



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 11:56 PM UTC

PDB ID : 3J4K / pdb_00003j4k
EMDB ID : EMD-5751
Title : Cryo-EM structures of the actin:tropomyosin filament reveal the mechanism for the transition from C- to M-state
Authors : Sousa, D.R.; Stagg, S.M.; Stroupe, M.E.
Deposited on : 2013-08-26
Resolution : 8.00 Å(reported)
Based on initial model : 4A7F

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

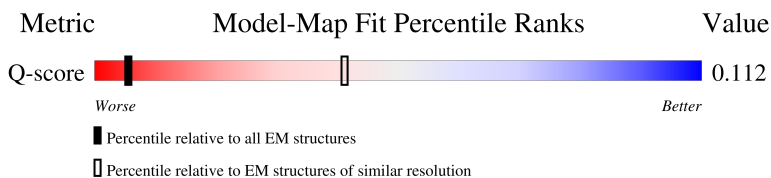
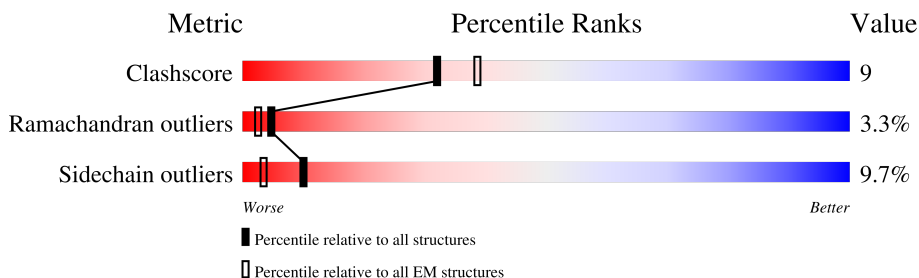
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 Å.

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



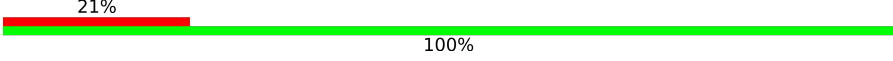
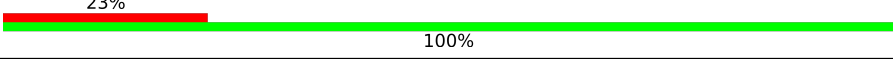
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	361 (7.50 - 8.50)

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	375	
1	B	375	
1	C	375	
1	D	375	

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Mol	Chain	Length	Quality of chain
1	E	375	
2	F	136	
2	G	136	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16160 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

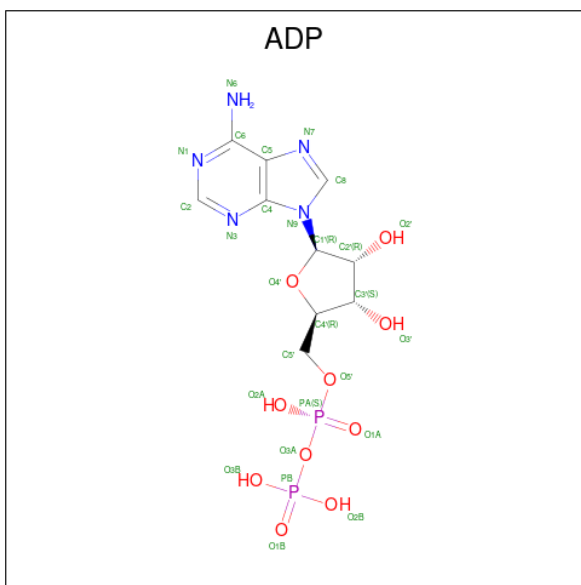
- Molecule 1 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	B	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	C	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	D	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	E	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		

- Molecule 2 is a protein called tropomyosin.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	F	136	Total	C	N	O	0	0
			680	408	136	136		
2	G	136	Total	C	N	O	0	0
			680	408	136	136		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

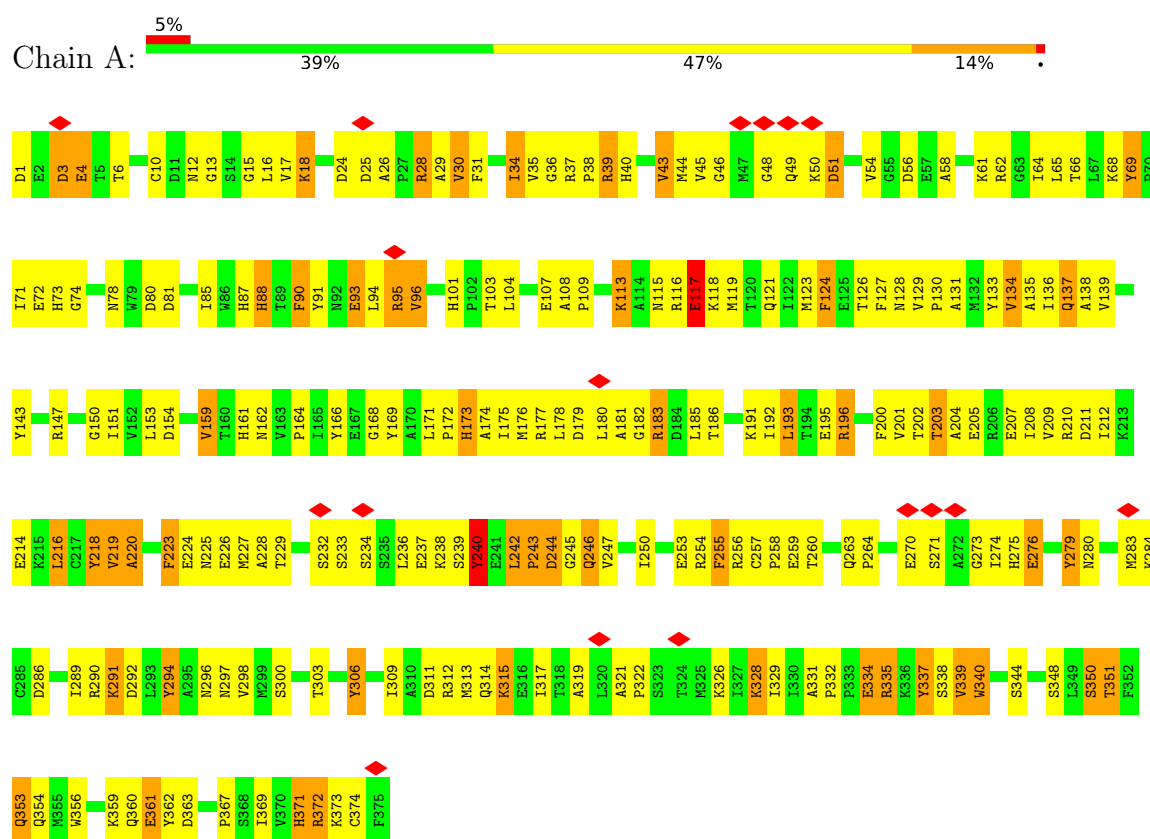


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0

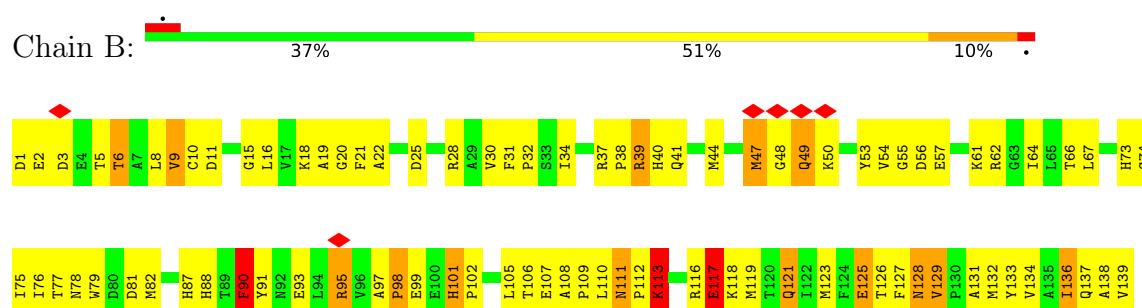
3 Residue-property plots

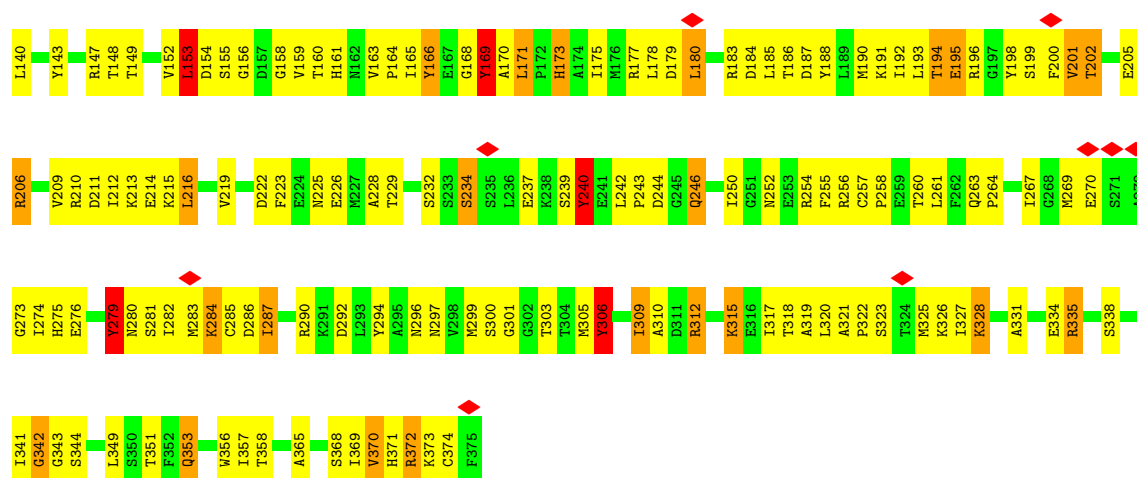
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Actin, alpha skeletal muscle



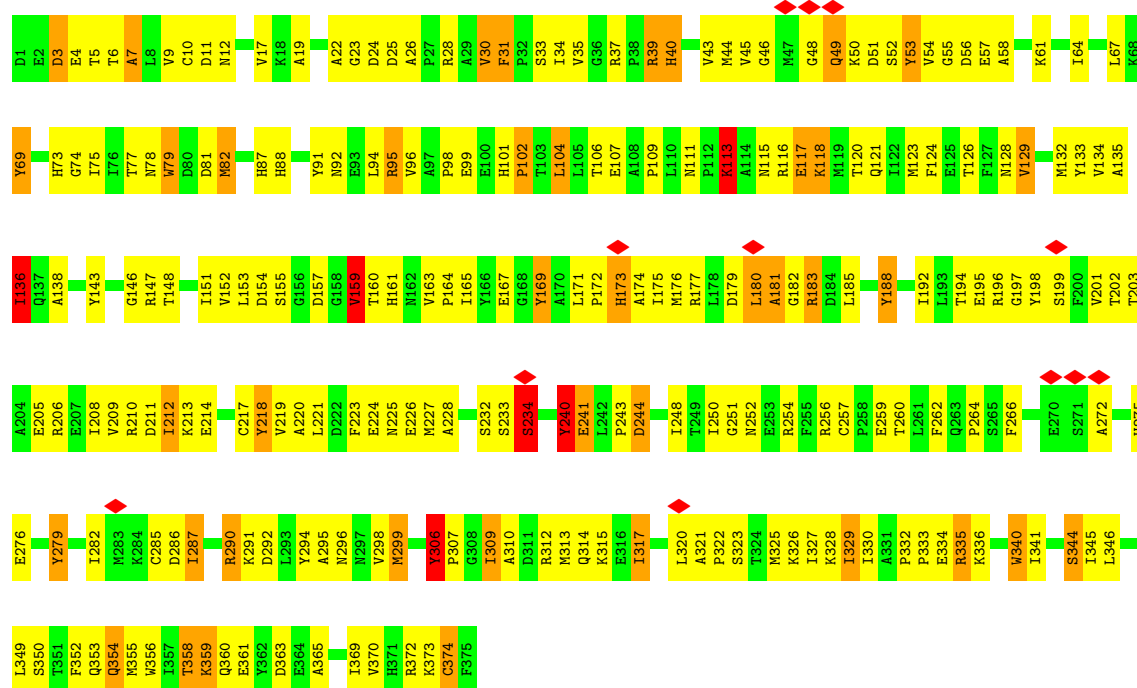
- Molecule 1: Actin, alpha skeletal muscle





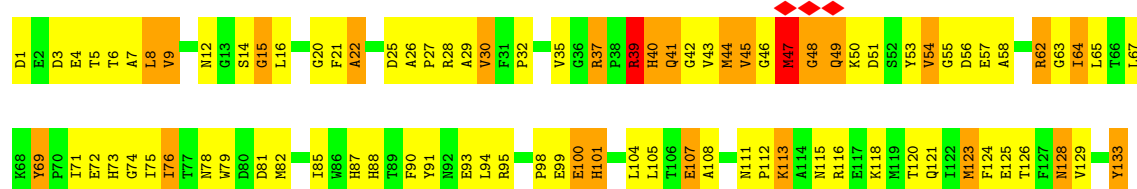
- Molecule 1: Actin, alpha skeletal muscle

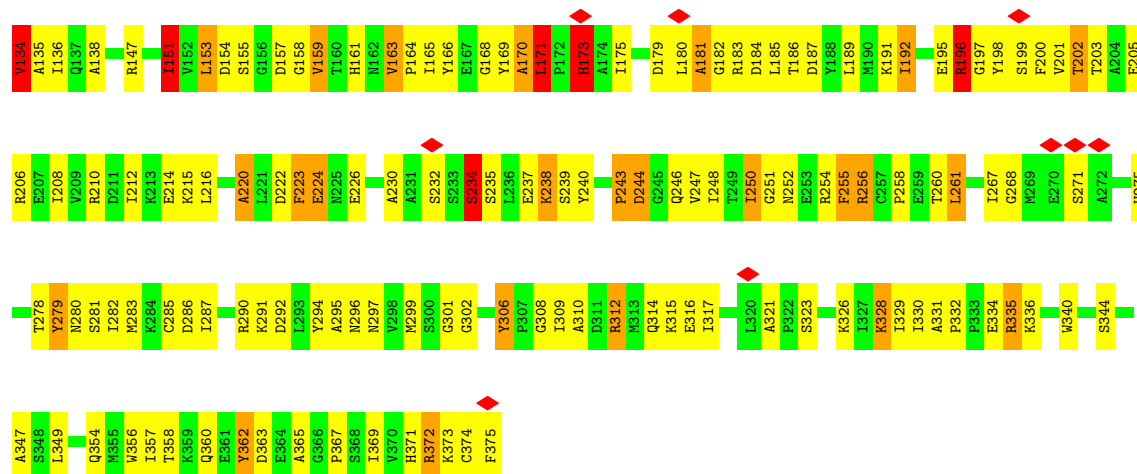
Chain C: 39% 49% 11%



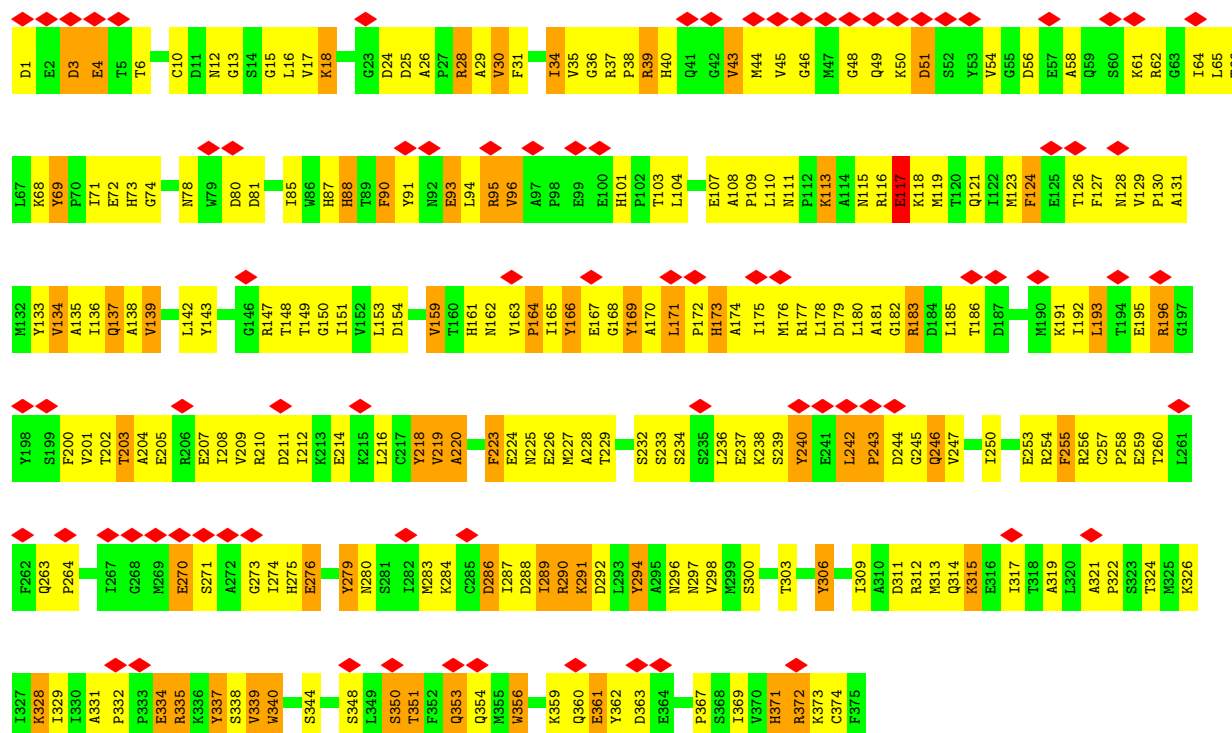
- Molecule 1: Actin, alpha skeletal muscle

Chain D: 38% 47% 13%

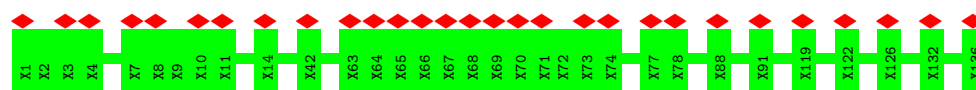




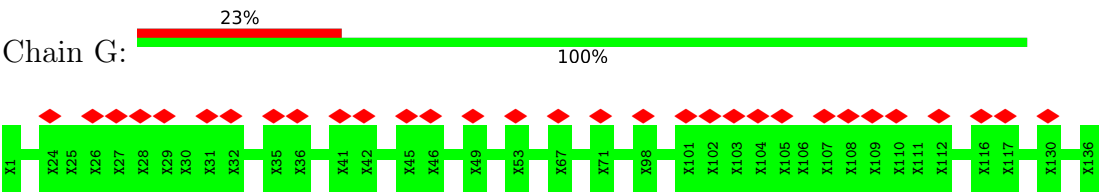
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 2: tropomyosin



- Molecule 2: tropomyosin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	HELICAL, twist=167°, rise=28 Å, axial sym=C1	Depositor
Number of particles used	224337	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	individual images	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	101555	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	32.032	Depositor
Minimum map value	-0.107	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.1	Depositor
Map size (Å)	378.112, 378.112, 378.112	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.477, 1.477, 1.477	Depositor

5 Model quality

5.1 Standard geometry

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

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	2.30	118/2996 (3.9%)	2.47	206/4058 (5.1%)
1	B	2.29	129/2996 (4.3%)	2.44	198/4058 (4.9%)
1	C	2.30	106/2996 (3.5%)	2.49	216/4058 (5.3%)
1	D	2.28	115/2996 (3.8%)	2.46	191/4058 (4.7%)
1	E	2.30	118/2996 (3.9%)	2.47	207/4058 (5.1%)
All	All	2.29	586/14980 (3.9%)	2.46	1018/20290 (5.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	15
1	B	0	11
1	C	0	12
1	D	0	8
1	E	0	15
All	All	0	61

All (586) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	ARG	NE-CZ	10.74	1.44	1.33
1	E	37	ARG	NE-CZ	10.73	1.44	1.33
1	B	95	ARG	CD-NE	9.93	1.60	1.46
1	E	71	ILE	CA-C	-9.56	1.40	1.52
1	A	71	ILE	CA-C	-9.54	1.40	1.52
1	A	296	ASN	CA-C	-9.19	1.39	1.53
1	A	179	ASP	N-CA	-9.19	1.34	1.46
1	E	179	ASP	N-CA	-9.15	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	296	ASN	CA-C	-9.15	1.39	1.53
1	C	19	ALA	CA-C	-9.01	1.42	1.52
1	C	219	VAL	CA-C	-8.97	1.42	1.52
1	B	153	LEU	CA-C	-8.80	1.41	1.53
1	D	373	LYS	CA-C	-8.77	1.42	1.53
1	C	327	ILE	N-CA	-8.69	1.35	1.46
1	A	173	HIS	ND1-CE1	8.66	1.41	1.32
1	C	232	SER	N-CA	-8.63	1.35	1.45
1	E	173	HIS	ND1-CE1	8.62	1.41	1.32
1	D	349	LEU	CA-C	-8.57	1.42	1.52
1	B	147	ARG	CD-NE	8.46	1.58	1.46
1	E	69	TYR	CA-C	-8.42	1.42	1.52
1	C	28	ARG	CA-C	-8.40	1.42	1.52
1	A	69	TYR	CA-C	-8.39	1.42	1.52
1	B	164	PRO	CA-C	-8.37	1.43	1.52
1	B	210	ARG	NE-CZ	8.29	1.42	1.33
1	C	10	CYS	CA-C	-8.29	1.42	1.52
1	E	353	GLN	CA-C	-8.23	1.41	1.52
1	A	353	GLN	CA-C	-8.18	1.41	1.52
1	D	29	ALA	C-N	8.18	1.44	1.33
1	B	11	ASP	CA-C	-8.17	1.40	1.53
1	D	136	ILE	CA-CB	8.13	1.62	1.53
1	B	327	ILE	N-CA	-8.12	1.35	1.46
1	D	12	ASN	C-N	8.02	1.41	1.33
1	B	40	HIS	ND1-CE1	8.00	1.40	1.32
1	D	154	ASP	CA-C	-7.97	1.43	1.52
1	C	52	SER	CA-C	-7.88	1.44	1.53
1	E	30	VAL	CA-C	-7.87	1.43	1.52
1	D	71	ILE	CA-C	-7.87	1.42	1.52
1	C	33	SER	CA-C	-7.86	1.44	1.53
1	A	30	VAL	CA-C	-7.84	1.43	1.52
1	D	20	GLY	N-CA	-7.77	1.36	1.45
1	D	128	ASN	C-N	7.76	1.42	1.33
1	D	250	ILE	C-N	7.72	1.44	1.33
1	B	306	TYR	CA-C	-7.68	1.45	1.53
1	D	104	LEU	CA-C	-7.62	1.43	1.52
1	B	206	ARG	CD-NE	7.58	1.56	1.46
1	E	236	LEU	CA-C	-7.58	1.42	1.52
1	C	147	ARG	CD-NE	7.58	1.56	1.46
1	A	236	LEU	CA-C	-7.57	1.42	1.52
1	C	350	SER	CA-C	-7.55	1.42	1.52
1	C	135	ALA	CA-CB	7.55	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	152	VAL	N-CA	-7.54	1.36	1.46
1	D	189	LEU	CA-CB	7.54	1.65	1.53
1	D	155	SER	CA-C	-7.54	1.43	1.53
1	D	98	PRO	CA-C	7.52	1.61	1.52
1	D	104	LEU	C-O	-7.52	1.15	1.24
1	A	317	ILE	CA-CB	-7.49	1.44	1.54
1	B	223	PHE	CA-CB	7.49	1.65	1.53
1	D	196	ARG	CA-C	-7.49	1.45	1.53
1	D	312	ARG	CD-NE	7.49	1.56	1.46
1	E	317	ILE	CA-CB	-7.49	1.44	1.54
1	D	47	MET	CA-C	-7.48	1.42	1.52
1	D	32	PRO	N-CD	-7.44	1.37	1.47
1	D	51	ASP	CA-C	-7.43	1.42	1.52
1	B	301	GLY	CA-C	-7.41	1.44	1.52
1	B	328	LYS	CA-C	-7.40	1.43	1.52
1	C	116	ARG	NE-CZ	7.36	1.41	1.33
1	C	134	VAL	CA-C	-7.31	1.43	1.52
1	A	219	VAL	CA-C	-7.29	1.43	1.52
1	B	22	ALA	CA-C	-7.29	1.43	1.52
1	D	112	PRO	CA-C	-7.27	1.43	1.52
1	E	219	VAL	CA-C	-7.25	1.43	1.52
1	B	88	HIS	ND1-CE1	7.25	1.39	1.32
1	C	163	VAL	CA-C	-7.25	1.45	1.52
1	D	69	TYR	N-CA	-7.25	1.39	1.46
1	C	188	TYR	CA-C	-7.23	1.42	1.52
1	E	256	ARG	NE-CZ	7.22	1.41	1.33
1	D	329	ILE	CA-C	-7.20	1.44	1.52
1	A	256	ARG	NE-CZ	7.20	1.41	1.33
1	B	148	THR	C-N	7.19	1.42	1.33
1	B	82	MET	CA-C	-7.18	1.43	1.52
1	E	131	ALA	CA-C	-7.16	1.44	1.52
1	C	320	LEU	CA-CB	7.15	1.63	1.53
1	B	273	GLY	CA-C	-7.14	1.41	1.52
1	B	90	PHE	CA-C	-7.14	1.44	1.52
1	A	131	ALA	CA-C	-7.13	1.44	1.52
1	E	17	VAL	N-CA	-7.12	1.37	1.47
1	A	17	VAL	CA-C	-7.10	1.46	1.53
1	A	17	VAL	N-CA	-7.08	1.37	1.47
1	A	39	ARG	NE-CZ	7.07	1.40	1.33
1	C	359	LYS	N-CA	-7.07	1.38	1.46
1	E	39	ARG	NE-CZ	7.06	1.40	1.33
1	E	17	VAL	CA-C	-7.06	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	161	HIS	CA-C	-7.05	1.43	1.52
1	D	76	ILE	CA-C	-7.04	1.45	1.53
1	B	6	THR	C-N	7.00	1.42	1.33
1	C	40	HIS	CE1-NE2	7.00	1.39	1.32
1	D	82	MET	CA-C	-6.99	1.43	1.52
1	C	206	ARG	CZ-NH1	6.99	1.42	1.32
1	A	61	LYS	N-CA	-6.98	1.37	1.46
1	B	20	GLY	CA-C	-6.97	1.43	1.51
1	E	61	LYS	N-CA	-6.96	1.37	1.46
1	A	218	TYR	CA-CB	6.95	1.65	1.53
1	E	218	TYR	CA-CB	6.95	1.65	1.53
1	C	251	GLY	N-CA	-6.95	1.40	1.45
1	C	257	CYS	C-N	6.92	1.42	1.33
1	B	199	SER	C-N	6.92	1.42	1.33
1	C	118	LYS	CA-CB	6.89	1.64	1.53
1	A	28	ARG	CA-C	-6.88	1.44	1.52
1	D	30	VAL	N-CA	-6.88	1.38	1.46
1	B	154	ASP	CA-C	-6.88	1.44	1.52
1	D	62	ARG	NE-CZ	6.83	1.40	1.33
1	C	104	LEU	CA-C	-6.83	1.44	1.52
1	A	229	THR	C-N	6.82	1.43	1.34
1	E	229	THR	C-N	6.82	1.43	1.34
1	E	28	ARG	CA-C	-6.81	1.44	1.52
1	A	58	ALA	CA-C	-6.80	1.44	1.52
1	E	58	ALA	CA-C	-6.80	1.44	1.52
1	E	372	ARG	CZ-NH1	6.80	1.42	1.32
1	E	360	GLN	CA-C	-6.80	1.44	1.52
1	E	210	ARG	C-N	6.80	1.43	1.33
1	C	256	ARG	NE-CZ	6.79	1.40	1.33
1	A	372	ARG	CZ-NH1	6.79	1.42	1.32
1	D	101	HIS	CA-C	-6.78	1.44	1.52
1	A	360	GLN	CA-C	-6.77	1.44	1.52
1	A	210	ARG	C-N	6.77	1.43	1.33
1	D	326	LYS	C-N	6.77	1.42	1.33
1	A	138	ALA	N-CA	-6.76	1.38	1.46
1	E	138	ALA	N-CA	-6.76	1.38	1.46
1	A	183	ARG	NE-CZ	6.73	1.40	1.33
1	A	131	ALA	N-CA	-6.72	1.38	1.46
1	E	131	ALA	N-CA	-6.71	1.38	1.46
1	B	206	ARG	CA-C	-6.71	1.43	1.52
1	D	12	ASN	N-CA	-6.70	1.38	1.46
1	E	294	TYR	C-N	6.67	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	341	ILE	CA-C	-6.67	1.44	1.52
1	A	28	ARG	NE-CZ	6.67	1.40	1.33
1	B	246	GLN	N-CA	-6.65	1.38	1.46
1	E	183	ARG	NE-CZ	6.64	1.40	1.33
1	A	31	PHE	N-CA	-6.64	1.39	1.46
1	E	31	PHE	N-CA	-6.63	1.39	1.46
1	C	61	LYS	N-CA	-6.63	1.38	1.45
1	A	294	TYR	C-N	6.62	1.42	1.33
1	E	28	ARG	NE-CZ	6.62	1.40	1.33
1	D	153	LEU	CA-C	-6.61	1.45	1.53
1	C	312	ARG	CA-C	-6.60	1.43	1.52
1	D	251	GLY	CA-C	-6.59	1.42	1.51
1	B	205	GLU	CA-C	-6.58	1.44	1.52
1	D	196	ARG	NE-CZ	6.58	1.40	1.33
1	D	25	ASP	C-N	6.56	1.40	1.33
1	E	309	ILE	CA-CB	-6.56	1.45	1.54
1	C	82	MET	CA-C	-6.54	1.44	1.52
1	E	207	GLU	CA-C	-6.51	1.44	1.52
1	A	309	ILE	CA-CB	-6.51	1.45	1.54
1	A	207	GLU	CA-C	-6.50	1.44	1.52
1	D	107	GLU	CA-C	-6.48	1.45	1.52
1	D	372	ARG	NE-CZ	6.48	1.40	1.33
1	D	138	ALA	C-N	6.47	1.42	1.34
1	A	81	ASP	CA-C	-6.47	1.43	1.52
1	E	81	ASP	CA-C	-6.45	1.43	1.52
1	A	247	VAL	CA-C	-6.44	1.45	1.52
1	A	131	ALA	C-N	-6.44	1.25	1.33
1	E	131	ALA	C-N	-6.43	1.25	1.33
1	E	247	VAL	CA-C	-6.41	1.45	1.52
1	C	155	SER	CA-C	-6.41	1.45	1.53
1	D	360	GLN	CA-C	-6.40	1.44	1.52
1	C	373	LYS	CA-C	-6.40	1.46	1.53
1	C	173	HIS	N-CA	-6.40	1.38	1.46
1	B	61	LYS	CA-C	-6.39	1.44	1.52
1	D	365	ALA	N-CA	-6.39	1.40	1.46
1	B	119	MET	CA-CB	6.38	1.63	1.53
1	E	72	GLU	CA-C	-6.38	1.45	1.52
1	D	116	ARG	N-CA	-6.37	1.38	1.46
1	C	118	LYS	CA-C	-6.36	1.44	1.52
1	E	259	GLU	C-N	6.35	1.42	1.34
1	B	77	THR	C-N	6.35	1.42	1.33
1	A	72	GLU	CA-C	-6.33	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	331	ALA	CA-C	-6.33	1.46	1.52
1	A	259	GLU	C-N	6.33	1.42	1.34
1	C	326	LYS	CA-C	-6.33	1.44	1.52
1	D	133	TYR	CA-C	-6.32	1.44	1.52
1	B	263	GLN	CA-C	-6.32	1.44	1.52
1	C	221	LEU	C-O	6.32	1.31	1.24
1	E	134	VAL	CA-CB	-6.31	1.45	1.54
1	D	51	ASP	N-CA	-6.31	1.38	1.46
1	C	163	VAL	CA-CB	-6.31	1.46	1.54
1	D	91	TYR	CA-CB	6.31	1.63	1.53
1	C	169	TYR	N-CA	-6.30	1.38	1.46
1	A	162	ASN	CA-C	-6.30	1.45	1.53
1	B	62	ARG	CD-NE	6.30	1.55	1.46
1	B	290	ARG	CZ-NH1	6.29	1.41	1.32
1	D	44	MET	CA-C	-6.29	1.45	1.52
1	A	134	VAL	CA-CB	-6.29	1.46	1.54
1	D	301	GLY	CA-C	-6.27	1.45	1.51
1	D	147	ARG	CZ-NH1	6.26	1.41	1.32
1	B	254	ARG	NE-CZ	6.26	1.40	1.33
1	D	275	HIS	CE1-NE2	6.25	1.38	1.32
1	E	175	ILE	N-CA	-6.24	1.39	1.46
1	E	162	ASN	CA-C	-6.23	1.45	1.53
1	C	49	GLN	C-N	6.23	1.41	1.33
1	B	369	ILE	C-O	-6.23	1.16	1.24
1	C	260	THR	C-N	6.23	1.42	1.33
1	C	299	MET	N-CA	-6.22	1.39	1.46
1	C	17	VAL	N-CA	-6.22	1.38	1.47
1	D	164	PRO	CA-CB	6.22	1.61	1.53
1	D	222	ASP	CA-C	-6.22	1.45	1.52
1	C	95	ARG	CD-NE	6.21	1.54	1.46
1	A	175	ILE	N-CA	-6.20	1.39	1.46
1	D	180	LEU	C-N	6.20	1.42	1.33
1	B	274	ILE	N-CA	-6.20	1.38	1.46
1	C	323	SER	CA-CB	6.20	1.63	1.53
1	E	212	ILE	CA-CB	-6.20	1.46	1.54
1	B	116	ARG	CD-NE	6.20	1.54	1.46
1	C	199	SER	CA-C	-6.20	1.45	1.52
1	B	357	ILE	CA-C	-6.18	1.45	1.52
1	A	212	ILE	CA-CB	-6.18	1.46	1.54
1	E	12	ASN	CA-C	6.16	1.60	1.53
1	C	370	VAL	CA-CB	-6.16	1.47	1.54
1	E	16	LEU	C-N	6.15	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	196	ARG	CZ-NH1	6.14	1.41	1.32
1	A	40	HIS	ND1-CE1	6.14	1.38	1.32
1	A	12	ASN	CA-C	6.13	1.60	1.53
1	A	16	LEU	C-N	6.13	1.39	1.33
1	C	345	ILE	C-N	6.13	1.42	1.34
1	A	18	LYS	N-CA	-6.11	1.39	1.46
1	E	18	LYS	N-CA	-6.11	1.39	1.46
1	C	148	THR	CA-C	-6.10	1.44	1.52
1	A	196	ARG	CZ-NH1	6.10	1.41	1.32
1	B	191	LYS	CA-CB	6.10	1.62	1.53
1	B	255	PHE	N-CA	-6.09	1.38	1.46
1	B	31	PHE	CA-C	-6.09	1.44	1.52
1	E	40	HIS	ND1-CE1	6.08	1.38	1.32
1	D	135	ALA	CA-C	-6.08	1.45	1.53
1	C	73	HIS	ND1-CE1	6.07	1.38	1.32
1	D	246	GLN	CA-C	-6.07	1.45	1.52
1	D	111	ASN	CA-C	-6.07	1.44	1.53
1	C	180	LEU	CA-C	-6.06	1.44	1.52
1	C	44	MET	C-N	6.04	1.41	1.33
1	D	28	ARG	CD-NE	6.04	1.54	1.46
1	A	24	ASP	C-O	-6.02	1.16	1.23
1	E	40	HIS	CA-C	-6.02	1.44	1.52
1	E	24	ASP	C-O	-6.01	1.16	1.23
1	B	50	LYS	N-CA	-6.01	1.38	1.45
1	B	129	VAL	C-O	-6.01	1.16	1.24
1	C	223	PHE	CA-CB	6.00	1.62	1.53
1	E	93	GLU	CA-C	6.00	1.60	1.52
1	D	14	SER	CA-CB	6.00	1.62	1.53
1	E	275	HIS	CB-CG	6.00	1.58	1.50
1	A	40	HIS	CA-C	-6.00	1.44	1.52
1	D	187	ASP	CA-C	-6.00	1.44	1.52
1	D	234	SER	N-CA	-6.00	1.38	1.46
1	A	93	GLU	CA-C	5.99	1.60	1.52
1	E	172	PRO	CA-C	-5.97	1.44	1.52
1	C	307	PRO	N-CA	-5.97	1.40	1.47
1	A	172	PRO	CA-C	-5.96	1.44	1.52
1	D	299	MET	N-CA	-5.96	1.39	1.46
1	B	154	ASP	N-CA	-5.96	1.39	1.46
1	E	202	THR	C-N	5.96	1.41	1.33
1	C	210	ARG	CA-CB	5.94	1.63	1.53
1	D	73	HIS	ND1-CE1	5.94	1.38	1.32
1	A	275	HIS	CB-CG	5.93	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	TYR	N-CA	-5.93	1.38	1.46
1	A	202	THR	C-N	5.93	1.41	1.33
1	B	44	MET	N-CA	-5.92	1.38	1.46
1	B	292	ASP	CA-C	-5.92	1.44	1.52
1	D	78	ASN	C-O	-5.92	1.17	1.23
1	B	125	GLU	N-CA	-5.90	1.38	1.46
1	A	136	ILE	N-CA	-5.89	1.39	1.46
1	E	371	HIS	CA-CB	5.89	1.64	1.53
1	C	95	ARG	NE-CZ	5.89	1.39	1.33
1	B	211	ASP	CA-CB	5.89	1.62	1.53
1	B	194	THR	C-N	5.88	1.41	1.33
1	D	220	ALA	CA-C	-5.88	1.45	1.52
1	B	179	ASP	CA-C	-5.88	1.45	1.52
1	E	136	ILE	N-CA	-5.87	1.39	1.46
1	D	57	GLU	CA-C	5.87	1.60	1.52
1	A	371	HIS	CA-CB	5.86	1.64	1.53
1	D	100	GLU	C-N	5.86	1.43	1.33
1	E	104	LEU	CA-C	-5.86	1.45	1.52
1	A	328	LYS	CA-C	-5.85	1.45	1.52
1	B	374	CYS	CA-C	-5.85	1.45	1.53
1	C	234	SER	CA-CB	5.85	1.63	1.53
1	A	104	LEU	CA-C	-5.84	1.45	1.52
1	D	335	ARG	N-CA	-5.84	1.42	1.47
1	D	158	GLY	C-N	5.84	1.41	1.33
1	D	279	TYR	N-CA	-5.84	1.39	1.46
1	B	283	MET	C-N	5.83	1.41	1.33
1	E	191	LYS	N-CA	-5.83	1.39	1.46
1	B	280	ASN	N-CA	-5.83	1.39	1.46
1	C	30	VAL	CA-C	-5.83	1.45	1.52
1	D	258	PRO	N-CA	-5.82	1.39	1.47
1	E	147	ARG	NE-CZ	5.82	1.39	1.33
1	E	237	GLU	C-O	-5.82	1.17	1.24
1	E	328	LYS	CA-C	-5.82	1.45	1.52
1	A	154	ASP	CA-C	-5.81	1.45	1.52
1	A	147	ARG	NE-CZ	5.80	1.39	1.33
1	A	191	LYS	N-CA	-5.80	1.39	1.46
1	C	354	GLN	C-N	5.79	1.41	1.33
1	A	237	GLU	C-O	-5.79	1.17	1.24
1	E	219	VAL	C-N	5.79	1.41	1.33
1	E	359	LYS	CA-C	-5.79	1.45	1.52
1	E	374	CYS	N-CA	5.79	1.53	1.46
1	E	154	ASP	CA-C	-5.78	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	75	ILE	N-CA	-5.78	1.39	1.46
1	C	154	ASP	N-CA	-5.78	1.39	1.46
1	C	220	ALA	CA-C	-5.78	1.45	1.53
1	A	219	VAL	C-N	5.77	1.41	1.33
1	C	213	LYS	C-N	5.77	1.41	1.33
1	D	40	HIS	CA-CB	5.77	1.62	1.53
1	B	67	LEU	C-N	5.77	1.41	1.33
1	B	254	ARG	CA-C	-5.77	1.44	1.52
1	D	285	CYS	CA-C	-5.77	1.45	1.53
1	C	275	HIS	C-N	5.76	1.42	1.33
1	D	81	ASP	CA-C	-5.76	1.44	1.52
1	D	113	LYS	CA-C	-5.75	1.44	1.52
1	D	155	SER	N-CA	-5.75	1.39	1.46
1	E	50	LYS	CA-CB	5.75	1.64	1.53
1	A	50	LYS	CA-CB	5.75	1.64	1.53
1	D	287	ILE	CA-CB	-5.75	1.47	1.54
1	A	374	CYS	N-CA	5.75	1.53	1.46
1	B	206	ARG	CZ-NH2	5.74	1.41	1.33
1	D	279	TYR	CA-C	-5.74	1.45	1.52
1	A	359	LYS	CA-C	-5.74	1.45	1.52
1	B	169	TYR	N-CA	-5.74	1.39	1.46
1	E	321	ALA	CA-C	5.74	1.59	1.53
1	A	109	PRO	C-N	5.73	1.41	1.33
1	E	173	HIS	CB-CG	5.73	1.58	1.50
1	E	109	PRO	C-N	5.72	1.41	1.33
1	E	183	ARG	CD-NE	5.72	1.54	1.46
1	A	183	ARG	CD-NE	5.72	1.54	1.46
1	E	371	HIS	ND1-CE1	5.72	1.38	1.32
1	E	300	SER	CA-C	-5.72	1.45	1.52
1	A	371	HIS	ND1-CE1	5.71	1.38	1.32
1	A	168	GLY	CA-C	-5.71	1.46	1.52
1	B	39	ARG	CZ-NH2	5.71	1.40	1.33
1	A	173	HIS	CB-CG	5.71	1.58	1.50
1	E	34	ILE	CA-CB	-5.70	1.47	1.54
1	A	34	ILE	CA-CB	-5.70	1.47	1.54
1	B	107	GLU	CA-C	-5.70	1.45	1.52
1	A	300	SER	CA-C	-5.70	1.45	1.52
1	E	168	GLY	CA-C	-5.70	1.46	1.52
1	A	243	PRO	N-CA	-5.69	1.40	1.47
1	B	323	SER	CA-CB	5.69	1.61	1.53
1	C	152	VAL	CA-C	-5.69	1.45	1.52
1	E	48	GLY	N-CA	-5.69	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	297	ASN	C-N	5.68	1.41	1.33
1	A	321	ALA	CA-C	5.68	1.59	1.53
1	A	48	GLY	N-CA	-5.67	1.36	1.45
1	B	335	ARG	CZ-NH1	5.67	1.40	1.32
1	C	209	VAL	CA-C	-5.66	1.45	1.52
1	B	365	ALA	CA-C	5.66	1.60	1.53
1	A	246	GLN	N-CA	-5.66	1.38	1.46
1	E	243	PRO	N-CA	-5.66	1.40	1.47
1	B	62	ARG	NE-CZ	5.65	1.39	1.33
1	B	371	HIS	C-N	5.65	1.42	1.33
1	D	191	LYS	CA-C	-5.65	1.45	1.52
1	D	261	LEU	C-N	5.64	1.42	1.33
1	D	45	VAL	C-N	5.64	1.41	1.33
1	A	29	ALA	CA-C	-5.64	1.45	1.52
1	E	29	ALA	CA-C	-5.63	1.45	1.52
1	C	208	ILE	N-CA	-5.63	1.39	1.46
1	A	49	GLN	CA-C	-5.63	1.45	1.52
1	A	62	ARG	CZ-NH2	5.62	1.40	1.33
1	B	275	HIS	CA-CB	5.62	1.63	1.53
1	E	62	ARG	CZ-NH2	5.62	1.40	1.33
1	C	329	ILE	C-O	5.62	1.29	1.24
1	D	335	ARG	NE-CZ	5.62	1.39	1.33
1	E	246	GLN	N-CA	-5.62	1.39	1.46
1	E	49	GLN	CA-C	-5.62	1.45	1.52
1	E	169	TYR	CA-C	5.62	1.59	1.52
1	B	353	GLN	CD-NE2	5.60	1.45	1.33
1	D	281	SER	CA-CB	5.59	1.62	1.53
1	A	169	TYR	CA-C	5.59	1.59	1.52
1	C	298	VAL	N-CA	-5.59	1.39	1.46
1	B	326	LYS	CA-C	5.58	1.60	1.52
1	D	330	ILE	CA-C	-5.58	1.46	1.52
1	B	201	VAL	C-O	5.57	1.30	1.24
1	C	285	CYS	C-N	5.57	1.40	1.33
1	C	11	ASP	N-CA	-5.56	1.39	1.46
1	D	20	GLY	CA-C	-5.56	1.44	1.51
1	B	76	ILE	N-CA	-5.56	1.40	1.46
1	B	254	ARG	C-N	5.55	1.41	1.33
1	B	56	ASP	CA-CB	5.55	1.62	1.53
1	A	373	LYS	N-CA	-5.55	1.39	1.46
1	B	101	HIS	ND1-CE1	5.54	1.38	1.32
1	C	126	THR	N-CA	5.53	1.53	1.46
1	B	118	LYS	CA-C	-5.53	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	256	ARG	N-CA	-5.53	1.39	1.46
1	B	10	CYS	N-CA	-5.52	1.39	1.46
1	E	196	ARG	CD-NE	5.52	1.53	1.46
1	B	335	ARG	CA-C	-5.52	1.48	1.52
1	E	129	VAL	N-CA	-5.52	1.39	1.46
1	B	9	VAL	CA-C	-5.52	1.45	1.52
1	D	171	LEU	C-O	5.52	1.30	1.23
1	B	179	ASP	CA-CB	5.51	1.60	1.53
1	C	195	GLU	C-N	5.51	1.41	1.33
1	C	282	ILE	C-N	5.51	1.41	1.33
1	C	53	TYR	C-N	5.51	1.40	1.33
1	C	185	LEU	CA-C	-5.51	1.45	1.52
1	E	205	GLU	CA-C	-5.51	1.45	1.52
1	A	256	ARG	CD-NE	5.50	1.53	1.46
1	E	256	ARG	CD-NE	5.50	1.53	1.46
1	A	64	ILE	CA-CB	-5.50	1.48	1.54
1	B	101	HIS	N-CA	-5.50	1.39	1.46
1	D	151	ILE	N-CA	-5.50	1.39	1.46
1	A	129	VAL	N-CA	-5.49	1.39	1.46
1	E	119	MET	N-CA	-5.49	1.39	1.46
1	B	237	GLU	C-N	5.49	1.40	1.33
1	C	91	TYR	CA-C	-5.49	1.45	1.52
1	D	28	ARG	CZ-NH2	5.49	1.40	1.33
1	A	205	GLU	CA-C	-5.49	1.45	1.52
1	E	373	LYS	N-CA	-5.48	1.39	1.46
1	A	196	ARG	CD-NE	5.48	1.53	1.46
1	D	292	ASP	C-O	-5.48	1.16	1.24
1	B	358	THR	N-CA	-5.47	1.38	1.45
1	A	119	MET	N-CA	-5.47	1.39	1.46
1	D	95	ARG	CD-NE	5.47	1.53	1.46
1	E	64	ILE	CA-CB	-5.46	1.48	1.54
1	D	357	ILE	CA-C	-5.46	1.45	1.52
1	B	105	LEU	C-N	5.46	1.41	1.33
1	D	87	HIS	ND1-CE1	5.46	1.38	1.32
1	B	187	ASP	CA-C	-5.45	1.45	1.52
1	E	68	LYS	N-CA	-5.45	1.39	1.45
1	D	232	SER	C-N	5.45	1.41	1.33
1	C	176	MET	CA-C	5.44	1.59	1.52
1	D	290	ARG	CD-NE	5.43	1.53	1.46
1	A	73	HIS	CA-C	-5.43	1.45	1.52
1	B	188	TYR	CA-CB	5.43	1.62	1.53
1	B	269	MET	CA-C	-5.43	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	228	ALA	C-N	5.43	1.41	1.33
1	D	301	GLY	C-N	5.43	1.40	1.33
1	B	296	ASN	CA-C	-5.42	1.46	1.53
1	C	312	ARG	NE-CZ	5.42	1.39	1.33
1	C	334	GLU	C-N	5.42	1.41	1.33
1	A	108	ALA	C-N	5.42	1.40	1.33
1	B	15	GLY	CA-C	-5.42	1.44	1.51
1	D	243	PRO	N-CD	5.41	1.55	1.47
1	D	335	ARG	C-O	-5.41	1.19	1.23
1	E	192	ILE	N-CA	-5.41	1.40	1.46
1	C	87	HIS	ND1-CE1	5.40	1.38	1.32
1	E	108	ALA	C-N	5.40	1.40	1.33
1	E	166	TYR	CA-C	-5.40	1.45	1.53
1	C	287	ILE	CA-CB	-5.39	1.47	1.54
1	E	73	HIS	CA-C	-5.39	1.45	1.52
1	B	18	LYS	CA-C	-5.39	1.46	1.52
1	A	192	ILE	N-CA	-5.38	1.40	1.46
1	B	149	THR	C-N	5.38	1.39	1.33
1	B	10	CYS	CA-C	-5.38	1.46	1.52
1	A	166	TYR	CA-C	-5.37	1.45	1.53
1	A	68	LYS	N-CA	-5.36	1.39	1.45
1	B	168	GLY	CA-C	-5.36	1.41	1.52
1	B	242	LEU	C-N	5.36	1.39	1.33
1	A	69	TYR	CA-CB	5.36	1.60	1.53
1	A	351	THR	N-CA	-5.36	1.39	1.46
1	C	173	HIS	CD2-NE2	5.35	1.43	1.37
1	B	77	THR	N-CA	-5.35	1.39	1.46
1	D	90	PHE	CA-CB	5.34	1.61	1.53
1	A	101	HIS	C-O	-5.34	1.18	1.24
1	E	69	TYR	CA-CB	5.34	1.60	1.53
1	C	57	GLU	C-N	5.33	1.41	1.33
1	C	67	LEU	C-N	5.33	1.40	1.33
1	A	78	ASN	CA-C	-5.33	1.46	1.52
1	C	167	GLU	CA-CB	5.33	1.61	1.53
1	C	128	ASN	C-N	5.32	1.39	1.33
1	B	105	LEU	CA-C	-5.32	1.46	1.52
1	B	75	ILE	CA-C	-5.32	1.46	1.52
1	E	78	ASN	CA-C	-5.32	1.46	1.52
1	B	214	GLU	CA-C	-5.31	1.46	1.52
1	E	280	ASN	C-O	-5.30	1.18	1.24
1	E	351	THR	N-CA	-5.30	1.39	1.46
1	E	101	HIS	C-O	-5.30	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	177	ARG	NE-CZ	5.30	1.38	1.33
1	C	39	ARG	CD-NE	5.30	1.53	1.46
1	A	280	ASN	C-O	-5.30	1.18	1.24
1	C	121	GLN	C-N	5.30	1.40	1.33
1	D	317	ILE	CA-C	-5.29	1.46	1.52
1	D	308	GLY	CA-C	-5.29	1.44	1.51
1	B	98	PRO	C-N	5.29	1.41	1.33
1	D	295	ALA	CA-CB	5.29	1.61	1.53
1	B	216	LEU	CA-C	-5.28	1.45	1.52
1	A	177	ARG	NE-CZ	5.28	1.38	1.33
1	A	334	GLU	CA-C	-5.28	1.46	1.52
1	E	334	GLU	CA-C	-5.28	1.46	1.52
1	B	113	LYS	N-CA	-5.27	1.39	1.46
1	C	254	ARG	CA-C	-5.27	1.45	1.52
1	E	367	PRO	CA-C	5.27	1.60	1.52
1	A	151	ILE	C-N	5.26	1.40	1.33
1	C	322	PRO	CA-C	5.26	1.59	1.52
1	D	67	LEU	CA-CB	5.26	1.60	1.53
1	C	46	GLY	C-O	-5.26	1.18	1.23
1	B	28	ARG	CD-NE	5.25	1.53	1.46
1	B	285	CYS	C-N	5.25	1.40	1.33
1	B	99	GLU	C-O	-5.25	1.17	1.24
1	A	367	PRO	CA-C	5.24	1.60	1.52
1	E	313	MET	CA-CB	-5.24	1.44	1.53
1	D	183	ARG	CZ-NH1	5.24	1.40	1.32
1	E	151	ILE	C-N	5.23	1.40	1.33
1	A	17	VAL	CA-CB	-5.23	1.46	1.53
1	B	170	ALA	N-CA	-5.23	1.39	1.46
1	B	338	SER	CA-CB	5.23	1.61	1.53
1	E	25	ASP	N-CA	-5.23	1.40	1.46
1	B	160	THR	CA-C	-5.22	1.46	1.52
1	B	258	PRO	N-CA	-5.22	1.40	1.47
1	C	111	ASN	CA-CB	5.22	1.61	1.53
1	D	124	PHE	CA-C	-5.22	1.46	1.52
1	D	159	VAL	CA-C	-5.21	1.46	1.52
1	E	137	GLN	CA-CB	5.21	1.62	1.53
1	A	25	ASP	N-CA	-5.21	1.40	1.46
1	D	335	ARG	CZ-NH1	5.21	1.40	1.32
1	C	336	LYS	N-CA	5.21	1.52	1.46
1	C	218	TYR	CA-C	-5.21	1.46	1.52
1	A	137	GLN	CA-CB	5.20	1.62	1.53
1	B	147	ARG	CA-CB	5.20	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	MET	CA-CB	-5.20	1.44	1.53
1	E	17	VAL	CA-CB	-5.20	1.46	1.53
1	A	117	GLU	CA-CB	5.20	1.61	1.53
1	D	49	GLN	N-CA	5.19	1.53	1.46
1	B	177	ARG	CD-NE	5.19	1.53	1.46
1	D	328	LYS	CA-C	-5.19	1.46	1.52
1	C	355	MET	C-N	5.18	1.40	1.33
1	B	240	TYR	CA-C	-5.18	1.47	1.53
1	E	117	GLU	CA-CB	5.17	1.61	1.53
1	D	39	ARG	CZ-NH1	5.17	1.40	1.32
1	D	224	GLU	N-CA	-5.17	1.39	1.46
1	A	1	ASP	C-N	5.17	1.40	1.33
1	B	206	ARG	CZ-NH1	5.16	1.40	1.32
1	B	243	PRO	CA-C	5.16	1.58	1.52
1	C	352	PHE	CA-C	5.16	1.59	1.52
1	D	254	ARG	CZ-NH1	5.16	1.40	1.32
1	B	312	ARG	CZ-NH1	5.15	1.40	1.32
1	C	161	HIS	CB-CG	-5.15	1.43	1.50
1	B	64	ILE	CA-CB	-5.15	1.48	1.54
1	B	372	ARG	CZ-NH2	5.15	1.40	1.33
1	A	154	ASP	N-CA	-5.14	1.40	1.46
1	E	154	ASP	N-CA	-5.14	1.40	1.46
1	D	247	VAL	CA-C	-5.14	1.46	1.52
1	E	1	ASP	C-N	5.14	1.40	1.33
1	B	79	TRP	CA-C	-5.13	1.45	1.52
1	B	173	HIS	CA-C	-5.13	1.45	1.52
1	E	283	MET	CG-SD	5.13	1.93	1.80
1	C	183	ARG	CZ-NH1	5.12	1.40	1.32
1	E	359	LYS	CA-CB	5.12	1.61	1.53
1	B	134	VAL	N-CA	-5.12	1.40	1.46
1	B	341	ILE	N-CA	-5.12	1.40	1.46
1	B	87	HIS	CA-CB	5.12	1.61	1.53
1	D	41	GLN	N-CA	-5.11	1.39	1.46
1	E	351	THR	C-N	5.11	1.41	1.33
1	B	111	ASN	CA-CB	5.10	1.60	1.53
1	A	123	MET	CA-C	-5.10	1.46	1.52
1	A	283	MET	CG-SD	5.10	1.93	1.80
1	B	31	PHE	N-CA	-5.10	1.40	1.46
1	C	233	SER	CA-CB	5.10	1.61	1.53
1	A	359	LYS	CA-CB	5.09	1.61	1.53
1	D	54	VAL	C-N	5.09	1.40	1.33
1	E	224	GLU	CA-C	-5.08	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	279	TYR	CA-C	-5.08	1.46	1.52
1	A	224	GLU	CA-C	-5.08	1.45	1.52
1	C	115	ASN	C-N	-5.08	1.27	1.33
1	E	123	MET	CA-C	-5.08	1.46	1.52
1	B	222	ASP	CA-C	-5.07	1.46	1.52
1	A	351	THR	C-N	5.06	1.41	1.33
1	D	27	PRO	N-CA	-5.06	1.40	1.47
1	A	279	TYR	CA-C	-5.05	1.46	1.52
1	C	183	ARG	CA-C	5.05	1.59	1.52
1	B	39	ARG	CA-C	-5.04	1.46	1.52
1	E	290	ARG	CZ-NH1	5.04	1.39	1.32
1	B	125	GLU	C-N	5.04	1.40	1.33
1	C	291	LYS	CA-CB	5.04	1.61	1.53
1	D	73	HIS	CG-ND1	5.04	1.43	1.38
1	A	62	ARG	CA-C	-5.04	1.45	1.52
1	C	210	ARG	CD-NE	5.04	1.53	1.46
1	A	65	LEU	CA-CB	5.03	1.64	1.54
1	C	244	ASP	CA-CB	5.03	1.61	1.53
1	B	256	ARG	CA-C	-5.02	1.46	1.52
1	C	117	GLU	CA-CB	5.02	1.61	1.53
1	C	182	GLY	C-N	5.02	1.40	1.34
1	D	15	GLY	CA-C	-5.02	1.44	1.51
1	C	175	ILE	CA-CB	-5.02	1.47	1.54
1	A	228	ALA	C-N	5.02	1.40	1.33
1	E	62	ARG	CA-C	-5.02	1.45	1.52
1	E	223	PHE	CB-CG	5.01	1.62	1.50
1	C	23	GLY	CA-C	5.01	1.59	1.51
1	A	290	ARG	CZ-NH1	5.01	1.39	1.32
1	E	228	ALA	C-N	5.01	1.40	1.33
1	C	272	ALA	C-N	5.01	1.37	1.33
1	A	223	PHE	CB-CG	5.00	1.62	1.50
1	E	65	LEU	CA-CB	5.00	1.64	1.54

All (1018) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	179	ASP	CA-CB-CG	-12.33	100.27	112.60
1	D	9	VAL	N-CA-C	-11.92	90.12	107.77
1	D	282	ILE	N-CA-C	-11.08	99.83	111.58
1	A	234	SER	N-CA-C	-11.05	102.02	114.62
1	E	234	SER	N-CA-C	-11.04	102.04	114.62
1	C	24	ASP	CA-CB-CG	-10.62	101.98	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	ILE	N-CA-C	-10.26	103.11	113.47
1	C	286	ASP	CA-C-N	10.12	134.32	120.46
1	C	286	ASP	C-N-CA	10.12	134.32	120.46
1	B	214	GLU	N-CA-C	10.09	122.36	111.36
1	D	26	ALA	O-C-N	-10.09	114.29	121.65
1	C	272	ALA	CA-C-N	10.07	129.59	119.92
1	C	272	ALA	C-N-CA	10.07	129.59	119.92
1	A	35	VAL	N-CA-C	-9.99	94.09	108.48
1	B	21	PHE	CA-CB-CG	-9.98	103.82	113.80
1	E	35	VAL	N-CA-C	-9.98	94.11	108.48
1	A	88	HIS	CA-CB-CG	9.92	123.72	113.80
1	E	88	HIS	CA-CB-CG	9.88	123.68	113.80
1	D	35	VAL	N-CA-C	-9.81	94.37	108.11
1	D	202	THR	CA-C-N	9.66	133.57	120.44
1	D	202	THR	C-N-CA	9.66	133.57	120.44
1	E	263	GLN	CA-C-N	9.66	129.28	119.82
1	E	263	GLN	C-N-CA	9.66	129.28	119.82
1	B	64	ILE	N-CA-C	-9.65	103.72	113.47
1	A	263	GLN	CA-C-N	9.64	129.26	119.82
1	A	263	GLN	C-N-CA	9.64	129.26	119.82
1	B	49	GLN	OE1-CD-NE2	9.55	132.15	122.60
1	E	26	ALA	CA-C-O	-9.55	109.48	119.22
1	A	26	ALA	CA-C-O	-9.52	109.51	119.22
1	A	39	ARG	NE-CZ-NH2	9.39	127.66	119.20
1	C	51	ASP	N-CA-C	-9.38	99.55	114.09
1	E	39	ARG	NE-CZ-NH2	9.36	127.62	119.20
1	B	98	PRO	N-CA-CB	9.33	112.14	103.46
1	E	64	ILE	N-CA-C	-9.30	104.07	113.47
1	D	196	ARG	NE-CZ-NH2	-9.29	110.83	119.20
1	A	64	ILE	N-CA-C	-9.29	104.09	113.47
1	E	297	ASN	CA-CB-CG	-9.20	103.40	112.60
1	A	297	ASN	CA-CB-CG	-9.19	103.41	112.60
1	C	164	PRO	CA-C-O	-9.08	110.67	121.03
1	C	353	GLN	CA-C-O	8.87	130.12	120.10
1	A	289	ILE	N-CA-C	-8.80	103.84	113.43
1	E	289	ILE	N-CA-C	-8.79	103.85	113.43
1	A	298	VAL	N-CA-CB	8.76	120.27	110.72
1	E	298	VAL	N-CA-CB	8.72	120.23	110.72
1	D	118	LYS	CA-C-N	8.71	131.76	120.44
1	D	118	LYS	C-N-CA	8.71	131.76	120.44
1	D	252	ASN	CA-C-N	8.69	132.79	120.28
1	D	252	ASN	C-N-CA	8.69	132.79	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	332	PRO	CA-C-O	-8.66	108.01	120.56
1	B	97	ALA	N-CA-C	-8.63	99.17	110.39
1	E	211	ASP	CA-CB-CG	-8.63	103.97	112.60
1	A	211	ASP	CA-CB-CG	-8.61	103.99	112.60
1	A	292	ASP	CA-C-O	8.61	128.61	119.14
1	E	292	ASP	CA-C-O	8.60	128.60	119.14
1	D	85	ILE	N-CA-C	8.54	119.33	110.62
1	B	222	ASP	CA-C-N	8.48	131.46	120.44
1	B	222	ASP	C-N-CA	8.48	131.46	120.44
1	C	172	PRO	N-CA-CB	8.48	107.67	102.92
1	C	173	HIS	CA-CB-CG	8.47	122.27	113.80
1	B	267	ILE	CB-CA-C	-8.45	100.91	112.24
1	C	252	ASN	CA-C-N	8.45	132.44	120.28
1	C	252	ASN	C-N-CA	8.45	132.44	120.28
1	C	124	PHE	CA-CB-CG	-8.41	105.39	113.80
1	B	243	PRO	O-C-N	8.41	132.14	122.98
1	C	92	ASN	CA-CB-CG	8.36	120.96	112.60
1	D	181	ALA	CA-C-N	8.34	129.41	119.99
1	D	181	ALA	C-N-CA	8.34	129.41	119.99
1	C	275	HIS	CE1-NE2-CD2	-8.26	100.75	109.00
1	A	108	ALA	CA-C-N	8.23	128.29	119.90
1	A	108	ALA	C-N-CA	8.23	128.29	119.90
1	C	244	ASP	CA-CB-CG	-8.22	104.38	112.60
1	B	371	HIS	CE1-NE2-CD2	-8.22	100.78	109.00
1	A	118	LYS	CA-C-N	8.21	131.11	120.44
1	A	118	LYS	C-N-CA	8.21	131.11	120.44
1	A	204	ALA	N-CA-C	8.21	122.39	112.38
1	E	108	ALA	CA-C-N	8.21	128.27	119.90
1	E	108	ALA	C-N-CA	8.21	128.27	119.90
1	E	118	LYS	CA-C-N	8.20	131.10	120.44
1	E	118	LYS	C-N-CA	8.20	131.10	120.44
1	E	204	ALA	N-CA-C	8.19	122.37	112.38
1	D	101	HIS	CE1-NE2-CD2	-8.15	100.85	109.00
1	E	348	SER	N-CA-C	-8.14	103.06	113.16
1	A	348	SER	N-CA-C	-8.14	103.07	113.16
1	C	75	ILE	N-CA-C	-8.11	96.75	108.11
1	C	344	SER	N-CA-CB	8.10	122.15	110.16
1	C	3	ASP	CA-CB-CG	8.09	120.69	112.60
1	C	182	GLY	N-CA-C	8.08	122.42	112.64
1	A	242	LEU	CA-C-O	-8.08	112.92	119.71
1	B	202	THR	CA-C-N	8.07	131.42	120.44
1	B	202	THR	C-N-CA	8.07	131.42	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	321	ALA	O-C-N	-8.05	110.87	121.34
1	E	182	GLY	CA-C-O	-8.05	112.76	121.05
1	D	62	ARG	NE-CZ-NH2	-8.03	111.97	119.20
1	E	242	LEU	CA-C-O	-8.03	112.97	119.71
1	C	87	HIS	CE1-NE2-CD2	-8.02	100.98	109.00
1	C	240	TYR	N-CA-CB	8.01	122.26	110.49
1	E	363	ASP	CA-CB-CG	8.00	120.60	112.60
1	C	345	ILE	O-C-N	8.00	129.75	121.91
1	C	333	PRO	O-C-N	8.00	130.82	122.18
1	A	182	GLY	CA-C-O	-7.99	112.83	121.05
1	D	260	THR	CA-C-N	7.98	131.31	120.38
1	D	260	THR	C-N-CA	7.98	131.31	120.38
1	A	363	ASP	CA-CB-CG	7.96	120.56	112.60
1	B	16	LEU	N-CA-C	-7.96	99.05	110.59
1	B	79	TRP	CG-CD2-CE3	-7.95	125.95	133.90
1	B	223	PHE	CA-CB-CG	7.84	121.64	113.80
1	A	332	PRO	N-CA-CB	7.84	110.68	103.08
1	E	332	PRO	N-CA-CB	7.83	110.67	103.08
1	C	210	ARG	CA-C-O	7.82	128.97	119.97
1	B	213	LYS	CA-C-N	-7.79	109.23	120.29
1	B	213	LYS	C-N-CA	-7.79	109.23	120.29
1	E	143	TYR	CA-C-N	7.78	130.56	120.44
1	E	143	TYR	C-N-CA	7.78	130.56	120.44
1	A	143	TYR	CA-C-N	7.77	130.55	120.44
1	A	143	TYR	C-N-CA	7.77	130.55	120.44
1	E	335	ARG	NE-CZ-NH1	-7.76	113.73	121.50
1	B	279	TYR	CA-C-N	7.76	130.68	120.28
1	B	279	TYR	C-N-CA	7.76	130.68	120.28
1	B	79	TRP	CB-CG-CD1	7.76	138.54	126.90
1	D	99	GLU	N-CA-C	-7.74	100.67	111.81
1	A	371	HIS	CA-CB-CG	7.74	121.54	113.80
1	A	335	ARG	NE-CZ-NH1	-7.73	113.77	121.50
1	C	136	ILE	CA-C-N	7.73	136.30	121.54
1	C	136	ILE	C-N-CA	7.73	136.30	121.54
1	E	371	HIS	CA-CB-CG	7.71	121.51	113.80
1	D	9	VAL	N-CA-CB	7.61	122.17	111.82
1	B	215	LYS	CB-CA-C	7.59	123.55	110.72
1	B	55	GLY	CA-C-N	7.59	130.78	120.38
1	B	55	GLY	C-N-CA	7.59	130.78	120.38
1	A	34	ILE	CA-CB-CG1	7.57	123.26	110.40
1	D	55	GLY	CA-C-N	7.56	130.74	120.38
1	D	55	GLY	C-N-CA	7.56	130.74	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	PHE	CB-CA-C	-7.56	100.50	111.23
1	C	226	GLU	CA-C-N	7.56	131.02	120.29
1	C	226	GLU	C-N-CA	7.56	131.02	120.29
1	E	34	ILE	CA-CB-CG1	7.54	123.21	110.40
1	E	200	PHE	CB-CA-C	-7.54	100.53	111.23
1	D	302	GLY	O-C-N	7.46	131.11	122.68
1	B	225	ASN	CA-CB-CG	-7.41	105.19	112.60
1	A	344	SER	CA-C-N	7.40	130.93	120.42
1	A	344	SER	C-N-CA	7.40	130.93	120.42
1	B	91	TYR	N-CA-C	7.40	119.43	111.36
1	B	186	THR	N-CA-C	-7.37	103.24	111.28
1	E	344	SER	CA-C-N	7.37	130.89	120.42
1	E	344	SER	C-N-CA	7.37	130.89	120.42
1	C	37	ARG	NE-CZ-NH2	7.36	125.82	119.20
1	A	39	ARG	NE-CZ-NH1	-7.36	114.14	121.50
1	C	9	VAL	N-CA-C	-7.35	96.90	107.77
1	D	226	GLU	CA-C-N	7.34	130.72	120.29
1	D	226	GLU	C-N-CA	7.34	130.72	120.29
1	E	39	ARG	NE-CZ-NH1	-7.34	114.16	121.50
1	C	330	ILE	N-CA-C	-7.34	96.58	107.51
1	D	16	LEU	N-CA-C	-7.33	97.87	109.23
1	C	276	GLU	N-CA-CB	7.32	121.10	110.20
1	E	255	PHE	N-CA-C	-7.31	102.91	112.41
1	A	255	PHE	N-CA-C	-7.29	102.93	112.41
1	B	252	ASN	CA-CB-CG	7.29	119.89	112.60
1	D	101	HIS	CG-CD2-NE2	7.28	114.48	107.20
1	B	121	GLN	N-CA-C	7.25	119.27	111.36
1	B	78	ASN	CA-CB-CG	-7.25	105.35	112.60
1	A	263	GLN	CB-CG-CD	7.24	124.91	112.60
1	A	173	HIS	CE1-NE2-CD2	-7.24	101.76	109.00
1	A	236	LEU	N-CA-C	-7.24	104.59	113.50
1	C	298	VAL	N-CA-CB	7.24	118.42	110.53
1	A	273	GLY	N-CA-C	-7.23	103.28	112.54
1	E	225	ASN	CA-CB-CG	-7.23	105.37	112.60
1	E	236	LEU	N-CA-C	-7.23	104.60	113.50
1	E	273	GLY	N-CA-C	-7.23	103.28	112.54
1	C	26	ALA	CA-C-O	-7.23	113.39	120.26
1	E	173	HIS	CE1-NE2-CD2	-7.22	101.78	109.00
1	A	64	ILE	N-CA-CB	-7.22	103.74	112.33
1	D	268	GLY	N-CA-C	-7.22	104.77	114.95
1	E	263	GLN	CB-CG-CD	7.22	124.87	112.60
1	E	64	ILE	N-CA-CB	-7.22	103.74	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	374	CYS	N-CA-C	-7.21	100.13	110.59
1	A	225	ASN	CA-CB-CG	-7.21	105.39	112.60
1	B	62	ARG	O-C-N	-7.17	114.80	122.19
1	C	73	HIS	ND1-CE1-NE2	7.16	115.56	108.40
1	D	354	GLN	N-CA-C	-7.16	104.58	113.38
1	D	88	HIS	CA-CB-CG	7.15	120.95	113.80
1	D	171	LEU	CA-C-O	-7.15	113.01	120.87
1	B	106	THR	CA-C-N	7.14	133.04	123.05
1	B	106	THR	C-N-CA	7.14	133.04	123.05
1	E	139	VAL	CA-C-N	7.13	130.42	120.29
1	E	139	VAL	C-N-CA	7.13	130.42	120.29
1	B	171	LEU	CA-C-O	-7.11	113.21	120.96
1	D	248	ILE	CA-C-N	7.11	132.03	121.72
1	D	248	ILE	C-N-CA	7.11	132.03	121.72
1	A	139	VAL	CA-C-N	7.11	130.38	120.29
1	A	139	VAL	C-N-CA	7.11	130.38	120.29
1	C	188	TYR	CA-C-O	-7.10	111.29	119.60
1	D	182	GLY	CA-C-O	-7.10	113.74	121.05
1	E	121	GLN	CA-C-N	7.10	131.94	120.30
1	E	121	GLN	C-N-CA	7.10	131.94	120.30
1	A	121	GLN	CA-C-N	7.09	131.93	120.30
1	A	121	GLN	C-N-CA	7.09	131.93	120.30
1	E	208	ILE	CA-C-N	7.09	130.17	120.46
1	E	208	ILE	C-N-CA	7.09	130.17	120.46
1	A	208	ILE	CA-C-N	7.08	130.16	120.46
1	A	208	ILE	C-N-CA	7.08	130.16	120.46
1	D	267	ILE	O-C-N	7.08	131.19	121.84
1	D	48	GLY	N-CA-C	-7.08	103.52	115.62
1	B	310	ALA	CA-C-O	7.06	127.90	120.42
1	C	228	ALA	CA-C-N	7.06	132.51	120.72
1	C	228	ALA	C-N-CA	7.06	132.51	120.72
1	E	319	ALA	CA-C-O	7.05	128.41	121.00
1	C	40	HIS	N-CA-C	-7.05	104.49	113.23
1	A	319	ALA	CA-C-O	7.04	128.39	121.00
1	B	138	ALA	O-C-N	7.03	129.31	122.07
1	C	205	GLU	CA-C-N	7.02	130.98	120.31
1	C	205	GLU	C-N-CA	7.02	130.98	120.31
1	D	202	THR	N-CA-CB	7.00	121.09	110.45
1	B	107	GLU	CA-C-O	-6.98	112.64	120.32
1	B	34	ILE	N-CA-C	-6.95	98.19	108.97
1	C	344	SER	CB-CA-C	-6.95	99.04	110.85
1	B	198	TYR	N-CA-CB	6.94	122.15	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	369	ILE	CA-C-N	6.94	129.37	120.70
1	C	369	ILE	C-N-CA	6.94	129.37	120.70
1	D	170	ALA	N-CA-CB	6.92	120.28	109.83
1	A	332	PRO	CA-C-N	6.92	128.49	119.84
1	A	332	PRO	C-N-CA	6.92	128.49	119.84
1	E	332	PRO	CA-C-N	6.91	128.47	119.84
1	E	332	PRO	C-N-CA	6.91	128.47	119.84
1	B	243	PRO	CA-C-O	-6.88	114.05	121.27
1	D	201	VAL	N-CA-C	6.88	117.39	110.23
1	A	4	GLU	CA-C-O	6.88	128.13	120.70
1	C	361	GLU	N-CA-CB	6.88	121.01	110.14
1	E	4	GLU	CA-C-O	6.87	128.12	120.70
1	C	279	TYR	N-CA-CB	6.86	120.02	110.07
1	E	159	VAL	CA-C-N	6.86	133.91	122.87
1	E	159	VAL	C-N-CA	6.86	133.91	122.87
1	A	159	VAL	CA-C-N	6.86	133.91	122.87
1	A	159	VAL	C-N-CA	6.86	133.91	122.87
1	C	248	ILE	CB-CA-C	-6.84	103.65	111.59
1	A	321	ALA	CA-C-N	6.83	128.38	119.84
1	A	321	ALA	C-N-CA	6.83	128.38	119.84
1	E	321	ALA	CA-C-N	6.83	128.38	119.84
1	E	321	ALA	C-N-CA	6.83	128.38	119.84
1	E	30	VAL	N-CA-C	-6.83	98.21	108.17
1	A	30	VAL	N-CA-C	-6.82	98.21	108.17
1	A	90	PHE	N-CA-C	-6.82	103.46	111.03
1	B	108	ALA	CA-C-O	-6.80	113.70	119.76
1	C	99	GLU	N-CA-C	-6.80	105.39	113.21
1	E	90	PHE	N-CA-C	-6.80	103.48	111.03
1	B	358	THR	N-CA-C	-6.78	101.40	110.55
1	C	113	LYS	CB-CG-CD	6.78	126.89	111.30
1	A	175	ILE	N-CA-C	-6.78	97.86	108.23
1	D	74	GLY	CA-C-N	6.76	132.00	123.14
1	D	74	GLY	C-N-CA	6.76	132.00	123.14
1	E	175	ILE	N-CA-C	-6.76	97.89	108.23
1	B	373	LYS	N-CA-CB	6.76	120.68	110.14
1	A	338	SER	N-CA-C	6.75	119.48	111.71
1	E	181	ALA	CA-C-N	6.75	127.61	119.99
1	E	181	ALA	C-N-CA	6.75	127.61	119.99
1	E	338	SER	N-CA-C	6.75	119.47	111.71
1	A	181	ALA	CA-C-N	6.75	127.61	119.99
1	A	181	ALA	C-N-CA	6.75	127.61	119.99
1	B	323	SER	N-CA-C	-6.74	104.95	112.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	147	ARG	N-CA-CB	6.73	119.98	110.36
1	C	79	TRP	CA-C-O	6.71	126.53	119.14
1	B	31	PHE	CB-CA-C	6.70	119.04	109.92
1	E	290	ARG	CA-C-N	6.70	129.93	120.28
1	E	290	ARG	C-N-CA	6.70	129.93	120.28
1	B	368	SER	CA-C-N	6.69	131.59	120.62
1	B	368	SER	C-N-CA	6.69	131.59	120.62
1	D	285	CYS	CA-C-N	6.69	130.86	120.75
1	D	285	CYS	C-N-CA	6.69	130.86	120.75
1	A	290	ARG	CA-C-N	6.68	129.90	120.28
1	A	290	ARG	C-N-CA	6.68	129.90	120.28
1	D	210	ARG	CA-C-N	6.68	129.77	120.29
1	D	210	ARG	C-N-CA	6.68	129.77	120.29
1	E	331	ALA	CA-C-N	6.66	127.24	120.38
1	E	331	ALA	C-N-CA	6.66	127.24	120.38
1	E	306	TYR	CA-C-N	6.65	127.69	119.98
1	E	306	TYR	C-N-CA	6.65	127.69	119.98
1	A	331	ALA	CA-C-N	6.64	127.22	120.38
1	A	331	ALA	C-N-CA	6.64	127.22	120.38
1	B	229	THR	CA-C-N	6.64	129.85	120.28
1	B	229	THR	C-N-CA	6.64	129.85	120.28
1	A	306	TYR	CA-C-N	6.64	127.68	119.98
1	A	306	TYR	C-N-CA	6.64	127.68	119.98
1	C	221	LEU	N-CA-C	-6.63	103.31	111.40
1	B	5	THR	CA-C-N	6.62	134.19	121.54
1	B	5	THR	C-N-CA	6.62	134.19	121.54
1	C	370	VAL	N-CA-CB	6.62	117.84	110.62
1	B	264	PRO	N-CA-C	-6.62	106.26	114.20
1	A	289	ILE	CB-CA-C	6.62	119.11	110.84
1	D	157	ASP	N-CA-C	-6.61	107.09	114.62
1	E	289	ILE	CB-CA-C	6.60	119.09	110.84
1	B	40	HIS	CA-CB-CG	6.60	120.40	113.80
1	A	232	SER	N-CA-C	-6.58	97.45	109.56
1	D	308	GLY	CA-C-N	6.58	128.85	120.56
1	D	308	GLY	C-N-CA	6.58	128.85	120.56
1	B	305	MET	N-CA-C	-6.58	104.85	114.39
1	E	232	SER	N-CA-C	-6.57	97.47	109.56
1	A	74	GLY	N-CA-C	-6.57	106.17	115.30
1	C	88	HIS	ND1-CE1-NE2	6.57	114.97	108.40
1	D	329	ILE	CA-C-N	6.56	130.70	122.43
1	D	329	ILE	C-N-CA	6.56	130.70	122.43
1	C	73	HIS	CA-CB-CG	-6.56	107.24	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	123	MET	N-CA-CB	6.56	119.84	110.13
1	E	74	GLY	N-CA-C	-6.56	106.19	115.30
1	A	339	VAL	N-CA-C	-6.55	102.66	111.44
1	E	339	VAL	N-CA-C	-6.55	102.66	111.44
1	B	40	HIS	ND1-CE1-NE2	6.53	114.93	108.40
1	E	329	ILE	N-CA-CB	6.53	117.64	110.53
1	C	164	PRO	O-C-N	6.52	130.41	123.10
1	D	278	THR	CA-C-O	6.52	127.46	120.55
1	C	73	HIS	CE1-NE2-CD2	-6.52	102.48	109.00
1	A	164	PRO	N-CA-CB	6.51	108.76	103.36
1	E	46	GLY	N-CA-C	-6.50	102.38	112.85
1	A	329	ILE	N-CA-CB	6.50	117.62	110.53
1	B	32	PRO	O-C-N	6.50	131.42	122.64
1	D	275	HIS	CG-CD2-NE2	6.50	113.70	107.20
1	E	12	ASN	CA-C-N	6.50	128.70	122.27
1	E	12	ASN	C-N-CA	6.50	128.70	122.27
1	E	164	PRO	N-CA-CB	6.50	108.75	103.36
1	A	12	ASN	CA-C-N	6.49	128.70	122.27
1	A	12	ASN	C-N-CA	6.49	128.70	122.27
1	B	40	HIS	CE1-NE2-CD2	-6.49	102.51	109.00
1	D	87	HIS	CA-CB-CG	-6.49	107.31	113.80
1	E	173	HIS	ND1-CE1-NE2	6.49	114.89	108.40
1	A	46	GLY	N-CA-C	-6.49	102.41	112.85
1	D	168	GLY	N-CA-C	-6.49	97.81	113.18
1	D	200	PHE	CA-CB-CG	-6.48	107.32	113.80
1	B	123	MET	N-CA-C	-6.48	102.71	112.04
1	A	226	GLU	N-CA-C	-6.47	105.39	113.28
1	C	360	GLN	CA-C-N	6.47	129.83	120.38
1	C	360	GLN	C-N-CA	6.47	129.83	120.38
1	B	79	TRP	CB-CG-CD2	-6.47	117.74	126.80
1	E	315	LYS	N-CA-C	-6.47	105.92	113.88
1	A	315	LYS	N-CA-C	-6.47	105.92	113.88
1	A	185	LEU	N-CA-C	-6.46	104.09	112.23
1	D	321	ALA	CA-C-N	6.46	127.35	120.11
1	D	321	ALA	C-N-CA	6.46	127.35	120.11
1	A	173	HIS	ND1-CE1-NE2	6.46	114.86	108.40
1	B	290	ARG	N-CA-C	6.46	119.31	111.82
1	E	226	GLU	N-CA-C	-6.45	105.41	113.28
1	B	284	LYS	N-CA-C	-6.45	104.33	111.36
1	E	185	LEU	N-CA-C	-6.44	104.11	112.23
1	B	170	ALA	N-CA-C	6.44	118.61	110.24
1	D	358	THR	CA-C-N	6.43	129.73	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	358	THR	C-N-CA	6.43	129.73	120.79
1	B	334	GLU	CB-CG-CD	6.43	123.53	112.60
1	D	21	PHE	N-CA-C	-6.42	100.96	110.46
1	C	101	HIS	CA-C-O	6.41	126.29	119.50
1	A	58	ALA	CA-C-N	6.41	129.50	120.28
1	A	58	ALA	C-N-CA	6.41	129.50	120.28
1	C	87	HIS	ND1-CE1-NE2	6.40	114.80	108.40
1	D	371	HIS	ND1-CE1-NE2	6.40	114.80	108.40
1	E	58	ALA	CA-C-N	6.40	129.50	120.28
1	E	58	ALA	C-N-CA	6.40	129.50	120.28
1	B	198	TYR	N-CA-C	-6.39	99.27	108.60
1	C	87	HIS	CB-CG-CD2	-6.39	122.89	131.20
1	C	202	THR	CA-C-N	6.39	128.84	120.28
1	C	202	THR	C-N-CA	6.39	128.84	120.28
1	C	264	PRO	CA-C-N	6.38	129.47	120.28
1	C	264	PRO	C-N-CA	6.38	129.47	120.28
1	C	227	MET	N-CA-C	-6.37	104.41	111.36
1	D	362	TYR	N-CA-C	-6.36	104.43	111.36
1	C	183	ARG	CA-C-N	6.35	129.97	120.31
1	C	183	ARG	C-N-CA	6.35	129.97	120.31
1	D	30	VAL	N-CA-C	-6.35	98.90	108.17
1	C	55	GLY	CA-C-N	6.35	128.78	120.28
1	C	55	GLY	C-N-CA	6.35	128.78	120.28
1	B	112	PRO	CA-C-N	6.34	129.40	120.28
1	B	112	PRO	C-N-CA	6.34	129.40	120.28
1	D	244	ASP	N-CA-C	-6.33	102.80	112.99
1	A	171	LEU	N-CA-C	-6.32	102.10	110.07
1	A	166	TYR	CA-C-O	-6.32	113.66	121.88
1	C	48	GLY	CA-C-N	6.32	133.61	121.54
1	C	48	GLY	C-N-CA	6.32	133.61	121.54
1	C	101	HIS	CB-CA-C	-6.32	100.29	109.45
1	E	166	TYR	CA-C-O	-6.31	113.68	121.88
1	B	371	HIS	CG-CD2-NE2	6.31	113.51	107.20
1	D	283	MET	N-CA-CB	6.30	120.85	110.39
1	A	66	THR	N-CA-C	-6.29	99.14	109.40
1	C	28	ARG	O-C-N	6.29	128.88	122.09
1	C	220	ALA	CA-C-O	-6.29	115.41	122.01
1	E	66	THR	N-CA-C	-6.29	99.16	109.40
1	E	171	LEU	N-CA-C	-6.28	102.16	110.07
1	D	237	GLU	CA-CB-CG	-6.28	101.54	114.10
1	C	160	THR	N-CA-C	-6.28	99.47	109.76
1	B	351	THR	N-CA-C	-6.27	104.54	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	37	ARG	NH1-CZ-NH2	-6.27	111.15	119.30
1	E	254	ARG	N-CA-C	6.27	118.92	111.71
1	A	73	HIS	CE1-NE2-CD2	-6.26	102.73	109.00
1	E	73	HIS	CE1-NE2-CD2	-6.26	102.74	109.00
1	A	254	ARG	N-CA-C	6.26	118.91	111.71
1	B	276	GLU	N-CA-C	-6.25	104.00	111.69
1	D	125	GLU	CB-CG-CD	-6.23	102.00	112.60
1	C	107	GLU	O-C-N	-6.22	115.29	123.13
1	C	208	ILE	N-CA-C	6.21	116.96	110.62
1	B	117	GLU	CA-C-N	6.21	128.60	120.28
1	B	117	GLU	C-N-CA	6.21	128.60	120.28
1	B	239	SER	CA-C-O	6.21	127.07	120.36
1	D	238	LYS	N-CA-CB	6.21	120.99	110.49
1	A	161	HIS	CE1-NE2-CD2	-6.21	102.79	109.00
1	B	216	LEU	O-C-N	-6.20	114.34	122.59
1	C	363	ASP	CA-C-N	6.20	131.99	121.14
1	C	363	ASP	C-N-CA	6.20	131.99	121.14
1	A	245	GLY	CA-C-N	6.20	133.37	121.54
1	A	245	GLY	C-N-CA	6.20	133.37	121.54
1	E	161	HIS	CE1-NE2-CD2	-6.20	102.81	109.00
1	E	245	GLY	CA-C-N	6.18	133.34	121.54
1	E	245	GLY	C-N-CA	6.18	133.34	121.54
1	B	31	PHE	N-CA-C	-6.17	100.15	108.11
1	A	214	GLU	N-CA-C	6.16	118.00	111.28
1	C	202	THR	O-C-N	-6.16	114.40	122.59
1	C	374	CYS	CA-C-O	6.16	127.49	120.84
1	D	363	ASP	CA-CB-CG	-6.14	106.46	112.60
1	A	239	SER	CA-C-O	6.12	126.97	120.36
1	A	260	THR	O-C-N	6.12	129.38	122.22
1	E	214	GLU	N-CA-C	6.12	117.95	111.28
1	B	54	VAL	CB-CA-C	6.11	121.28	110.71
1	D	206	ARG	NE-CZ-NH1	-6.11	115.39	121.50
1	E	239	SER	CA-C-O	6.11	126.95	120.36
1	E	212	ILE	CB-CA-C	-6.11	103.90	112.14
1	A	212	ILE	CB-CA-C	-6.09	103.91	112.14
1	A	117	GLU	CA-C-N	6.09	128.44	120.28
1	A	117	GLU	C-N-CA	6.09	128.44	120.28
1	E	260	THR	O-C-N	6.09	129.35	122.22
1	C	259	GLU	CA-C-N	6.09	129.05	120.28
1	C	259	GLU	C-N-CA	6.09	129.05	120.28
1	B	48	GLY	CA-C-N	6.09	133.17	121.54
1	B	48	GLY	C-N-CA	6.09	133.17	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ASP	CA-C-N	6.08	129.04	120.28
1	A	56	ASP	C-N-CA	6.08	129.04	120.28
1	C	17	VAL	O-C-N	6.08	129.11	122.36
1	C	117	GLU	CA-C-N	6.08	128.42	120.28
1	C	117	GLU	C-N-CA	6.08	128.42	120.28
1	E	56	ASP	CA-C-N	6.08	129.03	120.28
1	E	56	ASP	C-N-CA	6.08	129.03	120.28
1	B	219	VAL	N-CA-CB	6.07	117.34	110.72
1	C	37	ARG	CA-C-N	6.07	126.91	120.11
1	C	37	ARG	C-N-CA	6.07	126.91	120.11
1	E	117	GLU	CA-C-N	6.07	128.41	120.28
1	E	117	GLU	C-N-CA	6.07	128.41	120.28
1	D	302	GLY	CA-C-O	-6.07	112.34	119.50
1	B	343	GLY	N-CA-C	-6.06	107.15	114.66
1	A	16	LEU	N-CA-CB	6.06	121.97	111.13
1	C	22	ALA	CA-C-O	-6.05	114.39	121.16
1	A	297	ASN	N-CA-CB	6.04	119.36	110.35
1	B	90	PHE	CA-CB-CG	-6.04	107.76	113.80
1	E	16	LEU	N-CA-CB	6.04	121.94	111.13
1	E	340	TRP	CE2-CD2-CE3	6.04	124.84	118.80
1	E	297	ASN	N-CA-CB	6.03	119.33	110.35
1	D	58	ALA	CA-C-N	6.02	130.24	120.60
1	D	58	ALA	C-N-CA	6.02	130.24	120.60
1	C	256	ARG	CD-NE-CZ	-6.02	115.97	124.40
1	C	369	ILE	O-C-N	-6.02	115.99	121.89
1	E	88	HIS	CE1-NE2-CD2	-6.02	102.98	109.00
1	A	88	HIS	CE1-NE2-CD2	-6.01	102.99	109.00
1	C	123	MET	N-CA-C	-6.01	103.38	112.04
1	E	238	LYS	N-CA-CB	6.01	121.06	111.56
1	B	179	ASP	N-CA-C	-6.01	98.94	108.73
1	B	8	LEU	N-CA-C	-6.00	101.10	110.17
1	A	340	TRP	CE2-CD2-CE3	6.00	124.80	118.80
1	C	356	TRP	CG-CD2-CE3	-6.00	127.90	133.90
1	D	235	SER	N-CA-C	-6.00	105.45	112.89
1	A	238	LYS	N-CA-CB	5.99	121.03	111.56
1	D	330	ILE	CA-C-N	5.99	129.79	122.42
1	D	330	ILE	C-N-CA	5.99	129.79	122.42
1	D	8	LEU	N-CA-CB	5.99	119.74	110.46
1	C	31	PHE	N-CA-CB	5.98	121.02	110.37
1	E	150	GLY	CA-C-O	5.98	127.01	120.97
1	A	150	GLY	CA-C-O	5.98	127.01	120.97
1	B	138	ALA	N-CA-C	5.98	117.47	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	146	GLY	N-CA-C	-5.98	107.15	114.92
1	E	50	LYS	N-CA-C	-5.96	100.08	108.96
1	B	260	THR	CA-CB-OG1	5.96	118.53	109.60
1	C	87	HIS	CG-CD2-NE2	5.96	113.16	107.20
1	A	185	LEU	CA-C-O	5.95	126.82	119.79
1	B	173	HIS	CE1-NE2-CD2	-5.95	103.05	109.00
1	D	166	TYR	CA-C-N	5.95	128.25	120.28
1	D	166	TYR	C-N-CA	5.95	128.25	120.28
1	E	10	CYS	N-CA-C	-5.95	98.16	108.69
1	E	185	LEU	CA-C-O	5.95	126.81	119.79
1	A	50	LYS	N-CA-C	-5.95	100.10	108.96
1	D	306	TYR	CA-C-O	-5.95	113.98	120.17
1	E	205	GLU	N-CA-C	-5.95	105.99	113.72
1	A	10	CYS	N-CA-C	-5.94	98.17	108.69
1	D	275	HIS	CE1-NE2-CD2	-5.94	103.06	109.00
1	A	205	GLU	N-CA-C	-5.94	106.00	113.72
1	D	78	ASN	N-CA-C	-5.94	97.92	108.13
1	C	221	LEU	CA-C-O	-5.94	114.20	120.55
1	A	361	GLU	N-CA-C	5.93	119.33	111.75
1	E	130	PRO	N-CD-CG	5.92	112.08	103.20
1	A	130	PRO	N-CD-CG	5.92	112.08	103.20
1	E	361	GLU	N-CA-C	5.92	119.33	111.75
1	B	81	ASP	CA-C-N	5.92	129.30	120.31
1	B	81	ASP	C-N-CA	5.92	129.30	120.31
1	B	180	LEU	N-CA-C	-5.92	98.20	110.80
1	E	127	PHE	CA-C-N	5.92	132.84	121.54
1	E	127	PHE	C-N-CA	5.92	132.84	121.54
1	B	127	PHE	CB-CG-CD1	-5.91	110.66	120.70
1	A	3	ASP	CA-C-N	5.91	131.80	122.94
1	A	3	ASP	C-N-CA	5.91	131.80	122.94
1	B	202	THR	N-CA-CB	5.91	120.47	110.49
1	A	127	PHE	CA-C-N	5.91	132.82	121.54
1	A	127	PHE	C-N-CA	5.91	132.82	121.54
1	B	138	ALA	CA-C-O	-5.91	114.62	120.82
1	B	56	ASP	O-C-N	-5.90	115.86	122.12
1	C	74	GLY	CA-C-O	5.90	127.19	119.69
1	B	219	VAL	CA-C-N	5.88	129.63	120.75
1	B	219	VAL	C-N-CA	5.88	129.63	120.75
1	C	5	THR	CA-C-N	5.88	132.78	121.54
1	C	5	THR	C-N-CA	5.88	132.78	121.54
1	E	3	ASP	CA-C-N	5.88	131.76	122.94
1	E	3	ASP	C-N-CA	5.88	131.76	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	HIS	CA-C-N	5.87	127.18	119.84
1	B	101	HIS	C-N-CA	5.87	127.18	119.84
1	C	94	LEU	N-CA-C	-5.87	106.28	113.50
1	C	275	HIS	CG-CD2-NE2	5.86	113.06	107.20
1	B	134	VAL	CA-C-O	5.85	128.09	120.78
1	D	101	HIS	ND1-CE1-NE2	5.85	114.25	108.40
1	C	52	SER	CA-C-N	5.85	129.01	120.71
1	C	52	SER	C-N-CA	5.85	129.01	120.71
1	C	317	ILE	O-C-N	5.84	127.98	121.90
1	A	108	ALA	N-CA-CB	5.84	119.53	110.01
1	E	108	ALA	N-CA-CB	5.84	119.53	110.01
1	D	331	ALA	O-C-N	-5.84	116.60	121.27
1	B	56	ASP	CA-C-O	5.84	126.93	120.63
1	B	349	LEU	N-CA-C	-5.83	100.38	109.72
1	B	257	CYS	CA-C-N	5.83	125.70	119.28
1	B	257	CYS	C-N-CA	5.83	125.70	119.28
1	E	109	PRO	N-CA-CB	5.82	108.37	103.25
1	A	109	PRO	N-CA-CB	5.82	108.37	103.25
1	A	38	PRO	N-CA-C	5.82	119.65	111.33
1	A	161	HIS	ND1-CE1-NE2	5.81	114.21	108.40
1	D	321	ALA	N-CA-CB	5.80	116.47	109.74
1	D	121	GLN	N-CA-C	5.80	117.60	111.28
1	A	233	SER	CB-CA-C	-5.79	97.66	109.65
1	B	356	TRP	CB-CG-CD2	-5.79	118.69	126.80
1	C	225	ASN	CA-CB-CG	-5.79	106.81	112.60
1	E	38	PRO	N-CA-C	5.79	119.61	111.33
1	E	161	HIS	ND1-CE1-NE2	5.79	114.19	108.40
1	B	200	PHE	N-CA-CB	5.79	120.32	110.71
1	E	233	SER	CB-CA-C	-5.78	97.68	109.65
1	D	5	THR	N-CA-C	5.78	118.32	111.33
1	B	297	ASN	N-CA-CB	5.77	119.03	110.49
1	A	247	VAL	N-CA-C	-5.77	100.16	108.53
1	E	247	VAL	N-CA-C	-5.77	100.17	108.53
1	B	239	SER	CA-C-N	5.76	131.88	123.12
1	B	239	SER	C-N-CA	5.76	131.88	123.12
1	B	315	LYS	N-CA-C	-5.75	106.81	113.88
1	C	64	ILE	N-CA-C	-5.75	107.52	113.10
1	A	332	PRO	CA-C-O	-5.75	112.23	120.56
1	E	202	THR	N-CA-C	5.75	123.04	110.80
1	A	193	LEU	N-CA-C	-5.74	106.23	113.18
1	A	202	THR	N-CA-C	5.74	123.03	110.80
1	A	209	VAL	O-C-N	5.74	127.44	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	124	PHE	N-CA-CB	5.74	118.62	110.13
1	C	257	CYS	CA-C-N	5.74	125.59	119.28
1	C	257	CYS	C-N-CA	5.74	125.59	119.28
1	E	193	LEU	N-CA-C	-5.74	106.24	113.18
1	A	243	PRO	N-CA-CB	-5.73	97.23	103.25
1	E	178	LEU	O-C-N	-5.73	116.70	123.41
1	A	290	ARG	NE-CZ-NH2	5.73	124.35	119.20
1	E	332	PRO	CA-C-O	-5.72	112.26	120.56
1	E	209	VAL	O-C-N	5.72	127.42	121.87
1	D	186	THR	CA-C-O	-5.71	114.50	120.55
1	D	37	ARG	CA-C-O	-5.71	113.45	119.50
1	E	243	PRO	N-CA-CB	-5.70	97.26	103.25
1	E	290	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	D	314	GLN	N-CA-C	-5.70	106.49	113.50
1	B	322	PRO	N-CD-CG	5.70	111.75	103.20
1	D	173	HIS	CA-C-O	5.70	128.66	120.51
1	D	271	SER	CA-C-O	-5.70	115.49	121.99
1	A	178	LEU	O-C-N	-5.70	116.74	123.41
1	D	199	SER	CA-C-O	-5.70	114.21	120.36
1	B	155	SER	N-CA-C	-5.69	95.19	107.49
1	C	69	TYR	CB-CA-C	5.69	117.76	110.13
1	B	107	GLU	N-CA-CB	5.69	119.48	110.55
1	B	226	GLU	N-CA-C	-5.69	106.34	113.28
1	A	326	LYS	CA-C-N	5.69	131.05	122.98
1	A	326	LYS	C-N-CA	5.69	131.05	122.98
1	E	326	LYS	CA-C-N	5.68	131.05	122.98
1	E	326	LYS	C-N-CA	5.68	131.05	122.98
1	D	136	ILE	CA-C-N	5.68	132.39	121.54
1	D	136	ILE	C-N-CA	5.68	132.39	121.54
1	C	34	ILE	CA-CB-CG2	-5.68	100.85	110.50
1	E	292	ASP	CA-CB-CG	5.66	118.26	112.60
1	C	25	ASP	CA-CB-CG	5.66	118.26	112.60
1	C	317	ILE	N-CA-CB	5.66	117.82	110.57
1	D	51	ASP	N-CA-C	-5.66	98.75	110.80
1	D	90	PHE	CA-C-N	5.66	128.32	120.29
1	D	90	PHE	C-N-CA	5.66	128.32	120.29
1	D	310	ALA	N-CA-C	5.66	117.53	111.36
1	C	77	THR	CA-C-O	-5.65	114.43	120.42
1	B	37	ARG	CA-C-N	5.64	126.89	119.84
1	B	37	ARG	C-N-CA	5.64	126.89	119.84
1	A	292	ASP	CA-CB-CG	5.64	118.24	112.60
1	B	252	ASN	CA-C-N	5.64	128.40	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	ASN	C-N-CA	5.64	128.40	120.28
1	C	203	THR	CA-C-N	5.64	128.40	120.28
1	C	203	THR	C-N-CA	5.64	128.40	120.28
1	B	290	ARG	CB-CA-C	-5.64	99.85	110.67
1	B	82	MET	CA-C-N	5.63	127.83	120.28
1	B	82	MET	C-N-CA	5.63	127.83	120.28
1	D	183	ARG	NE-CZ-NH1	-5.63	115.87	121.50
1	B	67	LEU	CB-CA-C	-5.63	101.62	110.79
1	B	287	ILE	CA-C-O	-5.62	114.55	120.57
1	D	98	PRO	N-CA-C	-5.62	105.19	114.75
1	E	283	MET	CG-SD-CE	-5.62	88.53	100.90
1	C	77	THR	O-C-N	5.62	128.56	122.15
1	C	87	HIS	CB-CG-ND1	5.62	131.13	122.70
1	D	280	ASN	O-C-N	5.62	127.94	122.09
1	A	283	MET	CG-SD-CE	-5.62	88.54	100.90
1	B	74	GLY	N-CA-C	-5.62	106.43	115.08
1	B	371	HIS	ND1-CE1-NE2	5.62	114.02	108.40
1	C	309	ILE	CA-CB-CG1	5.61	119.94	110.40
1	A	51	ASP	CA-C-N	5.61	130.91	123.00
1	A	51	ASP	C-N-CA	5.61	130.91	123.00
1	D	316	GLU	CB-CA-C	-5.61	101.31	110.85
1	A	115	ASN	CA-C-N	5.60	127.79	120.28
1	A	115	ASN	C-N-CA	5.60	127.79	120.28
1	B	228	ALA	CA-C-N	5.60	130.08	120.72
1	B	228	ALA	C-N-CA	5.60	130.08	120.72
1	E	51	ASP	CA-C-N	5.60	130.90	123.00
1	E	51	ASP	C-N-CA	5.60	130.90	123.00
1	A	138	ALA	CB-CA-C	-5.60	101.49	110.79
1	B	318	THR	CA-C-N	5.60	128.04	120.65
1	B	318	THR	C-N-CA	5.60	128.04	120.65
1	C	126	THR	N-CA-C	-5.60	106.99	113.88
1	E	138	ALA	CB-CA-C	-5.59	101.50	110.79
1	A	220	ALA	N-CA-CB	5.59	118.22	110.17
1	D	81	ASP	N-CA-CB	5.59	118.91	110.30
1	A	276	GLU	CA-C-N	5.59	128.33	120.28
1	A	276	GLU	C-N-CA	5.59	128.33	120.28
1	C	262	PHE	N-CA-C	-5.59	106.23	113.16
1	E	115	ASN	CA-C-N	5.59	127.77	120.28
1	E	115	ASN	C-N-CA	5.59	127.77	120.28
1	B	325	MET	N-CA-CB	5.58	120.87	110.99
1	E	220	ALA	N-CA-CB	5.58	118.20	110.17
1	B	168	GLY	N-CA-C	-5.58	104.16	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	159	VAL	CA-C-O	5.58	126.51	120.43
1	D	290	ARG	NE-CZ-NH1	5.58	127.08	121.50
1	A	289	ILE	O-C-N	-5.57	116.62	122.25
1	E	276	GLU	CA-C-N	5.57	128.30	120.28
1	E	276	GLU	C-N-CA	5.57	128.30	120.28
1	B	282	ILE	N-CA-C	-5.57	105.68	111.58
1	C	88	HIS	CE1-NE2-CD2	-5.57	103.44	109.00
1	E	80	ASP	CB-CA-C	-5.57	101.55	110.79
1	A	80	ASP	CB-CA-C	-5.56	101.56	110.79
1	C	115	ASN	CA-CB-CG	-5.56	107.04	112.60
1	E	239	SER	N-CA-C	-5.56	99.84	108.90
1	E	34	ILE	CB-CA-C	-5.55	102.37	110.81
1	E	351	THR	CA-CB-OG1	5.55	117.93	109.60
1	A	195	GLU	N-CA-C	-5.55	106.55	113.38
1	C	325	MET	CA-C-N	5.55	130.32	121.66
1	C	325	MET	C-N-CA	5.55	130.32	121.66
1	D	32	PRO	CA-C-O	-5.55	114.49	122.31
1	E	171	LEU	CA-C-O	-5.55	115.53	120.19
1	E	289	ILE	O-C-N	-5.54	116.65	122.25
1	A	351	THR	CA-CB-OG1	5.54	117.91	109.60
1	B	317	ILE	CA-C-O	5.54	127.20	121.05
1	C	104	LEU	N-CA-CB	5.54	119.25	110.55
1	A	34	ILE	CB-CA-C	-5.54	102.39	110.81
1	D	369	ILE	CA-CB-CG1	5.54	119.81	110.40
1	E	18	LYS	N-CA-CB	5.53	118.68	110.49
1	A	239	SER	N-CA-C	-5.53	99.89	108.90
1	E	183	ARG	CB-CG-CD	5.53	124.02	111.30
1	A	183	ARG	CB-CG-CD	5.53	124.02	111.30
1	B	175	ILE	CA-CB-CG1	5.53	119.80	110.40
1	C	275	HIS	ND1-CE1-NE2	5.53	113.93	108.40
1	D	78	ASN	OD1-CG-ND2	5.53	128.13	122.60
1	D	367	PRO	O-C-N	5.53	129.81	122.30
1	D	179	ASP	CA-C-O	-5.52	114.67	120.58
1	A	18	LYS	N-CA-CB	5.51	118.65	110.49
1	C	234	SER	CA-C-N	5.51	131.03	122.26
1	C	234	SER	C-N-CA	5.51	131.03	122.26
1	B	99	GLU	CA-C-O	5.51	126.34	119.12
1	E	195	GLU	N-CA-C	-5.51	106.61	113.38
1	E	219	VAL	CA-C-O	5.51	126.59	120.59
1	B	5	THR	CA-CB-OG1	5.51	117.86	109.60
1	C	120	THR	CA-C-N	5.50	127.66	120.28
1	C	120	THR	C-N-CA	5.50	127.66	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	PHE	CA-CB-CG	-5.49	108.31	113.80
1	C	138	ALA	CA-C-N	5.49	128.28	120.53
1	C	138	ALA	C-N-CA	5.49	128.28	120.53
1	E	303	THR	O-C-N	-5.49	115.25	122.39
1	A	219	VAL	CA-C-O	5.49	126.57	120.59
1	B	47	MET	N-CA-C	-5.48	100.18	108.52
1	A	96	VAL	N-CA-C	5.48	118.00	108.95
1	C	194	THR	O-C-N	5.48	130.34	122.28
1	C	341	ILE	CB-CA-C	-5.48	104.66	112.22
1	D	94	LEU	N-CA-C	-5.48	107.60	114.56
1	C	35	VAL	N-CA-C	-5.48	100.58	108.53
1	E	96	VAL	N-CA-C	5.48	117.99	108.95
1	C	129	VAL	CA-C-N	5.48	125.31	119.28
1	C	129	VAL	C-N-CA	5.48	125.31	119.28
1	B	152	VAL	CB-CA-C	-5.48	103.48	110.98
1	B	50	LYS	CA-C-N	5.47	128.07	120.63
1	B	50	LYS	C-N-CA	5.47	128.07	120.63
1	B	148	THR	CA-C-O	5.47	124.97	118.79
1	C	306	TYR	CB-CA-C	5.47	118.17	109.52
1	A	171	LEU	CA-C-O	-5.47	115.60	120.19
1	A	303	THR	O-C-N	-5.46	115.29	122.39
1	D	47	MET	N-CA-CB	5.46	119.72	110.49
1	C	45	VAL	N-CA-C	-5.46	97.99	109.34
1	C	295	ALA	CA-C-N	-5.46	115.67	123.20
1	C	295	ALA	C-N-CA	-5.46	115.67	123.20
1	D	88	HIS	CE1-NE2-CD2	-5.46	103.54	109.00
1	B	242	LEU	CA-C-N	5.45	126.31	119.98
1	B	242	LEU	C-N-CA	5.45	126.31	119.98
1	C	290	ARG	CA-C-N	5.45	127.58	120.28
1	C	290	ARG	C-N-CA	5.45	127.58	120.28
1	A	108	ALA	CA-C-O	-5.45	114.91	119.76
1	E	108	ALA	CA-C-O	-5.45	114.91	119.76
1	B	37	ARG	O-C-N	-5.44	116.51	122.06
1	C	115	ASN	CA-C-N	5.44	127.57	120.28
1	C	115	ASN	C-N-CA	5.44	127.57	120.28
1	D	340	TRP	CG-CD2-CE3	-5.44	128.46	133.90
1	B	212	ILE	N-CA-C	-5.44	105.07	110.62
1	C	290	ARG	CB-CA-C	-5.44	99.29	110.38
1	C	61	LYS	N-CA-C	-5.44	101.42	110.17
1	B	370	VAL	N-CA-C	-5.43	105.03	110.30
1	E	71	ILE	CA-C-O	-5.43	114.99	120.31
1	A	71	ILE	CA-C-O	-5.43	114.99	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	253	GLU	N-CA-C	5.43	117.95	111.71
1	B	279	TYR	CB-CA-C	-5.43	102.33	110.90
1	D	118	LYS	N-CA-C	-5.43	105.26	111.07
1	D	331	ALA	CA-C-N	5.42	125.97	120.38
1	D	331	ALA	C-N-CA	5.42	125.97	120.38
1	B	246	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	C	109	PRO	O-C-N	5.42	129.87	122.99
1	E	176	MET	CA-C-N	5.42	131.50	122.73
1	E	176	MET	C-N-CA	5.42	131.50	122.73
1	A	253	GLU	N-CA-C	5.41	117.94	111.71
1	C	4	GLU	N-CA-C	-5.41	100.08	108.42
1	E	103	THR	CB-CA-C	-5.41	102.35	110.24
1	C	199	SER	CB-CA-C	-5.40	100.20	109.65
1	D	76	ILE	N-CA-C	-5.40	99.83	107.98
1	C	115	ASN	CB-CA-C	-5.40	101.67	110.85
1	A	314	GLN	OE1-CD-NE2	5.40	128.00	122.60
1	A	54	VAL	CA-C-N	5.39	128.79	120.00
1	A	54	VAL	C-N-CA	5.39	128.79	120.00
1	B	292	ASP	N-CA-C	-5.39	106.75	113.38
1	A	176	MET	CA-C-N	5.39	131.46	122.73
1	A	176	MET	C-N-CA	5.39	131.46	122.73
1	A	164	PRO	CB-CA-C	-5.39	104.81	111.11
1	E	54	VAL	CA-C-N	5.39	128.78	120.00
1	E	54	VAL	C-N-CA	5.39	128.78	120.00
1	E	212	ILE	O-C-N	-5.39	116.65	121.87
1	E	240	TYR	N-CA-C	-5.39	96.53	107.41
1	E	164	PRO	CB-CA-C	-5.38	104.81	111.11
1	A	103	THR	CB-CA-C	-5.38	102.38	110.24
1	C	314	GLN	N-CA-C	-5.38	106.88	113.50
1	C	102	PRO	CB-CA-C	-5.38	102.69	111.56
1	B	127	PHE	CB-CG-CD2	5.38	129.84	120.70
1	A	212	ILE	O-C-N	-5.37	116.66	121.87
1	A	240	TYR	N-CA-C	-5.37	96.56	107.41
1	C	346	LEU	CA-C-O	5.37	126.15	119.97
1	D	271	SER	O-C-N	5.37	129.20	122.65
1	E	314	GLN	OE1-CD-NE2	5.37	127.97	122.60
1	B	98	PRO	N-CA-C	-5.37	106.72	114.18
1	C	157	ASP	N-CA-C	-5.37	108.50	114.62
1	B	185	LEU	CB-CA-C	-5.37	100.37	110.67
1	D	223	PHE	CA-CB-CG	5.37	119.17	113.80
1	B	184	ASP	CA-C-N	5.36	128.46	120.31
1	B	184	ASP	C-N-CA	5.36	128.46	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	214	GLU	N-CA-C	5.36	117.12	111.28
1	D	185	LEU	O-C-N	-5.36	115.68	122.27
1	C	332	PRO	CA-C-N	5.36	124.81	119.24
1	C	332	PRO	C-N-CA	5.36	124.81	119.24
1	D	296	ASN	OD1-CG-ND2	5.36	127.96	122.60
1	B	209	VAL	N-CA-CB	5.35	117.82	110.54
1	C	279	TYR	CB-CA-C	-5.35	102.44	110.90
1	B	270	GLU	O-C-N	5.35	128.85	122.27
1	D	334	GLU	N-CA-C	-5.35	99.22	108.69
1	B	269	MET	CA-C-N	5.35	128.44	120.31
1	B	269	MET	C-N-CA	5.35	128.44	120.31
1	B	131	ALA	CB-CA-C	-5.34	101.33	110.95
1	C	49	GLN	CG-CD-NE2	-5.34	108.38	116.40
1	C	78	ASN	CA-CB-CG	5.34	117.94	112.60
1	A	173	HIS	CG-CD2-NE2	5.34	112.54	107.20
1	A	340	TRP	CG-CD2-CE3	-5.34	128.56	133.90
1	E	356	TRP	CA-CB-CG	5.34	123.74	113.60
1	A	356	TRP	CA-CB-CG	5.34	123.74	113.60
1	C	358	THR	CA-C-N	5.34	128.21	120.79
1	C	358	THR	C-N-CA	5.34	128.21	120.79
1	C	279	TYR	N-CA-C	-5.33	105.38	111.14
1	D	254	ARG	CB-CA-C	-5.33	100.77	110.63
1	C	241	GLU	O-C-N	5.33	129.67	122.59
1	C	243	PRO	CA-C-N	5.32	131.71	121.54
1	C	243	PRO	C-N-CA	5.32	131.71	121.54
1	C	323	SER	CB-CA-C	-5.32	101.48	110.64
1	D	161	HIS	ND1-CE1-NE2	5.32	113.72	108.40
1	C	296	ASN	CB-CA-C	-5.32	103.83	111.70
1	E	340	TRP	CG-CD2-CE3	-5.32	128.58	133.90
1	E	350	SER	CA-C-O	5.32	124.90	119.05
1	A	350	SER	CA-C-O	5.32	124.90	119.05
1	B	163	VAL	CA-C-O	-5.32	112.82	119.95
1	D	163	VAL	CA-CB-CG2	-5.32	101.36	110.40
1	D	191	LYS	N-CA-C	-5.32	105.40	111.14
1	C	43	VAL	CA-CB-CG2	5.31	119.43	110.40
1	C	134	VAL	CB-CA-C	5.31	120.00	111.29
1	A	65	LEU	N-CA-CB	-5.31	102.31	111.55
1	D	4	GLU	N-CA-CB	-5.31	102.79	111.66
1	D	118	LYS	CB-CA-C	5.31	119.22	110.88
1	C	358	THR	N-CA-C	-5.31	103.39	110.55
1	D	71	ILE	CA-C-O	-5.30	115.11	120.31
1	E	173	HIS	CG-CD2-NE2	5.30	112.50	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	LYS	CA-C-N	5.30	128.97	121.66
1	B	328	LYS	C-N-CA	5.30	128.97	121.66
1	C	201	VAL	CA-C-N	5.30	131.66	121.54
1	C	201	VAL	C-N-CA	5.30	131.66	121.54
1	E	65	LEU	N-CA-CB	-5.29	102.34	111.55
1	D	255	PHE	N-CA-C	-5.29	105.14	113.02
1	B	126	THR	CA-CB-OG1	5.29	117.53	109.60
1	D	286	ASP	N-CA-C	5.29	117.54	110.35
1	C	224	GLU	N-CA-C	5.28	117.04	111.28
1	B	240	TYR	O-C-N	-5.28	117.04	122.64
1	B	178	LEU	CA-C-N	5.28	129.79	122.77
1	B	178	LEU	C-N-CA	5.28	129.79	122.77
1	E	124	PHE	CA-C-O	5.28	126.20	120.55
1	A	223	PHE	CA-C-N	5.28	127.88	120.28
1	A	223	PHE	C-N-CA	5.28	127.88	120.28
1	D	154	ASP	CA-CB-CG	5.28	117.88	112.60
1	B	331	ALA	CB-CA-C	-5.27	102.30	109.42
1	C	164	PRO	CB-CA-C	-5.27	105.08	111.46
1	A	350	SER	N-CA-C	-5.27	106.87	113.72
1	C	374	CYS	O-C-N	-5.27	116.39	122.87
1	D	292	ASP	CA-CB-CG	5.27	117.87	112.60
1	D	22	ALA	N-CA-CB	5.27	118.02	110.06
1	B	173	HIS	ND1-CE1-NE2	5.27	113.67	108.40
1	C	199	SER	N-CA-CB	5.27	119.66	110.81
1	A	227	MET	N-CA-C	-5.26	105.62	111.36
1	A	124	PHE	CA-C-O	5.26	126.18	120.55
1	A	87	HIS	CA-CB-CG	5.26	119.06	113.80
1	E	227	MET	N-CA-C	-5.26	105.63	111.36
1	E	270	GLU	N-CA-C	-5.25	106.26	113.30
1	D	214	GLU	CA-C-O	5.25	125.99	120.42
1	E	203	THR	CB-CA-C	-5.25	102.60	110.90
1	E	223	PHE	CA-C-N	5.25	127.84	120.28
1	E	223	PHE	C-N-CA	5.25	127.84	120.28
1	C	349	LEU	O-C-N	-5.24	116.55	123.16
1	D	169	TYR	CB-CG-CD1	5.24	128.66	120.80
1	E	271	SER	CA-C-O	-5.24	115.99	121.55
1	E	350	SER	N-CA-C	-5.24	106.90	113.72
1	B	136	ILE	CA-C-N	5.24	131.55	121.54
1	B	136	ILE	C-N-CA	5.24	131.55	121.54
1	E	87	HIS	CA-CB-CG	5.24	119.04	113.80
1	D	290	ARG	NE-CZ-NH2	-5.24	114.49	119.20
1	D	208	ILE	CA-C-N	5.24	127.64	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	208	ILE	C-N-CA	5.24	127.64	120.46
1	D	356	TRP	CA-CB-CG	5.24	123.55	113.60
1	B	232	SER	CA-C-N	5.23	128.14	120.71
1	B	232	SER	C-N-CA	5.23	128.14	120.71
1	D	138	ALA	N-CA-C	-5.23	105.66	111.36
1	D	173	HIS	ND1-CE1-NE2	5.23	113.63	108.40
1	E	186	THR	N-CA-C	-5.23	105.66	111.36
1	A	186	THR	N-CA-C	-5.23	105.66	111.36
1	A	216	LEU	CB-CA-C	-5.22	102.33	109.28
1	A	203	THR	CB-CA-C	-5.22	102.65	110.90
1	D	309	ILE	N-CA-CB	5.22	116.66	110.55
1	A	270	GLU	N-CA-C	-5.21	106.31	113.30
1	E	94	LEU	N-CA-C	-5.21	106.07	112.90
1	A	94	LEU	N-CA-C	-5.21	106.07	112.90
1	E	286	ASP	O-C-N	-5.21	116.15	122.82
1	D	214	GLU	N-CA-CB	5.21	117.87	110.16
1	E	216	LEU	CB-CA-C	-5.21	102.35	109.28
1	C	181	ALA	CA-C-N	5.21	125.87	119.99
1	C	181	ALA	C-N-CA	5.21	125.87	119.99
1	D	256	ARG	N-CA-C	-5.20	105.22	112.45
1	C	361	GLU	CB-CA-C	-5.20	100.37	110.46
1	B	173	HIS	CA-CB-CG	5.20	119.00	113.80
1	C	292	ASP	CA-C-O	5.20	125.08	119.15
1	D	206	ARG	CA-C-N	5.20	127.67	120.29
1	D	206	ARG	C-N-CA	5.20	127.67	120.29
1	B	112	PRO	O-C-N	5.20	128.92	123.10
1	D	192	ILE	N-CA-C	-5.20	105.27	112.50
1	A	271	SER	CA-C-O	-5.20	116.04	121.55
1	D	120	THR	O-C-N	5.20	127.63	122.12
1	B	281	SER	N-CA-C	-5.19	105.80	111.82
1	A	147	ARG	N-CA-CB	5.19	117.78	110.36
1	D	75	ILE	CA-C-O	-5.19	114.94	120.39
1	D	134	VAL	CG1-CB-CG2	5.19	122.22	110.80
1	B	286	ASP	CA-C-N	5.18	128.66	120.47
1	B	286	ASP	C-N-CA	5.18	128.66	120.47
1	E	147	ARG	N-CA-CB	5.18	117.77	110.36
1	D	239	SER	CA-C-N	5.18	130.44	122.77
1	D	239	SER	C-N-CA	5.18	130.44	122.77
1	B	112	PRO	CA-C-O	-5.18	115.13	121.03
1	A	286	ASP	O-C-N	-5.18	116.19	122.82
1	C	159	VAL	CA-C-N	5.17	130.36	122.65
1	C	159	VAL	C-N-CA	5.17	130.36	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	275	HIS	N-CA-C	-5.17	106.97	113.28
1	A	275	HIS	N-CA-C	-5.17	106.97	113.28
1	E	36	GLY	CA-C-O	-5.17	113.83	121.58
1	A	95	ARG	CA-C-N	5.17	130.84	122.68
1	A	95	ARG	C-N-CA	5.17	130.84	122.68
1	C	81	ASP	CA-C-N	5.17	128.16	120.31
1	C	81	ASP	C-N-CA	5.17	128.16	120.31
1	B	169	TYR	CB-CG-CD2	-5.16	113.06	120.80
1	E	337	TYR	CA-C-N	5.16	127.71	120.28
1	E	337	TYR	C-N-CA	5.16	127.71	120.28
1	C	185	LEU	CA-C-O	5.16	125.90	119.97
1	E	95	ARG	CA-C-N	5.16	130.83	122.68
1	E	95	ARG	C-N-CA	5.16	130.83	122.68
1	B	56	ASP	CA-C-N	5.16	127.70	120.28
1	B	56	ASP	C-N-CA	5.16	127.70	120.28
1	B	148	THR	N-CA-C	-5.15	106.10	114.09
1	B	270	GLU	CA-C-N	5.15	131.38	121.54
1	B	270	GLU	C-N-CA	5.15	131.38	121.54
1	C	107	GLU	CB-CA-C	5.15	119.18	110.79
1	B	169	TYR	CG-CD2-CE2	-5.14	113.49	121.20
1	C	143	TYR	CA-C-N	5.14	127.17	120.28
1	C	143	TYR	C-N-CA	5.14	127.17	120.28
1	A	337	TYR	CA-C-N	5.14	127.68	120.28
1	A	337	TYR	C-N-CA	5.14	127.68	120.28
1	B	31	PHE	O-C-N	-5.14	117.82	121.83
1	D	169	TYR	N-CA-CB	5.14	118.14	109.92
1	C	211	ASP	CA-CB-CG	5.14	117.74	112.60
1	C	212	ILE	O-C-N	-5.14	116.68	121.87
1	A	18	LYS	CB-CA-C	-5.13	103.06	111.68
1	A	130	PRO	N-CA-CB	5.13	108.96	103.52
1	B	319	ALA	N-CA-CB	5.13	117.40	109.91
1	C	217	CYS	N-CA-CB	5.13	117.61	109.51
1	C	233	SER	CB-CA-C	-5.12	102.25	110.14
1	E	233	SER	CA-C-O	-5.12	116.24	121.87
1	A	36	GLY	CA-C-O	-5.12	113.90	121.58
1	D	14	SER	O-C-N	-5.12	115.82	122.37
1	D	166	TYR	CA-C-O	-5.12	115.64	121.58
1	E	62	ARG	NE-CZ-NH2	-5.12	114.59	119.20
1	D	27	PRO	CA-C-N	5.12	127.09	120.44
1	D	27	PRO	C-N-CA	5.12	127.09	120.44
1	D	173	HIS	O-C-N	-5.12	115.79	122.59
1	E	18	LYS	CB-CA-C	-5.12	103.08	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	ILE	CA-C-O	-5.11	115.02	120.39
1	D	332	PRO	CA-C-N	5.11	124.78	119.56
1	D	332	PRO	C-N-CA	5.11	124.78	119.56
1	A	233	SER	CA-C-O	-5.11	116.25	121.87
1	B	19	ALA	CA-C-N	5.11	129.14	120.86
1	B	19	ALA	C-N-CA	5.11	129.14	120.86
1	C	98	PRO	N-CA-C	-5.11	107.54	114.80
1	D	323	SER	N-CA-C	-5.11	106.36	112.59
1	C	165	ILE	CA-C-O	5.11	126.65	120.67
1	C	334	GLU	CA-C-O	-5.11	115.14	121.06
1	A	201	VAL	CA-C-N	5.10	131.28	121.54
1	A	201	VAL	C-N-CA	5.10	131.28	121.54
1	A	270	GLU	CB-CG-CD	5.10	121.27	112.60
1	D	222	ASP	CA-C-O	5.10	126.42	120.20
1	E	286	ASP	CA-C-N	5.10	127.44	120.46
1	E	286	ASP	C-N-CA	5.10	127.44	120.46
1	C	50	LYS	N-CA-C	-5.10	101.16	108.60
1	D	279	TYR	CB-CG-CD2	-5.09	113.17	120.80
1	E	270	GLU	CB-CG-CD	5.09	121.25	112.60
1	E	201	VAL	CA-C-N	5.09	131.25	121.54
1	E	201	VAL	C-N-CA	5.09	131.25	121.54
1	A	38	PRO	CA-C-O	-5.08	114.99	122.31
1	A	286	ASP	CA-C-N	5.08	127.42	120.46
1	A	286	ASP	C-N-CA	5.08	127.42	120.46
1	A	291	LYS	CA-C-O	-5.08	114.36	120.10
1	A	371	HIS	ND1-CE1-NE2	5.08	113.48	108.40
1	C	310	ALA	N-CA-CB	5.08	117.65	110.13
1	D	375	PHE	CA-CB-CG	-5.08	108.72	113.80
1	E	38	PRO	CA-C-O	-5.08	114.99	122.31
1	E	311	ASP	N-CA-CB	5.08	118.82	110.39
1	B	232	SER	CA-C-O	5.08	125.81	120.33
1	E	13	GLY	CA-C-O	-5.08	117.20	122.28
1	E	130	PRO	N-CA-CB	5.08	108.90	103.52
1	D	108	ALA	CA-C-N	5.08	126.19	119.84
1	D	108	ALA	C-N-CA	5.08	126.19	119.84
1	C	132	MET	CA-C-O	-5.07	115.52	121.10
1	D	165	ILE	CA-C-O	5.07	126.61	120.67
1	D	115	ASN	O-C-N	5.07	127.49	122.12
1	E	291	LYS	CA-C-O	-5.07	114.37	120.10
1	D	105	LEU	CA-C-O	-5.07	115.29	121.78
1	A	80	ASP	CA-C-N	5.07	129.29	120.68
1	A	80	ASP	C-N-CA	5.07	129.29	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ARG	NE-CZ-NH2	-5.07	114.64	119.20
1	E	80	ASP	CA-C-N	5.07	129.29	120.68
1	E	80	ASP	C-N-CA	5.07	129.29	120.68
1	A	311	ASP	N-CA-CB	5.06	118.80	110.39
1	C	365	ALA	CA-C-O	5.06	124.73	119.97
1	B	73	HIS	ND1-CE1-NE2	5.06	113.46	108.40
1	B	342	GLY	CA-C-N	5.06	129.64	120.79
1	B	342	GLY	C-N-CA	5.06	129.64	120.79
1	E	371	HIS	ND1-CE1-NE2	5.06	113.46	108.40
1	A	13	GLY	CA-C-O	-5.05	117.22	122.28
1	A	196	ARG	N-CA-C	-5.05	100.03	110.80
1	D	328	LYS	N-CA-C	-5.05	99.87	108.26
1	D	371	HIS	CE1-NE2-CD2	-5.05	103.95	109.00
1	C	340	TRP	CB-CG-CD2	-5.05	119.73	126.80
1	D	250	ILE	CA-C-N	5.05	131.31	121.41
1	D	250	ILE	C-N-CA	5.05	131.31	121.41
1	E	196	ARG	N-CA-C	-5.05	100.04	110.80
1	D	336	LYS	CA-C-N	5.05	130.85	122.73
1	D	336	LYS	C-N-CA	5.05	130.85	122.73
1	D	123	MET	CG-SD-CE	-5.04	89.81	100.90
1	C	209	VAL	CA-C-N	5.04	127.97	120.31
1	C	209	VAL	C-N-CA	5.04	127.97	120.31
1	D	205	GLU	N-CA-CB	5.04	118.22	110.61
1	D	238	LYS	N-CA-C	-5.04	100.07	110.80
1	E	326	LYS	CB-CG-CD	5.04	122.88	111.30
1	D	205	GLU	O-C-N	5.03	128.33	122.24
1	A	326	LYS	CB-CG-CD	5.03	122.87	111.30
1	B	211	ASP	CA-C-N	5.03	127.35	120.46
1	B	211	ASP	C-N-CA	5.03	127.35	120.46
1	B	321	ALA	N-CA-C	-5.03	102.41	110.10
1	E	351	THR	O-C-N	-5.03	116.09	122.27
1	D	3	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	240	TYR	O-C-N	-5.02	116.81	122.84
1	B	127	PHE	N-CA-CB	5.02	118.98	110.49
1	B	132	MET	CG-SD-CE	-5.02	89.85	100.90
1	B	190	MET	O-C-N	5.02	128.10	122.22
1	D	203	THR	CA-CB-CG2	-5.02	101.96	110.50
1	E	297	ASN	CB-CA-C	-5.02	102.76	111.30
1	C	211	ASP	N-CA-CB	5.02	117.59	110.16
1	C	96	VAL	CA-CB-CG1	5.02	118.93	110.40
1	A	297	ASN	CB-CA-C	-5.02	102.77	111.30
1	D	230	ALA	N-CA-CB	5.01	118.06	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	49	GLN	O-C-N	-5.01	113.96	122.03
1	E	240	TYR	O-C-N	-5.01	116.82	122.84
1	C	94	LEU	CA-C-O	5.01	124.65	119.14
1	C	198	TYR	CB-CA-C	-5.00	101.36	111.17

There are no chirality outliers.

All (61) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	PHE	Sidechain
1	A	218	TYR	Sidechain
1	A	223	PHE	Sidechain
1	A	240	TYR	Sidechain
1	A	279	TYR	Sidechain
1	A	28	ARG	Sidechain
1	A	294	TYR	Sidechain
1	A	306	TYR	Sidechain
1	A	335	ARG	Sidechain
1	A	337	TYR	Sidechain
1	A	362	TYR	Sidechain
1	A	69	TYR	Sidechain
1	A	88	HIS	Sidechain
1	A	91	TYR	Sidechain
1	A	95	ARG	Sidechain
1	B	133	TYR	Sidechain
1	B	143	TYR	Sidechain
1	B	169	TYR	Sidechain
1	B	206	ARG	Sidechain
1	B	240	TYR	Sidechain
1	B	279	TYR	Sidechain
1	B	294	TYR	Sidechain
1	B	306	TYR	Sidechain
1	B	53	TYR	Sidechain
1	B	90	PHE	Sidechain
1	B	95	ARG	Sidechain
1	C	169	TYR	Sidechain
1	C	188	TYR	Sidechain
1	C	218	TYR	Sidechain
1	C	240	TYR	Sidechain
1	C	266	PHE	Sidechain
1	C	279	TYR	Sidechain
1	C	290	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	294	TYR	Sidechain
1	C	306	TYR	Sidechain
1	C	335	ARG	Sidechain
1	C	69	TYR	Sidechain
1	C	95	ARG	Sidechain
1	D	133	TYR	Sidechain
1	D	198	TYR	Sidechain
1	D	256	ARG	Sidechain
1	D	279	TYR	Sidechain
1	D	294	TYR	Sidechain
1	D	362	TYR	Sidechain
1	D	372	ARG	Sidechain
1	D	69	TYR	Sidechain
1	E	124	PHE	Sidechain
1	E	218	TYR	Sidechain
1	E	223	PHE	Sidechain
1	E	240	TYR	Sidechain
1	E	279	TYR	Sidechain
1	E	28	ARG	Sidechain
1	E	294	TYR	Sidechain
1	E	306	TYR	Sidechain
1	E	335	ARG	Sidechain
1	E	337	TYR	Sidechain
1	E	362	TYR	Sidechain
1	E	69	TYR	Sidechain
1	E	88	HIS	Sidechain
1	E	91	TYR	Sidechain
1	E	95	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2933	0	2894	18	0
1	B	2933	0	2894	27	0
1	C	2933	0	2894	16	0
1	D	2933	0	2893	192	0
1	E	2933	0	2893	199	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	680	0	138	0	0
2	G	680	0	138	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	2	0
3	E	27	0	12	0	0
All	All	16160	0	14804	266	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 9.

All (266) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:HIS:CD2	1:E:166:TYR:CD1	1.88	1.62
1:D:43:VAL:CG1	1:E:139:VAL:HG22	1.35	1.54
1:D:40:HIS:CD2	1:E:166:TYR:HD1	1.17	1.53
1:D:64:ILE:HD11	1:E:289:ILE:CG2	1.38	1.51
1:D:243:PRO:C	1:E:324:THR:HG21	1.36	1.50
1:D:64:ILE:CD1	1:E:289:ILE:HG21	1.43	1.43
1:D:243:PRO:CA	1:E:324:THR:CG2	2.00	1.39
1:D:64:ILE:CD1	1:E:289:ILE:CG2	1.97	1.39
1:B:195:GLU:HG2	1:E:110:LEU:CB	1.57	1.33
1:D:243:PRO:HA	1:E:324:THR:CG2	1.59	1.31
1:D:243:PRO:C	1:E:324:THR:CG2	2.04	1.30
1:D:40:HIS:CG	1:E:166:TYR:HB2	1.66	1.30
1:D:40:HIS:HD2	1:E:166:TYR:CD1	1.35	1.28
1:D:39:ARG:HH21	1:E:286:ASP:CG	1.41	1.27
1:D:244:ASP:N	1:E:324:THR:HG21	1.50	1.25
1:D:243:PRO:CA	1:E:324:THR:HG21	1.58	1.25
1:D:44:MET:O	1:E:169:TYR:CD1	1.91	1.24
1:D:64:ILE:HG21	1:E:166:TYR:CE1	1.71	1.23
1:D:40:HIS:CG	1:E:166:TYR:CD1	2.26	1.23
1:D:64:ILE:CG2	1:E:166:TYR:HE1	1.52	1.20
1:D:63:GLY:N	1:E:288:ASP:HB3	1.57	1.19
1:D:63:GLY:HA2	1:E:286:ASP:OD2	1.39	1.18
1:B:195:GLU:CG	1:E:110:LEU:HB3	1.73	1.18
1:D:44:MET:H	1:E:169:TYR:HA	1.05	1.17
1:D:64:ILE:CG2	1:E:166:TYR:CE1	2.28	1.16
1:D:243:PRO:O	1:E:324:THR:CB	1.94	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:HIS:HB2	1:E:166:TYR:CD1	1.83	1.12
1:D:40:HIS:CB	1:E:166:TYR:CD1	2.32	1.12
1:D:43:VAL:CG1	1:E:139:VAL:CG2	2.27	1.11
1:D:43:VAL:HG11	1:E:139:VAL:CG2	1.80	1.11
1:D:63:GLY:HA2	1:E:286:ASP:CG	1.75	1.11
1:D:64:ILE:HD13	1:E:289:ILE:HG21	1.13	1.10
1:D:43:VAL:HG13	1:E:139:VAL:HG22	1.29	1.10
1:D:244:ASP:HB3	1:E:290:ARG:NH1	1.67	1.10
1:D:40:HIS:CD2	1:E:166:TYR:CG	2.40	1.08
1:D:40:HIS:CG	1:E:166:TYR:CB	2.36	1.07
1:D:64:ILE:HD13	1:E:289:ILE:HD13	1.30	1.06
1:D:243:PRO:HB2	1:E:324:THR:HB	1.37	1.06
1:D:243:PRO:O	1:E:324:THR:HB	1.54	1.06
1:D:243:PRO:C	1:E:324:THR:CB	2.29	1.06
1:D:64:ILE:HG12	1:E:289:ILE:HG12	1.10	1.05
1:D:41:GLN:HB3	1:E:171:LEU:O	1.54	1.05
1:D:243:PRO:CA	1:E:324:THR:HG22	1.82	1.04
1:D:40:HIS:CG	1:E:166:TYR:HD1	1.64	1.03
1:D:63:GLY:CA	1:E:286:ASP:OD2	1.98	1.03
1:D:39:ARG:NH2	1:E:286:ASP:CG	2.16	1.02
1:D:46:GLY:N	1:E:167:GLU:O	1.89	1.02
1:D:47:MET:C	1:E:167:GLU:CG	2.29	1.01
1:D:64:ILE:HD11	1:E:289:ILE:HG23	1.04	1.01
1:D:243:PRO:HA	1:E:324:THR:HG22	1.35	1.00
1:D:62:ARG:HB2	1:E:288:ASP:HB2	1.42	1.00
1:B:195:GLU:OE1	1:E:111:ASN:C	2.06	0.99
1:D:43:VAL:HB	1:E:165:ILE:HB	1.45	0.99
1:D:64:ILE:HG21	1:E:166:TYR:HE1	0.82	0.98
1:D:64:ILE:HG12	1:E:289:ILE:CG1	1.90	0.98
1:D:43:VAL:HG11	1:E:139:VAL:HG22	0.98	0.97
1:D:63:GLY:H	1:E:288:ASP:HB3	1.23	0.97
1:D:44:MET:N	1:E:169:TYR:HA	1.67	0.96
1:D:40:HIS:CG	1:E:166:TYR:CG	2.53	0.95
1:B:195:GLU:HG2	1:E:110:LEU:HB3	0.96	0.95
1:D:44:MET:HA	1:E:166:TYR:O	1.67	0.95
1:D:47:MET:O	1:E:167:GLU:OE2	1.85	0.95
1:D:62:ARG:HB2	1:E:288:ASP:CB	1.97	0.95
1:D:63:GLY:C	1:E:286:ASP:HB3	1.92	0.95
1:D:64:ILE:CG1	1:E:289:ILE:HG12	1.98	0.93
1:D:47:MET:C	1:E:167:GLU:HG3	1.93	0.93
1:D:243:PRO:O	1:E:324:THR:OG1	1.85	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:GLY:O	1:E:286:ASP:HB3	1.67	0.93
1:D:40:HIS:CD2	1:E:166:TYR:CB	2.54	0.90
1:D:243:PRO:CB	1:E:324:THR:HG22	2.02	0.90
1:D:43:VAL:HG12	1:E:165:ILE:HG12	1.53	0.89
1:D:63:GLY:HA3	1:E:289:ILE:N	1.86	0.89
1:D:43:VAL:HG13	1:E:139:VAL:CG2	1.97	0.88
1:D:39:ARG:NH2	1:E:286:ASP:OD1	2.08	0.87
1:D:64:ILE:HD13	1:E:289:ILE:CD1	2.04	0.87
1:D:47:MET:O	1:E:167:GLU:CG	2.23	0.86
1:D:39:ARG:CZ	1:E:286:ASP:HB2	2.05	0.85
1:D:243:PRO:CB	1:E:324:THR:CG2	2.54	0.85
1:D:243:PRO:HA	1:E:324:THR:HG21	1.26	0.85
1:D:41:GLN:O	1:E:170:ALA:CB	2.24	0.85
1:D:40:HIS:ND1	1:E:166:TYR:HB2	1.93	0.84
1:D:63:GLY:HA2	1:E:286:ASP:CB	2.08	0.84
1:D:47:MET:O	1:E:167:GLU:CD	2.21	0.83
1:D:243:PRO:HB2	1:E:324:THR:CB	2.09	0.82
1:D:39:ARG:NE	1:E:286:ASP:HB2	1.95	0.81
1:D:64:ILE:CD1	1:E:289:ILE:HG23	1.86	0.79
1:D:244:ASP:HB3	1:E:290:ARG:HH12	1.46	0.78
1:D:44:MET:H	1:E:169:TYR:CA	1.91	0.78
1:D:64:ILE:CG1	1:E:289:ILE:CG1	2.59	0.77
1:B:195:GLU:OE1	1:E:111:ASN:O	2.03	0.77
1:D:40:HIS:CB	1:E:166:TYR:CG	2.66	0.77
1:D:40:HIS:NE2	1:E:149:THR:HG23	2.00	0.77
1:D:46:GLY:HA3	1:E:148:THR:HB	1.66	0.76
1:D:44:MET:O	1:E:169:TYR:HD1	1.69	0.75
1:D:48:GLY:N	1:E:167:GLU:HG3	2.02	0.75
1:D:41:GLN:HA	1:E:171:LEU:H	1.52	0.75
1:D:64:ILE:CD1	1:E:289:ILE:HD13	1.98	0.74
1:D:243:PRO:CB	1:E:324:THR:HB	2.16	0.74
1:D:39:ARG:NH2	1:E:286:ASP:CB	2.51	0.73
1:D:63:GLY:HA3	1:E:288:ASP:C	2.12	0.73
1:D:43:VAL:HG12	1:E:165:ILE:CG1	2.18	0.73
1:D:40:HIS:NE2	1:E:166:TYR:HA	2.03	0.73
1:D:45:VAL:CG2	1:E:139:VAL:HG13	2.18	0.73
1:D:63:GLY:CA	1:E:286:ASP:HB3	2.18	0.73
1:D:244:ASP:HB3	1:E:290:ARG:HH11	1.55	0.72
1:D:39:ARG:NH2	1:E:286:ASP:HB2	2.06	0.71
1:D:53:TYR:OH	1:E:166:TYR:OH	2.05	0.71
1:D:43:VAL:CG1	1:E:165:ILE:HD13	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:GLY:N	1:E:288:ASP:CB	2.47	0.71
1:D:46:GLY:CA	1:E:167:GLU:HA	2.22	0.70
1:D:44:MET:O	1:E:169:TYR:CG	2.44	0.69
1:D:64:ILE:HG23	1:E:166:TYR:CE1	2.23	0.69
1:B:195:GLU:HG2	1:E:110:LEU:HB2	1.71	0.68
1:D:45:VAL:HG21	1:E:139:VAL:HG13	1.76	0.68
1:D:64:ILE:HD13	1:E:289:ILE:CG2	1.89	0.68
1:D:47:MET:O	1:E:167:GLU:HG3	1.92	0.67
1:D:243:PRO:CB	1:E:324:THR:CB	2.72	0.65
1:B:195:GLU:HG2	1:E:110:LEU:CA	2.24	0.65
1:D:40:HIS:CD2	1:E:166:TYR:HA	2.30	0.65
1:D:244:ASP:N	1:E:324:THR:CG2	2.39	0.65
1:D:40:HIS:CE1	1:E:165:ILE:C	2.75	0.64
1:D:64:ILE:CD1	1:E:289:ILE:CD1	2.72	0.64
1:D:62:ARG:CB	1:E:288:ASP:HB2	2.24	0.64
1:D:244:ASP:CB	1:E:290:ARG:NH1	2.55	0.63
1:C:40:HIS:CE1	1:D:170:ALA:HA	2.33	0.63
1:D:63:GLY:HA2	1:E:286:ASP:HB3	1.74	0.63
1:D:45:VAL:HG21	1:E:139:VAL:CG1	2.31	0.61
1:D:40:HIS:CD2	1:E:166:TYR:CA	2.84	0.60
1:D:42:GLY:HA3	1:E:164:PRO:O	2.02	0.60
1:D:46:GLY:HA3	1:E:167:GLU:HA	1.82	0.60
1:D:41:GLN:O	1:E:170:ALA:HB2	2.01	0.59
1:C:12:ASN:HD21	1:C:82:MET:HE2	1.67	0.59
1:D:44:MET:O	1:E:169:TYR:HA	2.03	0.59
1:D:45:VAL:C	1:E:167:GLU:O	2.45	0.59
1:D:43:VAL:HG21	1:E:163:VAL:HG11	1.85	0.58
1:D:244:ASP:HA	1:E:324:THR:OG1	2.04	0.58
1:D:107:GLU:HB2	1:D:134:VAL:HG22	1.85	0.57
1:D:45:VAL:CG2	1:E:139:VAL:CG1	2.82	0.57
1:D:243:PRO:C	1:E:324:THR:HB	2.12	0.57
1:D:244:ASP:CG	1:E:287:ILE:HG23	2.30	0.57
1:D:40:HIS:HB2	1:E:166:TYR:CE1	2.38	0.57
1:D:306:TYR:CZ	3:D:401:ADP:H2	2.23	0.56
1:C:212:ILE:HG12	1:C:240:TYR:CE2	2.41	0.56
1:D:47:MET:N	1:E:167:GLU:OE2	2.36	0.56
1:D:48:GLY:CA	1:E:167:GLU:HG3	2.35	0.56
1:C:136:ILE:HD12	1:C:136:ILE:N	2.21	0.56
1:D:64:ILE:CD1	1:E:289:ILE:CG1	2.82	0.55
1:D:244:ASP:OD1	1:E:287:ILE:HG23	2.08	0.54
1:D:40:HIS:HB3	1:E:166:TYR:CG	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:VAL:HB	1:E:142:LEU:HD23	1.90	0.54
1:E:107:GLU:HB2	1:E:134:VAL:HG22	1.91	0.53
1:B:202:THR:HG21	1:E:270:GLU:HG2	1.91	0.53
1:D:43:VAL:CB	1:E:165:ILE:HB	2.25	0.53
1:D:44:MET:O	1:E:169:TYR:CA	2.56	0.53
1:B:9:VAL:HG21	1:B:344:SER:HA	1.91	0.53
1:D:39:ARG:HH21	1:E:286:ASP:CB	2.07	0.53
1:A:107:GLU:HB2	1:A:134:VAL:HG22	1.91	0.52
1:E:43:VAL:HG12	1:E:44:MET:H	1.74	0.52
1:E:173:HIS:CG	1:E:174:ALA:H	2.26	0.52
1:A:43:VAL:HG12	1:A:44:MET:H	1.74	0.52
1:D:171:LEU:HD13	1:D:173:HIS:HB3	1.91	0.52
1:D:46:GLY:CA	1:E:148:THR:HB	2.37	0.52
1:D:9:VAL:HG23	1:D:22:ALA:HA	1.91	0.52
1:A:173:HIS:CG	1:A:174:ALA:H	2.26	0.51
1:D:40:HIS:CE1	1:E:166:TYR:CA	2.93	0.51
1:D:40:HIS:NE2	1:E:166:TYR:CA	2.72	0.51
1:D:62:ARG:CB	1:E:288:ASP:CB	2.81	0.51
1:A:173:HIS:CD2	1:A:174:ALA:H	2.30	0.50
1:B:102:PRO:HA	1:B:129:VAL:HG12	1.93	0.50
1:D:244:ASP:OD1	1:E:290:ARG:HD2	2.11	0.50
1:D:43:VAL:CG2	1:E:163:VAL:CG1	2.89	0.50
1:D:244:ASP:OD2	1:E:287:ILE:HG23	2.12	0.50
1:D:64:ILE:CD1	1:E:289:ILE:CB	2.86	0.49
1:D:243:PRO:HB3	1:E:324:THR:HG22	1.90	0.49
1:D:41:GLN:CA	1:E:171:LEU:H	2.24	0.49
1:D:151:ILE:HG23	1:D:297:ASN:HA	1.94	0.49
1:E:173:HIS:CD2	1:E:174:ALA:H	2.30	0.49
1:A:18:LYS:O	1:A:340:TRP:CD1	2.66	0.49
1:D:43:VAL:CG1	1:E:165:ILE:CD1	2.83	0.49
1:D:62:ARG:HB2	1:E:288:ASP:CG	2.37	0.49
1:D:1:ASP:OD2	1:D:101:HIS:CE1	2.66	0.48
1:D:40:HIS:CE1	1:E:165:ILE:O	2.66	0.48
1:B:113:LYS:HE2	1:D:196:ARG:HH21	1.77	0.48
1:D:40:HIS:CD2	1:E:166:TYR:HB2	2.26	0.48
1:D:44:MET:C	1:E:169:TYR:HA	2.26	0.48
1:E:18:LYS:O	1:E:340:TRP:CD1	2.66	0.48
1:B:121:GLN:O	1:B:125:GLU:HB2	2.14	0.48
1:D:62:ARG:C	1:E:288:ASP:HB3	2.32	0.48
1:D:64:ILE:HD13	1:E:289:ILE:CG1	2.42	0.48
1:D:212:ILE:HG12	1:D:240:TYR:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:HIS:CE1	1:E:166:TYR:N	2.82	0.47
1:D:40:HIS:CB	1:E:166:TYR:HB2	2.39	0.47
1:D:215:LYS:HG3	1:D:216:LEU:HD12	1.96	0.47
1:D:43:VAL:HG12	1:E:165:ILE:CD1	2.39	0.47
1:E:133:TYR:CE2	1:E:135:ALA:HA	2.50	0.47
1:C:7:ALA:HB2	1:C:102:PRO:HB2	1.97	0.47
1:D:9:VAL:HG21	1:D:344:SER:HA	1.98	0.46
1:A:133:TYR:CE2	1:A:135:ALA:HA	2.50	0.46
1:B:1:ASP:OD2	1:B:101:HIS:CE1	2.68	0.46
1:E:220:ALA:HB2	1:E:255:PHE:HB2	1.98	0.46
1:A:90:PHE:CD2	1:A:96:VAL:HG23	2.52	0.45
1:A:220:ALA:HB2	1:A:255:PHE:HB2	1.98	0.45
1:C:53:TYR:HB3	1:C:58:ALA:HA	1.98	0.45
1:B:216:LEU:HD11	1:B:240:TYR:CD1	2.52	0.45
1:B:279:TYR:CZ	1:B:320:LEU:HB2	2.51	0.45
1:D:40:HIS:CE1	1:E:166:TYR:HB2	2.50	0.45
1:B:117:GLU:HA	1:B:370:VAL:HG21	1.99	0.45
1:C:306:TYR:O	1:C:309:ILE:HG22	2.16	0.45
1:D:306:TYR:CE1	3:D:401:ADP:C2	3.04	0.45
1:D:41:GLN:HE22	1:E:171:LEU:HD22	1.82	0.45
1:E:90:PHE:CD2	1:E:96:VAL:HG23	2.52	0.45
1:B:139:VAL:HG11	1:B:169:TYR:CE2	2.52	0.45
1:B:165:ILE:HD12	1:B:165:ILE:HA	1.79	0.44
1:B:306:TYR:O	1:B:309:ILE:HG22	2.17	0.44
1:C:317:ILE:O	1:C:321:ALA:HB3	2.16	0.44
1:D:43:VAL:CG2	1:E:163:VAL:HG11	2.48	0.44
1:C:159:VAL:HG11	1:C:177:ARG:HD2	2.00	0.44
1:D:220:ALA:HB2	1:D:255:PHE:HB2	1.98	0.44
1:E:113:LYS:O	1:E:371:HIS:HE1	2.01	0.44
1:A:137:GLN:HG3	1:A:339:VAL:HG11	2.00	0.44
1:D:22:ALA:HB1	1:D:347:ALA:HB1	2.00	0.44
1:D:49:GLN:O	1:D:50:LYS:HG2	2.17	0.44
1:E:361:GLU:HB3	1:E:369:ILE:HG12	2.00	0.44
1:C:340:TRP:CZ3	1:C:344:SER:OG	2.70	0.43
1:E:117:GLU:OE1	1:E:371:HIS:CE1	2.71	0.43
1:D:76:ILE:HG21	1:D:79:TRP:CD2	2.53	0.43
1:C:79:TRP:CE2	1:C:118:LYS:HG2	2.54	0.43
1:A:113:LYS:O	1:A:371:HIS:HE1	2.01	0.43
1:A:117:GLU:OE1	1:A:371:HIS:CE1	2.71	0.43
1:A:350:SER:O	1:A:353:GLN:HB3	2.19	0.43
1:D:48:GLY:HA2	1:E:167:GLU:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:CYS:HB3	1:E:258:PRO:HD3	2.01	0.43
1:E:116:ARG:HD2	1:E:371:HIS:CE1	2.54	0.43
1:D:76:ILE:HG21	1:D:79:TRP:CE3	2.53	0.43
1:B:90:PHE:CD2	1:B:98:PRO:HA	2.54	0.42
1:B:195:GLU:OE1	1:E:111:ASN:CA	2.62	0.42
1:D:41:GLN:CB	1:E:171:LEU:O	2.45	0.42
1:E:350:SER:O	1:E:353:GLN:HB3	2.19	0.42
1:B:195:GLU:CB	1:E:110:LEU:O	2.46	0.42
1:E:137:GLN:HG3	1:E:339:VAL:HG11	2.00	0.42
1:A:116:ARG:HD2	1:A:371:HIS:CE1	2.54	0.42
1:A:361:GLU:HB3	1:A:369:ILE:HG12	2.00	0.42
1:B:202:THR:CG2	1:E:270:GLU:HG2	2.50	0.42
1:C:299:MET:HE2	1:C:313:MET:HG3	2.02	0.42
1:D:45:VAL:HG23	1:E:139:VAL:HG13	2.01	0.42
1:B:159:VAL:HG23	1:B:161:HIS:CE1	2.54	0.42
1:C:287:ILE:H	1:C:287:ILE:HG13	1.60	0.42
1:C:113:LYS:H	1:C:113:LYS:HD2	1.85	0.42
1:A:244:ASP:HB3	1:B:287:ILE:HG22	2.01	0.41
1:A:351:THR:HA	1:A:354:GLN:HG2	2.02	0.41
1:D:44:MET:CA	1:E:166:TYR:O	2.51	0.41
1:D:72:GLU:HA	1:D:72:GLU:OE1	2.20	0.41
1:A:257:CYS:HB3	1:A:258:PRO:HD3	2.01	0.41
1:B:140:LEU:O	1:B:342:GLY:HA3	2.20	0.41
1:C:104:LEU:HD12	1:C:133:TYR:O	2.20	0.41
1:D:41:GLN:C	1:E:170:ALA:CA	2.83	0.41
1:D:64:ILE:HD13	1:E:289:ILE:CB	2.47	0.41
1:D:163:VAL:HA	1:D:175:ILE:HG22	2.03	0.41
1:A:216:LEU:HD11	1:A:240:TYR:CD1	2.56	0.41
1:C:136:ILE:N	1:C:136:ILE:CD1	2.84	0.41
1:D:41:GLN:NE2	1:E:171:LEU:HD22	2.36	0.40
1:D:101:HIS:O	1:D:129:VAL:HG13	2.22	0.40
1:B:153:LEU:HD13	1:B:299:MET:HE1	2.04	0.40
1:D:63:GLY:C	1:E:286:ASP:CB	2.81	0.40
1:E:351:THR:HA	1:E:354:GLN:HG2	2.02	0.40
1:D:43:VAL:N	1:E:165:ILE:HA	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	373/375 (100%)	321 (86%)	40 (11%)	12 (3%)	3	21
1	B	373/375 (100%)	326 (87%)	33 (9%)	14 (4%)	2	19
1	C	373/375 (100%)	322 (86%)	39 (10%)	12 (3%)	3	21
1	D	373/375 (100%)	325 (87%)	37 (10%)	11 (3%)	3	23
1	E	373/375 (100%)	321 (86%)	40 (11%)	12 (3%)	3	21
All	All	1865/1875 (100%)	1615 (87%)	189 (10%)	61 (3%)	5	21

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	246	GLN
1	B	6	THR
1	B	39	ARG
1	B	128	ASN
1	B	173	HIS
1	B	180	LEU
1	C	6	THR
1	C	234	SER
1	C	244	ASP
1	D	6	THR
1	E	6	THR
1	E	246	GLN
1	A	3	ASP
1	A	128	ASN
1	A	180	LEU
1	B	156	GLY
1	B	244	ASP
1	C	174	ALA
1	C	197	GLY
1	D	7	ALA

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Mol	Chain	Res	Type
1	D	39	ARG
1	D	100	GLU
1	E	3	ASP
1	E	128	ASN
1	E	180	LEU
1	A	39	ARG
1	B	158	GLY
1	C	7	ALA
1	C	49	GLN
1	C	180	LEU
1	C	181	ALA
1	D	47	MET
1	D	197	GLY
1	D	238	LYS
1	E	39	ARG
1	A	51	ASP
1	A	244	ASP
1	B	3	ASP
1	B	49	GLN
1	B	234	SER
1	C	173	HIS
1	D	234	SER
1	E	51	ASP
1	E	244	ASP
1	B	194	THR
1	C	129	VAL
1	D	173	HIS
1	B	137	GLN
1	C	3	ASP
1	D	181	ALA
1	A	45	VAL
1	A	322	PRO
1	B	201	VAL
1	E	45	VAL
1	E	322	PRO
1	A	243	PRO
1	E	243	PRO
1	A	15	GLY
1	D	15	GLY
1	E	15	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	318/318 (100%)	290 (91%)	28 (9%)	9	28
1	B	318/318 (100%)	280 (88%)	38 (12%)	5	18
1	C	318/318 (100%)	290 (91%)	28 (9%)	9	28
1	D	318/318 (100%)	286 (90%)	32 (10%)	7	23
1	E	318/318 (100%)	289 (91%)	29 (9%)	9	27
All	All	1590/1590 (100%)	1435 (90%)	155 (10%)	10	24

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	30	VAL
1	A	34	ILE
1	A	43	VAL
1	A	85	ILE
1	A	93	GLU
1	A	113	LYS
1	A	117	GLU
1	A	126	THR
1	A	153	LEU
1	A	159	VAL
1	A	183	ARG
1	A	193	LEU
1	A	196	ARG
1	A	203	THR
1	A	219	VAL
1	A	242	LEU
1	A	250	ILE
1	A	264	PRO
1	A	274	ILE
1	A	276	GLU
1	A	284	LYS
1	A	291	LYS

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Mol	Chain	Res	Type
1	A	312	ARG
1	A	315	LYS
1	A	328	LYS
1	A	334	GLU
1	A	372	ARG
1	B	2	GLU
1	B	25	ASP
1	B	30	VAL
1	B	38	PRO
1	B	41	GLN
1	B	47	MET
1	B	57	GLU
1	B	66	THR
1	B	93	GLU
1	B	109	PRO
1	B	110	LEU
1	B	111	ASN
1	B	113	LYS
1	B	117	GLU
1	B	128	ASN
1	B	136	ILE
1	B	153	LEU
1	B	166	TYR
1	B	171	LEU
1	B	183	ARG
1	B	192	ILE
1	B	193	LEU
1	B	195	GLU
1	B	196	ARG
1	B	234	SER
1	B	246	GLN
1	B	250	ILE
1	B	261	LEU
1	B	284	LYS
1	B	300	SER
1	B	303	THR
1	B	309	ILE
1	B	312	ARG
1	B	315	LYS
1	B	328	LYS
1	B	335	ARG
1	B	353	GLN

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Mol	Chain	Res	Type
1	B	372	ARG
1	C	30	VAL
1	C	31	PHE
1	C	39	ARG
1	C	54	VAL
1	C	56	ASP
1	C	106	THR
1	C	113	LYS
1	C	117	GLU
1	C	136	ILE
1	C	151	ILE
1	C	153	LEU
1	C	159	VAL
1	C	171	LEU
1	C	183	ARG
1	C	192	ILE
1	C	196	ARG
1	C	234	SER
1	C	241	GLU
1	C	250	ILE
1	C	315	LYS
1	C	328	LYS
1	C	329	ILE
1	C	335	ARG
1	C	354	GLN
1	C	358	THR
1	C	359	LYS
1	C	372	ARG
1	C	374	CYS
1	D	8	LEU
1	D	30	VAL
1	D	37	ARG
1	D	47	MET
1	D	54	VAL
1	D	56	ASP
1	D	65	LEU
1	D	93	GLU
1	D	113	LYS
1	D	123	MET
1	D	126	THR
1	D	128	ASN
1	D	134	VAL

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Mol	Chain	Res	Type
1	D	151	ILE
1	D	153	LEU
1	D	159	VAL
1	D	171	LEU
1	D	184	ASP
1	D	192	ILE
1	D	195	GLU
1	D	196	ARG
1	D	202	THR
1	D	223	PHE
1	D	224	GLU
1	D	234	SER
1	D	250	ILE
1	D	261	LEU
1	D	291	LYS
1	D	312	ARG
1	D	315	LYS
1	D	328	LYS
1	D	335	ARG
1	E	4	GLU
1	E	30	VAL
1	E	34	ILE
1	E	43	VAL
1	E	85	ILE
1	E	93	GLU
1	E	113	LYS
1	E	117	GLU
1	E	126	THR
1	E	153	LEU
1	E	159	VAL
1	E	183	ARG
1	E	193	LEU
1	E	196	ARG
1	E	203	THR
1	E	219	VAL
1	E	242	LEU
1	E	250	ILE
1	E	264	PRO
1	E	274	ILE
1	E	276	GLU
1	E	284	LYS
1	E	291	LYS

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Mol	Chain	Res	Type
1	E	312	ARG
1	E	315	LYS
1	E	328	LYS
1	E	334	GLU
1	E	356	TRP
1	E	372	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	41	GLN
1	A	101	HIS
1	A	173	HIS
1	A	225	ASN
1	A	314	GLN
1	A	360	GLN
1	A	371	HIS
1	B	12	ASN
1	B	78	ASN
1	B	87	HIS
1	B	101	HIS
1	B	161	HIS
1	B	225	ASN
1	B	263	GLN
1	B	360	GLN
1	C	12	ASN
1	C	40	HIS
1	C	111	ASN
1	C	137	GLN
1	C	161	HIS
1	C	252	ASN
1	C	275	HIS
1	D	40	HIS
1	D	78	ASN
1	D	87	HIS
1	D	92	ASN
1	D	101	HIS
1	D	111	ASN
1	D	137	GLN
1	D	246	GLN
1	D	314	GLN

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Mol	Chain	Res	Type
1	D	360	GLN
1	E	40	HIS
1	E	41	GLN
1	E	101	HIS
1	E	173	HIS
1	E	225	ASN
1	E	314	GLN
1	E	360	GLN
1	E	371	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	C	401	-	28,29,29	1.20	2 (7%)	43,45,45	1.57	11 (25%)
3	ADP	E	401	-	28,29,29	1.90	5 (17%)	43,45,45	1.44	7 (16%)
3	ADP	A	401	-	28,29,29	1.91	5 (17%)	43,45,45	1.43	7 (16%)
3	ADP	B	401	-	28,29,29	1.40	3 (10%)	43,45,45	1.89	12 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	D	401	-	28,29,29	1.42	4 (14%)	43,45,45	2.06	12 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	C	401	-	-	4/16/32/32	0/3/3/3
3	ADP	E	401	-	-	3/16/32/32	0/3/3/3
3	ADP	A	401	-	-	3/16/32/32	0/3/3/3
3	ADP	B	401	-	-	10/16/32/32	0/3/3/3
3	ADP	D	401	-	-	3/16/32/32	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	ADP	PA-O3A	7.29	1.67	1.59
3	E	401	ADP	PA-O3A	7.24	1.67	1.59
3	B	401	ADP	C4-N9	3.95	1.45	1.37
3	D	401	ADP	O2'-C2'	3.28	1.51	1.43
3	D	401	ADP	C4-N3	3.18	1.40	1.34
3	C	401	ADP	O4'-C4'	3.04	1.51	1.45
3	D	401	ADP	PA-O3A	2.82	1.62	1.59
3	E	401	ADP	O4'-C1'	2.69	1.48	1.42
3	A	401	ADP	O4'-C1'	2.66	1.48	1.42
3	E	401	ADP	C5-C4	-2.54	1.34	1.39
3	E	401	ADP	C2-N3	2.53	1.38	1.33
3	A	401	ADP	C5-C4	-2.52	1.34	1.39
3	A	401	ADP	C2-N3	2.49	1.38	1.33
3	E	401	ADP	C4-N9	2.44	1.42	1.37
3	A	401	ADP	C4-N9	2.41	1.42	1.37
3	B	401	ADP	C2'-C1'	-2.21	1.46	1.53
3	B	401	ADP	PA-O3A	2.20	1.61	1.59
3	C	401	ADP	O3'-C3'	-2.06	1.37	1.43
3	D	401	ADP	C8-N9	2.04	1.41	1.37

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	ADP	N6-C6-N1	5.90	131.51	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	ADP	O4'-C1'-N9	4.61	116.95	108.09
3	D	401	ADP	C5-C6-N6	-4.27	112.70	123.29
3	B	401	ADP	O4'-C1'-N9	4.17	116.10	108.09
3	C	401	ADP	N6-C6-N1	4.12	127.56	118.38
3	D	401	ADP	N3-C2-N1	4.04	134.70	128.58
3	B	401	ADP	C3'-C2'-C1'	4.00	109.02	101.46
3	C	401	ADP	C4-N9-C8	-3.88	101.67	105.74
3	B	401	ADP	C4-N9-C8	-3.83	101.72	105.74
3	B	401	ADP	C5-C4-N3	-3.75	121.55	126.72
3	E	401	ADP	O4'-C1'-N9	3.69	115.18	108.09
3	A	401	ADP	O4'-C1'-N9	3.68	115.16	108.09
3	C	401	ADP	C5'-C4'-C3'	-3.44	102.84	115.21
3	B	401	ADP	C6-C5-C4	3.32	121.71	117.18
3	D	401	ADP	O3B-PB-O2B	3.27	120.06	107.80
3	D	401	ADP	C5-C4-N9	3.14	109.24	105.81
3	B	401	ADP	C6-C5-N7	-3.12	126.07	132.09
3	D	401	ADP	C5'-C4'-C3'	-3.06	104.18	115.21
3	E	401	ADP	C6-C5-N7	-3.06	126.20	132.09
3	A	401	ADP	C6-C5-N7	-3.02	126.28	132.09
3	B	401	ADP	N6-C6-N1	2.75	124.51	118.38
3	E	401	ADP	C5'-C4'-C3'	-2.74	105.34	115.21
3	A	401	ADP	C5'-C4'-C3'	-2.74	105.36	115.21
3	D	401	ADP	C2-N3-C4	-2.68	105.29	111.83
3	C	401	ADP	C5-C6-N6	-2.64	116.75	123.29
3	E	401	ADP	C4-C5-N7	2.64	113.60	110.58
3	A	401	ADP	C4-C5-N7	2.62	113.58	110.58
3	D	401	ADP	O4'-C4'-C5'	2.62	117.71	109.33
3	E	401	ADP	N6-C6-N1	2.60	124.17	118.38
3	C	401	ADP	O4'-C1'-N9	2.59	113.06	108.09
3	A	401	ADP	N6-C6-N1	2.59	124.14	118.38
3	B	401	ADP	N3-C4-N9	2.45	131.33	127.17
3	C	401	ADP	O3A-PB-O1B	-2.43	98.26	111.04
3	B	401	ADP	O3B-PB-O3A	-2.41	96.56	104.64
3	A	401	ADP	C2'-C3'-C4'	2.35	107.15	102.61
3	C	401	ADP	O3B-PB-O1B	2.34	119.97	110.83
3	E	401	ADP	C2'-C3'-C4'	2.34	107.13	102.61
3	C	401	ADP	O4'-C4'-C3'	-2.33	100.53	105.15
3	B	401	ADP	C1'-N9-C8	2.31	132.22	127.09
3	D	401	ADP	O3A-PA-O1A	-2.30	103.78	110.70
3	E	401	ADP	O3B-PB-O1B	2.22	119.47	110.83
3	A	401	ADP	O3B-PB-O1B	2.22	119.47	110.83
3	C	401	ADP	C5-C4-N9	2.20	108.21	105.81

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	ADP	O3'-C3'-C4'	-2.20	104.77	111.08
3	B	401	ADP	O2B-PB-O3A	2.18	111.95	104.64
3	B	401	ADP	C5'-C4'-C3'	-2.18	107.38	115.21
3	D	401	ADP	C4-N9-C8	-2.16	103.47	105.74
3	C	401	ADP	O4'-C4'-C5'	2.07	115.96	109.33
3	C	401	ADP	C4-N9-C1'	2.03	131.37	126.63

There are no chirality outliers.

All (23) torsion outliers are listed below:

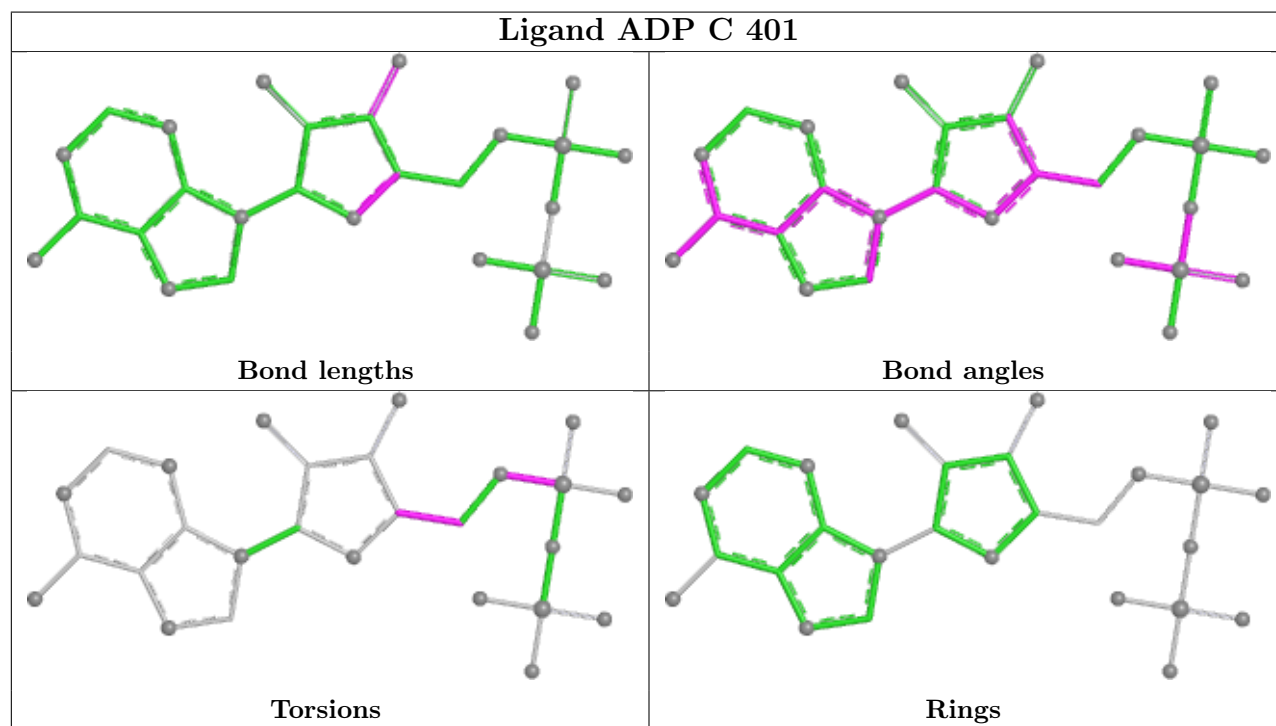
Mol	Chain	Res	Type	Atoms
3	A	401	ADP	C5'-O5'-PA-O1A
3	A	401	ADP	C5'-O5'-PA-O2A
3	A	401	ADP	C5'-O5'-PA-O3A
3	B	401	ADP	PA-O3A-PB-O3B
3	B	401	ADP	C4'-C5'-O5'-PA
3	B	401	ADP	O4'-C1'-N9-C8
3	B	401	ADP	O4'-C1'-N9-C4
3	C	401	ADP	C5'-O5'-PA-O1A
3	C	401	ADP	C5'-O5'-PA-O2A
3	C	401	ADP	C5'-O5'-PA-O3A
3	E	401	ADP	C5'-O5'-PA-O1A
3	E	401	ADP	C5'-O5'-PA-O2A
3	E	401	ADP	C5'-O5'-PA-O3A
3	D	401	ADP	O4'-C1'-N9-C8
3	B	401	ADP	O4'-C4'-C5'-O5'
3	D	401	ADP	O4'-C1'-N9-C4
3	B	401	ADP	C3'-C4'-C5'-O5'
3	C	401	ADP	O4'-C4'-C5'-O5'
3	B	401	ADP	PA-O3A-PB-O1B
3	B	401	ADP	PA-O3A-PB-O2B
3	B	401	ADP	PB-O3A-PA-O1A
3	B	401	ADP	PB-O3A-PA-O2A
3	D	401	ADP	C2'-C1'-N9-C8

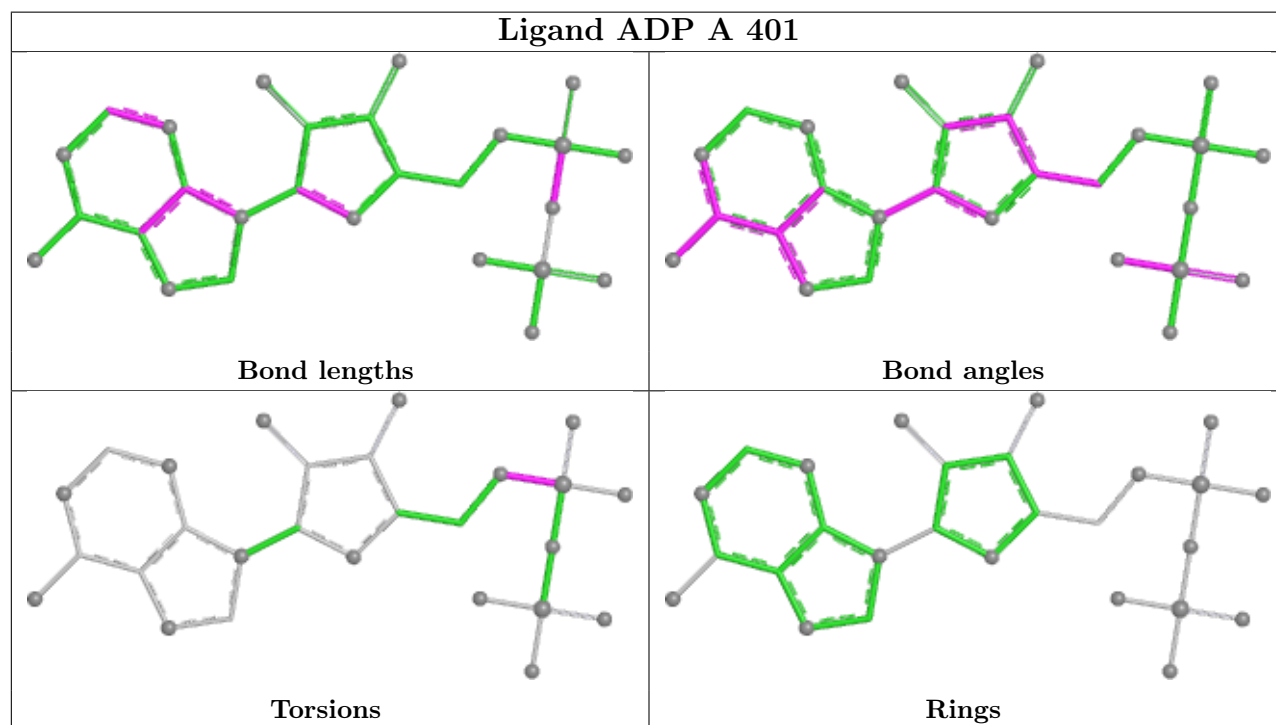
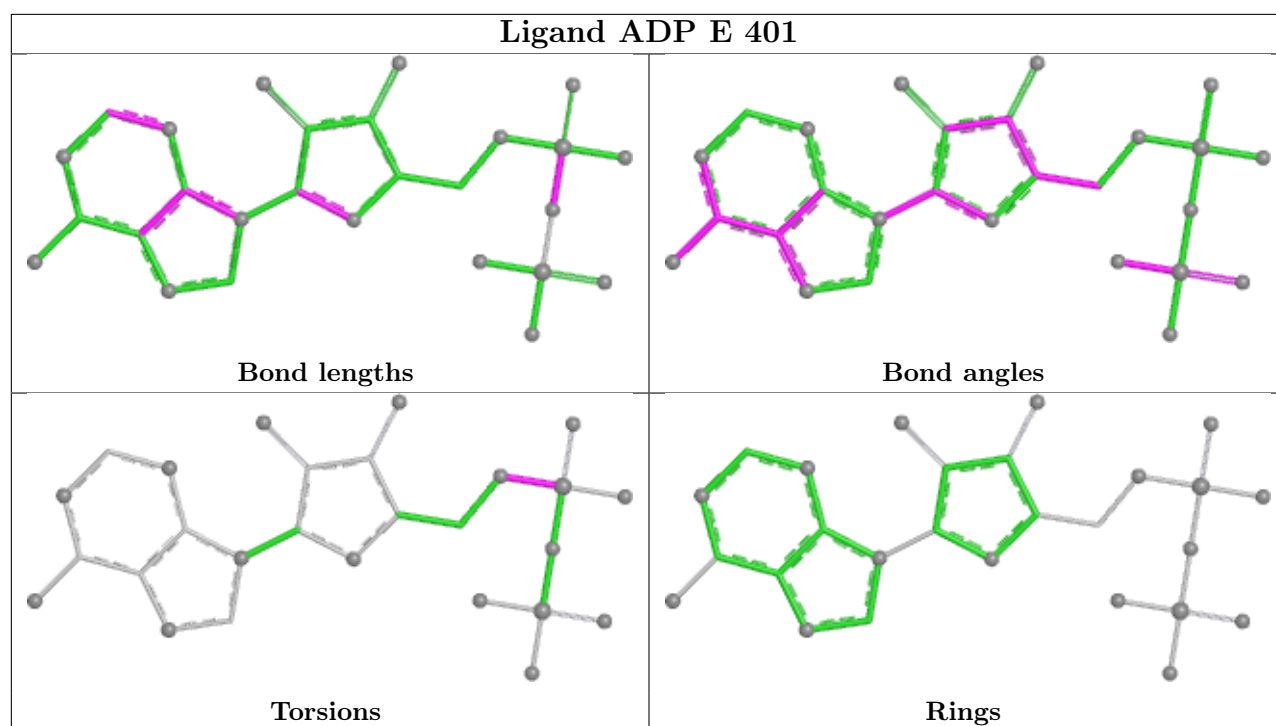
There are no ring outliers.

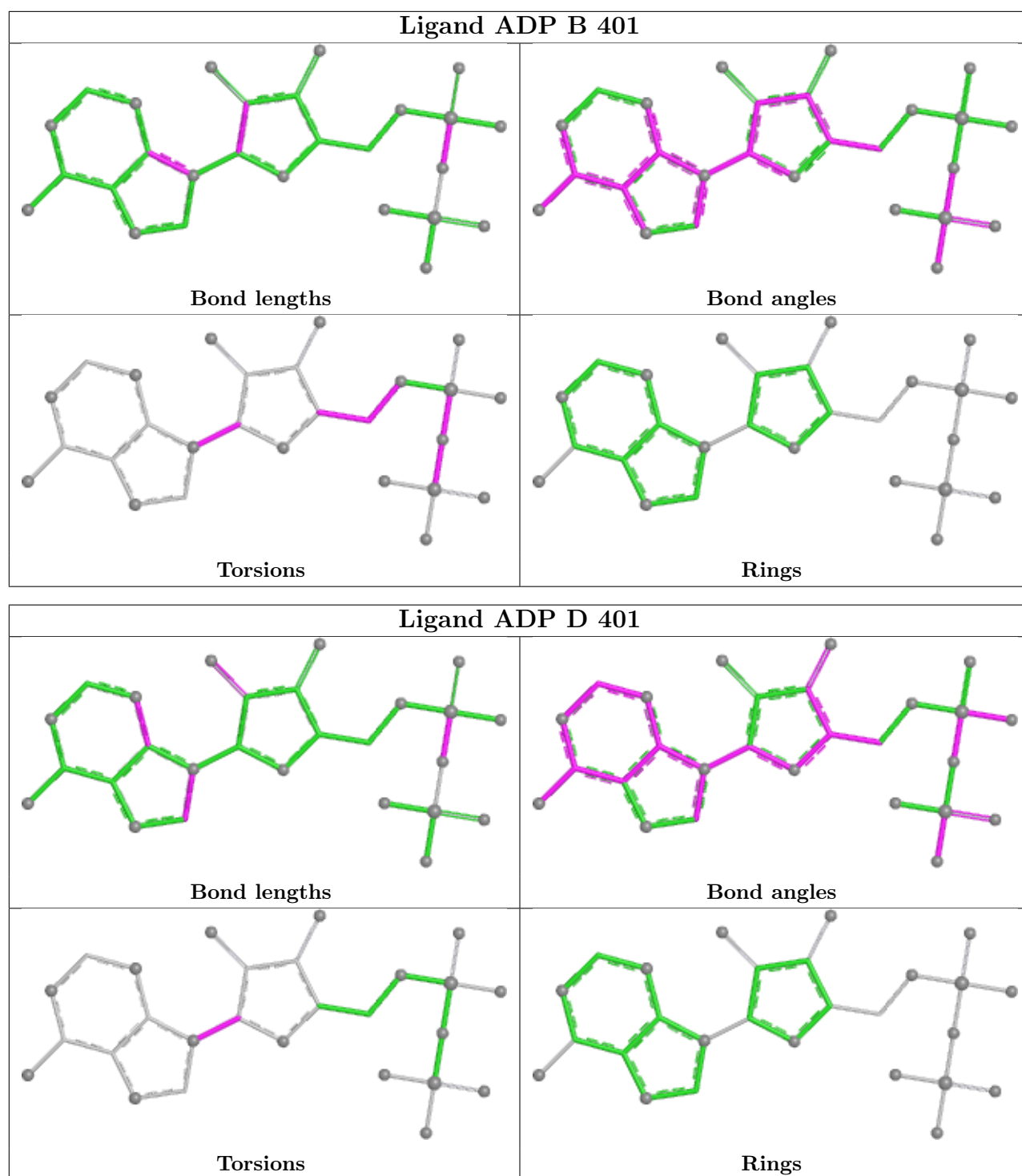
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	ADP	2	0

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







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

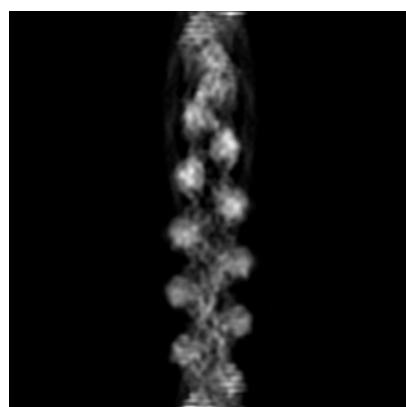
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5751. These allow visual inspection of the internal detail of the map and identification of artifacts.

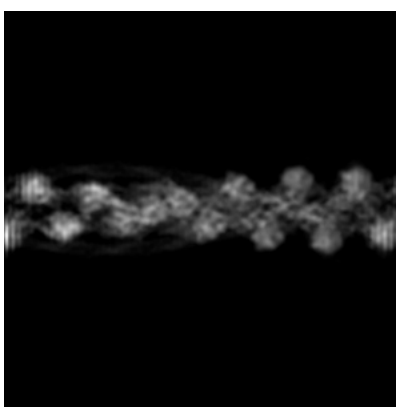
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

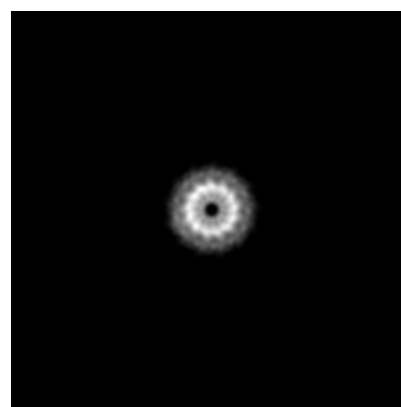
6.1.1 Primary map



X



Y

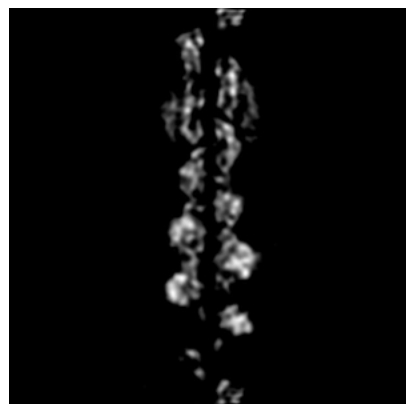


Z

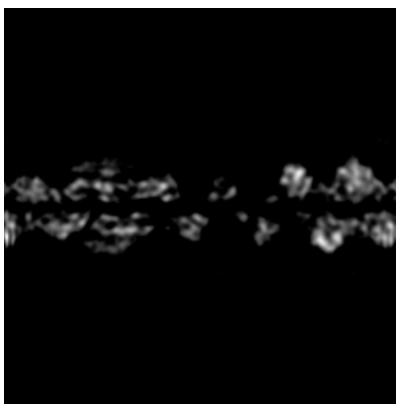
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 128



Y Index: 128

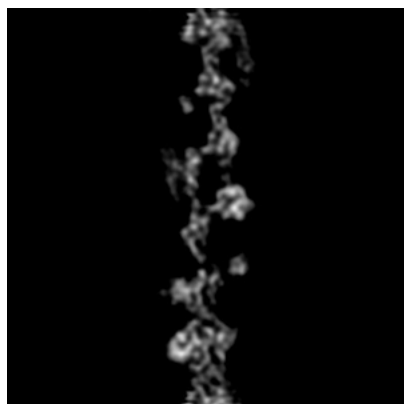


Z Index: 128

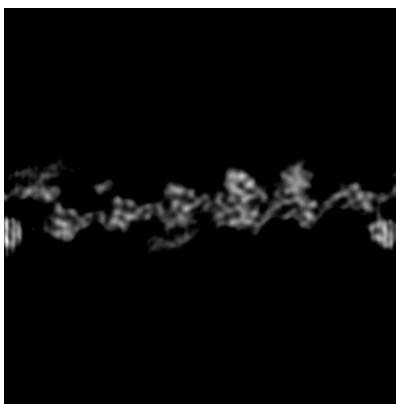
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

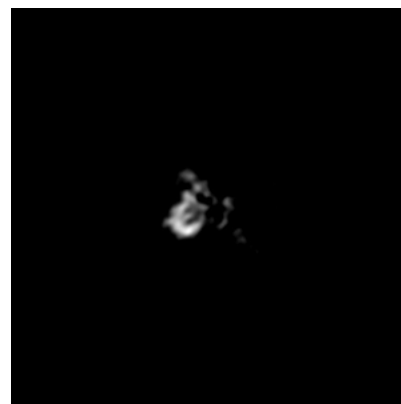
6.3.1 Primary map



X Index: 117



Y Index: 116

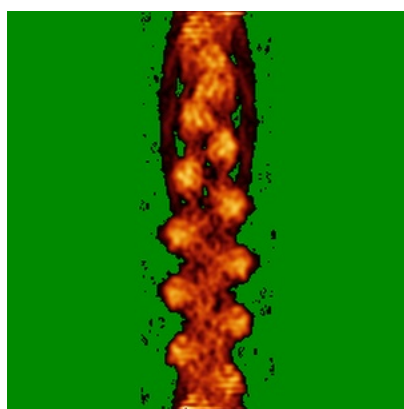


Z Index: 1

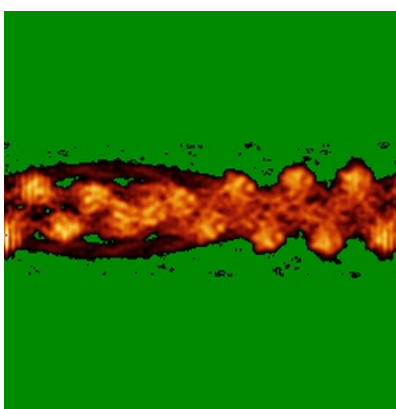
The images above show the largest variance slices of the map in three orthogonal directions.

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

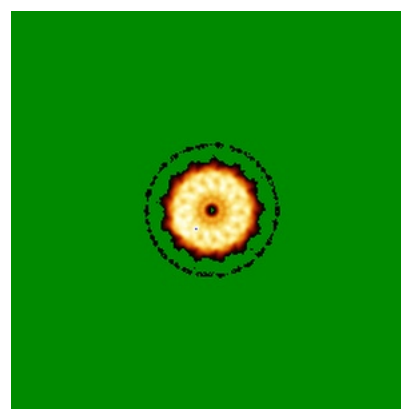
6.4.1 Primary map



X



Y

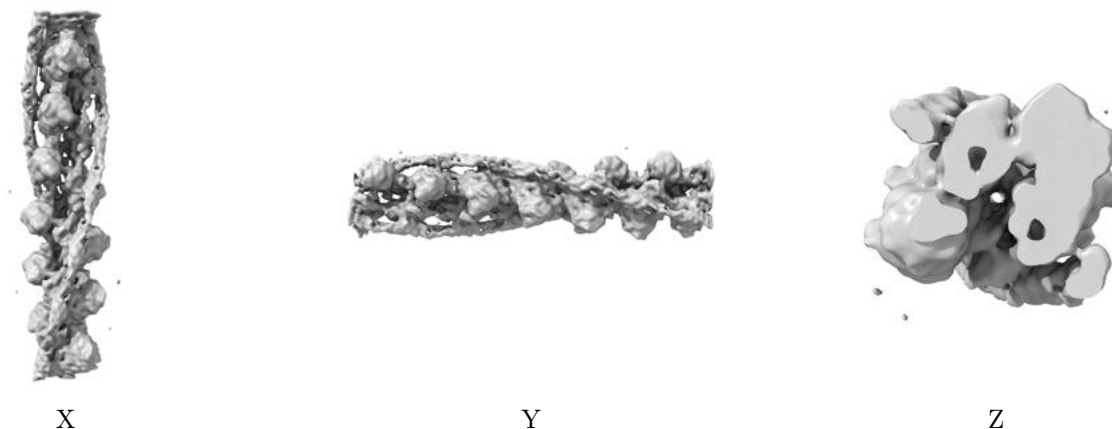


Z

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 2.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

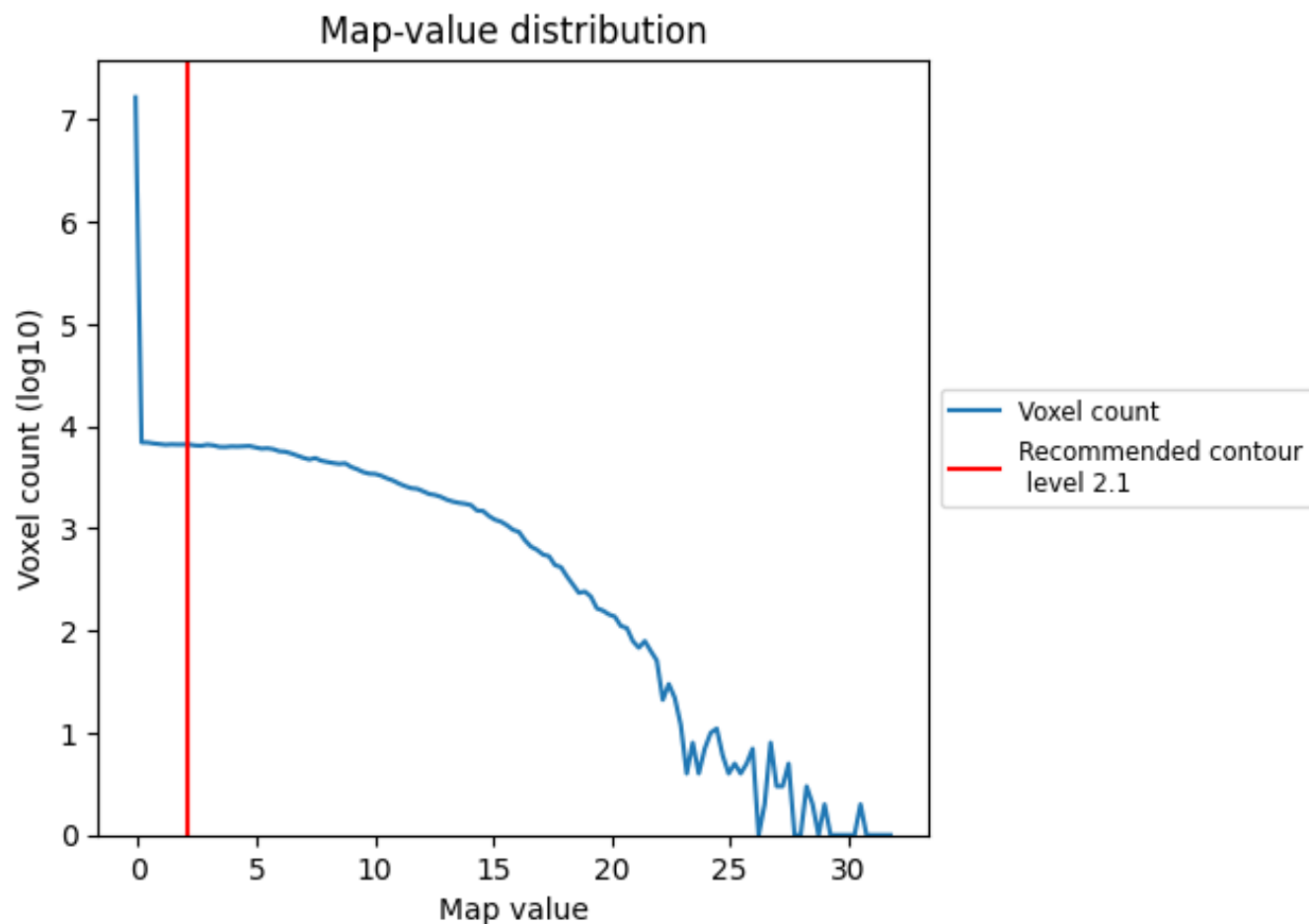
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

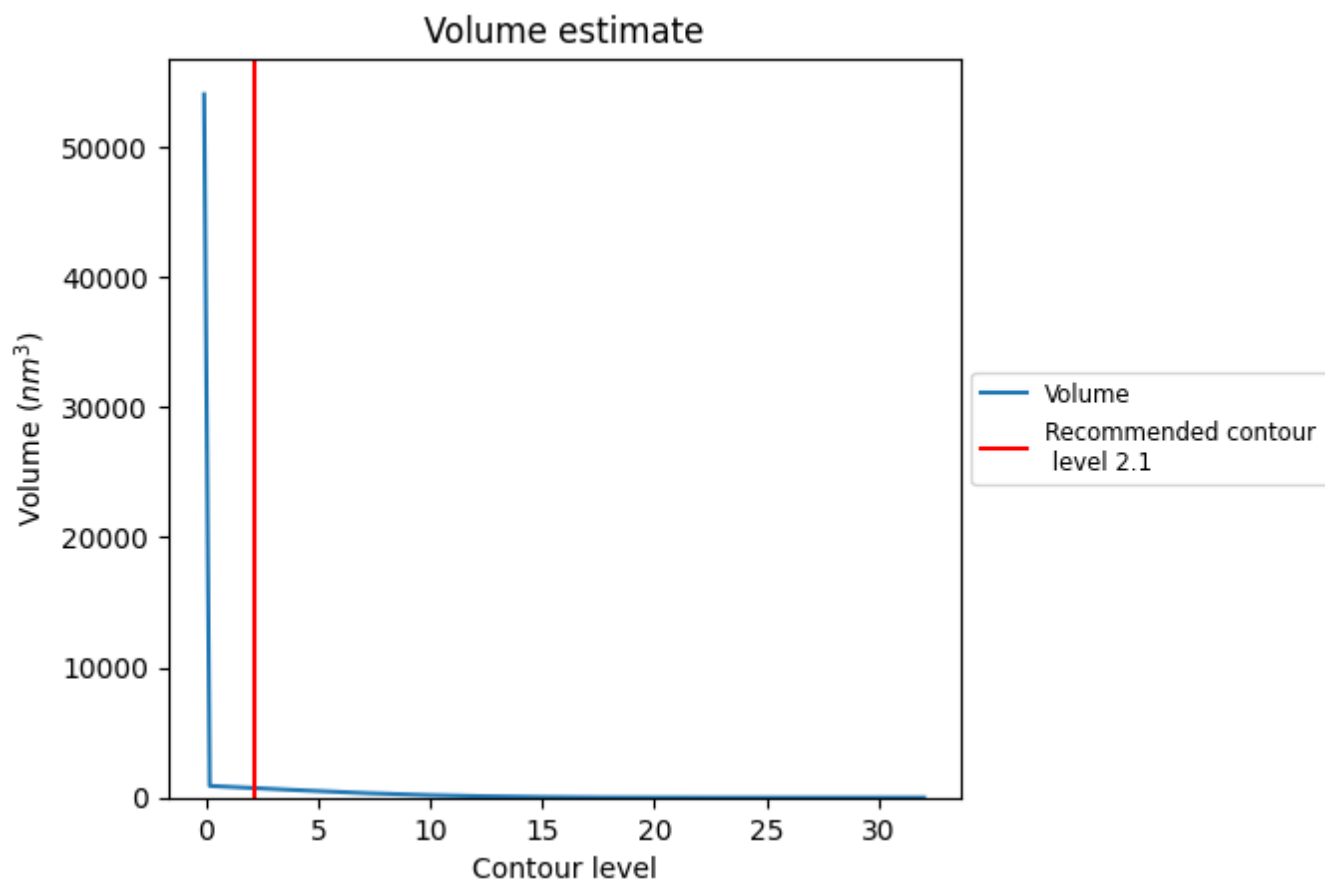
This section contains the results of statistical analysis of the map.

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.

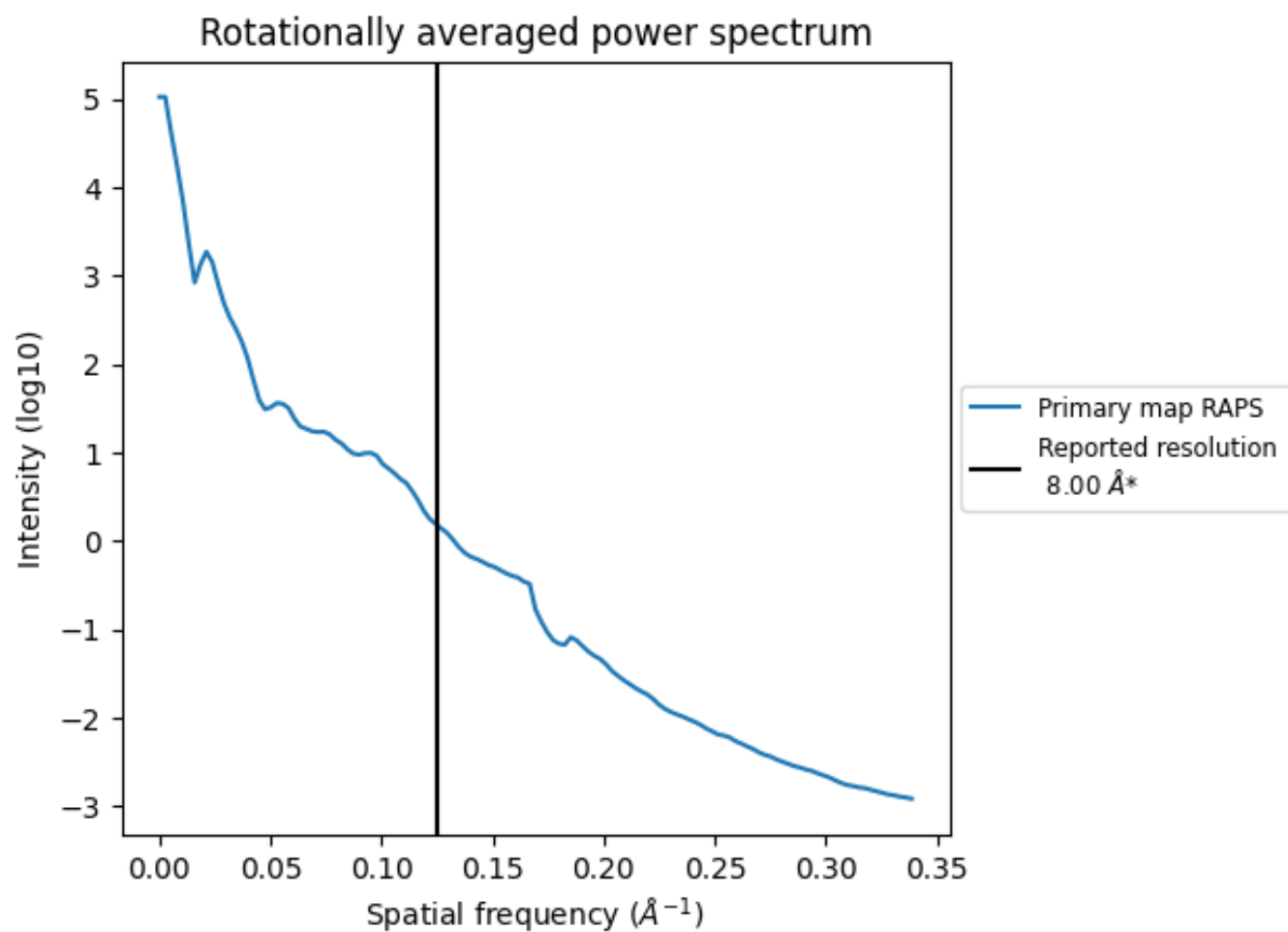
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 730 nm³; this corresponds to an approximate mass of 659 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.125 Å⁻¹

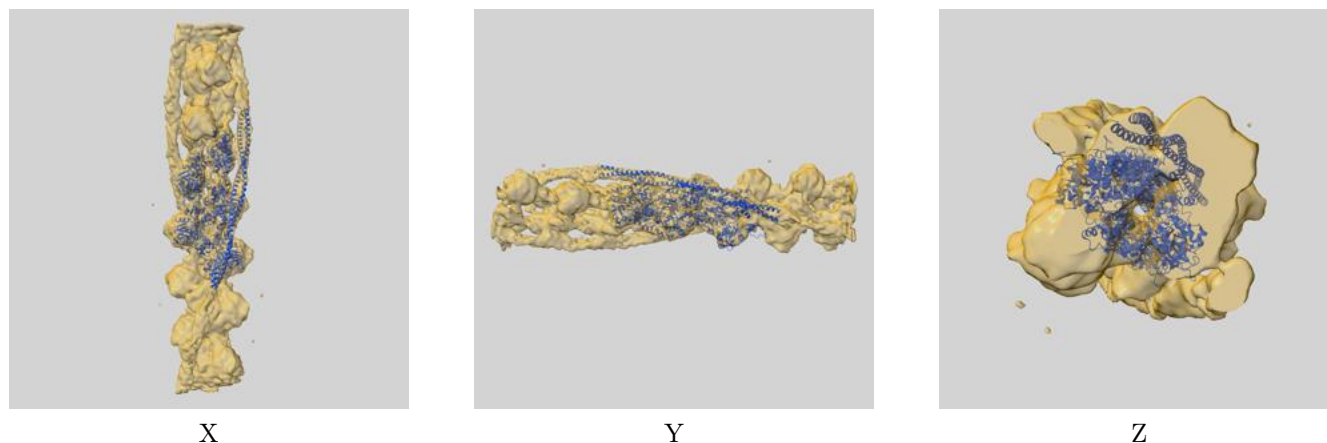
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

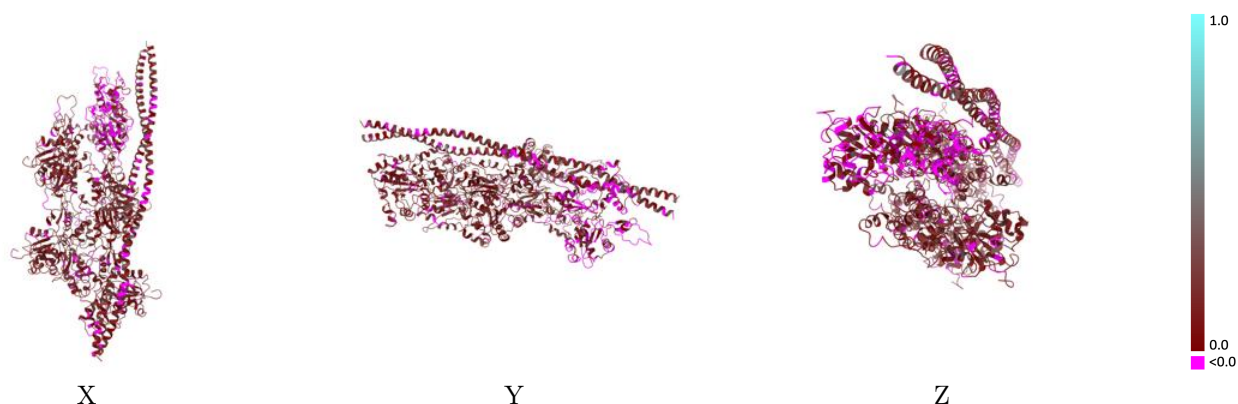
This section contains information regarding the fit between EMDB map EMD-5751 and PDB model 3J4K. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



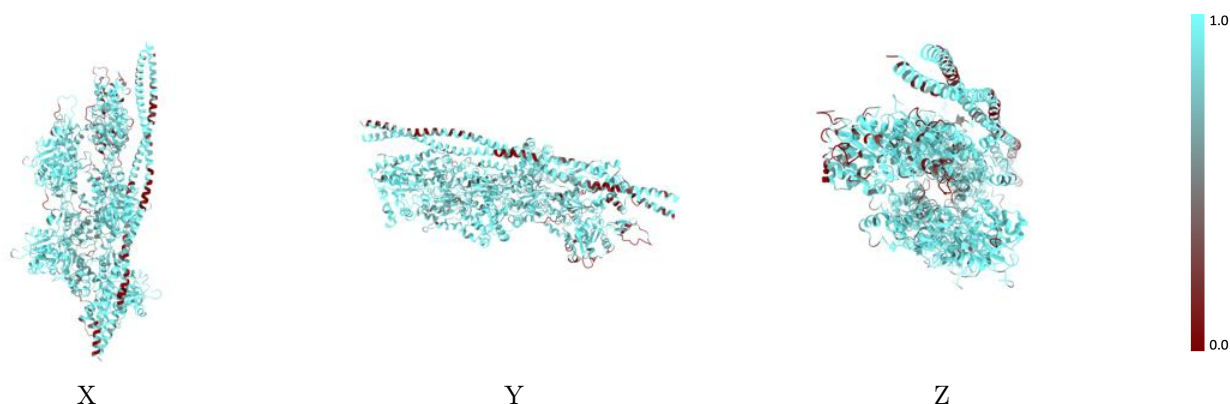
The images above show the 3D surface view of the map at the recommended contour level 2.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



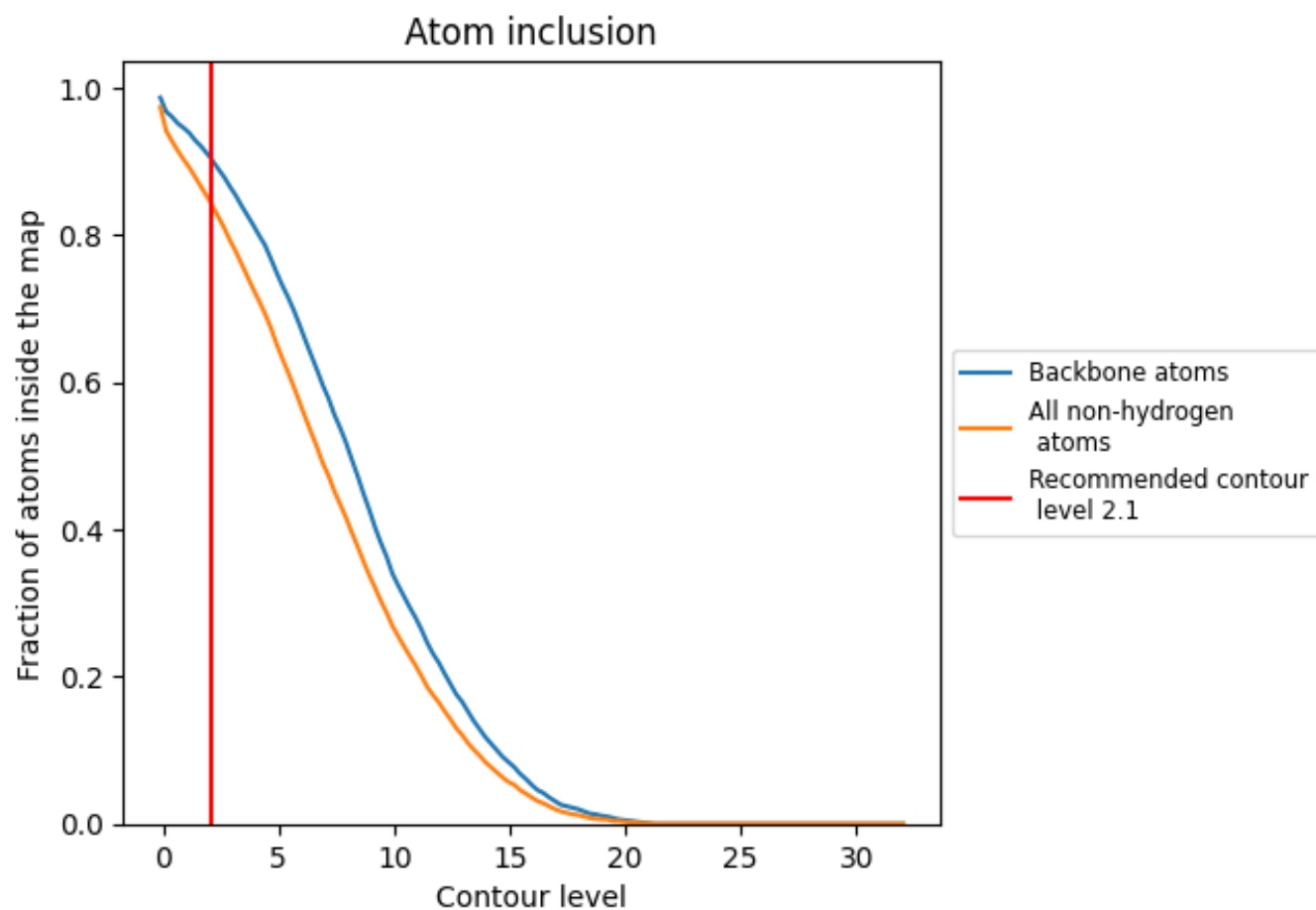
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (2.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8430	0.1120
A	0.8790	0.1350
B	0.8870	0.1390
C	0.8890	0.1370
D	0.8900	0.1370
E	0.7160	-0.0050
F	0.7590	0.1590
G	0.7180	0.1390

1.0

0.0

<0.0