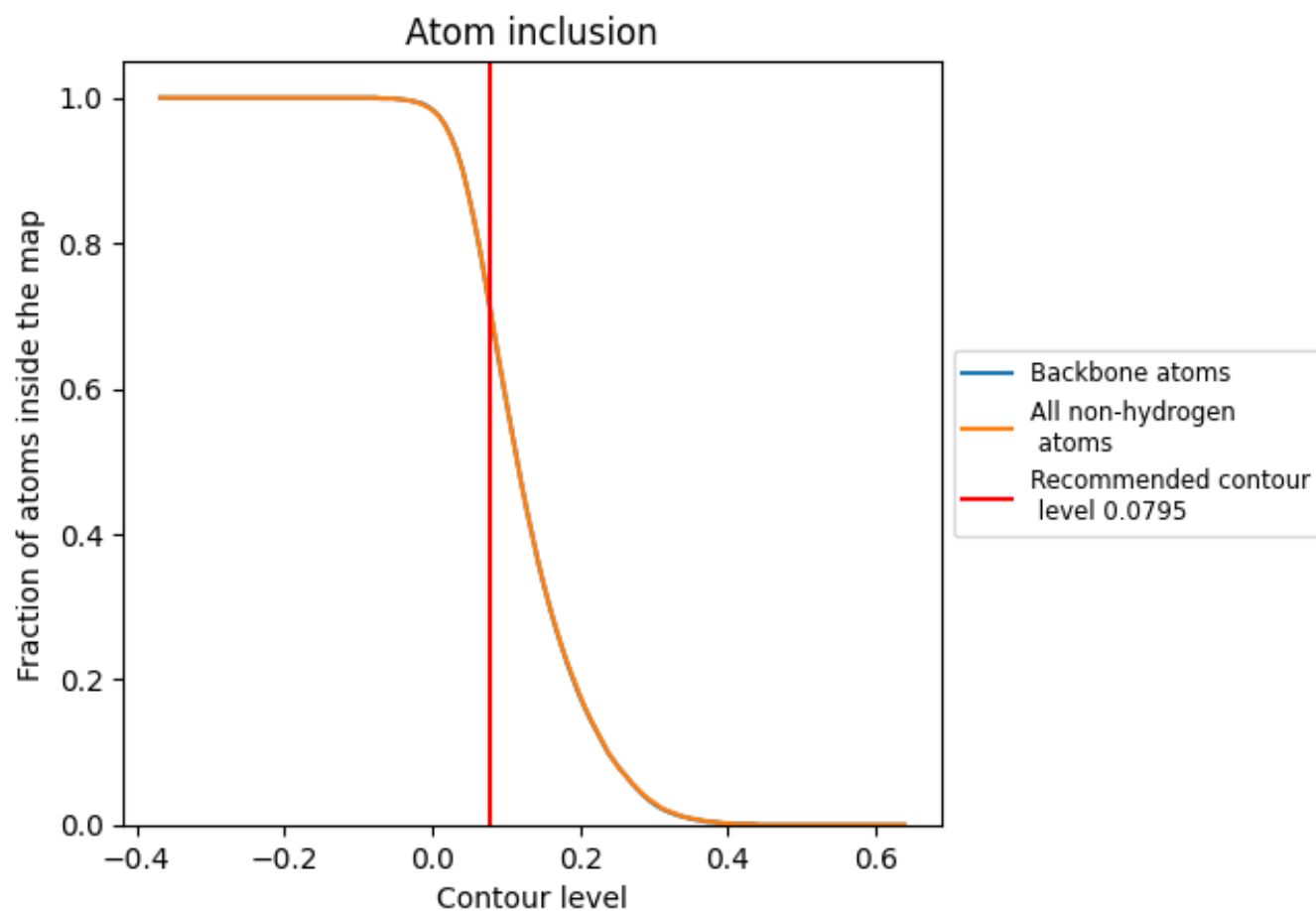
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0795).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 70% 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 (0.0795) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7050	0.2410
A	0.7150	0.2410
B	0.7150	0.2410
C	0.7150	0.2410
D	0.7150	0.2400
E	0.6570	0.2310
F	0.6580	0.2300
G	0.6560	0.2330
H	0.6590	0.2320

1.0

0.0

<0.0