



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 11:51 PM UTC

PDB ID : 8DFA / pdb_00008dfa
EMDB ID : EMD-27403
Title : type I-C Cascade bound to ssDNA target
Authors : O'Brien, R.E.; Bravo, J.P.K.; Ramos, D.; Hibshman, G.N.; Wright, J.T.; Taylor, D.W.
Deposited on : 2022-06-21
Resolution : 2.80 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:

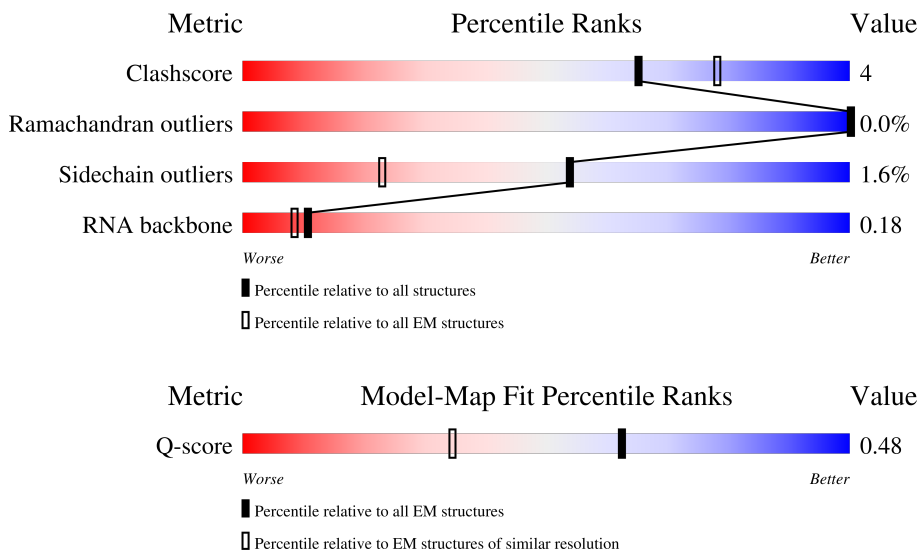
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	227	
2	B	290	
2	C	290	

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Mol	Chain	Length	Quality of chain
2	D	290	
2	E	290	
2	F	290	
2	G	290	
2	H	290	
3	I	612	
4	J	124	
4	K	124	
5	L	46	
6	N	18	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 46813 atoms, of which 23023 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 pre-crRNA processing endonuclease.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	220	3535	1123	1761	323	318	10	0	0

- Molecule 2 is a protein called CRISPR-associated protein, TM1801 family.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	B	270	4193	1324	2081	378	397	13	0	0
2	C	286	4462	1406	2224	399	419	14	0	0
2	D	286	4462	1406	2224	399	419	14	0	0
2	E	286	4462	1406	2224	399	419	14	0	0
2	F	286	4462	1406	2224	399	419	14	0	0
2	G	286	4462	1406	2224	399	419	14	0	0
2	H	286	4462	1406	2224	399	419	14	0	0

- Molecule 3 is a protein called CRISPR-associated protein, CT1133 family.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	I	415	6536	2067	3269	586	599	15	0	0

- Molecule 4 is a protein called CRISPR-associated protein, CT1133 family.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	J	117	1863	589	933	164	172	5	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	K	117	1863	589	933	164	172	5	0	0

- Molecule 5 is a RNA chain called RNA (46-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
5	L	46	1480	438	500	178	319	45	0	0

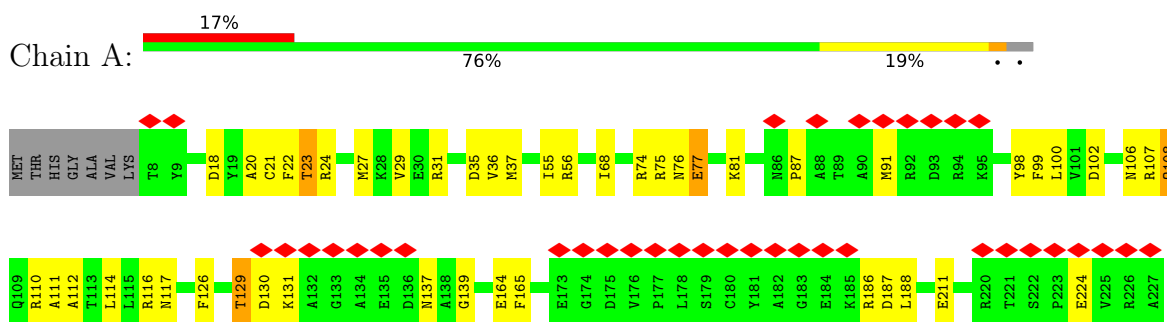
- Molecule 6 is DNA/RNA hybrid called TS.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
6	N	18	571	174	202	69	108	18	0	0

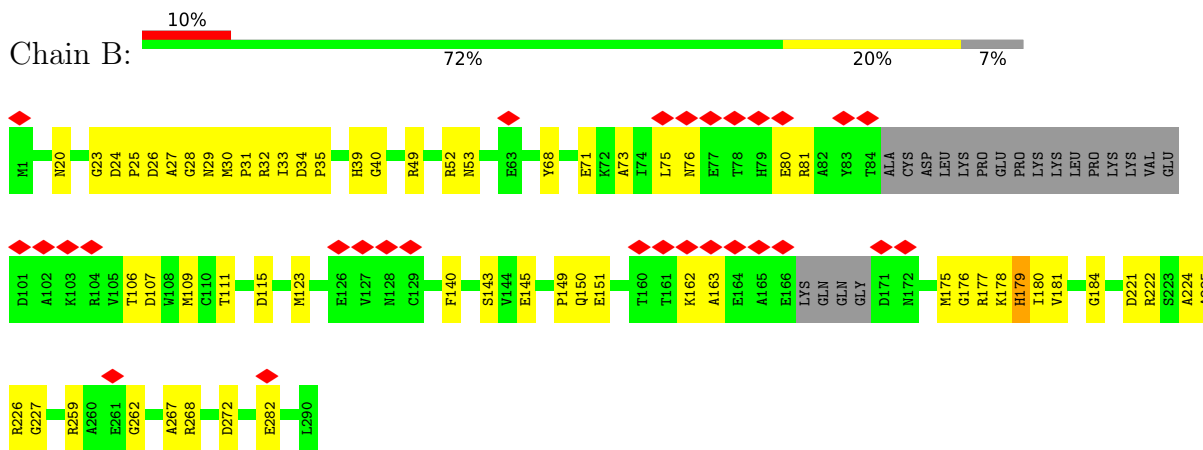
3 Residue-property plots [i](#)

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

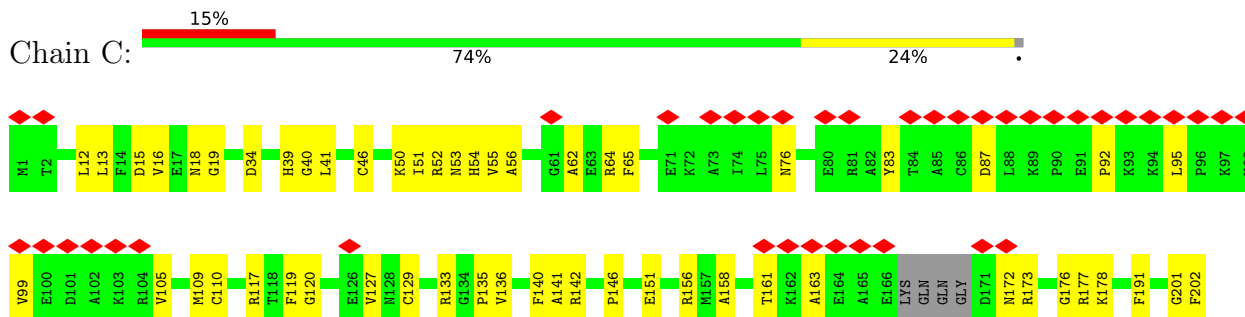
- Molecule 1: pre-crRNA processing endonuclease

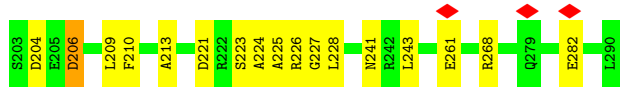


- Molecule 2: CRISPR-associated protein, TM1801 family

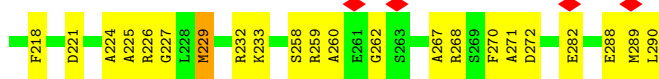
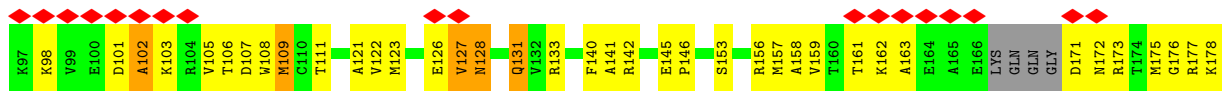
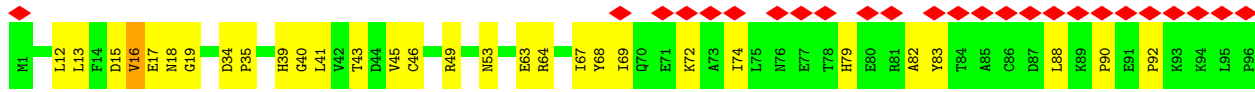


- Molecule 2: CRISPR-associated protein, TM1801 family

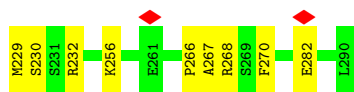
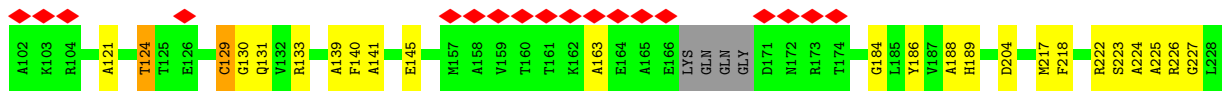
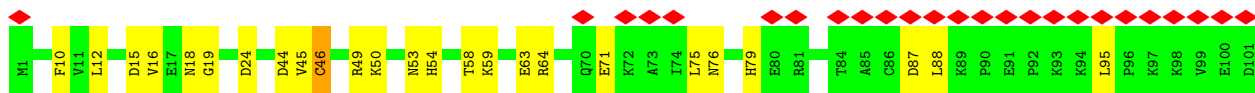
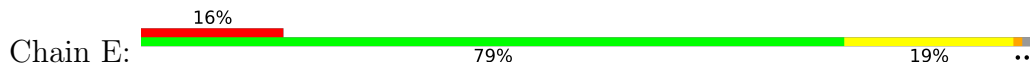




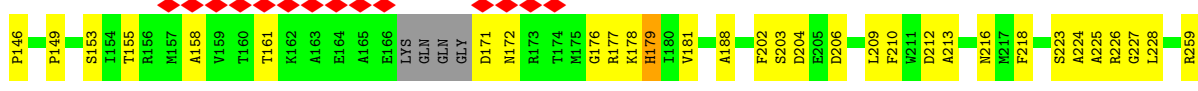
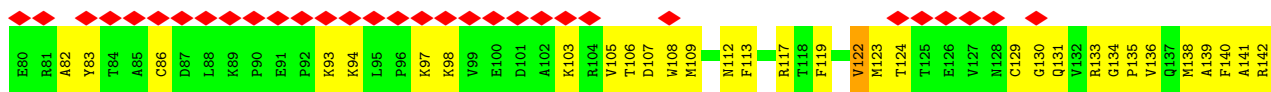
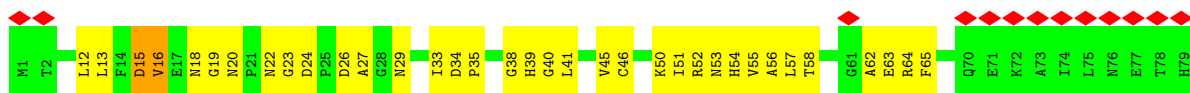
• Molecule 2: CRISPR-associated protein, TM1801 family



• Molecule 2: CRISPR-associated protein, TM1801 family

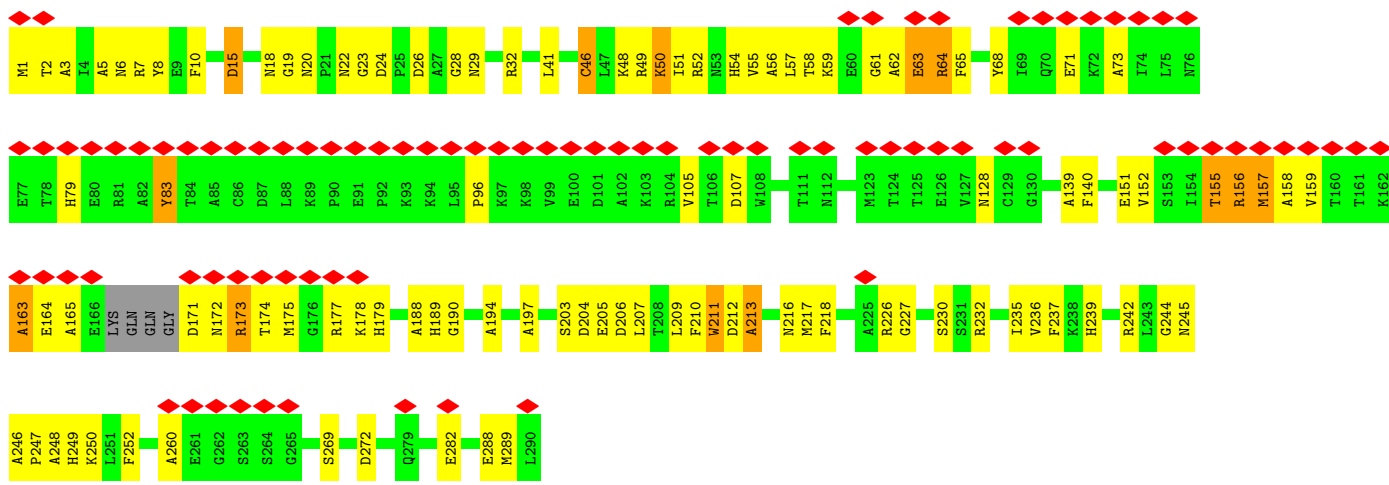


• Molecule 2: CRISPR-associated protein, TM1801 family

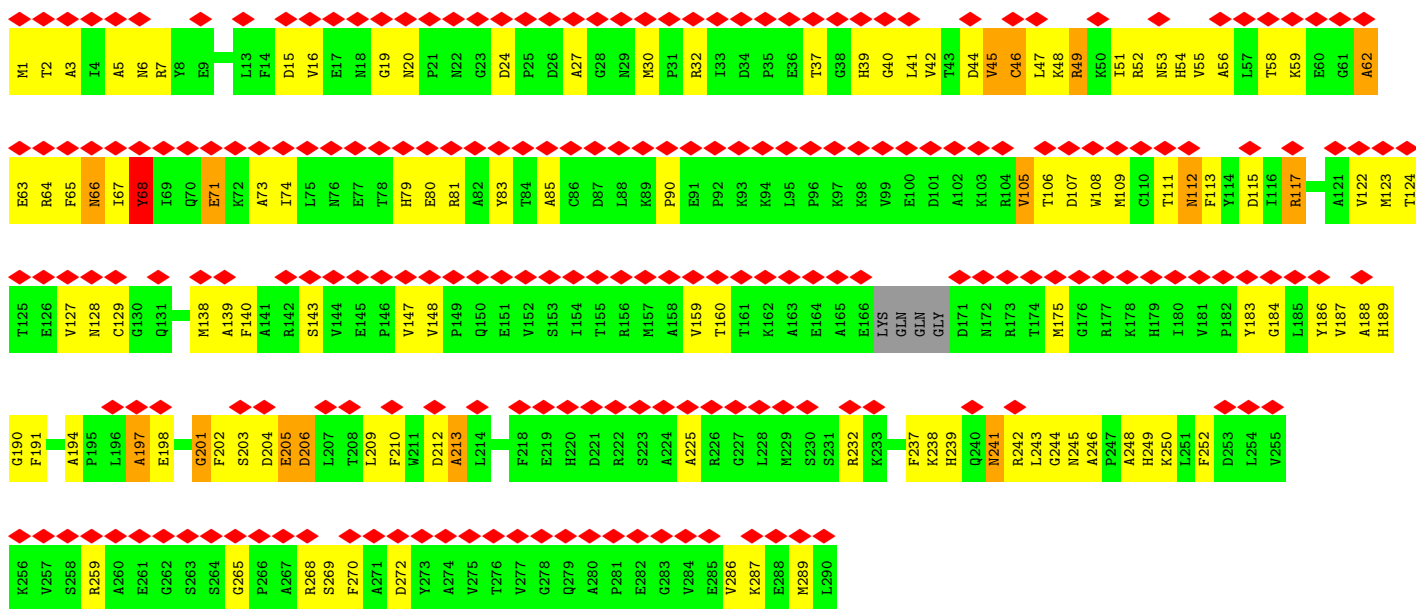
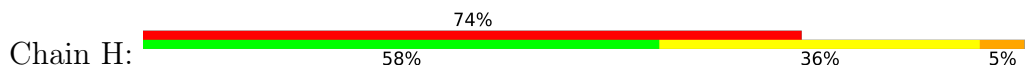




• Molecule 2: CRISPR-associated protein, TM1801 family



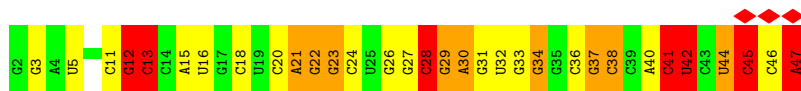
• Molecule 2: CRISPR-associated protein, TM1801 family



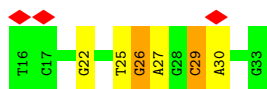
• Molecule 3: CRISPR-associated protein, CT1133 family



• Molecule 5: RNA (46-MER)



• Molecule 6: TS



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	174004	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.5	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	11.064	Depositor
Minimum map value	-4.191	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.171	Depositor
Recommended contour level	1.55	Depositor
Map size (\AA)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	Depositor

5 Model quality i

5.1 Standard geometry i

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	1.51	27/1817 (1.5%)	1.47	56/2460 (2.3%)
2	B	1.61	42/2153 (2.0%)	1.52	50/2909 (1.7%)
2	C	1.83	41/2283 (1.8%)	1.80	68/3085 (2.2%)
2	D	1.79	45/2283 (2.0%)	1.67	66/3085 (2.1%)
2	E	1.60	32/2283 (1.4%)	1.55	53/3085 (1.7%)
2	F	1.97	39/2283 (1.7%)	1.97	108/3085 (3.5%)
2	G	2.14	55/2283 (2.4%)	2.12	124/3085 (4.0%)
2	H	1.83	43/2283 (1.9%)	1.85	98/3085 (3.2%)
3	I	2.01	68/3334 (2.0%)	1.97	117/4506 (2.6%)
4	J	2.43	28/947 (3.0%)	2.28	58/1274 (4.6%)
4	K	2.29	27/947 (2.9%)	2.20	39/1274 (3.1%)
5	L	1.40	9/1095 (0.8%)	1.33	11/1706 (0.6%)
6	N	1.40	3/413 (0.7%)	1.95	3/635 (0.5%)
All	All	1.86	459/24404 (1.9%)	1.82	851/33274 (2.6%)

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	F	0	1
2	G	0	4
2	H	0	3
3	I	0	1
5	L	0	3
All	All	0	12

All (459) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	189	HIS	CE1-NE2	-8.92	1.23	1.32
2	G	239	HIS	CE1-NE2	-8.91	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	353	HIS	CE1-NE2	-8.89	1.23	1.32
2	B	179	HIS	CE1-NE2	-8.88	1.23	1.32
2	G	54	HIS	CE1-NE2	-8.87	1.23	1.32
3	I	550	HIS	CE1-NE2	-8.87	1.23	1.32
2	B	39	HIS	CE1-NE2	-8.85	1.23	1.32
2	E	79	HIS	ND1-CE1	-8.85	1.23	1.32
2	F	179	HIS	ND1-CE1	-8.85	1.23	1.32
4	K	111	HIS	CE1-NE2	-8.84	1.23	1.32
2	D	39	HIS	CE1-NE2	-8.84	1.23	1.32
2	F	54	HIS	ND1-CE1	-8.84	1.23	1.32
2	B	27	ALA	CA-CB	-8.82	1.42	1.52
2	C	54	HIS	CE1-NE2	-8.81	1.23	1.32
4	K	53	HIS	CE1-NE2	-8.80	1.23	1.32
3	I	376	HIS	ND1-CE1	-8.80	1.23	1.32
4	J	62	HIS	CE1-NE2	-8.79	1.23	1.32
2	H	249	HIS	CE1-NE2	-8.77	1.23	1.32
2	G	249	HIS	CE1-NE2	-8.76	1.23	1.32
3	I	541	HIS	CE1-NE2	-8.74	1.23	1.32
2	F	39	HIS	ND1-CE1	-8.74	1.23	1.32
2	H	239	HIS	ND1-CE1	-8.71	1.23	1.32
2	G	189	HIS	ND1-CE1	-8.71	1.23	1.32
2	C	39	HIS	ND1-CE1	-8.70	1.23	1.32
4	K	62	HIS	CE1-NE2	-8.68	1.23	1.32
2	H	189	HIS	CE1-NE2	-8.68	1.23	1.32
2	F	176	GLY	N-CA	-8.62	1.38	1.44
2	G	179	HIS	ND1-CE1	-8.60	1.24	1.32
1	A	107	ARG	CZ-NH2	-8.25	1.22	1.33
2	G	49	ARG	CZ-NH2	-8.24	1.22	1.33
2	E	226	ARG	CZ-NH2	-8.20	1.22	1.33
1	A	74	ARG	CZ-NH2	-8.20	1.22	1.33
2	C	117	ARG	CZ-NH2	-8.20	1.22	1.33
2	B	32	ARG	CZ-NH2	-8.19	1.22	1.33
1	A	110	ARG	CZ-NH2	-8.19	1.22	1.33
2	C	156	ARG	CZ-NH2	-8.19	1.22	1.33
2	D	226	ARG	CZ-NH2	-8.18	1.22	1.33
3	I	550	HIS	CD2-NE2	-8.18	1.28	1.37
2	H	249	HIS	CD2-NE2	-8.17	1.28	1.37
1	A	24	ARG	CZ-NH2	-8.16	1.22	1.33
1	A	75	ARG	CZ-NH2	-8.16	1.22	1.33
4	J	67	ARG	CZ-NH2	-8.16	1.22	1.33
2	C	133	ARG	CZ-NH2	-8.16	1.22	1.33
2	C	226	ARG	CZ-NH2	-8.16	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	49	ARG	CZ-NH2	-8.15	1.22	1.33
2	D	142	ARG	CZ-NH2	-8.15	1.22	1.33
2	G	7	ARG	CZ-NH2	-8.14	1.22	1.33
2	G	249	HIS	CD2-NE2	-8.14	1.28	1.37
2	D	49	ARG	CZ-NH2	-8.14	1.22	1.33
4	J	113	ARG	CZ-NH2	-8.14	1.22	1.33
2	G	52	ARG	CZ-NH2	-8.14	1.22	1.33
2	D	133	ARG	CZ-NH2	-8.13	1.22	1.33
2	E	133	ARG	CZ-NH2	-8.13	1.22	1.33
2	C	268	ARG	CZ-NH2	-8.13	1.22	1.33
1	A	116	ARG	CZ-NH2	-8.13	1.22	1.33
2	G	64	ARG	CZ-NH2	-8.12	1.22	1.33
2	C	54	HIS	CD2-NE2	-8.12	1.28	1.37
4	K	39	ARG	CZ-NH2	-8.12	1.22	1.33
1	A	31	ARG	CZ-NH2	-8.11	1.23	1.33
4	J	62	HIS	CD2-NE2	-8.12	1.28	1.37
2	B	39	HIS	CD2-NE2	-8.11	1.28	1.37
3	I	351	ARG	CZ-NH2	-8.11	1.23	1.33
3	I	541	HIS	CD2-NE2	-8.10	1.28	1.37
1	A	186	ARG	CZ-NH2	-8.10	1.23	1.33
4	K	62	HIS	CD2-NE2	-8.09	1.28	1.37
2	G	54	HIS	CD2-NE2	-8.09	1.28	1.37
4	K	53	HIS	CD2-NE2	-8.08	1.28	1.37
4	K	111	HIS	CD2-NE2	-8.08	1.28	1.37
2	D	177	ARG	CZ-NH2	-8.07	1.23	1.33
2	F	142	ARG	CZ-NH2	-8.06	1.23	1.33
2	B	179	HIS	CD2-NE2	-8.05	1.28	1.37
2	H	189	HIS	CD2-NE2	-8.05	1.28	1.37
2	C	173	ARG	CZ-NH2	-8.04	1.23	1.33
2	D	39	HIS	CD2-NE2	-8.04	1.29	1.37
2	D	156	ARG	CZ-NH2	-8.04	1.23	1.33
2	D	173	ARG	CZ-NH2	-8.04	1.23	1.33
2	E	189	HIS	CD2-NE2	-8.04	1.29	1.37
2	G	239	HIS	CD2-NE2	-8.03	1.29	1.37
3	I	353	HIS	CD2-NE2	-8.02	1.29	1.37
2	F	64	ARG	CZ-NH2	-8.02	1.23	1.33
2	B	259	ARG	CZ-NH2	-8.01	1.23	1.33
4	J	34	ALA	CA-CB	-7.99	1.43	1.53
2	B	268	ARG	CZ-NH2	-7.99	1.23	1.33
4	K	113	ARG	CZ-NH2	-7.99	1.23	1.33
3	I	383	ARG	CZ-NH2	-7.99	1.23	1.33
4	J	10	ARG	CZ-NH2	-7.98	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	338	ARG	CZ-NH2	-7.97	1.23	1.33
3	I	386	ARG	CZ-NH2	-7.97	1.23	1.33
3	I	259	ARG	CZ-NH2	-7.96	1.23	1.33
3	I	504	ARG	CZ-NH2	-7.96	1.23	1.33
2	G	32	ARG	CZ-NH2	-7.95	1.23	1.33
2	D	259	ARG	CZ-NH2	-7.94	1.23	1.33
2	B	226	ARG	CZ-NH2	-7.93	1.23	1.33
2	F	177	ARG	CZ-NH2	-7.93	1.23	1.33
2	B	222	ARG	CZ-NH2	-7.93	1.23	1.33
2	C	64	ARG	CZ-NH2	-7.93	1.23	1.33
3	I	448	ARG	CZ-NH2	-7.93	1.23	1.33
3	I	12	ARG	CZ-NH2	-7.92	1.23	1.33
4	K	10	ARG	CZ-NH2	-7.92	1.23	1.33
2	G	242	ARG	CZ-NH2	-7.92	1.23	1.33
2	E	268	ARG	CZ-NH2	-7.90	1.23	1.33
2	F	133	ARG	CZ-NH2	-7.90	1.23	1.33
2	E	232	ARG	CZ-NH2	-7.89	1.23	1.33
2	F	117	ARG	CZ-NH2	-7.88	1.23	1.33
2	E	49	ARG	CZ-NH2	-7.88	1.23	1.33
2	D	232	ARG	CZ-NH2	-7.87	1.23	1.33
3	I	408	ARG	CZ-NH2	-7.86	1.23	1.33
2	H	52	ARG	CZ-NH2	-7.86	1.23	1.33
2	C	142	ARG	CZ-NH2	-7.86	1.23	1.33
2	H	32	ARG	CZ-NH2	-7.85	1.23	1.33
2	H	64	ARG	CZ-NH2	-7.83	1.23	1.33
2	H	7	ARG	CZ-NH2	-7.83	1.23	1.33
2	E	222	ARG	CZ-NH2	-7.82	1.23	1.33
2	H	242	ARG	CZ-NH2	-7.82	1.23	1.33
4	J	7	ARG	CZ-NH2	-7.82	1.23	1.33
3	I	363	ARG	CZ-NH2	-7.80	1.23	1.33
2	H	81	ARG	CZ-NH2	-7.77	1.23	1.33
2	H	49	ARG	CZ-NH2	-7.77	1.23	1.33
3	I	205	ARG	CZ-NH2	-7.76	1.23	1.33
2	G	173	ARG	CZ-NH2	-7.75	1.23	1.33
2	G	194	ALA	CA-CB	-7.72	1.43	1.53
2	C	19	GLY	N-CA	-7.63	1.37	1.45
2	D	19	GLY	N-CA	-7.61	1.37	1.45
2	D	141	ALA	CA-CB	-7.51	1.42	1.53
2	F	27	ALA	CA-CB	-7.43	1.42	1.53
2	D	163	ALA	CA-CB	-7.42	1.42	1.52
2	H	194	ALA	CA-CB	-7.41	1.43	1.53
2	F	141	ALA	CA-CB	-7.40	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	19	GLY	N-CA	-7.35	1.37	1.45
2	E	19	GLY	N-CA	-7.31	1.37	1.45
2	H	139	ALA	CA-CB	-7.25	1.42	1.53
2	D	158	ALA	CA-CB	-7.20	1.43	1.53
2	F	139	ALA	CA-CB	-7.18	1.43	1.53
2	G	246	ALA	CA-CB	-7.14	1.43	1.54
2	C	141	ALA	CA-CB	-7.07	1.42	1.53
2	G	5	ALA	CA-CB	-7.01	1.43	1.53
2	G	56	ALA	CA-CB	-7.01	1.42	1.53
2	H	213	ALA	CA-CB	-6.99	1.42	1.53
2	E	141	ALA	CA-CB	-6.99	1.42	1.53
3	I	5	ALA	CA-CB	-6.98	1.42	1.53
3	I	273	ALA	CA-CB	-6.96	1.42	1.53
2	F	224	ALA	CA-CB	-6.94	1.42	1.53
2	D	260	ALA	CA-CB	-6.92	1.42	1.53
2	G	3	ALA	CA-CB	-6.90	1.42	1.53
2	D	176	GLY	N-CA	-6.90	1.38	1.45
2	G	139	ALA	CA-CB	-6.89	1.43	1.53
2	C	176	GLY	N-CA	-6.89	1.38	1.45
2	H	246	ALA	CA-CB	-6.87	1.43	1.54
2	H	3	ALA	CA-CB	-6.82	1.43	1.53
2	C	224	ALA	CA-CB	-6.82	1.42	1.53
2	F	19	GLY	N-CA	-6.82	1.38	1.45
2	G	213	ALA	CA-CB	-6.80	1.42	1.53
2	D	267	ALA	CA-CB	-6.79	1.43	1.53
2	G	248	ALA	CA-CB	-6.79	1.42	1.53
4	J	46	ALA	CA-CB	-6.78	1.42	1.53
2	D	224	ALA	CA-CB	-6.78	1.42	1.53
2	G	190	GLY	N-CA	-6.76	1.38	1.45
2	B	176	GLY	N-CA	-6.75	1.38	1.45
2	F	158	ALA	CA-CB	-6.75	1.42	1.53
4	J	42	ALA	CA-CB	-6.75	1.42	1.53
3	I	552	ALA	CA-CB	-6.74	1.43	1.53
3	I	512	ALA	CA-CB	-6.74	1.43	1.53
2	F	56	ALA	CA-CB	-6.73	1.43	1.53
2	F	213	ALA	CA-CB	-6.72	1.43	1.53
2	H	190	GLY	N-CA	-6.72	1.37	1.45
4	J	44	ALA	CA-CB	-6.72	1.43	1.53
3	I	473	ALA	CA-CB	-6.71	1.43	1.53
3	I	444	ALA	CA-CB	-6.70	1.43	1.53
2	E	267	ALA	CA-CB	-6.70	1.43	1.53
4	K	44	ALA	CA-CB	-6.70	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	19	ALA	CA-CB	-6.69	1.44	1.53
3	I	507	ALA	CA-CB	-6.67	1.43	1.53
2	E	139	ALA	CA-CB	-6.67	1.43	1.53
3	I	477	ALA	CA-CB	-6.67	1.42	1.53
2	B	32	ARG	CZ-NH1	-6.65	1.23	1.32
4	K	115	ALA	CA-CB	-6.65	1.43	1.53
2	G	49	ARG	CZ-NH1	-6.64	1.23	1.32
4	K	28	ALA	CA-CB	-6.64	1.43	1.53
2	E	224	ALA	CA-CB	-6.64	1.43	1.53
4	J	28	ALA	CA-CB	-6.63	1.43	1.53
4	K	19	ALA	CA-CB	-6.62	1.43	1.53
3	I	603	ALA	CA-CB	-6.62	1.43	1.53
4	J	64	ALA	CA-CB	-6.62	1.43	1.53
2	G	52	ARG	CZ-NH1	-6.61	1.23	1.32
2	C	268	ARG	CZ-NH1	-6.61	1.23	1.32
2	H	85	ALA	CA-CB	-6.61	1.43	1.53
3	I	351	ARG	CZ-NH1	-6.61	1.23	1.32
2	E	163	ALA	CA-CB	-6.60	1.45	1.53
2	E	226	ARG	CZ-NH1	-6.59	1.23	1.32
1	A	107	ARG	CZ-NH1	-6.59	1.23	1.32
2	G	62	ALA	CA-CB	-6.59	1.42	1.53
2	D	142	ARG	CZ-NH1	-6.59	1.23	1.32
1	A	75	ARG	CZ-NH1	-6.58	1.23	1.32
1	A	110	ARG	CZ-NH1	-6.58	1.23	1.32
4	K	6	ALA	CA-CB	-6.58	1.43	1.53
2	G	64	ARG	CZ-NH1	-6.58	1.23	1.32
2	B	163	ALA	CA-CB	-6.58	1.43	1.53
2	C	117	ARG	CZ-NH1	-6.57	1.23	1.32
2	D	156	ARG	CZ-NH1	-6.57	1.23	1.32
2	C	156	ARG	CZ-NH1	-6.57	1.23	1.32
2	D	49	ARG	CZ-NH1	-6.57	1.23	1.32
4	J	59	ALA	CA-CB	-6.57	1.43	1.53
4	J	67	ARG	CZ-NH1	-6.57	1.23	1.32
1	A	116	ARG	CZ-NH1	-6.57	1.23	1.32
2	B	49	ARG	CZ-NH1	-6.57	1.23	1.32
3	I	494	ALA	CA-CB	-6.56	1.43	1.53
1	A	20	ALA	CA-CB	-6.56	1.42	1.53
1	A	31	ARG	CZ-NH1	-6.56	1.23	1.32
2	C	226	ARG	CZ-NH1	-6.56	1.23	1.32
3	I	279	ALA	CA-CB	-6.56	1.43	1.53
1	A	186	ARG	CZ-NH1	-6.56	1.23	1.32
2	C	56	ALA	CA-CB	-6.55	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	24	ALA	CA-CB	-6.55	1.43	1.53
1	A	74	ARG	CZ-NH1	-6.55	1.23	1.32
2	D	226	ARG	CZ-NH1	-6.54	1.23	1.32
2	B	225	ALA	CA-CB	-6.53	1.43	1.53
2	F	142	ARG	CZ-NH1	-6.53	1.23	1.32
2	C	173	ARG	CZ-NH1	-6.53	1.23	1.32
1	A	111	ALA	CA-CB	-6.52	1.42	1.53
2	D	173	ARG	CZ-NH1	-6.52	1.23	1.32
4	K	39	ARG	CZ-NH1	-6.52	1.23	1.32
3	I	249	ALA	CA-CB	-6.52	1.43	1.53
6	N	26	DG	P-OP2	6.52	1.61	1.48
6	N	29	DC	P-OP1	6.52	1.61	1.48
2	H	5	ALA	CA-CB	-6.51	1.43	1.53
2	D	177	ARG	CZ-NH1	-6.51	1.23	1.32
2	C	133	ARG	CZ-NH1	-6.51	1.23	1.32
2	E	133	ARG	CZ-NH1	-6.50	1.23	1.32
4	J	113	ARG	CZ-NH1	-6.50	1.23	1.32
1	A	24	ARG	CZ-NH1	-6.50	1.23	1.32
2	H	248	ALA	CA-CB	-6.49	1.43	1.53
2	G	165	ALA	CA-CB	-6.49	1.43	1.53
2	D	133	ARG	CZ-NH1	-6.48	1.23	1.32
2	H	197	ALA	CA-CB	-6.47	1.43	1.53
4	K	10	ARG	CZ-NH1	-6.47	1.23	1.32
4	J	32	ALA	CA-CB	-6.47	1.43	1.53
2	C	225	ALA	CA-CB	-6.47	1.43	1.53
2	G	7	ARG	CZ-NH1	-6.46	1.23	1.32
3	I	386	ARG	CZ-NH1	-6.45	1.23	1.32
3	I	448	ARG	CZ-NH1	-6.45	1.23	1.32
3	I	259	ARG	CZ-NH1	-6.45	1.23	1.32
2	G	242	ARG	CZ-NH1	-6.44	1.23	1.32
3	I	383	ARG	CZ-NH1	-6.44	1.23	1.32
2	F	62	ALA	CA-CB	-6.44	1.43	1.53
2	G	32	ARG	CZ-NH1	-6.44	1.23	1.32
4	J	10	ARG	CZ-NH1	-6.43	1.23	1.32
2	H	62	ALA	CA-CB	-6.43	1.43	1.53
3	I	338	ARG	CZ-NH1	-6.42	1.23	1.32
4	K	113	ARG	CZ-NH1	-6.42	1.23	1.32
4	J	7	ARG	CZ-NH1	-6.42	1.23	1.32
3	I	516	ALA	CA-CB	-6.42	1.43	1.53
2	C	213	ALA	CA-CB	-6.41	1.43	1.53
2	B	222	ARG	CZ-NH1	-6.38	1.23	1.32
2	H	49	ARG	CZ-NH1	-6.38	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	232	ARG	CZ-NH1	-6.37	1.23	1.32
2	E	268	ARG	CZ-NH1	-6.36	1.23	1.32
2	F	64	ARG	CZ-NH1	-6.36	1.23	1.32
2	F	177	ARG	CZ-NH1	-6.36	1.23	1.32
2	D	102	ALA	CA-CB	-6.35	1.43	1.53
2	D	232	ARG	CZ-NH1	-6.35	1.23	1.32
3	I	363	ARG	CZ-NH1	-6.35	1.23	1.32
2	E	49	ARG	CZ-NH1	-6.35	1.23	1.32
2	B	268	ARG	CZ-NH1	-6.34	1.23	1.32
2	B	226	ARG	CZ-NH1	-6.34	1.23	1.32
2	C	64	ARG	CZ-NH1	-6.34	1.23	1.32
2	F	117	ARG	CZ-NH1	-6.34	1.23	1.32
2	B	259	ARG	CZ-NH1	-6.33	1.23	1.32
1	A	112	ALA	CA-CB	-6.33	1.43	1.53
2	H	64	ARG	CZ-NH1	-6.33	1.23	1.32
2	E	222	ARG	CZ-NH1	-6.32	1.24	1.32
2	H	242	ARG	CZ-NH1	-6.32	1.24	1.32
3	I	382	GLY	N-CA	-6.32	1.38	1.45
3	I	504	ARG	CZ-NH1	-6.32	1.24	1.32
2	C	142	ARG	CZ-NH1	-6.31	1.24	1.32
2	G	173	ARG	CZ-NH1	-6.31	1.24	1.32
3	I	12	ARG	CZ-NH1	-6.31	1.24	1.32
2	G	23	GLY	N-CA	-6.30	1.38	1.45
3	I	213	ALA	CA-CB	-6.30	1.43	1.53
2	D	259	ARG	CZ-NH1	-6.30	1.24	1.32
3	I	408	ARG	CZ-NH1	-6.30	1.24	1.32
2	B	267	ALA	CA-CB	-6.29	1.42	1.53
2	G	73	ALA	CA-CB	-6.29	1.42	1.53
2	H	52	ARG	CZ-NH1	-6.28	1.24	1.32
2	H	81	ARG	CZ-NH1	-6.28	1.24	1.32
2	D	225	ALA	CA-CB	-6.28	1.43	1.53
2	F	133	ARG	CZ-NH1	-6.27	1.24	1.32
2	H	73	ALA	CA-CB	-6.27	1.43	1.53
2	E	225	ALA	CA-CB	-6.26	1.43	1.53
2	H	7	ARG	CZ-NH1	-6.26	1.24	1.32
2	F	225	ALA	CA-CB	-6.26	1.43	1.53
2	H	32	ARG	CZ-NH1	-6.25	1.24	1.32
3	I	205	ARG	CZ-NH1	-6.25	1.24	1.32
3	I	547	ALA	CA-CB	-6.23	1.42	1.53
4	J	103	GLY	N-CA	-6.23	1.38	1.45
2	G	158	ALA	CA-CB	-6.20	1.43	1.53
3	I	211	ALA	CA-CB	-6.14	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	62	ALA	CA-CB	-6.13	1.43	1.53
2	C	158	ALA	CA-CB	-6.08	1.43	1.53
2	B	73	ALA	CA-CB	-6.07	1.43	1.53
2	G	188	ALA	CA-CB	-6.07	1.43	1.53
4	K	32	ALA	CA-CB	-6.05	1.43	1.53
2	B	224	ALA	CA-CB	-6.01	1.43	1.53
3	I	411	ALA	CA-CB	-5.96	1.43	1.53
4	J	108	GLY	N-CA	-5.94	1.38	1.45
3	I	447	GLY	N-CA	-5.93	1.38	1.45
4	K	15	GLY	N-CA	-5.88	1.38	1.45
2	B	181	VAL	N-CA	-5.88	1.42	1.46
2	G	163	ALA	CA-CB	-5.86	1.43	1.53
2	D	271	ALA	CA-CB	-5.81	1.43	1.53
2	D	40	GLY	N-CA	-5.79	1.37	1.45
4	K	64	ALA	CA-CB	-5.78	1.44	1.53
2	C	226	ARG	CD-NE	-5.72	1.38	1.46
2	H	56	ALA	CA-CB	-5.69	1.43	1.53
3	I	362	ALA	CA-CB	-5.69	1.43	1.53
2	B	227	GLY	N-CA	-5.64	1.37	1.45
2	D	173	ARG	CD-NE	-5.62	1.38	1.46
2	B	226	ARG	CD-NE	-5.61	1.38	1.46
4	K	49	GLY	N-CA	-5.61	1.38	1.45
2	G	156	ARG	C-O	-5.60	1.17	1.23
4	J	113	ARG	CD-NE	-5.60	1.38	1.46
2	D	156	ARG	CD-NE	-5.59	1.38	1.46
2	B	40	GLY	N-CA	-5.59	1.37	1.45
2	D	226	ARG	CD-NE	-5.58	1.38	1.46
2	B	28	GLY	N-CA	-5.57	1.37	1.45
2	B	32	ARG	CD-NE	-5.56	1.38	1.46
4	J	67	ARG	CD-NE	-5.56	1.38	1.46
2	B	23	GLY	N-CA	-5.56	1.37	1.45
2	F	177	ARG	CD-NE	-5.53	1.38	1.46
4	K	39	ARG	CD-NE	-5.52	1.38	1.46
3	I	448	ARG	CD-NE	-5.52	1.38	1.46
2	G	28	GLY	N-CA	-5.52	1.37	1.45
2	G	244	GLY	N-CA	-5.51	1.37	1.45
2	G	20	ASN	CA-CB	-5.50	1.46	1.53
4	K	113	ARG	CD-NE	-5.49	1.38	1.46
2	B	262	GLY	N-CA	-5.49	1.38	1.45
2	C	227	GLY	N-CA	-5.49	1.37	1.45
2	C	268	ARG	CD-NE	-5.49	1.38	1.46
2	H	201	GLY	N-CA	-5.49	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	142	ARG	CD-NE	-5.48	1.38	1.46
3	I	361	ALA	CA-CB	-5.48	1.42	1.52
3	I	205	ARG	CD-NE	-5.47	1.38	1.46
2	F	227	GLY	N-CA	-5.47	1.37	1.45
2	B	180	ILE	C-N	-5.47	1.28	1.33
2	E	227	GLY	N-CA	-5.47	1.37	1.45
3	I	351	ARG	CD-NE	-5.47	1.38	1.46
1	A	31	ARG	CD-NE	-5.46	1.38	1.46
2	H	52	ARG	CD-NE	-5.45	1.38	1.46
2	B	20	ASN	CA-CB	-5.45	1.46	1.53
2	C	173	ARG	CD-NE	-5.45	1.38	1.46
3	I	492	ASP	CA-CB	-5.45	1.46	1.53
2	C	156	ARG	CD-NE	-5.44	1.38	1.46
2	E	226	ARG	CD-NE	-5.44	1.38	1.46
4	J	7	ARG	CD-NE	-5.44	1.38	1.46
2	F	142	ARG	CD-NE	-5.44	1.38	1.46
1	A	116	ARG	CD-NE	-5.44	1.38	1.46
2	G	52	ARG	CD-NE	-5.44	1.38	1.46
2	E	268	ARG	CD-NE	-5.43	1.38	1.46
2	F	117	ARG	CD-NE	-5.43	1.38	1.46
2	B	268	ARG	CD-NE	-5.42	1.38	1.46
1	A	75	ARG	CD-NE	-5.42	1.38	1.46
2	D	259	ARG	CD-NE	-5.42	1.38	1.46
2	F	134	GLY	N-CA	-5.42	1.37	1.44
3	I	259	ARG	CD-NE	-5.40	1.38	1.46
2	C	142	ARG	CD-NE	-5.40	1.38	1.46
2	H	32	ARG	CD-NE	-5.39	1.38	1.46
2	B	49	ARG	CD-NE	-5.39	1.38	1.46
2	F	188	ALA	CA-CB	-5.38	1.43	1.53
2	E	49	ARG	CD-NE	-5.37	1.38	1.46
2	G	242	ARG	CD-NE	-5.36	1.38	1.46
1	A	74	ARG	CD-NE	-5.36	1.38	1.46
2	G	32	ARG	CD-NE	-5.36	1.38	1.46
2	D	49	ARG	CD-NE	-5.36	1.38	1.46
2	D	232	ARG	CD-NE	-5.35	1.38	1.46
2	H	244	GLY	N-CA	-5.35	1.37	1.45
2	F	181	VAL	N-CA	-5.34	1.42	1.46
2	G	227	GLY	N-CA	-5.33	1.37	1.45
2	H	242	ARG	CD-NE	-5.33	1.38	1.46
2	D	177	ARG	CD-NE	-5.33	1.38	1.46
1	A	24	ARG	CD-NE	-5.33	1.38	1.46
3	I	386	ARG	CD-NE	-5.33	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	338	ARG	CD-NE	-5.32	1.38	1.46
2	C	117	ARG	CD-NE	-5.32	1.38	1.46
1	A	110	ARG	CD-NE	-5.32	1.38	1.46
2	D	133	ARG	CD-NE	-5.32	1.38	1.46
2	F	40	GLY	N-CA	-5.31	1.37	1.45
2	H	64	ARG	CD-NE	-5.31	1.38	1.46
3	I	504	ARG	CD-NE	-5.31	1.38	1.46
3	I	392	PRO	CA-CB	-5.31	1.46	1.53
2	G	64	ARG	CD-NE	-5.30	1.38	1.46
2	C	120	GLY	N-CA	-5.30	1.38	1.45
2	G	49	ARG	CD-NE	-5.28	1.38	1.46
2	G	7	ARG	CD-NE	-5.28	1.38	1.46
3	I	383	ARG	CD-NE	-5.27	1.38	1.46
1	A	186	ARG	CD-NE	-5.26	1.38	1.46
2	E	133	ARG	CD-NE	-5.26	1.38	1.46
2	E	232	ARG	CD-NE	-5.26	1.38	1.46
2	G	173	ARG	CD-NE	-5.25	1.38	1.46
2	C	64	ARG	CD-NE	-5.25	1.39	1.46
2	E	222	ARG	CD-NE	-5.25	1.39	1.46
3	I	375	GLY	N-CA	-5.25	1.37	1.45
2	D	145	GLU	CA-CB	-5.24	1.47	1.53
5	L	33	G	C2-N2	-5.24	1.24	1.34
2	G	194	ALA	N-CA	-5.23	1.41	1.46
2	F	130	GLY	N-CA	-5.23	1.37	1.45
2	C	133	ARG	CD-NE	-5.23	1.39	1.46
1	A	107	ARG	CD-NE	-5.22	1.39	1.46
2	B	222	ARG	CD-NE	-5.22	1.39	1.46
2	H	7	ARG	CD-NE	-5.22	1.39	1.46
2	H	49	ARG	CD-NE	-5.21	1.39	1.46
2	D	262	GLY	N-CA	-5.21	1.37	1.45
2	G	1	MET	N-CA	-5.21	1.38	1.49
3	I	285	GLY	N-CA	-5.21	1.37	1.45
2	B	259	ARG	CD-NE	-5.19	1.39	1.46
4	J	10	ARG	CD-NE	-5.18	1.39	1.46
2	F	64	ARG	CD-NE	-5.18	1.39	1.46
5	L	21	A	C6-N6	-5.17	1.23	1.33
5	L	22	G	C2-N2	-5.17	1.24	1.34
2	B	145	GLU	N-CA	-5.17	1.41	1.46
3	I	363	ARG	CD-NE	-5.16	1.39	1.46
3	I	408	ARG	CD-NE	-5.16	1.39	1.46
4	K	10	ARG	CD-NE	-5.16	1.39	1.46
2	F	38	GLY	N-CA	-5.15	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	MET	N-CA	-5.15	1.38	1.49
2	E	188	ALA	CA-CB	-5.14	1.43	1.54
3	I	12	ARG	CD-NE	-5.13	1.39	1.46
4	J	47	ASN	CA-CB	-5.13	1.47	1.53
2	D	35	PRO	CA-CB	-5.12	1.46	1.53
2	E	145	GLU	CA-CB	-5.12	1.47	1.53
2	G	61	GLY	N-CA	-5.12	1.38	1.45
2	F	149	PRO	CA-CB	-5.12	1.46	1.53
2	B	31	PRO	CA-CB	-5.11	1.46	1.53
2	F	133	ARG	CD-NE	-5.10	1.39	1.46
2	B	149	PRO	CA-CB	-5.10	1.46	1.53
4	K	10	ARG	N-CA	-5.10	1.41	1.46
2	H	81	ARG	CD-NE	-5.10	1.39	1.46
2	C	19	GLY	CA-C	-5.09	1.47	1.52
2	C	40	GLY	N-CA	-5.09	1.37	1.45
2	C	201	GLY	N-CA	-5.09	1.38	1.45
2	B	184	GLY	N-CA	-5.08	1.38	1.45
2	G	20	ASN	N-CA	-5.08	1.41	1.46
5	L	11	C	C4-N4	-5.08	1.23	1.33
4	J	10	ARG	CA-CB	-5.07	1.47	1.53
5	L	12	G	C2-N2	-5.07	1.24	1.34
5	L	13	C	C4-N4	-5.07	1.23	1.33
4	K	1	VAL	N-CA	-5.06	1.39	1.49
4	J	10	ARG	N-CA	-5.06	1.41	1.46
4	K	10	ARG	CA-CB	-5.04	1.48	1.53
2	F	24	ASP	CA-CB	-5.04	1.46	1.53
5	L	23	G	C2-N2	-5.04	1.24	1.34
2	E	266	PRO	CA-CB	-5.03	1.47	1.53
6	N	22	DG	C2-N2	-5.02	1.24	1.34
2	F	23	GLY	N-CA	-5.02	1.38	1.45
3	I	518	PRO	CA-CB	-5.02	1.47	1.53
2	D	162	LYS	CA-CB	-5.02	1.46	1.52
5	L	15	A	C6-N6	-5.02	1.24	1.33
2	H	194	ALA	N-CA	-5.01	1.42	1.46
3	I	256	PRO	CA-CB	-5.01	1.46	1.53
5	L	28	C	C4-N4	-5.01	1.24	1.33
2	B	35	PRO	CA-CB	-5.00	1.46	1.53

All (851) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	25	DT	OP2-P-O3'	-33.35	7.94	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	45	C	O4'-C1'-N1	10.31	123.97	108.50
6	N	26	DG	P-O3'-C3'	-9.86	105.41	120.20
2	H	127	VAL	N-CA-C	8.38	121.34	112.96
2	G	156	ARG	CA-C-N	8.29	139.39	122.55
2	G	156	ARG	C-N-CA	8.29	139.39	122.55
2	H	67	ILE	O-C-N	-8.22	114.17	122.97
2	G	156	ARG	O-C-N	-7.93	113.54	123.06
2	G	178	LYS	CA-C-N	7.68	134.57	122.74
2	G	178	LYS	C-N-CA	7.68	134.57	122.74
2	H	189	HIS	CA-C-N	7.62	129.19	121.35
2	H	189	HIS	C-N-CA	7.62	129.19	121.35
2	F	140	PHE	CA-CB-CG	7.42	121.22	113.80
2	G	245	ASN	CA-CB-CG	7.39	119.99	112.60
2	G	29	ASN	CA-CB-CG	7.38	119.98	112.60
2	H	140	PHE	CA-CB-CG	7.35	121.15	113.80
2	C	140	PHE	CA-CB-CG	7.30	121.10	113.80
4	J	18	PHE	CA-CB-CG	7.29	121.09	113.80
2	E	76	ASN	CA-CB-CG	7.26	119.86	112.60
2	D	140	PHE	CA-CB-CG	7.25	121.05	113.80
2	E	121	ALA	CA-C-N	7.25	130.56	122.59
2	E	121	ALA	C-N-CA	7.25	130.56	122.59
2	C	18	ASN	CA-C-N	7.25	129.16	121.48
2	C	18	ASN	C-N-CA	7.25	129.16	121.48
2	B	180	ILE	CA-C-N	7.23	131.09	122.85
2	B	180	ILE	C-N-CA	7.23	131.09	122.85
2	B	140	PHE	CA-CB-CG	7.20	121.00	113.80
2	E	140	PHE	CA-CB-CG	7.17	120.97	113.80
2	F	171	ASP	CA-CB-CG	7.16	119.76	112.60
2	C	221	ASP	CA-CB-CG	7.15	119.75	112.60
2	D	18	ASN	CA-C-N	7.14	129.05	121.48
2	D	18	ASN	C-N-CA	7.14	129.05	121.48
2	G	15	ASP	CA-CB-CG	7.13	119.73	112.60
2	G	79	HIS	CA-CB-CG	7.13	120.93	113.80
2	G	140	PHE	CA-CB-CG	7.12	120.92	113.80
2	H	210	PHE	CA-CB-CG	7.10	120.90	113.80
3	I	251	ASN	CA-CB-CG	7.10	119.70	112.60
2	C	172	ASN	CA-CB-CG	7.06	119.66	112.60
1	A	117	ASN	CA-CB-CG	7.05	119.65	112.60
2	F	172	ASN	CA-CB-CG	7.03	119.63	112.60
2	F	18	ASN	CA-CB-CG	6.99	119.59	112.60
2	B	26	ASP	CA-CB-CG	6.97	119.58	112.60
3	I	352	PHE	CA-CB-CG	6.97	120.77	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	33	ASN	CA-CB-CG	6.97	119.57	112.60
1	A	76	ASN	CA-CB-CG	6.96	119.56	112.60
2	H	53	ASN	CA-CB-CG	6.95	119.55	112.60
6	N	25	DT	P-O3'-C3'	-6.95	109.77	120.20
3	I	372	ASP	CA-CB-CG	6.95	119.55	112.60
2	D	221	ASP	CA-CB-CG	6.92	119.52	112.60
2	G	172	ASN	CA-CB-CG	6.91	119.51	112.60
2	F	39	HIS	CA-CB-CG	6.90	120.70	113.80
3	I	414	ASN	CA-CB-CG	6.90	119.50	112.60
4	J	117	PHE	CA-CB-CG	6.90	120.70	113.80
4	K	111	HIS	CA-CB-CG	6.90	120.70	113.80
2	B	29	ASN	CA-CB-CG	6.88	119.48	112.60
4	K	52	PHE	CA-CB-CG	6.86	120.66	113.80
4	J	52	PHE	CA-CB-CG	6.86	120.66	113.80
2	F	202	PHE	CA-CB-CG	6.83	120.63	113.80
2	E	18	ASN	CA-CB-CG	6.81	119.41	112.60
2	D	39	HIS	CA-CB-CG	6.81	120.61	113.80
3	I	515	ASP	CA-CB-CG	6.79	119.39	112.60
2	B	53	ASN	CA-CB-CG	6.78	119.38	112.60
2	E	79	HIS	CA-CB-CG	6.78	120.58	113.80
2	C	119	PHE	CA-CB-CG	6.77	120.57	113.80
1	A	102	ASP	CA-CB-CG	6.75	119.35	112.60
2	C	18	ASN	CA-CB-CG	6.75	119.35	112.60
5	L	37	G	C5'-C4'-C3'	-6.75	105.88	116.00
1	A	18	ASP	CA-CB-CG	6.72	119.32	112.60
2	G	252	PHE	CA-CB-CG	6.70	120.50	113.80
2	G	218	PHE	CA-CB-CG	6.70	120.50	113.80
2	F	26	ASP	CA-CB-CG	6.70	119.30	112.60
3	I	379	ASP	CA-CB-CG	6.69	119.29	112.60
1	A	106	ASN	CA-CB-CG	6.69	119.29	112.60
2	H	113	PHE	CA-CB-CG	6.69	120.49	113.80
3	I	482	ASN	CA-CB-CG	6.69	119.29	112.60
2	H	239	HIS	CA-CB-CG	6.69	120.49	113.80
2	B	24	ASP	CA-CB-CG	6.68	119.28	112.60
2	B	221	ASP	CA-CB-CG	6.67	119.27	112.60
4	J	47	ASN	CA-CB-CG	6.64	119.24	112.60
2	B	39	HIS	CA-CB-CG	6.64	120.44	113.80
2	D	18	ASN	CA-CB-CG	6.63	119.23	112.60
2	C	202	PHE	CA-CB-CG	6.63	120.43	113.80
3	I	353	HIS	CA-CB-CG	6.63	120.43	113.80
2	G	107	ASP	CA-CB-CG	6.62	119.22	112.60
2	D	53	ASN	CA-CB-CG	6.61	119.21	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	6	ASN	CA-CB-CG	6.61	119.21	112.60
1	A	35	ASP	CA-C-N	6.61	129.51	122.11
1	A	35	ASP	C-N-CA	6.61	129.51	122.11
2	G	210	PHE	CA-CB-CG	6.61	120.41	113.80
2	G	15	ASP	CA-C-N	6.59	130.80	121.96
2	G	15	ASP	C-N-CA	6.59	130.80	121.96
2	C	210	PHE	CA-CB-CG	6.59	120.39	113.80
2	H	73	ALA	CA-C-N	6.59	130.61	122.37
2	H	73	ALA	C-N-CA	6.59	130.61	122.37
4	K	93	PHE	CA-CB-CG	6.59	120.39	113.80
2	F	22	ASN	CA-CB-CG	6.57	119.17	112.60
2	C	53	ASN	CA-CB-CG	6.57	119.17	112.60
2	C	39	HIS	CA-CB-CG	6.57	120.37	113.80
2	H	202	PHE	CA-CB-CG	6.55	120.35	113.80
2	D	34	ASP	CA-CB-CG	6.54	119.14	112.60
2	D	218	PHE	CA-CB-CG	6.53	120.33	113.80
2	B	20	ASN	CA-CB-CG	6.53	119.12	112.60
2	F	24	ASP	CA-CB-CG	6.50	119.10	112.60
4	J	105	PHE	CA-CB-CG	6.50	120.30	113.80
2	C	15	ASP	CA-C-N	6.50	130.66	121.96
2	C	15	ASP	C-N-CA	6.50	130.66	121.96
4	K	18	PHE	CA-CB-CG	6.50	120.30	113.80
2	H	252	PHE	CA-CB-CG	6.50	120.30	113.80
2	G	18	ASN	CA-CB-CG	6.49	119.08	112.60
2	F	53	ASN	CA-CB-CG	6.48	119.08	112.60
2	D	128	ASN	CA-CB-CG	6.47	119.07	112.60
2	G	216	ASN	CA-CB-CG	6.46	119.06	112.60
2	G	237	PHE	CA-CB-CG	6.44	120.24	113.80
2	F	34	ASP	CA-CB-CG	6.43	119.03	112.60
2	G	20	ASN	CA-CB-CG	6.43	119.03	112.60
2	H	66	ASN	CA-CB-CG	6.43	119.03	112.60
3	I	255	ASN	CA-CB-CG	6.42	119.03	112.60
1	A	77	GLU	CA-C-N	6.41	131.69	122.45
1	A	77	GLU	C-N-CA	6.41	131.69	122.45
2	E	53	ASN	CA-CB-CG	6.40	119.00	112.60
2	F	119	PHE	CA-CB-CG	6.40	120.20	113.80
2	G	155	THR	O-C-N	-6.39	113.86	122.68
2	F	20	ASN	CA-CB-CG	6.39	118.99	112.60
1	A	187	ASP	CA-CB-CG	6.38	118.98	112.60
2	G	22	ASN	CA-CB-CG	6.37	118.97	112.60
2	G	171	ASP	CA-CB-CG	6.37	118.97	112.60
2	G	197	ALA	CA-C-N	6.36	128.81	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	197	ALA	C-N-CA	6.36	128.81	120.28
4	J	69	ASP	CA-CB-CG	6.36	118.95	112.60
2	F	15	ASP	CA-CB-CG	6.35	118.95	112.60
2	C	65	PHE	CA-CB-CG	6.34	120.14	113.80
2	B	175	MET	CA-C-N	6.33	132.94	120.84
2	B	175	MET	C-N-CA	6.33	132.94	120.84
3	I	225	PHE	CA-CB-CG	6.33	120.13	113.80
2	F	210	PHE	CA-CB-CG	6.33	120.12	113.80
2	B	68	TYR	CA-C-N	6.32	130.27	122.37
2	B	68	TYR	C-N-CA	6.32	130.27	122.37
2	G	239	HIS	CA-CB-CG	6.32	120.12	113.80
2	D	272	ASP	CA-CB-CG	6.31	118.91	112.60
2	D	121	ALA	CA-C-N	6.30	130.25	122.37
2	D	121	ALA	C-N-CA	6.30	130.25	122.37
2	H	189	HIS	CA-CB-CG	6.30	120.10	113.80
3	I	546	ASN	CA-CB-CG	6.30	118.90	112.60
4	J	62	HIS	CA-CB-CG	6.30	120.10	113.80
2	B	34	ASP	CA-CB-CG	6.28	118.88	112.60
5	L	41	C	C4'-C3'-C2'	-6.27	96.33	102.60
3	I	376	HIS	CA-CB-CG	6.26	120.06	113.80
1	A	99	PHE	CA-CB-CG	6.26	120.06	113.80
2	D	153	SER	CA-C-N	6.25	131.62	122.94
2	D	153	SER	C-N-CA	6.25	131.62	122.94
2	F	218	PHE	CA-CB-CG	6.24	120.04	113.80
4	J	89	ASN	CA-CB-CG	6.24	118.84	112.60
2	E	189	HIS	CA-CB-CG	6.24	120.04	113.80
4	J	46	ALA	CA-C-N	6.23	129.70	122.85
4	J	46	ALA	C-N-CA	6.23	129.70	122.85
2	C	52	ARG	NE-CZ-NH2	6.23	124.81	119.20
1	A	35	ASP	CA-CB-CG	6.23	118.83	112.60
2	G	156	ARG	NE-CZ-NH2	6.22	124.80	119.20
4	K	117	PHE	CA-CB-CG	6.22	120.03	113.80
2	B	76	ASN	CA-CB-CG	6.20	118.80	112.60
4	K	62	HIS	CA-CB-CG	6.18	119.98	113.80
3	I	492	ASP	CA-CB-CG	6.17	118.77	112.60
3	I	347	ASP	CA-CB-CG	6.17	118.77	112.60
3	I	418	ASN	CA-CB-CG	6.17	118.77	112.60
2	F	65	PHE	CA-CB-CG	6.16	119.96	113.80
3	I	213	ALA	CA-C-N	6.15	131.28	123.10
3	I	213	ALA	C-N-CA	6.15	131.28	123.10
1	A	75	ARG	CD-NE-CZ	6.15	133.01	124.40
1	A	165	PHE	CA-CB-CG	6.14	119.94	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	122	VAL	N-CA-CB	6.14	118.15	110.47
4	K	4	ASP	CA-CB-CG	6.14	118.74	112.60
4	K	61	ASN	CA-CB-CG	6.14	118.74	112.60
4	J	89	ASN	CA-C-N	6.14	130.29	122.37
4	J	89	ASN	C-N-CA	6.14	130.29	122.37
3	I	281	ASP	CA-CB-CG	6.14	118.74	112.60
2	H	107	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	22	PHE	CA-CB-CG	6.11	119.91	113.80
3	I	12	ARG	CD-NE-CZ	6.11	132.95	124.40
5	L	45	C	C1'-O4'-C4'	-6.11	103.79	109.90
2	C	34	ASP	CA-CB-CG	6.11	118.71	112.60
2	G	26	ASP	CA-CB-CG	6.11	118.70	112.60
1	A	100	LEU	CA-C-N	6.10	128.25	120.56
1	A	100	LEU	C-N-CA	6.10	128.25	120.56
2	H	7	ARG	CD-NE-CZ	6.10	132.94	124.40
1	A	110	ARG	CD-NE-CZ	6.09	132.93	124.40
2	F	54	HIS	CA-CB-CG	6.09	119.89	113.80
2	E	270	PHE	CA-CB-CG	6.08	119.88	113.80
2	G	24	ASP	CA-CB-CG	6.08	118.68	112.60
2	G	79	HIS	CB-CG-CD2	-6.07	123.31	131.20
2	H	79	HIS	CA-C-N	6.06	128.40	120.28
2	H	79	HIS	C-N-CA	6.06	128.40	120.28
3	I	200	SER	CA-C-N	6.06	131.42	123.06
3	I	200	SER	C-N-CA	6.06	131.42	123.06
2	G	65	PHE	CA-CB-CG	6.06	119.86	113.80
2	F	216	ASN	CA-CB-CG	6.05	118.66	112.60
2	D	171	ASP	CA-C-N	6.05	130.70	122.84
2	D	171	ASP	C-N-CA	6.05	130.70	122.84
4	J	33	ASN	CA-CB-CG	6.05	118.65	112.60
2	E	218	PHE	CA-CB-CG	6.05	119.85	113.80
2	D	158	ALA	CA-C-N	6.04	131.39	122.99
2	D	158	ALA	C-N-CA	6.04	131.39	122.99
3	I	383	ARG	CD-NE-CZ	6.04	132.86	124.40
4	K	47	ASN	CA-CB-CG	6.03	118.63	112.60
2	G	7	ARG	CD-NE-CZ	6.02	132.83	124.40
4	J	7	ARG	CD-NE-CZ	6.02	132.82	124.40
3	I	365	SER	CA-C-N	6.01	131.10	123.10
3	I	365	SER	C-N-CA	6.01	131.10	123.10
4	K	67	ARG	NE-CZ-NH2	6.01	124.61	119.20
2	G	49	ARG	CD-NE-CZ	6.01	132.81	124.40
2	F	216	ASN	CA-C-N	6.00	128.57	120.65
2	F	216	ASN	C-N-CA	6.00	128.57	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	550	HIS	CA-CB-CG	6.00	119.80	113.80
2	B	272	ASP	CA-CB-CG	6.00	118.60	112.60
2	E	222	ARG	CD-NE-CZ	6.00	132.80	124.40
1	A	107	ARG	CD-NE-CZ	5.99	132.79	124.40
2	E	133	ARG	CD-NE-CZ	5.99	132.79	124.40
3	I	577	ASN	CA-CB-CG	5.99	118.59	112.60
2	D	270	PHE	CA-CB-CG	5.99	119.79	113.80
4	J	38	ASP	CA-CB-CG	5.99	118.59	112.60
2	H	81	ARG	CD-NE-CZ	5.98	132.77	124.40
4	J	58	ASN	CA-CB-CG	5.98	118.58	112.60
2	F	133	ARG	CD-NE-CZ	5.97	132.76	124.40
3	I	386	ARG	CD-NE-CZ	5.97	132.76	124.40
2	F	161	THR	CA-C-N	5.97	129.19	120.71
2	F	161	THR	C-N-CA	5.97	129.19	120.71
4	J	88	ASP	CA-CB-CG	5.97	118.57	112.60
2	F	29	ASN	CA-C-N	5.96	129.16	120.51
2	F	29	ASN	C-N-CA	5.96	129.16	120.51
2	B	49	ARG	CD-NE-CZ	5.96	132.75	124.40
2	G	206	ASP	CA-CB-CG	5.96	118.56	112.60
2	F	135	PRO	CA-C-N	5.96	130.58	123.19
2	F	135	PRO	C-N-CA	5.96	130.58	123.19
3	I	341	ASP	CA-CB-CG	5.96	118.56	112.60
2	B	75	LEU	CA-C-N	5.96	130.34	122.42
2	B	75	LEU	C-N-CA	5.96	130.34	122.42
2	C	133	ARG	CD-NE-CZ	5.96	132.74	124.40
2	H	206	ASP	CA-CB-CG	5.96	118.56	112.60
2	F	107	ASP	CA-CB-CG	5.95	118.55	112.60
3	I	222	ASN	CA-CB-CG	5.94	118.54	112.60
2	G	189	HIS	CA-CB-CG	5.94	119.74	113.80
2	H	49	ARG	CD-NE-CZ	5.93	132.71	124.40
2	F	206	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	74	ARG	CD-NE-CZ	5.93	132.70	124.40
3	I	504	ARG	CD-NE-CZ	5.93	132.70	124.40
2	D	133	ARG	CD-NE-CZ	5.92	132.69	124.40
2	B	35	PRO	CA-C-N	5.92	128.70	120.29
2	B	35	PRO	C-N-CA	5.92	128.70	120.29
3	I	408	ARG	CD-NE-CZ	5.92	132.69	124.40
1	A	24	ARG	CD-NE-CZ	5.92	132.69	124.40
2	D	49	ARG	CD-NE-CZ	5.92	132.69	124.40
3	I	395	ASN	CA-CB-CG	5.92	118.52	112.60
2	C	209	LEU	CA-C-N	5.91	128.13	120.44
2	C	209	LEU	C-N-CA	5.91	128.13	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	173	ARG	CD-NE-CZ	5.91	132.67	124.40
4	K	42	ALA	CA-C-N	5.91	128.12	120.44
4	K	42	ALA	C-N-CA	5.91	128.12	120.44
2	E	232	ARG	CD-NE-CZ	5.91	132.67	124.40
2	D	172	ASN	CA-CB-CG	5.90	118.50	112.60
4	K	58	ASN	CA-CB-CG	5.90	118.50	112.60
2	B	73	ALA	CA-C-N	5.89	128.53	120.35
2	B	73	ALA	C-N-CA	5.89	128.53	120.35
4	K	10	ARG	CD-NE-CZ	5.89	132.64	124.40
2	C	156	ARG	CD-NE-CZ	5.88	132.64	124.40
5	L	44	U	C3'-C2'-C1'	5.88	107.19	101.30
2	G	204	ASP	CA-CB-CG	5.88	118.48	112.60
2	F	177	ARG	CA-C-N	5.88	131.76	122.94
2	F	177	ARG	C-N-CA	5.88	131.76	122.94
1	A	186	ARG	CD-NE-CZ	5.88	132.63	124.40
4	K	38	ASP	CA-CB-CG	5.88	118.48	112.60
2	E	49	ARG	CD-NE-CZ	5.87	132.62	124.40
4	J	10	ARG	CD-NE-CZ	5.86	132.61	124.40
2	D	127	VAL	CA-C-N	5.86	130.21	122.30
2	D	127	VAL	C-N-CA	5.86	130.21	122.30
2	F	33	ILE	CA-C-N	5.86	129.47	121.74
2	F	33	ILE	C-N-CA	5.86	129.47	121.74
2	D	232	ARG	CD-NE-CZ	5.86	132.60	124.40
2	B	222	ARG	CD-NE-CZ	5.86	132.60	124.40
3	I	605	PHE	CA-CB-CG	5.86	119.66	113.80
2	G	236	VAL	CA-C-N	5.85	131.25	123.05
2	G	236	VAL	C-N-CA	5.85	131.25	123.05
2	D	175	MET	CA-C-N	5.85	130.88	121.17
2	D	175	MET	C-N-CA	5.85	130.88	121.17
2	F	212	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	81	LYS	CA-C-N	5.84	129.29	121.23
1	A	81	LYS	C-N-CA	5.84	129.29	121.23
2	E	10	PHE	CA-C-N	5.84	131.23	122.75
2	E	10	PHE	C-N-CA	5.84	131.23	122.75
2	F	34	ASP	N-CA-CB	5.84	117.59	110.17
2	G	32	ARG	CD-NE-CZ	5.83	132.56	124.40
3	I	569	ILE	CA-C-N	5.81	128.39	120.54
3	I	569	ILE	C-N-CA	5.81	128.39	120.54
1	A	75	ARG	CA-C-N	5.81	130.69	122.09
1	A	75	ARG	C-N-CA	5.81	130.69	122.09
2	H	209	LEU	CA-C-N	5.80	127.98	120.44
2	H	209	LEU	C-N-CA	5.80	127.98	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	345	ASP	CA-CB-CG	5.80	118.41	112.60
1	A	31	ARG	CA-C-N	5.80	131.06	122.99
1	A	31	ARG	C-N-CA	5.80	131.06	122.99
2	B	25	PRO	CA-C-N	5.80	129.77	121.71
2	B	25	PRO	C-N-CA	5.80	129.77	121.71
2	F	103	LYS	N-CA-CB	5.80	118.64	110.12
2	F	109	MET	CA-C-N	5.80	128.53	120.29
2	F	109	MET	C-N-CA	5.80	128.53	120.29
2	F	146	PRO	CA-C-N	5.80	131.00	122.94
2	F	146	PRO	C-N-CA	5.80	131.00	122.94
2	H	245	ASN	CA-CB-CG	5.79	118.39	112.60
2	C	54	HIS	CA-CB-CG	5.79	119.59	113.80
2	H	191	PHE	CA-CB-CG	5.79	119.59	113.80
1	A	164	GLU	CA-C-N	5.79	131.27	123.46
1	A	164	GLU	C-N-CA	5.79	131.27	123.46
2	H	111	THR	CA-C-N	5.79	128.31	120.44
2	H	111	THR	C-N-CA	5.79	128.31	120.44
2	F	224	ALA	CA-C-N	5.78	128.31	120.44
2	F	224	ALA	C-N-CA	5.78	128.31	120.44
2	B	259	ARG	CD-NE-CZ	5.77	132.47	124.40
2	D	131	GLN	CA-C-N	5.76	131.01	122.71
2	D	131	GLN	C-N-CA	5.76	131.01	122.71
2	H	65	PHE	CA-CB-CG	5.75	119.56	113.80
2	G	235	ILE	CA-C-N	5.75	130.67	123.14
2	G	235	ILE	C-N-CA	5.75	130.67	123.14
2	H	204	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	98	TYR	CA-C-N	5.73	131.07	123.00
1	A	98	TYR	C-N-CA	5.73	131.07	123.00
2	G	10	PHE	CA-C-N	5.73	130.90	122.94
2	G	10	PHE	C-N-CA	5.73	130.90	122.94
2	G	209	LEU	CA-C-N	5.72	127.88	120.44
2	G	209	LEU	C-N-CA	5.72	127.88	120.44
2	D	159	VAL	CA-C-N	5.72	128.22	120.44
2	D	159	VAL	C-N-CA	5.72	128.22	120.44
2	F	64	ARG	CD-NE-CZ	5.72	132.40	124.40
4	K	53	HIS	CA-CB-CG	5.72	119.52	113.80
2	B	33	ILE	CA-C-N	5.71	130.41	121.17
2	B	33	ILE	C-N-CA	5.71	130.41	121.17
2	C	206	ASP	CA-CB-CG	5.71	118.31	112.60
3	I	580	ASP	CA-CB-CG	5.70	118.30	112.60
2	G	29	ASN	CA-C-N	5.68	128.74	120.51
2	G	29	ASN	C-N-CA	5.68	128.74	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	54	HIS	N-CA-CB	5.68	118.24	110.01
2	C	54	HIS	N-CA-CB	5.66	118.22	110.01
2	E	227	GLY	CA-C-N	5.64	130.95	123.05
2	E	227	GLY	C-N-CA	5.64	130.95	123.05
2	B	178	LYS	CA-C-N	5.64	130.94	122.99
2	B	178	LYS	C-N-CA	5.64	130.94	122.99
2	F	57	LEU	CA-C-N	5.63	128.29	120.63
2	F	57	LEU	C-N-CA	5.63	128.29	120.63
2	H	6	ASN	CA-C-N	5.63	129.55	121.50
2	H	6	ASN	C-N-CA	5.63	129.55	121.50
2	B	151	GLU	CA-C-N	5.62	130.57	123.10
2	B	151	GLU	C-N-CA	5.62	130.57	123.10
2	F	103	LYS	CB-CG-CD	5.62	124.21	111.30
2	H	191	PHE	CA-C-N	5.61	130.78	122.99
2	H	191	PHE	C-N-CA	5.61	130.78	122.99
2	G	64	ARG	CD-NE-CZ	5.61	132.25	124.40
1	A	77	GLU	N-CA-C	5.60	116.76	108.86
2	C	135	PRO	CA-C-N	5.60	130.40	123.12
2	C	135	PRO	C-N-CA	5.60	130.40	123.12
3	I	401	PRO	CA-C-N	5.60	128.82	120.87
3	I	401	PRO	C-N-CA	5.60	128.82	120.87
2	C	41	LEU	CA-C-N	5.60	130.87	122.75
2	C	41	LEU	C-N-CA	5.60	130.87	122.75
2	G	41	LEU	CA-C-N	5.60	130.93	122.98
2	G	41	LEU	C-N-CA	5.60	130.93	122.98
2	H	6	ASN	CA-CB-CG	5.58	118.18	112.60
2	F	58	THR	CA-C-N	5.58	127.76	120.28
2	F	58	THR	C-N-CA	5.58	127.76	120.28
2	G	151	GLU	N-CA-CB	5.58	118.17	109.97
2	H	203	SER	CA-C-N	5.58	127.75	120.28
2	H	203	SER	C-N-CA	5.58	127.75	120.28
2	H	205	GLU	CA-C-N	5.57	127.69	120.44
2	H	205	GLU	C-N-CA	5.57	127.69	120.44
2	G	203	SER	CA-C-N	5.57	127.74	120.28
2	G	203	SER	C-N-CA	5.57	127.74	120.28
2	E	256	LYS	CA-C-N	5.56	130.72	122.99
2	E	256	LYS	C-N-CA	5.56	130.72	122.99
2	H	190	GLY	N-CA-C	5.56	119.25	110.96
2	B	177	ARG	NE-CZ-NH2	5.56	124.21	119.20
2	F	52	ARG	NE-CZ-NH2	5.56	124.21	119.20
3	I	257	SER	CA-C-N	5.56	130.67	123.00
3	I	257	SER	C-N-CA	5.56	130.67	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	41	LEU	CA-C-N	5.56	130.72	122.99
2	D	41	LEU	C-N-CA	5.56	130.72	122.99
1	A	23	THR	CA-C-N	5.56	128.11	120.39
1	A	23	THR	C-N-CA	5.56	128.11	120.39
4	J	12	TYR	CA-C-N	5.54	127.64	120.44
4	J	12	TYR	C-N-CA	5.54	127.64	120.44
2	E	16	VAL	CA-C-N	5.53	130.58	122.39
2	E	16	VAL	C-N-CA	5.53	130.58	122.39
2	G	212	ASP	CA-CB-CG	5.53	118.13	112.60
4	K	32	ALA	CA-C-N	5.53	127.69	120.28
4	K	32	ALA	C-N-CA	5.53	127.69	120.28
2	H	55	VAL	N-CA-CB	5.51	116.63	110.62
2	H	80	GLU	CA-C-N	5.51	127.61	120.44
2	H	80	GLU	C-N-CA	5.51	127.61	120.44
4	J	25	GLN	N-CA-CB	5.51	118.00	110.01
2	H	51	ILE	N-CA-CB	5.50	116.62	110.62
2	H	52	ARG	CA-C-N	5.50	127.59	120.44
2	H	52	ARG	C-N-CA	5.50	127.59	120.44
2	G	179	HIS	CA-CB-CG	5.49	119.29	113.80
3	I	334	ARG	CA-C-N	5.48	127.56	120.44
3	I	334	ARG	C-N-CA	5.48	127.56	120.44
2	H	41	LEU	CA-C-N	5.47	130.60	122.99
2	H	41	LEU	C-N-CA	5.47	130.60	122.99
2	H	239	HIS	CE1-NE2-CD2	-5.47	103.53	109.00
4	J	90	ILE	N-CA-CB	5.47	116.68	110.72
2	G	151	GLU	CA-C-N	5.47	130.54	122.94
2	G	151	GLU	C-N-CA	5.47	130.54	122.94
5	L	30	A	O4'-C1'-C2'	-5.46	100.34	105.80
2	G	246	ALA	N-CA-C	5.46	113.13	108.22
2	F	54	HIS	N-CA-CB	5.45	117.92	110.01
3	I	514	GLU	CA-C-N	5.45	128.03	120.29
3	I	514	GLU	C-N-CA	5.45	128.03	120.29
2	D	227	GLY	CA-C-N	5.45	130.68	123.05
2	D	227	GLY	C-N-CA	5.45	130.68	123.05
2	E	12	LEU	CA-C-N	5.45	131.11	122.94
2	E	12	LEU	C-N-CA	5.45	131.11	122.94
2	E	230	SER	CA-C-N	5.45	130.77	122.65
2	E	230	SER	C-N-CA	5.45	130.77	122.65
2	G	177	ARG	NE-CZ-NH2	5.45	124.10	119.20
2	H	64	ARG	CD-NE-CZ	5.45	132.03	124.40
2	F	16	VAL	CA-C-N	5.44	129.98	121.76
2	F	16	VAL	C-N-CA	5.44	129.98	121.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	85	GLU	CA-C-N	5.44	127.50	120.70
4	J	85	GLU	C-N-CA	5.44	127.50	120.70
2	D	16	VAL	CA-C-N	5.44	130.44	122.39
2	D	16	VAL	C-N-CA	5.44	130.44	122.39
2	F	179	HIS	CE1-NE2-CD2	-5.44	103.56	109.00
2	H	241	ASN	CA-C-N	5.43	127.50	120.44
2	H	241	ASN	C-N-CA	5.43	127.50	120.44
3	I	376	HIS	CE1-NE2-CD2	-5.43	103.56	109.00
2	D	15	ASP	CA-C-N	5.43	130.41	122.69
2	D	15	ASP	C-N-CA	5.43	130.41	122.69
2	H	48	LYS	CB-CG-CD	5.43	123.79	111.30
2	C	39	HIS	CE1-NE2-CD2	-5.43	103.57	109.00
4	K	64	ALA	CA-C-N	5.43	127.49	120.44
4	K	64	ALA	C-N-CA	5.43	127.49	120.44
2	E	184	GLY	CA-C-N	5.42	131.09	122.74
2	E	184	GLY	C-N-CA	5.42	131.09	122.74
2	E	44	ASP	CA-C-N	5.42	127.39	120.56
2	E	44	ASP	C-N-CA	5.42	127.39	120.56
2	G	188	ALA	CA-C-N	5.42	131.07	122.62
2	G	188	ALA	C-N-CA	5.42	131.07	122.62
2	G	189	HIS	CE1-NE2-CD2	-5.42	103.58	109.00
3	I	372	ASP	N-CA-CB	5.42	117.66	110.29
2	H	212	ASP	CA-C-N	5.41	127.48	120.44
2	H	212	ASP	C-N-CA	5.41	127.48	120.44
2	B	150	GLN	CA-C-N	5.41	130.62	122.99
2	B	150	GLN	C-N-CA	5.41	130.62	122.99
2	F	106	THR	CA-C-N	5.41	127.47	120.44
2	F	106	THR	C-N-CA	5.41	127.47	120.44
2	H	49	ARG	N-CA-CB	5.41	117.85	110.01
2	F	209	LEU	CA-C-N	5.41	127.84	120.54
2	F	209	LEU	C-N-CA	5.41	127.84	120.54
1	A	21	CYS	CA-C-N	5.40	131.33	123.12
1	A	21	CYS	C-N-CA	5.40	131.33	123.12
2	E	163	ALA	CA-C-N	5.40	127.46	120.44
2	E	163	ALA	C-N-CA	5.40	127.46	120.44
2	C	227	GLY	CA-C-N	5.39	130.60	123.05
2	C	227	GLY	C-N-CA	5.39	130.60	123.05
2	F	39	HIS	CE1-NE2-CD2	-5.39	103.61	109.00
2	D	19	GLY	N-CA-C	5.39	118.97	111.10
2	H	71	GLU	N-CA-CB	5.39	117.83	109.48
2	E	79	HIS	CE1-NE2-CD2	-5.39	103.61	109.00
3	I	373	THR	CA-C-N	5.38	127.34	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	373	THR	C-N-CA	5.38	127.34	120.56
2	D	177	ARG	CA-C-N	5.38	131.16	122.29
2	D	177	ARG	C-N-CA	5.38	131.16	122.29
2	D	177	ARG	CD-NE-CZ	5.38	131.93	124.40
2	G	57	LEU	CA-C-N	5.38	127.43	120.44
2	G	57	LEU	C-N-CA	5.38	127.43	120.44
2	H	68	TYR	CA-CB-CG	5.38	123.58	113.90
2	G	52	ARG	CA-CB-CG	5.38	124.85	114.10
4	J	86	ILE	N-CA-CB	5.38	116.48	110.62
2	G	206	ASP	CA-C-N	5.38	127.43	120.44
2	G	206	ASP	C-N-CA	5.38	127.43	120.44
2	H	242	ARG	CA-C-N	5.38	130.72	122.93
2	H	242	ARG	C-N-CA	5.38	130.72	122.93
2	F	98	LYS	N-CA-CB	5.37	118.44	110.49
3	I	573	GLU	CA-C-N	5.37	127.33	120.56
3	I	573	GLU	C-N-CA	5.37	127.33	120.56
2	F	54	HIS	CE1-NE2-CD2	-5.36	103.64	109.00
5	L	47	A	C5'-C4'-O4'	5.36	117.85	109.80
2	G	179	HIS	CE1-NE2-CD2	-5.36	103.64	109.00
2	H	244	GLY	CA-C-N	5.36	130.34	121.99
2	H	244	GLY	C-N-CA	5.36	130.34	121.99
4	K	25	GLN	N-CA-CB	5.35	117.99	110.12
2	H	239	HIS	CG-CD2-NE2	5.35	112.55	107.20
3	I	280	GLU	CA-C-N	5.35	127.39	120.44
3	I	280	GLU	C-N-CA	5.35	127.39	120.44
4	J	107	ILE	N-CA-CB	5.34	116.44	110.51
2	G	50	LYS	CA-C-N	5.34	127.29	120.56
2	G	50	LYS	C-N-CA	5.34	127.29	120.56
2	H	206	ASP	CA-C-N	5.34	127.38	120.44
2	H	206	ASP	C-N-CA	5.34	127.38	120.44
2	G	63	GLU	N-CA-CB	5.34	117.89	109.83
2	C	19	GLY	N-CA-C	5.33	118.89	111.10
1	A	24	ARG	CA-CB-CG	5.33	124.76	114.10
2	H	188	ALA	CA-C-N	5.33	130.93	122.94
2	H	188	ALA	C-N-CA	5.33	130.93	122.94
4	J	41	LEU	N-CA-CB	5.32	117.73	110.01
2	G	139	ALA	CA-C-N	5.32	128.26	120.71
2	G	139	ALA	C-N-CA	5.32	128.26	120.71
3	I	515	ASP	CA-C-N	5.32	127.35	120.44
3	I	515	ASP	C-N-CA	5.32	127.35	120.44
2	B	179	HIS	CA-CB-CG	5.31	119.11	113.80
4	K	113	ARG	N-CA-CB	5.31	117.71	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	55	VAL	N-CA-CB	5.31	116.76	110.55
2	G	19	GLY	N-CA-C	5.31	119.25	110.55
3	I	11	GLN	CA-C-N	5.31	127.34	120.44
3	I	11	GLN	C-N-CA	5.31	127.34	120.44
4	K	53	HIS	CA-C-N	5.31	127.66	120.44
4	K	53	HIS	C-N-CA	5.31	127.66	120.44
1	A	108	GLN	CA-C-N	5.30	130.47	122.99
1	A	108	GLN	C-N-CA	5.30	130.47	122.99
2	C	92	PRO	CA-C-N	5.30	128.12	120.38
2	C	92	PRO	C-N-CA	5.30	128.12	120.38
2	F	228	LEU	CA-C-N	5.30	130.89	122.94
2	F	228	LEU	C-N-CA	5.30	130.89	122.94
2	G	244	GLY	CA-C-N	5.30	130.09	121.98
2	G	244	GLY	C-N-CA	5.30	130.09	121.98
2	H	107	ASP	CA-C-N	5.30	127.38	120.28
2	H	107	ASP	C-N-CA	5.30	127.38	120.28
4	K	41	LEU	N-CA-CB	5.30	117.69	110.01
2	H	7	ARG	CA-CB-CG	5.29	124.69	114.10
1	A	68	ILE	CA-C-N	5.29	130.56	122.25
1	A	68	ILE	C-N-CA	5.29	130.56	122.25
2	G	46	CYS	CA-C-N	5.29	127.32	120.44
2	G	46	CYS	C-N-CA	5.29	127.32	120.44
2	H	105	VAL	N-CA-CB	5.29	117.74	110.54
2	E	188	ALA	CA-C-N	5.29	131.12	122.81
2	E	188	ALA	C-N-CA	5.29	131.12	122.81
2	G	71	GLU	N-CA-CB	5.29	117.78	109.69
2	C	110	CYS	CA-C-N	5.28	127.62	120.65
2	C	110	CYS	C-N-CA	5.28	127.62	120.65
2	G	189	HIS	CG-CD2-NE2	5.28	112.48	107.20
2	G	55	VAL	N-CA-CB	5.28	116.73	110.55
4	J	113	ARG	N-CA-CB	5.28	117.81	109.94
2	H	239	HIS	ND1-CG-CD2	-5.28	100.82	106.10
3	I	252	TYR	N-CA-CB	5.28	117.67	110.01
2	F	41	LEU	CA-C-N	5.28	130.77	122.70
2	F	41	LEU	C-N-CA	5.28	130.77	122.70
2	H	108	TRP	N-CA-CB	5.28	117.88	110.12
2	C	56	ALA	CA-C-N	5.28	127.30	120.44
2	C	56	ALA	C-N-CA	5.28	127.30	120.44
2	F	50	LYS	CA-C-N	5.28	127.21	120.56
2	F	50	LYS	C-N-CA	5.28	127.21	120.56
2	G	172	ASN	N-CA-CB	5.28	117.80	110.04
2	H	113	PHE	CA-C-N	5.27	127.66	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	113	PHE	C-N-CA	5.27	127.66	120.54
2	B	49	ARG	CA-C-N	5.27	127.29	120.44
2	B	49	ARG	C-N-CA	5.27	127.29	120.44
2	D	178	LYS	CA-CB-CG	5.27	124.64	114.10
2	F	97	LYS	CA-C-N	5.27	130.77	122.34
2	F	97	LYS	C-N-CA	5.27	130.77	122.34
2	D	146	PRO	CA-C-N	5.27	130.58	122.68
2	D	146	PRO	C-N-CA	5.27	130.58	122.68
3	I	247	VAL	CA-C-N	5.27	127.29	120.44
3	I	247	VAL	C-N-CA	5.27	127.29	120.44
2	G	24	ASP	N-CA-CB	5.26	117.13	110.23
2	C	39	HIS	CG-CD2-NE2	5.26	112.46	107.20
4	J	16	ARG	CA-C-N	5.26	127.28	120.44
4	J	16	ARG	C-N-CA	5.26	127.28	120.44
3	I	245	SER	CA-C-N	5.26	128.10	120.79
3	I	245	SER	C-N-CA	5.26	128.10	120.79
1	A	186	ARG	CA-C-N	5.26	130.82	122.94
1	A	186	ARG	C-N-CA	5.26	130.82	122.94
2	G	216	ASN	CA-C-N	5.25	127.27	120.44
2	G	216	ASN	C-N-CA	5.25	127.27	120.44
2	G	2	THR	CA-C-N	5.25	128.93	121.42
2	G	2	THR	C-N-CA	5.25	128.93	121.42
2	F	39	HIS	ND1-CG-CD2	-5.25	100.85	106.10
3	I	201	ILE	CA-C-N	5.25	128.23	120.82
3	I	201	ILE	C-N-CA	5.25	128.23	120.82
2	F	179	HIS	ND1-CG-CD2	-5.25	100.85	106.10
3	I	4	GLN	CB-CG-CD	5.25	121.53	112.60
2	G	205	GLU	CA-C-N	5.25	127.26	120.44
2	G	205	GLU	C-N-CA	5.25	127.26	120.44
1	A	22	PHE	CA-C-N	5.24	128.21	120.82
1	A	22	PHE	C-N-CA	5.24	128.21	120.82
2	C	228	LEU	CA-C-N	5.24	130.80	122.62
2	C	228	LEU	C-N-CA	5.24	130.80	122.62
2	F	179	HIS	CG-CD2-NE2	5.24	112.44	107.20
2	F	39	HIS	CG-CD2-NE2	5.24	112.44	107.20
2	G	189	HIS	ND1-CG-CD2	-5.24	100.86	106.10
2	E	223	SER	CA-C-N	5.24	127.25	120.44
2	E	223	SER	C-N-CA	5.24	127.25	120.44
4	J	59	ALA	CA-C-N	5.24	127.25	120.44
4	J	59	ALA	C-N-CA	5.24	127.25	120.44
2	G	54	HIS	CA-CB-CG	5.23	119.03	113.80
1	A	29	VAL	CA-C-N	5.23	131.07	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	VAL	C-N-CA	5.23	131.07	123.12
2	B	29	ASN	CA-C-N	5.23	127.66	120.39
2	B	29	ASN	C-N-CA	5.23	127.66	120.39
2	C	142	ARG	CD-NE-CZ	5.23	131.72	124.40
2	D	268	ARG	NE-CZ-NH2	5.23	123.91	119.20
2	C	39	HIS	ND1-CG-CD2	-5.23	100.87	106.10
4	J	22	GLU	N-CA-CB	5.23	117.59	110.01
2	F	54	HIS	ND1-CG-CD2	-5.22	100.88	106.10
2	G	237	PHE	CA-C-N	5.22	130.37	123.00
2	G	237	PHE	C-N-CA	5.22	130.37	123.00
3	I	376	HIS	CG-CD2-NE2	5.22	112.42	107.20
2	F	94	LYS	CA-CB-CG	5.22	124.55	114.10
2	H	139	ALA	CA-C-N	5.22	128.18	120.82
2	H	139	ALA	C-N-CA	5.22	128.18	120.82
2	E	79	HIS	ND1-CG-CD2	-5.21	100.89	106.10
2	G	8	TYR	CA-C-N	5.21	131.17	122.73
2	G	8	TYR	C-N-CA	5.21	131.17	122.73
2	B	262	GLY	CA-C-N	5.21	128.10	120.71
2	B	262	GLY	C-N-CA	5.21	128.10	120.71
2	H	1	MET	CA-C-N	5.21	128.27	120.87
2	H	1	MET	C-N-CA	5.21	128.27	120.87
3	I	469	TYR	CA-C-N	5.20	127.52	120.44
3	I	469	TYR	C-N-CA	5.20	127.52	120.44
2	C	64	ARG	CD-NE-CZ	5.20	131.68	124.40
2	H	74	ILE	N-CA-CB	5.20	116.93	111.00
2	C	55	VAL	N-CA-CB	5.20	116.64	110.55
3	I	205	ARG	CA-C-N	5.20	127.20	120.44
3	I	205	ARG	C-N-CA	5.20	127.20	120.44
3	I	411	ALA	CA-C-N	5.20	127.31	120.60
3	I	411	ALA	C-N-CA	5.20	127.31	120.60
2	G	48	LYS	CA-C-N	5.20	127.20	120.44
2	G	48	LYS	C-N-CA	5.20	127.20	120.44
3	I	249	ALA	CA-C-N	5.20	127.20	120.44
3	I	249	ALA	C-N-CA	5.20	127.20	120.44
5	L	29	G	C5'-C4'-C3'	5.19	123.79	116.00
2	F	178	LYS	CA-CB-CG	5.19	124.48	114.10
2	F	54	HIS	CG-CD2-NE2	5.19	112.39	107.20
5	L	34	G	O5'-C5'-C4'	5.19	119.48	111.70
2	E	79	HIS	CG-CD2-NE2	5.19	112.39	107.20
2	F	131	GLN	CA-C-N	5.18	129.69	122.23
2	F	131	GLN	C-N-CA	5.18	129.69	122.23
2	G	7	ARG	CA-CB-CG	5.18	124.47	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	376	HIS	ND1-CG-CD2	-5.18	100.92	106.10
2	F	19	GLY	CA-C-N	5.18	130.76	123.30
2	F	19	GLY	C-N-CA	5.18	130.76	123.30
2	G	173	ARG	CA-C-N	5.18	128.44	120.82
2	G	173	ARG	C-N-CA	5.18	128.44	120.82
2	H	46	CYS	N-CA-CB	5.18	117.66	109.94
4	J	98	SER	N-CA-CB	5.18	117.77	110.36
2	H	90	PRO	CA-C-N	5.17	128.68	122.89
2	H	90	PRO	C-N-CA	5.17	128.68	122.89
4	J	108	GLY	CA-C-N	5.17	127.16	120.44
4	J	108	GLY	C-N-CA	5.17	127.16	120.44
4	K	65	LYS	CA-CB-CG	5.17	124.44	114.10
2	C	151	GLU	CA-C-N	5.17	129.91	123.14
2	C	151	GLU	C-N-CA	5.17	129.91	123.14
2	G	230	SER	CA-C-N	5.17	128.18	120.95
2	G	230	SER	C-N-CA	5.17	128.18	120.95
4	J	35	THR	CA-C-N	5.17	127.54	120.46
4	J	35	THR	C-N-CA	5.17	127.54	120.46
2	G	179	HIS	CG-CD2-NE2	5.16	112.36	107.20
2	H	47	LEU	CA-C-N	5.16	127.62	120.29
2	H	47	LEU	C-N-CA	5.16	127.62	120.29
2	H	202	PHE	N-CA-CB	5.16	117.54	109.85
2	G	242	ARG	CD-NE-CZ	5.16	131.63	124.40
2	G	247	PRO	CA-C-N	5.16	127.15	120.44
2	G	247	PRO	C-N-CA	5.16	127.15	120.44
4	K	116	LEU	CA-C-N	5.16	127.19	120.28
4	K	116	LEU	C-N-CA	5.16	127.19	120.28
2	D	98	LYS	CA-C-N	5.16	127.25	120.60
2	D	98	LYS	C-N-CA	5.16	127.25	120.60
3	I	4	GLN	CA-C-N	5.16	127.14	120.44
3	I	4	GLN	C-N-CA	5.16	127.14	120.44
2	F	153	SER	CA-C-N	5.15	130.82	122.68
2	F	153	SER	C-N-CA	5.15	130.82	122.68
2	D	72	LYS	CB-CG-CD	5.15	123.14	111.30
2	D	46	CYS	CA-C-N	5.15	127.13	120.44
2	D	46	CYS	C-N-CA	5.15	127.13	120.44
2	G	152	VAL	CA-C-N	5.15	130.89	122.81
2	G	152	VAL	C-N-CA	5.15	130.89	122.81
4	J	63	THR	CA-C-N	5.14	127.13	120.44
4	J	63	THR	C-N-CA	5.14	127.13	120.44
4	K	114	LYS	N-CA-CB	5.14	117.46	110.01
2	F	57	LEU	N-CA-CB	5.14	117.46	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	177	ARG	NE-CZ-NH2	5.13	123.82	119.20
2	E	46	CYS	CA-C-N	5.13	127.11	120.44
2	E	46	CYS	C-N-CA	5.13	127.11	120.44
3	I	444	ALA	CA-C-N	5.13	127.03	120.56
3	I	444	ALA	C-N-CA	5.13	127.03	120.56
3	I	471	ARG	NE-CZ-NH2	5.13	123.82	119.20
2	C	50	LYS	CA-C-N	5.13	127.03	120.56
2	C	50	LYS	C-N-CA	5.13	127.03	120.56
4	J	41	LEU	CA-C-N	5.13	127.42	120.65
4	J	41	LEU	C-N-CA	5.13	127.42	120.65
3	I	5	ALA	CA-C-N	5.13	127.11	120.44
3	I	5	ALA	C-N-CA	5.13	127.11	120.44
2	C	140	PHE	CA-C-N	5.13	130.08	123.00
2	C	140	PHE	C-N-CA	5.13	130.08	123.00
3	I	543	LEU	CA-C-N	5.13	127.11	120.44
3	I	543	LEU	C-N-CA	5.13	127.11	120.44
2	D	156	ARG	CA-C-N	5.12	127.91	120.79
2	D	156	ARG	C-N-CA	5.12	127.91	120.79
2	H	238	LYS	CA-C-N	5.12	129.90	121.39
2	H	238	LYS	C-N-CA	5.12	129.90	121.39
2	F	171	ASP	CA-C-N	5.12	129.67	122.09
2	F	171	ASP	C-N-CA	5.12	129.67	122.09
2	C	46	CYS	CA-C-N	5.12	127.09	120.44
2	C	46	CYS	C-N-CA	5.12	127.09	120.44
2	G	6	ASN	CA-C-N	5.12	129.41	122.19
2	G	6	ASN	C-N-CA	5.12	129.41	122.19
2	D	157	MET	CA-CB-CG	5.12	124.33	114.10
3	I	398	GLN	CA-CB-CG	5.12	124.33	114.10
2	F	45	VAL	CA-C-N	5.11	127.09	120.44
2	F	45	VAL	C-N-CA	5.11	127.09	120.44
2	G	250	LYS	CA-C-N	5.11	127.09	120.44
2	G	250	LYS	C-N-CA	5.11	127.09	120.44
2	F	35	PRO	CA-C-N	5.11	128.08	120.31
2	F	35	PRO	C-N-CA	5.11	128.08	120.31
1	A	107	ARG	N-CA-CB	5.11	117.46	109.85
2	D	258	SER	CA-C-N	5.11	127.97	120.71
2	D	258	SER	C-N-CA	5.11	127.97	120.71
2	E	71	GLU	N-CA-CB	5.11	117.50	109.69
2	B	162	LYS	CA-C-N	5.11	127.38	120.44
2	B	162	LYS	C-N-CA	5.11	127.38	120.44
4	J	66	LEU	CA-C-N	5.11	127.12	120.28
4	J	66	LEU	C-N-CA	5.11	127.12	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	THR	CA-C-N	5.10	128.72	121.42
2	H	2	THR	C-N-CA	5.10	128.72	121.42
3	I	9	TYR	N-CA-CB	5.10	117.41	110.01
2	G	179	HIS	ND1-CG-CD2	-5.10	101.00	106.10
4	J	45	SER	CA-C-N	5.10	127.07	120.44
4	J	45	SER	C-N-CA	5.10	127.07	120.44
4	K	57	LYS	CA-C-N	5.10	127.11	120.28
4	K	57	LYS	C-N-CA	5.10	127.11	120.28
1	A	74	ARG	CA-CB-CG	5.10	124.29	114.10
2	F	51	ILE	N-CA-CB	5.10	116.52	110.55
1	A	186	ARG	CA-CB-CG	5.10	124.29	114.10
3	I	513	GLN	N-CA-CB	5.10	117.40	110.01
3	I	476	LYS	CA-C-N	5.09	127.11	120.28
3	I	476	LYS	C-N-CA	5.09	127.11	120.28
2	G	1	MET	CA-C-N	5.09	127.94	120.71
2	G	1	MET	C-N-CA	5.09	127.94	120.71
2	H	45	VAL	CA-C-N	5.09	127.41	120.54
2	H	45	VAL	C-N-CA	5.09	127.41	120.54
3	I	541	HIS	CA-C-N	5.09	127.52	120.29
3	I	541	HIS	C-N-CA	5.09	127.52	120.29
1	A	186	ARG	CG-CD-NE	5.09	123.20	112.00
2	C	51	ILE	N-CA-CB	5.09	116.50	110.55
3	I	288	ASP	CA-C-N	5.09	125.62	120.38
3	I	288	ASP	C-N-CA	5.09	125.62	120.38
2	E	226	ARG	CD-NE-CZ	5.08	131.52	124.40
4	J	44	ALA	CA-C-N	5.08	127.05	120.44
4	J	44	ALA	C-N-CA	5.08	127.05	120.44
2	C	223	SER	CA-C-N	5.08	127.05	120.44
2	C	223	SER	C-N-CA	5.08	127.05	120.44
3	I	3	LEU	CA-C-N	5.08	127.80	120.38
3	I	3	LEU	C-N-CA	5.08	127.80	120.38
4	K	49	GLY	CA-C-N	5.08	127.36	120.65
4	K	49	GLY	C-N-CA	5.08	127.36	120.65
2	B	143	SER	N-CA-CB	5.08	117.62	110.36
2	E	140	PHE	CA-C-N	5.08	128.76	121.50
2	E	140	PHE	C-N-CA	5.08	128.76	121.50
2	F	212	ASP	CA-C-N	5.08	127.04	120.44
2	F	212	ASP	C-N-CA	5.08	127.04	120.44
3	I	374	VAL	N-CA-CB	5.08	116.49	110.55
3	I	602	LYS	N-CA-CB	5.08	117.58	110.12
2	C	16	VAL	CA-C-N	5.07	129.42	121.76
2	C	16	VAL	C-N-CA	5.07	129.42	121.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	101	ASP	CA-C-N	5.07	127.04	120.44
2	D	101	ASP	C-N-CA	5.07	127.04	120.44
3	I	577	ASN	CA-C-N	5.07	130.81	122.64
3	I	577	ASN	C-N-CA	5.07	130.81	122.64
3	I	212	GLN	N-CA-CB	5.07	117.49	110.04
4	J	42	ALA	CA-C-N	5.07	127.03	120.44
4	J	42	ALA	C-N-CA	5.07	127.03	120.44
2	C	64	ARG	CA-C-N	5.07	130.60	122.14
2	C	64	ARG	C-N-CA	5.07	130.60	122.14
2	H	198	GLU	CA-C-N	5.07	129.30	120.68
2	H	198	GLU	C-N-CA	5.07	129.30	120.68
3	I	256	PRO	CA-C-N	5.07	127.58	120.28
3	I	256	PRO	C-N-CA	5.07	127.58	120.28
2	C	178	LYS	CA-CB-CG	5.07	124.23	114.10
2	F	94	LYS	CG-CD-CE	5.07	122.95	111.30
2	G	211	TRP	CA-C-N	5.06	127.02	120.44
2	G	211	TRP	C-N-CA	5.06	127.02	120.44
2	E	130	GLY	CA-C-N	5.06	130.52	122.62
2	E	130	GLY	C-N-CA	5.06	130.52	122.62
2	C	146	PRO	CA-C-N	5.06	130.27	122.68
2	C	146	PRO	C-N-CA	5.06	130.27	122.68
4	J	105	PHE	CA-C-N	5.06	127.02	120.44
4	J	105	PHE	C-N-CA	5.06	127.02	120.44
2	E	15	ASP	CA-C-N	5.06	130.73	122.69
2	E	15	ASP	C-N-CA	5.06	130.73	122.69
5	L	44	U	C4'-C3'-C2'	-5.06	97.54	102.60
2	F	223	SER	CA-C-N	5.05	127.31	120.44
2	F	223	SER	C-N-CA	5.05	127.31	120.44
2	C	109	MET	CA-C-N	5.05	127.47	120.29
2	C	109	MET	C-N-CA	5.05	127.47	120.29
2	E	186	TYR	CA-C-N	5.05	129.96	122.94
2	E	186	TYR	C-N-CA	5.05	129.96	122.94
2	F	178	LYS	CA-C-N	5.05	129.69	122.72
2	F	178	LYS	C-N-CA	5.05	129.69	122.72
3	I	505	LEU	N-CA-CB	5.05	117.46	109.94
4	J	65	LYS	CA-C-N	5.04	127.49	120.63
4	J	65	LYS	C-N-CA	5.04	127.49	120.63
2	B	52	ARG	CA-C-N	5.04	127.00	120.44
2	B	52	ARG	C-N-CA	5.04	127.00	120.44
2	D	45	VAL	CA-C-N	5.04	127.00	120.44
2	D	45	VAL	C-N-CA	5.04	127.00	120.44
3	I	447	GLY	CA-C-N	5.04	127.00	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	447	GLY	C-N-CA	5.04	127.00	120.44
2	C	117	ARG	CD-NE-CZ	5.04	131.45	124.40
3	I	491	LEU	N-CA-CB	5.03	117.28	109.48
3	I	544	LEU	CA-C-N	5.03	126.98	120.44
3	I	544	LEU	C-N-CA	5.03	126.98	120.44
4	K	117	PHE	N-CA-CB	5.03	117.52	110.12
2	H	250	LYS	CA-C-N	5.03	126.98	120.44
2	H	250	LYS	C-N-CA	5.03	126.98	120.44
3	I	572	GLN	N-CA-CB	5.03	117.30	110.01
2	D	161	THR	CA-C-N	5.03	129.65	122.21
2	D	161	THR	C-N-CA	5.03	129.65	122.21
4	J	113	ARG	CB-CG-CD	5.03	122.86	111.30
2	F	54	HIS	CA-C-N	5.02	126.89	120.56
2	F	54	HIS	C-N-CA	5.02	126.89	120.56
4	K	68	LYS	N-CA-CB	5.02	117.24	109.91
5	L	42	U	O5'-C5'-C4'	5.02	119.23	111.70
2	C	136	VAL	CA-C-N	5.02	130.47	122.59
2	C	136	VAL	C-N-CA	5.02	130.47	122.59
2	E	45	VAL	CA-C-N	5.02	126.97	120.44
2	E	45	VAL	C-N-CA	5.02	126.97	120.44
4	J	27	ASP	CA-C-N	5.02	126.97	120.44
4	J	27	ASP	C-N-CA	5.02	126.97	120.44
1	A	187	ASP	CA-C-N	5.02	130.34	122.11
1	A	187	ASP	C-N-CA	5.02	130.34	122.11
2	B	32	ARG	CA-CB-CG	5.02	124.13	114.10
2	G	51	ILE	N-CA-CB	5.02	116.42	110.55
3	I	375	GLY	CA-C-N	5.02	126.96	120.44
3	I	375	GLY	C-N-CA	5.02	126.96	120.44
3	I	8	GLY	CA-C-N	5.02	126.96	120.44
3	I	8	GLY	C-N-CA	5.02	126.96	120.44
4	K	3	LEU	N-CA-CB	5.02	117.26	109.48
2	F	136	VAL	CA-C-N	5.01	130.56	122.29
2	F	136	VAL	C-N-CA	5.01	130.56	122.29
2	H	187	VAL	CA-C-N	5.01	130.85	122.73
2	H	187	VAL	C-N-CA	5.01	130.85	122.73
1	A	106	ASN	CA-C-N	5.01	127.97	120.95
1	A	106	ASN	C-N-CA	5.01	127.97	120.95
2	F	15	ASP	CA-C-N	5.01	130.66	122.69
2	F	15	ASP	C-N-CA	5.01	130.66	122.69
4	J	7	ARG	N-CA-CB	5.01	117.34	110.07
2	G	164	GLU	CA-C-N	5.01	127.30	120.54
2	G	164	GLU	C-N-CA	5.01	127.30	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	386	ARG	CA-C-N	5.01	127.41	120.29
3	I	386	ARG	C-N-CA	5.01	127.41	120.29
2	D	43	THR	CA-C-N	5.01	127.49	120.28
2	D	43	THR	C-N-CA	5.01	127.49	120.28
2	F	46	CYS	CA-C-N	5.00	126.94	120.44
2	F	46	CYS	C-N-CA	5.00	126.94	120.44
3	I	281	ASP	N-CA-CB	5.00	117.27	110.01
3	I	510	GLU	N-CA-CB	5.00	117.56	110.16
4	K	54	MET	CA-C-N	5.00	126.98	120.28
4	K	54	MET	C-N-CA	5.00	126.98	120.28

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	226	ARG	Sidechain
2	G	155	THR	Mainchain
2	G	226	ARG	Sidechain
2	G	68	TYR	Sidechain
2	G	83	TYR	Sidechain
2	H	117	ARG	Sidechain
2	H	123	MET	Peptide
2	H	83	TYR	Sidechain
3	I	498	ARG	Sidechain
5	L	41	C	Sidechain
5	L	44	U	Sidechain
5	L	45	C	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1774	1761	1762	13	0
2	B	2112	2081	2079	9	0
2	C	2238	2224	2223	9	0
2	D	2238	2224	2223	28	0
2	E	2238	2224	2223	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2238	2224	2223	14	0
2	G	2238	2224	2223	19	0
2	H	2238	2224	2223	47	0
3	I	3267	3269	3261	16	0
4	J	930	933	931	6	0
4	K	930	933	931	2	0
5	L	980	500	459	14	0
6	N	369	202	188	8	0
All	All	23790	23023	22949	184	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 4.

All (184) 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)
3:I:590:GLN:O	3:I:591:GLY:N	1.67	1.27
3:I:588:ASP:O	3:I:589:GLU:N	1.78	1.16
4:K:100:ASP:O	4:K:101:GLU:N	1.80	1.13
2:E:282:GLU:OE1	2:E:282:GLU:N	2.12	0.81
2:F:282:GLU:N	2:F:282:GLU:OE1	2.13	0.81
2:D:282:GLU:OE1	2:D:282:GLU:N	2.13	0.80
1:A:211:GLU:N	1:A:211:GLU:OE1	2.16	0.78
2:B:282:GLU:N	2:B:282:GLU:OE1	2.14	0.78
2:F:155:THR:OG1	5:L:42:U:OP2	2.03	0.77
2:C:261:GLU:N	2:C:261:GLU:OE1	2.17	0.77
2:B:107:ASP:O	2:B:111:THR:HG23	1.84	0.76
6:N:26:DG:C8	6:N:26:DG:H5'	2.22	0.75
6:N:26:DG:H2'	6:N:27:DA:C8	2.22	0.75
2:C:282:GLU:N	2:C:282:GLU:OE1	2.20	0.73
2:H:289:MET:HE3	2:H:289:MET:H	1.51	0.73
2:G:282:GLU:N	2:G:282:GLU:OE1	2.20	0.72
2:D:109:MET:HE3	2:D:123:MET:SD	2.31	0.70
2:E:63:GLU:OE1	2:E:64:ARG:N	2.27	0.67
2:H:45:VAL:HG22	5:L:47:A:O3'	1.95	0.67
2:E:217:MET:HA	2:E:217:MET:HE3	1.76	0.67
2:H:45:VAL:O	5:L:47:A:O3'	2.04	0.67
6:N:29:DC:H4'	6:N:30:DA:OP2	1.95	0.66
4:J:83:MET:O	4:J:87:ILE:HG22	1.95	0.66
2:D:83:TYR:OH	2:D:128:ASN:O	2.03	0.66
2:E:131:GLN:NE2	5:L:26:G:N3	2.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:107:ASP:O	2:D:111:THR:HG23	1.96	0.66
2:H:20:ASN:N	2:H:225:ALA:O	2.30	0.65
1:A:224:GLU:N	1:A:224:GLU:OE1	2.31	0.64
2:C:161:THR:OG1	2:D:126:GLU:OE2	2.17	0.62
2:H:63:GLU:O	2:H:66:ASN:ND2	2.33	0.61
2:D:289:MET:SD	2:D:289:MET:N	2.74	0.61
2:H:46:CYS:O	5:L:47:A:O2'	2.18	0.61
2:D:79:HIS:HA	2:D:109:MET:HE1	1.82	0.61
5:L:12:G:O2'	5:L:13:C:OP2	2.15	0.61
2:B:80:GLU:OE1	2:B:81:ARG:N	2.31	0.60
2:C:161:THR:HG22	2:C:163:ALA:H	1.66	0.60
2:D:102:ALA:O	2:D:105:VAL:HG22	2.02	0.60
2:H:16:VAL:HG12	2:H:184:GLY:O	2.02	0.59
6:N:26:DG:H2''	6:N:27:DA:O4'	2.01	0.59
2:D:131:GLN:NE2	5:L:20:C:O2	2.36	0.58
2:H:66:ASN:N	2:H:112:ASN:O	2.35	0.58
2:H:15:ASP:OD2	2:H:232:ARG:NE	2.37	0.58
2:H:138:MET:C	2:H:138:MET:HE2	2.29	0.57
2:G:46:CYS:SG	2:G:50:LYS:NZ	2.77	0.57
3:I:399:GLU:N	3:I:399:GLU:OE1	2.37	0.57
4:J:7:ARG:O	4:J:8:THR:OG1	2.17	0.57
3:I:240:GLN:N	3:I:240:GLN:OE1	2.38	0.56
4:J:101:GLU:OE1	4:J:101:GLU:N	2.38	0.56
2:H:40:GLY:N	2:H:143:SER:OG	2.33	0.56
1:A:55:ILE:HD13	1:A:126:PHE:CZ	2.41	0.56
2:H:269:SER:N	2:H:272:ASP:OD2	2.35	0.55
2:H:42:VAL:HG23	2:H:186:TYR:CE2	2.41	0.55
2:H:128:ASN:CG	2:H:129:CYS:H	2.14	0.55
2:G:157:MET:SD	2:G:157:MET:N	2.80	0.55
3:I:542:MET:HE2	3:I:542:MET:C	2.32	0.55
3:I:13:MET:C	3:I:13:MET:HE2	2.32	0.54
2:B:30:MET:SD	2:B:179:HIS:ND1	2.80	0.54
2:H:241:ASN:ND2	2:H:243:LEU:O	2.41	0.54
2:C:12:LEU:C	2:C:13:LEU:HD12	2.33	0.54
2:D:82:ALA:HB2	2:D:108:TRP:CE3	2.42	0.54
2:G:173:ARG:NH1	2:H:71:GLU:OE2	2.40	0.54
2:E:54:HIS:HB2	2:E:217:MET:HE1	1.90	0.53
3:I:4:GLN:HA	3:I:186:ILE:HD11	1.89	0.53
6:N:26:DG:C4	6:N:27:DA:C6	2.97	0.53
1:A:55:ILE:HD12	1:A:56:ARG:N	2.23	0.53
3:I:22:PRO:N	3:I:23:PRO:CD	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:24:ASP:N	2:H:30:MET:O	2.36	0.52
2:H:16:VAL:HG12	2:H:184:GLY:C	2.36	0.51
2:E:46:CYS:SG	2:E:50:LYS:NZ	2.83	0.51
2:B:115:ASP:N	2:B:115:ASP:OD1	2.43	0.51
2:D:103:LYS:O	2:D:106:THR:OG1	2.27	0.51
2:H:159:VAL:HG22	2:H:160:THR:H	1.75	0.51
2:D:83:TYR:O	2:D:88:LEU:N	2.40	0.51
4:J:98:SER:N	4:J:101:GLU:OE1	2.44	0.50
2:D:122:VAL:HG21	5:L:21:A:C2	2.47	0.50
2:F:105:VAL:HG11	2:F:129:CYS:SG	2.51	0.50
2:B:109:MET:HE1	2:B:123:MET:SD	2.52	0.50
3:I:20:GLY:C	3:I:21:MET:HE3	2.36	0.50
2:H:44:ASP:O	2:H:138:MET:HE1	2.12	0.49
2:H:289:MET:HE3	2:H:289:MET:N	2.25	0.49
3:I:588:ASP:C	3:I:589:GLU:N	2.64	0.49
2:E:87:ASP:O	2:E:88:LEU:HD13	2.12	0.49
6:N:26:DG:H1'	6:N:27:DA:C4	2.46	0.49
3:I:184:CYS:O	3:I:188:GLY:N	2.44	0.49
2:E:95:LEU:HD21	2:E:129:CYS:HA	1.95	0.48
2:E:124:THR:O	2:E:124:THR:HG23	2.12	0.48
2:F:15:ASP:OD1	2:F:16:VAL:N	2.46	0.48
2:G:63:GLU:OE2	2:G:64:ARG:N	2.46	0.48
2:G:156:ARG:O	2:G:174:THR:N	2.46	0.48
2:H:46:CYS:HA	5:L:47:A:H2'	1.95	0.48
3:I:371:VAL:HG12	3:I:371:VAL:O	2.12	0.48
2:C:204:ASP:N	2:C:204:ASP:OD1	2.45	0.47
2:D:12:LEU:C	2:D:13:LEU:HD12	2.39	0.47
5:L:27:G:O2'	5:L:28:C:OP2	2.23	0.47
2:H:175:MET:C	2:H:175:MET:SD	2.97	0.47
2:B:106:THR:HA	2:B:109:MET:HE2	1.97	0.47
1:A:91:MET:SD	1:A:91:MET:N	2.76	0.47
2:H:268:ARG:N	2:H:272:ASP:OD2	2.46	0.47
2:H:16:VAL:HG22	2:H:16:VAL:O	2.14	0.47
2:H:287:LYS:HB2	2:H:289:MET:HE1	1.97	0.46
4:J:98:SER:O	4:J:101:GLU:N	2.48	0.46
2:H:68:TYR:N	2:H:115:ASP:OD2	2.47	0.46
2:F:259:ARG:NH1	2:F:265:GLY:O	2.38	0.46
2:G:15:ASP:OD2	2:G:232:ARG:NE	2.39	0.46
2:F:63:GLU:N	2:F:63:GLU:OE1	2.49	0.46
2:D:289:MET:H	2:D:289:MET:CE	2.29	0.46
2:H:117:ARG:HE	2:H:206:ASP:CG	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:184:CYS:SG	3:I:187:THR:OG1	2.71	0.46
2:E:217:MET:HE3	2:E:217:MET:O	2.15	0.46
2:D:290:LEU:HD12	2:D:290:LEU:H	1.81	0.45
2:H:15:ASP:CG	2:H:232:ARG:HE	2.23	0.45
2:D:74:ILE:HD12	2:D:74:ILE:N	2.32	0.45
2:D:92:PRO:HA	2:D:127:VAL:HA	1.98	0.45
2:H:205:GLU:CD	2:H:205:GLU:C	2.84	0.45
2:F:82:ALA:C	2:F:105:VAL:HG13	2.42	0.45
2:H:148:VAL:HG13	2:H:148:VAL:O	2.17	0.45
2:G:156:ARG:N	2:G:174:THR:O	2.50	0.45
1:A:129:THR:OG1	1:A:130:ASP:N	2.50	0.45
2:E:217:MET:HE3	2:E:217:MET:CA	2.44	0.44
2:D:67:ILE:O	2:D:67:ILE:HG23	2.17	0.44
2:D:126:GLU:OE1	2:D:126:GLU:N	2.45	0.44
2:H:37:THR:OG1	2:H:39:HIS:ND1	2.45	0.44
1:A:87:PRO:O	1:A:91:MET:HE1	2.18	0.44
2:B:71:GLU:O	2:B:71:GLU:HG3	2.17	0.44
2:G:269:SER:N	2:G:272:ASP:OD2	2.45	0.44
1:A:77:GLU:N	1:A:108:GLN:O	2.47	0.44
2:H:16:VAL:HG22	2:H:19:GLY:O	2.18	0.44
1:A:27:MET:SD	1:A:27:MET:N	2.91	0.44
6:N:26:DG:C5	6:N:27:DA:N6	2.86	0.43
2:B:109:MET:HE1	2:B:123:MET:CE	2.48	0.43
2:D:105:VAL:O	2:D:109:MET:HE2	2.18	0.43
2:H:58:THR:HG23	2:H:59:LYS:N	2.33	0.43
2:C:76:ASN:ND2	2:C:127:VAL:H	2.15	0.43
2:H:45:VAL:O	5:L:47:A:O2'	2.36	0.43
2:D:83:TYR:CG	2:D:90:PRO:HA	2.53	0.43
2:G:83:TYR:CE2	2:G:96:PRO:HD3	2.53	0.43
2:D:63:GLU:OE2	2:D:64:ARG:N	2.49	0.43
2:D:16:VAL:HG22	2:D:17:GLU:N	2.33	0.43
4:K:84:GLN:HA	4:K:87:ILE:HG22	2.01	0.43
2:F:203:SER:OG	2:F:204:ASP:N	2.52	0.43
2:H:147:VAL:O	2:H:148:VAL:C	2.62	0.43
2:E:204:ASP:N	2:E:204:ASP:OD1	2.52	0.42
1:A:36:VAL:HG22	1:A:37:MET:N	2.35	0.42
2:G:288:GLU:O	2:G:289:MET:C	2.60	0.42
3:I:206:ASP:N	3:I:206:ASP:OD1	2.52	0.42
2:G:213:ALA:O	2:G:217:MET:HB3	2.19	0.42
2:E:58:THR:HG23	2:E:59:LYS:N	2.33	0.42
2:C:241:ASN:ND2	2:C:243:LEU:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:233:LYS:NZ	2:D:288:GLU:OE2	2.43	0.42
2:F:86:CYS:SG	2:F:105:VAL:HA	2.59	0.42
2:F:93:LYS:O	2:F:124:THR:HG23	2.20	0.42
2:H:54:HIS:ND1	2:H:213:ALA:HA	2.35	0.42
2:D:68:TYR:O	2:D:69:ILE:C	2.62	0.42
2:H:27:ALA:HB3	2:H:30:MET:HB2	2.01	0.42
2:H:183:TYR:CZ	2:H:270:PHE:HA	2.55	0.42
2:F:112:ASN:OD1	2:F:113:PHE:N	2.53	0.41
2:G:58:THR:HG23	2:G:59:LYS:N	2.35	0.41
2:G:207:LEU:HD11	2:G:211:TRP:CZ2	2.55	0.41
2:H:106:THR:HA	2:H:109:MET:HE2	2.02	0.41
6:N:26:DG:C2'	6:N:27:DA:C8	3.00	0.41
2:C:99:VAL:HG21	2:C:105:VAL:CG2	2.51	0.41
2:H:49:ARG:HB2	5:L:47:A:H4'	2.02	0.41
1:A:131:LYS:HD2	1:A:131:LYS:O	2.21	0.41
2:H:45:VAL:HG13	5:L:47:A:O3'	2.20	0.41
2:H:237:PHE:CD2	2:H:286:VAL:HG22	2.55	0.41
2:D:12:LEU:O	2:D:13:LEU:HD12	2.21	0.41
2:G:128:ASN:C	5:L:38:C:C2	2.98	0.41
2:G:260:ALA:N	2:G:272:ASP:O	2.44	0.41
2:H:289:MET:H	2:H:289:MET:CE	2.27	0.41
1:A:55:ILE:HD12	1:A:55:ILE:C	2.46	0.41
2:G:156:ARG:O	2:G:174:THR:HB	2.22	0.41
2:G:157:MET:HE3	2:G:173:ARG:HG3	2.02	0.40
3:I:13:MET:HE3	3:I:19:ALA:HB3	2.03	0.40
2:H:62:ALA:O	2:H:63:GLU:C	2.62	0.40
3:I:22:PRO:CD	3:I:23:PRO:HD3	2.51	0.40
2:H:259:ARG:NH2	2:H:265:GLY:O	2.42	0.40
2:F:82:ALA:HA	2:F:108:TRP:CZ3	2.56	0.40
2:G:159:VAL:HG21	2:G:163:ALA:HB3	2.03	0.40
1:A:137:ASN:OD1	1:A:139:GLY:N	2.55	0.40
2:D:16:VAL:HG23	2:D:229:MET:HG2	2.03	0.40
2:F:12:LEU:C	2:F:13:LEU:HD12	2.47	0.40
2:F:286:VAL:O	2:F:286:VAL:HG13	2.20	0.40
2:H:197:ALA:O	2:H:201:GLY:N	2.52	0.40
4:J:81:ILE:O	4:J:85:GLU:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	218/227 (96%)	210 (96%)	8 (4%)	0	100	100
2	B	264/290 (91%)	253 (96%)	11 (4%)	0	100	100
2	C	282/290 (97%)	266 (94%)	16 (6%)	0	100	100
2	D	282/290 (97%)	266 (94%)	16 (6%)	0	100	100
2	E	282/290 (97%)	267 (95%)	15 (5%)	0	100	100
2	F	282/290 (97%)	265 (94%)	17 (6%)	0	100	100
2	G	282/290 (97%)	262 (93%)	20 (7%)	0	100	100
2	H	282/290 (97%)	259 (92%)	22 (8%)	1 (0%)	30	60
3	I	402/612 (66%)	383 (95%)	19 (5%)	0	100	100
4	J	111/124 (90%)	108 (97%)	3 (3%)	0	100	100
4	K	111/124 (90%)	109 (98%)	2 (2%)	0	100	100
All	All	2798/3117 (90%)	2648 (95%)	149 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	122	VAL

5.3.2 Protein sidechains [i](#)

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	189/194 (97%)	185 (98%)	4 (2%)	47	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	224/242 (93%)	224 (100%)	0	100	100
2	C	239/242 (99%)	233 (98%)	6 (2%)	42	76
2	D	239/242 (99%)	237 (99%)	2 (1%)	73	90
2	E	239/242 (99%)	234 (98%)	5 (2%)	47	79
2	F	239/242 (99%)	234 (98%)	5 (2%)	47	79
2	G	239/242 (99%)	236 (99%)	3 (1%)	61	86
2	H	239/242 (99%)	235 (98%)	4 (2%)	53	83
3	I	347/508 (68%)	339 (98%)	8 (2%)	44	78
4	J	99/105 (94%)	98 (99%)	1 (1%)	68	88
4	K	99/105 (94%)	98 (99%)	1 (1%)	68	88
All	All	2392/2606 (92%)	2353 (98%)	39 (2%)	54	83

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	THR
1	A	114	LEU
1	A	129	THR
1	A	188	LEU
2	C	83	TYR
2	C	87	ASP
2	C	95	LEU
2	C	129	CYS
2	C	191	PHE
2	C	206	ASP
2	D	109	MET
2	D	229	MET
2	E	24	ASP
2	E	75	LEU
2	E	124	THR
2	E	129	CYS
2	E	229	MET
2	F	83	TYR
2	F	122	VAL
2	F	123	MET
2	F	138	MET
2	F	179	HIS
2	G	105	VAL

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Mol	Chain	Res	Type
2	G	157	MET
2	G	175	MET
2	H	68	TYR
2	H	105	VAL
2	H	112	ASN
2	H	124	THR
3	I	287	PHE
3	I	341	ASP
3	I	402	SER
3	I	413	LEU
3	I	432	LEU
3	I	561	LYS
3	I	571	MET
3	I	580	ASP
4	J	101	GLU
4	K	38	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
2	B	39	HIS
2	B	66	ASN
2	B	79	HIS
2	B	189	HIS
2	C	150	GLN
2	C	189	HIS
2	D	241	ASN
2	E	22	ASN
2	E	179	HIS
2	E	189	HIS
2	E	249	HIS
2	F	18	ASN
2	F	29	ASN
2	F	179	HIS
2	G	76	ASN
2	G	79	HIS
2	G	112	ASN
2	G	179	HIS
2	G	220	HIS
2	H	20	ASN
2	H	22	ASN

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Mol	Chain	Res	Type
2	H	245	ASN
4	J	84	GLN
4	J	102	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	L	45/46 (97%)	24 (53%)	3 (6%)
6	N	0/18	-	-
All	All	45/64 (70%)	24 (53%)	3 (6%)

All (24) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	L	3	G
5	L	5	U
5	L	12	G
5	L	13	C
5	L	16	U
5	L	18	C
5	L	22	G
5	L	23	G
5	L	24	C
5	L	28	C
5	L	29	G
5	L	30	A
5	L	31	G
5	L	32	U
5	L	34	G
5	L	36	C
5	L	37	G
5	L	38	C
5	L	40	A
5	L	41	C
5	L	42	U
5	L	45	C
5	L	46	C
5	L	47	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	L	30	A
5	L	36	C
5	L	46	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	I	3
4	J	1
4	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	325:ARG	C	326:MET	N	4.99
1	J	100:ASP	C	101:GLU	N	3.12
1	K	100:ASP	C	101:GLU	N	2.76
1	I	590:GLN	C	591:GLY	N	2.65
1	I	588:ASP	C	589:GLU	N	2.64

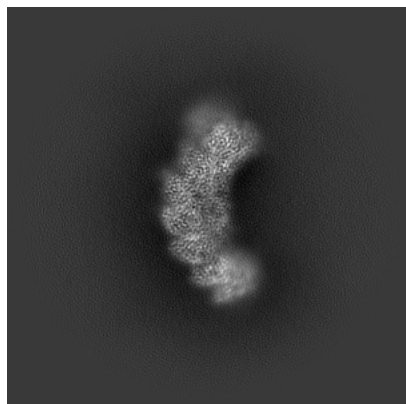
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27403. These allow visual inspection of the internal detail of the map and identification of artifacts.

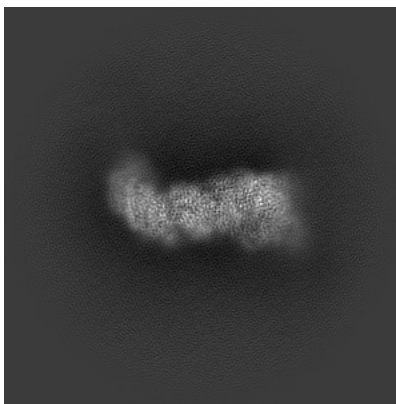
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

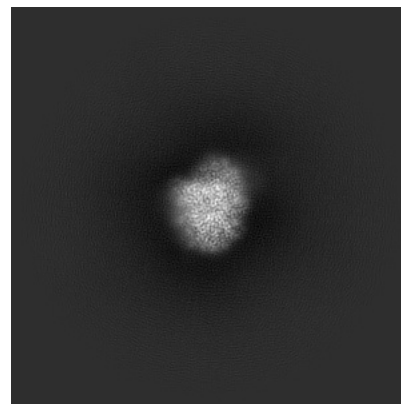
6.1.1 Primary map



X

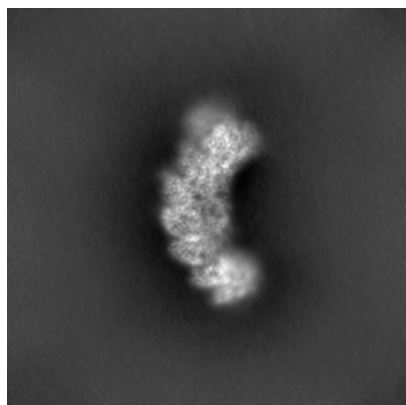


Y

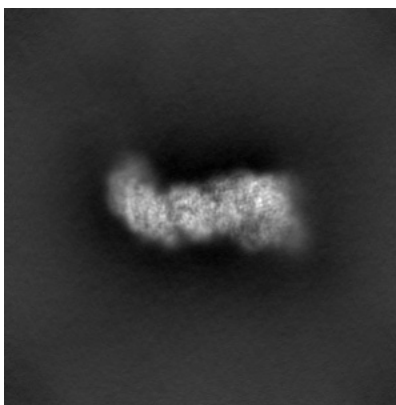


Z

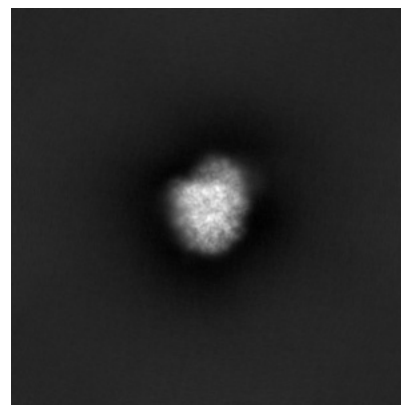
6.1.2 Raw map



X



Y

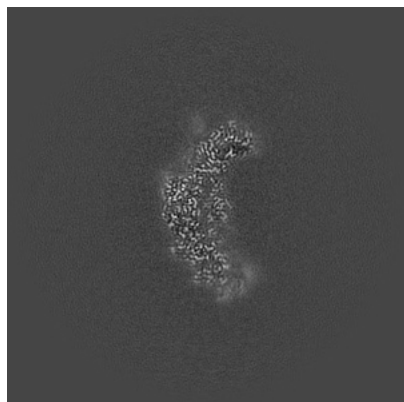


Z

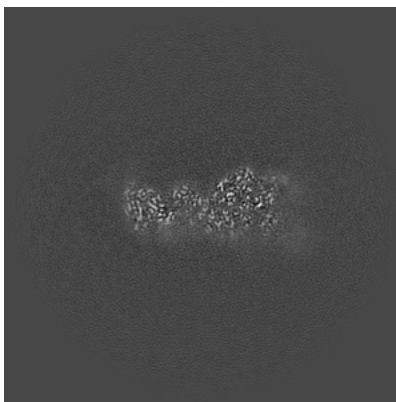
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

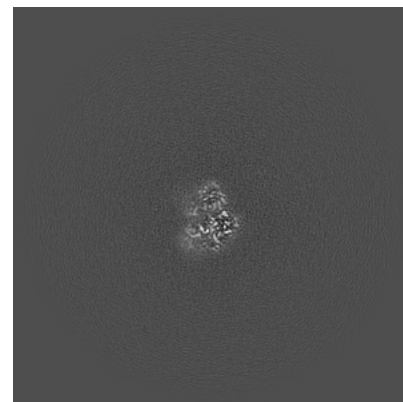
6.2.1 Primary map



X Index: 192

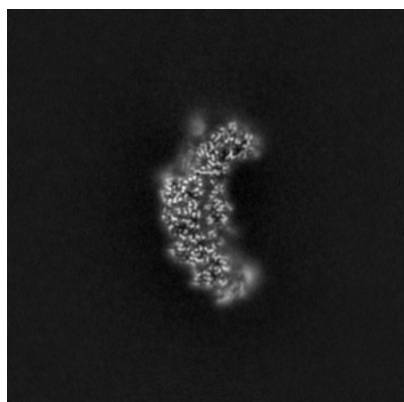


Y Index: 192

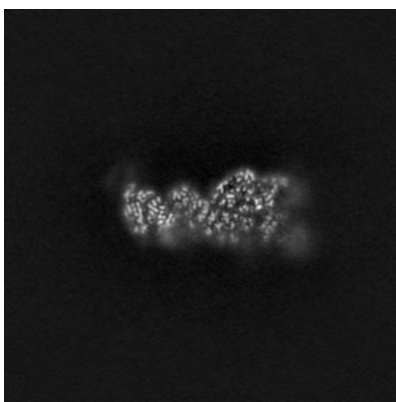


Z Index: 192

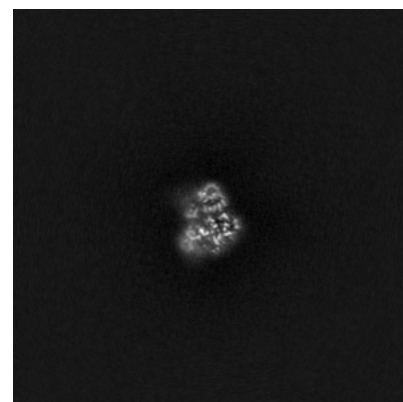
6.2.2 Raw map



X Index: 192



Y Index: 192

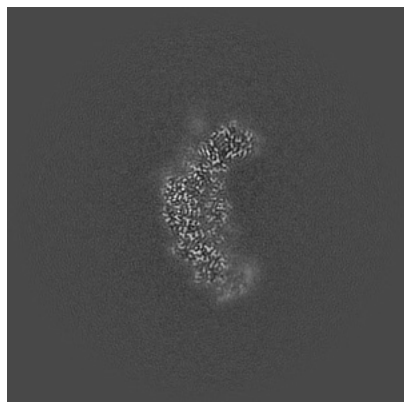


Z Index: 192

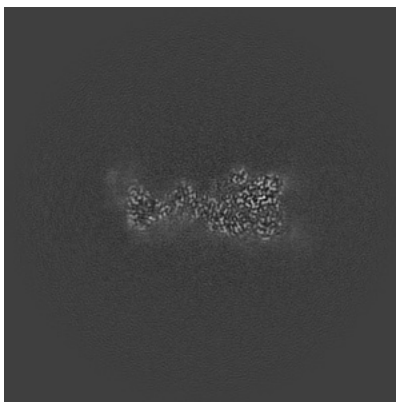
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

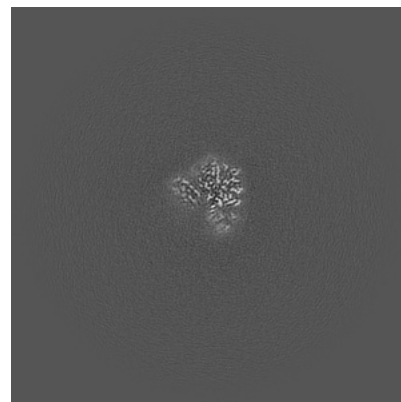
6.3.1 Primary map



X Index: 193

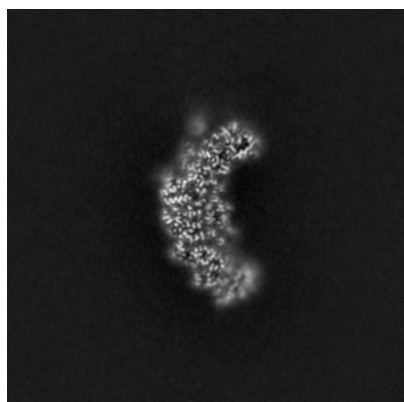


Y Index: 198

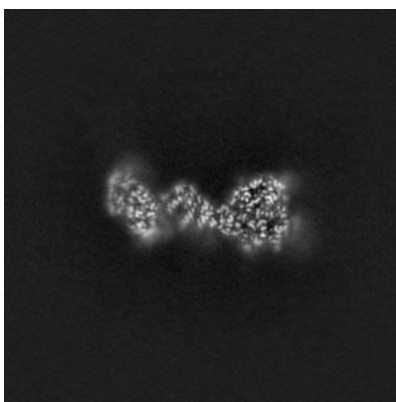


Z Index: 245

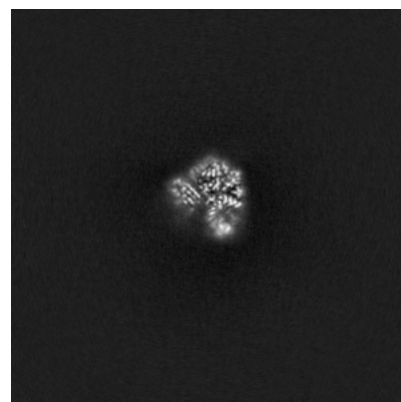
6.3.2 Raw map



X Index: 194



Y Index: 205

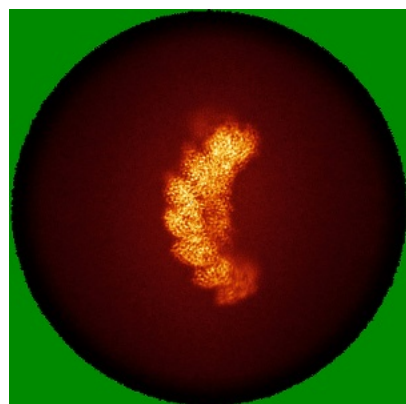


Z Index: 246

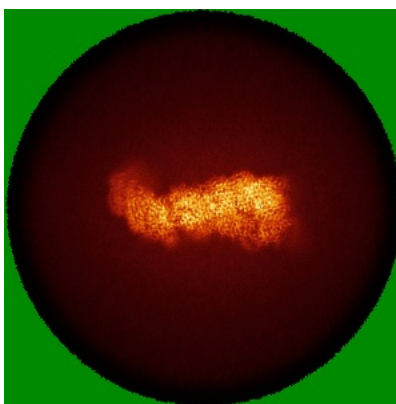
The images above show the largest variance slices of the map in three orthogonal directions.

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

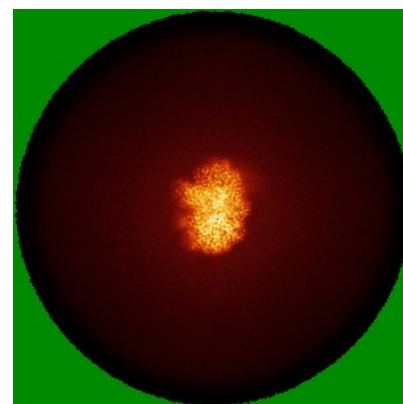
6.4.1 Primary map



X

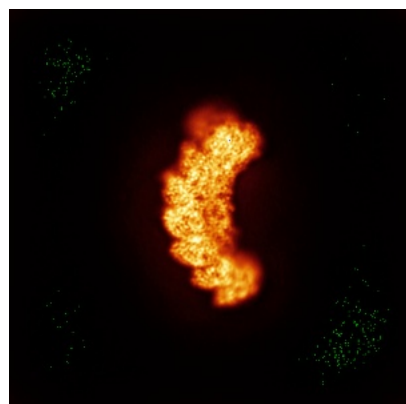


Y

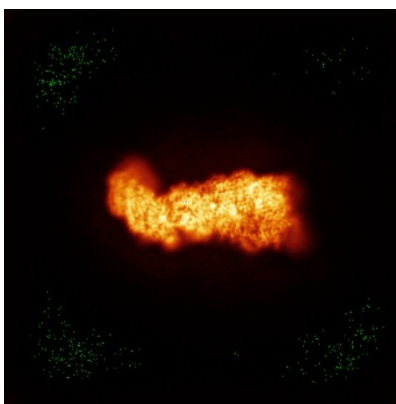


Z

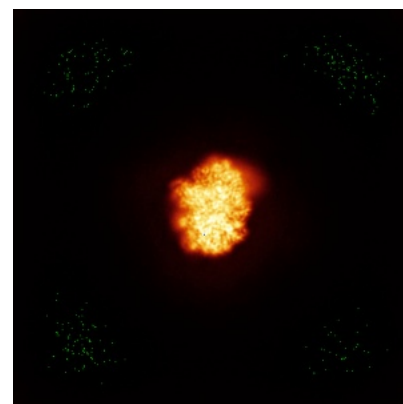
6.4.2 Raw map



X



Y

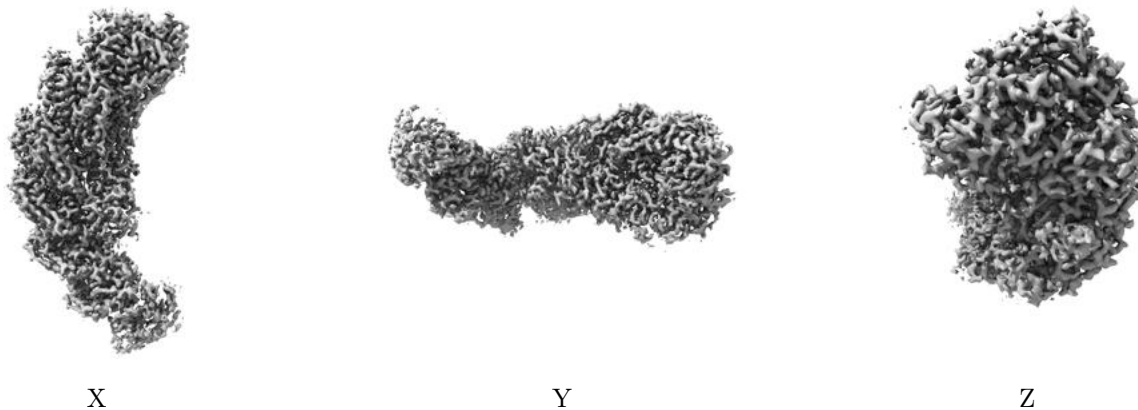


Z

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.

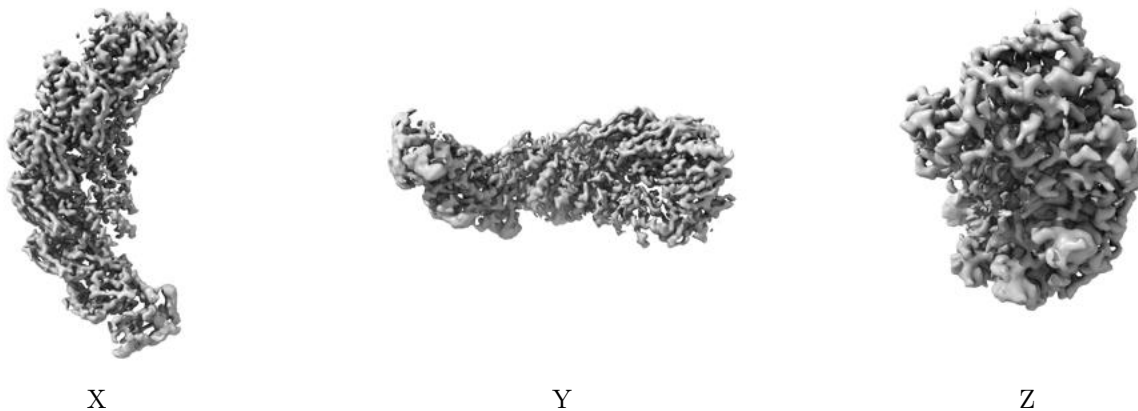
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.55. 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.

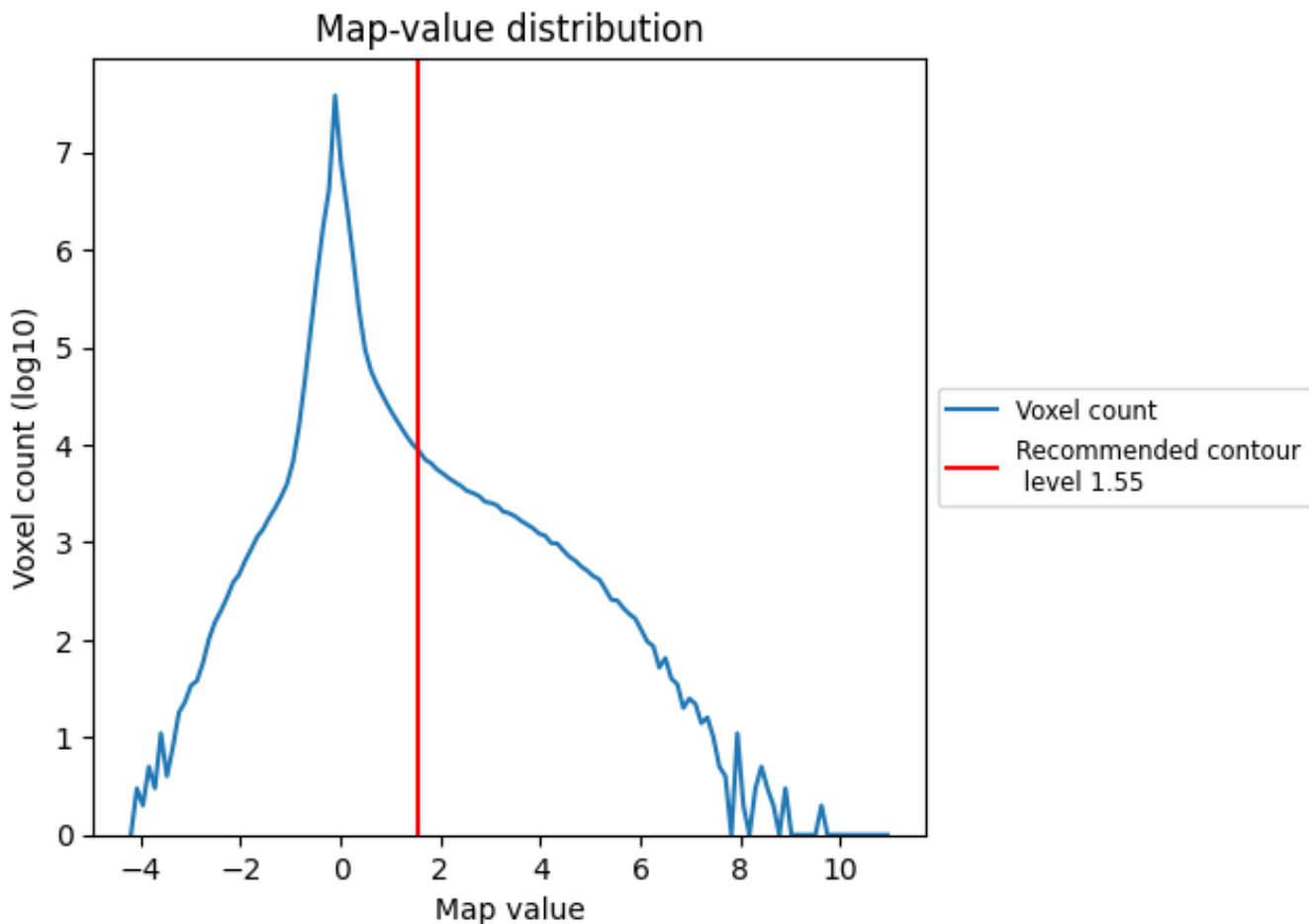
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

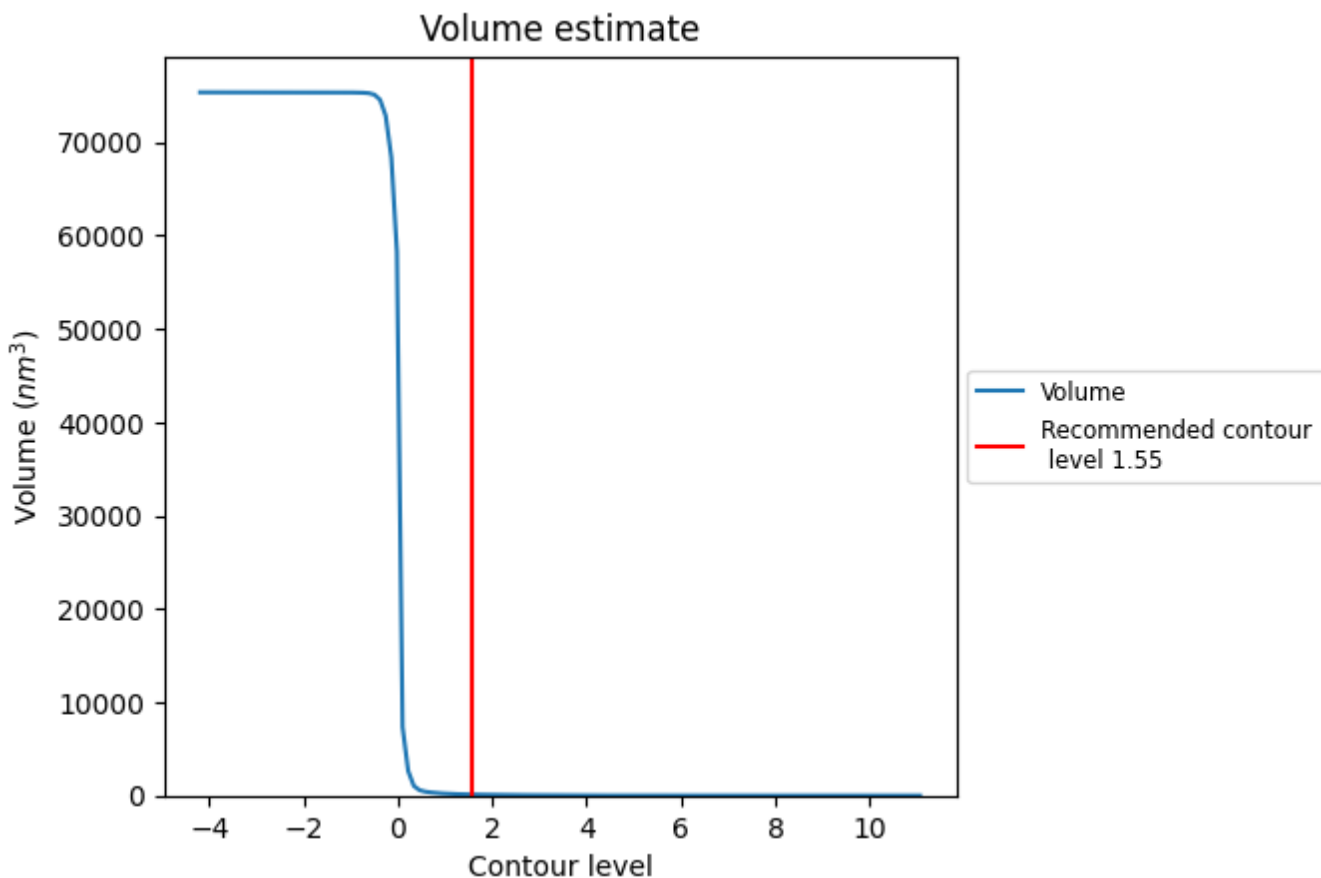
This section contains the results of statistical analysis of the map.

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.

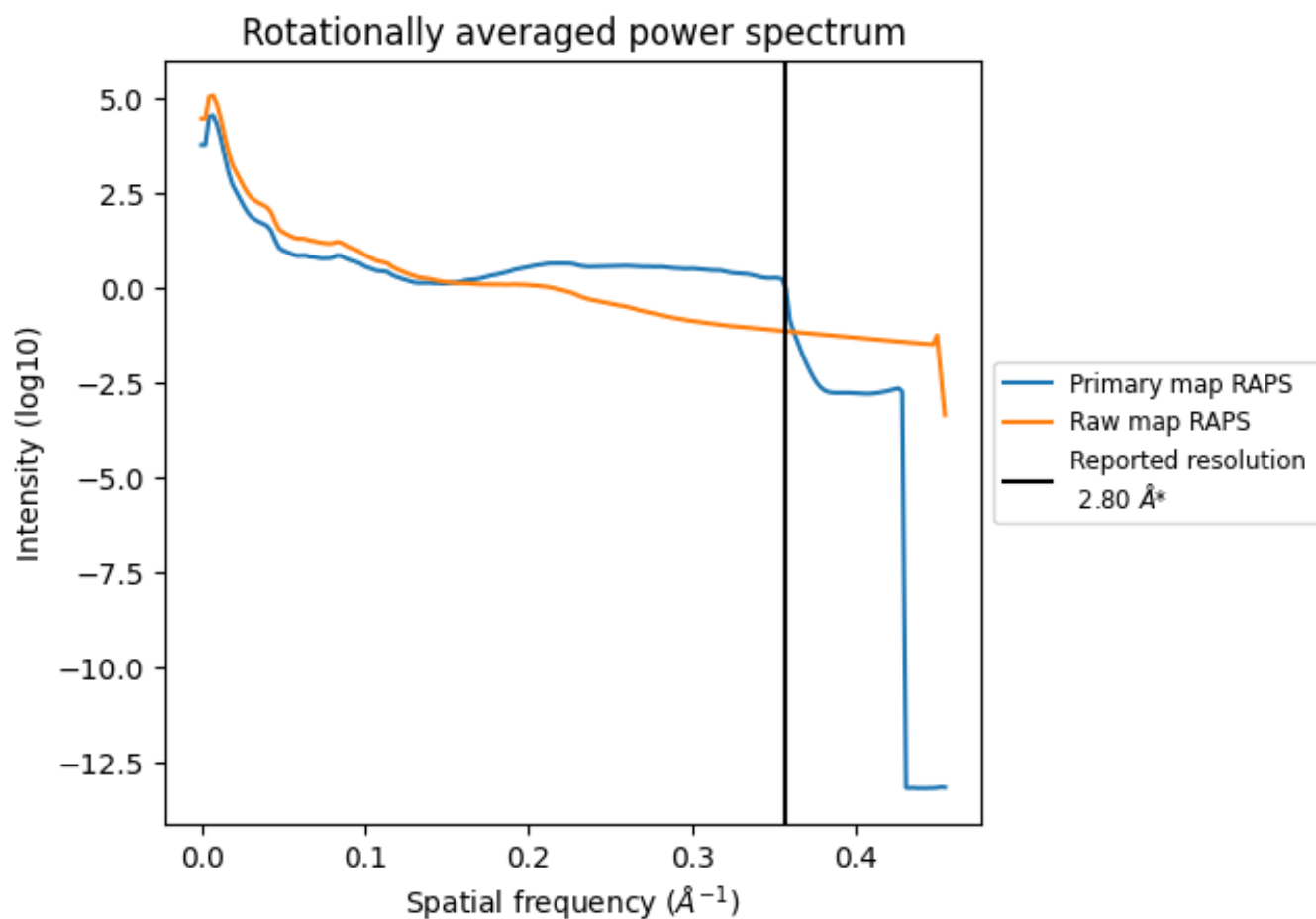
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 114 nm³; this corresponds to an approximate mass of 103 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

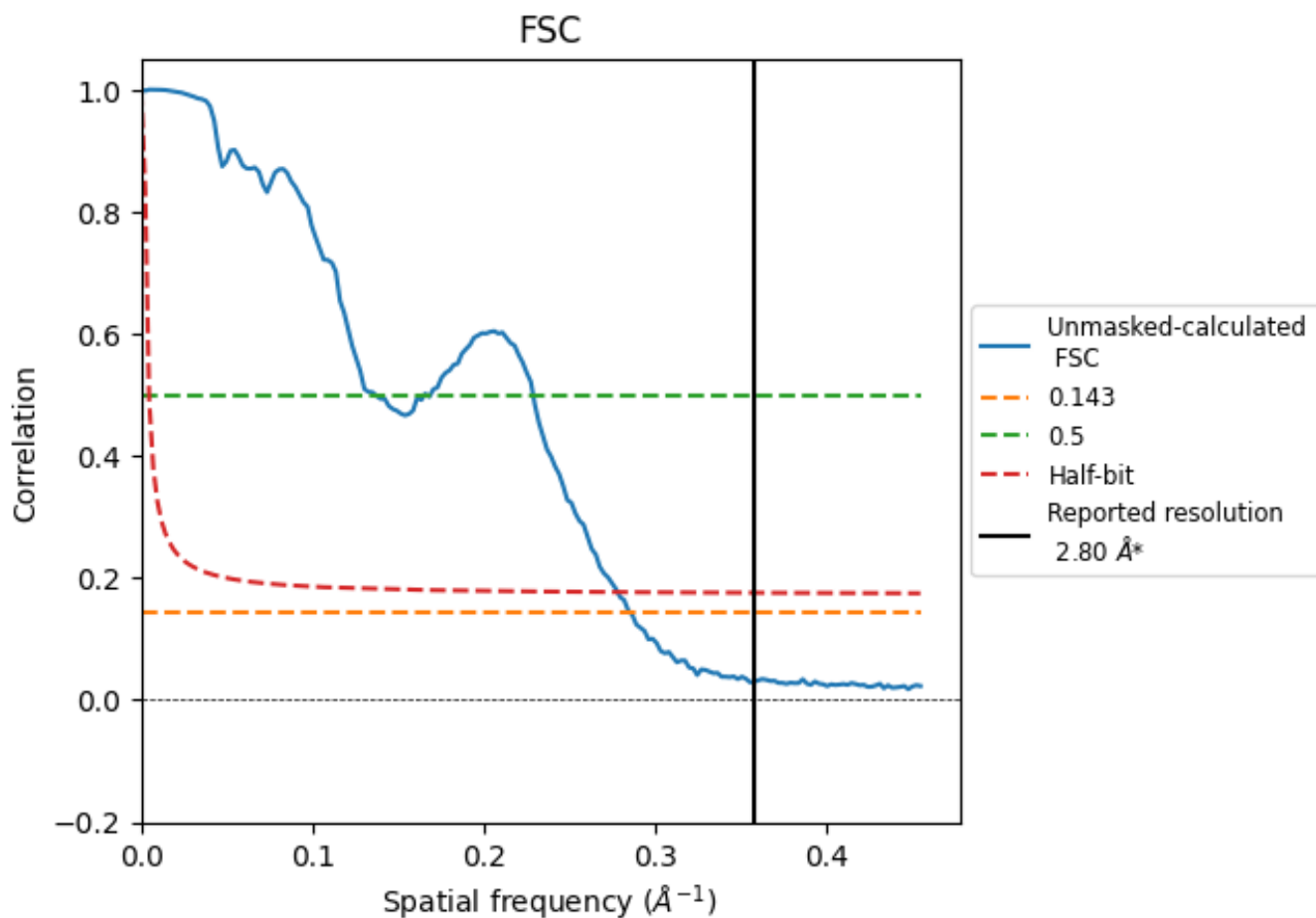


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

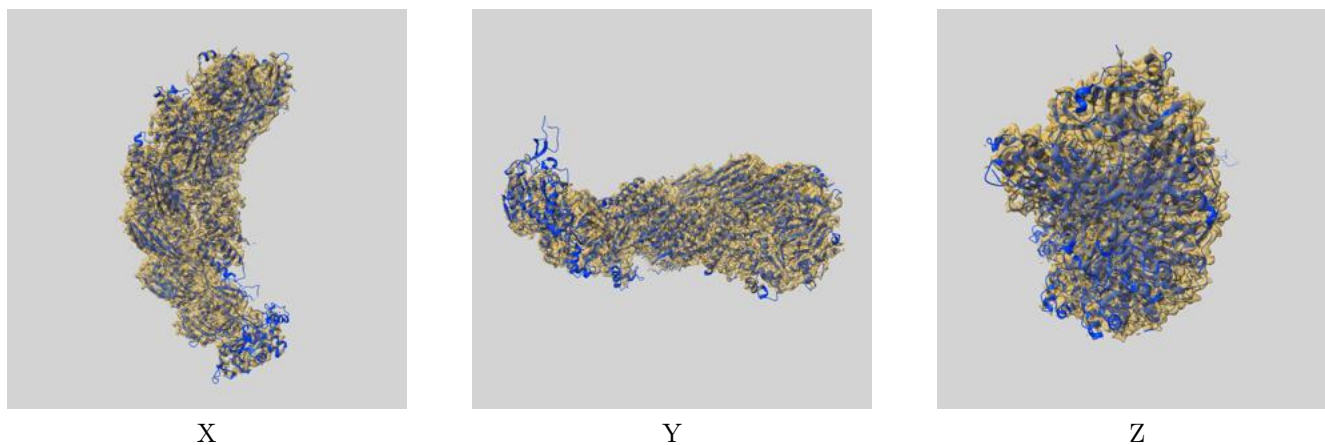
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.51	7.33	3.60

*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 3.51 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

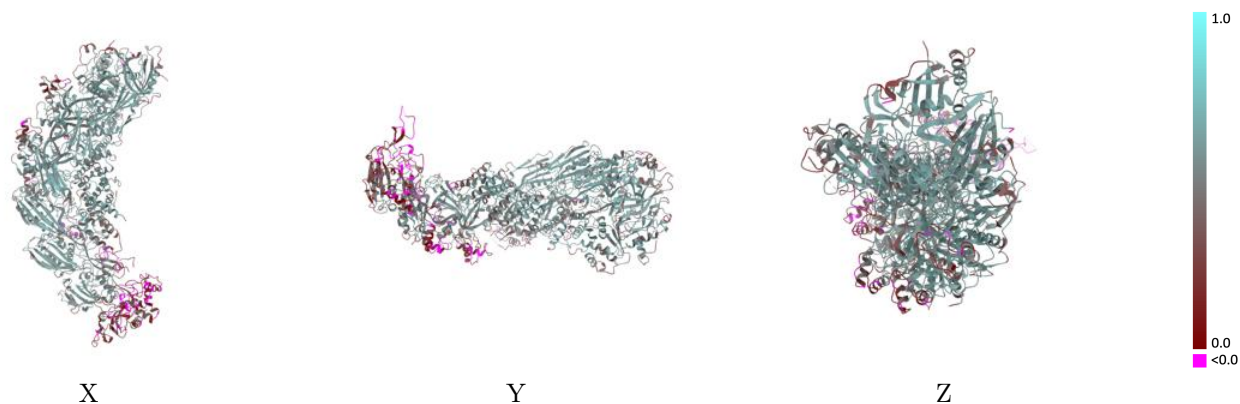
This section contains information regarding the fit between EMDB map EMD-27403 and PDB model 8DFA. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



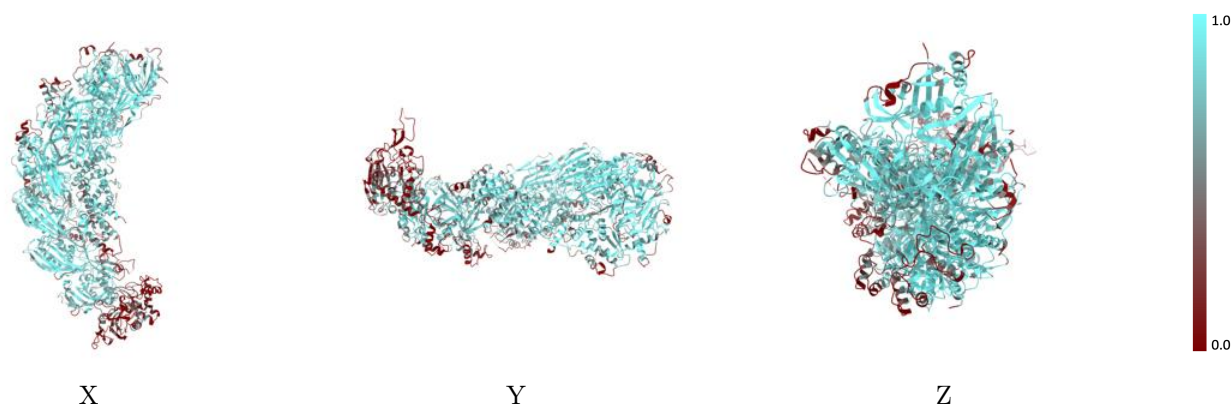
The images above show the 3D surface view of the map at the recommended contour level 1.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



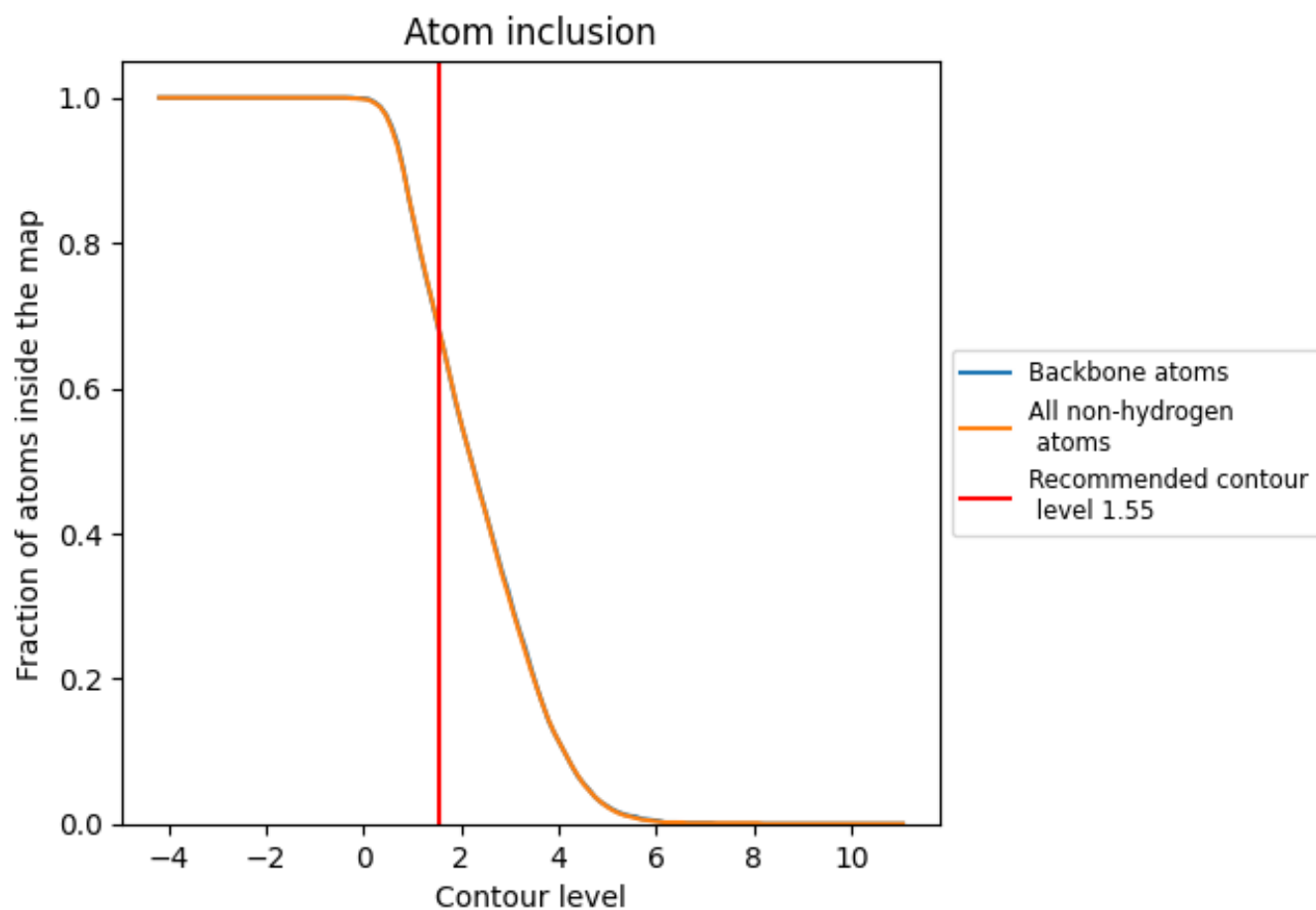
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.55).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 68% 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 (1.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6790	 0.4800
A	 0.7520	 0.5310
B	 0.8030	 0.5560
C	 0.7740	 0.5360
D	 0.7590	 0.5160
E	 0.7560	 0.5200
F	 0.6920	 0.4610
G	 0.5820	 0.4140
H	 0.2250	 0.2260
I	 0.7120	 0.5170
J	 0.6810	 0.5140
K	 0.6340	 0.4900
L	 0.9000	 0.5570
N	 0.6370	 0.4470

