



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:14 PM UTC

PDB ID : 1J4T / pdb_00001j4t
Title : Structure of Artocarpin: a Lectin with Mannose Specificity (Form 2)
Authors : Pratap, J.V.; Jeyaprakash, A.A.; Rani, P.G.; Sekar, K.; Surolia, A.; Vijayan, M.
Deposited on : 2001-10-30
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

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

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

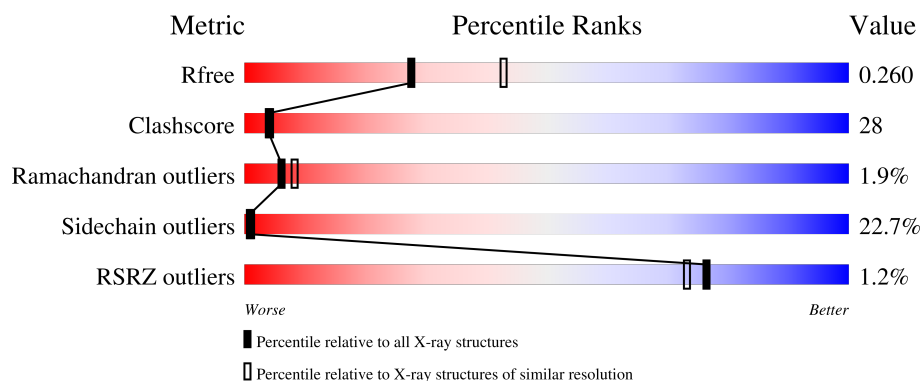
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	149	5% 51% 34% 10%
1	B	149	7% 46% 36% 10%
1	C	149	12% 42% 36% 10%
1	D	149	5% 49% 36% 11%
1	E	149	9% 53% 31% 7%

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Mol	Chain	Length	Quality of chain
1	F	149	
1	G	149	
1	H	149	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	AYA	A	1	X	X	-	-
1	AYA	B	1	X	X	X	-
1	AYA	C	1	X	X	-	-
1	AYA	E	1	X	-	-	-
1	AYA	F	1	-	X	-	-
1	AYA	G	1	X	-	-	-
1	AYA	H	1	X	X	-	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9922 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Artocarpin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			
1	B	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			
1	C	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			
1	D	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			
1	E	149	Total	C	N	O	S	0	0	0
			1128	724	181	222	1			
1	F	149	Total	C	N	O	S	0	0	0
			1128	724	181	222	1			
1	G	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			
1	H	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	AYA	ALA	modified residue	UNP Q7M1T4
A	9	SER	PRO	conflict	UNP Q7M1T4
A	20	GLU	ASP	conflict	UNP Q7M1T4
A	49	ASP	GLU	conflict	UNP Q7M1T4
A	70	LYS	ARG	conflict	UNP Q7M1T4
A	84	GLY	ALA	conflict	UNP Q7M1T4
A	145	ILE	VAL	conflict	UNP Q7M1T4
A	148	SER	ALA	conflict	UNP Q7M1T4
B	1	AYA	ALA	modified residue	UNP Q7M1T4
B	9	SER	PRO	conflict	UNP Q7M1T4
B	20	GLU	ASP	conflict	UNP Q7M1T4
B	49	ASP	GLU	conflict	UNP Q7M1T4
B	70	LYS	ARG	conflict	UNP Q7M1T4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	84	GLY	ALA	conflict	UNP Q7M1T4
B	145	ILE	VAL	conflict	UNP Q7M1T4
B	148	SER	ALA	conflict	UNP Q7M1T4
C	1	AYA	ALA	modified residue	UNP Q7M1T4
C	9	SER	PRO	conflict	UNP Q7M1T4
C	20	GLU	ASP	conflict	UNP Q7M1T4
C	49	ASP	GLU	conflict	UNP Q7M1T4
C	70	LYS	ARG	conflict	UNP Q7M1T4
C	84	GLY	ALA	conflict	UNP Q7M1T4
C	145	ILE	VAL	conflict	UNP Q7M1T4
C	148	SER	ALA	conflict	UNP Q7M1T4
D	1	AYA	ALA	modified residue	UNP Q7M1T4
D	9	SER	PRO	conflict	UNP Q7M1T4
D	20	GLU	ASP	conflict	UNP Q7M1T4
D	49	ASP	GLU	conflict	UNP Q7M1T4
D	70	LYS	ARG	conflict	UNP Q7M1T4
D	84	GLY	ALA	conflict	UNP Q7M1T4
D	145	ILE	VAL	conflict	UNP Q7M1T4
D	148	SER	ALA	conflict	UNP Q7M1T4
E	1	AYA	ALA	modified residue	UNP Q7M1T4
E	9	SER	PRO	conflict	UNP Q7M1T4
E	20	GLU	ASP	conflict	UNP Q7M1T4
E	49	ASP	GLU	conflict	UNP Q7M1T4
E	70	LYS	ARG	conflict	UNP Q7M1T4
E	84	GLY	ALA	conflict	UNP Q7M1T4
E	145	ILE	VAL	conflict	UNP Q7M1T4
E	148	SER	ALA	conflict	UNP Q7M1T4
F	1	AYA	ALA	modified residue	UNP Q7M1T4
F	9	SER	PRO	conflict	UNP Q7M1T4
F	20	GLU	ASP	conflict	UNP Q7M1T4
F	49	ASP	GLU	conflict	UNP Q7M1T4
F	70	LYS	ARG	conflict	UNP Q7M1T4
F	84	GLY	ALA	conflict	UNP Q7M1T4
F	145	ILE	VAL	conflict	UNP Q7M1T4
F	148	SER	ALA	conflict	UNP Q7M1T4
G	1	AYA	ALA	modified residue	UNP Q7M1T4
G	9	SER	PRO	conflict	UNP Q7M1T4
G	20	GLU	ASP	conflict	UNP Q7M1T4
G	49	ASP	GLU	conflict	UNP Q7M1T4
G	70	LYS	ARG	conflict	UNP Q7M1T4
G	84	GLY	ALA	conflict	UNP Q7M1T4
G	145	ILE	VAL	conflict	UNP Q7M1T4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	148	SER	ALA	conflict	UNP Q7M1T4
H	1	AYA	ALA	modified residue	UNP Q7M1T4
H	9	SER	PRO	conflict	UNP Q7M1T4
H	20	GLU	ASP	conflict	UNP Q7M1T4
H	49	ASP	GLU	conflict	UNP Q7M1T4
H	70	LYS	ARG	conflict	UNP Q7M1T4
H	84	GLY	ALA	conflict	UNP Q7M1T4
H	145	ILE	VAL	conflict	UNP Q7M1T4
H	148	SER	ALA	conflict	UNP Q7M1T4

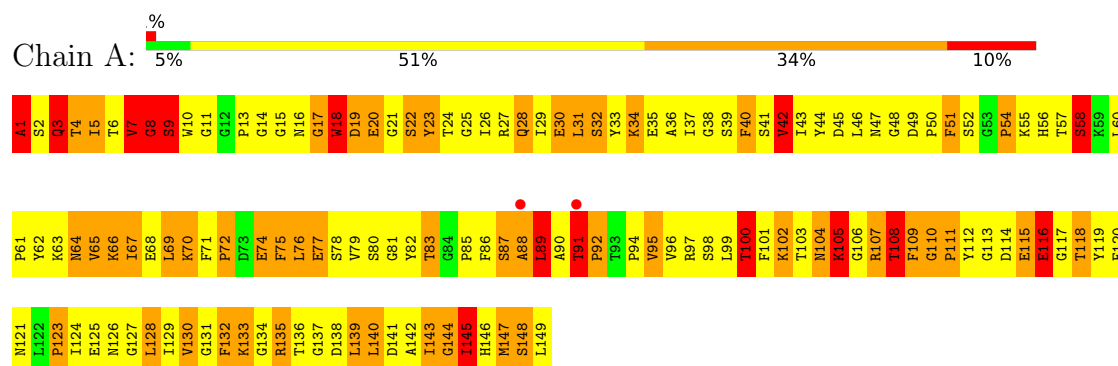
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	118	Total O 118 118	0	0
2	B	123	Total O 123 123	0	0
2	C	121	Total O 121 121	0	0
2	D	121	Total O 121 121	0	0
2	E	93	Total O 93 93	0	0
2	F	115	Total O 115 115	0	0
2	G	102	Total O 102 102	0	0
2	H	81	Total O 81 81	0	0

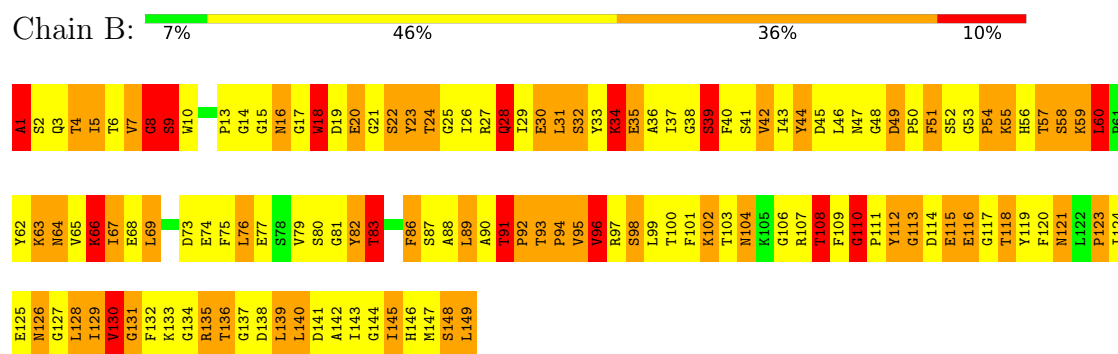
3 Residue-property plots

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

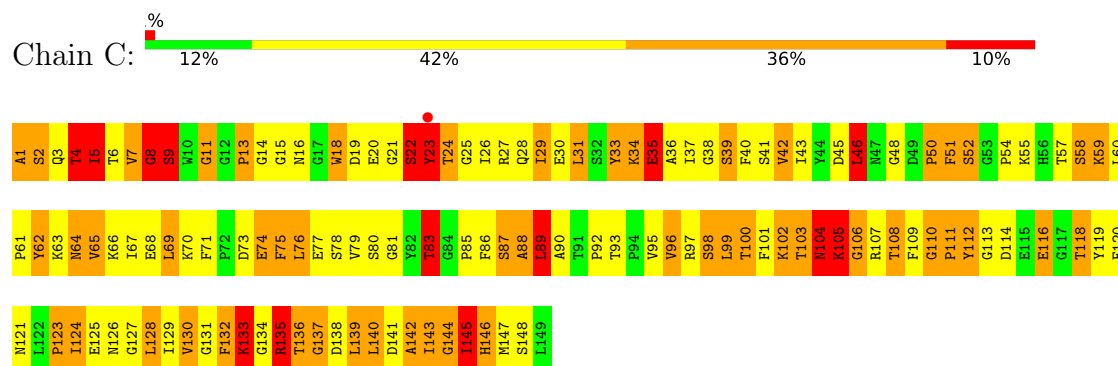
• Molecule 1: Artocarpin



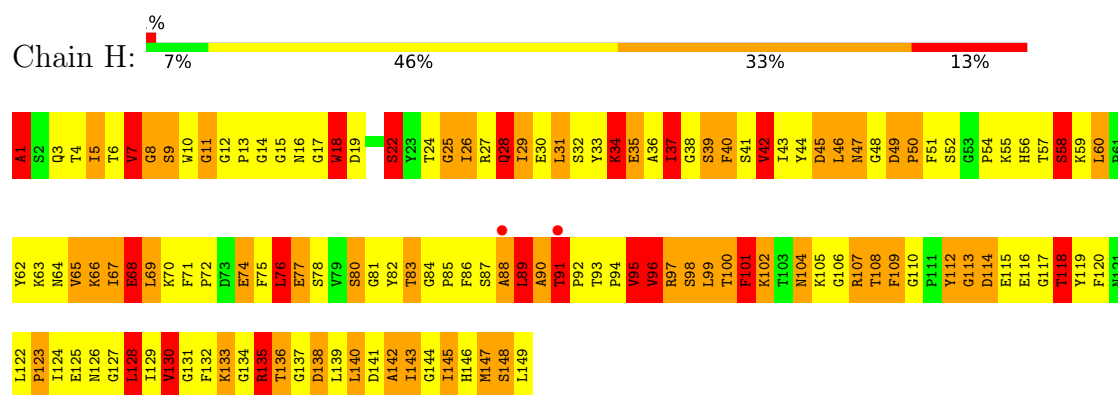
• Molecule 1: Artocarpin



• Molecule 1: Artocarpin



• Molecule 1: Artocarpin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.69Å 72.19Å 92.63Å 90.00° 101.15° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.40) 82.3 (20.00-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.41Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.191 , 0.258 0.203 , 0.260	Depositor DCC
R_{free} test set	1536 reflections (4.18%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtrriage
Anisotropy	0.137	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 72.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9922	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.0588e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.33	3/1155 (0.3%)	2.79	154/1569 (9.8%)
1	B	1.34	6/1155 (0.5%)	2.86	151/1569 (9.6%)
1	C	1.35	5/1155 (0.4%)	2.92	158/1569 (10.1%)
1	D	1.24	7/1155 (0.6%)	3.14	156/1569 (9.9%)
1	E	1.20	5/1151 (0.4%)	3.09	148/1565 (9.5%)
1	F	1.63	9/1151 (0.8%)	2.90	151/1565 (9.6%)
1	G	1.59	7/1155 (0.6%)	2.72	138/1569 (8.8%)
1	H	1.24	7/1155 (0.6%)	3.00	144/1569 (9.2%)
All	All	1.37	49/9232 (0.5%)	2.93	1200/12544 (9.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	8
1	B	1	4
1	C	1	8
1	D	0	5
1	E	1	5
1	F	0	7
1	G	1	5
1	H	1	4
All	All	6	46

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	70	LYS	CD-CE	32.69	2.50	1.52
1	F	70	LYS	CD-CE	30.66	2.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	33	TYR	C-N	18.56	1.59	1.33
1	A	34	LYS	C-N	16.98	1.58	1.33
1	C	33	TYR	C-N	15.29	1.55	1.33
1	F	90	ALA	C-N	-15.00	1.15	1.33
1	F	34	LYS	C-N	13.09	1.53	1.33
1	F	22	SER	C-N	-11.02	1.20	1.33
1	D	8	GLY	C-N	-11.01	1.20	1.33
1	B	89	LEU	C-N	-11.00	1.19	1.33
1	C	22	SER	C-N	-10.63	1.20	1.33
1	E	33	TYR	C-N	10.53	1.48	1.33
1	G	96	VAL	CA-CB	10.22	1.65	1.53
1	B	59	LYS	C-O	-9.43	1.11	1.24
1	F	9	SER	C-N	-9.41	1.20	1.33
1	D	33	TYR	C-N	-8.64	1.21	1.33
1	D	22	SER	C-N	-8.32	1.22	1.33
1	H	33	TYR	C-N	7.88	1.44	1.33
1	H	8	GLY	C-N	-7.85	1.22	1.33
1	D	34	LYS	C-N	-7.53	1.22	1.33
1	E	34	LYS	C-N	-6.99	1.23	1.33
1	A	33	TYR	C-N	6.90	1.43	1.33
1	B	96	VAL	CA-CB	6.88	1.61	1.53
1	F	89	LEU	C-N	-6.67	1.24	1.33
1	G	89	LEU	C-N	6.66	1.43	1.33
1	H	82	TYR	CA-C	-6.63	1.44	1.52
1	G	34	LYS	C-N	6.59	1.43	1.33
1	E	37	ILE	CA-CB	6.44	1.61	1.54
1	B	90	ALA	C-N	-6.38	1.25	1.33
1	A	91	THR	CA-CB	6.37	1.64	1.54
1	E	9	SER	C-N	-6.33	1.24	1.33
1	G	57	THR	CA-CB	6.11	1.62	1.53
1	G	90	ALA	C-N	6.05	1.42	1.33
1	D	100	THR	CA-CB	5.89	1.62	1.53
1	C	136	THR	CA-CB	5.84	1.62	1.53
1	B	143	ILE	CA-CB	5.80	1.62	1.54
1	G	68	GLU	CA-C	-5.64	1.45	1.52
1	D	90	ALA	CA-CB	5.58	1.61	1.53
1	F	37	ILE	CA-CB	5.48	1.61	1.54
1	H	43	ILE	CA-CB	5.47	1.59	1.53
1	C	90	ALA	C-N	-5.39	1.26	1.33
1	H	90	ALA	C-O	5.38	1.30	1.24
1	C	133	LYS	CE-NZ	5.21	1.65	1.49
1	H	6	THR	CA-CB	-5.16	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	89	LEU	CB-CG	5.12	1.63	1.53
1	D	70	LYS	CA-CB	5.11	1.58	1.52
1	E	91	THR	CA-CB	5.11	1.62	1.53
1	F	90	ALA	CA-C	-5.09	1.46	1.52
1	F	70	LYS	CE-NZ	-5.03	1.34	1.49

All (1200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	34	LYS	O-C-N	-43.70	64.47	122.59
1	D	34	LYS	O-C-N	-33.93	77.46	122.59
1	H	9	SER	O-C-N	-33.53	77.99	122.59
1	H	89	LEU	O-C-N	-31.42	91.07	122.18
1	B	8	GLY	O-C-N	-27.23	100.28	122.88
1	D	8	GLY	O-C-N	-26.65	95.60	123.05
1	D	8	GLY	CA-C-N	26.55	164.58	121.58
1	D	8	GLY	C-N-CA	26.55	164.58	121.58
1	G	70	LYS	CD-CE-NZ	-25.79	29.38	111.90
1	F	70	LYS	CD-CE-NZ	-25.34	30.80	111.90
1	C	89	LEU	O-C-N	-22.57	93.07	122.19
1	A	33	TYR	O-C-N	-22.50	97.90	123.33
1	E	8	GLY	O-C-N	-22.06	96.96	123.21
1	C	9	SER	O-C-N	-22.05	93.26	122.59
1	F	9	SER	O-C-N	-21.23	94.35	122.59
1	D	33	TYR	O-C-N	-21.20	100.74	123.42
1	B	9	SER	O-C-N	-20.11	95.85	122.59
1	E	8	GLY	CA-C-N	18.62	157.10	121.54
1	E	8	GLY	C-N-CA	18.62	157.10	121.54
1	G	8	GLY	O-C-N	-18.30	102.54	122.67
1	A	34	LYS	O-C-N	-17.92	98.76	122.59
1	C	23	TYR	O-C-N	-17.74	104.63	123.26
1	F	90	ALA	O-C-N	-17.43	99.40	122.59
1	E	33	TYR	CA-C-N	-15.43	92.07	121.54
1	E	33	TYR	C-N-CA	-15.43	92.07	121.54
1	B	34	LYS	O-C-N	-15.39	102.12	122.59
1	B	89	LEU	CA-C-N	15.21	144.42	122.82
1	B	89	LEU	C-N-CA	15.21	144.42	122.82
1	H	90	ALA	O-C-N	14.86	142.36	122.59
1	D	9	SER	O-C-N	-14.69	105.05	123.26
1	C	89	LEU	CA-C-N	14.57	143.53	122.40
1	C	89	LEU	C-N-CA	14.57	143.53	122.40
1	B	144	GLY	O-C-N	-14.51	112.78	123.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	LEU	N-CA-C	-14.18	96.90	113.21
1	H	8	GLY	O-C-N	-14.18	108.44	123.05
1	D	22	SER	O-C-N	-14.16	106.82	123.10
1	H	90	ALA	CA-C-N	-13.83	105.35	122.64
1	H	90	ALA	C-N-CA	-13.83	105.35	122.64
1	H	9	SER	CA-C-N	13.56	142.03	123.05
1	H	9	SER	C-N-CA	13.56	142.03	123.05
1	H	144	GLY	O-C-N	-13.53	113.53	123.95
1	E	34	LYS	CB-CA-C	-13.39	83.77	110.42
1	E	9	SER	O-C-N	-13.02	105.27	122.59
1	A	8	GLY	O-C-N	-12.87	108.70	122.98
1	F	70	LYS	CG-CD-CE	12.81	140.76	111.30
1	B	8	GLY	CA-C-N	12.55	145.52	121.54
1	B	8	GLY	C-N-CA	12.55	145.52	121.54
1	E	34	LYS	CA-C-N	12.45	145.85	121.58
1	E	34	LYS	C-N-CA	12.45	145.85	121.58
1	C	8	GLY	O-C-N	-12.31	107.19	122.58
1	D	123	PRO	O-C-N	-12.23	111.07	122.93
1	F	144	GLY	O-C-N	-12.12	113.06	123.60
1	B	33	TYR	CA-C-N	-12.02	98.59	121.54
1	B	33	TYR	C-N-CA	-12.02	98.59	121.54
1	B	134	GLY	O-C-N	-11.95	112.53	123.88
1	G	88	ALA	O-C-N	-11.67	109.75	122.12
1	F	89	LEU	CA-C-N	11.64	143.78	121.54
1	F	89	LEU	C-N-CA	11.64	143.78	121.54
1	A	127	GLY	O-C-N	-11.57	112.55	123.78
1	H	113	GLY	O-C-N	-11.45	111.67	123.00
1	H	89	LEU	N-CA-C	-11.44	96.91	110.41
1	E	144	GLY	O-C-N	-11.40	115.17	123.95
1	F	22	SER	O-C-N	-11.29	110.11	123.10
1	F	138	ASP	N-CA-C	-11.28	98.12	112.90
1	E	134	GLY	O-C-N	-11.19	114.51	123.80
1	D	25	GLY	O-C-N	-11.05	113.31	123.92
1	G	29	ILE	O-C-N	-11.01	111.62	123.18
1	G	8	GLY	CA-C-N	10.95	142.45	121.54
1	G	8	GLY	C-N-CA	10.95	142.45	121.54
1	D	9	SER	N-CA-C	-10.92	89.91	107.93
1	F	29	ILE	O-C-N	-10.91	112.13	122.71
1	C	22	SER	O-C-N	-10.74	109.62	123.16
1	G	15	GLY	O-C-N	-10.66	112.07	123.05
1	D	34	LYS	CA-C-N	10.58	138.85	122.24
1	D	34	LYS	C-N-CA	10.58	138.85	122.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	33	TYR	O-C-N	-10.57	112.16	123.26
1	D	22	SER	CA-C-N	10.47	139.05	121.87
1	D	22	SER	C-N-CA	10.47	139.05	121.87
1	F	127	GLY	O-C-N	-10.47	114.53	123.43
1	A	81	GLY	O-C-N	-10.47	111.47	123.61
1	F	25	GLY	O-C-N	-10.43	113.38	123.81
1	H	146	HIS	O-C-N	-10.28	111.55	123.06
1	F	134	GLY	O-C-N	-10.27	112.65	124.15
1	E	95	VAL	O-C-N	-10.21	111.77	123.00
1	B	129	ILE	N-CA-C	-10.15	96.48	109.58
1	H	129	ILE	N-CA-C	-10.15	96.49	109.58
1	F	130	VAL	O-C-N	-10.13	112.03	122.06
1	C	8	GLY	CA-C-N	10.10	140.84	121.54
1	C	8	GLY	C-N-CA	10.10	140.84	121.54
1	F	33	TYR	O-C-N	-10.07	110.06	123.15
1	A	113	GLY	O-C-N	-10.05	112.04	122.70
1	G	4	THR	O-C-N	-10.04	112.03	123.48
1	C	145	ILE	N-CA-C	9.98	121.53	108.35
1	C	90	ALA	N-CA-C	9.92	124.94	112.24
1	F	91	THR	CA-C-N	9.90	129.56	119.56
1	F	91	THR	C-N-CA	9.90	129.56	119.56
1	A	14	GLY	O-C-N	-9.87	113.50	122.88
1	A	25	GLY	O-C-N	-9.85	114.47	123.92
1	D	83	THR	O-C-N	-9.85	111.67	123.29
1	C	148	SER	O-C-N	-9.83	113.46	123.29
1	H	8	GLY	CA-C-N	9.83	140.31	121.54
1	H	8	GLY	C-N-CA	9.83	140.31	121.54
1	E	130	VAL	O-C-N	-9.82	113.22	122.16
1	H	34	LYS	O-C-N	-9.79	109.58	122.59
1	A	130	VAL	O-C-N	-9.74	113.30	122.16
1	G	9	SER	N-CA-C	-9.73	90.07	110.80
1	C	95	VAL	O-C-N	-9.71	112.05	123.02
1	H	35	GLU	N-CA-C	-9.68	101.02	113.12
1	B	89	LEU	O-C-N	-9.67	109.83	122.20
1	C	134	GLY	O-C-N	-9.63	114.43	123.96
1	F	69	LEU	O-C-N	-9.58	112.33	123.06
1	B	29	ILE	O-C-N	-9.55	112.86	123.18
1	C	25	GLY	O-C-N	-9.55	114.51	123.96
1	H	9	SER	N-CA-C	-9.47	90.63	110.80
1	E	89	LEU	N-CA-C	-9.46	101.25	113.17
1	H	120	PHE	O-C-N	-9.46	112.64	123.33
1	C	114	ASP	O-C-N	-9.41	112.50	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	SER	O-C-N	-9.40	111.68	123.24
1	H	32	SER	O-C-N	-9.38	112.43	123.41
1	C	99	LEU	O-C-N	-9.37	111.84	123.27
1	A	134	GLY	N-CA-C	9.36	123.29	110.56
1	B	133	LYS	O-C-N	-9.33	112.78	123.33
1	F	131	GLY	O-C-N	-9.32	115.10	123.76
1	C	22	SER	CA-C-N	9.28	137.67	121.80
1	C	22	SER	C-N-CA	9.28	137.67	121.80
1	D	65	VAL	O-C-N	-9.28	113.04	122.97
1	D	129	ILE	O-C-N	-9.25	111.01	122.57
1	G	6	THR	O-C-N	-9.25	112.30	123.30
1	D	100	THR	O-C-N	-9.21	112.59	123.27
1	H	105	LYS	N-CA-C	-9.19	101.33	112.54
1	A	117	GLY	O-C-N	-9.18	114.13	122.85
1	A	37	ILE	O-C-N	-9.17	111.75	122.94
1	E	55	LYS	O-C-N	-9.16	112.33	123.04
1	E	81	GLY	O-C-N	-9.12	110.84	122.70
1	F	89	LEU	O-C-N	-9.11	110.70	121.99
1	E	100	THR	O-C-N	-9.10	112.55	123.29
1	E	18	TRP	O-C-N	-9.05	113.97	123.56
1	H	123	PRO	O-C-N	-9.04	114.16	122.93
1	G	138	ASP	N-CA-C	-9.04	102.38	113.41
1	G	25	GLY	O-C-N	-9.01	114.80	123.81
1	C	135	ARG	O-C-N	-8.99	112.84	123.27
1	A	134	GLY	O-C-N	-8.95	114.09	123.58
1	G	99	LEU	O-C-N	-8.95	112.44	123.36
1	F	95	VAL	O-C-N	-8.95	112.91	123.02
1	E	101	PHE	O-C-N	-8.94	111.89	123.16
1	H	99	LEU	O-C-N	-8.92	113.31	123.48
1	F	81	GLY	O-C-N	-8.92	115.36	123.92
1	F	55	LYS	O-C-N	-8.91	112.88	123.13
1	A	146	HIS	O-C-N	-8.90	112.77	123.27
1	F	89	LEU	CA-CB-CG	8.85	147.26	116.30
1	E	146	HIS	O-C-N	-8.84	112.91	123.16
1	E	9	SER	N-CA-C	-8.82	92.02	110.80
1	H	138	ASP	N-CA-C	-8.81	102.27	113.72
1	C	129	ILE	O-C-N	-8.80	112.33	122.72
1	D	18	TRP	O-C-N	-8.80	113.06	123.27
1	D	142	ALA	O-C-N	-8.80	113.62	123.48
1	B	21	GLY	O-C-N	-8.76	114.36	122.86
1	E	123	PRO	O-C-N	-8.76	112.02	123.06
1	G	101	PHE	O-C-N	-8.74	113.02	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	6	THR	O-C-N	-8.73	113.40	123.27
1	C	79	VAL	O-C-N	-8.72	114.05	123.03
1	A	74	GLU	O-C-N	-8.71	113.01	123.29
1	D	145	ILE	O-C-N	-8.71	113.78	123.10
1	C	51	PHE	O-C-N	-8.68	113.20	123.27
1	A	16	ASN	O-C-N	-8.68	113.33	123.22
1	C	29	ILE	O-C-N	-8.66	113.73	123.00
1	C	130	VAL	O-C-N	-8.64	112.88	121.78
1	E	75	PHE	O-C-N	-8.64	114.17	123.42
1	D	5	ILE	O-C-N	-8.62	114.42	122.79
1	H	102	LYS	O-C-N	-8.62	113.04	123.30
1	G	76	LEU	O-C-N	-8.62	112.26	122.95
1	C	28	GLN	O-C-N	-8.60	113.84	123.48
1	D	131	GLY	O-C-N	-8.60	115.76	123.76
1	D	113	GLY	O-C-N	-8.59	113.58	122.60
1	H	128	LEU	O-C-N	-8.58	112.89	123.36
1	C	15	GLY	O-C-N	-8.57	113.51	122.68
1	F	4	THR	O-C-N	-8.57	114.25	123.42
1	G	79	VAL	O-C-N	-8.57	114.21	123.03
1	D	53	GLY	CA-C-N	8.56	130.55	119.84
1	D	53	GLY	C-N-CA	8.56	130.55	119.84
1	E	62	TYR	O-C-N	-8.56	112.73	122.75
1	F	38	GLY	O-C-N	-8.55	111.58	122.70
1	B	121	ASN	O-C-N	-8.54	113.28	123.27
1	D	95	VAL	O-C-N	-8.51	113.64	123.00
1	A	15	GLY	O-C-N	-8.49	114.71	122.77
1	F	45	ASP	O-C-N	-8.49	113.68	123.27
1	G	129	ILE	N-CA-C	-8.48	96.23	108.36
1	B	124	ILE	O-C-N	-8.47	113.92	122.99
1	C	45	ASP	O-C-N	-8.47	113.70	123.27
1	G	127	GLY	O-C-N	-8.46	113.92	123.23
1	E	135	ARG	O-C-N	-8.46	113.84	123.48
1	F	36	ALA	O-C-N	-8.45	114.38	123.42
1	G	42	VAL	O-C-N	-8.45	113.71	123.00
1	B	119	TYR	O-C-N	-8.43	113.18	123.04
1	A	17	GLY	O-C-N	-8.43	111.75	122.70
1	H	78	SER	O-C-N	-8.42	114.63	123.56
1	B	143	ILE	O-C-N	-8.41	112.06	122.57
1	E	50	PRO	O-C-N	-8.41	113.68	123.10
1	C	139	LEU	O-C-N	-8.39	112.19	122.68
1	E	81	GLY	N-CA-C	8.38	133.03	113.18
1	B	101	PHE	O-C-N	-8.34	113.44	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	82	TYR	O-C-N	-8.32	113.39	123.30
1	E	7	VAL	O-C-N	-8.31	114.31	123.03
1	A	29	ILE	O-C-N	-8.30	114.22	123.18
1	H	129	ILE	O-C-N	-8.29	113.58	122.61
1	D	114	ASP	O-C-N	-8.28	112.75	122.93
1	G	40	PHE	O-C-N	-8.26	113.28	123.44
1	H	95	VAL	O-C-N	-8.26	113.87	123.04
1	C	36	ALA	O-C-N	-8.25	114.16	122.99
1	G	5	ILE	O-C-N	-8.25	113.61	122.61
1	A	79	VAL	O-C-N	-8.24	114.61	123.18
1	A	95	VAL	O-C-N	-8.24	113.60	123.00
1	F	79	VAL	O-C-N	-8.24	114.30	123.20
1	G	51	PHE	O-C-N	-8.24	112.73	123.28
1	G	62	TYR	O-C-N	-8.24	113.28	122.84
1	H	117	GLY	O-C-N	-8.23	115.03	122.85
1	E	63	LYS	O-C-N	-8.23	113.66	122.96
1	G	121	ASN	O-C-N	-8.23	112.75	123.28
1	B	15	GLY	O-C-N	-8.22	113.22	122.68
1	C	131	GLY	O-C-N	-8.22	115.56	123.87
1	A	31	LEU	O-C-N	-8.22	113.64	123.10
1	F	76	LEU	O-C-N	-8.21	112.87	122.89
1	H	101	PHE	O-C-N	-8.19	113.61	123.19
1	A	11	GLY	O-C-N	-8.18	114.09	124.15
1	A	22	SER	O-C-N	-8.18	114.03	123.27
1	C	90	ALA	CA-C-N	-8.17	109.08	122.65
1	C	90	ALA	C-N-CA	-8.17	109.08	122.65
1	A	35	GLU	N-CA-C	-8.17	103.51	113.97
1	G	95	VAL	O-C-N	-8.17	113.88	122.95
1	B	138	ASP	N-CA-C	-8.16	103.12	113.72
1	F	15	GLY	O-C-N	-8.15	113.31	122.68
1	E	141	ASP	O-C-N	-8.14	112.86	122.15
1	H	89	LEU	CA-C-O	8.13	128.34	121.02
1	F	48	GLY	O-C-N	-8.12	113.78	122.56
1	H	54	PRO	O-C-N	-8.12	112.96	122.71
1	A	144	GLY	O-C-N	-8.12	114.84	123.45
1	D	30	GLU	O-C-N	-8.12	113.85	123.27
1	E	69	LEU	O-C-N	-8.12	113.43	123.01
1	D	120	PHE	O-C-N	-8.11	113.52	123.33
1	G	55	LYS	O-C-N	-8.10	113.45	123.01
1	B	80	SER	O-C-N	-8.09	114.77	123.26
1	C	16	ASN	O-C-N	-8.09	113.73	123.19
1	D	51	PHE	O-C-N	-8.09	113.89	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	86	PHE	O-C-N	-8.08	113.73	123.27
1	C	130	VAL	CA-C-O	8.08	125.76	119.46
1	A	101	PHE	O-C-N	-8.08	113.76	123.29
1	H	46	LEU	O-C-N	-8.07	112.52	123.01
1	F	91	THR	N-CA-C	-8.06	93.69	108.85
1	D	101	PHE	O-C-N	-8.05	112.97	122.87
1	A	9	SER	N-CA-C	-8.05	93.66	110.80
1	C	37	ILE	O-C-N	-8.04	113.50	122.83
1	A	99	LEU	O-C-N	-8.04	113.30	123.26
1	F	143	ILE	O-C-N	-8.04	114.82	123.18
1	G	130	VAL	O-C-N	-8.04	113.33	122.09
1	D	4	THR	O-C-N	-8.03	114.01	123.41
1	F	21	GLY	O-C-N	-8.03	113.65	123.21
1	C	18	TRP	O-C-N	-8.03	113.46	123.17
1	G	41	SER	O-C-N	-8.01	114.11	123.25
1	H	5	ILE	O-C-N	-8.01	113.67	122.64
1	B	100	THR	O-C-N	-7.99	113.96	123.31
1	B	86	PHE	O-C-N	-7.99	112.81	123.19
1	E	25	GLY	O-C-N	-7.96	114.47	123.62
1	F	146	HIS	O-C-N	-7.96	113.90	123.29
1	A	42	VAL	O-C-N	-7.96	114.49	123.00
1	A	63	LYS	O-C-N	-7.95	114.16	123.22
1	C	42	VAL	O-C-N	-7.95	113.63	122.69
1	B	60	LEU	CA-C-N	7.94	129.77	119.84
1	B	60	LEU	C-N-CA	7.94	129.77	119.84
1	D	80	SER	O-C-N	-7.94	112.95	122.96
1	H	106	GLY	O-C-N	-7.94	113.69	122.50
1	D	145	ILE	N-CA-C	7.93	120.28	108.46
1	E	127	GLY	O-C-N	-7.92	114.51	123.23
1	B	44	TYR	O-C-N	-7.91	113.83	122.85
1	G	143	ILE	O-C-N	-7.91	113.94	123.03
1	C	26	ILE	O-C-N	-7.89	114.56	123.00
1	E	143	ILE	O-C-N	-7.89	114.30	123.05
1	A	68	GLU	O-C-N	-7.88	112.67	122.68
1	A	33	TYR	CA-C-N	7.88	136.59	121.54
1	A	33	TYR	C-N-CA	7.88	136.59	121.54
1	A	7	VAL	O-C-N	-7.87	114.68	123.10
1	C	106	GLY	O-C-N	-7.86	112.48	122.70
1	G	66	LYS	O-C-N	-7.86	113.01	123.23
1	B	95	VAL	O-C-N	-7.86	114.32	123.04
1	B	57	THR	N-CA-C	7.86	122.65	109.76
1	E	142	ALA	O-C-N	-7.86	114.29	123.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	VAL	O-C-N	-7.86	114.36	123.00
1	E	29	ILE	O-C-N	-7.85	114.61	122.93
1	D	45	ASP	O-C-N	-7.83	114.29	123.22
1	F	100	THR	O-C-N	-7.83	114.11	123.27
1	A	4	THR	O-C-N	-7.82	111.76	122.94
1	F	78	SER	O-C-N	-7.82	114.57	123.48
1	F	27	ARG	O-C-N	-7.81	112.97	122.19
1	C	89	LEU	N-CA-C	-7.81	103.75	112.57
1	H	96	VAL	O-C-N	-7.81	114.09	122.83
1	D	102	LYS	O-C-N	-7.80	113.66	122.86
1	H	135	ARG	O-C-N	-7.80	112.66	123.34
1	F	140	LEU	O-C-N	-7.79	112.79	122.68
1	H	51	PHE	O-C-N	-7.79	114.20	123.31
1	E	42	VAL	O-C-N	-7.79	114.77	123.10
1	C	14	GLY	O-C-N	-7.79	112.90	122.71
1	E	107	ARG	O-C-N	-7.79	113.67	122.86
1	C	113	GLY	O-C-N	-7.78	114.93	123.10
1	D	57	THR	O-C-N	-7.77	113.84	123.01
1	B	106	GLY	O-C-N	-7.77	112.52	122.39
1	G	107	ARG	O-C-N	-7.76	113.85	123.01
1	E	126	ASN	O-C-N	-7.76	114.19	123.27
1	F	62	TYR	O-C-N	-7.76	114.26	123.03
1	F	141	ASP	O-C-N	-7.74	113.73	122.09
1	B	45	ASP	O-C-N	-7.73	114.15	123.27
1	F	113	GLY	O-C-N	-7.73	114.49	122.60
1	B	18	TRP	O-C-N	-7.73	113.82	123.17
1	D	90	ALA	O-C-N	-7.72	113.72	122.91
1	A	64	ASN	O-C-N	-7.72	114.29	122.94
1	B	136	THR	O-C-N	-7.72	114.38	123.41
1	C	145	ILE	O-C-N	-7.72	114.14	123.09
1	D	67	ILE	O-C-N	-7.72	114.07	123.10
1	D	134	GLY	O-C-N	-7.71	116.52	123.92
1	H	81	GLY	O-C-N	-7.70	114.73	123.67
1	E	37	ILE	O-C-N	-7.70	114.28	122.67
1	C	31	LEU	O-C-N	-7.70	114.48	123.25
1	G	63	LYS	O-C-N	-7.69	114.45	123.22
1	H	76	LEU	O-C-N	-7.69	113.59	122.97
1	E	17	GLY	O-C-N	-7.69	112.70	122.70
1	E	124	ILE	O-C-N	-7.69	114.11	123.10
1	G	28	GLN	O-C-N	-7.68	114.66	123.42
1	C	130	VAL	N-CA-C	-7.68	105.83	113.20
1	H	58	SER	O-C-N	-7.68	114.21	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	83	THR	O-C-N	-7.66	113.27	123.23
1	H	15	GLY	O-C-N	-7.66	114.59	123.17
1	F	32	SER	O-C-N	-7.66	114.19	123.30
1	A	6	THR	O-C-N	-7.64	114.20	123.30
1	D	108	THR	O-C-N	-7.63	112.88	123.34
1	E	22	SER	O-C-N	-7.63	114.26	123.19
1	F	128	LEU	O-C-N	-7.63	114.05	123.36
1	F	135	ARG	O-C-N	-7.63	114.09	123.33
1	A	28	GLN	O-C-N	-7.62	114.79	123.48
1	A	133	LYS	O-C-N	-7.62	111.78	122.76
1	H	55	LYS	O-C-N	-7.62	114.53	123.22
1	A	107	ARG	O-C-N	-7.62	113.67	122.97
1	D	76	LEU	O-C-N	-7.61	113.93	123.06
1	D	74	GLU	O-C-N	-7.61	114.30	123.27
1	F	63	LYS	O-C-N	-7.60	113.61	122.89
1	B	89	LEU	CB-CA-C	7.60	123.36	111.13
1	E	16	ASN	O-C-N	-7.60	114.15	123.04
1	E	136	THR	O-C-N	-7.60	113.41	123.14
1	G	94	PRO	O-C-N	-7.60	113.59	123.01
1	F	41	SER	O-C-N	-7.58	114.84	123.48
1	C	81	GLY	O-C-N	-7.57	114.91	123.62
1	C	119	TYR	N-CA-C	7.57	121.38	110.10
1	D	19	ASP	O-C-N	-7.57	113.30	123.14
1	B	17	GLY	O-C-N	-7.56	113.61	122.91
1	H	45	ASP	O-C-N	-7.55	114.61	123.22
1	F	91	THR	CB-CA-C	7.55	120.24	110.13
1	H	124	ILE	O-C-N	-7.53	113.44	122.77
1	D	41	SER	O-C-N	-7.52	114.68	123.25
1	A	57	THR	O-C-N	-7.51	114.47	122.96
1	H	62	TYR	O-C-N	-7.51	114.13	122.84
1	B	63	LYS	O-C-N	-7.51	113.70	122.93
1	D	146	HIS	O-C-N	-7.50	114.46	123.16
1	A	132	PHE	O-C-N	-7.50	113.48	123.23
1	E	130	VAL	CA-C-O	7.50	127.22	119.35
1	D	99	LEU	O-C-N	-7.49	114.50	123.27
1	A	69	LEU	O-C-N	-7.49	114.31	122.85
1	A	136	THR	O-C-N	-7.49	114.51	123.27
1	D	43	ILE	O-C-N	-7.48	115.40	123.18
1	C	77	GLU	O-C-N	-7.48	113.15	122.35
1	B	146	HIS	O-C-N	-7.48	114.82	123.27
1	E	102	LYS	O-C-N	-7.48	114.24	123.36
1	D	24	THR	O-C-N	-7.47	112.15	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	71	PHE	N-CA-C	-7.46	100.36	109.83
1	G	81	GLY	O-C-N	-7.46	113.42	123.64
1	D	144	GLY	O-C-N	-7.45	116.64	123.57
1	C	6	THR	O-C-N	-7.45	114.50	123.29
1	H	98	SER	O-C-N	-7.45	112.73	122.94
1	G	10	TRP	O-C-N	-7.44	114.86	123.27
1	H	142	ALA	O-C-N	-7.44	114.92	123.33
1	D	107	ARG	O-C-N	-7.44	113.90	122.68
1	E	79	VAL	O-C-N	-7.44	115.44	123.18
1	E	113	GLY	O-C-N	-7.43	114.14	122.68
1	G	133	LYS	O-C-N	-7.42	113.81	123.16
1	B	114	ASP	O-C-N	-7.41	114.90	123.27
1	F	30	GLU	O-C-N	-7.41	114.27	123.01
1	F	119	TYR	O-C-N	-7.41	114.27	123.01
1	D	6	THR	O-C-N	-7.40	114.68	123.27
1	F	66	LYS	O-C-N	-7.40	114.90	123.27
1	C	21	GLY	O-C-N	-7.39	115.34	123.10
1	C	88	ALA	O-C-N	-7.39	114.40	122.09
1	H	18	TRP	O-C-N	-7.38	114.83	123.25
1	B	31	LEU	O-C-N	-7.38	115.53	123.42
1	G	106	GLY	O-C-N	-7.37	113.04	122.39
1	A	124	ILE	O-C-N	-7.36	114.49	123.10
1	E	6	THR	O-C-N	-7.36	114.58	123.27
1	G	102	LYS	O-C-N	-7.36	114.30	123.27
1	H	114	ASP	O-C-N	-7.36	114.67	123.13
1	B	130	VAL	O-C-N	-7.35	113.38	122.57
1	C	141	ASP	O-C-N	-7.35	114.15	122.09
1	E	114	ASP	O-C-N	-7.35	113.70	122.96
1	C	144	GLY	O-C-N	-7.35	113.15	122.70
1	E	90	ALA	O-C-N	-7.35	113.76	122.58
1	F	130	VAL	CA-C-O	7.34	125.77	119.38
1	H	24	THR	N-CA-C	-7.34	104.57	113.97
1	F	3	GLN	O-C-N	-7.34	112.96	122.72
1	F	31	LEU	O-C-N	-7.34	115.04	123.33
1	A	131	GLY	O-C-N	-7.34	115.16	123.67
1	D	124	ILE	O-C-N	-7.34	114.89	123.03
1	B	65	VAL	O-C-N	-7.34	115.28	123.20
1	D	94	PRO	O-C-N	-7.34	114.30	123.10
1	A	123	PRO	O-C-N	-7.33	113.82	123.06
1	C	74	GLU	O-C-N	-7.33	113.66	123.19
1	D	58	SER	O-C-N	-7.33	114.67	123.10
1	A	58	SER	O-C-N	-7.33	114.33	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	37	ILE	O-C-N	-7.33	114.68	122.81
1	F	83	THR	O-C-N	-7.32	114.66	123.29
1	C	124	ILE	O-C-N	-7.32	115.45	123.20
1	D	42	VAL	O-C-N	-7.31	114.83	122.95
1	C	40	PHE	O-C-N	-7.31	113.33	123.34
1	E	116	GLU	N-CA-C	7.31	120.39	108.26
1	C	41	SER	O-C-N	-7.31	113.33	123.34
1	D	64	ASN	O-C-N	-7.30	114.73	123.13
1	F	19	ASP	O-C-N	-7.30	113.48	123.12
1	A	66	LYS	O-C-N	-7.30	114.61	123.30
1	C	76	LEU	O-C-N	-7.30	113.95	122.93
1	D	32	SER	O-C-N	-7.30	114.26	123.24
1	C	146	HIS	O-C-N	-7.29	114.66	123.19
1	C	68	GLU	O-C-N	-7.29	114.06	123.02
1	C	63	LYS	O-C-N	-7.29	114.71	123.16
1	H	14	GLY	O-C-N	-7.29	115.75	122.96
1	C	126	ASN	O-C-N	-7.28	112.90	122.59
1	B	99	LEU	O-C-N	-7.28	113.96	123.28
1	C	110	GLY	CA-C-N	7.28	128.93	119.84
1	C	110	GLY	C-N-CA	7.28	128.93	119.84
1	H	88	ALA	O-C-N	-7.28	112.42	122.46
1	C	121	ASN	O-C-N	-7.27	114.53	123.33
1	A	129	ILE	O-C-N	-7.27	114.30	122.66
1	F	64	ASN	O-C-N	-7.26	114.75	123.10
1	G	100	THR	O-C-N	-7.26	114.77	123.27
1	B	90	ALA	N-CA-C	7.25	121.39	111.17
1	C	66	LYS	O-C-N	-7.25	114.75	123.16
1	E	35	GLU	N-CA-C	-7.25	104.41	113.18
1	E	148	SER	O-C-N	-7.25	115.66	123.42
1	A	45	ASP	O-C-N	-7.24	114.73	123.27
1	H	127	GLY	O-C-N	-7.24	115.91	123.58
1	E	104	ASN	O-C-N	-7.23	112.93	122.33
1	D	55	LYS	O-C-N	-7.23	113.42	122.82
1	D	118	THR	O-C-N	-7.22	114.99	123.22
1	C	133	LYS	O-C-N	-7.22	113.77	123.15
1	H	133	LYS	O-C-N	-7.22	113.86	122.96
1	H	39	SER	O-C-N	-7.22	114.62	122.85
1	B	28	GLN	O-C-N	-7.21	114.98	123.41
1	C	85	PRO	O-C-N	-7.21	114.21	123.00
1	G	80	SER	O-C-N	-7.20	114.46	123.17
1	G	124	ILE	O-C-N	-7.20	114.68	123.10
1	B	112	TYR	O-C-N	-7.19	114.77	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	75	PHE	O-C-N	-7.19	115.71	123.26
1	C	128	LEU	O-C-N	-7.19	115.28	123.48
1	A	86	PHE	O-C-N	-7.19	113.94	123.14
1	A	76	LEU	O-C-N	-7.18	114.12	122.89
1	D	128	LEU	O-C-N	-7.18	113.81	123.15
1	F	120	PHE	O-C-N	-7.18	113.89	123.23
1	C	9	SER	N-CA-C	-7.18	95.51	110.80
1	B	19	ASP	O-C-N	-7.18	114.61	123.44
1	H	45	ASP	N-CA-C	-7.17	97.04	108.73
1	B	24	THR	O-C-N	-7.17	113.38	122.34
1	E	67	ILE	O-C-N	-7.17	114.23	122.62
1	C	48	GLY	O-C-N	-7.16	113.65	122.46
1	B	123	PRO	O-C-N	-7.16	113.46	123.05
1	E	51	PHE	O-C-N	-7.16	114.97	123.27
1	D	135	ARG	O-C-N	-7.16	113.83	123.14
1	D	116	GLU	O-C-N	-7.15	114.79	123.30
1	G	120	PHE	O-C-N	-7.15	114.39	123.26
1	H	131	GLY	O-C-N	-7.15	115.39	123.61
1	C	107	ARG	O-C-N	-7.15	114.87	123.16
1	E	28	GLN	O-C-N	-7.15	114.65	123.44
1	E	108	THR	O-C-N	-7.15	114.13	123.28
1	A	125	GLU	O-C-N	-7.14	113.53	122.17
1	A	112	TYR	N-CA-C	-7.14	98.10	109.59
1	B	52	SER	O-C-N	-7.14	114.92	123.13
1	A	147	MET	O-C-N	-7.13	114.47	123.24
1	H	85	PRO	O-C-N	-7.12	114.45	123.14
1	A	41	SER	O-C-N	-7.12	115.08	123.41
1	B	137	GLY	O-C-N	-7.12	113.45	122.70
1	A	11	GLY	CA-C-O	7.11	125.82	120.91
1	A	27	ARG	O-C-N	-7.11	113.72	122.25
1	C	102	LYS	O-C-N	-7.10	114.60	123.27
1	E	41	SER	O-C-N	-7.10	115.10	123.41
1	B	37	ILE	O-C-N	-7.10	114.59	122.83
1	B	64	ASN	N-CA-C	7.10	121.25	109.46
1	G	144	GLY	O-C-N	-7.10	113.47	122.70
1	D	87	SER	O-C-N	-7.10	112.92	122.43
1	C	80	SER	O-C-N	-7.09	114.02	122.96
1	E	70	LYS	O-C-N	-7.09	113.01	122.38
1	C	119	TYR	O-C-N	-7.09	114.15	122.95
1	A	132	PHE	N-CA-C	7.09	120.95	109.40
1	G	38	GLY	O-C-N	-7.09	113.49	122.70
1	H	57	THR	N-CA-C	7.08	120.99	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	77	GLU	O-C-N	-7.07	113.16	122.42
1	F	114	ASP	O-C-N	-7.07	114.97	122.96
1	H	25	GLY	O-C-N	-7.07	115.49	123.62
1	B	67	ILE	O-C-N	-7.07	114.01	122.77
1	D	26	ILE	O-C-N	-7.07	115.83	123.18
1	B	113	GLY	O-C-N	-7.06	113.63	123.02
1	F	16	ASN	O-C-N	-7.06	115.02	123.13
1	G	36	ALA	O-C-N	-7.05	114.07	122.96
1	D	78	SER	O-C-N	-7.05	116.48	123.46
1	H	41	SER	O-C-N	-7.04	114.66	123.17
1	E	52	SER	O-C-N	-7.03	113.28	122.77
1	F	37	ILE	O-C-N	-7.03	114.42	122.72
1	E	10	TRP	O-C-N	-7.02	115.33	123.27
1	D	77	GLU	N-CA-C	-7.02	103.82	112.88
1	D	143	ILE	CB-CA-C	-7.02	100.79	110.90
1	H	118	THR	O-C-N	-7.02	115.05	123.13
1	A	8	GLY	CA-C-N	7.02	134.95	121.54
1	A	8	GLY	C-N-CA	7.02	134.95	121.54
1	F	28	GLN	O-C-N	-7.02	114.68	123.17
1	H	80	SER	O-C-N	-7.01	112.91	122.94
1	A	98	SER	O-C-N	-7.01	114.69	123.17
1	E	129	ILE	O-C-N	-7.01	114.98	122.83
1	A	130	VAL	N-CA-CB	-7.01	103.22	112.26
1	A	40	PHE	O-C-N	-7.00	114.03	123.14
1	E	103	THR	O-C-N	-7.00	114.33	123.16
1	H	26	ILE	O-C-N	-7.00	115.64	123.20
1	D	62	TYR	O-C-N	-7.00	114.34	123.16
1	G	78	SER	O-C-N	-7.00	115.22	123.41
1	A	51	PHE	O-C-N	-7.00	113.88	123.12
1	D	40	PHE	O-C-N	-6.99	114.33	123.28
1	F	132	PHE	O-C-N	-6.99	114.83	123.36
1	C	127	GLY	O-C-N	-6.99	113.62	122.70
1	G	67	ILE	O-C-N	-6.99	113.73	122.88
1	E	15	GLY	O-C-N	-6.98	113.62	122.70
1	H	107	ARG	O-C-N	-6.98	114.77	123.01
1	G	46	LEU	O-C-N	-6.98	113.93	123.01
1	D	46	LEU	O-C-N	-6.97	115.25	122.64
1	A	50	PRO	O-C-N	-6.97	114.28	123.06
1	E	145	ILE	O-C-N	-6.96	115.55	123.07
1	F	102	LYS	O-C-N	-6.96	114.78	123.27
1	E	97	ARG	N-CA-C	6.96	119.89	111.40
1	D	28	GLN	O-C-N	-6.96	114.68	123.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	126	ASN	O-C-N	-6.96	114.37	123.28
1	B	117	GLY	O-C-N	-6.96	113.66	122.70
1	D	23	TYR	O-C-N	-6.95	115.10	123.10
1	G	77	GLU	O-C-N	-6.95	113.83	122.24
1	C	38	GLY	O-C-N	-6.95	113.67	122.70
1	G	7	VAL	O-C-N	-6.94	115.84	123.20
1	E	78	SER	O-C-N	-6.94	115.29	123.41
1	H	134	GLY	O-C-N	-6.94	117.29	123.88
1	C	87	SER	O-C-N	-6.93	114.77	122.12
1	H	29	ILE	O-C-N	-6.92	115.00	123.10
1	B	79	VAL	O-C-N	-6.92	115.37	123.05
1	F	23	TYR	O-C-N	-6.92	113.81	122.73
1	G	141	ASP	O-C-N	-6.92	113.80	122.17
1	B	90	ALA	O-C-N	-6.91	114.56	122.86
1	B	118	THR	O-C-N	-6.91	115.34	123.22
1	E	30	GLU	O-C-N	-6.91	115.22	123.31
1	A	5	ILE	O-C-N	-6.91	114.57	122.72
1	D	35	GLU	O-C-N	-6.90	114.75	122.34
1	B	55	LYS	O-C-N	-6.89	114.87	123.01
1	B	81	GLY	O-C-N	-6.89	117.30	123.92
1	G	75	PHE	O-C-N	-6.87	115.42	123.25
1	G	18	TRP	O-C-N	-6.87	114.86	123.17
1	E	133	LYS	O-C-N	-6.86	113.43	122.97
1	D	66	LYS	O-C-N	-6.86	115.29	123.31
1	G	148	SER	O-C-N	-6.86	114.90	122.92
1	B	145	ILE	O-C-N	-6.85	115.77	123.10
1	D	11	GLY	O-C-N	-6.85	113.80	122.70
1	F	79	VAL	N-CA-C	-6.85	98.26	108.12
1	B	30	GLU	O-C-N	-6.84	114.33	123.23
1	D	63	LYS	O-C-N	-6.84	114.54	122.89
1	C	55	LYS	O-C-N	-6.83	115.27	123.13
1	H	48	GLY	O-C-N	-6.83	113.71	122.25
1	E	66	LYS	O-C-N	-6.83	114.11	123.12
1	C	52	SER	O-C-N	-6.83	113.51	122.59
1	D	84	GLY	N-CA-C	-6.82	98.43	112.34
1	G	109	PHE	O-C-N	-6.82	114.55	123.21
1	E	121	ASN	O-C-N	-6.82	115.05	123.44
1	G	118	THR	O-C-N	-6.81	115.30	123.13
1	E	32	SER	O-C-N	-6.81	114.38	123.23
1	F	40	PHE	O-C-N	-6.81	114.01	123.34
1	B	36	ALA	O-C-N	-6.81	115.27	123.10
1	B	138	ASP	O-C-N	-6.80	113.98	122.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	69	LEU	O-C-N	-6.80	115.27	123.16
1	B	25	GLY	O-C-N	-6.80	115.37	123.46
1	F	105	LYS	O-C-N	-6.79	113.92	122.27
1	E	87	SER	O-C-N	-6.78	113.24	122.33
1	G	74	GLU	O-C-N	-6.78	115.38	123.31
1	A	115	GLU	O-C-N	-6.77	113.69	122.56
1	B	64	ASN	O-C-N	-6.77	115.50	123.22
1	B	88	ALA	O-C-N	-6.77	113.26	122.33
1	C	24	THR	O-C-N	-6.77	113.03	122.37
1	E	145	ILE	N-CA-C	6.77	118.05	108.17
1	G	96	VAL	N-CA-CB	6.76	119.63	111.31
1	C	101	PHE	O-C-N	-6.76	115.32	123.16
1	D	97	ARG	O-C-N	-6.76	113.17	122.30
1	C	100	THR	O-C-N	-6.75	114.21	123.12
1	G	140	LEU	O-C-N	-6.75	114.04	122.82
1	C	24	THR	CA-C-O	6.75	127.44	119.28
1	F	124	ILE	N-CA-C	6.75	117.56	107.51
1	C	143	ILE	O-C-N	-6.74	115.28	123.03
1	B	129	ILE	O-C-N	-6.73	115.27	122.61
1	E	132	PHE	O-C-N	-6.73	115.29	123.30
1	G	57	THR	N-CA-C	6.73	120.21	109.24
1	D	117	GLY	O-C-N	-6.73	113.23	123.93
1	A	34	LYS	CA-C-N	6.72	133.13	122.11
1	A	34	LYS	C-N-CA	6.72	133.13	122.11
1	D	59	LYS	O-C-N	-6.72	113.94	122.34
1	G	45	ASP	O-C-N	-6.72	115.34	123.27
1	F	58	SER	O-C-N	-6.72	114.46	123.19
1	A	100	THR	O-C-N	-6.71	114.50	123.23
1	G	146	HIS	O-C-N	-6.71	115.33	123.19
1	G	17	GLY	O-C-N	-6.71	113.97	122.70
1	E	68	GLU	O-C-N	-6.70	115.08	123.05
1	F	133	LYS	O-C-N	-6.70	113.77	122.94
1	D	7	VAL	O-C-N	-6.69	115.81	122.76
1	C	11	GLY	O-C-N	-6.68	114.01	122.70
1	B	125	GLU	O-C-N	-6.68	113.55	122.23
1	H	108	THR	O-C-N	-6.68	114.55	123.23
1	D	57	THR	N-CA-C	6.66	120.72	110.20
1	B	112	TYR	N-CA-C	-6.66	98.84	109.76
1	F	74	GLU	O-C-N	-6.66	115.43	123.29
1	G	39	SER	O-C-N	-6.66	115.00	122.86
1	D	39	SER	O-C-N	-6.65	114.69	122.87
1	B	69	LEU	O-C-N	-6.65	115.44	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	52	SER	O-C-N	-6.65	114.84	123.02
1	B	115	GLU	O-C-N	-6.65	113.84	122.61
1	C	57	THR	O-C-N	-6.64	115.46	123.10
1	C	5	ILE	O-C-N	-6.64	115.02	122.66
1	H	126	ASN	O-C-N	-6.64	113.76	122.59
1	E	137	GLY	O-C-N	-6.64	114.07	122.70
1	E	130	VAL	N-CA-CB	-6.64	103.70	112.26
1	F	22	SER	CA-C-N	6.64	133.62	122.20
1	F	22	SER	C-N-CA	6.64	133.62	122.20
1	B	103	THR	O-C-N	-6.63	114.22	123.11
1	H	119	TYR	O-C-N	-6.63	115.23	122.79
1	D	68	GLU	O-C-N	-6.63	115.58	123.27
1	G	70	LYS	CG-CD-CE	6.63	126.55	111.30
1	F	12	GLY	CA-C-N	6.63	128.69	121.00
1	F	12	GLY	C-N-CA	6.63	128.69	121.00
1	E	85	PRO	O-C-N	-6.63	114.64	122.86
1	A	140	LEU	O-C-N	-6.62	114.21	122.82
1	H	64	ASN	N-CA-C	6.62	119.38	109.25
1	F	88	ALA	O-C-N	-6.61	113.63	122.43
1	H	69	LEU	O-C-N	-6.61	115.49	122.96
1	C	61	PRO	O-C-N	-6.61	113.72	122.64
1	H	63	LYS	O-C-N	-6.61	114.89	123.02
1	H	91	THR	N-CA-C	-6.61	94.46	108.73
1	E	119	TYR	O-C-N	-6.60	114.81	122.93
1	G	132	PHE	O-C-N	-6.60	115.44	123.30
1	H	4	THR	O-C-N	-6.60	115.18	123.17
1	A	13	PRO	O-C-N	-6.60	112.60	122.83
1	E	106	GLY	O-C-N	-6.59	113.77	122.28
1	G	70	LYS	O-C-N	-6.59	113.67	122.38
1	B	89	LEU	CA-C-O	6.59	128.53	120.55
1	C	4	THR	O-C-N	-6.59	115.88	123.33
1	E	39	SER	O-C-N	-6.59	115.52	123.16
1	G	24	THR	O-C-N	-6.59	113.79	122.42
1	G	139	LEU	O-C-N	-6.58	114.24	122.73
1	A	145	ILE	N-CA-C	6.58	119.47	108.81
1	H	3	GLN	O-C-N	-6.58	113.83	122.97
1	C	30	GLU	O-C-N	-6.57	115.25	123.27
1	F	148	SER	O-C-N	-6.56	115.24	122.92
1	F	118	THR	O-C-N	-6.56	115.52	123.19
1	H	140	LEU	O-C-N	-6.56	115.06	122.93
1	B	83	THR	O-C-N	-6.55	115.50	123.30
1	A	20	GLU	O-C-N	-6.55	113.42	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	48	GLY	O-C-N	-6.54	114.41	122.46
1	A	108	THR	O-C-N	-6.54	115.29	123.27
1	D	29	ILE	O-C-N	-6.54	116.14	123.20
1	G	114	ASP	O-C-N	-6.54	115.39	123.04
1	A	75	PHE	O-C-N	-6.54	114.72	122.96
1	C	120	PHE	O-C-N	-6.54	114.73	123.23
1	E	139	LEU	O-C-N	-6.53	114.73	122.96
1	B	62	TYR	O-C-N	-6.53	115.59	123.10
1	F	117	GLY	O-C-N	-6.53	114.35	123.56
1	D	36	ALA	O-C-N	-6.53	114.73	122.96
1	H	28	GLN	O-C-N	-6.53	115.77	123.41
1	E	103	THR	N-CA-C	6.53	120.33	109.95
1	H	17	GLY	O-C-N	-6.53	113.87	122.81
1	F	34	LYS	CA-C-N	6.53	132.64	122.26
1	F	34	LYS	C-N-CA	6.53	132.64	122.26
1	D	101	PHE	N-CA-C	6.52	119.88	107.75
1	F	18	TRP	O-C-N	-6.52	115.96	123.33
1	E	4	THR	O-C-N	-6.52	114.68	123.15
1	B	127	GLY	O-C-N	-6.51	116.06	123.23
1	E	88	ALA	O-C-N	-6.51	113.48	122.46
1	A	83	THR	O-C-N	-6.50	115.72	123.27
1	E	74	GLU	O-C-N	-6.50	114.95	123.21
1	A	88	ALA	O-C-N	-6.50	113.78	122.23
1	E	52	SER	N-CA-C	6.50	118.50	109.15
1	E	19	ASP	O-C-N	-6.49	115.57	123.36
1	F	68	GLU	O-C-N	-6.49	115.14	122.93
1	C	123	PRO	O-C-N	-6.48	114.90	123.06
1	D	96	VAL	O-C-N	-6.48	115.56	122.95
1	E	112	TYR	O-C-N	-6.48	115.84	123.22
1	H	105	LYS	O-C-N	-6.48	113.75	122.43
1	E	62	TYR	N-CA-C	6.47	118.91	110.43
1	E	76	LEU	O-C-N	-6.47	114.40	123.01
1	H	57	THR	O-C-N	-6.47	114.99	123.21
1	H	42	VAL	O-C-N	-6.47	115.59	123.09
1	F	52	SER	O-C-N	-6.47	113.69	122.48
1	F	123	PRO	O-C-N	-6.46	113.91	122.64
1	G	54	PRO	O-C-N	-6.46	115.11	123.06
1	H	66	LYS	O-C-N	-6.45	115.02	123.28
1	F	125	GLU	O-C-N	-6.44	114.38	122.17
1	E	26	ILE	O-C-N	-6.44	116.25	123.20
1	F	57	THR	N-CA-C	6.43	120.04	110.52
1	G	130	VAL	CA-C-O	6.43	125.82	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	SER	O-C-N	-6.42	115.05	122.89
1	B	94	PRO	O-C-N	-6.42	115.01	122.85
1	A	145	ILE	O-C-N	-6.42	115.68	123.00
1	G	136	THR	O-C-N	-6.40	115.58	123.33
1	D	112	TYR	O-C-N	-6.40	114.92	123.23
1	C	137	GLY	N-CA-C	-6.39	98.02	113.18
1	A	30	GLU	O-C-N	-6.39	115.83	123.31
1	A	148	SER	O-C-N	-6.39	116.55	123.26
1	F	5	ILE	O-C-N	-6.39	115.64	122.61
1	B	35	GLU	N-CA-C	-6.39	105.53	113.38
1	A	128	LEU	O-C-N	-6.38	115.59	123.44
1	F	99	LEU	O-C-N	-6.38	115.11	123.28
1	H	10	TRP	O-C-N	-6.38	115.74	123.27
1	D	38	GLY	O-C-N	-6.38	114.41	122.70
1	F	57	THR	O-C-N	-6.38	115.80	122.94
1	E	13	PRO	O-C-N	-6.37	114.04	122.64
1	G	129	ILE	O-C-N	-6.37	115.95	123.03
1	A	102	LYS	O-C-N	-6.37	115.72	123.30
1	C	140	LEU	O-C-N	-6.37	114.03	122.57
1	F	86	PHE	O-C-N	-6.37	115.77	123.29
1	H	143	ILE	O-C-N	-6.37	115.98	123.05
1	C	54	PRO	O-C-N	-6.36	115.46	123.10
1	H	130	VAL	O-C-N	-6.36	114.62	122.57
1	G	32	SER	O-C-N	-6.36	115.47	123.17
1	B	134	GLY	N-CA-C	6.35	119.44	110.74
1	D	3	GLN	O-C-N	-6.35	113.62	122.76
1	F	39	SER	O-C-N	-6.35	115.37	122.86
1	G	31	LEU	O-C-N	-6.35	114.44	122.43
1	B	91	THR	N-CA-C	-6.34	96.92	108.85
1	E	43	ILE	O-C-N	-6.34	114.90	122.77
1	E	115	GLU	O-C-N	-6.34	114.15	122.59
1	C	105	LYS	O-C-N	-6.34	114.16	122.59
1	A	44	TYR	O-C-N	-6.34	113.80	122.23
1	F	112	TYR	N-CA-C	-6.34	99.07	109.40
1	F	42	VAL	O-C-N	-6.33	116.39	123.03
1	A	32	SER	O-C-N	-6.33	115.46	123.24
1	A	126	ASN	O-C-N	-6.33	114.91	123.14
1	D	130	VAL	O-C-N	-6.33	114.66	122.57
1	F	115	GLU	O-C-N	-6.32	113.06	122.67
1	D	31	LEU	O-C-N	-6.32	114.28	122.94
1	B	140	LEU	O-C-N	-6.32	114.24	122.77
1	F	137	GLY	O-C-N	-6.31	114.49	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	96	VAL	O-C-N	-6.30	114.96	122.77
1	A	137	GLY	N-CA-C	-6.30	98.26	113.18
1	D	52	SER	N-CA-C	6.30	118.55	108.41
1	B	40	PHE	O-C-N	-6.29	115.09	123.14
1	F	8	GLY	O-C-N	-6.29	115.50	122.61
1	D	140	LEU	O-C-N	-6.28	115.57	123.05
1	F	126	ASN	O-C-N	-6.28	115.70	123.36
1	B	68	GLU	O-C-N	-6.27	114.85	123.01
1	B	124	ILE	N-CA-C	6.27	117.25	107.28
1	H	148	SER	O-C-N	-6.27	116.28	122.99
1	G	64	ASN	O-C-N	-6.27	115.70	122.85
1	A	119	TYR	O-C-N	-6.27	115.22	122.93
1	F	100	THR	CA-C-O	6.27	126.88	120.24
1	C	142	ALA	O-C-N	-6.26	115.59	123.17
1	A	112	TYR	O-C-N	-6.26	115.26	123.21
1	D	14	GLY	O-C-N	-6.25	114.83	122.71
1	D	35	GLU	N-CA-C	-6.25	106.25	114.31
1	A	105	LYS	N-CA-C	-6.25	105.51	112.57
1	C	118	THR	O-C-N	-6.25	116.10	123.22
1	A	55	LYS	O-C-N	-6.24	115.74	123.04
1	A	106	GLY	O-C-N	-6.24	114.59	122.70
1	H	37	ILE	O-C-N	-6.23	114.75	122.97
1	D	95	VAL	N-CA-CB	-6.23	103.80	112.52
1	G	85	PRO	O-C-N	-6.23	115.40	123.00
1	H	89	LEU	CB-CG-CD1	6.23	129.38	110.70
1	A	54	PRO	O-C-N	-6.22	115.51	123.03
1	E	56	HIS	O-C-N	-6.22	116.05	122.64
1	H	31	LEU	O-C-N	-6.21	114.46	122.72
1	F	89	LEU	CB-CA-C	6.21	122.03	111.35
1	H	65	VAL	O-C-N	-6.20	116.31	122.76
1	F	85	PRO	O-C-N	-6.20	115.43	123.06
1	F	98	SER	O-C-N	-6.20	115.61	123.24
1	F	75	PHE	O-C-N	-6.20	115.67	123.17
1	G	65	VAL	O-C-N	-6.19	116.19	123.00
1	B	138	ASP	CA-C-O	6.18	125.85	119.05
1	B	32	SER	O-C-N	-6.17	115.20	123.23
1	A	97	ARG	O-C-N	-6.17	114.21	122.23
1	A	120	PHE	O-C-N	-6.17	115.17	123.19
1	E	83	THR	O-C-N	-6.16	115.39	123.21
1	A	18	TRP	O-C-N	-6.15	114.08	122.81
1	C	34	LYS	CG-CD-CE	6.15	125.45	111.30
1	E	65	VAL	O-C-N	-6.15	116.21	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	117	GLY	O-C-N	-6.15	114.70	122.70
1	B	108	THR	O-C-N	-6.15	116.04	123.29
1	G	19	ASP	O-C-N	-6.15	115.13	123.24
1	G	52	SER	O-C-N	-6.14	115.22	122.96
1	E	140	LEU	O-C-N	-6.14	114.13	122.48
1	G	93	THR	CA-C-N	6.14	126.10	119.78
1	G	93	THR	C-N-CA	6.14	126.10	119.78
1	F	80	SER	O-C-N	-6.13	116.05	123.10
1	G	112	TYR	O-C-N	-6.13	115.03	123.12
1	H	70	LYS	O-C-N	-6.13	114.52	122.61
1	F	43	ILE	O-C-N	-6.12	115.19	122.77
1	H	145	ILE	O-C-N	-6.12	116.00	123.03
1	A	143	ILE	O-C-N	-6.12	116.03	123.00
1	H	112	TYR	O-C-N	-6.12	113.82	122.87
1	A	80	SER	O-C-N	-6.11	115.77	123.17
1	F	47	ASN	O-C-N	-6.11	115.25	122.58
1	E	36	ALA	O-C-N	-6.11	116.08	123.10
1	B	137	GLY	N-CA-C	-6.10	98.72	113.18
1	B	87	SER	O-C-N	-6.10	115.19	122.27
1	C	50	PRO	O-C-N	-6.09	116.01	123.01
1	G	92	PRO	O-C-N	-6.09	114.42	122.64
1	B	66	LYS	O-C-N	-6.08	115.81	123.05
1	D	106	GLY	O-C-N	-6.08	114.80	122.70
1	D	82	TYR	O-C-N	-6.07	115.97	123.44
1	B	9	SER	N-CA-C	-6.07	97.87	110.80
1	F	58	SER	N-CA-C	-6.07	100.00	109.72
1	A	3	GLN	O-C-N	-6.07	115.30	123.19
1	A	82	TYR	O-C-N	-6.07	115.34	123.23
1	A	118	THR	CA-C-N	6.07	129.45	120.95
1	A	118	THR	C-N-CA	6.07	129.45	120.95
1	D	143	ILE	O-C-N	-6.07	116.48	122.97
1	D	69	LEU	O-C-N	-6.06	116.09	123.19
1	E	64	ASN	O-C-N	-6.06	116.10	123.19
1	D	119	TYR	O-C-N	-6.05	115.72	122.86
1	B	16	ASN	O-C-N	-6.05	116.44	123.27
1	B	145	ILE	N-CA-C	6.05	117.47	108.46
1	B	77	GLU	O-C-N	-6.04	115.06	122.25
1	B	59	LYS	N-CA-C	-6.04	105.74	113.23
1	B	147	MET	O-C-N	-6.04	115.29	123.15
1	A	48	GLY	O-C-N	-6.04	114.76	122.43
1	D	70	LYS	O-C-N	-6.04	114.64	122.61
1	E	5	ILE	O-C-N	-6.04	115.72	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	32	SER	N-CA-C	-6.03	99.57	109.40
1	C	34	LYS	O-C-N	-6.03	114.57	122.59
1	H	38	GLY	O-C-N	-6.03	114.86	122.70
1	G	88	ALA	CA-C-N	-6.03	114.19	123.17
1	G	88	ALA	C-N-CA	-6.03	114.19	123.17
1	F	112	TYR	O-C-N	-6.02	115.40	123.23
1	C	64	ASN	O-C-N	-6.01	116.18	123.16
1	C	100	THR	CB-CA-C	6.01	119.69	110.62
1	E	116	GLU	O-C-N	-6.01	115.59	123.28
1	F	129	ILE	O-C-N	-6.00	115.76	122.66
1	A	78	SER	O-C-N	-6.00	117.20	123.56
1	C	136	THR	N-CA-C	-5.99	101.34	110.14
1	C	58	SER	O-C-N	-5.98	116.23	123.29
1	D	85	PRO	O-C-N	-5.98	115.70	123.00
1	E	21	GLY	O-C-N	-5.98	115.06	123.02
1	B	48	GLY	O-C-N	-5.98	115.11	122.46
1	A	24	THR	O-C-N	-5.97	114.28	122.46
1	C	116	GLU	O-C-N	-5.97	115.47	123.23
1	F	60	LEU	CA-C-N	5.97	131.15	120.88
1	F	60	LEU	C-N-CA	5.97	131.15	120.88
1	B	3	GLN	O-C-N	-5.96	114.41	122.94
1	A	115	GLU	N-CA-C	5.96	118.87	109.39
1	G	135	ARG	O-C-N	-5.96	114.66	122.59
1	G	145	ILE	O-C-N	-5.96	115.12	122.57
1	D	64	ASN	N-CA-C	5.96	118.44	108.96
1	B	135	ARG	O-C-N	-5.96	115.91	123.24
1	E	54	PRO	O-C-N	-5.96	115.82	123.03
1	C	43	ILE	O-C-N	-5.95	116.13	123.10
1	A	103	THR	O-C-N	-5.95	115.72	122.68
1	G	3	GLN	O-C-N	-5.95	114.52	122.14
1	A	114	ASP	O-C-N	-5.95	116.40	123.06
1	H	99	LEU	N-CA-C	-5.95	98.92	108.55
1	B	126	ASN	O-C-N	-5.93	115.69	123.28
1	C	57	THR	N-CA-C	5.92	119.71	110.17
1	B	38	GLY	O-C-N	-5.92	115.01	122.70
1	D	141	ASP	O-C-N	-5.92	114.54	122.23
1	A	116	GLU	O-C-N	-5.91	115.54	123.23
1	H	116	GLU	O-C-N	-5.91	116.18	123.33
1	A	129	ILE	N-CA-C	-5.91	101.04	108.84
1	D	133	LYS	O-C-N	-5.91	114.85	122.94
1	E	61	PRO	O-C-N	-5.91	114.67	122.64
1	C	77	GLU	N-CA-C	-5.90	106.05	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	120	PHE	O-C-N	-5.90	115.56	123.23
1	B	7	VAL	O-C-N	-5.90	116.83	123.20
1	B	76	LEU	O-C-N	-5.90	115.76	123.02
1	F	139	LEU	O-C-N	-5.90	114.74	122.59
1	G	37	ILE	N-CA-C	-5.90	101.19	109.21
1	E	67	ILE	CB-CA-C	-5.89	104.28	111.88
1	E	120	PHE	O-C-N	-5.89	115.53	123.19
1	G	47	ASN	O-C-N	-5.89	115.25	122.55
1	G	30	GLU	O-C-N	-5.88	114.16	122.87
1	G	113	GLY	O-C-N	-5.88	116.14	123.37
1	B	75	PHE	O-C-N	-5.87	115.56	122.96
1	B	102	LYS	O-C-N	-5.87	115.77	123.16
1	F	35	GLU	CA-C-O	5.87	125.50	119.05
1	G	7	VAL	N-CA-C	5.86	116.31	107.75
1	A	23	TYR	O-C-N	-5.86	114.80	122.59
1	D	81	GLY	O-C-N	-5.86	116.96	123.58
1	H	77	GLU	N-CA-C	-5.86	104.29	113.02
1	D	103	THR	O-C-N	-5.85	114.57	122.94
1	E	65	VAL	CB-CA-C	-5.84	101.67	110.55
1	G	126	ASN	O-C-N	-5.84	116.02	123.26
1	C	39	SER	O-C-N	-5.84	115.97	122.86
1	C	42	VAL	N-CA-C	5.84	118.02	108.97
1	F	109	PHE	O-C-N	-5.84	115.41	123.12
1	B	46	LEU	O-C-N	-5.84	115.42	123.01
1	C	96	VAL	N-CA-CB	5.84	117.65	111.00
1	E	94	PRO	O-C-N	-5.84	115.73	122.85
1	B	128	LEU	O-C-N	-5.83	116.48	123.31
1	H	97	ARG	O-C-N	-5.83	114.42	122.30
1	D	49	ASP	CA-C-N	5.83	126.17	119.93
1	D	49	ASP	C-N-CA	5.83	126.17	119.93
1	H	83	THR	O-C-N	-5.82	116.17	123.27
1	E	27	ARG	O-C-N	-5.81	113.41	122.13
1	D	59	LYS	CA-C-O	5.81	126.15	119.35
1	B	54	PRO	O-C-N	-5.81	116.00	123.03
1	G	83	THR	O-C-N	-5.81	116.53	123.27
1	E	14	GLY	O-C-N	-5.80	115.15	122.70
1	G	115	GLU	O-C-N	-5.80	114.95	122.61
1	B	107	ARG	O-C-N	-5.80	116.61	123.22
1	F	35	GLU	O-C-N	-5.80	115.22	122.35
1	F	108	THR	O-C-N	-5.80	116.11	123.24
1	A	36	ALA	O-C-N	-5.79	115.01	122.94
1	H	11	GLY	O-C-N	-5.77	113.00	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	136	THR	O-C-N	-5.77	116.23	123.27
1	D	88	ALA	O-C-N	-5.76	114.73	122.23
1	F	8	GLY	N-CA-C	5.76	121.53	111.50
1	C	2	SER	O-C-N	-5.76	113.78	123.00
1	H	44	TYR	O-C-N	-5.76	116.28	122.85
1	B	59	LYS	CA-C-O	5.76	126.01	119.27
1	D	15	GLY	O-C-N	-5.76	115.21	122.70
1	G	96	VAL	O-C-N	-5.76	115.63	122.77
1	B	27	ARG	O-C-N	-5.76	114.65	122.19
1	C	136	THR	O-C-N	-5.76	114.97	122.97
1	B	6	THR	O-C-N	-5.75	116.46	123.30
1	D	32	SER	N-CA-C	-5.75	100.42	109.50
1	F	51	PHE	O-C-N	-5.74	115.93	123.28
1	H	68	GLU	O-C-N	-5.74	116.22	123.05
1	F	10	TRP	O-C-N	-5.73	116.79	123.27
1	H	137	GLY	N-CA-C	-5.73	99.60	113.18
1	H	147	MET	O-C-N	-5.73	116.24	123.17
1	B	39	SER	O-C-N	-5.72	116.26	123.01
1	F	9	SER	N-CA-C	-5.72	98.62	110.80
1	G	22	SER	O-C-N	-5.71	115.96	123.16
1	C	137	GLY	O-C-N	-5.71	115.28	122.70
1	E	98	SER	O-C-N	-5.71	114.78	122.94
1	D	33	TYR	CA-C-N	5.71	132.44	121.54
1	D	33	TYR	C-N-CA	5.71	132.44	121.54
1	A	137	GLY	O-C-N	-5.70	115.28	122.70
1	C	112	TYR	O-C-N	-5.70	115.94	123.13
1	H	106	GLY	CA-C-O	5.70	125.12	118.96
1	A	105	LYS	O-C-N	-5.70	114.83	122.19
1	B	58	SER	N-CA-C	-5.70	101.26	110.32
1	A	135	ARG	O-C-N	-5.69	116.44	123.44
1	B	10	TRP	O-C-N	-5.69	116.84	123.27
1	D	16	ASN	O-C-N	-5.69	116.30	123.01
1	E	45	ASP	O-C-N	-5.68	116.57	123.27
1	A	94	PRO	O-C-N	-5.68	116.16	123.03
1	D	61	PRO	O-C-N	-5.68	114.98	122.64
1	F	101	PHE	O-C-N	-5.68	116.00	123.21
1	G	8	GLY	N-CA-C	5.68	122.58	112.02
1	B	50	PRO	O-C-N	-5.67	115.69	122.89
1	A	142	ALA	O-C-N	-5.67	116.78	123.25
1	H	137	GLY	O-C-N	-5.67	115.33	122.70
1	B	5	ILE	O-C-N	-5.67	116.52	122.81
1	G	57	THR	O-C-N	-5.67	116.87	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	64	ASN	O-C-N	-5.67	116.05	123.02
1	D	75	PHE	O-C-N	-5.66	116.28	123.24
1	F	24	THR	O-C-N	-5.66	114.65	122.46
1	A	48	GLY	CA-C-O	5.66	125.39	119.06
1	A	87	SER	O-C-N	-5.65	115.61	122.22
1	F	65	VAL	O-C-N	-5.65	116.54	123.03
1	A	38	GLY	O-C-N	-5.64	115.37	122.70
1	D	48	GLY	O-C-N	-5.63	115.38	122.70
1	E	111	PRO	O-C-N	-5.63	116.79	123.10
1	H	40	PHE	O-C-N	-5.63	116.61	123.36
1	H	50	PRO	O-C-N	-5.63	116.54	123.01
1	D	79	VAL	O-C-N	-5.62	115.54	122.57
1	H	90	ALA	N-CA-C	5.62	122.77	110.80
1	F	147	MET	O-C-N	-5.62	115.85	123.15
1	G	142	ALA	O-C-N	-5.61	115.25	122.94
1	B	74	GLU	O-C-N	-5.60	116.68	123.29
1	C	125	GLU	O-C-N	-5.60	114.79	122.46
1	E	47	ASN	O-C-N	-5.58	116.16	122.86
1	H	59	LYS	O-C-N	-5.58	115.17	122.59
1	D	50	PRO	O-C-N	-5.57	116.05	122.85
1	D	105	LYS	O-C-N	-5.57	116.23	122.03
1	B	110	GLY	N-CA-C	5.57	123.71	112.34
1	G	43	ILE	N-CA-C	-5.57	98.42	107.28
1	A	2	SER	O-C-N	-5.57	114.10	123.00
1	A	40	PHE	CA-CB-CG	-5.56	108.24	113.80
1	F	48	GLY	CA-C-O	5.56	124.89	119.27
1	H	92	PRO	O-C-N	-5.56	115.04	122.22
1	A	92	PRO	O-C-N	-5.56	115.14	122.64
1	D	136	THR	O-C-N	-5.56	115.97	123.19
1	C	58	SER	N-CA-C	-5.55	100.13	109.07
1	H	132	PHE	O-C-N	-5.55	115.67	123.11
1	H	130	VAL	N-CA-CB	-5.55	102.07	111.23
1	H	77	GLU	O-C-N	-5.55	115.21	122.20
1	F	103	THR	O-C-N	-5.54	115.95	123.10
1	B	73	ASP	O-C-N	-5.54	115.45	122.27
1	G	113	GLY	N-CA-C	-5.54	104.61	111.70
1	D	148	SER	O-C-N	-5.53	116.45	122.92
1	D	115	GLU	O-C-N	-5.53	115.23	122.59
1	D	137	GLY	O-C-N	-5.53	115.51	122.70
1	B	89	LEU	N-CA-C	-5.53	104.97	112.26
1	B	55	LYS	N-CA-C	-5.52	101.47	110.20
1	H	5	ILE	CB-CA-C	-5.52	105.33	111.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	33	TYR	CA-C-N	-5.52	111.00	121.54
1	C	33	TYR	C-N-CA	-5.52	111.00	121.54
1	C	69	LEU	O-C-N	-5.52	116.20	123.21
1	C	140	LEU	CA-C-O	5.52	126.94	120.98
1	G	125	GLU	O-C-N	-5.51	114.53	122.36
1	A	111	PRO	O-C-N	-5.51	116.13	122.85
1	B	34	LYS	N-CA-CB	5.51	119.80	110.49
1	G	135	ARG	N-CA-C	-5.51	99.07	110.80
1	H	19	ASP	O-C-N	-5.50	115.98	123.24
1	G	138	ASP	CA-C-O	5.50	125.62	119.41
1	D	58	SER	N-CA-C	-5.49	101.33	110.17
1	C	62	TYR	O-C-N	-5.49	115.01	122.36
1	H	75	PHE	O-C-N	-5.49	117.34	123.48
1	D	137	GLY	N-CA-C	-5.48	100.18	113.18
1	G	103	THR	O-C-N	-5.48	116.03	123.10
1	E	147	MET	O-C-N	-5.48	116.03	123.15
1	D	43	ILE	N-CA-C	-5.48	99.66	107.77
1	C	7	VAL	O-C-N	-5.48	117.34	123.26
1	C	130	VAL	CB-CA-C	5.48	116.12	110.70
1	D	127	GLY	O-C-N	-5.47	115.58	122.70
1	E	118	THR	O-C-N	-5.47	116.83	123.29
1	G	26	ILE	O-C-N	-5.47	117.35	123.26
1	C	98	SER	O-C-N	-5.47	116.92	123.27
1	C	35	GLU	O-C-N	-5.47	115.75	122.20
1	E	119	TYR	N-CA-C	5.47	118.16	109.96
1	A	46	LEU	O-C-N	-5.47	115.90	123.01
1	G	59	LYS	O-C-N	-5.46	114.92	122.46
1	D	52	SER	O-C-N	-5.46	116.38	122.93
1	E	93	THR	N-CA-C	5.46	117.83	110.29
1	D	27	ARG	O-C-N	-5.46	115.04	122.19
1	G	137	GLY	O-C-N	-5.46	115.61	122.70
1	G	48	GLY	O-C-N	-5.45	115.59	122.41
1	H	22	SER	O-C-N	-5.45	116.84	123.16
1	B	51	PHE	O-C-N	-5.45	116.31	123.28
1	F	60	LEU	N-CA-C	5.44	117.41	109.84
1	H	145	ILE	N-CA-C	5.43	115.72	108.27
1	C	27	ARG	O-C-N	-5.43	114.82	122.10
1	D	47	ASN	O-C-N	-5.43	116.45	122.91
1	F	145	ILE	N-CA-C	5.43	117.61	108.81
1	B	53	GLY	CA-C-N	5.42	125.35	119.76
1	B	53	GLY	C-N-CA	5.42	125.35	119.76
1	G	122	LEU	CA-C-N	-5.42	114.13	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	122	LEU	C-N-CA	-5.42	114.13	119.99
1	A	26	ILE	O-C-N	-5.42	117.33	123.18
1	B	20	GLU	O-C-N	-5.41	115.58	122.34
1	C	132	PHE	CA-C-O	5.41	126.54	120.70
1	D	56	HIS	O-C-N	-5.41	115.75	122.83
1	E	46	LEU	O-C-N	-5.40	114.76	122.96
1	F	52	SER	N-CA-C	5.40	117.27	108.63
1	B	26	ILE	O-C-N	-5.40	117.43	123.26
1	A	52	SER	O-C-N	-5.39	115.42	122.59
1	D	89	LEU	N-CA-C	-5.39	106.73	113.15
1	A	19	ASP	O-C-N	-5.39	115.42	122.59
1	E	99	LEU	O-C-N	-5.39	115.42	122.59
1	B	48	GLY	CA-C-O	5.39	124.87	119.27
1	B	104	ASN	O-C-N	-5.39	115.92	122.22
1	H	74	GLU	O-C-N	-5.38	116.19	123.19
1	D	111	PRO	O-C-N	-5.38	115.38	122.64
1	F	145	ILE	O-C-N	-5.38	116.87	123.00
1	G	131	GLY	O-C-N	-5.38	114.09	122.91
1	H	36	ALA	O-C-N	-5.38	115.17	122.81
1	C	106	GLY	N-CA-C	5.38	125.92	113.18
1	G	9	SER	O-C-N	-5.38	115.44	122.59
1	D	132	PHE	O-C-N	-5.37	116.21	123.19
1	E	86	PHE	O-C-N	-5.37	116.15	123.24
1	H	67	ILE	O-C-N	-5.37	115.10	122.62
1	E	10	TRP	N-CA-C	-5.37	100.49	109.24
1	C	138	ASP	CA-C-O	5.36	125.47	119.41
1	E	89	LEU	CA-C-O	5.35	125.61	119.35
1	G	123	PRO	O-C-N	-5.35	116.32	123.06
1	H	25	GLY	CA-C-O	5.35	127.00	121.38
1	F	104	ASN	O-C-N	-5.35	115.44	122.39
1	C	7	VAL	N-CA-C	5.34	115.59	108.11
1	A	81	GLY	CA-C-O	5.34	126.70	121.63
1	C	103	THR	CA-C-N	5.33	127.43	120.28
1	C	103	THR	C-N-CA	5.33	127.43	120.28
1	G	37	ILE	O-C-N	-5.33	116.43	122.72
1	A	141	ASP	O-C-N	-5.33	115.11	122.46
1	F	73	ASP	N-CA-C	-5.33	105.47	111.28
1	H	30	GLU	O-C-N	-5.33	116.09	123.12
1	B	148	SER	O-C-N	-5.32	115.87	122.73
1	E	80	SER	O-C-N	-5.32	116.24	123.15
1	E	40	PHE	O-C-N	-5.31	116.06	123.34
1	F	50	PRO	O-C-N	-5.31	116.42	123.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	29	ILE	CB-CA-C	-5.30	105.20	111.09
1	A	77	GLU	O-C-N	-5.30	115.95	122.20
1	A	109	PHE	CA-C-N	5.29	130.18	121.87
1	A	109	PHE	C-N-CA	5.29	130.18	121.87
1	D	121	ASN	O-C-N	-5.29	116.25	123.24
1	D	77	GLU	O-C-N	-5.29	115.95	122.25
1	H	51	PHE	CA-C-O	5.29	126.19	120.32
1	E	145	ILE	CA-C-O	5.29	126.19	120.43
1	D	13	PRO	O-C-N	-5.29	114.06	122.52
1	B	116	GLU	O-C-N	-5.28	116.36	123.23
1	C	46	LEU	O-C-N	-5.28	115.05	122.87
1	C	111	PRO	O-C-N	-5.28	115.51	122.64
1	D	134	GLY	CA-C-O	5.28	126.89	121.35
1	E	44	TYR	O-C-N	-5.28	115.66	122.20
1	E	38	GLY	O-C-N	-5.27	115.85	122.70
1	E	77	GLU	CA-C-O	5.27	125.16	119.15
1	C	19	ASP	O-C-N	-5.27	116.29	123.24
1	G	128	LEU	O-C-N	-5.27	116.30	123.15
1	A	62	TYR	O-C-N	-5.27	116.85	122.85
1	F	136	THR	O-C-N	-5.26	116.85	123.27
1	F	54	PRO	O-C-N	-5.26	116.66	123.03
1	B	92	PRO	CA-C-O	5.26	125.39	118.98
1	B	2	SER	O-C-N	-5.25	114.60	123.00
1	E	128	LEU	O-C-N	-5.25	116.98	123.44
1	E	138	ASP	N-CA-C	-5.25	106.90	113.72
1	A	70	LYS	O-C-N	-5.24	115.44	122.68
1	C	78	SER	O-C-N	-5.24	117.41	123.33
1	B	132	PHE	O-C-N	-5.24	116.38	123.19
1	G	73	ASP	O-C-N	-5.23	115.42	122.43
1	D	104	ASN	O-C-N	-5.23	115.84	122.27
1	C	20	GLU	O-C-N	-5.22	115.43	122.43
1	H	118	THR	CB-CA-C	5.22	118.95	110.22
1	A	7	VAL	CA-C-O	5.22	126.52	120.67
1	A	116	GLU	N-CA-C	5.22	117.91	109.40
1	G	98	SER	O-C-N	-5.22	116.82	123.24
1	H	47	ASN	O-C-N	-5.22	116.31	122.58
1	A	21	GLY	O-C-N	-5.21	116.27	122.68
1	G	21	GLY	O-C-N	-5.21	117.96	122.91
1	B	79	VAL	CB-CA-C	-5.20	101.71	110.71
1	C	55	LYS	N-CA-C	5.20	117.23	108.96
1	B	57	THR	O-C-N	-5.20	117.10	123.19
1	H	141	ASP	O-C-N	-5.20	115.47	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	73	ASP	O-C-N	-5.19	115.88	122.27
1	A	67	ILE	O-C-N	-5.19	116.33	122.66
1	C	108	THR	O-C-N	-5.19	117.25	123.27
1	G	105	LYS	O-C-N	-5.19	114.06	122.42
1	C	59	LYS	O-C-N	-5.19	115.30	122.46
1	C	7	VAL	CA-C-O	5.19	125.83	120.39
1	B	47	ASN	O-C-N	-5.18	116.12	122.55
1	G	7	VAL	CA-C-O	5.18	125.78	120.39
1	H	24	THR	CA-C-O	5.18	124.52	118.97
1	C	3	GLN	O-C-N	-5.18	115.59	122.74
1	A	139	LEU	O-C-N	-5.18	115.46	122.81
1	E	2	SER	O-C-N	-5.17	114.72	123.00
1	H	109	PHE	CA-CB-CG	-5.17	108.63	113.80
1	H	127	GLY	N-CA-C	-5.17	103.53	110.56
1	D	119	TYR	N-CA-C	5.17	117.79	110.50
1	F	74	GLU	N-CA-C	5.17	117.39	109.07
1	E	91	THR	CB-CA-C	5.17	117.05	110.13
1	C	43	ILE	N-CA-C	-5.16	100.32	107.80
1	F	122	LEU	CA-C-N	5.16	126.28	119.84
1	F	122	LEU	C-N-CA	5.16	126.28	119.84
1	A	85	PRO	O-C-N	-5.15	115.68	122.64
1	D	21	GLY	O-C-N	-5.15	117.08	123.21
1	E	73	ASP	O-C-N	-5.15	115.43	122.33
1	B	42	VAL	O-C-N	-5.15	117.13	123.00
1	H	7	VAL	O-C-N	-5.15	117.46	122.97
1	B	22	SER	O-C-N	-5.15	116.94	123.17
1	E	82	TYR	O-C-N	-5.14	115.75	122.59
1	F	6	THR	O-C-N	-5.14	116.33	123.12
1	B	98	SER	O-C-N	-5.14	116.51	123.19
1	A	119	TYR	N-CA-C	5.14	117.67	109.96
1	A	141	ASP	CA-C-O	5.13	125.68	119.31
1	F	73	ASP	O-C-N	-5.13	116.68	122.12
1	G	132	PHE	CA-C-O	5.13	125.90	120.36
1	G	14	GLY	O-C-N	-5.12	116.08	122.84
1	B	23	TYR	O-C-N	-5.12	113.61	122.11
1	F	61	PRO	N-CA-C	-5.12	105.57	112.48
1	H	33	TYR	O-C-N	-5.12	116.51	122.96
1	A	45	ASP	CA-C-O	5.12	125.95	120.32
1	H	119	TYR	N-CA-C	5.10	117.27	110.53
1	H	133	LYS	N-CA-C	-5.10	101.54	109.14
1	C	48	GLY	CA-C-O	5.10	124.58	119.27
1	F	44	TYR	O-C-N	-5.10	117.23	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	33	TYR	N-CA-C	5.09	116.04	108.60
1	D	98	SER	O-C-N	-5.09	116.98	123.24
1	H	115	GLU	O-C-N	-5.09	115.82	122.59
1	G	50	PRO	O-C-N	-5.09	116.53	122.99
1	D	17	GLY	O-C-N	-5.08	115.84	122.81
1	A	121	ASN	O-C-N	-5.08	117.19	123.44
1	C	96	VAL	O-C-N	-5.08	116.75	122.94
1	F	59	LYS	O-C-N	-5.08	115.02	122.43
1	A	108	THR	N-CA-C	-5.07	100.78	109.24
1	A	10	TRP	O-C-N	-5.06	116.24	122.82
1	D	144	GLY	N-CA-C	-5.06	103.42	110.96
1	B	14	GLY	N-CA-C	-5.06	104.97	113.02
1	C	68	GLU	CA-C-N	-5.06	115.59	122.93
1	C	68	GLU	C-N-CA	-5.06	115.59	122.93
1	F	2	SER	O-C-N	-5.06	114.91	123.00
1	G	13	PRO	O-C-N	-5.06	115.81	122.64
1	A	74	GLU	N-CA-C	5.05	117.21	109.07
1	B	131	GLY	O-C-N	-5.05	116.14	122.70
1	F	7	VAL	CA-C-O	5.05	126.09	120.59
1	G	32	SER	N-CA-C	-5.04	101.62	109.24
1	G	43	ILE	O-C-N	-5.04	117.60	122.99
1	C	118	THR	CA-C-N	5.03	127.92	120.82
1	C	118	THR	C-N-CA	5.03	127.92	120.82
1	G	11	GLY	O-C-N	-5.03	114.05	123.36
1	C	92	PRO	O-C-N	-5.03	115.47	122.30
1	C	104	ASN	O-C-N	-5.02	116.80	122.12
1	E	6	THR	CA-C-O	5.02	125.84	120.32
1	E	105	LYS	O-C-N	-5.02	115.92	122.39
1	D	125	GLU	O-C-N	-5.01	114.88	122.20
1	G	10	TRP	N-CA-C	-5.01	101.08	109.24
1	E	31	LEU	O-C-N	-5.00	116.65	122.96
1	D	10	TRP	O-C-N	-5.00	117.39	123.29
1	B	82	TYR	O-C-N	-5.00	117.46	123.31

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	AYA	CA
1	B	1	AYA	CA
1	C	1	AYA	CA
1	E	1	AYA	CA
1	G	1	AYA	CA

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Mol	Chain	Res	Type	Atom
1	H	1	AYA	CA

All (46) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	AYA	Mainchain
1	A	115	GLU	Mainchain
1	A	34	LYS	Mainchain
1	A	42	VAL	Mainchain
1	A	72	PRO	Mainchain
1	A	8	GLY	Peptide,Mainchain
1	A	9	SER	Mainchain
1	B	1	AYA	Mainchain
1	B	34	LYS	Mainchain
1	B	8	GLY	Mainchain
1	B	9	SER	Mainchain
1	C	109	PHE	Mainchain
1	C	144	GLY	Mainchain
1	C	23	TYR	Mainchain
1	C	34	LYS	Mainchain
1	C	7	VAL	Mainchain
1	C	8	GLY	Mainchain
1	C	89	LEU	Mainchain
1	C	9	SER	Mainchain
1	D	1	AYA	Mainchain
1	D	23	TYR	Mainchain
1	D	34	LYS	Mainchain
1	D	8	GLY	Peptide,Mainchain
1	E	34	LYS	Peptide,Mainchain
1	E	8	GLY	Peptide
1	E	9	SER	Mainchain
1	E	99	LEU	Mainchain
1	F	23	TYR	Mainchain
1	F	7	VAL	Mainchain
1	F	8	GLY	Mainchain
1	F	88	ALA	Mainchain
1	F	89	LEU	Mainchain
1	F	9	SER	Mainchain
1	F	90	ALA	Mainchain
1	G	3	GLN	Mainchain
1	G	33	TYR	Mainchain
1	G	7	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	G	8	GLY	Mainchain
1	G	89	LEU	Mainchain
1	H	1	AYA	Mainchain
1	H	118	THR	Mainchain
1	H	89	LEU	Mainchain
1	H	9	SER	Mainchain

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	1132	0	1084	72	0
1	B	1132	0	1084	60	0
1	C	1132	0	1084	59	0
1	D	1132	0	1081	86	0
1	E	1128	0	1071	50	0
1	F	1128	0	1068	70	0
1	G	1132	0	1082	57	0
1	H	1132	0	1083	75	0
2	A	118	0	0	7	0
2	B	123	0	0	9	0
2	C	121	0	0	4	0
2	D	121	0	0	7	0
2	E	93	0	0	4	0
2	F	115	0	0	6	0
2	G	102	0	0	6	0
2	H	81	0	0	6	0
All	All	9922	0	8637	493	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 28.

All (493) 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:C:8:GLY:HA2	1:D:123:PRO:HG2	1.22	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:TRP:HZ3	1:D:136:THR:HG23	0.98	1.10
1:D:18:TRP:CZ3	1:D:136:THR:HG23	1.89	1.07
1:A:61:PRO:HD2	2:A:181:HOH:O	1.57	1.04
1:E:60:LEU:HD11	1:E:89:LEU:HD11	1.47	0.97
1:F:28:GLN:HG2	1:F:43:ILE:HB	1.47	0.95
1:D:20:GLU:HG2	1:D:54:PRO:HD2	1.50	0.92
1:D:74:GLU:HA	1:D:104:ASN:HD21	1.33	0.92
1:D:99:LEU:HD11	1:D:143:ILE:HD11	1.51	0.91
1:C:8:GLY:CA	1:D:123:PRO:HG2	2.00	0.90
1:A:92:PRO:HD2	2:A:240:HOH:O	1.72	0.88
1:H:86:PHE:CZ	1:H:88:ALA:HB3	2.10	0.86
1:C:60:LEU:HD11	1:C:89:LEU:HD11	1.56	0.86
1:G:123:PRO:HG2	1:H:8:GLY:HA2	1.55	0.86
1:G:8:GLY:HA2	1:H:123:PRO:HB2	1.55	0.86
1:H:74:GLU:HA	1:H:104:ASN:HD21	1.42	0.84
1:D:18:TRP:HZ3	1:D:136:THR:CG2	1.88	0.84
1:D:60:LEU:HD12	1:D:139:LEU:HD13	1.59	0.83
1:D:14:GLY:O	1:D:135:ARG:HG2	1.78	0.82
1:G:34:LYS:HG3	2:G:246:HOH:O	1.78	0.82
1:F:79:VAL:HG13	1:F:101:PHE:CE1	2.14	0.82
1:C:74:GLU:HA	1:C:104:ASN:HD21	1.43	0.82
2:B:212:HOH:O	1:D:1:AYA:HM3	1.82	0.80
1:E:86:PHE:HD2	1:E:89:LEU:HB2	1.46	0.78
1:E:86:PHE:CD2	1:E:89:LEU:HB2	2.19	0.78
1:F:60:LEU:HD22	1:F:60:LEU:H	1.48	0.78
1:D:60:LEU:HD12	1:D:139:LEU:CD1	2.14	0.78
1:E:123:PRO:HG2	1:F:8:GLY:HA2	1.66	0.78
1:F:67:ILE:HG23	1:F:109:PHE:CD2	2.19	0.77
1:F:75:PHE:H	1:F:104:ASN:ND2	1.83	0.76
1:A:133:LYS:HE3	1:A:144:GLY:HA3	1.66	0.76
1:A:89:LEU:O	1:A:91:THR:HG22	1.86	0.76
1:D:41:SER:OG	1:D:55:LYS:HD3	1.86	0.76
1:H:18:TRP:HZ3	1:H:136:THR:HG1	1.32	0.76
1:D:75:PHE:H	1:D:104:ASN:ND2	1.84	0.75
1:A:88:ALA:C	1:A:90:ALA:H	1.90	0.75
1:H:18:TRP:HZ3	1:H:136:THR:OG1	1.71	0.74
1:E:52:SER:HB2	2:E:153:HOH:O	1.87	0.74
1:A:102:LYS:HG2	1:A:108:THR:HB	1.70	0.73
1:D:60:LEU:CD1	1:D:139:LEU:HD13	2.17	0.73
1:H:91:THR:HG21	1:H:95:VAL:HG21	1.69	0.73
1:G:74:GLU:HA	1:G:104:ASN:HD21	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:7:VAL:HG12	1:F:145:ILE:HG22	1.69	0.73
1:A:100:THR:HG22	1:A:111:PRO:HA	1.70	0.73
1:C:8:GLY:HA2	1:D:123:PRO:CG	2.12	0.73
1:B:20:GLU:HG2	1:B:54:PRO:HD2	1.69	0.72
1:C:35:GLU:HG3	1:C:86:PHE:CZ	2.24	0.72
1:C:133:LYS:HE2	2:C:218:HOH:O	1.90	0.72
1:E:48:GLY:HA3	2:E:172:HOH:O	1.89	0.72
1:F:20:GLU:HG2	1:F:54:PRO:HD2	1.71	0.72
1:H:109:PHE:HB3	1:H:112:TYR:OH	1.90	0.71
1:D:89:LEU:HA	2:D:223:HOH:O	1.90	0.71
1:C:4:THR:HG21	1:C:146:HIS:HB3	1.73	0.71
1:B:39:SER:HB3	1:B:57:THR:HA	1.73	0.71
1:E:60:LEU:CD1	1:E:89:LEU:HD11	2.20	0.70
1:B:28:GLN:HG2	1:B:43:ILE:HG13	1.74	0.70
1:G:133:LYS:HE3	1:H:125:GLU:OE2	1.92	0.69
1:C:65:VAL:HG21	1:C:112:TYR:CE1	2.28	0.68
1:H:135:ARG:HD2	2:H:205:HOH:O	1.95	0.67
1:A:60:LEU:HD22	1:A:60:LEU:H	1.59	0.67
1:C:74:GLU:HB2	1:C:105:LYS:HG3	1.75	0.67
1:F:67:ILE:HG23	1:F:109:PHE:CE2	2.30	0.67
1:H:71:PHE:CD1	1:H:72:PRO:HA	2.30	0.66
1:D:78:SER:HB3	1:D:102:LYS:HB2	1.77	0.66
1:F:34:LYS:HD2	1:F:62:TYR:HA	1.76	0.66
1:B:30:GLU:OE2	1:B:66:LYS:HG3	1.95	0.66
1:F:79:VAL:HG13	1:F:101:PHE:HE1	1.57	0.66
1:F:89:LEU:O	1:F:91:THR:HG22	1.94	0.66
1:A:92:PRO:HD3	2:A:256:HOH:O	1.95	0.66
1:D:136:THR:HG22	1:D:140:LEU:HD12	1.78	0.66
1:G:83:THR:HG22	1:G:118:THR:HG23	1.77	0.66
1:G:18:TRP:HZ3	1:G:136:THR:OG1	1.78	0.66
1:C:18:TRP:HH2	1:C:140:LEU:CD1	2.09	0.65
1:F:74:GLU:HA	1:F:104:ASN:HD21	1.60	0.65
1:E:82:TYR:HB2	1:E:98:SER:HB3	1.79	0.65
1:C:5:ILE:HD13	1:D:5:ILE:HD12	1.77	0.65
1:G:104:ASN:HD22	1:G:104:ASN:H	1.45	0.65
1:D:74:GLU:OE2	1:D:103:THR:HG21	1.98	0.64
1:D:60:LEU:HD11	1:D:89:LEU:HD11	1.78	0.64
1:G:18:TRP:HZ3	1:G:136:THR:HG1	1.44	0.64
1:E:123:PRO:HG2	1:F:8:GLY:CA	2.26	0.64
1:H:58:SER:HB2	1:H:138:ASP:O	1.98	0.64
1:D:60:LEU:CD1	1:D:89:LEU:HD11	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:GLU:HB2	1:F:132:PHE:O	1.98	0.63
1:D:99:LEU:HD11	1:D:143:ILE:CD1	2.28	0.63
1:B:1:AYA:H	1:D:128:LEU:HD21	1.63	0.63
1:A:1:AYA:HM3	1:C:128:LEU:HD11	1.81	0.63
1:B:89:LEU:O	1:B:91:THR:HG22	1.99	0.63
1:D:74:GLU:OE2	1:D:107:ARG:HD3	1.99	0.63
1:H:18:TRP:CZ3	1:H:136:THR:OG1	2.48	0.63
1:A:132:PHE:CE1	1:A:145:ILE:HD11	2.33	0.63
1:A:20:GLU:HG2	1:A:54:PRO:HD2	1.80	0.63
1:F:34:LYS:CD	1:F:62:TYR:HA	2.29	0.63
1:F:1:AYA:HM2	1:H:128:LEU:HG	1.81	0.62
1:D:37:ILE:O	1:D:139:LEU:HG	1.99	0.62
1:C:86:PHE:CZ	1:C:88:ALA:HB3	2.35	0.62
1:G:116:GLU:HB3	2:G:203:HOH:O	1.97	0.62
1:G:18:TRP:CD1	1:G:18:TRP:C	2.78	0.61
1:E:82:TYR:CE2	1:E:115:GLU:HG2	2.34	0.61
1:E:81:GLY:O	1:E:98:SER:HB3	2.00	0.61
1:A:40:PHE:O	1:A:56:HIS:HB2	2.00	0.61
1:B:102:LYS:HD3	1:B:108:THR:HB	1.81	0.61
1:C:11:GLY:HA2	1:C:83:THR:HG21	1.83	0.61
1:A:8:GLY:HA2	1:B:123:PRO:HD2	1.82	0.61
1:B:130:VAL:HG11	1:B:148:SER:OG	2.01	0.60
1:H:60:LEU:HD21	2:H:227:HOH:O	2.01	0.60
1:F:34:LYS:HB2	1:F:62:TYR:CD1	2.35	0.60
1:A:60:LEU:HD11	1:A:89:LEU:HD11	1.83	0.60
1:A:88:ALA:C	1:A:90:ALA:N	2.60	0.60
1:D:98:SER:HA	1:D:112:TYR:O	2.01	0.60
1:D:59:LYS:HG3	2:D:186:HOH:O	2.00	0.59
1:G:18:TRP:HH2	1:G:140:LEU:HD13	1.66	0.59
1:B:135:ARG:HB2	1:B:141:ASP:HB2	1.85	0.59
1:D:67:ILE:HG23	1:D:109:PHE:CD2	2.37	0.59
1:E:20:GLU:HG2	1:E:54:PRO:HD2	1.84	0.59
1:H:28:GLN:NE2	1:H:66:LYS:HE3	2.17	0.59
1:A:123:PRO:HD2	1:B:8:GLY:HA2	1.84	0.59
1:H:74:GLU:OE2	1:H:107:ARG:HD3	2.03	0.59
1:D:13:PRO:HB3	2:D:162:HOH:O	2.02	0.58
1:D:136:THR:CG2	1:D:140:LEU:HD12	2.34	0.58
1:B:128:LEU:HD12	1:D:2:SER:HB3	1.85	0.58
1:C:135:ARG:CG	1:C:142:ALA:HB3	2.34	0.58
1:D:74:GLU:CA	1:D:104:ASN:HD21	2.11	0.58
1:B:98:SER:HA	1:B:112:TYR:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:LYS:NZ	2:E:166:HOH:O	2.37	0.58
1:A:49:ASP:HB3	2:A:172:HOH:O	2.03	0.58
1:H:28:GLN:HE22	1:H:66:LYS:HE3	1.68	0.58
1:A:18:TRP:CD1	1:A:19:ASP:N	2.72	0.58
1:B:23:TYR:HE2	1:B:51:PHE:CE2	2.21	0.58
1:A:18:TRP:HD1	1:A:19:ASP:N	2.02	0.57
1:B:1:AYA:HM3	2:D:150:HOH:O	2.04	0.57
1:C:135:ARG:HG3	1:C:142:ALA:HB3	1.84	0.57
1:D:58:SER:HB2	1:D:138:ASP:O	2.04	0.57
1:D:18:TRP:HH2	1:D:140:LEU:HD11	1.69	0.57
1:D:136:THR:HG22	1:D:140:LEU:HA	1.86	0.57
1:F:96:VAL:HG21	1:F:140:LEU:HD23	1.86	0.57
1:G:139:LEU:HD23	2:G:212:HOH:O	2.03	0.57
1:H:86:PHE:CE2	1:H:88:ALA:HB3	2.39	0.57
1:D:75:PHE:N	1:D:104:ASN:ND2	2.52	0.57
1:D:99:LEU:CD1	1:D:143:ILE:HD11	2.32	0.57
1:H:18:TRP:CD1	1:H:18:TRP:C	2.81	0.57
1:H:27:ARG:HD3	1:H:71:PHE:CD2	2.40	0.57
1:F:104:ASN:H	1:F:104:ASN:HD22	1.51	0.57
1:G:78:SER:HB3	1:G:102:LYS:HB3	1.86	0.57
1:G:135:ARG:HB2	1:G:142:ALA:HB3	1.87	0.57
1:G:121:ASN:HB3	2:G:214:HOH:O	2.04	0.57
1:C:60:LEU:CD1	1:C:89:LEU:HD11	2.31	0.56
1:B:83:THR:O	1:B:118:THR:HG22	2.05	0.56
1:B:35:GLU:HB2	1:B:86:PHE:CZ	2.40	0.56
1:F:8:GLY:O	1:F:9:SER:HB2	2.04	0.56
1:A:74:GLU:HA	1:A:104:ASN:HD21	1.70	0.56
1:D:36:ALA:HB3	1:D:139:LEU:HD21	1.88	0.56
1:A:17:GLY:HA2	1:A:135:ARG:HG2	1.87	0.56
1:C:11:GLY:HA2	1:C:83:THR:CG2	2.36	0.56
1:G:139:LEU:HD23	1:G:139:LEU:N	2.20	0.56
1:H:138:ASP:HB2	1:H:139:LEU:HD12	1.88	0.56
1:C:46:LEU:HB2	1:C:51:PHE:HB2	1.88	0.56
1:B:93:THR:CG2	2:B:195:HOH:O	2.53	0.56
1:H:26:ILE:HG23	1:H:42:VAL:HG23	1.87	0.56
1:H:104:ASN:HD22	1:H:104:ASN:H	1.52	0.56
1:D:11:GLY:HA2	1:D:83:THR:OG1	2.06	0.55
1:D:132:PHE:CE1	1:D:145:ILE:HD12	2.41	0.55
1:D:74:GLU:HG3	1:D:105:LYS:HG2	1.88	0.55
1:G:74:GLU:OE2	1:G:107:ARG:HD3	2.06	0.55
1:A:28:GLN:NE2	1:A:66:LYS:HE3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLN:NE2	1:A:66:LYS:CE	2.69	0.55
1:B:22:SER:HB2	2:B:156:HOH:O	2.07	0.55
1:C:67:ILE:O	1:C:67:ILE:HG22	2.06	0.55
1:F:23:TYR:O	1:F:130:VAL:HG22	2.07	0.55
1:F:19:ASP:HA	1:F:133:LYS:HB2	1.87	0.55
1:E:75:PHE:H	1:E:104:ASN:ND2	2.04	0.55
1:B:102:LYS:CD	1:B:108:THR:HB	2.36	0.55
1:E:104:ASN:N	1:E:104:ASN:HD22	2.03	0.55
1:D:18:TRP:CD1	1:D:18:TRP:C	2.85	0.55
1:G:34:LYS:NZ	1:G:34:LYS:HB3	2.22	0.54
1:C:22:SER:C	1:C:23:TYR:CD1	2.85	0.54
1:H:13:PRO:HD2	1:H:93:THR:OG1	2.07	0.54
1:A:7:VAL:HG12	1:A:145:ILE:HG22	1.88	0.54
1:A:23:TYR:HE2	1:A:51:PHE:CE2	2.25	0.54
1:A:104:ASN:H	1:A:104:ASN:HD22	1.54	0.54
1:E:11:GLY:HA2	1:E:83:THR:CG2	2.36	0.54
1:E:60:LEU:HD22	1:E:60:LEU:H	1.72	0.54
1:H:101:PHE:CD1	1:H:101:PHE:N	2.74	0.54
1:F:1:AYA:HM3	2:H:153:HOH:O	2.07	0.54
1:G:18:TRP:CZ3	1:G:136:THR:OG1	2.54	0.54
1:H:28:GLN:HB2	1:H:68:GLU:HA	1.89	0.53
1:A:23:TYR:CE2	1:A:51:PHE:CD2	2.95	0.53
1:C:11:GLY:HA3	1:C:142:ALA:HA	1.90	0.53
1:G:139:LEU:HD23	1:G:139:LEU:H	1.74	0.53
1:B:92:PRO:HD3	2:B:245:HOH:O	2.07	0.53
1:G:104:ASN:HD22	1:G:104:ASN:N	2.05	0.53
1:E:114:ASP:O	1:E:116:GLU:N	2.42	0.53
1:F:74:GLU:HG3	1:F:105:LYS:HG2	1.91	0.53
1:D:40:PHE:O	1:D:56:HIS:HB2	2.09	0.53
1:A:89:LEU:O	1:A:90:ALA:C	2.51	0.53
1:D:96:VAL:HG12	1:D:140:LEU:O	2.09	0.53
1:H:18:TRP:HH2	1:H:140:LEU:CD1	2.22	0.53
1:A:89:LEU:HG	1:A:139:LEU:HD21	1.91	0.53
1:C:18:TRP:CZ3	1:C:136:THR:OG1	2.55	0.53
1:D:20:GLU:OE1	1:D:44:TYR:OH	2.27	0.53
1:F:104:ASN:HD22	1:F:104:ASN:N	2.07	0.53
1:A:60:LEU:HD22	1:A:60:LEU:N	2.23	0.52
1:B:97:ARG:O	1:B:113:GLY:HA3	2.09	0.52
1:G:125:GLU:OE2	1:H:133:LYS:HE3	2.09	0.52
1:C:31:LEU:HA	1:C:39:SER:O	2.10	0.52
1:C:35:GLU:HG3	1:C:86:PHE:HZ	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:LEU:CD1	1:D:139:LEU:HD22	2.39	0.52
1:H:11:GLY:HA3	1:H:142:ALA:HA	1.91	0.52
1:B:23:TYR:CE2	1:B:51:PHE:CE2	2.98	0.52
1:B:135:ARG:HD2	2:B:268:HOH:O	2.08	0.52
1:D:14:GLY:O	1:D:135:ARG:CG	2.53	0.52
1:E:11:GLY:HA2	1:E:83:THR:HG23	1.91	0.52
1:E:18:TRP:CD1	1:E:18:TRP:C	2.87	0.52
1:E:60:LEU:HD11	1:E:89:LEU:CD1	2.30	0.52
1:D:100:THR:HG22	1:D:111:PRO:HA	1.92	0.52
1:A:5:ILE:HG13	1:B:149:LEU:HD13	1.92	0.52
1:D:132:PHE:CE1	1:D:145:ILE:CD1	2.93	0.52
1:F:31:LEU:HD12	1:F:31:LEU:C	2.35	0.52
1:G:83:THR:HG22	1:G:118:THR:CG2	2.40	0.52
1:G:71:PHE:C	1:G:71:PHE:CD1	2.88	0.52
1:C:124:ILE:HG12	1:C:147:MET:HE1	1.91	0.51
1:H:27:ARG:HH21	1:H:49:ASP:C	2.18	0.51
1:A:28:GLN:NE2	1:A:43:ILE:HD12	2.25	0.51
1:F:58:SER:HB2	1:F:138:ASP:O	2.11	0.51
1:F:32:SER:HA	1:F:63:LYS:O	2.10	0.51
1:G:130:VAL:HG21	1:G:148:SER:HB3	1.93	0.51
1:D:31:LEU:C	1:D:31:LEU:HD12	2.36	0.51
1:D:33:TYR:N	1:D:33:TYR:CD1	2.79	0.51
1:D:86:PHE:CD2	1:D:89:LEU:HG	2.46	0.51
1:B:18:TRP:CD1	1:B:18:TRP:C	2.89	0.51
1:D:60:LEU:HD11	1:D:89:LEU:CD1	2.41	0.51
1:D:86:PHE:HD2	1:D:89:LEU:HG	1.75	0.50
1:G:36:ALA:HA	1:G:97:ARG:HA	1.93	0.50
1:H:35:GLU:HA	1:H:114:ASP:OD2	2.11	0.50
1:H:31:LEU:HA	1:H:39:SER:O	2.11	0.50
1:G:33:TYR:O	1:G:62:TYR:HB3	2.12	0.50
1:B:18:TRP:CZ3	1:B:136:THR:OG1	2.63	0.50
1:F:41:SER:HB3	1:F:55:LYS:HA	1.94	0.50
1:F:47:ASN:ND2	1:H:22:SER:H	2.09	0.50
1:F:100:THR:HG22	2:F:202:HOH:O	2.10	0.50
1:H:135:ARG:HG3	1:H:142:ALA:HB3	1.93	0.50
1:C:60:LEU:HD11	1:C:89:LEU:CD1	2.35	0.49
1:C:22:SER:O	1:C:23:TYR:CD1	2.65	0.49
1:C:97:ARG:HH12	1:C:116:GLU:CD	2.20	0.49
1:F:18:TRP:C	1:F:18:TRP:CD1	2.89	0.49
1:F:27:ARG:HB2	1:F:43:ILE:HG22	1.93	0.49
1:C:75:PHE:H	1:C:104:ASN:ND2	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:VAL:HG13	1:E:44:TYR:CE2	2.47	0.49
1:B:89:LEU:HD11	1:B:139:LEU:CD2	2.43	0.49
1:E:62:TYR:CD1	1:E:62:TYR:N	2.80	0.49
1:F:106:GLY:HA2	2:F:209:HOH:O	2.11	0.49
1:B:18:TRP:HH2	1:B:140:LEU:CD1	2.26	0.49
1:H:12:GLY:HA2	1:H:94:PRO:HG2	1.94	0.49
1:D:71:PHE:HE2	2:D:177:HOH:O	1.96	0.49
1:A:18:TRP:CD1	1:A:18:TRP:C	2.91	0.49
1:C:18:TRP:HH2	1:C:140:LEU:HD13	1.78	0.49
1:C:71:PHE:CD1	1:C:71:PHE:C	2.91	0.49
1:F:47:ASN:HD21	1:H:22:SER:H	1.61	0.49
1:B:18:TRP:CD1	1:B:56:HIS:NE2	2.81	0.49
1:B:96:VAL:HG13	1:B:140:LEU:O	2.13	0.49
1:E:60:LEU:CG	1:E:89:LEU:HD11	2.43	0.49
1:G:63:LYS:CB	2:G:246:HOH:O	2.61	0.49
1:H:83:THR:HG22	1:H:118:THR:O	2.12	0.49
1:F:18:TRP:CG	1:F:56:HIS:CE1	3.01	0.48
1:F:89:LEU:HD11	1:F:139:LEU:HD11	1.95	0.48
1:G:31:LEU:C	1:G:31:LEU:HD12	2.38	0.48
1:H:74:GLU:OE1	1:H:107:ARG:NH1	2.45	0.48
1:C:97:ARG:NH1	1:C:116:GLU:HG3	2.27	0.48
1:E:84:GLY:O	1:E:95:VAL:HG12	2.14	0.48
1:D:36:ALA:HB3	1:D:139:LEU:CD2	2.43	0.48
1:D:94:PRO:HD2	2:D:236:HOH:O	2.12	0.48
1:A:3:GLN:HG3	1:B:126:ASN:ND2	2.28	0.48
1:G:102:LYS:HD3	1:G:108:THR:HB	1.95	0.48
1:F:21:GLY:O	1:F:131:GLY:HA3	2.14	0.48
1:G:8:GLY:N	1:H:123:PRO:O	2.46	0.48
1:E:18:TRP:CG	1:E:56:HIS:CE1	3.02	0.48
1:H:67:ILE:HG12	1:H:109:PHE:CD2	2.48	0.48
1:A:60:LEU:H	1:A:60:LEU:CD2	2.25	0.48
1:B:44:TYR:CE1	1:B:131:GLY:HA2	2.49	0.47
1:C:13:PRO:HD2	1:C:93:THR:OG1	2.14	0.47
1:D:18:TRP:CH2	1:D:140:LEU:HD11	2.49	0.47
1:H:71:PHE:CE1	1:H:72:PRO:HB3	2.50	0.47
1:B:34:LYS:HG2	1:B:35:GLU:CD	2.39	0.47
1:D:7:VAL:CG1	1:D:8:GLY:N	2.77	0.47
1:E:5:ILE:HG13	1:F:149:LEU:HD13	1.96	0.47
1:F:17:GLY:HA2	1:F:135:ARG:HG2	1.96	0.47
1:G:95:VAL:HG13	1:G:140:LEU:O	2.14	0.47
1:H:27:ARG:HH21	1:H:50:PRO:N	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:TRP:CH2	1:B:140:LEU:CD1	2.98	0.47
1:B:34:LYS:NZ	2:B:170:HOH:O	2.26	0.47
1:A:4:THR:HG21	1:A:22:SER:OG	2.14	0.47
1:E:1:AYA:OT	1:G:71:PHE:CE2	2.68	0.47
1:F:33:TYR:HD2	1:F:113:GLY:H	1.62	0.47
1:G:59:LYS:O	1:G:60:LEU:C	2.57	0.47
1:A:23:TYR:HE2	1:A:51:PHE:CD2	2.32	0.47
1:A:132:PHE:CE1	1:A:145:ILE:CD1	2.98	0.47
1:A:148:SER:HA	1:B:5:ILE:HD11	1.97	0.47
1:G:11:GLY:HA2	1:G:83:THR:OG1	2.15	0.47
1:G:35:GLU:HB3	1:G:97:ARG:HH21	1.79	0.47
1:G:75:PHE:H	1:G:104:ASN:ND2	2.13	0.47
1:H:40:PHE:O	1:H:56:HIS:HB2	2.15	0.47
1:H:58:SER:OG	1:H:60:LEU:HB2	2.15	0.47
1:C:58:SER:OG	1:C:60:LEU:HD12	2.15	0.46
1:D:99:LEU:HD12	1:D:99:LEU:HA	1.78	0.46
1:E:24:THR:O	1:G:2:SER:OG	2.33	0.46
1:F:60:LEU:H	1:F:60:LEU:CD2	2.24	0.46
1:D:74:GLU:HA	1:D:104:ASN:ND2	2.16	0.46
1:F:110:GLY:HA2	2:F:210:HOH:O	2.14	0.46
1:A:58:SER:HB2	1:A:138:ASP:O	2.16	0.46
1:C:74:GLU:CA	1:C:104:ASN:HD21	2.19	0.46
1:H:147:MET:HB3	1:H:147:MET:HE2	1.70	0.46
1:A:67:ILE:HG23	1:A:109:PHE:CE2	2.51	0.46
1:D:45:ASP:CG	1:D:71:PHE:CZ	2.93	0.46
1:A:28:GLN:NE2	1:A:66:LYS:HE2	2.30	0.46
1:A:67:ILE:HG23	1:A:109:PHE:CD2	2.51	0.46
1:B:93:THR:HG22	2:B:195:HOH:O	2.15	0.46
1:C:46:LEU:HD23	1:C:46:LEU:HA	1.86	0.46
1:F:98:SER:HA	1:F:112:TYR:O	2.15	0.46
1:G:17:GLY:HA2	1:G:135:ARG:HG2	1.97	0.46
1:B:135:ARG:HG3	1:B:142:ALA:HB3	1.98	0.46
1:D:7:VAL:HG13	1:D:8:GLY:N	2.31	0.46
1:G:139:LEU:N	1:G:139:LEU:CD2	2.78	0.46
1:H:27:ARG:NH2	1:H:50:PRO:N	2.64	0.46
1:F:71:PHE:HE1	1:H:1:AYA:HM3	1.81	0.45
1:G:4:THR:HG21	1:G:146:HIS:ND1	2.31	0.45
1:H:16:ASN:O	1:H:135:ARG:HA	2.15	0.45
1:H:99:LEU:O	1:H:100:THR:HG22	2.16	0.45
1:C:64:ASN:HB3	2:C:172:HOH:O	2.17	0.45
1:C:87:SER:O	1:C:88:ALA:C	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:PHE:HB3	1:B:112:TYR:OH	2.16	0.45
1:C:33:TYR:C	1:C:62:TYR:HB3	2.41	0.45
1:F:75:PHE:H	1:F:104:ASN:HD21	1.57	0.45
1:F:76:LEU:HD11	1:F:101:PHE:HB3	1.99	0.45
1:H:18:TRP:CH2	1:H:140:LEU:CD1	3.00	0.45
1:F:90:ALA:HA	2:F:248:HOH:O	2.16	0.45
1:H:96:VAL:HG12	1:H:140:LEU:O	2.16	0.45
1:A:28:GLN:HB3	1:A:43:ILE:HB	1.98	0.45
1:E:62:TYR:N	1:E:62:TYR:HD1	2.14	0.45
1:F:58:SER:HB2	1:F:60:LEU:HD23	1.98	0.45
1:B:23:TYR:O	1:B:130:VAL:HG22	2.16	0.45
1:A:74:GLU:HG3	1:A:105:LYS:HB2	1.99	0.45
1:F:44:TYR:O	1:F:51:PHE:N	2.45	0.45
1:A:31:LEU:HD12	1:A:31:LEU:C	2.42	0.45
1:E:37:ILE:HG21	1:E:140:LEU:HD23	1.99	0.45
1:G:24:THR:O	1:G:24:THR:HG22	2.17	0.45
1:G:130:VAL:O	1:G:130:VAL:CG1	2.64	0.45
1:D:18:TRP:CZ3	1:D:136:THR:CG2	2.77	0.45
1:F:121:ASN:C	1:F:123:PRO:HD3	2.41	0.45
1:A:104:ASN:HD22	1:A:104:ASN:N	2.15	0.45
1:H:37:ILE:HD12	1:H:99:LEU:HD22	1.99	0.45
1:G:26:ILE:HG22	1:G:69:LEU:HD12	1.98	0.44
1:A:89:LEU:CG	1:A:139:LEU:HD21	2.47	0.44
1:G:45:ASP:CG	1:G:71:PHE:CZ	2.96	0.44
1:A:89:LEU:HA	1:A:89:LEU:HD22	1.63	0.44
1:F:34:LYS:HB2	1:F:62:TYR:CG	2.52	0.44
1:A:116:GLU:HG3	2:A:208:HOH:O	2.17	0.44
1:D:54:PRO:HG2	2:D:164:HOH:O	2.16	0.44
1:E:18:TRP:CD1	1:E:56:HIS:CE1	3.05	0.44
1:H:84:GLY:HA2	2:H:202:HOH:O	2.17	0.44
1:B:18:TRP:HZ3	1:B:136:THR:OG1	1.99	0.44
1:E:87:SER:O	1:E:90:ALA:N	2.44	0.44
1:B:32:SER:HB3	1:B:64:ASN:ND2	2.33	0.44
1:C:18:TRP:HZ3	1:C:136:THR:N	2.16	0.44
1:H:97:ARG:O	1:H:113:GLY:HA3	2.17	0.44
1:A:110:GLY:HA3	2:A:203:HOH:O	2.18	0.44
1:E:47:ASN:CG	1:G:21:GLY:HA3	2.42	0.44
1:E:60:LEU:HD21	1:E:89:LEU:HD11	2.00	0.44
1:F:68:GLU:HB3	2:F:154:HOH:O	2.18	0.44
1:A:30:GLU:HG2	1:A:66:LYS:HG3	2.00	0.43
1:A:96:VAL:HG22	1:A:140:LEU:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ILE:HG22	1:B:69:LEU:HD22	1.99	0.43
1:B:89:LEU:HD11	1:B:139:LEU:HD22	2.00	0.43
1:D:103:THR:HG23	1:D:105:LYS:H	1.84	0.43
1:E:134:GLY:O	1:E:135:ARG:HG3	2.18	0.43
1:F:74:GLU:OE2	1:F:107:ARG:HD3	2.17	0.43
1:C:8:GLY:O	1:C:9:SER:HB2	2.18	0.43
1:C:97:ARG:NH1	1:C:116:GLU:CG	2.82	0.43
1:E:34:LYS:HB2	1:E:62:TYR:CD1	2.53	0.43
1:F:45:ASP:CG	1:F:71:PHE:CZ	2.96	0.43
1:F:71:PHE:O	2:F:182:HOH:O	2.21	0.43
1:G:18:TRP:CH2	1:G:140:LEU:CD1	3.02	0.43
1:F:18:TRP:CH2	1:F:140:LEU:HD11	2.54	0.43
1:D:86:PHE:CZ	1:D:88:ALA:HB3	2.53	0.43
1:A:77:GLU:HG2	1:A:77:GLU:O	2.17	0.43
1:B:39:SER:HB3	1:B:57:THR:CA	2.47	0.43
1:C:5:ILE:HG13	1:D:149:LEU:HD13	2.00	0.43
1:D:67:ILE:HG23	1:D:109:PHE:CE2	2.54	0.43
1:E:33:TYR:HE1	1:E:65:VAL:HG22	1.84	0.43
1:F:24:THR:O	1:F:24:THR:HG22	2.19	0.43
1:C:105:LYS:HB3	1:C:105:LYS:HE2	1.62	0.43
1:D:43:ILE:HG12	1:D:52:SER:HB3	2.01	0.43
1:A:132:PHE:HE1	1:A:145:ILE:HD11	1.82	0.43
1:B:31:LEU:HA	1:B:39:SER:O	2.19	0.43
1:A:75:PHE:H	1:A:104:ASN:ND2	2.16	0.42
1:B:1:AYA:HM2	1:D:128:LEU:HD21	2.01	0.42
1:D:139:LEU:HD12	1:D:139:LEU:HA	1.78	0.42
1:A:20:GLU:CG	1:A:54:PRO:HD2	2.47	0.42
1:B:104:ASN:OD1	1:B:104:ASN:N	2.51	0.42
1:C:104:ASN:N	1:C:104:ASN:HD22	2.17	0.42
1:D:18:TRP:HH2	1:D:140:LEU:CD1	2.33	0.42
1:D:69:LEU:HD12	1:D:69:LEU:HA	1.79	0.42
1:E:75:PHE:H	1:E:104:ASN:HD21	1.66	0.42
1:B:32:SER:HA	1:B:63:LYS:O	2.19	0.42
1:H:122:LEU:HA	1:H:122:LEU:HD12	1.77	0.42
1:F:46:LEU:HD12	1:F:46:LEU:HA	1.70	0.42
1:G:20:GLU:OE1	1:G:44:TYR:OH	2.25	0.42
1:G:100:THR:HG21	2:G:224:HOH:O	2.18	0.42
1:B:13:PRO:HB2	2:B:160:HOH:O	2.20	0.42
1:B:121:ASN:ND2	1:B:123:PRO:HG3	2.35	0.42
1:G:20:GLU:HG2	1:G:54:PRO:HD2	2.00	0.42
1:H:96:VAL:CG1	1:H:140:LEU:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLY:O	1:A:111:PRO:C	2.61	0.42
1:B:23:TYR:CD1	1:B:23:TYR:N	2.87	0.42
1:B:93:THR:HA	1:B:94:PRO:HD3	1.99	0.42
1:E:81:GLY:O	1:E:82:TYR:HB2	2.20	0.42
1:H:58:SER:C	1:H:60:LEU:H	2.27	0.42
1:C:93:THR:HG23	2:C:200:HOH:O	2.20	0.42
1:D:37:ILE:HD13	1:D:37:ILE:HA	1.87	0.42
1:F:34:LYS:HD3	1:F:62:TYR:HA	2.02	0.42
1:G:8:GLY:HA2	1:H:123:PRO:CB	2.36	0.42
1:H:27:ARG:CZ	1:H:50:PRO:HG3	2.50	0.42
1:H:46:LEU:O	1:H:47:ASN:C	2.59	0.42
1:A:47:ASN:OD1	1:C:23:TYR:CE1	2.73	0.42
1:C:59:LYS:NZ	2:C:188:HOH:O	2.51	0.42
1:H:74:GLU:HA	1:H:104:ASN:ND2	2.21	0.42
1:A:23:TYR:CE2	1:A:51:PHE:CE2	3.06	0.42
1:A:32:SER:HA	1:A:64:ASN:HA	2.02	0.42
1:B:82:TYR:HE1	1:B:115:GLU:OE1	2.02	0.42
1:C:33:TYR:O	1:C:62:TYR:HB3	2.20	0.42
1:G:140:LEU:HD11	1:G:142:ALA:O	2.20	0.42
1:H:27:ARG:NH2	1:H:45:ASP:OD1	2.53	0.42
1:H:60:LEU:HA	1:H:60:LEU:HD12	1.70	0.42
1:C:104:ASN:HD22	1:C:104:ASN:H	1.66	0.42
1:D:65:VAL:HG21	1:D:112:TYR:CE1	2.55	0.42
1:F:29:ILE:HB	1:F:67:ILE:HD12	2.01	0.42
1:H:26:ILE:HG23	1:H:42:VAL:CG2	2.49	0.42
1:H:89:LEU:O	1:H:90:ALA:C	2.63	0.42
1:A:18:TRP:CE2	1:A:56:HIS:CD2	3.07	0.41
1:B:49:ASP:HB3	2:B:230:HOH:O	2.20	0.41
1:C:50:PRO:O	1:C:50:PRO:HG2	2.19	0.41
1:E:60:LEU:HD23	1:E:139:LEU:HD12	2.01	0.41
1:A:74:GLU:OE2	1:A:107:ARG:HD3	2.20	0.41
1:B:1:AYA:H	1:D:128:LEU:CD2	2.30	0.41
1:E:42:VAL:CG1	1:E:44:TYR:CZ	3.03	0.41
1:F:58:SER:HB2	1:F:60:LEU:CD2	2.50	0.41
1:F:121:ASN:O	1:F:123:PRO:HD3	2.20	0.41
1:H:67:ILE:HG23	1:H:109:PHE:CE2	2.55	0.41
1:F:35:GLU:O	1:F:97:ARG:NE	2.53	0.41
1:G:96:VAL:HG22	1:G:140:LEU:HD23	2.02	0.41
1:H:130:VAL:HG21	1:H:148:SER:HB3	2.02	0.41
1:C:135:ARG:HG3	1:C:142:ALA:CB	2.49	0.41
1:D:89:LEU:HD11	1:D:139:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:PHE:CD1	1:D:109:PHE:N	2.88	0.41
1:H:12:GLY:CA	1:H:94:PRO:HG2	2.49	0.41
1:A:31:LEU:HD12	1:A:65:VAL:HG12	2.03	0.41
1:D:129:ILE:HG12	1:D:145:ILE:HG12	2.03	0.41
1:E:34:LYS:HB2	1:E:62:TYR:CG	2.55	0.41
1:F:129:ILE:HG21	1:F:129:ILE:HD13	1.81	0.41
1:B:58:SER:OG	1:B:60:LEU:HB2	2.21	0.41
1:D:74:GLU:CG	1:D:105:LYS:HG2	2.51	0.41
1:F:36:ALA:HA	1:F:97:ARG:HA	2.01	0.41
1:H:7:VAL:HG13	1:H:8:GLY:N	2.35	0.41
1:A:96:VAL:HG21	1:A:140:LEU:HD23	2.02	0.41
1:C:29:ILE:HG12	1:C:42:VAL:HG13	2.02	0.41
1:F:82:TYR:CD1	1:F:115:GLU:HG2	2.56	0.41
1:A:128:LEU:HD21	1:C:1:AYA:CT	2.51	0.41
1:D:120:PHE:CD1	1:D:120:PHE:C	2.98	0.41
1:H:71:PHE:CD1	1:H:72:PRO:CA	3.02	0.41
1:E:89:LEU:O	1:E:90:ALA:HB3	2.21	0.41
1:F:71:PHE:CE1	1:H:1:AYA:HM3	2.55	0.41
1:G:119:TYR:CE2	1:G:121:ASN:HB2	2.56	0.41
1:H:29:ILE:HD11	1:H:76:LEU:HD21	2.02	0.41
1:B:4:THR:HG23	1:B:5:ILE:O	2.21	0.41
1:B:110:GLY:O	1:B:111:PRO:C	2.64	0.41
1:E:37:ILE:HG23	1:E:37:ILE:HD12	1.82	0.41
1:A:87:SER:O	1:A:90:ALA:HA	2.21	0.40
1:C:123:PRO:HD2	1:D:8:GLY:HA2	2.03	0.40
1:D:6:THR:HG23	1:D:146:HIS:ND1	2.36	0.40
1:E:125:GLU:HG3	2:E:226:HOH:O	2.20	0.40
1:F:60:LEU:HB3	1:F:61:PRO:HD2	2.02	0.40
1:A:64:ASN:ND2	2:A:244:HOH:O	2.53	0.40
1:A:70:LYS:O	1:A:71:PHE:C	2.63	0.40
1:C:132:PHE:CE1	1:C:145:ILE:HD11	2.57	0.40
1:E:82:TYR:CD2	1:E:115:GLU:HG2	2.55	0.40
1:G:104:ASN:N	1:G:104:ASN:ND2	2.70	0.40
1:H:25:GLY:HA2	2:H:153:HOH:O	2.22	0.40
1:A:47:ASN:HD21	1:C:22:SER:H	1.67	0.40
1:E:18:TRP:CD1	1:E:19:ASP:N	2.90	0.40
1:H:100:THR:CG2	2:H:196:HOH:O	2.69	0.40
1:A:147:MET:HE2	1:A:147:MET:HB3	1.83	0.40
1:E:89:LEU:HA	1:E:89:LEU:HD22	1.68	0.40
1:G:95:VAL:HG11	1:G:139:LEU:HG	2.04	0.40
1:E:59:LYS:O	1:E:60:LEU:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	147/149 (99%)	133 (90%)	12 (8%)	2 (1%)	9	13
1	B	147/149 (99%)	136 (92%)	8 (5%)	3 (2%)	6	7
1	C	147/149 (99%)	131 (89%)	11 (8%)	5 (3%)	3	2
1	D	147/149 (99%)	132 (90%)	12 (8%)	3 (2%)	6	7
1	E	147/149 (99%)	131 (89%)	12 (8%)	4 (3%)	4	4
1	F	147/149 (99%)	135 (92%)	11 (8%)	1 (1%)	18	28
1	G	147/149 (99%)	139 (95%)	6 (4%)	2 (1%)	9	13
1	H	147/149 (99%)	128 (87%)	17 (12%)	2 (1%)	9	13
All	All	1176/1192 (99%)	1065 (91%)	89 (8%)	22 (2%)	6	8

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	110	GLY
1	B	9	SER
1	B	110	GLY
1	C	9	SER
1	C	110	GLY
1	D	110	GLY
1	E	110	GLY
1	F	9	SER
1	H	110	GLY
1	C	70	LYS
1	D	130	VAL
1	G	90	ALA
1	B	34	LYS

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Mol	Chain	Res	Type
1	C	106	GLY
1	E	34	LYS
1	E	81	GLY
1	D	34	LYS
1	H	34	LYS
1	G	34	LYS
1	E	13	PRO
1	C	137	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 X-ray entries followed by that with respect to entries of similar resolution.

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	120/122 (98%)	97 (81%)	23 (19%)	1	2
1	B	120/122 (98%)	93 (78%)	27 (22%)	1	1
1	C	120/122 (98%)	90 (75%)	30 (25%)	0	1
1	D	120/122 (98%)	93 (78%)	27 (22%)	1	1
1	E	119/122 (98%)	91 (76%)	28 (24%)	1	1
1	F	119/122 (98%)	96 (81%)	23 (19%)	1	2
1	G	120/122 (98%)	96 (80%)	24 (20%)	1	2
1	H	120/122 (98%)	85 (71%)	35 (29%)	0	0
All	All	958/976 (98%)	741 (77%)	217 (23%)	1	1

All (217) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	7	VAL
1	A	9	SER
1	A	18	TRP
1	A	42	VAL
1	A	58	SER
1	A	69	LEU

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Mol	Chain	Res	Type
1	A	72	PRO
1	A	76	LEU
1	A	83	THR
1	A	89	LEU
1	A	91	THR
1	A	95	VAL
1	A	100	THR
1	A	104	ASN
1	A	105	LYS
1	A	108	THR
1	A	116	GLU
1	A	118	THR
1	A	130	VAL
1	A	143	ILE
1	A	145	ILE
1	A	149	LEU
1	B	4	THR
1	B	7	VAL
1	B	16	ASN
1	B	18	TRP
1	B	24	THR
1	B	28	GLN
1	B	34	LYS
1	B	39	SER
1	B	42	VAL
1	B	49	ASP
1	B	55	LYS
1	B	59	LYS
1	B	60	LEU
1	B	66	LYS
1	B	76	LEU
1	B	83	THR
1	B	91	THR
1	B	93	THR
1	B	95	VAL
1	B	96	VAL
1	B	108	THR
1	B	116	GLU
1	B	129	ILE
1	B	130	VAL
1	B	139	LEU
1	B	145	ILE

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Mol	Chain	Res	Type
1	B	149	LEU
1	C	2	SER
1	C	4	THR
1	C	5	ILE
1	C	13	PRO
1	C	22	SER
1	C	24	THR
1	C	35	GLU
1	C	46	LEU
1	C	52	SER
1	C	65	VAL
1	C	69	LEU
1	C	76	LEU
1	C	83	THR
1	C	96	VAL
1	C	98	SER
1	C	99	LEU
1	C	100	THR
1	C	102	LYS
1	C	103	THR
1	C	104	ASN
1	C	105	LYS
1	C	108	THR
1	C	111	PRO
1	C	118	THR
1	C	130	VAL
1	C	133	LYS
1	C	135	ARG
1	C	139	LEU
1	C	143	ILE
1	C	145	ILE
1	D	7	VAL
1	D	16	ASN
1	D	18	TRP
1	D	22	SER
1	D	34	LYS
1	D	42	VAL
1	D	49	ASP
1	D	50	PRO
1	D	69	LEU
1	D	76	LEU
1	D	80	SER

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Mol	Chain	Res	Type
1	D	93	THR
1	D	95	VAL
1	D	96	VAL
1	D	98	SER
1	D	99	LEU
1	D	100	THR
1	D	103	THR
1	D	104	ASN
1	D	108	THR
1	D	118	THR
1	D	120	PHE
1	D	130	VAL
1	D	143	ILE
1	D	145	ILE
1	D	148	SER
1	D	149	LEU
1	E	5	ILE
1	E	7	VAL
1	E	13	PRO
1	E	18	TRP
1	E	24	THR
1	E	42	VAL
1	E	57	THR
1	E	65	VAL
1	E	69	LEU
1	E	76	LEU
1	E	89	LEU
1	E	93	THR
1	E	95	VAL
1	E	103	THR
1	E	104	ASN
1	E	107	ARG
1	E	108	THR
1	E	115	GLU
1	E	118	THR
1	E	125	GLU
1	E	130	VAL
1	E	136	THR
1	E	138	ASP
1	E	141	ASP
1	E	143	ILE
1	E	145	ILE

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Mol	Chain	Res	Type
1	E	148	SER
1	E	149	LEU
1	F	5	ILE
1	F	7	VAL
1	F	18	TRP
1	F	28	GLN
1	F	42	VAL
1	F	43	ILE
1	F	57	THR
1	F	60	LEU
1	F	70	LYS
1	F	72	PRO
1	F	76	LEU
1	F	80	SER
1	F	87	SER
1	F	89	LEU
1	F	94	PRO
1	F	95	VAL
1	F	102	LYS
1	F	104	ASN
1	F	130	VAL
1	F	141	ASP
1	F	145	ILE
1	F	148	SER
1	F	149	LEU
1	G	2	SER
1	G	4	THR
1	G	5	ILE
1	G	34	LYS
1	G	49	ASP
1	G	68	GLU
1	G	70	LYS
1	G	72	PRO
1	G	76	LEU
1	G	83	THR
1	G	89	LEU
1	G	96	VAL
1	G	100	THR
1	G	102	LYS
1	G	104	ASN
1	G	105	LYS
1	G	108	THR

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Mol	Chain	Res	Type
1	G	120	PHE
1	G	125	GLU
1	G	128	LEU
1	G	130	VAL
1	G	133	LYS
1	G	139	LEU
1	G	145	ILE
1	H	5	ILE
1	H	7	VAL
1	H	18	TRP
1	H	22	SER
1	H	28	GLN
1	H	34	LYS
1	H	37	ILE
1	H	42	VAL
1	H	49	ASP
1	H	58	SER
1	H	60	LEU
1	H	65	VAL
1	H	68	GLU
1	H	69	LEU
1	H	76	LEU
1	H	77	GLU
1	H	80	SER
1	H	87	SER
1	H	89	LEU
1	H	91	THR
1	H	95	VAL
1	H	96	VAL
1	H	98	SER
1	H	100	THR
1	H	101	PHE
1	H	102	LYS
1	H	104	ASN
1	H	108	THR
1	H	118	THR
1	H	128	LEU
1	H	130	VAL
1	H	135	ARG
1	H	143	ILE
1	H	145	ILE
1	H	149	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	16	ASN
1	A	28	GLN
1	A	47	ASN
1	A	104	ASN
1	B	16	ASN
1	B	47	ASN
1	B	64	ASN
1	B	126	ASN
1	C	16	ASN
1	C	28	GLN
1	C	47	ASN
1	C	104	ASN
1	D	28	GLN
1	D	104	ASN
1	D	121	ASN
1	E	47	ASN
1	E	56	HIS
1	E	104	ASN
1	F	47	ASN
1	F	64	ASN
1	F	104	ASN
1	G	3	GLN
1	G	16	ASN
1	G	47	ASN
1	G	104	ASN
1	H	47	ASN
1	H	104	ASN
1	H	121	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	AYA	H	1	1	6,7,8	1.44	1 (16%)	6,8,10	10.82	6 (100%)
1	AYA	F	1	1	6,7,8	1.65	1 (16%)	6,8,10	10.99	6 (100%)
1	AYA	C	1	1	6,7,8	1.26	1 (16%)	6,8,10	11.40	5 (83%)
1	AYA	A	1	1	6,7,8	1.08	0	6,8,10	11.15	5 (83%)
1	AYA	G	1	1	6,7,8	2.44	1 (16%)	6,8,10	10.67	3 (50%)
1	AYA	E	1	1	6,7,8	0.81	0	6,8,10	10.73	3 (50%)
1	AYA	D	1	1	6,7,8	1.81	1 (16%)	6,8,10	11.61	3 (50%)
1	AYA	B	1	1	6,7,8	1.68	2 (33%)	6,8,10	10.46	6 (100%)

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
1	AYA	H	1	1	1/1/2/4	5/5/6/8	-
1	AYA	F	1	1	-	5/5/6/8	-
1	AYA	C	1	1	1/1/2/4	5/5/6/8	-
1	AYA	A	1	1	1/1/2/4	5/5/6/8	-
1	AYA	G	1	1	1/1/2/4	4/5/6/8	-
1	AYA	E	1	1	1/1/2/4	4/5/6/8	-
1	AYA	D	1	1	-	4/5/6/8	-
1	AYA	B	1	1	1/1/2/4	3/5/6/8	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1	AYA	CA-N	-5.46	1.40	1.46
1	D	1	AYA	CA-N	3.62	1.50	1.46
1	F	1	AYA	CA-N	3.22	1.50	1.46
1	H	1	AYA	OT-CT	2.90	1.29	1.23
1	B	1	AYA	CA-N	-2.82	1.43	1.46
1	C	1	AYA	CM-CT	2.51	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	AYA	CM-CT	2.38	1.55	1.50

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1	AYA	CB-CA-N	23.84	136.60	109.68
1	C	1	AYA	CB-CA-N	23.71	136.45	109.68
1	G	1	AYA	CB-CA-N	23.22	135.89	109.68
1	A	1	AYA	CB-CA-N	23.01	135.66	109.68
1	E	1	AYA	CB-CA-N	21.68	134.16	109.68
1	B	1	AYA	CB-CA-N	21.43	133.88	109.68
1	H	1	AYA	CB-CA-N	21.37	133.81	109.68
1	F	1	AYA	CB-CA-N	21.25	133.68	109.68
1	D	1	AYA	CA-N-CT	14.40	140.09	121.50
1	F	1	AYA	CA-N-CT	13.88	139.41	121.50
1	H	1	AYA	CA-N-CT	13.65	139.12	121.50
1	E	1	AYA	CA-N-CT	13.40	138.80	121.50
1	A	1	AYA	CA-N-CT	13.01	138.30	121.50
1	C	1	AYA	CA-N-CT	12.63	137.80	121.50
1	G	1	AYA	CA-N-CT	10.15	134.61	121.50
1	B	1	AYA	CA-N-CT	8.60	132.60	121.50
1	B	1	AYA	OT-CT-N	-6.87	109.83	121.98
1	F	1	AYA	O-C-CA	-6.77	102.84	123.94
1	B	1	AYA	O-C-CA	-6.54	103.57	123.94
1	C	1	AYA	O-C-CA	-6.21	104.58	123.94
1	H	1	AYA	O-C-CA	-6.10	104.93	123.94
1	G	1	AYA	O-C-CA	-5.95	105.41	123.94
1	E	1	AYA	O-C-CA	-5.81	105.82	123.94
1	A	1	AYA	O-C-CA	-5.75	106.03	123.94
1	D	1	AYA	O-C-CA	-5.59	106.53	123.94
1	B	1	AYA	CM-CT-N	5.02	124.45	116.12
1	F	1	AYA	CM-CT-N	4.54	123.65	116.12
1	H	1	AYA	OT-CT-N	-3.38	116.01	121.98
1	C	1	AYA	CM-CT-N	3.05	121.18	116.12
1	C	1	AYA	OT-CT-CM	-2.99	116.72	122.05
1	F	1	AYA	OT-CT-N	-2.92	116.82	121.98
1	B	1	AYA	OT-CT-CM	-2.82	117.03	122.05
1	A	1	AYA	CM-CT-N	2.54	120.33	116.12
1	H	1	AYA	CM-CT-N	2.47	120.22	116.12
1	F	1	AYA	OT-CT-CM	-2.41	117.75	122.05
1	A	1	AYA	OT-CT-CM	-2.34	117.89	122.05
1	H	1	AYA	OT-CT-CM	-2.19	118.16	122.05

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	AYA	CA
1	B	1	AYA	CA
1	C	1	AYA	CA
1	E	1	AYA	CA
1	G	1	AYA	CA
1	H	1	AYA	CA

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	AYA	CB-CA-N-CT
1	A	1	AYA	OT-CT-N-CA
1	A	1	AYA	CM-CT-N-CA
1	A	1	AYA	O-C-CA-CB
1	B	1	AYA	CB-CA-N-CT
1	C	1	AYA	CB-CA-N-CT
1	C	1	AYA	C-CA-N-CT
1	C	1	AYA	OT-CT-N-CA
1	C	1	AYA	CM-CT-N-CA
1	C	1	AYA	O-C-CA-CB
1	D	1	AYA	CB-CA-N-CT
1	D	1	AYA	OT-CT-N-CA
1	D	1	AYA	CM-CT-N-CA
1	E	1	AYA	CB-CA-N-CT
1	E	1	AYA	C-CA-N-CT
1	E	1	AYA	OT-CT-N-CA
1	E	1	AYA	CM-CT-N-CA
1	F	1	AYA	CB-CA-N-CT
1	F	1	AYA	O-C-CA-CB
1	G	1	AYA	CB-CA-N-CT
1	G	1	AYA	C-CA-N-CT
1	G	1	AYA	OT-CT-N-CA
1	G	1	AYA	CM-CT-N-CA
1	H	1	AYA	CB-CA-N-CT
1	H	1	AYA	C-CA-N-CT
1	H	1	AYA	OT-CT-N-CA
1	H	1	AYA	CM-CT-N-CA
1	H	1	AYA	O-C-CA-CB
1	B	1	AYA	OT-CT-N-CA
1	F	1	AYA	OT-CT-N-CA
1	A	1	AYA	C-CA-N-CT
1	B	1	AYA	C-CA-N-CT

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Mol	Chain	Res	Type	Atoms
1	D	1	AYA	C-CA-N-CT
1	F	1	AYA	C-CA-N-CT
1	F	1	AYA	CM-CT-N-CA

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	1	AYA	2	0
1	F	1	AYA	2	0
1	C	1	AYA	1	0
1	A	1	AYA	1	0
1	E	1	AYA	1	0
1	D	1	AYA	1	0
1	B	1	AYA	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	2
1	C	1
1	D	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	22:SER	C	23:TYR	N	1.20
1	D	8:GLY	C	9:SER	N	1.20
1	F	9:SER	C	10:TRP	N	1.20
1	B	89:LEU	C	90:ALA	N	1.18
1	F	90:ALA	C	91:THR	N	1.14

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	148/149 (99%)	-0.63	2 (1%) 73 69	7, 20, 37, 60	0
1	B	148/149 (99%)	-0.54	0 100 100	11, 24, 37, 46	0
1	C	148/149 (99%)	-0.62	1 (0%) 84 81	7, 22, 34, 57	0
1	D	148/149 (99%)	-0.38	2 (1%) 73 69	11, 26, 44, 66	0
1	E	148/149 (99%)	-0.54	2 (1%) 73 69	8, 23, 47, 61	0
1	F	148/149 (99%)	-0.41	4 (2%) 56 52	9, 26, 44, 63	0
1	G	148/149 (99%)	-0.69	1 (0%) 84 81	10, 21, 33, 52	0
1	H	148/149 (99%)	-0.48	2 (1%) 73 69	11, 26, 40, 60	0
All	All	1184/1192 (99%)	-0.54	14 (1%) 76 73	7, 24, 43, 66	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	91	THR	4.8
1	C	23	TYR	4.1
1	F	91	THR	3.6
1	A	91	THR	3.1
1	D	89	LEU	2.9
1	H	88	ALA	2.8
1	E	91	THR	2.7
1	D	91	THR	2.4
1	A	88	ALA	2.4
1	F	90	ALA	2.4
1	E	88	ALA	2.1
1	G	88	ALA	2.1
1	F	89	LEU	2.1
1	F	88	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	AYA	A	1	8/9	0.91	0.07	24,26,31,35	0
1	AYA	E	1	8/9	0.91	0.06	12,20,22,22	0
1	AYA	B	1	8/9	0.92	0.08	30,33,37,38	0
1	AYA	F	1	8/9	0.92	0.06	17,23,32,32	0
1	AYA	D	1	8/9	0.93	0.07	22,28,32,34	0
1	AYA	H	1	8/9	0.93	0.06	23,25,30,32	0
1	AYA	G	1	8/9	0.94	0.05	22,26,31,31	0
1	AYA	C	1	8/9	0.95	0.06	18,23,29,34	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.