



Full wwPDB EM Validation Report ⓘ

Aug 3, 2026 – 06:32 pm BST

PDB ID : 9S4L / pdb_00009s4l
EMDB ID : EMD-54569
Title : Down class, Activated-state RyR1 with activating ligand mixture (Calcium/ACP/Caffeine) in the native membrane
Authors : Mikirtumov, V.
Deposited on : 2025-07-28
Resolution : 4.92 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

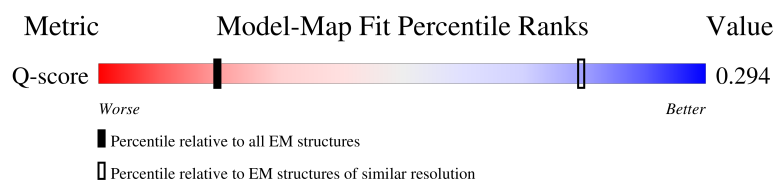
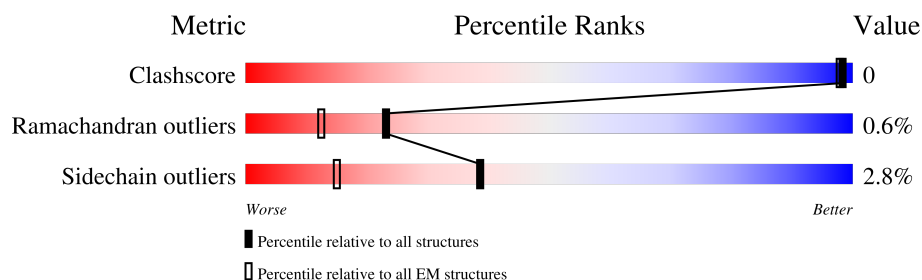
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.92 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	1071 (4.42 - 5.42)

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	
1	B	5037	
1	C	5037	
1	D	5037	

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Mol	Chain	Length	Quality of chain
2	E	108	19% 94% 6%
2	F	108	18% 93% 6%
2	G	108	19% 90% 9%
2	H	108	19% 91% 7%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 285952 atoms, of which 142272 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
			69827	22323	34739	6046	6482	237		
1	B	4404	Total	C	H	N	O	S	0	0
			69827	22323	34739	6046	6482	237		
1	C	4404	Total	C	H	N	O	S	0	0
			69827	22323	34739	6046	6482	237		
1	D	4404	Total	C	H	N	O	S	0	0
			69827	22323	34739	6046	6482	237		

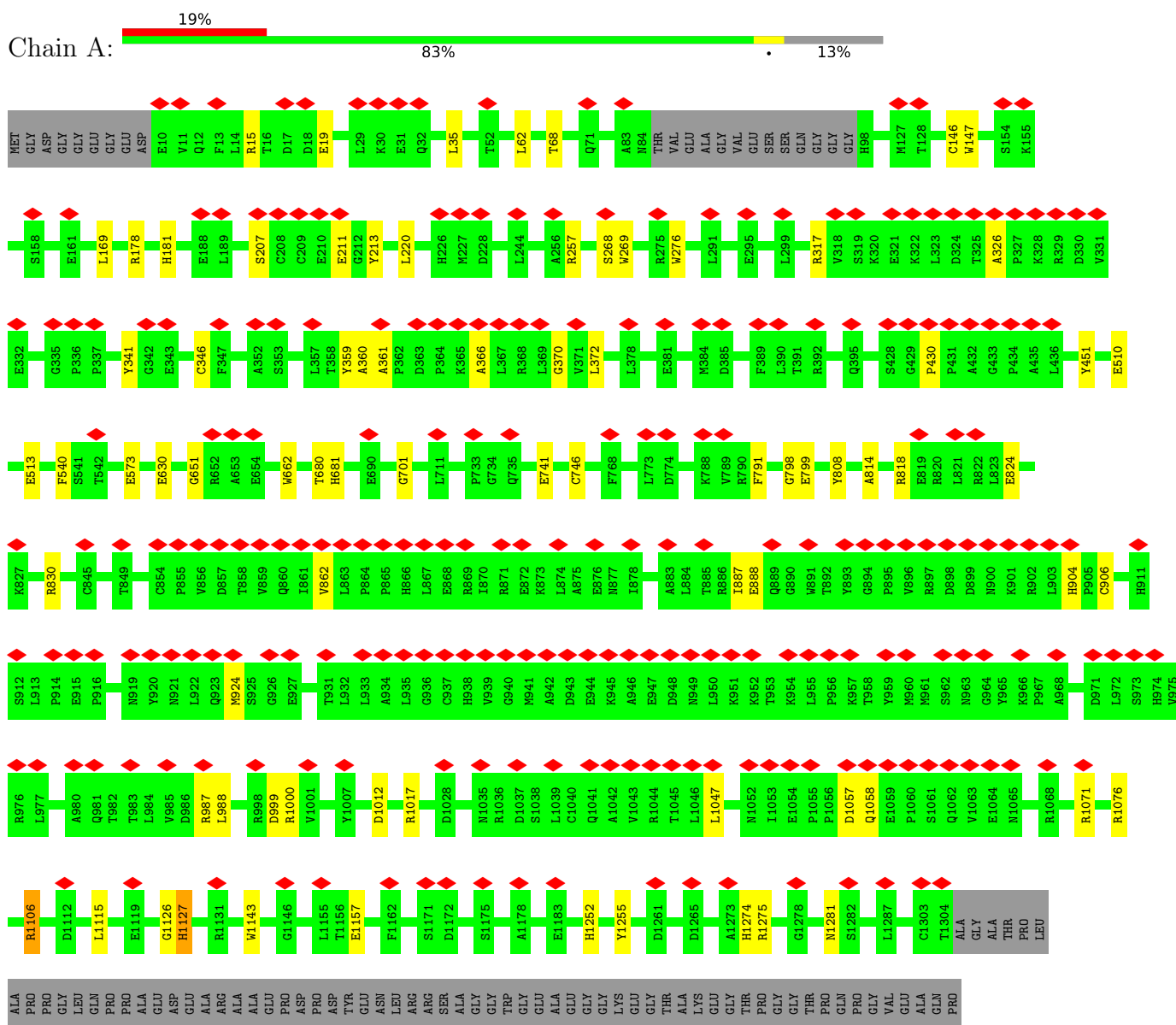
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

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		

3 Residue-property plots

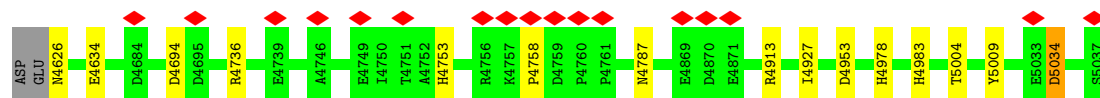
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Ryanodine receptor 1

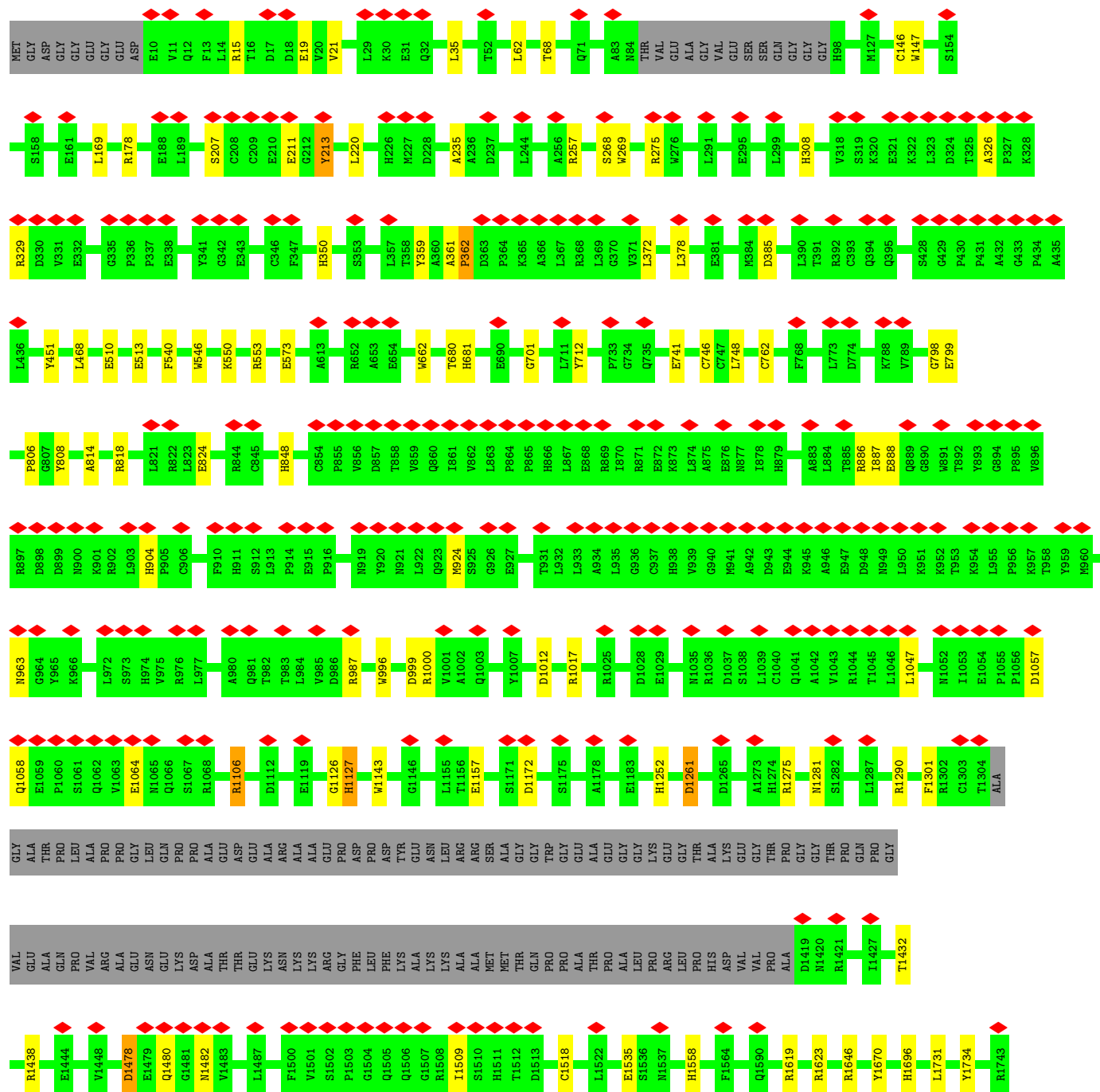
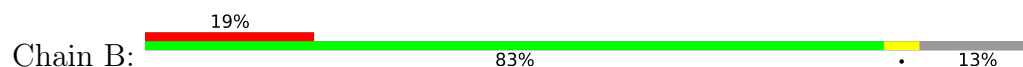


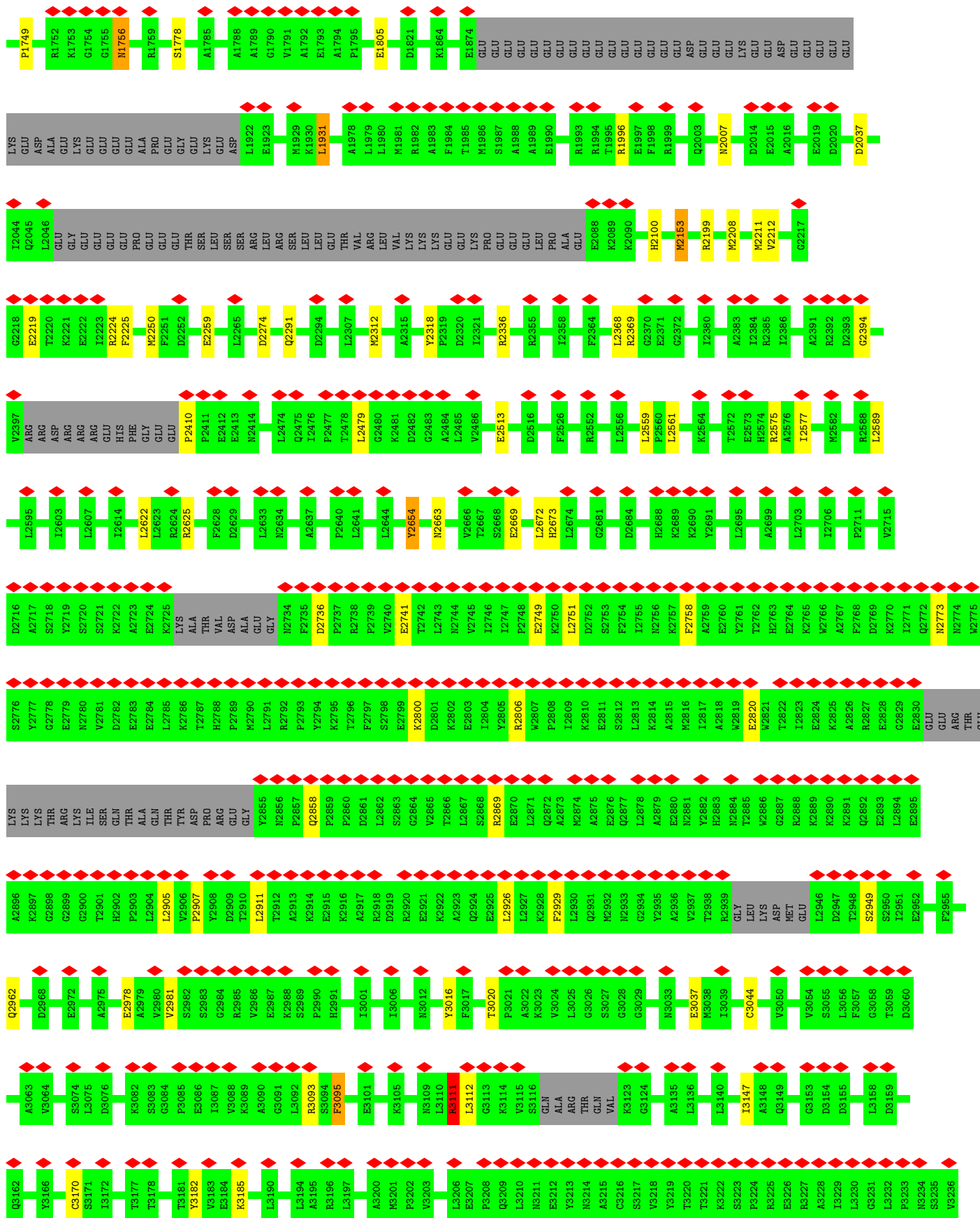




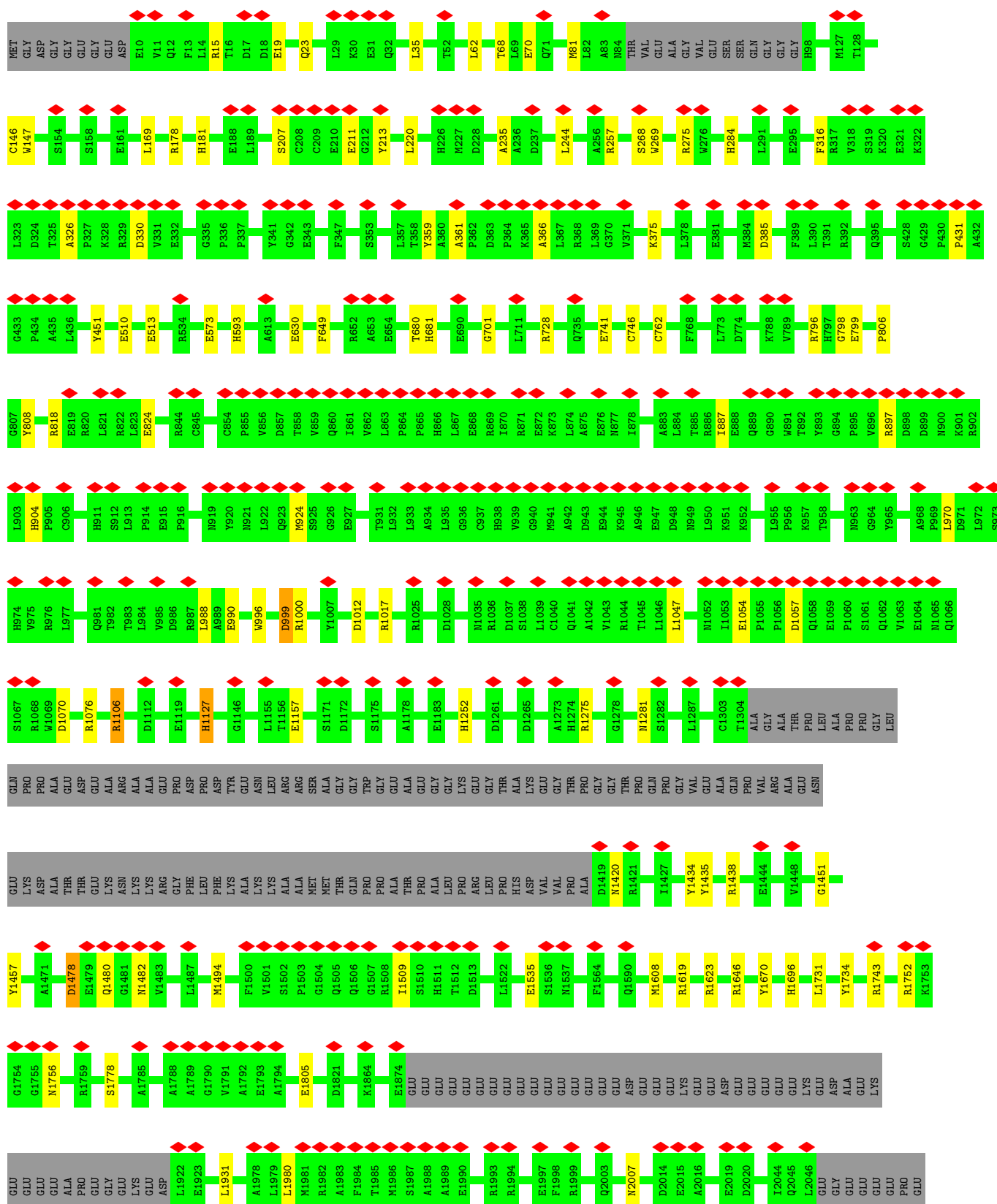
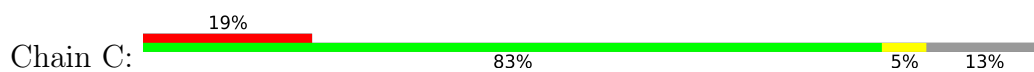


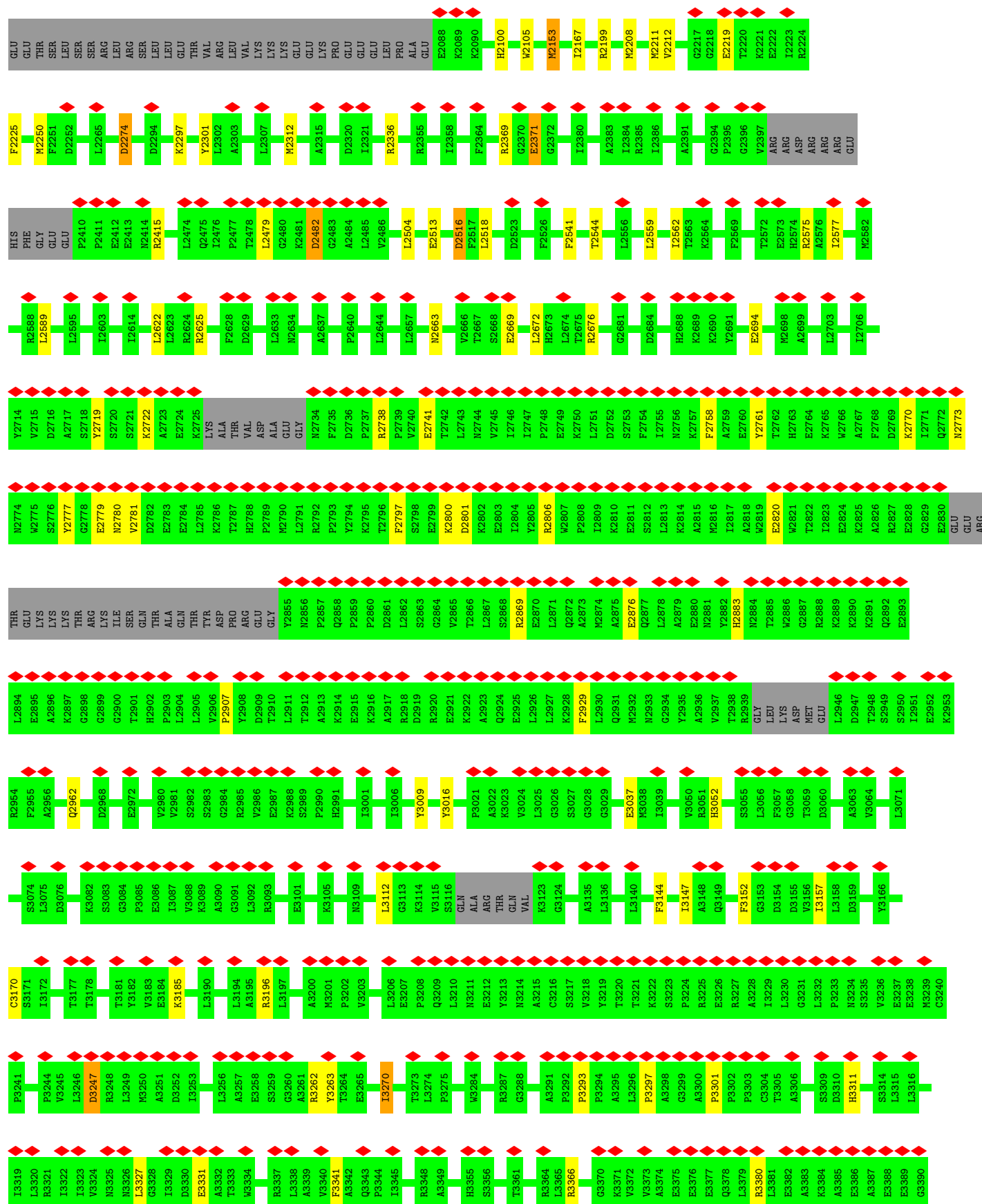
● Molecule 1: Ryanodine receptor 1

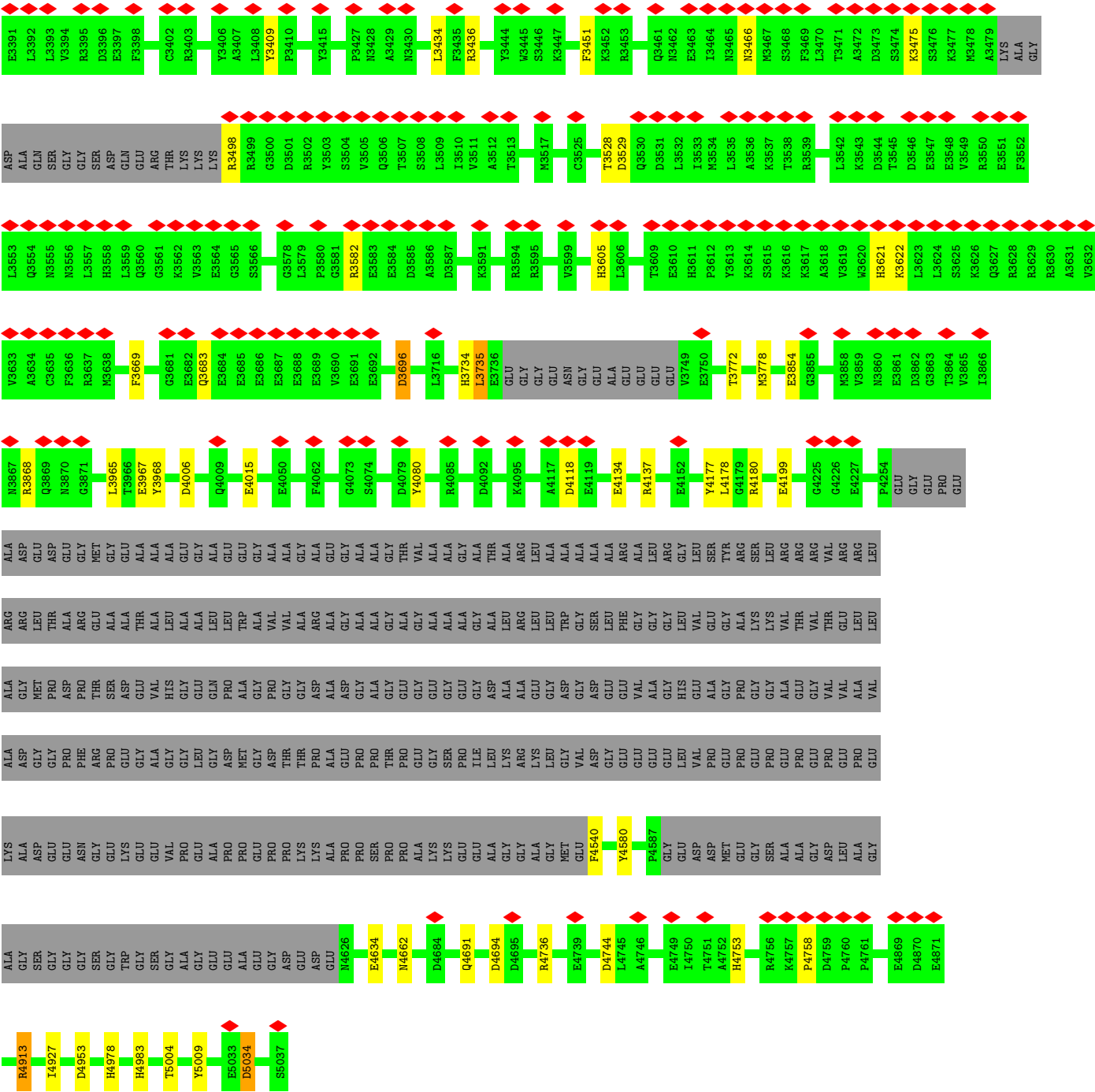




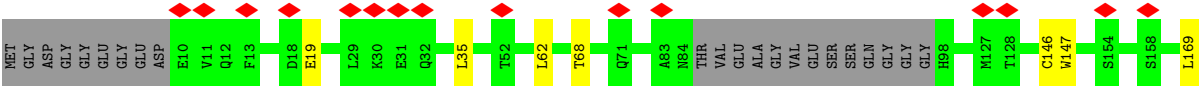
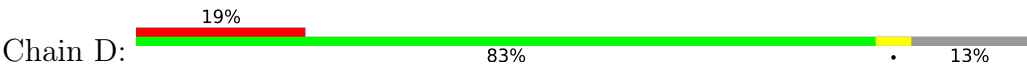






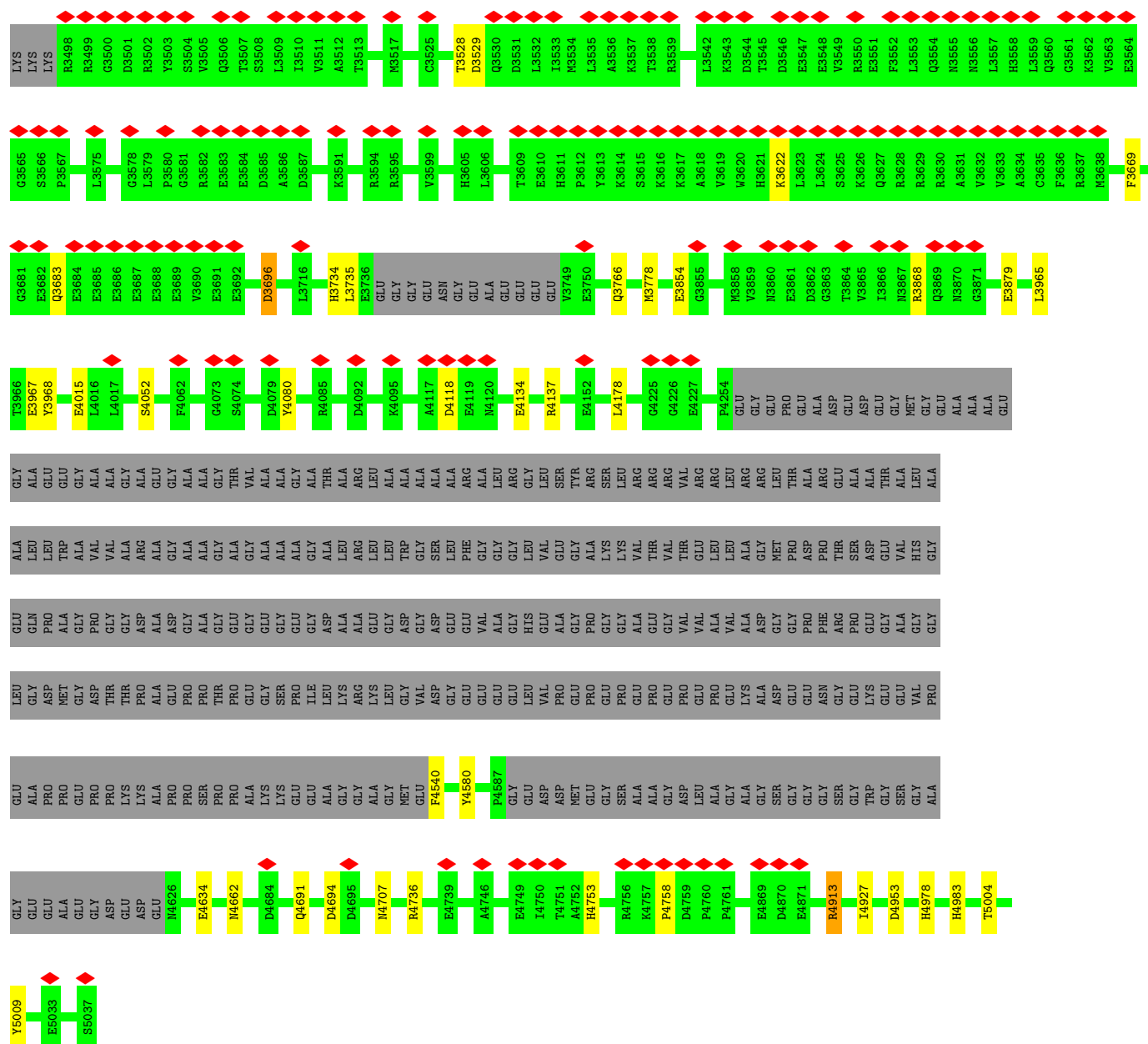


● Molecule 1: Ryanodine receptor 1

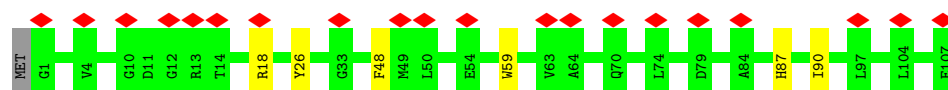






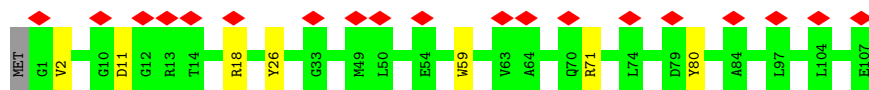


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

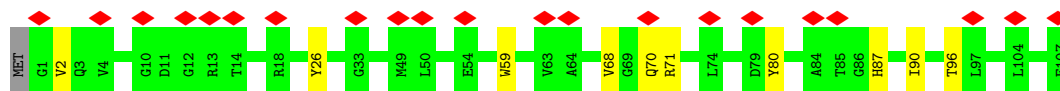
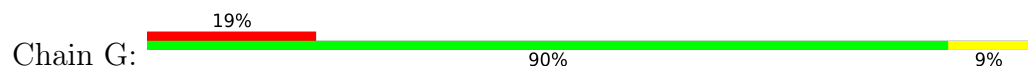


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

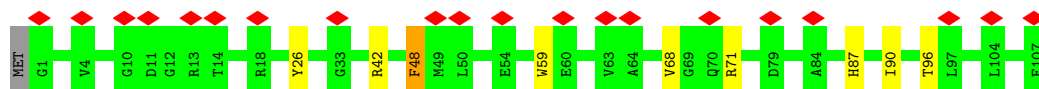
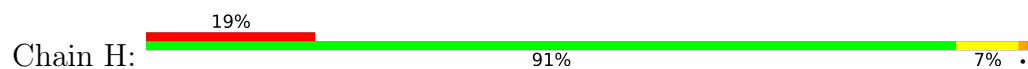




- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	16369	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 ($e^-/\text{\AA}^2$)	67.44	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.028	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00538	Depositor
Map size (Å)	601.04004, 601.04004, 601.04004	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.366, 1.366, 1.366	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	1.33	77/48603 (0.2%)
1	B	0.78	0/35885	1.33	91/48603 (0.2%)
1	C	0.78	0/35885	1.33	82/48603 (0.2%)
1	D	0.78	0/35885	1.33	75/48603 (0.2%)
2	E	0.80	0/851	1.36	1/1146 (0.1%)
2	F	0.81	0/851	1.37	3/1146 (0.3%)
2	G	0.80	0/851	1.34	2/1146 (0.2%)
2	H	0.79	0/851	1.37	3/1146 (0.3%)
All	All	0.78	0/146944	1.33	334/198996 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	22
1	B	0	20
1	C	0	22
1	D	0	16
2	E	0	1
2	F	0	2
2	G	0	2
2	H	0	1
All	All	0	86

There are no bond length outliers.

All (334) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2773	ASN	CA-CB-CG	8.43	121.03	112.60
1	C	2516	ASP	CA-CB-CG	8.35	120.95	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2773	ASN	CA-CB-CG	8.19	120.79	112.60
1	B	1012	ASP	CA-C-N	7.87	125.20	120.24
1	B	1012	ASP	C-N-CA	7.87	125.20	120.24
1	A	1012	ASP	CA-C-N	7.76	125.13	120.24
1	A	1012	ASP	C-N-CA	7.76	125.13	120.24
1	D	1012	ASP	CA-C-N	7.58	125.02	120.24
1	D	1012	ASP	C-N-CA	7.58	125.02	120.24
1	C	999	ASP	CA-CB-CG	7.51	120.11	112.60
1	B	904	HIS	CA-CB-CG	7.50	121.30	113.80
1	D	3696	ASP	CA-CB-CG	7.32	119.92	112.60
1	B	3341	PHE	CA-CB-CG	7.22	121.02	113.80
1	D	3341	PHE	CA-CB-CG	7.21	121.02	113.80
1	B	3696	ASP	CA-CB-CG	7.07	119.67	112.60
1	D	2274	ASP	CA-CB-CG	6.99	119.59	112.60
1	C	1012	ASP	CA-C-N	6.93	124.60	120.24
1	C	1012	ASP	C-N-CA	6.93	124.60	120.24
1	C	2773	ASN	CA-CB-CG	6.89	119.49	112.60
1	C	3696	ASP	CA-CB-CG	6.76	119.36	112.60
1	A	3696	ASP	CA-CB-CG	6.75	119.35	112.60
1	B	1017	ARG	NE-CZ-NH2	6.62	125.15	119.20
1	A	1275	ARG	NE-CZ-NH2	6.57	125.12	119.20
1	C	1275	ARG	NE-CZ-NH2	6.51	125.06	119.20
1	C	3270	ILE	N-CA-CB	6.49	118.15	110.55
1	D	1017	ARG	NE-CZ-NH2	6.49	125.04	119.20
1	B	904	HIS	CB-CG-CD2	-6.47	122.79	131.20
1	D	1275	ARG	NE-CZ-NH2	6.42	124.98	119.20
1	A	1017	ARG	NE-CZ-NH2	6.42	124.97	119.20
1	B	3270	ILE	N-CA-CB	6.37	118.00	110.55
1	B	1275	ARG	NE-CZ-NH2	6.36	124.92	119.20
1	A	1106	ARG	NE-CZ-NH2	6.35	124.91	119.20
1	B	1127	HIS	CB-CG-CD2	-6.33	122.97	131.20
1	D	1106	ARG	NE-CZ-NH2	6.32	124.89	119.20
1	B	1106	ARG	NE-CZ-NH2	6.32	124.89	119.20
1	D	3451	PHE	CA-CB-CG	6.29	120.09	113.80
1	A	3102	ASP	CA-CB-CG	-6.28	106.33	112.60
1	A	3270	ILE	N-CA-CB	6.23	117.84	110.55
1	B	1261	ASP	CA-CB-CG	6.21	118.81	112.60
1	C	1127	HIS	CB-CG-CD2	-6.21	123.13	131.20
1	A	1127	HIS	CB-CG-CD2	-6.18	123.16	131.20
1	D	3270	ILE	N-CA-CB	6.18	117.78	110.55
1	D	1127	HIS	CB-CG-CD2	-6.17	123.18	131.20
1	B	257	ARG	NE-CZ-NH2	6.16	124.74	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3111	ARG	CD-NE-CZ	6.11	132.95	124.40
1	B	2869	ARG	NE-CZ-NH2	6.11	124.70	119.20
1	A	2741	GLU	CA-C-N	6.07	128.70	120.38
1	A	2741	GLU	C-N-CA	6.07	128.70	120.38
1	A	257	ARG	NE-CZ-NH2	6.07	124.66	119.20
1	A	824	GLU	N-CA-C	6.04	115.25	108.25
1	A	4118	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	904	HIS	CB-CG-CD2	-6.01	123.39	131.20
1	D	3152	PHE	CA-CB-CG	6.00	119.80	113.80
1	B	3684	GLU	CA-C-N	5.99	130.72	120.72
1	B	3684	GLU	C-N-CA	5.99	130.72	120.72
2	F	18	ARG	NE-CZ-NH2	5.98	124.58	119.20
1	C	1017	ARG	NE-CZ-NH2	5.97	124.58	119.20
1	A	3684	GLU	CA-C-N	5.97	130.68	120.72
1	A	3684	GLU	C-N-CA	5.97	130.68	120.72
1	C	3247	ASP	CA-CB-CG	5.97	118.57	112.60
1	D	257	ARG	NE-CZ-NH2	5.96	124.56	119.20
1	C	904	HIS	CB-CG-CD2	-5.96	123.46	131.20
1	C	1106	ARG	NE-CZ-NH2	5.93	124.54	119.20
1	C	2741	GLU	CA-C-N	5.92	128.49	120.38
1	C	2741	GLU	C-N-CA	5.92	128.49	120.38
1	A	317	ARG	NE-CZ-NH2	5.92	124.53	119.20
1	A	3451	PHE	CA-CB-CG	5.91	119.71	113.80
1	C	3498	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	A	1274	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	D	1057	ASP	CA-CB-CG	5.89	118.49	112.60
1	C	1646	ARG	NE-CZ-NH2	5.89	124.50	119.20
1	B	2736	ASP	CA-CB-CG	5.88	118.48	112.60
1	B	2905	LEU	CA-C-N	5.87	132.99	122.13
1	B	2905	LEU	C-N-CA	5.87	132.99	122.13
1	B	4118	ASP	CA-CB-CG	5.87	118.47	112.60
1	D	2736	ASP	CA-CB-CG	5.85	118.45	112.60
1	D	3283	ARG	NE-CZ-NH2	5.85	124.46	119.20
1	C	824	GLU	N-CA-C	5.84	115.03	108.25
1	D	824	GLU	N-CA-C	5.83	115.02	108.25
1	B	1057	ASP	CA-CB-CG	5.83	118.43	112.60
1	B	2625	ARG	NE-CZ-NH2	5.83	124.44	119.20
1	A	1057	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	1646	ARG	NE-CZ-NH2	5.79	124.41	119.20
1	B	1438	ARG	NE-CZ-NH2	5.78	124.40	119.20
1	D	1478	ASP	CA-CB-CG	5.77	118.37	112.60
1	D	1646	ARG	NE-CZ-NH2	5.77	124.39	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1646	ARG	NE-CZ-NH2	5.77	124.39	119.20
1	C	2225	PHE	CB-CA-C	5.77	116.02	111.00
1	D	3247	ASP	CA-CB-CG	5.77	118.37	112.60
1	D	904	HIS	CB-CG-CD2	-5.75	123.72	131.20
1	B	326	ALA	N-CA-C	5.75	115.53	108.11
1	B	4927	ILE	N-CA-C	5.75	115.97	110.74
1	D	3125	VAL	N-CA-C	5.75	116.53	110.72
1	B	361	ALA	CA-C-N	5.74	127.02	119.84
1	B	361	ALA	C-N-CA	5.74	127.02	119.84
1	D	2738	ARG	NE-CZ-NH2	5.74	124.36	119.20
1	D	1438	ARG	NE-CZ-NH2	5.73	124.36	119.20
1	C	4118	ASP	CA-CB-CG	5.73	118.33	112.60
1	A	904	HIS	CA-CB-CG	5.72	119.52	113.80
1	A	2225	PHE	CB-CA-C	5.72	116.08	110.71
2	F	11	ASP	CA-CB-CG	5.71	118.31	112.60
1	C	2274	ASP	CA-CB-CG	5.71	118.31	112.60
1	C	2907	PRO	CA-C-N	5.71	128.20	120.38
1	C	2907	PRO	C-N-CA	5.71	128.20	120.38
1	A	3529	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	326	ALA	N-CA-C	5.70	115.47	108.11
1	A	4927	ILE	N-CA-C	5.70	115.92	110.74
1	C	3144	PHE	CA-CB-CG	-5.70	108.10	113.80
1	D	3529	ASP	CA-CB-CG	5.69	118.29	112.60
2	E	18	ARG	NE-CZ-NH2	5.69	124.33	119.20
1	D	681	HIS	CB-CG-CD2	-5.69	123.81	131.20
1	D	4118	ASP	CA-CB-CG	5.68	118.28	112.60
1	C	4927	ILE	N-CA-C	5.68	115.91	110.74
1	A	3247	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	2905	LEU	CA-C-N	5.67	132.62	122.13
1	A	2905	LEU	C-N-CA	5.67	132.62	122.13
1	B	824	GLU	N-CA-C	5.67	114.83	108.25
1	B	1172	ASP	CA-C-N	5.66	131.48	121.80
1	B	1172	ASP	C-N-CA	5.66	131.48	121.80
1	B	3451	PHE	CA-CB-CG	5.64	119.44	113.80
1	C	2738	ARG	NE-CZ-NH2	5.63	124.27	119.20
1	B	2907	PRO	CA-C-N	5.61	128.07	120.38
1	B	2907	PRO	C-N-CA	5.61	128.07	120.38
1	A	2736	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	3311	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	A	2973	PHE	CA-CB-CG	5.60	119.40	113.80
1	B	2410	PRO	CA-C-N	5.60	125.31	119.82
1	B	2410	PRO	C-N-CA	5.60	125.31	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1057	ASP	CA-CB-CG	5.60	118.20	112.60
1	C	3301	PRO	N-CA-CB	5.59	106.32	103.19
1	D	326	ALA	N-CA-C	5.59	115.32	108.11
1	B	2225	PHE	CB-CA-C	5.58	115.86	111.00
1	B	3436	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	A	1252	HIS	CB-CG-CD2	-5.57	123.95	131.20
1	C	1070	ASP	CA-CB-CG	5.57	118.17	112.60
1	C	178	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	D	3436	ARG	NE-CZ-NH2	5.55	124.19	119.20
1	A	1976	ARG	NE-CZ-NH2	5.55	124.19	119.20
1	C	3293	PRO	N-CA-C	5.55	117.47	110.70
1	D	2907	PRO	CA-C-N	5.54	127.70	120.28
1	D	2907	PRO	C-N-CA	5.54	127.70	120.28
1	C	1438	ARG	NE-CZ-NH2	5.53	124.18	119.20
2	H	42	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	A	3436	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	A	681	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	C	326	ALA	N-CA-C	5.52	115.23	108.11
1	C	5034	ASP	CA-CB-CG	5.52	118.12	112.60
1	B	2673	HIS	CA-CB-CG	-5.52	108.28	113.80
1	D	818	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	A	3111	ARG	CD-NE-CZ	5.50	132.10	124.40
1	A	651	GLY	N-CA-C	5.50	118.52	110.38
1	C	3436	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	D	4927	ILE	N-CA-C	5.49	115.74	110.74
1	A	2907	PRO	CA-C-N	5.49	127.63	120.28
1	A	2907	PRO	C-N-CA	5.49	127.63	120.28
1	D	3366	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	C	2482	ASP	CA-CB-CG	5.47	118.07	112.60
1	D	796	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	C	681	HIS	CB-CG-CD2	-5.44	124.13	131.20
1	C	796	ARG	NE-CZ-NH2	5.44	124.10	119.20
1	D	791	PHE	CA-CB-CG	5.44	119.24	113.80
1	D	4736	ARG	NE-CZ-NH2	5.44	124.09	119.20
1	D	2625	ARG	NE-CZ-NH2	5.44	124.09	119.20
1	A	4753	HIS	CB-CG-CD2	-5.43	124.13	131.20
1	A	1071	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	C	3582	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	D	181	HIS	N-CA-C	5.43	118.41	109.72
1	D	4052	SER	N-CA-C	5.43	117.20	111.28
1	B	5034	ASP	CA-CB-CG	5.42	118.03	112.60
1	B	1778	SER	N-CA-C	5.42	114.54	108.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3529	ASP	CA-CB-CG	5.42	118.02	112.60
1	D	862	VAL	N-CA-C	5.41	117.85	111.09
1	A	1778	SER	N-CA-C	5.41	114.52	108.25
1	B	4753	HIS	CB-CG-CD2	-5.40	124.17	131.20
1	B	4736	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	C	904	HIS	CA-CB-CG	5.39	119.19	113.80
1	B	178	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	C	2625	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	A	3111	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	D	2741	GLU	CA-C-N	5.36	127.78	120.54
1	D	2741	GLU	C-N-CA	5.36	127.78	120.54
1	C	1619	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	C	3451	PHE	CA-CB-CG	5.36	119.16	113.80
1	D	1071	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	C	818	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	D	3111	ARG	NE-CZ-NH2	5.36	124.02	119.20
2	H	48	PHE	CA-CB-CG	5.36	119.16	113.80
1	D	178	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	D	2773	ASN	CA-CB-CG	5.35	117.95	112.60
1	C	1696	HIS	CB-CG-CD2	-5.34	124.26	131.20
1	B	762	CYS	CA-C-N	5.34	125.33	120.21
1	B	762	CYS	C-N-CA	5.34	125.33	120.21
1	A	3341	PHE	CA-CB-CG	5.33	119.13	113.80
1	B	3529	ASP	CA-CB-CG	5.33	117.93	112.60
1	D	4753	HIS	CB-CG-CD2	-5.32	124.28	131.20
1	C	3341	PHE	CA-CB-CG	5.32	119.12	113.80
1	B	3111	ARG	CD-NE-CZ	5.32	131.84	124.40
1	B	2741	GLU	CA-C-N	5.31	127.65	120.38
1	B	2741	GLU	C-N-CA	5.31	127.65	120.38
1	A	818	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	B	681	HIS	CB-CG-CD2	-5.30	124.31	131.20
1	A	178	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	D	1772	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	B	4773	VAL	N-CA-C	5.29	116.02	110.62
1	C	4736	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	B	4180	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	A	4787	ASN	CA-CB-CG	5.28	117.88	112.60
1	B	2100	HIS	CA-CB-CG	5.28	119.08	113.80
1	A	5034	ASP	CA-CB-CG	5.28	117.88	112.60
1	D	999	ASP	CA-CB-CG	5.28	117.88	112.60
1	C	385	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	4137	ARG	N-CA-C	5.27	116.83	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1478	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	1478	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	540	PHE	CA-CB-CG	-5.25	108.55	113.80
1	B	329	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	B	886	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	D	385	ASP	CA-CB-CG	5.25	117.85	112.60
1	C	1778	SER	N-CA-C	5.25	114.34	108.25
1	A	181	HIS	N-CA-C	5.25	118.11	109.72
1	C	1743	ARG	NE-CZ-NH2	5.25	123.92	119.20
2	F	71	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	A	430	PRO	CA-C-N	5.24	126.39	119.84
1	A	430	PRO	C-N-CA	5.24	126.39	119.84
1	D	2905	LEU	CA-C-N	5.24	131.82	122.13
1	D	2905	LEU	C-N-CA	5.24	131.82	122.13
1	A	1438	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	B	3683	GLN	OE1-CD-NE2	-5.23	117.37	122.60
1	A	1076	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	C	4913	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	C	2797	PHE	CA-CB-CG	5.22	119.02	113.80
1	D	1608	MET	CA-C-N	5.22	125.50	119.92
1	D	1608	MET	C-N-CA	5.22	125.50	119.92
1	B	4052	SER	N-CA-C	5.22	116.97	111.28
1	B	3093	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	D	1558	HIS	CB-CG-CD2	-5.21	124.43	131.20
1	A	1752	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	C	887	ILE	CB-CA-C	-5.20	105.32	111.97
1	B	1252	HIS	CB-CG-CD2	-5.19	124.45	131.20
1	D	1619	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	B	3095	PHE	CA-CB-CG	5.19	118.99	113.80
1	B	1749	PRO	N-CA-CB	5.19	106.09	103.19
1	A	2625	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	C	3311	HIS	CB-CG-CD2	-5.18	124.47	131.20
1	D	2291	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	C	3621	HIS	CB-CG-CD2	-5.18	124.47	131.20
1	A	4736	ARG	NE-CZ-NH2	5.17	123.86	119.20
1	B	3350	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	C	4180	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	A	3366	ARG	NE-CZ-NH2	5.16	123.85	119.20
1	D	316	PHE	CA-CB-CG	5.16	118.96	113.80
1	D	2884	ASN	CA-CB-CG	5.15	117.75	112.60
1	C	4137	ARG	N-CA-C	5.15	116.70	111.14
2	G	70	GLN	OE1-CD-NE2	-5.15	117.45	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	818	ARG	NE-CZ-NH2	5.15	123.83	119.20
1	A	1749	PRO	N-CA-CB	5.15	106.07	103.19
1	C	1252	HIS	CB-CG-CD2	-5.15	124.51	131.20
2	H	71	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	C	257	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	C	316	PHE	CA-CB-CG	5.14	118.94	113.80
1	D	3766	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	A	1558	HIS	CB-CG-CD2	-5.14	124.52	131.20
1	A	3144	PHE	CA-CB-CG	-5.14	108.66	113.80
1	D	1054	GLU	CA-C-N	5.14	123.36	119.66
1	D	1054	GLU	C-N-CA	5.14	123.36	119.66
1	A	3582	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	B	1619	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	D	4137	ARG	N-CA-C	5.13	116.73	111.03
1	C	1608	MET	CA-C-N	5.13	125.41	119.92
1	C	1608	MET	C-N-CA	5.13	125.41	119.92
1	B	2291	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	B	3766	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	C	181	HIS	N-CA-C	5.13	118.10	109.95
1	B	999	ASP	CA-CB-CG	-5.12	107.47	112.60
1	B	2749	GLU	CA-C-N	5.12	127.96	119.35
1	B	2749	GLU	C-N-CA	5.12	127.96	119.35
1	C	1478	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	3366	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	B	2806	ARG	N-CA-C	5.12	117.98	111.69
1	C	2167	ILE	N-CA-C	5.11	117.09	111.77
1	B	385	ASP	CA-CB-CG	5.11	117.71	112.60
1	B	1558	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	B	3311	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	D	1252	HIS	CB-CG-CD2	-5.10	124.58	131.20
1	C	4753	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	A	999	ASP	CA-CB-CG	-5.09	107.51	112.60
1	C	3366	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	D	1696	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	B	4583	SER	CA-C-N	5.09	127.51	120.29
1	B	4583	SER	C-N-CA	5.09	127.51	120.29
1	C	593	HIS	CB-CG-CD2	-5.08	124.59	131.20
1	A	3498	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	C	2100	HIS	CA-CB-CG	5.08	118.88	113.80
1	B	4892	ARG	NE-CZ-NH2	5.07	123.77	119.20
1	A	862	VAL	N-CA-C	5.07	118.23	111.44
1	A	1619	ARG	NE-CZ-NH2	5.07	123.76	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2100	HIS	CA-CB-CG	5.07	118.87	113.80
1	B	848	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	B	1696	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	B	4913	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	C	728	ARG	NE-CZ-NH2	5.06	123.76	119.20
1	C	1076	ARG	NE-CZ-NH2	5.06	123.76	119.20
1	D	4913	ARG	NE-CZ-NH2	5.06	123.76	119.20
1	C	330	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	361	ALA	CB-CA-C	5.06	114.79	111.20
1	D	2167	ILE	N-CA-C	5.06	117.03	111.77
1	A	2801	ASP	N-CA-C	5.05	117.68	111.82
1	C	1054	GLU	CA-C-N	5.05	123.30	119.66
1	C	1054	GLU	C-N-CA	5.05	123.30	119.66
1	D	2973	PHE	CA-CB-CG	5.05	118.85	113.80
1	B	3270	ILE	CA-CB-CG1	5.05	118.98	110.40
1	C	2806	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	D	308	HIS	CA-C-N	5.05	131.19	121.54
1	D	308	HIS	C-N-CA	5.05	131.19	121.54
1	D	350	HIS	CB-CG-CD2	-5.05	124.64	131.20
1	B	540	PHE	CA-CB-CG	-5.04	108.76	113.80
1	C	284	HIS	CB-CG-CD2	-5.04	124.64	131.20
1	A	791	PHE	CA-CB-CG	5.04	118.84	113.80
1	B	3854	GLU	CA-C-N	5.04	125.55	120.00
1	B	3854	GLU	C-N-CA	5.04	125.55	120.00
1	C	3152	PHE	CA-CB-CG	5.04	118.84	113.80
1	B	3111	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	B	350	HIS	CB-CG-CD2	-5.03	124.66	131.20
1	C	361	ALA	CB-CA-C	5.03	114.77	111.20
1	B	1301	PHE	CA-CB-CG	5.03	118.83	113.80
1	C	762	CYS	CA-C-N	5.03	125.04	120.21
1	C	762	CYS	C-N-CA	5.03	125.04	120.21
1	B	2224	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	C	2801	ASP	N-CA-C	5.02	117.64	111.82
1	D	540	PHE	CA-CB-CG	-5.02	108.78	113.80
1	D	3419	ASN	CA-CB-CG	5.02	117.62	112.60
1	A	3621	HIS	CB-CG-CD2	-5.01	124.68	131.20
2	G	71	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	A	830	ARG	NE-CZ-NH2	5.00	123.70	119.20

There are no chirality outliers.

All (86) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1000	ARG	Sidechain
1	A	1106	ARG	Sidechain
1	A	1127	HIS	Sidechain
1	A	1255	TYR	Sidechain
1	A	1670	TYR	Sidechain
1	A	1734	TYR	Sidechain
1	A	2336	ARG	Sidechain
1	A	2415	ARG	Sidechain
1	A	2654	TYR	Sidechain
1	A	3009	TYR	Sidechain
1	A	3262	ARG	Sidechain
1	A	3409	TYR	Sidechain
1	A	341	TYR	Sidechain
1	A	3902	TYR	Sidechain
1	A	4080	TYR	Sidechain
1	A	4177	TYR	Sidechain
1	A	4180	ARG	Sidechain
1	A	451	TYR	Sidechain
1	A	4560	TYR	Sidechain
1	A	4913	ARG	Sidechain
1	A	5009	TYR	Sidechain
1	A	808	TYR	Sidechain
1	B	1000	ARG	Sidechain
1	B	1106	ARG	Sidechain
1	B	1127	HIS	Sidechain
1	B	1290	ARG	Sidechain
1	B	1670	TYR	Sidechain
1	B	1734	TYR	Sidechain
1	B	213	TYR	Sidechain
1	B	2199	ARG	Sidechain
1	B	2336	ARG	Sidechain
1	B	2654	TYR	Sidechain
1	B	3406	TYR	Sidechain
1	B	4080	TYR	Sidechain
1	B	4177	TYR	Sidechain
1	B	4180	ARG	Sidechain
1	B	451	TYR	Sidechain
1	B	4560	TYR	Sidechain
1	B	4913	ARG	Sidechain
1	B	5009	TYR	Sidechain
1	B	712	TYR	Sidechain
1	B	808	TYR	Sidechain
1	C	1000	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	1106	ARG	Sidechain
1	C	1127	HIS	Sidechain
1	C	1434	TYR	Sidechain
1	C	1457	TYR	Sidechain
1	C	1670	TYR	Sidechain
1	C	1734	TYR	Sidechain
1	C	2199	ARG	Sidechain
1	C	2301	TYR	Sidechain
1	C	2336	ARG	Sidechain
1	C	2415	ARG	Sidechain
1	C	2676	ARG	Sidechain
1	C	3009	TYR	Sidechain
1	C	3262	ARG	Sidechain
1	C	3380	ARG	Sidechain
1	C	3409	TYR	Sidechain
1	C	4080	TYR	Sidechain
1	C	4177	TYR	Sidechain
1	C	451	TYR	Sidechain
1	C	4913	ARG	Sidechain
1	C	5009	TYR	Sidechain
1	C	808	TYR	Sidechain
1	D	1000	ARG	Sidechain
1	D	1106	ARG	Sidechain
1	D	1127	HIS	Sidechain
1	D	1434	TYR	Sidechain
1	D	1670	TYR	Sidechain
1	D	1734	TYR	Sidechain
1	D	2199	ARG	Sidechain
1	D	2336	ARG	Sidechain
1	D	2714	TYR	Sidechain
1	D	3409	TYR	Sidechain
1	D	4080	TYR	Sidechain
1	D	451	TYR	Sidechain
1	D	4913	ARG	Sidechain
1	D	5009	TYR	Sidechain
1	D	663	TYR	Sidechain
1	D	808	TYR	Sidechain
2	E	26	TYR	Sidechain
2	F	26	TYR	Sidechain
2	F	80	TYR	Sidechain
2	G	26	TYR	Sidechain
2	G	80	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	H	26	TYR	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	34739	34717	19	0
1	B	35088	34739	34717	22	0
1	C	35088	34739	34717	19	0
1	D	35088	34739	34717	19	0
2	E	832	829	831	1	0
2	F	832	829	831	0	0
2	G	832	829	831	1	0
2	H	832	829	831	1	0
All	All	143680	142272	142192	82	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 0.

All (82) 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:D:146:CYS:HG	1:D:147:TRP:CD1	2.16	0.64
1:B:146:CYS:HG	1:B:147:TRP:CD1	2.20	0.59
1:C:146:CYS:HG	1:C:147:TRP:CD1	2.21	0.59
1:A:146:CYS:HG	1:A:147:TRP:CD1	2.21	0.58
1:A:1931:LEU:H	1:A:1931:LEU:HD22	1.71	0.56
1:B:1931:LEU:H	1:B:1931:LEU:HD22	1.69	0.56
1:C:1931:LEU:HD22	1:C:1931:LEU:H	1.71	0.55
1:D:1931:LEU:H	1:D:1931:LEU:HD22	1.74	0.53
1:C:2153:MET:HA	1:C:2153:MET:HE2	1.90	0.53
1:B:2318:TYR:CD2	1:B:2394:GLY:HA2	2.44	0.53
1:B:3997:ALA:HB1	1:B:4057:MET:HE3	1.90	0.53
1:A:1805:GLU:H	1:A:1805:GLU:CD	2.17	0.52
1:C:2577:ILE:H	1:C:2577:ILE:HD12	1.74	0.52
1:B:2153:MET:HA	1:B:2153:MET:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2153:MET:HE2	1:D:2153:MET:HA	1.92	0.51
1:A:2153:MET:HA	1:A:2153:MET:HE2	1.91	0.51
1:B:2577:ILE:HD12	1:B:2577:ILE:H	1.78	0.48
1:A:573:GLU:H	1:A:573:GLU:CD	2.22	0.48
1:A:2577:ILE:HD12	1:A:2577:ILE:H	1.78	0.48
1:C:1805:GLU:H	1:C:1805:GLU:CD	2.22	0.47
1:B:1805:GLU:H	1:B:1805:GLU:CD	2.21	0.47
1:C:573:GLU:H	1:C:573:GLU:CD	2.21	0.47
1:C:2371:GLU:H	1:C:2371:GLU:CD	2.23	0.47
1:A:2318:TYR:CE2	1:A:2394:GLY:HA2	2.50	0.47
1:B:573:GLU:CD	1:B:573:GLU:H	2.23	0.46
1:B:3044:CYS:HA	1:B:3095:PHE:CE2	2.50	0.46
1:D:2371:GLU:H	1:D:2371:GLU:CD	2.24	0.46
1:D:4978:HIS:CE1	1:D:4983:HIS:CD2	3.05	0.45
1:D:1126:GLY:HA3	1:D:1143:TRP:CZ3	2.51	0.45
1:D:2672:LEU:HD12	1:D:2672:LEU:H	1.81	0.45
1:C:244:LEU:HD12	1:C:375:LYS:HE2	1.99	0.45
1:C:2758:PHE:HB2	1:C:2929:PHE:CE1	2.52	0.45
1:A:3734:HIS:CG	1:A:3735:LEU:N	2.85	0.45
1:C:2211:MET:C	1:C:2211:MET:SD	3.01	0.44
1:C:2672:LEU:H	1:C:2672:LEU:HD12	1.81	0.44
1:A:1126:GLY:HA3	1:A:1143:TRP:CZ3	2.53	0.44
1:B:3734:HIS:CG	1:B:3735:LEU:N	2.86	0.44
1:D:573:GLU:H	1:D:573:GLU:CD	2.25	0.44
1:B:2211:MET:SD	1:B:2211:MET:C	3.01	0.44
1:B:662:TRP:CH2	1:B:814:ALA:HB2	2.52	0.44
1:C:3734:HIS:CG	1:C:3735:LEU:N	2.85	0.44
1:C:19:GLU:HG2	1:C:68:THR:HG22	2.00	0.44
1:A:2211:MET:SD	1:A:2211:MET:C	3.00	0.44
1:A:2672:LEU:HD12	1:A:2672:LEU:H	1.83	0.44
1:B:3371:LYS:HA	1:B:3371:LYS:HE3	2.00	0.44
1:A:19:GLU:HG2	1:A:68:THR:HG22	2.00	0.43
1:C:2541:PHE:HA	1:C:2544:THR:HG23	2.00	0.43
2:H:87:HIS:CD2	2:H:90:ILE:HD12	2.54	0.43
1:A:2758:PHE:HB2	1:A:2929:PHE:CE1	2.54	0.43
1:B:1126:GLY:HA3	1:B:1143:TRP:CZ3	2.53	0.43
1:C:4978:HIS:CE1	1:C:4983:HIS:CD2	3.07	0.43
1:A:4978:HIS:CE1	1:A:4983:HIS:CD2	3.06	0.43
1:D:3734:HIS:CG	1:D:3735:LEU:N	2.86	0.43
1:D:2211:MET:C	1:D:2211:MET:SD	3.02	0.43
1:A:1558:HIS:CG	1:A:1559:GLN:H	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1126:GLY:HA3	1:D:1143:TRP:CE3	2.54	0.42
1:D:2318:TYR:CD2	1:D:2394:GLY:HA2	2.55	0.42
2:G:87:HIS:CD2	2:G:90:ILE:HD12	2.54	0.42
1:C:1451:GLY:HA3	1:C:1494:MET:HG2	2.02	0.42
1:B:4978:HIS:CE1	1:B:4983:HIS:CD2	3.07	0.42
1:C:2869:ARG:HG2	1:C:2869:ARG:HH21	1.84	0.42
1:A:1126:GLY:HA3	1:A:1143:TRP:CE3	2.55	0.42
1:D:2758:PHE:HB2	1:D:2929:PHE:CE1	2.54	0.42
1:B:546:TRP:CZ2	1:B:550:LYS:HE2	2.55	0.41
1:B:19:GLU:HG2	1:B:68:THR:HG22	2.03	0.41
1:D:19:GLU:HG2	1:D:68:THR:HG22	2.02	0.41
1:D:3965:LEU:HA	1:D:3968:TYR:CD2	2.55	0.41
1:B:2758:PHE:HB2	1:B:2929:PHE:CE1	2.55	0.41
1:B:3768:SER:HA	1:B:3771:HIS:CD2	2.56	0.41
1:B:4711:PHE:CD1	1:B:4711:PHE:C	2.99	0.41
1:A:662:TRP:CH2	1:A:814:ALA:HB2	2.56	0.41
1:C:2770:LYS:N	1:C:2770:LYS:HE2	2.36	0.41
1:A:3965:LEU:HA	1:A:3968:TYR:CD2	2.56	0.41
1:D:546:TRP:CZ2	1:D:550:LYS:HE2	2.56	0.41
1:D:3371:LYS:HE3	1:D:3371:LYS:HA	2.02	0.41
1:A:3620:TRP:CG	1:A:3621:HIS:H	2.39	0.40
1:B:3965:LEU:HA	1:B:3968:TYR:CD2	2.56	0.40
1:D:2204:HIS:CD2	1:D:2204:HIS:C	2.99	0.40
1:B:2672:LEU:HD12	1:B:2672:LEU:H	1.85	0.40
1:C:3965:LEU:HA	1:C:3968:TYR:CD2	2.56	0.40
1:D:2089:LYS:HA	1:D:2089:LYS:HE2	2.04	0.40
2:E:87:HIS:CD2	2:E:90:ILE:HD12	2.56	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%)	4115 (94%)	238 (5%)	23 (0%)	24	62
1	B	4376/5037 (87%)	4114 (94%)	234 (5%)	28 (1%)	21	58
1	C	4376/5037 (87%)	4121 (94%)	225 (5%)	30 (1%)	18	55
1	D	4376/5037 (87%)	4117 (94%)	233 (5%)	26 (1%)	21	58
2	E	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	F	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
2	G	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
2	H	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
All	All	17924/20580 (87%)	16858 (94%)	959 (5%)	107 (1%)	23	58

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3868	ARG
1	B	3868	ARG
1	C	3868	ARG
1	D	3868	ARG
1	A	1482	ASN
1	A	3304	CYS
1	A	4694	ASP
1	B	308	HIS
1	B	3304	CYS
1	C	2719	TYR
1	C	4694	ASP
1	D	2219	GLU
1	D	3304	CYS
1	D	4694	ASP
1	A	211	GLU
1	A	906	CYS
1	A	2663	ASN
1	A	2820	GLU
1	A	3669	PHE
1	B	211	GLU
1	B	1064	GLU
1	B	1756	ASN
1	B	2820	GLU
1	B	3669	PHE
1	B	4694	ASP
1	C	211	GLU
1	C	268	SER

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Mol	Chain	Res	Type
1	C	366	ALA
1	C	2800	LYS
1	C	3669	PHE
1	D	211	GLU
1	D	1482	ASN
1	D	2663	ASN
1	D	2820	GLU
1	D	3669	PHE
1	D	4134	GLU
1	A	207	SER
1	A	213	TYR
1	A	366	ALA
1	A	2219	GLU
1	A	2750	LYS
1	A	2800	LYS
1	A	4134	GLU
1	B	207	SER
1	B	213	TYR
1	B	268	SER
1	B	553	ARG
1	B	1482	ASN
1	B	2219	GLU
1	B	2663	ASN
1	B	2800	LYS
1	B	3111	ARG
1	B	3466	ASN
1	B	3623	LEU
1	B	4134	GLU
1	C	207	SER
1	C	213	TYR
1	C	431	PRO
1	C	2663	ASN
1	C	2722	LYS
1	C	2820	GLU
1	C	3052	HIS
1	C	3157	ILE
1	C	3466	ASN
1	C	3622	LYS
1	C	4134	GLU
1	D	207	SER
1	D	213	TYR
1	D	268	SER

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Mol	Chain	Res	Type
1	D	366	ALA
1	D	1756	ASN
1	D	2750	LYS
1	D	3622	LYS
1	A	3622	LYS
1	B	235	ALA
1	B	362	PRO
1	B	2669	GLU
1	B	3735	LEU
1	C	235	ALA
1	C	701	GLY
1	C	1482	ASN
1	C	2219	GLU
1	C	3735	LEU
1	D	360	ALA
1	D	3111	ARG
1	A	268	SER
1	A	360	ALA
1	C	2669	GLU
1	A	701	GLY
1	B	701	GLY
1	D	431	PRO
1	D	3157	ILE
1	D	3464	ILE
1	C	806	PRO
1	D	701	GLY
1	D	798	GLY
1	D	4758	PRO
1	A	798	GLY
1	B	798	GLY
1	B	806	PRO
1	C	798	GLY
1	C	3297	PRO
1	C	4691	GLN
1	D	4691	GLN
1	A	370	GLY
1	A	4758	PRO
1	C	4758	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3827/4276 (90%)	3718 (97%)	109 (3%)	38	59
1	B	3827/4276 (90%)	3721 (97%)	106 (3%)	38	59
1	C	3827/4276 (90%)	3722 (97%)	105 (3%)	39	60
1	D	3827/4276 (90%)	3726 (97%)	101 (3%)	40	61
2	E	89/90 (99%)	87 (98%)	2 (2%)	45	64
2	F	89/90 (99%)	87 (98%)	2 (2%)	45	64
2	G	89/90 (99%)	85 (96%)	4 (4%)	24	46
2	H	89/90 (99%)	85 (96%)	4 (4%)	24	46
All	All	15664/17464 (90%)	15231 (97%)	433 (3%)	38	59

All (433) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	35	LEU
1	A	62	LEU
1	A	169	LEU
1	A	220	LEU
1	A	269	TRP
1	A	276	TRP
1	A	346	CYS
1	A	359	TYR
1	A	372	LEU
1	A	510	GLU
1	A	513	GLU
1	A	630	GLU
1	A	680	THR
1	A	741	GLU
1	A	746	CYS
1	A	799	GLU
1	A	887	ILE
1	A	888	GLU

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Mol	Chain	Res	Type
1	A	924	MET
1	A	987	ARG
1	A	988	LEU
1	A	1047	LEU
1	A	1058	GLN
1	A	1115	LEU
1	A	1157	GLU
1	A	1281	ASN
1	A	1420	ASN
1	A	1432	THR
1	A	1478	ASP
1	A	1480	GLN
1	A	1509	ILE
1	A	1535	GLU
1	A	1569	GLN
1	A	1623	ARG
1	A	1731	LEU
1	A	1752	ARG
1	A	1756	ASN
1	A	1980	LEU
1	A	1982	ARG
1	A	1986	MET
1	A	1996	ARG
1	A	2005	GLN
1	A	2007	ASN
1	A	2105	TRP
1	A	2153	MET
1	A	2250	MET
1	A	2274	ASP
1	A	2297	LYS
1	A	2312	MET
1	A	2369	ARG
1	A	2479	LEU
1	A	2504	LEU
1	A	2513	GLU
1	A	2559	LEU
1	A	2561	LEU
1	A	2589	LEU
1	A	2622	LEU
1	A	2751	LEU
1	A	2774	ASN
1	A	2775	TRP

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Mol	Chain	Res	Type
1	A	2777	TYR
1	A	2801	ASP
1	A	2858	GLN
1	A	2867	LEU
1	A	2883	HIS
1	A	2891	LYS
1	A	2906	VAL
1	A	2911	LEU
1	A	2962	GLN
1	A	2981	VAL
1	A	3007	ASN
1	A	3016	TYR
1	A	3037	GLU
1	A	3111	ARG
1	A	3112	LEU
1	A	3132	THR
1	A	3147	ILE
1	A	3170	CYS
1	A	3182	TYR
1	A	3185	LYS
1	A	3196	ARG
1	A	3247	ASP
1	A	3250	MET
1	A	3263	TYR
1	A	3270	ILE
1	A	3331	GLU
1	A	3346	VAL
1	A	3434	LEU
1	A	3461	GLN
1	A	3475	LYS
1	A	3478	MET
1	A	3528	THR
1	A	3683	GLN
1	A	3696	ASP
1	A	3778	MET
1	A	3854	GLU
1	A	3856	LEU
1	A	3967	GLU
1	A	4015	GLU
1	A	4178	LEU
1	A	4199	GLU
1	A	4540	PHE

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Mol	Chain	Res	Type
1	A	4580	TYR
1	A	4626	ASN
1	A	4634	GLU
1	A	4953	ASP
1	A	5004	THR
1	A	5034	ASP
1	B	15	ARG
1	B	21	VAL
1	B	35	LEU
1	B	62	LEU
1	B	169	LEU
1	B	220	LEU
1	B	269	TRP
1	B	275	ARG
1	B	359	TYR
1	B	362	PRO
1	B	372	LEU
1	B	378	LEU
1	B	468	LEU
1	B	510	GLU
1	B	513	GLU
1	B	680	THR
1	B	741	GLU
1	B	746	CYS
1	B	748	LEU
1	B	799	GLU
1	B	887	ILE
1	B	888	GLU
1	B	924	MET
1	B	963	ASN
1	B	987	ARG
1	B	996	TRP
1	B	1047	LEU
1	B	1058	GLN
1	B	1157	GLU
1	B	1261	ASP
1	B	1281	ASN
1	B	1432	THR
1	B	1478	ASP
1	B	1480	GLN
1	B	1509	ILE
1	B	1518	CYS

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Mol	Chain	Res	Type
1	B	1535	GLU
1	B	1623	ARG
1	B	1731	LEU
1	B	1756	ASN
1	B	1931	LEU
1	B	1996	ARG
1	B	2007	ASN
1	B	2037	ASP
1	B	2153	MET
1	B	2208	MET
1	B	2212	VAL
1	B	2250	MET
1	B	2259	GLU
1	B	2274	ASP
1	B	2312	MET
1	B	2368	LEU
1	B	2369	ARG
1	B	2479	LEU
1	B	2513	GLU
1	B	2559	LEU
1	B	2561	LEU
1	B	2575	ARG
1	B	2589	LEU
1	B	2622	LEU
1	B	2654	TYR
1	B	2751	LEU
1	B	2858	GLN
1	B	2911	LEU
1	B	2926	LEU
1	B	2949	SER
1	B	2962	GLN
1	B	2978	GLU
1	B	2981	VAL
1	B	3016	TYR
1	B	3020	THR
1	B	3037	GLU
1	B	3111	ARG
1	B	3112	LEU
1	B	3147	ILE
1	B	3170	CYS
1	B	3182	TYR
1	B	3185	LYS

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Mol	Chain	Res	Type
1	B	3250	MET
1	B	3262	ARG
1	B	3263	TYR
1	B	3270	ILE
1	B	3331	GLU
1	B	3346	VAL
1	B	3391	GLU
1	B	3434	LEU
1	B	3461	GLN
1	B	3475	LYS
1	B	3478	MET
1	B	3528	THR
1	B	3605	HIS
1	B	3683	GLN
1	B	3696	ASP
1	B	3778	MET
1	B	3854	GLU
1	B	3879	GLU
1	B	3967	GLU
1	B	4015	GLU
1	B	4540	PHE
1	B	4580	TYR
1	B	4626	ASN
1	B	4634	GLU
1	B	4662	ASN
1	B	4953	ASP
1	B	5004	THR
1	B	5034	ASP
1	C	15	ARG
1	C	23	GLN
1	C	35	LEU
1	C	62	LEU
1	C	70	GLU
1	C	81	MET
1	C	169	LEU
1	C	220	LEU
1	C	269	TRP
1	C	275	ARG
1	C	359	TYR
1	C	510	GLU
1	C	513	GLU
1	C	630	GLU

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Mol	Chain	Res	Type
1	C	649	PHE
1	C	680	THR
1	C	741	GLU
1	C	746	CYS
1	C	799	GLU
1	C	897	ARG
1	C	924	MET
1	C	970	LEU
1	C	988	LEU
1	C	990	GLU
1	C	996	TRP
1	C	999	ASP
1	C	1047	LEU
1	C	1157	GLU
1	C	1281	ASN
1	C	1420	ASN
1	C	1435	TYR
1	C	1478	ASP
1	C	1480	GLN
1	C	1509	ILE
1	C	1535	GLU
1	C	1623	ARG
1	C	1731	LEU
1	C	1752	ARG
1	C	1756	ASN
1	C	1980	LEU
1	C	2007	ASN
1	C	2105	TRP
1	C	2153	MET
1	C	2208	MET
1	C	2212	VAL
1	C	2250	MET
1	C	2274	ASP
1	C	2297	LYS
1	C	2312	MET
1	C	2369	ARG
1	C	2371	GLU
1	C	2479	LEU
1	C	2482	ASP
1	C	2504	LEU
1	C	2513	GLU
1	C	2516	ASP

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Mol	Chain	Res	Type
1	C	2518	LEU
1	C	2559	LEU
1	C	2562	ILE
1	C	2575	ARG
1	C	2589	LEU
1	C	2622	LEU
1	C	2694	GLU
1	C	2761	TYR
1	C	2777	TYR
1	C	2779	GLU
1	C	2780	ASN
1	C	2781	VAL
1	C	2876	GLU
1	C	2883	HIS
1	C	2962	GLN
1	C	3016	TYR
1	C	3037	GLU
1	C	3112	LEU
1	C	3147	ILE
1	C	3170	CYS
1	C	3185	LYS
1	C	3196	ARG
1	C	3247	ASP
1	C	3263	TYR
1	C	3270	ILE
1	C	3327	LEU
1	C	3331	GLU
1	C	3434	LEU
1	C	3475	LYS
1	C	3528	THR
1	C	3605	HIS
1	C	3683	GLN
1	C	3696	ASP
1	C	3772	THR
1	C	3778	MET
1	C	3854	GLU
1	C	3967	GLU
1	C	4006	ASP
1	C	4015	GLU
1	C	4178	LEU
1	C	4199	GLU
1	C	4540	PHE

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Mol	Chain	Res	Type
1	C	4580	TYR
1	C	4634	GLU
1	C	4662	ASN
1	C	4744	ASP
1	C	4953	ASP
1	C	5004	THR
1	C	5034	ASP
1	D	35	LEU
1	D	62	LEU
1	D	169	LEU
1	D	220	LEU
1	D	269	TRP
1	D	275	ARG
1	D	359	TYR
1	D	372	LEU
1	D	513	GLU
1	D	680	THR
1	D	741	GLU
1	D	746	CYS
1	D	748	LEU
1	D	799	GLU
1	D	886	ARG
1	D	887	ILE
1	D	888	GLU
1	D	987	ARG
1	D	990	GLU
1	D	996	TRP
1	D	999	ASP
1	D	1047	LEU
1	D	1058	GLN
1	D	1157	GLU
1	D	1281	ASN
1	D	1420	ASN
1	D	1432	THR
1	D	1478	ASP
1	D	1480	GLN
1	D	1509	ILE
1	D	1518	CYS
1	D	1535	GLU
1	D	1623	ARG
1	D	1731	LEU
1	D	1756	ASN

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Mol	Chain	Res	Type
1	D	1980	LEU
1	D	1996	ARG
1	D	2007	ASN
1	D	2037	ASP
1	D	2105	TRP
1	D	2153	MET
1	D	2212	VAL
1	D	2250	MET
1	D	2271	THR
1	D	2274	ASP
1	D	2297	LYS
1	D	2368	LEU
1	D	2369	ARG
1	D	2371	GLU
1	D	2429	LEU
1	D	2479	LEU
1	D	2513	GLU
1	D	2559	LEU
1	D	2561	LEU
1	D	2589	LEU
1	D	2622	LEU
1	D	2654	TYR
1	D	2670	GLU
1	D	2777	TYR
1	D	2787	THR
1	D	2883	HIS
1	D	2906	VAL
1	D	2911	LEU
1	D	2962	GLN
1	D	2985	ARG
1	D	3007	ASN
1	D	3037	GLU
1	D	3111	ARG
1	D	3112	LEU
1	D	3170	CYS
1	D	3182	TYR
1	D	3185	LYS
1	D	3196	ARG
1	D	3247	ASP
1	D	3250	MET
1	D	3262	ARG
1	D	3263	TYR

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Mol	Chain	Res	Type
1	D	3270	ILE
1	D	3315	LEU
1	D	3331	GLU
1	D	3346	VAL
1	D	3414	ARG
1	D	3434	LEU
1	D	3475	LYS
1	D	3478	MET
1	D	3528	THR
1	D	3683	GLN
1	D	3696	ASP
1	D	3778	MET
1	D	3854	GLU
1	D	3879	GLU
1	D	3967	GLU
1	D	4015	GLU
1	D	4178	LEU
1	D	4540	PHE
1	D	4580	TYR
1	D	4634	GLU
1	D	4662	ASN
1	D	4707	ASN
1	D	4953	ASP
1	D	5004	THR
2	E	48	PHE
2	E	59	TRP
2	F	2	VAL
2	F	59	TRP
2	G	2	VAL
2	G	59	TRP
2	G	68	VAL
2	G	96	THR
2	H	48	PHE
2	H	59	TRP
2	H	68	VAL
2	H	96	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (177) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	105	HIS

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Mol	Chain	Res	Type
1	A	495	ASN
1	A	579	GLN
1	A	581	ASN
1	A	582	HIS
1	A	921	ASN
1	A	963	ASN
1	A	1158	ASN
1	A	1165	ASN
1	A	1220	GLN
1	A	1229	ASN
1	A	1459	GLN
1	A	1545	ASN
1	A	1563	GLN
1	A	1590	GLN
1	A	1688	HIS
1	A	1691	GLN
1	A	1776	HIS
1	A	1973	GLN
1	A	2095	GLN
1	A	2127	GLN
1	A	2180	GLN
1	A	2193	GLN
1	A	2204	HIS
1	A	2487	GLN
1	A	2515	GLN
1	A	2520	HIS
1	A	2634	ASN
1	A	2856	ASN
1	A	2881	ASN
1	A	2962	GLN
1	A	2971	GLN
1	A	3109	ASN
1	A	3150	HIS
1	A	3180	ASN
1	A	3466	ASN
1	A	3560	GLN
1	A	3572	GLN
1	A	3700	GLN
1	A	3781	GLN
1	A	4037	ASN
1	A	4100	GLN
1	A	4102	GLN

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Mol	Chain	Res	Type
1	A	4753	HIS
1	A	5035	GLN
1	B	105	HIS
1	B	582	HIS
1	B	919	ASN
1	B	921	ASN
1	B	963	ASN
1	B	1165	ASN
1	B	1229	ASN
1	B	1254	HIS
1	B	1459	GLN
1	B	1545	ASN
1	B	1563	GLN
1	B	1590	GLN
1	B	1663	HIS
1	B	1688	HIS
1	B	1775	HIS
1	B	1973	GLN
1	B	2095	GLN
1	B	2127	GLN
1	B	2180	GLN
1	B	2204	HIS
1	B	2253	HIS
1	B	2291	GLN
1	B	2487	GLN
1	B	2515	GLN
1	B	2520	HIS
1	B	2663	ASN
1	B	2744	ASN
1	B	2856	ASN
1	B	3150	HIS
1	B	3162	GLN
1	B	3180	ASN
1	B	3418	ASN
1	B	3560	GLN
1	B	3572	GLN
1	B	3700	GLN
1	B	3850	GLN
1	B	4037	ASN
1	B	4100	GLN
1	B	4102	GLN
1	B	4626	ASN

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Mol	Chain	Res	Type
1	B	4753	HIS
1	B	5035	GLN
1	C	79	GLN
1	C	113	HIS
1	C	218	HIS
1	C	413	GLN
1	C	579	GLN
1	C	581	ASN
1	C	582	HIS
1	C	963	ASN
1	C	993	HIS
1	C	1035	ASN
1	C	1041	GLN
1	C	1158	ASN
1	C	1165	ASN
1	C	1229	ASN
1	C	1254	HIS
1	C	1545	ASN
1	C	1563	GLN
1	C	1663	HIS
1	C	1691	GLN
1	C	1775	HIS
1	C	1973	GLN
1	C	2095	GLN
1	C	2180	GLN
1	C	2204	HIS
1	C	2253	HIS
1	C	2291	GLN
1	C	2487	GLN
1	C	2515	GLN
1	C	2881	ASN
1	C	2883	HIS
1	C	2931	GLN
1	C	3013	HIS
1	C	3149	GLN
1	C	3150	HIS
1	C	3180	ASN
1	C	3313	ASN
1	C	3466	ASN
1	C	3523	ASN
1	C	3560	GLN
1	C	3572	GLN

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Mol	Chain	Res	Type
1	C	3700	GLN
1	C	3781	GLN
1	C	3850	GLN
1	C	4100	GLN
1	C	4102	GLN
1	C	4753	HIS
1	D	105	HIS
1	D	579	GLN
1	D	581	ASN
1	D	582	HIS
1	D	919	ASN
1	D	921	ASN
1	D	963	ASN
1	D	1041	GLN
1	D	1133	HIS
1	D	1459	GLN
1	D	1545	ASN
1	D	1563	GLN
1	D	1590	GLN
1	D	1688	HIS
1	D	1775	HIS
1	D	2095	GLN
1	D	2127	GLN
1	D	2180	GLN
1	D	2253	HIS
1	D	2291	GLN
1	D	2487	GLN
1	D	2520	HIS
1	D	2993	GLN
1	D	3109	ASN
1	D	3128	ASN
1	D	3150	HIS
1	D	3180	ASN
1	D	3211	ASN
1	D	3466	ASN
1	D	3560	GLN
1	D	3572	GLN
1	D	3683	GLN
1	D	3781	GLN
1	D	3850	GLN
1	D	3897	ASN
1	D	4102	GLN

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Mol	Chain	Res	Type
1	D	4626	ASN
1	D	4753	HIS
2	E	87	HIS
2	F	87	HIS
2	G	87	HIS
2	H	87	HIS
2	H	94	HIS

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.

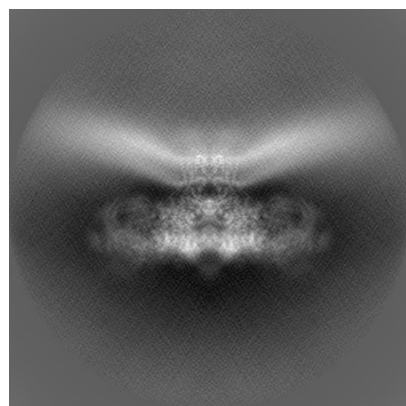
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54569. These allow visual inspection of the internal detail of the map and identification of artifacts.

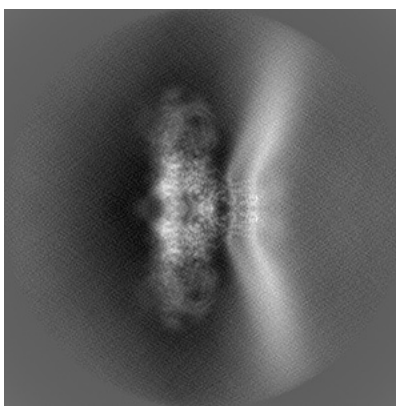
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

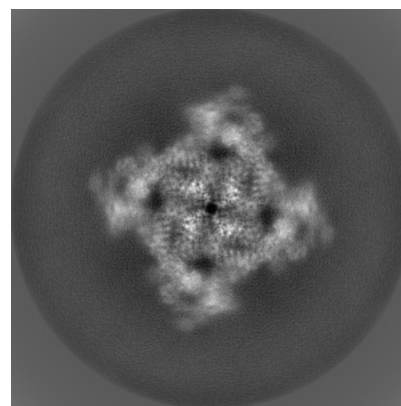
6.1.1 Primary map



X

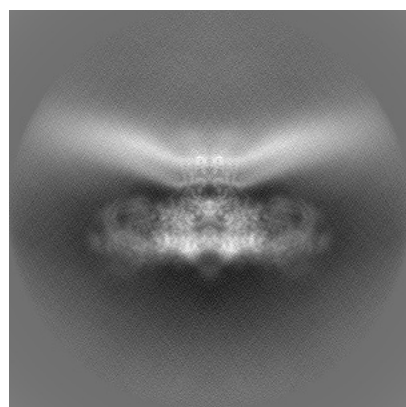


Y

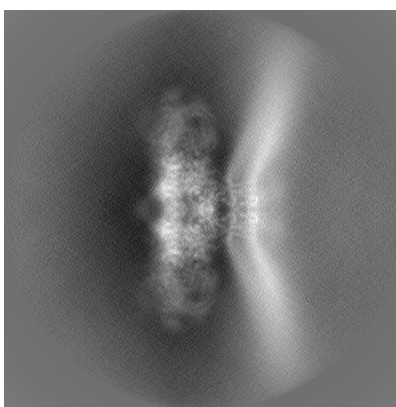


Z

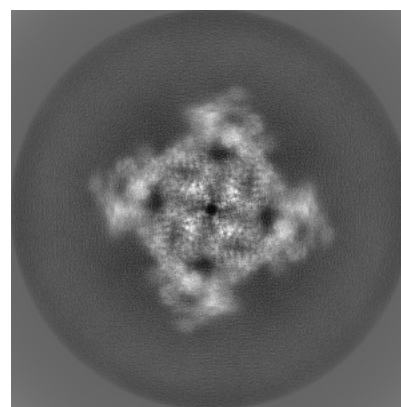
6.1.2 Raw map



X



Y

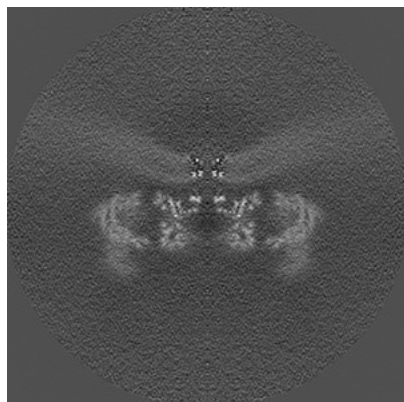


Z

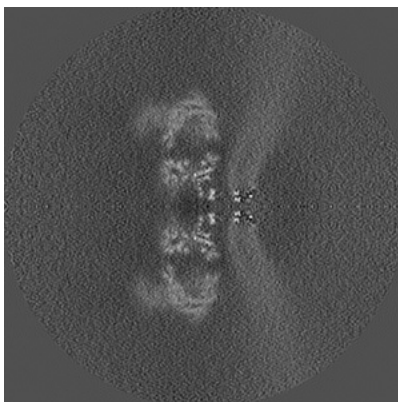
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

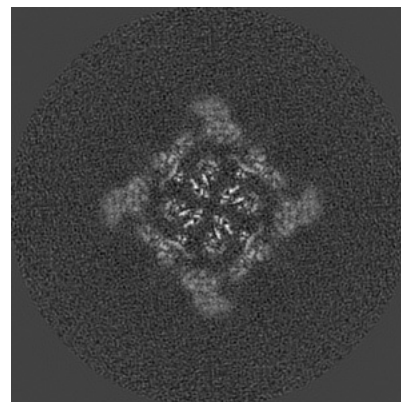
6.2.1 Primary map



X Index: 220

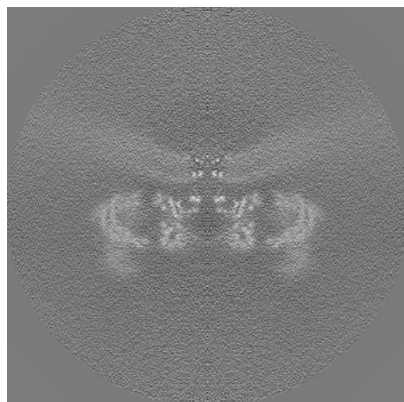


Y Index: 220

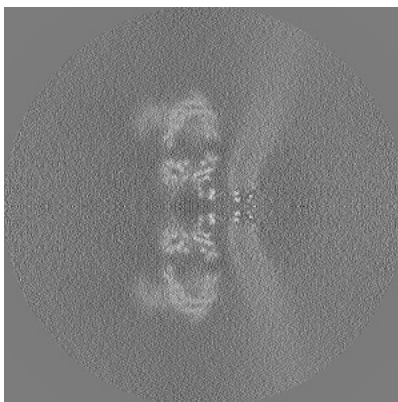


Z Index: 220

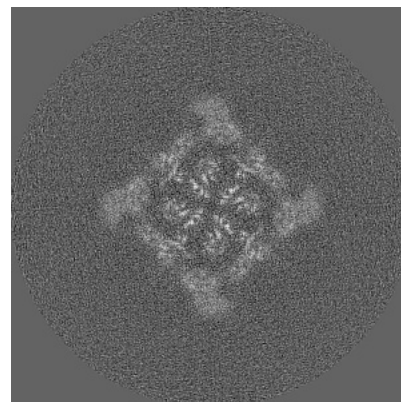
6.2.2 Raw map



X Index: 220



Y Index: 220

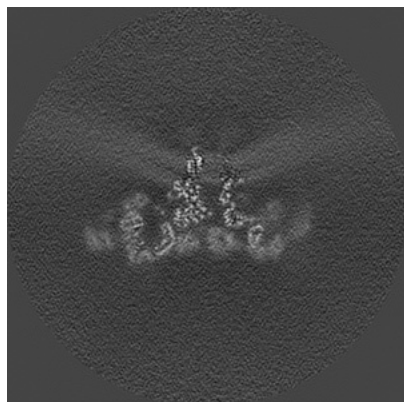


Z Index: 220

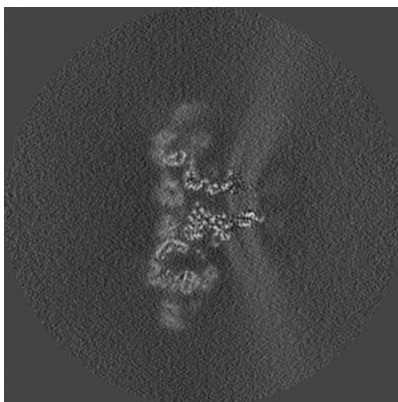
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

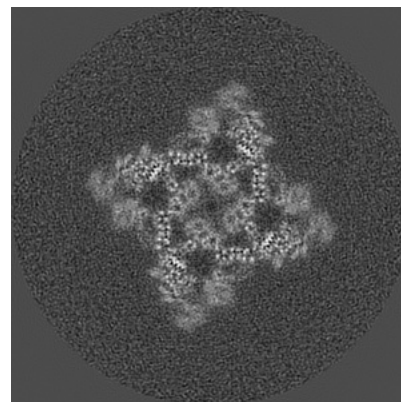
6.3.1 Primary map



X Index: 197

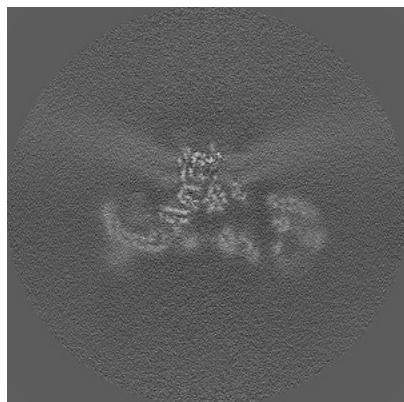


Y Index: 243

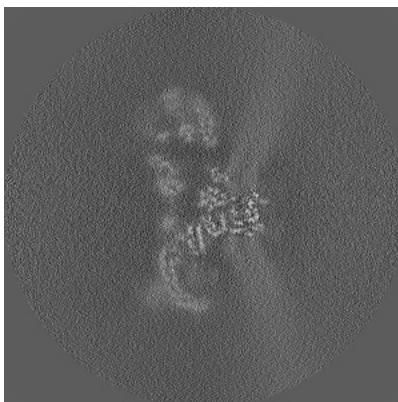


Z Index: 188

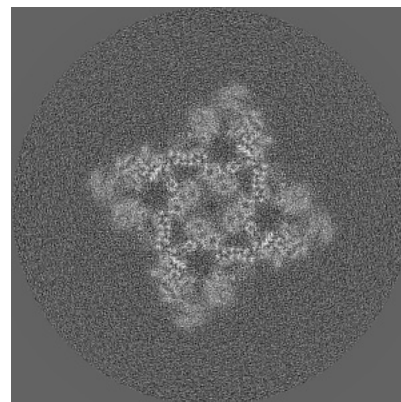
6.3.2 Raw map



X Index: 232



Y Index: 208

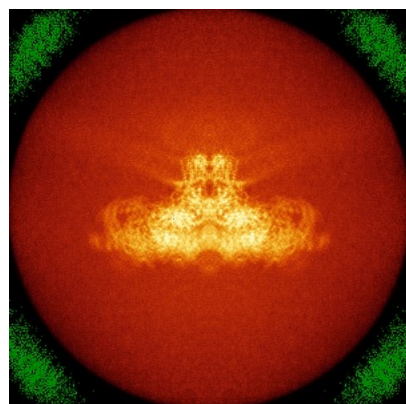


Z Index: 188

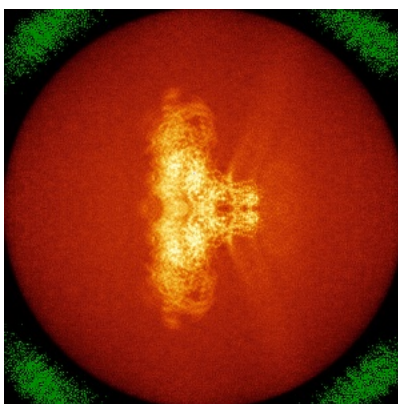
The images above show the largest variance slices of the map in three orthogonal directions.

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

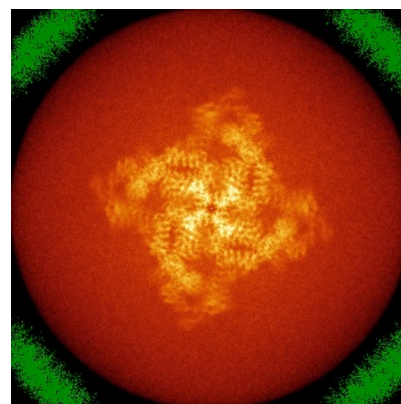
6.4.1 Primary map



X

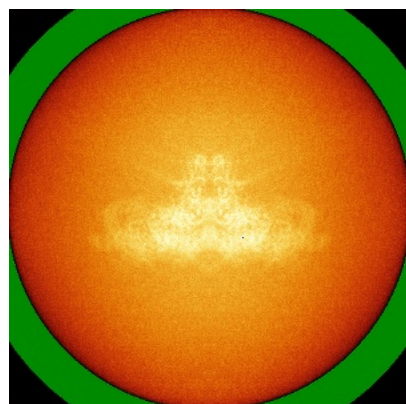


Y

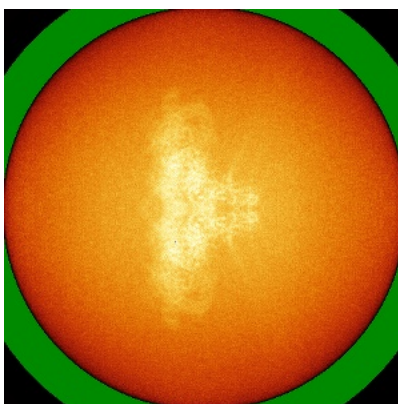


Z

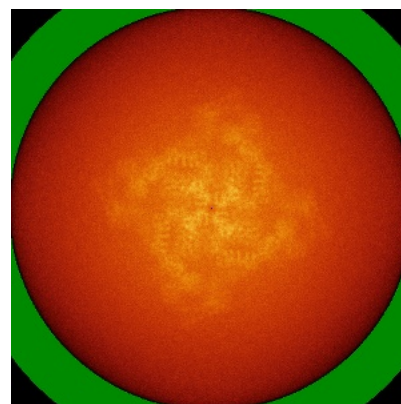
6.4.2 Raw map



X



Y

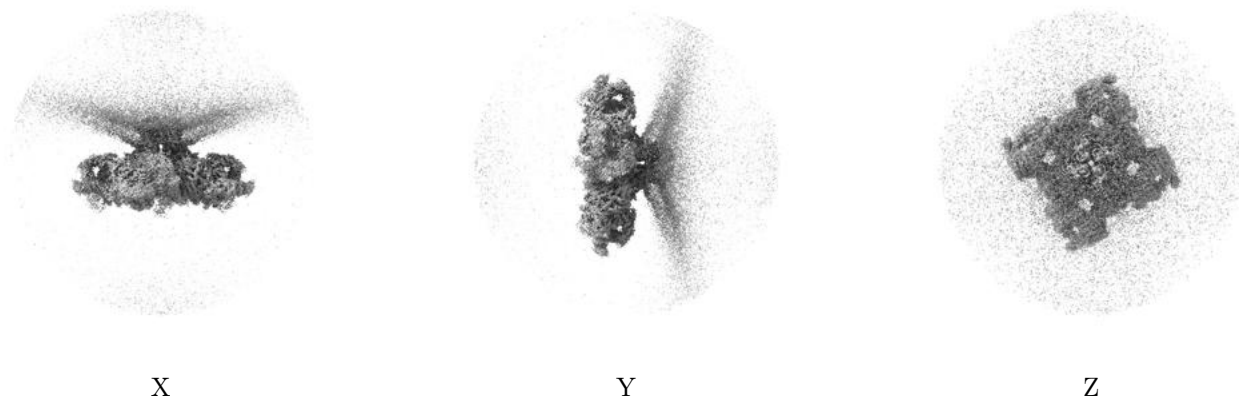


Z

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.

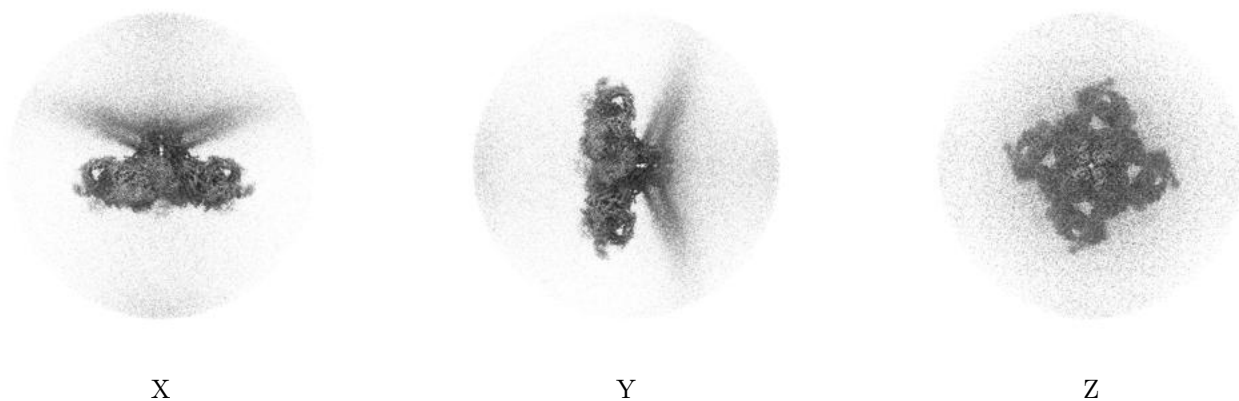
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00538. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

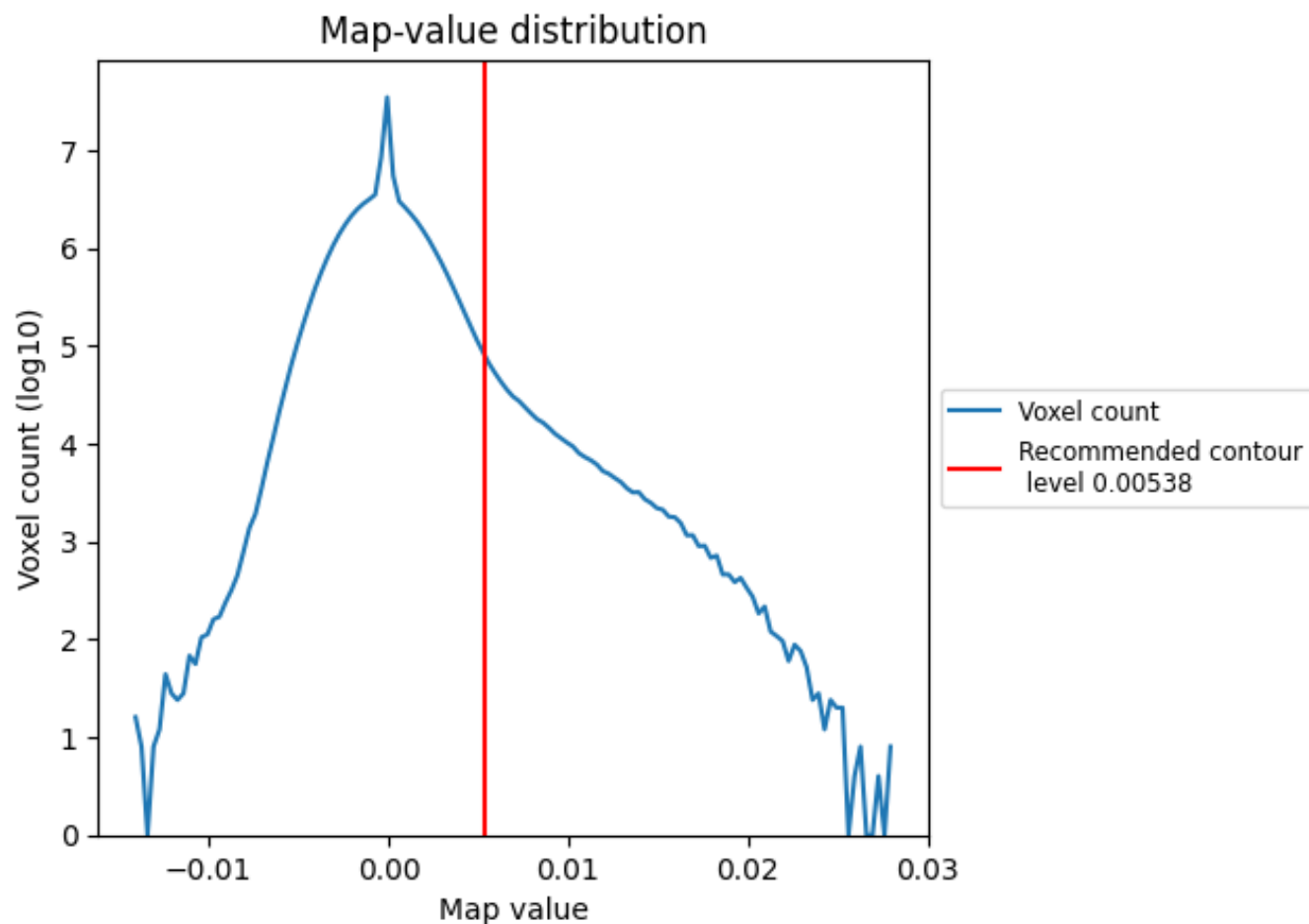
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

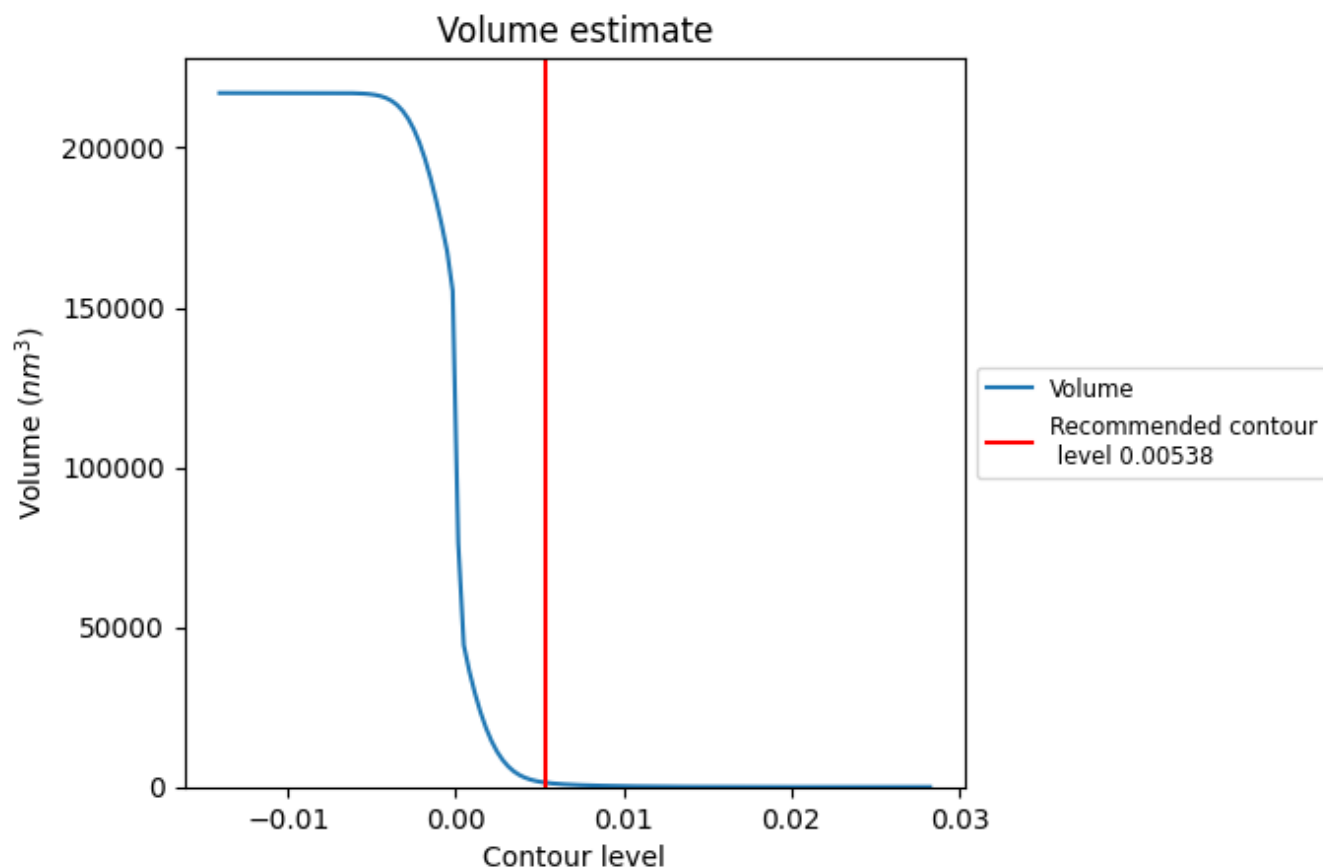
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

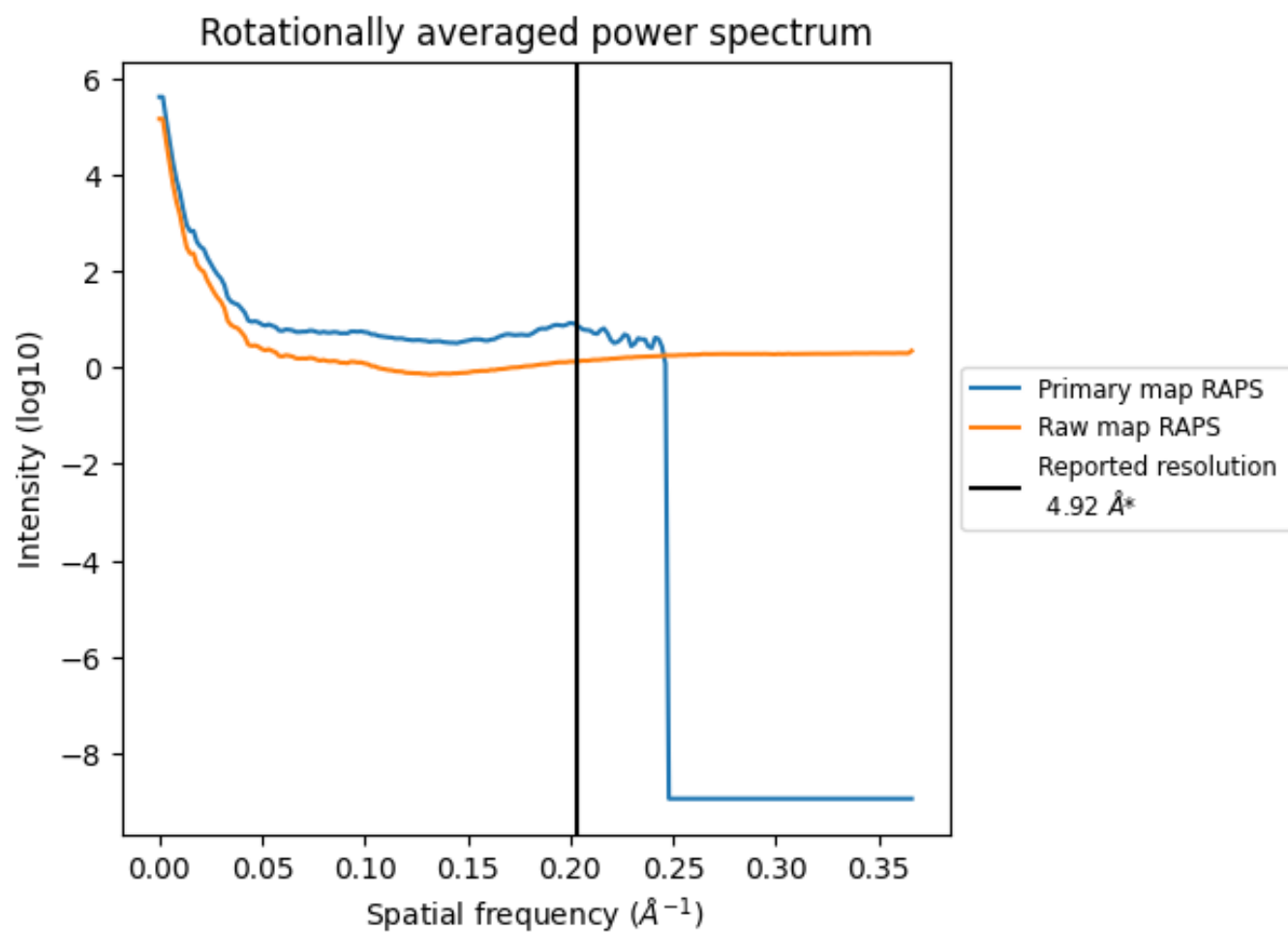
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1339 nm³; this corresponds to an approximate mass of 1210 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 ⓘ

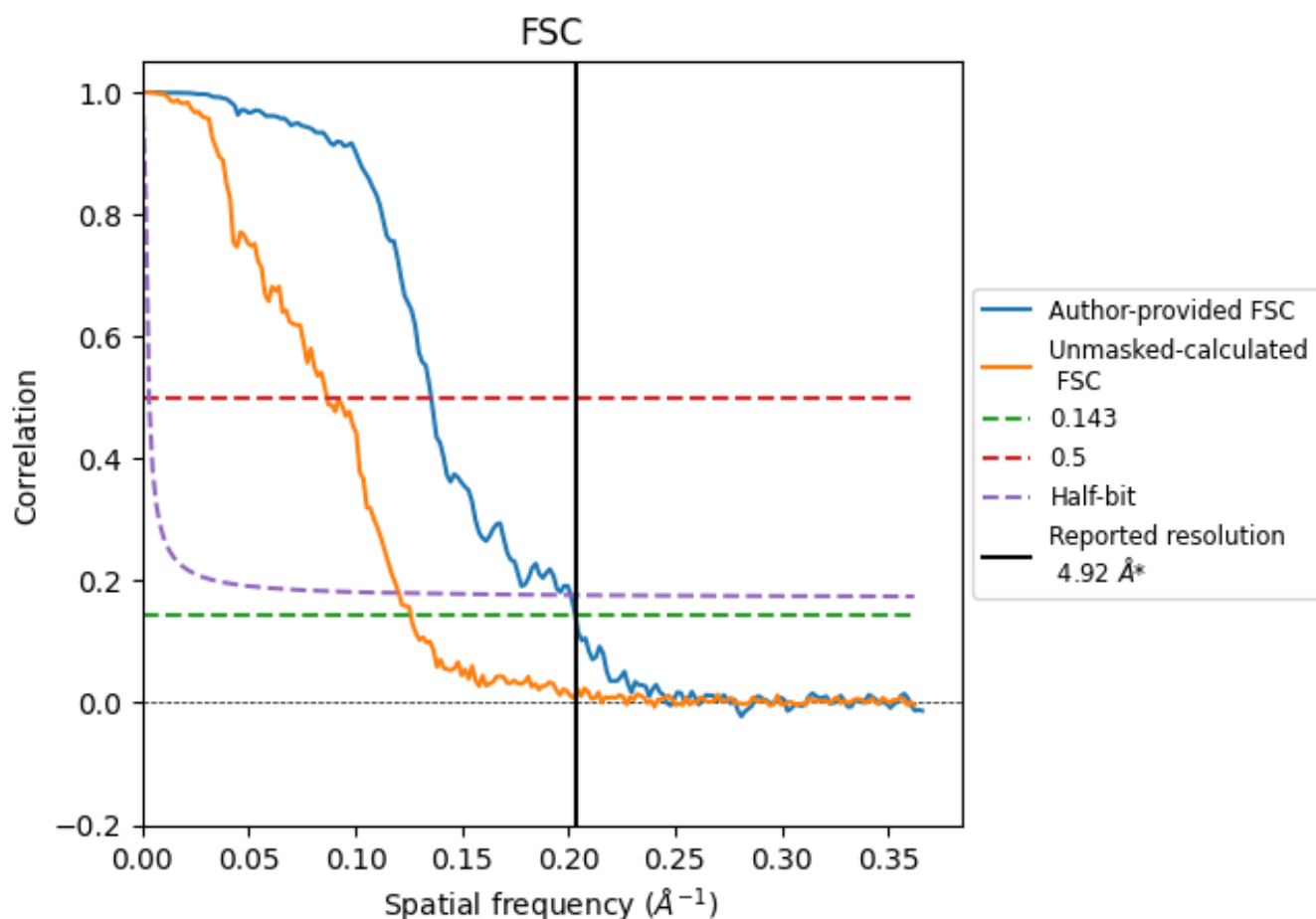


*Reported resolution corresponds to spatial frequency of $0.203 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.203 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

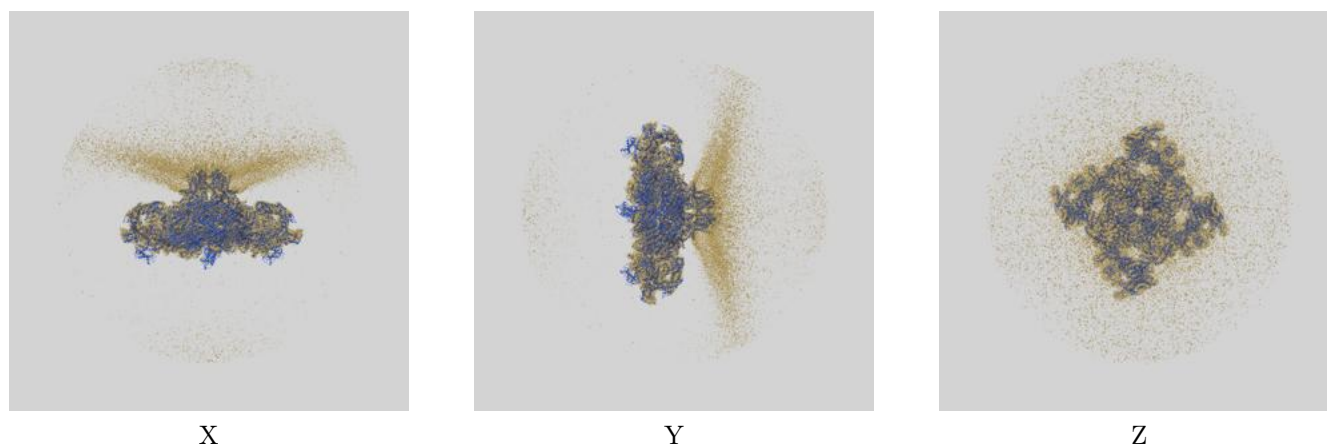
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.92	-	-
Author-provided FSC curve	4.92	7.37	4.97
Unmasked-calculated*	7.94	11.55	8.31

*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 7.94 differs from the reported value 4.92 by more than 10 %

9 Map-model fit [i](#)

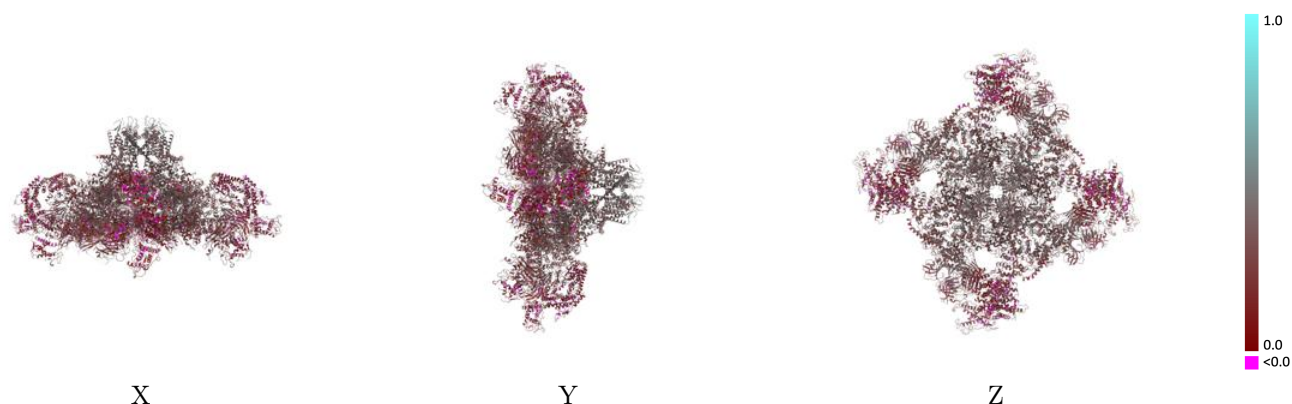
This section contains information regarding the fit between EMDB map EMD-54569 and PDB model 9S4L. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



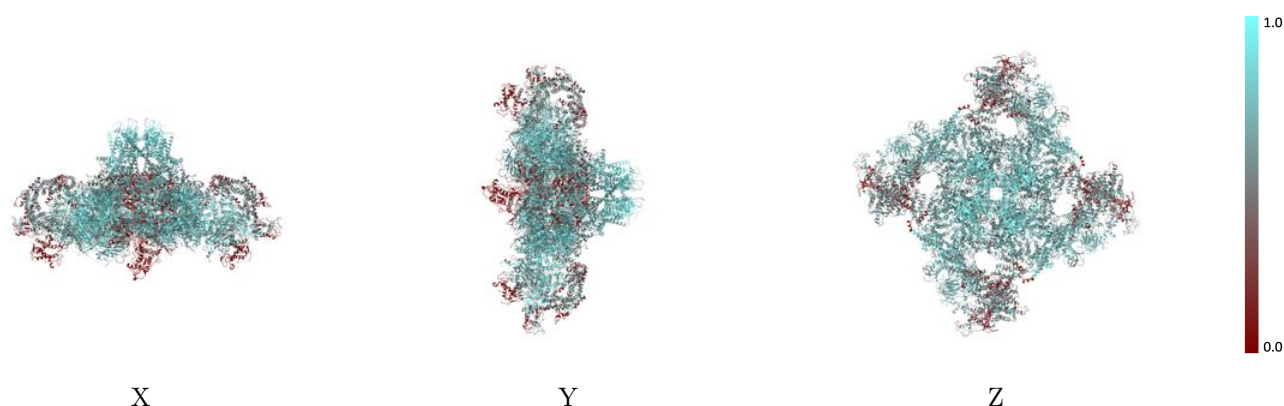
The images above show the 3D surface view of the map at the recommended contour level 0.00538 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



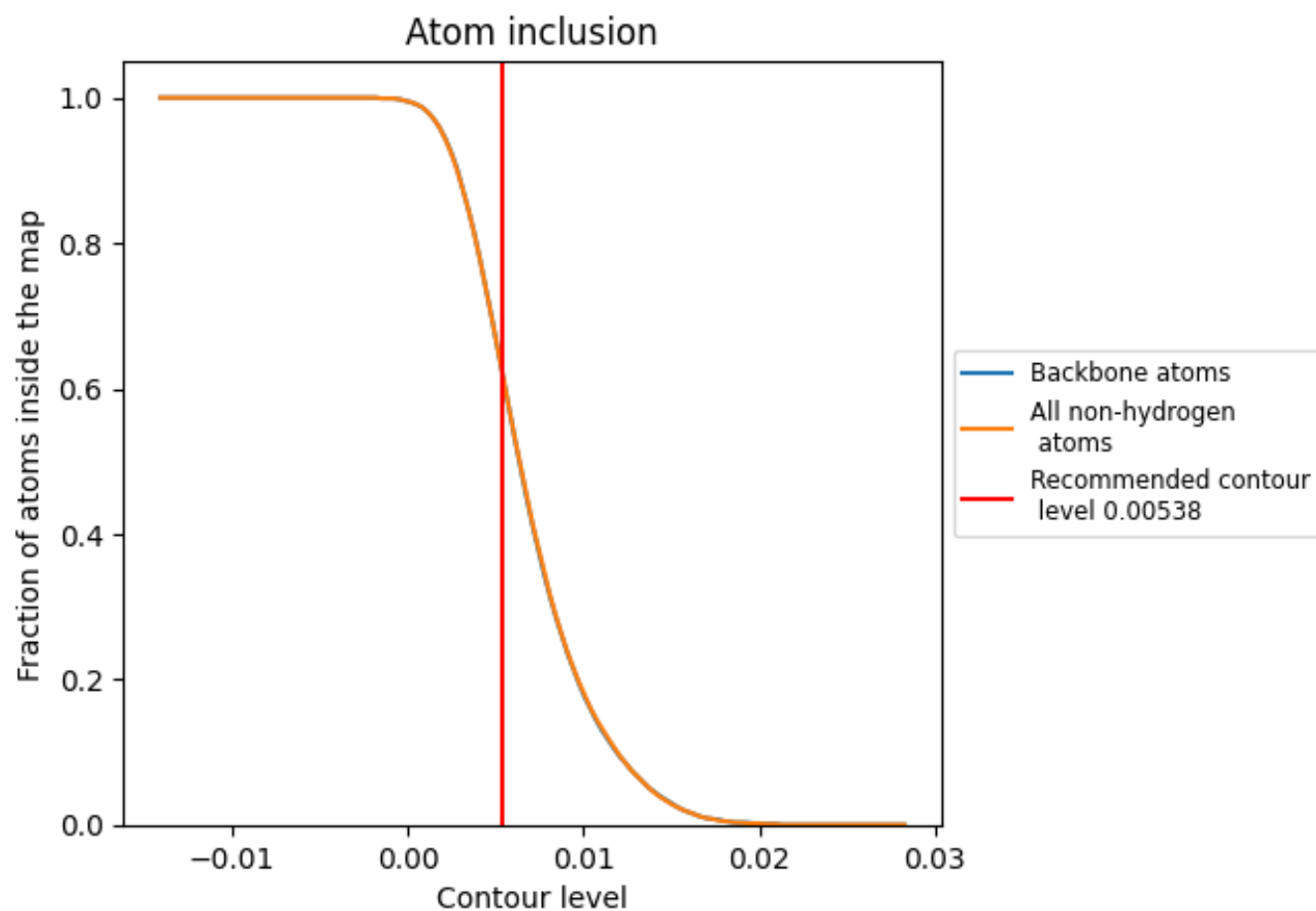
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00538).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 62% 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 (0.00538) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6210	0.2940
A	0.6260	0.2940
B	0.6270	0.2930
C	0.6270	0.2930
D	0.6260	0.2930
E	0.6430	0.3010
F	0.6460	0.3020
G	0.6380	0.3010
H	0.6430	0.3030

1.0

0.0

<0.0