



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 01:14 AM UTC

PDB ID : 8EZA / pdb_00008eza
EMDB ID : EMD-28732
Title : NHEJ Long-range complex with PAXX
Authors : Chen, S.; He, Y.
Deposited on : 2022-10-31
Resolution : 4.39 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:

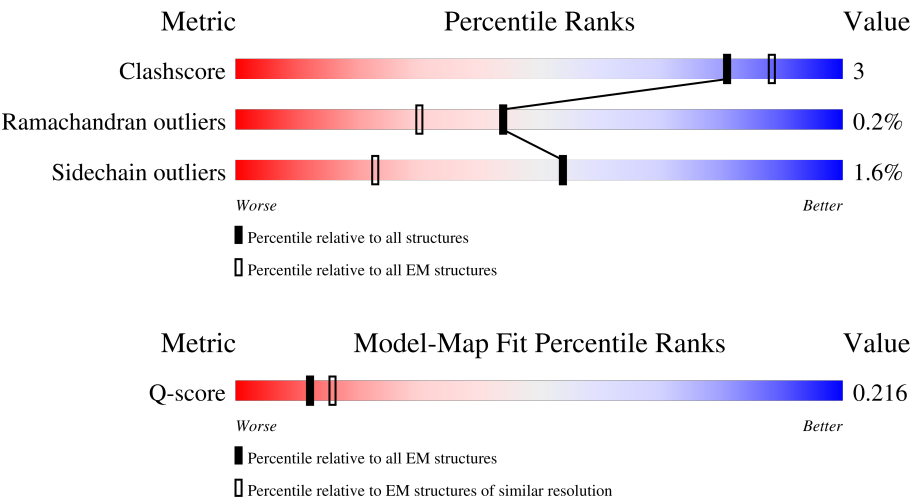
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.39 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.



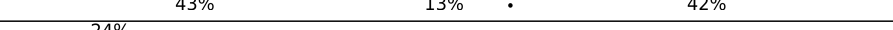
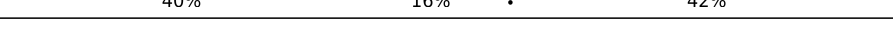
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3667 (3.89 - 4.88)

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	S	204	8% 89%
1	T	204	8% 89%
2	A	609	72% 9% 18%
2	J	609	72% 9% 18%

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Mol	Chain	Length	Quality of chain
3	B	732	
3	K	732	
4	C	4128	
4	L	4128	
5	Q	20	
5	R	20	
6	D	31	
6	M	31	
7	E	30	
7	N	30	
8	H	299	
8	I	299	
9	F	336	
9	G	336	
9	O	336	
9	P	336	
10	X	911	
10	Y	911	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 93588 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Protein PAXX.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S	23	Total	C	N	O	S	0	0
			168	107	30	30	1		
1	T	23	Total	C	N	O	S	0	0
			168	107	30	30	1		

- Molecule 2 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	497	Total	C	N	O	S	0	0
			4021	2577	680	746	18		
2	A	497	Total	C	N	O	S	0	0
			4021	2577	680	746	18		

- Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	531	Total	C	N	O	S	0	0
			4259	2723	711	801	24		
3	B	531	Total	C	N	O	S	0	0
			4259	2723	711	801	24		

- Molecule 4 is a protein called DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	3720	Total	C	N	O	S	0	0
			29811	19106	5059	5451	195		
4	C	3720	Total	C	N	O	S	0	0
			29811	19106	5059	5451	195		

- Molecule 5 is a protein called PRKDC_HUMAN DNA-dependent protein kinase catalytic subunit – Unknown region.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	R	20	Total	C	N	O	0	0
			101	60	20	21		
5	Q	20	Total	C	N	O	0	0
			101	60	20	21		

- Molecule 6 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	31	Total	C	N	O	P	0	0
			634	304	113	186	31		
6	D	31	Total	C	N	O	P	0	0
			634	304	113	186	31		

- Molecule 7 is a DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	30	Total	C	N	O	P	0	0
			616	295	110	181	30		
7	E	30	Total	C	N	O	P	0	0
			616	295	110	181	30		

- Molecule 8 is a protein called Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	223	Total	C	N	O	S	0	0
			1779	1140	298	326	15		
8	I	218	Total	C	N	O	S	0	0
			1737	1111	290	321	15		

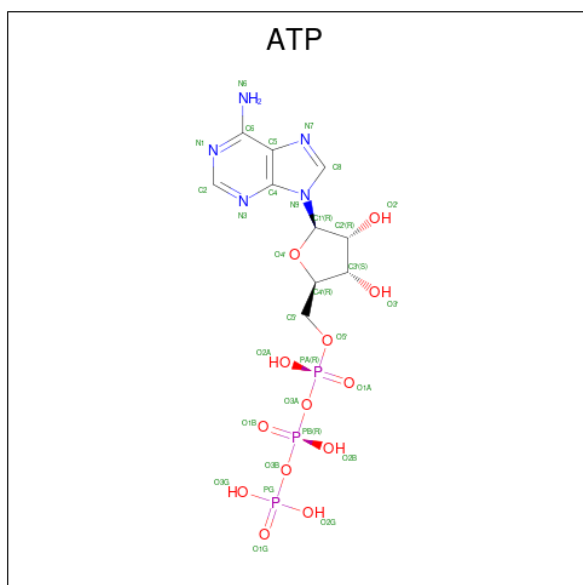
- Molecule 9 is a protein called DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	213	Total	C	N	O	S	0	0
			1736	1093	308	327	8		
9	G	195	Total	C	N	O	S	0	0
			1595	1012	272	304	7		
9	O	213	Total	C	N	O	S	0	0
			1736	1093	308	327	8		
9	P	195	Total	C	N	O	S	0	0
			1595	1012	272	304	7		

- Molecule 10 is a protein called DNA ligase 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	254	Total	C	N	O	S	0	0
			2064	1314	348	389	13		
10	Y	254	Total	C	N	O	S	0	0
			2064	1314	348	389	13		

- Molecule 11 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

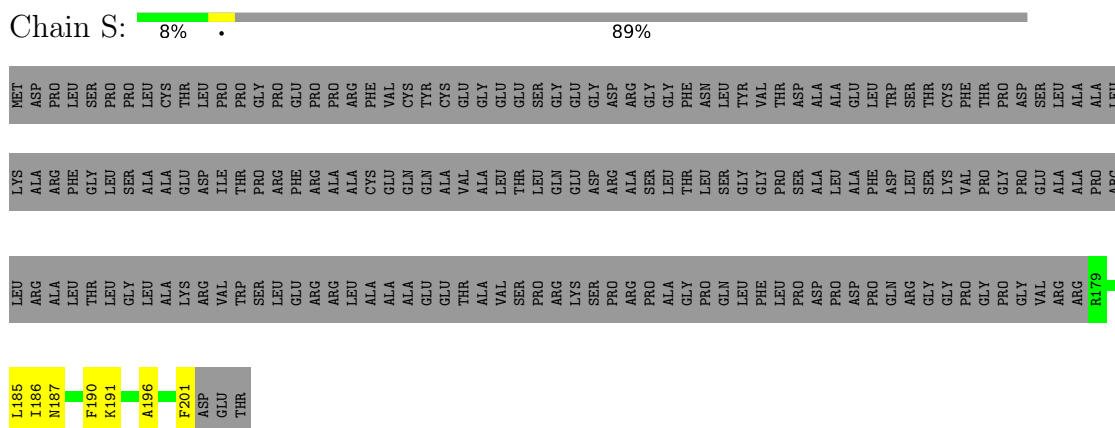


Mol	Chain	Residues	Atoms					AltConf
11	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
11	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

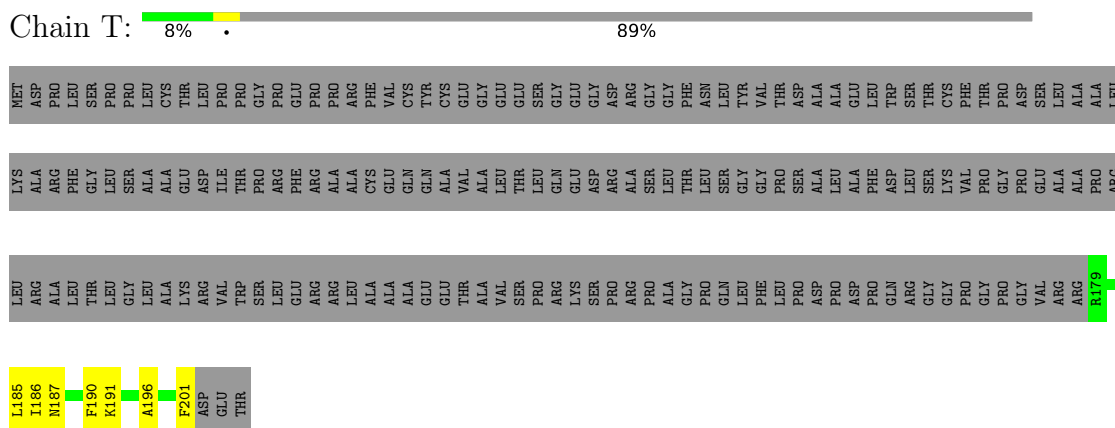
3 Residue-property plots

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.

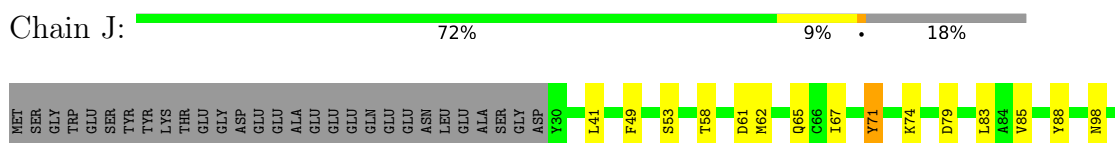
• Molecule 1: Protein PAXX

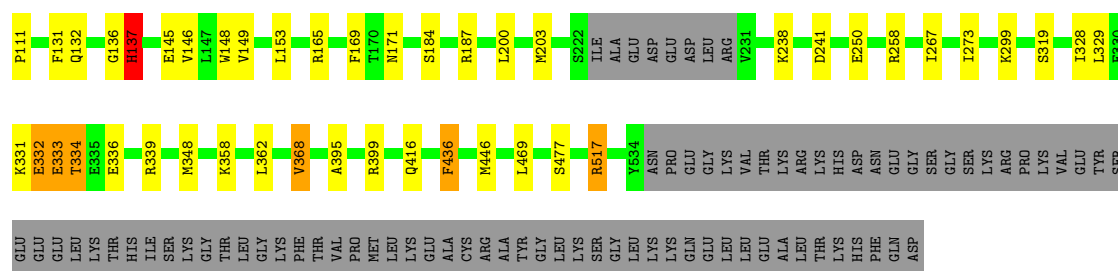


• Molecule 1: Protein PAXX



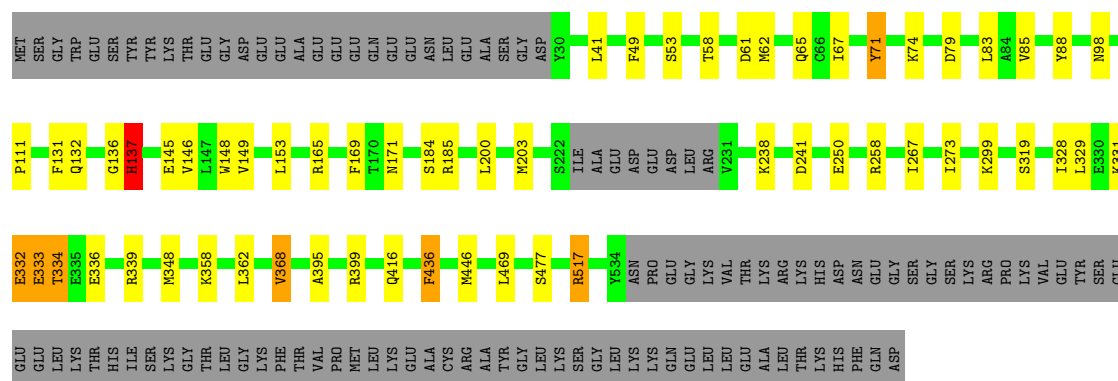
• Molecule 2: X-ray repair cross-complementing protein 6





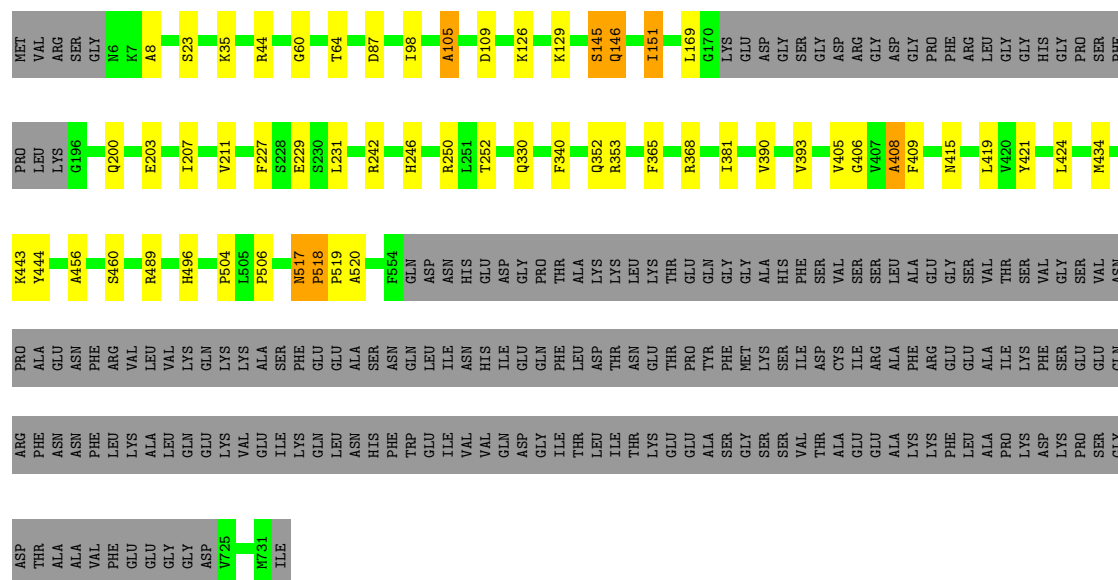
• Molecule 2: X-ray repair cross-complementing protein 6

Chain A: 72% 9% 18%



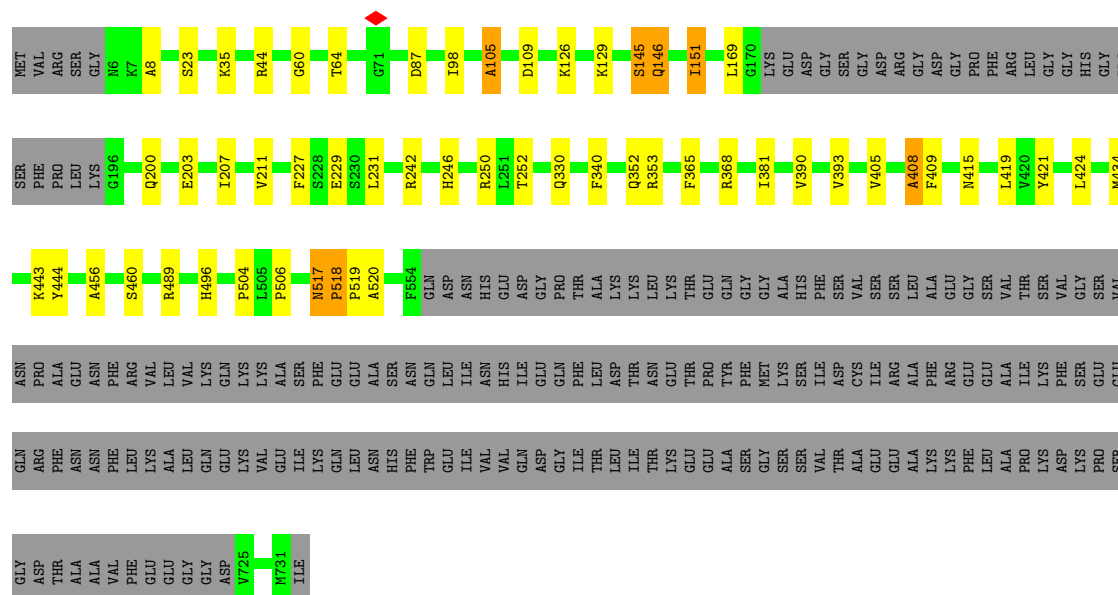
• Molecule 3: X-ray repair cross-complementing protein 5

Chain K: 65% 7% 27%



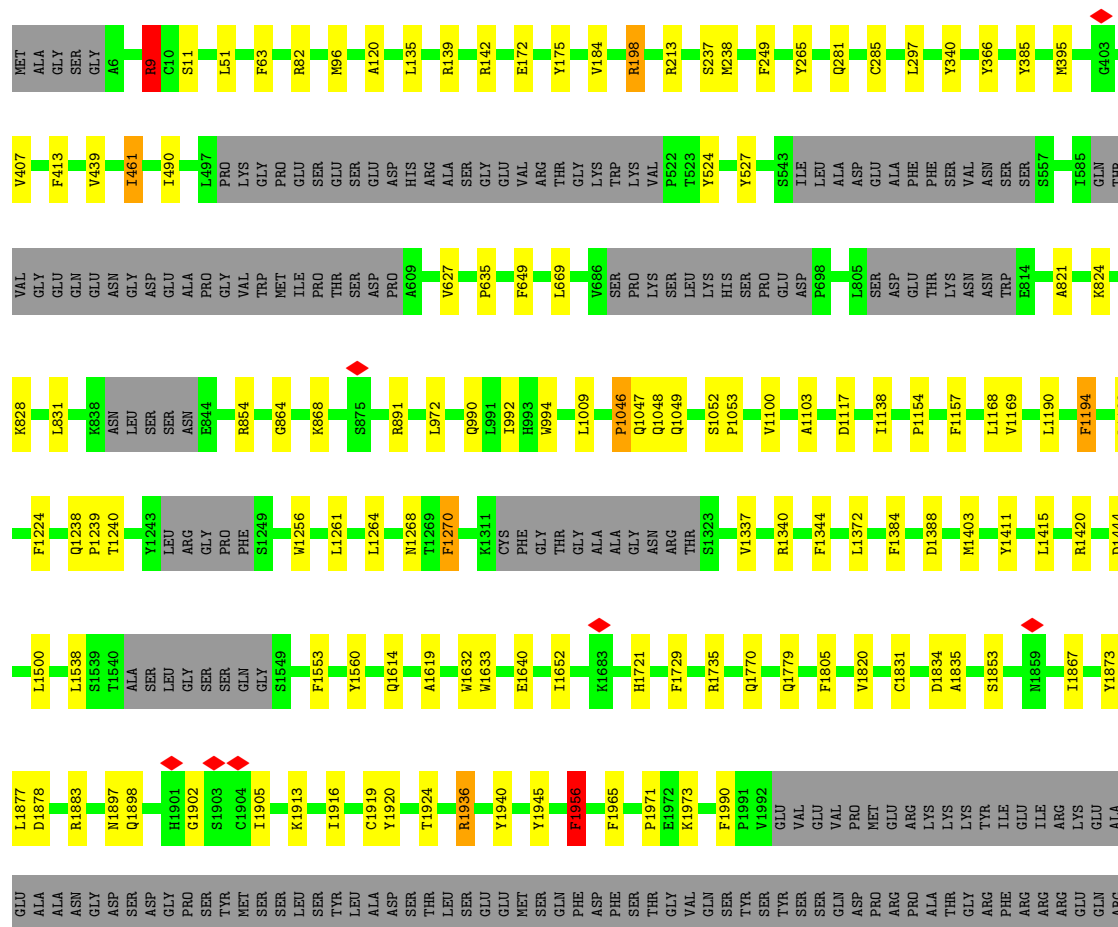
• Molecule 3: X-ray repair cross-complementing protein 5

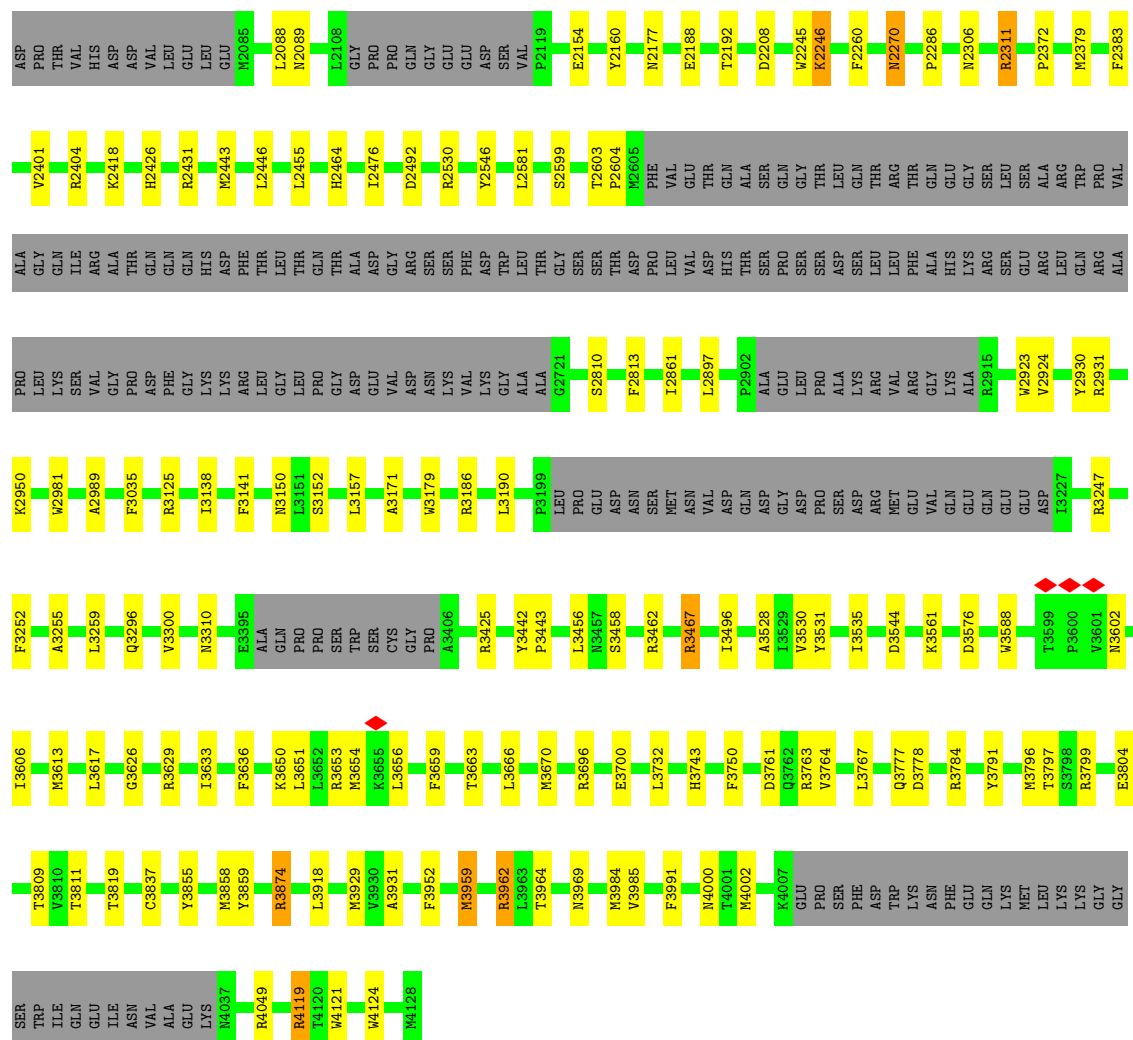
Chain B: 65% 7% 27%



• Molecule 4: DNA-dependent protein kinase catalytic subunit

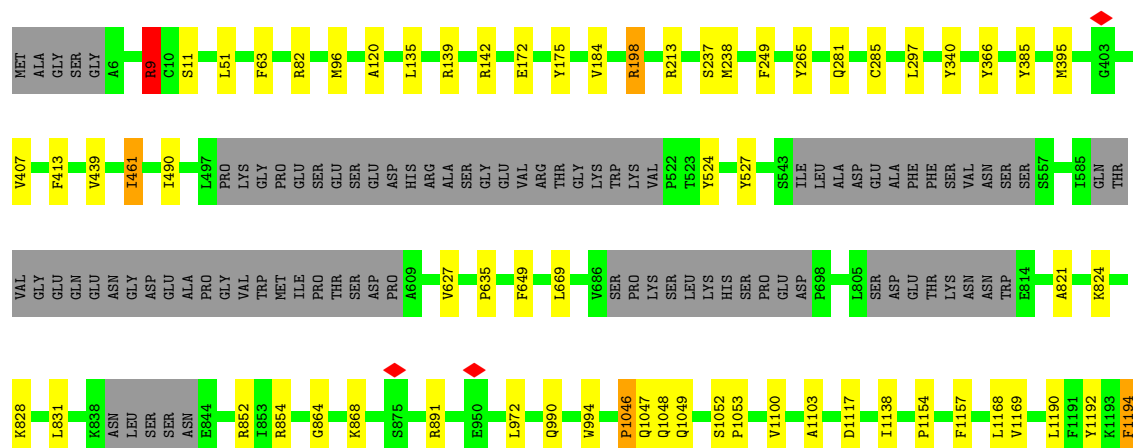
Chain L: 84% 6% 10%



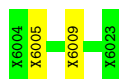


● Molecule 4: DNA-dependent protein kinase catalytic subunit

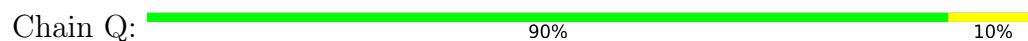
Chain C: 84% 6% 10%







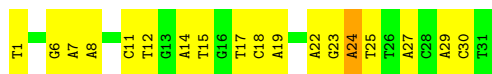
- Molecule 5: PRKDC_HUMAN DNA-dependent protein kinase catalytic subunit – Unknown region



- Molecule 6: DNA (31-MER)



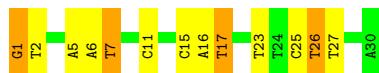
- Molecule 6: DNA (31-MER)



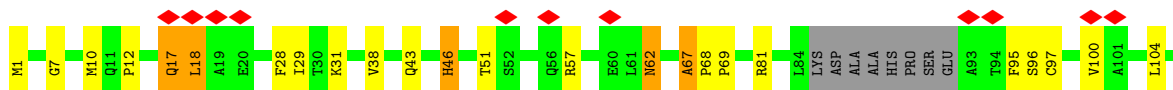
- Molecule 7: DNA (30-MER)

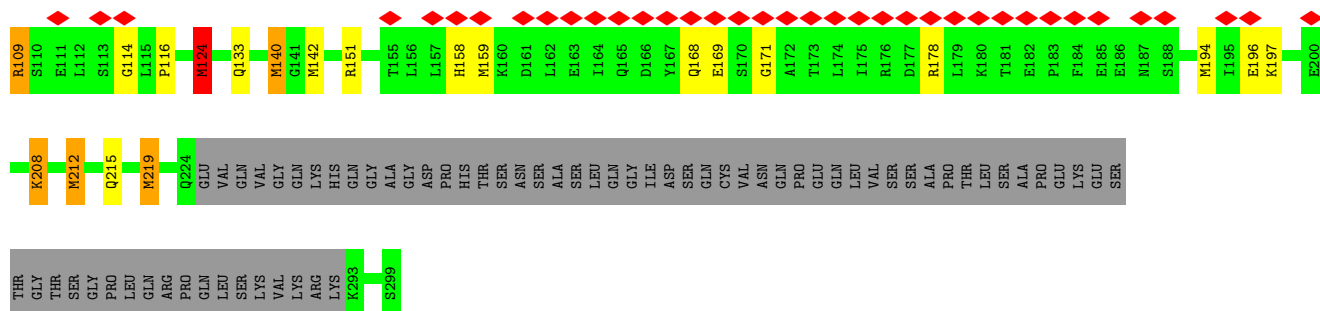


- Molecule 7: DNA (30-MER)

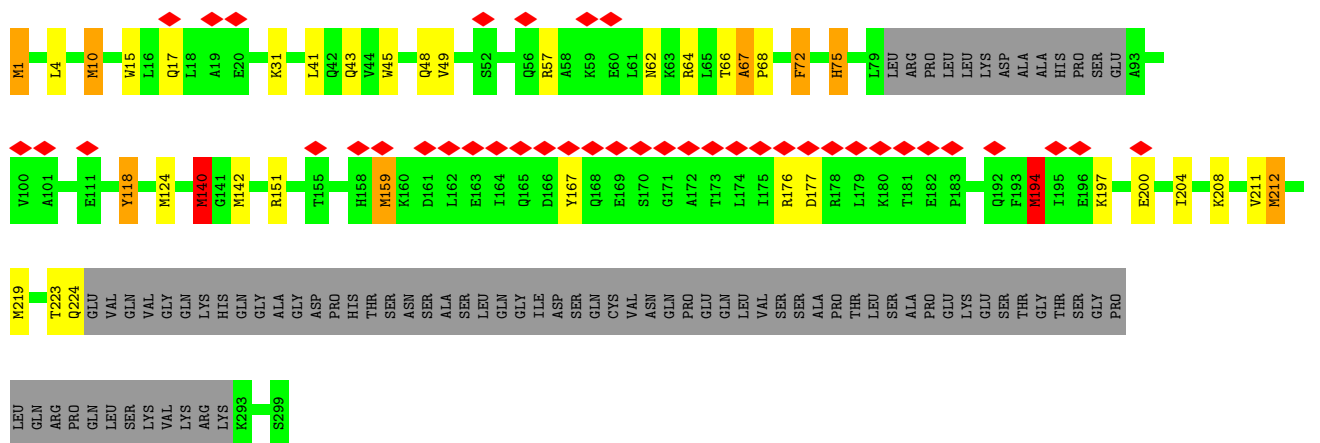


- Molecule 8: Non-homologous end-joining factor 1

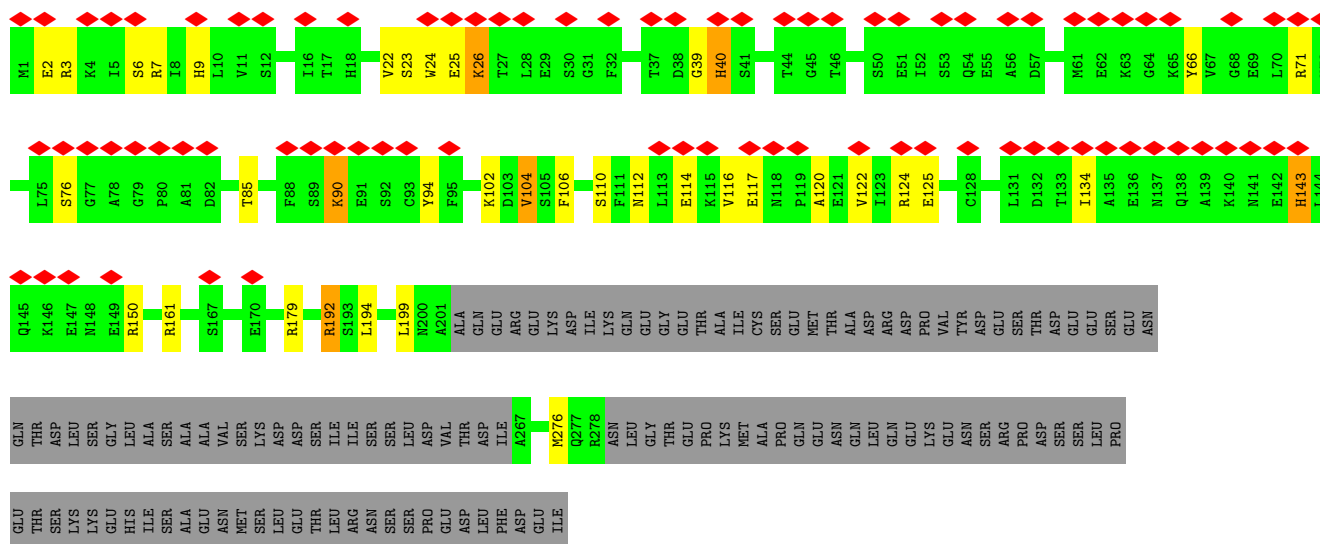




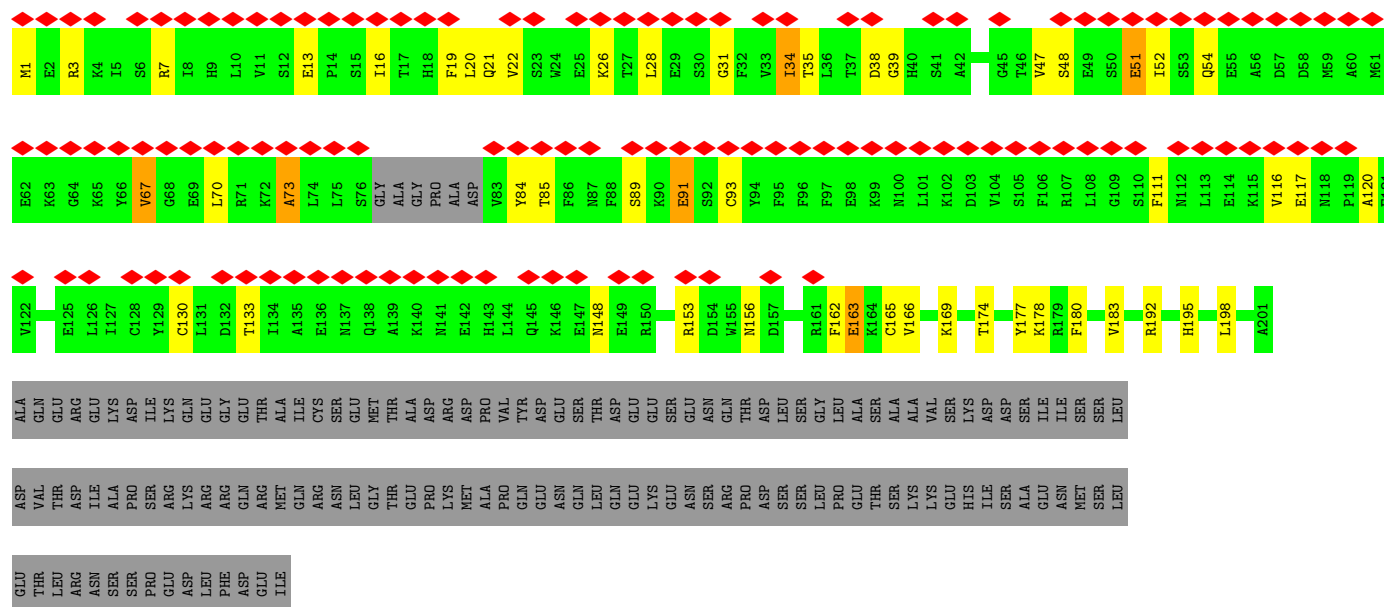
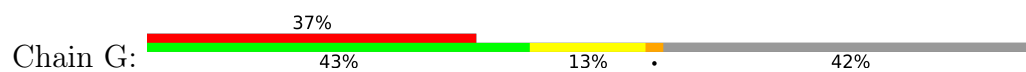
• Molecule 8: Non-homologous end-joining factor 1



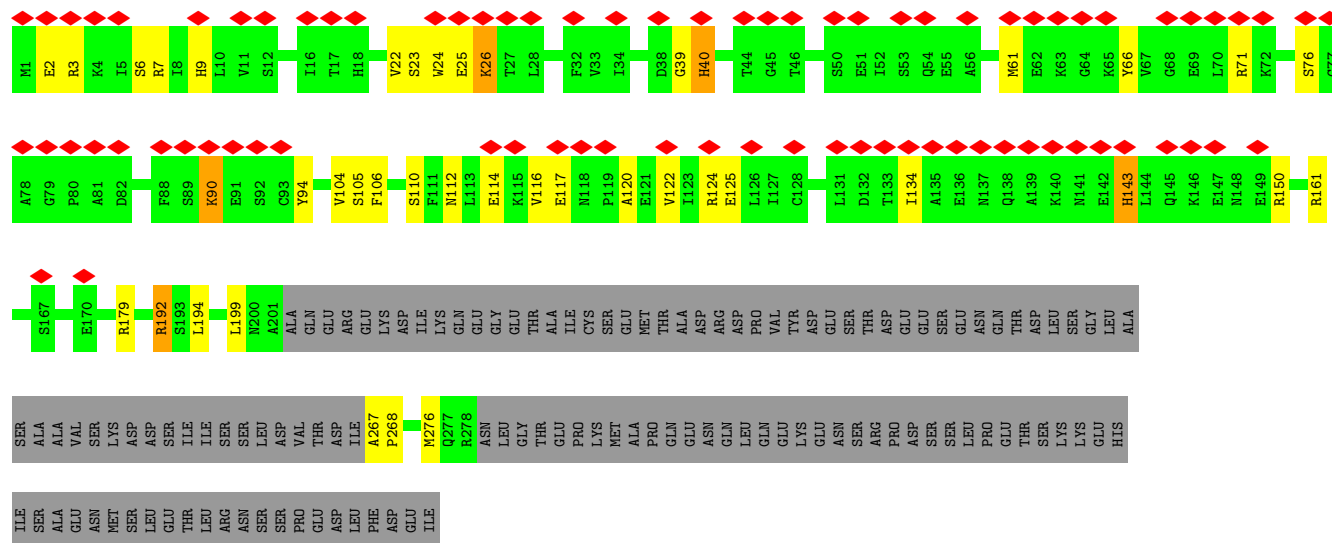
• Molecule 9: DNA repair protein XRCC4



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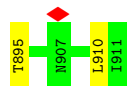
• Molecule 9: DNA repair protein XRCC4



• Molecule 9: DNA repair protein XRCC4







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	138252	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.123	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	517.92, 517.92, 517.92	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.079, 1.079, 1.079	Depositor

5 Model quality

5.1 Standard geometry

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

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	S	0.75	0/172	1.44	0/229
1	T	0.79	0/172	1.49	0/229
2	A	1.40	11/4101 (0.3%)	1.53	35/5523 (0.6%)
2	J	1.40	10/4101 (0.2%)	1.53	36/5523 (0.7%)
3	B	0.81	1/4340 (0.0%)	1.51	34/5853 (0.6%)
3	K	0.81	1/4340 (0.0%)	1.51	35/5853 (0.6%)
4	C	0.80	9/30414 (0.0%)	1.36	103/41079 (0.3%)
4	L	0.80	9/30414 (0.0%)	1.36	99/41079 (0.2%)
6	D	0.70	0/710	1.41	0/1093
6	M	0.70	0/710	1.41	0/1093
7	E	0.73	0/690	1.30	0/1063
7	N	0.73	0/690	1.29	0/1063
8	H	0.97	18/1814 (1.0%)	1.47	21/2454 (0.9%)
8	I	0.96	16/1771 (0.9%)	1.37	8/2395 (0.3%)
9	F	0.77	0/1765	1.44	13/2367 (0.5%)
9	G	0.84	0/1622	1.59	18/2178 (0.8%)
9	O	0.77	0/1765	1.43	11/2367 (0.5%)
9	P	0.84	0/1622	1.59	19/2178 (0.9%)
10	X	0.81	0/2112	1.41	12/2851 (0.4%)
10	Y	0.81	0/2112	1.41	12/2851 (0.4%)
All	All	0.87	75/95437 (0.1%)	1.40	456/129321 (0.4%)

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
2	A	0	3
2	J	0	3
3	B	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	K	0	5
4	C	0	27
4	L	0	28
6	D	0	15
6	M	0	15
7	E	0	11
7	N	0	11
8	H	0	2
8	I	0	4
9	F	0	5
9	G	0	3
9	O	0	5
9	P	0	3
All	All	0	145

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	334	THR	N-CA	43.55	2.08	1.46
2	A	334	THR	N-CA	43.53	2.08	1.46
2	A	334	THR	CB-CG2	39.49	2.82	1.52
2	J	334	THR	CB-CG2	39.45	2.82	1.52
2	J	334	THR	CB-OG1	21.37	1.77	1.43
2	A	334	THR	CB-OG1	21.24	1.77	1.43
2	J	333	GLU	CB-CG	17.71	2.05	1.52
2	A	333	GLU	CB-CG	17.70	2.05	1.52
2	J	333	GLU	CA-C	17.56	1.77	1.52
2	A	333	GLU	CA-C	17.51	1.77	1.52
2	A	333	GLU	CA-CB	17.15	1.83	1.53
2	J	333	GLU	CA-CB	17.13	1.82	1.53
2	J	333	GLU	N-CA	16.86	1.68	1.46
2	A	333	GLU	N-CA	16.80	1.68	1.46
4	C	9	ARG	CZ-NH1	-16.36	1.09	1.32
4	L	9	ARG	CZ-NH1	-16.35	1.09	1.32
2	A	333	GLU	C-N	14.58	1.56	1.33
2	J	333	GLU	C-N	14.54	1.56	1.33
4	L	2446	LEU	CG-CD1	-10.59	1.17	1.52
4	C	2446	LEU	CG-CD1	-10.59	1.17	1.52
4	C	2446	LEU	CG-CD2	-8.59	1.24	1.52
4	L	2446	LEU	CG-CD2	-8.59	1.24	1.52
2	J	333	GLU	CG-CD	8.48	1.73	1.52
2	A	333	GLU	CG-CD	8.47	1.73	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1835	ALA	CA-CB	-7.91	1.41	1.53
4	L	1835	ALA	CA-CB	-7.91	1.41	1.53
4	L	9	ARG	CZ-NH2	-7.06	1.24	1.33
4	C	9	ARG	CZ-NH2	-7.06	1.24	1.33
8	H	1	MET	CG-SD	7.00	1.98	1.80
8	H	159	MET	SD-CE	6.62	1.96	1.79
8	H	140	MET	CG-SD	6.60	1.97	1.80
8	H	10	MET	CG-SD	6.59	1.97	1.80
8	I	140	MET	SD-CE	6.57	1.96	1.79
3	B	443	LYS	CA-C	6.56	1.61	1.52
8	H	1	MET	SD-CE	6.56	1.96	1.79
8	I	1	MET	CG-SD	6.49	1.97	1.80
3	K	443	LYS	CA-C	6.48	1.61	1.52
8	H	212	MET	SD-CE	6.47	1.95	1.79
8	H	140	MET	SD-CE	6.46	1.95	1.79
8	I	212	MET	SD-CE	6.41	1.95	1.79
8	H	194	MET	SD-CE	6.40	1.95	1.79
8	I	124	MET	CG-SD	6.40	1.96	1.80
8	H	124	MET	SD-CE	6.37	1.95	1.79
8	H	219	MET	SD-CE	6.37	1.95	1.79
8	I	124	MET	SD-CE	6.34	1.95	1.79
8	I	140	MET	CG-SD	6.33	1.96	1.80
8	I	10	MET	SD-CE	6.27	1.95	1.79
8	I	194	MET	CG-SD	6.25	1.96	1.80
8	H	10	MET	SD-CE	6.21	1.95	1.79
8	H	212	MET	CG-SD	6.16	1.96	1.80
8	I	159	MET	SD-CE	6.14	1.95	1.79
8	I	219	MET	SD-CE	6.02	1.94	1.79
8	I	212	MET	CG-SD	6.02	1.95	1.80
8	I	194	MET	SD-CE	6.00	1.94	1.79
8	H	124	MET	CG-SD	5.99	1.95	1.80
8	I	142	MET	SD-CE	5.91	1.94	1.79
8	I	159	MET	CG-SD	5.83	1.95	1.80
8	H	142	MET	SD-CE	5.79	1.94	1.79
8	H	194	MET	CG-SD	5.76	1.95	1.80
8	I	1	MET	SD-CE	5.76	1.94	1.79
8	H	159	MET	CG-SD	5.71	1.95	1.80
2	J	334	THR	CA-C	-5.68	1.42	1.52
2	A	334	THR	CA-C	-5.68	1.42	1.52
8	H	68	PRO	CA-C	5.34	1.54	1.51
4	L	1919	CYS	C-N	-5.29	1.27	1.33
8	I	142	MET	CG-SD	5.26	1.94	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1919	CYS	C-N	-5.22	1.27	1.33
4	L	2286	PRO	CA-C	5.21	1.54	1.51
4	C	2286	PRO	CA-C	5.16	1.54	1.51
4	C	2599	SER	CB-OG	-5.13	1.31	1.42
4	L	2599	SER	CB-OG	-5.10	1.31	1.42
4	C	3777	GLN	C-N	-5.10	1.26	1.33
2	A	185	ARG	N-CA	-5.09	1.40	1.46
8	H	142	MET	CG-SD	5.09	1.93	1.80
4	L	3777	GLN	C-N	-5.02	1.26	1.33

All (456) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	334	THR	CA-CB-OG1	-16.58	84.73	109.60
2	A	334	THR	CA-CB-OG1	-16.56	84.76	109.60
2	J	333	GLU	CA-CB-CG	-14.73	84.64	114.10
2	A	333	GLU	CA-CB-CG	-14.72	84.67	114.10
2	J	334	THR	N-CA-CB	-14.46	84.97	110.42
2	A	334	THR	N-CA-CB	-14.43	85.03	110.42
4	C	3985	VAL	N-CA-CB	13.45	126.29	110.55
4	L	3985	VAL	N-CA-CB	13.43	126.27	110.55
2	J	333	GLU	CA-C-N	-12.98	91.15	121.52
2	J	333	GLU	C-N-CA	-12.98	91.15	121.52
2	A	333	GLU	CA-C-N	-12.96	91.19	121.52
2	A	333	GLU	C-N-CA	-12.96	91.19	121.52
2	J	333	GLU	CB-CA-C	-11.96	87.38	110.11
2	A	333	GLU	CB-CA-C	-11.96	87.39	110.11
4	C	3985	VAL	N-CA-C	-11.86	99.03	110.42
4	L	3985	VAL	N-CA-C	-11.82	99.07	110.42
3	K	23	SER	N-CA-C	11.64	126.30	108.96
3	B	23	SER	N-CA-C	11.63	126.29	108.96
2	J	333	GLU	O-C-N	11.39	139.24	122.39
2	A	333	GLU	O-C-N	11.35	139.18	122.39
2	J	137	HIS	CA-CB-CG	-11.23	102.56	113.80
2	A	137	HIS	CA-CB-CG	-11.21	102.59	113.80
3	B	105	ALA	N-CA-C	11.06	124.00	108.74
3	K	105	ALA	N-CA-C	11.03	123.96	108.74
4	C	3984	MET	CA-C-N	10.56	133.86	120.56
4	C	3984	MET	C-N-CA	10.56	133.86	120.56
2	J	333	GLU	N-CA-CB	-10.50	93.41	110.42
4	L	3984	MET	CA-C-N	10.49	133.78	120.56
4	L	3984	MET	C-N-CA	10.49	133.78	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	333	GLU	N-CA-CB	-10.47	93.45	110.42
8	H	18	LEU	CD1-CG-CD2	9.93	132.64	110.80
3	K	98	ILE	N-CA-C	9.83	122.18	109.30
3	B	98	ILE	N-CA-C	9.81	122.15	109.30
3	B	381	ILE	CA-CB-CG1	9.79	127.04	110.40
3	K	381	ILE	CA-CB-CG1	9.74	126.97	110.40
2	J	416	GLN	N-CA-C	9.68	124.79	109.50
2	A	416	GLN	N-CA-C	9.66	124.76	109.50
2	J	333	GLU	CB-CG-CD	-9.37	96.67	112.60
2	A	333	GLU	CB-CG-CD	-9.36	96.69	112.60
3	K	169	LEU	N-CA-C	9.34	123.99	112.59
3	B	169	LEU	N-CA-C	9.33	123.98	112.59
3	K	504	PRO	N-CA-C	9.25	125.67	111.34
3	B	504	PRO	N-CA-C	9.18	125.56	111.34
3	B	126	LYS	N-CA-C	9.09	123.94	110.48
3	K	126	LYS	N-CA-C	9.07	123.91	110.48
2	J	333	GLU	CG-CD-OE2	-9.01	97.69	118.40
2	A	333	GLU	CG-CD-OE2	-9.01	97.69	118.40
9	O	143	HIS	CB-CG-CD2	-8.98	119.53	131.20
9	F	143	HIS	CB-CG-CD2	-8.97	119.54	131.20
4	L	1919	CYS	CA-C-N	8.95	132.63	120.54
4	L	1919	CYS	C-N-CA	8.95	132.63	120.54
4	C	1919	CYS	CA-C-N	8.94	132.60	120.54
4	C	1919	CYS	C-N-CA	8.94	132.60	120.54
2	J	333	GLU	CG-CD-OE1	8.76	138.55	118.40
2	A	333	GLU	CG-CD-OE1	8.74	138.51	118.40
3	K	8	ALA	N-CA-C	8.74	123.46	110.52
3	B	8	ALA	N-CA-C	8.74	123.45	110.52
2	J	334	THR	N-CA-C	-8.72	102.81	113.19
2	A	334	THR	N-CA-C	-8.69	102.85	113.19
3	K	415	ASN	N-CA-C	8.68	123.87	113.28
2	J	137	HIS	N-CA-C	8.64	123.36	108.76
2	A	137	HIS	N-CA-C	8.62	123.34	108.76
3	B	415	ASN	N-CA-C	8.60	123.77	113.28
3	K	207	ILE	N-CA-C	8.54	119.33	110.62
3	B	207	ILE	N-CA-C	8.51	119.30	110.62
3	B	211	VAL	N-CA-C	8.51	119.30	110.62
2	J	334	THR	CB-CA-C	8.50	126.75	110.27
3	K	211	VAL	N-CA-C	8.50	119.29	110.62
2	A	334	THR	CB-CA-C	8.49	126.75	110.27
3	K	151	ILE	CA-CB-CG1	8.25	124.42	110.40
3	B	151	ILE	CA-CB-CG1	8.24	124.41	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	250	ARG	N-CA-C	8.20	124.81	107.67
3	K	252	THR	N-CA-C	8.19	124.78	107.67
3	B	250	ARG	N-CA-C	8.18	124.77	107.67
3	B	252	THR	N-CA-C	8.17	124.74	107.67
3	B	456	ALA	N-CA-C	7.91	122.70	112.89
3	K	456	ALA	N-CA-C	7.89	122.67	112.89
9	G	67	VAL	CA-C-N	7.88	128.69	119.94
9	G	67	VAL	C-N-CA	7.88	128.69	119.94
3	B	352	GLN	CA-C-N	7.81	130.59	120.44
3	B	352	GLN	C-N-CA	7.81	130.59	120.44
3	B	129	LYS	N-CA-C	7.77	122.68	110.32
3	K	129	LYS	N-CA-C	7.76	122.66	110.32
3	K	352	GLN	CA-C-N	7.75	130.51	120.44
3	K	352	GLN	C-N-CA	7.75	130.51	120.44
4	L	1834	ASP	CA-C-N	7.74	134.68	122.61
4	L	1834	ASP	C-N-CA	7.74	134.68	122.61
4	C	1834	ASP	CA-C-N	7.67	134.58	122.61
4	C	1834	ASP	C-N-CA	7.67	134.58	122.61
3	K	460	SER	N-CA-C	7.62	120.55	111.33
9	P	148	ASN	CB-CA-C	7.62	122.90	109.65
9	G	148	ASN	CB-CA-C	7.60	122.88	109.65
3	B	460	SER	N-CA-C	7.58	120.51	111.33
3	B	231	LEU	CB-CG-CD1	7.49	133.17	110.70
3	K	231	LEU	CB-CG-CD1	7.48	133.13	110.70
4	C	3952	PHE	CA-C-N	7.34	133.14	121.62
4	C	3952	PHE	C-N-CA	7.34	133.14	121.62
9	G	21	GLN	OE1-CD-NE2	-7.33	115.28	122.60
3	K	200	GLN	N-CA-C	7.32	121.12	111.75
4	L	3952	PHE	CA-C-N	7.32	133.10	121.62
4	L	3952	PHE	C-N-CA	7.32	133.10	121.62
9	P	21	GLN	OE1-CD-NE2	-7.31	115.29	122.60
3	B	200	GLN	N-CA-C	7.30	121.09	111.75
4	C	2089	ASN	CA-C-N	7.19	132.11	120.60
4	C	2089	ASN	C-N-CA	7.19	132.11	120.60
4	L	2089	ASN	CA-C-N	7.19	132.10	120.60
4	L	2089	ASN	C-N-CA	7.19	132.10	120.60
4	C	1046	PRO	CA-N-CD	-7.17	101.96	112.00
4	L	1046	PRO	CA-N-CD	-7.14	102.00	112.00
3	K	146	GLN	N-CA-C	7.02	125.75	110.80
4	L	1936	ARG	NE-CZ-NH2	7.01	125.51	119.20
3	B	146	GLN	N-CA-C	7.00	125.71	110.80
4	L	3777	GLN	CA-C-N	6.98	133.50	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	3777	GLN	C-N-CA	6.98	133.50	122.74
3	B	87	ASP	CA-CB-CG	6.95	119.55	112.60
4	C	3777	GLN	CA-C-N	6.94	133.43	122.74
4	C	3777	GLN	C-N-CA	6.94	133.43	122.74
4	C	1936	ARG	NE-CZ-NH2	6.94	125.45	119.20
3	K	87	ASP	CA-CB-CG	6.93	119.53	112.60
3	B	145	SER	N-CA-C	6.87	125.42	110.80
3	K	145	SER	N-CA-C	6.85	125.39	110.80
4	C	142	ARG	NE-CZ-NH2	6.77	125.30	119.20
4	L	142	ARG	NE-CZ-NH2	6.74	125.27	119.20
4	C	82	ARG	NE-CZ-NH2	6.65	125.18	119.20
4	L	82	ARG	NE-CZ-NH2	6.63	125.17	119.20
9	P	67	VAL	CA-C-N	6.62	127.16	119.94
9	P	67	VAL	C-N-CA	6.62	127.16	119.94
2	J	184	SER	CA-C-N	6.61	129.03	120.44
2	J	184	SER	C-N-CA	6.61	129.03	120.44
2	A	184	SER	CA-C-N	6.60	129.01	120.44
2	A	184	SER	C-N-CA	6.60	129.01	120.44
2	J	332	GLU	CA-C-N	-6.54	108.86	121.94
2	J	332	GLU	C-N-CA	-6.54	108.86	121.94
2	J	258	ARG	NE-CZ-NH2	6.52	125.07	119.20
2	A	332	GLU	CA-C-N	-6.52	108.90	121.94
2	A	332	GLU	C-N-CA	-6.52	108.90	121.94
8	H	109	ARG	NE-CZ-NH2	6.52	125.07	119.20
8	H	17	GLN	CA-C-N	6.51	132.13	121.58
8	H	17	GLN	C-N-CA	6.51	132.13	121.58
8	I	176	ARG	NE-CZ-NH2	6.49	125.04	119.20
2	A	258	ARG	NE-CZ-NH2	6.45	125.00	119.20
3	B	353	ARG	NE-CZ-NH2	6.37	124.94	119.20
3	K	353	ARG	NE-CZ-NH2	6.37	124.93	119.20
2	J	171	ASN	CA-CB-CG	6.36	118.95	112.60
2	A	171	ASN	CA-CB-CG	6.29	118.89	112.60
10	X	910	LEU	CA-C-N	6.25	132.95	121.70
10	X	910	LEU	C-N-CA	6.25	132.95	121.70
10	Y	910	LEU	CA-C-N	6.24	132.93	121.70
10	Y	910	LEU	C-N-CA	6.24	132.93	121.70
4	C	1831	CYS	CA-C-N	6.21	130.12	120.75
4	C	1831	CYS	C-N-CA	6.21	130.12	120.75
10	Y	814	ARG	NE-CZ-NH2	6.20	124.78	119.20
4	L	1831	CYS	CA-C-N	6.20	130.11	120.75
4	L	1831	CYS	C-N-CA	6.20	130.11	120.75
10	X	814	ARG	NE-CZ-NH2	6.18	124.76	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	9	HIS	CB-CG-CD2	-6.09	123.29	131.20
9	O	9	HIS	CB-CG-CD2	-6.09	123.29	131.20
9	P	156	ASN	OD1-CG-ND2	-6.09	116.51	122.60
4	L	1956	PHE	CA-CB-CG	6.08	119.88	113.80
2	A	319	SER	N-CA-C	6.08	117.47	108.60
2	J	334	THR	OG1-CB-CG2	6.08	121.45	109.30
2	A	334	THR	OG1-CB-CG2	6.07	121.44	109.30
4	L	3576	ASP	O-C-N	6.06	128.34	122.03
4	C	1956	PHE	CA-CB-CG	6.06	119.86	113.80
9	G	156	ASN	OD1-CG-ND2	-6.05	116.55	122.60
4	C	3576	ASP	O-C-N	6.05	128.32	122.03
2	J	319	SER	N-CA-C	6.04	117.42	108.60
9	P	73	ALA	CA-C-N	6.03	129.93	120.89
9	P	73	ALA	C-N-CA	6.03	129.93	120.89
4	L	3964	THR	CA-C-N	6.02	130.76	121.19
4	L	3964	THR	C-N-CA	6.02	130.76	121.19
4	C	3969	ASN	CA-CB-CG	6.02	118.62	112.60
3	K	409	PHE	CA-CB-CG	6.01	119.81	113.80
8	I	57	ARG	NE-CZ-NH2	6.01	124.61	119.20
9	G	73	ALA	CA-C-N	6.01	129.91	120.89
9	G	73	ALA	C-N-CA	6.01	129.91	120.89
4	C	3964	THR	CA-C-N	6.01	130.74	121.19
4	C	3964	THR	C-N-CA	6.01	130.74	121.19
4	L	2177	ASN	CA-CB-CG	6.01	118.61	112.60
4	C	1444	ASP	CA-CB-CG	5.99	118.59	112.60
2	A	184	SER	O-C-N	-5.99	115.21	122.22
3	B	409	PHE	CA-CB-CG	5.99	119.79	113.80
10	Y	871	ARG	NE-CZ-NH2	5.98	124.58	119.20
3	B	517	ASN	CA-C-N	5.96	126.52	120.38
3	B	517	ASN	C-N-CA	5.96	126.52	120.38
10	X	871	ARG	NE-CZ-NH2	5.95	124.56	119.20
3	K	517	ASN	CA-C-N	5.95	126.51	120.38
3	K	517	ASN	C-N-CA	5.95	126.51	120.38
2	J	184	SER	O-C-N	-5.94	115.27	122.22
4	L	3969	ASN	CA-CB-CG	5.94	118.54	112.60
4	C	2177	ASN	CA-CB-CG	5.93	118.53	112.60
4	C	3964	THR	O-C-N	5.92	129.54	122.20
4	C	2372	PRO	N-CA-C	5.91	117.92	110.70
4	L	1444	ASP	CA-CB-CG	5.91	118.51	112.60
8	H	17	GLN	O-C-N	5.88	130.28	123.17
4	L	2372	PRO	N-CA-C	5.87	117.86	110.70
9	F	3	ARG	NE-CZ-NH2	5.86	124.47	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	3985	VAL	O-C-N	-5.86	116.17	121.91
4	C	3985	VAL	O-C-N	-5.85	116.18	121.91
9	O	3	ARG	NE-CZ-NH2	5.84	124.46	119.20
4	L	3152	SER	CA-C-N	5.84	131.70	122.36
4	L	3152	SER	C-N-CA	5.84	131.70	122.36
4	C	2577	PHE	O-C-N	-5.84	116.15	123.27
4	L	3964	THR	O-C-N	5.83	129.43	122.20
9	F	102	LYS	CA-C-N	5.83	130.86	122.40
9	F	102	LYS	C-N-CA	5.83	130.86	122.40
4	C	3152	SER	CA-C-N	5.83	131.69	122.36
4	C	3152	SER	C-N-CA	5.83	131.69	122.36
4	C	649	PHE	CA-CB-CG	5.80	119.60	113.80
4	L	1919	CYS	O-C-N	-5.80	116.10	122.07
4	L	649	PHE	CA-CB-CG	5.78	119.58	113.80
8	I	67	ALA	N-CA-CB	-5.78	105.03	111.10
4	C	1919	CYS	O-C-N	-5.78	116.12	122.07
10	X	879	ARG	NE-CZ-NH2	5.77	124.39	119.20
8	H	57	ARG	NE-CZ-NH2	5.76	124.39	119.20
4	C	3778	ASP	CA-C-N	5.75	128.25	120.38
4	C	3778	ASP	C-N-CA	5.75	128.25	120.38
8	H	151	ARG	NE-CZ-NH2	5.74	124.36	119.20
9	F	150	ARG	NE-CZ-NH2	5.74	124.36	119.20
9	O	150	ARG	NE-CZ-NH2	5.73	124.36	119.20
4	L	3778	ASP	CA-C-N	5.73	128.23	120.38
4	L	3778	ASP	C-N-CA	5.73	128.23	120.38
9	P	7	ARG	NE-CZ-NH2	5.72	124.35	119.20
9	G	7	ARG	NE-CZ-NH2	5.72	124.35	119.20
10	Y	879	ARG	NE-CZ-NH2	5.71	124.34	119.20
2	J	395	ALA	N-CA-C	5.70	119.35	110.17
4	C	3458	SER	N-CA-C	5.70	119.53	112.47
2	A	395	ALA	N-CA-C	5.70	119.34	110.17
4	L	4049	ARG	NE-CZ-NH2	5.69	124.32	119.20
4	C	2578	GLU	N-CA-C	5.69	117.48	111.28
10	Y	770	ASP	CA-C-N	5.67	128.67	120.79
10	Y	770	ASP	C-N-CA	5.67	128.67	120.79
10	X	770	ASP	CA-C-N	5.66	128.66	120.79
10	X	770	ASP	C-N-CA	5.66	128.66	120.79
8	H	62	ASN	CA-C-N	5.65	128.16	120.54
8	H	62	ASN	C-N-CA	5.65	128.16	120.54
4	C	2208	ASP	CA-CB-CG	5.64	118.24	112.60
4	L	2208	ASP	CA-CB-CG	5.64	118.24	112.60
10	X	862	HIS	CB-CG-CD2	-5.62	123.89	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	63	PHE	CA-CB-CG	5.62	119.42	113.80
4	L	3458	SER	N-CA-C	5.62	119.44	112.47
4	C	3125	ARG	NE-CZ-NH2	5.62	124.26	119.20
4	C	2246	LYS	N-CA-C	5.61	118.24	108.76
4	L	2246	LYS	N-CA-C	5.60	118.22	108.76
4	C	4049	ARG	NE-CZ-NH2	5.60	124.24	119.20
4	L	3125	ARG	NE-CZ-NH2	5.59	124.23	119.20
8	I	75	HIS	CB-CG-CD2	-5.58	123.94	131.20
10	Y	862	HIS	CB-CG-CD2	-5.58	123.94	131.20
3	K	405	VAL	N-CA-C	5.57	117.94	108.86
4	L	1117	ASP	CA-CB-CG	5.55	118.15	112.60
2	A	358	LYS	O-C-N	-5.55	113.53	122.41
4	C	2464	HIS	CB-CG-CD2	-5.55	123.99	131.20
4	C	1117	ASP	CA-CB-CG	5.54	118.14	112.60
4	L	3732	LEU	N-CA-C	5.54	118.85	111.75
3	B	405	VAL	N-CA-C	5.53	117.88	108.86
4	C	63	PHE	CA-CB-CG	5.52	119.32	113.80
2	A	165	ARG	NE-CZ-NH2	5.51	124.16	119.20
4	C	2260	PHE	CA-CB-CG	5.51	119.31	113.80
4	C	120	ALA	CA-C-N	5.51	127.92	120.38
4	C	120	ALA	C-N-CA	5.51	127.92	120.38
4	L	120	ALA	CA-C-N	5.50	127.92	120.38
4	L	120	ALA	C-N-CA	5.50	127.92	120.38
4	L	385	TYR	CA-C-N	5.50	127.69	120.60
4	L	385	TYR	C-N-CA	5.50	127.69	120.60
4	C	172	GLU	CB-CA-C	-5.50	102.25	110.88
4	C	2580	PRO	CA-C-N	5.50	127.65	120.28
4	C	2580	PRO	C-N-CA	5.50	127.65	120.28
9	F	143	HIS	CA-CB-CG	-5.50	108.30	113.80
4	L	2464	HIS	CB-CG-CD2	-5.48	124.07	131.20
2	J	53	SER	CA-C-N	5.48	130.90	121.86
2	J	53	SER	C-N-CA	5.48	130.90	121.86
4	C	1834	ASP	CA-CB-CG	5.48	118.08	112.60
9	G	153	ARG	NE-CZ-NH2	5.48	124.13	119.20
4	L	172	GLU	CB-CA-C	-5.47	102.29	110.88
8	H	178	ARG	NE-CZ-NH2	5.47	124.12	119.20
2	A	53	SER	CA-C-N	5.47	130.88	121.86
2	A	53	SER	C-N-CA	5.47	130.88	121.86
9	P	153	ARG	NE-CZ-NH2	5.47	124.12	119.20
4	C	3763	ARG	NE-CZ-NH2	5.46	124.12	119.20
9	G	133	THR	CA-C-N	5.46	127.93	120.77
9	G	133	THR	C-N-CA	5.46	127.93	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	64	ARG	NE-CZ-NH2	5.46	124.11	119.20
2	J	165	ARG	NE-CZ-NH2	5.46	124.11	119.20
2	J	358	LYS	O-C-N	-5.46	113.67	122.41
9	O	143	HIS	CA-CB-CG	-5.46	108.34	113.80
8	H	67	ALA	CA-C-N	5.46	123.64	119.66
8	H	67	ALA	C-N-CA	5.46	123.64	119.66
8	H	46	HIS	CB-CG-CD2	-5.46	124.11	131.20
4	C	3530	VAL	N-CA-C	5.46	115.90	110.23
9	O	161	ARG	NE-CZ-NH2	5.45	124.11	119.20
4	L	407	VAL	N-CA-C	5.45	116.18	110.62
9	P	133	THR	CA-C-N	5.45	127.91	120.77
9	P	133	THR	C-N-CA	5.45	127.91	120.77
4	L	3530	VAL	N-CA-C	5.45	115.89	110.23
10	X	711	ASN	CA-CB-CG	5.44	118.04	112.60
4	C	385	TYR	CA-C-N	5.44	127.62	120.60
4	C	385	TYR	C-N-CA	5.44	127.62	120.60
10	Y	711	ASN	CA-CB-CG	5.44	118.04	112.60
9	P	183	VAL	CA-C-N	5.44	127.51	120.44
9	P	183	VAL	C-N-CA	5.44	127.51	120.44
4	L	213	ARG	NE-CZ-NH2	5.44	124.09	119.20
4	L	1384	PHE	CA-CB-CG	5.44	119.24	113.80
4	C	407	VAL	N-CA-C	5.44	116.17	110.62
9	G	183	VAL	CA-C-N	5.43	127.50	120.44
9	G	183	VAL	C-N-CA	5.43	127.50	120.44
9	F	161	ARG	NE-CZ-NH2	5.42	124.08	119.20
4	L	2260	PHE	CA-CB-CG	5.42	119.22	113.80
4	L	1834	ASP	CA-CB-CG	5.42	118.02	112.60
4	L	3763	ARG	NE-CZ-NH2	5.41	124.07	119.20
8	H	62	ASN	CA-CB-CG	5.41	118.01	112.60
4	C	3991	PHE	CA-CB-CG	5.40	119.20	113.80
4	L	198	ARG	NE-CZ-NH2	5.39	124.05	119.20
4	C	1384	PHE	CA-CB-CG	5.39	119.19	113.80
3	K	390	VAL	N-CA-C	5.39	117.15	108.85
4	L	1916	ILE	CA-C-N	5.37	128.22	120.38
4	L	1916	ILE	C-N-CA	5.37	128.22	120.38
8	I	151	ARG	NE-CZ-NH2	5.37	124.03	119.20
4	C	213	ARG	NE-CZ-NH2	5.37	124.03	119.20
3	K	227	PHE	CA-CB-CG	5.37	119.17	113.80
4	L	3991	PHE	CA-CB-CG	5.36	119.16	113.80
3	B	390	VAL	N-CA-C	5.36	117.11	108.85
4	C	3186	ARG	NE-CZ-NH2	5.36	124.02	119.20
4	C	1916	ILE	CA-C-N	5.35	128.19	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1916	ILE	C-N-CA	5.35	128.19	120.38
4	C	2088	LEU	O-C-N	-5.35	116.68	122.19
4	L	3462	ARG	NE-CZ-NH2	5.35	124.01	119.20
4	L	3777	GLN	O-C-N	-5.34	114.94	122.26
3	B	227	PHE	CA-CB-CG	5.34	119.14	113.80
4	L	3700	GLU	CB-CG-CD	5.33	121.66	112.60
4	L	3252	PHE	N-CA-C	5.33	116.89	111.14
4	C	3700	GLU	CB-CG-CD	5.32	121.64	112.60
4	L	11	SER	O-C-N	-5.31	116.60	122.07
4	C	3462	ARG	NE-CZ-NH2	5.31	123.98	119.20
4	C	3777	GLN	O-C-N	-5.31	114.99	122.26
4	C	3252	PHE	N-CA-C	5.30	116.86	111.14
4	L	2426	HIS	O-C-N	-5.29	115.62	122.77
4	C	11	SER	O-C-N	-5.29	116.62	122.07
4	C	2426	HIS	O-C-N	-5.29	115.63	122.77
8	H	133	GLN	OE1-CD-NE2	-5.29	117.31	122.60
3	B	109	ASP	N-CA-C	5.28	122.06	110.80
4	L	990	GLN	OE1-CD-NE2	-5.28	117.32	122.60
4	C	1971	PRO	N-CA-C	5.27	120.78	113.98
2	A	339	ARG	NE-CZ-NH2	5.27	123.94	119.20
4	L	3247	ARG	NE-CZ-NH2	5.27	123.94	119.20
4	L	2088	LEU	O-C-N	-5.27	116.76	122.19
4	C	198	ARG	NE-CZ-NH2	5.27	123.94	119.20
3	B	408	ALA	CA-C-N	5.26	128.68	121.74
3	B	408	ALA	C-N-CA	5.26	128.68	121.74
4	L	1729	PHE	CA-CB-CG	5.25	119.05	113.80
4	L	3186	ARG	NE-CZ-NH2	5.25	123.93	119.20
3	K	408	ALA	CA-C-N	5.25	128.67	121.74
3	K	408	ALA	C-N-CA	5.25	128.67	121.74
9	F	179	ARG	NE-CZ-NH2	5.25	123.92	119.20
4	C	1729	PHE	CA-CB-CG	5.25	119.05	113.80
9	O	179	ARG	NE-CZ-NH2	5.25	123.92	119.20
3	K	109	ASP	N-CA-C	5.24	121.97	110.80
4	C	990	GLN	OE1-CD-NE2	-5.24	117.36	122.60
4	C	635	PRO	CA-C-N	5.23	129.55	122.07
4	C	635	PRO	C-N-CA	5.23	129.55	122.07
2	J	517	ARG	NE-CZ-NH2	5.22	123.90	119.20
4	C	3743	HIS	CB-CG-CD2	-5.22	124.41	131.20
10	X	846	ARG	NE-CZ-NH2	5.22	123.90	119.20
4	C	1735	ARG	NE-CZ-NH2	5.21	123.89	119.20
4	L	1388	ASP	CA-CB-CG	5.21	117.81	112.60
4	L	1735	ARG	NE-CZ-NH2	5.21	123.89	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	195	HIS	CB-CG-CD2	-5.21	124.43	131.20
4	L	3962	ARG	NE-CZ-NH2	5.21	123.89	119.20
8	H	43	GLN	OE1-CD-NE2	-5.21	117.39	122.60
2	J	339	ARG	NE-CZ-NH2	5.20	123.88	119.20
4	L	1971	PRO	N-CA-C	5.19	120.68	113.98
9	O	90	LYS	CA-C-N	5.19	127.49	120.44
9	O	90	LYS	C-N-CA	5.19	127.49	120.44
4	L	3743	HIS	CB-CG-CD2	-5.18	124.46	131.20
9	G	195	HIS	CB-CG-CD2	-5.18	124.46	131.20
2	J	79	ASP	CA-C-N	5.18	129.48	120.68
2	J	79	ASP	C-N-CA	5.18	129.48	120.68
4	C	63	PHE	N-CA-CB	-5.17	103.44	111.35
2	A	79	ASP	CA-C-N	5.17	129.47	120.68
2	A	79	ASP	C-N-CA	5.17	129.47	120.68
10	Y	846	ARG	NE-CZ-NH2	5.17	123.85	119.20
9	O	25	GLU	CA-C-N	5.17	131.41	121.54
9	O	25	GLU	C-N-CA	5.17	131.41	121.54
9	F	25	GLU	CA-C-N	5.16	131.40	121.54
9	F	25	GLU	C-N-CA	5.16	131.40	121.54
4	L	1853	SER	N-CA-C	5.16	114.85	108.19
4	L	63	PHE	N-CA-CB	-5.16	103.46	111.35
9	F	90	LYS	CA-C-N	5.16	127.45	120.44
9	F	90	LYS	C-N-CA	5.16	127.45	120.44
4	C	1388	ASP	CA-CB-CG	5.16	117.75	112.60
4	C	3247	ARG	NE-CZ-NH2	5.16	123.84	119.20
4	L	635	PRO	CA-C-N	5.15	129.43	122.07
4	L	635	PRO	C-N-CA	5.15	129.43	122.07
4	C	3962	ARG	NE-CZ-NH2	5.15	123.83	119.20
2	J	436	PHE	CA-CB-CG	5.15	118.95	113.80
2	A	436	PHE	CA-CB-CG	5.14	118.94	113.80
9	P	61	MET	N-CA-C	5.14	118.08	109.96
4	C	1973	LYS	CA-C-N	5.14	127.44	120.65
4	C	1973	LYS	C-N-CA	5.14	127.44	120.65
10	X	821	ASP	CA-CB-CG	5.14	117.74	112.60
4	C	1853	SER	N-CA-C	5.13	114.81	108.19
4	L	172	GLU	N-CA-CB	5.13	117.45	110.01
4	L	1973	LYS	CA-C-N	5.12	127.41	120.65
4	L	1973	LYS	C-N-CA	5.12	127.41	120.65
4	L	891	ARG	NE-CZ-NH2	5.12	123.80	119.20
4	L	1194	PHE	CA-C-N	5.12	124.42	120.33
4	L	1194	PHE	C-N-CA	5.12	124.42	120.33
4	C	3696	ARG	NE-CZ-NH2	5.12	123.81	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	62	ASN	CA-C-N	5.11	128.49	120.82
8	I	62	ASN	C-N-CA	5.11	128.49	120.82
10	Y	821	ASP	CA-CB-CG	5.11	117.71	112.60
4	L	1340	ARG	NE-CZ-NH2	5.10	123.79	119.20
4	L	854	ARG	NE-CZ-NH2	5.10	123.79	119.20
4	C	1194	PHE	CA-C-N	5.10	124.41	120.33
4	C	1194	PHE	C-N-CA	5.10	124.41	120.33
4	L	2492	ASP	CA-CB-CG	5.10	117.70	112.60
4	L	3696	ARG	NE-CZ-NH2	5.10	123.79	119.20
4	C	2922	ARG	NE-CZ-NH2	5.09	123.78	119.20
2	A	517	ARG	NE-CZ-NH2	5.09	123.78	119.20
4	C	172	GLU	N-CA-CB	5.09	117.39	110.01
10	X	661	ASP	CA-CB-CG	5.09	117.69	112.60
4	L	238	MET	N-CA-C	5.08	118.97	112.87
9	G	180	PHE	CA-C-N	5.08	127.15	120.60
9	G	180	PHE	C-N-CA	5.08	127.15	120.60
4	L	1614	GLN	OE1-CD-NE2	-5.08	117.52	122.60
4	L	1721	HIS	CB-CG-CD2	-5.08	124.60	131.20
9	G	13	GLU	CA-C-N	5.08	124.69	119.56
9	G	13	GLU	C-N-CA	5.08	124.69	119.56
10	Y	661	ASP	CA-CB-CG	5.07	117.67	112.60
4	C	238	MET	N-CA-C	5.07	118.95	112.87
4	C	1340	ARG	NE-CZ-NH2	5.07	123.76	119.20
4	C	1883	ARG	NE-CZ-NH2	5.07	123.76	119.20
8	H	68	PRO	N-CA-CB	5.06	106.03	103.19
4	C	1711	ARG	NE-CZ-NH2	5.06	123.76	119.20
4	C	1614	GLN	OE1-CD-NE2	-5.06	117.54	122.60
4	L	1883	ARG	NE-CZ-NH2	5.06	123.75	119.20
2	J	187	ARG	NE-CZ-NH2	5.06	123.75	119.20
4	C	854	ARG	NE-CZ-NH2	5.05	123.75	119.20
4	C	1721	HIS	CB-CG-CD2	-5.05	124.63	131.20
4	C	891	ARG	NE-CZ-NH2	5.05	123.75	119.20
4	C	2492	ASP	CA-CB-CG	5.05	117.65	112.60
9	P	13	GLU	CA-C-N	5.05	124.66	119.56
9	P	13	GLU	C-N-CA	5.05	124.66	119.56
9	P	180	PHE	CA-C-N	5.05	127.11	120.60
9	P	180	PHE	C-N-CA	5.05	127.11	120.60
4	L	972	LEU	N-CA-CB	-5.04	103.92	110.88
4	L	3150	ASN	CA-CB-CG	5.04	117.64	112.60
4	L	3138	ILE	CA-CB-CG1	5.04	118.97	110.40
8	H	171	GLY	CA-C-N	5.03	129.50	122.36
8	H	171	GLY	C-N-CA	5.03	129.50	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	972	LEU	N-CA-CB	-5.03	103.94	110.88
4	L	2404	ARG	NE-CZ-NH2	5.02	123.72	119.20
8	H	18	LEU	N-CA-C	5.01	116.20	107.93
3	K	406	GLY	N-CA-C	5.01	116.80	110.38
4	C	1819	PHE	CA-CB-CG	5.01	118.81	113.80
8	H	158	HIS	CB-CG-CD2	-5.01	124.69	131.20
4	C	2404	ARG	NE-CZ-NH2	5.00	123.70	119.20

There are no chirality outliers.

All (145) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	137	HIS	Sidechain
2	A	71	TYR	Sidechain
2	A	88	TYR	Sidechain
3	B	242	ARG	Sidechain
3	B	421	TYR	Sidechain
3	B	44	ARG	Sidechain
3	B	444	TYR	Sidechain
3	B	489	ARG	Sidechain
4	C	1270	PHE	Sidechain
4	C	139	ARG	Sidechain
4	C	1420	ARG	Sidechain
4	C	1560	TYR	Sidechain
4	C	175	TYR	Sidechain
4	C	1873	TYR	Sidechain
4	C	1936	ARG	Sidechain
4	C	1945	TYR	Sidechain
4	C	1956	PHE	Sidechain
4	C	1965	PHE	Sidechain
4	C	198	ARG	Sidechain
4	C	2160	TYR	Sidechain
4	C	2431	ARG	Sidechain
4	C	2530	ARG	Sidechain
4	C	2546	TYR	Sidechain
4	C	265	TYR	Sidechain
4	C	2930	TYR	Sidechain
4	C	2931	ARG	Sidechain
4	C	340	TYR	Sidechain
4	C	3467	ARG	Sidechain
4	C	366	TYR	Sidechain
4	C	3784	ARG	Sidechain

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Mol	Chain	Res	Type	Group
4	C	3791	TYR	Sidechain
4	C	3874	ARG	Sidechain
4	C	3962	ARG	Sidechain
4	C	4119	ARG	Sidechain
4	C	9	ARG	Sidechain
6	D	1	DT	Sidechain
6	D	11	DC	Sidechain
6	D	12	DT	Sidechain
6	D	17	DT	Sidechain
6	D	18	DC	Sidechain
6	D	19	DA	Sidechain
6	D	22	DA	Sidechain
6	D	23	DG	Sidechain
6	D	24	DA	Sidechain
6	D	27	DA	Sidechain
6	D	29	DA	Sidechain
6	D	30	DC	Sidechain
6	D	6	DG	Sidechain
6	D	7	DA	Sidechain
6	D	8	DA	Sidechain
7	E	1	DG	Sidechain
7	E	11	DC	Sidechain
7	E	15	DC	Sidechain
7	E	16	DA	Sidechain
7	E	17	DT	Sidechain
7	E	23	DT	Sidechain
7	E	25	DC	Sidechain
7	E	26	DT	Sidechain
7	E	5	DA	Sidechain
7	E	6	DA	Sidechain
7	E	7	DT	Sidechain
9	F	143	HIS	Sidechain
9	F	192	ARG	Sidechain
9	F	66	TYR	Sidechain
9	F	7	ARG	Sidechain
9	F	94	TYR	Sidechain
9	G	111	PHE	Sidechain
9	G	192	ARG	Sidechain
9	G	3	ARG	Sidechain
8	H	17	GLN	Mainchain
8	H	81	ARG	Sidechain
8	I	118	TYR	Sidechain

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Mol	Chain	Res	Type	Group
8	I	167	TYR	Sidechain
8	I	72	PHE	Sidechain
8	I	75	HIS	Sidechain
2	J	137	HIS	Sidechain
2	J	71	TYR	Sidechain
2	J	88	TYR	Sidechain
3	K	242	ARG	Sidechain
3	K	421	TYR	Sidechain
3	K	44	ARG	Sidechain
3	K	444	TYR	Sidechain
3	K	489	ARG	Sidechain
4	L	1270	PHE	Sidechain
4	L	139	ARG	Sidechain
4	L	1420	ARG	Sidechain
4	L	1560	TYR	Sidechain
4	L	175	TYR	Sidechain
4	L	1873	TYR	Sidechain
4	L	1936	ARG	Sidechain
4	L	1945	TYR	Sidechain
4	L	1956	PHE	Sidechain
4	L	1965	PHE	Sidechain
4	L	198	ARG	Sidechain
4	L	2160	TYR	Sidechain
4	L	2311	ARG	Sidechain
4	L	2431	ARG	Sidechain
4	L	2530	ARG	Sidechain
4	L	2546	TYR	Sidechain
4	L	265	TYR	Sidechain
4	L	2930	TYR	Sidechain
4	L	2931	ARG	Sidechain
4	L	340	TYR	Sidechain
4	L	3467	ARG	Sidechain
4	L	366	TYR	Sidechain
4	L	3784	ARG	Sidechain
4	L	3791	TYR	Sidechain
4	L	3874	ARG	Sidechain
4	L	3962	ARG	Sidechain
4	L	4119	ARG	Sidechain
4	L	9	ARG	Sidechain
6	M	1	DT	Sidechain
6	M	11	DC	Sidechain
6	M	12	DT	Sidechain

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Mol	Chain	Res	Type	Group
6	M	17	DT	Sidechain
6	M	18	DC	Sidechain
6	M	19	DA	Sidechain
6	M	22	DA	Sidechain
6	M	23	DG	Sidechain
6	M	24	DA	Sidechain
6	M	27	DA	Sidechain
6	M	29	DA	Sidechain
6	M	30	DC	Sidechain
6	M	6	DG	Sidechain
6	M	7	DA	Sidechain
6	M	8	DA	Sidechain
7	N	1	DG	Sidechain
7	N	11	DC	Sidechain
7	N	15	DC	Sidechain
7	N	16	DA	Sidechain
7	N	17	DT	Sidechain
7	N	23	DT	Sidechain
7	N	25	DC	Sidechain
7	N	26	DT	Sidechain
7	N	5	DA	Sidechain
7	N	6	DA	Sidechain
7	N	7	DT	Sidechain
9	O	143	HIS	Sidechain
9	O	192	ARG	Sidechain
9	O	66	TYR	Sidechain
9	O	7	ARG	Sidechain
9	O	94	TYR	Sidechain
9	P	111	PHE	Sidechain
9	P	192	ARG	Sidechain
9	P	3	ARG	Sidechain

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	S	168	0	169	15	0
1	T	168	0	169	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4021	0	4100	57	0
2	J	4021	0	4100	58	0
3	B	4259	0	4301	9	0
3	K	4259	0	4301	8	0
4	C	29811	0	30286	111	0
4	L	29811	0	30286	108	0
5	Q	101	0	23	1	0
5	R	101	0	23	1	0
6	D	634	0	348	4	0
6	M	634	0	348	4	0
7	E	616	0	339	5	0
7	N	616	0	339	5	0
8	H	1779	0	1797	19	0
8	I	1737	0	1744	13	0
9	F	1736	0	1739	22	0
9	G	1595	0	1592	34	0
9	O	1736	0	1739	27	0
9	P	1595	0	1592	36	0
10	X	2064	0	2012	14	0
10	Y	2064	0	2012	14	0
11	C	31	0	12	0	0
11	L	31	0	12	0	0
All	All	93588	0	93383	479	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 3.

All (479) 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)
2:J:333:GLU:C	2:J:333:GLU:CA	1.77	1.57
2:A:333:GLU:CB	2:A:333:GLU:CA	1.83	1.57
2:J:333:GLU:CA	2:J:333:GLU:CB	1.83	1.56
2:A:333:GLU:CA	2:A:333:GLU:N	1.68	1.56
2:A:333:GLU:CA	2:A:333:GLU:C	1.77	1.53
2:J:333:GLU:CA	2:J:333:GLU:N	1.68	1.50
2:A:333:GLU:CB	2:A:333:GLU:CG	2.05	1.35
2:J:334:THR:OG1	2:J:334:THR:CB	1.77	1.32
2:J:333:GLU:CB	2:J:333:GLU:CG	2.05	1.32
2:A:334:THR:CB	2:A:334:THR:OG1	1.77	1.30
2:J:334:THR:N	2:J:334:THR:CA	2.08	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:334:THR:N	2:A:334:THR:CA	2.08	1.17
9:O:40:HIS:CG	9:P:120:ALA:HB2	2.05	0.91
9:F:40:HIS:CG	9:G:120:ALA:HB2	2.05	0.91
2:J:332:GLU:C	2:J:333:GLU:CA	2.46	0.89
8:I:66:THR:O	9:F:106:PHE:CE1	2.26	0.89
8:I:15:TRP:HB2	8:I:211:VAL:HG21	1.55	0.88
2:A:332:GLU:C	2:A:333:GLU:CA	2.46	0.88
1:S:196:ALA:O	2:A:477:SER:O	1.93	0.86
2:J:477:SER:O	1:T:196:ALA:O	1.93	0.86
2:A:333:GLU:CB	2:A:333:GLU:C	2.48	0.86
2:J:333:GLU:C	2:J:333:GLU:CB	2.48	0.85
2:A:334:THR:OG1	2:A:334:THR:CA	2.24	0.85
2:J:334:THR:OG1	2:J:334:THR:CA	2.24	0.85
4:C:3617:LEU:HB3	4:C:3633:ILE:HD13	1.61	0.81
4:L:3617:LEU:HB3	4:L:3633:ILE:HD13	1.61	0.81
8:I:211:VAL:HG23	8:I:212:MET:SD	2.20	0.81
9:F:40:HIS:CD2	9:G:120:ALA:HB2	2.15	0.80
9:O:40:HIS:CD2	9:P:120:ALA:HB2	2.15	0.80
9:F:124:ARG:CZ	9:G:38:ASP:O	2.31	0.79
9:O:124:ARG:CZ	9:P:38:ASP:O	2.31	0.79
2:J:333:GLU:CA	2:J:333:GLU:CG	2.62	0.78
4:L:3855:TYR:HA	4:L:3858:MET:HE3	1.66	0.78
2:A:333:GLU:CA	2:A:333:GLU:CG	2.62	0.78
2:A:334:THR:CB	2:A:334:THR:N	2.48	0.77
2:J:334:THR:CB	2:J:334:THR:N	2.48	0.76
4:C:3855:TYR:HA	4:C:3858:MET:HE3	1.66	0.76
2:J:331:LYS:O	2:J:334:THR:HG22	1.89	0.73
2:A:331:LYS:O	2:A:334:THR:HG22	1.89	0.72
2:A:333:GLU:C	2:A:334:THR:CA	2.62	0.72
2:J:333:GLU:C	2:J:334:THR:CA	2.62	0.72
9:F:120:ALA:HB1	9:G:39:GLY:C	2.14	0.71
9:O:120:ALA:HB1	9:P:39:GLY:C	2.14	0.71
1:S:186:ILE:O	2:A:74:LYS:HE3	1.91	0.71
9:F:40:HIS:CD2	9:G:120:ALA:CB	2.75	0.69
2:J:74:LYS:HE3	1:T:186:ILE:O	1.92	0.69
9:O:40:HIS:CD2	9:P:120:ALA:CB	2.75	0.69
9:F:39:GLY:O	9:G:120:ALA:HA	1.92	0.69
9:O:124:ARG:HG2	9:P:19:PHE:HE2	1.58	0.69
2:J:250:GLU:HG2	1:T:187:ASN:HD21	1.58	0.69
2:A:333:GLU:CB	2:A:333:GLU:N	2.55	0.69
9:O:39:GLY:O	9:P:120:ALA:HA	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:333:GLU:CB	2:J:333:GLU:N	2.55	0.68
8:H:116:PRO:HD3	9:O:61:MET:HE3	1.76	0.67
4:L:3764:VAL:HA	4:L:3767:LEU:HD12	1.77	0.67
2:J:333:GLU:CA	2:J:334:THR:N	2.58	0.67
1:S:187:ASN:HD21	2:A:250:GLU:HG2	1.58	0.66
9:F:124:ARG:HG2	9:G:19:PHE:HE2	1.58	0.66
8:H:116:PRO:HD3	9:O:61:MET:CE	2.26	0.66
4:C:1897:ASN:N	4:C:1898:GLN:OE1	2.28	0.66
4:L:1897:ASN:N	4:L:1898:GLN:OE1	2.28	0.66
2:J:58:THR:HB	2:J:61:ASP:HB2	1.77	0.65
4:C:3764:VAL:HA	4:C:3767:LEU:HD12	1.77	0.65
2:A:58:THR:HB	2:A:61:ASP:HB2	1.77	0.65
2:A:333:GLU:CA	2:A:334:THR:N	2.58	0.64
4:C:3653:ARG:C	4:C:3654:MET:HE2	2.23	0.64
1:S:186:ILE:O	2:A:74:LYS:CE	2.45	0.64
4:L:3653:ARG:C	4:L:3654:MET:HE2	2.23	0.64
4:L:1224:PHE:CZ	4:L:1270:PHE:CZ	2.86	0.63
4:C:1403:MET:HE2	4:C:1403:MET:HA	1.81	0.63
1:S:191:LYS:NZ	3:B:434:MET:HG2	2.14	0.63
10:X:843:LEU:HD21	9:G:163:GLU:HA	1.81	0.63
4:C:1046:PRO:HA	4:C:1049:GLN:HB3	1.80	0.63
2:J:74:LYS:CE	1:T:186:ILE:O	2.47	0.62
4:L:1403:MET:HA	4:L:1403:MET:HE2	1.80	0.62
3:K:434:MET:HG2	1:T:191:LYS:NZ	2.14	0.62
4:C:1224:PHE:CZ	4:C:1270:PHE:CZ	2.88	0.62
10:Y:843:LEU:HD21	9:P:163:GLU:HA	1.81	0.62
4:L:1046:PRO:HA	4:L:1049:GLN:HB3	1.80	0.62
2:A:131:PHE:CE2	2:A:137:HIS:CE1	2.89	0.61
4:C:1897:ASN:OD1	4:C:1898:GLN:NE2	2.33	0.61
2:J:131:PHE:CE2	2:J:137:HIS:CE1	2.89	0.61
10:X:792:MET:SD	9:G:178:LYS:HG3	2.41	0.61
4:C:1046:PRO:HD2	4:C:1047:GLN:H	1.64	0.61
10:X:843:LEU:CD2	9:G:163:GLU:HA	2.31	0.61
4:L:1046:PRO:HD2	4:L:1047:GLN:H	1.65	0.61
9:G:20:LEU:HD11	9:G:34:ILE:HD11	1.83	0.61
4:L:1240:THR:HG21	4:L:1256:TRP:CD1	2.36	0.60
9:P:20:LEU:HD11	9:P:34:ILE:HD11	1.83	0.60
10:Y:843:LEU:CD2	9:P:163:GLU:HA	2.31	0.60
10:Y:792:MET:SD	9:P:178:LYS:HG3	2.41	0.60
4:L:1897:ASN:OD1	4:L:1898:GLN:NE2	2.33	0.60
4:L:1619:ALA:HA	4:L:1652:ILE:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1619:ALA:HA	4:C:1652:ILE:HD11	1.83	0.59
4:C:1240:THR:HG21	4:C:1256:TRP:CD1	2.36	0.59
4:C:1632:TRP:CD1	4:C:1633:TRP:H	2.20	0.59
9:O:124:ARG:HG2	9:P:19:PHE:CE2	2.38	0.59
4:L:1632:TRP:CD1	4:L:1633:TRP:H	2.20	0.59
9:F:124:ARG:HG2	9:G:19:PHE:CE2	2.38	0.58
2:J:334:THR:CB	2:J:334:THR:CG2	2.82	0.58
9:G:116:VAL:HG12	9:G:117:GLU:H	1.69	0.58
2:A:334:THR:CB	2:A:334:THR:CG2	2.82	0.57
2:J:241:ASP:O	1:T:186:ILE:HD11	2.04	0.57
9:P:116:VAL:HG12	9:P:117:GLU:H	1.69	0.57
4:C:1046:PRO:HD2	4:C:1047:GLN:N	2.20	0.57
4:L:1046:PRO:HD2	4:L:1047:GLN:N	2.20	0.56
8:H:208:LYS:HG2	8:H:212:MET:HE1	1.86	0.56
1:S:196:ALA:O	2:A:477:SER:C	2.48	0.56
2:J:477:SER:C	1:T:196:ALA:O	2.48	0.56
2:A:333:GLU:HA	2:A:336:GLU:HB3	1.87	0.56
1:S:186:ILE:HD11	2:A:241:ASP:O	2.06	0.56
3:K:434:MET:HG2	1:T:191:LYS:HZ2	1.69	0.56
4:C:490:ILE:HD13	4:C:527:TYR:CD1	2.41	0.56
4:C:490:ILE:HD11	4:C:524:TYR:HA	1.88	0.56
9:F:120:ALA:CB	9:G:39:GLY:C	2.79	0.55
4:L:490:ILE:HD13	4:L:527:TYR:CD1	2.41	0.55
9:O:120:ALA:CB	9:P:39:GLY:C	2.79	0.55
2:J:333:GLU:HA	2:J:336:GLU:HB3	1.87	0.55
2:A:49:PHE:CD2	2:A:137:HIS:ND1	2.75	0.55
8:H:18:LEU:HD13	8:H:96:SER:HA	1.87	0.55
2:J:49:PHE:CD2	2:J:137:HIS:ND1	2.75	0.55
4:L:1770:GLN:OE1	4:L:1770:GLN:N	2.33	0.55
8:I:10:MET:SD	8:I:223:THR:HA	2.47	0.55
4:C:1372:LEU:HD11	4:C:1403:MET:HE3	1.89	0.55
4:L:1372:LEU:HD11	4:L:1403:MET:HE3	1.89	0.55
4:L:490:ILE:HD11	4:L:524:TYR:HA	1.88	0.54
10:Y:847:PHE:O	9:P:169:LYS:CE	2.56	0.54
2:J:132:GLN:OE1	2:J:137:HIS:CD2	2.60	0.54
2:A:132:GLN:OE1	2:A:137:HIS:CD2	2.60	0.54
9:O:117:GLU:CD	9:O:117:GLU:H	2.15	0.54
1:S:187:ASN:ND2	2:A:250:GLU:HG2	2.23	0.54
4:L:135:LEU:HD12	4:L:184:VAL:HG21	1.89	0.54
4:L:1048:GLN:O	4:L:1053:PRO:HD3	2.07	0.54
10:X:847:PHE:O	9:G:169:LYS:CE	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:117:GLU:CD	9:F:117:GLU:H	2.15	0.54
4:L:3296:GLN:O	4:L:3300:VAL:HG12	2.08	0.54
8:H:12:PRO:HB3	8:H:219:MET:SD	2.48	0.54
4:C:1048:GLN:O	4:C:1053:PRO:HD3	2.07	0.54
4:L:1048:GLN:HB2	4:L:1052:SER:HB3	1.90	0.54
4:L:2245:TRP:CD2	4:L:2246:LYS:HE2	2.43	0.54
10:X:847:PHE:O	9:G:169:LYS:HE3	2.08	0.54
2:A:362:LEU:HD23	2:A:436:PHE:HB3	1.90	0.53
4:C:135:LEU:HD12	4:C:184:VAL:HG21	1.89	0.53
4:C:2245:TRP:CD2	4:C:2246:LYS:HE2	2.43	0.53
4:C:3296:GLN:O	4:C:3300:VAL:HG12	2.08	0.53
4:L:2379:MET:HE1	4:L:2401:VAL:HA	1.91	0.53
10:Y:847:PHE:O	9:P:169:LYS:HE3	2.08	0.53
4:C:1048:GLN:HB2	4:C:1052:SER:HB3	1.90	0.53
4:C:1867:ILE:HD11	4:C:1940:TYR:CG	2.44	0.53
4:L:1224:PHE:CE1	4:L:1270:PHE:CZ	2.97	0.52
4:L:1867:ILE:HD11	4:L:1940:TYR:CG	2.44	0.52
2:J:250:GLU:HG2	1:T:187:ASN:ND2	2.23	0.52
4:C:1046:PRO:HA	4:C:1049:GLN:CB	2.40	0.52
9:O:104:VAL:HG12	9:O:105:SER:H	1.74	0.52
2:J:362:LEU:HD23	2:J:436:PHE:HB3	1.90	0.52
4:L:1898:GLN:OE1	4:L:1898:GLN:N	2.43	0.52
8:I:10:MET:SD	8:I:223:THR:HG22	2.50	0.52
4:C:1538:LEU:HD12	4:C:1553:PHE:CE2	2.45	0.52
2:J:169:PHE:CE2	2:J:203:MET:SD	3.03	0.52
4:L:51:LEU:HD21	4:L:96:MET:HE1	1.92	0.52
4:C:1898:GLN:OE1	4:C:1898:GLN:N	2.43	0.52
2:A:267:ILE:HD12	2:A:267:ILE:H	1.75	0.52
4:C:2379:MET:HE1	4:C:2401:VAL:HA	1.91	0.52
4:C:1190:LEU:HD21	4:C:1194:PHE:CZ	2.45	0.52
4:C:2950:LYS:HE3	4:C:2981:TRP:CE3	2.45	0.52
10:Y:792:MET:SD	9:P:178:LYS:CG	2.98	0.52
4:C:1224:PHE:CE1	4:C:1270:PHE:CZ	2.98	0.51
4:C:3837:CYS:SG	4:C:3874:ARG:HB2	2.51	0.51
4:C:51:LEU:HD21	4:C:96:MET:HE1	1.91	0.51
4:C:3797:THR:HG23	4:C:3799:ARG:H	1.76	0.51
4:L:1190:LEU:HD21	4:L:1194:PHE:CZ	2.45	0.51
4:L:3797:THR:HG23	4:L:3799:ARG:H	1.76	0.51
4:C:3588:TRP:CH2	4:C:3613:MET:HG2	2.46	0.51
2:A:446:MET:HE1	3:B:365:PHE:CZ	2.46	0.51
4:L:3837:CYS:SG	4:L:3874:ARG:HB2	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:169:PHE:CE2	2:A:203:MET:SD	3.03	0.51
3:K:340:PHE:CE1	3:K:393:VAL:HG11	2.46	0.51
2:A:334:THR:OG1	2:A:334:THR:HA	2.11	0.51
4:L:1538:LEU:HD12	4:L:1553:PHE:CE2	2.45	0.51
10:Y:847:PHE:O	9:P:169:LYS:NZ	2.44	0.51
4:L:2311:ARG:HH11	7:N:7:DT:P	2.34	0.51
4:L:3626:GLY:HA3	4:L:3629:ARG:HB2	1.93	0.51
3:B:60:GLY:H	3:B:105:ALA:HB3	1.76	0.51
10:X:847:PHE:O	9:G:169:LYS:NZ	2.44	0.51
2:J:333:GLU:CB	2:J:333:GLU:CD	2.83	0.50
4:C:2311:ARG:HH11	7:E:7:DT:P	2.34	0.50
4:L:2950:LYS:HE3	4:L:2981:TRP:CE3	2.45	0.50
3:B:340:PHE:CE1	3:B:393:VAL:HG11	2.46	0.50
4:C:2379:MET:CE	4:C:2401:VAL:HA	2.42	0.50
4:C:3626:GLY:HA3	4:C:3629:ARG:HB2	1.94	0.50
4:L:1046:PRO:HA	4:L:1049:GLN:CB	2.40	0.50
3:B:408:ALA:HB1	3:B:419:LEU:HD21	1.93	0.50
10:X:792:MET:SD	9:G:178:LYS:CG	2.98	0.50
2:J:267:ILE:HD12	2:J:267:ILE:H	1.75	0.50
3:K:60:GLY:H	3:K:105:ALA:HB3	1.76	0.50
4:L:2379:MET:CE	4:L:2401:VAL:HA	2.42	0.50
4:L:3588:TRP:CH2	4:L:3613:MET:HG2	2.46	0.50
4:L:3666:LEU:O	4:L:3670:MET:HG2	2.12	0.50
2:J:58:THR:O	2:J:62:MET:N	2.45	0.50
4:C:3666:LEU:O	4:C:3670:MET:HG2	2.12	0.50
2:J:446:MET:HE1	3:K:365:PHE:CZ	2.46	0.49
2:A:58:THR:O	2:A:62:MET:N	2.45	0.49
3:K:408:ALA:HB1	3:K:419:LEU:HD21	1.93	0.49
6:M:14:DA:N6	7:N:17:DT:H3	2.11	0.49
2:A:333:GLU:CB	2:A:333:GLU:CD	2.83	0.49
4:L:3157:LEU:C	4:L:3157:LEU:HD23	2.38	0.49
2:J:136:GLY:C	2:J:137:HIS:CD2	2.91	0.49
8:I:68:PRO:HD3	9:F:104:VAL:HG11	1.95	0.49
2:A:67:ILE:O	2:A:71:TYR:HB2	2.13	0.49
2:A:136:GLY:C	2:A:137:HIS:CD2	2.91	0.49
4:C:2154:GLU:OE2	4:C:2192:THR:HG22	2.13	0.49
6:D:14:DA:N6	7:E:17:DT:H3	2.11	0.49
4:L:2154:GLU:OE2	4:L:2192:THR:HG22	2.13	0.48
8:H:97:CYS:SG	8:H:104:LEU:HD11	2.53	0.48
4:C:1100:VAL:HA	4:C:1103:ALA:HB3	1.95	0.48
4:C:1770:GLN:OE1	4:C:1770:GLN:N	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:3157:LEU:HD23	4:C:3157:LEU:C	2.38	0.48
2:J:67:ILE:O	2:J:71:TYR:HB2	2.13	0.48
4:L:1100:VAL:HA	4:L:1103:ALA:HB3	1.95	0.48
8:H:208:LYS:CG	8:H:212:MET:HE1	2.42	0.48
4:L:2897:LEU:HD22	4:L:2923:TRP:CD1	2.49	0.48
8:I:140:MET:SD	8:I:140:MET:C	2.97	0.48
9:P:91:GLU:CD	9:P:91:GLU:H	2.22	0.48
2:J:517:ARG:HH11	1:T:201:PHE:HB2	1.79	0.48
4:L:828:LYS:HA	4:L:831:LEU:HD13	1.95	0.48
2:J:131:PHE:CE2	2:J:137:HIS:NE2	2.82	0.48
2:J:238:LYS:HG2	1:T:185:LEU:HD13	1.94	0.48
2:J:334:THR:OG1	2:J:334:THR:HA	2.11	0.48
4:C:439:VAL:HG13	4:C:461:ILE:HD11	1.95	0.48
10:Y:796:ILE:HG12	9:P:177:TYR:CG	2.49	0.48
10:X:796:ILE:HG12	9:G:177:TYR:CG	2.49	0.48
1:S:191:LYS:HZ2	3:B:434:MET:HG2	1.77	0.48
4:L:439:VAL:HG13	4:L:461:ILE:HD11	1.95	0.48
4:C:828:LYS:HA	4:C:831:LEU:HD13	1.95	0.48
4:C:2188:GLU:O	4:C:2192:THR:HG23	2.14	0.48
2:A:131:PHE:CE2	2:A:137:HIS:NE2	2.82	0.47
4:L:3859:TYR:HA	4:L:4119:ARG:HH21	1.79	0.47
9:O:40:HIS:CB	9:P:120:ALA:HB2	2.44	0.47
1:S:201:PHE:CZ	2:A:469:LEU:HD13	2.49	0.47
4:C:1138:ILE:HD12	4:C:1194:PHE:CZ	2.49	0.47
4:C:3659:PHE:O	4:C:3663:THR:HG23	2.13	0.47
4:L:3659:PHE:O	4:L:3663:THR:HG23	2.13	0.47
1:S:191:LYS:HZ1	3:B:434:MET:HG2	1.79	0.47
4:C:3859:TYR:HA	4:C:4119:ARG:HH21	1.79	0.47
9:F:40:HIS:CB	9:G:120:ALA:HB2	2.44	0.47
2:A:145:GLU:O	2:A:149:VAL:HG23	2.15	0.47
4:L:1138:ILE:HD12	4:L:1194:PHE:CZ	2.49	0.47
4:C:3141:PHE:CD1	4:C:3141:PHE:C	2.93	0.47
1:S:185:LEU:HD13	2:A:238:LYS:HG2	1.96	0.47
4:L:2188:GLU:O	4:L:2192:THR:HG23	2.15	0.47
2:J:469:LEU:HD13	1:T:201:PHE:CZ	2.49	0.47
4:L:828:LYS:HA	4:L:831:LEU:CD1	2.45	0.47
4:L:3650:LYS:O	4:L:3650:LYS:HD3	2.15	0.47
6:M:24:DA:C2	6:M:25:DT:C2	3.03	0.47
8:H:116:PRO:CD	9:O:61:MET:HE3	2.42	0.47
4:C:828:LYS:HA	4:C:831:LEU:CD1	2.45	0.47
4:C:2897:LEU:HD22	4:C:2923:TRP:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:149:VAL:O	2:A:153:LEU:HD23	2.15	0.47
4:C:3650:LYS:O	4:C:3650:LYS:HD3	2.15	0.47
2:J:145:GLU:O	2:J:149:VAL:HG23	2.15	0.47
4:L:1877:LEU:HD12	4:L:1878:ASP:N	2.30	0.47
4:L:3141:PHE:CD1	4:L:3141:PHE:C	2.93	0.47
8:H:51:THR:HG23	8:H:69:PRO:CG	2.45	0.47
2:A:348:MET:HE2	2:A:399:ARG:HD3	1.97	0.46
6:D:24:DA:C2	6:D:25:DT:C2	3.03	0.46
9:O:194:LEU:HD23	9:P:198:LEU:HD13	1.96	0.46
2:J:348:MET:HE2	2:J:399:ARG:HD3	1.98	0.46
3:B:246:HIS:CD2	3:B:368:ARG:HH22	2.33	0.46
4:C:395:MET:HG3	4:C:413:PHE:CE2	2.50	0.46
9:F:194:LEU:HD23	9:G:198:LEU:HD13	1.96	0.46
9:G:91:GLU:CD	9:G:91:GLU:H	2.22	0.46
9:P:34:ILE:HD13	9:P:35:THR:N	2.30	0.46
10:X:843:LEU:HB3	9:G:166:VAL:HG21	1.98	0.46
9:G:34:ILE:HD13	9:G:35:THR:N	2.30	0.46
4:C:3809:THR:HG22	4:C:3931:ALA:HA	1.98	0.46
4:C:1261:LEU:HD13	4:C:1337:VAL:HA	1.98	0.46
10:Y:843:LEU:HB3	9:P:166:VAL:HG21	1.98	0.46
3:K:496:HIS:CD2	3:K:506:PRO:HD3	2.51	0.46
4:L:395:MET:HG3	4:L:413:PHE:CE2	2.50	0.46
3:B:496:HIS:CD2	3:B:506:PRO:HD3	2.51	0.46
4:C:237:SER:HB2	4:C:281:GLN:HA	1.98	0.46
1:S:186:ILE:O	2:A:74:LYS:HE2	2.16	0.46
4:L:3425:ARG:HA	4:L:3425:ARG:NE	2.31	0.46
4:C:1271:ILE:HD12	4:C:1271:ILE:H	1.81	0.46
3:K:246:HIS:CD2	3:K:368:ARG:HH22	2.33	0.46
4:L:1261:LEU:HD13	4:L:1337:VAL:HA	1.98	0.46
8:I:194:MET:SD	8:I:194:MET:N	2.89	0.46
4:L:237:SER:HB2	4:L:281:GLN:HA	1.98	0.45
2:J:333:GLU:N	2:J:334:THR:N	2.64	0.45
4:C:1877:LEU:HD12	4:C:1878:ASP:N	2.30	0.45
4:C:3425:ARG:HA	4:C:3425:ARG:NE	2.31	0.45
4:L:1805:PHE:CD1	4:L:1820:VAL:HG23	2.51	0.45
10:X:846:ARG:NH2	9:G:166:VAL:HG12	2.32	0.45
2:A:333:GLU:N	2:A:334:THR:N	2.64	0.45
1:S:201:PHE:HB2	2:A:517:ARG:HH11	1.81	0.45
4:C:1805:PHE:CD1	4:C:1820:VAL:HG23	2.51	0.45
4:C:3496:ILE:HD11	4:C:3528:ALA:HB1	1.99	0.45
4:L:2810:SER:HA	4:L:2861:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:51:THR:HG23	8:H:69:PRO:HG3	1.99	0.45
4:C:1913:LYS:HB3	4:C:1956:PHE:CZ	2.52	0.45
4:L:249:PHE:CE2	4:L:285:CYS:HB3	2.52	0.45
4:C:2810:SER:HA	4:C:2861:ILE:HD11	1.98	0.45
4:C:3767:LEU:HD11	4:C:4002:MET:SD	2.57	0.45
10:Y:846:ARG:NH2	9:P:166:VAL:HG12	2.32	0.45
2:J:132:GLN:OE1	2:J:137:HIS:CG	2.70	0.45
4:L:1049:GLN:HA	4:L:1053:PRO:CG	2.47	0.45
4:L:1913:LYS:HB3	4:L:1956:PHE:CZ	2.52	0.45
4:L:3809:THR:HG22	4:L:3931:ALA:HA	1.98	0.45
4:C:249:PHE:CE2	4:C:285:CYS:HB3	2.52	0.45
4:C:1240:THR:HG21	4:C:1256:TRP:CG	2.52	0.45
10:Y:843:LEU:HD13	9:P:162:PHE:CD2	2.52	0.45
4:L:627:VAL:HG22	4:L:669:LEU:CD1	2.48	0.44
8:H:18:LEU:CD2	8:H:95:PHE:O	2.65	0.44
4:C:461:ILE:HD12	4:C:461:ILE:HA	1.90	0.44
9:F:40:HIS:CD2	9:G:120:ALA:HB3	2.53	0.44
2:J:200:LEU:C	2:J:200:LEU:HD23	2.43	0.44
8:H:140:MET:C	8:H:140:MET:SD	3.01	0.44
2:J:149:VAL:O	2:J:153:LEU:HD23	2.15	0.44
4:L:1240:THR:HG21	4:L:1256:TRP:CG	2.52	0.44
4:L:3171:ALA:HA	4:L:3179:TRP:CZ3	2.53	0.44
8:I:67:ALA:HB3	8:I:72:PHE:CE2	2.52	0.44
2:A:132:GLN:OE1	2:A:137:HIS:CG	2.70	0.44
2:A:200:LEU:C	2:A:200:LEU:HD23	2.43	0.44
4:L:3496:ILE:HD11	4:L:3528:ALA:HB1	1.99	0.44
4:L:3651:LEU:C	4:L:3654:MET:HE3	2.43	0.44
4:L:3767:LEU:HD11	4:L:4002:MET:SD	2.57	0.44
7:N:26:DT:H2'	7:N:27:DT:C6	2.53	0.44
4:L:2383:PHE:O	4:L:2418:LYS:HE2	2.18	0.44
10:X:843:LEU:HD13	9:G:162:PHE:CD2	2.52	0.44
4:L:3767:LEU:HD13	4:L:3918:LEU:HD13	2.00	0.44
4:C:1805:PHE:CG	4:C:1820:VAL:HG23	2.53	0.44
4:C:1920:TYR:CE1	4:C:1924:THR:HG21	2.53	0.44
8:H:67:ALA:HB2	9:O:106:PHE:CZ	2.53	0.43
4:C:2813:PHE:CD1	4:C:2861:ILE:HD12	2.53	0.43
2:J:74:LYS:HE2	1:T:186:ILE:O	2.18	0.43
2:A:332:GLU:O	2:A:333:GLU:CA	2.66	0.43
4:C:3171:ALA:HA	4:C:3179:TRP:CZ3	2.53	0.43
4:L:1169:VAL:HG21	4:L:1198:LEU:HD21	1.99	0.43
4:L:1920:TYR:CE1	4:L:1924:THR:HG21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:46:HIS:HB3	8:H:124:MET:SD	2.59	0.43
4:C:1049:GLN:HA	4:C:1053:PRO:CG	2.47	0.43
4:C:1169:VAL:HG21	4:C:1198:LEU:HD21	1.99	0.43
4:C:2443:MET:HE3	4:C:2476:ILE:HG23	2.00	0.43
4:C:3535:ILE:HD11	4:C:3797:THR:HA	2.00	0.43
4:C:3651:LEU:C	4:C:3654:MET:HE3	2.43	0.43
9:O:124:ARG:NE	9:P:38:ASP:O	2.51	0.43
9:P:51:GLU:HA	9:P:54:GLN:HB3	2.00	0.43
4:L:3535:ILE:HD11	4:L:3797:THR:HA	2.00	0.43
4:C:627:VAL:HG22	4:C:669:LEU:CD1	2.48	0.43
4:C:3496:ILE:CD1	4:C:3528:ALA:HB1	2.48	0.43
10:X:758:TYR:HA	10:X:764:SER:HA	2.00	0.43
9:G:51:GLU:HA	9:G:54:GLN:HB3	2.00	0.43
9:P:116:VAL:CG1	9:P:117:GLU:H	2.31	0.43
2:J:328:ILE:C	2:J:329:LEU:HD12	2.43	0.43
4:L:1157:PHE:CE1	4:L:1168:LEU:HG	2.54	0.43
4:L:3496:ILE:CD1	4:L:3528:ALA:HB1	2.48	0.43
2:A:273:ILE:HD13	2:A:368:VAL:HG22	2.01	0.43
4:L:2924:VAL:HG11	4:L:2989:ALA:HB1	1.99	0.43
8:I:1:MET:SD	8:I:4:LEU:HB2	2.59	0.43
2:A:328:ILE:C	2:A:329:LEU:HD12	2.43	0.43
4:C:3767:LEU:HD13	4:C:3918:LEU:HD13	2.00	0.43
7:E:26:DT:H2'	7:E:27:DT:C6	2.53	0.43
9:O:125:GLU:C	9:O:125:GLU:CD	2.87	0.43
10:Y:725:TRP:CD1	10:Y:742:PHE:CD2	3.07	0.43
10:Y:758:TYR:HA	10:Y:764:SER:HA	2.00	0.43
4:L:1805:PHE:CG	4:L:1820:VAL:HG23	2.53	0.43
4:L:2443:MET:HE3	4:L:2476:ILE:HG23	2.00	0.43
4:L:2813:PHE:CD1	4:L:2861:ILE:HD12	2.53	0.43
9:F:120:ALA:CB	9:G:39:GLY:O	2.67	0.43
1:S:190:PHE:CG	2:A:250:GLU:HG2	2.54	0.42
4:L:3035:PHE:CD2	9:O:276:MET:HE3	2.54	0.42
4:L:3636:PHE:CZ	4:L:3666:LEU:HG	2.54	0.42
4:L:9:ARG:CZ	4:L:9:ARG:CB	2.97	0.42
4:C:51:LEU:HD23	4:C:51:LEU:C	2.44	0.42
4:C:3636:PHE:CZ	4:C:3666:LEU:HG	2.54	0.42
4:C:3811:THR:HA	4:C:3929:MET:HG2	2.02	0.42
9:F:124:ARG:NE	9:G:38:ASP:O	2.51	0.42
10:X:725:TRP:CD1	10:X:742:PHE:CD2	3.07	0.42
2:J:98:ASN:HD22	2:J:148:TRP:CD1	2.37	0.42
4:L:1902:GLY:HA2	4:L:1905:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:3255:ALA:O	4:L:3259:LEU:HD23	2.20	0.42
4:C:2924:VAL:HG11	4:C:2989:ALA:HB1	1.99	0.42
4:C:3035:PHE:CD2	9:F:276:MET:HE3	2.54	0.42
4:L:3761:ASP:HA	4:L:3764:VAL:HG12	2.01	0.42
4:C:9:ARG:CZ	4:C:9:ARG:CB	2.97	0.42
4:C:3467:ARG:CZ	4:C:4000:ASN:HD21	2.33	0.42
9:P:68:GLY:HA2	9:P:71:ARG:HG2	2.01	0.42
2:J:332:GLU:O	2:J:333:GLU:CA	2.66	0.42
4:L:51:LEU:C	4:L:51:LEU:HD23	2.44	0.42
8:H:7:GLY:HA3	8:H:28:PHE:CE2	2.55	0.42
8:H:18:LEU:HD22	8:H:95:PHE:O	2.19	0.42
9:F:125:GLU:CD	9:F:125:GLU:C	2.87	0.42
9:P:73:ALA:HA	9:P:84:TYR:CD2	2.55	0.42
2:J:83:LEU:HD23	2:J:111:PRO:HB3	2.02	0.42
2:J:250:GLU:HG2	1:T:190:PHE:CG	2.54	0.42
8:I:208:LYS:HG2	8:I:212:MET:SD	2.59	0.42
4:C:1224:PHE:CE1	4:C:1270:PHE:CE1	3.08	0.42
9:F:134:ILE:HD11	9:G:130:CYS:HA	2.02	0.42
9:O:120:ALA:CB	9:P:39:GLY:O	2.67	0.42
2:J:41:LEU:HD21	2:J:146:VAL:HG12	2.01	0.42
4:L:3467:ARG:CZ	4:L:4000:ASN:HD21	2.33	0.42
4:L:3811:THR:HA	4:L:3929:MET:HG2	2.01	0.42
5:R:6005:UNK:O	5:R:6009:UNK:N	2.53	0.42
4:C:1157:PHE:CE1	4:C:1168:LEU:HG	2.54	0.42
5:Q:6005:UNK:O	5:Q:6009:UNK:N	2.53	0.42
2:J:333:GLU:N	2:J:333:GLU:CG	2.83	0.42
4:C:1154:PRO:HB2	4:C:1157:PHE:CD2	2.55	0.42
9:O:40:HIS:CD2	9:P:120:ALA:HB3	2.53	0.42
2:A:98:ASN:HD22	2:A:148:TRP:CD1	2.37	0.42
4:L:1500:LEU:CD1	4:L:1538:LEU:HD13	2.50	0.42
4:C:3750:PHE:CD1	4:C:3804:GLU:HA	2.55	0.42
4:L:3602:ASN:O	4:L:3606:ILE:HG12	2.20	0.41
4:L:3855:TYR:CZ	4:L:4121:TRP:HA	2.55	0.41
4:L:3959:MET:HE2	4:L:4124:TRP:CE2	2.55	0.41
6:M:14:DA:C2	6:M:15:DT:C2	3.08	0.41
8:H:215:GLN:O	8:H:219:MET:SD	2.78	0.41
4:C:1902:GLY:HA2	4:C:1905:ILE:HG23	2.01	0.41
4:C:2383:PHE:O	4:C:2418:LYS:HE2	2.18	0.41
9:G:116:VAL:CG1	9:G:117:GLU:H	2.31	0.41
4:L:1154:PRO:HB2	4:L:1157:PHE:CD2	2.55	0.41
4:C:3602:ASN:O	4:C:3606:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:3959:MET:HE2	4:C:4124:TRP:CE2	2.55	0.41
9:G:31:GLY:HA3	9:G:48:SER:HA	2.02	0.41
2:A:83:LEU:HD23	2:A:111:PRO:HB3	2.02	0.41
9:O:267:ALA:HA	9:O:268:PRO:HD3	1.95	0.41
4:C:1224:PHE:CZ	4:C:1270:PHE:CE2	3.09	0.41
4:C:2270:ASN:HD21	4:C:2306:ASN:CG	2.28	0.41
4:C:3255:ALA:O	4:C:3259:LEU:HD23	2.20	0.41
4:C:1500:LEU:CD1	4:C:1538:LEU:HD13	2.50	0.41
9:O:134:ILE:HD11	9:P:130:CYS:HA	2.02	0.41
2:A:41:LEU:HD21	2:A:146:VAL:HG12	2.01	0.41
4:L:2270:ASN:HD21	4:L:2306:ASN:CG	2.28	0.41
4:L:3750:PHE:CD1	4:L:3804:GLU:HA	2.55	0.41
4:C:864:GLY:O	4:C:868:LYS:HE3	2.21	0.41
4:C:1344:PHE:CD1	4:C:1344:PHE:C	2.99	0.41
9:F:2:GLU:HB2	9:F:24:TRP:CZ2	2.56	0.41
9:P:31:GLY:HA3	9:P:48:SER:HA	2.02	0.41
2:J:273:ILE:HD13	2:J:368:VAL:HG22	2.01	0.41
2:A:65:GLN:OE1	2:A:65:GLN:HA	2.21	0.41
8:H:208:LYS:O	8:H:212:MET:SD	2.78	0.41
4:C:1238:GLN:N	4:C:1239:PRO:HD2	2.36	0.41
4:C:3761:ASP:HA	4:C:3764:VAL:HG12	2.02	0.41
4:C:3855:TYR:CZ	4:C:4121:TRP:HA	2.55	0.41
6:D:14:DA:C2	6:D:15:DT:C2	3.08	0.41
9:G:73:ALA:HA	9:G:84:TYR:CD2	2.55	0.41
2:A:333:GLU:N	2:A:333:GLU:CG	2.83	0.41
4:L:864:GLY:O	4:L:868:LYS:HE3	2.21	0.41
4:L:1238:GLN:N	4:L:1239:PRO:HD2	2.36	0.41
4:C:1192:TYR:OH	4:C:1270:PHE:CE2	2.71	0.41
4:L:821:ALA:O	4:L:824:LYS:HG3	2.21	0.41
4:C:821:ALA:O	4:C:824:LYS:HG3	2.21	0.41
4:C:2861:ILE:HD13	4:C:2861:ILE:HA	1.93	0.41
2:J:241:ASP:HB2	1:T:185:LEU:HD21	2.03	0.41
4:L:1224:PHE:CZ	4:L:1270:PHE:CE2	3.08	0.41
4:C:395:MET:HG3	4:C:413:PHE:CZ	2.56	0.41
9:F:192:ARG:HD3	10:X:766:PHE:HA	2.03	0.41
9:O:192:ARG:HD3	10:Y:766:PHE:HA	2.03	0.41
4:L:1344:PHE:CD1	4:L:1344:PHE:C	2.98	0.40
7:N:1:DG:N2	7:N:2:DT:C2	2.89	0.40
9:O:2:GLU:HB2	9:O:24:TRP:CZ2	2.56	0.40
4:L:3531:TYR:CD1	4:L:3796:MET:HE1	2.56	0.40
4:L:3656:LEU:H	4:L:3656:LEU:HD23	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:43:TRP:CD1	9:P:115:LYS:HB2	2.57	0.40
4:L:992:ILE:HD13	4:L:1009:LEU:HD21	2.03	0.40
4:L:2603:THR:HB	4:L:2604:PRO:HD3	2.03	0.40
6:M:24:DA:N6	7:N:6:DA:H61	2.20	0.40
4:C:1046:PRO:CD	4:C:1047:GLN:N	2.84	0.40
4:C:1261:LEU:HD11	4:C:1340:ARG:HG3	2.03	0.40
2:J:65:GLN:OE1	2:J:65:GLN:HA	2.21	0.40
4:L:994:TRP:CZ3	4:L:2581:LEU:HB3	2.57	0.40
8:H:116:PRO:HD3	9:O:61:MET:HE1	2.02	0.40
8:I:208:LYS:CG	8:I:212:MET:SD	3.10	0.40
4:C:852:ARG:HD3	4:C:3111:MET:HE1	2.03	0.40
4:C:994:TRP:CZ3	4:C:2581:LEU:HB3	2.57	0.40
6:D:14:DA:H61	7:E:17:DT:H3	1.70	0.40
7:E:1:DG:N2	7:E:2:DT:C2	2.89	0.40
4:L:1154:PRO:HB2	4:L:1157:PHE:HD2	1.87	0.40
4:L:3442:TYR:HB2	4:L:3443:PRO:HD3	2.04	0.40
8:I:43:GLN:HB2	8:I:45:TRP:CH2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	21/204 (10%)	18 (86%)	3 (14%)	0	100	100
1	T	21/204 (10%)	17 (81%)	4 (19%)	0	100	100
2	A	493/609 (81%)	461 (94%)	32 (6%)	0	100	100
2	J	493/609 (81%)	460 (93%)	33 (7%)	0	100	100
3	B	525/732 (72%)	477 (91%)	42 (8%)	6 (1%)	11	45
3	K	525/732 (72%)	476 (91%)	43 (8%)	6 (1%)	11	45
4	C	3686/4128 (89%)	3440 (93%)	245 (7%)	1 (0%)	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	3686/4128 (89%)	3442 (93%)	243 (7%)	1 (0%)	100	100
8	H	217/299 (73%)	202 (93%)	13 (6%)	2 (1%)	14	49
8	I	212/299 (71%)	201 (95%)	10 (5%)	1 (0%)	24	62
9	F	209/336 (62%)	201 (96%)	7 (3%)	1 (0%)	24	62
9	G	191/336 (57%)	178 (93%)	12 (6%)	1 (0%)	24	62
9	O	209/336 (62%)	201 (96%)	7 (3%)	1 (0%)	24	62
9	P	191/336 (57%)	176 (92%)	12 (6%)	3 (2%)	7	36
10	X	250/911 (27%)	241 (96%)	9 (4%)	0	100	100
10	Y	250/911 (27%)	241 (96%)	9 (4%)	0	100	100
All	All	11179/15110 (74%)	10432 (93%)	724 (6%)	23 (0%)	44	77

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	145	SER
3	K	146	GLN
3	K	518	PRO
3	K	520	ALA
3	B	145	SER
3	B	146	GLN
3	B	518	PRO
3	B	520	ALA
9	F	26	LYS
9	O	26	LYS
8	H	114	GLY
8	H	208	LYS
9	G	26	LYS
9	P	26	LYS
9	P	64	GLY
3	K	519	PRO
4	L	3544	ASP
8	I	177	ASP
3	B	519	PRO
4	C	3544	ASP
9	P	60	ALA
3	K	517	ASN
3	B	517	ASN

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	S	18/160 (11%)	18 (100%)	0	100	100
1	T	18/160 (11%)	18 (100%)	0	100	100
2	A	452/548 (82%)	449 (99%)	3 (1%)	76	79
2	J	452/548 (82%)	449 (99%)	3 (1%)	76	79
3	B	481/649 (74%)	473 (98%)	8 (2%)	53	67
3	K	481/649 (74%)	473 (98%)	8 (2%)	53	67
4	C	3325/3671 (91%)	3308 (100%)	17 (0%)	81	81
4	L	3325/3671 (91%)	3308 (100%)	17 (0%)	81	81
8	H	198/262 (76%)	187 (94%)	11 (6%)	19	41
8	I	193/262 (74%)	180 (93%)	13 (7%)	15	37
9	F	191/303 (63%)	175 (92%)	16 (8%)	10	30
9	G	178/303 (59%)	161 (90%)	17 (10%)	8	25
9	O	191/303 (63%)	177 (93%)	14 (7%)	13	34
9	P	178/303 (59%)	160 (90%)	18 (10%)	7	23
10	X	230/808 (28%)	223 (97%)	7 (3%)	36	57
10	Y	230/808 (28%)	223 (97%)	7 (3%)	36	57
All	All	10141/13408 (76%)	9982 (98%)	159 (2%)	54	69

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	85	VAL
2	J	299	LYS
2	J	368	VAL
2	A	85	VAL
2	A	299	LYS
2	A	368	VAL
3	K	35	LYS
3	K	64	THR

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Mol	Chain	Res	Type
3	K	151	ILE
3	K	203	GLU
3	K	229	GLU
3	K	330	GLN
3	K	424	LEU
3	K	518	PRO
4	L	297	LEU
4	L	461	ILE
4	L	1264	LEU
4	L	1268	ASN
4	L	1411	TYR
4	L	1415	LEU
4	L	1640	GLU
4	L	1779	GLN
4	L	1990	PHE
4	L	2270	ASN
4	L	2455	LEU
4	L	3190	LEU
4	L	3310	ASN
4	L	3456	LEU
4	L	3561	LYS
4	L	3819	THR
4	L	3959	MET
8	H	29	ILE
8	H	31	LYS
8	H	38	VAL
8	H	62	ASN
8	H	100	VAL
8	H	109	ARG
8	H	124	MET
8	H	168	GLN
8	H	169	GLU
8	H	196	GLU
8	H	197	LYS
8	I	17	GLN
8	I	31	LYS
8	I	41	LEU
8	I	48	GLN
8	I	49	VAL
8	I	118	TYR
8	I	140	MET
8	I	159	MET

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Mol	Chain	Res	Type
8	I	194	MET
8	I	197	LYS
8	I	200	GLU
8	I	204	ILE
8	I	224	GLN
3	B	35	LYS
3	B	64	THR
3	B	151	ILE
3	B	203	GLU
3	B	229	GLU
3	B	330	GLN
3	B	424	LEU
3	B	518	PRO
4	C	297	LEU
4	C	461	ILE
4	C	1264	LEU
4	C	1268	ASN
4	C	1411	TYR
4	C	1415	LEU
4	C	1640	GLU
4	C	1779	GLN
4	C	1990	PHE
4	C	2270	ASN
4	C	2455	LEU
4	C	3190	LEU
4	C	3310	ASN
4	C	3456	LEU
4	C	3561	LYS
4	C	3819	THR
4	C	3959	MET
9	F	6	SER
9	F	22	VAL
9	F	23	SER
9	F	26	LYS
9	F	40	HIS
9	F	71	ARG
9	F	76	SER
9	F	85	THR
9	F	90	LYS
9	F	104	VAL
9	F	110	SER
9	F	112	ASN

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Mol	Chain	Res	Type
9	F	114	GLU
9	F	116	VAL
9	F	122	VAL
9	F	199	LEU
10	X	661	ASP
10	X	783	ASN
10	X	788	THR
10	X	792	MET
10	X	830	SER
10	X	856	LEU
10	X	895	THR
9	G	1	MET
9	G	16	ILE
9	G	22	VAL
9	G	28	LEU
9	G	34	ILE
9	G	47	VAL
9	G	51	GLU
9	G	52	ILE
9	G	67	VAL
9	G	70	LEU
9	G	85	THR
9	G	89	SER
9	G	91	GLU
9	G	93	CYS
9	G	163	GLU
9	G	165	CYS
9	G	174	THR
9	O	6	SER
9	O	22	VAL
9	O	23	SER
9	O	26	LYS
9	O	40	HIS
9	O	71	ARG
9	O	76	SER
9	O	90	LYS
9	O	110	SER
9	O	112	ASN
9	O	114	GLU
9	O	116	VAL
9	O	122	VAL
9	O	199	LEU

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Mol	Chain	Res	Type
10	Y	661	ASP
10	Y	783	ASN
10	Y	788	THR
10	Y	792	MET
10	Y	830	SER
10	Y	856	LEU
10	Y	895	THR
9	P	1	MET
9	P	16	ILE
9	P	22	VAL
9	P	28	LEU
9	P	34	ILE
9	P	47	VAL
9	P	51	GLU
9	P	52	ILE
9	P	65	LYS
9	P	67	VAL
9	P	70	LEU
9	P	85	THR
9	P	89	SER
9	P	91	GLU
9	P	93	CYS
9	P	163	GLU
9	P	165	CYS
9	P	174	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (137) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	187	ASN
2	J	68	GLN
2	J	128	GLN
2	J	176	HIS
2	J	278	GLN
2	J	405	ASN
2	J	433	GLN
2	A	68	GLN
2	A	176	HIS
2	A	278	GLN
2	A	405	ASN
2	A	426	GLN
2	A	433	GLN

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Mol	Chain	Res	Type
3	K	33	GLN
3	K	76	ASN
3	K	246	HIS
3	K	500	HIS
3	K	514	ASN
3	K	517	ASN
4	L	40	GLN
4	L	289	ASN
4	L	448	GLN
4	L	738	HIS
4	L	739	ASN
4	L	753	GLN
4	L	1146	ASN
4	L	1205	ASN
4	L	1231	GLN
4	L	1457	GLN
4	L	1568	ASN
4	L	1611	GLN
4	L	1721	HIS
4	L	1725	GLN
4	L	1738	ASN
4	L	2089	ASN
4	L	2222	HIS
4	L	2270	ASN
4	L	2283	ASN
4	L	2306	ASN
4	L	2353	GLN
4	L	2432	GLN
4	L	2481	HIS
4	L	2483	ASN
4	L	2553	HIS
4	L	2560	ASN
4	L	2859	GLN
4	L	3093	GLN
4	L	3166	ASN
4	L	3249	GLN
4	L	3263	HIS
4	L	3551	ASN
4	L	3573	ASN
4	L	3602	ASN
4	L	3605	ASN
4	L	3704	GLN

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Mol	Chain	Res	Type
4	L	3777	GLN
4	L	4103	GLN
8	H	42	GLN
8	H	78	ASN
8	H	149	GLN
8	H	158	HIS
8	I	21	ASN
8	I	46	HIS
8	I	48	GLN
8	I	213	ASN
3	B	33	GLN
3	B	119	GLN
3	B	246	HIS
3	B	500	HIS
3	B	517	ASN
4	C	289	ASN
4	C	448	GLN
4	C	738	HIS
4	C	739	ASN
4	C	753	GLN
4	C	1146	ASN
4	C	1205	ASN
4	C	1231	GLN
4	C	1457	GLN
4	C	1568	ASN
4	C	1611	GLN
4	C	1721	HIS
4	C	1725	GLN
4	C	2089	ASN
4	C	2213	ASN
4	C	2222	HIS
4	C	2270	ASN
4	C	2283	ASN
4	C	2306	ASN
4	C	2353	GLN
4	C	2432	GLN
4	C	2481	HIS
4	C	2483	ASN
4	C	2553	HIS
4	C	2560	ASN
4	C	2859	GLN
4	C	2954	GLN

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Mol	Chain	Res	Type
4	C	3093	GLN
4	C	3166	ASN
4	C	3249	GLN
4	C	3263	HIS
4	C	3564	GLN
4	C	3573	ASN
4	C	3602	ASN
4	C	3605	ASN
4	C	3704	GLN
4	C	3777	GLN
4	C	4103	GLN
9	F	40	HIS
9	F	137	ASN
9	F	141	ASN
9	F	145	GLN
9	F	159	GLN
9	F	196	ASN
10	X	673	GLN
10	X	772	ASN
10	X	848	HIS
10	X	908	GLN
9	G	21	GLN
9	G	138	GLN
9	G	145	GLN
1	T	187	ASN
9	O	40	HIS
9	O	137	ASN
9	O	141	ASN
9	O	145	GLN
9	O	196	ASN
10	Y	673	GLN
10	Y	772	ASN
10	Y	848	HIS
10	Y	908	GLN
9	P	21	GLN
9	P	138	GLN
9	P	143	HIS
9	P	145	GLN
9	P	156	ASN
9	P	159	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
11	ATP	L	4201	-	32,33,33	1.09	0	48,52,52	1.31	5 (10%)
11	ATP	C	4201	-	32,33,33	1.08	1 (3%)	48,52,52	1.22	4 (8%)

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
11	ATP	L	4201	-	-	6/22/38/38	0/3/3/3
11	ATP	C	4201	-	-	3/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	4201	ATP	PB-O3B	-2.06	1.57	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	4201	ATP	C5-C4-N3	-3.38	122.06	126.72
11	C	4201	ATP	C5-C4-N3	-2.85	122.79	126.72
11	L	4201	ATP	C4-C5-N7	2.78	113.76	110.58
11	C	4201	ATP	C4-C5-N7	2.75	113.72	110.58
11	L	4201	ATP	N3-C4-N9	2.31	131.09	127.17
11	L	4201	ATP	C2-N1-C6	-2.07	115.32	118.73
11	C	4201	ATP	O2G-PG-O3B	2.06	111.54	104.64
11	L	4201	ATP	O2G-PG-O3B	2.04	111.47	104.64
11	C	4201	ATP	O3A-PA-O1A	2.02	116.79	110.70

There are no chirality outliers.

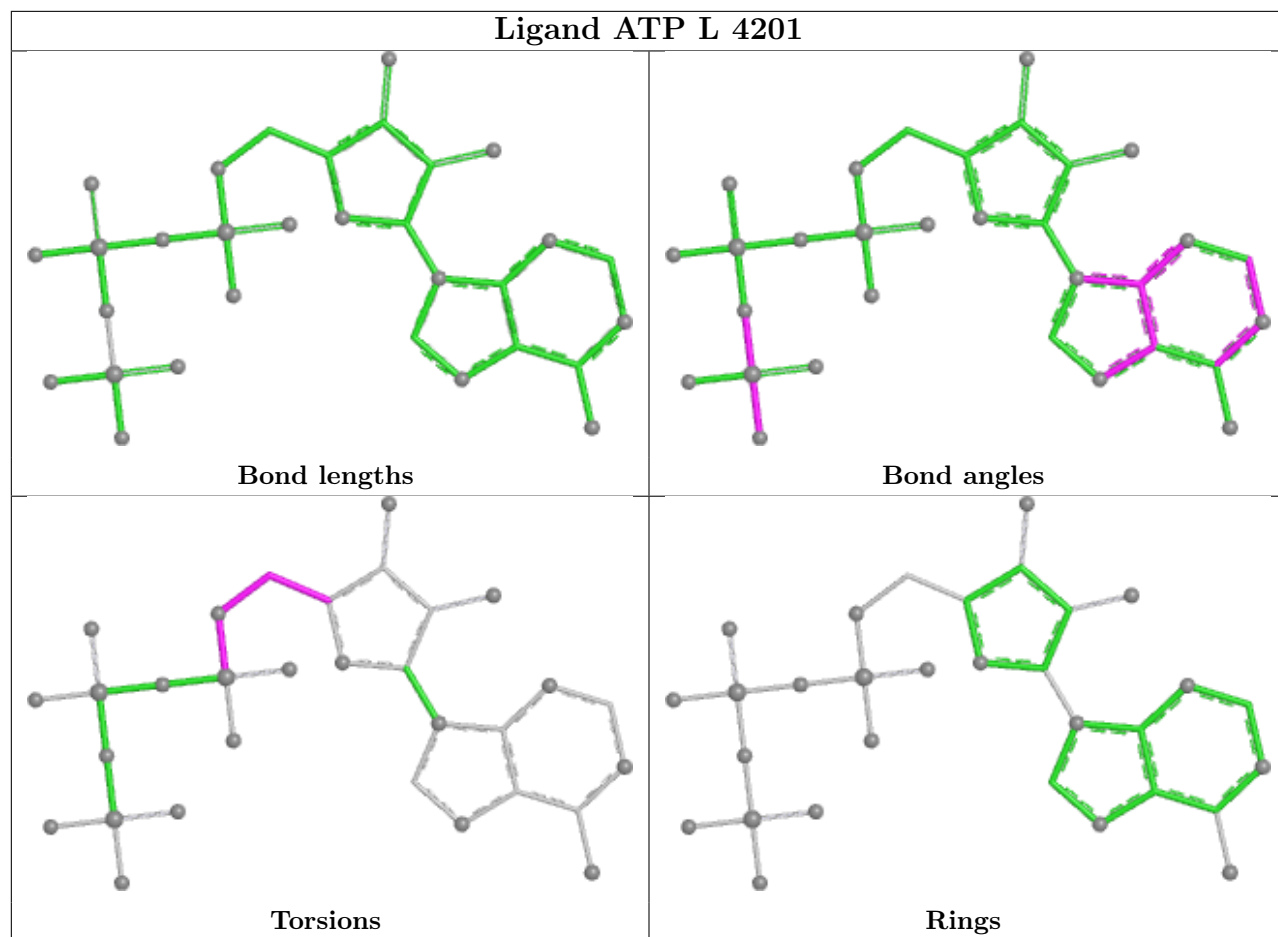
All (9) torsion outliers are listed below:

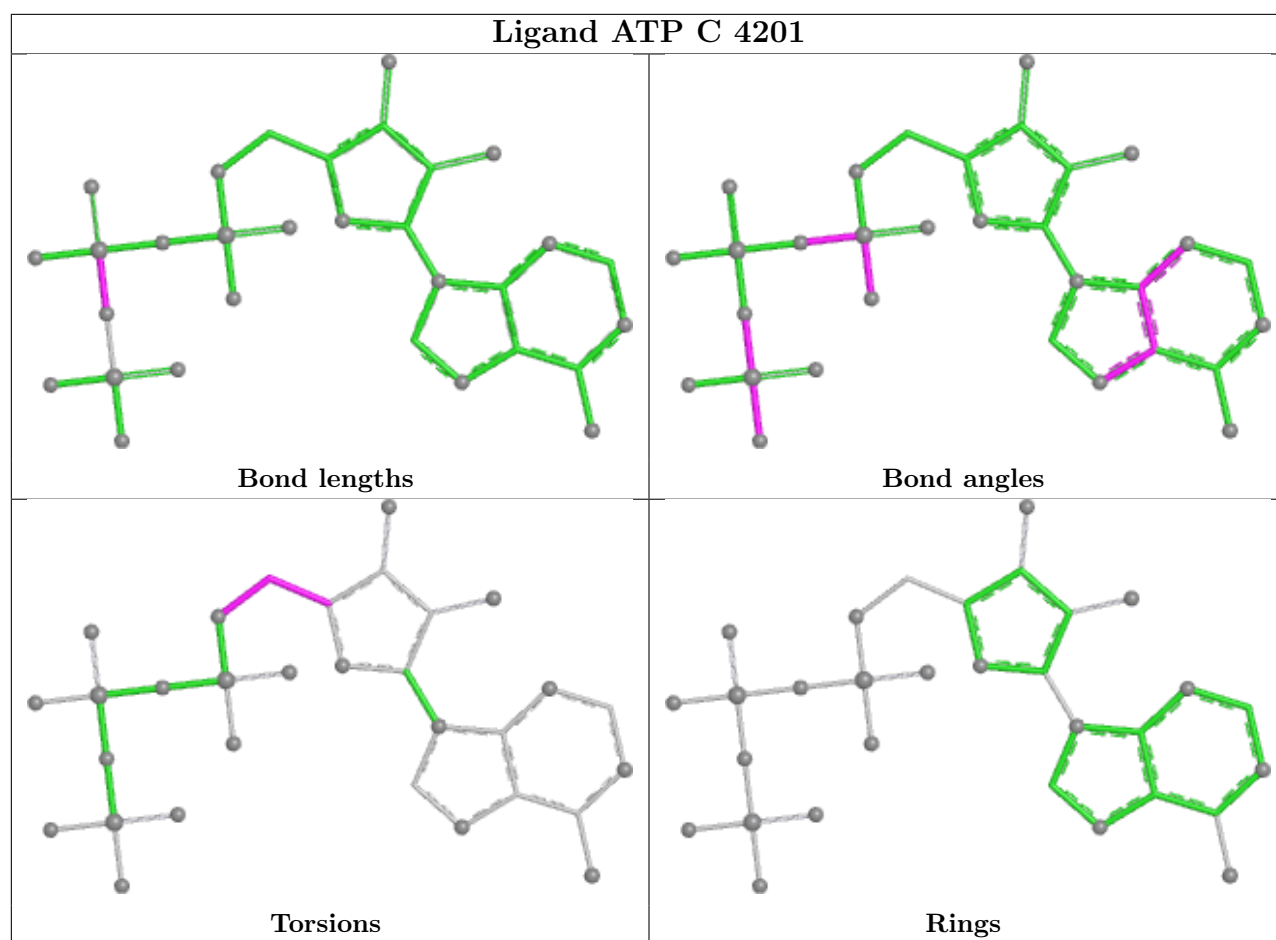
Mol	Chain	Res	Type	Atoms
11	L	4201	ATP	C5'-O5'-PA-O1A
11	L	4201	ATP	C5'-O5'-PA-O3A
11	L	4201	ATP	O4'-C4'-C5'-O5'
11	C	4201	ATP	O4'-C4'-C5'-O5'
11	L	4201	ATP	C3'-C4'-C5'-O5'
11	C	4201	ATP	C3'-C4'-C5'-O5'
11	L	4201	ATP	C5'-O5'-PA-O2A
11	L	4201	ATP	C4'-C5'-O5'-PA
11	C	4201	ATP	C4'-C5'-O5'-PA

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 than 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.





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.

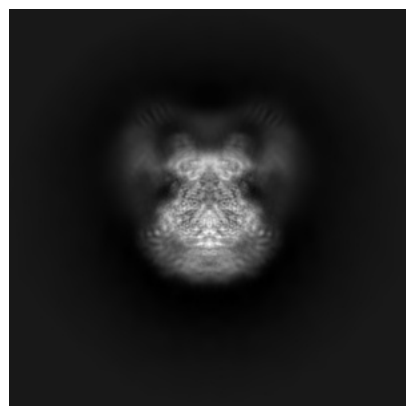
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28732. These allow visual inspection of the internal detail of the map and identification of artifacts.

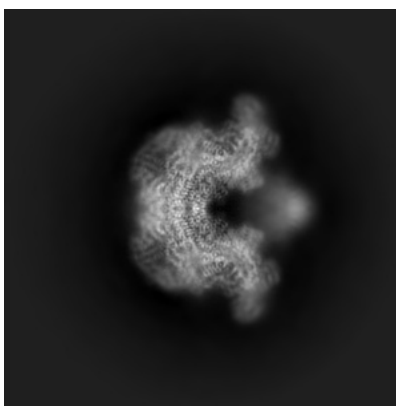
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

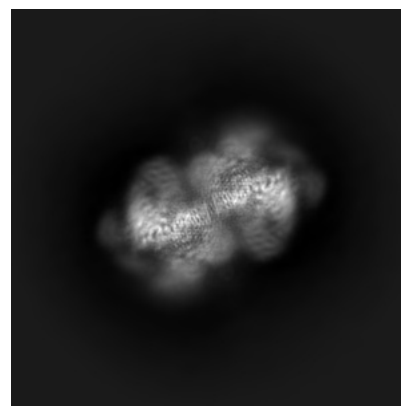
6.1.1 Primary map



X

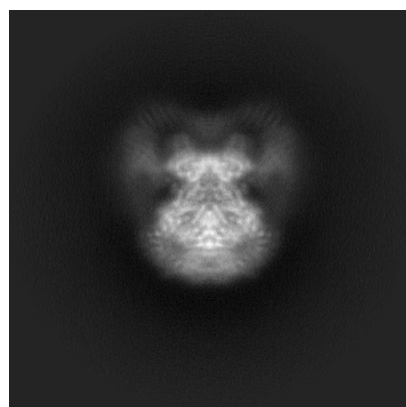


Y

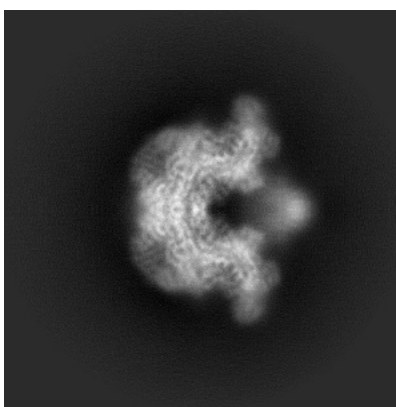


Z

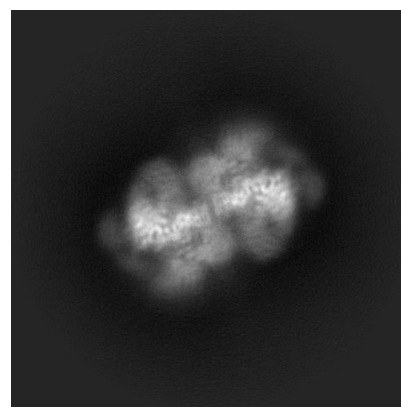
6.1.2 Raw map



X



Y

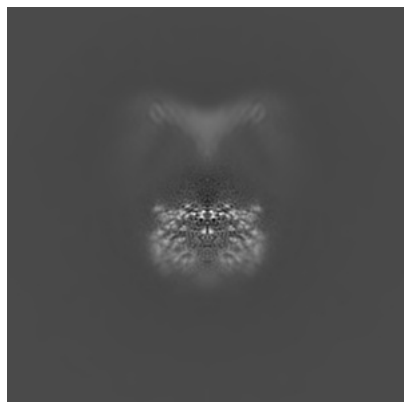


Z

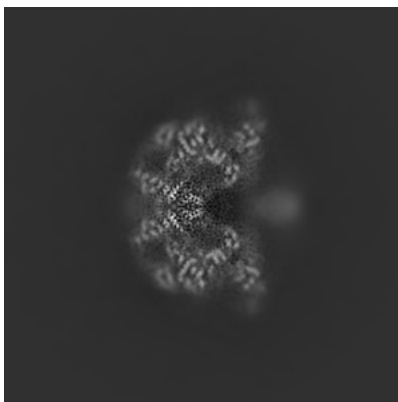
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

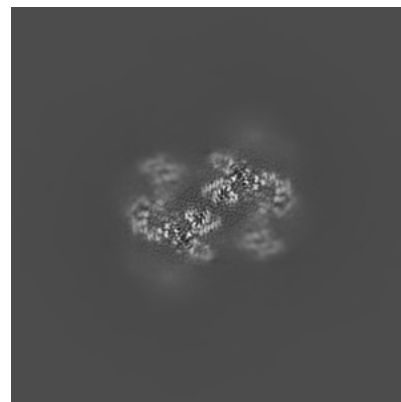
6.2.1 Primary map



X Index: 240

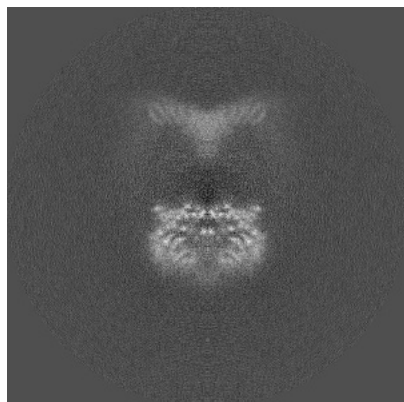


Y Index: 240

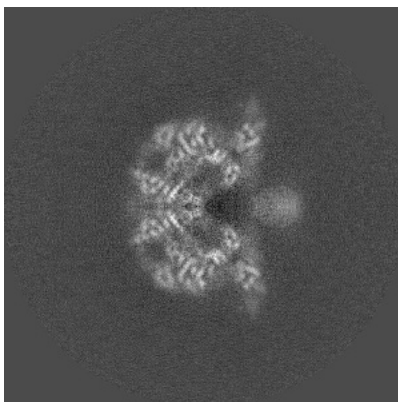


Z Index: 240

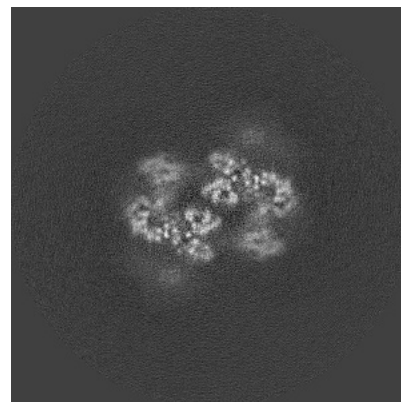
6.2.2 Raw map



X Index: 240



Y Index: 240

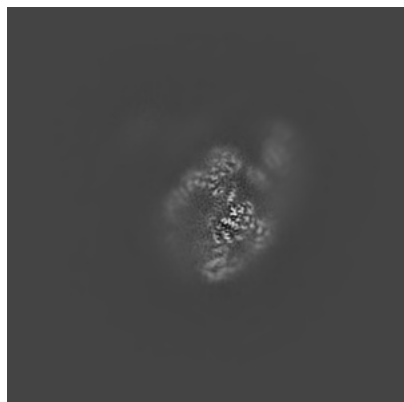


Z Index: 240

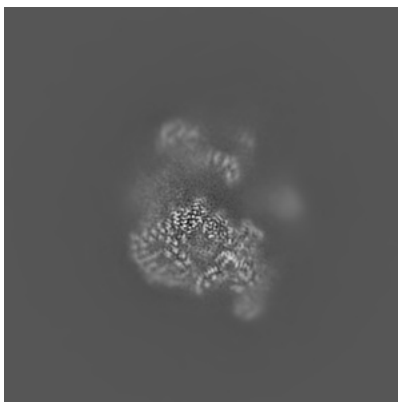
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

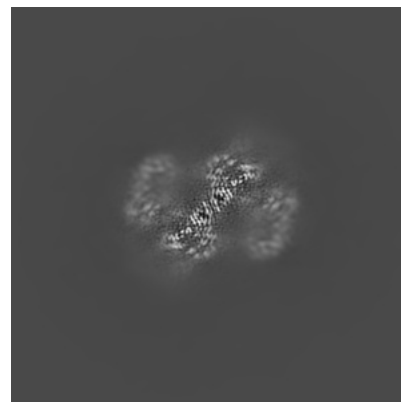
6.3.1 Primary map



X Index: 278

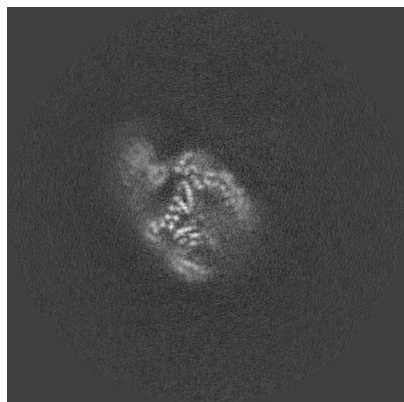


Y Index: 226

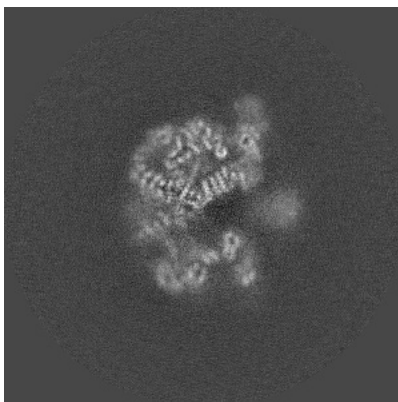


Z Index: 227

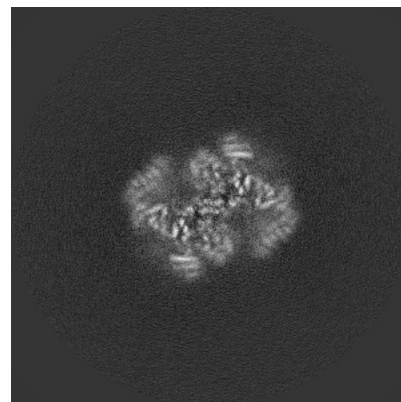
6.3.2 Raw map



X Index: 196



Y Index: 247

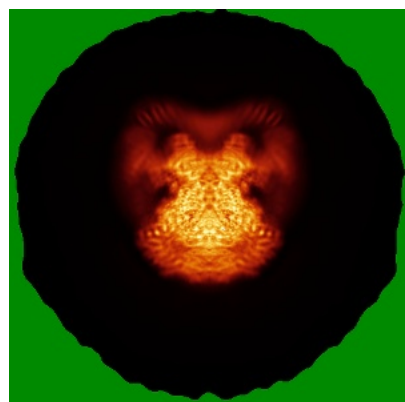


Z Index: 211

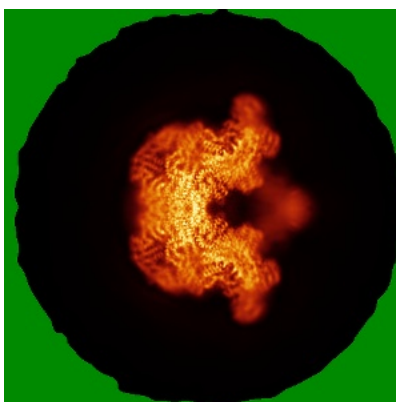
The images above show the largest variance slices of the map in three orthogonal directions.

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

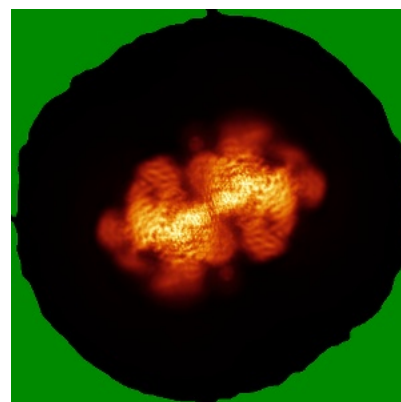
6.4.1 Primary map



X

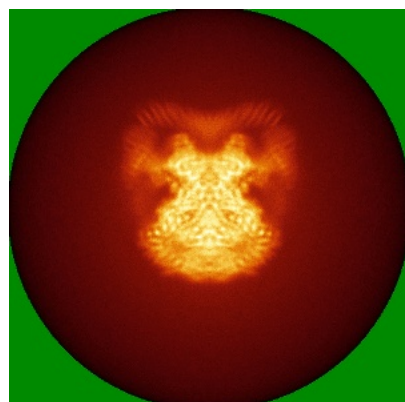


Y

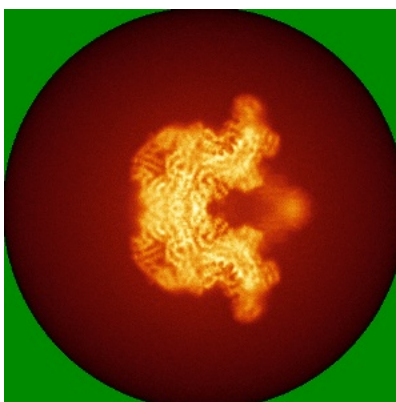


Z

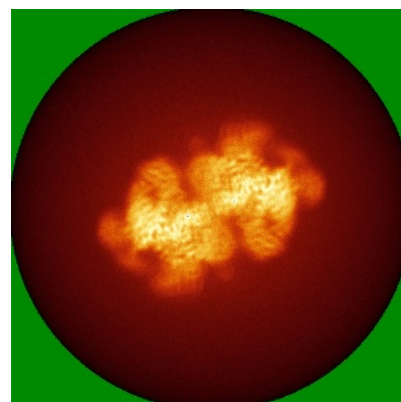
6.4.2 Raw map



X



Y

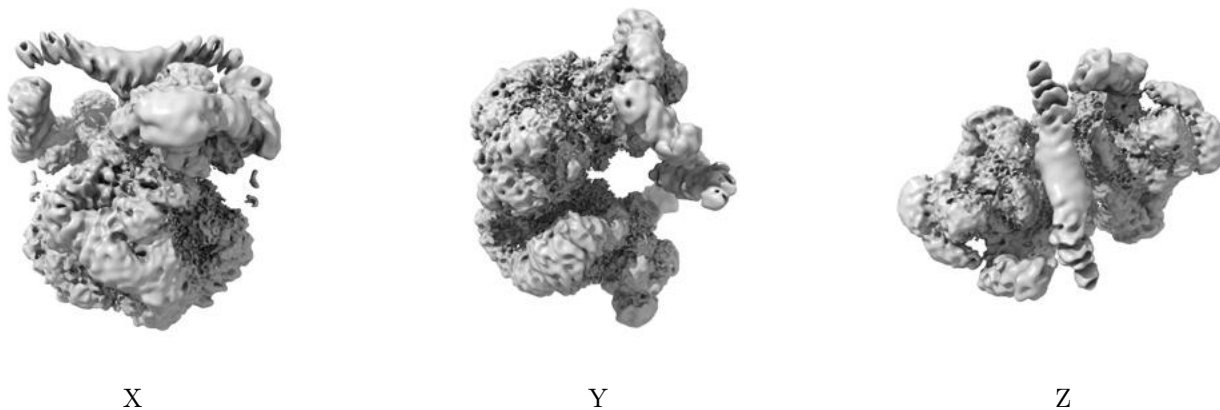


Z

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.

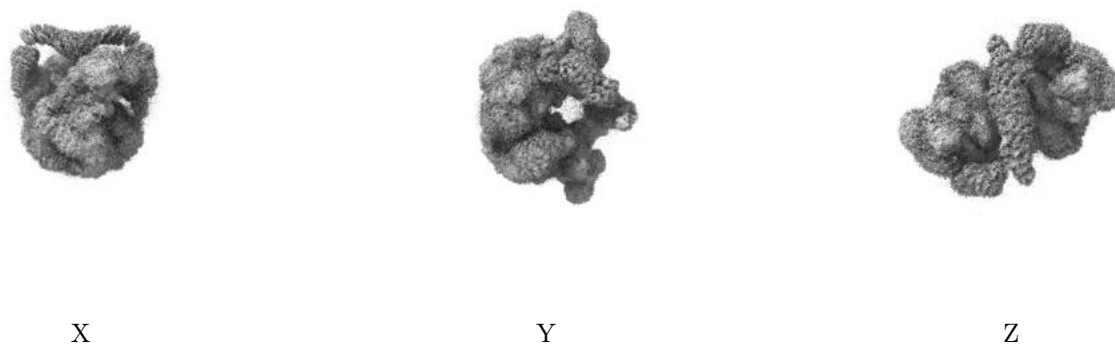
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

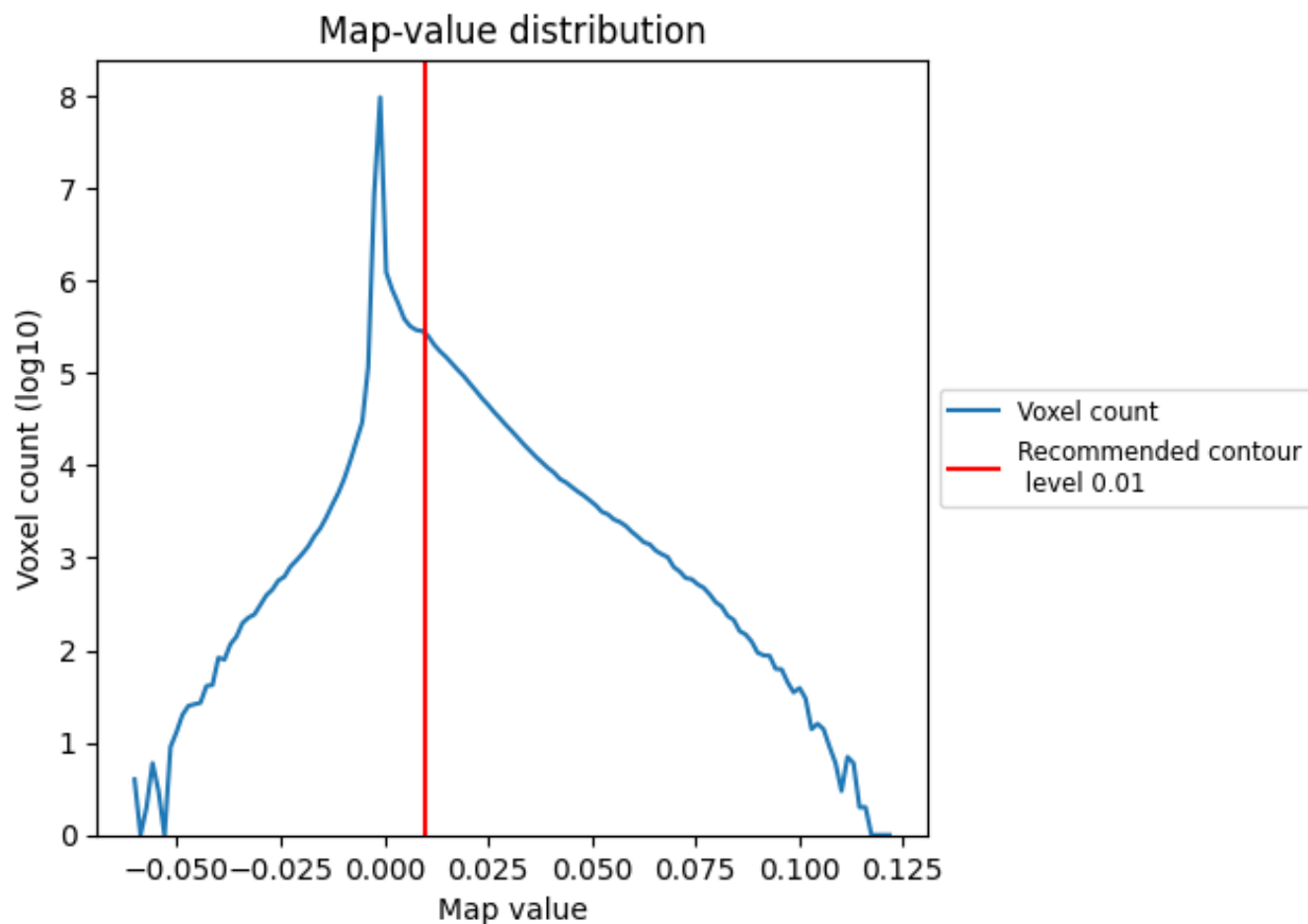
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

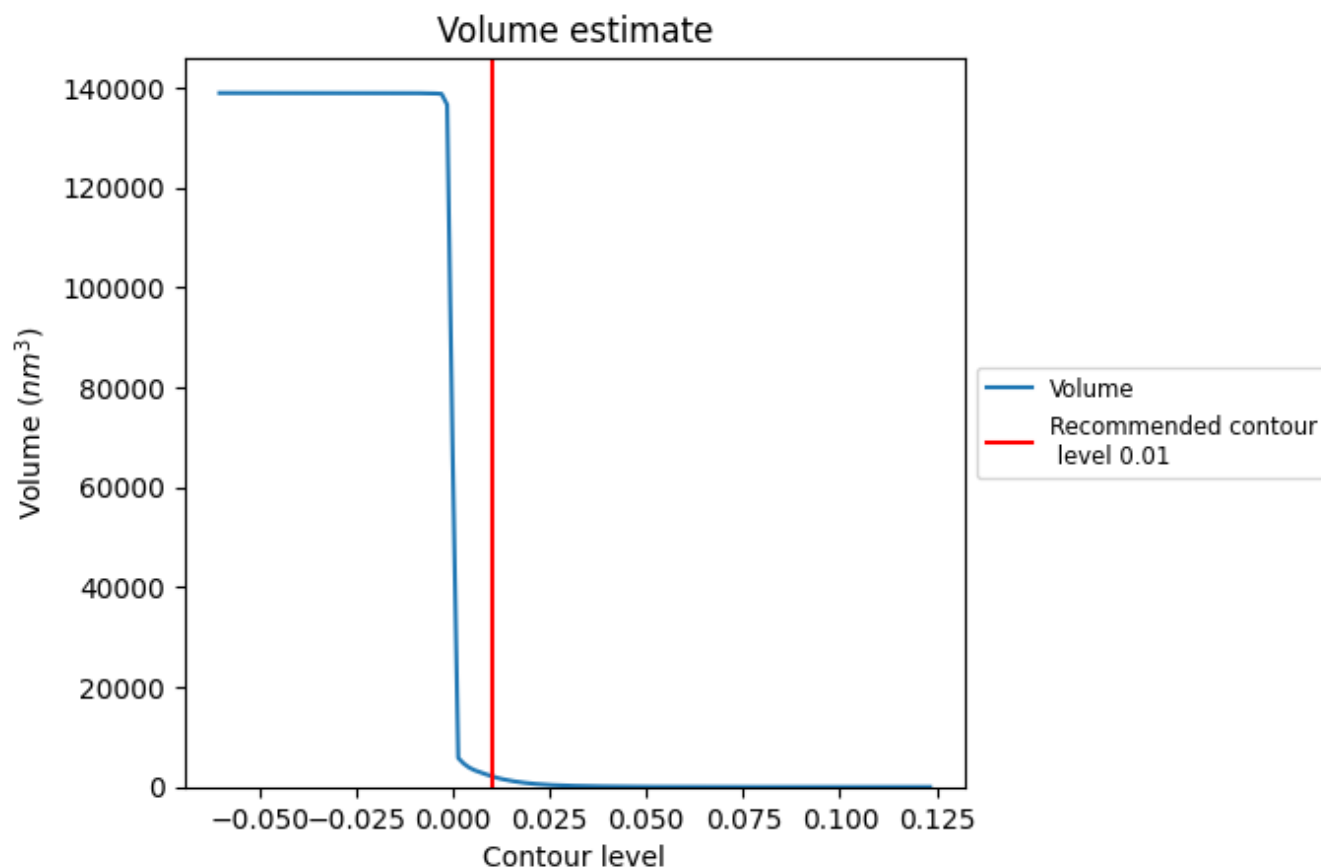
This section contains the results of statistical analysis of the map.

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.

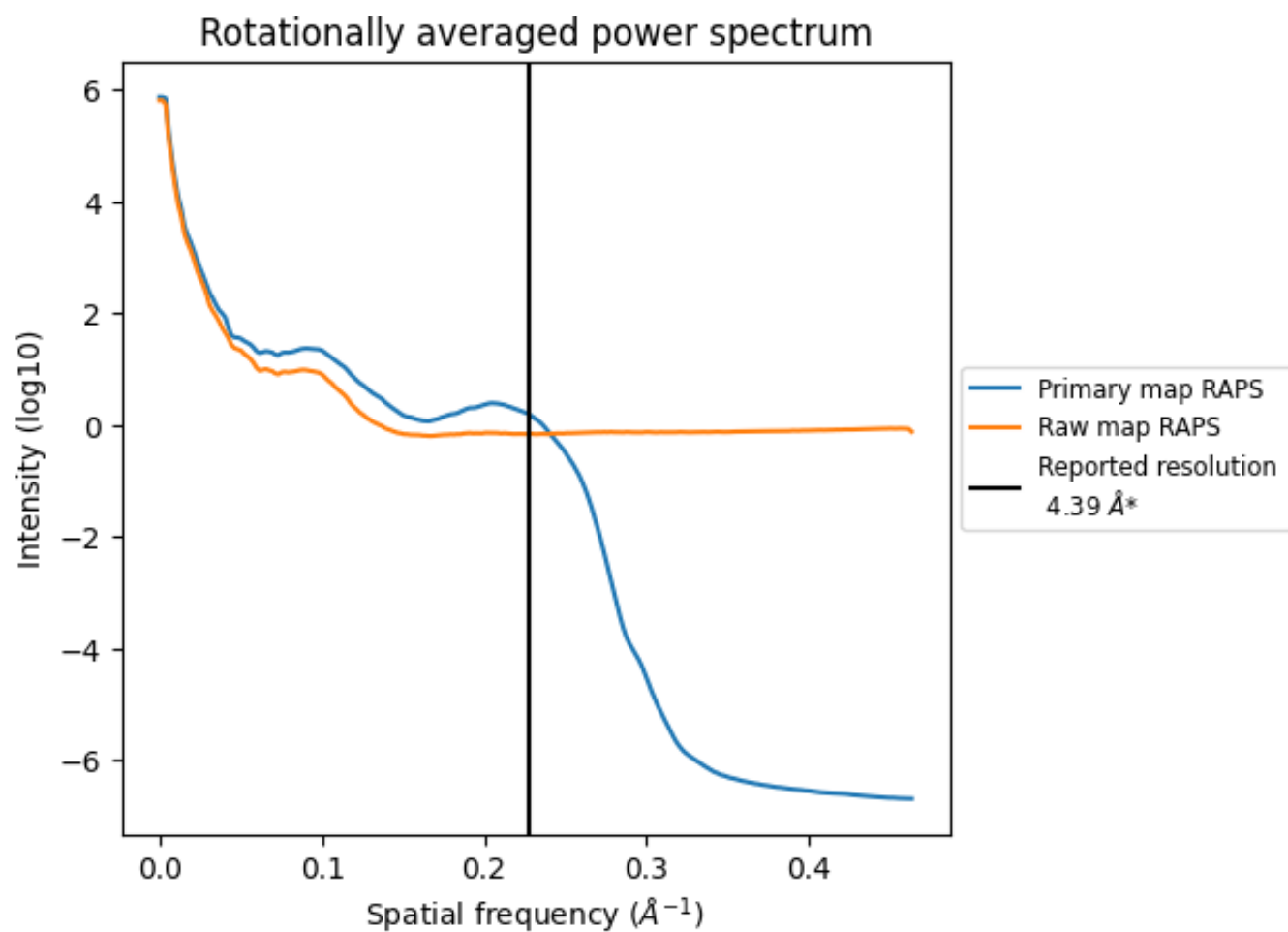
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2174 nm^3 ; this corresponds to an approximate mass of 1964 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](#)

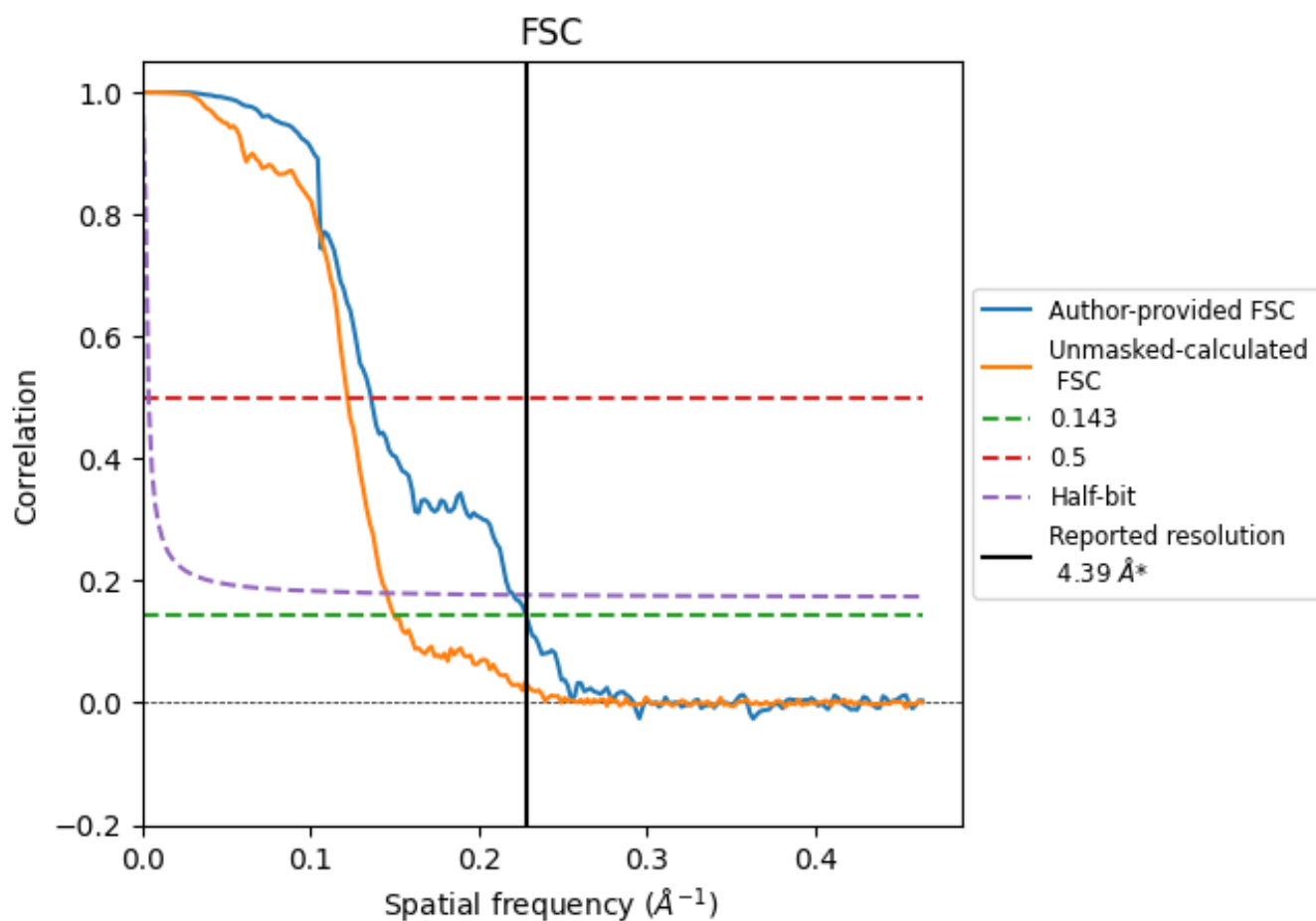


*Reported resolution corresponds to spatial frequency of 0.228 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.228 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

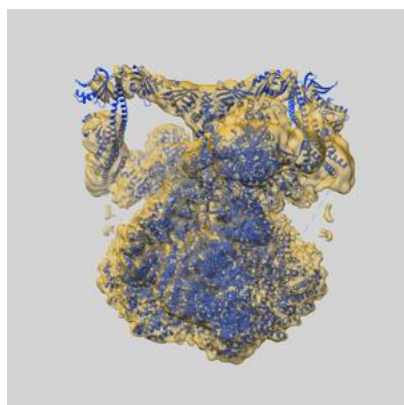
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.39	-	-
Author-provided FSC curve	4.38	7.36	4.53
Unmasked-calculated*	6.68	8.19	6.88

*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 6.68 differs from the reported value 4.39 by more than 10 %

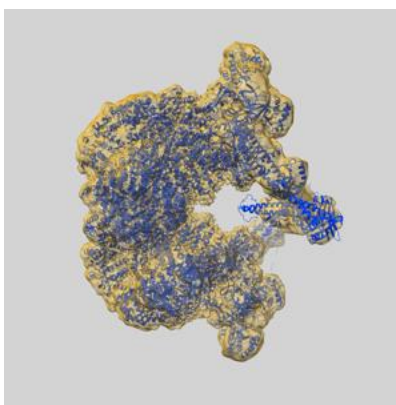
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28732 and PDB model 8EZA. Per-residue inclusion information can be found in section 3 on page 7.

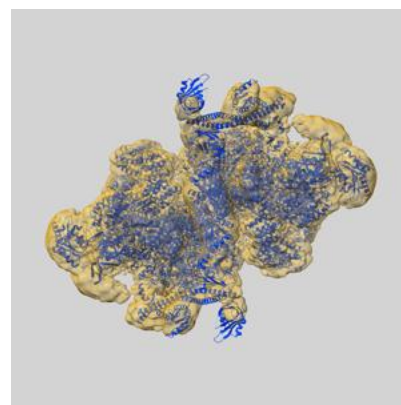
9.1 Map-model overlay [i](#)



X



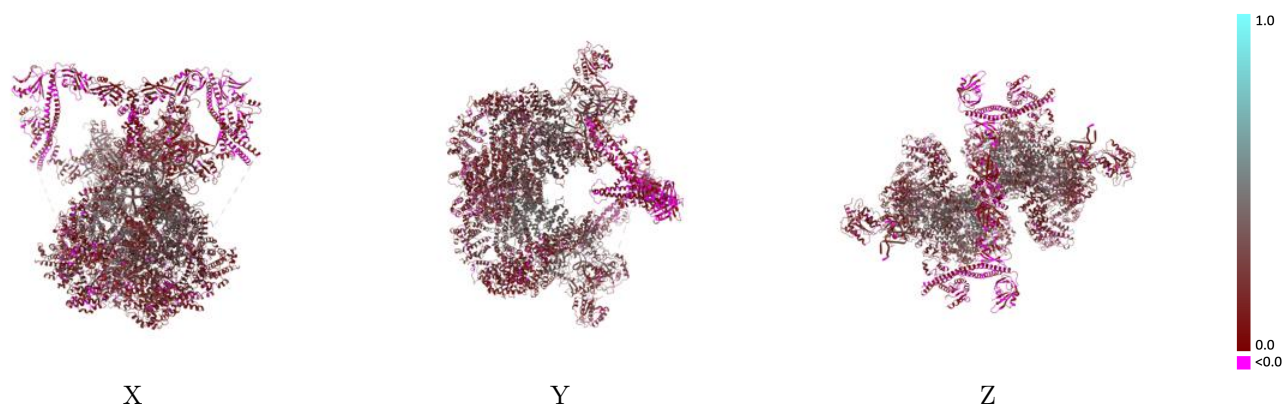
Y



Z

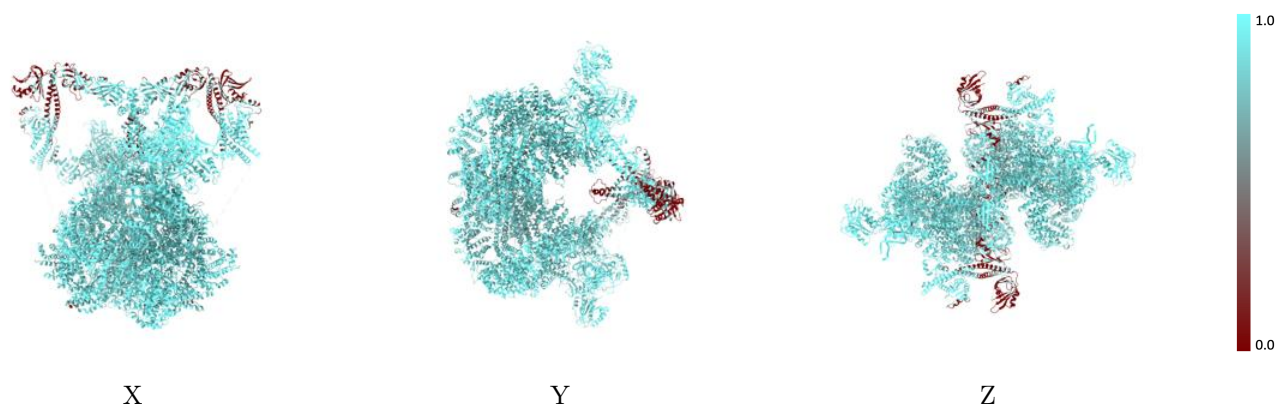
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



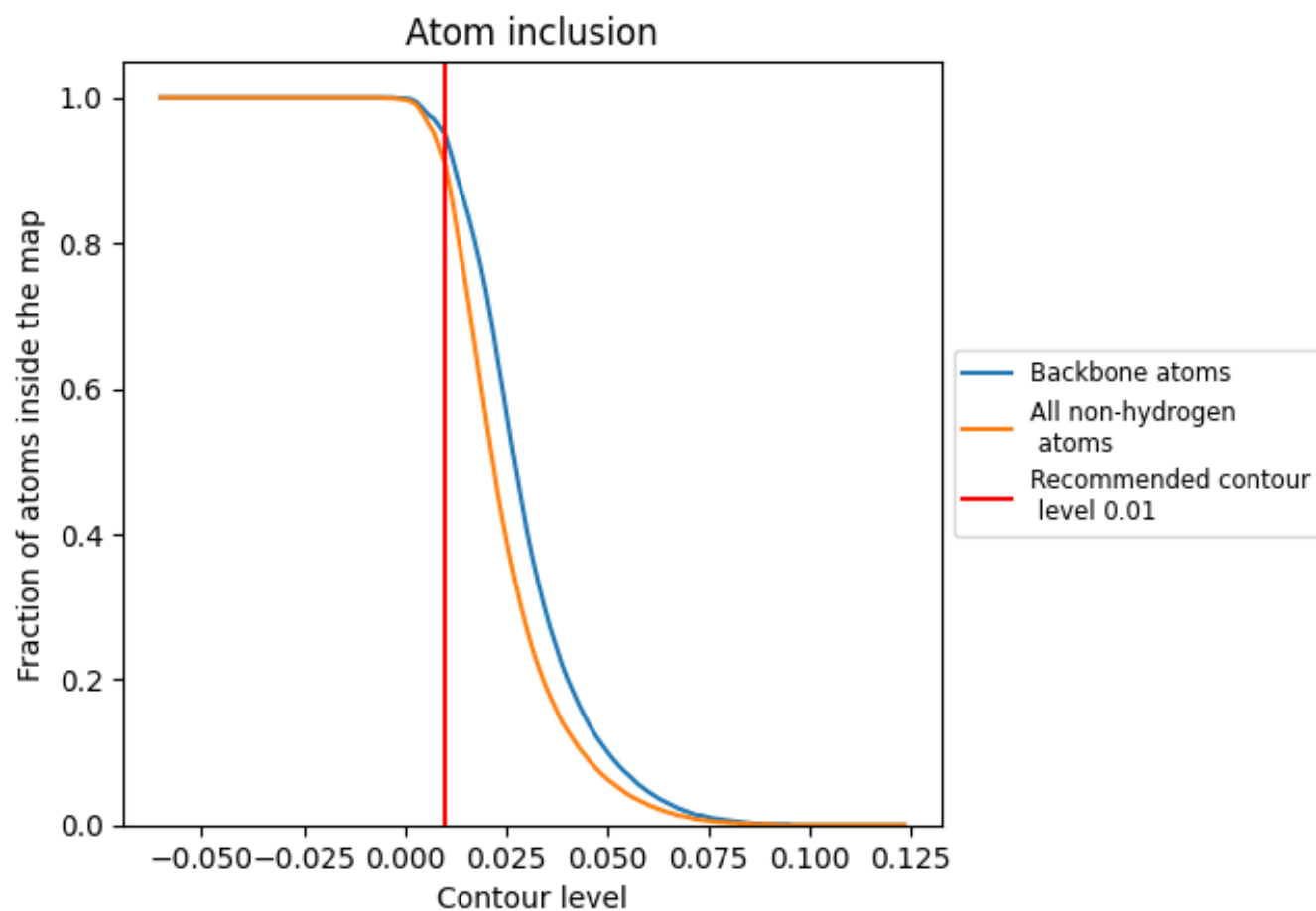
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9080	 0.2160
A	 0.9600	 0.2620
B	 0.9690	 0.2070
C	 0.9430	 0.2350
D	 0.9980	 0.3170
E	 0.9970	 0.3350
F	 0.5590	 0.0430
G	 0.3530	 0.0410
H	 0.7720	 0.0650
I	 0.7740	 0.0580
J	 0.9650	 0.2640
K	 0.9700	 0.2060
L	 0.9470	 0.2500
M	 0.9950	 0.3240
N	 0.9970	 0.3330
O	 0.5650	 0.0420
P	 0.3530	 0.0440
Q	 0.9700	 0.2200
R	 0.9700	 0.2180
S	 0.9760	 0.2800
T	 0.9760	 0.2830
X	 0.9170	 0.1090
Y	 0.9120	 0.1110

