



Full wwPDB EM Validation Report ⓘ

Jun 9, 2024 – 01:16 PM EDT

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

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

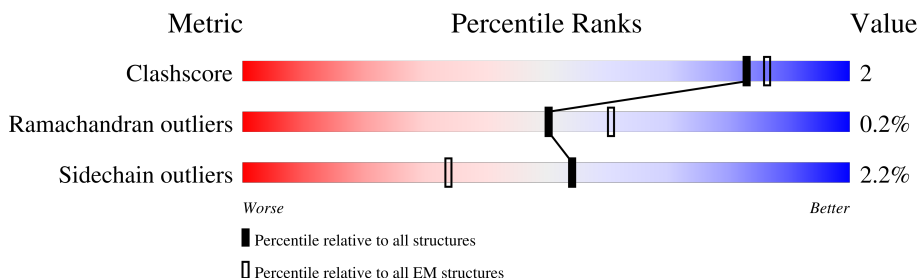
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.39 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	S	204	
1	T	204	
2	A	609	
2	J	609	
3	B	732	
3	K	732	
4	C	4128	
4	L	4128	

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Mol	Chain	Length	Quality of chain
5	Q	20	 90% 10%
5	R	20	 90% 10%
6	D	31	 48% 48% .
6	M	31	 45% 52% .
7	E	30	 13% 47% 33% 7%
7	N	30	 13% 47% 30% 10%
8	H	299	 16% 61% 11% . 25%
8	I	299	 13% 61% 10% .. 27%
9	F	336	 25% 54% 7% .. 37%
9	G	336	 37% 43% 14% . 42%
9	O	336	 24% 52% 9% .. 37%
9	P	336	 38% 41% 15% . 42%
10	X	911	 25% . 72%
10	Y	911	 25% . 72%

2 Entry composition

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

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

- Molecule 1 is a protein called Protein PAXX.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

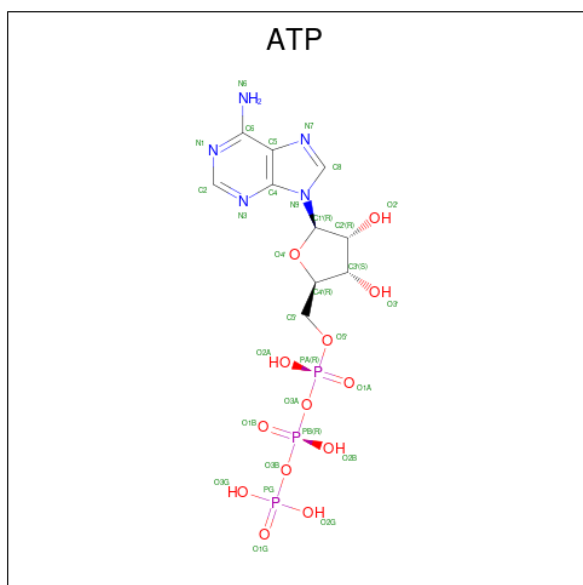
- Molecule 9 is a protein called DNA repair protein XRCC4.

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

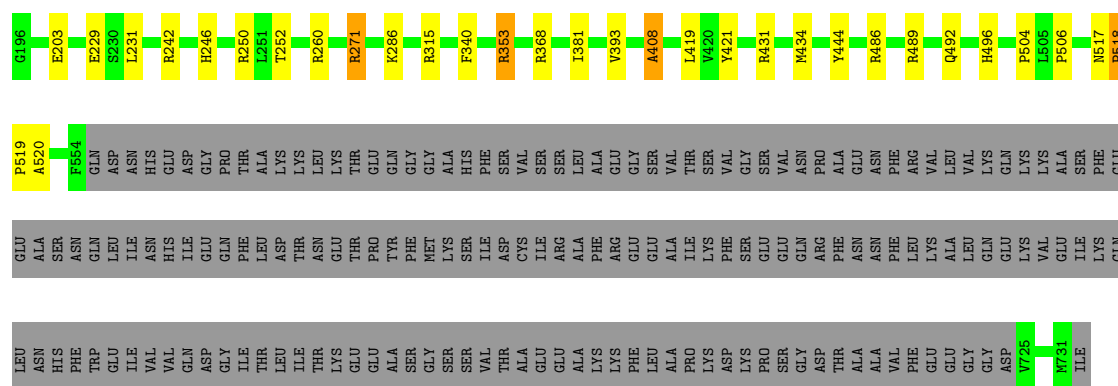
- Molecule 10 is a protein called DNA ligase 4.

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

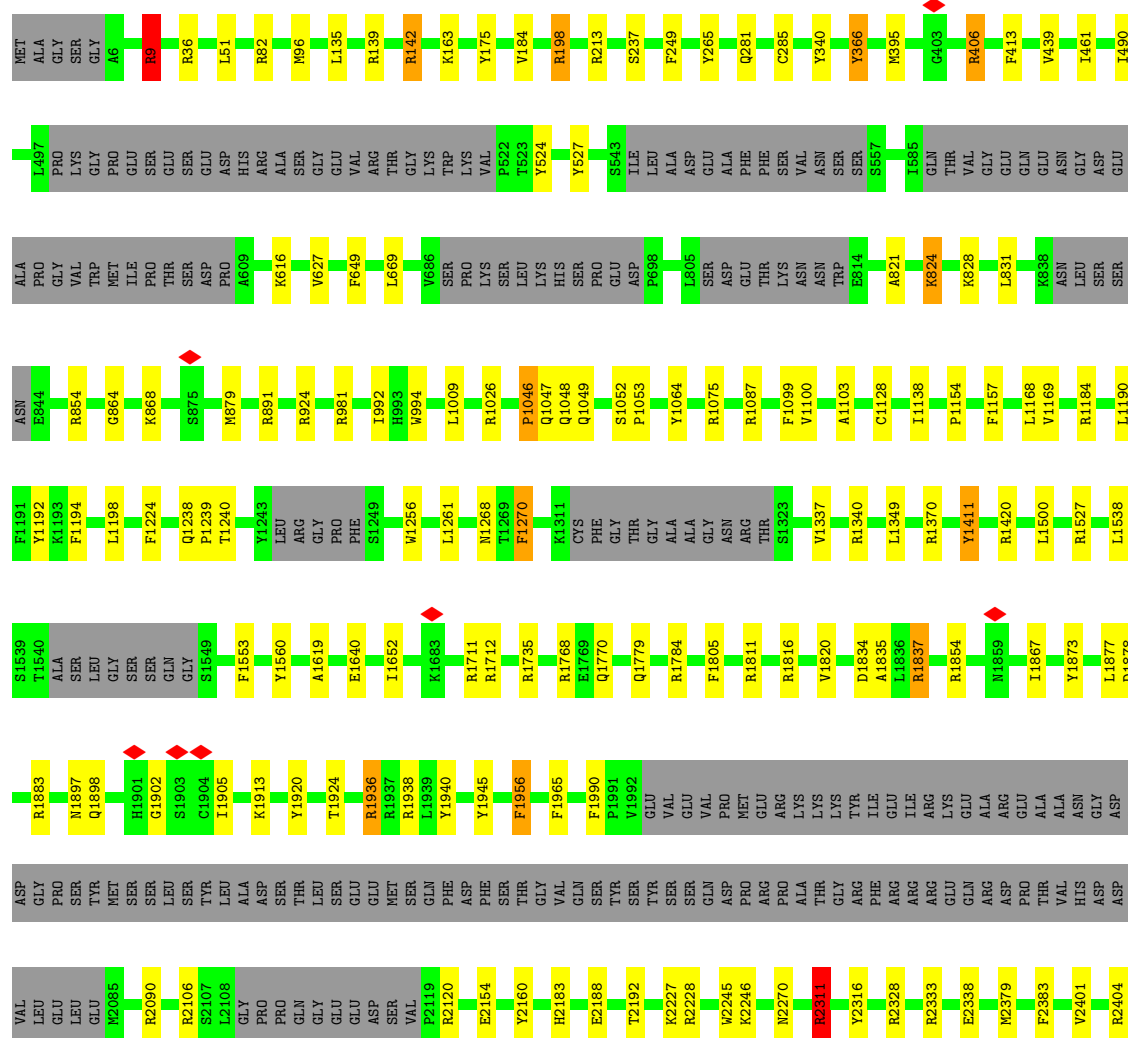
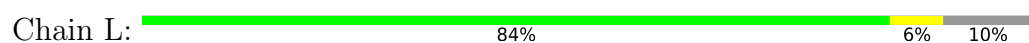
- Molecule 11 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

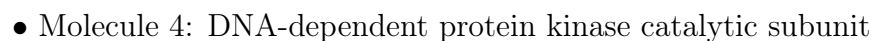


Mol	Chain	Residues	Atoms					AltConf
11	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
11	C	1	Total	C	N	O	P	0
			31	10	5	13	3	



● Molecule 4: DNA-dependent protein kinase catalytic subunit





Response	Percentage
Yes, the U.S. is a democracy	84%
No, the U.S. is not a democracy	6%
Don't know	10%





- Molecule 6: DNA (31-MER)

Chain M: 45% 52%



- Molecule 6: DNA (31-MER)

Chain D: 48% 48%



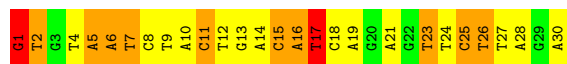
- Molecule 7: DNA (30-MER)

Chain N: 13% 47% 30% 10%



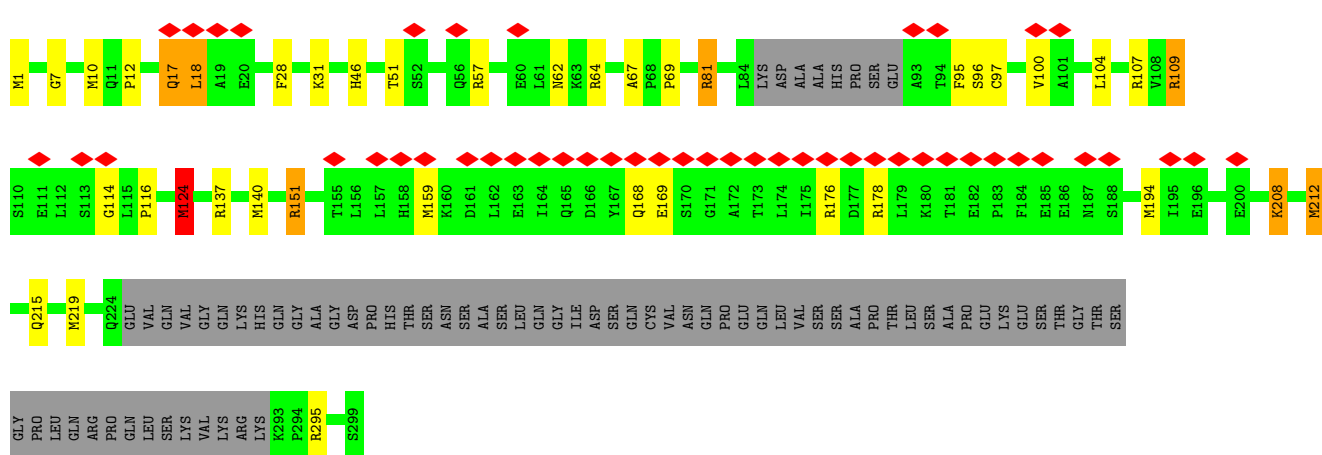
- Molecule 7: DNA (30-MER)

Chain E: 13% 47% 33% 7%



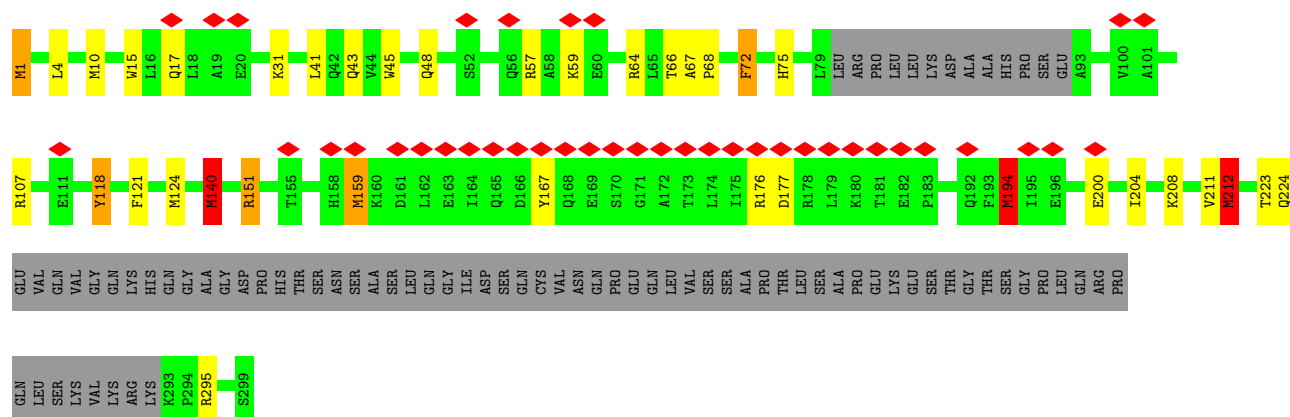
- Molecule 8: Non-homologous end-joining factor 1

Chain H: 16% 61% 11% 25%

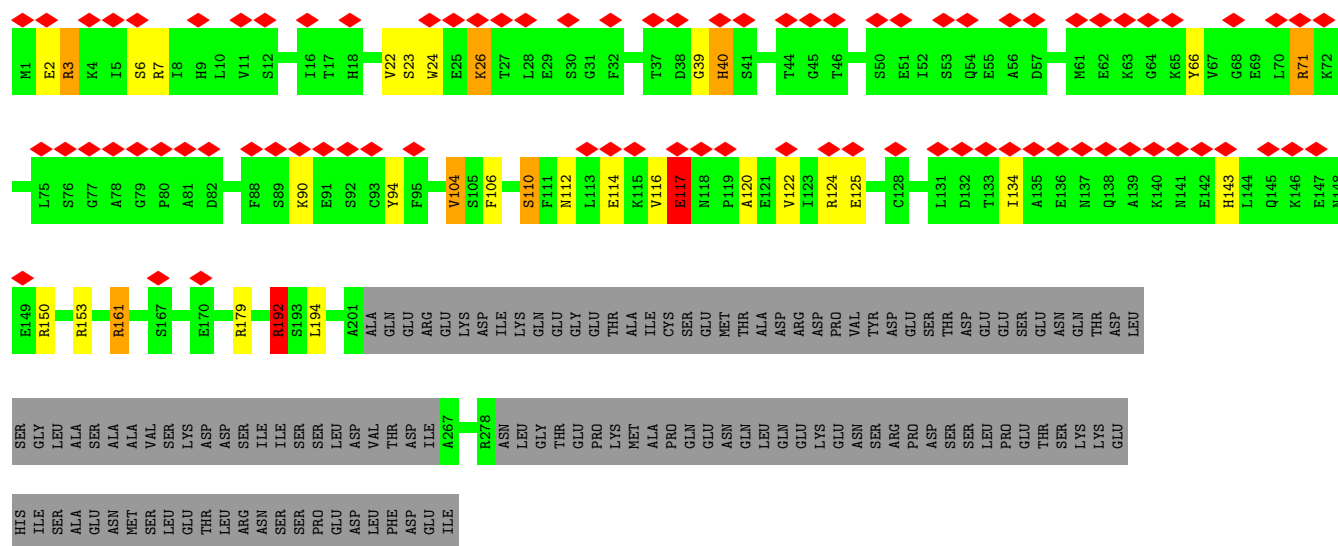


- Molecule 8: Non-homologous end-joining factor 1

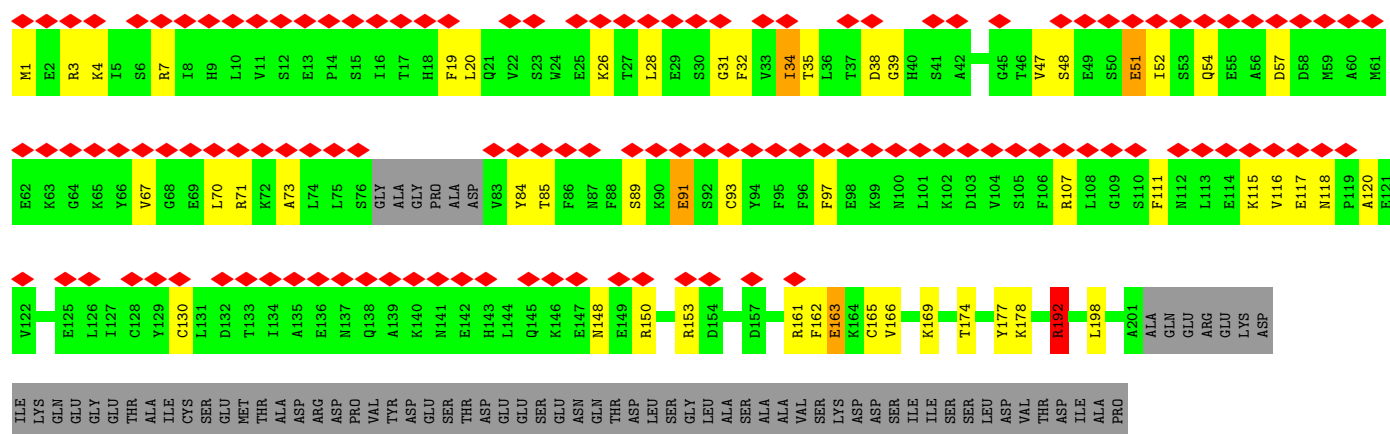
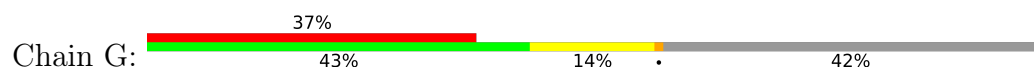
Chain I: 13% 61% 10% 27%



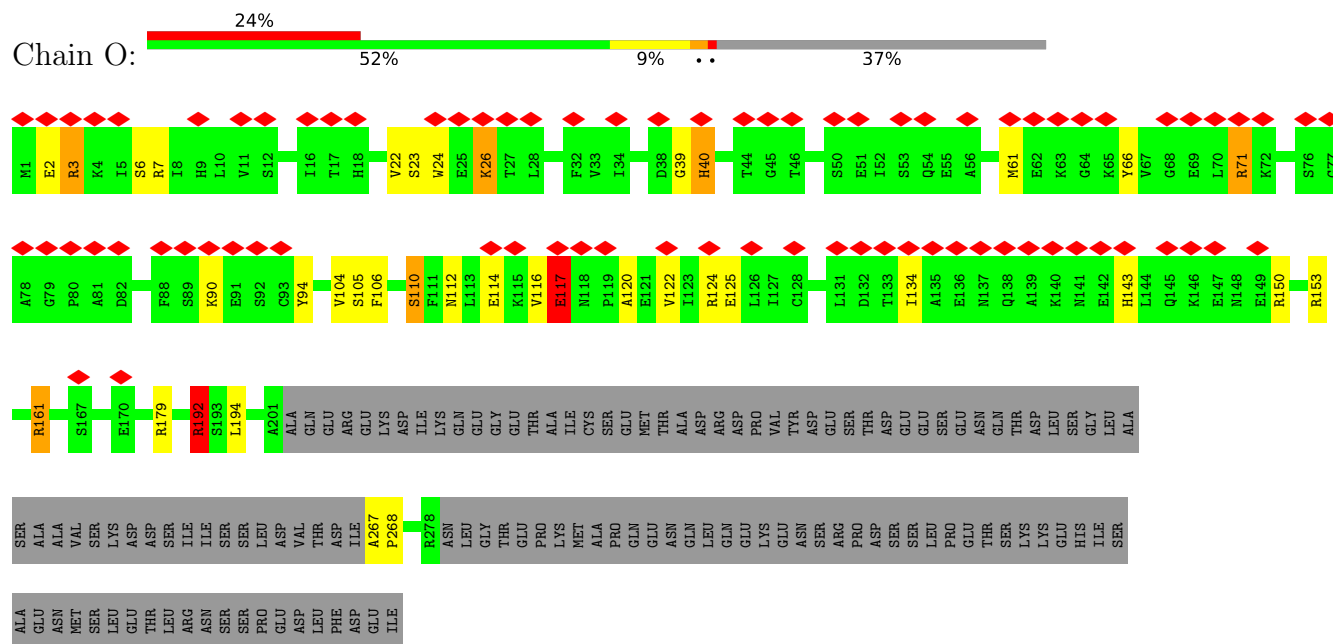
• Molecule 9: DNA repair protein XRCC4



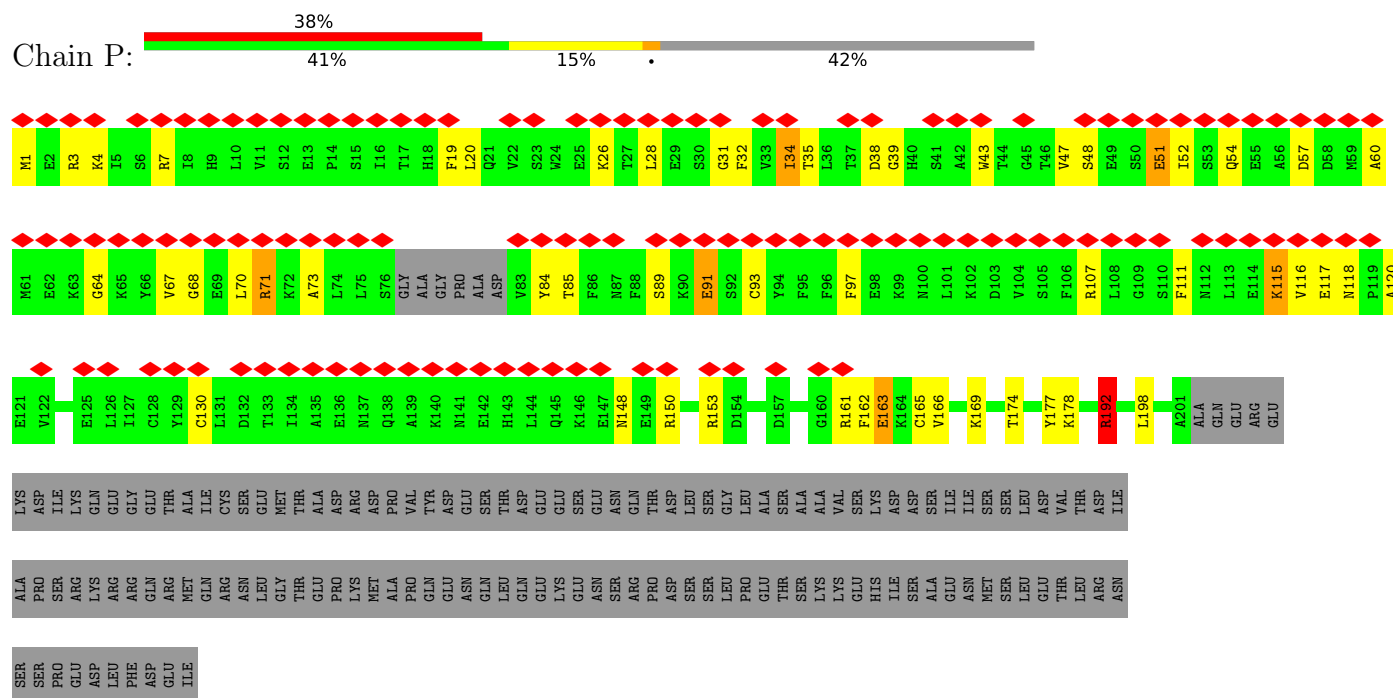
• Molecule 9: DNA repair protein XRCC4



- Molecule 9: DNA repair protein XRCC4



- Molecule 9: DNA repair protein XRCC4



- Molecule 10: DNA ligase 4





4 Experimental information

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	S	0.66	0/172	1.01	0/229
1	T	0.67	0/172	1.04	0/229
2	A	1.23	9/4101 (0.2%)	1.20	34/5523 (0.6%)
2	J	1.23	9/4101 (0.2%)	1.20	34/5523 (0.6%)
3	B	0.66	0/4340	1.08	17/5853 (0.3%)
3	K	0.66	0/4340	1.08	17/5853 (0.3%)
4	C	0.68	8/30414 (0.0%)	1.05	91/41079 (0.2%)
4	L	0.68	8/30414 (0.0%)	1.05	85/41079 (0.2%)
6	D	1.64	7/710 (1.0%)	2.57	73/1093 (6.7%)
6	M	1.64	6/710 (0.8%)	2.57	73/1093 (6.7%)
7	E	1.69	4/690 (0.6%)	2.32	53/1063 (5.0%)
7	N	1.68	4/690 (0.6%)	2.32	55/1063 (5.2%)
8	H	0.79	7/1814 (0.4%)	1.18	14/2454 (0.6%)
8	I	0.79	6/1771 (0.3%)	1.11	6/2395 (0.3%)
9	F	0.70	2/1765 (0.1%)	1.11	8/2367 (0.3%)
9	G	0.71	0/1622	1.17	10/2178 (0.5%)
9	O	0.70	2/1765 (0.1%)	1.11	8/2367 (0.3%)
9	P	0.72	0/1622	1.19	10/2178 (0.5%)
10	X	0.73	1/2112 (0.0%)	1.11	9/2851 (0.3%)
10	Y	0.73	1/2112 (0.0%)	1.11	9/2851 (0.3%)
All	All	0.79	74/95437 (0.1%)	1.15	606/129321 (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
2	A	0	3
2	J	0	3
3	B	0	5

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

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	334	THR	CB-CG2	39.55	2.82	1.52
2	J	334	THR	CB-CG2	39.51	2.82	1.52
2	J	334	THR	N-CA	30.85	2.08	1.46
2	A	334	THR	N-CA	30.84	2.08	1.46
2	J	333	GLU	CB-CG	28.12	2.05	1.52
2	A	333	GLU	CB-CG	28.11	2.05	1.52
4	C	9	ARG	CZ-NH1	-17.85	1.09	1.33
4	L	9	ARG	CZ-NH1	-17.84	1.09	1.33
2	J	334	THR	CB-OG1	17.35	1.77	1.43
2	A	334	THR	CB-OG1	17.24	1.77	1.43
2	J	333	GLU	CG-CD	14.19	1.73	1.51
2	A	333	GLU	CG-CD	14.18	1.73	1.51
2	A	333	GLU	CA-CB	13.22	1.83	1.53
2	J	333	GLU	CA-CB	13.20	1.82	1.53
2	J	333	GLU	N-CA	11.02	1.68	1.46
2	A	333	GLU	N-CA	10.98	1.68	1.46
2	A	333	GLU	C-N	9.77	1.56	1.34
2	J	333	GLU	C-N	9.74	1.56	1.34
2	J	333	GLU	CA-C	9.43	1.77	1.52
2	A	333	GLU	CA-C	9.40	1.77	1.52
4	L	2446	LEU	CG-CD1	-9.25	1.17	1.51
4	C	2446	LEU	CG-CD1	-9.25	1.17	1.51
4	C	2599	SER	CB-OG	-7.97	1.31	1.42
4	L	2599	SER	CB-OG	-7.92	1.31	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2446	LEU	CG-CD2	-7.47	1.24	1.51
4	L	2446	LEU	CG-CD2	-7.47	1.24	1.51
4	L	2513	GLU	CD-OE2	-6.86	1.18	1.25
4	C	2513	GLU	CD-OE1	-6.86	1.18	1.25
4	L	2513	GLU	CD-OE1	-6.86	1.18	1.25
4	C	2513	GLU	CD-OE2	-6.85	1.18	1.25
4	L	9	ARG	CZ-NH2	-6.75	1.24	1.33
4	C	9	ARG	CZ-NH2	-6.75	1.24	1.33
8	H	1	MET	CG-SD	6.58	1.98	1.81
9	F	117	GLU	CD-OE1	-6.42	1.18	1.25
9	O	117	GLU	CD-OE1	-6.41	1.18	1.25
8	H	140	MET	CG-SD	6.20	1.97	1.81
8	H	10	MET	CG-SD	6.18	1.97	1.81
8	I	1	MET	CG-SD	6.08	1.97	1.81
8	I	124	MET	CG-SD	6.00	1.96	1.81
8	I	140	MET	CG-SD	5.93	1.96	1.81
8	I	194	MET	CG-SD	5.86	1.96	1.81
8	H	212	MET	CG-SD	5.77	1.96	1.81
8	I	212	MET	CG-SD	5.63	1.95	1.81
8	H	124	MET	CG-SD	5.61	1.95	1.81
6	D	22	DA	C5-C4	-5.54	1.34	1.38
8	I	159	MET	CG-SD	5.45	1.95	1.81
7	E	16	DA	C5-C4	-5.45	1.34	1.38
7	N	16	DA	C5-C4	-5.42	1.34	1.38
8	H	194	MET	CG-SD	5.39	1.95	1.81
6	M	22	DA	C5-C4	-5.38	1.34	1.38
10	Y	790	GLU	CD-OE2	-5.38	1.19	1.25
7	E	5	DA	C5-C4	-5.35	1.35	1.38
10	X	790	GLU	CD-OE2	-5.35	1.19	1.25
7	N	5	DA	C5-C4	-5.34	1.35	1.38
8	H	159	MET	CG-SD	5.34	1.95	1.81
9	O	110	SER	CB-OG	-5.28	1.35	1.42
9	F	110	SER	CB-OG	-5.26	1.35	1.42
6	M	24	DA	C5-C4	-5.24	1.35	1.38
6	D	24	DA	C5-C4	-5.16	1.35	1.38
6	M	27	DA	C5-C4	-5.16	1.35	1.38
6	D	6	DG	C2-N2	-5.15	1.29	1.34
6	M	6	DG	C2-N2	-5.14	1.29	1.34
6	D	20	DG	C2-N2	-5.13	1.29	1.34
7	N	10	DA	C5-C4	-5.12	1.35	1.38
4	C	1835	ALA	CA-CB	-5.12	1.41	1.52
4	L	1835	ALA	CA-CB	-5.12	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	27	DA	C5-C4	-5.08	1.35	1.38
6	D	29	DA	C5-C4	-5.08	1.35	1.38
7	E	18	DC	C4-N4	-5.07	1.29	1.33
7	E	10	DA	C5-C4	-5.07	1.35	1.38
6	M	20	DG	C2-N2	-5.05	1.29	1.34
6	M	29	DA	C5-C4	-5.03	1.35	1.38
7	N	18	DC	C4-N4	-5.02	1.29	1.33
6	D	14	DA	C5-C4	-5.01	1.35	1.38

All (606) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	334	THR	N-CA-CB	-13.33	84.97	110.30
2	A	334	THR	N-CA-CB	-13.30	85.03	110.30
2	J	333	GLU	CA-CB-CG	-13.07	84.64	113.40
2	A	333	GLU	CA-CB-CG	-13.06	84.67	113.40
3	B	231	LEU	CB-CG-CD1	13.04	133.17	111.00
3	K	231	LEU	CB-CG-CD1	13.02	133.13	111.00
2	J	333	GLU	C-N-CA	-12.22	91.15	121.70
2	A	333	GLU	C-N-CA	-12.20	91.19	121.70
2	J	334	THR	CA-CB-OG1	-11.56	84.73	109.00
2	A	334	THR	CA-CB-OG1	-11.54	84.76	109.00
2	J	333	GLU	CB-CA-C	-11.51	87.38	110.40
2	A	333	GLU	CB-CA-C	-11.50	87.39	110.40
4	L	1936	ARG	NE-CZ-NH2	10.42	125.51	120.30
2	J	333	GLU	O-C-N	10.34	139.24	122.70
2	J	333	GLU	CG-CD-OE2	-10.31	97.69	118.30
2	A	333	GLU	CG-CD-OE2	-10.31	97.69	118.30
2	A	333	GLU	O-C-N	10.30	139.18	122.70
4	C	1936	ARG	NE-CZ-NH2	10.29	125.45	120.30
2	J	333	GLU	CG-CD-OE1	10.13	138.55	118.30
2	A	333	GLU	CG-CD-OE1	10.11	138.51	118.30
4	C	142	ARG	NE-CZ-NH2	9.99	125.30	120.30
4	L	142	ARG	NE-CZ-NH2	9.93	125.27	120.30
4	C	82	ARG	NE-CZ-NH2	9.77	125.18	120.30
4	L	82	ARG	NE-CZ-NH2	9.73	125.17	120.30
2	J	333	GLU	N-CA-CB	-9.55	93.41	110.60
2	J	258	ARG	NE-CZ-NH2	9.53	125.07	120.30
8	H	109	ARG	NE-CZ-NH2	9.54	125.07	120.30
2	A	333	GLU	N-CA-CB	-9.53	93.45	110.60
6	D	5	DA	N1-C6-N6	-9.50	112.90	118.60
8	I	176	ARG	NE-CZ-NH2	9.49	125.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	7	DA	C5-C6-N1	9.48	122.44	117.70
6	D	7	DA	C5-C6-N1	9.48	122.44	117.70
2	A	258	ARG	NE-CZ-NH2	9.40	125.00	120.30
6	M	5	DA	N1-C6-N6	-9.32	113.01	118.60
3	B	353	ARG	NE-CZ-NH2	9.27	124.94	120.30
3	K	353	ARG	NE-CZ-NH2	9.26	124.93	120.30
10	Y	814	ARG	NE-CZ-NH2	8.96	124.78	120.30
6	D	8	DA	N1-C6-N6	-8.96	113.22	118.60
6	M	8	DA	N1-C6-N6	-8.95	113.23	118.60
10	X	814	ARG	NE-CZ-NH2	8.92	124.76	120.30
6	M	29	DA	C5-C6-N1	8.75	122.08	117.70
6	D	19	DA	N1-C6-N6	-8.70	113.38	118.60
6	M	19	DA	N1-C6-N6	-8.63	113.42	118.60
6	D	29	DA	C5-C6-N1	8.63	122.01	117.70
8	I	57	ARG	NE-CZ-NH2	8.62	124.61	120.30
6	D	4	DA	C5-C6-N1	8.59	121.99	117.70
6	M	4	DA	C5-C6-N1	8.56	121.98	117.70
10	Y	871	ARG	NE-CZ-NH2	8.56	124.58	120.30
6	M	27	DA	C5-C6-N1	8.54	121.97	117.70
10	X	871	ARG	NE-CZ-NH2	8.51	124.56	120.30
6	D	27	DA	C5-C6-N1	8.51	121.95	117.70
6	D	18	DC	N3-C2-O2	-8.51	115.94	121.90
3	B	381	ILE	CA-CB-CG1	8.44	127.04	111.00
7	E	5	DA	C5-C6-N1	8.43	121.92	117.70
3	K	381	ILE	CA-CB-CG1	8.40	126.97	111.00
7	N	10	DA	O4'-C4'-C3'	-8.38	100.97	106.00
6	M	18	DC	N3-C2-O2	-8.37	116.05	121.90
6	D	7	DA	N1-C6-N6	-8.36	113.58	118.60
9	F	3	ARG	NE-CZ-NH2	8.35	124.47	120.30
9	O	3	ARG	NE-CZ-NH2	8.32	124.46	120.30
7	E	10	DA	O4'-C4'-C3'	-8.29	101.03	106.00
7	N	5	DA	C5-C6-N1	8.21	121.81	117.70
7	E	14	DA	N1-C6-N6	-8.21	113.67	118.60
7	N	14	DA	N1-C6-N6	-8.19	113.68	118.60
7	N	15	DC	N3-C2-O2	-8.20	116.16	121.90
10	X	879	ARG	NE-CZ-NH2	8.19	124.39	120.30
7	E	15	DC	N3-C2-O2	-8.18	116.17	121.90
6	M	7	DA	N1-C6-N6	-8.18	113.69	118.60
8	H	57	ARG	NE-CZ-NH2	8.17	124.39	120.30
9	F	150	ARG	NE-CZ-NH2	8.13	124.36	120.30
8	H	151	ARG	NE-CZ-NH2	8.13	124.36	120.30
6	D	30	DC	O4'-C1'-N1	8.13	113.69	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	O	150	ARG	NE-CZ-NH2	8.11	124.36	120.30
6	M	30	DC	O4'-C1'-N1	8.11	113.68	108.00
9	P	7	ARG	NE-CZ-NH2	8.10	124.35	120.30
9	G	7	ARG	NE-CZ-NH2	8.10	124.35	120.30
6	M	8	DA	C4-C5-C6	-8.07	112.96	117.00
10	Y	879	ARG	NE-CZ-NH2	8.07	124.34	120.30
4	L	4049	ARG	NE-CZ-NH2	8.05	124.32	120.30
6	D	14	DA	C5-C6-N1	8.04	121.72	117.70
6	M	22	DA	C5-C6-N1	8.01	121.70	117.70
6	D	8	DA	C4-C5-C6	-7.99	113.01	117.00
6	D	14	DA	N1-C6-N6	-7.96	113.83	118.60
6	M	14	DA	C5-C6-N1	7.95	121.67	117.70
6	D	24	DA	C5-C6-N1	7.95	121.67	117.70
7	N	19	DA	C5-C6-N1	7.92	121.66	117.70
4	C	3125	ARG	NE-CZ-NH2	7.91	124.26	120.30
6	M	24	DA	C5-C6-N1	7.90	121.65	117.70
6	M	14	DA	N1-C6-N6	-7.89	113.87	118.60
4	C	4049	ARG	NE-CZ-NH2	7.88	124.24	120.30
4	L	3125	ARG	NE-CZ-NH2	7.85	124.23	120.30
6	D	22	DA	C5-C6-N1	7.80	121.60	117.70
7	E	19	DA	C5-C6-N1	7.77	121.59	117.70
7	N	16	DA	C4-C5-C6	-7.73	113.14	117.00
2	A	165	ARG	NE-CZ-NH2	7.71	124.16	120.30
6	M	8	DA	C5-C6-N1	7.70	121.55	117.70
7	N	30	DA	N1-C6-N6	-7.69	113.99	118.60
9	G	153	ARG	NE-CZ-NH2	7.66	124.13	120.30
7	E	30	DA	N1-C6-N6	-7.66	114.01	118.60
7	E	16	DA	C4-C5-C6	-7.65	113.18	117.00
8	H	178	ARG	NE-CZ-NH2	7.64	124.12	120.30
9	P	153	ARG	NE-CZ-NH2	7.64	124.12	120.30
4	C	3763	ARG	NE-CZ-NH2	7.63	124.12	120.30
8	I	64	ARG	NE-CZ-NH2	7.63	124.11	120.30
2	J	165	ARG	NE-CZ-NH2	7.63	124.11	120.30
9	O	161	ARG	NE-CZ-NH2	7.62	124.11	120.30
6	D	8	DA	C5-C6-N1	7.59	121.49	117.70
4	L	213	ARG	NE-CZ-NH2	7.59	124.09	120.30
6	D	24	DA	C4-C5-C6	-7.58	113.21	117.00
6	M	24	DA	C4-C5-C6	-7.58	113.21	117.00
7	E	30	DA	C5-C6-N1	7.58	121.49	117.70
7	N	30	DA	C5-C6-N1	7.57	121.49	117.70
9	F	161	ARG	NE-CZ-NH2	7.56	124.08	120.30
7	N	28	DA	C5-C6-N1	7.55	121.47	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	3763	ARG	NE-CZ-NH2	7.54	124.07	120.30
6	M	29	DA	C4-C5-C6	-7.53	113.23	117.00
6	D	19	DA	C5-C6-N1	7.52	121.46	117.70
7	E	28	DA	C5-C6-N1	7.52	121.46	117.70
4	L	198	ARG	NE-CZ-NH2	7.50	124.05	120.30
6	D	4	DA	N1-C6-N6	-7.49	114.10	118.60
6	M	19	DA	C5-C6-N1	7.49	121.44	117.70
6	D	19	DA	C4-C5-C6	-7.47	113.26	117.00
6	M	19	DA	C4-C5-C6	-7.47	113.27	117.00
8	I	151	ARG	NE-CZ-NH2	7.47	124.03	120.30
4	C	213	ARG	NE-CZ-NH2	7.46	124.03	120.30
6	M	4	DA	N1-C6-N6	-7.45	114.13	118.60
6	M	31	DT	C6-C5-C7	-7.45	118.43	122.90
6	M	27	DA	C4-C5-C6	-7.45	113.28	117.00
6	M	1	DT	N3-C2-O2	-7.45	117.83	122.30
4	C	3186	ARG	NE-CZ-NH2	7.44	124.02	120.30
6	D	31	DT	C6-C5-C7	-7.44	118.44	122.90
7	E	14	DA	C4-C5-C6	-7.43	113.28	117.00
4	L	3462	ARG	NE-CZ-NH2	7.42	124.01	120.30
6	D	29	DA	C4-C5-C6	-7.40	113.30	117.00
6	D	5	DA	C5-C6-N1	7.40	121.40	117.70
7	N	18	DC	N3-C4-C5	7.38	124.85	121.90
8	H	18	LEU	CD1-CG-CD2	7.38	132.64	110.50
7	N	14	DA	C4-C5-C6	-7.37	113.31	117.00
4	C	3462	ARG	NE-CZ-NH2	7.36	123.98	120.30
6	D	1	DT	N3-C2-O2	-7.34	117.90	122.30
6	M	9	DC	N3-C2-O2	-7.33	116.77	121.90
6	D	29	DA	O4'-C1'-N9	7.32	113.12	108.00
6	D	27	DA	C4-C5-C6	-7.31	113.34	117.00
2	A	339	ARG	NE-CZ-NH2	7.29	123.94	120.30
4	L	3247	ARG	NE-CZ-NH2	7.29	123.94	120.30
7	E	18	DC	N3-C4-C5	7.28	124.81	121.90
4	C	198	ARG	NE-CZ-NH2	7.28	123.94	120.30
7	N	16	DA	C5-C6-N1	7.27	121.33	117.70
4	L	3186	ARG	NE-CZ-NH2	7.26	123.93	120.30
7	N	10	DA	C4-C5-C6	-7.25	113.38	117.00
9	F	179	ARG	NE-CZ-NH2	7.25	123.92	120.30
9	O	179	ARG	NE-CZ-NH2	7.24	123.92	120.30
6	D	9	DC	N3-C2-O2	-7.23	116.84	121.90
7	N	10	DA	N1-C6-N6	-7.21	114.27	118.60
6	M	7	DA	C4-C5-C6	-7.21	113.39	117.00
2	J	517	ARG	NE-CZ-NH2	7.20	123.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	29	DA	O4'-C1'-N9	7.19	113.04	108.00
10	X	846	ARG	NE-CZ-NH2	7.19	123.90	120.30
6	M	14	DA	C4-C5-C6	-7.19	113.41	117.00
4	C	1735	ARG	NE-CZ-NH2	7.18	123.89	120.30
4	L	1735	ARG	NE-CZ-NH2	7.18	123.89	120.30
7	E	10	DA	C4-C5-C6	-7.18	113.41	117.00
4	L	3962	ARG	NE-CZ-NH2	7.17	123.89	120.30
6	D	28	DC	N3-C2-O2	-7.17	116.88	121.90
2	J	339	ARG	NE-CZ-NH2	7.16	123.88	120.30
2	A	333	GLU	CA-C-N	-7.16	101.44	117.20
6	M	5	DA	C5-C6-N1	7.16	121.28	117.70
7	E	16	DA	C5-C6-N1	7.16	121.28	117.70
2	J	333	GLU	CA-C-N	-7.16	101.46	117.20
6	D	7	DA	C4-C5-C6	-7.11	113.44	117.00
10	Y	846	ARG	NE-CZ-NH2	7.10	123.85	120.30
4	C	3247	ARG	NE-CZ-NH2	7.08	123.84	120.30
6	M	9	DC	O4'-C4'-C3'	7.07	110.24	106.00
4	C	3962	ARG	NE-CZ-NH2	7.07	123.83	120.30
3	K	151	ILE	CA-CB-CG1	7.06	124.42	111.00
3	B	151	ILE	CA-CB-CG1	7.06	124.41	111.00
6	M	28	DC	N3-C2-O2	-7.06	116.96	121.90
6	D	14	DA	C4-C5-C6	-7.03	113.49	117.00
7	E	10	DA	N1-C6-N6	-7.02	114.39	118.60
4	C	3696	ARG	NE-CZ-NH2	7.01	123.81	120.30
4	L	891	ARG	NE-CZ-NH2	7.01	123.80	120.30
4	L	1340	ARG	NE-CZ-NH2	6.99	123.79	120.30
4	L	854	ARG	NE-CZ-NH2	6.98	123.79	120.30
4	L	3696	ARG	NE-CZ-NH2	6.98	123.79	120.30
4	C	2922	ARG	NE-CZ-NH2	6.97	123.78	120.30
2	A	517	ARG	NE-CZ-NH2	6.96	123.78	120.30
6	D	9	DC	O4'-C4'-C3'	6.95	110.17	106.00
6	D	31	DT	N3-C2-O2	-6.94	118.13	122.30
7	E	21	DA	C5-C6-N1	6.94	121.17	117.70
6	M	22	DA	C4-C5-C6	-6.94	113.53	117.00
4	C	1340	ARG	NE-CZ-NH2	6.92	123.76	120.30
4	C	1711	ARG	NE-CZ-NH2	6.92	123.76	120.30
4	C	1883	ARG	NE-CZ-NH2	6.92	123.76	120.30
7	N	21	DA	C5-C6-N1	6.91	121.16	117.70
4	L	1883	ARG	NE-CZ-NH2	6.91	123.75	120.30
2	J	187	ARG	NE-CZ-NH2	6.90	123.75	120.30
4	C	854	ARG	NE-CZ-NH2	6.90	123.75	120.30
4	C	891	ARG	NE-CZ-NH2	6.89	123.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	31	DT	N3-C2-O2	-6.88	118.17	122.30
4	L	2404	ARG	NE-CZ-NH2	6.83	123.72	120.30
6	D	22	DA	C4-C5-C6	-6.82	113.59	117.00
4	C	1046	PRO	CA-N-CD	-6.82	101.96	111.50
6	D	6	DG	O4'-C1'-N9	6.82	112.77	108.00
4	C	2404	ARG	NE-CZ-NH2	6.81	123.70	120.30
6	M	6	DG	O4'-C1'-N9	6.80	112.76	108.00
6	D	4	DA	C4-C5-C6	-6.79	113.61	117.00
4	L	1046	PRO	CA-N-CD	-6.79	102.00	111.50
2	A	218	ARG	NE-CZ-NH2	6.78	123.69	120.30
2	A	187	ARG	NE-CZ-NH2	6.77	123.69	120.30
8	H	176	ARG	NE-CZ-NH2	6.77	123.69	120.30
4	C	924	ARG	NE-CZ-NH2	6.76	123.68	120.30
4	L	2922	ARG	NE-CZ-NH2	6.76	123.68	120.30
2	J	218	ARG	NE-CZ-NH2	6.76	123.68	120.30
4	L	1711	ARG	NE-CZ-NH2	6.76	123.68	120.30
6	M	4	DA	C4-C5-C6	-6.75	113.63	117.00
2	J	290	ARG	NE-CZ-NH2	6.74	123.67	120.30
4	L	2446	LEU	CB-CG-CD1	6.74	122.46	111.00
9	O	192	ARG	NE-CZ-NH2	6.74	123.67	120.30
4	C	2446	LEU	CB-CG-CD1	6.73	122.44	111.00
4	C	3985	VAL	N-CA-CB	6.72	126.29	111.50
2	A	290	ARG	NE-CZ-NH2	6.72	123.66	120.30
7	E	28	DA	C4-C5-C6	-6.71	113.64	117.00
4	L	3985	VAL	N-CA-CB	6.71	126.27	111.50
4	L	924	ARG	NE-CZ-NH2	6.70	123.65	120.30
7	E	17	DT	C5-C6-N1	-6.69	119.69	123.70
9	F	192	ARG	NE-CZ-NH2	6.69	123.64	120.30
7	N	17	DT	C5-C6-N1	-6.66	119.70	123.70
4	C	1075	ARG	NE-CZ-NH2	6.62	123.61	120.30
4	C	1816	ARG	NE-CZ-NH2	6.62	123.61	120.30
4	L	1816	ARG	NE-CZ-NH2	6.62	123.61	120.30
7	N	10	DA	C5-C6-N1	6.61	121.00	117.70
7	N	28	DA	C4-C5-C6	-6.60	113.70	117.00
7	E	21	DA	N1-C6-N6	-6.59	114.64	118.60
7	N	21	DA	C4-C5-C6	-6.59	113.70	117.00
6	D	1	DT	O4'-C1'-N1	6.55	112.59	108.00
4	L	1075	ARG	NE-CZ-NH2	6.55	123.57	120.30
7	N	19	DA	C4-C5-C6	-6.50	113.75	117.00
7	N	21	DA	N1-C6-N6	-6.50	114.70	118.60
2	J	333	GLU	CB-CG-CD	-6.49	96.67	114.20
4	C	981	ARG	NE-CZ-NH2	6.49	123.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	137	HIS	CA-CB-CG	-6.49	102.56	113.60
2	A	333	GLU	CB-CG-CD	-6.48	96.69	114.20
7	E	10	DA	C5-C6-N1	6.48	120.94	117.70
4	C	1064	TYR	CB-CG-CD2	-6.48	117.11	121.00
4	C	2228	ARG	NE-CZ-NH2	6.48	123.54	120.30
2	A	137	HIS	CA-CB-CG	-6.47	102.59	113.60
10	X	758	TYR	CB-CG-CD2	-6.47	117.12	121.00
4	L	1064	TYR	CB-CG-CD2	-6.47	117.12	121.00
6	D	6	DG	N3-C2-N2	-6.46	115.38	119.90
10	Y	758	TYR	CB-CG-CD2	-6.46	117.13	121.00
7	E	21	DA	C4-C5-C6	-6.45	113.78	117.00
7	E	19	DA	C4-C5-C6	-6.44	113.78	117.00
6	M	1	DT	O4'-C1'-N1	6.43	112.50	108.00
2	A	444	ARG	NE-CZ-NH2	6.42	123.51	120.30
6	D	5	DA	C4-C5-C6	-6.41	113.79	117.00
2	J	444	ARG	NE-CZ-NH2	6.39	123.49	120.30
4	L	2228	ARG	NE-CZ-NH2	6.38	123.49	120.30
7	N	25	DC	N3-C4-C5	6.38	124.45	121.90
6	M	18	DC	N1-C2-O2	6.38	122.72	118.90
10	X	802	ARG	NE-CZ-NH2	6.38	123.49	120.30
7	E	6	DA	C4-C5-C6	-6.37	113.81	117.00
6	D	18	DC	N1-C2-O2	6.37	122.72	118.90
4	L	3442	TYR	CB-CG-CD2	-6.36	117.18	121.00
4	C	3442	TYR	CB-CG-CD2	-6.35	117.19	121.00
7	E	4	DT	C6-C5-C7	-6.35	119.09	122.90
10	Y	802	ARG	NE-CZ-NH2	6.35	123.47	120.30
7	N	4	DT	C6-C5-C7	-6.34	119.09	122.90
8	H	137	ARG	NE-CZ-NH2	6.34	123.47	120.30
9	F	71	ARG	NE-CZ-NH2	6.34	123.47	120.30
4	L	981	ARG	NE-CZ-NH2	6.33	123.47	120.30
4	L	1837	ARG	NE-CZ-NH2	6.33	123.46	120.30
4	C	1784	ARG	NE-CZ-NH2	6.33	123.46	120.30
9	O	71	ARG	NE-CZ-NH2	6.32	123.46	120.30
4	L	3981	TYR	CB-CG-CD1	-6.31	117.21	121.00
4	L	1075	ARG	NE-CZ-NH1	6.31	123.45	120.30
7	N	6	DA	C4-C5-C6	-6.30	113.85	117.00
7	E	6	DA	C5-N7-C8	-6.28	100.76	103.90
4	L	1784	ARG	NE-CZ-NH2	6.26	123.43	120.30
9	P	148	ASN	CB-CA-C	6.25	122.90	110.40
9	G	148	ASN	CB-CA-C	6.24	122.88	110.40
6	M	6	DG	N3-C2-N2	-6.23	115.54	119.90
4	C	1837	ARG	NE-CZ-NH2	6.23	123.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	24	DA	N1-C6-N6	-6.23	114.86	118.60
6	M	3	DT	C6-C5-C7	-6.23	119.16	122.90
6	D	24	DA	N1-C6-N6	-6.21	114.87	118.60
7	N	25	DC	C2-N3-C4	-6.21	116.79	119.90
4	C	3981	TYR	CB-CG-CD1	-6.19	117.29	121.00
6	D	2	DC	N3-C2-O2	-6.18	117.57	121.90
7	E	5	DA	C4-C5-C6	-6.16	113.92	117.00
8	H	109	ARG	NE-CZ-NH1	-6.14	117.23	120.30
4	C	3784	ARG	NE-CZ-NH2	6.14	123.37	120.30
6	D	3	DT	C6-C5-C7	-6.14	119.22	122.90
7	N	6	DA	C5-N7-C8	-6.14	100.83	103.90
7	N	23	DT	C6-C5-C7	-6.14	119.22	122.90
4	L	3467	ARG	NE-CZ-NH2	6.13	123.37	120.30
7	E	25	DC	N3-C4-C5	6.13	124.35	121.90
7	N	8	DC	N3-C4-C5	6.13	124.35	121.90
4	C	1411	TYR	CB-CG-CD2	-6.13	117.32	121.00
3	K	431	ARG	NE-CZ-NH2	6.13	123.36	120.30
4	C	1075	ARG	NE-CZ-NH1	6.12	123.36	120.30
7	E	8	DC	N3-C4-C5	6.12	124.35	121.90
6	M	5	DA	C4-C5-C6	-6.11	113.95	117.00
6	M	30	DC	N3-C4-C5	6.10	124.34	121.90
4	C	3467	ARG	NE-CZ-NH2	6.10	123.35	120.30
7	N	5	DA	C4-C5-C6	-6.09	113.95	117.00
6	D	25	DT	N3-C2-O2	-6.09	118.65	122.30
3	B	431	ARG	NE-CZ-NH2	6.08	123.34	120.30
7	E	18	DC	N3-C4-N4	-6.08	113.75	118.00
6	M	2	DC	N3-C2-O2	-6.06	117.66	121.90
7	N	18	DC	N3-C4-N4	-6.05	113.76	118.00
7	E	14	DA	C5-C6-N1	6.05	120.73	117.70
4	L	3784	ARG	NE-CZ-NH2	6.05	123.33	120.30
4	L	1411	TYR	CB-CG-CD2	-6.03	117.38	121.00
7	N	14	DA	C5-C6-N1	6.03	120.71	117.70
6	M	25	DT	N3-C2-O2	-6.02	118.69	122.30
7	E	25	DC	C2-N3-C4	-6.02	116.89	119.90
7	E	30	DA	C4-C5-C6	-6.00	114.00	117.00
6	D	27	DA	N1-C6-N6	-6.00	115.00	118.60
6	M	27	DA	N1-C6-N6	-6.00	115.00	118.60
6	D	30	DC	N3-C4-C5	5.99	124.30	121.90
6	M	30	DC	C1'-O4'-C4'	-5.98	104.12	110.10
6	D	30	DC	C1'-O4'-C4'	-5.97	104.13	110.10
7	E	23	DT	C6-C5-C7	-5.97	119.32	122.90
7	N	30	DA	C4-C5-C6	-5.96	114.02	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3715	TYR	CB-CG-CD2	-5.95	117.43	121.00
6	M	20	DG	O4'-C4'-C3'	5.95	109.57	106.00
4	L	3715	TYR	CB-CG-CD2	-5.95	117.43	121.00
6	D	1	DT	C6-C5-C7	-5.94	119.33	122.90
4	L	36	ARG	NE-CZ-NH2	5.94	123.27	120.30
9	P	97	PHE	CB-CG-CD2	-5.94	116.64	120.80
9	G	97	PHE	CB-CG-CD2	-5.93	116.65	120.80
6	M	12	DT	C6-C5-C7	-5.91	119.35	122.90
7	N	2	DT	N3-C2-O2	-5.91	118.76	122.30
6	M	29	DA	N1-C6-N6	-5.90	115.06	118.60
4	L	3324	ARG	NE-CZ-NH2	5.90	123.25	120.30
3	B	260	ARG	NE-CZ-NH2	5.90	123.25	120.30
6	D	23	DG	C5-C6-N1	5.90	114.45	111.50
4	C	36	ARG	NE-CZ-NH2	5.88	123.24	120.30
6	D	20	DG	O4'-C4'-C3'	5.86	109.52	106.00
4	L	1075	ARG	NH1-CZ-NH2	-5.86	112.96	119.40
4	L	2311	ARG	NE-CZ-NH2	5.86	123.23	120.30
6	D	29	DA	N1-C6-N6	-5.85	115.09	118.60
6	M	23	DG	C5-C6-N1	5.84	114.42	111.50
2	A	363	ARG	NE-CZ-NH2	5.83	123.22	120.30
7	E	2	DT	N3-C2-O2	-5.83	118.81	122.30
6	D	23	DG	N3-C2-N2	-5.82	115.83	119.90
9	P	161	ARG	NE-CZ-NH2	5.81	123.21	120.30
6	M	1	DT	C6-C5-C7	-5.81	119.42	122.90
4	C	1075	ARG	NH1-CZ-NH2	-5.81	113.01	119.40
3	K	408	ALA	CB-CA-C	5.80	118.79	110.10
4	C	2773	ARG	NE-CZ-NH2	5.79	123.20	120.30
4	L	3040	TYR	CB-CG-CD1	-5.79	117.53	121.00
3	B	408	ALA	CB-CA-C	5.79	118.78	110.10
9	F	150	ARG	NE-CZ-NH1	-5.78	117.41	120.30
2	A	165	ARG	NE-CZ-NH1	-5.77	117.41	120.30
4	C	1768	ARG	NE-CZ-NH2	5.77	123.19	120.30
2	A	254	ARG	NE-CZ-NH2	5.76	123.18	120.30
4	C	3040	TYR	CB-CG-CD1	-5.76	117.54	121.00
9	G	161	ARG	NE-CZ-NH2	5.76	123.18	120.30
6	M	23	DG	N3-C2-N2	-5.76	115.87	119.90
4	C	2311	ARG	NE-CZ-NH2	5.76	123.18	120.30
4	L	1370	ARG	NE-CZ-NH2	5.75	123.18	120.30
4	C	3324	ARG	NE-CZ-NH2	5.75	123.18	120.30
2	J	363	ARG	NE-CZ-NH2	5.75	123.18	120.30
7	E	24	DT	C6-C5-C7	-5.74	119.45	122.90
6	D	12	DT	C6-C5-C7	-5.74	119.46	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2328	ARG	NE-CZ-NH2	5.73	123.17	120.30
2	J	517	ARG	NE-CZ-NH1	-5.73	117.43	120.30
2	A	358	LYS	O-C-N	-5.73	113.53	122.70
3	K	260	ARG	NE-CZ-NH2	5.72	123.16	120.30
4	C	1370	ARG	NE-CZ-NH2	5.72	123.16	120.30
4	L	2090	ARG	NE-CZ-NH2	5.72	123.16	120.30
7	N	11	DC	N3-C4-C5	5.72	124.19	121.90
7	N	24	DT	C6-C5-C7	-5.71	119.47	122.90
4	L	3046	ARG	NE-CZ-NH2	5.71	123.15	120.30
7	E	18	DC	O4'-C1'-N1	5.70	111.99	108.00
4	L	2773	ARG	NE-CZ-NH2	5.69	123.15	120.30
4	C	3557	ARG	NE-CZ-NH2	5.69	123.14	120.30
8	H	17	GLN	CA-C-N	-5.68	104.69	117.20
7	E	18	DC	C3'-C2'-C1'	-5.67	95.70	102.50
3	K	23	SER	N-CA-C	5.67	126.30	111.00
9	O	150	ARG	NE-CZ-NH1	-5.67	117.47	120.30
6	D	17	DT	N3-C2-O2	-5.66	118.90	122.30
7	E	11	DC	N3-C4-C5	5.66	124.17	121.90
7	N	19	DA	N1-C6-N6	-5.66	115.20	118.60
3	B	23	SER	N-CA-C	5.66	126.29	111.00
4	L	1768	ARG	NE-CZ-NH2	5.66	123.13	120.30
7	N	18	DC	C3'-C2'-C1'	-5.65	95.72	102.50
7	N	18	DC	O4'-C1'-N1	5.65	111.96	108.00
9	G	150	ARG	NE-CZ-NH2	5.65	123.12	120.30
2	J	165	ARG	NE-CZ-NH1	-5.64	117.48	120.30
2	J	358	LYS	O-C-N	-5.64	113.67	122.70
4	C	1938	ARG	NE-CZ-NH2	5.64	123.12	120.30
4	L	2328	ARG	NE-CZ-NH2	5.63	123.12	120.30
6	D	26	DT	C6-C5-C7	-5.63	119.52	122.90
4	L	366	TYR	CB-CG-CD2	-5.63	117.62	121.00
4	L	3557	ARG	NE-CZ-NH2	5.62	123.11	120.30
7	E	19	DA	N1-C6-N6	-5.62	115.23	118.60
2	J	334	THR	CB-CA-C	5.61	126.75	111.60
6	M	26	DT	C6-C5-C7	-5.61	119.53	122.90
2	A	334	THR	CB-CA-C	5.61	126.75	111.60
4	C	2530	ARG	NE-CZ-NH2	5.61	123.10	120.30
9	P	150	ARG	NE-CZ-NH2	5.60	123.10	120.30
4	L	3759	ARG	NE-CZ-NH2	5.59	123.09	120.30
4	C	2729	ARG	NE-CZ-NH2	5.59	123.09	120.30
2	A	517	ARG	NE-CZ-NH1	-5.58	117.51	120.30
4	L	1026	ARG	NE-CZ-NH2	5.57	123.09	120.30
3	B	315	ARG	NE-CZ-NH2	5.57	123.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	4	DT	C5-C6-N1	-5.57	120.36	123.70
7	E	1	DG	N1-C6-O6	-5.57	116.56	119.90
7	N	1	DG	N1-C6-O6	-5.57	116.56	119.90
4	C	2090	ARG	NE-CZ-NH2	5.56	123.08	120.30
4	C	366	TYR	CB-CG-CD2	-5.56	117.67	121.00
7	E	12	DT	C6-C5-C7	-5.55	119.57	122.90
4	C	3759	ARG	NE-CZ-NH2	5.55	123.08	120.30
4	L	1938	ARG	NE-CZ-NH2	5.54	123.07	120.30
9	P	71	ARG	NE-CZ-NH2	5.54	123.07	120.30
4	L	2729	ARG	NE-CZ-NH2	5.54	123.07	120.30
6	M	10	DT	C6-C5-C7	-5.54	119.58	122.90
4	L	2106	ARG	NE-CZ-NH2	5.53	123.06	120.30
2	J	254	ARG	NE-CZ-NH2	5.51	123.06	120.30
7	N	4	DT	C5-C6-N1	-5.51	120.40	123.70
6	M	17	DT	N3-C2-O2	-5.50	119.00	122.30
7	E	18	DC	N1-C2-O2	5.50	122.20	118.90
6	M	13	DG	O4'-C4'-C3'	5.49	109.29	106.00
7	N	18	DC	N1-C2-O2	5.48	122.19	118.90
4	L	3763	ARG	CD-NE-CZ	5.48	131.28	123.60
4	C	3046	ARG	NE-CZ-NH2	5.48	123.04	120.30
10	Y	880	ARG	NE-CZ-NH2	5.48	123.04	120.30
7	E	5	DA	N1-C6-N6	-5.48	115.31	118.60
9	P	192	ARG	NE-CZ-NH2	5.48	123.04	120.30
2	J	488	ARG	NE-CZ-NH2	5.47	123.04	120.30
4	C	1026	ARG	NE-CZ-NH2	5.47	123.04	120.30
9	G	71	ARG	NE-CZ-NH2	5.47	123.04	120.30
10	X	880	ARG	NE-CZ-NH2	5.47	123.03	120.30
3	K	146	GLN	N-CA-C	5.46	125.75	111.00
3	K	486	ARG	NE-CZ-NH2	5.46	123.03	120.30
7	E	16	DA	N1-C6-N6	-5.46	115.33	118.60
6	D	13	DG	O4'-C4'-C3'	5.45	109.27	106.00
4	C	3833	ARG	NE-CZ-NH2	5.45	123.02	120.30
3	B	146	GLN	N-CA-C	5.45	125.71	111.00
7	N	16	DA	N1-C6-N6	-5.45	115.33	118.60
3	B	486	ARG	NE-CZ-NH2	5.44	123.02	120.30
3	K	315	ARG	NE-CZ-NH2	5.44	123.02	120.30
9	G	192	ARG	NE-CZ-NH2	5.44	123.02	120.30
4	C	2106	ARG	NE-CZ-NH2	5.44	123.02	120.30
7	N	18	DC	N3-C2-O2	-5.43	118.10	121.90
4	C	1087	ARG	NE-CZ-NH2	5.43	123.02	120.30
4	C	3763	ARG	CD-NE-CZ	5.43	131.20	123.60
2	A	194	ARG	NE-CZ-NH2	5.42	123.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	2530	ARG	NE-CZ-NH2	5.42	123.01	120.30
7	N	9	DT	N3-C2-O2	-5.42	119.05	122.30
6	D	2	DC	N1-C2-O2	5.41	122.15	118.90
6	D	9	DC	N1-C2-O2	5.41	122.15	118.90
7	E	18	DC	N3-C2-O2	-5.41	118.11	121.90
6	M	6	DG	C4'-C3'-C2'	-5.41	98.23	103.10
4	C	1854	ARG	NE-CZ-NH2	5.40	123.00	120.30
6	D	10	DT	C6-C5-C7	-5.40	119.66	122.90
4	L	1087	ARG	NE-CZ-NH2	5.40	123.00	120.30
3	B	271	ARG	NE-CZ-NH2	5.39	123.00	120.30
8	H	57	ARG	NH1-CZ-NH2	-5.39	113.47	119.40
8	I	107	ARG	NE-CZ-NH2	5.39	123.00	120.30
4	L	1184	ARG	NE-CZ-NH2	5.39	122.99	120.30
6	D	23	DG	N1-C6-O6	-5.39	116.67	119.90
9	G	107	ARG	NE-CZ-NH2	5.38	122.99	120.30
2	J	404	ARG	NE-CZ-NH2	5.38	122.99	120.30
7	E	24	DT	N3-C2-O2	-5.37	119.08	122.30
8	H	18	LEU	CB-CG-CD1	-5.37	101.87	111.00
4	C	1712	ARG	NE-CZ-NH2	5.37	122.98	120.30
6	D	12	DT	N3-C2-O2	-5.37	119.08	122.30
3	B	141	ARG	NE-CZ-NH2	5.37	122.98	120.30
4	C	1811	ARG	NE-CZ-NH2	5.37	122.98	120.30
6	M	23	DG	N1-C6-O6	-5.36	116.68	119.90
9	P	107	ARG	NE-CZ-NH2	5.36	122.98	120.30
8	H	64	ARG	NE-CZ-NH2	5.35	122.97	120.30
7	N	12	DT	N3-C2-O2	-5.35	119.09	122.30
7	E	9	DT	C6-C5-C7	-5.35	119.69	122.90
7	E	12	DT	N3-C2-O2	-5.35	119.09	122.30
4	C	2333	ARG	NE-CZ-NH2	5.34	122.97	120.30
7	E	12	DT	C5-C6-N1	-5.34	120.49	123.70
3	B	145	SER	N-CA-C	5.34	125.42	111.00
4	C	3737	ARG	NE-CZ-NH2	5.34	122.97	120.30
6	M	9	DC	N1-C2-O2	5.34	122.10	118.90
6	D	21	DT	C6-C5-C7	-5.33	119.70	122.90
3	K	145	SER	N-CA-C	5.33	125.39	111.00
6	D	6	DG	C4'-C3'-C2'	-5.33	98.30	103.10
4	C	1184	ARG	NE-CZ-NH2	5.33	122.96	120.30
7	E	9	DT	N3-C2-O2	-5.33	119.11	122.30
4	L	3833	ARG	NE-CZ-NH2	5.32	122.96	120.30
4	L	1712	ARG	NE-CZ-NH2	5.32	122.96	120.30
2	J	194	ARG	NE-CZ-NH2	5.31	122.96	120.30
4	L	1854	ARG	NE-CZ-NH2	5.31	122.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	2722	ARG	NE-CZ-NH2	5.30	122.95	120.30
7	N	13	DG	C5-C6-N1	5.30	114.15	111.50
2	A	488	ARG	NE-CZ-NH2	5.30	122.95	120.30
4	L	3737	ARG	NE-CZ-NH2	5.30	122.95	120.30
7	E	13	DG	C5-C6-N1	5.30	114.15	111.50
3	K	141	ARG	NE-CZ-NH2	5.30	122.95	120.30
4	C	3159	ARG	NE-CZ-NH2	5.28	122.94	120.30
10	X	815	ARG	NE-CZ-NH2	5.28	122.94	120.30
2	J	130	ARG	NE-CZ-NH2	5.28	122.94	120.30
3	K	271	ARG	NE-CZ-NH2	5.28	122.94	120.30
6	M	16	DG	N1-C6-O6	-5.28	116.73	119.90
6	M	29	DA	O4'-C1'-C2'	-5.27	101.69	105.90
7	N	12	DT	C6-C5-C7	-5.27	119.74	122.90
7	N	24	DT	N3-C2-O2	-5.27	119.14	122.30
6	D	1	DT	O4'-C1'-C2'	-5.26	101.69	105.90
6	D	29	DA	O4'-C1'-C2'	-5.26	101.69	105.90
7	N	5	DA	N1-C6-N6	-5.25	115.45	118.60
4	C	3872	ARG	NE-CZ-NH2	5.25	122.92	120.30
2	A	301	ARG	NE-CZ-NH2	5.24	122.92	120.30
4	L	1811	ARG	NE-CZ-NH2	5.24	122.92	120.30
10	Y	815	ARG	NE-CZ-NH2	5.24	122.92	120.30
4	C	2722	ARG	NE-CZ-NH2	5.23	122.92	120.30
2	J	301	ARG	NE-CZ-NH2	5.23	122.92	120.30
7	N	12	DT	C5-C6-N1	-5.23	120.56	123.70
10	X	741	ARG	NE-CZ-NH2	5.23	122.91	120.30
6	M	1	DT	O4'-C1'-C2'	-5.23	101.72	105.90
6	M	2	DC	N1-C2-O2	5.22	122.03	118.90
3	K	504	PRO	N-CA-C	5.22	125.67	112.10
4	L	3159	ARG	NE-CZ-NH2	5.22	122.91	120.30
2	A	130	ARG	NE-CZ-NH2	5.21	122.91	120.30
2	A	404	ARG	NE-CZ-NH2	5.21	122.91	120.30
6	M	21	DT	C6-C5-C7	-5.21	119.78	122.90
4	L	4075	ARG	NE-CZ-NH2	5.21	122.90	120.30
4	L	2333	ARG	NE-CZ-NH2	5.20	122.90	120.30
4	C	3746	ARG	NE-CZ-NH2	5.20	122.90	120.30
6	M	8	DA	C6-C5-N7	5.20	135.94	132.30
6	M	12	DT	N3-C2-O2	-5.19	119.18	122.30
6	D	22	DA	C5-N7-C8	-5.19	101.30	103.90
9	F	153	ARG	NE-CZ-NH2	5.19	122.90	120.30
4	L	1834	ASP	C-N-CA	5.19	134.68	121.70
7	E	9	DT	C5-C6-N1	-5.19	120.59	123.70
10	Y	741	ARG	NE-CZ-NH2	5.19	122.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	25	DT	C6-C5-C7	-5.18	119.79	122.90
8	H	107	ARG	NE-CZ-NH2	5.18	122.89	120.30
3	B	504	PRO	N-CA-C	5.18	125.56	112.10
6	M	22	DA	C5-N7-C8	-5.18	101.31	103.90
6	D	9	DC	N3-C4-C5	5.17	123.97	121.90
6	D	25	DT	C6-C5-C7	-5.17	119.80	122.90
8	H	81	ARG	NE-CZ-NH2	5.17	122.88	120.30
4	L	3746	ARG	NE-CZ-NH2	5.16	122.88	120.30
4	L	3733	ARG	NE-CZ-NH2	5.16	122.88	120.30
9	G	32	PHE	CB-CG-CD2	-5.16	117.19	120.80
4	C	1834	ASP	C-N-CA	5.15	134.58	121.70
7	N	9	DT	C6-C5-C7	-5.15	119.81	122.90
6	M	9	DC	N3-C4-C5	5.15	123.96	121.90
4	C	3474	ARG	NE-CZ-NH2	5.15	122.87	120.30
6	D	16	DG	N1-C6-O6	-5.15	116.81	119.90
4	C	4075	ARG	NE-CZ-NH2	5.15	122.87	120.30
4	L	3872	ARG	NE-CZ-NH2	5.14	122.87	120.30
9	O	153	ARG	NE-CZ-NH2	5.14	122.87	120.30
2	J	332	GLU	C-N-CA	-5.14	108.86	121.70
4	C	2962	ARG	NE-CZ-NH2	5.13	122.86	120.30
9	P	32	PHE	CB-CG-CD2	-5.13	117.21	120.80
4	L	2513	GLU	OE1-CD-OE2	-5.12	117.15	123.30
4	L	3462	ARG	CD-NE-CZ	5.12	130.77	123.60
4	C	1936	ARG	CD-NE-CZ	5.12	130.77	123.60
4	L	3358	ARG	NE-CZ-NH2	5.12	122.86	120.30
7	N	9	DT	C5-C6-N1	-5.12	120.63	123.70
2	A	332	GLU	C-N-CA	-5.12	108.90	121.70
3	K	250	ARG	N-CA-C	5.12	124.81	111.00
4	C	2730	ARG	NE-CZ-NH2	5.12	122.86	120.30
6	D	8	DA	C6-C5-N7	5.12	135.88	132.30
4	C	2513	GLU	OE1-CD-OE2	-5.11	117.16	123.30
6	M	3	DT	O4'-C1'-N1	5.11	111.58	108.00
2	J	416	GLN	N-CA-C	5.11	124.79	111.00
3	K	252	THR	N-CA-C	5.10	124.78	111.00
4	C	350	ARG	NE-CZ-NH2	5.10	122.85	120.30
3	B	250	ARG	N-CA-C	5.10	124.77	111.00
2	A	416	GLN	N-CA-C	5.10	124.76	111.00
4	C	3733	ARG	NE-CZ-NH2	5.10	122.85	120.30
6	M	25	DT	C5-C6-N1	-5.10	120.64	123.70
6	D	3	DT	O4'-C1'-N1	5.10	111.57	108.00
4	L	1936	ARG	CD-NE-CZ	5.09	130.73	123.60
3	B	252	THR	N-CA-C	5.09	124.74	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3874	ARG	NE-CZ-NH2	5.09	122.84	120.30
6	D	25	DT	C5-C6-N1	-5.08	120.65	123.70
7	E	17	DT	C6-C5-C7	-5.07	119.86	122.90
7	N	17	DT	C6-C5-C7	-5.07	119.86	122.90
4	L	2120	ARG	NE-CZ-NH2	5.07	122.83	120.30
4	L	2800	ARG	NE-CZ-NH2	5.07	122.83	120.30
4	L	3474	ARG	NE-CZ-NH2	5.06	122.83	120.30
4	L	1527	ARG	NE-CZ-NH2	5.05	122.83	120.30
6	M	27	DA	C4'-C3'-C2'	-5.05	98.56	103.10
8	I	121	PHE	CB-CG-CD1	-5.05	117.27	120.80
4	C	3462	ARG	CD-NE-CZ	5.05	130.66	123.60
4	C	2158	ARG	NE-CZ-NH2	5.04	122.82	120.30
4	L	924	ARG	NE-CZ-NH1	-5.04	117.78	120.30
6	D	27	DA	C4'-C3'-C2'	-5.03	98.57	103.10
6	M	11	DC	N3-C4-C5	5.03	123.91	121.90
2	A	252	ARG	NE-CZ-NH2	5.03	122.81	120.30
7	N	15	DC	N1-C2-O2	5.03	121.92	118.90
4	C	924	ARG	NE-CZ-NH1	-5.03	117.79	120.30
4	C	3232	ARG	NE-CZ-NH2	5.03	122.81	120.30
2	J	252	ARG	NE-CZ-NH2	5.02	122.81	120.30
4	C	79	ARG	NE-CZ-NH1	-5.02	117.79	120.30
4	C	3734	ARG	NE-CZ-NH2	5.02	122.81	120.30
4	L	406	ARG	NE-CZ-NH2	5.01	122.81	120.30
4	C	1788	ARG	NE-CZ-NH2	5.01	122.81	120.30
4	C	2915	ARG	NE-CZ-NH2	5.01	122.81	120.30
4	L	3232	ARG	NE-CZ-NH2	5.01	122.81	120.30
4	C	1527	ARG	NE-CZ-NH2	5.01	122.80	120.30
6	D	13	DG	N1-C6-O6	-5.01	116.90	119.90
4	C	1937	ARG	NE-CZ-NH2	5.00	122.80	120.30
7	N	6	DA	C5-C6-N1	5.00	120.20	117.70

There are no chirality outliers.

All (145) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	137	HIS	Sidechain
2	A	71	TYR	Sidechain
2	A	88	TYR	Sidechain
3	B	242	ARG	Sidechain
3	B	421	TYR	Sidechain
3	B	44	ARG	Sidechain
3	B	444	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	B	489	ARG	Sidechain
4	C	1270	PHE	Sidechain
4	C	139	ARG	Sidechain
4	C	1420	ARG	Sidechain
4	C	1560	TYR	Sidechain
4	C	175	TYR	Sidechain
4	C	1873	TYR	Sidechain
4	C	1936	ARG	Sidechain
4	C	1945	TYR	Sidechain
4	C	1956	PHE	Sidechain
4	C	1965	PHE	Sidechain
4	C	198	ARG	Sidechain
4	C	2160	TYR	Sidechain
4	C	2431	ARG	Sidechain
4	C	2530	ARG	Sidechain
4	C	2546	TYR	Sidechain
4	C	265	TYR	Sidechain
4	C	2930	TYR	Sidechain
4	C	2931	ARG	Sidechain
4	C	340	TYR	Sidechain
4	C	3467	ARG	Sidechain
4	C	366	TYR	Sidechain
4	C	3784	ARG	Sidechain
4	C	3791	TYR	Sidechain
4	C	3874	ARG	Sidechain
4	C	3962	ARG	Sidechain
4	C	4119	ARG	Sidechain
4	C	9	ARG	Sidechain
6	D	1	DT	Sidechain
6	D	11	DC	Sidechain
6	D	12	DT	Sidechain
6	D	17	DT	Sidechain
6	D	18	DC	Sidechain
6	D	19	DA	Sidechain
6	D	22	DA	Sidechain
6	D	23	DG	Sidechain
6	D	24	DA	Sidechain
6	D	27	DA	Sidechain
6	D	29	DA	Sidechain
6	D	30	DC	Sidechain
6	D	6	DG	Sidechain
6	D	7	DA	Sidechain

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Mol	Chain	Res	Type	Group
6	D	8	DA	Sidechain
7	E	1	DG	Sidechain
7	E	11	DC	Sidechain
7	E	15	DC	Sidechain
7	E	16	DA	Sidechain
7	E	17	DT	Sidechain
7	E	23	DT	Sidechain
7	E	25	DC	Sidechain
7	E	26	DT	Sidechain
7	E	5	DA	Sidechain
7	E	6	DA	Sidechain
7	E	7	DT	Sidechain
9	F	143	HIS	Sidechain
9	F	192	ARG	Sidechain
9	F	66	TYR	Sidechain
9	F	7	ARG	Sidechain
9	F	94	TYR	Sidechain
9	G	111	PHE	Sidechain
9	G	192	ARG	Sidechain
9	G	3	ARG	Sidechain
8	H	17	GLN	Mainchain
8	H	81	ARG	Sidechain
8	I	118	TYR	Sidechain
8	I	167	TYR	Sidechain
8	I	72	PHE	Sidechain
8	I	75	HIS	Sidechain
2	J	137	HIS	Sidechain
2	J	71	TYR	Sidechain
2	J	88	TYR	Sidechain
3	K	242	ARG	Sidechain
3	K	421	TYR	Sidechain
3	K	44	ARG	Sidechain
3	K	444	TYR	Sidechain
3	K	489	ARG	Sidechain
4	L	1270	PHE	Sidechain
4	L	139	ARG	Sidechain
4	L	1420	ARG	Sidechain
4	L	1560	TYR	Sidechain
4	L	175	TYR	Sidechain
4	L	1873	TYR	Sidechain
4	L	1936	ARG	Sidechain
4	L	1945	TYR	Sidechain

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Mol	Chain	Res	Type	Group
4	L	1956	PHE	Sidechain
4	L	1965	PHE	Sidechain
4	L	198	ARG	Sidechain
4	L	2160	TYR	Sidechain
4	L	2311	ARG	Sidechain
4	L	2431	ARG	Sidechain
4	L	2530	ARG	Sidechain
4	L	2546	TYR	Sidechain
4	L	265	TYR	Sidechain
4	L	2930	TYR	Sidechain
4	L	2931	ARG	Sidechain
4	L	340	TYR	Sidechain
4	L	3467	ARG	Sidechain
4	L	366	TYR	Sidechain
4	L	3784	ARG	Sidechain
4	L	3791	TYR	Sidechain
4	L	3874	ARG	Sidechain
4	L	3962	ARG	Sidechain
4	L	4119	ARG	Sidechain
4	L	9	ARG	Sidechain
6	M	1	DT	Sidechain
6	M	11	DC	Sidechain
6	M	12	DT	Sidechain
6	M	17	DT	Sidechain
6	M	18	DC	Sidechain
6	M	19	DA	Sidechain
6	M	22	DA	Sidechain
6	M	23	DG	Sidechain
6	M	24	DA	Sidechain
6	M	27	DA	Sidechain
6	M	29	DA	Sidechain
6	M	30	DC	Sidechain
6	M	6	DG	Sidechain
6	M	7	DA	Sidechain
6	M	8	DA	Sidechain
7	N	1	DG	Sidechain
7	N	11	DC	Sidechain
7	N	15	DC	Sidechain
7	N	16	DA	Sidechain
7	N	17	DT	Sidechain
7	N	23	DT	Sidechain
7	N	25	DC	Sidechain

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Mol	Chain	Res	Type	Group
7	N	26	DT	Sidechain
7	N	5	DA	Sidechain
7	N	6	DA	Sidechain
7	N	7	DT	Sidechain
9	O	143	HIS	Sidechain
9	O	192	ARG	Sidechain
9	O	66	TYR	Sidechain
9	O	7	ARG	Sidechain
9	O	94	TYR	Sidechain
9	P	111	PHE	Sidechain
9	P	192	ARG	Sidechain
9	P	3	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S	168	0	169	15	0
1	T	168	0	169	16	0
2	A	4021	0	4100	52	0
2	J	4021	0	4100	53	0
3	B	4259	0	4301	8	0
3	K	4259	0	4301	8	0
4	C	29811	0	30286	98	0
4	L	29811	0	30286	97	0
5	Q	101	0	23	1	0
5	R	101	0	23	1	0
6	D	634	0	348	4	0
6	M	634	0	348	4	0
7	E	616	0	339	5	0
7	N	616	0	339	5	0
8	H	1779	0	1797	15	0
8	I	1737	0	1744	13	0
9	F	1736	0	1739	20	0
9	G	1595	0	1592	34	0
9	O	1736	0	1739	24	0
9	P	1595	0	1592	36	0
10	X	2064	0	2012	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	Y	2064	0	2012	14	0
11	C	31	0	12	0	0
11	L	31	0	12	0	0
All	All	93588	0	93383	440	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (440) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:333:GLU:CB	2:A:333:GLU:CA	1.83	1.57
2:J:333:GLU:CA	2:J:333:GLU:CB	1.83	1.56
2:A:333:GLU:CA	2:A:333:GLU:N	1.68	1.56
2:J:333:GLU:CA	2:J:333:GLU:C	1.77	1.52
2:J:333:GLU:CA	2:J:333:GLU:N	1.68	1.50
2:A:333:GLU:CA	2:A:333:GLU:C	1.77	1.49
2:A:333:GLU:CB	2:A:333:GLU:CG	2.05	1.35
2:J:334:THR:OG1	2:J:334:THR:CB	1.77	1.32
2:J:333:GLU:CB	2:J:333:GLU:CG	2.05	1.32
2:A:334:THR:CB	2:A:334:THR:OG1	1.77	1.30
2:J:334:THR:N	2:J:334:THR:CA	2.08	1.17
2:A:334:THR:N	2:A:334:THR:CA	2.08	1.17
9:O:40:HIS:CG	9:P:120:ALA:HB2	2.05	0.91
9:F:40:HIS:CG	9:G:120:ALA:HB2	2.05	0.91
8:I:66:THR:O	9:F:106:PHE:CE1	2.26	0.89
8:I:15:TRP:HB2	8:I:211:VAL:HG21	1.55	0.88
1:S:196:ALA:O	2:A:477:SER:O	1.93	0.86
2:J:477:SER:O	1:T:196:ALA:O	1.93	0.86
2:A:334:THR:OG1	2:A:334:THR:CA	2.24	0.85
2:J:334:THR:OG1	2:J:334:THR:CA	2.24	0.85
2:J:332:GLU:C	2:J:333:GLU:CA	2.46	0.84
2:A:332:GLU:C	2:A:333:GLU:CA	2.46	0.83
2:J:333:GLU:CB	2:J:333:GLU:C	2.48	0.81
2:A:333:GLU:CB	2:A:333:GLU:C	2.48	0.81
4:C:3617:LEU:HB3	4:C:3633:ILE:HD13	1.61	0.81
4:L:3617:LEU:HB3	4:L:3633:ILE:HD13	1.61	0.81
8:I:211:VAL:HG23	8:I:212:MET:SD	2.20	0.81
9:F:40:HIS:CD2	9:G:120:ALA:HB2	2.15	0.80
9:O:40:HIS:CD2	9:P:120:ALA:HB2	2.15	0.80
9:F:124:ARG:CZ	9:G:38:ASP:O	2.31	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:124:ARG:CZ	9:P:38:ASP:O	2.31	0.79
2:J:333:GLU:CA	2:J:333:GLU:CG	2.62	0.78
2:A:333:GLU:CA	2:A:333:GLU:CG	2.62	0.78
8:H:116:PRO:HD3	9:O:61:MET:HE3	1.65	0.77
2:A:334:THR:CB	2:A:334:THR:N	2.48	0.77
2:J:334:THR:CB	2:J:334:THR:N	2.48	0.76
4:L:3855:TYR:HD1	4:L:3858:MET:HE3	1.49	0.76
2:J:331:LYS:O	2:J:334:THR:HG22	1.89	0.73
4:C:3855:TYR:HD1	4:C:3858:MET:HE3	1.54	0.73
2:A:331:LYS:O	2:A:334:THR:HG22	1.89	0.72
1:S:186:ILE:O	2:A:74:LYS:HE3	1.91	0.71
9:F:40:HIS:CD2	9:G:120:ALA:CB	2.75	0.69
2:J:74:LYS:HE3	1:T:186:ILE:O	1.92	0.69
9:O:40:HIS:CD2	9:P:120:ALA:CB	2.75	0.69
9:F:39:GLY:O	9:G:120:ALA:HA	1.92	0.69
9:O:124:ARG:HG2	9:P:19:PHE:HE2	1.58	0.69
2:J:250:GLU:HG2	1:T:187:ASN:HD21	1.58	0.69
2:A:333:GLU:CB	2:A:333:GLU:N	2.55	0.69
9:O:39:GLY:O	9:P:120:ALA:HA	1.92	0.69
2:J:333:GLU:CB	2:J:333:GLU:N	2.55	0.68
2:A:333:GLU:C	2:A:334:THR:CA	2.62	0.67
2:J:333:GLU:C	2:J:334:THR:CA	2.62	0.67
9:F:120:ALA:HB1	9:G:39:GLY:C	2.14	0.67
4:L:3764:VAL:HA	4:L:3767:LEU:HD12	1.77	0.67
2:J:333:GLU:CA	2:J:334:THR:N	2.58	0.67
9:O:120:ALA:HB1	9:P:39:GLY:C	2.14	0.67
1:S:187:ASN:HD21	2:A:250:GLU:HG2	1.58	0.66
9:F:124:ARG:HG2	9:G:19:PHE:HE2	1.58	0.66
4:C:1897:ASN:N	4:C:1898:GLN:OE1	2.28	0.66
4:L:1897:ASN:N	4:L:1898:GLN:OE1	2.28	0.66
2:J:58:THR:HB	2:J:61:ASP:HB2	1.77	0.65
4:C:3764:VAL:HA	4:C:3767:LEU:HD12	1.77	0.65
2:A:58:THR:HB	2:A:61:ASP:HB2	1.77	0.65
8:H:116:PRO:HD3	9:O:61:MET:CE	2.26	0.65
2:A:333:GLU:CA	2:A:334:THR:N	2.58	0.65
1:S:186:ILE:O	2:A:74:LYS:CE	2.45	0.64
4:L:1224:PHE:CZ	4:L:1270:PHE:CZ	2.86	0.63
1:S:191:LYS:NZ	3:B:434:MET:HG2	2.14	0.63
10:X:843:LEU:HD21	9:G:163:GLU:HA	1.81	0.63
4:C:1046:PRO:HA	4:C:1049:GLN:HB3	1.80	0.63
2:J:74:LYS:CE	1:T:186:ILE:O	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:434:MET:HG2	1:T:191:LYS:NZ	2.14	0.62
4:C:1224:PHE:CZ	4:C:1270:PHE:CZ	2.88	0.62
10:Y:843:LEU:HD21	9:P:163:GLU:HA	1.81	0.62
4:L:1046:PRO:HA	4:L:1049:GLN:HB3	1.80	0.62
2:A:131:PHE:CE2	2:A:137:HIS:CE1	2.89	0.61
4:C:1897:ASN:OD1	4:C:1898:GLN:NE2	2.33	0.61
2:J:131:PHE:CE2	2:J:137:HIS:CE1	2.89	0.61
10:X:792:MET:SD	9:G:178:LYS:HG3	2.41	0.61
4:C:1046:PRO:HD2	4:C:1047:GLN:H	1.64	0.61
10:X:843:LEU:CD2	9:G:163:GLU:HA	2.31	0.61
4:L:1046:PRO:HD2	4:L:1047:GLN:H	1.65	0.61
9:G:20:LEU:HD11	9:G:34:ILE:HD11	1.83	0.61
4:L:1240:THR:HG21	4:L:1256:TRP:CD1	2.36	0.60
9:P:20:LEU:HD11	9:P:34:ILE:HD11	1.83	0.60
10:Y:843:LEU:CD2	9:P:163:GLU:HA	2.31	0.60
10:Y:792:MET:SD	9:P:178:LYS:HG3	2.41	0.60
4:L:1897:ASN:OD1	4:L:1898:GLN:NE2	2.33	0.60
4:L:1619:ALA:HA	4:L:1652:ILE:HD11	1.83	0.60
4:C:1619:ALA:HA	4:C:1652:ILE:HD11	1.83	0.59
4:C:1240:THR:HG21	4:C:1256:TRP:CD1	2.36	0.59
9:O:124:ARG:HG2	9:P:19:PHE:CE2	2.38	0.59
9:F:124:ARG:HG2	9:G:19:PHE:CE2	2.38	0.58
2:J:334:THR:CB	2:J:334:THR:CG2	2.82	0.58
9:G:116:VAL:HG12	9:G:117:GLU:H	1.69	0.58
2:A:334:THR:CB	2:A:334:THR:CG2	2.82	0.57
2:J:241:ASP:O	1:T:186:ILE:HD11	2.04	0.57
9:P:116:VAL:HG12	9:P:117:GLU:H	1.69	0.57
8:H:116:PRO:CD	9:O:61:MET:HE3	2.32	0.57
4:C:1046:PRO:HD2	4:C:1047:GLN:N	2.20	0.57
4:L:1046:PRO:HD2	4:L:1047:GLN:N	2.20	0.56
2:A:333:GLU:HA	2:A:336:GLU:HB3	1.87	0.56
1:S:186:ILE:HD11	2:A:241:ASP:O	2.06	0.56
4:C:490:ILE:HD13	4:C:527:TYR:CD1	2.41	0.56
4:C:490:ILE:HD11	4:C:524:TYR:HA	1.88	0.56
4:L:490:ILE:HD13	4:L:527:TYR:CD1	2.41	0.55
2:J:333:GLU:HA	2:J:336:GLU:HB3	1.87	0.55
2:A:49:PHE:CD2	2:A:137:HIS:ND1	2.75	0.55
8:H:18:LEU:HD13	8:H:96:SER:HA	1.87	0.55
2:J:49:PHE:CD2	2:J:137:HIS:ND1	2.75	0.55
4:L:1770:GLN:OE1	4:L:1770:GLN:N	2.33	0.55
8:I:10:MET:SD	8:I:223:THR:HA	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:490:ILE:HD11	4:L:524:TYR:HA	1.88	0.54
10:Y:847:PHE:O	9:P:169:LYS:CE	2.56	0.54
2:J:132:GLN:OE1	2:J:137:HIS:CD2	2.60	0.54
2:A:132:GLN:OE1	2:A:137:HIS:CD2	2.60	0.54
1:S:187:ASN:ND2	2:A:250:GLU:HG2	2.23	0.54
4:L:135:LEU:HD12	4:L:184:VAL:HG21	1.89	0.54
4:L:1048:GLN:O	4:L:1053:PRO:HD3	2.07	0.54
10:X:847:PHE:O	9:G:169:LYS:CE	2.56	0.54
4:L:3296:GLN:O	4:L:3300:VAL:HG12	2.08	0.54
8:H:12:PRO:HB3	8:H:219:MET:SD	2.48	0.54
4:C:1048:GLN:O	4:C:1053:PRO:HD3	2.07	0.54
4:L:1048:GLN:HB2	4:L:1052:SER:HB3	1.90	0.54
4:L:2245:TRP:CD2	4:L:2246:LYS:HE2	2.43	0.54
10:X:847:PHE:O	9:G:169:LYS:HE3	2.08	0.54
2:A:362:LEU:HD23	2:A:436:PHE:HB3	1.90	0.53
4:C:135:LEU:HD12	4:C:184:VAL:HG21	1.89	0.53
4:C:2245:TRP:CD2	4:C:2246:LYS:HE2	2.43	0.53
4:C:3296:GLN:O	4:C:3300:VAL:HG12	2.08	0.53
10:Y:847:PHE:O	9:P:169:LYS:HE3	2.08	0.53
4:C:1048:GLN:HB2	4:C:1052:SER:HB3	1.90	0.53
4:C:1867:ILE:HD11	4:C:1940:TYR:CG	2.44	0.53
4:L:1224:PHE:CE1	4:L:1270:PHE:CZ	2.97	0.52
4:L:1867:ILE:HD11	4:L:1940:TYR:CG	2.44	0.52
2:J:250:GLU:HG2	1:T:187:ASN:ND2	2.23	0.52
4:C:1046:PRO:HA	4:C:1049:GLN:CB	2.40	0.52
9:O:104:VAL:HG12	9:O:105:SER:H	1.74	0.52
2:J:362:LEU:HD23	2:J:436:PHE:HB3	1.90	0.52
4:L:1898:GLN:OE1	4:L:1898:GLN:N	2.43	0.52
8:I:10:MET:SD	8:I:223:THR:HG22	2.50	0.52
4:C:1538:LEU:HD12	4:C:1553:PHE:CE2	2.45	0.52
2:J:169:PHE:CE2	2:J:203:MET:SD	3.03	0.52
4:C:1898:GLN:OE1	4:C:1898:GLN:N	2.43	0.52
2:A:267:ILE:HD12	2:A:267:ILE:H	1.75	0.52
4:C:1190:LEU:HD21	4:C:1194:PHE:CZ	2.45	0.52
4:C:2950:LYS:HE3	4:C:2981:TRP:CE3	2.45	0.52
10:Y:792:MET:SD	9:P:178:LYS:CG	2.98	0.52
4:C:1224:PHE:CE1	4:C:1270:PHE:CZ	2.98	0.51
4:C:3837:CYS:SG	4:C:3874:ARG:HB2	2.51	0.51
4:C:3855:TYR:HA	4:C:3858:MET:HE2	1.91	0.51
1:S:196:ALA:O	2:A:477:SER:C	2.48	0.51
2:J:477:SER:C	1:T:196:ALA:O	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:3797:THR:HG23	4:C:3799:ARG:H	1.76	0.51
3:K:434:MET:HG2	1:T:191:LYS:HZ1	1.74	0.51
4:L:1190:LEU:HD21	4:L:1194:PHE:CZ	2.45	0.51
4:L:3797:THR:HG23	4:L:3799:ARG:H	1.76	0.51
4:C:3588:TRP:CH2	4:C:3613:MET:HG2	2.46	0.51
4:L:3837:CYS:SG	4:L:3874:ARG:HB2	2.51	0.51
2:A:169:PHE:CE2	2:A:203:MET:SD	3.03	0.51
3:K:340:PHE:CE1	3:K:393:VAL:HG11	2.46	0.51
9:F:120:ALA:CB	9:G:39:GLY:C	2.79	0.51
2:A:334:THR:OG1	2:A:334:THR:HA	2.11	0.51
4:L:1538:LEU:HD12	4:L:1553:PHE:CE2	2.45	0.51
9:O:120:ALA:CB	9:P:39:GLY:C	2.79	0.51
10:Y:847:PHE:O	9:P:169:LYS:NZ	2.44	0.51
4:L:2311:ARG:HH11	7:N:7:DT:P	2.34	0.51
4:L:3626:GLY:HA3	4:L:3629:ARG:HB2	1.93	0.51
3:B:60:GLY:H	3:B:105:ALA:HB3	1.76	0.51
10:X:847:PHE:O	9:G:169:LYS:NZ	2.44	0.51
4:C:2311:ARG:HH11	7:E:7:DT:P	2.34	0.50
4:L:2950:LYS:HE3	4:L:2981:TRP:CE3	2.45	0.50
3:B:340:PHE:CE1	3:B:393:VAL:HG11	2.46	0.50
4:C:2379:MET:CE	4:C:2401:VAL:HA	2.42	0.50
4:C:3626:GLY:HA3	4:C:3629:ARG:HB2	1.94	0.50
4:L:1046:PRO:HA	4:L:1049:GLN:CB	2.40	0.50
3:B:408:ALA:HB1	3:B:419:LEU:HD21	1.93	0.50
10:X:792:MET:SD	9:G:178:LYS:CG	2.98	0.50
2:J:267:ILE:HD12	2:J:267:ILE:H	1.75	0.50
3:K:60:GLY:H	3:K:105:ALA:HB3	1.76	0.50
4:L:2379:MET:CE	4:L:2401:VAL:HA	2.42	0.50
4:L:3588:TRP:CH2	4:L:3613:MET:HG2	2.46	0.50
4:L:3666:LEU:O	4:L:3670:MET:HG2	2.12	0.50
2:J:58:THR:O	2:J:62:MET:N	2.45	0.50
4:C:3666:LEU:O	4:C:3670:MET:HG2	2.12	0.50
9:O:117:GLU:CD	9:O:117:GLU:H	2.15	0.49
2:A:58:THR:O	2:A:62:MET:N	2.45	0.49
9:F:117:GLU:CD	9:F:117:GLU:H	2.15	0.49
3:K:408:ALA:HB1	3:K:419:LEU:HD21	1.93	0.49
6:M:14:DA:N6	7:N:17:DT:H3	2.11	0.49
8:I:68:PRO:HD3	9:F:104:VAL:HG11	1.95	0.49
2:A:67:ILE:O	2:A:71:TYR:HB2	2.13	0.49
4:C:2154:GLU:OE2	4:C:2192:THR:HG22	2.13	0.49
6:D:14:DA:N6	7:E:17:DT:H3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:2154:GLU:OE2	4:L:2192:THR:HG22	2.13	0.48
8:H:97:CYS:SG	8:H:104:LEU:HD11	2.53	0.48
4:C:1100:VAL:HA	4:C:1103:ALA:HB3	1.95	0.48
4:C:1770:GLN:OE1	4:C:1770:GLN:N	2.33	0.48
2:J:67:ILE:O	2:J:71:TYR:HB2	2.13	0.48
4:L:1100:VAL:HA	4:L:1103:ALA:HB3	1.95	0.48
4:L:2897:LEU:HD22	4:L:2923:TRP:CD1	2.49	0.48
2:J:517:ARG:HH11	1:T:201:PHE:HB2	1.79	0.48
4:L:828:LYS:HA	4:L:831:LEU:HD13	1.95	0.48
2:J:131:PHE:CE2	2:J:137:HIS:NE2	2.82	0.48
2:J:238:LYS:HG2	1:T:185:LEU:HD13	1.94	0.48
2:J:334:THR:OG1	2:J:334:THR:HA	2.11	0.48
4:C:439:VAL:HG13	4:C:461:ILE:HD11	1.95	0.48
10:Y:796:ILE:HG12	9:P:177:TYR:CG	2.49	0.48
10:X:796:ILE:HG12	9:G:177:TYR:CG	2.49	0.48
1:S:191:LYS:HZ2	3:B:434:MET:HG2	1.77	0.48
4:L:439:VAL:HG13	4:L:461:ILE:HD11	1.95	0.48
4:C:828:LYS:HA	4:C:831:LEU:HD13	1.95	0.48
4:C:2188:GLU:O	4:C:2192:THR:HG23	2.14	0.48
2:A:131:PHE:CE2	2:A:137:HIS:NE2	2.82	0.47
4:L:3859:TYR:HA	4:L:4119:ARG:HH21	1.79	0.47
9:O:40:HIS:CB	9:P:120:ALA:HB2	2.44	0.47
1:S:201:PHE:CZ	2:A:469:LEU:HD13	2.49	0.47
4:C:1138:ILE:HD12	4:C:1194:PHE:CZ	2.49	0.47
4:C:3659:PHE:O	4:C:3663:THR:HG23	2.13	0.47
4:L:3659:PHE:O	4:L:3663:THR:HG23	2.13	0.47
1:S:191:LYS:HZ1	3:B:434:MET:HG2	1.79	0.47
4:C:3859:TYR:HA	4:C:4119:ARG:HH21	1.79	0.47
9:F:40:HIS:CB	9:G:120:ALA:HB2	2.44	0.47
2:A:145:GLU:O	2:A:149:VAL:HG23	2.15	0.47
4:L:1138:ILE:HD12	4:L:1194:PHE:CZ	2.49	0.47
1:S:185:LEU:HD13	2:A:238:LYS:HG2	1.96	0.47
4:L:2188:GLU:O	4:L:2192:THR:HG23	2.15	0.47
2:J:469:LEU:HD13	1:T:201:PHE:CZ	2.49	0.47
4:L:828:LYS:HA	4:L:831:LEU:CD1	2.45	0.47
4:L:3650:LYS:O	4:L:3650:LYS:HD3	2.15	0.47
6:M:24:DA:C2	6:M:25:DT:C2	3.03	0.47
4:C:828:LYS:HA	4:C:831:LEU:CD1	2.45	0.47
4:C:2897:LEU:HD22	4:C:2923:TRP:CD1	2.49	0.47
2:A:149:VAL:O	2:A:153:LEU:HD23	2.15	0.47
4:C:3650:LYS:O	4:C:3650:LYS:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:145:GLU:O	2:J:149:VAL:HG23	2.15	0.47
4:L:1877:LEU:HD12	4:L:1878:ASP:N	2.30	0.47
8:H:51:THR:HG23	8:H:69:PRO:CG	2.45	0.47
6:D:24:DA:C2	6:D:25:DT:C2	3.03	0.46
9:O:194:LEU:HD23	9:P:198:LEU:HD13	1.96	0.46
3:B:246:HIS:CD2	3:B:368:ARG:HH22	2.33	0.46
4:C:395:MET:HG3	4:C:413:PHE:CE2	2.50	0.46
9:F:194:LEU:HD23	9:G:198:LEU:HD13	1.96	0.46
9:P:34:ILE:HD13	9:P:35:THR:N	2.30	0.46
10:X:843:LEU:HB3	9:G:166:VAL:HG21	1.98	0.46
9:G:34:ILE:HD13	9:G:35:THR:N	2.30	0.46
4:C:3809:THR:HG22	4:C:3931:ALA:HA	1.98	0.46
4:C:1261:LEU:HD13	4:C:1337:VAL:HA	1.98	0.46
10:Y:843:LEU:HB3	9:P:166:VAL:HG21	1.98	0.46
3:K:496:HIS:CD2	3:K:506:PRO:HD3	2.51	0.46
4:L:395:MET:HG3	4:L:413:PHE:CE2	2.50	0.46
3:B:496:HIS:CD2	3:B:506:PRO:HD3	2.51	0.46
4:C:237:SER:HB2	4:C:281:GLN:HA	1.98	0.46
1:S:186:ILE:O	2:A:74:LYS:HE2	2.16	0.46
2:J:333:GLU:CB	2:J:333:GLU:CD	2.83	0.46
4:L:3425:ARG:HA	4:L:3425:ARG:NE	2.31	0.46
4:C:1271:ILE:HD12	4:C:1271:ILE:H	1.81	0.46
3:K:246:HIS:CD2	3:K:368:ARG:HH22	2.33	0.46
4:L:1261:LEU:HD13	4:L:1337:VAL:HA	1.98	0.46
8:I:194:MET:SD	8:I:194:MET:N	2.89	0.46
4:L:237:SER:HB2	4:L:281:GLN:HA	1.98	0.45
2:J:333:GLU:N	2:J:334:THR:N	2.64	0.45
4:C:1877:LEU:HD12	4:C:1878:ASP:N	2.30	0.45
4:C:3425:ARG:HA	4:C:3425:ARG:NE	2.31	0.45
4:L:1805:PHE:CD1	4:L:1820:VAL:HG23	2.51	0.45
10:X:846:ARG:NH2	9:G:166:VAL:HG12	2.32	0.45
2:A:333:GLU:N	2:A:334:THR:N	2.64	0.45
1:S:201:PHE:HB2	2:A:517:ARG:HH11	1.81	0.45
4:C:1805:PHE:CD1	4:C:1820:VAL:HG23	2.51	0.45
4:C:3496:ILE:HD11	4:C:3528:ALA:HB1	1.99	0.45
4:L:2810:SER:HA	4:L:2861:ILE:HD11	1.98	0.45
8:H:51:THR:HG23	8:H:69:PRO:HG3	1.99	0.45
4:C:1913:LYS:HB3	4:C:1956:PHE:CZ	2.52	0.45
4:L:249:PHE:CE2	4:L:285:CYS:HB3	2.52	0.45
4:C:2810:SER:HA	4:C:2861:ILE:HD11	1.98	0.45
4:C:3767:LEU:HD11	4:C:4002:MET:SD	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:846:ARG:NH2	9:P:166:VAL:HG12	2.32	0.45
2:J:132:GLN:OE1	2:J:137:HIS:CG	2.70	0.45
4:L:1049:GLN:HA	4:L:1053:PRO:CG	2.47	0.45
4:L:1913:LYS:HB3	4:L:1956:PHE:CZ	2.52	0.45
4:L:3809:THR:HG22	4:L:3931:ALA:HA	1.98	0.45
4:C:249:PHE:CE2	4:C:285:CYS:HB3	2.52	0.45
4:C:1240:THR:HG21	4:C:1256:TRP:CG	2.52	0.45
10:Y:843:LEU:HD13	9:P:162:PHE:CD2	2.52	0.45
4:L:627:VAL:HG22	4:L:669:LEU:CD1	2.48	0.44
8:H:18:LEU:CD2	8:H:95:PHE:O	2.65	0.44
4:C:461:ILE:HD12	4:C:461:ILE:HA	1.90	0.44
9:F:40:HIS:CD2	9:G:120:ALA:HB3	2.53	0.44
2:A:333:GLU:CB	2:A:333:GLU:CD	2.83	0.44
4:L:3157:LEU:C	4:L:3157:LEU:HD23	2.38	0.44
2:J:136:GLY:C	2:J:137:HIS:CD2	2.91	0.44
2:J:149:VAL:O	2:J:153:LEU:HD23	2.15	0.44
4:L:1240:THR:HG21	4:L:1256:TRP:CG	2.52	0.44
4:L:3171:ALA:HA	4:L:3179:TRP:CZ3	2.53	0.44
8:I:67:ALA:HB3	8:I:72:PHE:CE2	2.52	0.44
2:A:132:GLN:OE1	2:A:137:HIS:CG	2.70	0.44
2:A:136:GLY:C	2:A:137:HIS:CD2	2.91	0.44
4:L:3496:ILE:HD11	4:L:3528:ALA:HB1	1.99	0.44
4:L:3767:LEU:HD11	4:L:4002:MET:SD	2.57	0.44
7:N:26:DT:H2'	7:N:27:DT:C6	2.53	0.44
4:L:2383:PHE:O	4:L:2418:LYS:HE2	2.18	0.44
10:X:843:LEU:HD13	9:G:162:PHE:CD2	2.52	0.44
4:L:3767:LEU:HD13	4:L:3918:LEU:HD13	2.00	0.44
4:C:1805:PHE:CG	4:C:1820:VAL:HG23	2.53	0.44
4:C:1920:TYR:CE1	4:C:1924:THR:HG21	2.53	0.44
4:C:3157:LEU:HD23	4:C:3157:LEU:C	2.38	0.44
8:H:67:ALA:HB2	9:O:106:PHE:CZ	2.53	0.43
4:C:2813:PHE:CD1	4:C:2861:ILE:HD12	2.53	0.43
2:J:74:LYS:HE2	1:T:186:ILE:O	2.18	0.43
2:A:332:GLU:O	2:A:333:GLU:CA	2.66	0.43
3:K:434:MET:HG2	1:T:191:LYS:HZ2	1.83	0.43
4:C:3171:ALA:HA	4:C:3179:TRP:CZ3	2.53	0.43
4:L:1169:VAL:HG21	4:L:1198:LEU:HD21	1.99	0.43
4:L:1920:TYR:CE1	4:L:1924:THR:HG21	2.53	0.43
8:H:46:HIS:HB3	8:H:124:MET:SD	2.59	0.43
4:C:1049:GLN:HA	4:C:1053:PRO:CG	2.47	0.43
4:C:1169:VAL:HG21	4:C:1198:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:3535:ILE:HD11	4:C:3797:THR:HA	2.00	0.43
9:O:124:ARG:NE	9:P:38:ASP:O	2.51	0.43
9:P:51:GLU:HA	9:P:54:GLN:HB3	2.00	0.43
9:P:91:GLU:CD	9:P:91:GLU:H	2.22	0.43
4:L:3535:ILE:HD11	4:L:3797:THR:HA	2.00	0.43
8:I:140:MET:SD	8:I:140:MET:C	2.97	0.43
4:C:627:VAL:HG22	4:C:669:LEU:CD1	2.48	0.43
4:C:3496:ILE:CD1	4:C:3528:ALA:HB1	2.48	0.43
10:X:758:TYR:HA	10:X:764:SER:HA	2.00	0.43
9:G:51:GLU:HA	9:G:54:GLN:HB3	2.00	0.43
9:P:116:VAL:CG1	9:P:117:GLU:H	2.31	0.43
4:L:1157:PHE:CE1	4:L:1168:LEU:HG	2.54	0.43
4:L:3496:ILE:CD1	4:L:3528:ALA:HB1	2.48	0.43
2:A:273:ILE:HD13	2:A:368:VAL:HG22	2.01	0.43
4:L:2924:VAL:HG11	4:L:2989:ALA:HB1	1.99	0.43
8:I:1:MET:SD	8:I:4:LEU:HB2	2.59	0.43
4:C:3767:LEU:HD13	4:C:3918:LEU:HD13	2.00	0.43
7:E:26:DT:H2'	7:E:27:DT:C6	2.53	0.43
9:G:91:GLU:CD	9:G:91:GLU:H	2.22	0.43
10:Y:725:TRP:CD1	10:Y:742:PHE:CD2	3.07	0.43
10:Y:758:TYR:HA	10:Y:764:SER:HA	2.00	0.43
4:L:1805:PHE:CG	4:L:1820:VAL:HG23	2.53	0.43
4:L:2813:PHE:CD1	4:L:2861:ILE:HD12	2.53	0.43
9:F:120:ALA:CB	9:G:39:GLY:O	2.67	0.43
1:S:190:PHE:CG	2:A:250:GLU:HG2	2.54	0.42
4:L:3636:PHE:CZ	4:L:3666:LEU:HG	2.54	0.42
4:L:9:ARG:CZ	4:L:9:ARG:CB	2.97	0.42
4:C:3141:PHE:CD1	4:C:3141:PHE:C	2.93	0.42
4:C:3636:PHE:CZ	4:C:3666:LEU:HG	2.54	0.42
4:C:3811:THR:HA	4:C:3929:MET:HG2	2.02	0.42
9:F:124:ARG:NE	9:G:38:ASP:O	2.51	0.42
10:X:725:TRP:CD1	10:X:742:PHE:CD2	3.07	0.42
4:L:1902:GLY:HA2	4:L:1905:ILE:HG23	2.01	0.42
4:L:3255:ALA:O	4:L:3259:LEU:HD23	2.20	0.42
4:C:2924:VAL:HG11	4:C:2989:ALA:HB1	1.99	0.42
4:L:3761:ASP:HA	4:L:3764:VAL:HG12	2.01	0.42
4:C:9:ARG:CZ	4:C:9:ARG:CB	2.97	0.42
4:C:3467:ARG:CZ	4:C:4000:ASN:HD21	2.33	0.42
9:P:68:GLY:HA2	9:P:71:ARG:HG2	2.01	0.42
4:L:51:LEU:HD21	4:L:96:MET:HE1	2.02	0.42
2:J:332:GLU:O	2:J:333:GLU:CA	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:7:GLY:HA3	8:H:28:PHE:CE2	2.55	0.42
8:H:18:LEU:HD22	8:H:95:PHE:O	2.19	0.42
9:P:73:ALA:HA	9:P:84:TYR:CD2	2.55	0.42
2:J:83:LEU:HD23	2:J:111:PRO:HB3	2.02	0.42
2:J:250:GLU:HG2	1:T:190:PHE:CG	2.54	0.42
8:I:208:LYS:HG2	8:I:212:MET:SD	2.59	0.42
4:C:1224:PHE:CE1	4:C:1270:PHE:CE1	3.08	0.42
9:F:134:ILE:HD11	9:G:130:CYS:HA	2.02	0.42
9:O:120:ALA:CB	9:P:39:GLY:O	2.67	0.42
2:J:41:LEU:HD21	2:J:146:VAL:HG12	2.01	0.42
4:L:3141:PHE:CD1	4:L:3141:PHE:C	2.93	0.42
4:L:3467:ARG:CZ	4:L:4000:ASN:HD21	2.33	0.42
4:L:3811:THR:HA	4:L:3929:MET:HG2	2.01	0.42
5:R:6005:UNK:O	5:R:6009:UNK:N	2.53	0.42
4:C:1157:PHE:CE1	4:C:1168:LEU:HG	2.54	0.42
5:Q:6005:UNK:O	5:Q:6009:UNK:N	2.53	0.42
2:J:333:GLU:N	2:J:333:GLU:CG	2.83	0.42
4:C:1154:PRO:HB2	4:C:1157:PHE:CD2	2.55	0.42
9:O:40:HIS:CD2	9:P:120:ALA:HB3	2.53	0.42
4:L:1500:LEU:CD1	4:L:1538:LEU:HD13	2.50	0.42
4:C:3750:PHE:CD1	4:C:3804:GLU:HA	2.55	0.42
4:L:3602:ASN:O	4:L:3606:ILE:HG12	2.20	0.41
4:L:3855:TYR:CZ	4:L:4121:TRP:HA	2.55	0.41
6:M:14:DA:C2	6:M:15:DT:C2	3.08	0.41
8:H:215:GLN:O	8:H:219:MET:SD	2.78	0.41
4:C:1902:GLY:HA2	4:C:1905:ILE:HG23	2.01	0.41
4:C:2383:PHE:O	4:C:2418:LYS:HE2	2.18	0.41
9:G:116:VAL:CG1	9:G:117:GLU:H	2.31	0.41
4:L:1154:PRO:HB2	4:L:1157:PHE:CD2	2.55	0.41
4:C:3602:ASN:O	4:C:3606:ILE:HG12	2.20	0.41
9:G:31:GLY:HA3	9:G:48:SER:HA	2.02	0.41
2:A:83:LEU:HD23	2:A:111:PRO:HB3	2.02	0.41
9:O:267:ALA:HA	9:O:268:PRO:HD3	1.95	0.41
4:L:1192:TYR:OH	4:L:1270:PHE:CE2	2.72	0.41
4:C:1224:PHE:CZ	4:C:1270:PHE:CE2	3.09	0.41
4:C:3255:ALA:O	4:C:3259:LEU:HD23	2.20	0.41
4:C:1500:LEU:CD1	4:C:1538:LEU:HD13	2.50	0.41
9:O:134:ILE:HD11	9:P:130:CYS:HA	2.02	0.41
2:A:41:LEU:HD21	2:A:146:VAL:HG12	2.01	0.41
4:L:3750:PHE:CD1	4:L:3804:GLU:HA	2.55	0.41
4:C:864:GLY:O	4:C:868:LYS:HE3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:2:GLU:HB2	9:F:24:TRP:CZ2	2.56	0.41
9:P:31:GLY:HA3	9:P:48:SER:HA	2.02	0.41
2:J:273:ILE:HD13	2:J:368:VAL:HG22	2.01	0.41
2:A:65:GLN:OE1	2:A:65:GLN:HA	2.21	0.41
8:H:208:LYS:O	8:H:212:MET:SD	2.78	0.41
4:C:1238:GLN:N	4:C:1239:PRO:HD2	2.36	0.41
4:C:3761:ASP:HA	4:C:3764:VAL:HG12	2.02	0.41
4:C:3855:TYR:CZ	4:C:4121:TRP:HA	2.55	0.41
6:D:14:DA:C2	6:D:15:DT:C2	3.08	0.41
9:G:73:ALA:HA	9:G:84:TYR:CD2	2.55	0.41
2:A:333:GLU:N	2:A:333:GLU:CG	2.83	0.41
4:L:864:GLY:O	4:L:868:LYS:HE3	2.21	0.41
4:L:1238:GLN:N	4:L:1239:PRO:HD2	2.36	0.41
4:C:1192:TYR:OH	4:C:1270:PHE:CE2	2.71	0.41
4:L:821:ALA:O	4:L:824:LYS:HG3	2.21	0.41
4:C:821:ALA:O	4:C:824:LYS:HG3	2.21	0.41
4:C:2861:ILE:HD13	4:C:2861:ILE:HA	1.93	0.41
2:J:241:ASP:HB2	1:T:185:LEU:HD21	2.03	0.41
4:L:1224:PHE:CZ	4:L:1270:PHE:CE2	3.08	0.41
4:C:395:MET:HG3	4:C:413:PHE:CZ	2.56	0.41
9:F:192:ARG:HD3	10:X:766:PHE:HA	2.03	0.41
9:O:192:ARG:HD3	10:Y:766:PHE:HA	2.03	0.41
4:L:3855:TYR:HA	4:L:3858:MET:HE2	2.03	0.40
7:N:1:DG:N2	7:N:2:DT:C2	2.89	0.40
9:O:2:GLU:HB2	9:O:24:TRP:CZ2	2.56	0.40
4:L:3656:LEU:H	4:L:3656:LEU:HD23	1.86	0.40
9:P:43:TRP:CD1	9:P:115:LYS:HB2	2.57	0.40
4:L:992:ILE:HD13	4:L:1009:LEU:HD21	2.03	0.40
4:L:2603:THR:HB	4:L:2604:PRO:HD3	2.03	0.40
6:M:24:DA:N6	7:N:6:DA:H61	2.20	0.40
4:C:1046:PRO:CD	4:C:1047:GLN:N	2.84	0.40
4:C:1261:LEU:HD11	4:C:1340:ARG:HG3	2.03	0.40
2:J:65:GLN:OE1	2:J:65:GLN:HA	2.21	0.40
4:L:994:TRP:CZ3	4:L:2581:LEU:HB3	2.57	0.40
8:I:208:LYS:CG	8:I:212:MET:SD	3.10	0.40
4:C:994:TRP:CZ3	4:C:2581:LEU:HB3	2.57	0.40
6:D:14:DA:H61	7:E:17:DT:H3	1.70	0.40
7:E:1:DG:N2	7:E:2:DT:C2	2.89	0.40
4:L:1154:PRO:HB2	4:L:1157:PHE:HD2	1.87	0.40
4:L:3442:TYR:HB2	4:L:3443:PRO:HD3	2.04	0.40
8:I:43:GLN:HB2	8:I:45:TRP:CH2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	21/204 (10%)	18 (86%)	3 (14%)	0	100	100
1	T	21/204 (10%)	17 (81%)	4 (19%)	0	100	100
2	A	493/609 (81%)	461 (94%)	32 (6%)	0	100	100
2	J	493/609 (81%)	460 (93%)	33 (7%)	0	100	100
3	B	525/732 (72%)	477 (91%)	42 (8%)	6 (1%)	14	52
3	K	525/732 (72%)	476 (91%)	43 (8%)	6 (1%)	14	52
4	C	3686/4128 (89%)	3440 (93%)	245 (7%)	1 (0%)	100	100
4	L	3686/4128 (89%)	3442 (93%)	243 (7%)	1 (0%)	100	100
8	H	217/299 (73%)	202 (93%)	13 (6%)	2 (1%)	17	56
8	I	212/299 (71%)	201 (95%)	10 (5%)	1 (0%)	29	68
9	F	209/336 (62%)	201 (96%)	7 (3%)	1 (0%)	29	68
9	G	191/336 (57%)	178 (93%)	12 (6%)	1 (0%)	29	68
9	O	209/336 (62%)	201 (96%)	7 (3%)	1 (0%)	29	68
9	P	191/336 (57%)	176 (92%)	12 (6%)	3 (2%)	9	45
10	X	250/911 (27%)	241 (96%)	9 (4%)	0	100	100
10	Y	250/911 (27%)	241 (96%)	9 (4%)	0	100	100
All	All	11179/15110 (74%)	10432 (93%)	724 (6%)	23 (0%)	50	81

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	145	SER
3	K	146	GLN
3	K	518	PRO

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	18/160 (11%)	18 (100%)	0	100	100
1	T	18/160 (11%)	18 (100%)	0	100	100
2	A	452/548 (82%)	446 (99%)	6 (1%)	69	82
2	J	452/548 (82%)	446 (99%)	6 (1%)	69	82
3	B	481/649 (74%)	468 (97%)	13 (3%)	44	66
3	K	481/649 (74%)	468 (97%)	13 (3%)	44	66
4	C	3325/3671 (91%)	3289 (99%)	36 (1%)	73	85
4	L	3325/3671 (91%)	3289 (99%)	36 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	198/262 (76%)	189 (96%)	9 (4%)	27	54
8	I	193/262 (74%)	178 (92%)	15 (8%)	12	38
9	F	191/303 (63%)	174 (91%)	17 (9%)	9	33
9	G	178/303 (59%)	158 (89%)	20 (11%)	6	25
9	O	191/303 (63%)	175 (92%)	16 (8%)	11	36
9	P	178/303 (59%)	158 (89%)	20 (11%)	6	25
10	X	230/808 (28%)	221 (96%)	9 (4%)	32	57
10	Y	230/808 (28%)	221 (96%)	9 (4%)	32	57
All	All	10141/13408 (76%)	9916 (98%)	225 (2%)	54	71

All (225) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	71	TYR
2	J	252	ARG
2	J	299	LYS
2	J	338	LYS
2	J	461	LYS
2	J	505	ASP
2	A	71	TYR
2	A	252	ARG
2	A	299	LYS
2	A	338	LYS
2	A	461	LYS
2	A	505	ASP
3	K	20	MET
3	K	35	LYS
3	K	81	ARG
3	K	97	LYS
3	K	130	ARG
3	K	151	ILE
3	K	203	GLU
3	K	229	GLU
3	K	271	ARG
3	K	286	LYS
3	K	353	ARG
3	K	492	GLN
3	K	518	PRO
4	L	142	ARG

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Mol	Chain	Res	Type
4	L	163	LYS
4	L	406	ARG
4	L	616	LYS
4	L	649	PHE
4	L	824	LYS
4	L	879	MET
4	L	1099	PHE
4	L	1128	CYS
4	L	1268	ASN
4	L	1349	LEU
4	L	1411	TYR
4	L	1640	GLU
4	L	1779	GLN
4	L	1837	ARG
4	L	1990	PHE
4	L	2183	HIS
4	L	2227	LYS
4	L	2270	ASN
4	L	2311	ARG
4	L	2316	TYR
4	L	2338	GLU
4	L	2455	LEU
4	L	2722	ARG
4	L	3179	TRP
4	L	3190	LEU
4	L	3310	ASN
4	L	3357	ARG
4	L	3586	LYS
4	L	3593	ARG
4	L	3750	PHE
4	L	3819	THR
4	L	3831	ASP
4	L	3959	MET
4	L	3969	ASN
4	L	3974	MET
8	H	31	LYS
8	H	62	ASN
8	H	100	VAL
8	H	109	ARG
8	H	124	MET
8	H	151	ARG
8	H	168	GLN

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Mol	Chain	Res	Type
8	H	169	GLU
8	H	295	ARG
8	I	17	GLN
8	I	31	LYS
8	I	41	LEU
8	I	48	GLN
8	I	59	LYS
8	I	118	TYR
8	I	140	MET
8	I	151	ARG
8	I	159	MET
8	I	194	MET
8	I	200	GLU
8	I	204	ILE
8	I	212	MET
8	I	224	GLN
8	I	295	ARG
3	B	20	MET
3	B	35	LYS
3	B	81	ARG
3	B	97	LYS
3	B	130	ARG
3	B	151	ILE
3	B	203	GLU
3	B	229	GLU
3	B	271	ARG
3	B	286	LYS
3	B	353	ARG
3	B	492	GLN
3	B	518	PRO
4	C	142	ARG
4	C	163	LYS
4	C	406	ARG
4	C	616	LYS
4	C	649	PHE
4	C	824	LYS
4	C	879	MET
4	C	1099	PHE
4	C	1128	CYS
4	C	1268	ASN
4	C	1349	LEU
4	C	1411	TYR

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Mol	Chain	Res	Type
4	C	1640	GLU
4	C	1779	GLN
4	C	1837	ARG
4	C	1990	PHE
4	C	2183	HIS
4	C	2227	LYS
4	C	2270	ASN
4	C	2311	ARG
4	C	2316	TYR
4	C	2338	GLU
4	C	2455	LEU
4	C	2722	ARG
4	C	3179	TRP
4	C	3190	LEU
4	C	3310	ASN
4	C	3357	ARG
4	C	3586	LYS
4	C	3593	ARG
4	C	3750	PHE
4	C	3819	THR
4	C	3831	ASP
4	C	3959	MET
4	C	3969	ASN
4	C	3974	MET
9	F	3	ARG
9	F	6	SER
9	F	22	VAL
9	F	23	SER
9	F	26	LYS
9	F	40	HIS
9	F	71	ARG
9	F	90	LYS
9	F	104	VAL
9	F	110	SER
9	F	112	ASN
9	F	114	GLU
9	F	116	VAL
9	F	117	GLU
9	F	122	VAL
9	F	125	GLU
9	F	161	ARG
10	X	661	ASP

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Mol	Chain	Res	Type
10	X	783	ASN
10	X	788	THR
10	X	792	MET
10	X	821	ASP
10	X	830	SER
10	X	837	ARG
10	X	856	LEU
10	X	862	HIS
9	G	1	MET
9	G	4	LYS
9	G	28	LEU
9	G	34	ILE
9	G	47	VAL
9	G	51	GLU
9	G	52	ILE
9	G	57	ASP
9	G	67	VAL
9	G	70	LEU
9	G	85	THR
9	G	89	SER
9	G	91	GLU
9	G	93	CYS
9	G	115	LYS
9	G	118	ASN
9	G	163	GLU
9	G	165	CYS
9	G	174	THR
9	G	192	ARG
9	O	3	ARG
9	O	6	SER
9	O	22	VAL
9	O	23	SER
9	O	26	LYS
9	O	40	HIS
9	O	71	ARG
9	O	90	LYS
9	O	110	SER
9	O	112	ASN
9	O	114	GLU
9	O	116	VAL
9	O	117	GLU
9	O	122	VAL

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Mol	Chain	Res	Type
9	O	125	GLU
9	O	161	ARG
10	Y	661	ASP
10	Y	783	ASN
10	Y	788	THR
10	Y	792	MET
10	Y	821	ASP
10	Y	830	SER
10	Y	837	ARG
10	Y	856	LEU
10	Y	862	HIS
9	P	1	MET
9	P	4	LYS
9	P	28	LEU
9	P	34	ILE
9	P	47	VAL
9	P	51	GLU
9	P	52	ILE
9	P	57	ASP
9	P	67	VAL
9	P	70	LEU
9	P	85	THR
9	P	89	SER
9	P	91	GLU
9	P	93	CYS
9	P	115	LYS
9	P	118	ASN
9	P	163	GLU
9	P	165	CYS
9	P	174	THR
9	P	192	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	187	ASN
2	J	68	GLN
2	J	405	ASN
2	A	68	GLN
2	A	405	ASN
3	K	246	HIS
4	L	739	ASN

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Mol	Chain	Res	Type
4	L	2270	ASN
4	L	2283	ASN
4	L	2306	ASN
4	L	2422	GLN
4	L	2481	HIS
4	L	2543	ASN
4	L	2859	GLN
4	L	4068	HIS
8	I	46	HIS
8	I	48	GLN
3	B	246	HIS
4	C	739	ASN
4	C	2270	ASN
4	C	2283	ASN
4	C	2306	ASN
4	C	2422	GLN
4	C	2859	GLN
4	C	4068	HIS
9	F	40	HIS
9	F	277	GLN
1	T	187	ASN
9	O	40	HIS
9	O	277	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	ATP	L	4201	-	26,33,33	1.25	2 (7%)	31,52,52	1.56	5 (16%)
11	ATP	C	4201	-	26,33,33	1.25	1 (3%)	31,52,52	1.49	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ATP	L	4201	-	-	6/18/38/38	0/3/3/3
11	ATP	C	4201	-	-	4/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	4201	ATP	O4'-C1'	3.75	1.46	1.41
11	L	4201	ATP	O4'-C1'	3.59	1.46	1.41
11	L	4201	ATP	C2'-C1'	2.10	1.56	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	4201	ATP	C4-C5-N7	4.18	113.76	109.40
11	C	4201	ATP	C4-C5-N7	4.15	113.72	109.40
11	L	4201	ATP	PB-O3B-PG	-3.44	121.03	132.83
11	C	4201	ATP	PB-O3B-PG	-3.27	121.62	132.83
11	L	4201	ATP	PA-O3A-PB	-2.87	122.97	132.83
11	C	4201	ATP	PA-O3A-PB	-2.87	122.97	132.83
11	C	4201	ATP	O2G-PG-O3B	2.06	111.54	104.64
11	L	4201	ATP	O2G-PG-O3B	2.04	111.47	104.64
11	L	4201	ATP	C2-N1-C6	-2.01	115.32	118.75

There are no chirality outliers.

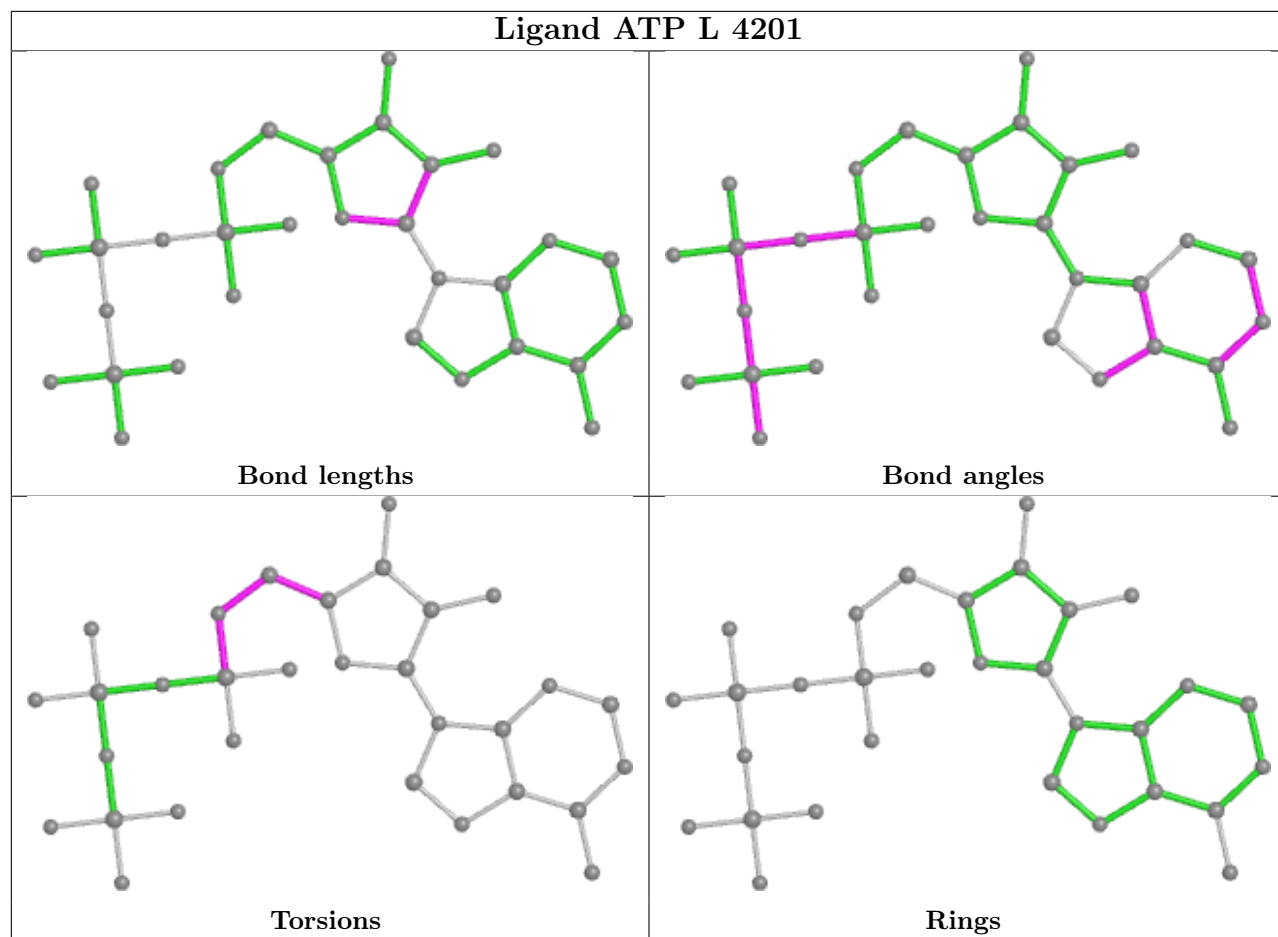
All (10) torsion outliers are listed below:

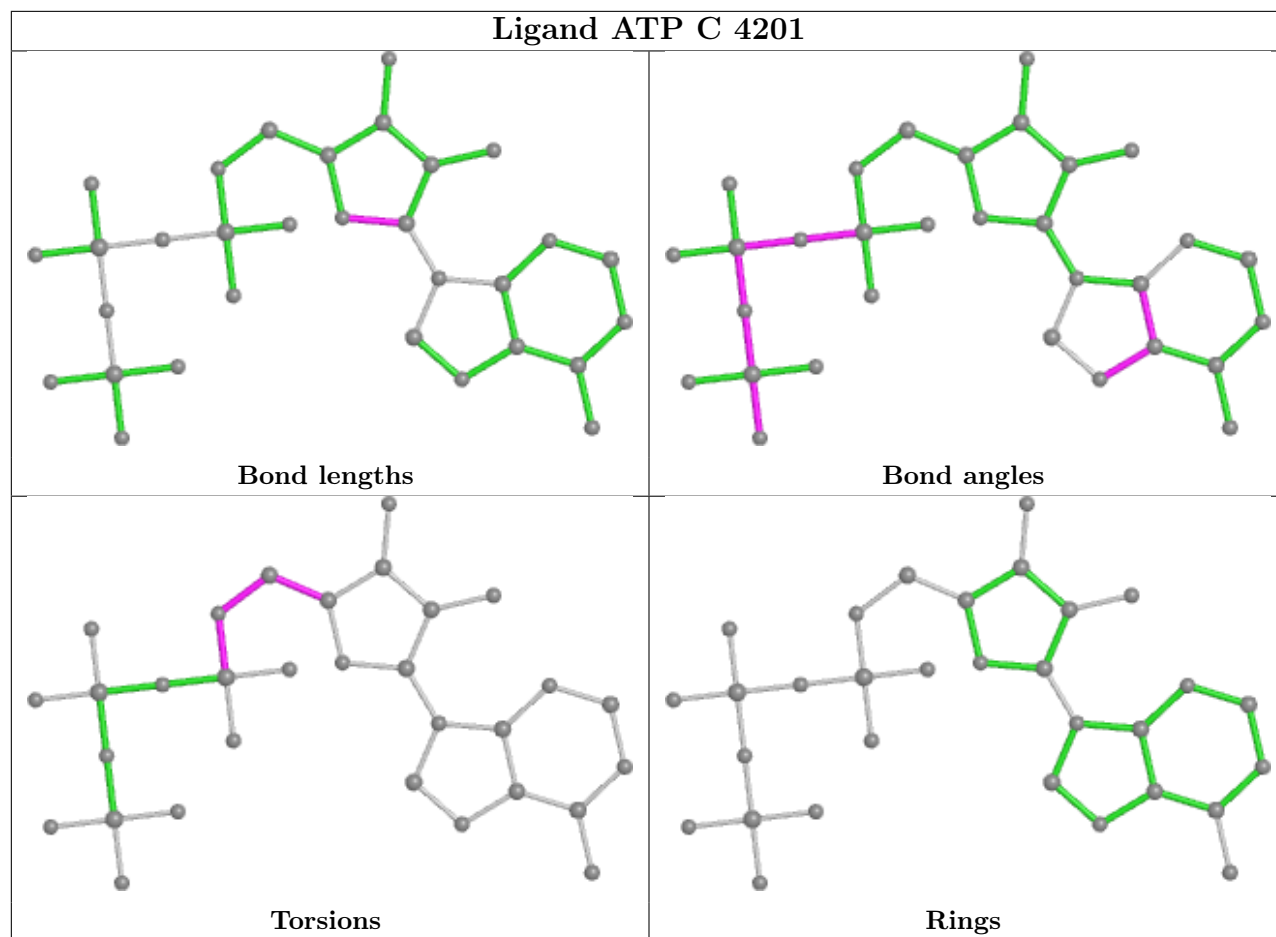
Mol	Chain	Res	Type	Atoms
11	L	4201	ATP	C5'-O5'-PA-O1A
11	L	4201	ATP	O4'-C4'-C5'-O5'
11	L	4201	ATP	C3'-C4'-C5'-O5'
11	C	4201	ATP	O4'-C4'-C5'-O5'
11	C	4201	ATP	C3'-C4'-C5'-O5'
11	C	4201	ATP	C4'-C5'-O5'-PA
11	L	4201	ATP	C5'-O5'-PA-O3A
11	L	4201	ATP	C5'-O5'-PA-O2A
11	L	4201	ATP	C4'-C5'-O5'-PA
11	C	4201	ATP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

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

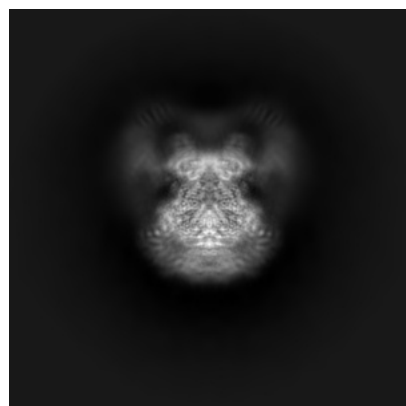
6 Map visualisation [i](#)

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

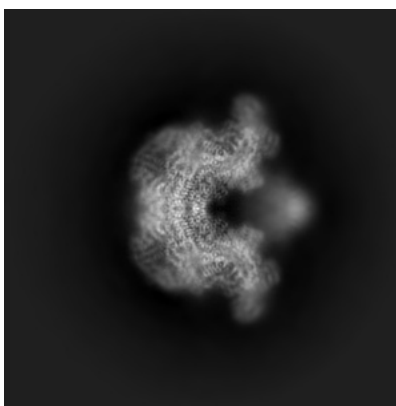
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

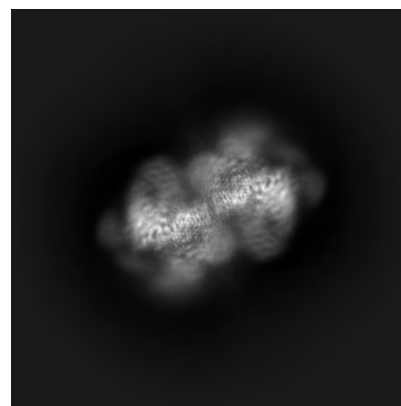
6.1.1 Primary map



X

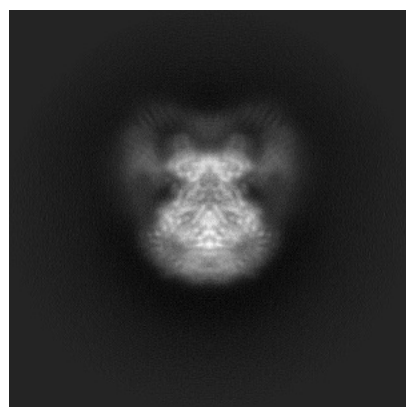


Y

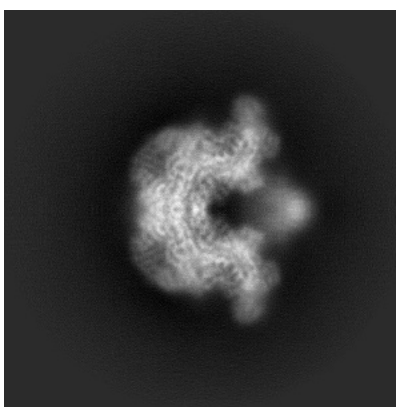


Z

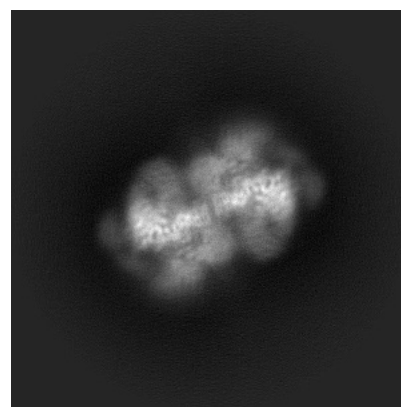
6.1.2 Raw map



X



Y

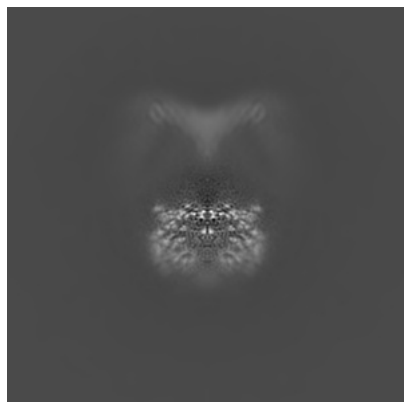


Z

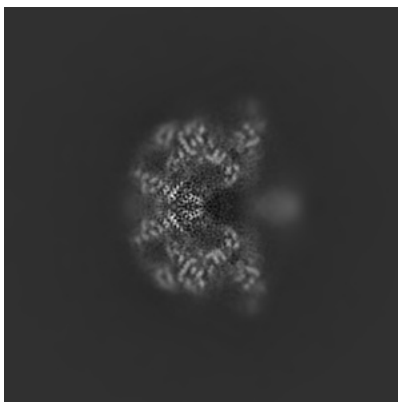
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

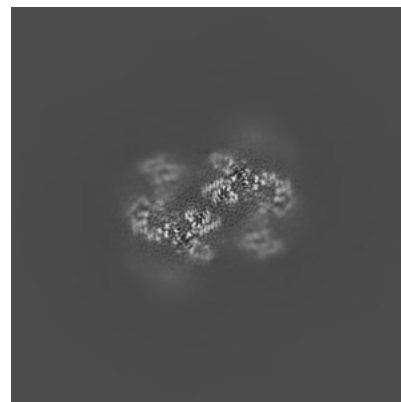
6.2.1 Primary map



X Index: 240

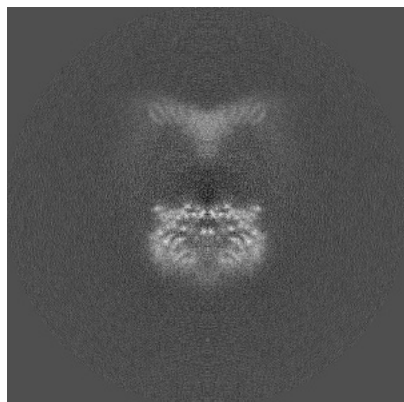


Y Index: 240

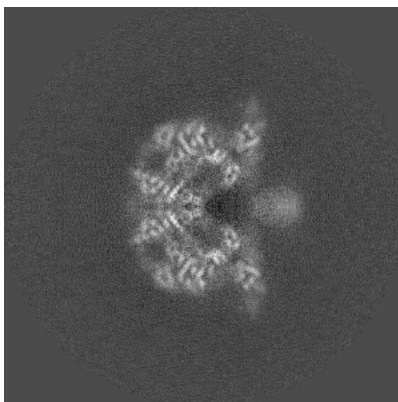


Z Index: 240

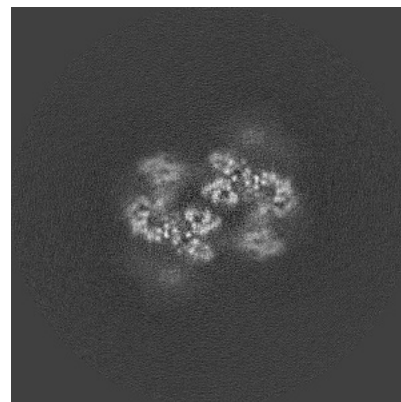
6.2.2 Raw map



X Index: 240



Y Index: 240

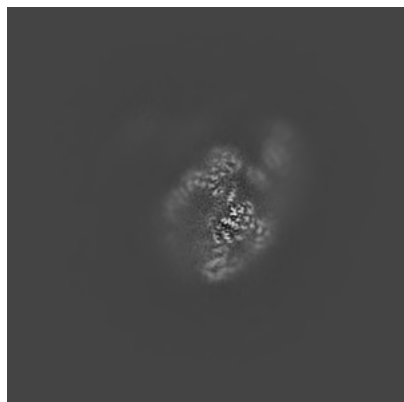


Z Index: 240

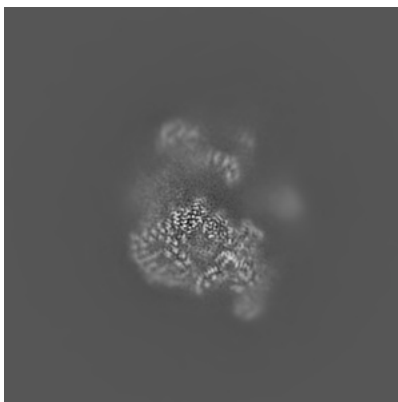
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

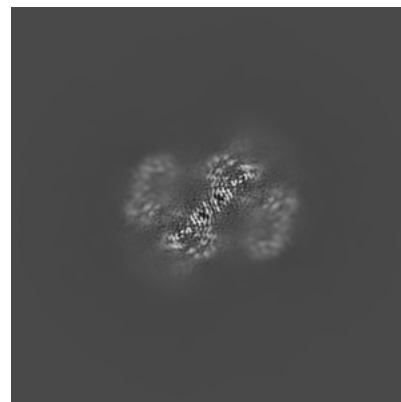
6.3.1 Primary map



X Index: 278

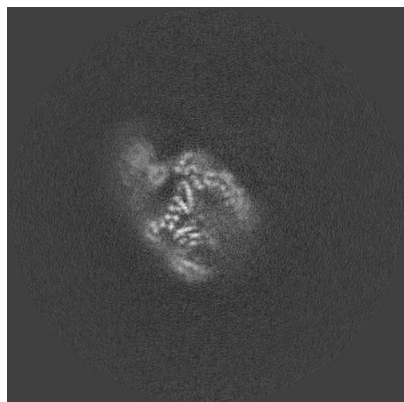


Y Index: 226

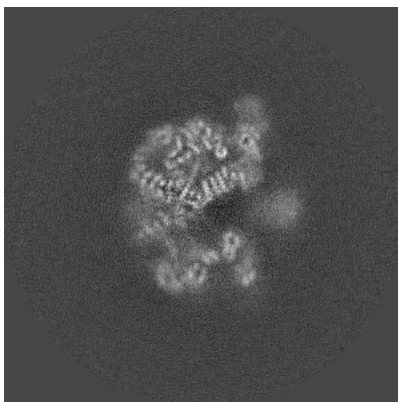


Z Index: 227

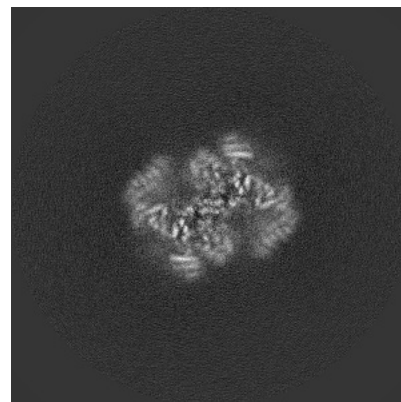
6.3.2 Raw map



X Index: 196



Y Index: 247

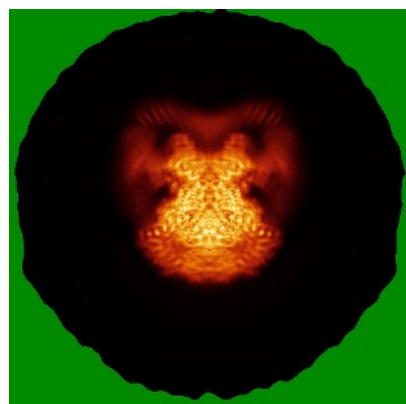


Z Index: 211

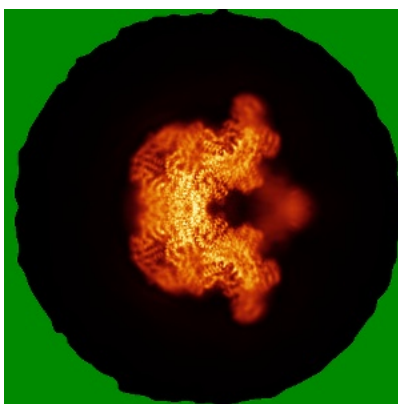
The images above show the largest variance slices of the map in three orthogonal directions.

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

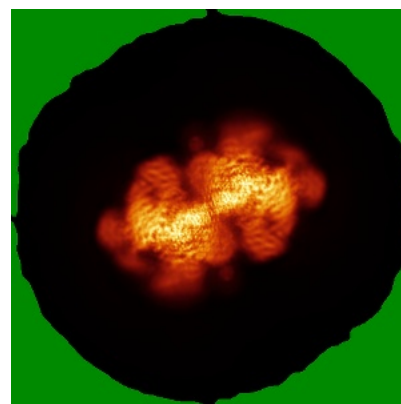
6.4.1 Primary map



X

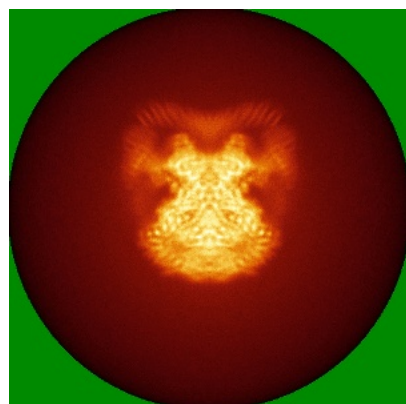


Y

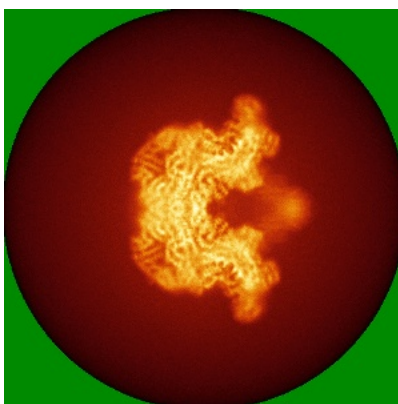


Z

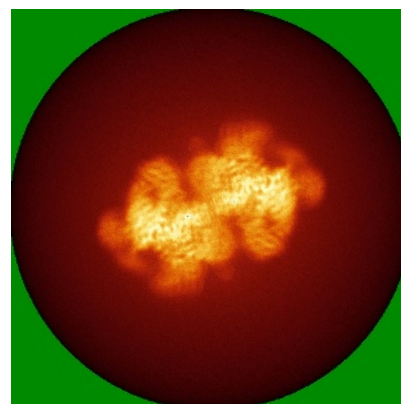
6.4.2 Raw map



X



Y

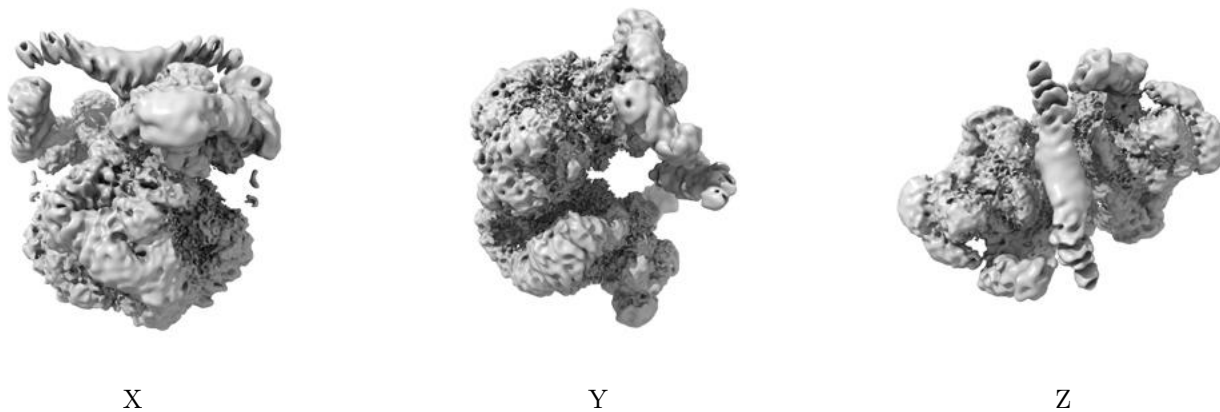


Z

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

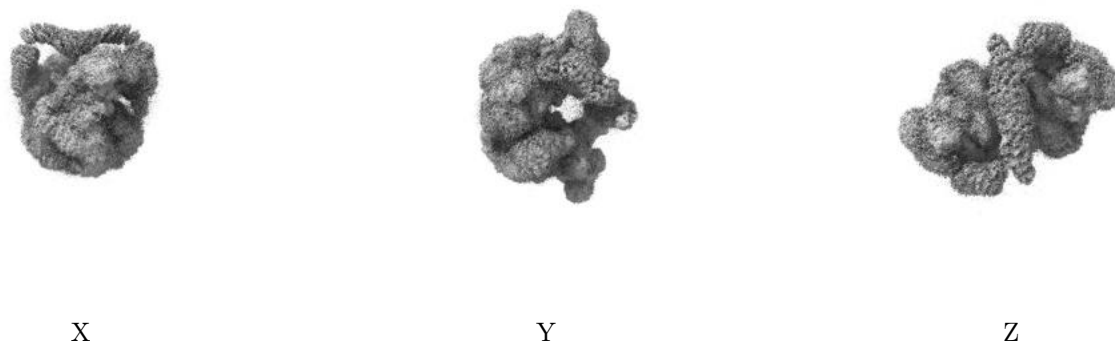
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

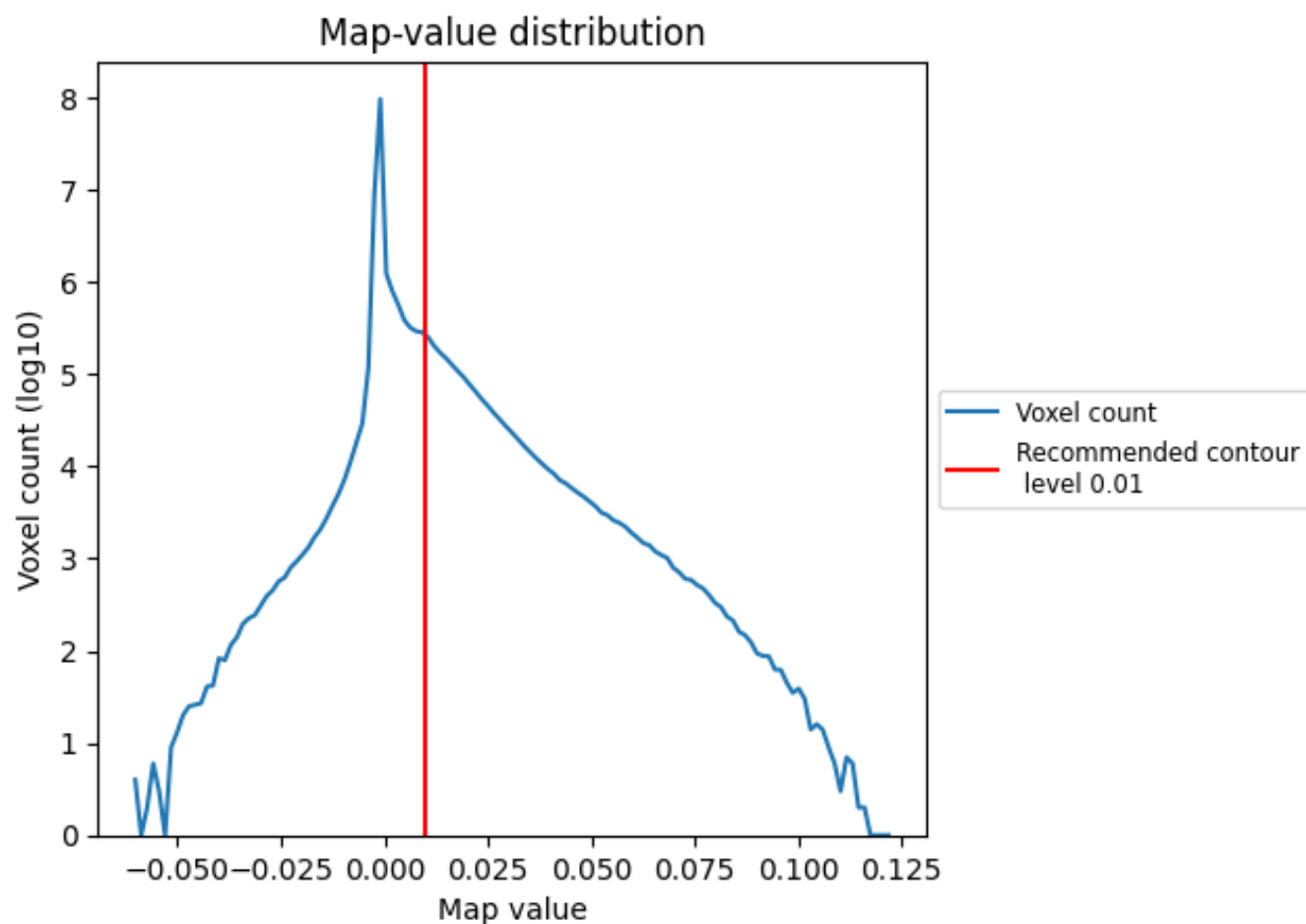
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

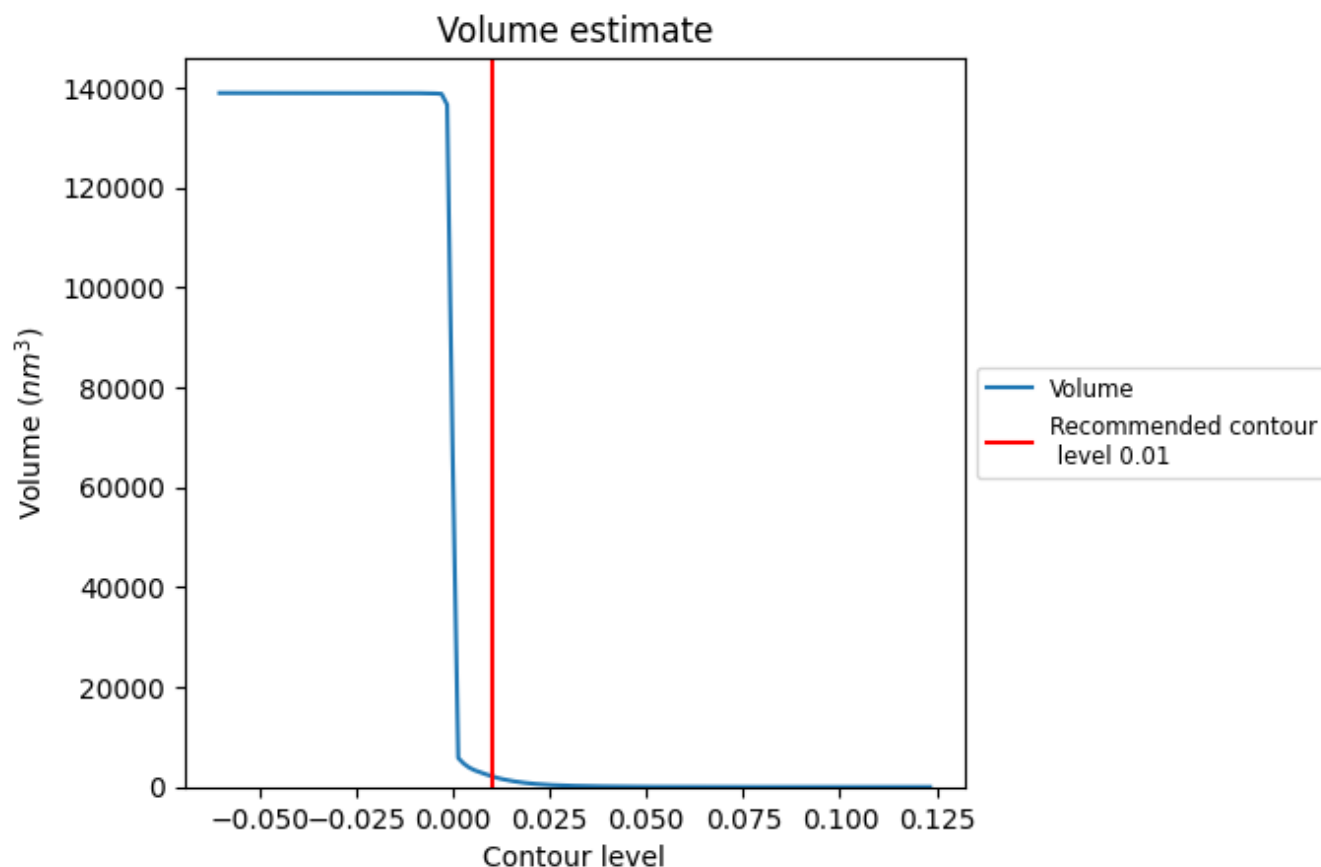
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

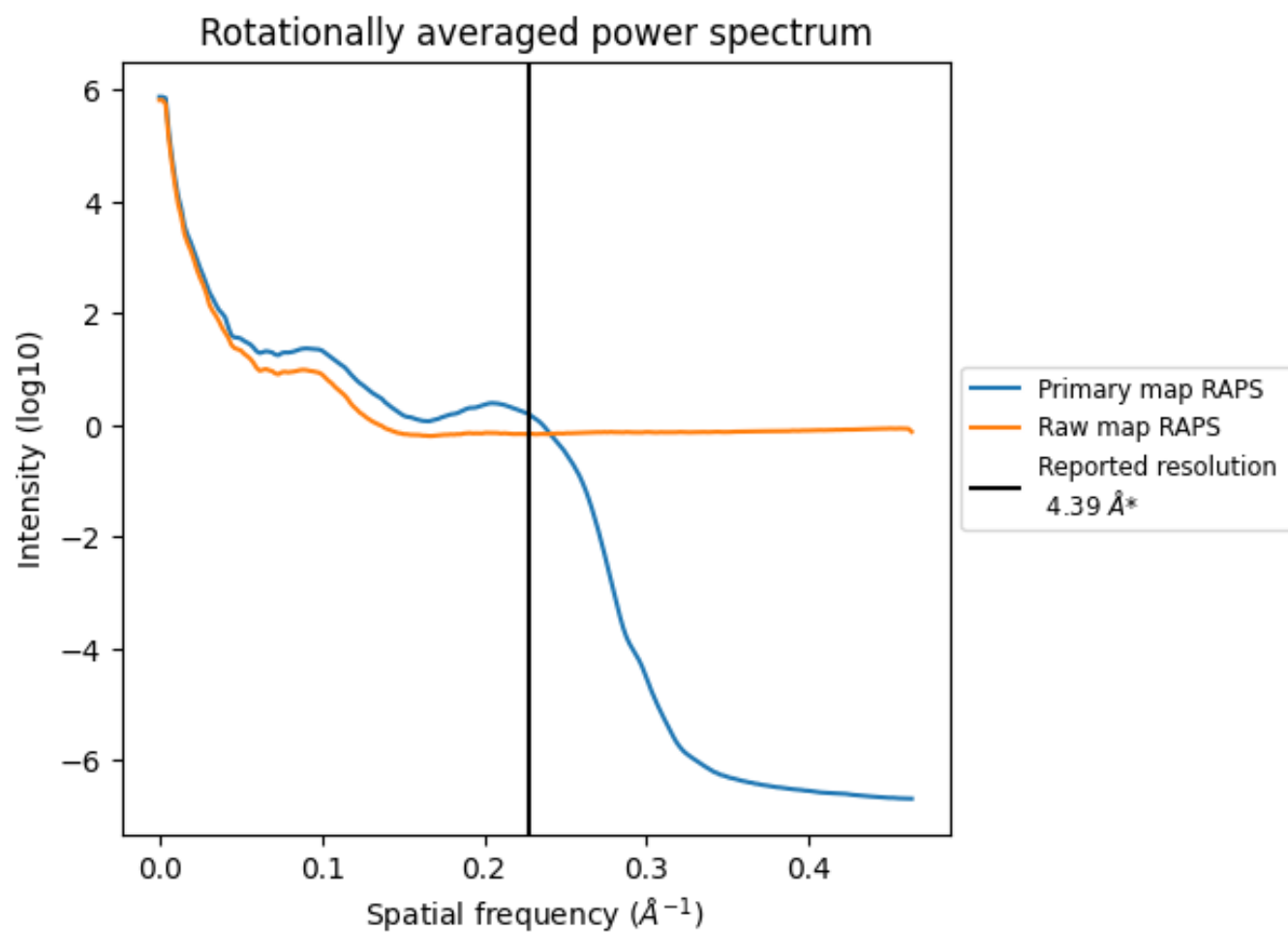
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2174 nm^3 ; this corresponds to an approximate mass of 1964 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

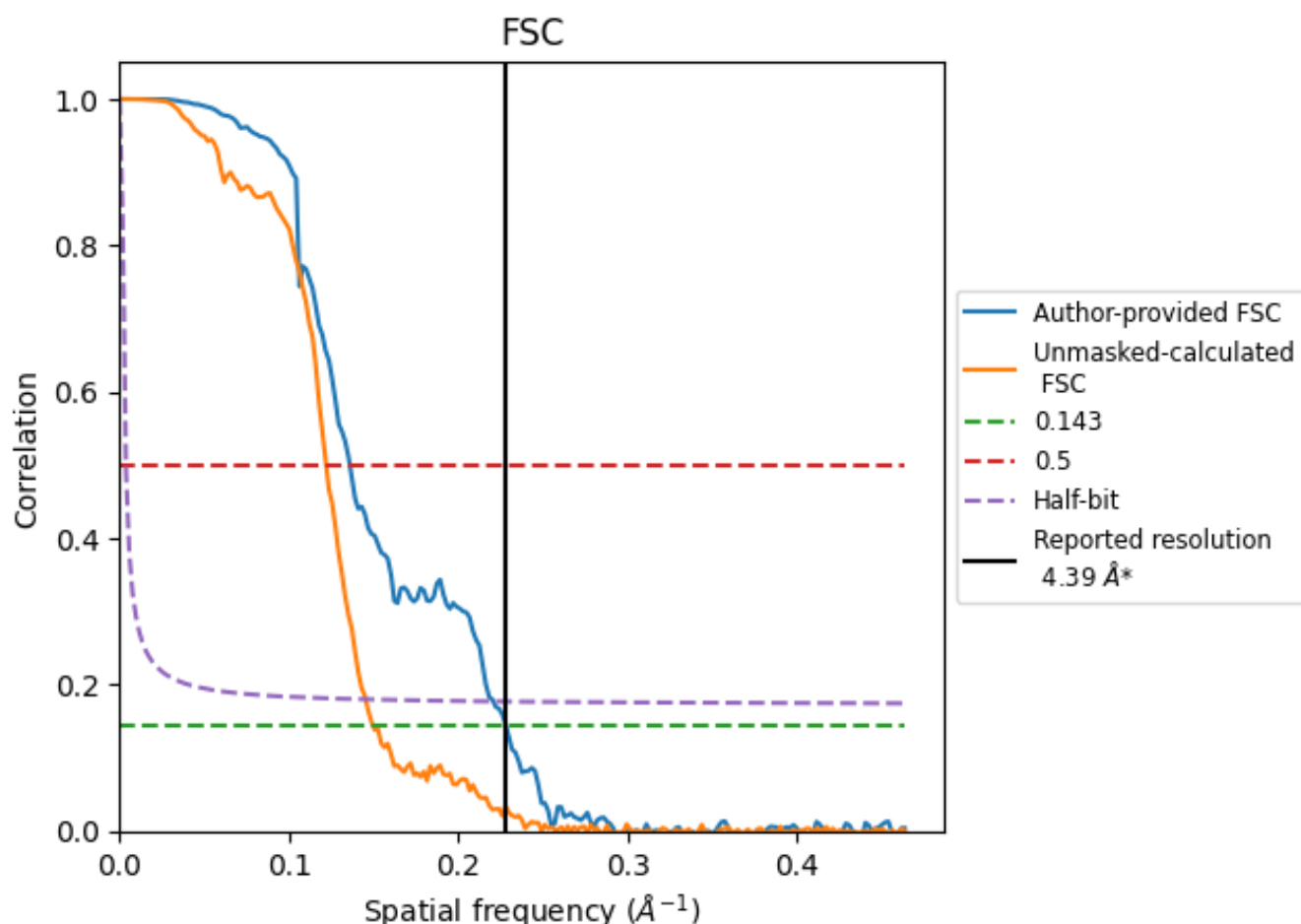


*Reported resolution corresponds to spatial frequency of 0.228 \AA^{-1}

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 0.228 Å⁻¹

8.2 Resolution estimates [i](#)

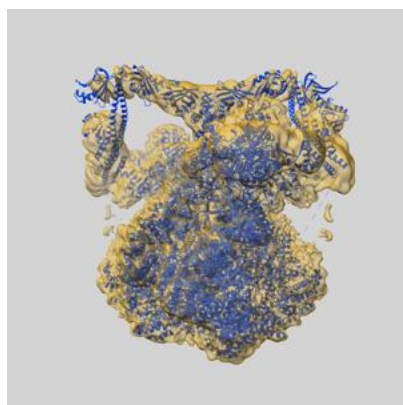
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.39	-	-
Author-provided FSC curve	4.38	7.36	4.53
Unmasked-calculated*	6.68	8.19	6.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.68 differs from the reported value 4.39 by more than 10 %

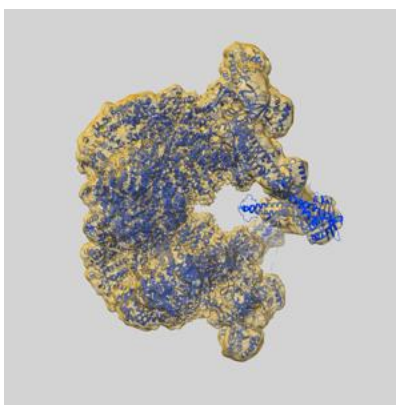
9 Map-model fit [i](#)

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

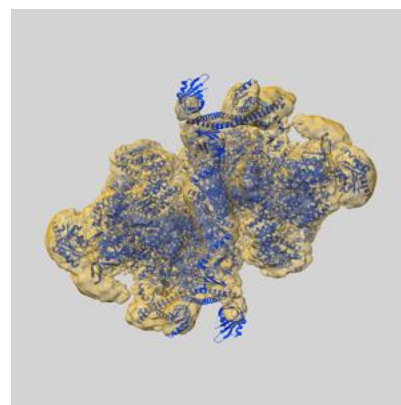
9.1 Map-model overlay [i](#)



X



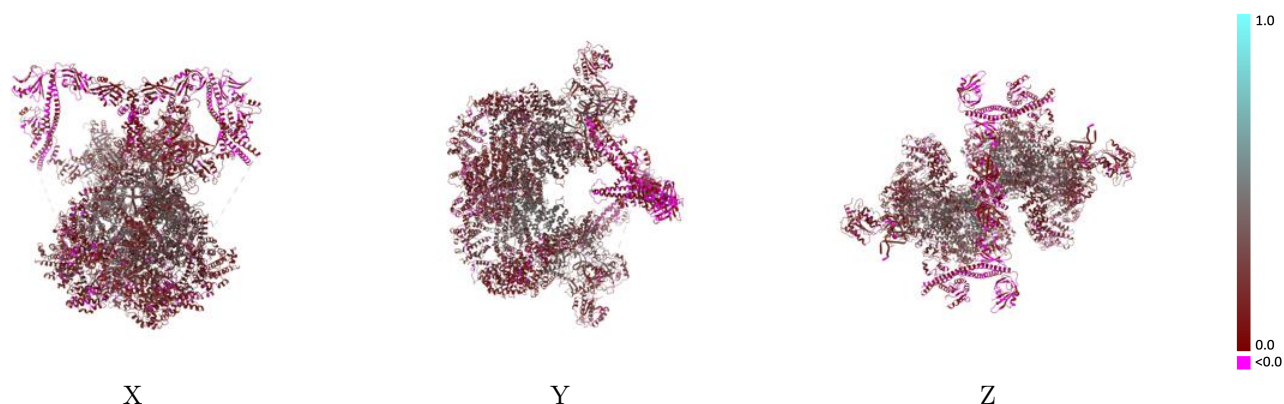
Y



Z

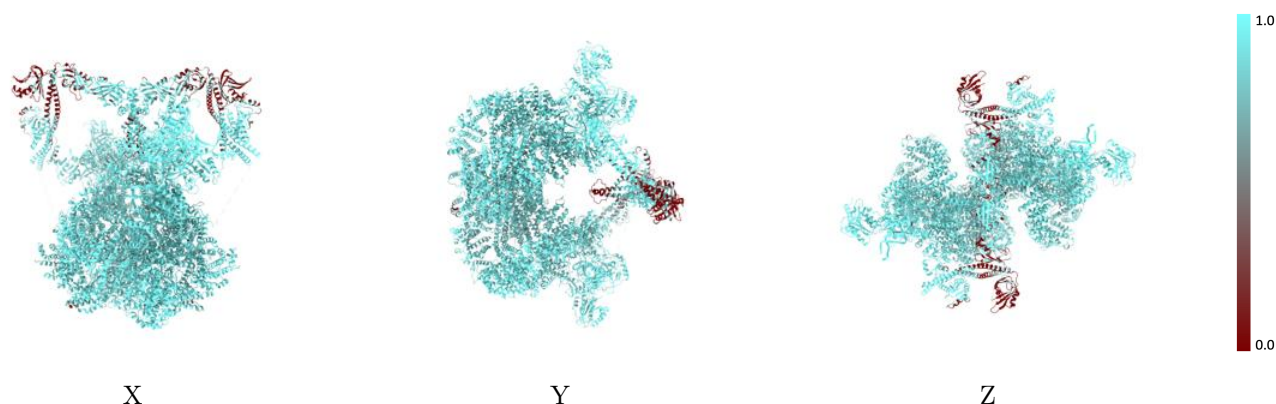
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



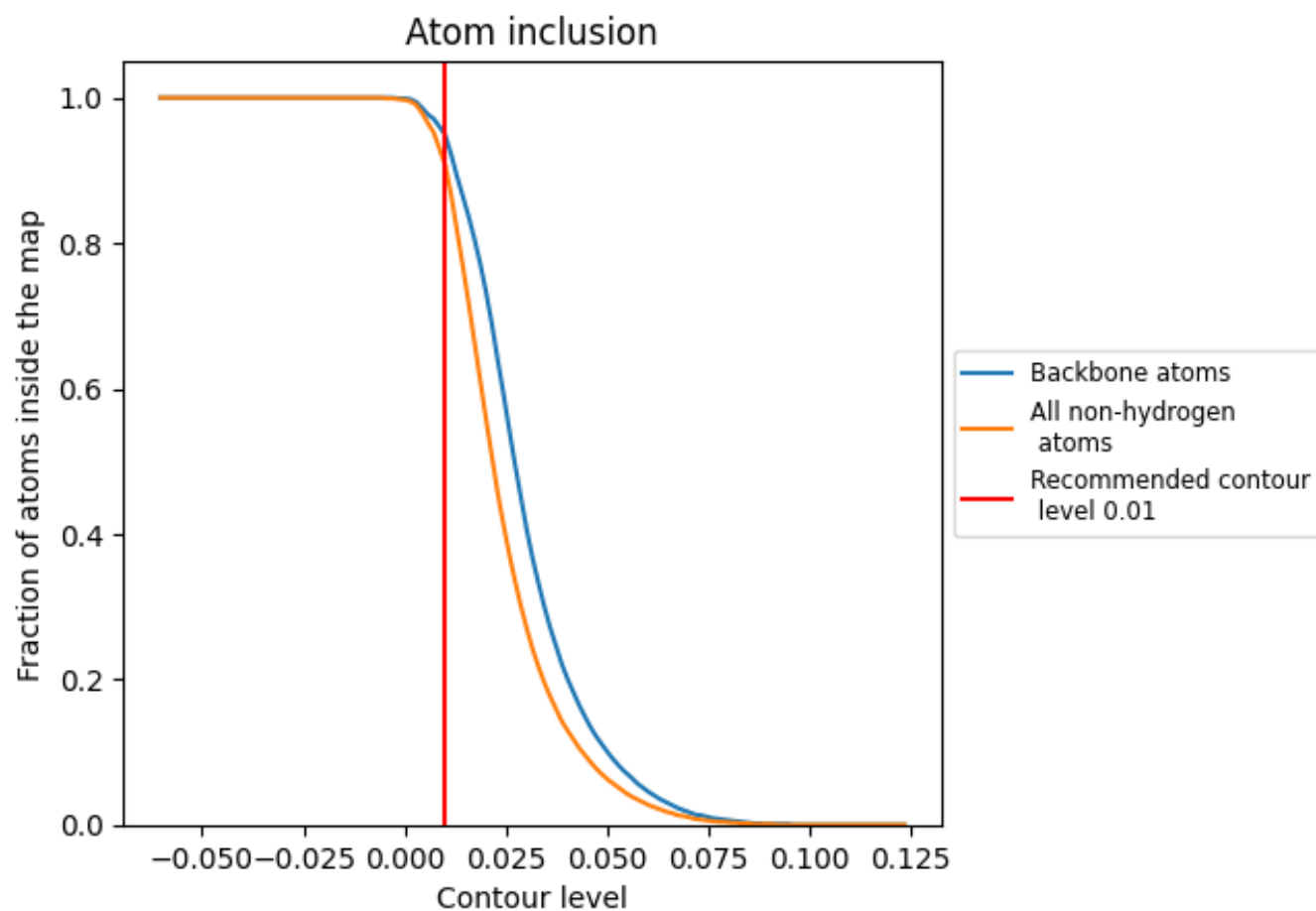
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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















































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

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

