Full wwPDB EM Validation Report

Jul 2, 2025 – 02:40 PM JST

PDB ID	:	9L4F / pdb_0000914f
EMDB ID	:	EMD-62812
Title	:	ATR-ATRIP bound with ATPgammaS
Authors	:	Wang, G.
Deposited on	:	2024-12-20
Resolution	:	6.22 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

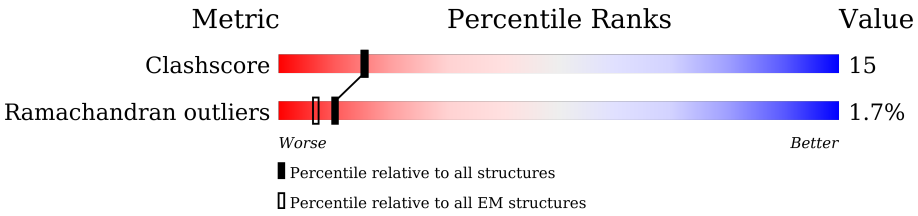
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.22 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835

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 <=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	2644	5% 75% 14% • 10%
1	B	2644	8% 70% 12% • 17%
2	C	791	6% 38% 6% 56%
2	D	791	8% 36% 7% • 57%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26137 atoms, of which 8 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.

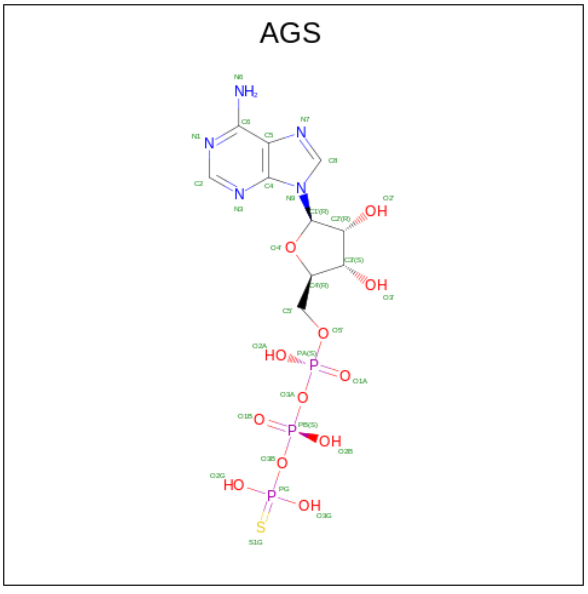
- Molecule 1 is a protein called Serine/threonine-protein kinase ATR.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	2383	Total 11815	C 7048	N 2383	O 2384	0	0
1	B	2188	Total 10846	C 6469	N 2188	O 2189	0	0

- Molecule 2 is a protein called ATR-interacting protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	339	Total 1678	C 1000	N 339	O 339	0	0
2	C	349	Total 1728	C 1030	N 349	O 349	0	0

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



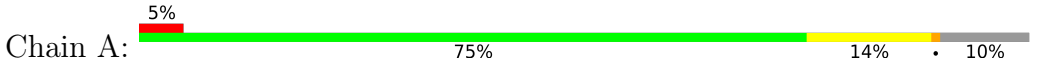
Mol	Chain	Residues	Atoms							AltConf
3	A	1	Total	C	H	N	O	P	S	0
			35	10	4	5	12	3	1	
3	B	1	Total	C	H	N	O	P	S	0
			35	10	4	5	12	3	1	

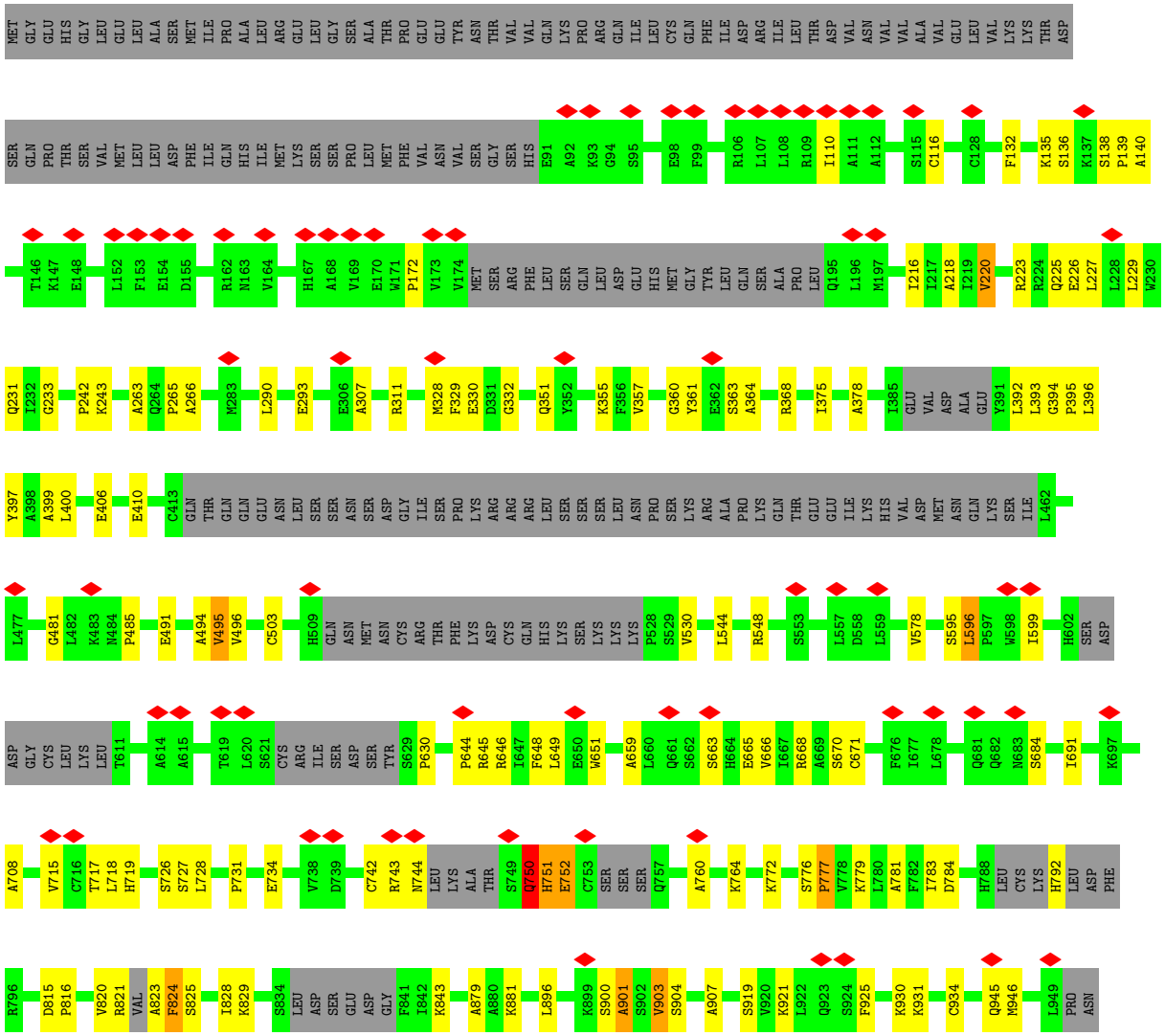
3 Residue-property plots (i)

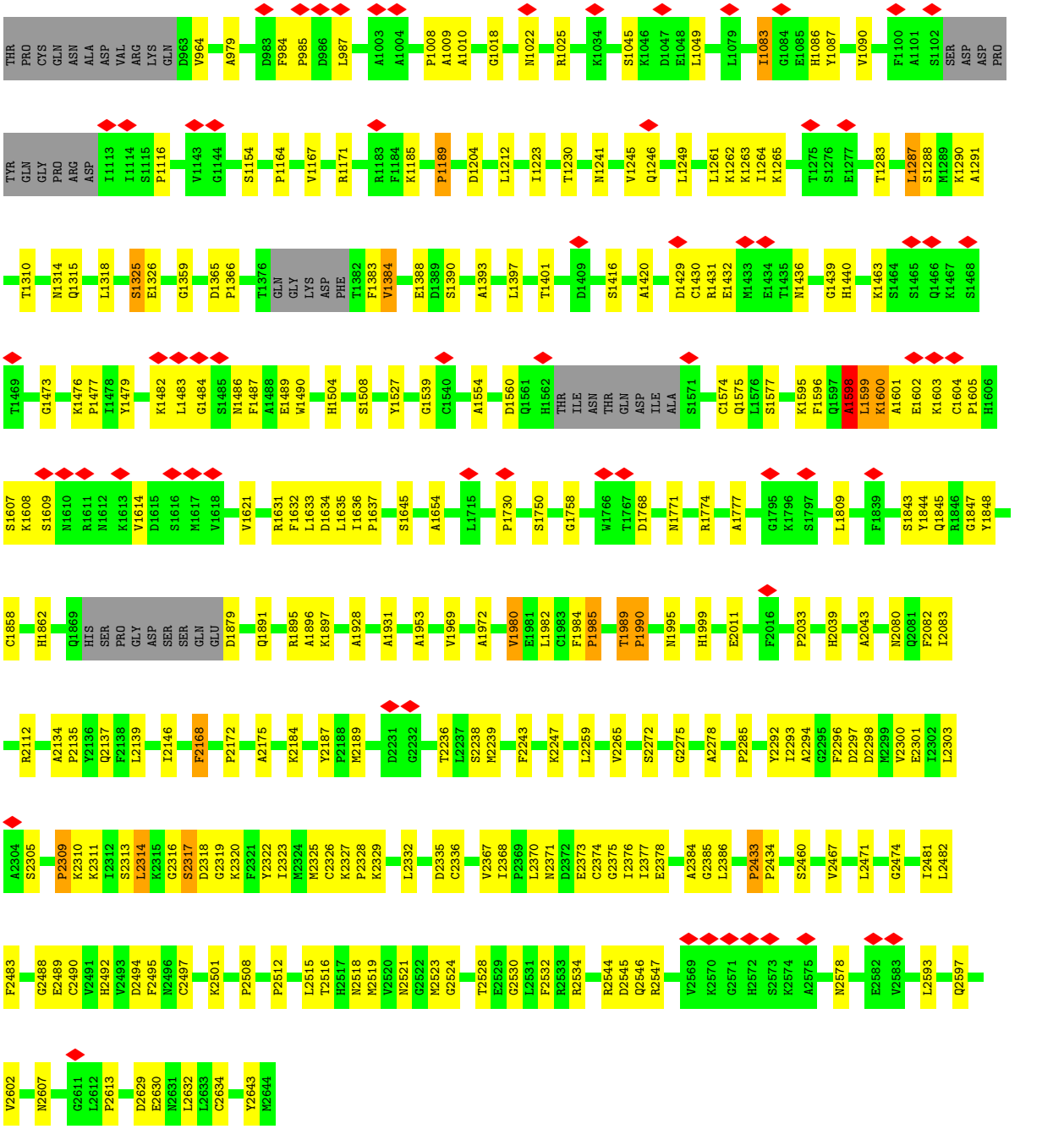
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Serine/threonine-protein kinase ATR

Chain A:

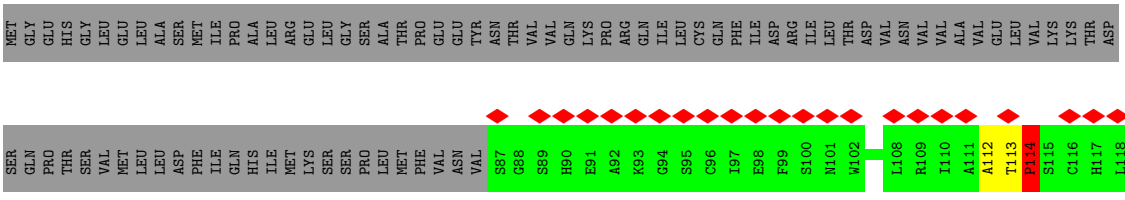


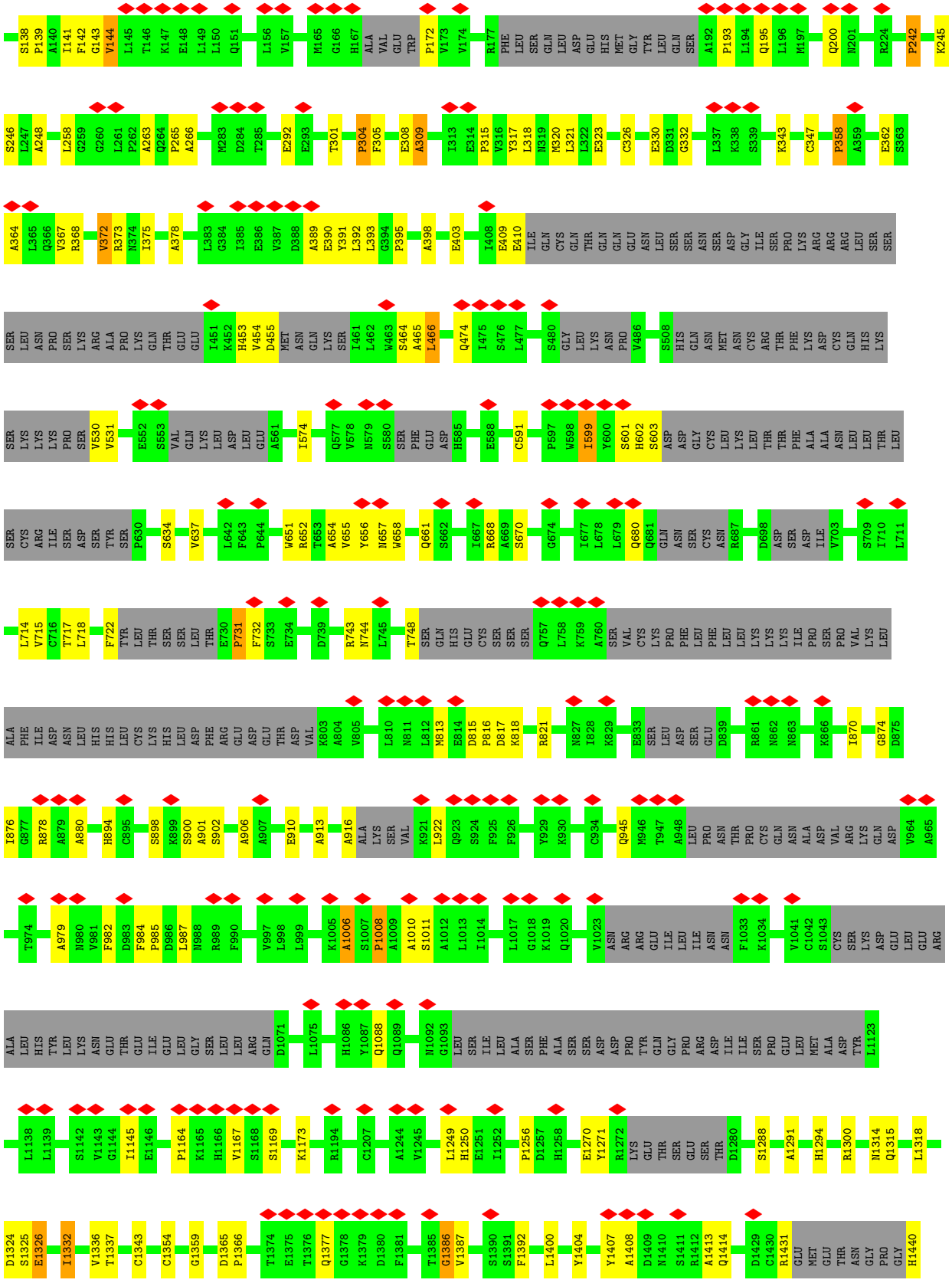


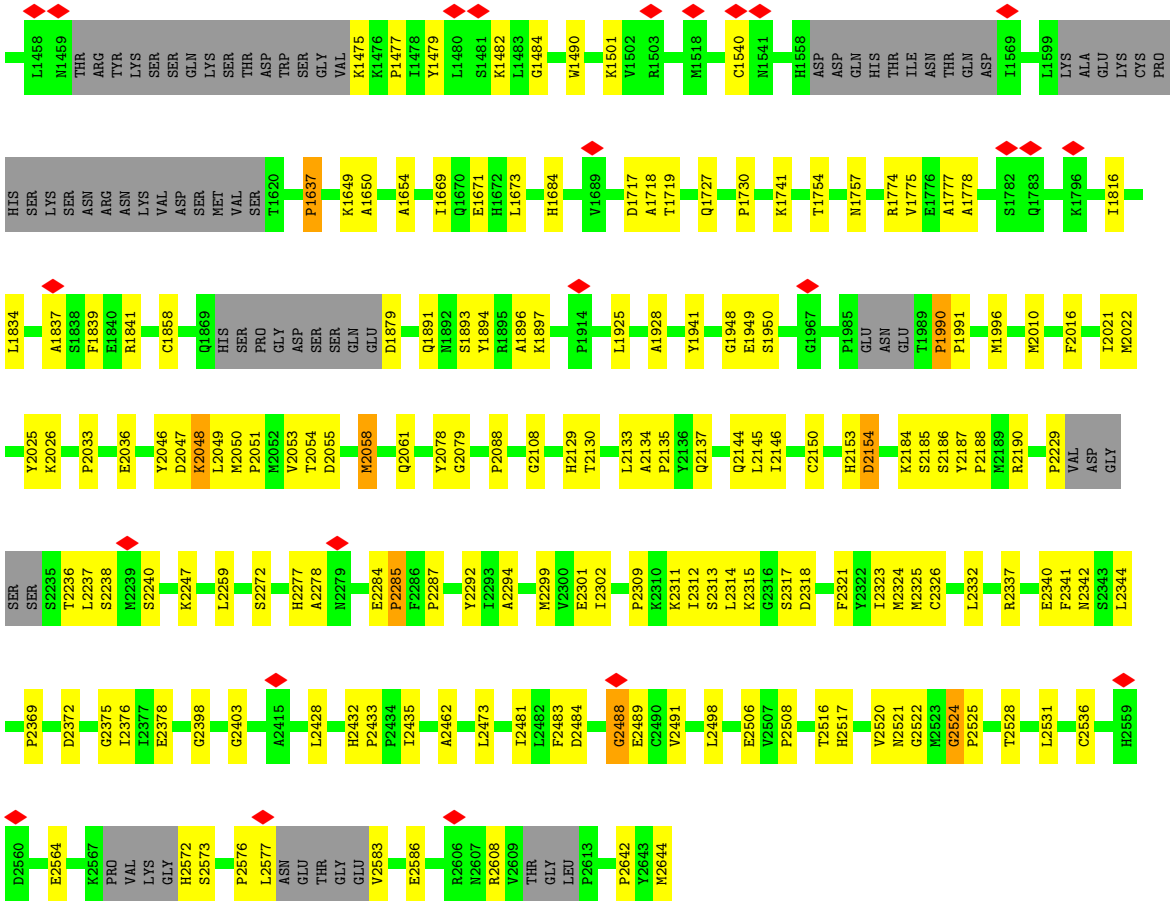


• Molecule 1: Serine/threonine-protein kinase ATR

Chain B:

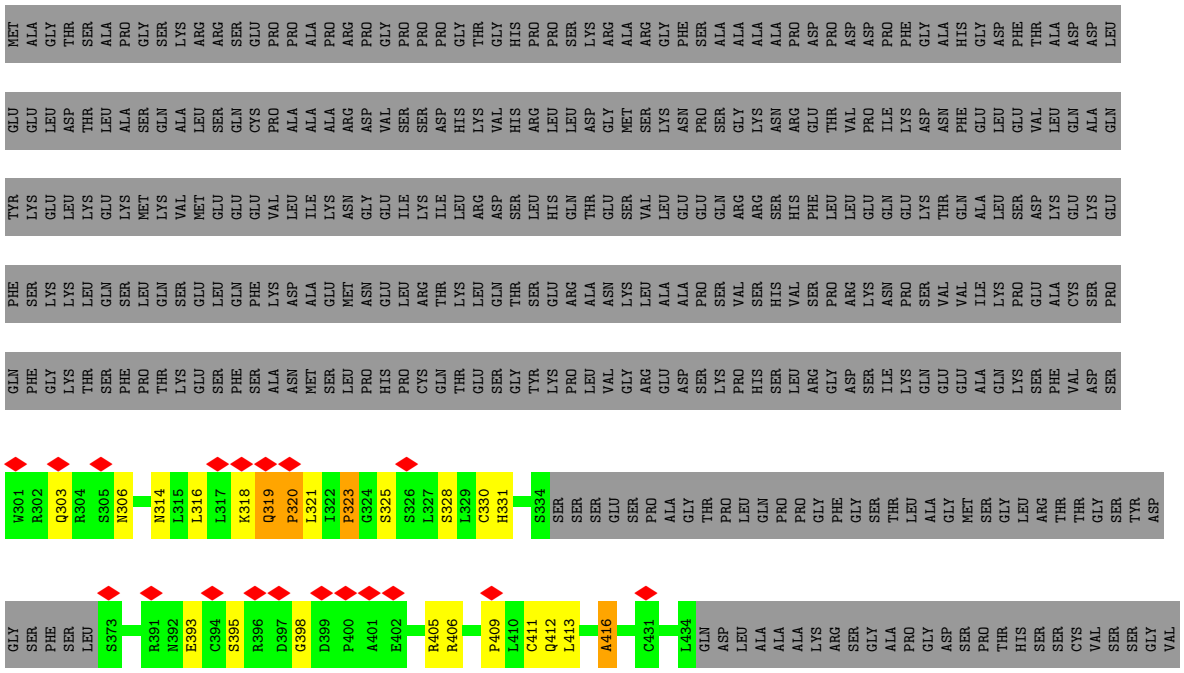


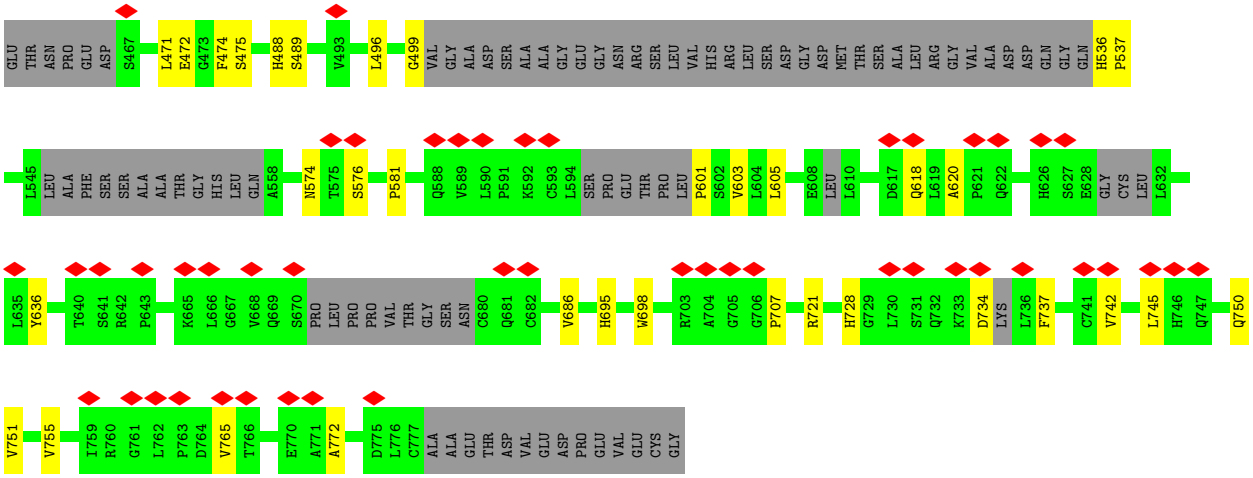




• Molecule 2: ATR-interacting protein

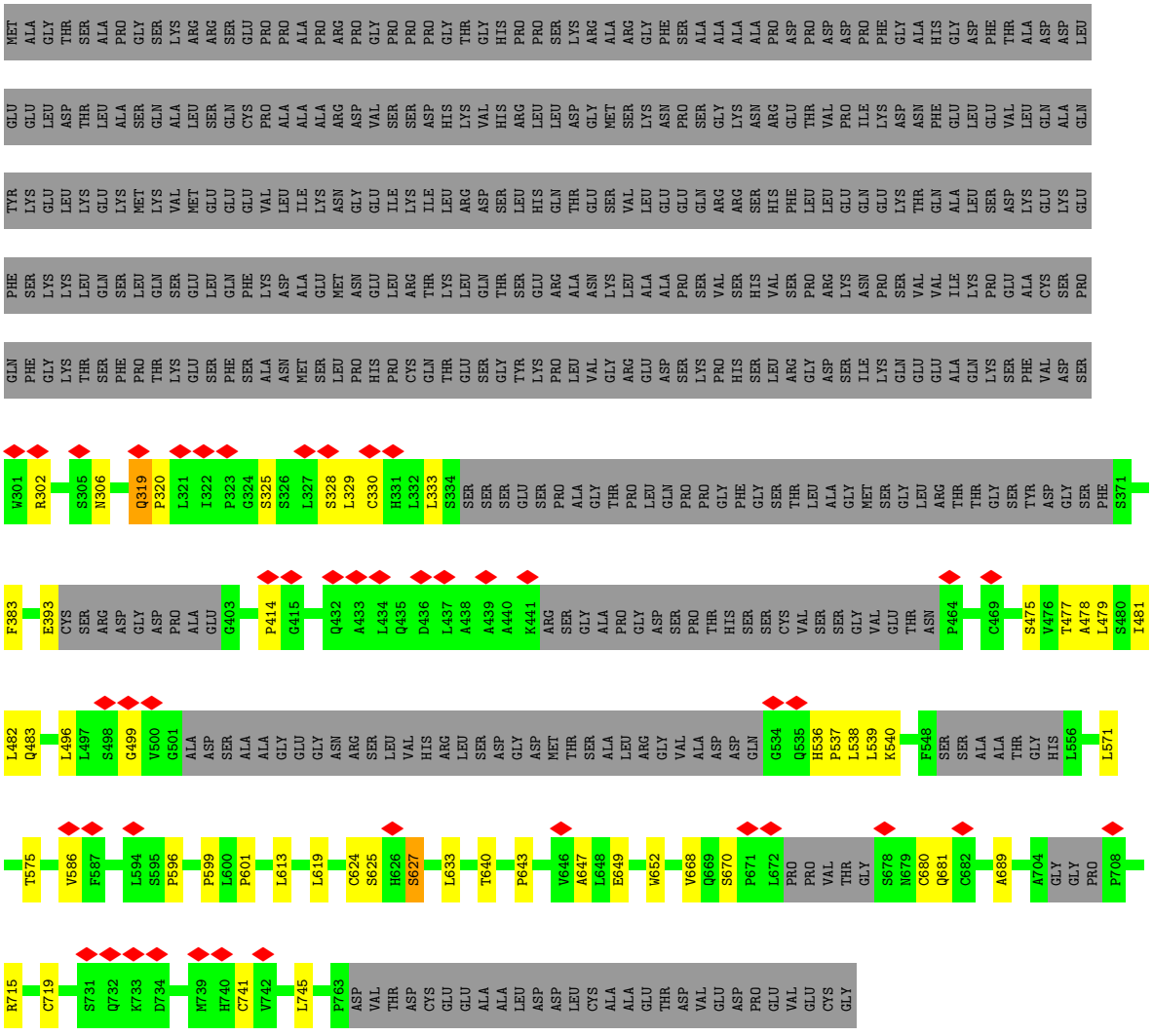
Chain D:





• Molecule 2: ATR-interacting protein

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40429	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.353	Depositor
Minimum map value	-0.770	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.27	Depositor
Map size (Å)	308.16, 308.16, 308.16	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.12	1/11797 (0.0%)	1.73	92/16425 (0.6%)
1	B	1.12	0/10814	1.70	74/15030 (0.5%)
2	C	1.11	0/1720	1.69	14/2385 (0.6%)
2	D	1.13	0/1668	1.66	9/2309 (0.4%)
All	All	1.12	1/25999 (0.0%)	1.71	189/36149 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
2	C	0	1
2	D	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	750	GLN	C-O	-11.34	1.09	1.24

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1477	PRO	N-CA-C	-13.47	95.67	114.80
2	C	586	VAL	N-CA-C	-13.21	97.38	110.72
1	B	2433	PRO	N-CA-C	-13.16	94.64	110.70
1	A	1598	ALA	CA-C-O	-12.29	107.52	120.55
1	A	752	GLU	N-CA-C	11.96	127.89	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2344	LEU	N-CA-C	-11.01	98.28	112.93
1	A	1189	PRO	N-CA-CB	-10.80	91.45	103.33
1	B	2285	PRO	N-CA-C	-10.36	99.14	113.53
1	A	750	GLN	CB-CA-C	10.32	130.97	110.42
1	A	1990	PRO	N-CA-C	10.31	123.27	110.70
1	A	2546	GLN	N-CA-C	-9.62	101.23	113.16
1	B	114	PRO	N-CA-C	-9.47	92.96	112.47
1	B	718	LEU	N-CA-C	9.25	121.36	111.28
1	A	752	GLU	CB-CA-C	-9.16	98.88	111.89
1	A	784	ASP	CB-CA-C	-9.01	106.17	116.63
1	A	2135	PRO	N-CA-C	-8.68	101.46	113.53
1	A	750	GLN	O-C-N	-8.66	111.07	122.59
1	A	919	SER	N-CA-C	-8.49	100.28	111.74
1	A	1985	PRO	N-CA-C	-8.42	101.82	113.53
1	A	751	HIS	N-CA-C	8.29	121.51	108.67
1	A	816	PRO	N-CA-C	-8.23	102.08	113.53
1	B	139	PRO	N-CA-C	-8.22	102.11	113.53
1	A	779	LYS	N-CA-C	-8.10	102.45	111.28
1	B	1649	LYS	N-CA-C	-8.08	101.90	112.24
1	B	358	PRO	N-CA-CB	8.07	111.72	103.25
1	A	394	GLY	N-CA-C	-8.02	105.03	115.22
2	D	707	PRO	N-CA-C	-7.84	102.19	110.58
1	A	1189	PRO	N-CA-C	7.79	124.36	113.53
1	A	485	PRO	N-CA-C	-7.77	99.02	111.14
1	B	574	ILE	N-CA-C	-7.75	102.89	110.72
1	A	1366	PRO	N-CA-C	-7.73	102.79	113.53
2	C	414	PRO	N-CA-C	-7.72	102.80	113.53
1	A	1008	PRO	N-CA-C	-7.70	102.83	113.53
1	A	1599	LEU	N-CA-CB	-7.66	100.23	110.57
1	B	1008	PRO	N-CA-CB	7.62	111.26	103.25
1	A	139	PRO	N-CA-C	-7.58	102.99	113.53
1	A	1022	ASN	N-CA-C	-7.56	101.54	111.74
1	B	373	ARG	N-CA-C	-7.53	104.06	113.55
1	A	750	GLN	CA-C-N	-7.40	110.97	121.99
1	A	750	GLN	C-N-CA	-7.40	110.97	121.99
1	A	2265	VAL	N-CA-C	-7.32	103.33	110.72
1	B	1719	THR	N-CA-C	-7.30	103.33	111.28
1	A	265	PRO	N-CA-C	-7.24	103.47	113.53
1	A	1897	LYS	N-CA-C	-7.22	103.41	111.28
1	B	2048	LYS	N-CA-C	-7.18	103.45	111.28
1	B	315	PRO	N-CA-C	-7.11	103.64	113.53
1	B	2317	SER	N-CA-C	-6.85	103.81	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	361	TYR	N-CA-C	-6.83	103.84	111.28
1	A	752	GLU	N-CA-CB	6.79	121.75	111.70
1	B	717	THR	CA-C-O	-6.73	113.23	121.11
2	C	537	PRO	N-CA-C	-6.67	104.25	113.53
1	B	2135	PRO	N-CA-C	-6.67	104.26	113.53
1	B	1006	ALA	CA-C-N	-6.66	116.71	123.10
1	B	1006	ALA	C-N-CA	-6.66	116.71	123.10
1	A	843	LYS	CB-CA-C	-6.59	99.85	110.79
2	C	596	PRO	N-CA-C	-6.58	104.38	113.53
1	A	772	LYS	N-CA-C	-6.53	104.17	111.28
1	A	2534	ARG	CB-CA-C	-6.48	109.09	116.54
1	A	2285	PRO	N-CA-C	-6.47	101.03	111.19
1	A	1263	LYS	N-CA-C	-6.47	104.22	111.28
1	B	2398	GLY	N-CA-C	-6.46	106.76	115.36
1	A	751	HIS	CA-C-N	6.37	131.41	122.36
1	A	751	HIS	C-N-CA	6.37	131.41	122.36
1	A	1087	TYR	CB-CA-C	-6.37	109.24	116.63
1	B	474	GLN	CB-CA-C	-6.34	109.28	116.63
1	B	2309	PRO	N-CA-C	-6.33	101.31	111.38
1	A	2168	PHE	N-CA-C	-6.32	104.39	111.28
1	B	591	CYS	CB-CA-C	-6.32	109.30	116.63
1	A	2433	PRO	N-CA-C	-6.29	103.03	110.70
1	B	2088	PRO	N-CA-C	-6.27	104.81	113.53
1	A	2530	GLY	CA-C-O	-6.22	116.83	122.24
2	C	481	ILE	N-CA-C	-6.19	104.31	110.62
1	A	750	GLN	N-CA-CB	-6.17	100.06	110.49
1	B	1894	TYR	N-CA-C	-6.15	104.58	111.28
1	B	292	GLU	CB-CA-C	-6.15	109.50	116.63
1	A	2488	GLY	N-CA-C	-6.12	107.22	115.36
1	A	328	MET	CB-CA-C	-6.12	108.91	117.23
1	B	1948	GLY	CA-C-O	-6.11	117.34	122.29
1	B	1990	PRO	N-CA-C	-6.07	103.30	110.70
1	A	1599	LEU	CA-C-O	-6.06	115.40	122.37
1	A	2112	ARG	CB-CA-C	-6.05	109.61	116.63
1	A	2317	SER	N-CA-C	-6.05	104.69	111.28
1	A	1116	PRO	N-CA-C	-6.03	105.15	113.53
1	B	265	PRO	N-CA-C	-6.01	105.17	113.53
1	B	1088	GLN	CB-CA-C	-6.00	109.64	116.54
2	D	323	PRO	N-CA-CB	6.00	109.55	103.25
1	B	1386	GLY	CA-C-O	-5.98	117.45	122.29
1	A	1326	GLU	N-CA-C	-5.98	104.76	111.28
2	C	302	ARG	CB-CA-C	-5.95	109.73	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	317	TYR	N-CA-C	-5.94	104.80	111.28
1	A	1482	LYS	N-CA-C	-5.91	104.84	111.28
1	A	760	ALA	N-CA-C	-5.89	104.86	111.28
1	A	293	GLU	N-CA-C	-5.87	104.82	113.16
1	B	358	PRO	N-CA-C	-5.87	100.39	112.47
2	D	330	CYS	N-CA-C	-5.83	104.92	111.28
1	A	481	GLY	N-CA-C	-5.83	105.74	112.73
2	D	409	PRO	N-CA-CB	-5.82	98.13	103.31
1	B	2586	GLU	N-CA-C	-5.80	104.95	111.28
1	B	1671	GLU	N-CA-C	-5.75	105.02	111.28
1	A	2146	ILE	N-CA-C	-5.74	104.76	110.62
1	B	2108	GLY	N-CA-C	-5.72	107.35	115.30
1	A	2607	ASN	N-CA-C	-5.72	106.07	113.16
1	B	2506	GLU	CB-CA-C	-5.72	110.00	116.63
1	A	2367	VAL	CA-C-N	-5.71	117.78	123.04
1	A	2367	VAL	C-N-CA	-5.71	117.78	123.04
2	C	643	PRO	N-CA-C	-5.70	105.61	113.53
1	B	1741	LYS	N-CA-C	-5.67	105.10	111.28
1	A	752	GLU	CA-C-O	-5.67	115.26	121.84
1	A	1634	ASP	N-CA-C	-5.65	105.12	111.28
2	D	409	PRO	N-CA-C	5.65	119.96	111.14
1	B	1475	LYS	CA-C-N	-5.65	116.32	123.15
1	B	1475	LYS	C-N-CA	-5.65	116.32	123.15
2	C	649	GLU	CB-CA-C	-5.64	110.08	116.63
1	A	1212	LEU	CB-CA-C	-5.64	110.06	116.54
1	B	114	PRO	N-CA-CB	5.64	109.17	103.25
2	C	627	SER	CB-CA-C	-5.61	110.12	116.63
1	B	2531	LEU	N-CA-C	-5.54	105.24	111.28
1	B	2229	PRO	N-CA-CB	-5.54	96.91	103.00
1	A	646	ARG	CB-CA-C	-5.51	110.24	116.63
1	A	630	PRO	N-CA-C	-5.49	105.90	113.53
1	B	1366	PRO	N-CA-C	-5.48	105.91	113.53
1	A	2630	GLU	N-CA-C	-5.48	105.30	111.28
1	A	2139	LEU	CB-CA-C	-5.47	110.25	116.54
2	C	330	CYS	CB-CA-C	-5.46	110.29	116.63
1	A	734	GLU	CB-CA-C	-5.46	110.30	116.63
1	A	783	ILE	N-CA-C	-5.46	105.05	110.62
1	B	1332	ILE	N-CA-C	-5.46	105.05	110.62
2	D	581	PRO	N-CA-C	-5.46	105.94	113.53
1	B	599	ILE	N-CA-C	-5.45	107.17	112.29
1	B	321	LEU	N-CA-C	-5.44	105.35	111.28
1	B	2522	GLY	N-CA-C	-5.44	106.21	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2079	GLY	CA-C-O	-5.43	117.89	122.29
2	D	416	ALA	N-CA-C	-5.43	105.36	111.28
1	A	496	VAL	N-CA-C	-5.41	105.25	110.72
1	A	2532	PHE	N-CA-C	-5.41	105.38	111.28
1	B	2058	MET	CB-CA-C	-5.40	110.37	116.63
1	A	1539	GLY	CA-C-O	-5.40	117.92	122.29
1	A	2033	PRO	N-CA-C	-5.40	106.17	113.40
1	A	1390	SER	CB-CA-C	-5.39	110.37	116.63
1	A	503	CYS	CB-CA-C	-5.39	109.90	117.23
1	B	258	LEU	N-CA-C	-5.38	105.42	111.28
1	B	391	TYR	N-CA-C	-5.37	105.43	111.28
1	B	390	GLU	CB-CA-C	-5.36	110.42	116.63
1	B	2053	VAL	N-CA-C	-5.36	105.31	110.72
2	C	538	LEU	N-CA-C	-5.33	105.47	111.28
1	A	2318	ASP	N-CA-C	-5.33	106.37	112.92
2	C	599	PRO	N-CA-C	5.32	119.40	111.41
1	B	818	LYS	CB-CA-C	-5.30	110.48	116.63
1	B	1326	GLU	N-CA-C	-5.29	105.52	111.28
1	B	403	GLU	N-CA-C	-5.28	105.53	111.28
1	A	330	GLU	N-CA-C	-5.27	105.53	111.28
1	A	1287	LEU	N-CA-C	-5.26	105.55	111.28
1	B	1482	LYS	CB-CA-C	-5.26	110.08	117.23
1	B	658	TRP	CB-CA-C	-5.24	110.55	116.63
1	B	2318	ASP	N-CA-C	-5.24	105.57	111.28
1	B	2055	ASP	N-CA-C	-5.22	104.69	111.74
1	A	1473	GLY	N-CA-C	-5.21	108.43	115.36
1	B	1684	HIS	N-CA-C	-5.21	104.71	111.74
1	A	2545	ASP	N-CA-C	-5.20	105.61	111.28
1	A	1290	LYS	N-CA-C	-5.20	105.62	111.28
1	A	665	GLU	CB-CA-C	-5.19	110.61	116.63
1	A	1989	THR	N-CA-C	-5.19	103.05	109.64
1	B	1008	PRO	CA-C-N	-5.18	115.48	123.04
1	B	1008	PRO	C-N-CA	-5.18	115.48	123.04
1	A	1980	VAL	N-CA-C	-5.17	105.35	110.62
1	A	332	GLY	N-CA-C	-5.14	108.22	115.32
1	B	1941	TYR	N-CA-C	-5.14	105.67	111.28
2	C	601	PRO	N-CA-C	-5.14	106.38	113.53
1	B	2403	GLY	N-CA-C	-5.12	106.59	112.73
1	A	2082	PHE	N-CA-C	-5.12	106.81	113.16
1	A	881	LYS	N-CA-C	-5.11	106.64	112.92
1	A	1436	ASN	N-CA-C	-5.11	106.83	113.16
1	B	2435	ILE	N-CA-C	-5.10	107.49	112.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1637	PRO	N-CA-C	-5.10	101.97	112.47
1	A	218	ALA	N-CA-C	-5.10	105.72	111.28
1	A	824	PHE	N-CA-C	-5.09	105.73	111.28
1	A	1809	LEU	CA-C-N	-5.09	114.67	122.21
1	A	1809	LEU	C-N-CA	-5.09	114.67	122.21
1	A	2172	PRO	N-CA-C	-5.09	106.46	113.53
1	B	2608	ARG	CB-CA-C	-5.09	110.73	116.63
1	A	2011	GLU	N-CA-C	-5.08	105.74	111.28
1	B	2033	PRO	N-CA-C	-5.08	106.59	113.40
1	A	2305	SER	CB-CA-C	-5.08	110.73	116.63
1	B	1164	PRO	N-CA-C	-5.06	106.49	113.53
1	B	1337	THR	N-CA-C	-5.05	105.78	111.28
1	B	2524	GLY	O-C-N	5.04	122.89	121.07
2	D	603	VAL	N-CA-C	-5.04	105.48	110.62
2	D	488	HIS	CA-C-O	-5.02	115.23	120.55
2	C	477	THR	N-CA-C	-5.01	105.82	111.28

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1476	LYS	Peptide
1	A	1598	ALA	Mainchain
1	A	750	GLN	Mainchain
1	A	777	PRO	Peptide
2	C	319	GLN	Peptide
2	D	319	GLN	Peptide

5.2 Too-close contacts (i)

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	11815	0	5242	251	0
1	B	10846	0	4821	221	0
2	C	1728	0	757	47	0
2	D	1678	0	732	39	0
3	A	31	4	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	4	12	0	0
All	All	26129	8	11576	550	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 15.

All (550) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2544:ARG:HA	1:A:2547:ARG:CB	1.35	1.55
2:C:320:PRO:CB	2:C:325:SER:O	1.71	1.37
1:A:2544:ARG:CA	1:A:2547:ARG:CB	2.08	1.32
2:D:303:GLN:HA	2:D:393:GLU:CB	1.61	1.31
1:B:135:LYS:N	1:B:142:PHE:CB	1.95	1.30
1:B:1250:HIS:CA	1:B:1271:TYR:HA	1.58	1.30
1:B:134:PHE:C	1:B:142:PHE:CB	2.05	1.29
1:A:1844:TYR:O	1:A:1848:TYR:N	1.62	1.29
1:B:1250:HIS:HA	1:B:1271:TYR:CA	1.63	1.27
1:A:2259:LEU:HA	1:A:2292:TYR:CA	1.64	1.25
1:A:2259:LEU:CA	1:A:2292:TYR:HA	1.67	1.23
1:A:1261:LEU:O	1:A:1265:LYS:N	1.77	1.18
1:A:728:LEU:CB	1:A:744:ASN:C	2.17	1.17
1:B:2369:PRO:HA	1:B:2375:GLY:HA2	1.22	1.15
1:A:1164:PRO:CB	1:A:1204:ASP:CB	2.24	1.14
1:A:2297:ASP:H	1:A:2314:LEU:HA	1.04	1.13
2:C:627:SER:HA	2:C:681:GLN:H	1.14	1.12
1:B:2524:GLY:CA	1:B:2528:THR:HA	1.78	1.11
1:A:2544:ARG:O	1:A:2547:ARG:CB	1.98	1.11
1:B:1650:ALA:HB3	1:B:1654:ALA:HB2	1.18	1.11
1:B:2259:LEU:HA	1:B:2292:TYR:HA	1.24	1.11
2:C:499:GLY:HA2	2:C:536:HIS:HA	1.17	1.09
2:C:536:HIS:O	2:C:540:LYS:N	1.86	1.09
1:B:2517:HIS:N	1:B:2644:MET:O	1.85	1.09
2:D:496:LEU:HA	2:D:536:HIS:HA	1.18	1.09
1:B:2312:ILE:C	1:B:2323:ILE:HA	1.78	1.09
2:C:647:ALA:HB1	2:C:652:TRP:HA	1.22	1.09
1:B:2150:CYS:HA	1:B:2577:LEU:HA	1.32	1.08
1:A:1045:SER:CB	1:A:1049:LEU:N	2.17	1.08
1:A:1045:SER:CB	1:A:1049:LEU:CA	2.31	1.07
2:D:496:LEU:HA	2:D:536:HIS:CA	1.84	1.07
1:B:135:LYS:CA	1:B:142:PHE:CB	2.32	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2483:PHE:HA	1:A:2490:CYS:HA	1.38	1.05
1:A:2184:LYS:HA	1:A:2371:ASN:HA	1.36	1.04
1:B:2313:SER:N	1:B:2323:ILE:HA	1.64	1.04
1:B:1359:GLY:HA3	1:B:1858:CYS:CB	1.88	1.02
1:A:1844:TYR:O	1:A:1848:TYR:CA	2.06	1.02
1:A:2544:ARG:C	1:A:2547:ARG:CB	2.32	1.02
1:B:2186:SER:H	1:B:2572:HIS:CB	1.73	1.02
1:A:1602:GLU:HA	1:A:1607:SER:HA	1.40	1.01
2:C:741:CYS:O	2:C:745:LEU:N	1.94	1.01
1:A:392:LEU:O	1:A:396:LEU:N	1.95	1.00
1:B:2369:PRO:HA	1:B:2375:GLY:CA	1.92	0.98
2:C:499:GLY:HA2	2:C:536:HIS:CA	1.93	0.98
1:B:2524:GLY:HA3	1:B:2528:THR:HA	1.41	0.97
2:C:320:PRO:CB	2:C:325:SER:C	2.38	0.97
1:A:1045:SER:CB	1:A:1049:LEU:CB	2.43	0.96
1:B:135:LYS:HA	1:B:142:PHE:CB	1.94	0.96
1:B:1669:ILE:O	1:B:1673:LEU:N	1.98	0.96
1:A:140:ALA:HB1	2:C:670:SER:HA	1.44	0.96
1:B:2186:SER:N	1:B:2572:HIS:CB	2.29	0.96
1:B:2236:THR:HA	1:B:2301:GLU:HA	1.48	0.95
2:D:306:ASN:CB	2:D:393:GLU:HA	1.97	0.94
1:A:2332:LEU:O	1:A:2336:CYS:N	1.99	0.93
2:D:496:LEU:CA	2:D:536:HIS:HA	1.98	0.93
1:B:661:GLN:HA	1:B:668:ARG:HA	1.50	0.93
1:A:2325:MET:H	1:A:2377:ILE:H	1.16	0.91
1:A:946:MET:HA	1:A:1009:ALA:HB3	1.53	0.91
1:B:2524:GLY:HA2	1:B:2528:THR:HA	1.50	0.91
1:B:134:PHE:CB	1:B:142:PHE:HA	2.02	0.90
2:D:303:GLN:CA	2:D:393:GLU:CB	2.49	0.89
1:B:2186:SER:CB	1:B:2573:SER:CB	2.51	0.88
1:A:666:VAL:O	1:A:670:SER:N	2.05	0.88
1:A:1045:SER:H	1:A:1049:LEU:CB	1.88	0.87
1:B:1359:GLY:CA	1:B:1858:CYS:CB	2.52	0.87
2:C:571:LEU:O	2:C:575:THR:N	2.05	0.87
1:B:2313:SER:N	1:B:2323:ILE:CA	2.38	0.86
2:C:640:THR:HA	2:C:689:ALA:HB2	1.56	0.86
1:A:648:PHE:CB	1:A:651:TRP:CB	2.53	0.86
1:A:393:LEU:O	1:A:397:TYR:N	2.09	0.86
1:A:2515:LEU:HA	1:A:2519:MET:CB	2.05	0.86
1:A:2297:ASP:N	1:A:2314:LEU:HA	1.90	0.86
2:C:499:GLY:CA	2:C:536:HIS:HA	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1991:PRO:HA	1:B:1996:MET:CB	2.05	0.85
1:A:2481:ILE:CB	1:A:2492:HIS:HA	2.06	0.85
1:A:1632:PHE:O	1:A:1636:ILE:N	2.09	0.85
2:C:319:GLN:HA	2:C:328:SER:H	1.40	0.85
1:A:2275:GLY:HA2	1:A:2278:ALA:HB3	1.59	0.85
1:A:2544:ARG:C	1:A:2547:ARG:H	1.85	0.83
1:B:2516:THR:C	1:B:2644:MET:O	2.21	0.83
1:A:2168:PHE:HA	1:A:2175:ALA:HB2	1.60	0.83
1:A:329:PHE:CB	1:A:378:ALA:HB1	2.08	0.83
1:A:750:GLN:O	1:A:792:HIS:N	2.12	0.82
1:A:1560:ASP:HA	1:A:1575:GLN:CB	2.09	0.82
1:B:1377:GLN:CB	1:B:1841:ARG:H	1.91	0.82
1:A:1844:TYR:O	1:A:1848:TYR:CB	2.29	0.81
1:A:396:LEU:O	1:A:400:LEU:N	2.11	0.81
1:A:1164:PRO:CB	1:A:1204:ASP:CA	2.59	0.81
1:A:1246:GLN:HA	1:A:1249:LEU:CB	2.11	0.81
1:A:1483:LEU:O	1:A:1489:GLU:CB	2.29	0.81
1:A:2297:ASP:H	1:A:2314:LEU:CA	1.92	0.80
2:C:647:ALA:CB	2:C:652:TRP:HA	2.10	0.79
1:A:2544:ARG:O	1:A:2547:ARG:N	2.16	0.79
1:B:2473:LEU:CB	1:B:2498:LEU:HA	2.11	0.79
1:B:2516:THR:CA	1:B:2644:MET:O	2.30	0.78
2:C:627:SER:CA	2:C:681:GLN:H	1.95	0.78
1:B:2517:HIS:O	1:B:2521:ASN:N	2.15	0.78
1:B:2520:VAL:O	1:B:2524:GLY:N	2.16	0.78
2:C:647:ALA:HB1	2:C:652:TRP:CA	2.07	0.78
1:B:2237:LEU:CB	1:B:2302:ILE:CB	2.62	0.77
1:B:134:PHE:C	1:B:142:PHE:CA	2.57	0.77
1:A:896:LEU:HA	1:A:904:SER:N	1.99	0.77
1:A:2386:LEU:H	1:A:2482:LEU:HA	1.48	0.77
1:A:2184:LYS:HA	1:A:2371:ASN:CA	2.14	0.76
2:C:741:CYS:O	2:C:745:LEU:CA	2.32	0.76
1:B:2524:GLY:HA2	1:B:2528:THR:CA	2.15	0.76
1:B:813:MET:HA	1:B:817:ASP:CB	2.17	0.75
1:A:2483:PHE:HA	1:A:2490:CYS:CA	2.15	0.74
1:B:330:GLU:HA	1:B:375:ILE:CA	2.17	0.74
1:B:2046:TYR:O	1:B:2050:MET:N	2.18	0.74
1:B:599:ILE:HA	1:B:655:VAL:O	1.86	0.74
2:C:536:HIS:CB	2:C:539:LEU:CB	2.65	0.74
1:B:602:HIS:N	1:B:657:ASN:HA	2.03	0.73
1:B:902:SER:HA	2:D:750:GLN:CB	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:479:LEU:O	2:C:483:GLN:N	2.21	0.73
1:B:2190:ARG:H	1:B:2576:PRO:CB	2.02	0.72
1:A:1045:SER:CB	1:A:1049:LEU:HA	2.19	0.72
1:B:878:ARG:HA	1:B:913:ALA:HB1	1.70	0.72
1:B:2369:PRO:CA	1:B:2375:GLY:CA	2.67	0.72
1:A:1980:VAL:O	1:A:1984:PHE:O	2.06	0.72
1:A:2184:LYS:CA	1:A:2371:ASN:HA	2.17	0.72
1:A:1045:SER:N	1:A:1049:LEU:CB	2.52	0.72
1:A:1487:PHE:CB	1:A:1574:CYS:HA	2.20	0.72
2:D:721:ARG:CB	2:D:765:VAL:HA	2.20	0.72
1:B:1407:TYR:O	1:B:1413:ALA:HB3	1.90	0.71
1:B:2369:PRO:CA	1:B:2375:GLY:HA2	2.13	0.71
1:A:2303:LEU:H	1:A:2309:PRO:N	1.88	0.71
2:D:406:ARG:CB	2:D:574:ASN:HA	2.20	0.71
1:A:2474:GLY:H	1:A:2497:CYS:CB	2.05	0.70
1:A:2187:TYR:CB	1:A:2578:ASN:HA	2.21	0.70
1:B:874:GLY:HA2	1:B:910:GLU:CB	2.22	0.70
1:A:1989:THR:HA	1:A:1999:HIS:CB	2.21	0.70
1:A:896:LEU:HA	1:A:903:VAL:C	2.16	0.70
1:A:1845:GLN:HA	1:A:1848:TYR:CB	2.21	0.70
1:A:2080:ASN:HA	1:A:2083:ILE:CB	2.22	0.70
1:A:2335:ASP:CB	1:A:2495:PHE:CB	2.70	0.69
1:A:1325:SER:HA	1:A:2272:SER:CB	2.22	0.69
1:A:2325:MET:H	1:A:2377:ILE:N	1.88	0.69
1:A:1758:GLY:HA2	1:B:1757:ASN:CB	2.22	0.69
1:B:134:PHE:O	1:B:142:PHE:CB	2.41	0.69
1:B:1332:ILE:O	1:B:1336:VAL:N	2.26	0.69
1:B:2259:LEU:CA	1:B:2292:TYR:HA	2.14	0.69
1:B:2150:CYS:HA	1:B:2577:LEU:CA	2.19	0.68
1:A:1325:SER:HA	1:A:2272:SER:CA	2.23	0.68
1:A:2474:GLY:HA3	1:A:2501:LYS:CB	2.23	0.68
1:B:2516:THR:CB	1:B:2644:MET:O	2.42	0.68
1:B:2021:ILE:O	1:B:2025:TYR:N	2.19	0.68
1:B:1325:SER:HA	1:B:2272:SER:N	2.09	0.67
1:B:603:SER:CB	1:B:656:TYR:H	2.08	0.67
1:B:2259:LEU:HA	1:B:2292:TYR:CA	2.15	0.67
2:C:536:HIS:H	2:C:539:LEU:CB	2.07	0.67
1:A:2313:SER:HA	1:A:2323:ILE:HA	1.77	0.67
1:B:1484:GLY:HA2	1:B:1490:TRP:N	2.09	0.67
1:B:1365:ASP:HA	1:B:1891:GLN:CB	2.26	0.66
1:A:684:SER:HA	1:A:719:HIS:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ALA:HB3	1:A:368:ARG:CA	2.26	0.66
1:B:2237:LEU:H	1:B:2302:ILE:CB	2.09	0.65
2:D:316:LEU:O	2:D:321:LEU:CB	2.44	0.65
1:B:330:GLU:HA	1:B:375:ILE:HA	1.79	0.65
1:A:2325:MET:N	1:A:2377:ILE:H	1.94	0.65
1:A:2368:ILE:H	1:A:2376:ILE:H	1.43	0.65
1:B:2150:CYS:CA	1:B:2577:LEU:HA	2.19	0.65
1:B:343:LYS:O	1:B:347:CYS:N	2.28	0.65
1:A:351:GLN:HA	1:A:355:LYS:CB	2.27	0.65
1:A:2544:ARG:O	1:A:2547:ARG:CA	2.44	0.65
1:B:637:VAL:CB	1:B:670:SER:CB	2.75	0.64
1:A:1045:SER:CA	1:A:1049:LEU:CB	2.74	0.64
1:A:2296:PHE:HA	1:A:2314:LEU:CB	2.26	0.64
1:A:1602:GLU:CA	1:A:1607:SER:HA	2.22	0.64
1:B:113:THR:O	1:B:114:PRO:C	2.39	0.64
1:A:2301:GLU:C	1:A:2310:LYS:HA	2.23	0.64
1:B:1650:ALA:CB	1:B:1654:ALA:HB2	2.11	0.64
2:D:601:PRO:O	2:D:605:LEU:N	2.29	0.63
2:D:734:ASP:CB	2:D:737:PHE:H	2.11	0.63
1:A:979:ALA:HB1	1:A:987:LEU:HA	1.79	0.63
1:A:2386:LEU:N	1:A:2482:LEU:HA	2.12	0.63
1:B:732:PHE:HA	1:B:744:ASN:CB	2.28	0.63
1:B:2186:SER:CB	1:B:2573:SER:H	2.11	0.63
1:A:307:ALA:HB1	1:A:311:ARG:CB	2.28	0.63
1:B:2517:HIS:H	1:B:2644:MET:C	2.05	0.63
2:D:411:CYS:O	2:D:489:SER:HA	1.97	0.63
1:A:708:ALA:HB1	1:A:781:ALA:HB3	1.81	0.63
1:B:1377:GLN:CB	1:B:1841:ARG:N	2.61	0.63
1:B:2323:ILE:O	1:B:2378:GLU:HA	1.98	0.62
2:D:314:ASN:O	2:D:318:LYS:N	2.31	0.62
2:C:741:CYS:O	2:C:745:LEU:CB	2.47	0.62
1:A:708:ALA:CB	1:A:781:ALA:HB3	2.29	0.62
1:B:2481:ILE:HA	1:B:2491:VAL:O	1.98	0.62
2:D:499:GLY:HA2	2:D:536:HIS:C	2.23	0.62
2:C:306:ASN:HA	2:C:393:GLU:HA	1.82	0.62
1:B:2186:SER:CB	1:B:2573:SER:N	2.63	0.62
2:C:613:LEU:HA	2:C:619:LEU:CB	2.29	0.62
1:B:601:SER:O	1:B:654:ALA:HB1	1.99	0.62
2:C:536:HIS:N	2:C:539:LEU:CB	2.62	0.62
1:A:663:SER:HA	1:A:668:ARG:HA	1.82	0.62
1:A:1325:SER:HA	1:A:2272:SER:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2329:LYS:H	1:A:2373:GLU:CB	2.13	0.61
1:A:2294:ALA:H	1:A:2317:SER:HA	1.65	0.61
1:A:2313:SER:HA	1:A:2322:TYR:O	2.01	0.61
2:C:320:PRO:CB	2:C:325:SER:CB	2.79	0.61
1:A:1262:LYS:HA	1:A:1265:LYS:CB	2.31	0.61
1:B:2312:ILE:C	1:B:2323:ILE:CA	2.64	0.61
1:A:2039:HIS:O	1:A:2043:ALA:N	2.27	0.61
1:A:360:GLY:HA2	1:A:363:SER:CB	2.31	0.60
1:B:913:ALA:O	1:B:916:ALA:HB3	2.00	0.60
1:A:2189:MET:H	1:A:2578:ASN:CB	2.15	0.60
1:B:1169:SER:O	1:B:1173:LYS:N	2.28	0.60
1:A:820:VAL:HA	1:A:823:ALA:CB	2.31	0.60
1:B:2337:ARG:O	1:B:2341:PHE:N	2.34	0.60
1:B:134:PHE:CB	1:B:142:PHE:CA	2.78	0.60
1:B:2238:SER:CB	1:B:2299:MET:HA	2.31	0.60
1:A:364:ALA:HB3	1:A:368:ARG:CB	2.32	0.59
1:B:2325:MET:C	1:B:2376:ILE:HA	2.26	0.59
2:C:627:SER:HA	2:C:681:GLN:N	2.00	0.59
1:B:454:VAL:CB	1:B:465:ALA:HB2	2.31	0.59
1:B:2340:GLU:C	1:B:2342:ASN:H	2.08	0.59
1:A:140:ALA:HA	2:C:668:VAL:O	2.02	0.59
1:A:2236:THR:CB	1:A:2300:VAL:H	2.16	0.59
1:A:2239:MET:H	1:A:2298:ASP:CB	2.16	0.59
1:A:820:VAL:HA	1:A:823:ALA:HB3	1.85	0.59
1:A:946:MET:HA	1:A:1009:ALA:CB	2.30	0.59
1:B:876:ILE:O	1:B:880:ALA:HB2	2.03	0.59
1:B:1650:ALA:HB3	1:B:1654:ALA:CB	2.12	0.59
1:B:2326:CYS:HA	1:B:2375:GLY:O	2.03	0.59
2:D:742:VAL:HA	2:D:745:LEU:CB	2.31	0.59
1:B:1479:TYR:HA	1:B:1490:TRP:CB	2.33	0.58
1:A:1768:ASP:HA	1:A:1771:ASN:CB	2.33	0.58
1:B:134:PHE:O	1:B:142:PHE:CA	2.51	0.58
1:B:172:PRO:HA	1:B:195:GLN:CB	2.33	0.58
1:B:453:HIS:HA	1:B:530:VAL:HA	1.83	0.58
1:B:651:TRP:O	1:B:655:VAL:N	2.36	0.58
1:A:1164:PRO:CB	1:A:1204:ASP:N	2.67	0.58
1:A:1432:GLU:HA	1:A:1440:HIS:O	2.03	0.58
1:A:2316:GLY:HA3	1:A:2320:LYS:N	2.18	0.58
1:A:2629:ASP:CB	1:A:2632:LEU:CB	2.81	0.58
1:B:134:PHE:C	1:B:142:PHE:HA	2.27	0.58
1:B:1343:CYS:HA	1:B:1354:CYS:CB	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2524:GLY:HA2	1:B:2528:THR:O	2.04	0.58
1:A:1595:LYS:O	1:A:1598:ALA:HB3	2.04	0.58
1:A:645:ARG:HA	1:A:649:LEU:CB	2.34	0.58
1:A:1607:SER:C	1:A:1609:SER:H	2.10	0.58
1:B:2010:MET:HA	1:B:2016:PHE:CB	2.33	0.58
1:A:223:ARG:C	1:A:225:GLN:H	2.12	0.58
1:A:1045:SER:CB	1:A:1049:LEU:H	2.12	0.58
1:B:1315:GLN:HA	1:B:1879:ASP:CB	2.34	0.58
1:B:1325:SER:HA	1:B:2272:SER:H	1.69	0.58
1:B:2524:GLY:HA2	1:B:2528:THR:C	2.29	0.58
1:B:2129:HIS:C	1:B:2133:LEU:CB	2.73	0.57
2:D:698:TRP:CB	2:D:755:VAL:HA	2.33	0.57
2:C:319:GLN:HA	2:C:328:SER:N	2.14	0.57
2:C:640:THR:CA	2:C:689:ALA:HB2	2.32	0.57
1:B:2325:MET:O	1:B:2376:ILE:HA	2.02	0.57
1:B:922:LEU:CB	1:B:982:PHE:HA	2.33	0.57
1:B:1386:GLY:HA2	1:B:1392:PHE:CB	2.35	0.57
1:A:2328:PRO:HA	1:A:2373:GLU:C	2.30	0.57
1:B:603:SER:H	1:B:654:ALA:HA	1.69	0.57
1:B:2369:PRO:CA	1:B:2375:GLY:HA3	2.35	0.57
1:A:921:LYS:H	1:A:925:PHE:CB	2.17	0.56
1:B:332:GLY:HA3	1:B:378:ALA:HB1	1.86	0.56
1:A:1223:ILE:HA	1:A:1230:THR:CB	2.36	0.56
1:A:1607:SER:C	1:A:1609:SER:N	2.61	0.56
1:B:112:ALA:HB1	1:B:200:GLN:CB	2.35	0.56
1:B:602:HIS:H	1:B:657:ASN:HA	1.71	0.56
1:A:132:PHE:O	1:A:136:SER:N	2.33	0.56
1:A:2602:VAL:CB	1:A:2613:PRO:HA	2.36	0.56
2:C:475:SER:O	2:C:478:ALA:HB3	2.06	0.56
1:A:1430:CYS:C	1:A:1440:HIS:HA	2.31	0.56
1:B:2369:PRO:CB	1:B:2375:GLY:HA3	2.36	0.56
1:A:1416:SER:O	1:A:1420:ALA:N	2.34	0.56
1:B:2184:LYS:CB	1:B:2372:ASP:H	2.19	0.56
1:B:603:SER:HA	1:B:656:TYR:CB	2.36	0.55
1:B:1408:ALA:HA	1:B:1414:GLN:HA	1.88	0.55
1:A:2460:SER:CB	1:A:2489:GLU:HA	2.36	0.55
1:A:904:SER:HA	1:A:907:ALA:HB3	1.88	0.55
1:B:1893:SER:H	1:B:1897:LYS:CB	2.19	0.55
1:B:2134:ALA:HB3	1:B:2137:GLN:CB	2.36	0.55
1:A:2293:ILE:HA	1:A:2317:SER:CB	2.37	0.55
1:A:2134:ALA:HB3	1:A:2137:GLN:CB	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:979:ALA:CB	1:B:987:LEU:H	2.18	0.55
2:C:319:GLN:CA	2:C:328:SER:H	2.18	0.55
1:B:389:ALA:HB1	1:B:393:LEU:CA	2.36	0.55
1:B:2313:SER:N	1:B:2323:ILE:CB	2.71	0.54
1:A:595:SER:O	1:A:596:LEU:C	2.50	0.54
1:A:1388:GLU:O	1:A:1393:ALA:HB2	2.07	0.54
1:A:1631:ARG:O	1:A:1635:LEU:N	2.34	0.54
2:D:695:HIS:HA	2:D:751:VAL:CB	2.37	0.54
1:A:717:THR:HA	1:A:751:HIS:C	2.33	0.54
1:B:2130:THR:HA	1:B:2133:LEU:CB	2.37	0.54
1:A:1430:CYS:HA	1:A:1439:GLY:C	2.32	0.54
1:B:138:SER:CB	1:B:141:ILE:H	2.20	0.54
1:A:1633:LEU:O	1:A:1636:ILE:O	2.25	0.54
1:A:393:LEU:HA	1:A:396:LEU:CB	2.38	0.53
1:A:896:LEU:CB	1:A:904:SER:HA	2.39	0.53
1:B:652:ARG:HA	1:B:655:VAL:CB	2.38	0.53
1:A:1758:GLY:HA3	1:B:1754:THR:HA	1.90	0.53
2:C:475:SER:O	2:C:479:LEU:N	2.41	0.53
1:A:2385:GLY:HA2	1:A:2482:LEU:CB	2.39	0.53
2:D:306:ASN:CB	2:D:393:GLU:CA	2.81	0.53
1:A:821:ARG:N	1:A:823:ALA:HB3	2.24	0.53
1:B:2236:THR:CA	1:B:2301:GLU:HA	2.30	0.53
1:A:2316:GLY:C	1:A:2319:GLY:H	2.17	0.53
1:A:1185:LYS:CB	1:A:1189:PRO:CB	2.86	0.53
1:A:1596:PHE:O	1:A:1599:LEU:C	2.51	0.53
1:B:1387:VAL:H	1:B:1392:PHE:CB	2.21	0.53
1:A:140:ALA:CB	2:C:670:SER:HA	2.31	0.52
1:B:455:ASP:HA	1:B:464:SER:O	2.09	0.52
1:B:894:HIS:O	1:B:898:SER:N	2.42	0.52
1:B:2483:PHE:HA	1:B:2489:GLU:O	2.10	0.52
2:D:471:LEU:O	2:D:472:GLU:C	2.53	0.52
1:A:1484:GLY:HA2	1:A:1490:TRP:CB	2.39	0.52
1:B:2188:PRO:N	1:B:2573:SER:HA	2.25	0.52
1:B:2311:LYS:HA	1:B:2324:MET:O	2.09	0.52
2:C:640:THR:HA	2:C:689:ALA:CB	2.33	0.52
1:A:2311:LYS:CB	1:A:2325:MET:HA	2.40	0.52
1:B:2047:ASP:O	1:B:2051:PRO:N	2.43	0.52
1:A:1241:ASN:CB	1:A:1245:VAL:CB	2.88	0.52
1:B:409:GLU:O	1:B:410:GLU:C	2.53	0.52
1:A:2168:PHE:CA	1:A:2175:ALA:HB2	2.36	0.52
1:B:2564:GLU:HA	1:B:2583:VAL:CB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:LEU:O	1:A:395:PRO:CB	2.58	0.51
1:A:945:GLN:CB	1:A:1010:ALA:HA	2.40	0.51
1:B:134:PHE:CA	1:B:142:PHE:HA	2.40	0.51
1:B:1315:GLN:CA	1:B:1879:ASP:HA	2.40	0.51
1:B:2340:GLU:C	1:B:2342:ASN:N	2.68	0.51
1:A:659:ALA:HB1	1:A:671:CYS:HA	1.91	0.51
1:B:2236:THR:HA	1:B:2301:GLU:CA	2.30	0.51
2:D:728:HIS:CB	2:D:772:ALA:HB2	2.41	0.51
1:A:1750:SER:H	1:B:1727:GLN:CB	2.23	0.51
1:B:2524:GLY:CA	1:B:2528:THR:CA	2.67	0.51
1:A:1045:SER:C	1:A:1049:LEU:H	2.19	0.51
2:D:398:GLY:HA3	2:D:412:GLN:CB	2.40	0.51
1:A:2294:ALA:N	1:A:2317:SER:HA	2.25	0.51
1:A:1596:PHE:O	1:A:1599:LEU:N	2.44	0.51
1:A:1645:SER:CB	1:A:1654:ALA:HA	2.40	0.51
1:B:2144:GLN:O	1:B:2146:ILE:N	2.44	0.51
2:C:625:SER:HA	2:C:680:CYS:CB	2.41	0.50
1:A:1429:ASP:O	1:A:1439:GLY:HA3	2.11	0.50
1:B:1484:GLY:HA2	1:B:1490:TRP:CA	2.41	0.50
1:B:2187:TYR:H	1:B:2572:HIS:C	2.19	0.50
2:D:471:LEU:O	2:D:475:SER:N	2.36	0.50
1:A:227:LEU:O	1:A:231:GLN:N	2.36	0.50
2:D:319:GLN:C	2:D:321:LEU:N	2.69	0.50
1:A:1359:GLY:HA3	1:A:1858:CYS:CB	2.41	0.50
1:A:2467:VAL:CB	1:A:2471:LEU:CB	2.89	0.50
1:B:301:THR:HA	1:B:305:PHE:CB	2.40	0.50
1:B:2314:LEU:O	1:B:2321:PHE:HA	2.12	0.50
1:A:1486:ASN:CB	1:A:1489:GLU:CB	2.90	0.50
2:D:405:ARG:HA	2:D:576:SER:HA	1.94	0.50
1:B:323:GLU:HA	1:B:326:CYS:CB	2.42	0.50
2:D:318:LYS:HA	2:C:383:PHE:CB	2.42	0.50
1:A:717:THR:HA	1:A:751:HIS:O	2.12	0.50
1:A:945:GLN:O	1:A:1009:ALA:HB1	2.11	0.50
1:A:979:ALA:CB	1:A:987:LEU:HA	2.40	0.50
1:A:2313:SER:CA	1:A:2323:ILE:HA	2.41	0.49
1:A:2326:CYS:HA	1:A:2375:GLY:O	2.12	0.49
1:A:2516:THR:CB	1:A:2643:TYR:HA	2.42	0.49
1:A:375:ILE:O	1:A:378:ALA:HB3	2.13	0.49
1:A:821:ARG:HA	1:A:824:PHE:CB	2.42	0.49
1:A:829:LYS:CB	1:A:879:ALA:HB2	2.42	0.49
1:A:1261:LEU:O	1:A:1264:ILE:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:328:SER:H	2:D:331:HIS:CB	2.25	0.49
1:A:708:ALA:HB1	1:A:781:ALA:C	2.38	0.49
1:A:821:ARG:C	1:A:825:SER:H	2.19	0.49
2:C:715:ARG:O	2:C:719:CYS:N	2.43	0.49
1:A:2384:ALA:HB3	1:A:2483:PHE:O	2.13	0.49
1:A:1288:SER:O	1:A:1291:ALA:HB3	2.12	0.49
1:B:2484:ASP:H	1:B:2489:GLU:H	1.60	0.49
2:D:471:LEU:O	2:D:474:PHE:N	2.46	0.49
1:A:900:SER:O	1:A:901:ALA:HB3	2.13	0.49
1:B:1315:GLN:CB	1:B:1879:ASP:HA	2.43	0.49
1:A:717:THR:CB	1:A:752:GLU:CB	2.91	0.48
1:A:1261:LEU:O	1:A:1264:ILE:N	2.45	0.48
1:A:2483:PHE:HA	1:A:2490:CYS:CB	2.42	0.48
1:B:320:MET:HA	1:B:323:GLU:CB	2.43	0.48
2:D:499:GLY:HA2	2:D:537:PRO:N	2.28	0.48
1:A:1164:PRO:HA	1:A:1204:ASP:H	1.78	0.48
1:A:1483:LEU:O	1:A:1490:TRP:N	2.46	0.48
1:A:2134:ALA:HB3	1:A:2137:GLN:H	1.78	0.48
1:B:308:GLU:O	1:B:309:ALA:HB3	2.12	0.48
1:B:2484:ASP:O	1:B:2488:GLY:HA2	2.13	0.48
2:D:413:LEU:CB	2:D:489:SER:CB	2.92	0.48
1:A:2301:GLU:O	1:A:2310:LYS:HA	2.13	0.48
1:B:680:GLN:HA	1:B:722:PHE:CB	2.43	0.48
1:B:2312:ILE:O	1:B:2323:ILE:HA	2.10	0.48
2:D:496:LEU:HA	2:D:536:HIS:CB	2.40	0.48
1:B:1314:ASN:CB	1:B:1318:LEU:CB	2.92	0.48
1:A:1953:ALA:HB2	1:A:1982:LEU:CB	2.43	0.48
1:B:1006:ALA:HB1	1:B:1011:SER:H	1.78	0.48
1:B:2054:THR:CB	1:B:2058:MET:H	2.26	0.48
2:D:636:TYR:CB	2:D:686:VAL:HA	2.44	0.48
1:A:110:ILE:O	1:A:116:CYS:CB	2.62	0.48
1:A:1283:THR:O	1:A:1287:LEU:N	2.41	0.48
1:A:2544:ARG:C	1:A:2547:ARG:N	2.60	0.48
1:A:727:SER:N	1:A:742:CYS:CB	2.77	0.48
1:A:2323:ILE:O	1:A:2378:GLU:HA	2.13	0.48
1:A:2327:LYS:H	1:A:2375:GLY:H	1.61	0.48
2:D:395:SER:CB	2:D:413:LEU:HA	2.43	0.48
1:A:726:SER:O	1:A:743:ARG:C	2.56	0.48
1:A:1365:ASP:HA	1:A:1891:GLN:CB	2.44	0.48
1:B:143:GLY:O	1:B:144:VAL:C	2.56	0.48
2:C:499:GLY:HA2	2:C:536:HIS:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2368:ILE:O	1:A:2375:GLY:HA2	2.14	0.47
1:B:389:ALA:HB1	1:B:393:LEU:HA	1.97	0.47
1:A:364:ALA:CB	1:A:368:ARG:N	2.77	0.47
1:B:263:ALA:O	1:B:266:ALA:HB2	2.14	0.47
1:B:395:PRO:O	1:B:398:ALA:HB3	2.14	0.47
1:B:2184:LYS:CB	1:B:2372:ASP:N	2.77	0.47
1:A:1083:ILE:CB	1:A:1154:SER:HA	2.44	0.47
1:A:1774:ARG:O	1:A:1777:ALA:HB3	2.13	0.47
1:B:2236:THR:HA	1:B:2302:ILE:H	1.79	0.47
1:A:396:LEU:HA	1:A:399:ALA:HB3	1.96	0.47
1:A:718:LEU:N	1:A:751:HIS:O	2.48	0.47
1:A:1086:HIS:CB	1:A:1090:VAL:CB	2.92	0.47
1:A:1383:PHE:O	1:A:1384:VAL:C	2.58	0.47
1:A:1479:TYR:CB	1:A:1554:ALA:HB1	2.44	0.47
1:A:2313:SER:HA	1:A:2322:TYR:C	2.40	0.47
1:B:1501:LYS:CB	1:B:1540:CYS:HA	2.45	0.47
1:A:216:ILE:O	1:A:220:VAL:N	2.44	0.47
1:A:1261:LEU:O	1:A:1264:ILE:CA	2.63	0.47
2:D:496:LEU:O	2:D:536:HIS:HA	2.15	0.46
1:B:2237:LEU:N	1:B:2302:ILE:CB	2.77	0.46
1:B:330:GLU:HA	1:B:375:ILE:N	2.30	0.46
1:A:1397:LEU:O	1:A:1401:THR:N	2.43	0.46
1:A:1862:HIS:HA	1:A:1879:ASP:N	2.31	0.46
1:B:389:ALA:CB	1:B:393:LEU:CB	2.92	0.46
1:B:817:ASP:CB	1:B:821:ARG:CB	2.93	0.46
1:B:2294:ALA:HB3	1:B:2315:LYS:O	2.16	0.46
1:A:243:LYS:H	1:A:290:LEU:CB	2.29	0.46
1:A:2593:LEU:O	1:A:2597:GLN:N	2.46	0.46
1:A:1018:GLY:HA3	1:A:1025:ARG:CB	2.46	0.46
1:A:1600:LYS:H	1:A:1614:VAL:CB	2.29	0.46
1:B:1249:LEU:CB	1:B:1270:GLU:CB	2.92	0.46
1:B:1717:ASP:O	1:B:1718:ALA:HB3	2.15	0.46
1:A:494:ALA:O	1:A:495:VAL:CB	2.63	0.46
1:A:824:PHE:O	1:A:828:ILE:CB	2.64	0.46
1:B:1774:ARG:O	1:B:1777:ALA:HB3	2.16	0.46
2:C:329:LEU:C	2:C:333:LEU:H	2.24	0.46
1:A:2327:LYS:CB	1:A:2375:GLY:HA3	2.45	0.46
1:B:722:PHE:C	1:B:748:THR:HA	2.41	0.46
1:A:1895:ARG:O	1:A:1896:ALA:HB3	2.17	0.45
1:B:599:ILE:CB	1:B:655:VAL:HA	2.45	0.45
2:D:496:LEU:C	2:D:536:HIS:HA	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ARG:C	1:A:225:GLN:N	2.74	0.45
1:A:930:LYS:CB	1:A:934:CYS:CB	2.94	0.45
1:A:1843:SER:O	1:A:1847:GLY:N	2.37	0.45
1:B:2134:ALA:HB3	1:B:2137:GLN:H	1.80	0.45
2:D:306:ASN:CB	2:D:393:GLU:CB	2.94	0.45
1:B:900:SER:O	1:B:901:ALA:HB3	2.16	0.45
1:A:1167:VAL:CB	1:A:1171:ARG:CB	2.95	0.45
1:A:2293:ILE:HA	1:A:2317:SER:CA	2.46	0.45
2:D:320:PRO:O	2:D:325:SER:O	2.35	0.45
1:A:2523:MET:CB	1:A:2528:THR:HA	2.47	0.45
1:A:491:GLU:O	1:A:494:ALA:HB3	2.16	0.45
2:C:536:HIS:CB	2:C:539:LEU:H	2.30	0.45
1:A:2243:PHE:CB	1:A:2247:LYS:CB	2.95	0.45
2:C:536:HIS:CA	2:C:539:LEU:CB	2.94	0.45
1:A:821:ARG:CA	1:A:824:PHE:H	2.30	0.44
1:B:1893:SER:CB	1:B:1896:ALA:H	2.29	0.44
1:B:2022:MET:O	1:B:2026:LYS:N	2.37	0.44
1:A:1602:GLU:O	1:A:1604:CYS:N	2.51	0.44
1:B:1834:LEU:O	1:B:1837:ALA:HB3	2.17	0.44
2:C:496:LEU:HA	2:C:536:HIS:CB	2.47	0.44
1:B:1288:SER:O	1:B:1291:ALA:HB3	2.18	0.44
1:A:2259:LEU:HA	1:A:2292:TYR:CB	2.41	0.44
1:B:2284:GLU:O	1:B:2285:PRO:C	2.59	0.44
1:A:1483:LEU:O	1:A:1489:GLU:C	2.61	0.43
1:B:242:PRO:C	1:B:246:SER:H	2.26	0.43
1:A:2434:PRO:HA	1:A:2518:ASN:N	2.33	0.43
1:B:722:PHE:O	1:B:748:THR:HA	2.18	0.43
1:A:229:LEU:O	1:A:233:GLY:N	2.50	0.43
1:A:544:LEU:O	1:A:548:ARG:N	2.45	0.43
1:A:1928:ALA:O	1:A:1931:ALA:HB3	2.17	0.43
1:B:601:SER:H	1:B:657:ASN:CB	2.31	0.43
1:B:2153:HIS:O	1:B:2154:ASP:CB	2.66	0.43
1:A:1487:PHE:CB	1:A:1577:SER:CB	2.97	0.43
1:B:2185:SER:C	1:B:2572:HIS:CB	2.91	0.43
1:B:330:GLU:O	1:B:378:ALA:HB2	2.18	0.43
1:B:389:ALA:HB3	1:B:393:LEU:CB	2.48	0.43
1:B:731:PRO:N	1:B:743:ARG:H	2.16	0.43
1:A:2134:ALA:CB	1:A:2137:GLN:H	2.32	0.43
1:B:368:ARG:O	1:B:372:VAL:N	2.51	0.43
1:B:389:ALA:O	1:B:392:LEU:CB	2.66	0.43
1:B:1294:HIS:CB	1:B:1300:ARG:CB	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1925:LEU:O	1:B:1928:ALA:HB3	2.18	0.43
1:A:1984:PHE:O	1:A:1985:PRO:C	2.61	0.42
1:B:2428:LEU:O	1:B:2432:HIS:N	2.39	0.42
1:A:2370:LEU:CB	1:A:2374:CYS:CB	2.97	0.42
1:B:634:SER:HA	1:B:670:SER:CB	2.48	0.42
1:A:364:ALA:HB3	1:A:368:ARG:HA	2.02	0.42
1:A:820:VAL:CA	1:A:823:ALA:HB3	2.50	0.42
1:A:1969:VAL:O	1:A:1972:ALA:HB3	2.19	0.42
1:A:2313:SER:HA	1:A:2323:ILE:CA	2.48	0.42
1:A:2301:GLU:H	1:A:2311:LYS:H	1.66	0.42
1:B:1949:GLU:O	1:B:1950:SER:C	2.62	0.42
1:B:2516:THR:HA	1:B:2644:MET:O	2.17	0.42
2:C:624:CYS:HA	2:C:633:LEU:N	2.34	0.42
1:A:2168:PHE:CB	1:A:2175:ALA:HB2	2.49	0.42
1:B:1431:ARG:O	1:B:1440:HIS:HA	2.19	0.42
1:A:135:LYS:HA	1:A:138:SER:O	2.20	0.42
1:B:1315:GLN:HA	1:B:1879:ASP:HA	2.02	0.42
1:B:2236:THR:HA	1:B:2302:ILE:N	2.35	0.42
1:B:2237:LEU:H	1:B:2302:ILE:N	2.18	0.42
1:B:2462:ALA:HB1	1:B:2536:CYS:CB	2.49	0.42
1:A:727:SER:HA	1:A:742:CYS:HA	2.01	0.42
1:A:708:ALA:HB1	1:A:781:ALA:CB	2.48	0.42
1:B:330:GLU:HA	1:B:375:ILE:CB	2.50	0.42
1:B:2048:LYS:O	1:B:2049:LEU:C	2.59	0.42
1:B:870:ILE:CB	1:B:906:ALA:HB3	2.50	0.42
1:B:1400:LEU:HA	1:B:1404:TYR:CB	2.50	0.42
1:B:2240:SER:HA	1:B:2247:LYS:CB	2.49	0.42
1:B:2315:LYS:HA	1:B:2321:PHE:CB	2.49	0.42
1:A:263:ALA:O	1:A:266:ALA:HB2	2.20	0.42
1:A:1083:ILE:CB	1:A:1154:SER:CB	2.98	0.42
1:B:304:PRO:HA	1:B:308:GLU:HA	2.02	0.42
1:B:453:HIS:CB	1:B:531:VAL:H	2.33	0.41
1:B:945:GLN:N	1:B:1010:ALA:HB2	2.35	0.41
2:C:320:PRO:HA	2:C:328:SER:N	2.35	0.41
2:C:479:LEU:O	2:C:482:LEU:CB	2.68	0.41
1:B:318:LEU:HA	1:B:362:GLU:CB	2.50	0.41
1:B:2036:GLU:CB	1:B:2078:TYR:CB	2.98	0.41
1:B:2185:SER:CB	1:B:2572:HIS:CB	2.98	0.41
1:B:2186:SER:CB	1:B:2573:SER:CA	2.98	0.41
1:B:1775:VAL:O	1:B:1778:ALA:HB3	2.20	0.41
2:C:627:SER:H	2:C:680:CYS:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1325:SER:CA	1:A:2272:SER:HA	2.49	0.41
1:B:134:PHE:O	1:B:142:PHE:N	2.53	0.41
1:B:245:LYS:O	1:B:248:ALA:HB3	2.19	0.41
1:A:1607:SER:O	1:A:1609:SER:N	2.54	0.41
1:B:364:ALA:HB3	1:B:367:VAL:CB	2.51	0.41
1:B:1250:HIS:HA	1:B:1271:TYR:HA	0.67	0.41
2:D:395:SER:CB	2:D:413:LEU:CA	2.99	0.41
1:A:406:GLU:O	1:A:410:GLU:CB	2.69	0.41
1:A:1314:ASN:HA	1:A:1318:LEU:CB	2.50	0.41
1:A:1314:ASN:O	1:A:1315:GLN:C	2.62	0.41
1:A:1504:HIS:CB	1:A:1508:SER:CB	2.99	0.41
1:A:1990:PRO:CB	1:A:1995:ASN:CB	2.98	0.41
1:B:1326:GLU:N	1:B:2272:SER:HA	2.36	0.41
1:B:465:ALA:O	1:B:466:LEU:C	2.63	0.41
1:B:2332:LEU:CB	1:B:2369:PRO:CB	2.99	0.41
1:A:2332:LEU:HA	1:A:2335:ASP:CB	2.51	0.40
1:A:2368:ILE:CB	1:A:2376:ILE:CB	2.99	0.40
1:A:2467:VAL:C	1:A:2471:LEU:H	2.29	0.40
1:A:751:HIS:C	1:A:792:HIS:O	2.64	0.40
1:A:2259:LEU:HA	1:A:2292:TYR:HA	0.70	0.40
1:A:2521:ASN:O	1:A:2524:GLY:N	2.54	0.40
1:B:2277:HIS:O	1:B:2278:ALA:HB3	2.22	0.40
2:C:479:LEU:HA	2:C:482:LEU:CB	2.52	0.40
1:A:364:ALA:HB3	1:A:368:ARG:N	2.34	0.40
1:A:1310:THR:O	1:A:1314:ASN:N	2.54	0.40
2:D:413:LEU:O	2:D:416:ALA:HB2	2.21	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	2348/2644 (89%)	2197 (94%)	104 (4%)	47 (2%)	6 31
1	B	2124/2644 (80%)	1992 (94%)	98 (5%)	34 (2%)	8 38
2	C	333/791 (42%)	324 (97%)	9 (3%)	0	100 100
2	D	319/791 (40%)	303 (95%)	12 (4%)	4 (1%)	10 42
All	All	5124/6870 (75%)	4816 (94%)	223 (4%)	85 (2%)	10 36

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	PRO
1	A	495	VAL
1	A	530	VAL
1	A	596	LEU
1	A	731	PRO
1	A	764	LYS
1	A	776	SER
1	A	777	PRO
1	A	931	LYS
1	A	984	PHE
1	A	985	PRO
1	A	1600	LYS
1	A	1605	PRO
1	A	1621	VAL
1	A	1730	PRO
1	A	2433	PRO
1	A	2512	PRO
1	B	114	PRO
1	B	144	VAL
1	B	242	PRO
1	B	304	PRO
1	B	358	PRO
1	B	466	LEU
1	B	715	VAL
1	B	815	ASP
1	B	816	PRO
1	B	984	PHE
1	B	985	PRO
1	B	1008	PRO
1	B	1167	VAL
1	B	1256	PRO
1	B	2525	PRO
2	D	323	PRO

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Mol	Chain	Res	Type
2	D	618	GLN
2	D	620	ALA
1	A	644	PRO
1	A	1384	VAL
1	A	1463	LYS
1	A	1603	LYS
1	A	2238	SER
1	B	2145	LEU
1	B	2488	GLY
1	B	2508	PRO
1	A	172	PRO
1	A	226	GLU
1	A	357	VAL
1	A	599	ILE
1	A	1431	ARG
1	A	1477	PRO
1	A	1527	TYR
1	A	2508	PRO
1	A	2634	CYS
1	B	193	PRO
1	B	731	PRO
1	B	1637	PRO
1	B	1730	PRO
1	B	1839	PHE
1	B	1990	PRO
1	B	2061	GLN
1	B	2287	PRO
1	A	578	VAL
1	A	691	ILE
1	A	715	VAL
1	A	815	ASP
1	A	901	ALA
1	A	903	VAL
1	A	964	VAL
1	A	1083	ILE
1	A	1325	SER
1	A	1608	LYS
1	A	2309	PRO
1	A	2494	ASP
1	B	309	ALA
1	B	714	LEU
1	B	1145	ILE

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Mol	Chain	Res	Type
1	B	1324	ASP
1	B	1816	ILE
1	A	1601	ALA
1	A	1637	PRO
1	B	372	VAL
1	B	2154	ASP
2	D	320	PRO
1	A	2314	LEU
1	B	2642	PRO
1	A	220	VAL

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	AGS	A	2701	-	26,33,33	0.82	1 (3%)	26,52,52	0.72	1 (3%)
3	AGS	B	2701	-	26,33,33	0.83	1 (3%)	26,52,52	0.73	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGS	A	2701	-	-	6/17/38/38	0/3/3/3
3	AGS	B	2701	-	-	6/17/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2701	AGS	PG-S1G	2.18	1.95	1.90
3	A	2701	AGS	PG-S1G	2.14	1.95	1.90

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2701	AGS	C5-C6-N6	2.20	123.70	120.35
3	A	2701	AGS	C5-C6-N6	2.17	123.65	120.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

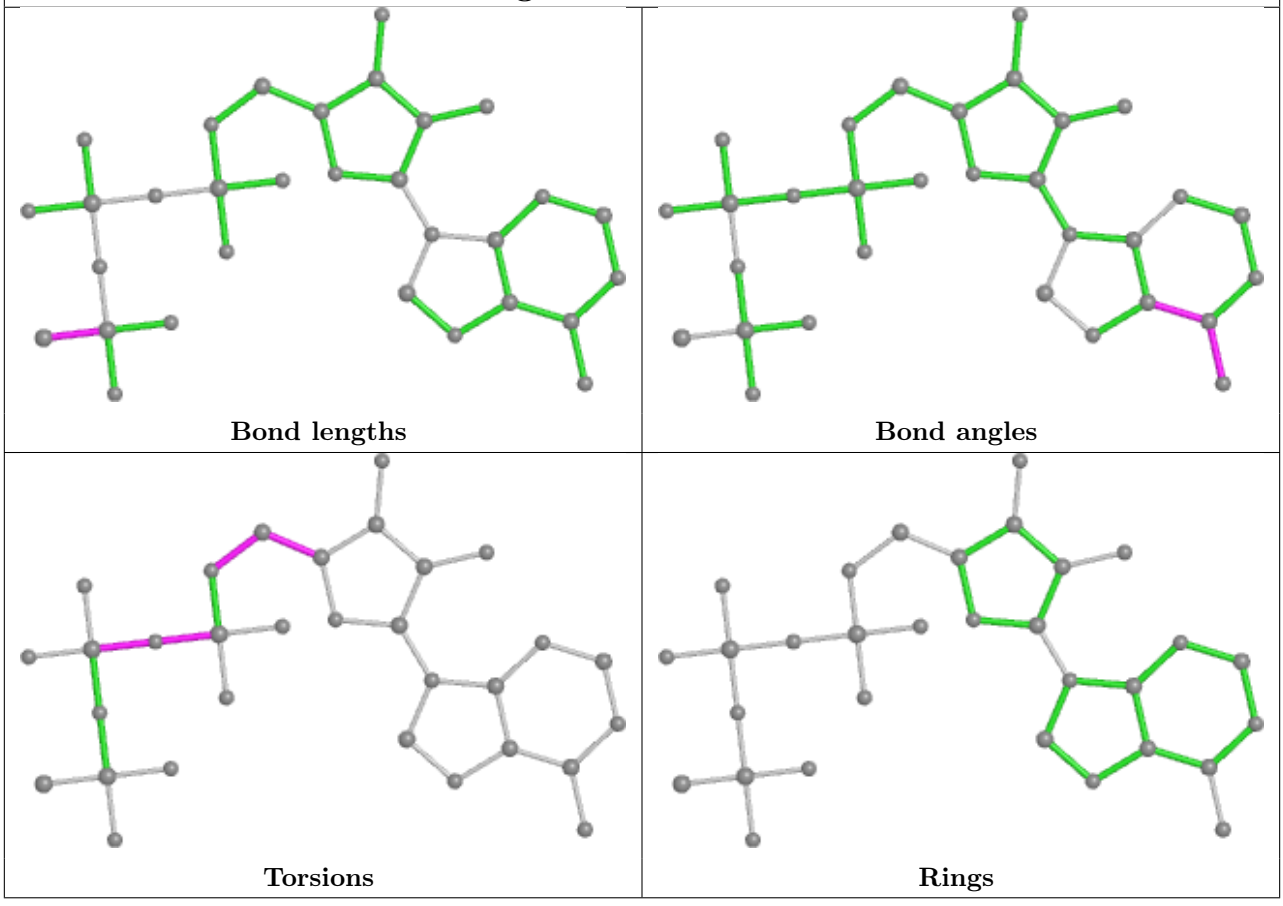
Mol	Chain	Res	Type	Atoms
3	A	2701	AGS	PB-O3A-PA-O5'
3	B	2701	AGS	C5'-O5'-PA-O2A
3	B	2701	AGS	C5'-O5'-PA-O3A
3	B	2701	AGS	O4'-C4'-C5'-O5'
3	A	2701	AGS	O4'-C4'-C5'-O5'
3	A	2701	AGS	C3'-C4'-C5'-O5'
3	B	2701	AGS	C3'-C4'-C5'-O5'
3	B	2701	AGS	C4'-C5'-O5'-PA
3	B	2701	AGS	PB-O3A-PA-O5'
3	A	2701	AGS	PA-O3A-PB-O2B
3	A	2701	AGS	C4'-C5'-O5'-PA
3	A	2701	AGS	PA-O3A-PB-O1B

There are no ring outliers.

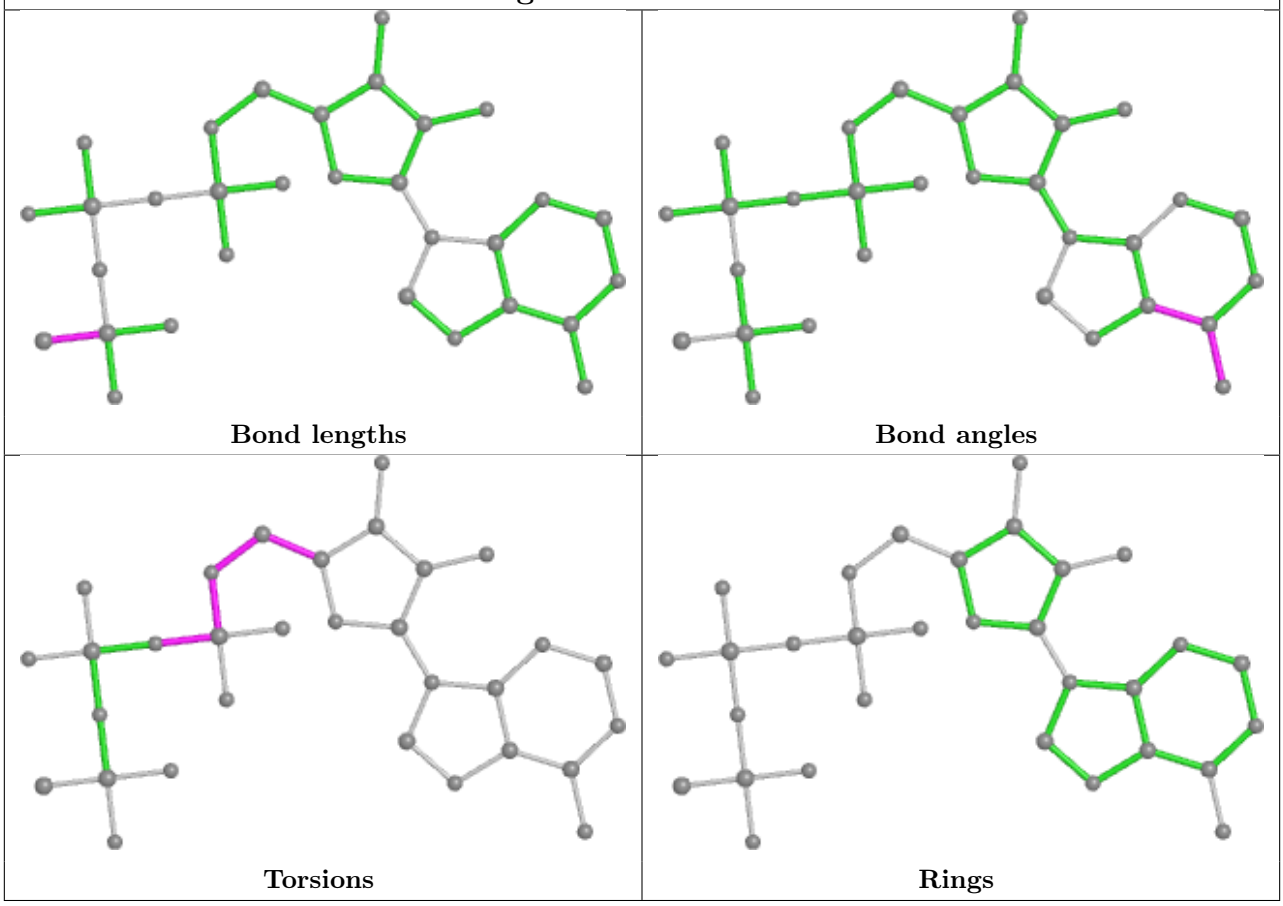
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand AGS A 2701



Ligand AGS B 2701



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.

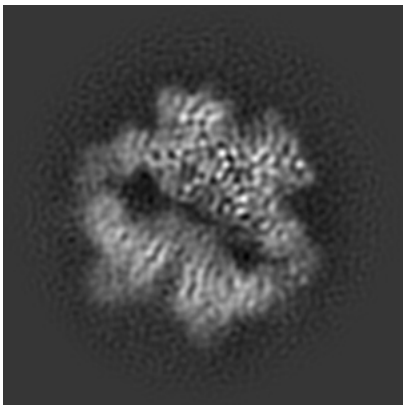
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-62812. These allow visual inspection of the internal detail of the map and identification of artifacts.

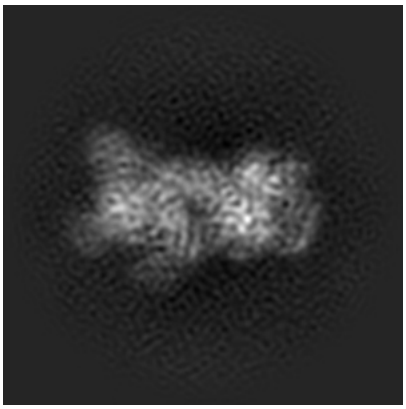
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

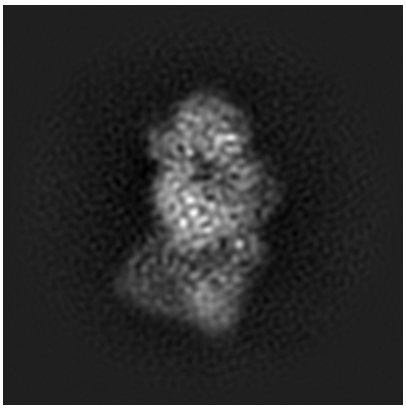
6.1.1 Primary map



X

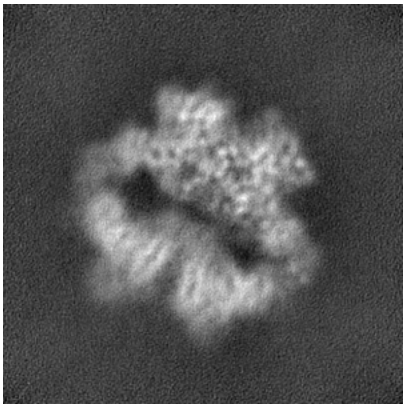


Y

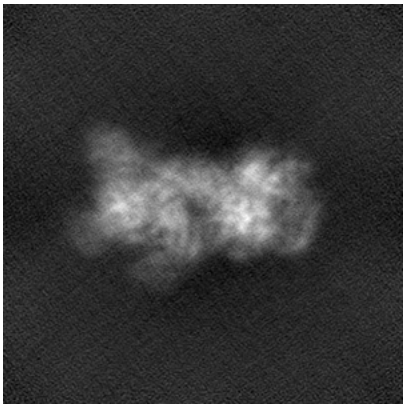


Z

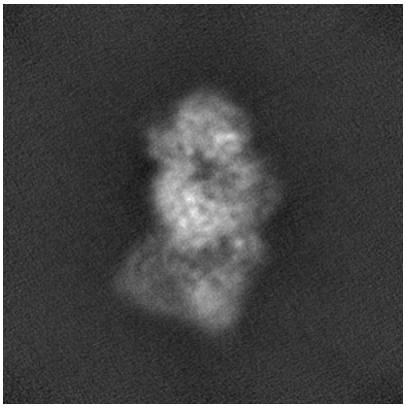
6.1.2 Raw map



X



Y

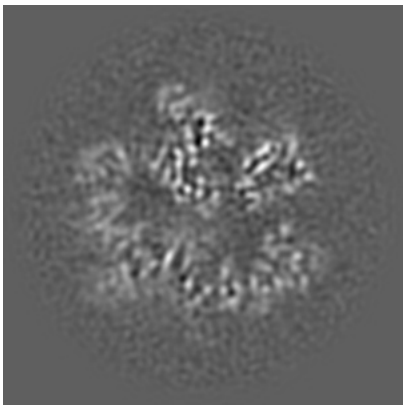


Z

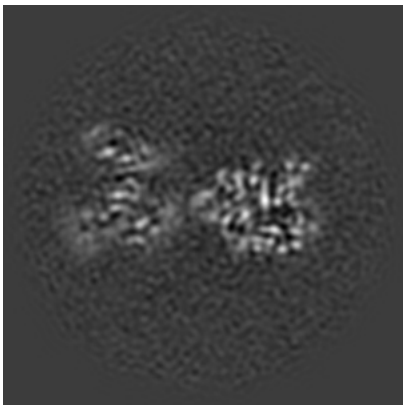
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

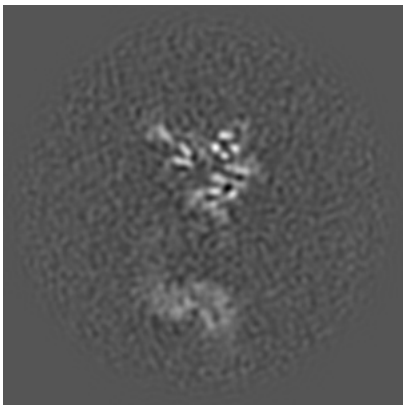
6.2.1 Primary map



X Index: 144

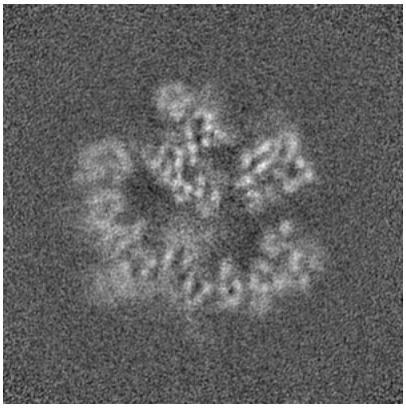


Y Index: 144

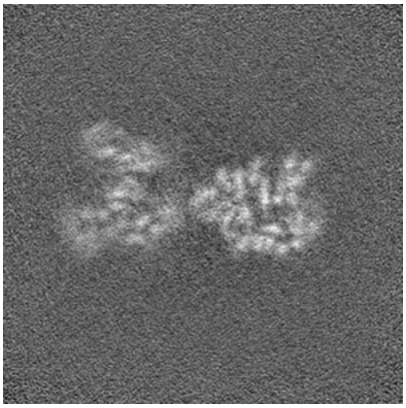


Z Index: 144

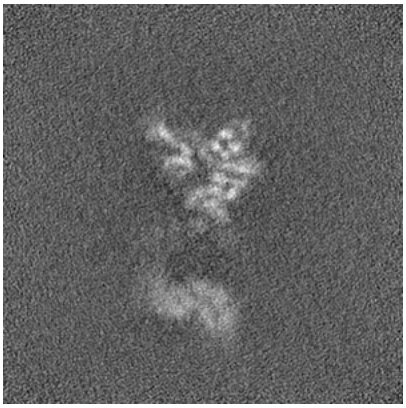
6.2.2 Raw map



X Index: 144



Y Index: 144

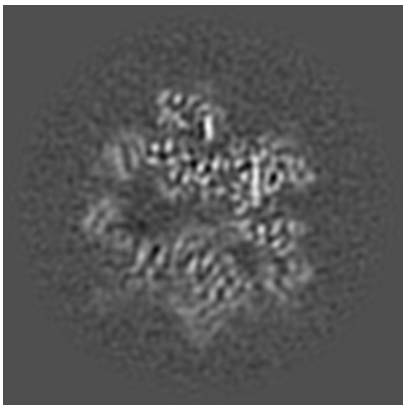


Z Index: 144

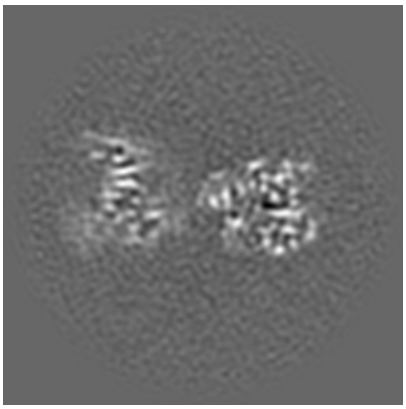
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

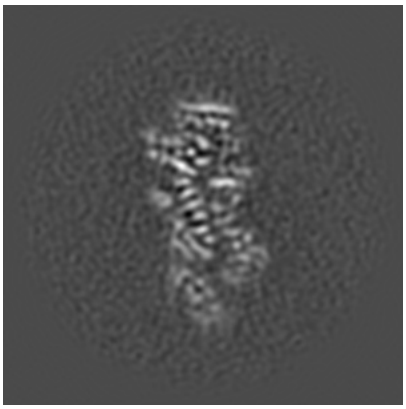
6.3.1 Primary map



X Index: 133

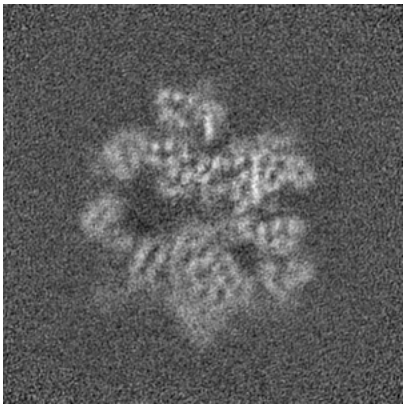


Y Index: 140

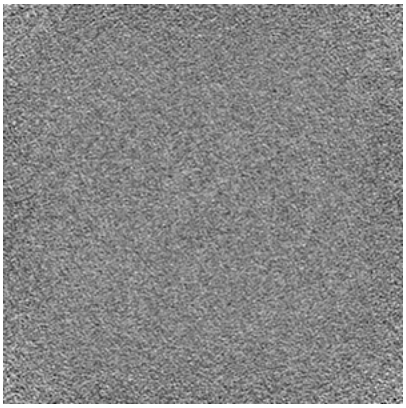


Z Index: 173

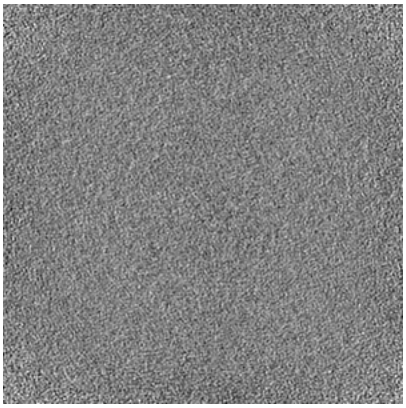
6.3.2 Raw map



X Index: 133



Y Index: 0

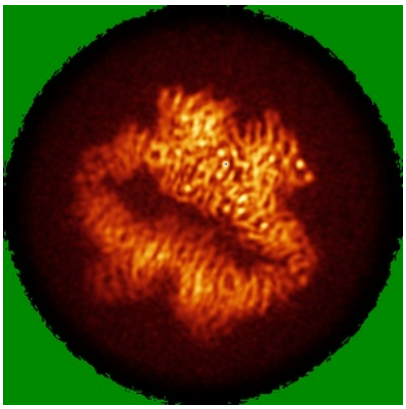


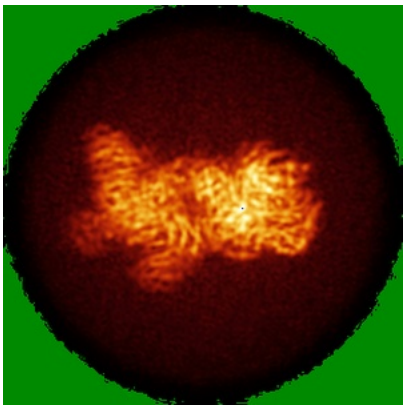
Z Index: 0

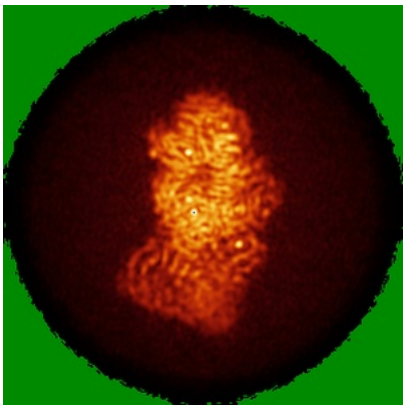
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

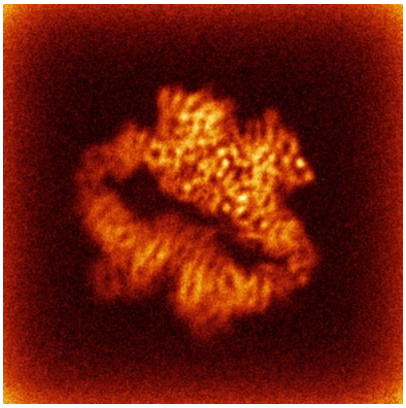
6.4.1 Primary map

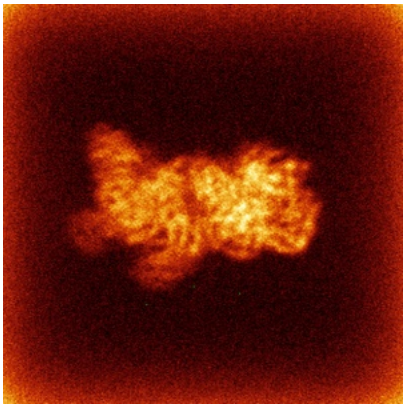

X

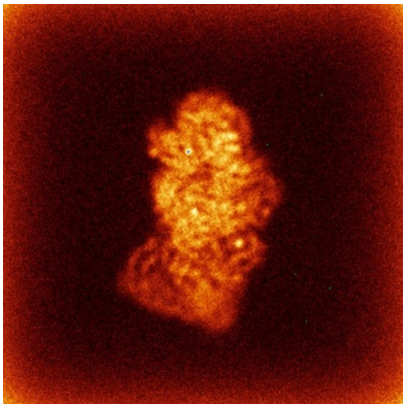

Y


Z

6.4.2 Raw map


X

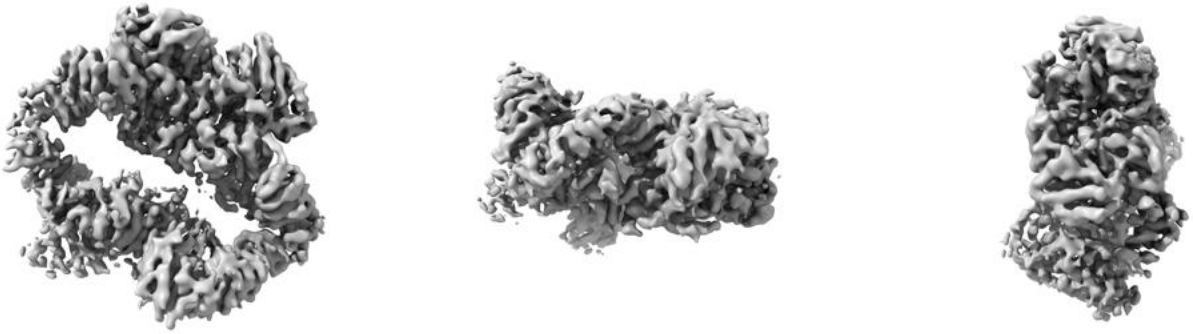

Y


Z

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

6.5 Orthogonal surface views (i)

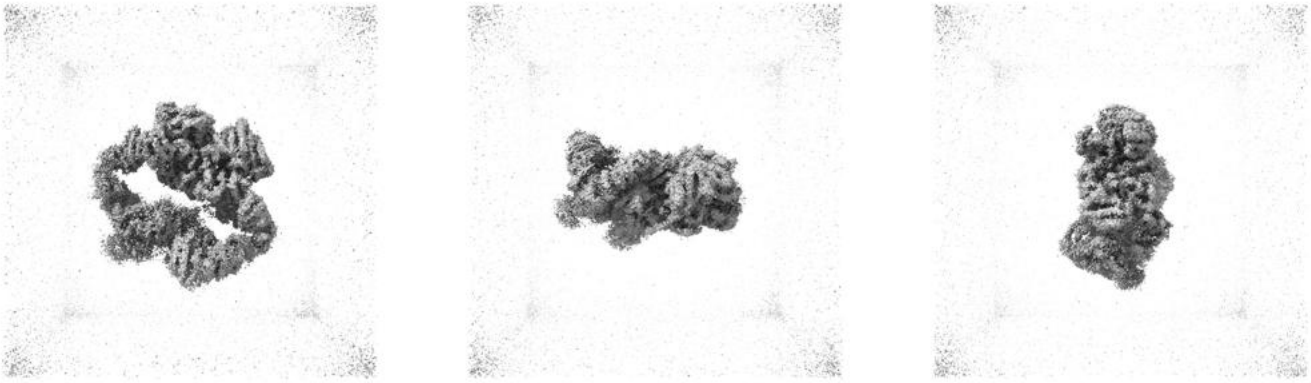
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.27. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

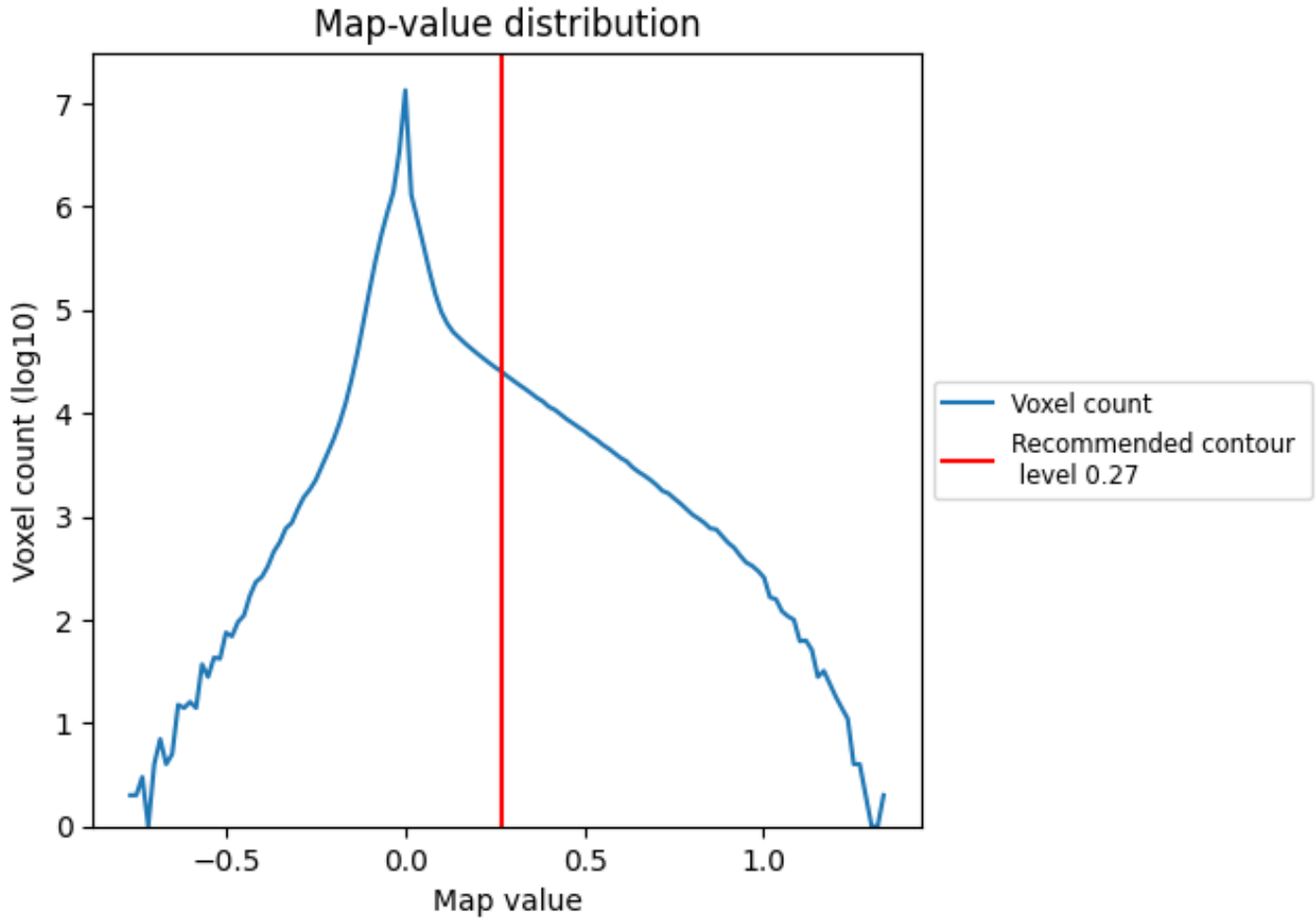
6.6 Mask visualisation (i)

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

7 Map analysis

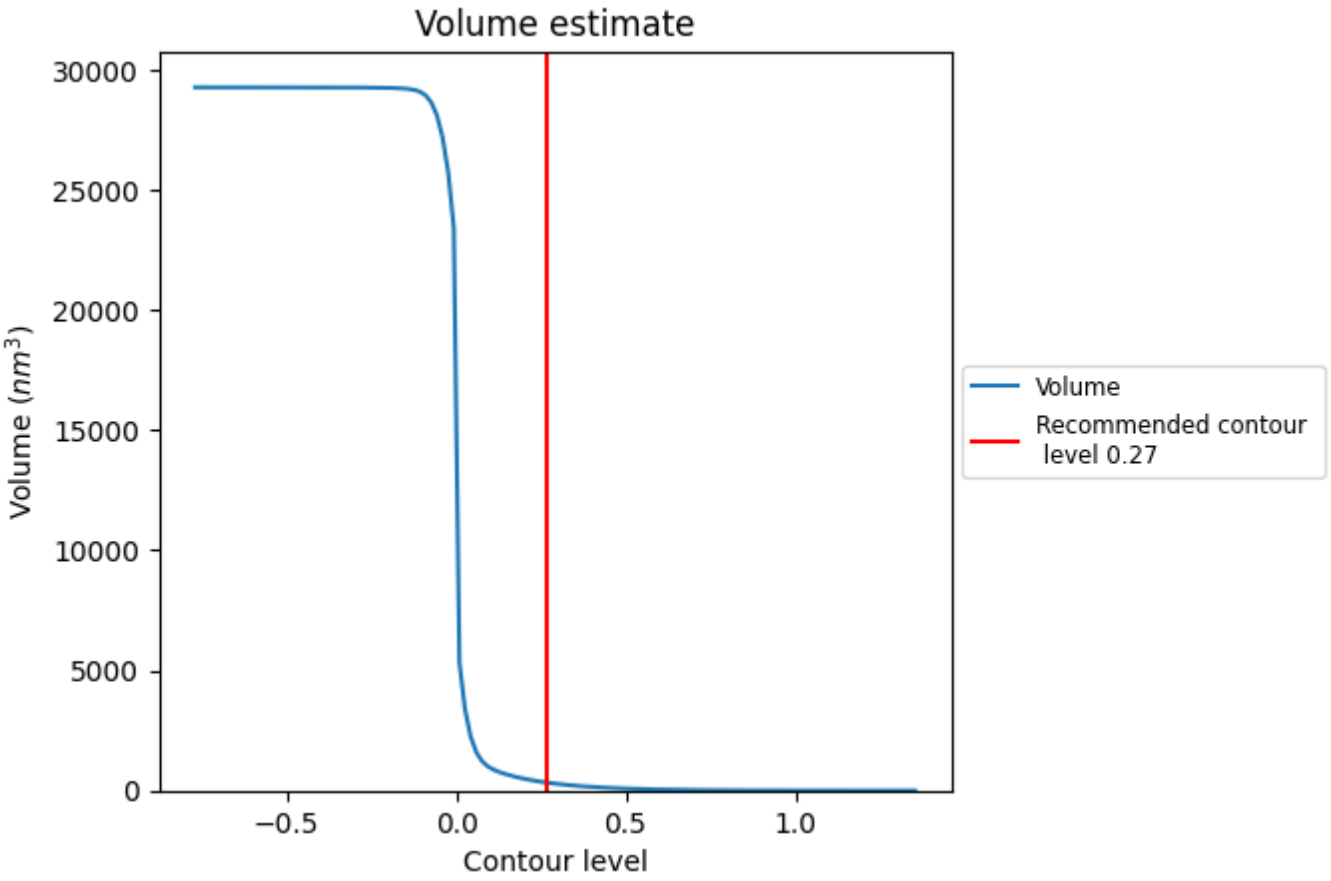
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

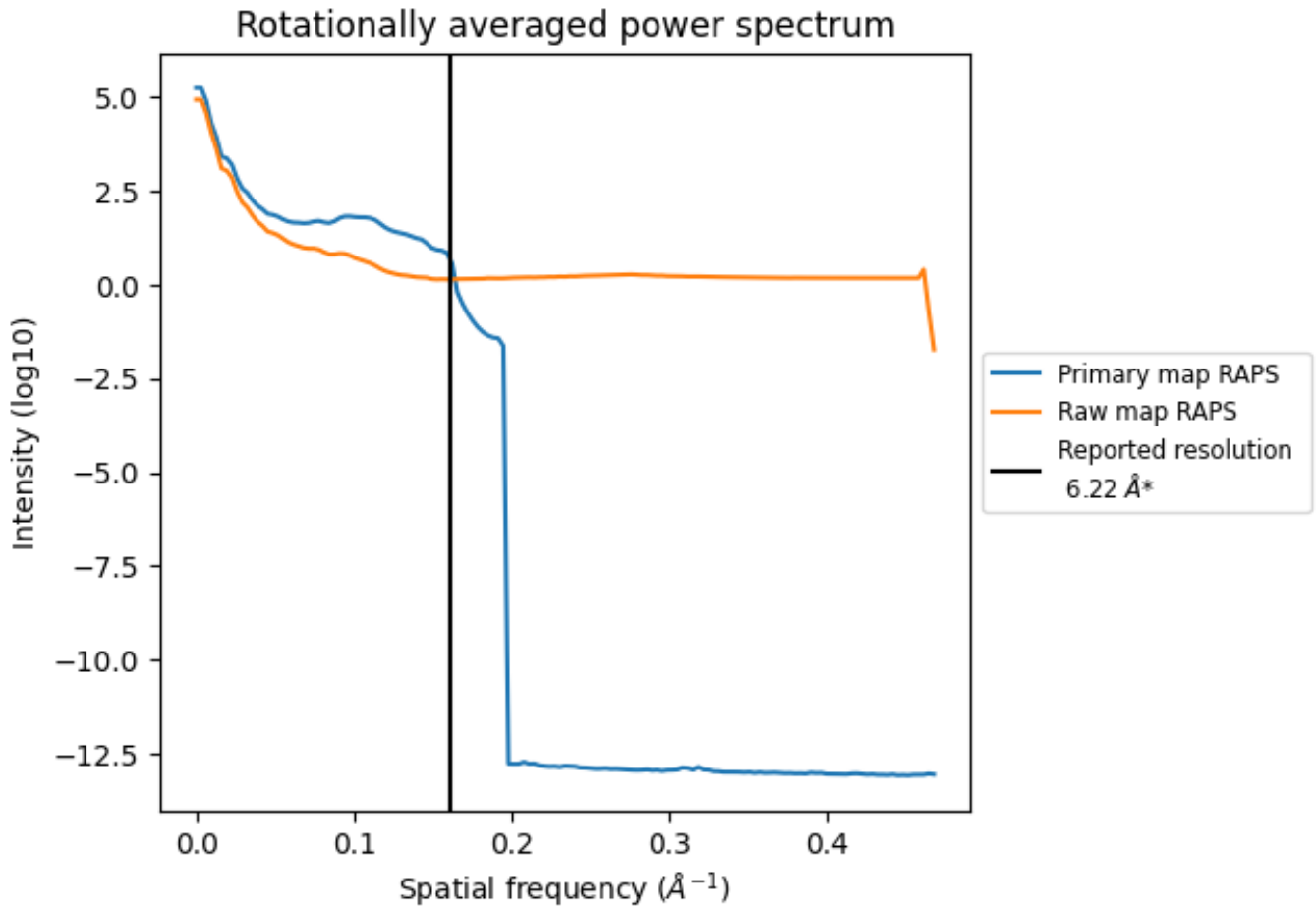
7.2 Volume estimate



The volume at the recommended contour level is 326 nm^3; this corresponds to an approximate mass of 295 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 (i)

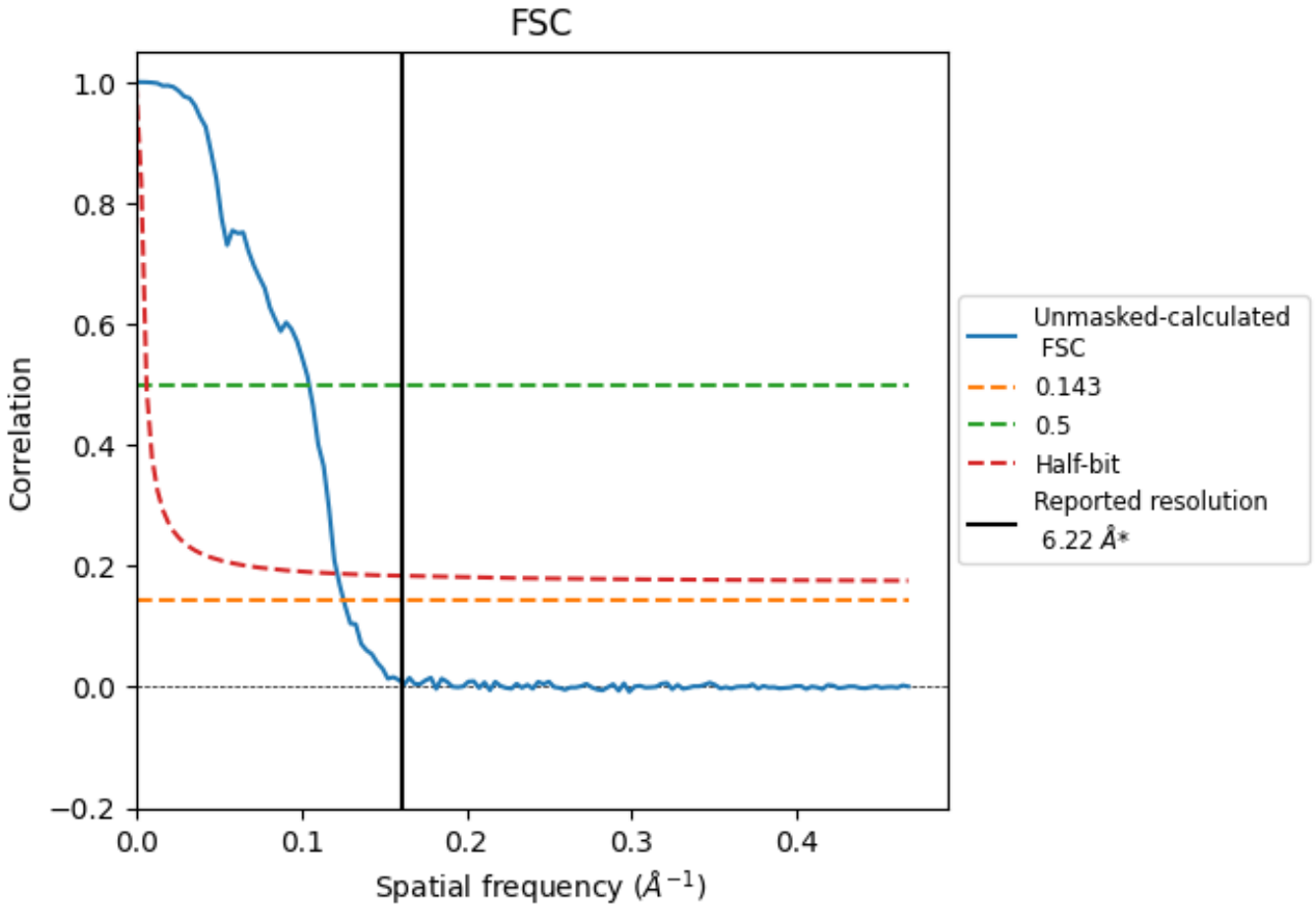


*Reported resolution corresponds to spatial frequency of 0.161 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.161 Å^{-1}

8.2 Resolution estimates (i)

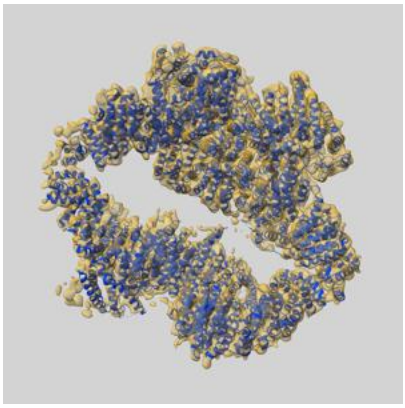
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.22	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.96	9.54	8.21

*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 7.96 differs from the reported value 6.22 by more than 10 %

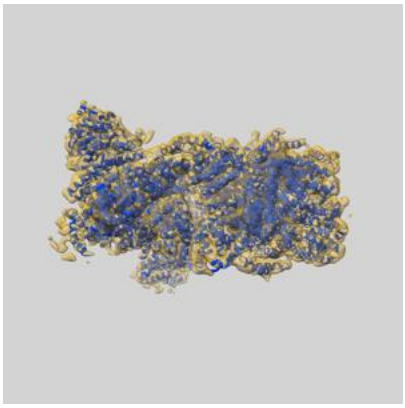
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-62812 and PDB model 9L4F. Per-residue inclusion information can be found in section 3 on page 5.

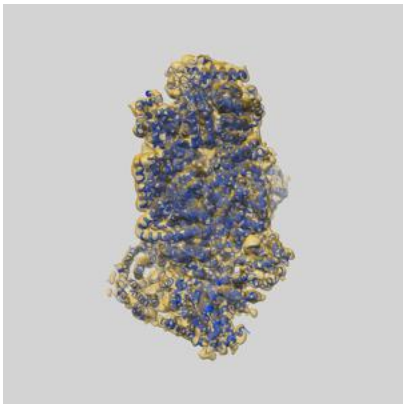
9.1 Map-model overlay



X



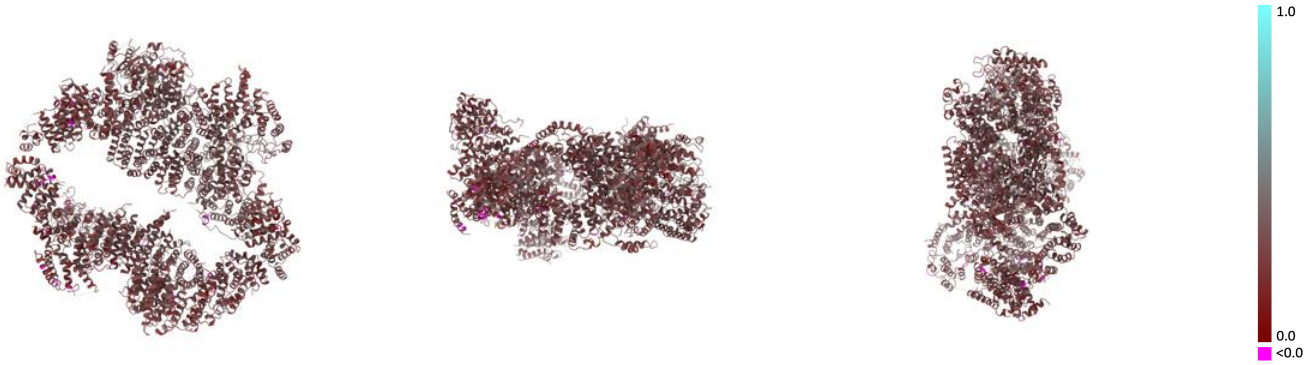
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.27 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.

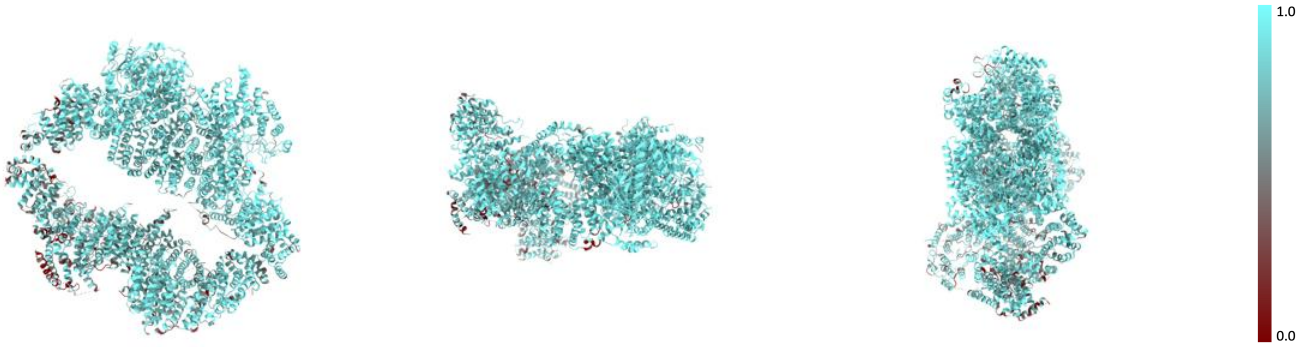
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

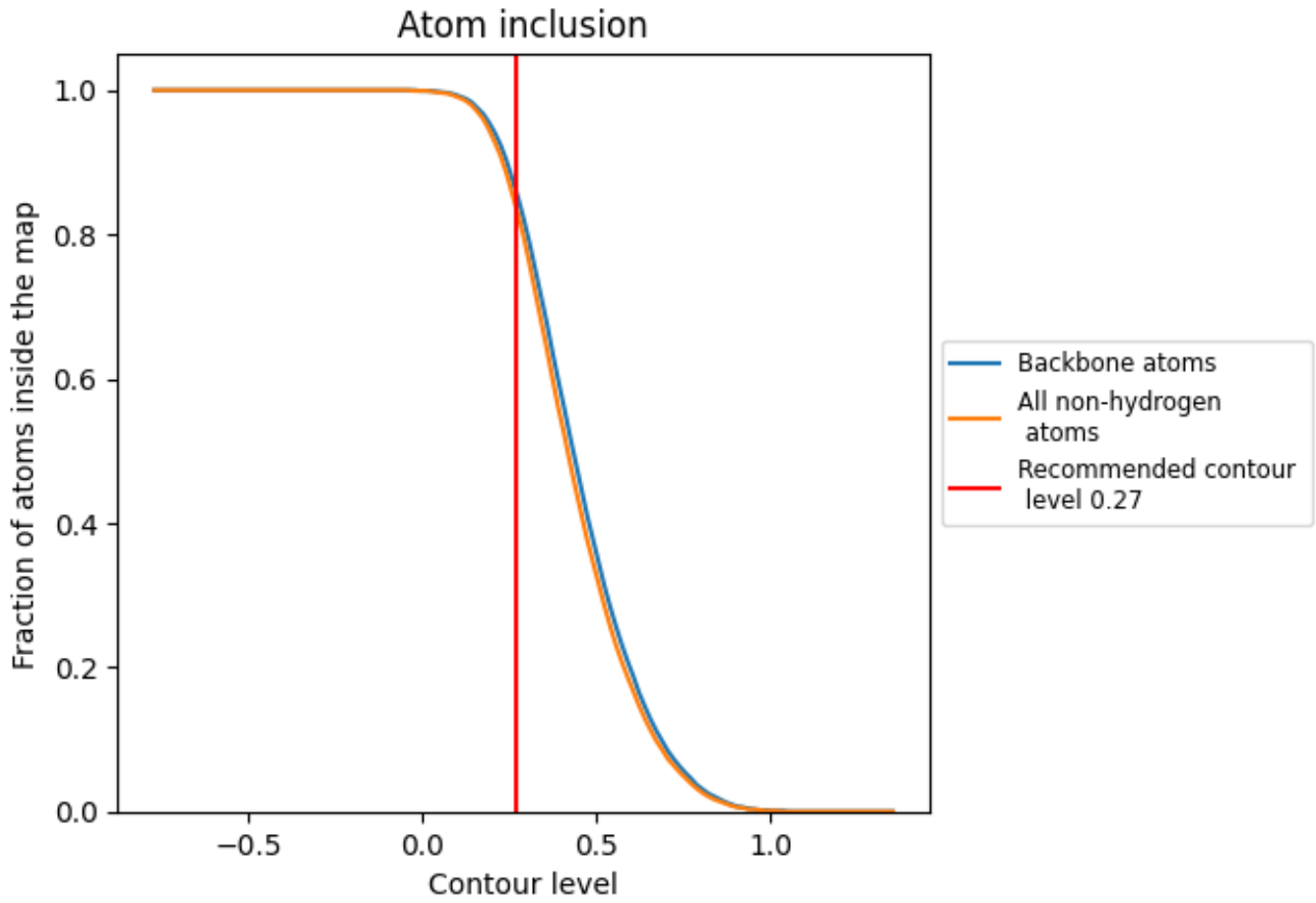
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.27).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.27) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8380	0.2850
A	0.8680	0.2910
B	0.8320	0.2840
C	0.7750	0.2670
D	0.7350	0.2640