



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:44 PM UTC

PDB ID : 2SOD / pdb_00002sod
Title : DETERMINATION AND ANALYSIS OF THE 2 ANGSTROM STRUCTURE OF COPPER, ZINC SUPEROXIDE DISMUTASE
Authors : Tainer, J.A.; Getzoff, E.D.; Richardson, J.S.; Richardson, D.C.
Deposited on : 1980-03-25
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

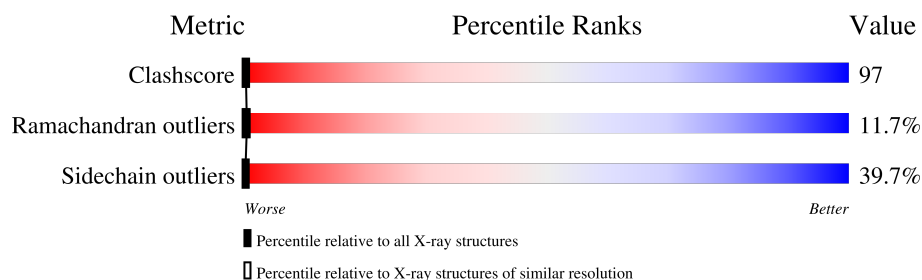
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	152	8% 31% 38% 24%
1	G	152	7% 20% 42% 32%
1	O	152	9% 22% 42% 26%
1	Y	152	• 26% 39% 32%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4392 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 COPPER,ZINC SUPEROXIDE DISMUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	152	Total	C	N	O	S	0	0	0
			1095	672	198	221	4			
1	Y	152	Total	C	N	O	S	0	0	0
			1095	672	198	221	4			
1	B	152	Total	C	N	O	S	0	0	0
			1095	672	198	221	4			
1	G	152	Total	C	N	O	S	0	0	0
			1095	672	198	221	4			

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	O	1	Total	Cu	0	0
			1	1		
2	Y	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		
2	G	1	Total	Cu	0	0
			1	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	1	Total	Zn	0	0
			1	1		
3	Y	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	G	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

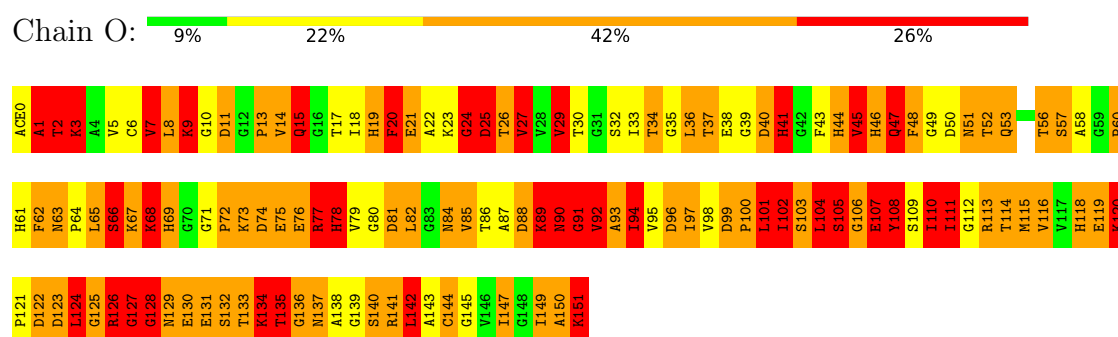
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	1	Total 1	O 1	0	0
4	Y	1	Total 1	O 1	0	0
4	B	1	Total 1	O 1	0	0
4	G	1	Total 1	O 1	0	0

3 Residue-property plots

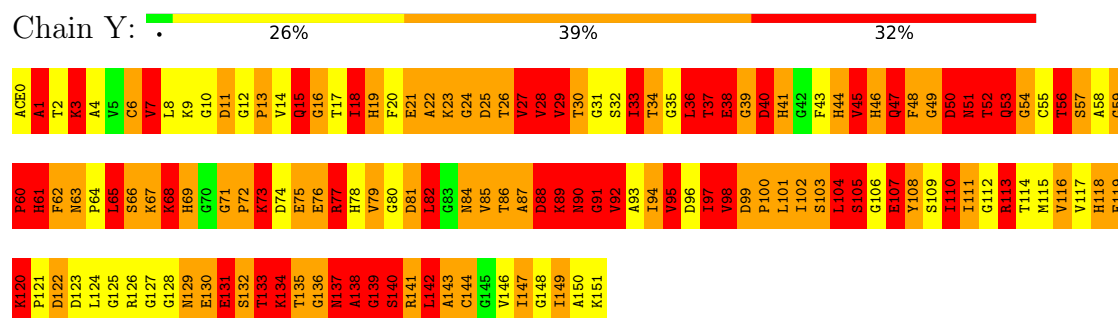
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

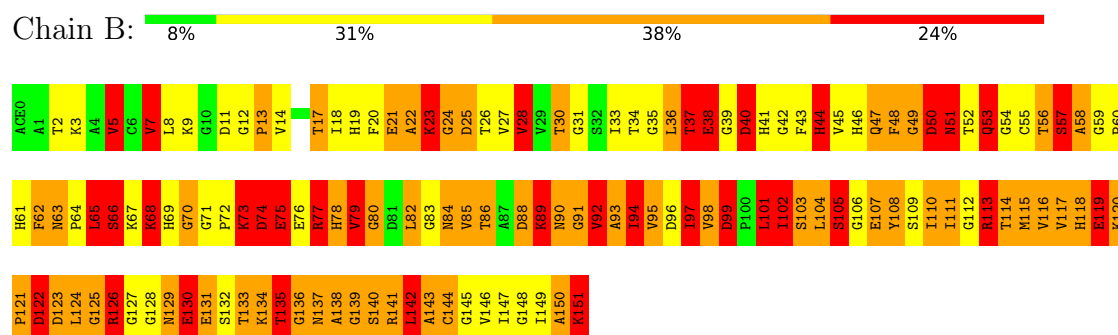
• Molecule 1: COPPER,ZINC SUPEROXIDE DISMUTASE



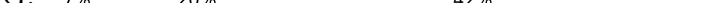
• Molecule 1: COPPER,ZINC SUPEROXIDE DISMUTASE

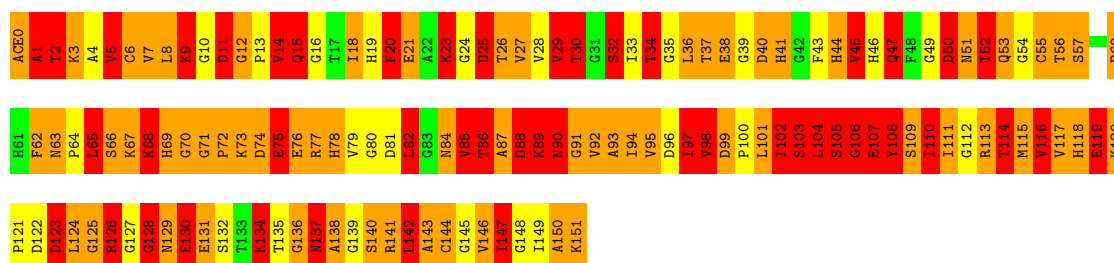


• Molecule 1: COPPER,ZINC SUPEROXIDE DISMUTASE



• Molecule 1: COPPER,ZINC SUPEROXIDE DISMUTASE

Chain G: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.65Å 90.33Å 71.65Å 90.00° 95.10° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.256 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4392	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, ACE, ZN

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	B	2.19	40/1111 (3.6%)	4.06	258/1501 (17.2%)
1	G	2.51	56/1111 (5.0%)	4.63	283/1501 (18.9%)
1	O	2.27	35/1111 (3.2%)	4.29	241/1501 (16.1%)
1	Y	2.45	58/1111 (5.2%)	5.03	307/1501 (20.5%)
All	All	2.36	189/4444 (4.3%)	4.52	1089/6004 (18.1%)

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	G	0	2
1	Y	0	2
All	All	0	4

All (189) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	88	ASP	CA-CB	14.16	1.76	1.53
1	G	141	ARG	N-CA	-12.59	1.30	1.46
1	O	89	LYS	CA-CB	11.62	1.73	1.54
1	G	141	ARG	CA-CB	11.52	1.67	1.53
1	Y	139	GLY	N-CA	-10.91	1.29	1.45
1	O	94	ILE	N-CA	-10.64	1.33	1.46
1	Y	60	PRO	C-O	10.50	1.37	1.24
1	G	108	TYR	N-CA	10.40	1.59	1.46
1	G	127	GLY	N-CA	10.32	1.60	1.45
1	B	95	VAL	N-CA	-10.31	1.33	1.46
1	Y	88	ASP	CA-CB	9.71	1.69	1.53
1	G	85	VAL	C-O	9.61	1.35	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	123	ASP	N-CA	9.51	1.58	1.46
1	B	57	SER	C-O	9.21	1.35	1.23
1	G	88	ASP	N-CA	-9.16	1.34	1.46
1	B	95	VAL	CA-CB	9.14	1.67	1.53
1	Y	118	HIS	CA-CB	8.86	1.69	1.53
1	G	66	SER	CA-C	-8.78	1.43	1.53
1	G	131	GLU	CA-C	8.68	1.61	1.52
1	Y	133	THR	CA-CB	8.63	1.68	1.53
1	O	104	LEU	N-CA	8.54	1.57	1.46
1	G	144	CYS	CA-CB	-8.47	1.39	1.53
1	B	136	GLY	N-CA	8.46	1.57	1.45
1	G	126	ARG	C-O	8.33	1.34	1.24
1	Y	89	LYS	N-CA	-8.33	1.35	1.46
1	G	68	LYS	C-N	-7.96	1.23	1.33
1	Y	139	GLY	CA-C	-7.71	1.41	1.51
1	Y	60	PRO	C-N	-7.69	1.23	1.33
1	O	127	GLY	C-O	7.68	1.34	1.23
1	Y	54	GLY	N-CA	-7.65	1.34	1.45
1	Y	22	ALA	N-CA	7.65	1.56	1.46
1	G	57	SER	C-N	-7.49	1.23	1.33
1	G	118	HIS	C-N	-7.46	1.23	1.33
1	B	94	ILE	C-N	-7.42	1.24	1.33
1	G	131	GLU	N-CA	-7.35	1.37	1.46
1	Y	24	GLY	N-CA	7.31	1.55	1.45
1	G	40	ASP	CA-CB	7.31	1.63	1.53
1	B	113	ARG	CD-NE	-7.29	1.36	1.46
1	Y	39	GLY	N-CA	-7.23	1.35	1.44
1	G	7	VAL	N-CA	7.16	1.54	1.46
1	O	90	ASN	N-CA	-7.15	1.36	1.46
1	G	128	GLY	N-CA	-7.14	1.35	1.45
1	Y	51	ASN	N-CA	-7.12	1.37	1.46
1	G	89	LYS	CA-C	7.07	1.62	1.52
1	O	94	ILE	CA-CB	7.04	1.64	1.54
1	G	12	GLY	N-CA	7.04	1.54	1.44
1	G	147	ILE	C-N	7.03	1.40	1.33
1	O	151	LYS	N-CA	6.90	1.59	1.46
1	Y	102	ILE	C-O	6.89	1.32	1.24
1	G	140	SER	CB-OG	6.89	1.55	1.42
1	Y	143	ALA	CA-CB	-6.86	1.42	1.53
1	Y	149	ILE	C-N	-6.85	1.23	1.33
1	Y	126	ARG	C-N	-6.83	1.23	1.33
1	Y	46	HIS	C-N	-6.72	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	94	ILE	C-O	6.71	1.32	1.24
1	G	103	SER	N-CA	-6.70	1.37	1.46
1	G	144	CYS	CA-C	6.69	1.60	1.52
1	B	94	ILE	CA-CB	6.69	1.63	1.54
1	B	144	CYS	N-CA	-6.61	1.37	1.45
1	B	148	GLY	CA-C	6.60	1.58	1.52
1	Y	106	GLY	N-CA	6.56	1.52	1.45
1	O	65	LEU	N-CA	6.55	1.56	1.46
1	B	142	LEU	CA-CB	6.54	1.65	1.53
1	Y	60	PRO	CA-C	-6.54	1.43	1.52
1	B	139	GLY	CA-C	-6.50	1.42	1.51
1	Y	38	GLU	N-CA	6.46	1.54	1.46
1	B	51	ASN	N-CA	-6.42	1.38	1.46
1	Y	140	SER	N-CA	6.41	1.54	1.46
1	G	109	SER	N-CA	-6.35	1.38	1.46
1	Y	98	VAL	N-CA	6.33	1.53	1.46
1	B	25	ASP	N-CA	6.33	1.53	1.46
1	B	56	THR	N-CA	6.30	1.54	1.46
1	G	56	THR	CA-CB	6.28	1.63	1.53
1	Y	26	THR	CA-CB	6.27	1.64	1.53
1	Y	126	ARG	CA-C	6.27	1.59	1.52
1	Y	22	ALA	CA-CB	-6.26	1.45	1.52
1	B	138	ALA	CA-CB	6.25	1.63	1.53
1	B	33	ILE	CB-CG1	6.22	1.65	1.53
1	B	140	SER	N-CA	6.20	1.54	1.45
1	O	127	GLY	N-CA	-6.19	1.36	1.45
1	O	81	ASP	C-O	-6.18	1.17	1.24
1	B	96	ASP	C-N	-6.17	1.26	1.33
1	G	10	GLY	N-CA	6.17	1.50	1.45
1	B	57	SER	C-N	-6.14	1.25	1.33
1	O	85	VAL	N-CA	6.12	1.53	1.46
1	O	25	ASP	C-O	6.11	1.31	1.24
1	B	77	ARG	CD-NE	-6.11	1.37	1.46
1	B	106	GLY	N-CA	6.10	1.53	1.45
1	B	140	SER	CA-CB	-6.10	1.43	1.53
1	Y	48	PHE	C-O	-6.08	1.16	1.23
1	Y	130	GLU	CA-CB	6.06	1.63	1.53
1	G	10	GLY	CA-C	6.05	1.58	1.52
1	Y	60	PRO	CA-CB	6.04	1.62	1.53
1	O	126	ARG	CA-C	6.03	1.60	1.52
1	Y	56	THR	CB-OG1	6.03	1.53	1.43
1	Y	52	THR	CB-OG1	6.02	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	135	THR	C-O	6.01	1.31	1.24
1	G	66	SER	N-CA	6.01	1.54	1.46
1	G	109	SER	C-N	-5.99	1.27	1.34
1	G	140	SER	C-O	-5.99	1.16	1.23
1	B	139	GLY	N-CA	-5.96	1.36	1.45
1	G	126	ARG	N-CA	-5.94	1.38	1.46
1	G	74	ASP	C-O	5.94	1.31	1.24
1	O	136	GLY	N-CA	5.93	1.53	1.45
1	B	149	ILE	CA-C	5.93	1.59	1.52
1	G	43	PHE	CA-CB	-5.92	1.44	1.53
1	Y	134	LYS	CA-CB	5.92	1.63	1.53
1	G	125	GLY	C-N	-5.91	1.25	1.33
1	Y	143	ALA	C-N	-5.88	1.26	1.33
1	G	87	ALA	C-N	-5.86	1.25	1.33
1	G	96	ASP	CA-C	-5.86	1.47	1.53
1	Y	74	ASP	CA-CB	5.85	1.63	1.53
1	G	108	TYR	CA-C	-5.85	1.46	1.53
1	G	76	GLU	CA-C	5.81	1.60	1.53
1	B	73	LYS	CA-CB	5.76	1.62	1.53
1	G	10	GLY	C-N	-5.73	1.25	1.33
1	O	46	HIS	CA-CB	5.72	1.60	1.53
1	B	80	GLY	C-N	-5.72	1.25	1.33
1	O	44	HIS	ND1-CE1	5.72	1.38	1.32
1	B	94	ILE	N-CA	-5.72	1.39	1.46
1	G	111	ILE	N-CA	5.71	1.53	1.46
1	Y	25	ASP	CB-CG	5.70	1.66	1.52
1	G	122	ASP	C-O	5.69	1.31	1.24
1	O	126	ARG	CD-NE	5.61	1.54	1.46
1	Y	49	GLY	N-CA	-5.61	1.37	1.45
1	Y	147	ILE	C-N	-5.61	1.26	1.33
1	B	139	GLY	C-O	5.60	1.31	1.23
1	Y	88	ASP	N-CA	-5.59	1.39	1.46
1	B	115	MET	CA-C	5.59	1.59	1.52
1	G	30	THR	CA-CB	5.54	1.64	1.54
1	Y	150	ALA	N-CA	-5.52	1.39	1.46
1	B	70	GLY	C-O	5.50	1.27	1.23
1	G	107	GLU	N-CA	-5.50	1.39	1.46
1	Y	127	GLY	CA-C	5.48	1.59	1.51
1	G	102	ILE	C-N	-5.47	1.26	1.33
1	O	96	ASP	N-CA	5.47	1.52	1.46
1	G	143	ALA	CA-CB	-5.46	1.44	1.53
1	O	103	SER	C-N	-5.45	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	135	THR	N-CA	-5.45	1.39	1.46
1	Y	139	GLY	C-O	5.44	1.31	1.23
1	G	122	ASP	CA-CB	-5.44	1.44	1.53
1	B	118	HIS	C-O	5.44	1.30	1.23
1	O	89	LYS	N-CA	-5.43	1.38	1.45
1	G	122	ASP	N-CA	5.42	1.53	1.46
1	Y	119	GLU	N-CA	5.42	1.52	1.45
1	G	106	GLY	C-N	-5.39	1.26	1.33
1	O	132	SER	CA-CB	-5.38	1.45	1.53
1	G	91	GLY	N-CA	-5.37	1.38	1.45
1	G	52	THR	C-O	5.34	1.30	1.24
1	B	110	ILE	CA-CB	5.34	1.61	1.54
1	Y	87	ALA	C-O	5.33	1.30	1.23
1	Y	30	THR	CA-CB	5.33	1.64	1.53
1	O	23	LYS	CA-CB	-5.33	1.44	1.53
1	B	93	ALA	C-N	-5.32	1.26	1.33
1	B	47	GLN	CA-CB	5.31	1.61	1.53
1	G	129	ASN	C-N	-5.31	1.26	1.33
1	G	130	GLU	N-CA	-5.30	1.39	1.46
1	O	33	ILE	CA-C	5.30	1.59	1.52
1	G	123	ASP	N-CA	5.29	1.53	1.46
1	Y	96	ASP	C-O	5.28	1.30	1.23
1	O	24	GLY	CA-C	-5.27	1.44	1.51
1	O	110	ILE	CA-CB	5.27	1.61	1.54
1	B	135	THR	C-O	5.26	1.30	1.24
1	Y	141	ARG	CD-NE	-5.26	1.38	1.46
1	B	48	PHE	C-O	-5.25	1.17	1.23
1	O	44	HIS	CA-CB	5.25	1.64	1.54
1	B	46	HIS	CD2-NE2	-5.24	1.32	1.37
1	B	9	LYS	CA-CB	5.23	1.63	1.53
1	Y	34	THR	CA-C	5.22	1.58	1.52
1	Y	105	SER	N-CA	-5.22	1.39	1.46
1	Y	51	ASN	C-N	-5.21	1.26	1.33
1	O	81	ASP	N-CA	5.21	1.52	1.46
1	B	38	GLU	C-O	5.20	1.30	1.24
1	Y	79	VAL	N-CA	5.20	1.53	1.46
1	O	78	HIS	CD2-NE2	-5.18	1.32	1.37
1	Y	87	ALA	C-N	-5.17	1.26	1.33
1	Y	24	GLY	C-N	-5.16	1.26	1.33
1	Y	46	HIS	CG-ND1	-5.13	1.32	1.38
1	Y	73	LYS	C-O	5.12	1.30	1.24
1	O	68	LYS	CA-CB	-5.12	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	41	HIS	CA-CB	5.11	1.65	1.53
1	Y	15	GLN	CA-CB	5.10	1.62	1.53
1	O	81	ASP	CA-CB	-5.09	1.45	1.53
1	Y	7	VAL	C-O	-5.08	1.18	1.24
1	O	101	LEU	N-CA	-5.07	1.40	1.46
1	O	132	SER	C-O	-5.06	1.18	1.24
1	G	26	THR	CA-CB	5.05	1.61	1.53
1	B	83	GLY	CA-C	-5.03	1.44	1.51
1	Y	65	LEU	N-CA	-5.02	1.40	1.46

All (1089) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	96	ASP	CA-CB-CG	65.40	178.00	112.60
1	B	77	ARG	CD-NE-CZ	35.75	174.45	124.40
1	O	89	LYS	N-CA-C	35.61	163.54	109.41
1	Y	38	GLU	CA-C-N	31.67	163.88	121.13
1	Y	38	GLU	C-N-CA	31.67	163.88	121.13
1	O	89	LYS	CA-C-N	30.41	179.62	121.54
1	O	89	LYS	C-N-CA	30.41	179.62	121.54
1	G	123	ASP	CA-CB-CG	28.49	141.09	112.60
1	O	89	LYS	CA-C-O	27.30	153.25	121.58
1	Y	25	ASP	CA-CB-CG	-26.41	86.19	112.60
1	G	119	GLU	CB-CG-CD	26.15	157.06	112.60
1	G	87	ALA	CA-C-N	25.31	163.71	120.68
1	G	87	ALA	C-N-CA	25.31	163.71	120.68
1	G	102	ILE	CA-C-N	24.30	167.96	121.54
1	G	102	ILE	C-N-CA	24.30	167.96	121.54
1	G	85	VAL	CA-C-O	-24.04	90.73	120.78
1	Y	88	ASP	CA-C-N	23.85	167.09	121.54
1	Y	88	ASP	C-N-CA	23.85	167.09	121.54
1	B	50	ASP	CA-C-N	23.37	166.18	121.54
1	B	50	ASP	C-N-CA	23.37	166.18	121.54
1	O	93	ALA	CA-C-N	22.61	162.67	121.97
1	O	93	ALA	C-N-CA	22.61	162.67	121.97
1	G	108	TYR	CB-CA-C	22.53	143.65	111.88
1	O	123	ASP	CA-CB-CG	22.27	134.87	112.60
1	B	113	ARG	CD-NE-CZ	20.81	153.54	124.40
1	Y	139	GLY	N-CA-C	20.70	162.25	113.18
1	Y	48	PHE	CA-CB-CG	19.80	133.60	113.80
1	Y	131	GLU	CB-CG-CD	19.56	145.86	112.60
1	Y	141	ARG	NE-CZ-NH1	19.20	140.70	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	149	ILE	CA-C-N	18.88	150.78	122.65
1	Y	149	ILE	C-N-CA	18.88	150.78	122.65
1	G	88	ASP	N-CA-C	18.64	135.72	112.23
1	Y	88	ASP	CA-CB-CG	-18.54	94.06	112.60
1	O	134	LYS	CA-C-N	18.16	156.22	121.54
1	O	134	LYS	C-N-CA	18.16	156.22	121.54
1	G	43	PHE	CA-CB-CG	18.15	131.95	113.80
1	G	85	VAL	O-C-N	-18.12	99.92	122.57
1	O	25	ASP	CA-CB-CG	18.00	130.60	112.60
1	G	89	LYS	N-CA-CB	17.77	140.53	110.49
1	Y	106	GLY	CA-C-O	-17.18	104.87	122.05
1	Y	25	ASP	CB-CA-C	17.14	150.86	111.77
1	G	108	TYR	CA-C-N	16.82	145.46	121.24
1	G	108	TYR	C-N-CA	16.82	145.46	121.24
1	B	94	ILE	CA-C-N	16.74	145.21	120.77
1	B	94	ILE	C-N-CA	16.74	145.21	120.77
1	Y	74	ASP	N-CA-C	16.53	132.83	110.35
1	Y	141	ARG	CD-NE-CZ	16.36	147.30	124.40
1	B	73	LYS	N-CA-C	16.16	131.57	111.69
1	B	113	ARG	NE-CZ-NH1	16.12	137.62	121.50
1	G	140	SER	CA-C-O	16.00	139.43	121.51
1	O	102	ILE	CB-CG1-CD1	15.99	147.39	113.80
1	G	86	THR	CA-C-N	15.86	148.40	122.87
1	G	86	THR	C-N-CA	15.86	148.40	122.87
1	Y	104	LEU	CA-C-N	15.77	144.47	120.82
1	Y	104	LEU	C-N-CA	15.77	144.47	120.82
1	B	40	ASP	CA-CB-CG	-15.61	96.99	112.60
1	G	41	HIS	CA-CB-CG	-15.60	98.20	113.80
1	G	40	ASP	CA-CB-CG	-15.50	97.10	112.60
1	G	77	ARG	NE-CZ-NH2	15.17	132.85	119.20
1	O	94	ILE	CA-C-N	-15.12	102.54	123.11
1	O	94	ILE	C-N-CA	-15.12	102.54	123.11
1	G	106	GLY	CA-C-N	15.09	150.37	121.54
1	G	106	GLY	C-N-CA	15.09	150.37	121.54
1	G	57	SER	CA-C-N	15.07	150.33	121.54
1	G	57	SER	C-N-CA	15.07	150.33	121.54
1	Y	50	ASP	CA-C-N	15.05	147.63	122.65
1	Y	50	ASP	C-N-CA	15.05	147.63	122.65
1	G	140	SER	CA-C-N	15.00	144.34	121.99
1	G	140	SER	C-N-CA	15.00	144.34	121.99
1	Y	60	PRO	O-C-N	-14.69	102.81	122.64
1	Y	74	ASP	CA-CB-CG	-14.46	98.14	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	24	GLY	O-C-N	14.13	141.07	122.70
1	O	23	LYS	N-CA-CB	14.13	134.47	111.58
1	B	95	VAL	N-CA-C	14.10	127.96	108.93
1	Y	25	ASP	N-CA-C	-14.08	93.54	110.44
1	Y	41	HIS	CA-CB-CG	-14.04	99.76	113.80
1	O	89	LYS	O-C-N	-13.66	104.22	122.94
1	G	20	PHE	CA-CB-CG	13.59	127.39	113.80
1	O	96	ASP	CA-CB-CG	13.54	126.14	112.60
1	O	113	ARG	NE-CZ-NH1	13.51	135.01	121.50
1	Y	48	PHE	CA-C-O	13.50	137.15	120.54
1	Y	51	ASN	N-CA-CB	13.50	129.19	110.56
1	Y	88	ASP	N-CA-C	13.46	139.46	110.80
1	O	112	GLY	N-CA-C	-13.32	96.19	115.64
1	Y	87	ALA	CA-C-N	13.32	146.98	121.54
1	Y	87	ALA	C-N-CA	13.32	146.98	121.54
1	B	17	THR	N-CA-CB	13.25	133.08	110.81
1	Y	92	VAL	N-CA-C	13.17	129.62	109.20
1	Y	113	ARG	CD-NE-CZ	-13.12	106.03	124.40
1	Y	106	GLY	O-C-N	13.08	137.62	123.23
1	O	128	GLY	CA-C-N	13.07	146.51	121.54
1	O	128	GLY	C-N-CA	13.07	146.51	121.54
1	O	125	GLY	CA-C-N	13.04	146.46	121.54
1	O	125	GLY	C-N-CA	13.04	146.46	121.54
1	B	139	GLY	N-CA-C	12.91	143.79	113.18
1	G	14	VAL	CA-C-O	12.91	135.82	120.84
1	Y	53	GLN	CA-C-N	12.89	140.50	120.65
1	Y	53	GLN	C-N-CA	12.89	140.50	120.65
1	B	138	ALA	CA-C-O	12.83	134.59	120.10
1	G	7	VAL	CB-CA-C	12.64	129.66	110.83
1	O	73	LYS	CB-CG-CD	12.63	140.36	111.30
1	G	130	GLU	CA-CB-CG	12.62	139.35	114.10
1	Y	106	GLY	N-CA-C	-12.61	95.95	110.96
1	B	96	ASP	CA-C-O	-12.57	106.36	120.32
1	Y	123	ASP	CB-CA-C	12.57	135.44	110.42
1	Y	25	ASP	CA-C-O	12.55	138.08	121.89
1	Y	84	ASN	CA-CB-CG	12.54	125.14	112.60
1	Y	126	ARG	CA-C-N	12.54	145.99	121.41
1	Y	126	ARG	C-N-CA	12.54	145.99	121.41
1	B	77	ARG	CG-CD-NE	12.54	139.59	112.00
1	Y	63	ASN	OD1-CG-ND2	12.52	135.12	122.60
1	G	108	TYR	CA-C-O	12.47	140.97	122.38
1	Y	110	ILE	CB-CG1-CD1	12.46	139.97	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	130	GLU	CA-C-N	12.37	144.72	122.46
1	G	130	GLU	C-N-CA	12.37	144.72	122.46
1	B	51	ASN	OD1-CG-ND2	-12.36	110.24	122.60
1	Y	75	GLU	CA-CB-CG	12.32	138.74	114.10
1	B	46	HIS	CA-CB-CG	-12.27	101.53	113.80
1	Y	123	ASP	CA-C-N	12.23	139.70	122.46
1	Y	123	ASP	C-N-CA	12.23	139.70	122.46
1	G	62	PHE	CA-C-O	12.23	134.67	120.49
1	O	119	GLU	CB-CG-CD	12.21	133.35	112.60
1	Y	36	LEU	N-CA-C	12.01	136.39	110.80
1	O	89	LYS	N-CA-CB	-11.89	92.52	111.43
1	O	113	ARG	NH1-CZ-NH2	-11.87	103.87	119.30
1	O	74	ASP	CA-CB-CG	11.86	124.46	112.60
1	G	128	GLY	CA-C-N	11.81	139.27	122.85
1	G	128	GLY	C-N-CA	11.81	139.27	122.85
1	O	127	GLY	N-CA-C	11.79	141.13	113.18
1	Y	33	ILE	N-CA-CB	11.77	132.34	111.63
1	Y	51	ASN	O-C-N	11.74	137.39	122.37
1	Y	126	ARG	CD-NE-CZ	11.70	140.79	124.40
1	B	74	ASP	CA-CB-CG	-11.70	100.91	112.60
1	O	129	ASN	CA-CB-CG	-11.69	100.91	112.60
1	G	109	SER	O-C-N	11.63	137.61	122.96
1	O	121	PRO	CA-C-N	11.57	138.04	121.50
1	O	121	PRO	C-N-CA	11.57	138.04	121.50
1	G	147	ILE	CA-C-O	11.49	133.11	120.59
1	O	15	GLN	CB-CG-CD	11.48	132.12	112.60
1	O	40	ASP	CA-CB-CG	-11.48	101.12	112.60
1	O	85	VAL	CB-CA-C	11.39	128.65	111.68
1	Y	89	LYS	N-CA-CB	11.37	129.71	110.49
1	G	57	SER	CA-C-O	-11.36	107.97	122.63
1	B	111	ILE	CB-CA-C	11.35	125.90	111.15
1	O	46	HIS	CA-CB-CG	-11.32	102.48	113.80
1	O	78	HIS	N-CA-CB	-11.29	91.20	110.17
1	G	107	GLU	CA-C-N	-11.26	105.20	122.08
1	G	107	GLU	C-N-CA	-11.26	105.20	122.08
1	O	44	HIS	N-CA-C	11.18	126.12	109.24
1	G	126	ARG	N-CA-C	11.18	127.04	113.41
1	O	110	ILE	N-CA-CB	-11.16	92.81	111.23
1	Y	127	GLY	N-CA-C	-11.15	86.76	113.18
1	O	131	GLU	CB-CA-C	-11.07	88.39	110.42
1	B	121	PRO	CB-CA-C	11.05	125.38	111.12
1	Y	48	PHE	N-CA-C	11.05	127.65	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	40	ASP	O-C-N	11.04	136.35	122.89
1	Y	73	LYS	CA-C-N	10.87	137.16	120.75
1	Y	73	LYS	C-N-CA	10.87	137.16	120.75
1	G	94	ILE	CA-C-N	10.86	136.65	121.66
1	G	94	ILE	C-N-CA	10.86	136.65	121.66
1	G	52	THR	CB-CA-C	10.81	131.93	110.42
1	B	135	THR	CA-CB-OG1	-10.80	93.41	109.60
1	Y	98	VAL	CB-CA-C	10.78	126.68	110.62
1	Y	14	VAL	CB-CA-C	10.77	125.15	111.15
1	O	96	ASP	CB-CA-C	10.74	125.93	110.24
1	G	66	SER	CB-CA-C	10.74	129.29	112.00
1	G	125	GLY	CA-C-N	10.72	141.28	122.09
1	G	125	GLY	C-N-CA	10.72	141.28	122.09
1	G	129	ASN	CA-C-O	-10.55	109.45	120.84
1	O	81	ASP	CA-C-N	10.54	139.93	122.54
1	O	81	ASP	C-N-CA	10.54	139.93	122.54
1	G	116	VAL	CA-C-N	10.53	137.11	123.10
1	G	116	VAL	C-N-CA	10.53	137.11	123.10
1	O	45	VAL	CB-CA-C	10.45	126.21	110.96
1	O	150	ALA	CA-C-N	-10.38	103.02	121.70
1	O	150	ALA	C-N-CA	-10.38	103.02	121.70
1	Y	143	ALA	N-CA-CB	10.35	129.30	110.99
1	O	80	GLY	CA-C-N	-10.34	108.19	122.77
1	O	80	GLY	C-N-CA	-10.34	108.19	122.77
1	Y	141	ARG	NH1-CZ-NH2	-10.33	105.86	119.30
1	G	40	ASP	N-CA-C	10.32	126.59	109.46
1	B	52	THR	CA-CB-OG1	-10.29	94.17	109.60
1	B	90	ASN	CA-CB-CG	-10.28	102.32	112.60
1	O	88	ASP	N-CA-CB	10.27	127.79	111.56
1	Y	88	ASP	N-CA-CB	-10.27	93.13	110.49
1	Y	48	PHE	CA-C-N	10.26	141.51	121.41
1	Y	48	PHE	C-N-CA	10.26	141.51	121.41
1	Y	135	THR	CA-CB-OG1	-10.19	94.31	109.60
1	B	48	PHE	CA-C-O	10.19	132.11	120.80
1	Y	60	PRO	N-CA-C	10.17	133.43	112.47
1	Y	92	VAL	CA-C-O	10.16	133.81	121.92
1	B	143	ALA	CA-C-N	10.15	138.46	122.62
1	B	143	ALA	C-N-CA	10.15	138.46	122.62
1	B	135	THR	CA-C-O	-10.14	106.00	120.51
1	Y	128	GLY	CA-C-N	10.12	140.87	121.54
1	Y	128	GLY	C-N-CA	10.12	140.87	121.54
1	G	63	ASN	CA-CB-CG	-10.09	102.51	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	131	GLU	CB-CA-C	-10.07	90.39	110.42
1	O	29	VAL	CB-CA-C	10.06	125.65	110.96
1	G	62	PHE	CB-CA-C	10.03	126.73	110.29
1	Y	108	TYR	CA-CB-CG	9.99	131.89	113.90
1	B	53	GLN	N-CA-C	-9.99	100.85	113.23
1	Y	2	THR	N-CA-CB	9.98	124.15	110.98
1	G	47	GLN	CG-CD-NE2	-9.97	101.44	116.40
1	Y	47	GLN	CA-CB-CG	9.96	134.01	114.10
1	G	92	VAL	CA-C-N	9.95	136.87	122.44
1	G	92	VAL	C-N-CA	9.95	136.87	122.44
1	Y	16	GLY	CA-C-O	-9.90	112.08	121.38
1	Y	97	ILE	N-CA-C	9.88	122.85	108.53
1	O	65	LEU	N-CA-CB	-9.86	99.31	110.35
1	G	63	ASN	OD1-CG-ND2	9.84	132.44	122.60
1	O	53	GLN	OE1-CD-NE2	9.82	132.42	122.60
1	G	85	VAL	CB-CA-C	9.80	127.36	111.29
1	O	81	ASP	CA-CB-CG	9.79	122.39	112.60
1	Y	143	ALA	N-CA-C	-9.77	92.72	108.55
1	O	122	ASP	CA-CB-CG	9.74	122.34	112.60
1	G	90	ASN	CA-CB-CG	-9.71	102.89	112.60
1	G	73	LYS	CA-C-N	9.70	140.38	121.18
1	G	73	LYS	C-N-CA	9.70	140.38	121.18
1	B	126	ARG	CB-CA-C	9.68	126.08	111.85
1	G	77	ARG	CD-NE-CZ	-9.67	110.86	124.40
1	B	57	SER	CA-C-O	-9.67	110.95	121.88
1	B	122	ASP	CA-C-N	9.66	134.19	120.28
1	B	122	ASP	C-N-CA	9.66	134.19	120.28
1	Y	3	LYS	O-C-N	9.65	134.29	123.48
1	G	144	CYS	N-CA-CB	9.65	127.78	111.66
1	O	94	ILE	CA-C-O	-9.65	108.72	120.78
1	O	113	ARG	CD-NE-CZ	9.63	137.89	124.40
1	O	81	ASP	CB-CA-C	9.61	125.52	110.14
1	Y	18	ILE	CB-CA-C	9.60	124.93	110.62
1	B	23	LYS	N-CA-CB	9.59	126.51	110.69
1	Y	61	HIS	N-CA-CB	9.58	126.67	110.49
1	G	70	GLY	O-C-N	9.58	135.15	122.70
1	B	53	GLN	CG-CD-NE2	-9.57	102.04	116.40
1	B	47	GLN	OE1-CD-NE2	-9.53	113.07	122.60
1	G	51	ASN	N-CA-CB	9.52	126.58	110.49
1	Y	133	THR	N-CA-CB	-9.50	94.44	110.49
1	G	38	GLU	CB-CG-CD	9.49	128.74	112.60
1	Y	144	CYS	O-C-N	9.49	133.57	123.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	88	ASP	CA-CB-CG	-9.49	103.11	112.60
1	G	89	LYS	N-CA-C	-9.49	90.59	110.80
1	Y	38	GLU	CB-CG-CD	9.48	128.72	112.60
1	G	3	LYS	N-CA-C	9.48	124.21	109.52
1	Y	11	ASP	CA-C-N	9.46	136.72	121.87
1	Y	11	ASP	C-N-CA	9.46	136.72	121.87
1	Y	134	LYS	N-CA-C	9.46	130.95	110.80
1	G	76	GLU	N-CA-CB	9.43	126.24	110.87
1	B	95	VAL	N-CA-CB	-9.41	99.67	110.49
1	Y	118	HIS	CA-CB-CG	-9.41	104.39	113.80
1	Y	135	THR	N-CA-CB	-9.35	96.84	110.40
1	B	77	ARG	CB-CG-CD	9.32	132.75	111.30
1	G	87	ALA	O-C-N	-9.31	111.43	123.16
1	Y	56	THR	CA-C-N	9.30	136.25	120.72
1	Y	56	THR	C-N-CA	9.30	136.25	120.72
1	B	108	TYR	CA-C-N	9.29	135.30	122.19
1	B	108	TYR	C-N-CA	9.29	135.30	122.19
1	G	90	ASN	OD1-CG-ND2	9.28	131.88	122.60
1	B	57	SER	N-CA-CB	-9.26	97.61	110.38
1	Y	138	ALA	CA-C-N	9.25	139.53	121.41
1	Y	138	ALA	C-N-CA	9.25	139.53	121.41
1	B	129	ASN	CB-CA-C	9.25	127.62	110.24
1	Y	132	SER	CA-C-O	9.23	130.50	120.80
1	G	142	LEU	CA-C-N	-9.23	108.73	122.39
1	G	142	LEU	C-N-CA	-9.23	108.73	122.39
1	B	51	ASN	CB-CG-ND2	9.20	130.20	116.40
1	Y	134	LYS	CA-C-N	9.19	139.15	122.79
1	Y	134	LYS	C-N-CA	9.19	139.15	122.79
1	Y	123	ASP	CA-C-O	9.19	133.65	120.51
1	G	116	VAL	CA-C-O	9.17	131.92	121.28
1	G	141	ARG	CD-NE-CZ	9.14	137.20	124.40
1	G	122	ASP	CA-CB-CG	9.14	121.74	112.60
1	Y	87	ALA	CA-C-O	-9.10	110.12	121.50
1	O	72	PRO	CA-C-O	9.10	135.22	119.84
1	G	84	ASN	OD1-CG-ND2	9.09	131.69	122.60
1	O	36	LEU	N-CA-CB	-9.09	96.13	111.31
1	G	29	VAL	CB-CA-C	9.07	124.06	110.63
1	G	6	CYS	CA-C-N	-9.06	111.95	123.19
1	G	6	CYS	C-N-CA	-9.06	111.95	123.19
1	G	47	GLN	OE1-CD-NE2	9.04	131.64	122.60
1	G	127	GLY	N-CA-C	-8.98	101.02	115.66
1	B	73	LYS	CA-CB-CG	-8.95	96.19	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	29	VAL	CB-CA-C	8.95	124.17	110.83
1	G	66	SER	N-CA-CB	-8.94	97.11	110.60
1	G	10	GLY	N-CA-C	-8.89	97.91	110.63
1	B	119	GLU	CB-CG-CD	8.89	127.71	112.60
1	G	101	LEU	CA-C-O	8.87	130.02	119.28
1	G	55	CYS	CA-C-N	8.87	132.50	120.44
1	G	55	CYS	C-N-CA	8.87	132.50	120.44
1	B	94	ILE	CA-CB-CG1	-8.87	95.32	110.40
1	G	88	ASP	N-CA-CB	-8.85	96.67	110.30
1	O	63	ASN	CB-CA-C	-8.84	97.35	111.14
1	O	67	LYS	N-CA-C	8.84	123.56	109.86
1	O	27	VAL	CB-CA-C	8.83	123.23	110.33
1	B	142	LEU	N-CA-C	8.82	124.04	113.28
1	O	43	PHE	CB-CA-C	8.81	123.49	110.62
1	G	126	ARG	NE-CZ-NH1	8.78	130.28	121.50
1	Y	99	ASP	CA-C-O	8.77	126.43	119.59
1	G	144	CYS	CA-CB-SG	8.77	134.57	114.40
1	B	47	GLN	CB-CG-CD	8.75	127.47	112.60
1	Y	13	PRO	CA-C-O	8.75	128.65	118.68
1	G	96	ASP	N-CA-CB	-8.73	96.56	110.79
1	O	107	GLU	CB-CG-CD	8.71	127.41	112.60
1	Y	132	SER	N-CA-C	-8.71	100.01	111.24
1	G	51	ASN	O-C-N	8.71	134.17	122.59
1	O	113	ARG	CB-CG-CD	8.70	131.30	111.30
1	B	9	LYS	N-CA-C	8.67	122.61	108.99
1	O	132	SER	N-CA-C	-8.64	98.34	111.56
1	G	131	GLU	CB-CA-C	-8.64	96.20	110.37
1	G	44	HIS	CA-C-O	8.63	131.15	121.40
1	Y	55	CYS	CA-C-N	8.62	132.53	120.29
1	Y	55	CYS	C-N-CA	8.62	132.53	120.29
1	G	143	ALA	N-CA-C	-8.60	93.98	108.26
1	Y	126	ARG	N-CA-CB	8.60	122.92	110.37
1	O	104	LEU	N-CA-C	-8.60	92.49	110.80
1	G	44	HIS	N-CA-C	8.60	122.22	109.24
1	G	91	GLY	N-CA-C	8.59	129.36	114.76
1	Y	21	GLU	O-C-N	8.59	133.31	123.27
1	G	84	ASN	O-C-N	8.59	134.61	123.11
1	Y	27	VAL	CB-CA-C	8.57	123.48	110.96
1	B	89	LYS	CG-CD-CE	8.57	131.02	111.30
1	G	2	THR	CA-CB-CG2	8.57	125.08	110.50
1	B	137	ASN	CA-C-N	8.57	132.62	120.28
1	B	137	ASN	C-N-CA	8.57	132.62	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	ASN	CA-CB-CG	8.56	121.16	112.60
1	B	99	ASP	O-C-N	8.54	127.83	121.85
1	O	91	GLY	O-C-N	8.54	133.80	122.70
1	B	50	ASP	CA-C-O	8.53	132.71	120.51
1	Y	134	LYS	CB-CA-C	-8.53	93.44	110.42
1	B	144	CYS	CB-CA-C	-8.52	91.57	109.38
1	B	113	ARG	NH1-CZ-NH2	-8.49	108.26	119.30
1	G	77	ARG	NH1-CZ-NH2	-8.49	108.27	119.30
1	G	86	THR	N-CA-CB	8.48	124.82	110.49
1	O	60	PRO	CA-C-N	8.45	132.74	120.82
1	O	60	PRO	C-N-CA	8.45	132.74	120.82
1	G	127	GLY	CA-C-N	8.45	137.97	121.41
1	G	127	GLY	C-N-CA	8.45	137.97	121.41
1	B	103	SER	CA-C-O	-8.44	111.69	121.06
1	Y	77	ARG	NE-CZ-NH1	8.44	129.94	121.50
1	B	28	VAL	CB-CA-C	8.43	122.53	110.98
1	B	84	ASN	CA-CB-CG	8.43	121.03	112.60
1	B	134	LYS	CA-C-N	8.41	137.60	121.54
1	B	134	LYS	C-N-CA	8.41	137.60	121.54
1	O	76	GLU	CA-C-O	8.41	131.00	121.58
1	G	130	GLU	CA-C-O	-8.37	108.54	120.51
1	O	73	LYS	N-CA-C	8.36	122.76	112.23
1	Y	37	THR	CA-C-N	-8.32	105.65	121.54
1	Y	37	THR	C-N-CA	-8.32	105.65	121.54
1	Y	126	ARG	NE-CZ-NH2	-8.31	111.72	119.20
1	G	101	LEU	CA-C-N	8.31	136.93	121.97
1	G	101	LEU	C-N-CA	8.31	136.93	121.97
1	B	7	VAL	N-CA-CB	8.31	120.93	111.21
1	O	24	GLY	N-CA-C	8.30	132.86	113.18
1	G	23	LYS	N-CA-CB	8.27	124.58	110.68
1	Y	132	SER	CA-C-N	8.27	137.33	121.54
1	Y	132	SER	C-N-CA	8.27	137.33	121.54
1	B	140	SER	N-CA-C	-8.25	100.26	110.41
1	Y	44	HIS	CA-CB-CG	8.23	122.03	113.80
1	Y	74	ASP	CA-C-O	8.22	130.26	121.55
1	B	38	GLU	N-CA-CB	-8.21	96.62	110.49
1	Y	127	GLY	CA-C-O	-8.21	106.29	120.57
1	G	109	SER	N-CA-C	-8.20	97.53	109.59
1	Y	12	GLY	N-CA-C	-8.19	95.64	112.34
1	G	98	VAL	CB-CA-C	8.19	123.25	110.81
1	B	140	SER	CA-CB-OG	8.18	127.47	111.10
1	Y	129	ASN	CA-C-O	8.16	132.18	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	118	HIS	CA-C-N	8.14	137.08	121.54
1	G	118	HIS	C-N-CA	8.14	137.08	121.54
1	Y	44	HIS	N-CA-C	8.13	122.88	109.06
1	O	34	THR	CA-CB-OG1	-8.12	97.42	109.60
1	O	81	ASP	CA-C-O	8.12	128.85	120.24
1	O	19	HIS	N-CA-CB	8.11	124.95	111.08
1	B	59	GLY	O-C-N	8.10	129.87	121.77
1	O	84	ASN	OD1-CG-ND2	-8.09	114.51	122.60
1	B	93	ALA	CA-C-N	8.09	136.53	121.97
1	B	93	ALA	C-N-CA	8.09	136.53	121.97
1	B	94	ILE	CB-CA-C	-8.08	98.03	111.29
1	B	53	GLN	CA-CB-CG	-8.08	97.94	114.10
1	O	94	ILE	CB-CA-C	-8.06	98.07	111.29
1	O	134	LYS	CG-CD-CE	8.06	129.84	111.30
1	O	111	ILE	O-C-N	8.05	131.96	123.26
1	B	89	LYS	CB-CA-C	8.04	126.42	110.42
1	Y	107	GLU	CB-CG-CD	8.04	126.27	112.60
1	O	104	LEU	N-CA-CB	-8.02	96.94	110.49
1	Y	34	THR	N-CA-CB	8.01	124.78	111.08
1	B	148	GLY	CA-C-N	8.01	132.04	120.91
1	B	148	GLY	C-N-CA	8.01	132.04	120.91
1	O	66	SER	CA-C-O	-8.00	109.06	120.51
1	Y	60	PRO	CA-C-N	8.00	136.82	121.54
1	Y	60	PRO	C-N-CA	8.00	136.82	121.54
1	G	78	HIS	CA-CB-CG	-8.00	105.80	113.80
1	G	50	ASP	CA-C-O	8.00	131.94	120.51
1	Y	21	GLU	CB-CG-CD	7.99	126.19	112.60
1	B	149	ILE	CA-C-O	7.99	129.78	121.23
1	O	151	LYS	CB-CA-C	7.99	125.27	110.10
1	O	116	VAL	CA-C-O	7.98	130.54	121.28
1	Y	148	GLY	CA-C-N	7.97	132.96	121.80
1	Y	148	GLY	C-N-CA	7.97	132.96	121.80
1	B	65	LEU	CB-CA-C	7.97	126.28	110.42
1	O	111	ILE	CB-CA-C	7.96	122.41	110.63
1	G	144	CYS	O-C-N	7.95	132.32	123.25
1	O	132	SER	CA-C-N	7.94	136.71	121.54
1	O	132	SER	C-N-CA	7.94	136.71	121.54
1	O	89	LYS	CB-CA-C	-7.93	94.60	110.30
1	Y	51	ASN	CB-CA-C	-7.91	97.13	110.81
1	B	122	ASP	CA-CB-CG	7.87	120.47	112.60
1	O	128	GLY	O-C-N	-7.87	112.47	122.70
1	O	106	GLY	O-C-N	7.87	129.41	122.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	63	ASN	O-C-N	7.86	128.33	121.34
1	O	11	ASP	N-CA-CB	7.85	123.59	110.41
1	O	65	LEU	CA-C-O	-7.85	111.99	122.51
1	G	108	TYR	N-CA-CB	-7.85	100.56	110.45
1	B	86	THR	CB-CA-C	7.84	123.33	110.78
1	B	98	VAL	O-C-N	7.84	131.67	123.20
1	G	71	GLY	N-CA-C	7.83	128.32	112.34
1	B	22	ALA	CB-CA-C	7.83	123.29	110.22
1	G	141	ARG	NH1-CZ-NH2	-7.82	109.13	119.30
1	B	98	VAL	CA-C-O	-7.82	112.07	120.36
1	O	15	GLN	OE1-CD-NE2	-7.81	114.79	122.60
1	O	122	ASP	CA-C-N	7.80	136.62	121.18
1	O	122	ASP	C-N-CA	7.80	136.62	121.18
1	B	110	ILE	N-CA-C	7.80	119.62	112.29
1	G	119	GLU	N-CA-CB	-7.79	97.33	110.49
1	Y	52	THR	N-CA-C	-7.78	94.23	110.80
1	O	94	ILE	N-CA-CB	7.78	124.06	111.23
1	B	46	HIS	CA-C-N	7.76	131.02	120.54
1	B	46	HIS	C-N-CA	7.76	131.02	120.54
1	B	61	HIS	CA-CB-CG	-7.75	106.05	113.80
1	G	81	ASP	CA-C-N	7.75	134.38	122.29
1	G	81	ASP	C-N-CA	7.75	134.38	122.29
1	G	107	GLU	N-CA-CB	7.73	123.55	110.49
1	Y	17	THR	CA-CB-CG2	7.70	123.58	110.50
1	B	138	ALA	N-CA-C	7.68	120.54	111.71
1	Y	135	THR	OG1-CB-CG2	7.66	124.62	109.30
1	B	141	ARG	O-C-N	7.65	133.22	123.12
1	G	75	GLU	CA-C-N	7.65	133.97	122.95
1	G	75	GLU	C-N-CA	7.65	133.97	122.95
1	B	38	GLU	CA-CB-CG	-7.63	98.84	114.10
1	O	23	LYS	CA-CB-CG	7.63	129.35	114.10
1	Y	6	CYS	CA-C-N	7.62	133.76	123.10
1	Y	6	CYS	C-N-CA	7.62	133.76	123.10
1	B	115	MET	N-CA-CB	7.61	122.83	110.43
1	B	143	ALA	N-CA-C	-7.60	94.61	110.80
1	Y	71	GLY	O-C-N	7.60	129.37	121.77
1	G	139	GLY	CA-C-N	-7.60	110.20	122.36
1	G	139	GLY	C-N-CA	-7.60	110.20	122.36
1	O	129	ASN	N-CA-CB	-7.60	97.65	110.49
1	O	25	ASP	CB-CA-C	7.58	125.51	110.42
1	O	112	GLY	O-C-N	7.58	130.91	122.50
1	Y	24	GLY	N-CA-C	-7.58	95.23	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	88	ASP	CB-CA-C	-7.57	94.94	110.38
1	G	88	ASP	CA-C-O	7.55	128.70	119.79
1	O	78	HIS	CA-CB-CG	7.55	121.35	113.80
1	G	8	LEU	N-CA-C	7.55	121.22	109.52
1	O	45	VAL	CA-C-O	7.54	128.60	120.53
1	B	124	LEU	CB-CA-C	7.53	124.72	110.35
1	Y	122	ASP	CA-C-N	-7.52	107.18	121.54
1	Y	122	ASP	C-N-CA	-7.52	107.18	121.54
1	G	102	ILE	CB-CA-C	-7.51	98.98	111.29
1	G	90	ASN	N-CA-C	-7.50	94.82	110.80
1	Y	56	THR	CA-CB-CG2	7.50	123.24	110.50
1	G	66	SER	CA-CB-OG	-7.50	96.11	111.10
1	G	105	SER	N-CA-CB	-7.49	98.46	111.04
1	G	137	ASN	CA-C-N	7.48	135.82	121.54
1	G	137	ASN	C-N-CA	7.48	135.82	121.54
1	O	63	ASN	N-CA-CB	-7.47	99.18	110.99
1	G	115	MET	CB-CA-C	7.47	122.44	110.19
1	G	95	VAL	O-C-N	7.45	131.08	122.81
1	B	75	GLU	CB-CA-C	-7.45	95.60	110.42
1	B	104	LEU	CA-C-N	7.45	135.76	121.54
1	B	104	LEU	C-N-CA	7.45	135.76	121.54
1	G	132	SER	CA-C-N	7.42	137.15	122.31
1	G	132	SER	C-N-CA	7.42	137.15	122.31
1	O	119	GLU	CA-C-O	-7.41	110.47	119.59
1	O	91	GLY	N-CA-C	-7.41	95.62	113.18
1	O	63	ASN	CA-C-O	-7.41	111.54	121.02
1	B	120	LYS	O-C-N	7.41	128.17	121.80
1	O	77	ARG	CA-C-O	7.40	129.33	121.33
1	Y	118	HIS	CB-CA-C	-7.40	95.83	109.37
1	Y	15	GLN	CA-CB-CG	-7.36	99.37	114.10
1	B	133	THR	CA-C-O	7.36	128.17	119.56
1	G	63	ASN	N-CA-CB	-7.36	101.22	110.79
1	Y	49	GLY	CA-C-N	-7.36	109.97	122.33
1	Y	49	GLY	C-N-CA	-7.36	109.97	122.33
1	B	139	GLY	CA-C-O	-7.35	107.78	120.57
1	G	74	ASP	CA-C-O	-7.35	109.50	119.05
1	Y	56	THR	CA-CB-OG1	-7.34	98.59	109.60
1	Y	113	ARG	NE-CZ-NH1	-7.34	114.16	121.50
1	O	126	ARG	CB-CA-C	-7.32	95.86	110.42
1	Y	101	LEU	N-CA-C	7.32	122.50	113.50
1	B	126	ARG	NH1-CZ-NH2	-7.31	109.79	119.30
1	O	147	ILE	CB-CA-C	7.31	119.97	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	51	ASN	N-CA-C	-7.31	95.23	110.80
1	G	141	ARG	NE-CZ-NH2	7.30	125.77	119.20
1	G	122	ASP	CB-CA-C	7.30	124.95	110.42
1	B	25	ASP	CB-CA-C	7.29	122.80	110.85
1	Y	120	LYS	O-C-N	7.26	129.67	121.32
1	B	11	ASP	N-CA-CB	7.26	120.96	110.65
1	O	34	THR	O-C-N	7.25	132.10	122.96
1	O	77	ARG	NH1-CZ-NH2	7.25	128.72	119.30
1	O	44	HIS	CB-CA-C	-7.24	94.14	110.07
1	Y	12	GLY	O-C-N	7.24	129.01	121.77
1	B	26	THR	CA-CB-OG1	-7.23	98.75	109.60
1	B	24	GLY	CA-C-O	-7.22	108.01	120.57
1	O	124	LEU	CB-CA-C	7.21	124.78	110.42
1	B	23	LYS	CB-CA-C	-7.21	99.11	111.23
1	B	94	ILE	CA-C-O	-7.21	111.77	120.78
1	Y	62	PHE	CA-CB-CG	7.20	121.00	113.80
1	Y	147	ILE	CA-C-N	7.20	127.77	121.58
1	Y	147	ILE	C-N-CA	7.20	127.77	121.58
1	G	78	HIS	N-CA-CB	7.19	120.52	110.17
1	O	101	LEU	N-CA-C	7.18	120.50	111.24
1	G	110	ILE	N-CA-C	-7.18	104.54	112.80
1	B	40	ASP	CB-CG-OD2	-7.17	101.91	118.40
1	G	60	PRO	CA-C-N	7.16	131.56	120.75
1	G	60	PRO	C-N-CA	7.16	131.56	120.75
1	G	94	ILE	CB-CA-C	7.16	121.62	111.81
1	B	110	ILE	O-C-N	7.15	128.53	122.09
1	O	118	HIS	CA-CB-CG	-7.15	106.65	113.80
1	B	12	GLY	O-C-N	7.14	128.91	121.77
1	B	36	LEU	N-CA-C	7.14	121.04	110.48
1	G	143	ALA	CB-CA-C	7.13	121.13	110.14
1	O	135	THR	CA-CB-CG2	7.13	122.62	110.50
1	B	40	ASP	N-CA-C	7.12	120.65	109.96
1	B	130	GLU	CA-C-O	-7.11	112.35	120.24
1	Y	60	PRO	N-CA-CB	-7.11	95.78	103.25
1	G	75	GLU	OE1-CD-OE2	7.11	139.96	122.90
1	O	108	TYR	N-CA-CB	7.10	122.48	110.49
1	B	90	ASN	N-CA-CB	7.08	124.80	112.27
1	B	107	GLU	CG-CD-OE2	-7.08	102.12	118.40
1	G	124	LEU	CB-CA-C	7.08	124.50	110.42
1	O	7	VAL	CA-CB-CG2	7.07	122.42	110.40
1	G	65	LEU	CA-C-N	-7.07	111.34	122.23
1	G	65	LEU	C-N-CA	-7.07	111.34	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	77	ARG	NE-CZ-NH1	-7.07	114.43	121.50
1	Y	134	LYS	N-CA-CB	-7.06	98.56	110.49
1	G	90	ASN	O-C-N	7.05	131.96	122.59
1	O	90	ASN	N-CA-CB	7.04	122.39	110.49
1	G	70	GLY	N-CA-C	-7.03	96.52	113.18
1	G	106	GLY	O-C-N	-7.03	113.56	122.70
1	B	105	SER	N-CA-CB	7.02	122.35	110.49
1	B	86	THR	N-CA-CB	-7.02	98.79	110.37
1	B	57	SER	CA-CB-OG	-7.01	97.08	111.10
1	Y	45	VAL	CB-CA-C	6.99	120.13	111.25
1	Y	72	PRO	CB-CA-C	6.99	123.10	111.56
1	G	114	THR	CB-CA-C	6.99	121.22	109.48
1	B	118	HIS	CA-C-N	-6.98	111.48	122.65
1	B	118	HIS	C-N-CA	-6.98	111.48	122.65
1	Y	55	CYS	CA-CB-SG	6.98	130.45	114.40
1	B	53	GLN	CA-C-O	6.98	127.44	119.27
1	B	136	GLY	N-CA-C	-6.97	96.66	113.18
1	Y	41	HIS	CA-C-O	-6.97	112.65	120.66
1	O	135	THR	CA-CB-OG1	-6.96	99.15	109.60
1	Y	88	ASP	O-C-N	-6.96	113.34	122.59
1	Y	35	GLY	CA-C-N	6.95	134.82	121.54
1	Y	35	GLY	C-N-CA	6.95	134.82	121.54
1	Y	131	GLU	O-C-N	6.95	131.83	122.59
1	G	1	ALA	N-CA-CB	6.95	120.82	110.40
1	Y	102	ILE	CB-CA-C	6.94	122.67	111.29
1	O	105	SER	N-CA-CB	-6.94	98.77	110.49
1	Y	58	ALA	CA-C-O	6.93	127.91	119.38
1	Y	15	GLN	OE1-CD-NE2	6.93	129.53	122.60
1	Y	78	HIS	O-C-N	6.93	130.75	122.85
1	G	27	VAL	CB-CA-C	6.92	120.60	110.77
1	O	123	ASP	CB-CA-C	-6.92	96.05	110.17
1	B	50	ASP	CA-CB-CG	-6.92	105.68	112.60
1	G	15	GLN	OE1-CD-NE2	6.92	129.52	122.60
1	B	113	ARG	CA-C-O	-6.92	113.23	121.60
1	G	150	ALA	CA-C-N	6.92	134.15	121.70
1	G	150	ALA	C-N-CA	6.92	134.15	121.70
1	Y	77	ARG	NH1-CZ-NH2	-6.91	110.31	119.30
1	G	11	ASP	CA-C-O	-6.91	110.62	120.51
1	G	45	VAL	CA-CB-CG1	6.91	122.15	110.40
1	O	135	THR	N-CA-CB	6.91	122.17	110.49
1	Y	29	VAL	CA-C-N	6.90	134.40	122.81
1	Y	29	VAL	C-N-CA	6.90	134.40	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	47	GLN	CA-C-N	-6.89	109.81	121.94
1	Y	47	GLN	C-N-CA	-6.89	109.81	121.94
1	B	62	PHE	CB-CA-C	6.89	121.15	110.67
1	Y	143	ALA	O-C-N	6.88	131.33	123.48
1	O	68	LYS	CA-CB-CG	6.88	127.86	114.10
1	Y	95	VAL	CB-CA-C	6.88	120.81	110.63
1	B	9	LYS	CB-CG-CD	6.88	127.12	111.30
1	B	57	SER	N-CA-C	-6.86	100.89	110.35
1	Y	62	PHE	CB-CA-C	6.85	121.53	110.29
1	Y	53	GLN	CB-CG-CD	-6.85	100.96	112.60
1	B	151	LYS	CA-CB-CG	-6.84	100.41	114.10
1	O	41	HIS	N-CA-CB	6.84	124.25	111.53
1	G	74	ASP	CA-CB-CG	-6.83	105.77	112.60
1	O	9	LYS	CA-C-O	-6.80	113.48	121.44
1	B	131	GLU	CG-CD-OE1	6.79	134.02	118.40
1	B	102	ILE	CB-CA-C	6.79	122.42	111.29
1	B	135	THR	CA-CB-CG2	6.79	122.03	110.50
1	G	75	GLU	CB-CG-CD	-6.79	101.06	112.60
1	G	117	VAL	CA-C-O	6.78	127.45	120.39
1	B	20	PHE	CA-CB-CG	6.78	120.58	113.80
1	G	109	SER	N-CA-CB	6.77	120.14	109.71
1	G	45	VAL	N-CA-CB	6.77	120.20	111.67
1	O	77	ARG	CD-NE-CZ	-6.77	114.93	124.40
1	Y	15	GLN	N-CA-C	6.76	118.79	108.52
1	O	57	SER	CA-C-N	6.75	129.87	120.29
1	O	57	SER	C-N-CA	6.75	129.87	120.29
1	B	85	VAL	O-C-N	6.74	130.54	123.26
1	G	131	GLU	CA-C-N	6.74	134.41	121.54
1	G	131	GLU	C-N-CA	6.74	134.41	121.54
1	O	140	SER	CA-C-O	6.72	130.12	120.51
1	Y	126	ARG	CG-CD-NE	-6.72	97.21	112.00
1	G	18	ILE	CA-C-N	6.72	133.36	122.81
1	G	18	ILE	C-N-CA	6.72	133.36	122.81
1	G	129	ASN	CA-C-N	6.71	134.36	121.54
1	G	129	ASN	C-N-CA	6.71	134.36	121.54
1	B	101	LEU	CA-C-N	6.71	134.04	121.97
1	B	101	LEU	C-N-CA	6.71	134.04	121.97
1	G	56	THR	N-CA-C	6.69	118.37	111.14
1	G	119	GLU	CG-CD-OE1	6.69	133.78	118.40
1	Y	77	ARG	CA-C-O	-6.69	114.08	121.23
1	Y	128	GLY	CA-C-O	6.69	130.26	121.83
1	O	126	ARG	CA-C-N	6.68	134.51	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	126	ARG	C-N-CA	6.68	134.51	121.41
1	G	130	GLU	CB-CA-C	-6.68	97.13	110.42
1	Y	22	ALA	CB-CA-C	6.68	122.34	111.05
1	Y	82	LEU	CA-C-O	6.67	126.57	119.03
1	B	47	GLN	N-CA-C	6.67	119.12	111.11
1	O	100	PRO	CB-CA-C	6.67	122.05	111.31
1	G	136	GLY	N-CA-C	-6.67	106.95	115.42
1	B	37	THR	CB-CA-C	6.67	120.56	109.89
1	B	92	VAL	CA-C-N	6.66	132.39	123.00
1	B	92	VAL	C-N-CA	6.66	132.39	123.00
1	Y	151	LYS	CA-CB-CG	6.65	127.40	114.10
1	O	44	HIS	CA-CB-CG	-6.65	107.15	113.80
1	O	32	SER	CA-CB-OG	6.64	124.38	111.10
1	B	140	SER	N-CA-CB	6.64	119.48	110.38
1	O	7	VAL	CA-C-O	6.63	127.29	120.39
1	O	51	ASN	CB-CG-OD1	6.61	134.02	120.80
1	Y	141	ARG	CG-CD-NE	6.61	126.54	112.00
1	G	93	ALA	CA-C-O	6.61	128.58	120.25
1	G	113	ARG	NE-CZ-NH1	-6.60	114.90	121.50
1	O	37	THR	CB-CA-C	6.58	120.85	110.19
1	B	40	ASP	CB-CA-C	6.58	120.42	109.89
1	G	73	LYS	CA-C-O	-6.58	111.86	119.56
1	G	73	LYS	N-CA-C	6.58	121.01	112.92
1	B	79	VAL	CA-CB-CG1	6.58	121.58	110.40
1	B	126	ARG	CA-C-O	6.57	134.23	121.35
1	Y	78	HIS	CB-CG-CD2	-6.57	122.66	131.20
1	G	141	ARG	N-CA-C	6.56	118.83	108.67
1	B	95	VAL	CB-CA-C	-6.55	101.47	111.69
1	B	144	CYS	O-C-N	6.54	131.28	123.24
1	Y	140	SER	CA-CB-OG	6.53	124.17	111.10
1	Y	126	ARG	CB-CG-CD	-6.53	96.28	111.30
1	G	21	GLU	N-CA-CB	6.53	121.78	110.81
1	O	13	PRO	CA-C-N	6.52	130.66	121.66
1	O	13	PRO	C-N-CA	6.52	130.66	121.66
1	Y	96	ASP	O-C-N	-6.52	113.15	121.83
1	B	53	GLN	CG-CD-OE1	6.52	133.84	120.80
1	O	43	PHE	CA-C-N	6.51	132.75	122.21
1	O	43	PHE	C-N-CA	6.51	132.75	122.21
1	B	12	GLY	N-CA-C	-6.51	99.06	112.34
1	Y	122	ASP	O-C-N	6.50	130.63	123.22
1	B	101	LEU	N-CA-C	6.50	118.36	111.28
1	B	60	PRO	CA-C-N	6.50	130.56	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	PRO	C-N-CA	6.50	130.56	120.75
1	B	37	THR	CA-C-O	6.50	128.28	120.81
1	G	47	GLN	N-CA-CB	-6.50	99.51	110.49
1	Y	50	ASP	CB-CA-C	6.49	121.02	109.65
1	Y	7	VAL	CB-CA-C	6.49	119.97	111.53
1	Y	18	ILE	CA-C-N	6.49	132.68	122.94
1	Y	18	ILE	C-N-CA	6.49	132.68	122.94
1	B	93	ALA	N-CA-C	-6.49	97.83	108.41
1	Y	63	ASN	CB-CG-OD1	-6.48	107.85	120.80
1	O	126	ARG	CD-NE-CZ	-6.47	115.33	124.40
1	Y	69	HIS	CA-C-O	6.47	128.41	121.16
1	O	19	HIS	O-C-N	6.47	131.60	123.19
1	B	38	GLU	CG-CD-OE2	-6.47	103.53	118.40
1	B	77	ARG	NE-CZ-NH2	6.45	125.01	119.20
1	G	142	LEU	N-CA-CB	6.45	121.39	110.49
1	O	23	LYS	N-CA-C	-6.45	94.07	107.67
1	B	40	ASP	N-CA-CB	-6.44	100.25	109.85
1	Y	67	LYS	N-CA-CB	6.44	121.46	110.65
1	O	129	ASN	OD1-CG-ND2	6.43	129.03	122.60
1	Y	56	THR	CA-C-O	6.43	127.23	120.42
1	O	29	VAL	CA-CB-CG1	6.42	121.32	110.40
1	B	92	VAL	CB-CA-C	6.42	120.40	110.83
1	O	51	ASN	CB-CG-ND2	-6.42	106.77	116.40
1	Y	141	ARG	NE-CZ-NH2	-6.41	113.43	119.20
1	Y	127	GLY	O-C-N	6.40	131.02	122.70
1	G	25	ASP	CA-C-N	6.40	134.18	122.92
1	G	25	ASP	C-N-CA	6.40	134.18	122.92
1	O	44	HIS	N-CA-CB	-6.39	100.57	111.69
1	G	7	VAL	CA-CB-CG1	6.39	121.26	110.40
1	Y	128	GLY	O-C-N	-6.37	116.68	122.86
1	Y	6	CYS	CB-CA-C	6.37	120.63	109.80
1	Y	91	GLY	N-CA-C	6.37	128.27	113.18
1	B	150	ALA	CA-C-O	6.37	128.47	121.40
1	G	129	ASN	N-CA-C	-6.37	95.91	107.75
1	Y	88	ASP	CA-C-O	6.36	129.61	120.51
1	Y	30	THR	CB-CA-C	-6.35	97.34	109.66
1	Y	117	VAL	CA-C-N	6.34	133.08	122.87
1	Y	117	VAL	C-N-CA	6.34	133.08	122.87
1	O	37	THR	N-CA-CB	-6.33	100.10	110.42
1	O	99	ASP	N-CA-C	6.33	119.53	109.40
1	B	88	ASP	CA-CB-CG	6.33	118.93	112.60
1	O	131	GLU	OE1-CD-OE2	6.30	138.02	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	68	LYS	CA-C-N	6.29	129.80	120.87
1	Y	68	LYS	C-N-CA	6.29	129.80	120.87
1	Y	105	SER	CB-CA-C	-6.28	100.32	110.74
1	Y	52	THR	CA-CB-CG2	6.27	121.17	110.50
1	Y	75	GLU	CB-CA-C	6.27	121.76	109.72
1	B	125	GLY	CA-C-N	-6.27	114.63	123.03
1	B	125	GLY	C-N-CA	-6.27	114.63	123.03
1	O	32	SER	N-CA-CB	6.26	122.76	111.37
1	Y	125	GLY	N-CA-C	6.25	123.65	115.40
1	O	48	PHE	N-CA-C	6.25	119.89	109.95
1	Y	122	ASP	N-CA-C	-6.25	98.55	108.73
1	O	53	GLN	CG-CD-OE1	-6.25	108.31	120.80
1	G	139	GLY	O-C-N	6.24	130.82	122.70
1	G	41	HIS	N-CA-C	6.24	119.57	109.40
1	B	48	PHE	CA-C-N	6.24	133.63	121.41
1	B	48	PHE	C-N-CA	6.24	133.63	121.41
1	Y	51	ASN	N-CA-C	-6.23	105.95	112.93
1	G	118	HIS	O-C-N	-6.22	116.13	123.22
1	B	117	VAL	O-C-N	6.22	129.65	123.18
1	G	141	ARG	CG-CD-NE	6.21	125.67	112.00
1	Y	63	ASN	CA-CB-CG	-6.21	106.39	112.60
1	B	146	VAL	N-CA-C	-6.20	101.00	109.55
1	Y	94	ILE	CA-C-N	-6.20	115.02	123.14
1	Y	94	ILE	C-N-CA	-6.20	115.02	123.14
1	G	15	GLN	CA-C-O	-6.20	114.30	120.80
1	G	131	GLU	CA-C-O	6.19	127.05	119.81
1	G	84	ASN	CA-C-O	-6.19	114.22	121.46
1	Y	28	VAL	CB-CA-C	6.18	118.44	110.96
1	O	120	LYS	N-CA-C	-6.18	102.57	108.13
1	B	128	GLY	N-CA-C	-6.18	106.89	114.92
1	O	142	LEU	CB-CA-C	6.17	120.40	110.09
1	Y	54	GLY	N-CA-C	6.17	122.95	112.22
1	G	38	GLU	CA-CB-CG	6.16	126.43	114.10
1	G	8	LEU	CA-C-O	6.15	128.64	121.44
1	O	21	GLU	CB-CG-CD	6.14	123.05	112.60
1	B	24	GLY	O-C-N	6.14	130.69	122.70
1	G	25	ASP	CA-C-O	6.14	129.29	120.51
1	B	131	GLU	CB-CA-C	-6.13	97.66	110.17
1	Y	49	GLY	CA-C-O	-6.13	109.90	120.57
1	Y	19	HIS	CA-CB-CG	-6.13	107.67	113.80
1	B	38	GLU	CG-CD-OE1	6.13	132.49	118.40
1	G	63	ASN	CB-CA-C	6.12	120.27	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	110	ILE	N-CA-CB	-6.12	104.14	112.28
1	Y	90	ASN	O-C-N	6.12	130.14	122.43
1	O	137	ASN	CB-CA-C	6.12	122.59	110.42
1	G	123	ASP	N-CA-CB	6.12	120.82	110.49
1	O	20	PHE	CA-CB-CG	6.11	119.91	113.80
1	B	49	GLY	CA-C-N	-6.11	109.87	121.54
1	B	49	GLY	C-N-CA	-6.11	109.87	121.54
1	G	94	ILE	N-CA-CB	-6.11	104.27	111.60
1	G	2	THR	CB-CA-C	6.11	122.58	110.42
1	G	119	GLU	OE1-CD-OE2	-6.10	108.25	122.90
1	G	122	ASP	CA-C-O	-6.10	111.79	120.51
1	O	140	SER	O-C-N	-6.09	114.49	122.59
1	Y	63	ASN	CB-CA-C	-6.09	101.64	111.14
1	G	108	TYR	O-C-N	-6.08	114.28	122.68
1	O	104	LEU	O-C-N	6.08	130.68	122.59
1	B	79	VAL	N-CA-C	-6.08	103.69	110.62
1	B	52	THR	O-C-N	6.07	130.63	122.49
1	G	56	THR	CB-CA-C	-6.07	101.31	110.90
1	B	101	LEU	N-CA-CB	-6.07	101.20	110.12
1	Y	113	ARG	NE-CZ-NH2	6.07	124.66	119.20
1	B	148	GLY	CA-C-O	6.06	126.57	121.11
1	O	140	SER	CA-C-N	6.06	132.37	122.07
1	O	140	SER	C-N-CA	6.06	132.37	122.07
1	Y	2	THR	CA-CB-OG1	-6.06	100.51	109.60
1	B	73	LYS	CB-CA-C	-6.05	99.64	110.70
1	G	103	SER	N-CA-CB	6.04	120.70	110.49
1	Y	40	ASP	CA-CB-CG	-6.04	106.56	112.60
1	B	141	ARG	N-CA-CB	6.04	120.20	110.65
1	Y	2	THR	N-CA-C	-6.04	105.64	114.39
1	B	150	ALA	CA-C-N	6.01	132.51	121.70
1	B	150	ALA	C-N-CA	6.01	132.51	121.70
1	G	123	ASP	OD1-CG-OD2	-6.01	108.48	122.90
1	G	0	ACE	O-C-N	-6.00	104.99	123.00
1	G	52	THR	CA-C-O	-6.00	111.93	120.51
1	O	149	ILE	CB-CA-C	5.99	118.74	111.13
1	O	56	THR	N-CA-CB	5.98	119.17	110.26
1	O	151	LYS	N-CA-CB	-5.97	100.36	110.50
1	Y	37	THR	N-CA-CB	5.96	120.57	110.49
1	B	5	VAL	CA-CB-CG1	5.96	120.54	110.40
1	B	78	HIS	CA-C-O	-5.96	114.21	121.36
1	O	11	ASP	O-C-N	5.95	131.12	122.43
1	O	114	THR	CA-C-N	5.95	130.69	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	114	THR	C-N-CA	5.95	130.69	122.77
1	G	128	GLY	N-CA-C	5.94	127.25	113.18
1	O	62	PHE	CA-C-O	5.93	127.68	120.62
1	G	99	ASP	CA-C-O	5.93	125.12	119.72
1	G	77	ARG	CG-CD-NE	5.93	125.04	112.00
1	B	137	ASN	OD1-CG-ND2	5.93	128.53	122.60
1	O	1	ALA	CA-C-N	5.92	132.84	121.54
1	O	1	ALA	C-N-CA	5.92	132.84	121.54
1	O	128	GLY	CA-C-O	5.92	130.87	120.57
1	Y	92	VAL	N-CA-CB	-5.91	101.55	112.43
1	B	12	GLY	CA-C-N	5.91	127.23	119.84
1	B	12	GLY	C-N-CA	5.91	127.23	119.84
1	B	8	LEU	N-CA-C	5.91	118.36	108.96
1	O	2	THR	CA-CB-CG2	5.91	120.55	110.50
1	Y	7	VAL	CA-C-O	5.90	128.71	120.86
1	B	12	GLY	CA-C-O	-5.90	113.08	121.52
1	B	118	HIS	CA-C-O	-5.90	114.20	121.88
1	G	32	SER	O-C-N	5.90	129.89	123.10
1	Y	33	ILE	CA-CB-CG1	5.89	120.41	110.40
1	B	13	PRO	N-CA-CB	-5.89	97.07	103.25
1	O	69	HIS	CA-CB-CG	-5.89	107.91	113.80
1	B	92	VAL	CA-CB-CG1	5.88	120.40	110.40
1	B	11	ASP	CA-C-N	5.88	131.09	121.87
1	B	11	ASP	C-N-CA	5.88	131.09	121.87
1	G	95	VAL	N-CA-C	5.87	116.64	108.89
1	Y	66	SER	CA-CB-OG	5.87	122.83	111.10
1	O	25	ASP	OD1-CG-OD2	-5.86	108.84	122.90
1	G	74	ASP	N-CA-C	5.85	120.03	113.01
1	B	74	ASP	CA-C-N	5.85	132.71	121.54
1	B	74	ASP	C-N-CA	5.85	132.71	121.54
1	Y	59	GLY	O-C-N	5.84	127.61	121.77
1	O	52	THR	CB-CA-C	5.84	122.29	110.38
1	Y	36	LEU	N-CA-CB	-5.84	100.62	110.49
1	G	97	ILE	N-CA-C	5.83	116.05	108.35
1	B	140	SER	CA-C-N	-5.82	114.58	123.07
1	B	140	SER	C-N-CA	-5.82	114.58	123.07
1	G	37	THR	CA-C-O	5.81	127.58	121.19
1	B	88	ASP	CA-C-N	-5.80	110.45	121.54
1	B	88	ASP	C-N-CA	-5.80	110.45	121.54
1	Y	50	ASP	O-C-N	5.79	130.43	123.36
1	Y	87	ALA	CB-CA-C	5.79	126.93	113.15
1	Y	41	HIS	O-C-N	5.79	130.33	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	56	THR	N-CA-C	5.78	117.66	111.36
1	G	3	LYS	N-CA-CB	-5.78	101.50	111.55
1	B	126	ARG	CA-C-N	5.78	132.73	121.41
1	B	126	ARG	C-N-CA	5.78	132.73	121.41
1	G	107	GLU	CB-CA-C	-5.77	98.93	110.42
1	G	102	ILE	O-C-N	5.77	129.78	122.57
1	O	22	ALA	CA-C-O	-5.76	114.19	120.81
1	Y	73	LYS	O-C-N	-5.75	114.94	122.59
1	O	111	ILE	CA-CB-CG1	5.75	120.17	110.40
1	Y	120	LYS	CB-CA-C	-5.74	98.86	110.17
1	G	47	GLN	N-CA-C	5.74	123.02	110.80
1	Y	92	VAL	CA-C-N	5.72	131.52	122.94
1	Y	92	VAL	C-N-CA	5.72	131.52	122.94
1	Y	120	LYS	CG-CD-CE	-5.72	98.15	111.30
1	O	68	LYS	N-CA-CB	5.72	119.71	110.51
1	O	72	PRO	CA-C-N	5.71	130.40	120.68
1	O	72	PRO	C-N-CA	5.71	130.40	120.68
1	Y	21	GLU	CA-C-N	-5.71	112.92	122.17
1	Y	21	GLU	C-N-CA	-5.71	112.92	122.17
1	B	111	ILE	CA-C-N	5.71	130.18	121.51
1	B	111	ILE	C-N-CA	5.71	130.18	121.51
1	B	24	GLY	CA-C-N	-5.70	112.62	122.14
1	B	24	GLY	C-N-CA	-5.70	112.62	122.14
1	Y	52	THR	CB-CA-C	5.70	121.76	110.42
1	O	113	ARG	CB-CA-C	5.69	120.49	110.36
1	Y	53	GLN	CG-CD-NE2	-5.69	107.86	116.40
1	O	81	ASP	CB-CG-OD1	-5.69	105.31	118.40
1	O	84	ASN	N-CA-C	5.68	118.67	109.40
1	B	113	ARG	NE-CZ-NH2	-5.68	114.09	119.20
1	G	146	VAL	O-C-N	5.68	129.43	122.72
1	Y	122	ASP	CA-C-O	-5.68	114.28	120.36
1	B	93	ALA	N-CA-CB	5.68	119.51	110.65
1	G	63	ASN	CB-CG-ND2	-5.68	107.88	116.40
1	O	116	VAL	CA-C-N	5.67	131.03	122.98
1	O	116	VAL	C-N-CA	5.67	131.03	122.98
1	B	30	THR	O-C-N	-5.65	116.33	123.17
1	G	35	GLY	CA-C-N	-5.65	113.72	122.59
1	G	35	GLY	C-N-CA	-5.65	113.72	122.59
1	G	143	ALA	CA-C-O	-5.65	113.31	120.20
1	B	61	HIS	O-C-N	5.65	129.76	122.81
1	G	134	LYS	CB-CA-C	5.65	121.66	110.42
1	O	93	ALA	CA-C-O	5.64	128.58	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	ASP	CB-CG-OD2	-5.64	105.42	118.40
1	Y	150	ALA	CA-C-O	5.64	127.06	120.80
1	B	36	LEU	CA-C-O	5.64	127.95	121.47
1	G	0	ACE	C-N-CA	5.63	138.59	121.70
1	G	9	LYS	CA-CB-CG	5.63	125.36	114.10
1	O	99	ASP	CB-CG-OD1	-5.62	105.47	118.40
1	Y	134	LYS	CA-C-O	5.62	128.54	120.51
1	Y	116	VAL	CG1-CB-CG2	-5.62	98.45	110.80
1	Y	88	ASP	CB-CA-C	-5.61	99.26	110.42
1	Y	104	LEU	N-CA-CB	-5.61	103.44	110.90
1	B	107	GLU	N-CA-C	5.61	119.38	112.54
1	B	85	VAL	N-CA-C	-5.61	100.26	108.11
1	G	99	ASP	CA-CB-CG	-5.60	107.00	112.60
1	O	92	VAL	N-CA-C	5.59	118.17	108.95
1	B	78	HIS	N-CA-CB	5.58	119.51	110.41
1	O	142	LEU	N-CA-CB	-5.58	102.23	110.49
1	Y	40	ASP	N-CA-C	-5.58	102.02	110.28
1	B	57	SER	O-C-N	-5.57	114.82	122.23
1	B	49	GLY	O-C-N	5.57	129.94	122.70
1	Y	1	ALA	N-CA-C	5.57	126.58	111.00
1	G	53	GLN	CA-C-N	5.57	129.07	120.00
1	G	53	GLN	C-N-CA	5.57	129.07	120.00
1	G	89	LYS	O-C-N	5.56	129.99	122.59
1	Y	129	ASN	CA-C-N	5.56	132.16	121.54
1	Y	129	ASN	C-N-CA	5.56	132.16	121.54
1	O	37	THR	CA-CB-OG1	-5.56	101.27	109.60
1	B	101	LEU	CB-CA-C	5.55	120.01	110.79
1	B	131	GLU	CG-CD-OE2	-5.54	105.65	118.40
1	Y	60	PRO	CA-C-O	-5.54	110.52	120.60
1	G	117	VAL	CA-C-N	5.54	130.13	122.77
1	G	117	VAL	C-N-CA	5.54	130.13	122.77
1	Y	81	ASP	CA-C-N	5.53	130.62	121.99
1	Y	81	ASP	C-N-CA	5.53	130.62	121.99
1	B	103	SER	O-C-N	5.53	128.39	123.41
1	O	73	LYS	N-CA-CB	-5.53	101.79	110.30
1	O	76	GLU	N-CA-CB	5.52	118.67	110.49
1	Y	61	HIS	O-C-N	5.52	129.93	122.59
1	Y	26	THR	CA-C-N	-5.52	115.95	123.12
1	Y	26	THR	C-N-CA	-5.52	115.95	123.12
1	O	11	ASP	CA-C-O	-5.51	112.05	119.11
1	Y	123	ASP	N-CA-CB	-5.51	101.17	110.49
1	O	43	PHE	CA-CB-CG	5.51	119.31	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	130	GLU	N-CA-C	5.51	122.54	110.80
1	Y	39	GLY	O-C-N	5.50	134.35	123.07
1	O	65	LEU	N-CA-C	-5.50	101.95	109.71
1	Y	116	VAL	CA-CB-CG2	5.50	119.75	110.40
1	G	14	VAL	CA-CB-CG1	5.50	119.75	110.40
1	O	58	ALA	CA-C-N	5.50	130.50	121.87
1	O	58	ALA	C-N-CA	5.50	130.50	121.87
1	Y	78	HIS	CA-C-O	-5.50	115.33	121.81
1	Y	2	THR	CA-CB-CG2	5.49	119.83	110.50
1	B	42	GLY	CA-C-O	5.49	126.52	121.58
1	B	56	THR	OG1-CB-CG2	5.49	120.28	109.30
1	O	103	SER	CA-C-O	5.49	128.35	120.51
1	O	131	GLU	CG-CD-OE2	-5.48	105.79	118.40
1	O	85	VAL	CA-CB-CG1	5.48	119.72	110.40
1	B	96	ASP	CA-C-N	5.48	130.12	122.23
1	B	96	ASP	C-N-CA	5.48	130.12	122.23
1	B	37	THR	CA-C-N	5.48	132.00	121.54
1	B	37	THR	C-N-CA	5.48	132.00	121.54
1	Y	113	ARG	CG-CD-NE	-5.48	99.95	112.00
1	O	67	LYS	CB-CA-C	-5.47	100.12	113.15
1	O	127	GLY	O-C-N	-5.47	115.59	122.70
1	B	66	SER	N-CA-CB	5.47	119.74	110.49
1	G	128	GLY	O-C-N	-5.46	115.61	122.70
1	Y	124	LEU	N-CA-C	5.46	118.72	111.30
1	G	10	GLY	O-C-N	5.45	129.36	123.96
1	G	90	ASN	CB-CG-ND2	-5.45	108.22	116.40
1	Y	32	SER	O-C-N	5.43	129.74	123.17
1	B	130	GLU	O-C-N	5.43	129.29	122.23
1	Y	15	GLN	N-CA-CB	-5.43	102.60	111.24
1	O	68	LYS	CA-C-O	5.42	128.93	121.88
1	O	67	LYS	CA-C-N	-5.42	113.04	122.64
1	O	67	LYS	C-N-CA	-5.42	113.04	122.64
1	B	14	VAL	CA-C-O	5.42	127.03	120.85
1	G	144	CYS	N-CA-C	-5.42	100.84	109.07
1	Y	142	LEU	O-C-N	5.41	129.78	122.59
1	G	69	HIS	O-C-N	5.41	129.42	123.25
1	Y	24	GLY	CA-C-O	-5.41	111.16	120.57
1	O	3	LYS	CB-CG-CD	-5.41	98.87	111.30
1	B	138	ALA	N-CA-CB	-5.40	101.91	110.22
1	O	74	ASP	O-C-N	5.39	129.00	122.85
1	Y	11	ASP	CA-CB-CG	5.39	117.99	112.60
1	G	2	THR	N-CA-C	-5.39	99.32	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	68	LYS	CB-CA-C	5.39	119.95	110.36
1	G	62	PHE	O-C-N	-5.39	116.39	123.02
1	G	115	MET	CA-CB-CG	5.37	124.85	114.10
1	B	135	THR	N-CA-CB	-5.37	101.41	110.49
1	Y	40	ASP	N-CA-CB	5.36	117.85	109.97
1	Y	61	HIS	N-CA-C	-5.36	99.39	110.80
1	G	140	SER	N-CA-CB	5.36	120.30	111.62
1	G	76	GLU	CB-CA-C	-5.35	102.92	111.17
1	O	144	CYS	O-C-N	5.35	129.15	123.42
1	G	21	GLU	CA-CB-CG	5.35	124.80	114.10
1	O	81	ASP	N-CA-C	5.35	117.11	108.34
1	O	91	GLY	CA-C-N	-5.34	114.24	122.68
1	O	91	GLY	C-N-CA	-5.34	114.24	122.68
1	G	72	PRO	CB-CA-C	5.34	120.37	111.56
1	B	115	MET	N-CA-C	-5.33	100.55	109.24
1	B	73	LYS	O-C-N	5.33	129.16	122.23
1	B	92	VAL	CA-C-O	5.33	126.13	120.48
1	B	144	CYS	N-CA-CB	-5.33	101.67	111.37
1	O	126	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	Y	23	LYS	CA-C-N	-5.33	110.97	121.41
1	Y	23	LYS	C-N-CA	-5.33	110.97	121.41
1	B	9	LYS	O-C-N	-5.32	117.31	123.33
1	O	45	VAL	CA-C-N	5.32	129.49	122.30
1	O	45	VAL	C-N-CA	5.32	129.49	122.30
1	O	37	THR	CA-C-N	5.32	128.65	121.05
1	O	37	THR	C-N-CA	5.32	128.65	121.05
1	B	35	GLY	CA-C-O	5.31	124.87	118.97
1	B	123	ASP	O-C-N	5.31	128.44	122.22
1	G	76	GLU	O-C-N	5.30	131.05	122.99
1	G	78	HIS	N-CA-C	-5.30	103.02	110.50
1	O	77	ARG	N-CA-CB	-5.30	102.80	111.66
1	G	143	ALA	O-C-N	5.30	130.06	123.28
1	G	128	GLY	CA-C-O	5.29	129.78	120.57
1	B	128	GLY	CA-C-N	-5.29	113.56	123.03
1	B	128	GLY	C-N-CA	-5.29	113.56	123.03
1	G	51	ASN	OD1-CG-ND2	5.29	127.89	122.60
1	G	45	VAL	CA-C-N	5.29	129.92	122.09
1	G	45	VAL	C-N-CA	5.29	129.92	122.09
1	Y	17	THR	CA-C-O	5.29	126.65	120.20
1	O	11	ASP	N-CA-C	-5.28	106.79	113.18
1	Y	126	ARG	CA-CB-CG	-5.28	103.54	114.10
1	Y	136	GLY	N-CA-C	-5.28	108.41	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	126	ARG	CB-CA-C	-5.27	100.01	109.24
1	G	14	VAL	N-CA-C	5.27	116.56	108.71
1	Y	103	SER	CA-C-N	5.26	130.50	122.24
1	Y	103	SER	C-N-CA	5.26	130.50	122.24
1	G	149	ILE	N-CA-CB	-5.25	103.32	110.56
1	B	44	HIS	N-CA-C	5.25	117.16	109.24
1	Y	3	LYS	N-CA-CB	5.24	120.57	111.39
1	Y	25	ASP	CB-CG-OD1	-5.24	106.35	118.40
1	O	39	GLY	O-C-N	-5.24	117.82	123.00
1	G	67	LYS	O-C-N	5.23	128.90	122.84
1	Y	50	ASP	CA-CB-CG	-5.22	107.38	112.60
1	B	104	LEU	N-CA-C	5.22	116.70	110.44
1	O	100	PRO	N-CA-C	-5.21	106.93	114.18
1	B	75	GLU	O-C-N	5.21	129.53	122.59
1	B	141	ARG	CD-NE-CZ	5.21	131.70	124.40
1	G	75	GLU	CA-C-O	5.21	127.97	120.51
1	O	96	ASP	N-CA-C	-5.21	99.18	108.13
1	G	82	LEU	CA-C-N	5.20	131.59	121.41
1	G	82	LEU	C-N-CA	5.20	131.59	121.41
1	O	119	GLU	CB-CA-C	-5.19	101.83	110.81
1	O	1	ALA	CB-CA-C	-5.19	102.71	110.50
1	B	9	LYS	CA-C-N	5.19	131.63	121.93
1	B	9	LYS	C-N-CA	5.19	131.63	121.93
1	B	99	ASP	CB-CA-C	5.19	117.70	109.55
1	Y	12	GLY	CA-C-O	-5.18	114.11	121.52
1	Y	46	HIS	CA-C-N	5.18	131.44	121.54
1	Y	46	HIS	C-N-CA	5.18	131.44	121.54
1	B	129	ASN	CA-CB-CG	5.18	117.78	112.60
1	G	78	HIS	CB-CG-CD2	-5.17	124.48	131.20
1	O	130	GLU	O-C-N	-5.17	115.71	122.59
1	Y	100	PRO	CA-C-N	5.17	130.86	121.92
1	Y	100	PRO	C-N-CA	5.17	130.86	121.92
1	O	75	GLU	O-C-N	5.17	128.62	122.27
1	B	39	GLY	CA-C-N	5.17	128.18	120.95
1	B	39	GLY	C-N-CA	5.17	128.18	120.95
1	O	75	GLU	N-CA-C	-5.16	105.83	111.82
1	G	29	VAL	CA-C-O	5.16	125.81	120.39
1	B	98	VAL	CA-C-N	-5.15	112.00	122.45
1	B	98	VAL	C-N-CA	-5.15	112.00	122.45
1	G	75	GLU	O-C-N	-5.15	115.75	122.59
1	G	141	ARG	O-C-N	5.15	129.51	122.82
1	B	63	ASN	CA-C-N	5.14	124.32	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	ASN	C-N-CA	5.14	124.32	118.97
1	Y	119	GLU	N-CA-C	-5.14	102.87	110.48
1	O	104	LEU	CA-C-O	-5.14	113.16	120.51
1	Y	151	LYS	CA-C-O	-5.14	105.58	121.00
1	B	31	GLY	CA-C-O	5.13	127.37	121.47
1	B	37	THR	CA-CB-OG1	-5.13	101.91	109.60
1	O	62	PHE	CB-CA-C	5.12	118.46	110.67
1	G	129	ASN	CA-CB-CG	-5.12	107.48	112.60
1	G	131	GLU	N-CA-CB	5.12	119.34	110.44
1	B	134	LYS	CA-C-O	5.11	125.02	119.40
1	Y	129	ASN	O-C-N	-5.11	115.79	122.59
1	O	36	LEU	CA-CB-CG	5.11	134.17	116.30
1	Y	68	LYS	O-C-N	-5.10	117.26	123.03
1	G	105	SER	CB-CA-C	5.10	125.54	115.28
1	O	37	THR	O-C-N	-5.10	117.41	123.22
1	B	126	ARG	NE-CZ-NH1	5.09	126.59	121.50
1	G	132	SER	O-C-N	-5.09	115.82	122.59
1	Y	143	ALA	CB-CA-C	5.09	119.02	109.86
1	O	134	LYS	CA-C-O	5.09	127.78	120.51
1	Y	34	THR	CA-C-N	-5.08	117.39	123.44
1	Y	34	THR	C-N-CA	-5.08	117.39	123.44
1	O	49	GLY	CA-C-N	5.08	129.16	122.30
1	O	49	GLY	C-N-CA	5.08	129.16	122.30
1	B	138	ALA	CA-C-N	5.08	131.37	121.41
1	B	138	ALA	C-N-CA	5.08	131.37	121.41
1	B	69	HIS	N-CA-C	5.08	117.79	110.28
1	G	69	HIS	CA-C-O	-5.07	115.85	121.33
1	Y	55	CYS	N-CA-C	-5.07	107.04	113.18
1	Y	85	VAL	CA-CB-CG1	5.07	119.02	110.40
1	B	135	THR	O-C-N	5.06	129.32	122.59
1	O	151	LYS	CG-CD-CE	5.06	122.94	111.30
1	Y	4	ALA	CA-C-N	5.06	130.07	122.58
1	Y	4	ALA	C-N-CA	5.06	130.07	122.58
1	B	98	VAL	CA-CB-CG2	5.06	119.00	110.40
1	Y	142	LEU	N-CA-C	5.05	121.56	110.80
1	G	5	VAL	CA-C-O	5.05	126.63	121.63
1	B	108	TYR	O-C-N	-5.04	113.96	121.63
1	Y	137	ASN	N-CA-CB	5.04	119.01	110.49
1	O	51	ASN	N-CA-CB	-5.04	102.91	111.17
1	Y	89	LYS	CA-C-O	-5.04	113.30	120.51
1	B	97	ILE	CA-CB-CG2	5.04	119.06	110.50
1	G	56	THR	CA-C-N	5.04	129.50	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	56	THR	C-N-CA	5.04	129.50	122.05
1	Y	96	ASP	N-CA-CB	-5.03	100.36	111.69
1	G	34	THR	O-C-N	5.03	129.30	122.96
1	O	75	GLU	CB-CG-CD	5.03	121.15	112.60
1	O	143	ALA	O-C-N	5.02	129.10	123.48
1	Y	136	GLY	O-C-N	5.02	128.32	122.65
1	G	72	PRO	O-C-N	5.01	129.41	122.64
1	Y	107	GLU	CG-CD-OE1	5.01	129.92	118.40
1	Y	125	GLY	CA-C-N	5.01	129.01	121.40
1	Y	125	GLY	C-N-CA	5.01	129.01	121.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	126	ARG	Sidechain
1	G	85	VAL	Mainchain
1	Y	113	ARG	Sidechain
1	Y	60	PRO	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1095	0	1065	165	26
1	G	1095	0	1062	249	7
1	O	1095	0	1064	214	22
1	Y	1095	0	1062	232	4
2	B	1	0	0	0	0
2	G	1	0	0	0	0
2	O	1	0	0	0	0
2	Y	1	0	0	0	0
3	B	1	0	0	0	0
3	G	1	0	0	0	0
3	O	1	0	0	0	0
3	Y	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	1	0	0	0	0
4	O	1	0	0	1	0
4	Y	1	0	0	0	0
All	All	4392	0	4253	842	30

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 97.

All (842) 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:G:88:ASP:CB	1:G:88:ASP:CA	1.76	1.60
1:B:119:GLU:HG2	1:B:142:LEU:CD2	1.48	1.43
1:G:65:LEU:HD13	1:G:66:SER:N	1.28	1.41
1:G:151:LYS:HA	1:G:151:LYS:CE	1.42	1.40
1:B:126:ARG:HB3	1:B:126:ARG:NH1	1.39	1.35
1:B:94:ILE:H	1:B:94:ILE:CD1	1.31	1.34
1:B:126:ARG:HH11	1:B:126:ARG:CB	1.39	1.33
1:O:74:ASP:OD1	1:O:125:GLY:HA3	1.30	1.29
1:Y:121:PRO:O	1:Y:138:ALA:HA	1.30	1.29
1:G:120:LYS:HB3	1:G:138:ALA:O	1.33	1.23
1:O:88:ASP:OD2	1:O:89:LYS:HG3	1.39	1.21
1:B:68:LYS:NZ	1:B:76:GLU:OE1	1.75	1.18
1:Y:109:SER:O	1:Y:113:ARG:NH2	1.75	1.18
1:B:151:LYS:HA	1:B:151:LYS:CE	1.69	1.14
1:Y:29:VAL:HG13	1:Y:97:ILE:HG12	1.30	1.14
1:B:94:ILE:N	1:B:94:ILE:HD12	1.41	1.14
1:Y:122:ASP:HA	1:Y:138:ALA:HB2	1.15	1.11
1:G:27:VAL:HG23	1:G:102:ILE:HG21	1.21	1.11
1:O:1:ALA:HA	1:O:104:LEU:HD21	1.13	1.11
1:G:89:LYS:C	1:G:90:ASN:HD22	1.56	1.11
1:O:150:ALA:O	1:O:151:LYS:HB2	1.35	1.10
1:G:151:LYS:HA	1:G:151:LYS:HE3	1.34	1.10
1:B:119:GLU:HG2	1:B:142:LEU:HD23	1.27	1.09
1:O:78:HIS:HE2	1:O:134:LYS:HD2	1.08	1.09
1:O:82:LEU:HG	1:O:97:ILE:HD11	1.25	1.09
1:G:51:ASN:O	1:G:53:GLN:N	1.85	1.09
1:G:151:LYS:HA	1:G:151:LYS:HE2	1.20	1.09
1:Y:53:GLN:O	1:Y:53:GLN:HG3	1.43	1.08
1:O:123:ASP:OD2	1:O:132:SER:OG	1.70	1.08
1:B:135:THR:HG22	1:B:137:ASN:H	1.12	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:23:LYS:CD	1:Y:28:VAL:HG21	1.84	1.07
1:Y:23:LYS:HD3	1:Y:28:VAL:HG21	1.23	1.07
1:O:104:LEU:HD22	1:O:104:LEU:O	1.52	1.07
1:B:123:ASP:OD1	1:B:137:ASN:HB2	1.55	1.07
1:B:99:ASP:HB3	1:B:102:ILE:CD1	1.83	1.07
1:G:65:LEU:CD1	1:G:66:SER:N	2.18	1.07
1:B:99:ASP:HB3	1:B:102:ILE:HD11	1.07	1.06
1:G:47:GLN:HG3	1:G:60:PRO:CD	1.86	1.06
1:Y:122:ASP:CA	1:Y:138:ALA:HB2	1.85	1.06
1:B:38:GLU:HB3	1:B:89:LYS:HG3	1.05	1.04
1:B:38:GLU:HB3	1:B:89:LYS:CG	1.87	1.04
1:G:27:VAL:HB	1:G:102:ILE:HG23	1.40	1.04
1:O:106:GLY:H	1:O:109:SER:HB2	1.19	1.03
1:O:105:SER:H	1:O:109:SER:HB2	1.23	1.03
1:G:27:VAL:CG2	1:G:102:ILE:CG2	2.36	1.03
1:Y:84:ASN:HD21	1:Y:122:ASP:N	1.57	1.02
1:G:47:GLN:HG3	1:G:60:PRO:HD2	1.06	1.02
1:G:117:VAL:CG1	1:G:143:ALA:HB3	1.90	1.02
1:G:151:LYS:CE	1:G:151:LYS:CA	2.38	1.02
1:Y:79:VAL:HG22	1:Y:101:LEU:HD12	1.40	1.01
1:B:119:GLU:HG2	1:B:142:LEU:CG	1.90	1.00
1:G:105:SER:O	1:G:109:SER:HB2	1.59	1.00
1:O:51:ASN:HB3	1:Y:7:VAL:HG11	1.41	1.00
1:O:125:GLY:O	1:O:126:ARG:HG2	1.62	1.00
1:O:120:LYS:HB2	1:O:138:ALA:O	1.61	0.99
1:G:64:PRO:HB3	1:G:108:TYR:CD2	1.99	0.98
1:G:23:LYS:O	1:G:26:THR:HG22	1.63	0.98
1:O:1:ALA:CA	1:O:104:LEU:HD21	1.94	0.97
1:G:77:ARG:NH2	1:G:99:ASP:OD2	1.96	0.97
1:O:1:ALA:HA	1:O:104:LEU:CD2	1.94	0.97
1:Y:118:HIS:HA	1:Y:140:SER:O	1.63	0.97
1:O:46:HIS:CD2	1:O:116:VAL:CG1	2.47	0.97
1:B:119:GLU:CG	1:B:142:LEU:CD2	2.41	0.97
1:G:123:ASP:HB2	1:G:136:GLY:O	1.65	0.97
1:Y:0:ACE:O	1:Y:1:ALA:HB2	1.64	0.96
1:B:99:ASP:CB	1:B:102:ILE:HD11	1.96	0.96
1:G:27:VAL:CG2	1:G:102:ILE:HG21	1.93	0.96
1:B:102:ILE:HD13	1:B:102:ILE:H	1.31	0.95
1:B:151:LYS:HA	1:B:151:LYS:HE2	1.45	0.95
1:G:27:VAL:HB	1:G:102:ILE:CG2	1.96	0.95
1:G:129:ASN:CG	1:G:129:ASN:O	2.10	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:27:VAL:HG23	1:G:102:ILE:CG2	1.96	0.94
1:O:119:GLU:O	1:O:119:GLU:HG2	1.66	0.94
1:B:151:LYS:HA	1:B:151:LYS:HE3	1.50	0.94
1:O:9:LYS:HD3	1:O:10:GLY:N	1.82	0.94
1:Y:131:GLU:H	1:Y:133:THR:HG22	1.33	0.94
1:G:20:PHE:HD1	1:G:29:VAL:HB	1.33	0.93
1:O:62:PHE:HE2	1:O:113:ARG:NH1	1.66	0.93
1:O:150:ALA:O	1:O:151:LYS:CB	2.16	0.93
1:B:38:GLU:CB	1:B:89:LYS:HG3	1.96	0.93
1:B:119:GLU:CG	1:B:142:LEU:HD23	1.97	0.93
1:G:120:LYS:HG3	1:G:121:PRO:HD2	1.48	0.92
1:G:142:LEU:O	1:G:142:LEU:HD12	1.69	0.92
1:G:88:ASP:CB	1:G:88:ASP:C	2.42	0.92
1:Y:65:LEU:N	1:Y:65:LEU:HD22	1.83	0.92
1:B:151:LYS:HE3	1:B:151:LYS:CA	2.00	0.92
1:Y:121:PRO:O	1:Y:138:ALA:CA	2.17	0.91
1:Y:84:ASN:ND2	1:Y:122:ASP:H	1.69	0.91
1:Y:119:GLU:O	1:Y:120:LYS:HG3	1.70	0.91
1:O:115:MET:HG2	1:O:147:ILE:HD11	1.52	0.91
1:G:88:ASP:CB	1:G:88:ASP:N	2.33	0.91
1:G:68:LYS:O	1:G:78:HIS:NE2	2.04	0.90
1:O:24:GLY:O	1:O:25:ASP:HB2	1.69	0.90
1:O:78:HIS:NE2	1:O:134:LYS:HD2	1.85	0.90
1:G:8:LEU:O	1:G:15:GLN:HB2	1.70	0.90
1:O:5:VAL:HG13	1:Y:50:ASP:CB	2.01	0.90
1:Y:84:ASN:HD21	1:Y:122:ASP:H	0.92	0.90
1:B:51:ASN:HA	1:B:54:GLY:O	1.72	0.90
1:G:151:LYS:HE2	1:G:151:LYS:CA	1.99	0.90
1:O:45:VAL:HG11	1:O:110:ILE:CD1	2.01	0.89
1:B:135:THR:HG22	1:B:137:ASN:N	1.87	0.89
1:B:151:LYS:CE	1:B:151:LYS:CA	2.47	0.89
1:G:51:ASN:O	1:G:54:GLY:N	2.05	0.89
1:G:12:GLY:H	1:G:142:LEU:HD13	1.38	0.89
1:G:89:LYS:HA	1:G:89:LYS:HE3	1.55	0.89
1:O:78:HIS:HE1	1:O:134:LYS:NZ	1.70	0.89
1:G:1:ALA:HB3	1:G:105:SER:OG	1.72	0.89
1:Y:38:GLU:HG3	1:Y:39:GLY:HA3	1.55	0.88
1:O:29:VAL:HG13	1:O:97:ILE:HG12	1.54	0.88
1:O:88:ASP:OD2	1:O:89:LYS:CG	2.20	0.88
1:B:7:VAL:HG11	1:G:51:ASN:CB	2.03	0.88
1:Y:137:ASN:O	1:Y:139:GLY:N	2.06	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:47:GLN:O	1:Y:113:ARG:HD3	1.74	0.88
1:G:27:VAL:CB	1:G:102:ILE:CG2	2.51	0.88
1:Y:0:ACE:O	1:Y:1:ALA:CB	2.22	0.87
1:O:86:THR:O	1:O:93:ALA:HB3	1.75	0.87
1:G:51:ASN:O	1:G:52:THR:C	2.17	0.87
1:G:47:GLN:CG	1:G:60:PRO:HD2	1.99	0.87
1:B:71:GLY:N	1:B:74:ASP:OD1	2.08	0.86
1:B:67:LYS:HD3	1:B:76:GLU:HA	1.57	0.86
1:Y:38:GLU:HG3	1:Y:39:GLY:CA	2.05	0.86
1:Y:18:ILE:HD11	1:Y:20:PHE:CZ	2.11	0.86
1:O:135:THR:HG23	1:O:136:GLY:H	1.41	0.86
1:O:88:ASP:CG	1:O:89:LYS:H	1.85	0.85
1:G:64:PRO:HB3	1:G:108:TYR:CE2	2.11	0.85
1:G:65:LEU:HD13	1:G:65:LEU:C	1.96	0.85
1:O:82:LEU:HG	1:O:97:ILE:CD1	2.07	0.85
1:O:46:HIS:CE1	1:O:141:ARG:HH21	1.94	0.85
1:B:85:VAL:HG12	1:B:93:ALA:HB1	1.57	0.85
1:G:70:GLY:HA2	1:G:124:LEU:O	1.75	0.85
1:O:104:LEU:HA	1:O:109:SER:OG	1.76	0.84
1:B:119:GLU:HG2	1:B:142:LEU:HD21	1.56	0.84
1:O:5:VAL:CG1	1:Y:50:ASP:CB	2.55	0.84
1:O:78:HIS:HE1	1:O:134:LYS:HZ3	1.24	0.83
1:O:131:GLU:O	1:O:135:THR:HG22	1.77	0.83
1:Y:44:HIS:NE2	1:Y:122:ASP:OD1	2.10	0.83
1:O:133:THR:O	1:O:134:LYS:HB2	1.79	0.83
1:Y:53:GLN:O	1:Y:53:GLN:CG	2.25	0.83
1:G:65:LEU:HD13	1:G:66:SER:H	0.98	0.82
1:O:62:PHE:CE2	1:O:113:ARG:NH1	2.47	0.82
1:G:3:LYS:HD3	1:G:151:LYS:HD2	1.61	0.82
1:G:119:GLU:OE2	1:G:142:LEU:HG	1.79	0.82
1:Y:23:LYS:HG2	1:Y:28:VAL:CG2	2.09	0.82
1:Y:38:GLU:CG	1:Y:39:GLY:N	2.34	0.82
1:G:107:GLU:C	1:G:109:SER:H	1.88	0.82
1:O:45:VAL:HG11	1:O:110:ILE:HD13	1.59	0.82
1:G:72:PRO:O	1:G:77:ARG:NH1	2.13	0.81
1:Y:119:GLU:HG2	1:Y:140:SER:HB3	1.62	0.81
1:B:70:GLY:HA2	1:B:124:LEU:O	1.80	0.81
1:G:6:CYS:HB2	1:G:147:ILE:HG22	1.61	0.81
1:G:89:LYS:C	1:G:90:ASN:ND2	2.39	0.81
1:B:68:LYS:HD3	1:B:68:LYS:N	1.94	0.81
1:Y:38:GLU:CG	1:Y:39:GLY:HA3	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:37:THR:HG22	1:Y:38:GLU:CD	2.05	0.81
1:B:38:GLU:O	1:B:89:LYS:HE3	1.79	0.80
1:G:90:ASN:HD22	1:G:90:ASN:N	1.72	0.80
1:O:103:SER:OG	1:O:104:LEU:N	2.13	0.80
1:O:5:VAL:CG1	1:Y:50:ASP:HB2	2.11	0.80
1:Y:131:GLU:N	1:Y:133:THR:HG22	1.97	0.80
1:O:129:ASN:H	1:O:129:ASN:ND2	1.77	0.80
1:B:3:LYS:HE3	1:B:21:GLU:HG3	1.63	0.79
1:B:94:ILE:H	1:B:94:ILE:HD12	0.63	0.79
1:G:14:VAL:HG22	1:G:143:ALA:HB2	1.64	0.79
1:G:20:PHE:CD1	1:G:29:VAL:HB	2.17	0.79
1:O:106:GLY:O	1:O:109:SER:N	2.15	0.79
1:Y:104:LEU:N	1:Y:104:LEU:HD22	1.98	0.79
1:Y:23:LYS:CG	1:Y:28:VAL:HG21	2.12	0.79
1:G:46:HIS:CD2	1:G:116:VAL:HG13	2.18	0.79
1:G:12:GLY:N	1:G:142:LEU:HD13	1.97	0.79
1:O:107:GLU:O	1:O:108:TYR:CD2	2.36	0.78
1:G:89:LYS:HA	1:G:89:LYS:CE	2.10	0.78
1:O:65:LEU:O	1:O:67:LYS:N	2.16	0.78
1:Y:37:THR:HG22	1:Y:38:GLU:CG	2.12	0.78
1:B:119:GLU:HG2	1:B:142:LEU:HG	1.65	0.78
1:G:117:VAL:HG13	1:G:143:ALA:HB3	1.65	0.78
1:G:27:VAL:CB	1:G:102:ILE:HG23	2.14	0.78
1:B:77:ARG:NH1	1:B:99:ASP:OD2	2.16	0.78
1:G:63:ASN:CG	1:G:78:HIS:HD2	1.92	0.78
1:Y:29:VAL:CG1	1:Y:97:ILE:HG12	2.14	0.78
1:B:43:PHE:CZ	1:B:115:MET:HE2	2.18	0.77
1:B:90:ASN:O	1:B:92:VAL:N	2.16	0.77
1:G:88:ASP:CA	1:G:88:ASP:CG	2.56	0.77
1:O:104:LEU:O	1:O:104:LEU:CD2	2.32	0.77
1:B:7:VAL:HG11	1:G:51:ASN:HB2	1.66	0.77
1:O:5:VAL:CG1	1:Y:50:ASP:HB3	2.14	0.77
1:Y:118:HIS:CA	1:Y:140:SER:O	2.32	0.77
1:O:40:ASP:OD2	1:O:40:ASP:N	2.16	0.76
1:O:47:GLN:OE1	1:O:48:PHE:CZ	2.37	0.76
1:G:117:VAL:HG12	1:G:143:ALA:HB3	1.67	0.76
1:G:113:ARG:O	1:G:147:ILE:HD13	1.85	0.76
1:G:72:PRO:HA	1:G:77:ARG:NH1	2.01	0.76
1:B:34:THR:HG22	1:B:92:VAL:HB	1.65	0.76
1:O:5:VAL:HG13	1:Y:50:ASP:HB3	1.66	0.76
1:G:53:GLN:HG2	1:G:56:THR:HB	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:GLU:OE1	1:B:130:GLU:N	2.14	0.75
1:O:119:GLU:O	1:O:120:LYS:HG3	1.86	0.75
1:O:78:HIS:CE1	1:O:134:LYS:HZ3	2.05	0.75
1:Y:38:GLU:CG	1:Y:39:GLY:CA	2.63	0.75
1:G:103:SER:HB3	1:G:108:TYR:C	2.11	0.75
1:Y:103:SER:HB2	1:Y:105:SER:HB2	1.68	0.75
1:G:67:LYS:HB3	1:G:76:GLU:HG3	1.68	0.75
1:Y:82:LEU:CD1	1:Y:97:ILE:HD11	2.17	0.75
1:B:151:LYS:HE3	1:B:151:LYS:N	2.01	0.75
1:G:62:PHE:HZ	1:G:108:TYR:CG	2.04	0.75
1:O:105:SER:N	1:O:109:SER:HB2	2.02	0.74
1:O:125:GLY:O	1:O:126:ARG:CG	2.33	0.74
1:Y:53:GLN:HE22	1:G:13:PRO:HB3	1.52	0.74
1:Y:88:ASP:HB2	1:Y:89:LYS:C	2.12	0.74
1:G:118:HIS:HA	1:G:140:SER:O	1.87	0.74
1:O:15:GLN:O	1:O:15:GLN:HG3	1.79	0.74
1:O:30:THR:HA	1:O:95:VAL:O	1.88	0.74
1:O:129:ASN:OD1	1:O:130:GLU:N	2.20	0.73
1:Y:137:ASN:O	1:Y:139:GLY:HA2	1.88	0.73
1:Y:82:LEU:HD12	1:Y:97:ILE:HD11	1.69	0.73
1:B:130:GLU:H	1:B:130:GLU:CD	1.96	0.73
1:O:36:LEU:HG	1:O:41:HIS:CE1	2.24	0.73
1:O:88:ASP:OD2	1:O:89:LYS:N	2.22	0.73
1:Y:135:THR:HG22	1:Y:137:ASN:H	1.54	0.73
1:G:120:LYS:CB	1:G:138:ALA:O	2.26	0.73
1:G:25:ASP:O	1:G:102:ILE:HD11	1.89	0.73
1:G:63:ASN:CG	1:G:78:HIS:CD2	2.66	0.73
1:G:123:ASP:CB	1:G:136:GLY:O	2.37	0.73
1:Y:22:ALA:HB2	1:Y:104:LEU:CD2	2.19	0.73
1:O:5:VAL:HG13	1:Y:50:ASP:HB2	1.69	0.72
1:G:53:GLN:HG2	1:G:53:GLN:O	1.89	0.72
1:O:68:LYS:HD2	1:O:133:THR:CG2	2.20	0.72
1:O:92:VAL:O	1:O:93:ALA:HB2	1.88	0.72
1:G:85:VAL:O	1:G:86:THR:OG1	2.07	0.72
1:O:103:SER:OG	1:O:105:SER:HB3	1.89	0.72
1:O:123:ASP:OD2	1:O:132:SER:CB	2.36	0.72
1:O:78:HIS:CE1	1:O:134:LYS:NZ	2.58	0.72
1:O:106:GLY:N	1:O:109:SER:HB2	2.00	0.72
1:Y:40:ASP:HB3	1:Y:84:ASN:HB3	1.70	0.72
1:B:34:THR:HA	1:B:91:GLY:O	1.87	0.72
1:B:64:PRO:O	1:B:65:LEU:O	2.08	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:123:ASP:C	1:G:125:GLY:H	1.95	0.72
1:O:69:HIS:CG	1:O:135:THR:O	2.42	0.72
1:O:64:PRO:HG3	1:O:108:TYR:CD1	2.25	0.71
1:Y:131:GLU:H	1:Y:133:THR:CG2	2.03	0.71
1:B:102:ILE:CD1	1:B:102:ILE:H	2.03	0.71
1:G:5:VAL:HG23	1:G:150:ALA:HB2	1.72	0.71
1:G:103:SER:O	1:G:109:SER:HA	1.89	0.71
1:O:86:THR:O	1:O:93:ALA:CB	2.39	0.71
1:Y:104:LEU:HD13	1:Y:110:ILE:HD11	1.72	0.71
1:Y:139:GLY:O	1:Y:140:SER:HB3	1.89	0.71
1:B:126:ARG:HB3	1:B:126:ARG:HH11	0.57	0.71
1:O:46:HIS:CD2	1:O:116:VAL:HG11	2.24	0.71
1:Y:38:GLU:HG2	1:Y:39:GLY:N	2.04	0.71
1:B:7:VAL:HG11	1:G:51:ASN:HB3	1.70	0.70
1:B:71:GLY:HA2	1:B:124:LEU:HD23	1.72	0.70
1:G:24:GLY:O	1:G:25:ASP:HB2	1.91	0.70
1:B:119:GLU:CB	1:B:142:LEU:HD23	2.21	0.70
1:Y:15:GLN:O	1:Y:15:GLN:HG3	1.90	0.70
1:B:49:GLY:O	1:B:50:ASP:HB2	1.90	0.70
1:Y:116:VAL:HG21	1:Y:141:ARG:HG2	1.73	0.70
1:Y:131:GLU:O	1:Y:135:THR:HB	1.91	0.70
1:Y:38:GLU:HG3	1:Y:39:GLY:N	2.07	0.70
1:G:89:LYS:HD3	1:G:90:ASN:H	1.55	0.70
1:B:43:PHE:HB2	1:B:85:VAL:HG23	1.74	0.70
1:O:46:HIS:CD2	1:O:116:VAL:HG12	2.26	0.69
1:O:93:ALA:HB1	1:O:94:ILE:CG1	2.22	0.69
1:Y:1:ALA:HB1	1:Y:104:LEU:C	2.17	0.69
1:B:30:THR:HA	1:B:95:VAL:O	1.93	0.69
1:G:5:VAL:HG13	1:G:19:HIS:CD2	2.28	0.69
1:Y:119:GLU:HG3	1:Y:120:LYS:HE2	1.74	0.69
1:O:9:LYS:HD3	1:O:9:LYS:C	2.16	0.69
1:Y:27:VAL:CG1	1:Y:102:ILE:HG13	2.21	0.69
1:Y:141:ARG:O	1:Y:142:LEU:HB2	1.92	0.69
1:B:5:VAL:HG13	1:B:150:ALA:HB2	1.75	0.69
1:B:67:LYS:NZ	1:B:75:GLU:O	2.21	0.69
1:G:89:LYS:O	1:G:90:ASN:HB2	1.91	0.69
1:G:105:SER:O	1:G:109:SER:CB	2.38	0.69
1:G:90:ASN:ND2	1:G:90:ASN:N	2.41	0.69
1:G:27:VAL:CG2	1:G:102:ILE:HG22	2.23	0.69
1:G:46:HIS:CD2	1:G:116:VAL:CG1	2.75	0.68
1:G:64:PRO:CB	1:G:108:TYR:CD2	2.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:65:LEU:CD1	1:G:66:SER:H	1.92	0.68
1:Y:65:LEU:HD22	1:Y:65:LEU:H	1.55	0.68
1:G:89:LYS:C	1:G:91:GLY:H	1.99	0.68
1:B:94:ILE:CD1	1:B:94:ILE:N	2.12	0.68
1:O:78:HIS:HE2	1:O:134:LYS:CD	1.97	0.68
1:B:48:PHE:O	1:B:114:THR:OG1	2.11	0.68
1:B:53:GLN:HG3	1:B:57:SER:OG	1.94	0.68
1:Y:1:ALA:HB1	1:Y:104:LEU:O	1.94	0.67
1:G:46:HIS:HD2	1:G:116:VAL:HG13	1.56	0.67
1:O:106:GLY:H	1:O:109:SER:CB	2.04	0.67
1:G:68:LYS:O	1:G:78:HIS:CE1	2.47	0.67
1:B:123:ASP:OD1	1:B:137:ASN:CB	2.38	0.67
1:O:45:VAL:HG21	1:O:110:ILE:CD1	2.25	0.67
1:G:1:ALA:CB	1:G:105:SER:OG	2.42	0.67
1:Y:131:GLU:HA	1:Y:134:LYS:HG3	1.77	0.67
1:O:62:PHE:HE1	1:O:79:VAL:HG11	1.60	0.67
1:Y:1:ALA:CB	1:Y:104:LEU:O	2.43	0.66
1:G:136:GLY:O	1:G:137:ASN:HB2	1.94	0.66
1:Y:27:VAL:HG13	1:Y:102:ILE:HG13	1.78	0.66
1:Y:65:LEU:N	1:Y:65:LEU:CD2	2.58	0.66
1:Y:111:ILE:HG21	1:Y:149:ILE:HG13	1.76	0.66
1:G:140:SER:OG	1:G:141:ARG:N	2.27	0.66
1:B:98:VAL:HG13	1:B:98:VAL:O	1.95	0.66
1:O:5:VAL:HG23	1:O:19:HIS:CD2	2.31	0.66
1:B:136:GLY:O	1:B:137:ASN:HB2	1.95	0.66
1:Y:52:THR:O	1:Y:53:GLN:HB3	1.94	0.66
1:G:126:ARG:C	1:G:128:GLY:H	2.00	0.66
1:B:73:LYS:HD2	1:B:73:LYS:N	2.12	0.65
1:O:93:ALA:HB1	1:O:94:ILE:HG12	1.78	0.65
1:Y:37:THR:CG2	1:Y:38:GLU:CD	2.69	0.65
1:B:49:GLY:HA3	1:B:112:GLY:O	1.95	0.65
1:G:25:ASP:O	1:G:102:ILE:CD1	2.44	0.65
1:O:45:VAL:HG11	1:O:110:ILE:HD11	1.78	0.65
1:B:67:LYS:C	1:B:68:LYS:HD3	2.22	0.65
1:G:134:LYS:HD3	1:G:135:THR:HG23	1.78	0.65
1:Y:24:GLY:O	1:Y:25:ASP:CG	2.39	0.65
1:O:88:ASP:CG	1:O:89:LYS:N	2.50	0.65
1:Y:77:ARG:HH21	1:Y:101:LEU:CB	2.10	0.65
1:B:82:LEU:HG	1:B:97:ILE:CD1	2.27	0.65
1:G:8:LEU:O	1:G:15:GLN:HA	1.97	0.65
1:G:6:CYS:CB	1:G:147:ILE:HG22	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:111:ILE:HD11	1:O:149:ILE:HG12	1.79	0.64
1:G:85:VAL:O	1:G:86:THR:CB	2.44	0.64
1:B:131:GLU:O	1:B:131:GLU:HG3	1.96	0.64
1:G:110:ILE:HD13	1:G:147:ILE:HG13	1.78	0.64
1:O:14:VAL:HG21	1:O:142:LEU:HG	1.79	0.64
1:Y:47:GLN:C	1:Y:113:ARG:HD3	2.22	0.64
1:Y:139:GLY:O	1:Y:140:SER:CB	2.45	0.64
1:B:82:LEU:HG	1:B:97:ILE:HD12	1.77	0.64
1:B:110:ILE:HA	1:B:113:ARG:HD2	1.79	0.64
1:G:131:GLU:HG2	1:G:137:ASN:OD1	1.97	0.64
1:Y:11:ASP:HB3	1:Y:142:LEU:HD11	1.80	0.64
1:O:0:ACE:H2	1:O:149:ILE:CD1	2.29	0.63
1:G:105:SER:C	1:G:109:SER:HB2	2.23	0.63
1:Y:36:LEU:HD13	1:Y:41:HIS:CD2	2.33	0.63
1:Y:103:SER:O	1:Y:110:ILE:HG12	1.98	0.63
1:B:103:SER:O	1:B:109:SER:HA	1.99	0.63
1:G:47:GLN:O	1:G:113:ARG:NH1	2.30	0.63
1:O:15:GLN:HG2	1:O:34:THR:OG1	1.98	0.63
1:O:76:GLU:OE2	1:O:76:GLU:HA	1.98	0.63
1:O:118:HIS:ND1	1:O:139:GLY:O	2.25	0.63
1:Y:92:VAL:HG23	1:Y:94:ILE:CD1	2.28	0.63
1:O:84:ASN:HD21	1:O:122:ASP:HB3	1.63	0.63
1:B:119:GLU:CG	1:B:142:LEU:HG	2.28	0.63
1:G:20:PHE:HA	1:G:28:VAL:O	1.97	0.63
1:Y:24:GLY:HA3	1:Y:26:THR:HG22	1.81	0.63
1:G:123:ASP:C	1:G:125:GLY:N	2.55	0.63
1:Y:10:GLY:HA3	1:Y:142:LEU:O	1.98	0.63
1:G:87:ALA:HA	1:G:92:VAL:O	1.98	0.63
1:Y:43:PHE:CE1	1:Y:115:MET:HE2	2.34	0.62
1:Y:53:GLN:O	1:Y:56:THR:OG1	2.15	0.62
1:G:65:LEU:CD1	1:G:65:LEU:C	2.60	0.62
1:O:45:VAL:HG12	1:O:115:MET:HE2	1.81	0.62
1:Y:23:LYS:CG	1:Y:28:VAL:CG2	2.74	0.62
1:G:129:ASN:O	1:G:129:ASN:ND2	2.32	0.62
1:Y:77:ARG:HH21	1:Y:101:LEU:HG	1.64	0.62
1:G:102:ILE:HB	1:G:103:SER:HA	1.82	0.62
1:B:85:VAL:HG13	1:B:95:VAL:HG22	1.81	0.62
1:G:110:ILE:O	1:G:147:ILE:CG1	2.47	0.62
1:Y:77:ARG:NH2	1:Y:101:LEU:HB2	2.15	0.62
1:G:8:LEU:O	1:G:15:GLN:CB	2.46	0.61
1:Y:37:THR:O	1:Y:38:GLU:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:67:LYS:HB3	1:G:76:GLU:CG	2.30	0.61
1:O:6:CYS:SG	1:O:115:MET:HB2	2.40	0.61
1:O:91:GLY:H	1:O:92:VAL:HG12	1.64	0.61
1:G:50:ASP:HB3	1:G:52:THR:OG1	2.00	0.61
1:O:111:ILE:HD11	1:O:149:ILE:CG1	2.31	0.61
1:G:53:GLN:HB3	1:G:57:SER:OG	2.01	0.61
1:O:45:VAL:CG1	1:O:110:ILE:HD11	2.31	0.61
1:Y:46:HIS:CD2	1:Y:116:VAL:CG1	2.83	0.61
1:Y:46:HIS:CE1	1:Y:116:VAL:HG11	2.36	0.61
1:O:0:ACE:H2	1:O:149:ILE:HD11	1.82	0.61
1:Y:18:ILE:HD12	1:Y:29:VAL:HG23	1.82	0.61
1:Y:22:ALA:HB2	1:Y:104:LEU:HD21	1.83	0.61
1:O:47:GLN:O	1:O:113:ARG:HG2	2.01	0.60
1:O:106:GLY:O	1:O:108:TYR:N	2.34	0.60
1:Y:77:ARG:HH21	1:Y:101:LEU:CG	2.14	0.60
1:Y:115:MET:O	1:Y:144:CYS:HA	2.00	0.60
1:B:51:ASN:CA	1:B:54:GLY:O	2.48	0.60
1:G:39:GLY:O	1:G:86:THR:HA	2.01	0.60
1:O:40:ASP:HA	1:O:85:VAL:O	2.01	0.60
1:G:103:SER:HB3	1:G:108:TYR:O	2.00	0.60
1:Y:119:GLU:C	1:Y:120:LYS:CG	2.75	0.60
1:B:40:ASP:O	1:B:121:PRO:HG3	2.01	0.60
1:B:118:HIS:HA	1:B:140:SER:O	2.02	0.60
1:B:77:ARG:NE	1:B:101:LEU:HD13	2.16	0.60
1:O:135:THR:HG23	1:O:136:GLY:N	2.13	0.60
1:O:47:GLN:OE1	1:O:48:PHE:CE2	2.54	0.60
1:Y:41:HIS:O	1:Y:84:ASN:HA	2.02	0.60
1:B:50:ASP:OD2	1:G:7:VAL:HG12	2.02	0.59
1:G:4:ALA:HB1	1:G:148:GLY:O	2.02	0.59
1:O:29:VAL:CG1	1:O:97:ILE:HG12	2.29	0.59
1:G:135:THR:C	1:G:137:ASN:H	2.09	0.59
1:B:3:LYS:CE	1:B:21:GLU:HG3	2.33	0.59
1:Y:34:THR:HA	1:Y:91:GLY:O	2.02	0.59
1:O:64:PRO:HG3	1:O:108:TYR:HD1	1.65	0.59
1:Y:51:ASN:HB3	1:Y:54:GLY:O	2.02	0.59
1:Y:122:ASP:HA	1:Y:138:ALA:CB	2.11	0.59
1:Y:119:GLU:C	1:Y:120:LYS:HG3	2.27	0.59
1:G:120:LYS:HG3	1:G:121:PRO:CD	2.29	0.59
1:O:133:THR:O	1:O:134:LYS:CB	2.50	0.59
1:G:103:SER:O	1:G:104:LEU:C	2.44	0.59
1:B:63:ASN:ND2	1:B:78:HIS:HD2	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:VAL:O	1:B:98:VAL:CG1	2.51	0.58
1:G:5:VAL:HG13	1:G:19:HIS:HD2	1.67	0.58
1:G:77:ARG:NH2	1:G:99:ASP:CG	2.60	0.58
1:Y:18:ILE:HD11	1:Y:20:PHE:CE2	2.38	0.58
1:Y:22:ALA:HB2	1:Y:104:LEU:HD23	1.85	0.58
1:Y:47:GLN:HG3	1:Y:48:PHE:HD2	1.67	0.58
1:Y:88:ASP:OD1	1:Y:88:ASP:N	2.25	0.58
1:G:14:VAL:HB	1:G:34:THR:O	2.03	0.58
1:Y:119:GLU:HG3	1:Y:120:LYS:CG	2.34	0.58
1:O:92:VAL:O	1:O:93:ALA:CB	2.51	0.58
1:Y:137:ASN:O	1:Y:139:GLY:CA	2.51	0.58
1:O:68:LYS:HD2	1:O:133:THR:HG22	1.85	0.58
1:O:78:HIS:NE2	1:O:134:LYS:CD	2.63	0.58
1:Y:38:GLU:O	1:Y:87:ALA:C	2.46	0.58
1:Y:46:HIS:CD2	1:Y:61:HIS:HD2	2.22	0.58
1:O:14:VAL:CG1	1:O:36:LEU:HD13	2.34	0.58
1:O:89:LYS:HB3	1:O:90:ASN:O	2.03	0.57
1:B:49:GLY:O	1:B:50:ASP:CB	2.51	0.57
1:O:46:HIS:CE1	1:O:141:ARG:NH2	2.69	0.57
1:Y:72:PRO:HA	1:Y:77:ARG:HH11	1.69	0.57
1:Y:84:ASN:ND2	1:Y:121:PRO:HA	2.18	0.57
1:G:5:VAL:HG12	1:G:6:CYS:H	1.68	0.57
1:G:89:LYS:O	1:G:90:ASN:CB	2.53	0.57
1:B:53:GLN:CG	1:B:57:SER:OG	2.53	0.57
1:Y:50:ASP:C	1:Y:52:THR:H	2.11	0.57
1:B:119:GLU:CD	1:B:142:LEU:HG	2.29	0.57
1:G:1:ALA:CB	1:G:105:SER:HG	2.17	0.57
1:Y:52:THR:O	1:Y:53:GLN:CB	2.52	0.57
1:G:62:PHE:CZ	1:G:108:TYR:CG	2.92	0.57
1:O:88:ASP:OD2	1:O:89:LYS:CD	2.52	0.57
1:G:53:GLN:HB3	1:G:57:SER:CB	2.33	0.57
1:Y:46:HIS:CD2	1:Y:116:VAL:HG12	2.39	0.57
1:G:6:CYS:SG	1:G:147:ILE:HG22	2.44	0.57
1:G:38:GLU:HB2	1:G:89:LYS:HZ2	1.70	0.57
1:G:114:THR:HA	1:G:145:GLY:O	2.04	0.57
1:Y:103:SER:O	1:Y:109:SER:HA	2.05	0.57
1:O:104:LEU:HA	1:O:109:SER:CB	2.35	0.56
1:G:26:THR:OG1	1:G:98:VAL:HG23	2.05	0.56
1:Y:103:SER:C	1:Y:104:LEU:HD22	2.30	0.56
1:B:38:GLU:HA	1:B:88:ASP:O	2.05	0.56
1:O:9:LYS:C	1:O:9:LYS:CD	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:84:ASN:ND2	1:Y:122:ASP:N	2.40	0.56
1:Y:71:GLY:O	1:Y:77:ARG:HD2	2.05	0.56
1:Y:129:ASN:O	1:Y:132:SER:HB3	2.05	0.56
1:G:27:VAL:HG22	1:G:104:LEU:HD22	1.86	0.56
1:Y:119:GLU:O	1:Y:120:LYS:CG	2.48	0.56
1:B:88:ASP:C	1:B:90:ASN:H	2.12	0.56
1:G:20:PHE:HD1	1:G:29:VAL:CB	2.11	0.56
1:B:22:ALA:HB2	1:B:27:VAL:HG22	1.88	0.56
1:G:9:LYS:HA	1:G:14:VAL:O	2.06	0.56
1:O:50:ASP:OD1	1:O:52:THR:HG23	2.06	0.55
1:Y:38:GLU:H	1:Y:87:ALA:HB3	1.69	0.55
1:G:68:LYS:O	1:G:78:HIS:CD2	2.58	0.55
1:G:45:VAL:HG13	1:G:80:GLY:HA2	1.89	0.55
1:O:119:GLU:O	1:O:119:GLU:CG	2.40	0.55
1:Y:11:ASP:H	1:Y:142:LEU:CD1	2.19	0.55
1:Y:53:GLN:NE2	1:G:13:PRO:HB3	2.19	0.55
1:B:3:LYS:HE3	1:B:21:GLU:CG	2.36	0.55
1:B:18:ILE:HG22	1:B:19:HIS:N	2.21	0.55
1:B:71:GLY:C	1:B:73:LYS:N	2.62	0.55
1:Y:104:LEU:N	1:Y:104:LEU:CD2	2.64	0.55
1:G:14:VAL:CG2	1:G:143:ALA:HB2	2.36	0.55
1:G:30:THR:HA	1:G:95:VAL:O	2.07	0.55
1:Y:122:ASP:CA	1:Y:138:ALA:CB	2.73	0.55
1:G:12:GLY:CA	1:G:142:LEU:HD13	2.37	0.55
1:G:142:LEU:O	1:G:142:LEU:CD1	2.50	0.55
1:G:45:VAL:HB	1:G:115:MET:HE2	1.89	0.55
1:G:134:LYS:HE2	1:G:135:THR:HG23	1.89	0.55
1:O:5:VAL:HG12	1:Y:50:ASP:HB2	1.88	0.55
1:B:126:ARG:NH1	1:B:126:ARG:CB	2.24	0.55
1:G:15:GLN:O	1:G:33:ILE:HG23	2.07	0.54
1:G:53:GLN:HB3	1:G:57:SER:HB3	1.89	0.54
1:O:119:GLU:HB2	1:O:140:SER:O	2.07	0.54
1:B:129:ASN:HB2	1:B:130:GLU:OE1	2.07	0.54
1:Y:29:VAL:HG13	1:Y:97:ILE:CG1	2.21	0.54
1:G:100:PRO:O	1:G:102:ILE:HG13	2.08	0.54
1:O:133:THR:O	1:O:133:THR:HG22	2.07	0.54
1:G:39:GLY:H	1:G:87:ALA:HB3	1.72	0.54
1:O:68:LYS:HD2	1:O:133:THR:HG23	1.89	0.54
1:O:65:LEU:HG	1:O:108:TYR:HE1	1.72	0.54
1:Y:85:VAL:HG13	1:Y:93:ALA:HB1	1.89	0.54
1:Y:68:LYS:HE2	1:Y:76:GLU:OE1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:102:ILE:HD12	1:Y:110:ILE:HD13	1.90	0.54
1:Y:132:SER:C	1:Y:134:LYS:H	2.15	0.54
1:B:5:VAL:HG13	1:B:150:ALA:CB	2.37	0.54
1:G:74:ASP:OD1	1:G:126:ARG:NH1	2.38	0.54
1:O:45:VAL:CG1	1:O:110:ILE:CD1	2.81	0.54
1:Y:18:ILE:CD1	1:Y:29:VAL:HG23	2.38	0.54
1:Y:46:HIS:CD2	1:Y:61:HIS:CD2	2.96	0.54
1:Y:103:SER:HA	1:Y:104:LEU:HD22	1.89	0.54
1:Y:122:ASP:CB	1:Y:138:ALA:HB2	2.38	0.54
1:O:14:VAL:HG13	1:O:36:LEU:HD13	1.90	0.53
1:O:65:LEU:O	1:O:67:LYS:HG3	2.08	0.53
1:O:69:HIS:HB3	1:O:134:LYS:N	2.23	0.53
1:Y:11:ASP:C	1:Y:142:LEU:HD12	2.34	0.53
1:G:36:LEU:C	1:G:36:LEU:HD23	2.33	0.53
1:G:47:GLN:N	1:G:60:PRO:O	2.30	0.53
1:Y:119:GLU:CG	1:Y:120:LYS:HE2	2.38	0.53
1:Y:50:ASP:O	1:Y:57:SER:HB2	2.08	0.53
1:B:37:THR:HA	1:B:38:GLU:HG2	1.89	0.53
1:Y:38:GLU:HG2	1:Y:39:GLY:CA	2.36	0.53
1:B:85:VAL:HG13	1:B:95:VAL:CG2	2.38	0.53
1:Y:131:GLU:C	1:Y:134:LYS:HB2	2.34	0.53
1:B:57:SER:O	1:B:58:ALA:HB3	2.09	0.53
1:Y:99:ASP:OD2	1:Y:101:LEU:HB2	2.09	0.53
1:B:71:GLY:HA2	1:B:124:LEU:CD2	2.38	0.53
1:G:3:LYS:HD3	1:G:151:LYS:CD	2.35	0.53
1:G:69:HIS:HB2	1:G:78:HIS:CE1	2.43	0.53
1:O:7:VAL:CG1	1:Y:50:ASP:OD2	2.56	0.53
1:Y:11:ASP:HB3	1:Y:142:LEU:CD1	2.38	0.53
1:Y:49:GLY:HA2	1:Y:112:GLY:O	2.08	0.53
1:Y:46:HIS:NE2	1:Y:116:VAL:HG11	2.24	0.53
1:G:2:THR:HG23	1:G:3:LYS:HG3	1.91	0.53
1:O:9:LYS:HD3	1:O:10:GLY:CA	2.38	0.52
1:O:103:SER:OG	1:O:105:SER:CB	2.57	0.52
1:G:41:HIS:O	1:G:85:VAL:N	2.42	0.52
1:G:51:ASN:O	1:G:53:GLN:C	2.52	0.52
1:G:70:GLY:HA2	1:G:124:LEU:C	2.33	0.52
1:O:111:ILE:CD1	1:O:149:ILE:HG12	2.39	0.52
1:O:142:LEU:HD22	1:O:142:LEU:H	1.73	0.52
1:G:38:GLU:HB2	1:G:89:LYS:NZ	2.24	0.52
1:G:103:SER:O	1:G:104:LEU:O	2.27	0.52
1:G:121:PRO:O	1:G:138:ALA:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:36:LEU:HG	1:O:41:HIS:HE1	1.74	0.52
1:O:106:GLY:O	1:O:107:GLU:C	2.51	0.52
1:Y:65:LEU:H	1:Y:65:LEU:CD2	2.22	0.52
1:G:8:LEU:O	1:G:15:GLN:CA	2.56	0.52
1:O:45:VAL:HG12	1:O:115:MET:CE	2.38	0.52
1:Y:23:LYS:HG3	1:Y:23:LYS:O	2.09	0.52
1:O:27:VAL:HG22	1:O:102:ILE:HD11	1.90	0.52
1:O:125:GLY:O	1:O:126:ARG:CD	2.58	0.52
1:Y:40:ASP:OD1	1:Y:40:ASP:N	2.43	0.52
1:Y:88:ASP:HB2	1:Y:90:ASN:N	2.24	0.52
1:O:116:VAL:CG2	1:O:141:ARG:HB3	2.39	0.52
1:O:26:THR:CG2	1:O:98:VAL:HG13	2.40	0.51
1:O:116:VAL:HG21	1:O:141:ARG:HB3	1.93	0.51
1:Y:103:SER:CA	1:Y:104:LEU:HD22	2.41	0.51
1:O:103:SER:HG	1:O:104:LEU:H	1.54	0.51
1:Y:82:LEU:HD13	1:Y:97:ILE:HD11	1.91	0.51
1:Y:120:LYS:CB	1:Y:121:PRO:CD	2.87	0.51
1:B:119:GLU:HB2	1:B:142:LEU:HD23	1.91	0.51
1:O:114:THR:HG23	1:O:145:GLY:C	2.36	0.51
1:Y:82:LEU:HD13	1:Y:97:ILE:CD1	2.40	0.51
1:B:85:VAL:HG12	1:B:93:ALA:CB	2.33	0.51
1:Y:38:GLU:N	1:Y:87:ALA:HB3	2.26	0.51
1:B:107:GLU:HG3	1:B:108:TYR:CD1	2.46	0.51
1:Y:16:GLY:HA3	1:Y:33:ILE:HG22	1.93	0.51
1:B:135:THR:HG22	1:B:137:ASN:CA	2.41	0.51
1:G:64:PRO:CB	1:G:108:TYR:HD2	2.22	0.51
1:G:126:ARG:C	1:G:128:GLY:N	2.68	0.51
1:O:69:HIS:NE2	1:O:122:ASP:OD1	2.36	0.51
1:O:69:HIS:CD2	1:O:135:THR:O	2.63	0.51
1:Y:40:ASP:N	1:Y:86:THR:HG23	2.26	0.51
1:G:110:ILE:O	1:G:147:ILE:HD11	2.11	0.51
1:G:71:GLY:O	1:G:77:ARG:HD2	2.11	0.50
1:O:129:ASN:H	1:O:129:ASN:HD22	1.54	0.50
1:B:38:GLU:O	1:B:89:LYS:CE	2.57	0.50
1:G:89:LYS:CD	1:G:90:ASN:H	2.22	0.50
1:O:77:ARG:NE	1:O:101:LEU:HD23	2.26	0.50
1:Y:141:ARG:O	1:Y:142:LEU:CB	2.59	0.50
1:Y:27:VAL:HG11	1:Y:102:ILE:HG13	1.93	0.50
1:B:64:PRO:O	1:B:65:LEU:C	2.55	0.50
1:O:24:GLY:O	1:O:25:ASP:CB	2.48	0.50
1:G:27:VAL:HG21	1:G:102:ILE:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:107:GLU:C	1:G:109:SER:N	2.63	0.50
1:O:14:VAL:HG22	1:O:35:GLY:O	2.12	0.50
1:O:45:VAL:HG21	1:O:110:ILE:HG12	1.93	0.50
1:O:62:PHE:CE1	1:O:79:VAL:HG11	2.45	0.50
1:G:107:GLU:CG	1:G:108:TYR:H	2.25	0.50
1:G:134:LYS:HE2	1:G:135:THR:CG2	2.42	0.50
1:Y:24:GLY:C	1:Y:25:ASP:CG	2.77	0.50
1:B:94:ILE:CD1	1:B:94:ILE:C	2.83	0.50
1:G:64:PRO:CB	1:G:108:TYR:CE2	2.91	0.50
1:Y:37:THR:HG22	1:Y:38:GLU:CB	2.41	0.49
1:Y:114:THR:CG2	1:Y:144:CYS:HB2	2.42	0.49
1:B:21:GLU:OE2	1:B:23:LYS:HD3	2.13	0.49
1:G:131:GLU:O	1:G:134:LYS:HD3	2.12	0.49
1:G:41:HIS:O	1:G:84:ASN:HA	2.12	0.49
1:O:84:ASN:ND2	1:O:122:ASP:HB3	2.26	0.49
1:G:105:SER:HA	1:G:109:SER:HB2	1.95	0.49
1:B:57:SER:O	1:B:58:ALA:CB	2.60	0.49
1:B:122:ASP:OD2	1:B:124:LEU:HG	2.13	0.49
1:G:134:LYS:CE	1:G:135:THR:HG23	2.42	0.49
1:B:122:ASP:OD2	1:B:124:LEU:N	2.44	0.49
1:G:134:LYS:CD	1:G:135:THR:HG23	2.41	0.49
1:B:41:HIS:O	1:B:84:ASN:HA	2.12	0.49
1:G:67:LYS:HD3	1:G:76:GLU:HG3	1.93	0.49
1:Y:43:PHE:CZ	1:Y:115:MET:HE2	2.47	0.49
1:Y:88:ASP:CB	1:Y:90:ASN:O	2.61	0.49
1:B:90:ASN:O	1:B:92:VAL:CG1	2.60	0.49
1:O:46:HIS:HE1	4:O:154:HOH:O	1.95	0.48
1:O:135:THR:HG23	1:O:137:ASN:H	1.78	0.48
1:Y:119:GLU:HG3	1:Y:120:LYS:HG3	1.94	0.48
1:Y:131:GLU:N	1:Y:133:THR:CG2	2.70	0.48
1:G:151:LYS:HE3	1:G:151:LYS:CA	2.24	0.48
1:O:15:GLN:HG2	1:O:34:THR:HG1	1.78	0.48
1:O:130:GLU:C	1:O:132:SER:H	2.21	0.48
1:Y:92:VAL:HG23	1:Y:94:ILE:HD12	1.93	0.48
1:Y:131:GLU:O	1:Y:134:LYS:HB2	2.13	0.48
1:Y:24:GLY:O	1:Y:25:ASP:OD2	2.31	0.48
1:G:5:VAL:HG23	1:G:150:ALA:CB	2.42	0.48
1:G:107:GLU:CG	1:G:108:TYR:N	2.75	0.48
1:O:89:LYS:H	1:O:89:LYS:HD2	1.78	0.48
1:B:63:ASN:CG	1:B:78:HIS:HD2	2.22	0.48
1:B:65:LEU:O	1:B:66:SER:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:47:GLN:HG3	1:G:60:PRO:CG	2.42	0.48
1:Y:118:HIS:ND1	1:Y:140:SER:O	2.44	0.48
1:G:32:SER:HA	1:G:93:ALA:O	2.14	0.48
1:G:89:LYS:O	1:G:90:ASN:ND2	2.44	0.48
1:O:104:LEU:CD2	1:O:104:LEU:C	2.83	0.48
1:Y:47:GLN:HG3	1:Y:48:PHE:CD2	2.48	0.48
1:B:135:THR:HG22	1:B:136:GLY:N	2.28	0.48
1:Y:84:ASN:HD21	1:Y:121:PRO:HA	1.77	0.48
1:Y:133:THR:HG23	1:Y:134:LYS:HG2	1.95	0.48
1:G:29:VAL:HG22	1:G:97:ILE:HD13	1.95	0.48
1:O:62:PHE:CE2	1:O:113:ARG:CZ	2.97	0.48
1:O:88:ASP:OD2	1:O:89:LYS:HD2	2.13	0.48
1:B:62:PHE:CE1	1:B:64:PRO:HD3	2.48	0.48
1:G:5:VAL:HG12	1:G:6:CYS:N	2.28	0.48
1:O:78:HIS:O	1:O:79:VAL:C	2.55	0.47
1:Y:64:PRO:HG2	1:Y:65:LEU:CD2	2.43	0.47
1:G:1:ALA:HB3	1:G:105:SER:CB	2.43	0.47
1:O:107:GLU:O	1:O:108:TYR:CG	2.67	0.47
1:Y:72:PRO:HA	1:Y:77:ARG:NH1	2.29	0.47
1:G:51:ASN:O	1:G:53:GLN:CA	2.62	0.47
1:G:117:VAL:CG1	1:G:143:ALA:CB	2.80	0.47
1:Y:47:GLN:HA	1:Y:62:PHE:HB2	1.96	0.47
1:B:123:ASP:OD1	1:B:136:GLY:O	2.32	0.47
1:G:123:ASP:O	1:G:125:GLY:N	2.47	0.47
1:O:101:LEU:HD12	1:O:101:LEU:O	2.14	0.47
1:B:62:PHE:CD1	1:B:64:PRO:HD3	2.49	0.47
1:G:142:LEU:HD12	1:G:142:LEU:C	2.39	0.47
1:O:135:THR:CG2	1:O:136:GLY:N	2.77	0.47
1:B:71:GLY:C	1:B:73:LYS:H	2.22	0.47
1:O:86:THR:O	1:O:94:ILE:HG13	2.15	0.47
1:O:36:LEU:HD23	1:O:87:ALA:HB2	1.97	0.47
1:O:45:VAL:HG21	1:O:110:ILE:CG1	2.44	0.47
1:O:92:VAL:CG2	1:O:93:ALA:N	2.78	0.47
1:Y:19:HIS:O	1:Y:29:VAL:HA	2.15	0.47
1:Y:26:THR:OG1	1:Y:98:VAL:HG23	2.14	0.47
1:Y:46:HIS:NE2	1:Y:116:VAL:CG1	2.78	0.47
1:B:71:GLY:CA	1:B:124:LEU:HD23	2.43	0.47
1:G:25:ASP:O	1:G:102:ILE:HG12	2.15	0.47
1:G:45:VAL:HB	1:G:115:MET:CE	2.44	0.47
1:Y:3:LYS:HE3	1:Y:3:LYS:HB2	1.76	0.47
1:Y:49:GLY:CA	1:Y:112:GLY:O	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:THR:HG22	1:B:145:GLY:O	2.15	0.47
1:G:131:GLU:HG3	1:G:135:THR:OG1	2.15	0.47
1:G:64:PRO:HG3	1:G:79:VAL:HG21	1.96	0.47
1:G:15:GLN:HG2	1:G:16:GLY:N	2.30	0.46
1:B:95:VAL:O	1:B:95:VAL:HG12	2.13	0.46
1:O:115:MET:O	1:O:144:CYS:HA	2.16	0.46
1:B:3:LYS:HD3	1:B:151:LYS:HD2	1.97	0.46
1:G:74:ASP:O	1:G:75:GLU:CB	2.64	0.46
1:Y:33:ILE:HG12	1:Y:93:ALA:HB3	1.97	0.46
1:Y:77:ARG:O	1:Y:77:ARG:HG3	2.16	0.46
1:G:49:GLY:HA2	1:G:114:THR:OG1	2.15	0.46
1:O:69:HIS:HB2	1:O:134:LYS:HA	1.97	0.46
1:Y:69:HIS:NE2	1:Y:136:GLY:HA3	2.31	0.46
1:G:65:LEU:HA	1:G:65:LEU:HD22	1.64	0.46
1:Y:137:ASN:O	1:Y:138:ALA:C	2.57	0.46
1:O:64:PRO:CG	1:O:108:TYR:CD1	2.96	0.46
1:O:65:LEU:O	1:O:66:SER:C	2.59	0.46
1:O:79:VAL:O	1:O:102:ILE:HG22	2.16	0.46
1:B:105:SER:H	1:B:109:SER:HB2	1.81	0.46
1:B:118:HIS:HB3	1:B:138:ALA:O	2.15	0.46
1:G:88:ASP:C	1:G:89:LYS:O	2.56	0.46
1:O:93:ALA:HB1	1:O:94:ILE:HG13	1.98	0.46
1:G:88:ASP:C	1:G:88:ASP:HB3	2.38	0.46
1:Y:9:LYS:O	1:Y:143:ALA:HA	2.16	0.46
1:G:50:ASP:OD1	1:G:50:ASP:N	2.49	0.46
1:B:114:THR:HG22	1:B:145:GLY:H	1.81	0.45
1:B:142:LEU:HD13	1:B:142:LEU:HA	1.17	0.45
1:G:99:ASP:HA	1:G:100:PRO:HD3	1.83	0.45
1:Y:43:PHE:O	1:Y:82:LEU:HB2	2.16	0.45
1:Y:62:PHE:HZ	1:Y:108:TYR:HA	1.80	0.45
1:O:15:GLN:CG	1:O:34:THR:OG1	2.62	0.45
1:O:51:ASN:HB3	1:Y:7:VAL:CG1	2.29	0.45
1:O:69:HIS:HB3	1:O:134:LYS:H	1.80	0.45
1:O:45:VAL:HG21	1:O:110:ILE:HD13	1.98	0.45
1:Y:103:SER:O	1:Y:110:ILE:CG1	2.64	0.45
1:Y:119:GLU:HG3	1:Y:120:LYS:HG2	1.98	0.45
1:O:8:LEU:HD12	1:O:144:CYS:CA	2.47	0.45
1:O:125:GLY:C	1:O:126:ARG:HG2	2.32	0.45
1:Y:24:GLY:CA	1:Y:26:THR:HG22	2.44	0.45
1:B:88:ASP:C	1:B:90:ASN:N	2.74	0.45
1:O:0:ACE:CH3	1:O:149:ILE:HD13	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:THR:HA	1:B:145:GLY:O	2.17	0.45
1:G:103:SER:O	1:G:109:SER:CA	2.62	0.45
1:G:63:ASN:HD22	1:G:63:ASN:HA	1.23	0.45
1:O:101:LEU:HD12	1:O:101:LEU:HA	1.58	0.45
1:B:72:PRO:HG3	1:B:82:LEU:C	2.41	0.45
1:B:115:MET:HG2	1:B:147:ILE:HD11	1.99	0.45
1:B:135:THR:CG2	1:B:136:GLY:N	2.80	0.45
1:G:51:ASN:C	1:G:53:GLN:N	2.61	0.45
1:Y:18:ILE:CD1	1:Y:20:PHE:CZ	2.94	0.45
1:B:64:PRO:HG2	1:B:79:VAL:HG21	1.99	0.45
1:Y:47:GLN:O	1:Y:48:PHE:HB3	2.17	0.45
1:Y:77:ARG:NH1	1:Y:81:ASP:O	2.50	0.45
1:B:27:VAL:HB	1:B:102:ILE:HG12	1.98	0.45
1:O:26:THR:HG21	1:O:98:VAL:HG13	1.99	0.44
1:O:46:HIS:ND1	1:O:141:ARG:NH2	2.66	0.44
1:Y:44:HIS:CE1	1:Y:61:HIS:CE1	3.06	0.44
1:O:122:ASP:C	1:O:124:LEU:H	2.24	0.44
1:Y:45:VAL:HG13	1:Y:80:GLY:HA2	1.99	0.44
1:Y:59:GLY:O	1:Y:141:ARG:NH2	2.49	0.44
1:B:18:ILE:CG2	1:B:19:HIS:N	2.81	0.44
1:B:36:LEU:O	1:B:91:GLY:HA2	2.17	0.44
1:G:106:GLY:O	1:G:107:GLU:HG2	2.18	0.44
1:Y:23:LYS:HG2	1:Y:28:VAL:HG22	1.97	0.44
1:Y:46:HIS:CE1	1:Y:141:ARG:HH21	2.36	0.44
1:Y:46:HIS:HA	1:Y:61:HIS:H	1.81	0.44
1:Y:51:ASN:HA	1:Y:54:GLY:O	2.18	0.44
1:Y:118:HIS:HD1	1:Y:140:SER:C	2.24	0.44
1:G:131:GLU:O	1:G:131:GLU:HG3	2.11	0.44
1:G:140:SER:OG	1:G:141:ARG:CB	2.66	0.44
1:O:68:LYS:HA	1:O:134:LYS:HG3	2.00	0.44
1:G:44:HIS:CE1	1:G:118:HIS:CD2	3.06	0.44
1:G:67:LYS:HD3	1:G:76:GLU:HA	1.99	0.44
1:B:38:GLU:HG2	1:B:38:GLU:H	0.69	0.44
1:G:88:ASP:HB3	1:G:89:LYS:O	2.17	0.44
1:Y:132:SER:O	1:Y:136:GLY:HA2	2.17	0.44
1:O:8:LEU:O	1:O:15:GLN:HA	2.17	0.44
1:B:23:LYS:HE3	1:B:28:VAL:HG11	1.99	0.44
1:B:23:LYS:CE	1:B:28:VAL:HG11	2.47	0.44
1:G:27:VAL:CG2	1:G:104:LEU:HD22	2.47	0.44
1:B:68:LYS:N	1:B:68:LYS:CD	2.71	0.43
1:O:78:HIS:HE1	1:O:134:LYS:HZ2	1.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:31:GLY:O	1:Y:95:VAL:HG13	2.17	0.43
1:Y:79:VAL:CG2	1:Y:101:LEU:HD12	2.29	0.43
1:B:120:LYS:HB3	1:B:121:PRO:CD	2.48	0.43
1:G:2:THR:CG2	1:G:3:LYS:HG3	2.48	0.43
1:G:114:THR:HG22	1:G:144:CYS:HB2	1.99	0.43
1:O:21:GLU:O	1:O:21:GLU:HG2	2.18	0.43
1:Y:18:ILE:CD1	1:Y:29:VAL:CG2	2.97	0.43
1:Y:38:GLU:HG2	1:Y:39:GLY:HA3	1.93	0.43
1:Y:135:THR:HG22	1:Y:137:ASN:N	2.28	0.43
1:G:71:GLY:H	1:G:74:ASP:HB2	1.82	0.43
1:G:82:LEU:HG	1:G:97:ILE:CD1	2.48	0.43
1:B:125:GLY:HA2	1:B:132:SER:O	2.19	0.43
1:Y:84:ASN:HD21	1:Y:121:PRO:CA	2.31	0.43
1:Y:141:ARG:O	1:Y:142:LEU:HD23	2.17	0.43
1:B:47:GLN:O	1:B:113:ARG:HG2	2.18	0.43
1:B:123:ASP:HB2	1:B:136:GLY:O	2.18	0.43
1:G:27:VAL:CB	1:G:102:ILE:HG22	2.45	0.43
1:O:90:ASN:HB3	1:O:91:GLY:H	1.63	0.43
1:Y:31:GLY:C	1:Y:95:VAL:HG13	2.44	0.43
1:B:56:THR:C	1:B:57:SER:O	2.59	0.43
1:O:0:ACE:H2	1:O:149:ILE:HD13	1.99	0.43
1:B:116:VAL:HG12	1:B:118:HIS:CD2	2.54	0.43
1:G:89:LYS:CG	1:G:90:ASN:H	2.31	0.43
1:G:105:SER:HA	1:G:109:SER:CB	2.49	0.43
1:O:63:ASN:ND2	1:O:78:HIS:CD2	2.87	0.43
1:Y:97:ILE:HD12	1:Y:97:ILE:HG21	1.58	0.43
1:B:23:LYS:HE3	1:B:28:VAL:CG1	2.48	0.43
1:O:71:GLY:O	1:O:77:ARG:HG3	2.19	0.43
1:O:99:ASP:HA	1:O:100:PRO:HD3	1.95	0.43
1:Y:49:GLY:O	1:Y:146:VAL:HG22	2.19	0.43
1:Y:104:LEU:HD22	1:Y:104:LEU:H	1.79	0.43
1:B:62:PHE:CZ	1:B:64:PRO:HG3	2.54	0.43
1:G:74:ASP:CG	1:G:126:ARG:HH12	2.26	0.43
1:G:77:ARG:HH22	1:G:99:ASP:CG	2.17	0.43
1:B:23:LYS:HE3	1:B:23:LYS:HB2	1.43	0.42
1:B:123:ASP:C	1:B:125:GLY:H	2.26	0.42
1:G:5:VAL:HG13	1:G:18:ILE:O	2.18	0.42
1:G:44:HIS:ND1	1:G:118:HIS:CD2	2.87	0.42
1:Y:36:LEU:CD1	1:Y:87:ALA:HB2	2.49	0.42
1:Y:101:LEU:N	1:Y:101:LEU:CD2	2.82	0.42
1:G:55:CYS:HB3	1:G:141:ARG:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:46:HIS:HD2	1:O:116:VAL:CG1	2.23	0.42
1:O:90:ASN:CB	1:O:92:VAL:HG12	2.49	0.42
1:Y:73:LYS:H	1:Y:73:LYS:HG2	1.60	0.42
1:B:117:VAL:HG12	1:B:143:ALA:HB3	2.01	0.42
1:G:25:ASP:O	1:G:102:ILE:CG1	2.67	0.42
1:G:100:PRO:C	1:G:102:ILE:HG13	2.43	0.42
1:B:77:ARG:CZ	1:B:101:LEU:HD13	2.48	0.42
1:O:47:GLN:HB2	1:O:60:PRO:O	2.20	0.42
1:O:62:PHE:HZ	1:O:108:TYR:HA	1.85	0.42
1:O:64:PRO:HG2	1:O:108:TYR:CE1	2.54	0.42
1:Y:36:LEU:CD1	1:Y:41:HIS:CD2	3.01	0.42
1:B:55:CYS:O	1:B:141:ARG:HD2	2.19	0.42
1:G:114:THR:CG2	1:G:144:CYS:HB2	2.50	0.42
1:O:14:VAL:HG21	1:O:142:LEU:CG	2.48	0.42
1:O:149:ILE:HG22	1:O:150:ALA:N	2.34	0.42
1:G:53:GLN:O	1:G:56:THR:HB	2.20	0.42
1:G:63:ASN:ND2	1:G:78:HIS:HD2	2.18	0.42
1:Y:99:ASP:HA	1:Y:100:PRO:HD3	1.66	0.42
1:B:72:PRO:HA	1:B:77:ARG:NH1	2.34	0.42
1:B:90:ASN:O	1:B:92:VAL:HG12	2.20	0.42
1:O:125:GLY:C	1:O:126:ARG:CG	2.90	0.42
1:Y:88:ASP:HB3	1:Y:90:ASN:O	2.19	0.42
1:G:36:LEU:HD23	1:G:36:LEU:O	2.18	0.42
1:G:113:ARG:O	1:G:146:VAL:HA	2.19	0.42
1:O:7:VAL:HG12	1:Y:50:ASP:CG	2.45	0.42
1:B:51:ASN:HA	1:B:57:SER:HB3	2.02	0.42
1:G:39:GLY:O	1:G:86:THR:CA	2.67	0.42
1:G:71:GLY:O	1:G:72:PRO:C	2.61	0.42
1:O:44:HIS:CE1	1:O:61:HIS:CE1	3.08	0.41
1:Y:79:VAL:HG22	1:Y:101:LEU:CD1	2.30	0.41
1:B:71:GLY:CA	1:B:124:LEU:CD2	2.98	0.41
1:B:131:GLU:HG3	1:B:135:THR:HB	2.02	0.41
1:O:45:VAL:CG1	1:O:115:MET:HE2	2.49	0.41
1:B:119:GLU:CG	1:B:142:LEU:CG	2.77	0.41
1:B:126:ARG:NH1	1:B:126:ARG:CG	2.83	0.41
1:Y:120:LYS:HG3	1:Y:139:GLY:HA3	2.02	0.41
1:Y:77:ARG:NH2	1:Y:101:LEU:CB	2.73	0.41
1:B:44:HIS:HB3	1:B:80:GLY:O	2.20	0.41
1:G:23:LYS:HB3	1:G:23:LYS:HE2	1.30	0.41
1:G:110:ILE:O	1:G:147:ILE:CD1	2.69	0.41
1:O:62:PHE:CZ	1:O:108:TYR:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:78:HIS:CE1	1:O:134:LYS:CD	3.04	0.41
1:Y:45:VAL:HG21	1:Y:110:ILE:HG22	2.02	0.41
1:Y:68:LYS:HD3	1:Y:68:LYS:N	2.36	0.41
1:G:11:ASP:O	1:G:11:ASP:CG	2.63	0.41
1:G:70:GLY:CA	1:G:124:LEU:O	2.57	0.41
1:G:82:LEU:HG	1:G:97:ILE:HD11	2.03	0.41
1:Y:37:THR:HG22	1:Y:38:GLU:HB3	2.03	0.41
1:B:77:ARG:HD3	1:B:101:LEU:HD13	2.01	0.41
1:O:72:PRO:O	1:O:77:ARG:NH1	2.54	0.41
1:O:119:GLU:N	1:O:140:SER:O	2.54	0.41
1:B:127:GLY:HA3	1:B:132:SER:CB	2.51	0.41
1:B:135:THR:CG2	1:B:136:GLY:H	2.34	0.41
1:G:8:LEU:HD13	1:G:143:ALA:HB1	2.01	0.41
1:O:3:LYS:HG2	1:O:150:ALA:HB3	2.03	0.41
1:O:69:HIS:CD2	1:O:69:HIS:C	2.98	0.41
1:O:78:HIS:O	1:O:81:ASP:N	2.50	0.41
1:Y:6:CYS:HB2	1:Y:147:ILE:HA	2.03	0.41
1:G:53:GLN:O	1:G:53:GLN:CG	2.62	0.41
1:G:105:SER:O	1:G:109:SER:CA	2.69	0.40
1:O:5:VAL:CG2	1:O:19:HIS:CD2	3.03	0.40
1:O:78:HIS:NE2	1:O:134:LYS:HG2	2.37	0.40
1:G:0:ACE:H2	1:G:1:ALA:O	2.21	0.40
1:O:7:VAL:HG11	1:Y:50:ASP:OD2	2.19	0.40
1:B:82:LEU:HG	1:B:97:ILE:HD11	2.02	0.40
1:G:112:GLY:N	1:G:147:ILE:O	2.46	0.40
1:O:3:LYS:HA	1:O:20:PHE:O	2.22	0.40
1:O:26:THR:HG23	1:O:98:VAL:HG13	2.02	0.40
1:B:120:LYS:HA	1:B:121:PRO:HD3	1.82	0.40
1:B:122:ASP:OD2	1:B:122:ASP:C	2.65	0.40
1:O:78:HIS:CE1	1:O:134:LYS:HD2	2.54	0.40
1:O:127:GLY:O	1:O:128:GLY:O	2.39	0.40
1:Y:121:PRO:C	1:Y:138:ALA:HA	2.27	0.40
1:G:110:ILE:C	1:G:110:ILE:CD1	2.95	0.40

All (30) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:ARG:NH2	1:G:75:GLU:OE2[3_445]	0.67	1.53
1:O:107:GLU:CD	1:B:24:GLY:O[1_554]	0.95	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:151:LYS:CE	1:B:130:GLU:OE2[4_455]	1.08	1.12
1:O:151:LYS:CE	1:B:130:GLU:CD[4_455]	1.15	1.05
1:O:107:GLU:OE1	1:B:24:GLY:O[1_554]	1.20	1.00
1:O:107:GLU:OE2	1:B:24:GLY:O[1_554]	1.35	0.85
1:B:126:ARG:NH2	1:G:75:GLU:CD[3_445]	1.42	0.78
1:Y:34:THR:CG2	1:B:90:ASN:OD1[2_455]	1.45	0.75
1:O:107:GLU:OE2	1:B:25:ASP:CA[1_554]	1.55	0.65
1:O:107:GLU:OE1	1:B:24:GLY:C[1_554]	1.61	0.59
1:O:107:GLU:OE2	1:B:24:GLY:C[1_554]	1.62	0.58
1:O:151:LYS:CD	1:B:130:GLU:OE1[4_455]	1.62	0.58
1:O:151:LYS:CE	1:B:130:GLU:OE1[4_455]	1.63	0.57
1:O:151:LYS:NZ	1:B:130:GLU:OE2[4_455]	1.75	0.45
1:O:151:LYS:CD	1:B:130:GLU:CD[4_455]	1.76	0.44
1:O:151:LYS:CG	1:B:130:GLU:OE1[4_455]	1.81	0.39
1:O:53:GLN:CD	1:G:129:ASN:ND2[4_445]	1.83	0.37
1:O:107:GLU:CD	1:B:24:GLY:C[1_554]	1.83	0.37
1:O:107:GLU:OE2	1:B:25:ASP:N[1_554]	1.84	0.36
1:Y:13:PRO:CG	1:Y:90:ASN:OD1[2_455]	1.84	0.36
1:O:53:GLN:NE2	1:G:129:ASN:ND2[4_445]	1.90	0.30
1:O:151:LYS:CD	1:B:130:GLU:OE2[4_455]	1.93	0.27
1:B:126:ARG:CZ	1:G:75:GLU:OE2[3_445]	2.01	0.19
1:O:107:GLU:OE1	1:B:24:GLY:N[1_554]	2.02	0.18
1:Y:34:THR:CG2	1:B:90:ASN:CG[2_455]	2.09	0.11
1:O:107:GLU:OE1	1:B:24:GLY:CA[1_554]	2.11	0.09
1:Y:68:LYS:CE	1:B:47:GLN:NE2[4_455]	2.13	0.07
1:O:53:GLN:OE1	1:G:129:ASN:ND2[4_445]	2.17	0.03
1:B:126:ARG:NH2	1:G:75:GLU:OE1[3_445]	2.18	0.02
1:O:151:LYS:CG	1:B:130:GLU:CD[4_455]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	B	150/152 (99%)	123 (82%)	18 (12%)	9 (6%)	1	0
1	G	150/152 (99%)	109 (73%)	20 (13%)	21 (14%)	0	0
1	O	150/152 (99%)	111 (74%)	18 (12%)	21 (14%)	0	0
1	Y	150/152 (99%)	114 (76%)	17 (11%)	19 (13%)	0	0
All	All	600/608 (99%)	457 (76%)	73 (12%)	70 (12%)	0	0

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	1	ALA
1	O	2	THR
1	O	3	LYS
1	O	66	SER
1	O	94	ILE
1	O	107	GLU
1	O	108	TYR
1	O	126	ARG
1	O	128	GLY
1	O	133	THR
1	O	134	LYS
1	O	135	THR
1	Y	1	ALA
1	Y	36	LEU
1	Y	53	GLN
1	Y	91	GLY
1	Y	130	GLU
1	Y	131	GLU
1	Y	138	ALA
1	Y	139	GLY
1	Y	140	SER
1	Y	142	LEU
1	B	38	GLU
1	B	65	LEU
1	B	66	SER
1	B	74	ASP
1	B	91	GLY
1	B	139	GLY
1	G	1	ALA
1	G	25	ASP
1	G	47	GLN
1	G	52	THR
1	G	86	THR

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Mol	Chain	Res	Type
1	G	102	ILE
1	G	106	GLY
1	G	107	GLU
1	G	128	GLY
1	G	130	GLU
1	O	25	ASP
1	O	90	ASN
1	O	124	LEU
1	O	127	GLY
1	Y	37	THR
1	Y	38	GLU
1	Y	47	GLN
1	Y	66	SER
1	Y	89	LYS
1	Y	137	ASN
1	B	105	SER
1	G	68	LYS
1	G	90	ASN
1	O	105	SER
1	Y	107	GLU
1	B	75	GLU
1	G	9	LYS
1	G	104	LEU
1	B	58	ALA
1	G	119	GLU
1	G	137	ASN
1	O	47	GLN
1	O	91	GLY
1	O	104	LEU
1	Y	61	HIS
1	Y	133	THR
1	G	11	ASP
1	G	103	SER
1	G	138	ALA
1	G	123	ASP
1	O	24	GLY
1	G	85	VAL

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	B	117/117 (100%)	71 (61%)	46 (39%)	0	0
1	G	117/117 (100%)	73 (62%)	44 (38%)	0	0
1	O	117/117 (100%)	69 (59%)	48 (41%)	0	0
1	Y	117/117 (100%)	69 (59%)	48 (41%)	0	0
All	All	468/468 (100%)	282 (60%)	186 (40%)	0	0

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	2	THR
1	O	7	VAL
1	O	8	LEU
1	O	9	LYS
1	O	11	ASP
1	O	13	PRO
1	O	14	VAL
1	O	15	GLN
1	O	17	THR
1	O	18	ILE
1	O	20	PHE
1	O	26	THR
1	O	27	VAL
1	O	29	VAL
1	O	37	THR
1	O	38	GLU
1	O	41	HIS
1	O	45	VAL
1	O	47	GLN
1	O	56	THR
1	O	57	SER
1	O	66	SER
1	O	68	LYS
1	O	73	LYS
1	O	75	GLU
1	O	77	ARG
1	O	78	HIS
1	O	82	LEU

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Mol	Chain	Res	Type
1	O	89	LYS
1	O	90	ASN
1	O	92	VAL
1	O	94	ILE
1	O	96	ASP
1	O	97	ILE
1	O	101	LEU
1	O	102	ILE
1	O	104	LEU
1	O	107	GLU
1	O	110	ILE
1	O	111	ILE
1	O	115	MET
1	O	120	LYS
1	O	124	LEU
1	O	134	LYS
1	O	135	THR
1	O	141	ARG
1	O	142	LEU
1	O	151	LYS
1	Y	3	LYS
1	Y	7	VAL
1	Y	8	LEU
1	Y	15	GLN
1	Y	18	ILE
1	Y	21	GLU
1	Y	27	VAL
1	Y	28	VAL
1	Y	29	VAL
1	Y	30	THR
1	Y	33	ILE
1	Y	36	LEU
1	Y	37	THR
1	Y	40	ASP
1	Y	45	VAL
1	Y	50	ASP
1	Y	51	ASN
1	Y	52	THR
1	Y	53	GLN
1	Y	56	THR
1	Y	57	SER
1	Y	60	PRO

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Mol	Chain	Res	Type
1	Y	63	ASN
1	Y	65	LEU
1	Y	67	LYS
1	Y	68	LYS
1	Y	73	LYS
1	Y	75	GLU
1	Y	76	GLU
1	Y	77	ARG
1	Y	82	LEU
1	Y	86	THR
1	Y	88	ASP
1	Y	89	LYS
1	Y	90	ASN
1	Y	92	VAL
1	Y	95	VAL
1	Y	97	ILE
1	Y	98	VAL
1	Y	104	LEU
1	Y	105	SER
1	Y	107	GLU
1	Y	110	ILE
1	Y	111	ILE
1	Y	120	LYS
1	Y	131	GLU
1	Y	133	THR
1	Y	134	LYS
1	B	2	THR
1	B	5	VAL
1	B	7	VAL
1	B	13	PRO
1	B	17	THR
1	B	21	GLU
1	B	23	LYS
1	B	28	VAL
1	B	37	THR
1	B	38	GLU
1	B	40	ASP
1	B	44	HIS
1	B	45	VAL
1	B	50	ASP
1	B	51	ASN
1	B	53	GLN

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Mol	Chain	Res	Type
1	B	57	SER
1	B	66	SER
1	B	68	LYS
1	B	73	LYS
1	B	77	ARG
1	B	79	VAL
1	B	82	LEU
1	B	86	THR
1	B	89	LYS
1	B	92	VAL
1	B	94	ILE
1	B	97	ILE
1	B	99	ASP
1	B	101	LEU
1	B	102	ILE
1	B	104	LEU
1	B	111	ILE
1	B	113	ARG
1	B	114	THR
1	B	116	VAL
1	B	119	GLU
1	B	122	ASP
1	B	126	ARG
1	B	130	GLU
1	B	133	THR
1	B	134	LYS
1	B	135	THR
1	B	142	LEU
1	B	144	CYS
1	B	151	LYS
1	G	2	THR
1	G	5	VAL
1	G	11	ASP
1	G	14	VAL
1	G	15	GLN
1	G	20	PHE
1	G	21	GLU
1	G	23	LYS
1	G	29	VAL
1	G	30	THR
1	G	32	SER
1	G	34	THR

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Mol	Chain	Res	Type
1	G	36	LEU
1	G	37	THR
1	G	40	ASP
1	G	45	VAL
1	G	50	ASP
1	G	65	LEU
1	G	73	LYS
1	G	75	GLU
1	G	82	LEU
1	G	86	THR
1	G	88	ASP
1	G	89	LYS
1	G	94	ILE
1	G	97	ILE
1	G	98	VAL
1	G	101	LEU
1	G	102	ILE
1	G	104	LEU
1	G	105	SER
1	G	107	GLU
1	G	108	TYR
1	G	110	ILE
1	G	111	ILE
1	G	114	THR
1	G	116	VAL
1	G	119	GLU
1	G	120	LYS
1	G	130	GLU
1	G	134	LYS
1	G	142	LEU
1	G	147	ILE
1	G	151	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	19	HIS
1	O	41	HIS
1	O	51	ASN
1	O	90	ASN
1	Y	15	GLN
1	Y	41	HIS

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Mol	Chain	Res	Type
1	Y	53	GLN
1	Y	63	ASN
1	Y	84	ASN
1	B	63	ASN
1	B	137	ASN
1	G	15	GLN
1	G	19	HIS
1	G	41	HIS
1	G	63	ASN
1	G	90	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.