



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:42 PM UTC

PDB ID : 8EZB / pdb_00008ezb
EMDB ID : EMD-28733
Title : NHEJ Long-range complex with ATP
Authors : Chen, S.; He, Y.
Deposited on : 2022-10-31
Resolution : 8.90 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:

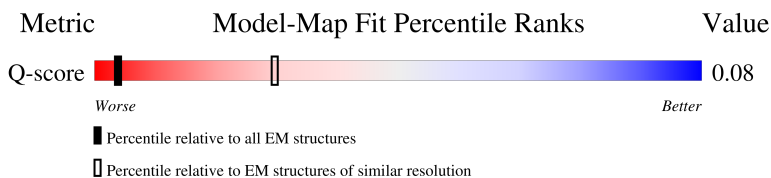
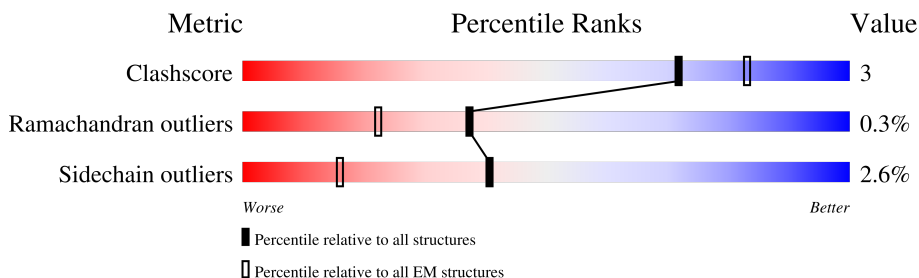
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 8.90 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.



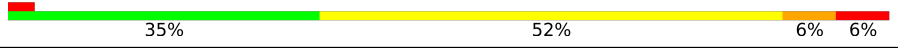
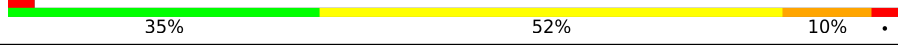
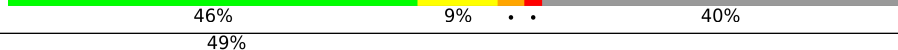
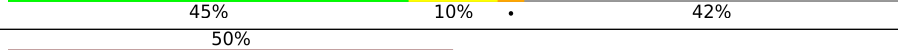
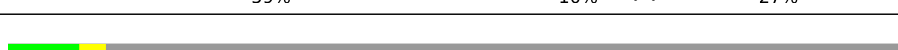
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	258 (8.40 - 9.40)

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

Mol	Chain	Length	Quality of chain
1	A	609	9% 72% 9% 18%
1	J	609	9% 72% 9% 18%
2	B	732	19% 64% 7% 28%
2	K	732	19% 63% 7% 28%

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Mol	Chain	Length	Quality of chain
3	C	4128	
3	L	4128	
4	D	31	
4	M	31	
5	E	30	
5	N	30	
6	F	336	
6	G	336	
6	O	336	
6	P	336	
7	H	299	
7	I	299	
8	S	204	
8	T	204	
9	X	911	
9	Y	911	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 93038 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 X-ray repair cross-complementing protein 6.

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

- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	524	Total	C	N	O	S	0	0
			4204	2689	704	788	23		
2	K	524	Total	C	N	O	S	0	0
			4204	2689	704	788	23		

- Molecule 3 is a protein called DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	3724	Total	C	N	O	S	0	0
			29799	19101	5041	5463	194		
3	L	3724	Total	C	N	O	S	0	0
			29799	19101	5041	5463	194		

- Molecule 4 is a DNA chain called DNA (31-MER).

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

- Molecule 5 is a DNA chain called DNA (30-MER).

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

- Molecule 6 is a protein called DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	201	Total	C	N	O	S	0	0
			1628	1031	278	312	7		
6	G	195	Total	C	N	O	S	0	0
			1595	1012	272	304	7		
6	O	201	Total	C	N	O	S	0	0
			1628	1031	278	312	7		
6	P	195	Total	C	N	O	S	0	0
			1595	1012	272	304	7		

- Molecule 7 is a protein called Non-homologous end-joining factor 1.

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

- Molecule 8 is a protein called Protein PAXX.

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

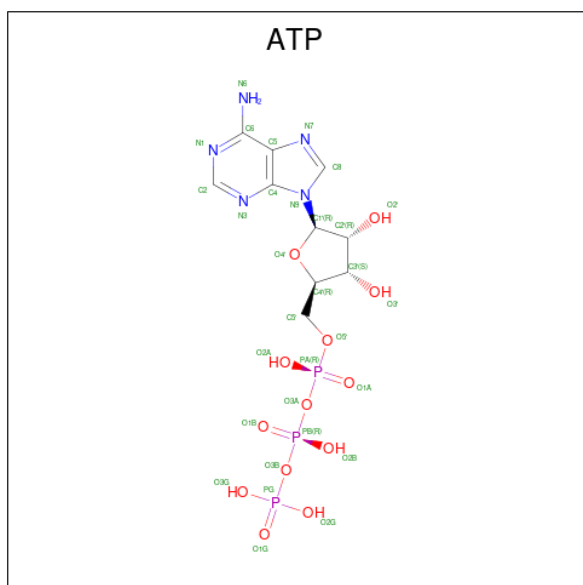
- Molecule 9 is a protein called DNA ligase 4.

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

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	C	1	Total	Mg	0
			1	1	
10	L	1	Total	Mg	0
			1	1	

- 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).

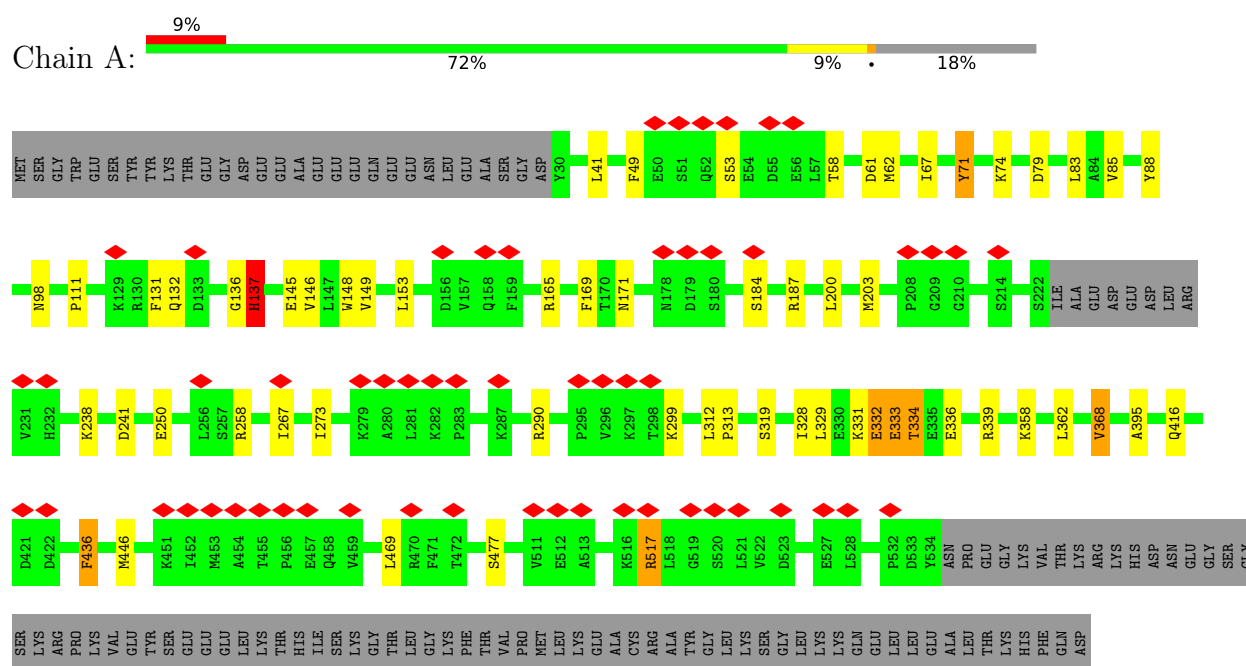


Mol	Chain	Residues	Atoms					AltConf
11	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
11	L	1	Total	C	N	O	P	0
			31	10	5	13	3	

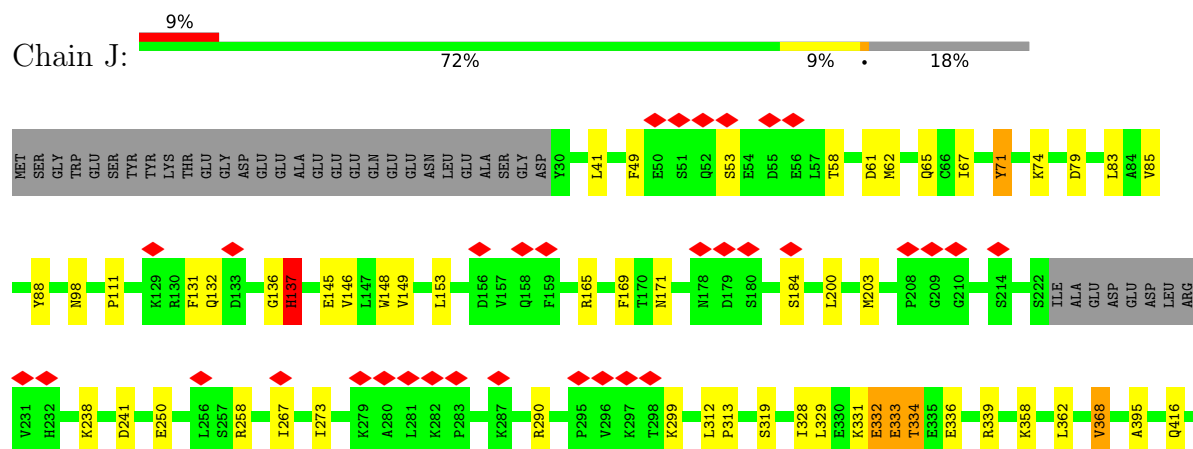
3 Residue-property plots

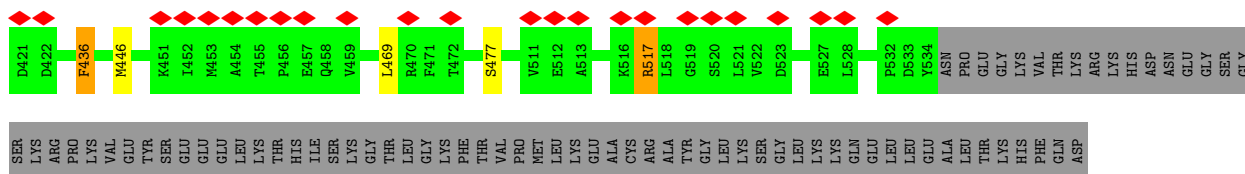
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: X-ray repair cross-complementing protein 6

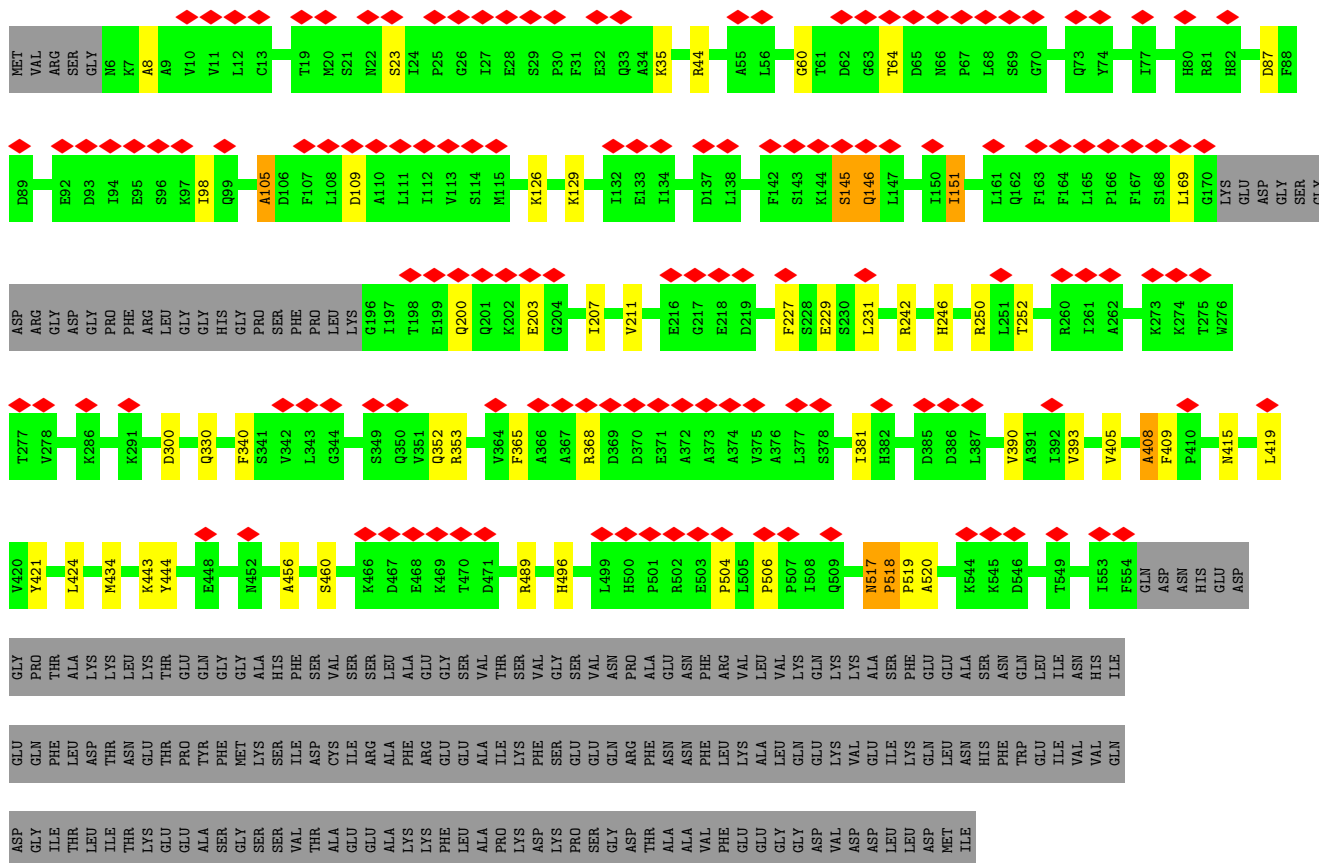


- Molecule 1: X-ray repair cross-complementing protein 6

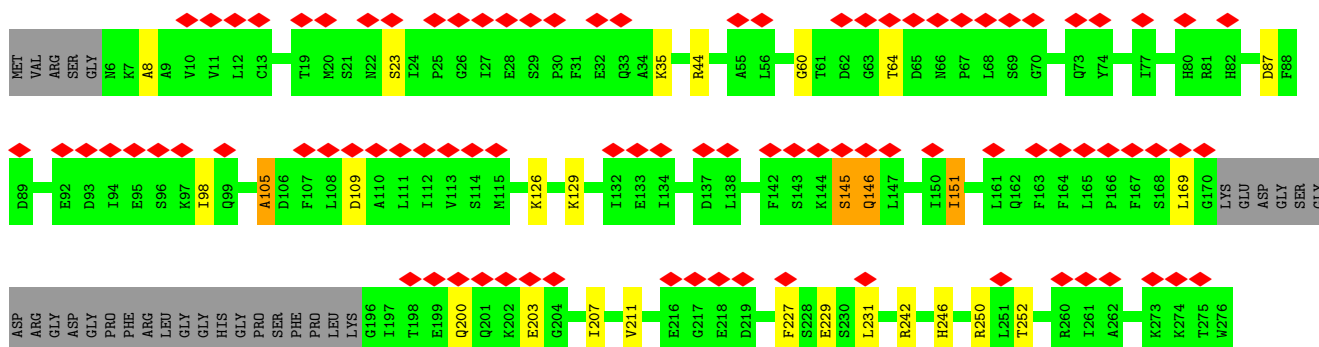


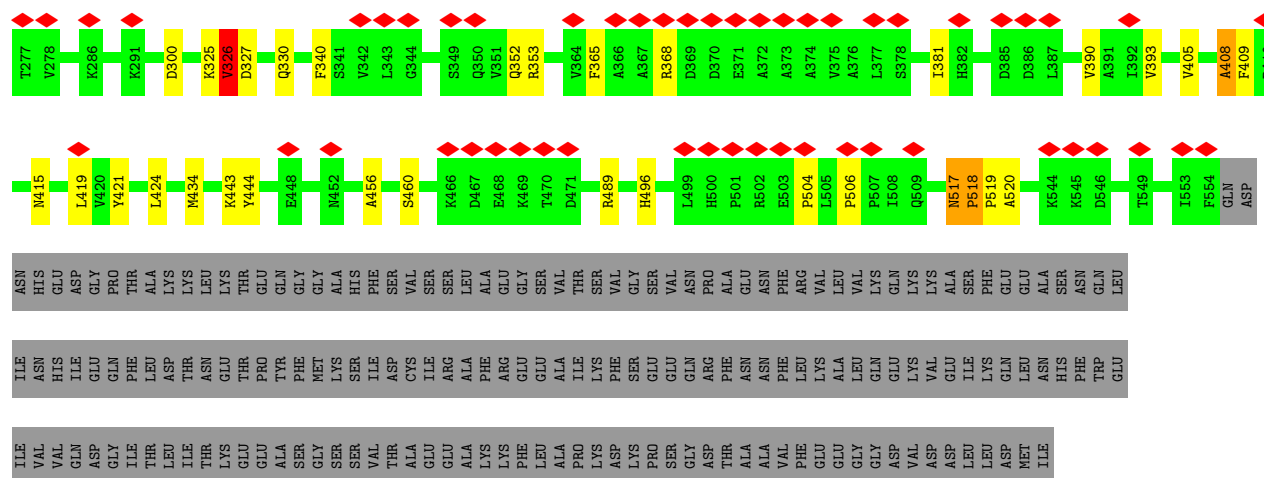


• Molecule 2: X-ray repair cross-complementing protein 5

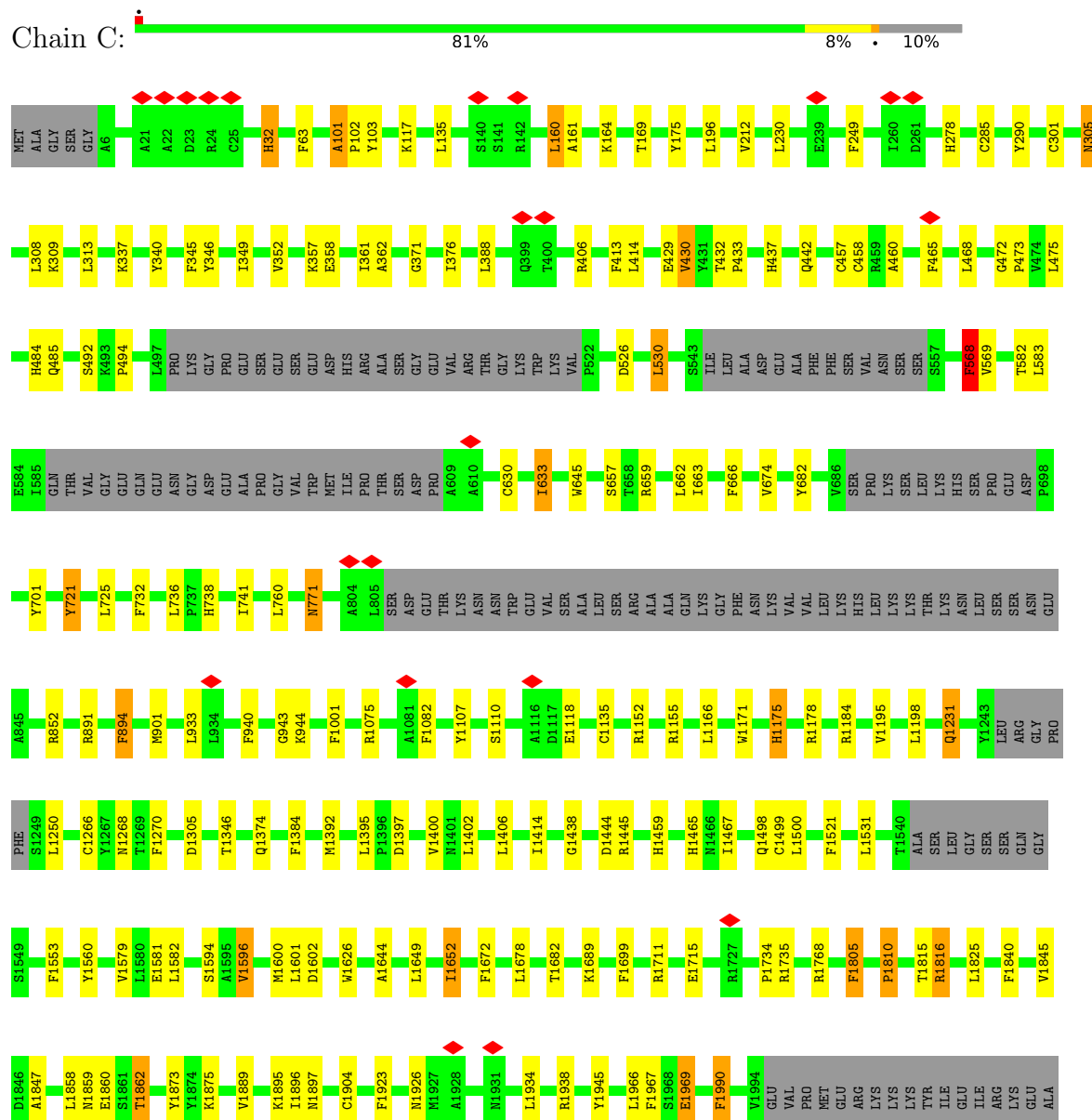


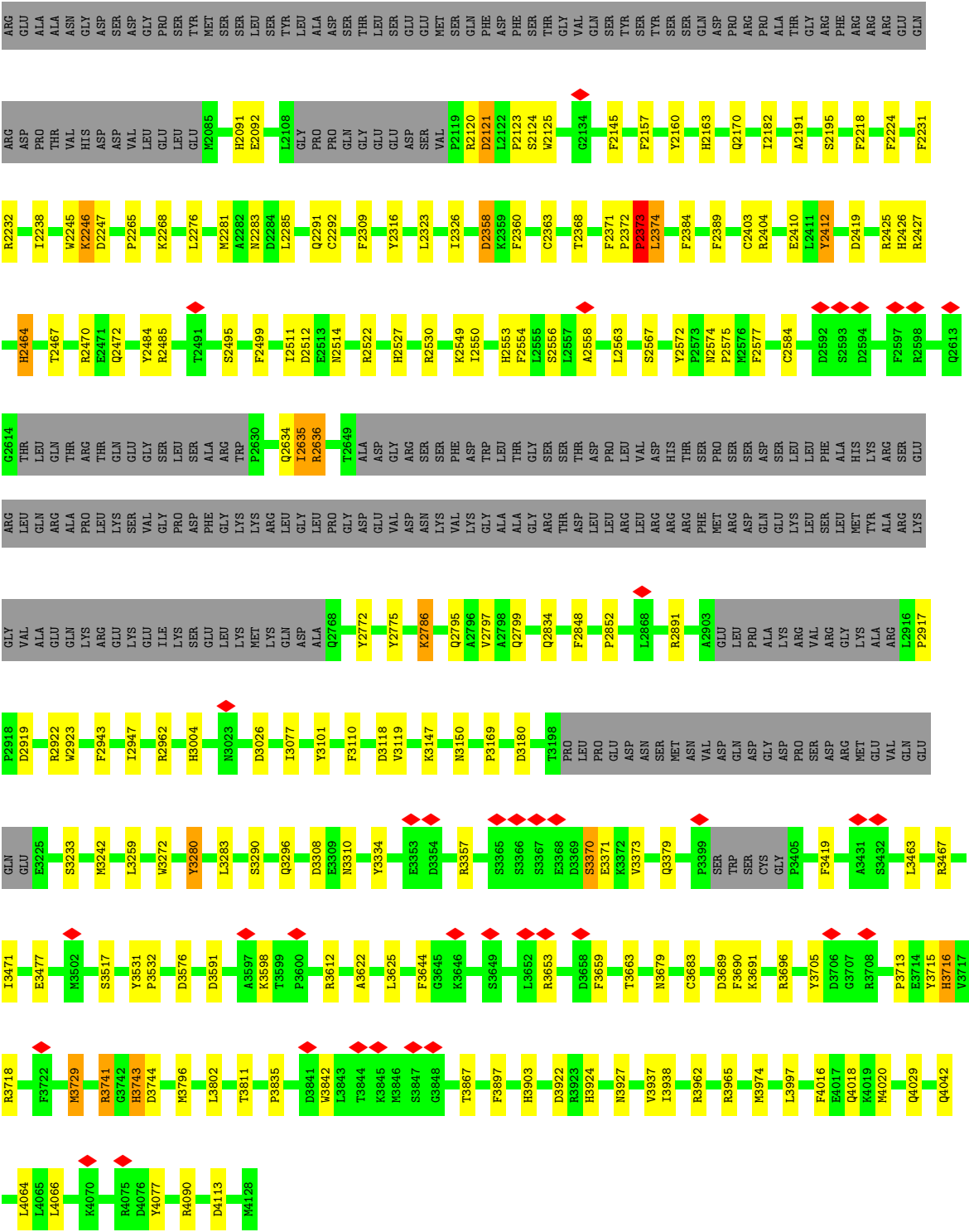
• Molecule 2: X-ray repair cross-complementing protein 5



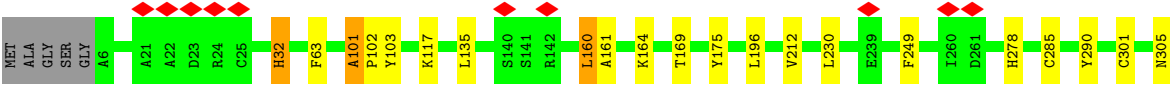
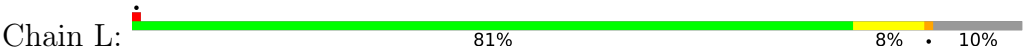


• Molecule 3: DNA-dependent protein kinase catalytic subunit

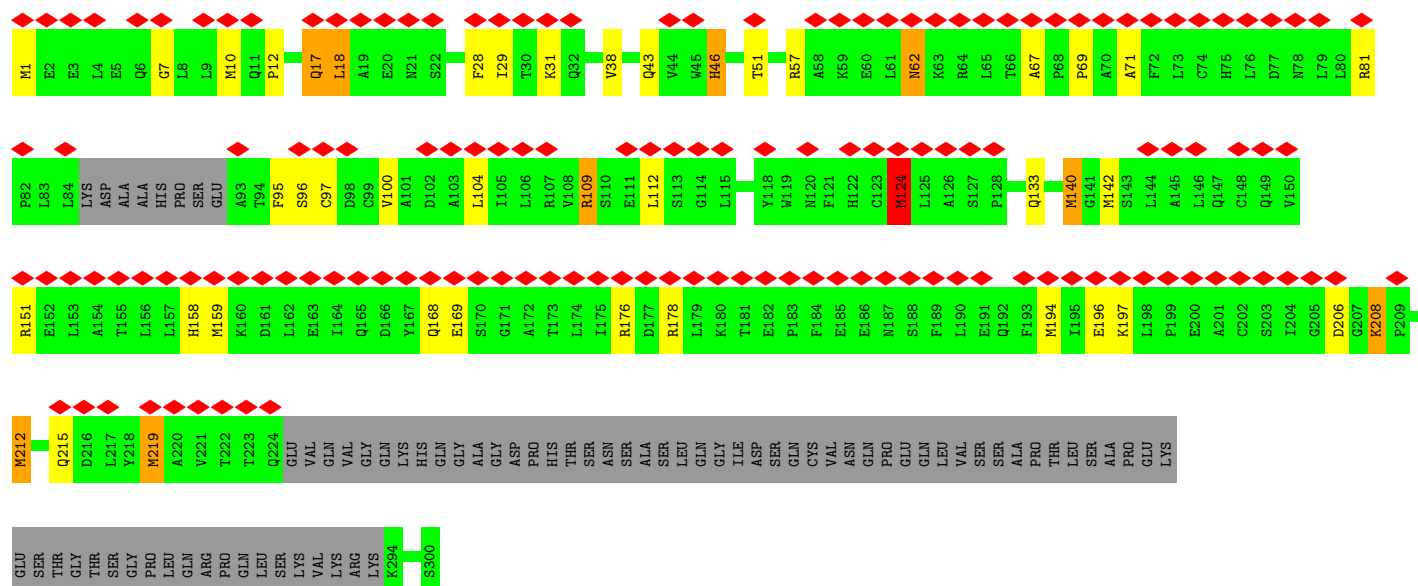




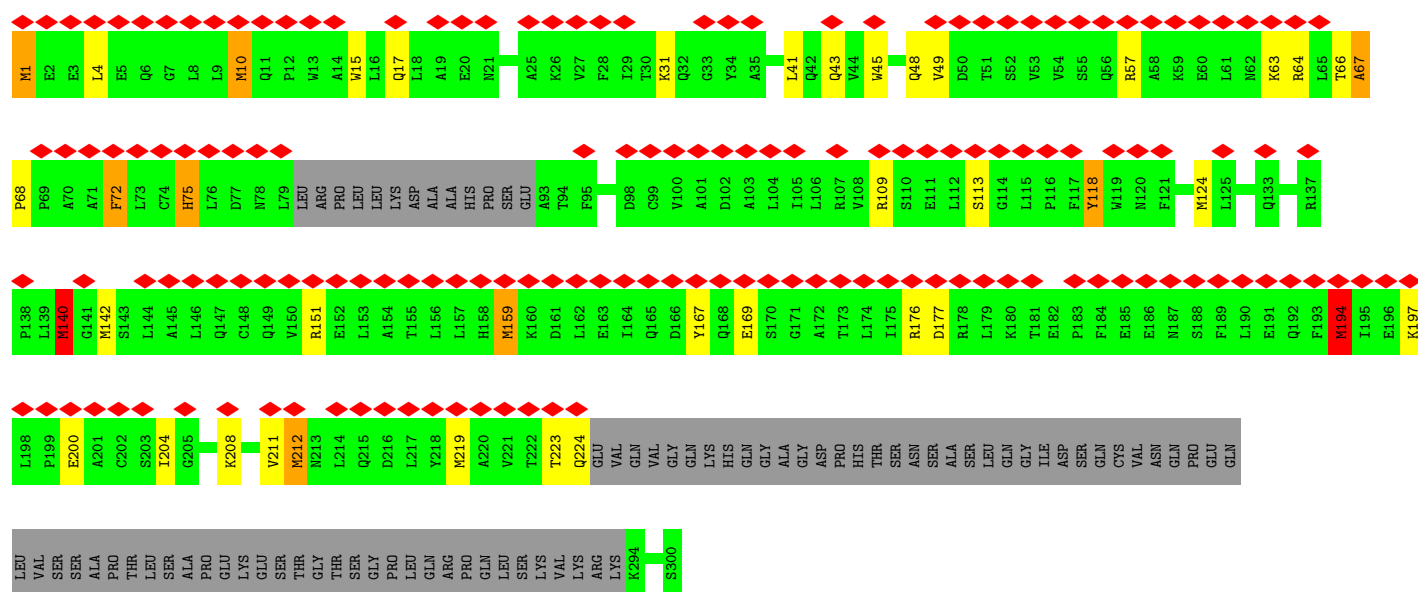
• Molecule 3: DNA-dependent protein kinase catalytic subunit



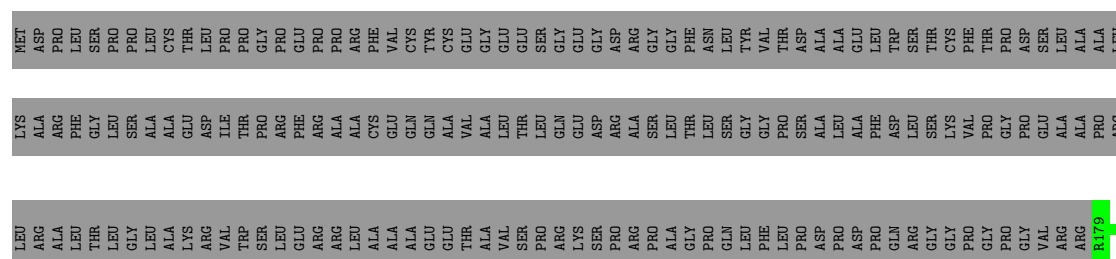


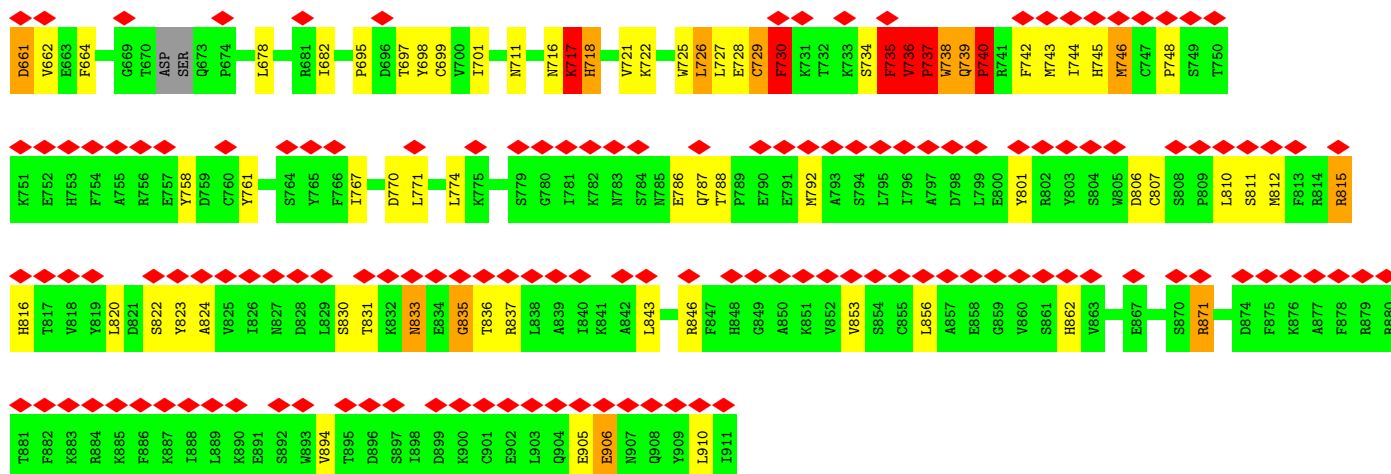


• Molecule 7: Non-homologous end-joining factor 1

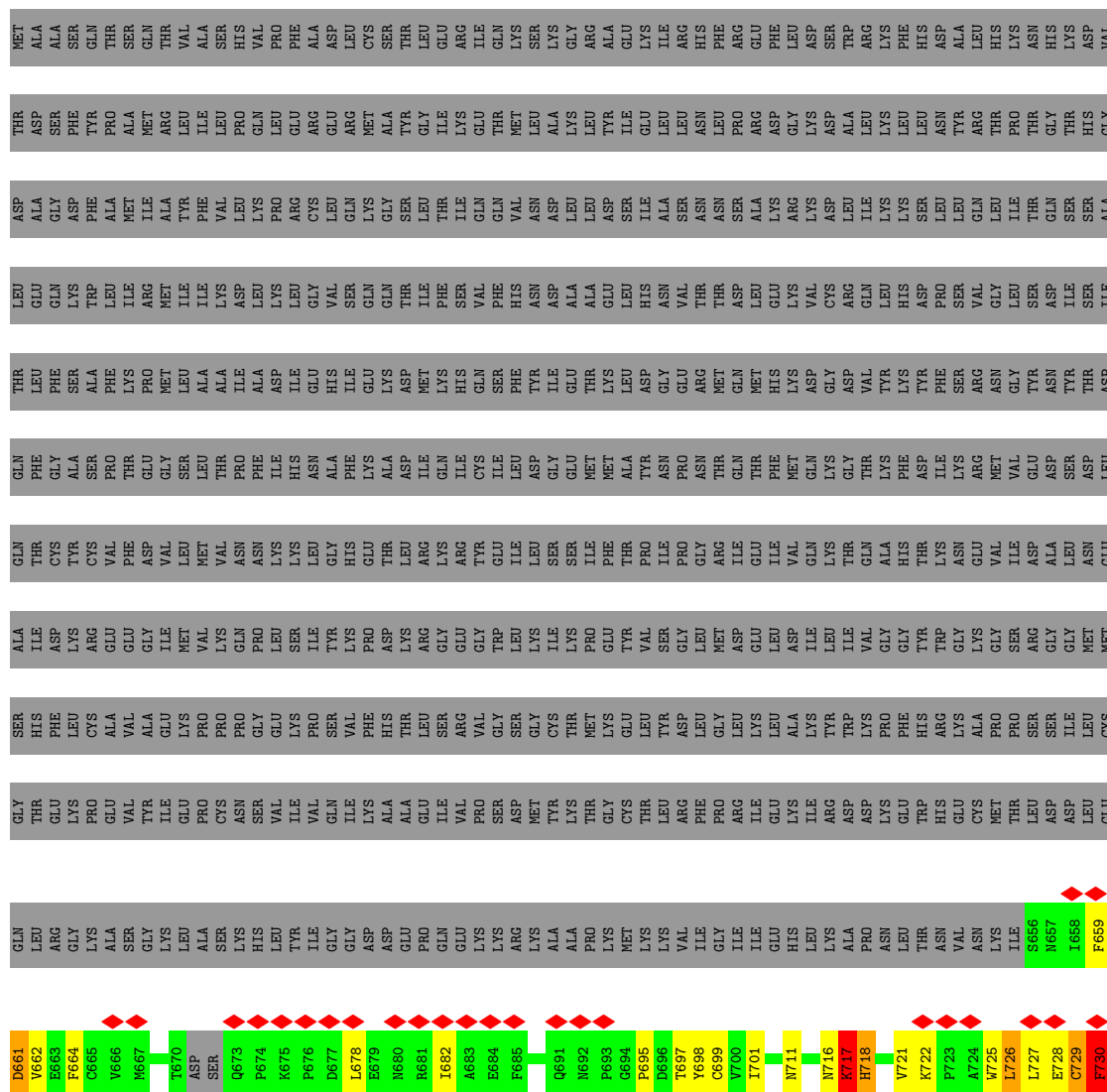


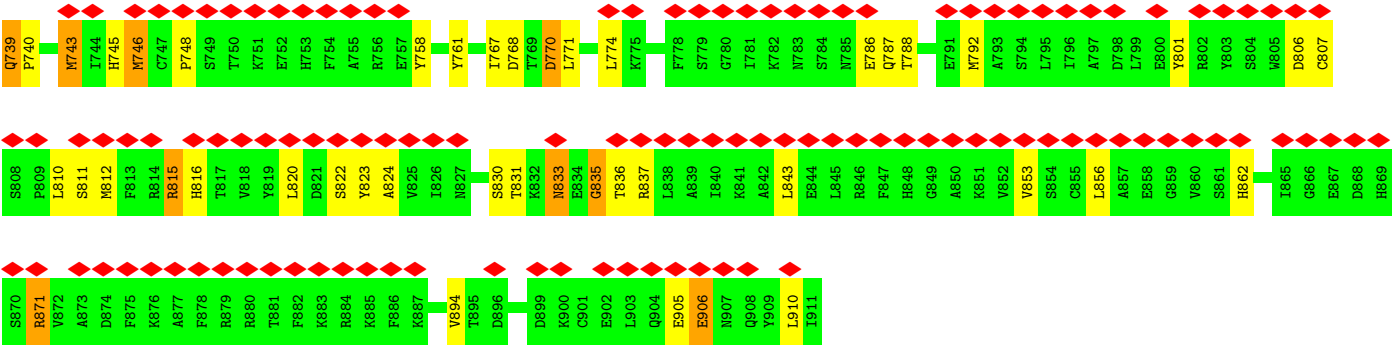
• Molecule 8: Protein PAXX





• Molecule 9: DNA ligase 4





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	495819	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	0.081	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	506.88, 506.88, 506.88	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.112, 2.112, 2.112	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, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.42	10/4101 (0.2%)	1.54	38/5523 (0.7%)
1	J	1.42	10/4101 (0.2%)	1.54	37/5523 (0.7%)
2	B	0.81	1/4286 (0.0%)	1.51	34/5781 (0.6%)
2	K	0.81	1/4286 (0.0%)	1.52	38/5781 (0.7%)
3	C	0.81	3/30414 (0.0%)	1.41	179/41106 (0.4%)
3	L	0.81	3/30414 (0.0%)	1.41	179/41106 (0.4%)
4	D	0.75	0/710	1.62	8/1093 (0.7%)
4	M	0.79	1/710 (0.1%)	1.79	8/1093 (0.7%)
5	E	0.73	0/690	1.29	0/1063
5	N	0.73	0/690	1.29	0/1063
6	F	0.90	1/1657 (0.1%)	1.65	18/2228 (0.8%)
6	G	0.84	0/1622	1.57	12/2178 (0.6%)
6	O	0.90	1/1657 (0.1%)	1.65	22/2228 (1.0%)
6	P	0.85	0/1622	1.57	12/2178 (0.6%)
7	H	0.95	17/1814 (0.9%)	1.43	15/2454 (0.6%)
7	I	0.96	16/1771 (0.9%)	1.37	5/2395 (0.2%)
8	S	0.79	0/172	1.46	0/229
8	T	0.79	0/172	1.46	0/229
9	X	1.00	5/2112 (0.2%)	1.79	49/2851 (1.7%)
9	Y	0.99	5/2112 (0.2%)	1.77	45/2851 (1.6%)
All	All	0.90	74/95113 (0.1%)	1.47	699/128953 (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	3
1	J	0	3
2	B	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	K	0	5
3	C	0	36
3	L	0	36
4	D	0	16
4	M	0	15
5	E	0	11
5	N	0	11
6	F	0	5
6	G	0	2
6	O	0	5
6	P	0	2
7	H	0	2
7	I	0	4
9	X	0	7
9	Y	0	8
All	All	0	176

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	334	THR	N-CA	45.84	2.08	1.46
1	A	334	THR	N-CA	45.77	2.08	1.46
1	A	334	THR	CB-CG2	39.41	2.82	1.52
1	J	334	THR	CB-CG2	39.41	2.82	1.52
1	J	334	THR	CB-OG1	21.39	1.77	1.43
1	A	334	THR	CB-OG1	21.32	1.77	1.43
1	A	333	GLU	CB-CG	17.76	2.05	1.52
1	J	333	GLU	CB-CG	17.72	2.05	1.52
1	J	333	GLU	CA-C	17.62	1.77	1.52
1	A	333	GLU	CA-C	17.55	1.77	1.52
1	J	333	GLU	CA-CB	17.20	1.83	1.53
1	A	333	GLU	CA-CB	17.16	1.83	1.53
1	A	333	GLU	N-CA	16.66	1.68	1.46
1	J	333	GLU	N-CA	16.66	1.68	1.46
1	A	333	GLU	C-N	16.42	1.56	1.33
1	J	333	GLU	C-N	16.41	1.56	1.33
9	Y	737	PRO	CA-C	9.70	1.66	1.52
9	X	737	PRO	CA-C	9.68	1.66	1.52
1	A	333	GLU	CG-CD	8.54	1.73	1.52
1	J	333	GLU	CG-CD	8.51	1.73	1.52
9	X	737	PRO	N-CA	8.35	1.58	1.47
9	Y	737	PRO	N-CA	8.30	1.57	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	334	THR	CA-C	-7.11	1.42	1.52
1	A	334	THR	CA-C	-7.11	1.42	1.52
7	H	1	MET	CG-SD	7.01	1.98	1.80
9	Y	739	GLN	CA-C	6.99	1.61	1.52
9	X	739	GLN	CA-C	6.98	1.61	1.52
7	H	159	MET	SD-CE	6.62	1.96	1.79
7	H	140	MET	CG-SD	6.60	1.97	1.80
7	H	10	MET	CG-SD	6.58	1.97	1.80
7	I	140	MET	SD-CE	6.58	1.96	1.79
7	H	1	MET	SD-CE	6.56	1.96	1.79
2	B	443	LYS	CA-C	6.53	1.61	1.52
9	X	739	GLN	N-CA	6.50	1.55	1.46
7	H	140	MET	SD-CE	6.50	1.95	1.79
2	K	443	LYS	CA-C	6.49	1.61	1.52
7	H	212	MET	SD-CE	6.49	1.95	1.79
7	I	212	MET	SD-CE	6.46	1.95	1.79
7	I	1	MET	CG-SD	6.45	1.96	1.80
9	Y	739	GLN	N-CA	6.44	1.55	1.46
7	H	194	MET	SD-CE	6.40	1.95	1.79
7	H	219	MET	SD-CE	6.38	1.95	1.79
7	I	124	MET	SD-CE	6.37	1.95	1.79
7	I	124	MET	CG-SD	6.35	1.96	1.80
7	I	140	MET	CG-SD	6.33	1.96	1.80
7	H	124	MET	SD-CE	6.32	1.95	1.79
7	I	10	MET	SD-CE	6.27	1.95	1.79
7	H	10	MET	SD-CE	6.25	1.95	1.79
7	I	194	MET	CG-SD	6.25	1.96	1.80
3	C	2247	ASP	N-CA	-6.20	1.38	1.46
3	L	2247	ASP	N-CA	-6.20	1.38	1.46
7	H	212	MET	CG-SD	6.15	1.96	1.80
7	I	159	MET	SD-CE	6.10	1.94	1.79
7	I	212	MET	CG-SD	6.04	1.95	1.80
7	I	219	MET	SD-CE	6.00	1.94	1.79
7	H	124	MET	CG-SD	5.99	1.95	1.80
7	I	194	MET	SD-CE	5.99	1.94	1.79
7	I	142	MET	SD-CE	5.95	1.94	1.79
7	I	159	MET	CG-SD	5.86	1.95	1.80
7	H	194	MET	CG-SD	5.79	1.95	1.80
7	H	142	MET	SD-CE	5.74	1.93	1.79
7	I	1	MET	SD-CE	5.71	1.93	1.79
7	H	159	MET	CG-SD	5.67	1.95	1.80
4	M	25	DT	O3'-P	-5.65	1.52	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	X	738	TRP	CA-C	5.36	1.59	1.52
9	Y	738	TRP	CA-C	5.29	1.59	1.52
7	I	142	MET	CG-SD	5.25	1.93	1.80
7	H	142	MET	CG-SD	5.12	1.93	1.80
6	O	47	VAL	N-CA	5.11	1.51	1.46
3	L	371	GLY	CA-C	5.08	1.55	1.51
6	F	47	VAL	N-CA	5.04	1.51	1.46
3	C	371	GLY	CA-C	5.03	1.55	1.51
3	C	2292	CYS	N-CA	-5.00	1.39	1.46
3	L	2292	CYS	N-CA	-5.00	1.39	1.46

All (699) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	25	DT	O3'-P-O5'	-25.51	65.73	104.00
1	J	334	THR	CA-CB-OG1	-16.52	84.82	109.60
1	A	334	THR	CA-CB-OG1	-16.50	84.85	109.60
4	M	26	DT	P-O5'-C5'	15.96	143.94	120.00
9	Y	735	PHE	CA-CB-CG	15.95	129.75	113.80
9	X	735	PHE	CA-CB-CG	15.95	129.75	113.80
9	Y	736	VAL	CA-C-N	15.23	138.88	119.84
9	Y	736	VAL	C-N-CA	15.23	138.88	119.84
9	X	736	VAL	CA-C-N	15.21	138.85	119.84
9	X	736	VAL	C-N-CA	15.21	138.85	119.84
1	J	333	GLU	CA-C-N	-15.17	91.14	121.18
1	J	333	GLU	C-N-CA	-15.17	91.14	121.18
1	A	333	GLU	CA-C-N	-15.16	91.17	121.18
1	A	333	GLU	C-N-CA	-15.16	91.17	121.18
1	J	333	GLU	CA-CB-CG	-14.74	84.62	114.10
1	A	333	GLU	CA-CB-CG	-14.72	84.66	114.10
1	J	334	THR	N-CA-CB	-14.50	85.01	110.39
1	A	334	THR	N-CA-CB	-14.49	85.04	110.39
6	F	58	ASP	CA-CB-CG	13.91	126.51	112.60
6	O	58	ASP	CA-CB-CG	13.89	126.49	112.60
4	D	25	DT	P-O3'-C3'	-13.09	100.56	120.20
9	Y	737	PRO	N-CA-C	12.31	137.83	112.47
9	X	737	PRO	N-CA-C	12.30	137.81	112.47
9	X	738	TRP	N-CA-C	12.04	125.36	108.74
9	Y	738	TRP	N-CA-C	12.04	125.35	108.74
1	A	333	GLU	CB-CA-C	-11.98	87.35	110.11
1	J	333	GLU	CB-CA-C	-11.98	87.35	110.11
2	K	326	VAL	CA-CB-CG1	11.69	130.27	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	23	SER	N-CA-C	11.69	126.37	108.96
2	K	23	SER	N-CA-C	11.67	126.35	108.96
1	J	333	GLU	O-C-N	11.39	139.25	122.39
1	A	333	GLU	O-C-N	11.35	139.19	122.39
1	A	137	HIS	CA-CB-CG	-11.21	102.59	113.80
1	J	137	HIS	CA-CB-CG	-11.20	102.61	113.80
2	B	105	ALA	N-CA-C	11.06	124.00	108.74
2	K	105	ALA	N-CA-C	11.05	124.00	108.74
3	C	1810	PRO	CA-C-N	10.70	141.97	121.54
3	C	1810	PRO	C-N-CA	10.70	141.97	121.54
1	J	333	GLU	N-CA-CB	-10.50	93.41	110.42
1	A	333	GLU	N-CA-CB	-10.49	93.43	110.42
9	X	736	VAL	CA-C-O	-10.39	106.02	119.95
9	Y	736	VAL	CA-C-O	-10.36	106.07	119.95
4	D	25	DT	OP1-P-O3'	-10.13	77.61	108.00
7	H	18	LEU	CD1-CG-CD2	9.93	132.64	110.80
2	B	98	ILE	N-CA-C	9.78	122.12	109.30
2	K	98	ILE	N-CA-C	9.78	122.12	109.30
2	K	381	ILE	CA-CB-CG1	9.75	126.98	110.40
2	B	381	ILE	CA-CB-CG1	9.72	126.93	110.40
1	J	416	GLN	N-CA-C	9.71	124.84	109.50
1	A	416	GLN	N-CA-C	9.70	124.82	109.50
9	X	770	ASP	N-CA-CB	-9.68	95.92	111.22
3	L	2291	GLN	CA-C-N	9.45	134.15	120.82
3	L	2291	GLN	C-N-CA	9.45	134.15	120.82
3	C	2291	GLN	CA-C-N	9.44	134.12	120.82
3	C	2291	GLN	C-N-CA	9.44	134.12	120.82
1	A	333	GLU	CB-CG-CD	-9.42	96.58	112.60
1	J	333	GLU	CB-CG-CD	-9.39	96.64	112.60
2	K	169	LEU	N-CA-C	9.35	124.00	112.59
2	B	169	LEU	N-CA-C	9.31	123.95	112.59
2	B	504	PRO	N-CA-C	9.29	125.73	111.34
2	K	504	PRO	N-CA-C	9.28	125.72	111.34
6	G	43	TRP	CB-CG-CD2	9.20	139.67	126.80
6	P	43	TRP	CB-CG-CD2	9.19	139.67	126.80
9	X	739	GLN	CA-C-N	9.14	131.26	119.84
9	X	739	GLN	C-N-CA	9.14	131.26	119.84
2	B	126	LYS	N-CA-C	9.06	123.89	110.48
1	A	333	GLU	CG-CD-OE2	-9.03	97.64	118.40
1	J	333	GLU	CG-CD-OE2	-9.03	97.64	118.40
2	K	126	LYS	N-CA-C	9.02	123.83	110.48
3	C	2427	ARG	N-CA-C	8.94	120.64	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	2427	ARG	N-CA-C	8.91	120.61	111.07
1	J	333	GLU	CG-CD-OE1	8.79	138.62	118.40
1	A	333	GLU	CG-CD-OE1	8.78	138.58	118.40
6	F	3	ARG	NE-CZ-NH2	8.77	127.09	119.20
2	K	8	ALA	N-CA-C	8.73	123.44	110.52
6	O	3	ARG	NE-CZ-NH2	8.72	127.05	119.20
2	B	8	ALA	N-CA-C	8.72	123.42	110.52
2	B	415	ASN	N-CA-C	8.69	123.88	113.28
2	K	415	ASN	N-CA-C	8.69	123.88	113.28
1	A	137	HIS	N-CA-C	8.68	123.43	108.76
1	J	137	HIS	N-CA-C	8.68	123.42	108.76
2	B	211	VAL	N-CA-C	8.59	119.38	110.62
2	K	211	VAL	N-CA-C	8.56	119.35	110.62
2	K	207	ILE	N-CA-C	8.55	119.34	110.62
2	B	207	ILE	N-CA-C	8.51	119.30	110.62
4	M	25	DT	P-O3'-C3'	-8.48	107.48	120.20
1	J	334	THR	N-CA-C	-8.47	102.84	113.01
1	A	334	THR	N-CA-C	-8.43	102.89	113.01
4	D	26	DT	C4'-C3'-O3'	8.39	122.58	110.00
9	Y	718	HIS	CA-CB-CG	8.34	122.14	113.80
9	X	718	HIS	CA-CB-CG	8.33	122.13	113.80
6	F	57	ASP	CA-C-N	8.31	132.24	120.28
6	F	57	ASP	C-N-CA	8.31	132.24	120.28
6	O	57	ASP	CA-C-N	8.30	132.23	120.28
6	O	57	ASP	C-N-CA	8.30	132.23	120.28
3	C	429	GLU	N-CA-C	8.29	123.43	107.44
3	L	429	GLU	N-CA-C	8.27	123.40	107.44
2	B	151	ILE	CA-CB-CG1	8.23	124.39	110.40
2	K	151	ILE	CA-CB-CG1	8.22	124.38	110.40
2	B	250	ARG	N-CA-C	8.20	124.81	107.67
9	X	718	HIS	CB-CG-CD2	-8.19	120.55	131.20
2	K	250	ARG	N-CA-C	8.19	124.78	107.67
3	C	568	PHE	CA-CB-CG	-8.18	105.62	113.80
1	J	334	THR	CB-CA-C	8.17	126.84	110.17
3	L	568	PHE	CA-CB-CG	-8.17	105.63	113.80
1	A	334	THR	CB-CA-C	8.17	126.83	110.17
9	Y	718	HIS	CB-CG-CD2	-8.16	120.59	131.20
3	L	305	ASN	OD1-CG-ND2	-8.13	114.47	122.60
2	K	252	THR	N-CA-C	8.10	124.61	107.67
2	B	252	THR	N-CA-C	8.10	124.59	107.67
3	L	63	PHE	CA-CB-CG	7.98	121.78	113.80
2	K	456	ALA	N-CA-C	7.96	122.77	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1268	ASN	CA-CB-CG	7.96	120.56	112.60
6	P	43	TRP	CB-CG-CD1	-7.94	114.98	126.90
3	L	1268	ASN	CA-CB-CG	7.94	120.54	112.60
2	B	456	ALA	N-CA-C	7.93	122.73	112.89
6	G	43	TRP	CB-CG-CD1	-7.93	115.01	126.90
9	Y	738	TRP	CG-CD2-CE3	7.91	141.81	133.90
3	C	63	PHE	CA-CB-CG	7.91	121.71	113.80
9	X	738	TRP	CG-CD2-CE3	7.83	141.73	133.90
2	K	352	GLN	CA-C-N	7.81	130.59	120.44
2	K	352	GLN	C-N-CA	7.81	130.59	120.44
2	B	129	LYS	N-CA-C	7.80	122.72	110.32
2	K	129	LYS	N-CA-C	7.80	122.72	110.32
2	B	352	GLN	CA-C-N	7.79	130.57	120.44
2	B	352	GLN	C-N-CA	7.79	130.57	120.44
3	L	1596	VAL	N-CA-CB	7.77	120.18	110.47
3	C	1596	VAL	N-CA-CB	7.76	120.17	110.47
3	L	430	VAL	CA-C-N	7.73	131.41	120.28
3	L	430	VAL	C-N-CA	7.73	131.41	120.28
3	C	430	VAL	CA-C-N	7.71	131.39	120.28
3	C	430	VAL	C-N-CA	7.71	131.39	120.28
9	Y	739	GLN	CA-C-N	7.66	129.42	119.84
9	Y	739	GLN	C-N-CA	7.66	129.42	119.84
9	Y	738	TRP	N-CA-CB	-7.64	98.45	111.21
2	B	460	SER	N-CA-C	7.63	120.56	111.33
9	X	738	TRP	N-CA-CB	-7.63	98.47	111.21
3	C	430	VAL	CB-CA-C	-7.60	100.95	112.05
3	L	430	VAL	CB-CA-C	-7.60	100.96	112.05
4	D	25	DT	O3'-P-O5'	-7.58	92.62	104.00
2	K	460	SER	N-CA-C	7.58	120.50	111.33
4	M	25	DT	OP1-P-O3'	-7.56	85.31	108.00
6	P	155	TRP	CB-CG-CD2	7.54	137.36	126.80
6	G	155	TRP	CB-CG-CD2	7.54	137.35	126.80
2	B	231	LEU	CB-CG-CD1	7.49	133.16	110.70
6	F	134	ILE	CA-CB-CG1	7.49	123.13	110.40
6	O	134	ILE	CA-CB-CG1	7.47	123.10	110.40
2	K	231	LEU	CB-CG-CD1	7.47	133.11	110.70
3	C	3903	HIS	CA-CB-CG	-7.47	106.33	113.80
3	L	3903	HIS	CA-CB-CG	-7.41	106.39	113.80
3	C	1175	HIS	CA-CB-CG	-7.38	106.42	113.80
3	L	1175	HIS	CA-CB-CG	-7.38	106.42	113.80
2	B	200	GLN	N-CA-C	7.38	121.19	111.75
2	K	200	GLN	N-CA-C	7.36	121.17	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Y	730	PHE	CA-CB-CG	-7.26	106.54	113.80
3	L	2218	PHE	CA-CB-CG	7.25	121.05	113.80
3	C	2218	PHE	CA-CB-CG	7.22	121.03	113.80
9	Y	738	TRP	CE2-CD2-CE3	-7.22	111.58	118.80
9	X	730	PHE	CA-CB-CG	-7.19	106.61	113.80
9	X	738	TRP	CE2-CD2-CE3	-7.18	111.62	118.80
9	X	738	TRP	CB-CG-CD2	7.17	136.83	126.80
3	L	2372	PRO	N-CA-C	7.16	119.44	110.70
9	Y	738	TRP	CB-CG-CD2	7.15	136.81	126.80
3	C	2384	PHE	CA-CB-CG	7.14	120.94	113.80
3	L	2384	PHE	CA-CB-CG	7.14	120.94	113.80
3	C	2372	PRO	N-CA-C	7.12	119.39	110.70
3	C	1810	PRO	O-C-N	7.06	130.68	122.98
4	D	26	DT	O5'-C5'-C4'	7.06	121.39	110.80
2	K	146	GLN	N-CA-C	7.03	125.78	110.80
2	B	146	GLN	N-CA-C	7.02	125.76	110.80
3	C	413	PHE	CA-CB-CG	6.98	120.78	113.80
3	L	413	PHE	CA-CB-CG	6.98	120.78	113.80
3	L	2943	PHE	CA-CB-CG	-6.95	106.86	113.80
9	X	770	ASP	N-CA-C	6.93	119.02	109.18
4	D	26	DT	O4'-C1'-C2'	-6.92	96.02	106.40
3	C	2943	PHE	CA-CB-CG	-6.91	106.89	113.80
2	B	87	ASP	CA-CB-CG	6.90	119.50	112.60
2	K	87	ASP	CA-CB-CG	6.90	119.50	112.60
2	B	145	SER	N-CA-C	6.88	125.45	110.80
2	K	145	SER	N-CA-C	6.86	125.42	110.80
3	L	2574	ASN	CA-C-N	6.85	126.89	119.90
3	L	2574	ASN	C-N-CA	6.85	126.89	119.90
3	C	2574	ASN	CA-C-N	6.79	126.82	119.90
3	C	2574	ASN	C-N-CA	6.79	126.82	119.90
6	F	137	ASN	CA-CB-CG	-6.79	105.81	112.60
3	C	771	ASN	CA-CB-CG	6.78	119.38	112.60
3	L	771	ASN	CA-CB-CG	6.78	119.38	112.60
3	C	2358	ASP	CA-CB-CG	6.78	119.38	112.60
3	L	2358	ASP	CA-CB-CG	6.78	119.38	112.60
9	X	740	PRO	CA-N-CD	-6.75	102.56	112.00
6	O	137	ASN	CA-CB-CG	-6.74	105.86	112.60
3	L	583	LEU	N-CA-C	6.73	120.68	111.39
3	C	583	LEU	N-CA-C	6.72	120.67	111.39
9	X	717	LYS	CA-CB-CG	6.70	127.50	114.10
9	Y	717	LYS	CA-CB-CG	6.68	127.47	114.10
3	C	1438	GLY	CA-C-N	6.62	126.20	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1438	GLY	C-N-CA	6.62	126.20	119.19
3	C	1001	PHE	N-CA-C	6.60	119.03	111.11
3	L	2786	LYS	CA-C-O	-6.60	113.50	121.28
3	L	1001	PHE	N-CA-C	6.59	119.02	111.11
3	L	1438	GLY	CA-C-N	6.59	126.17	119.19
3	L	1438	GLY	C-N-CA	6.59	126.17	119.19
3	C	2291	GLN	O-C-N	-6.58	113.84	122.59
3	L	2291	GLN	O-C-N	-6.57	113.85	122.59
1	A	184	SER	CA-C-N	6.57	128.98	120.44
1	A	184	SER	C-N-CA	6.57	128.98	120.44
6	P	155	TRP	CB-CG-CD1	-6.57	117.05	126.90
3	C	2786	LYS	CA-C-O	-6.57	113.53	121.28
6	G	155	TRP	CB-CG-CD1	-6.56	117.06	126.90
4	M	26	DT	O5'-P-OP1	6.56	128.69	109.00
7	I	176	ARG	NE-CZ-NH2	6.55	125.10	119.20
1	J	184	SER	CA-C-N	6.53	128.93	120.44
1	J	184	SER	C-N-CA	6.53	128.93	120.44
7	H	17	GLN	CA-C-N	6.53	132.15	121.58
7	H	17	GLN	C-N-CA	6.53	132.15	121.58
1	J	332	GLU	CA-C-N	-6.53	108.89	121.94
1	J	332	GLU	C-N-CA	-6.53	108.89	121.94
1	A	332	GLU	CA-C-N	-6.51	108.92	121.94
1	A	332	GLU	C-N-CA	-6.51	108.92	121.94
1	J	258	ARG	NE-CZ-NH2	6.50	125.05	119.20
3	L	2512	ASP	N-CA-C	6.50	118.41	110.41
3	C	1082	PHE	CA-CB-CG	-6.50	107.30	113.80
3	L	1082	PHE	CA-CB-CG	-6.50	107.30	113.80
3	C	2512	ASP	N-CA-C	6.49	118.39	110.41
6	O	106	PHE	CA-CB-CG	-6.48	107.32	113.80
1	A	258	ARG	NE-CZ-NH2	6.46	125.02	119.20
7	H	109	ARG	NE-CZ-NH2	6.45	125.00	119.20
9	X	736	VAL	O-C-N	6.43	128.44	121.10
3	C	278	HIS	CA-CB-CG	-6.43	107.37	113.80
3	C	3370	SER	CA-C-N	6.41	129.19	120.54
3	C	3370	SER	C-N-CA	6.41	129.19	120.54
3	C	1445	ARG	NE-CZ-NH2	6.41	124.97	119.20
3	L	1445	ARG	NE-CZ-NH2	6.41	124.97	119.20
3	L	278	HIS	CA-CB-CG	-6.40	107.40	113.80
9	Y	736	VAL	O-C-N	6.38	128.37	121.10
3	C	2917	PRO	N-CA-C	6.37	118.47	110.70
4	M	27	DA	O3'-P-O5'	6.37	113.56	104.00
3	L	2917	PRO	N-CA-C	6.37	118.47	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	171	ASN	CA-CB-CG	6.36	118.96	112.60
6	F	157	ASP	CA-CB-CG	-6.36	106.24	112.60
3	L	3370	SER	CA-C-N	6.36	129.12	120.54
3	L	3370	SER	C-N-CA	6.36	129.12	120.54
3	L	1231	GLN	CB-CA-C	6.35	117.25	110.65
3	L	2231	PHE	CA-CB-CG	6.35	120.15	113.80
3	C	1231	GLN	CB-CA-C	6.35	117.25	110.65
1	A	171	ASN	CA-CB-CG	6.33	118.93	112.60
6	O	157	ASP	CA-CB-CG	-6.33	106.27	112.60
2	K	353	ARG	NE-CZ-NH2	6.33	124.89	119.20
3	C	2231	PHE	CA-CB-CG	6.32	120.12	113.80
3	C	2472	GLN	OE1-CD-NE2	-6.29	116.31	122.60
3	L	2472	GLN	OE1-CD-NE2	-6.29	116.31	122.60
3	C	1735	ARG	NE-CZ-NH2	6.29	124.86	119.20
2	B	353	ARG	NE-CZ-NH2	6.28	124.85	119.20
3	C	2634	GLN	CA-C-N	6.28	131.45	123.10
3	C	2634	GLN	C-N-CA	6.28	131.45	123.10
9	Y	905	GLU	CA-C-N	6.27	129.53	120.38
9	Y	905	GLU	C-N-CA	6.27	129.53	120.38
9	X	905	GLU	CA-C-N	6.26	129.52	120.38
9	X	905	GLU	C-N-CA	6.26	129.52	120.38
6	F	13	GLU	CA-C-N	6.25	125.48	118.97
6	F	13	GLU	C-N-CA	6.25	125.48	118.97
3	L	2634	GLN	CA-C-N	6.25	131.42	123.10
3	L	2634	GLN	C-N-CA	6.25	131.42	123.10
3	L	494	PRO	CA-C-N	6.24	130.68	122.51
3	L	494	PRO	C-N-CA	6.24	130.68	122.51
9	Y	833	ASN	CA-CB-CG	6.23	118.83	112.60
3	C	494	PRO	CA-C-N	6.22	130.66	122.51
3	C	494	PRO	C-N-CA	6.22	130.66	122.51
4	D	26	DT	O5'-P-OP1	6.22	127.66	109.00
6	O	13	GLU	CA-C-N	6.21	125.43	118.97
6	O	13	GLU	C-N-CA	6.21	125.43	118.97
3	C	2120	ARG	CA-C-N	6.19	130.90	120.88
3	C	2120	ARG	C-N-CA	6.19	130.90	120.88
3	L	2120	ARG	CA-C-N	6.19	130.90	120.88
3	L	2120	ARG	C-N-CA	6.19	130.90	120.88
3	L	1735	ARG	NE-CZ-NH2	6.17	124.76	119.20
9	X	833	ASN	CA-CB-CG	6.17	118.77	112.60
3	C	1195	VAL	CB-CA-C	-6.12	107.89	113.70
3	L	429	GLU	CA-C-N	6.11	130.65	120.62
3	L	429	GLU	C-N-CA	6.11	130.65	120.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	429	GLU	CA-C-N	6.11	130.64	120.62
3	C	429	GLU	C-N-CA	6.11	130.64	120.62
9	X	871	ARG	NE-CZ-NH2	6.10	124.69	119.20
3	C	361	ILE	CB-CA-C	-6.10	104.17	111.97
3	C	582	THR	N-CA-C	6.10	117.56	107.20
6	G	197	LYS	CB-CG-CD	6.09	125.32	111.30
3	L	2426	HIS	CA-C-N	6.09	128.36	120.44
3	L	2426	HIS	C-N-CA	6.09	128.36	120.44
3	L	1990	PHE	CA-CB-CG	-6.09	107.71	113.80
9	Y	871	ARG	NE-CZ-NH2	6.09	124.68	119.20
3	L	2848	PHE	CA-C-N	6.08	131.02	120.68
3	L	2848	PHE	C-N-CA	6.08	131.02	120.68
3	L	2527	HIS	CB-CG-CD2	-6.08	123.29	131.20
3	C	852	ARG	NE-CZ-NH2	6.08	124.67	119.20
3	L	852	ARG	NE-CZ-NH2	6.08	124.67	119.20
1	A	334	THR	OG1-CB-CG2	6.08	121.45	109.30
2	K	409	PHE	CA-CB-CG	6.08	119.88	113.80
3	L	582	THR	N-CA-C	6.08	117.53	107.20
3	C	1990	PHE	CA-CB-CG	-6.07	107.73	113.80
1	J	334	THR	OG1-CB-CG2	6.07	121.44	109.30
6	P	91	GLU	CA-C-N	6.07	129.02	120.28
6	P	91	GLU	C-N-CA	6.07	129.02	120.28
6	P	197	LYS	CB-CG-CD	6.07	125.27	111.30
3	L	1195	VAL	CB-CA-C	-6.07	107.93	113.70
3	L	657	SER	CA-C-N	6.07	128.69	120.38
3	L	657	SER	C-N-CA	6.07	128.69	120.38
3	C	1195	VAL	N-CA-CB	6.07	114.58	110.52
3	L	361	ILE	CB-CA-C	-6.07	104.20	111.97
3	C	2848	PHE	CA-C-N	6.06	130.99	120.68
3	C	2848	PHE	C-N-CA	6.06	130.99	120.68
3	L	3026	ASP	N-CA-CB	6.06	118.88	109.85
3	C	2527	HIS	CB-CG-CD2	-6.06	123.32	131.20
6	G	91	GLU	CA-C-N	6.06	129.00	120.28
6	G	91	GLU	C-N-CA	6.06	129.00	120.28
2	B	409	PHE	CA-CB-CG	6.05	119.85	113.80
3	C	657	SER	CA-C-N	6.05	128.67	120.38
3	C	657	SER	C-N-CA	6.05	128.67	120.38
3	C	2426	HIS	CA-C-N	6.05	128.31	120.44
3	C	2426	HIS	C-N-CA	6.05	128.31	120.44
9	X	737	PRO	O-C-N	-6.05	114.47	122.64
6	F	40	HIS	CA-CB-CG	6.05	119.85	113.80
3	C	2389	PHE	CA-CB-CG	6.04	119.84	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	2389	PHE	CA-CB-CG	6.04	119.84	113.80
1	A	319	SER	N-CA-C	6.04	117.42	108.60
1	J	319	SER	N-CA-C	6.04	117.41	108.60
3	C	1178	ARG	NE-CZ-NH2	6.04	124.63	119.20
3	C	1500	LEU	CA-C-N	6.03	125.97	119.76
3	C	1500	LEU	C-N-CA	6.03	125.97	119.76
3	L	1500	LEU	CA-C-N	6.03	125.97	119.76
3	L	1500	LEU	C-N-CA	6.03	125.97	119.76
3	C	3026	ASP	N-CA-CB	6.03	118.83	109.85
3	L	1195	VAL	N-CA-CB	6.01	114.55	110.52
9	Y	862	HIS	CB-CG-CD2	-6.00	123.40	131.20
9	Y	737	PRO	O-C-N	-6.00	114.55	122.64
6	O	40	HIS	CA-CB-CG	6.00	119.80	113.80
9	Y	718	HIS	N-CA-CB	-5.99	101.90	111.43
7	I	57	ARG	NE-CZ-NH2	5.99	124.59	119.20
3	L	1178	ARG	NE-CZ-NH2	5.98	124.58	119.20
9	X	718	HIS	N-CA-CB	-5.97	101.93	111.43
1	A	184	SER	O-C-N	-5.97	115.24	122.22
9	X	862	HIS	CB-CG-CD2	-5.97	123.44	131.20
3	C	894	PHE	CA-CB-CG	-5.96	107.84	113.80
3	L	894	PHE	CA-CB-CG	-5.95	107.85	113.80
6	F	55	GLU	CA-CB-CG	5.94	125.99	114.10
6	O	55	GLU	CA-CB-CG	5.94	125.99	114.10
6	O	102	LYS	CA-C-N	5.92	132.53	123.47
6	O	102	LYS	C-N-CA	5.92	132.53	123.47
7	H	17	GLN	O-C-N	5.91	130.32	123.17
1	J	184	SER	O-C-N	-5.91	115.31	122.22
2	B	517	ASN	CA-C-N	5.89	126.44	120.38
2	B	517	ASN	C-N-CA	5.89	126.44	120.38
2	K	517	ASN	CA-C-N	5.89	126.44	120.38
2	K	517	ASN	C-N-CA	5.89	126.44	120.38
3	L	3357	ARG	NE-CZ-NH2	5.87	124.49	119.20
6	O	111	PHE	CA-CB-CG	5.87	119.67	113.80
6	F	111	PHE	CA-CB-CG	5.86	119.66	113.80
9	X	748	PRO	N-CA-CB	5.86	109.40	103.25
3	C	2464	HIS	CB-CG-CD2	-5.86	123.59	131.20
9	Y	748	PRO	N-CA-CB	5.86	109.40	103.25
9	X	758	TYR	CA-CB-CG	5.85	124.43	113.90
3	C	1734	PRO	CA-C-N	5.85	128.39	120.38
3	C	1734	PRO	C-N-CA	5.85	128.39	120.38
3	L	101	ALA	CA-C-N	5.84	126.60	120.12
3	L	101	ALA	C-N-CA	5.84	126.60	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	345	PHE	CA-CB-CG	5.82	119.62	113.80
3	C	345	PHE	CA-CB-CG	5.82	119.62	113.80
9	Y	758	TYR	CA-CB-CG	5.82	124.37	113.90
3	L	2464	HIS	CB-CG-CD2	-5.81	123.64	131.20
9	X	745	HIS	CB-CG-CD2	-5.81	123.64	131.20
3	L	1734	PRO	CA-C-N	5.81	128.34	120.38
3	L	1734	PRO	C-N-CA	5.81	128.34	120.38
3	C	3357	ARG	NE-CZ-NH2	5.81	124.43	119.20
3	C	2170	GLN	OE1-CD-NE2	-5.81	116.79	122.60
3	L	2170	GLN	OE1-CD-NE2	-5.81	116.79	122.60
7	H	57	ARG	NE-CZ-NH2	5.80	124.42	119.20
3	C	101	ALA	CA-C-N	5.79	126.55	120.12
3	C	101	ALA	C-N-CA	5.79	126.55	120.12
3	L	3026	ASP	CA-C-N	5.78	130.51	120.68
3	L	3026	ASP	C-N-CA	5.78	130.51	120.68
9	Y	745	HIS	CB-CG-CD2	-5.78	123.68	131.20
3	C	2246	LYS	O-C-N	-5.78	116.26	122.85
3	L	2246	LYS	O-C-N	-5.78	116.26	122.85
7	I	67	ALA	N-CA-CB	-5.77	105.04	111.10
3	C	2283	ASN	CA-CB-CG	5.76	118.36	112.60
9	X	770	ASP	CA-C-O	-5.76	114.81	121.49
3	L	3897	PHE	CA-CB-CG	-5.76	108.04	113.80
3	C	1601	LEU	CB-CA-C	5.75	120.61	110.37
3	L	484	HIS	N-CA-C	5.75	117.35	111.14
3	L	1601	LEU	CB-CA-C	5.75	120.60	110.37
3	C	3026	ASP	CA-C-N	5.73	130.43	120.68
3	C	3026	ASP	C-N-CA	5.73	130.43	120.68
7	H	151	ARG	NE-CZ-NH2	5.73	124.36	119.20
1	A	395	ALA	N-CA-C	5.72	119.38	110.17
1	J	395	ALA	N-CA-C	5.72	119.38	110.17
3	C	484	HIS	N-CA-C	5.71	117.31	111.14
3	L	1465	HIS	CA-CB-CG	5.71	119.51	113.80
3	L	2283	ASN	CA-CB-CG	5.71	118.31	112.60
3	C	3741	ARG	NE-CZ-NH2	5.70	124.33	119.20
3	C	1465	HIS	CA-CB-CG	5.69	119.49	113.80
3	C	1858	LEU	CA-C-N	5.69	128.37	120.29
3	C	1858	LEU	C-N-CA	5.69	128.37	120.29
3	L	472	GLY	CA-C-N	5.68	126.06	119.47
3	L	472	GLY	C-N-CA	5.68	126.06	119.47
3	C	472	GLY	CA-C-N	5.66	126.03	119.47
3	C	472	GLY	C-N-CA	5.66	126.03	119.47
3	C	3897	PHE	CA-CB-CG	-5.66	108.14	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	X	910	LEU	CA-C-N	5.66	131.88	121.70
9	X	910	LEU	C-N-CA	5.66	131.88	121.70
3	L	891	ARG	N-CA-C	5.65	118.29	111.40
3	L	1810	PRO	CA-C-N	5.64	134.51	121.87
3	L	1810	PRO	C-N-CA	5.64	134.51	121.87
3	L	3741	ARG	NE-CZ-NH2	5.64	124.28	119.20
3	C	3696	ARG	NE-CZ-NH2	5.63	124.27	119.20
3	C	305	ASN	OD1-CG-ND2	-5.63	116.97	122.60
3	C	891	ARG	N-CA-C	5.63	118.27	111.40
3	L	492	SER	CA-C-N	5.63	128.49	120.49
3	L	492	SER	C-N-CA	5.63	128.49	120.49
3	L	1858	LEU	CA-C-N	5.63	128.29	120.29
3	L	1858	LEU	C-N-CA	5.63	128.29	120.29
9	Y	905	GLU	CB-CA-C	5.62	119.50	109.38
9	Y	910	LEU	CA-C-N	5.62	131.81	121.70
9	Y	910	LEU	C-N-CA	5.62	131.81	121.70
3	L	1553	PHE	CA-CB-CG	5.61	119.41	113.80
3	L	3308	ASP	CA-CB-CG	5.60	118.20	112.60
4	D	27	DA	O3'-P-O5'	5.60	112.40	104.00
9	X	905	GLU	CB-CA-C	5.60	119.46	109.38
3	C	492	SER	CA-C-N	5.60	128.44	120.49
3	C	492	SER	C-N-CA	5.60	128.44	120.49
9	X	716	ASN	CA-C-N	5.59	132.22	121.54
9	X	716	ASN	C-N-CA	5.59	132.22	121.54
9	Y	716	ASN	CA-C-N	5.59	132.22	121.54
9	Y	716	ASN	C-N-CA	5.59	132.22	121.54
2	K	405	VAL	N-CA-C	5.58	117.95	108.86
7	I	75	HIS	CB-CG-CD2	-5.57	123.96	131.20
3	C	32	HIS	CB-CG-CD2	-5.57	123.96	131.20
3	C	1553	PHE	CA-CB-CG	5.57	119.37	113.80
3	C	3308	ASP	CA-CB-CG	5.57	118.17	112.60
2	B	405	VAL	N-CA-C	5.57	117.93	108.86
3	L	2120	ARG	NE-CZ-NH2	5.57	124.21	119.20
3	L	32	HIS	CB-CG-CD2	-5.56	123.97	131.20
3	L	3696	ARG	NE-CZ-NH2	5.56	124.21	119.20
6	P	148	ASN	CB-CA-C	5.56	120.40	109.72
3	C	2470	ARG	NE-CZ-NH2	5.56	124.20	119.20
3	L	1305	ASP	CA-CB-CG	5.55	118.16	112.60
3	C	1498	GLN	CA-C-N	5.54	129.57	121.31
3	C	1498	GLN	C-N-CA	5.54	129.57	121.31
3	C	1305	ASP	CA-CB-CG	5.54	118.14	112.60
3	L	444	ASP	CA-CB-CG	5.54	118.14	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	148	ASN	CB-CA-C	5.53	120.33	109.72
3	L	3419	PHE	CA-CB-CG	-5.53	108.27	113.80
3	C	1816	ARG	NE-CZ-NH2	5.52	124.17	119.20
3	L	1498	GLN	CA-C-N	5.52	129.54	121.31
3	L	1498	GLN	C-N-CA	5.52	129.54	121.31
3	C	2120	ARG	NE-CZ-NH2	5.52	124.17	119.20
4	M	26	DT	C5'-C4'-C3'	5.52	123.18	114.90
6	O	107	ARG	CB-CA-C	5.51	118.58	109.70
9	Y	831	THR	N-CA-C	-5.51	104.98	112.26
3	C	2224	PHE	CA-CB-CG	5.51	119.31	113.80
1	A	165	ARG	NE-CZ-NH2	5.51	124.16	119.20
3	C	2373	PRO	N-CA-C	5.51	123.81	112.47
3	L	1816	ARG	NE-CZ-NH2	5.51	124.16	119.20
3	L	2373	PRO	N-CA-C	5.51	123.81	112.47
3	C	3598	LYS	CA-C-N	5.50	130.04	122.06
3	C	3598	LYS	C-N-CA	5.50	130.04	122.06
1	J	334	THR	CA-C-O	-5.50	111.90	119.05
3	L	3598	LYS	CA-C-N	5.50	130.04	122.06
3	L	3598	LYS	C-N-CA	5.50	130.04	122.06
7	H	178	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	J	165	ARG	NE-CZ-NH2	5.49	124.14	119.20
7	H	46	HIS	CB-CG-CD2	-5.48	124.08	131.20
3	L	2470	ARG	NE-CZ-NH2	5.48	124.13	119.20
4	M	26	DT	C4'-C3'-O3'	5.48	118.22	110.00
3	C	3419	PHE	CA-CB-CG	-5.47	108.33	113.80
2	K	327	ASP	CA-CB-CG	5.47	118.07	112.60
9	X	831	THR	N-CA-C	-5.47	105.04	112.26
3	L	2224	PHE	CA-CB-CG	5.47	119.27	113.80
1	J	53	SER	CA-C-N	5.46	130.88	121.86
1	J	53	SER	C-N-CA	5.46	130.88	121.86
3	L	3811	THR	N-CA-CB	5.46	118.04	110.17
1	A	334	THR	CA-C-O	-5.46	111.95	119.05
1	A	53	SER	CA-C-N	5.45	130.86	121.86
1	A	53	SER	C-N-CA	5.45	130.86	121.86
9	Y	711	ASN	CA-CB-CG	5.45	118.05	112.60
1	A	358	LYS	O-C-N	-5.45	113.69	122.41
3	C	3811	THR	N-CA-CB	5.45	118.01	110.17
7	H	62	ASN	CA-CB-CG	5.44	118.04	112.60
1	J	358	LYS	O-C-N	-5.44	113.71	122.41
3	L	1652	ILE	N-CA-CB	5.43	116.54	110.62
3	C	1652	ILE	N-CA-CB	5.43	116.54	110.62
3	C	1862	THR	CA-CB-OG1	-5.43	101.46	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	352	VAL	N-CA-C	5.42	116.58	109.58
3	C	721	TYR	N-CA-C	5.42	117.53	110.53
3	L	352	VAL	N-CA-C	5.42	116.58	109.58
3	L	1075	ARG	NE-CZ-NH2	5.42	124.08	119.20
2	B	227	PHE	CA-CB-CG	5.41	119.20	113.80
9	X	711	ASN	CA-CB-CG	5.40	118.00	112.60
3	L	3690	PHE	CA-CB-CG	-5.40	108.40	113.80
3	C	1075	ARG	NE-CZ-NH2	5.40	124.06	119.20
3	C	3169	PRO	CA-C-N	5.40	129.59	122.30
3	C	3169	PRO	C-N-CA	5.40	129.59	122.30
3	C	3690	PHE	CA-CB-CG	-5.39	108.41	113.80
9	Y	726	LEU	CA-C-N	5.39	130.02	121.44
9	Y	726	LEU	C-N-CA	5.39	130.02	121.44
2	K	227	PHE	CA-CB-CG	5.39	119.19	113.80
3	L	305	ASN	CA-C-N	-5.39	111.93	120.55
3	L	305	ASN	C-N-CA	-5.39	111.93	120.55
3	L	721	TYR	N-CA-C	5.39	117.48	110.53
3	L	3169	PRO	CA-C-N	5.38	129.56	122.30
3	L	3169	PRO	C-N-CA	5.38	129.56	122.30
3	C	1384	PHE	CA-C-N	5.38	129.21	120.60
3	C	1384	PHE	C-N-CA	5.38	129.21	120.60
3	C	1711	ARG	NE-CZ-NH2	5.38	124.04	119.20
3	L	1711	ARG	NE-CZ-NH2	5.38	124.04	119.20
3	C	3974	MET	N-CA-CB	-5.38	102.55	111.96
9	X	726	LEU	CA-C-N	5.37	129.97	121.44
9	X	726	LEU	C-N-CA	5.37	129.97	121.44
9	Y	722	LYS	CA-C-N	5.37	124.82	119.24
9	Y	722	LYS	C-N-CA	5.37	124.82	119.24
6	P	118	ASN	CA-CB-CG	5.36	117.96	112.60
6	G	118	ASN	CA-CB-CG	5.36	117.96	112.60
3	C	2522	ARG	NE-CZ-NH2	5.35	124.02	119.20
3	L	1384	PHE	CA-C-N	5.34	129.15	120.60
3	L	1384	PHE	C-N-CA	5.34	129.15	120.60
3	L	3974	MET	N-CA-CB	-5.34	102.61	111.96
2	B	390	VAL	N-CA-C	5.34	117.07	108.85
3	L	3689	ASP	CA-CB-CG	5.34	117.94	112.60
1	J	339	ARG	NE-CZ-NH2	5.33	124.00	119.20
3	C	1689	LYS	CA-C-N	5.32	125.85	119.94
3	C	1689	LYS	C-N-CA	5.32	125.85	119.94
9	X	722	LYS	CA-C-N	5.32	124.77	119.24
9	X	722	LYS	C-N-CA	5.32	124.77	119.24
3	C	2163	HIS	CA-CB-CG	5.31	119.11	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	3716	HIS	CA-CB-CG	5.31	119.11	113.80
2	K	390	VAL	N-CA-C	5.31	117.03	108.85
3	L	1689	LYS	CA-C-N	5.31	125.83	119.94
3	L	1689	LYS	C-N-CA	5.31	125.83	119.94
3	L	2962	ARG	NE-CZ-NH2	5.31	123.98	119.20
3	L	2636	ARG	NE-CZ-NH2	5.30	123.97	119.20
3	C	437	HIS	CB-CG-CD2	-5.30	124.31	131.20
7	I	151	ARG	NE-CZ-NH2	5.30	123.97	119.20
3	L	2522	ARG	NE-CZ-NH2	5.30	123.97	119.20
3	C	3689	ASP	CA-CB-CG	5.29	117.89	112.60
6	G	21	GLN	OE1-CD-NE2	-5.29	117.31	122.60
3	C	2962	ARG	NE-CZ-NH2	5.29	123.96	119.20
3	L	526	ASP	N-CA-C	5.29	116.85	111.14
6	O	25	GLU	CA-C-N	5.29	131.64	121.54
6	O	25	GLU	C-N-CA	5.29	131.64	121.54
3	C	3716	HIS	CA-CB-CG	5.29	119.09	113.80
6	F	161	ARG	NE-CZ-NH2	5.29	123.96	119.20
3	L	2163	HIS	CA-CB-CG	5.29	119.09	113.80
3	C	1926	ASN	CA-CB-CG	5.28	117.88	112.60
3	C	2635	ILE	N-CA-CB	-5.28	104.77	111.64
6	O	34	ILE	CB-CA-C	5.28	118.64	110.50
7	H	43	GLN	OE1-CD-NE2	-5.28	117.33	122.60
1	A	339	ARG	NE-CZ-NH2	5.27	123.95	119.20
3	C	1581	GLU	CA-C-N	5.27	127.60	120.38
3	C	1581	GLU	C-N-CA	5.27	127.60	120.38
3	L	1581	GLU	CA-C-N	5.27	127.60	120.38
3	L	1581	GLU	C-N-CA	5.27	127.60	120.38
3	C	2636	ARG	NE-CZ-NH2	5.27	123.94	119.20
6	P	21	GLN	OE1-CD-NE2	-5.27	117.33	122.60
7	H	133	GLN	OE1-CD-NE2	-5.27	117.33	122.60
3	L	2891	ARG	NE-CZ-NH2	5.27	123.94	119.20
3	C	2121	ASP	N-CA-CB	-5.27	102.33	110.07
3	L	2121	ASP	N-CA-CB	-5.27	102.33	110.07
3	L	1406	LEU	CA-C-N	5.26	127.28	120.44
3	L	1406	LEU	C-N-CA	5.26	127.28	120.44
6	F	34	ILE	CB-CA-C	5.26	118.60	110.50
3	L	437	HIS	CB-CG-CD2	-5.26	124.36	131.20
9	X	835	GLY	CA-C-N	5.26	128.34	120.87
9	X	835	GLY	C-N-CA	5.26	128.34	120.87
3	C	526	ASP	N-CA-C	5.26	116.82	111.14
3	C	582	THR	CB-CA-C	-5.26	104.91	111.43
6	O	161	ARG	NE-CZ-NH2	5.26	123.93	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Y	835	GLY	CA-C-N	5.25	128.33	120.87
9	Y	835	GLY	C-N-CA	5.25	128.33	120.87
3	C	2891	ARG	NE-CZ-NH2	5.25	123.92	119.20
6	F	25	GLU	CA-C-N	5.25	131.56	121.54
6	F	25	GLU	C-N-CA	5.25	131.56	121.54
3	C	3743	HIS	CB-CG-CD2	-5.24	124.39	131.20
6	O	40	HIS	CB-CG-CD2	-5.24	124.39	131.20
2	B	408	ALA	CA-C-N	5.24	128.65	121.74
2	B	408	ALA	C-N-CA	5.24	128.65	121.74
2	K	408	ALA	CA-C-N	5.24	128.65	121.74
2	K	408	ALA	C-N-CA	5.24	128.65	121.74
3	L	3743	HIS	CB-CG-CD2	-5.24	124.39	131.20
2	B	109	ASP	N-CA-C	5.23	121.95	110.80
6	F	40	HIS	CB-CG-CD2	-5.23	124.40	131.20
2	K	325	LYS	CA-C-N	5.23	129.62	121.35
2	K	325	LYS	C-N-CA	5.23	129.62	121.35
3	L	2635	ILE	N-CA-CB	-5.23	104.84	111.64
3	C	1406	LEU	CA-C-N	5.23	127.24	120.44
3	C	1406	LEU	C-N-CA	5.23	127.24	120.44
2	K	109	ASP	N-CA-C	5.23	121.93	110.80
3	C	3744	ASP	CA-CB-CG	-5.21	107.39	112.60
3	L	582	THR	CB-CA-C	-5.21	104.97	111.43
3	L	3835	PRO	N-CA-C	5.21	117.06	110.70
3	L	3744	ASP	CA-CB-CG	-5.21	107.39	112.60
3	L	1926	ASN	CA-CB-CG	5.20	117.80	112.60
3	C	3835	PRO	N-CA-C	5.20	117.04	110.70
3	C	4018	GLN	OE1-CD-NE2	-5.19	117.41	122.60
3	L	4018	GLN	OE1-CD-NE2	-5.19	117.41	122.60
3	C	1521	PHE	CA-C-N	5.19	125.27	120.34
3	C	1521	PHE	C-N-CA	5.19	125.27	120.34
3	C	3296	GLN	OE1-CD-NE2	-5.19	117.41	122.60
3	C	1444	ASP	CA-CB-CG	5.18	117.78	112.60
3	L	1521	PHE	CA-C-N	5.18	125.26	120.34
3	L	1521	PHE	C-N-CA	5.18	125.26	120.34
3	L	3296	GLN	OE1-CD-NE2	-5.18	117.42	122.60
3	C	2268	LYS	CA-C-N	5.17	127.47	120.38
3	C	2268	LYS	C-N-CA	5.17	127.47	120.38
3	L	2268	LYS	CA-C-N	5.17	127.47	120.38
3	L	2268	LYS	C-N-CA	5.17	127.47	120.38
3	L	485	GLN	OE1-CD-NE2	-5.17	117.43	122.60
3	L	3903	HIS	CB-CG-CD2	-5.17	124.48	131.20
3	C	465	PHE	CA-CB-CG	5.17	118.97	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	79	ASP	CA-C-N	5.17	129.46	120.68
1	J	79	ASP	C-N-CA	5.17	129.46	120.68
3	L	278	HIS	CB-CG-CD2	-5.15	124.50	131.20
1	A	79	ASP	CA-C-N	5.14	129.43	120.68
1	A	79	ASP	C-N-CA	5.14	129.43	120.68
1	A	436	PHE	CA-CB-CG	5.14	118.94	113.80
1	J	436	PHE	CA-CB-CG	5.14	118.94	113.80
3	L	2092	GLU	N-CA-C	5.14	117.62	111.71
9	X	815	ARG	CB-CA-C	5.14	119.02	111.06
3	C	485	GLN	OE1-CD-NE2	-5.14	117.46	122.60
3	C	2092	GLU	N-CA-C	5.14	117.62	111.71
3	L	465	PHE	CA-CB-CG	5.14	118.94	113.80
3	L	1444	ASP	CA-CB-CG	5.13	117.73	112.60
3	L	2852	PRO	N-CA-C	5.12	116.95	110.70
9	Y	815	ARG	CB-CA-C	5.12	119.00	111.06
3	C	3689	ASP	N-CA-CB	5.12	118.25	110.42
3	L	738	HIS	CB-CG-CD2	-5.12	124.55	131.20
1	J	517	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	A	517	ARG	NE-CZ-NH2	5.11	123.80	119.20
3	L	2232	ARG	NE-CZ-NH2	5.11	123.80	119.20
9	Y	661	ASP	CA-CB-CG	5.11	117.71	112.60
3	C	3903	HIS	CB-CG-CD2	-5.10	124.56	131.20
3	C	2232	ARG	NE-CZ-NH2	5.10	123.79	119.20
3	L	2425	ARG	NE-CZ-NH2	5.10	123.79	119.20
3	L	3004	HIS	CB-CG-CD2	-5.09	124.58	131.20
3	C	278	HIS	CB-CG-CD2	-5.09	124.58	131.20
3	C	160	LEU	CA-C-N	5.08	127.80	120.38
3	C	160	LEU	C-N-CA	5.08	127.80	120.38
3	C	2852	PRO	N-CA-C	5.08	116.90	110.70
9	X	661	ASP	CA-CB-CG	5.08	117.68	112.60
3	L	2464	HIS	N-CA-C	5.08	116.05	109.65
3	L	2584	CYS	N-CA-C	5.08	118.77	112.47
3	L	3689	ASP	N-CA-CB	5.08	118.19	110.42
3	C	1184	ARG	NE-CZ-NH2	5.07	123.77	119.20
3	C	2584	CYS	N-CA-C	5.07	118.76	112.47
3	C	3004	HIS	CB-CG-CD2	-5.07	124.60	131.20
6	G	28	LEU	CA-C-N	5.07	127.59	120.28
6	G	28	LEU	C-N-CA	5.07	127.59	120.28
3	L	1184	ARG	NE-CZ-NH2	5.07	123.77	119.20
3	C	2425	ARG	NE-CZ-NH2	5.07	123.76	119.20
3	L	3653	ARG	CA-C-N	5.07	128.87	121.31
3	L	3653	ARG	C-N-CA	5.07	128.87	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Y	770	ASP	CA-C-O	-5.07	114.73	121.47
9	Y	816	HIS	CB-CG-CD2	-5.07	124.61	131.20
3	C	3591	ASP	CA-CB-CG	5.07	117.67	112.60
3	C	738	HIS	CB-CG-CD2	-5.07	124.61	131.20
9	X	816	HIS	CB-CG-CD2	-5.07	124.61	131.20
6	F	7	ARG	CB-CA-C	5.06	118.50	109.38
7	H	18	LEU	N-CA-C	5.06	116.29	107.93
3	L	3591	ASP	CA-CB-CG	5.06	117.66	112.60
7	H	176	ARG	NE-CZ-NH2	5.06	123.75	119.20
9	X	846	ARG	NE-CZ-NH2	5.06	123.75	119.20
3	L	4029	GLN	N-CA-C	5.05	116.48	110.97
3	C	3653	ARG	CA-C-N	5.05	128.84	121.31
3	C	3653	ARG	C-N-CA	5.05	128.84	121.31
3	L	3962	ARG	NE-CZ-NH2	5.05	123.75	119.20
6	P	28	LEU	CA-C-N	5.05	127.55	120.28
6	P	28	LEU	C-N-CA	5.05	127.55	120.28
9	Y	906	GLU	N-CA-C	5.05	118.22	111.75
6	O	7	ARG	CB-CA-C	5.05	118.47	109.38
7	H	158	HIS	CB-CG-CD2	-5.05	124.64	131.20
3	C	473	PRO	N-CA-C	5.04	121.12	113.81
3	C	2464	HIS	N-CA-C	5.04	116.00	109.65
3	L	473	PRO	N-CA-C	5.04	121.11	113.81
3	L	1805	PHE	CA-C-N	5.04	127.03	120.28
3	L	1805	PHE	C-N-CA	5.04	127.03	120.28
9	X	906	GLU	N-CA-C	5.04	118.20	111.75
3	L	1459	HIS	CA-CB-CG	-5.04	108.76	113.80
1	A	290	ARG	NE-CZ-NH2	5.03	123.73	119.20
3	C	2530	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	A	187	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	J	290	ARG	NE-CZ-NH2	5.03	123.72	119.20
3	C	4029	GLN	N-CA-C	5.02	116.44	110.97
3	L	2374	LEU	N-CA-C	5.02	117.48	111.71
3	C	2374	LEU	N-CA-C	5.01	117.47	111.71
3	C	3962	ARG	NE-CZ-NH2	5.01	123.70	119.20
3	C	1175	HIS	CB-CG-CD2	-5.00	124.70	131.20
3	C	1459	HIS	CA-CB-CG	-5.00	108.80	113.80
3	C	1805	PHE	CA-C-N	5.00	126.98	120.28
3	C	1805	PHE	C-N-CA	5.00	126.98	120.28
3	L	160	LEU	CA-C-N	5.00	127.68	120.38
3	L	160	LEU	C-N-CA	5.00	127.68	120.38
3	L	1175	HIS	CB-CG-CD2	-5.00	124.70	131.20

There are no chirality outliers.

All (176) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	HIS	Sidechain
1	A	71	TYR	Sidechain
1	A	88	TYR	Sidechain
2	B	242	ARG	Sidechain
2	B	421	TYR	Sidechain
2	B	44	ARG	Sidechain
2	B	444	TYR	Sidechain
2	B	489	ARG	Sidechain
3	C	103	TYR	Sidechain
3	C	1107	TYR	Sidechain
3	C	1152	ARG	Sidechain
3	C	1155	ARG	Sidechain
3	C	1414	ILE	Mainchain
3	C	1682	THR	Mainchain
3	C	175	TYR	Sidechain
3	C	1768	ARG	Sidechain
3	C	1969	GLU	Peptide
3	C	1990	PHE	Sidechain
3	C	2160	TYR	Sidechain
3	C	2316	TYR	Sidechain
3	C	2410	GLU	Peptide
3	C	2412	TYR	Sidechain
3	C	2464	HIS	Sidechain
3	C	2484	TYR	Sidechain
3	C	2495	SER	Peptide
3	C	3101	TYR	Sidechain
3	C	32	HIS	Sidechain
3	C	3280	TYR	Sidechain
3	C	3290	SER	Peptide
3	C	3334	TYR	Sidechain
3	C	340	TYR	Sidechain
3	C	346	TYR	Sidechain
3	C	3467	ARG	Sidechain
3	C	3612	ARG	Sidechain
3	C	3705	TYR	Sidechain
3	C	3715	TYR	Sidechain
3	C	3741	ARG	Sidechain
3	C	3965	ARG	Sidechain
3	C	568	PHE	Sidechain
3	C	659	ARG	Sidechain
3	C	682	TYR	Sidechain
3	C	701	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	C	721	TYR	Sidechain
3	C	894	PHE	Sidechain
4	D	1	DT	Sidechain
4	D	11	DC	Sidechain
4	D	12	DT	Sidechain
4	D	17	DT	Sidechain
4	D	18	DC	Sidechain
4	D	19	DA	Sidechain
4	D	22	DA	Sidechain
4	D	23	DG	Sidechain
4	D	24	DA	Sidechain
4	D	26	DT	Sidechain
4	D	27	DA	Sidechain
4	D	29	DA	Sidechain
4	D	30	DC	Sidechain
4	D	6	DG	Sidechain
4	D	7	DA	Sidechain
4	D	8	DA	Sidechain
5	E	1	DG	Sidechain
5	E	11	DC	Sidechain
5	E	15	DC	Sidechain
5	E	16	DA	Sidechain
5	E	17	DT	Sidechain
5	E	23	DT	Sidechain
5	E	25	DC	Sidechain
5	E	26	DT	Sidechain
5	E	5	DA	Sidechain
5	E	6	DA	Sidechain
5	E	7	DT	Sidechain
6	F	129	TYR	Sidechain
6	F	195	HIS	Sidechain
6	F	3	ARG	Sidechain
6	F	66	TYR	Sidechain
6	F	7	ARG	Sidechain
6	G	32	PHE	Sidechain
6	G	95	PHE	Sidechain
7	H	17	GLN	Mainchain
7	H	81	ARG	Sidechain
7	I	118	TYR	Sidechain
7	I	167	TYR	Sidechain
7	I	72	PHE	Sidechain
7	I	75	HIS	Sidechain

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Mol	Chain	Res	Type	Group
1	J	137	HIS	Sidechain
1	J	71	TYR	Sidechain
1	J	88	TYR	Sidechain
2	K	242	ARG	Sidechain
2	K	421	TYR	Sidechain
2	K	44	ARG	Sidechain
2	K	444	TYR	Sidechain
2	K	489	ARG	Sidechain
3	L	103	TYR	Sidechain
3	L	1107	TYR	Sidechain
3	L	1152	ARG	Sidechain
3	L	1155	ARG	Sidechain
3	L	1414	ILE	Mainchain
3	L	1682	THR	Mainchain
3	L	175	TYR	Sidechain
3	L	1768	ARG	Sidechain
3	L	1969	GLU	Peptide
3	L	1990	PHE	Sidechain
3	L	2160	TYR	Sidechain
3	L	2316	TYR	Sidechain
3	L	2410	GLU	Peptide
3	L	2412	TYR	Sidechain
3	L	2464	HIS	Sidechain
3	L	2484	TYR	Sidechain
3	L	2495	SER	Peptide
3	L	3101	TYR	Sidechain
3	L	32	HIS	Sidechain
3	L	3280	TYR	Sidechain
3	L	3290	SER	Peptide
3	L	3334	TYR	Sidechain
3	L	340	TYR	Sidechain
3	L	346	TYR	Sidechain
3	L	3467	ARG	Sidechain
3	L	3612	ARG	Sidechain
3	L	3705	TYR	Sidechain
3	L	3715	TYR	Sidechain
3	L	3741	ARG	Sidechain
3	L	3965	ARG	Sidechain
3	L	568	PHE	Sidechain
3	L	659	ARG	Sidechain
3	L	682	TYR	Sidechain
3	L	701	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	L	721	TYR	Sidechain
3	L	894	PHE	Sidechain
4	M	1	DT	Sidechain
4	M	11	DC	Sidechain
4	M	12	DT	Sidechain
4	M	17	DT	Sidechain
4	M	18	DC	Sidechain
4	M	19	DA	Sidechain
4	M	22	DA	Sidechain
4	M	23	DG	Sidechain
4	M	24	DA	Sidechain
4	M	27	DA	Sidechain
4	M	29	DA	Sidechain
4	M	30	DC	Sidechain
4	M	6	DG	Sidechain
4	M	7	DA	Sidechain
4	M	8	DA	Sidechain
5	N	1	DG	Sidechain
5	N	11	DC	Sidechain
5	N	15	DC	Sidechain
5	N	16	DA	Sidechain
5	N	17	DT	Sidechain
5	N	23	DT	Sidechain
5	N	25	DC	Sidechain
5	N	26	DT	Sidechain
5	N	5	DA	Sidechain
5	N	6	DA	Sidechain
5	N	7	DT	Sidechain
6	O	129	TYR	Sidechain
6	O	195	HIS	Sidechain
6	O	3	ARG	Sidechain
6	O	66	TYR	Sidechain
6	O	7	ARG	Sidechain
6	P	32	PHE	Sidechain
6	P	95	PHE	Sidechain
9	X	718	HIS	Sidechain
9	X	730	PHE	Sidechain
9	X	735	PHE	Sidechain
9	X	737	PRO	Peptide
9	X	761	TYR	Sidechain
9	X	801	TYR	Sidechain
9	X	823	TYR	Sidechain

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Mol	Chain	Res	Type	Group
9	Y	718	HIS	Sidechain
9	Y	730	PHE	Sidechain
9	Y	735	PHE	Sidechain
9	Y	737	PRO	Peptide
9	Y	761	TYR	Sidechain
9	Y	770	ASP	Peptide
9	Y	801	TYR	Sidechain
9	Y	823	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4021	0	4100	68	0
1	J	4021	0	4100	70	0
2	B	4204	0	4250	11	0
2	K	4204	0	4250	11	0
3	C	29799	0	30190	149	0
3	L	29799	0	30190	145	0
4	D	634	0	350	12	0
4	M	634	0	350	8	0
5	E	616	0	337	4	0
5	N	616	0	337	4	0
6	F	1628	0	1620	36	0
6	G	1595	0	1592	24	0
6	O	1628	0	1620	30	0
6	P	1595	0	1592	24	0
7	H	1779	0	1797	20	0
7	I	1737	0	1744	23	0
8	S	168	0	169	15	0
8	T	168	0	169	15	0
9	X	2064	0	2012	48	0
9	Y	2064	0	2012	50	0
10	C	1	0	0	0	0
10	L	1	0	0	0	0
11	C	31	0	12	0	0
11	L	31	0	12	0	0
All	All	93038	0	92805	635	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 (635) 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:J:333:GLU:CA	1:J:333:GLU:CB	1.83	1.56
1:A:333:GLU:C	1:A:333:GLU:CA	1.77	1.55
1:J:333:GLU:CA	1:J:333:GLU:C	1.77	1.54
1:J:333:GLU:CA	1:J:333:GLU:N	1.68	1.54
1:A:333:GLU:CA	1:A:333:GLU:N	1.68	1.51
1:A:333:GLU:CA	1:A:333:GLU:CB	1.83	1.51
1:J:333:GLU:CB	1:J:333:GLU:CG	2.05	1.35
1:A:333:GLU:CB	1:A:333:GLU:CG	2.05	1.32
1:A:334:THR:CB	1:A:334:THR:OG1	1.77	1.32
1:J:334:THR:OG1	1:J:334:THR:CB	1.78	1.31
1:A:334:THR:N	1:A:334:THR:CA	2.07	1.17
1:J:334:THR:N	1:J:334:THR:CA	2.08	1.15
3:C:1815:THR:HG21	3:L:1860:GLU:HG3	1.46	0.94
3:C:1860:GLU:HG3	3:L:1815:THR:HG21	1.47	0.94
7:H:71:ALA:HB1	6:O:104:VAL:HG21	1.49	0.94
3:C:1815:THR:HG21	3:L:1860:GLU:CG	2.01	0.90
3:C:1860:GLU:CG	3:L:1815:THR:HG21	2.01	0.90
1:J:332:GLU:C	1:J:333:GLU:CA	2.46	0.89
1:A:332:GLU:HB3	3:C:212:VAL:HG13	1.54	0.89
1:J:313:PRO:HG3	3:L:164:LYS:HD3	1.56	0.88
1:A:332:GLU:C	1:A:333:GLU:CA	2.46	0.88
1:A:333:GLU:C	1:A:333:GLU:CB	2.48	0.87
1:J:332:GLU:HB3	3:L:212:VAL:HG13	1.54	0.87
7:I:15:TRP:HB2	7:I:211:VAL:HG21	1.55	0.86
1:A:477:SER:O	8:S:196:ALA:O	1.93	0.86
1:J:477:SER:O	8:T:196:ALA:O	1.93	0.86
1:J:333:GLU:CB	1:J:333:GLU:C	2.48	0.86
1:A:334:THR:OG1	1:A:334:THR:CA	2.24	0.85
1:J:334:THR:OG1	1:J:334:THR:CA	2.24	0.85
1:A:313:PRO:HG3	3:C:164:LYS:HD3	1.56	0.85
9:Y:664:PHE:CE2	9:Y:726:LEU:HD11	2.13	0.83
9:X:664:PHE:CE2	9:X:726:LEU:HD11	2.13	0.83
9:X:698:TYR:O	9:X:737:PRO:HA	1.79	0.82
1:A:332:GLU:HB3	3:C:212:VAL:CG1	2.09	0.82
7:H:71:ALA:CB	6:O:104:VAL:HG21	2.09	0.82
9:Y:698:TYR:O	9:Y:737:PRO:HA	1.79	0.82
1:A:332:GLU:CA	3:C:212:VAL:HG11	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:211:VAL:HG23	7:I:212:MET:SD	2.20	0.81
1:J:332:GLU:HB3	3:L:212:VAL:CG1	2.09	0.81
1:J:332:GLU:CA	3:L:212:VAL:HG11	2.10	0.81
2:B:300:ASP:OD2	3:C:117:LYS:HE2	1.81	0.81
1:J:332:GLU:HA	3:L:212:VAL:HG11	1.64	0.80
1:A:332:GLU:HA	3:C:212:VAL:HG11	1.64	0.80
6:F:134:ILE:HD11	6:G:130:CYS:HA	1.63	0.80
6:O:134:ILE:HD11	6:P:130:CYS:HA	1.63	0.80
2:K:300:ASP:OD2	3:L:117:LYS:HE2	1.81	0.79
6:F:101:LEU:HD22	7:I:113:SER:HA	1.64	0.78
9:X:664:PHE:CZ	9:X:726:LEU:HD11	2.17	0.78
6:O:40:HIS:CG	6:P:120:ALA:HB2	2.19	0.78
1:J:333:GLU:CA	1:J:333:GLU:CG	2.62	0.78
9:Y:664:PHE:CZ	9:Y:726:LEU:HD11	2.17	0.78
1:A:334:THR:CB	1:A:334:THR:N	2.48	0.77
9:Y:664:PHE:CD2	9:Y:726:LEU:HD21	2.19	0.77
1:A:333:GLU:CA	1:A:333:GLU:CG	2.62	0.77
6:F:40:HIS:CG	6:G:120:ALA:HB2	2.19	0.77
9:X:664:PHE:CD2	9:X:726:LEU:HD21	2.19	0.77
6:O:104:VAL:HB	6:O:106:PHE:CE2	2.20	0.76
1:J:334:THR:CB	1:J:334:THR:N	2.48	0.76
9:Y:699:CYS:SG	9:Y:725:TRP:CH2	2.80	0.75
9:X:699:CYS:SG	9:X:725:TRP:CH2	2.80	0.75
9:X:659:PHE:CZ	9:X:729:CYS:HB3	2.21	0.74
9:Y:659:PHE:CZ	9:Y:729:CYS:HB3	2.21	0.74
1:A:313:PRO:CG	3:C:164:LYS:HD3	2.18	0.73
1:A:331:LYS:O	1:A:334:THR:HG22	1.89	0.73
9:X:701:ILE:HG12	9:X:726:LEU:HD22	1.71	0.73
1:J:313:PRO:CG	3:L:164:LYS:HD3	2.18	0.73
1:J:333:GLU:C	1:J:334:THR:CA	2.62	0.73
1:J:331:LYS:O	1:J:334:THR:HG22	1.89	0.72
3:L:2368:THR:HG23	3:L:2404:ARG:HB2	1.71	0.72
3:C:2563:LEU:HD12	3:C:2795:GLN:HE22	1.55	0.72
9:Y:701:ILE:HG12	9:Y:726:LEU:HD22	1.71	0.72
1:A:333:GLU:C	1:A:334:THR:CA	2.62	0.72
3:C:1392:MET:HA	3:C:1395:LEU:CD2	2.20	0.72
3:L:1392:MET:HA	3:L:1395:LEU:CD2	2.20	0.71
3:L:2563:LEU:HD12	3:L:2795:GLN:HE22	1.55	0.71
3:C:2368:THR:HG23	3:C:2404:ARG:HB2	1.71	0.71
6:F:101:LEU:HB2	7:I:113:SER:HB2	1.70	0.71
1:A:74:LYS:HE3	8:S:186:ILE:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Y:721:VAL:HG11	9:Y:725:TRP:CD2	2.27	0.70
1:J:74:LYS:HE3	8:T:186:ILE:O	1.92	0.69
1:J:333:GLU:CB	1:J:333:GLU:N	2.55	0.69
1:A:333:GLU:N	1:A:333:GLU:CB	2.55	0.69
9:X:721:VAL:HG11	9:X:725:TRP:CD2	2.27	0.69
1:A:250:GLU:HG2	8:S:187:ASN:HD21	1.57	0.69
9:X:725:TRP:CZ3	9:X:726:LEU:HD13	2.29	0.68
1:J:250:GLU:HG2	8:T:187:ASN:HD21	1.58	0.68
9:Y:725:TRP:CZ3	9:Y:726:LEU:HD13	2.29	0.67
1:J:333:GLU:CA	1:J:334:THR:N	2.58	0.67
1:J:58:THR:HB	1:J:61:ASP:HB2	1.77	0.66
1:A:58:THR:HB	1:A:61:ASP:HB2	1.77	0.66
1:A:333:GLU:CA	1:A:334:THR:N	2.58	0.65
6:O:130:CYS:HB3	6:P:130:CYS:HB3	1.78	0.65
9:X:662:VAL:HG21	9:X:735:PHE:CD1	2.32	0.64
3:C:1815:THR:CG2	3:L:1860:GLU:HG3	2.22	0.64
1:A:74:LYS:CE	8:S:186:ILE:O	2.45	0.64
6:F:130:CYS:HB3	6:G:130:CYS:HB3	1.78	0.64
3:C:3924:HIS:CE1	3:C:3927:ASN:ND2	2.66	0.64
1:A:332:GLU:CB	3:C:212:VAL:CG1	2.76	0.64
9:Y:662:VAL:HG21	9:Y:735:PHE:CD1	2.32	0.64
3:C:1860:GLU:HG3	3:L:1815:THR:CG2	2.24	0.64
3:C:305:ASN:HA	4:D:26:DT:H2'	1.79	0.63
3:L:3924:HIS:CE1	3:L:3927:ASN:ND2	2.66	0.63
2:B:434:MET:HG2	8:S:191:LYS:NZ	2.14	0.63
6:O:130:CYS:HB3	6:P:130:CYS:CB	2.28	0.63
1:J:332:GLU:CB	3:L:212:VAL:CG1	2.76	0.63
3:C:3922:ASP:O	3:C:3927:ASN:ND2	2.32	0.62
3:L:1346:THR:OG1	3:L:1402:LEU:HD13	1.99	0.62
3:L:3922:ASP:O	3:L:3927:ASN:ND2	2.32	0.62
6:F:130:CYS:HB3	6:G:130:CYS:CB	2.28	0.62
1:J:74:LYS:CE	8:T:186:ILE:O	2.47	0.62
3:C:2368:THR:HG22	3:C:2403:CYS:HB2	1.81	0.62
2:K:434:MET:HG2	8:T:191:LYS:NZ	2.14	0.61
3:L:2368:THR:HG22	3:L:2403:CYS:HB2	1.82	0.61
3:C:1346:THR:OG1	3:C:1402:LEU:HD13	1.99	0.61
6:F:59:MET:HE3	7:I:64:ARG:NH1	2.16	0.61
3:L:2635:ILE:HD11	3:L:2775:TYR:CD1	2.36	0.61
9:X:659:PHE:CZ	9:X:729:CYS:CB	2.83	0.61
9:Y:659:PHE:CZ	9:Y:729:CYS:CB	2.83	0.61
3:C:2635:ILE:HD11	3:C:2775:TYR:CD1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Y:806:ASP:CB	9:Y:815:ARG:HH21	2.14	0.61
3:L:430:VAL:HG22	3:L:1499:CYS:H	1.65	0.60
1:A:131:PHE:CE2	1:A:137:HIS:CE1	2.89	0.60
3:C:430:VAL:HG22	3:C:1499:CYS:H	1.65	0.60
6:F:134:ILE:CG1	6:G:134:ILE:HG13	2.31	0.60
6:O:134:ILE:CG1	6:P:134:ILE:HG13	2.31	0.60
9:Y:721:VAL:HG11	9:Y:725:TRP:CG	2.36	0.60
9:Y:725:TRP:CE3	9:Y:726:LEU:HD13	2.37	0.60
9:X:806:ASP:CB	9:X:815:ARG:HH21	2.14	0.60
1:J:131:PHE:CE2	1:J:137:HIS:CE1	2.89	0.60
1:J:312:LEU:HD21	3:L:161:ALA:HA	1.84	0.60
4:M:25:DT:H2''	4:M:26:DT:O5'	2.02	0.60
3:C:2191:ALA:HB1	3:C:2195:SER:HB2	1.84	0.59
9:X:721:VAL:HG11	9:X:725:TRP:CG	2.36	0.59
9:X:725:TRP:CE3	9:X:726:LEU:HD13	2.37	0.59
3:C:1859:ASN:HD21	3:L:1715:GLU:HB3	1.68	0.59
1:A:312:LEU:HD21	3:C:161:ALA:HA	1.84	0.59
9:Y:787:GLN:HB2	9:Y:792:MET:HG2	1.85	0.58
3:L:2191:ALA:HB1	3:L:2195:SER:HB2	1.84	0.58
9:X:787:GLN:HB2	9:X:792:MET:HG2	1.85	0.58
3:C:1392:MET:HA	3:C:1395:LEU:HD21	1.85	0.58
3:L:1392:MET:HA	3:L:1395:LEU:HD21	1.85	0.58
4:D:25:DT:H2''	4:D:26:DT:O5'	2.03	0.58
3:C:169:THR:HG23	5:E:11:DC:OP1	2.04	0.58
1:J:241:ASP:O	8:T:186:ILE:HD11	2.04	0.58
9:X:721:VAL:HG12	9:X:725:TRP:HB3	1.85	0.58
1:A:312:LEU:HD22	3:C:160:LEU:O	2.04	0.57
3:C:1923:PHE:CZ	3:C:1966:LEU:HD23	2.39	0.57
1:J:334:THR:CB	1:J:334:THR:CG2	2.82	0.57
1:A:334:THR:CB	1:A:334:THR:CG2	2.82	0.57
3:C:2575:PRO:HA	3:C:2786:LYS:HA	1.87	0.57
7:H:67:ALA:HB1	6:O:104:VAL:HG11	1.86	0.57
1:J:312:LEU:HD22	3:L:160:LEU:O	2.04	0.57
9:Y:721:VAL:HG12	9:Y:725:TRP:HB3	1.85	0.57
3:C:414:LEU:HB2	3:C:460:ALA:HB1	1.86	0.57
3:C:2567:SER:HA	3:C:2572:TYR:CD1	2.40	0.57
3:L:1923:PHE:CZ	3:L:1966:LEU:HD23	2.39	0.57
1:J:477:SER:C	8:T:196:ALA:O	2.48	0.57
1:J:333:GLU:HA	1:J:336:GLU:HB3	1.87	0.56
3:L:169:THR:HG23	5:N:11:DC:OP1	2.04	0.56
3:L:2567:SER:HA	3:L:2572:TYR:CD1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:18:LEU:HD13	7:H:96:SER:HA	1.87	0.56
1:A:333:GLU:HA	1:A:336:GLU:HB3	1.87	0.56
1:A:477:SER:C	8:S:196:ALA:O	2.48	0.56
6:F:101:LEU:HB2	7:I:113:SER:CB	2.34	0.56
6:F:107:ARG:H	7:I:66:THR:HG22	1.71	0.56
9:X:721:VAL:CG1	9:X:725:TRP:CG	2.89	0.56
7:H:208:LYS:HG2	7:H:212:MET:HE1	1.86	0.56
1:A:241:ASP:O	8:S:186:ILE:HD11	2.06	0.56
3:L:2575:PRO:HA	3:L:2786:LYS:HA	1.87	0.56
1:J:312:LEU:CD2	3:L:160:LEU:O	2.54	0.56
3:L:442:GLN:HG3	3:L:457:CYS:SG	2.46	0.56
1:A:312:LEU:CD2	3:C:160:LEU:O	2.54	0.56
3:C:732:PHE:CZ	3:C:736:LEU:HD21	2.41	0.56
3:L:414:LEU:HB2	3:L:460:ALA:HB1	1.86	0.56
9:Y:824:ALA:HB2	9:Y:833:ASN:HD21	1.71	0.56
3:C:349:ILE:HD11	3:C:362:ALA:C	2.31	0.55
3:L:732:PHE:CZ	3:L:736:LEU:HD21	2.41	0.55
9:Y:721:VAL:CG1	9:Y:725:TRP:CG	2.89	0.55
6:F:40:HIS:CD2	6:G:120:ALA:HB2	2.41	0.55
1:J:49:PHE:CD2	1:J:137:HIS:ND1	2.75	0.55
6:O:40:HIS:CD2	6:P:120:ALA:HB2	2.40	0.55
3:C:1715:GLU:HB3	3:L:1859:ASN:HD21	1.71	0.55
3:L:349:ILE:HD11	3:L:362:ALA:C	2.31	0.55
1:A:332:GLU:CB	3:C:212:VAL:HG11	2.36	0.55
3:C:442:GLN:HG3	3:C:457:CYS:SG	2.46	0.55
4:D:25:DT:H2''	4:D:26:DT:C5'	2.36	0.55
4:D:27:DA:C2'	4:D:28:DC:H5''	2.37	0.55
7:I:10:MET:SD	7:I:223:THR:HA	2.47	0.55
1:J:332:GLU:CB	3:L:212:VAL:HG11	2.36	0.55
6:G:31:GLY:HA3	6:G:48:SER:HA	1.89	0.54
1:J:132:GLN:OE1	1:J:137:HIS:CD2	2.60	0.54
1:A:49:PHE:CD2	1:A:137:HIS:ND1	2.75	0.54
3:C:943:GLY:HA3	3:C:2577:PHE:CZ	2.43	0.54
3:C:430:VAL:CG2	3:C:1499:CYS:H	2.21	0.54
3:C:1560:TYR:OH	3:C:1596:VAL:HA	2.08	0.54
2:K:434:MET:HG2	8:T:191:LYS:HZ1	1.71	0.54
9:X:824:ALA:HB2	9:X:833:ASN:HD21	1.71	0.54
3:C:2923:TRP:CG	3:C:2947:ILE:HD11	2.43	0.54
3:L:1945:TYR:CZ	3:L:1966:LEU:HD22	2.43	0.54
3:L:3622:ALA:HB3	3:L:3625:LEU:HB2	1.88	0.54
1:A:132:GLN:OE1	1:A:137:HIS:CD2	2.60	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:12:PRO:HB3	7:H:219:MET:SD	2.48	0.53
3:L:940:PHE:CZ	3:L:944:LYS:HE2	2.44	0.53
3:C:940:PHE:CZ	3:C:944:LYS:HE2	2.44	0.53
3:L:430:VAL:CG2	3:L:1499:CYS:H	2.21	0.53
3:C:3622:ALA:HB3	3:C:3625:LEU:HB2	1.88	0.53
3:C:3842:TRP:CZ2	3:C:3867:THR:HA	2.44	0.53
3:L:1560:TYR:OH	3:L:1596:VAL:HA	2.08	0.53
1:J:250:GLU:HG2	8:T:187:ASN:ND2	2.23	0.53
2:K:326:VAL:HG21	9:Y:743:MET:H	1.74	0.53
6:F:101:LEU:HD13	7:I:113:SER:O	2.08	0.53
3:L:943:GLY:HA3	3:L:2577:PHE:CZ	2.43	0.53
6:P:31:GLY:HA3	6:P:48:SER:HA	1.89	0.53
1:A:362:LEU:HD23	1:A:436:PHE:HB3	1.90	0.53
3:C:1945:TYR:CZ	3:C:1966:LEU:HD22	2.43	0.53
3:L:568:PHE:CE1	3:L:633:ILE:CG2	2.92	0.53
3:L:2923:TRP:CG	3:L:2947:ILE:HD11	2.43	0.53
3:L:3371:GLU:H	3:L:3371:GLU:CD	2.17	0.53
6:O:8:ILE:HB	6:O:86:PHE:CD1	2.44	0.53
3:L:1934:LEU:HD12	3:L:1934:LEU:H	1.74	0.52
1:A:332:GLU:CB	3:C:212:VAL:HG13	2.33	0.52
3:L:1938:ARG:HH22	3:L:2091:HIS:CE1	2.27	0.52
3:C:568:PHE:CE1	3:C:633:ILE:CG2	2.92	0.52
3:C:1934:LEU:HD12	3:C:1934:LEU:H	1.74	0.52
7:I:10:MET:SD	7:I:223:THR:HG22	2.49	0.52
1:J:362:LEU:HD23	1:J:436:PHE:HB3	1.91	0.52
9:Y:662:VAL:HG21	9:Y:735:PHE:CG	2.45	0.52
3:C:2635:ILE:HD11	3:C:2775:TYR:CE1	2.45	0.52
2:K:300:ASP:OD1	3:L:117:LYS:HG2	2.10	0.52
3:L:3842:TRP:CZ2	3:L:3867:THR:HA	2.44	0.52
3:C:1250:LEU:H	3:C:1250:LEU:HD12	1.75	0.52
3:C:3371:GLU:CD	3:C:3371:GLU:H	2.17	0.52
3:L:2635:ILE:HD11	3:L:2775:TYR:CE1	2.45	0.52
6:P:155:TRP:CZ3	9:Y:835:GLY:HA2	2.45	0.52
1:A:250:GLU:HG2	8:S:187:ASN:ND2	2.23	0.52
2:B:300:ASP:OD1	3:C:117:LYS:HG2	2.10	0.52
3:C:940:PHE:CE1	3:C:944:LYS:HE2	2.45	0.52
3:C:1938:ARG:HH22	3:C:2091:HIS:CE1	2.27	0.52
3:C:2923:TRP:CD1	3:C:2947:ILE:HD11	2.45	0.52
3:C:3233:SER:HA	3:C:3272:TRP:CZ2	2.45	0.52
6:G:155:TRP:CZ3	9:X:835:GLY:HA2	2.45	0.52
1:J:169:PHE:CE2	1:J:203:MET:SD	3.03	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:940:PHE:CE1	3:L:944:LYS:HE2	2.45	0.52
1:A:333:GLU:CB	1:A:333:GLU:CD	2.83	0.51
3:C:3370:SER:HA	3:C:3373:VAL:CG2	2.40	0.51
3:C:3659:PHE:CZ	3:C:3663:THR:HG21	2.45	0.51
3:L:3233:SER:HA	3:L:3272:TRP:CZ2	2.45	0.51
1:A:169:PHE:CE2	1:A:203:MET:SD	3.03	0.51
1:J:446:MET:HE1	2:K:365:PHE:CZ	2.46	0.51
3:L:3659:PHE:CZ	3:L:3663:THR:HG21	2.45	0.51
9:X:662:VAL:HG21	9:X:735:PHE:CG	2.45	0.51
1:A:446:MET:HE1	2:B:365:PHE:CZ	2.46	0.51
6:F:8:ILE:HB	6:F:86:PHE:CD1	2.44	0.51
1:J:334:THR:OG1	1:J:334:THR:HA	2.11	0.51
9:Y:806:ASP:HB3	9:Y:815:ARG:HH21	1.74	0.51
1:J:267:ILE:HD12	1:J:267:ILE:H	1.75	0.51
3:L:3370:SER:HA	3:L:3373:VAL:CG2	2.40	0.51
3:L:2360:PHE:HA	3:L:2363:CYS:HB3	1.93	0.51
6:P:155:TRP:CE3	9:Y:835:GLY:HA2	2.46	0.51
2:B:340:PHE:CE1	2:B:393:VAL:HG11	2.46	0.51
2:B:434:MET:HG2	8:S:191:LYS:HZ1	1.73	0.51
3:C:1860:GLU:CG	3:L:1815:THR:CG2	2.82	0.51
3:L:2467:THR:HG21	3:L:2514:ASN:HD22	1.76	0.51
3:L:3370:SER:HA	3:L:3373:VAL:HG22	1.93	0.51
4:M:27:DA:C2'	4:M:28:DC:H5''	2.41	0.51
9:X:806:ASP:HB3	9:X:815:ARG:HH21	1.74	0.51
3:C:1815:THR:CG2	3:L:1860:GLU:CG	2.81	0.51
6:F:109:GLY:HA2	7:I:64:ARG:HH21	1.76	0.51
3:L:1250:LEU:HD12	3:L:1250:LEU:H	1.75	0.51
3:L:2511:ILE:CG2	3:L:2550:ILE:HD12	2.41	0.51
3:C:2511:ILE:CG2	3:C:2550:ILE:HD12	2.41	0.51
3:L:2923:TRP:CD1	3:L:2947:ILE:HD11	2.45	0.50
2:B:408:ALA:HB1	2:B:419:LEU:HD21	1.93	0.50
3:C:2373:PRO:HA	3:C:2404:ARG:CZ	2.42	0.50
3:C:2467:THR:HG21	3:C:2514:ASN:HD22	1.76	0.50
2:K:340:PHE:CE1	2:K:393:VAL:HG11	2.46	0.50
3:L:2373:PRO:HA	3:L:2404:ARG:CZ	2.41	0.50
6:G:155:TRP:CE3	9:X:835:GLY:HA2	2.46	0.50
3:C:2276:LEU:C	3:C:2276:LEU:HD23	2.37	0.50
3:C:4064:LEU:HD13	3:C:4077:TYR:HB3	1.94	0.50
9:X:807:CYS:HA	9:X:812:MET:HA	1.93	0.50
3:C:2360:PHE:HA	3:C:2363:CYS:HB3	1.93	0.50
6:F:102:LYS:HE2	6:F:102:LYS:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Y:730:PHE:CD1	9:Y:730:PHE:N	2.80	0.50
3:C:1810:PRO:HA	3:L:1810:PRO:HA	1.93	0.50
9:Y:726:LEU:HD12	9:Y:729:CYS:HB2	1.94	0.50
1:A:267:ILE:HD12	1:A:267:ILE:H	1.75	0.49
4:D:25:DT:H1'	4:D:26:DT:H5'	1.93	0.49
7:H:208:LYS:CG	7:H:212:MET:HE1	2.42	0.49
4:M:26:DT:H2''	4:M:27:DA:C8	2.46	0.49
3:C:3370:SER:HA	3:C:3373:VAL:HG22	1.93	0.49
1:J:333:GLU:CB	1:J:333:GLU:CD	2.83	0.49
2:K:60:GLY:H	2:K:105:ALA:HB3	1.76	0.49
1:A:58:THR:O	1:A:62:MET:N	2.45	0.49
1:A:67:ILE:O	1:A:71:TYR:HB2	2.13	0.49
2:B:60:GLY:H	2:B:105:ALA:HB3	1.76	0.49
6:O:134:ILE:HG13	6:P:134:ILE:HG13	1.94	0.49
9:Y:807:CYS:HA	9:Y:812:MET:HA	1.93	0.49
3:C:1266:CYS:C	3:C:1270:PHE:CE2	2.91	0.49
3:L:2276:LEU:HD23	3:L:2276:LEU:C	2.37	0.49
9:X:698:TYR:O	9:X:737:PRO:CA	2.54	0.49
3:C:2554:PHE:CE1	3:C:2558:ALA:HB2	2.48	0.49
4:D:14:DA:N6	5:E:17:DT:H3	2.11	0.49
4:D:26:DT:H2''	4:D:27:DA:C8	2.48	0.49
4:M:14:DA:N6	5:N:17:DT:H3	2.11	0.49
6:P:91:GLU:CD	6:P:91:GLU:H	2.21	0.49
9:Y:659:PHE:CE2	9:Y:729:CYS:HB3	2.48	0.49
1:J:67:ILE:O	1:J:71:TYR:HB2	2.13	0.48
1:J:238:LYS:HG2	8:T:185:LEU:HD13	1.95	0.48
3:L:1266:CYS:C	3:L:1270:PHE:CE2	2.91	0.48
9:X:659:PHE:CE2	9:X:729:CYS:HB3	2.48	0.48
9:Y:698:TYR:O	9:Y:737:PRO:CA	2.54	0.48
1:A:136:GLY:C	1:A:137:HIS:CD2	2.91	0.48
7:H:97:CYS:SG	7:H:104:LEU:HD11	2.53	0.48
3:L:4064:LEU:HD13	3:L:4077:TYR:HB3	1.94	0.48
9:Y:678:LEU:HD22	9:Y:727:LEU:HD21	1.96	0.48
1:A:131:PHE:CE2	1:A:137:HIS:NE2	2.82	0.48
1:J:58:THR:O	1:J:62:MET:N	2.45	0.48
2:K:408:ALA:HB1	2:K:419:LEU:HD21	1.93	0.48
3:L:1889:VAL:HA	3:L:1896:ILE:HD11	1.96	0.48
3:C:2485:ARG:HA	3:C:2499:PHE:CZ	2.48	0.48
3:L:2245:TRP:CD1	3:L:2246:LYS:H	2.32	0.48
3:C:3718:ARG:HH11	3:C:3743:HIS:CD2	2.32	0.48
6:G:91:GLU:CD	6:G:91:GLU:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:43:TRP:CH2	6:G:115:LYS:HD2	2.49	0.48
1:J:517:ARG:HH11	8:T:201:PHE:HB2	1.79	0.48
6:F:127:ILE:HD12	6:G:126:LEU:HD22	1.96	0.48
3:L:3180:ASP:HA	3:L:3242:MET:HE1	1.96	0.48
9:X:726:LEU:HD12	9:X:729:CYS:HB2	1.94	0.48
3:C:442:GLN:CD	3:C:457:CYS:SG	2.97	0.48
3:C:1889:VAL:HA	3:C:1896:ILE:HD11	1.96	0.48
6:F:134:ILE:HG13	6:G:134:ILE:HG13	1.94	0.48
3:L:2554:PHE:CE1	3:L:2558:ALA:HB2	2.48	0.48
3:L:2636:ARG:HG3	3:L:2772:TYR:CZ	2.49	0.48
1:A:469:LEU:HD13	8:S:201:PHE:CZ	2.49	0.48
3:C:3180:ASP:HA	3:C:3242:MET:HE1	1.96	0.48
1:J:136:GLY:C	1:J:137:HIS:CD2	2.91	0.48
9:X:695:PRO:O	9:X:738:TRP:CD1	2.67	0.48
3:C:249:PHE:CE2	3:C:285:CYS:HB3	2.48	0.48
3:C:2636:ARG:HG3	3:C:2772:TYR:CZ	2.49	0.48
7:I:140:MET:SD	7:I:140:MET:C	2.97	0.48
3:L:249:PHE:CE2	3:L:285:CYS:HB3	2.48	0.48
3:L:2485:ARG:HA	3:L:2499:PHE:CZ	2.48	0.48
3:C:2245:TRP:CD1	3:C:2246:LYS:H	2.32	0.47
3:C:3924:HIS:CE1	3:C:3927:ASN:HD21	2.32	0.47
3:L:4016:PHE:CE1	3:L:4020:MET:HE3	2.49	0.47
6:P:43:TRP:CH2	6:P:115:LYS:HD2	2.49	0.47
1:J:469:LEU:HD13	8:T:201:PHE:CZ	2.49	0.47
3:L:3718:ARG:HH11	3:L:3743:HIS:CD2	2.32	0.47
9:Y:738:TRP:CZ2	9:Y:767:ILE:HD12	2.49	0.47
4:D:24:DA:C2	4:D:25:DT:C2	3.03	0.47
3:L:1626:TRP:HE1	3:L:1652:ILE:HD11	1.79	0.47
6:P:24:TRP:CD1	6:P:27:THR:C	2.93	0.47
1:A:238:LYS:HG2	8:S:185:LEU:HD13	1.96	0.47
1:J:131:PHE:CE2	1:J:137:HIS:NE2	2.82	0.47
9:X:678:LEU:HD22	9:X:727:LEU:HD21	1.95	0.47
9:Y:695:PRO:O	9:Y:738:TRP:CD1	2.67	0.47
1:A:145:GLU:O	1:A:149:VAL:HG23	2.15	0.47
3:L:1560:TYR:CZ	3:L:1596:VAL:HA	2.50	0.47
9:X:738:TRP:CZ2	9:X:767:ILE:HD12	2.49	0.47
3:C:1560:TYR:CZ	3:C:1596:VAL:HA	2.50	0.47
3:C:1626:TRP:HE1	3:C:1652:ILE:HD11	1.80	0.47
3:C:3259:LEU:HD11	3:C:3283:LEU:HD23	1.97	0.47
3:C:4016:PHE:CE1	3:C:4020:MET:HE3	2.49	0.47
3:L:442:GLN:CD	3:L:457:CYS:SG	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3729:MET:HE2	3:L:3729:MET:HA	1.97	0.47
6:O:127:ILE:HG22	6:P:127:ILE:HG12	1.97	0.47
9:X:695:PRO:O	9:X:738:TRP:CG	2.68	0.47
9:Y:721:VAL:CG1	9:Y:725:TRP:CB	2.93	0.47
3:C:3729:MET:HA	3:C:3729:MET:HE2	1.97	0.47
3:L:3924:HIS:CE1	3:L:3927:ASN:HD21	2.32	0.47
4:M:27:DA:H2''	4:M:28:DC:H5''	1.97	0.47
1:A:149:VAL:O	1:A:153:LEU:HD23	2.15	0.47
6:G:24:TRP:CD1	6:G:27:THR:C	2.93	0.47
1:J:145:GLU:O	1:J:149:VAL:HG23	2.15	0.47
9:X:730:PHE:CD1	9:X:730:PHE:N	2.80	0.47
6:F:127:ILE:HG22	6:G:127:ILE:HG12	1.97	0.47
9:X:697:THR:O	9:X:738:TRP:CE3	2.68	0.46
3:C:313:LEU:HD13	3:C:357:LYS:HB2	1.98	0.46
3:C:933:LEU:HD11	3:C:2797:VAL:HG11	1.98	0.46
2:K:246:HIS:CD2	2:K:368:ARG:HH22	2.33	0.46
1:J:149:VAL:O	1:J:153:LEU:HD23	2.15	0.46
2:B:246:HIS:CD2	2:B:368:ARG:HH22	2.33	0.46
2:B:496:HIS:CD2	2:B:506:PRO:HD3	2.51	0.46
4:D:27:DA:H2''	4:D:28:DC:H5''	1.96	0.46
3:L:568:PHE:CE1	3:L:633:ILE:HG21	2.50	0.46
4:M:24:DA:C2	4:M:25:DT:C2	3.03	0.46
4:D:25:DT:C2'	4:D:26:DT:H5'	2.46	0.46
6:P:32:PHE:CE2	6:P:47:VAL:HG23	2.51	0.46
1:A:74:LYS:HE2	8:S:186:ILE:O	2.16	0.46
7:I:194:MET:SD	7:I:194:MET:N	2.89	0.46
3:L:4042:GLN:HG2	3:L:4066:LEU:HD21	1.97	0.46
6:O:127:ILE:HD12	6:P:126:LEU:HD22	1.96	0.46
9:X:721:VAL:CG1	9:X:725:TRP:CB	2.93	0.46
1:J:333:GLU:N	1:J:334:THR:N	2.64	0.46
3:L:933:LEU:HD11	3:L:2797:VAL:HG11	1.98	0.46
3:L:3118:ASP:OD1	3:L:3119:VAL:N	2.49	0.46
3:L:3259:LEU:HD11	3:L:3283:LEU:HD23	1.97	0.46
9:Y:695:PRO:O	9:Y:738:TRP:CG	2.68	0.46
3:C:290:TYR:CE1	3:C:337:LYS:HE3	2.51	0.46
6:O:134:ILE:HD11	6:P:130:CYS:CA	2.41	0.46
9:X:721:VAL:CG1	9:X:725:TRP:HB3	2.46	0.46
9:Y:682:ILE:HD11	9:Y:726:LEU:HD23	1.97	0.46
6:F:134:ILE:HD11	6:G:130:CYS:CA	2.41	0.46
3:L:290:TYR:CE1	3:L:337:LYS:HE3	2.51	0.46
6:F:104:VAL:CG1	7:I:68:PRO:HD3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:313:LEU:HD13	3:L:357:LYS:HB2	1.98	0.46
3:C:568:PHE:CE1	3:C:633:ILE:HG21	2.50	0.45
3:C:3118:ASP:OD1	3:C:3119:VAL:N	2.49	0.45
6:F:88:PHE:CE1	6:F:93:CYS:HA	2.51	0.45
1:J:332:GLU:CB	3:L:212:VAL:HG13	2.33	0.45
3:L:388:LEU:HD13	3:L:388:LEU:C	2.41	0.45
9:Y:721:VAL:CG1	9:Y:725:TRP:HB3	2.46	0.45
1:A:334:THR:OG1	1:A:334:THR:HA	2.11	0.45
9:X:682:ILE:HD11	9:X:726:LEU:HD23	1.97	0.45
9:Y:697:THR:O	9:Y:738:TRP:CE3	2.69	0.45
1:A:333:GLU:N	1:A:334:THR:N	2.64	0.45
3:C:388:LEU:C	3:C:388:LEU:HD13	2.41	0.45
3:C:2323:LEU:HD23	3:C:2326:ILE:HD12	1.99	0.45
6:O:88:PHE:CE1	6:O:93:CYS:HA	2.52	0.45
6:P:2:GLU:HB2	6:P:24:TRP:CE2	2.51	0.45
2:K:496:HIS:CD2	2:K:506:PRO:HD3	2.51	0.45
6:O:181:ILE:HD11	9:Y:771:LEU:HA	1.99	0.45
3:C:4042:GLN:HG2	3:C:4066:LEU:HD21	1.97	0.45
1:J:132:GLN:OE1	1:J:137:HIS:CG	2.70	0.45
3:C:301:CYS:HB3	3:C:358:GLU:HG2	1.98	0.45
6:G:32:PHE:CE2	6:G:47:VAL:HG23	2.51	0.45
4:M:25:DT:C2'	4:M:26:DT:O5'	2.61	0.45
7:H:51:THR:HG23	7:H:69:PRO:CG	2.47	0.45
1:A:517:ARG:HH11	8:S:201:PHE:HB2	1.81	0.45
3:C:2511:ILE:HG21	3:C:2550:ILE:HD12	1.98	0.45
6:F:123:ILE:O	6:F:127:ILE:HG23	2.17	0.45
3:C:2556:SER:HB2	3:C:2799:GLN:HA	1.99	0.45
7:I:67:ALA:HB3	7:I:72:PHE:CE2	2.52	0.45
3:C:432:THR:HB	3:C:433:PRO:HD3	1.98	0.44
6:G:2:GLU:HB2	6:G:24:TRP:CE2	2.51	0.44
3:L:2323:LEU:HD23	3:L:2326:ILE:HD12	1.99	0.44
9:X:742:PHE:CZ	9:X:744:ILE:HB	2.52	0.44
1:A:332:GLU:O	1:A:333:GLU:CA	2.66	0.44
3:C:1860:GLU:CD	3:L:1815:THR:HG21	2.42	0.44
6:O:61:MET:HE2	6:O:65:LYS:HE2	1.98	0.44
6:O:97:PHE:O	6:O:107:ARG:HA	2.16	0.44
7:H:140:MET:C	7:H:140:MET:SD	3.01	0.44
1:J:200:LEU:C	1:J:200:LEU:HD23	2.43	0.44
3:L:313:LEU:HD13	3:L:357:LYS:CB	2.48	0.44
9:X:662:VAL:HG21	9:X:735:PHE:CE1	2.53	0.44
3:C:313:LEU:HD13	3:C:357:LYS:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:468:LEU:HB3	3:C:475:LEU:HD13	2.00	0.44
3:L:1171:TRP:CE2	3:L:1175:HIS:CD2	3.06	0.44
3:L:3147:LYS:HB2	3:L:3150:ASN:ND2	2.32	0.44
1:A:200:LEU:C	1:A:200:LEU:HD23	2.43	0.44
3:C:2919:ASP:HA	3:C:2922:ARG:HD2	2.00	0.44
6:F:181:ILE:HD11	9:X:771:LEU:HA	1.98	0.44
3:L:940:PHE:CZ	3:L:944:LYS:CE	3.00	0.44
3:L:2511:ILE:HG21	3:L:2550:ILE:HD12	1.98	0.44
9:Y:662:VAL:HG21	9:Y:735:PHE:CE1	2.53	0.44
9:Y:721:VAL:HG12	9:Y:725:TRP:CB	2.48	0.44
1:A:132:GLN:OE1	1:A:137:HIS:CG	2.70	0.44
3:C:305:ASN:HB3	3:C:308:LEU:HB3	2.00	0.44
3:C:3110:PHE:CD2	3:C:3110:PHE:C	2.96	0.44
3:L:2919:ASP:HA	3:L:2922:ARG:HD2	2.00	0.44
3:C:940:PHE:CZ	3:C:944:LYS:CE	3.00	0.44
3:L:3531:TYR:HB2	3:L:3532:PRO:HD3	2.00	0.44
5:N:26:DT:H2'	5:N:27:DT:C6	2.53	0.44
3:C:1649:LEU:HD12	3:C:1652:ILE:HD12	1.99	0.44
1:J:328:ILE:C	1:J:329:LEU:HD12	2.43	0.44
3:L:468:LEU:HB3	3:L:475:LEU:HD13	2.00	0.44
3:C:3147:LYS:HB2	3:C:3150:ASN:ND2	2.32	0.44
3:C:3531:TYR:HB2	3:C:3532:PRO:HD3	2.00	0.44
3:L:301:CYS:HB3	3:L:358:GLU:HG2	1.99	0.44
6:O:90:LYS:HE3	6:O:90:LYS:H	1.83	0.44
6:O:123:ILE:O	6:O:127:ILE:HG23	2.17	0.44
3:C:1171:TRP:CE2	3:C:1175:HIS:CD2	3.06	0.43
3:C:1815:THR:HG21	3:L:1860:GLU:CD	2.43	0.43
6:F:104:VAL:HG11	7:I:67:ALA:HA	2.00	0.43
6:G:126:LEU:C	6:G:126:LEU:HD23	2.42	0.43
7:H:18:LEU:CD2	7:H:95:PHE:O	2.65	0.43
3:L:1847:ALA:HB1	3:L:1873:TYR:CD1	2.53	0.43
1:A:328:ILE:C	1:A:329:LEU:HD12	2.43	0.43
1:J:98:ASN:HD22	1:J:148:TRP:CD1	2.37	0.43
3:C:2265:PRO:HD2	3:C:2309:PHE:CE2	2.53	0.43
3:L:1649:LEU:HD12	3:L:1652:ILE:HD12	1.99	0.43
3:L:1810:PRO:C	3:L:1811:ARG:HG3	2.43	0.43
1:A:98:ASN:HD22	1:A:148:TRP:CD1	2.37	0.43
6:F:58:ASP:CB	7:I:63:LYS:HD3	2.49	0.43
9:X:698:TYR:O	9:X:736:VAL:O	2.37	0.43
3:C:662:LEU:HA	3:C:725:LEU:HD22	2.00	0.43
3:L:432:THR:HB	3:L:433:PRO:HD3	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:2556:SER:HB2	3:L:2799:GLN:HA	1.99	0.43
3:L:2567:SER:HA	3:L:2572:TYR:CG	2.54	0.43
9:Y:698:TYR:O	9:Y:736:VAL:O	2.37	0.43
3:L:2549:LYS:O	3:L:2550:ILE:HD13	2.18	0.43
6:P:126:LEU:C	6:P:126:LEU:HD23	2.43	0.43
5:E:26:DT:H2'	5:E:27:DT:C6	2.53	0.43
6:F:90:LYS:H	6:F:90:LYS:HE3	1.83	0.43
9:X:721:VAL:HG12	9:X:725:TRP:CB	2.48	0.43
9:X:729:CYS:SG	9:X:734:SER:HB2	2.59	0.43
1:A:250:GLU:HG2	8:S:190:PHE:CG	2.54	0.43
3:C:1166:LEU:HA	3:C:1198:LEU:HD21	2.01	0.43
3:C:2549:LYS:O	3:C:2550:ILE:HD13	2.18	0.43
7:H:71:ALA:CB	6:O:104:VAL:CG2	2.89	0.43
7:H:112:LEU:HD22	6:O:106:PHE:CZ	2.53	0.43
3:L:1397:ASP:HA	3:L:1400:VAL:HG22	2.00	0.43
3:L:3463:LEU:HB3	3:L:3997:LEU:HD11	2.00	0.43
3:C:1672:PHE:CD1	3:C:1699:PHE:CD2	3.07	0.43
1:J:41:LEU:HD21	1:J:146:VAL:HG12	2.01	0.43
3:C:2567:SER:HA	3:C:2572:TYR:CG	2.54	0.43
3:L:630:CYS:HA	3:L:633:ILE:HB	2.01	0.43
3:L:3110:PHE:CD2	3:L:3110:PHE:C	2.96	0.43
3:C:1847:ALA:HB1	3:C:1873:TYR:CD1	2.53	0.42
3:C:3477:GLU:CD	3:C:3477:GLU:H	2.26	0.42
1:J:250:GLU:HG2	8:T:190:PHE:CG	2.54	0.42
1:J:273:ILE:HD13	1:J:368:VAL:HG22	2.01	0.42
3:L:3477:GLU:CD	3:L:3477:GLU:H	2.26	0.42
3:L:3713:PRO:HA	3:L:3716:HIS:CG	2.54	0.42
9:Y:729:CYS:SG	9:Y:734:SER:HB2	2.59	0.42
3:C:3463:LEU:HB3	3:C:3997:LEU:HD11	2.00	0.42
3:C:4090:ARG:NH1	3:C:4113:ASP:OD2	2.38	0.42
3:L:1600:MET:HE3	3:L:1600:MET:HA	2.00	0.42
9:X:725:TRP:CH2	9:X:734:SER:O	2.73	0.42
3:C:2121:ASP:HB3	3:C:2125:TRP:CE2	2.55	0.42
7:H:7:GLY:HA3	7:H:28:PHE:CE2	2.55	0.42
6:O:55:GLU:HA	6:O:58:ASP:HB3	2.01	0.42
2:B:434:MET:HG2	8:S:191:LYS:HZ2	1.83	0.42
3:L:569:VAL:HG11	3:L:645:TRP:CE3	2.54	0.42
3:L:662:LEU:HA	3:L:725:LEU:HD22	2.00	0.42
3:L:2265:PRO:HD2	3:L:2309:PHE:CE2	2.53	0.42
3:C:630:CYS:HA	3:C:633:ILE:HB	2.01	0.42
7:I:1:MET:SD	7:I:4:LEU:HB2	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:208:LYS:HG2	7:I:212:MET:SD	2.59	0.42
6:F:55:GLU:HA	6:F:58:ASP:HB3	2.01	0.42
7:H:46:HIS:HB3	7:H:124:MET:SD	2.59	0.42
1:A:273:ILE:HD13	1:A:368:VAL:HG22	2.01	0.42
3:C:1600:MET:HE3	3:C:1600:MET:HA	2.00	0.42
3:C:3796:MET:HE1	3:C:3802:LEU:HG	2.02	0.42
6:F:104:VAL:HG11	7:I:68:PRO:HD3	2.00	0.42
7:H:18:LEU:HD22	7:H:95:PHE:O	2.19	0.42
6:P:42:ALA:HB3	6:P:116:VAL:O	2.20	0.42
9:X:682:ILE:HD11	9:X:726:LEU:CD2	2.50	0.42
9:Y:697:THR:O	9:Y:738:TRP:HB3	2.20	0.42
1:A:333:GLU:N	1:A:333:GLU:CG	2.83	0.42
3:L:1166:LEU:HA	3:L:1198:LEU:HD21	2.01	0.42
3:L:1672:PHE:CD1	3:L:1699:PHE:CD2	3.07	0.42
3:L:1967:PHE:CD2	3:L:2123:PRO:HB3	2.55	0.42
9:X:697:THR:O	9:X:738:TRP:HB3	2.20	0.42
9:Y:725:TRP:CH2	9:Y:734:SER:O	2.73	0.42
1:A:312:LEU:CD2	3:C:161:ALA:HA	2.50	0.42
3:C:569:VAL:HG11	3:C:645:TRP:CE3	2.54	0.42
3:C:1579:VAL:HA	3:C:1582:LEU:HB2	2.02	0.42
3:L:2121:ASP:HB3	3:L:2125:TRP:CE2	2.55	0.42
9:X:725:TRP:O	9:X:729:CYS:HB2	2.20	0.42
3:C:309:LYS:HG2	3:C:313:LEU:HD12	2.02	0.42
3:C:1397:ASP:HA	3:C:1400:VAL:HG22	2.00	0.42
3:L:1579:VAL:HA	3:L:1582:LEU:HB2	2.02	0.42
3:L:3796:MET:HE1	3:L:3802:LEU:HG	2.02	0.42
6:F:90:LYS:HE3	6:F:91:GLU:OE2	2.20	0.41
6:F:101:LEU:CD2	7:I:113:SER:HA	2.42	0.41
6:F:130:CYS:HB3	6:G:130:CYS:HB2	2.02	0.41
4:M:14:DA:C2	4:M:15:DT:C2	3.08	0.41
6:O:90:LYS:HE3	6:O:91:GLU:OE2	2.20	0.41
9:Y:682:ILE:HD11	9:Y:726:LEU:CD2	2.50	0.41
9:Y:725:TRP:O	9:Y:729:CYS:HB2	2.20	0.41
3:C:1967:PHE:CD2	3:C:2123:PRO:HB3	2.55	0.41
1:J:332:GLU:O	1:J:333:GLU:CA	2.66	0.41
6:P:170:GLU:O	6:P:174:THR:HG22	2.20	0.41
9:Y:726:LEU:HD12	9:Y:726:LEU:HA	1.78	0.41
3:C:196:LEU:CD2	3:C:230:LEU:HD22	2.50	0.41
6:G:42:ALA:HB3	6:G:116:VAL:O	2.20	0.41
6:G:169:LYS:NZ	9:X:810:LEU:O	2.53	0.41
1:J:83:LEU:HD23	1:J:111:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:130:CYS:HB3	6:P:130:CYS:HB2	2.02	0.41
1:A:41:LEU:HD21	1:A:146:VAL:HG12	2.01	0.41
3:C:663:ILE:HG21	3:C:666:PHE:CE2	2.55	0.41
4:D:14:DA:C2	4:D:15:DT:C2	3.08	0.41
1:J:333:GLU:N	1:J:333:GLU:CG	2.83	0.41
3:L:196:LEU:CD2	3:L:230:LEU:HD22	2.50	0.41
1:A:83:LEU:HD23	1:A:111:PRO:HB3	2.02	0.41
3:C:1171:TRP:NE1	3:C:1175:HIS:HE2	2.18	0.41
6:F:102:LYS:HA	6:F:102:LYS:CE	2.50	0.41
1:J:74:LYS:HE2	8:T:186:ILE:O	2.18	0.41
3:L:2371:PHE:CD2	3:L:2373:PRO:HD2	2.56	0.41
3:C:2371:PHE:CD2	3:C:2373:PRO:HD2	2.56	0.41
1:J:312:LEU:CD2	3:L:161:ALA:HA	2.50	0.41
3:L:1594:SER:HB2	3:L:1644:ALA:HB1	2.03	0.41
3:C:458:CYS:SG	3:C:530:LEU:HD22	2.61	0.41
1:J:65:GLN:OE1	1:J:65:GLN:HA	2.21	0.41
3:L:1825:LEU:HD11	3:L:1875:LYS:HB3	2.01	0.41
6:P:169:LYS:NZ	9:Y:810:LEU:O	2.53	0.41
6:F:59:MET:HE3	7:I:64:ARG:HH11	1.84	0.41
6:G:170:GLU:O	6:G:174:THR:HG22	2.20	0.41
7:H:208:LYS:O	7:H:212:MET:SD	2.78	0.41
3:L:442:GLN:CG	3:L:457:CYS:SG	3.09	0.41
3:L:663:ILE:HG21	3:L:666:PHE:CE2	2.55	0.41
3:L:741:ILE:HG22	3:L:741:ILE:O	2.21	0.41
3:L:1171:TRP:NE1	3:L:1175:HIS:HE2	2.18	0.41
3:L:3937:VAL:C	3:L:3938:ILE:HG13	2.46	0.41
9:X:717:LYS:HA	9:X:739:GLN:HB2	2.03	0.41
9:Y:717:LYS:HA	9:Y:739:GLN:HB2	2.03	0.41
3:C:101:ALA:N	3:C:102:PRO:HD2	2.36	0.41
3:C:1825:LEU:HD11	3:C:1875:LYS:HB3	2.02	0.41
3:C:1840:PHE:CE1	3:C:1895:LYS:HD2	2.56	0.41
3:C:3713:PRO:HA	3:C:3716:HIS:CG	2.54	0.41
3:L:309:LYS:HG2	3:L:313:LEU:HD12	2.02	0.41
3:L:3626:GLY:HA2	3:L:3685:PRO:CD	2.51	0.41
5:E:23:DT:C2	5:E:24:DT:C4	3.09	0.40
1:J:241:ASP:HB2	8:T:185:LEU:HD21	2.03	0.40
3:L:101:ALA:N	3:L:102:PRO:HD2	2.36	0.40
5:N:1:DG:N2	5:N:2:DT:C2	2.89	0.40
6:O:3:ARG:HH11	6:O:129:TYR:CB	2.34	0.40
9:Y:725:TRP:CE2	9:Y:734:SER:HB2	2.56	0.40
3:C:1594:SER:HB2	3:C:1644:ALA:HB1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1805:PHE:CE1	3:C:1816:ARG:HG2	2.56	0.40
3:C:3280:TYR:CD2	3:C:3280:TYR:C	2.99	0.40
3:C:3937:VAL:C	3:C:3938:ILE:HG13	2.46	0.40
4:D:27:DA:H2'	4:D:28:DC:H5''	2.03	0.40
3:L:1805:PHE:CE1	3:L:1816:ARG:HG2	2.56	0.40
3:L:3280:TYR:CD2	3:L:3280:TYR:C	2.99	0.40
6:O:8:ILE:HG12	6:O:18:HIS:HB2	2.03	0.40
6:O:151:LEU:HB3	6:P:151:LEU:HB3	2.03	0.40
3:C:442:GLN:CG	3:C:457:CYS:SG	3.09	0.40
3:C:1897:ASN:HA	3:C:1904:CYS:SG	2.62	0.40
3:C:3679:ASN:C	3:C:3683:CYS:HG	2.29	0.40
6:F:8:ILE:HG12	6:F:18:HIS:HB2	2.03	0.40
7:H:215:GLN:O	7:H:219:MET:SD	2.78	0.40
3:C:2485:ARG:HA	3:C:2499:PHE:CE1	2.57	0.40
7:H:112:LEU:CD2	6:O:106:PHE:CZ	3.05	0.40
3:L:2485:ARG:HA	3:L:2499:PHE:CE1	2.56	0.40
9:X:726:LEU:HD12	9:X:729:CYS:CB	2.52	0.40
3:C:741:ILE:HG22	3:C:741:ILE:O	2.21	0.40
6:F:3:ARG:HH11	6:F:129:TYR:CB	2.34	0.40
6:F:151:LEU:HB3	6:G:151:LEU:HB3	2.03	0.40
7:H:206:ASP:C	7:H:208:LYS:H	2.29	0.40
7:I:43:GLN:HB2	7:I:45:TRP:CH2	2.57	0.40
3:L:4121:TRP:CD1	3:L:4123:GLY:H	2.40	0.40
9:Y:767:ILE:HG22	9:Y:768:ASP:O	2.22	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	493/609 (81%)	460 (93%)	33 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	493/609 (81%)	460 (93%)	33 (7%)	0	100	100
2	B	520/732 (71%)	473 (91%)	41 (8%)	6 (1%)	10	44
2	K	520/732 (71%)	474 (91%)	40 (8%)	6 (1%)	10	44
3	C	3694/4128 (90%)	3400 (92%)	294 (8%)	0	100	100
3	L	3694/4128 (90%)	3398 (92%)	296 (8%)	0	100	100
6	F	199/336 (59%)	192 (96%)	6 (3%)	1 (0%)	24	63
6	G	191/336 (57%)	177 (93%)	10 (5%)	4 (2%)	5	30
6	O	199/336 (59%)	193 (97%)	6 (3%)	0	100	100
6	P	191/336 (57%)	177 (93%)	10 (5%)	4 (2%)	5	30
7	H	217/299 (73%)	203 (94%)	13 (6%)	1 (0%)	24	63
7	I	212/299 (71%)	201 (95%)	10 (5%)	1 (0%)	24	63
8	S	21/204 (10%)	18 (86%)	3 (14%)	0	100	100
8	T	21/204 (10%)	18 (86%)	3 (14%)	0	100	100
9	X	250/911 (27%)	222 (89%)	24 (10%)	4 (2%)	7	38
9	Y	250/911 (27%)	222 (89%)	24 (10%)	4 (2%)	7	38
All	All	11165/15110 (74%)	10288 (92%)	846 (8%)	31 (0%)	37	72

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	145	SER
2	B	146	GLN
2	B	518	PRO
2	B	520	ALA
6	G	26	LYS
2	K	145	SER
2	K	146	GLN
2	K	518	PRO
2	K	520	ALA
6	P	26	LYS
9	X	717	LYS
9	X	737	PRO
9	X	740	PRO
9	X	746	MET
9	Y	717	LYS
9	Y	737	PRO
9	Y	746	MET

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Mol	Chain	Res	Type
7	H	208	LYS
9	Y	740	PRO
6	F	107	ARG
6	G	49	GLU
6	P	49	GLU
2	B	519	PRO
6	G	64	GLY
7	I	177	ASP
2	K	519	PRO
6	P	64	GLY
6	G	60	ALA
6	P	60	ALA
2	B	517	ASN
2	K	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	A	452/548 (82%)	449 (99%)	3 (1%)	76	81
1	J	452/548 (82%)	449 (99%)	3 (1%)	76	81
2	B	474/649 (73%)	466 (98%)	8 (2%)	53	69
2	K	474/649 (73%)	465 (98%)	9 (2%)	50	67
3	C	3322/3671 (90%)	3278 (99%)	44 (1%)	61	74
3	L	3322/3671 (90%)	3279 (99%)	43 (1%)	61	74
6	F	180/303 (59%)	157 (87%)	23 (13%)	4	15
6	G	178/303 (59%)	159 (89%)	19 (11%)	6	21
6	O	180/303 (59%)	159 (88%)	21 (12%)	5	18
6	P	178/303 (59%)	159 (89%)	19 (11%)	6	21
7	H	198/262 (76%)	187 (94%)	11 (6%)	19	40
7	I	193/262 (74%)	178 (92%)	15 (8%)	11	32
8	S	18/160 (11%)	18 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	T	18/160 (11%)	18 (100%)	0	100	100
9	X	230/808 (28%)	207 (90%)	23 (10%)	7	24
9	Y	230/808 (28%)	208 (90%)	22 (10%)	8	25
All	All	10099/13408 (75%)	9836 (97%)	263 (3%)	41	62

All (263) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	VAL
1	A	299	LYS
1	A	368	VAL
2	B	35	LYS
2	B	64	THR
2	B	151	ILE
2	B	203	GLU
2	B	229	GLU
2	B	330	GLN
2	B	424	LEU
2	B	518	PRO
3	C	135	LEU
3	C	376	ILE
3	C	406	ARG
3	C	530	LEU
3	C	633	ILE
3	C	674	VAL
3	C	760	LEU
3	C	771	ASN
3	C	901	MET
3	C	1110	SER
3	C	1118	GLU
3	C	1135	CYS
3	C	1231	GLN
3	C	1374	GLN
3	C	1467	ILE
3	C	1531	LEU
3	C	1602	ASP
3	C	1678	LEU
3	C	1845	VAL
3	C	1862	THR
3	C	1969	GLU
3	C	2124	SER

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Mol	Chain	Res	Type
3	C	2145	PHE
3	C	2157	PHE
3	C	2182	ILE
3	C	2238	ILE
3	C	2281	MET
3	C	2285	LEU
3	C	2358	ASP
3	C	2373	PRO
3	C	2374	LEU
3	C	2412	TYR
3	C	2419	ASP
3	C	2553	HIS
3	C	2834	GLN
3	C	3077	ILE
3	C	3310	ASN
3	C	3379	GLN
3	C	3471	ILE
3	C	3517	SER
3	C	3576	ASP
3	C	3644	PHE
3	C	3691	LYS
3	C	3729	MET
6	F	3	ARG
6	F	6	SER
6	F	7	ARG
6	F	8	ILE
6	F	22	VAL
6	F	23	SER
6	F	26	LYS
6	F	40	HIS
6	F	55	GLU
6	F	58	ASP
6	F	85	THR
6	F	90	LYS
6	F	101	LEU
6	F	104	VAL
6	F	110	SER
6	F	112	ASN
6	F	114	GLU
6	F	116	VAL
6	F	127	ILE
6	F	129	TYR

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Mol	Chain	Res	Type
6	F	157	ASP
6	F	191	ILE
6	F	195	HIS
6	G	1	MET
6	G	21	GLN
6	G	22	VAL
6	G	28	LEU
6	G	34	ILE
6	G	47	VAL
6	G	49	GLU
6	G	52	ILE
6	G	67	VAL
6	G	71	ARG
6	G	85	THR
6	G	89	SER
6	G	90	LYS
6	G	91	GLU
6	G	115	LYS
6	G	128	CYS
6	G	163	GLU
6	G	174	THR
6	G	186	GLU
7	H	29	ILE
7	H	31	LYS
7	H	38	VAL
7	H	62	ASN
7	H	100	VAL
7	H	109	ARG
7	H	124	MET
7	H	168	GLN
7	H	169	GLU
7	H	196	GLU
7	H	197	LYS
7	I	17	GLN
7	I	31	LYS
7	I	41	LEU
7	I	48	GLN
7	I	49	VAL
7	I	109	ARG
7	I	118	TYR
7	I	140	MET
7	I	159	MET

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Mol	Chain	Res	Type
7	I	169	GLU
7	I	194	MET
7	I	197	LYS
7	I	200	GLU
7	I	204	ILE
7	I	224	GLN
1	J	85	VAL
1	J	299	LYS
1	J	368	VAL
2	K	35	LYS
2	K	64	THR
2	K	151	ILE
2	K	203	GLU
2	K	229	GLU
2	K	326	VAL
2	K	330	GLN
2	K	424	LEU
2	K	518	PRO
3	L	135	LEU
3	L	376	ILE
3	L	406	ARG
3	L	530	LEU
3	L	633	ILE
3	L	674	VAL
3	L	760	LEU
3	L	771	ASN
3	L	901	MET
3	L	1110	SER
3	L	1118	GLU
3	L	1135	CYS
3	L	1231	GLN
3	L	1374	GLN
3	L	1467	ILE
3	L	1531	LEU
3	L	1602	ASP
3	L	1678	LEU
3	L	1845	VAL
3	L	1969	GLU
3	L	2124	SER
3	L	2145	PHE
3	L	2157	PHE
3	L	2182	ILE

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Mol	Chain	Res	Type
3	L	2238	ILE
3	L	2281	MET
3	L	2285	LEU
3	L	2358	ASP
3	L	2373	PRO
3	L	2374	LEU
3	L	2412	TYR
3	L	2419	ASP
3	L	2553	HIS
3	L	2834	GLN
3	L	3077	ILE
3	L	3310	ASN
3	L	3379	GLN
3	L	3471	ILE
3	L	3517	SER
3	L	3576	ASP
3	L	3644	PHE
3	L	3691	LYS
3	L	3729	MET
6	O	3	ARG
6	O	6	SER
6	O	7	ARG
6	O	8	ILE
6	O	22	VAL
6	O	23	SER
6	O	26	LYS
6	O	40	HIS
6	O	55	GLU
6	O	58	ASP
6	O	85	THR
6	O	90	LYS
6	O	104	VAL
6	O	112	ASN
6	O	114	GLU
6	O	116	VAL
6	O	127	ILE
6	O	129	TYR
6	O	157	ASP
6	O	191	ILE
6	O	195	HIS
6	P	1	MET
6	P	21	GLN

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Mol	Chain	Res	Type
6	P	22	VAL
6	P	28	LEU
6	P	34	ILE
6	P	47	VAL
6	P	49	GLU
6	P	52	ILE
6	P	67	VAL
6	P	71	ARG
6	P	85	THR
6	P	89	SER
6	P	90	LYS
6	P	91	GLU
6	P	115	LYS
6	P	128	CYS
6	P	163	GLU
6	P	174	THR
6	P	186	GLU
9	X	661	ASP
9	X	728	GLU
9	X	729	CYS
9	X	736	VAL
9	X	737	PRO
9	X	740	PRO
9	X	743	MET
9	X	746	MET
9	X	774	LEU
9	X	786	GLU
9	X	788	THR
9	X	811	SER
9	X	820	LEU
9	X	822	SER
9	X	830	SER
9	X	836	THR
9	X	837	ARG
9	X	843	LEU
9	X	853	VAL
9	X	856	LEU
9	X	871	ARG
9	X	894	VAL
9	X	906	GLU
9	Y	661	ASP
9	Y	728	GLU

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Mol	Chain	Res	Type
9	Y	729	CYS
9	Y	736	VAL
9	Y	737	PRO
9	Y	743	MET
9	Y	746	MET
9	Y	774	LEU
9	Y	786	GLU
9	Y	788	THR
9	Y	811	SER
9	Y	820	LEU
9	Y	822	SER
9	Y	830	SER
9	Y	836	THR
9	Y	837	ARG
9	Y	843	LEU
9	Y	853	VAL
9	Y	856	LEU
9	Y	871	ARG
9	Y	894	VAL
9	Y	906	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (163) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	128	GLN
1	A	176	HIS
1	A	278	GLN
1	A	433	GLN
2	B	33	GLN
2	B	76	ASN
2	B	119	GLN
2	B	246	HIS
2	B	500	HIS
2	B	514	ASN
3	C	16	GLN
3	C	185	HIS
3	C	278	HIS
3	C	289	ASN
3	C	442	GLN
3	C	448	GLN
3	C	484	HIS

Continued on next page...

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Mol	Chain	Res	Type
3	C	539	GLN
3	C	771	ASN
3	C	786	GLN
3	C	982	GLN
3	C	993	HIS
3	C	1004	GLN
3	C	1133	HIS
3	C	1304	HIS
3	C	1374	GLN
3	C	1465	HIS
3	C	1574	ASN
3	C	1598	ASN
3	C	1603	GLN
3	C	1738	ASN
3	C	1901	HIS
3	C	1980	ASN
3	C	2141	ASN
3	C	2283	ASN
3	C	2301	GLN
3	C	2305	ASN
3	C	2351	GLN
3	C	2426	HIS
3	C	2432	GLN
3	C	2481	HIS
3	C	2483	ASN
3	C	2493	ASN
3	C	2613	GLN
3	C	2640	GLN
3	C	2784	GLN
3	C	2795	GLN
3	C	2831	ASN
3	C	2838	GLN
3	C	2885	GLN
3	C	3004	HIS
3	C	3028	ASN
3	C	3054	GLN
3	C	3081	HIS
3	C	3105	ASN
3	C	3319	ASN
3	C	3577	GLN
3	C	3605	ASN
3	C	3766	GLN

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Mol	Chain	Res	Type
3	C	3908	HIS
3	C	3915	HIS
3	C	3986	HIS
3	C	4015	ASN
3	C	4088	ASN
3	C	4110	GLN
6	F	40	HIS
6	F	138	GLN
6	F	141	ASN
6	F	143	HIS
6	F	159	GLN
6	G	118	ASN
6	G	137	ASN
6	G	156	ASN
6	G	159	GLN
7	H	42	GLN
7	H	149	GLN
7	H	158	HIS
7	I	21	ASN
7	I	46	HIS
7	I	48	GLN
7	I	56	GLN
7	I	75	HIS
7	I	168	GLN
7	I	213	ASN
1	J	68	GLN
1	J	121	GLN
1	J	128	GLN
1	J	176	HIS
1	J	278	GLN
1	J	433	GLN
2	K	33	GLN
2	K	119	GLN
2	K	246	HIS
2	K	500	HIS
2	K	517	ASN
3	L	185	HIS
3	L	278	HIS
3	L	289	ASN
3	L	442	GLN
3	L	448	GLN
3	L	484	HIS

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Mol	Chain	Res	Type
3	L	539	GLN
3	L	771	ASN
3	L	786	GLN
3	L	982	GLN
3	L	993	HIS
3	L	1133	HIS
3	L	1304	HIS
3	L	1374	GLN
3	L	1465	HIS
3	L	1574	ASN
3	L	1598	ASN
3	L	1603	GLN
3	L	1738	ASN
3	L	1754	GLN
3	L	1901	HIS
3	L	2283	ASN
3	L	2301	GLN
3	L	2305	ASN
3	L	2351	GLN
3	L	2426	HIS
3	L	2432	GLN
3	L	2481	HIS
3	L	2483	ASN
3	L	2493	ASN
3	L	2613	GLN
3	L	2634	GLN
3	L	2640	GLN
3	L	2784	GLN
3	L	2795	GLN
3	L	2831	ASN
3	L	2838	GLN
3	L	2885	GLN
3	L	3004	HIS
3	L	3028	ASN
3	L	3054	GLN
3	L	3319	ASN
3	L	3577	GLN
3	L	3605	ASN
3	L	3643	HIS
3	L	3766	GLN
3	L	3850	HIS
3	L	3915	HIS

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Mol	Chain	Res	Type
3	L	3986	HIS
3	L	4015	ASN
3	L	4088	ASN
3	L	4110	GLN
6	O	40	HIS
6	O	138	GLN
6	O	141	ASN
6	O	143	HIS
6	O	159	GLN
6	P	118	ASN
6	P	137	ASN
6	P	156	ASN
6	P	159	GLN
8	S	187	ASN
8	T	187	ASN
9	X	739	GLN
9	X	833	ASN
9	Y	739	GLN
9	Y	833	ASN

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	C	4201	10	32,33,33	0.67	1 (3%)	48,52,52	0.57	0
11	ATP	L	4201	10	32,33,33	0.66	1 (3%)	48,52,52	0.56	0

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	C	4201	10	-	4/22/38/38	0/3/3/3
11	ATP	L	4201	10	-	4/22/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	4201	ATP	C6-N6	-2.09	1.28	1.34
11	L	4201	ATP	C6-N6	-2.06	1.28	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

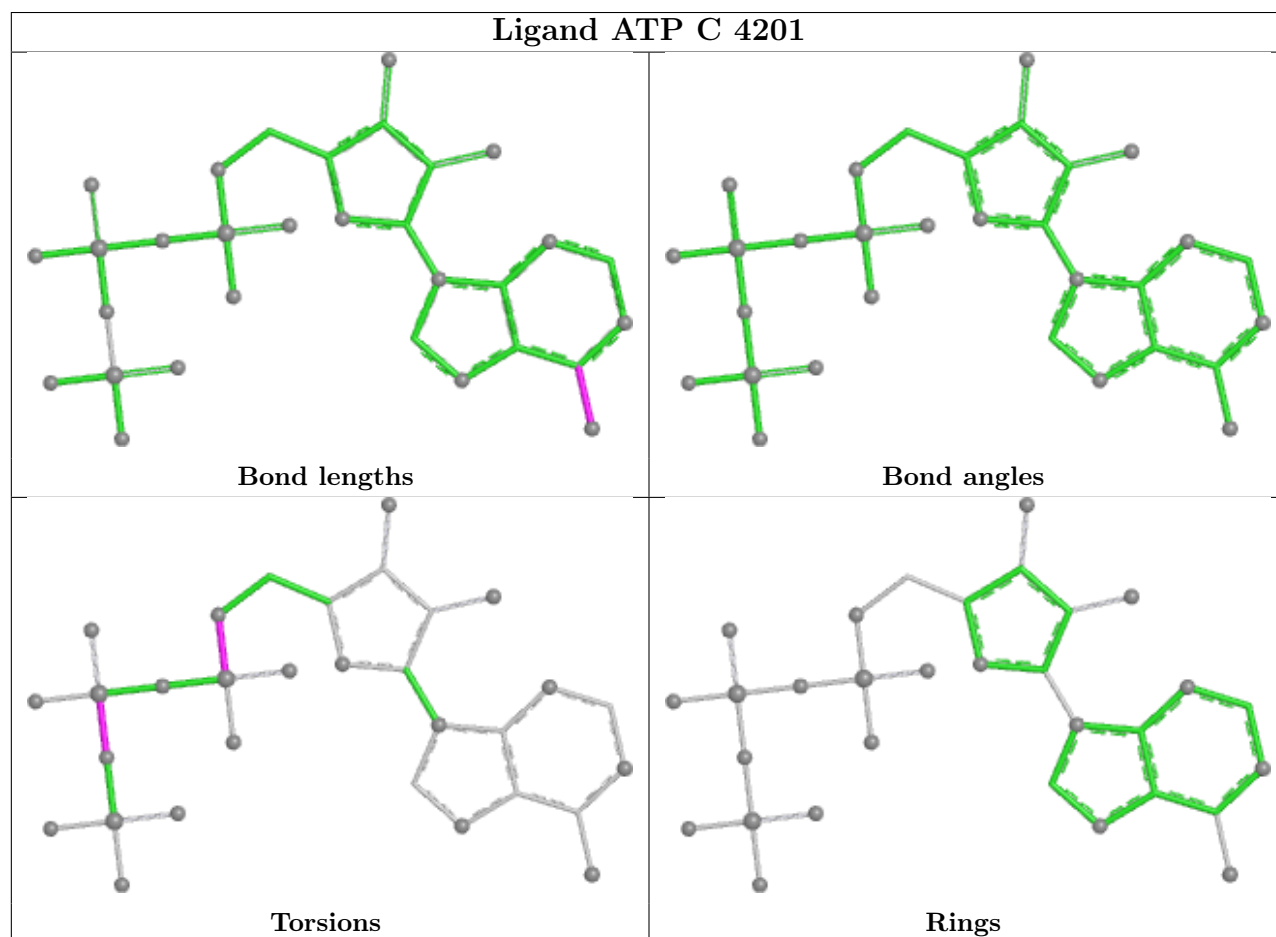
Mol	Chain	Res	Type	Atoms
11	C	4201	ATP	C5'-O5'-PA-O1A
11	C	4201	ATP	C5'-O5'-PA-O2A
11	C	4201	ATP	C5'-O5'-PA-O3A
11	L	4201	ATP	C5'-O5'-PA-O1A
11	L	4201	ATP	C5'-O5'-PA-O2A
11	L	4201	ATP	C5'-O5'-PA-O3A
11	C	4201	ATP	PG-O3B-PB-O1B
11	L	4201	ATP	PG-O3B-PB-O1B

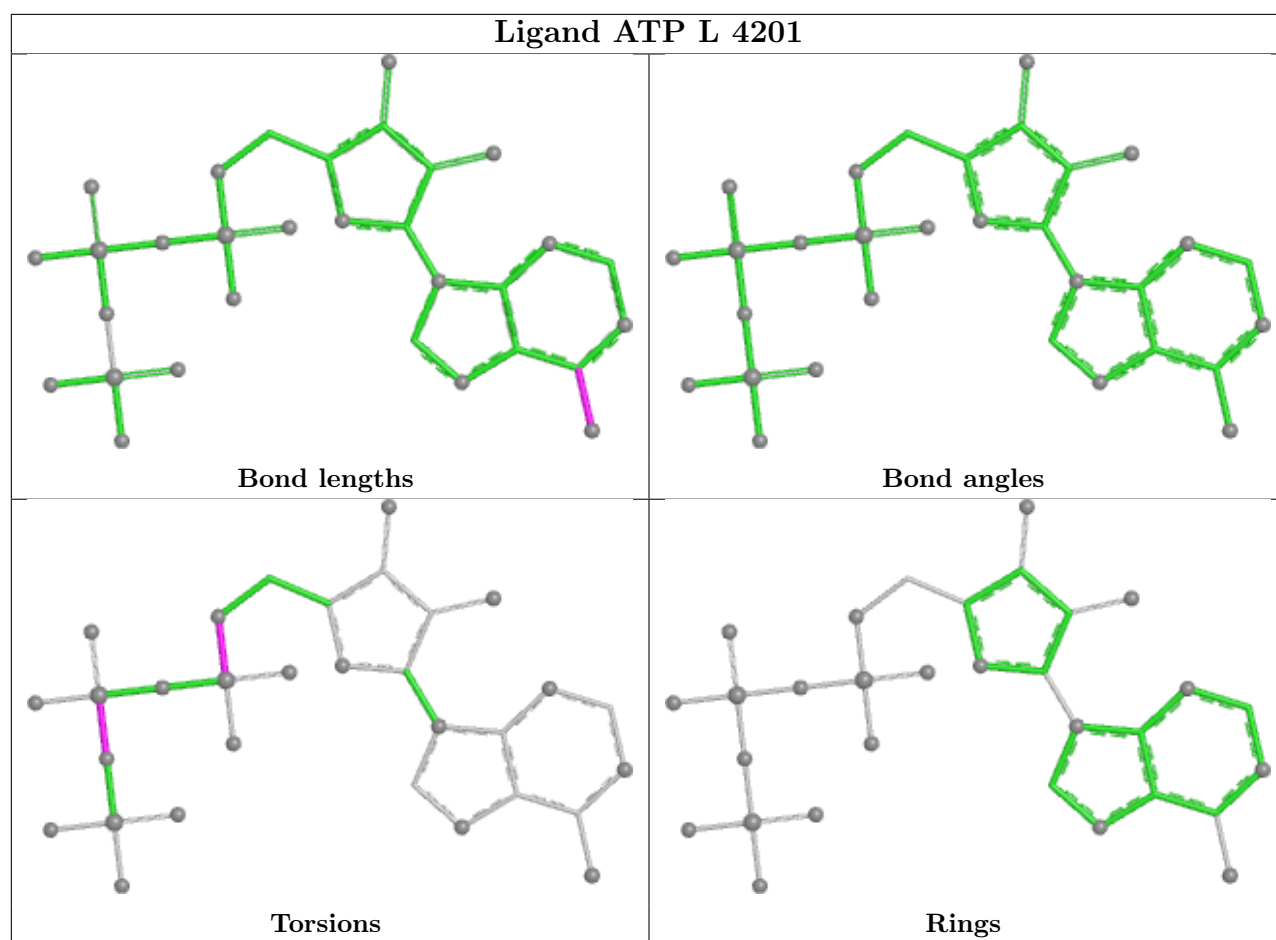
There are no ring outliers.

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 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.

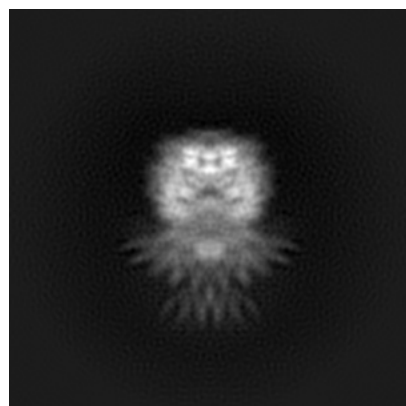
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28733. These allow visual inspection of the internal detail of the map and identification of artifacts.

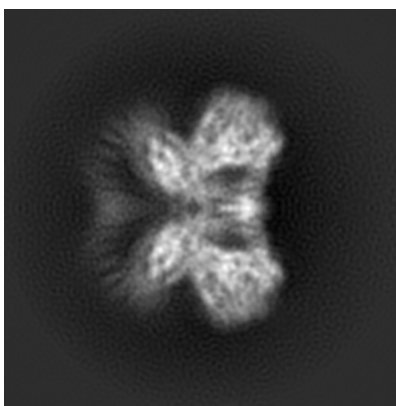
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

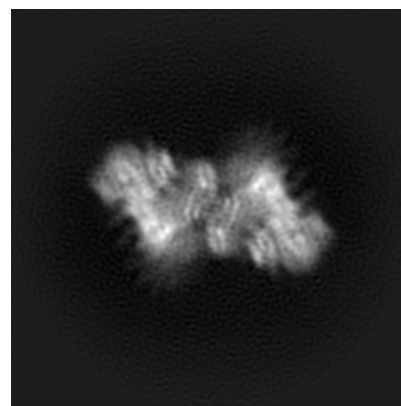
6.1.1 Primary map



X



Y

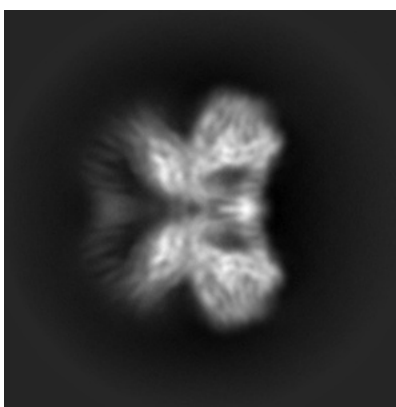


Z

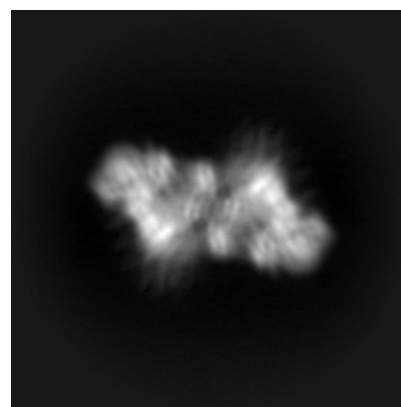
6.1.2 Raw map



X



Y

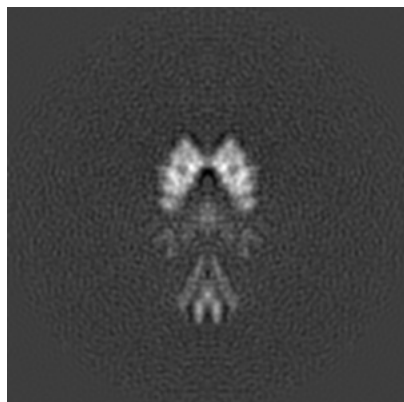


Z

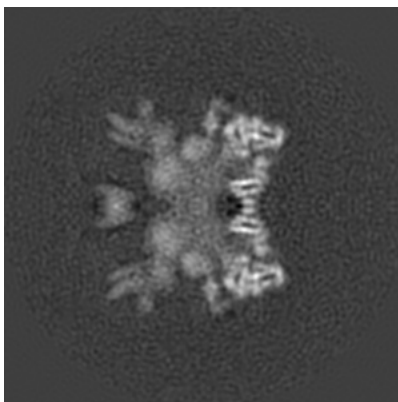
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

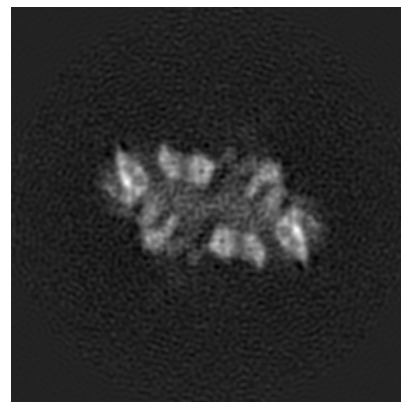
6.2.1 Primary map



X Index: 120

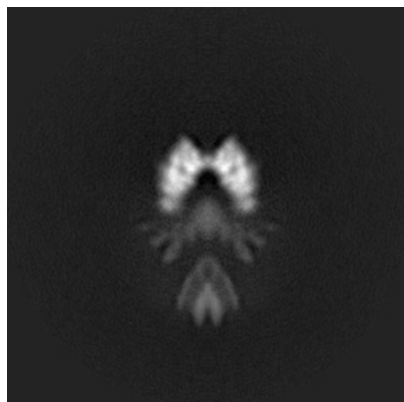


Y Index: 120

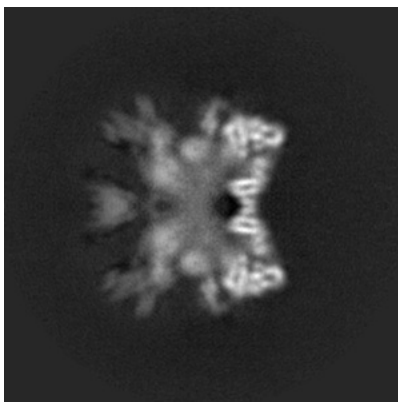


Z Index: 120

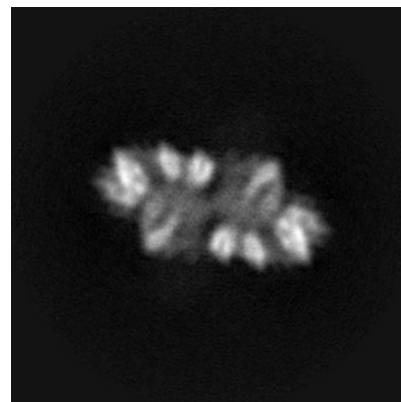
6.2.2 Raw map



X Index: 120



Y Index: 120

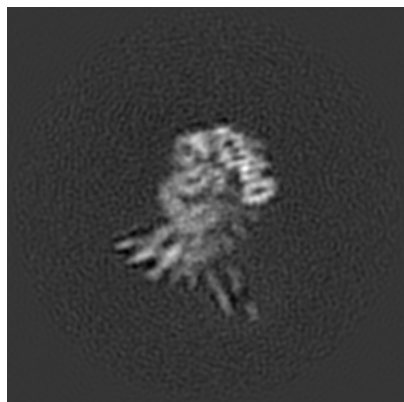


Z Index: 120

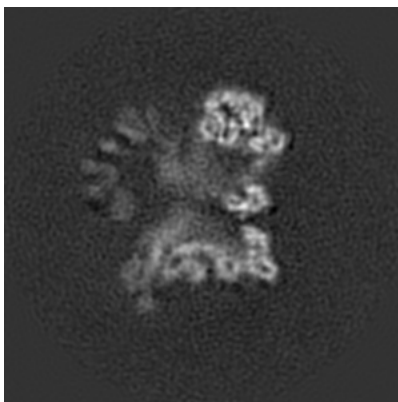
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

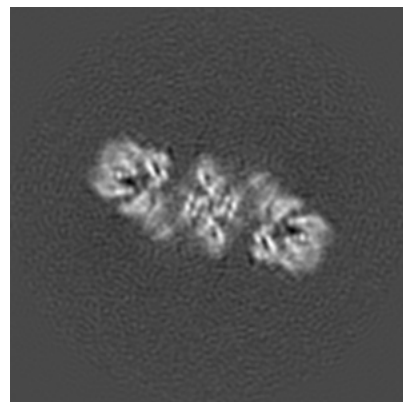
6.3.1 Primary map



X Index: 84

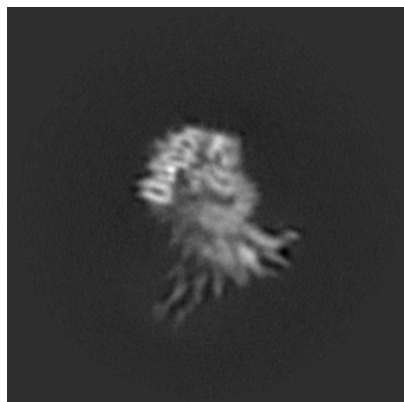


Y Index: 110

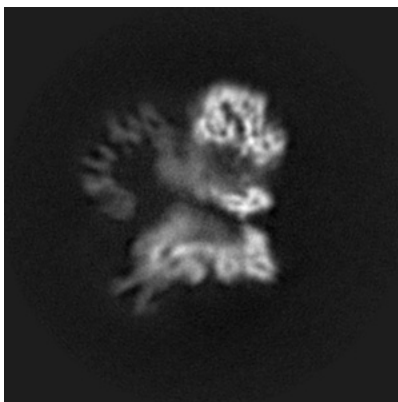


Z Index: 143

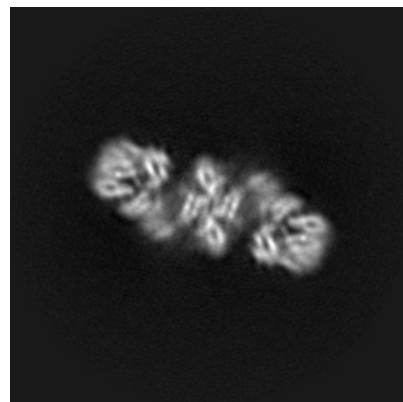
6.3.2 Raw map



X Index: 156



Y Index: 108

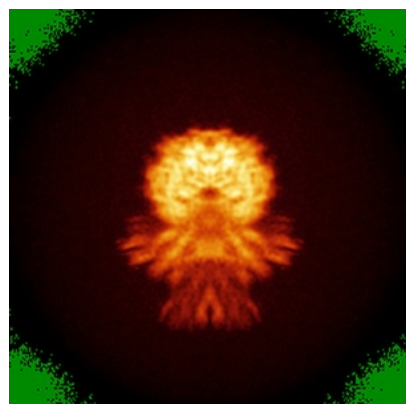


Z Index: 143

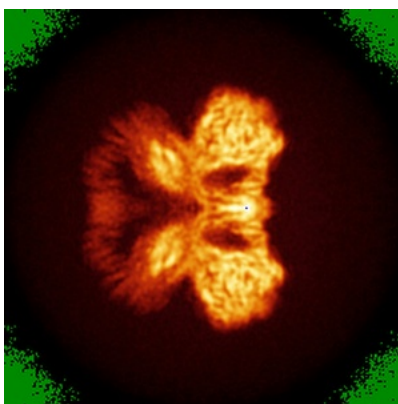
The images above show the largest variance slices of the map in three orthogonal directions.

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

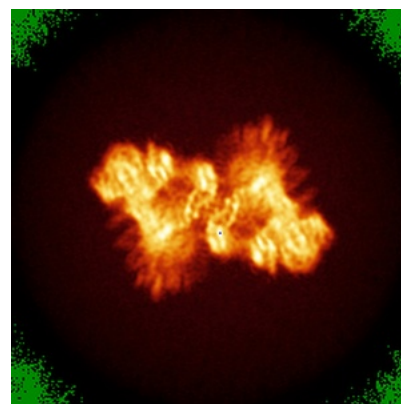
6.4.1 Primary map



X



Y

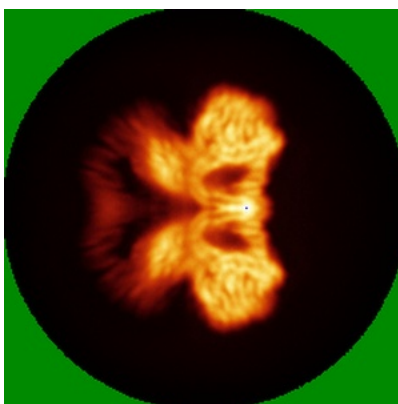


Z

6.4.2 Raw map



X



Y

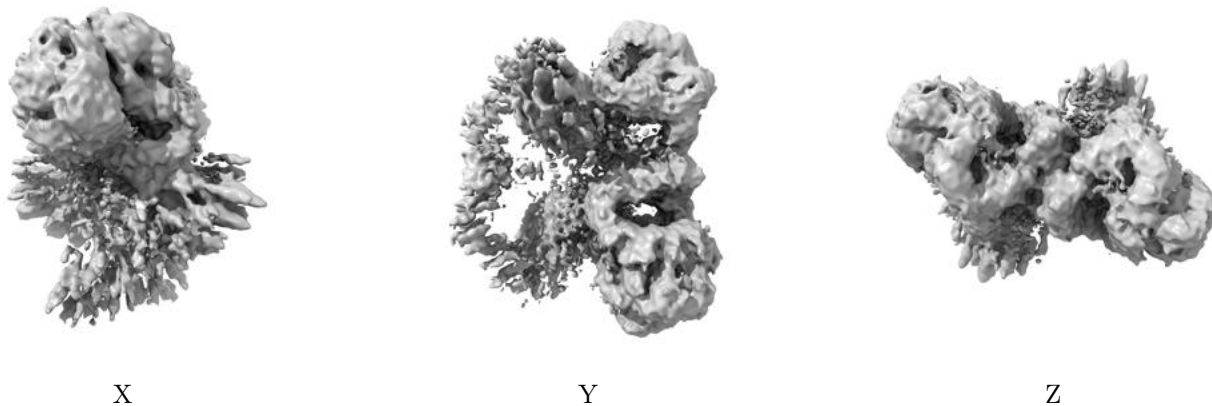


Z

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.

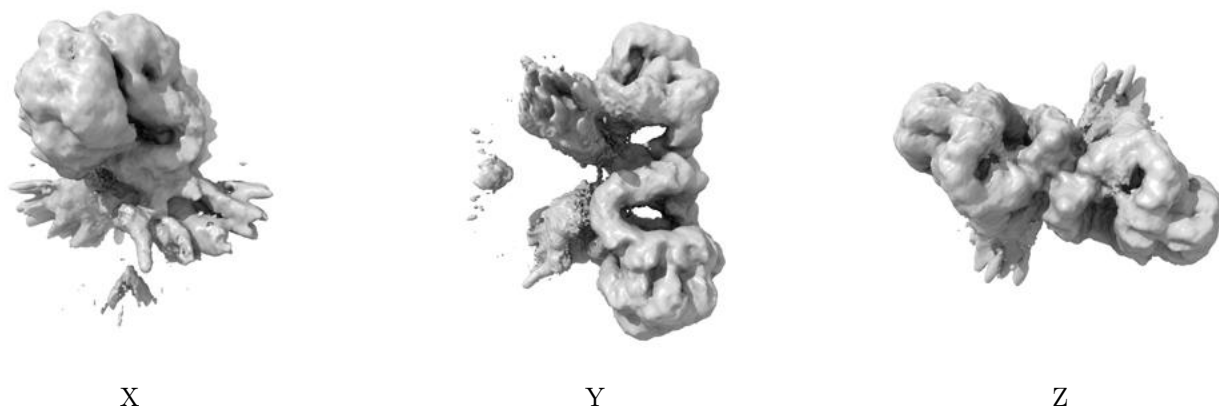
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. 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.

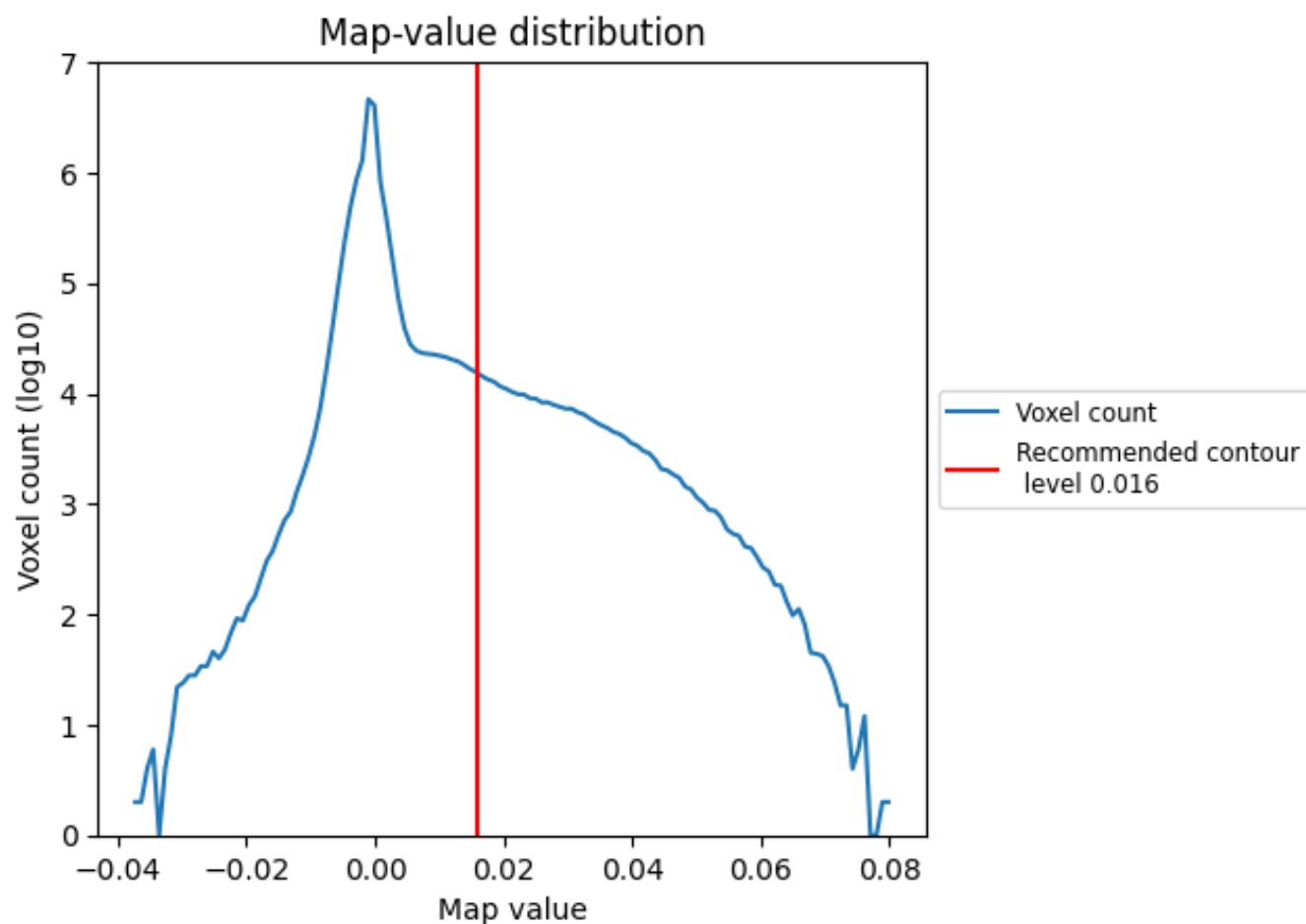
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

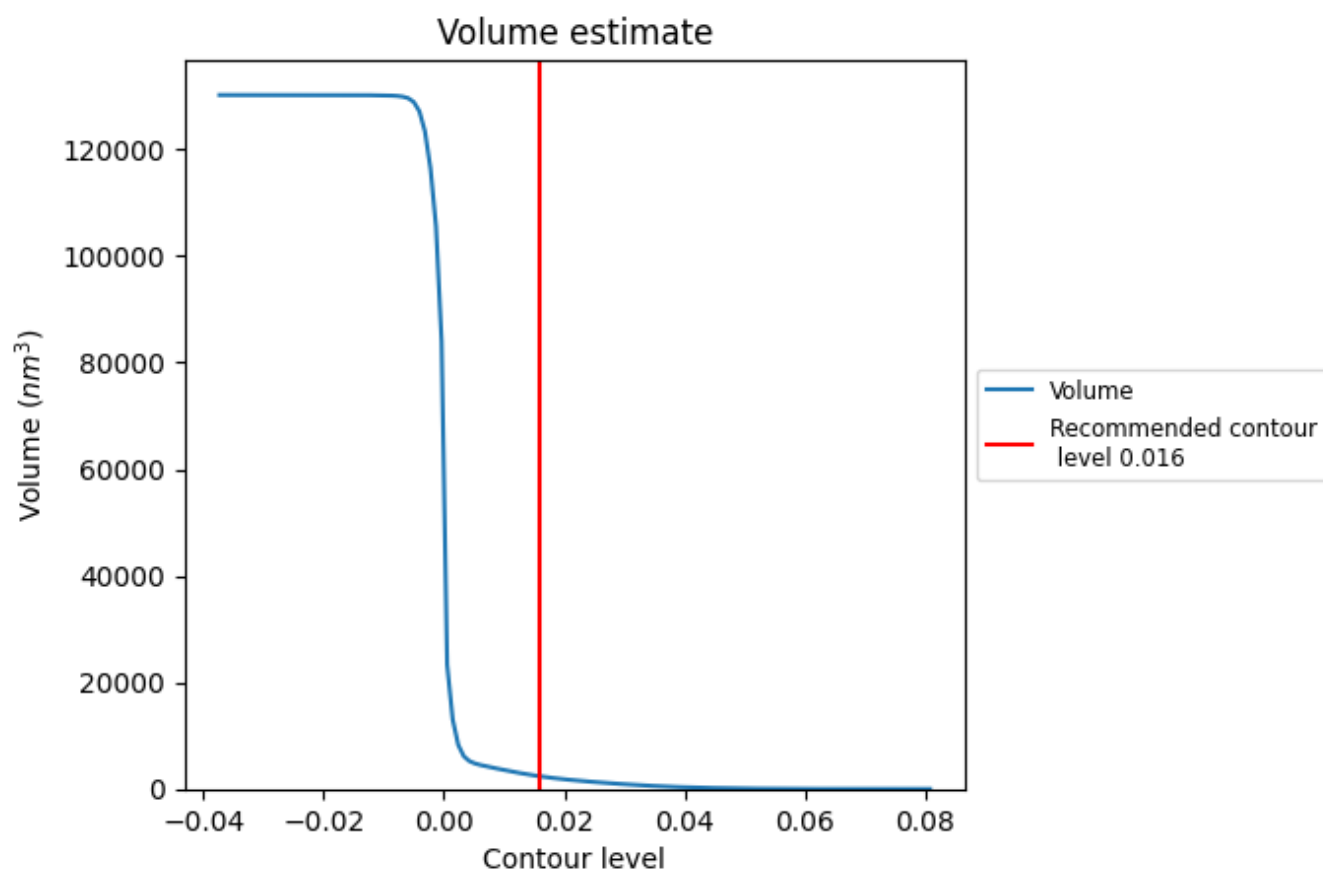
This section contains the results of statistical analysis of the map.

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.

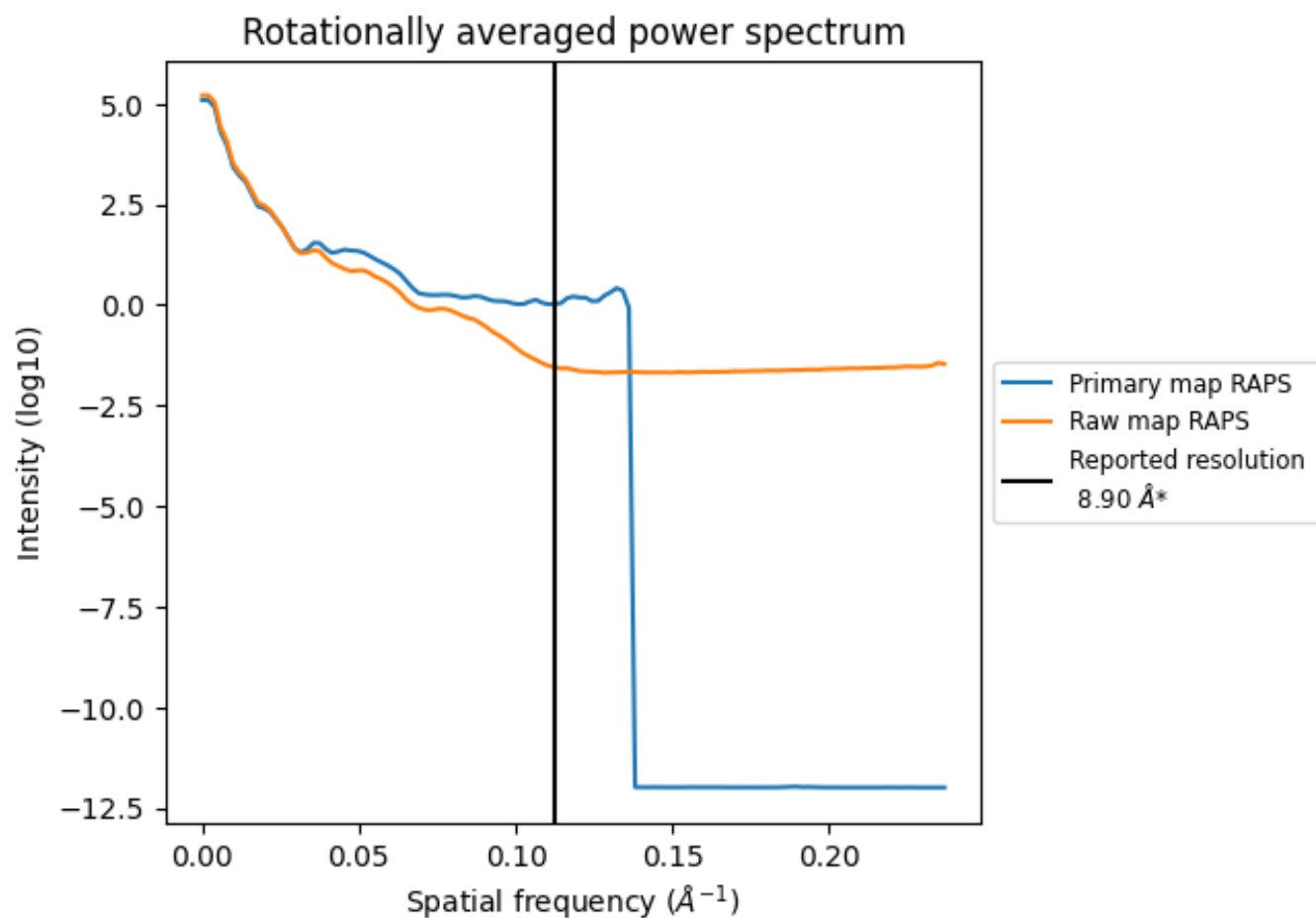
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2367 nm³; this corresponds to an approximate mass of 2138 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

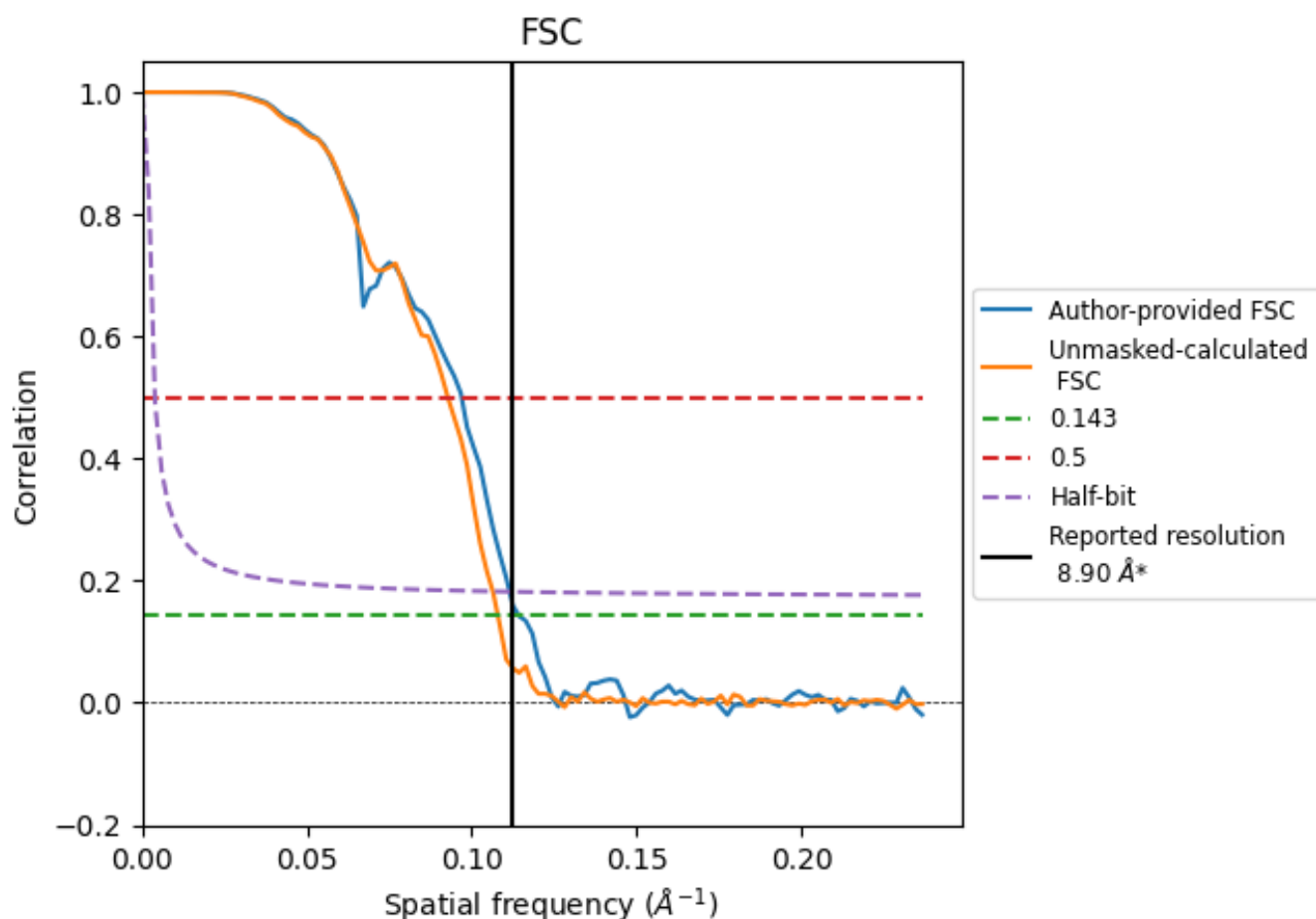


*Reported resolution corresponds to spatial frequency of $0.112 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.112 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

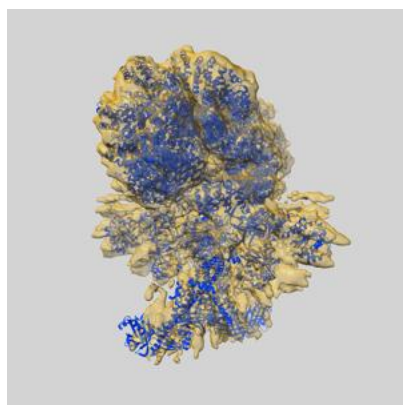
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.90	-	-
Author-provided FSC curve	8.75	10.32	8.97
Unmasked-calculated*	9.27	10.78	9.40

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

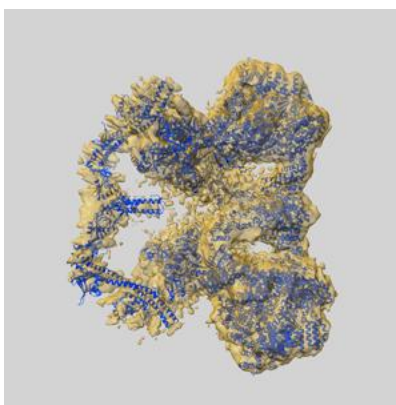
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28733 and PDB model 8EZB. Per-residue inclusion information can be found in section [3](#) on page [7](#).

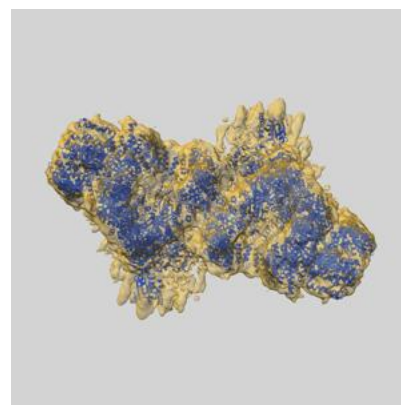
9.1 Map-model overlay [i](#)



X



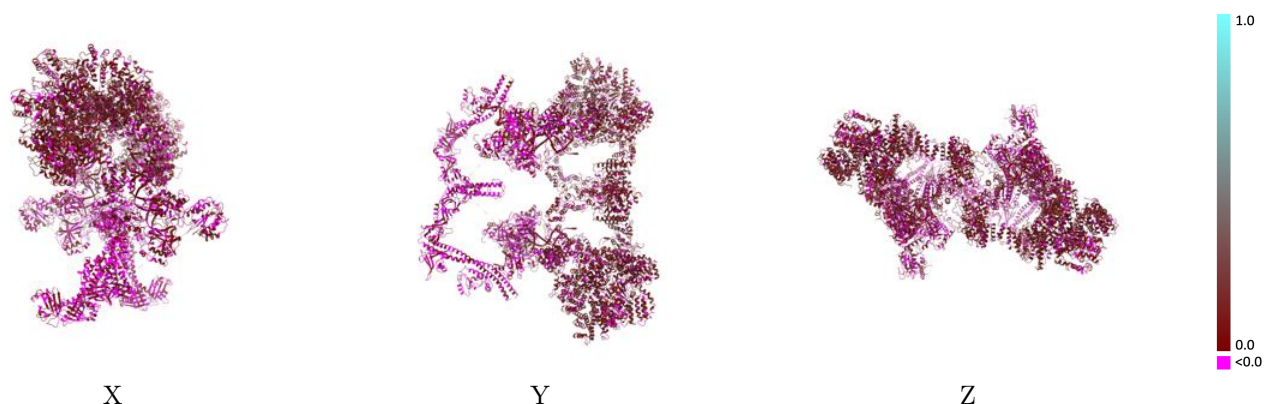
Y



Z

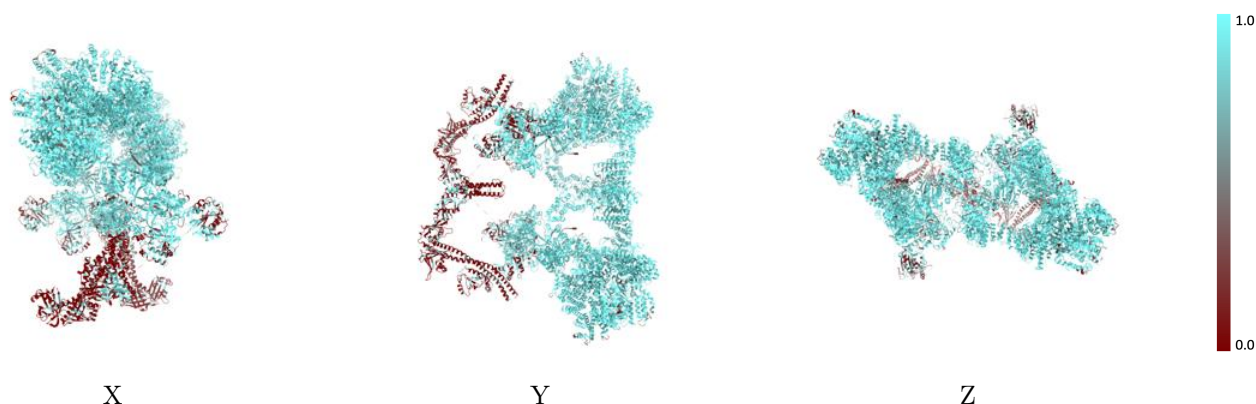
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



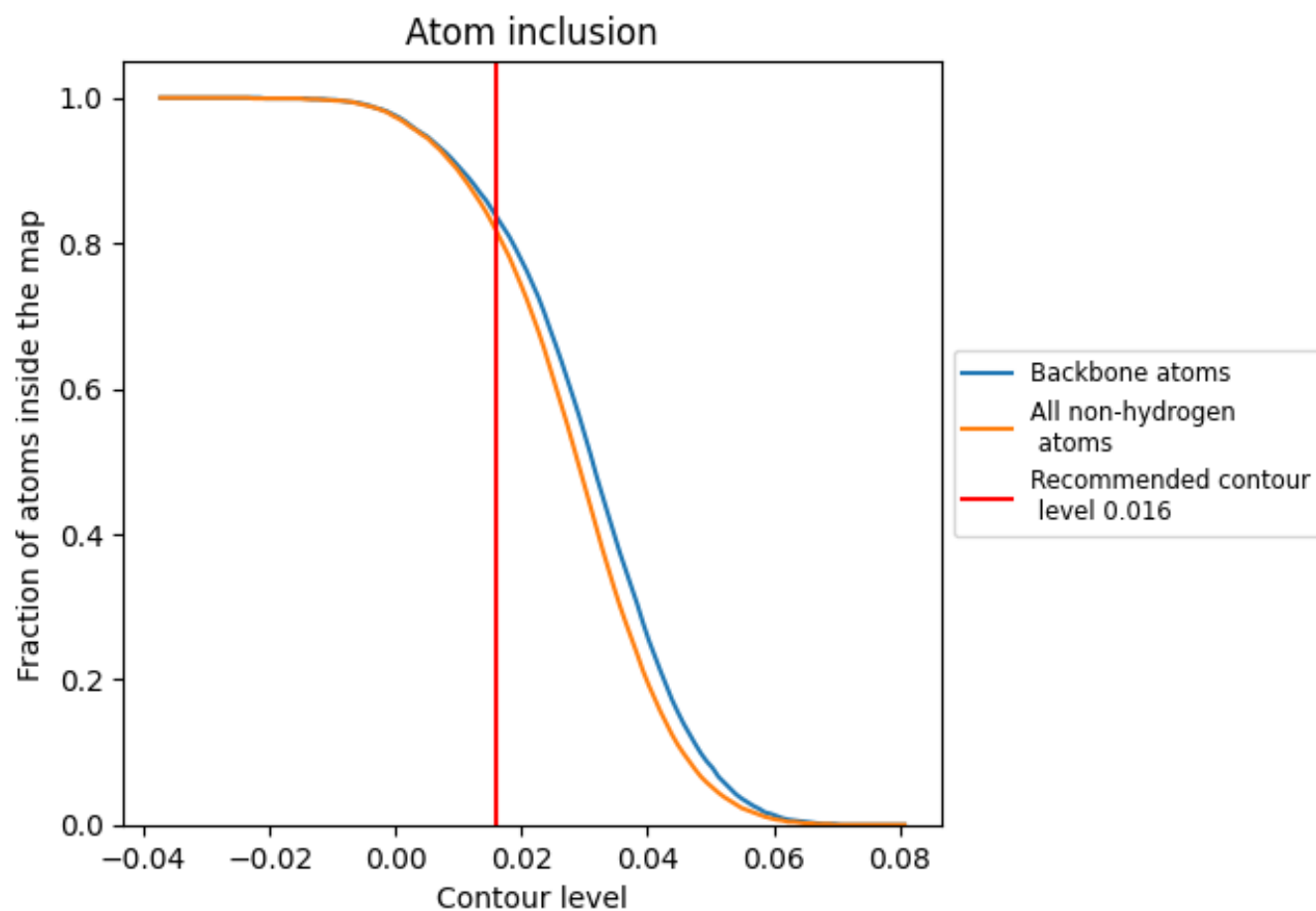
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 82% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8170	 0.0800
A	 0.8530	 0.0310
B	 0.6950	 0.0360
C	 0.9550	 0.1100
D	 0.8600	 0.0720
E	 0.9460	 0.0990
F	 0.1300	 0.0040
G	 0.1540	 0.0100
H	 0.3560	 0.0070
I	 0.2660	 -0.0090
J	 0.8520	 0.0300
K	 0.6950	 0.0350
L	 0.9550	 0.1100
M	 0.8600	 0.0680
N	 0.9460	 0.0980
O	 0.1490	 0.0070
P	 0.1700	 0.0110
S	 0.9340	 0.0300
T	 0.9340	 0.0220
X	 0.4000	 0.0220
Y	 0.4060	 0.0110

