



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:44 am BST

PDB ID : 3SOD
Title : CHANGES IN CRYSTALLOGRAPHIC STRUCTURE AND THERMOSTABILITY OF A CU,ZN SUPEROXIDE DISMUTASE MUTANT RESULTING FROM THE REMOVAL OF BURIED CYSTEINE
Authors : Mcree, D.E.; Redford, S.M.; Getzoff, E.D.; Lepock, J.R.; Hallewell, R.A.; Tainer, J.A.
Deposited on : 1990-06-26
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

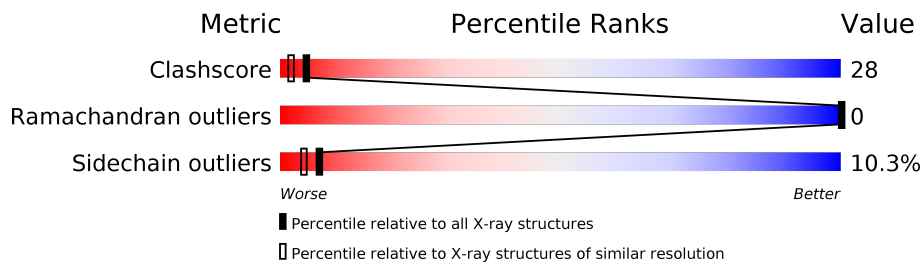
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 on 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	B	152	
1	G	152	
1	O	152	
1	Y	152	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4384 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
			Total	C	N	O	S			
1	O	152	1094	672	198	221	3	0	0	0
1	Y	152	1094	672	198	221	3	0	0	0
1	G	152	1094	672	198	221	3	0	0	0
1	B	152	1094	672	198	221	3	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	6	ALA	CYS	CONFLICT	UNP P00442
Y	6	ALA	CYS	CONFLICT	UNP P00442
G	6	ALA	CYS	CONFLICT	UNP P00442
B	6	ALA	CYS	CONFLICT	UNP P00442

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

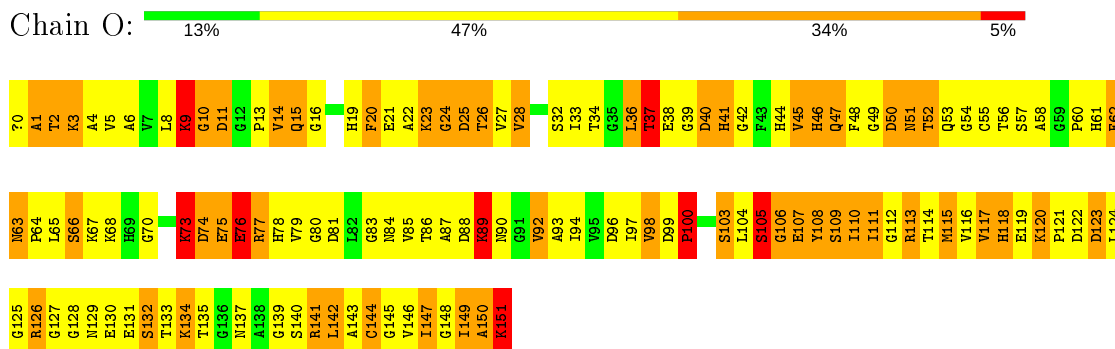
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

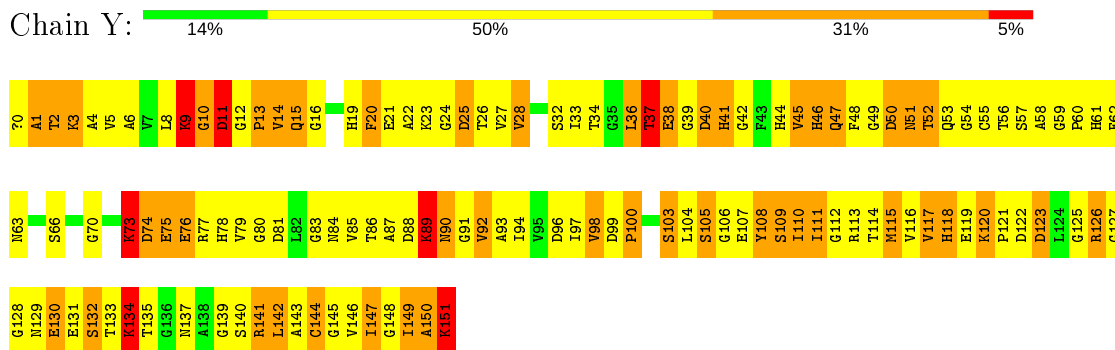
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

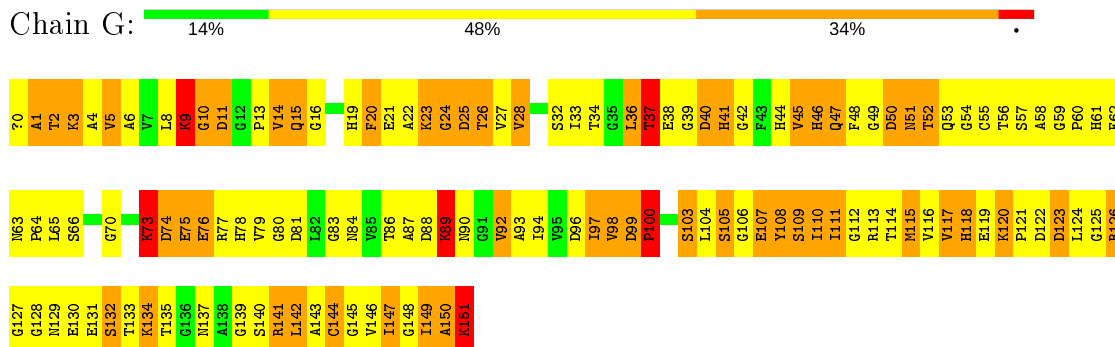
- Molecule 1: COPPER,ZINC SUPEROXIDE DISMUTASE



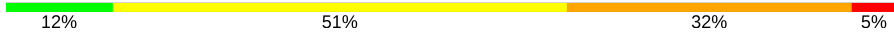
- Molecule 1: COPPER,ZINC SUPEROXIDE DISMUTASE

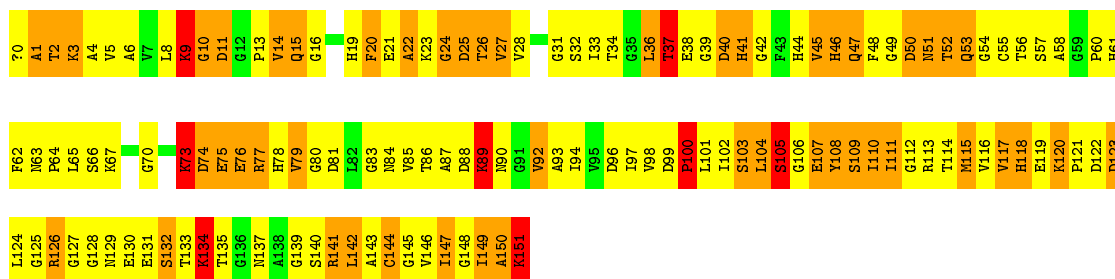


- Molecule 1: COPPER,ZINC SUPEROXIDE DISMUTASE



- Molecule 1: COPPER,ZINC SUPEROXIDE DISMUTASE

Chain B:  12% 51% 32% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.50 Å 89.40 Å 70.50 Å 90.00° 95.70° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.10 45.78 – 2.06	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.10) 52.8 (45.78-2.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.190 , (Not available) 0.445 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtrriage
Anisotropy	0.418	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 1.4	EDS
L-test for twinning ¹	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.43	EDS
Total number of atoms	4384	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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

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	2.35	40/1110 (3.6%)	3.86	213/1500 (14.2%)
1	G	2.35	37/1110 (3.3%)	3.86	213/1500 (14.2%)
1	O	2.35	39/1110 (3.5%)	3.86	214/1500 (14.3%)
1	Y	2.35	39/1110 (3.5%)	3.86	212/1500 (14.1%)
All	All	2.35	155/4440 (3.5%)	3.86	852/6000 (14.2%)

All (155) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	76	GLU	CB-CG	10.56	1.72	1.52
1	O	76	GLU	CB-CG	10.56	1.72	1.52
1	Y	76	GLU	CB-CG	10.55	1.72	1.52
1	G	76	GLU	CB-CG	10.54	1.72	1.52
1	Y	20	PHE	CD2-CE2	8.23	1.55	1.39
1	G	20	PHE	CD2-CE2	8.23	1.55	1.39
1	O	20	PHE	CD2-CE2	8.22	1.55	1.39
1	B	20	PHE	CD2-CE2	8.22	1.55	1.39
1	O	141	ARG	NE-CZ	-7.65	1.23	1.33
1	G	151	LYS	CA-CB	7.63	1.70	1.53
1	Y	141	ARG	NE-CZ	-7.62	1.23	1.33
1	G	141	ARG	NE-CZ	-7.60	1.23	1.33
1	B	141	ARG	NE-CZ	-7.59	1.23	1.33
1	O	151	LYS	CA-CB	7.58	1.70	1.53
1	Y	151	LYS	CA-CB	7.57	1.70	1.53
1	B	151	LYS	CA-CB	7.56	1.70	1.53
1	B	134	LYS	C-O	-7.54	1.09	1.23
1	O	134	LYS	C-O	-7.53	1.09	1.23
1	Y	134	LYS	C-O	-7.51	1.09	1.23
1	G	134	LYS	C-O	-7.49	1.09	1.23
1	Y	77	ARG	NE-CZ	7.21	1.42	1.33
1	G	77	ARG	NE-CZ	7.20	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	78	HIS	CA-CB	-7.17	1.38	1.53
1	O	77	ARG	NE-CZ	7.16	1.42	1.33
1	O	141	ARG	CZ-NH2	7.16	1.42	1.33
1	G	141	ARG	CZ-NH2	7.15	1.42	1.33
1	B	78	HIS	CA-CB	-7.15	1.38	1.53
1	B	141	ARG	CZ-NH2	7.14	1.42	1.33
1	O	78	HIS	CA-CB	-7.13	1.38	1.53
1	Y	141	ARG	CZ-NH2	7.13	1.42	1.33
1	B	77	ARG	NE-CZ	7.13	1.42	1.33
1	Y	78	HIS	CA-CB	-7.10	1.38	1.53
1	O	103	SER	CA-CB	7.09	1.63	1.52
1	O	75	GLU	CD-OE2	7.08	1.33	1.25
1	Y	103	SER	CA-CB	7.08	1.63	1.52
1	B	75	GLU	CD-OE2	7.08	1.33	1.25
1	B	103	SER	CA-CB	7.07	1.63	1.52
1	G	103	SER	CA-CB	7.05	1.63	1.52
1	G	75	GLU	CD-OE2	7.04	1.33	1.25
1	Y	75	GLU	CD-OE2	7.03	1.33	1.25
1	Y	62	PHE	CE1-CZ	7.00	1.50	1.37
1	B	62	PHE	CE1-CZ	6.99	1.50	1.37
1	O	62	PHE	CE1-CZ	6.97	1.50	1.37
1	G	62	PHE	CE1-CZ	6.94	1.50	1.37
1	O	110	ILE	C-O	6.92	1.36	1.23
1	B	110	ILE	C-O	6.91	1.36	1.23
1	G	110	ILE	C-O	6.91	1.36	1.23
1	Y	110	ILE	C-O	6.90	1.36	1.23
1	Y	42	GLY	CA-C	6.72	1.62	1.51
1	B	42	GLY	CA-C	6.69	1.62	1.51
1	O	42	GLY	CA-C	6.68	1.62	1.51
1	G	42	GLY	CA-C	6.67	1.62	1.51
1	B	66	SER	CB-OG	-6.61	1.33	1.42
1	Y	5	VAL	CB-CG1	6.60	1.66	1.52
1	G	5	VAL	CB-CG1	6.59	1.66	1.52
1	Y	66	SER	CB-OG	-6.59	1.33	1.42
1	O	5	VAL	CB-CG1	6.58	1.66	1.52
1	G	66	SER	CB-OG	-6.58	1.33	1.42
1	B	5	VAL	CB-CG1	6.58	1.66	1.52
1	B	141	ARG	CD-NE	-6.56	1.35	1.46
1	O	66	SER	CB-OG	-6.56	1.33	1.42
1	Y	141	ARG	CD-NE	-6.54	1.35	1.46
1	G	141	ARG	CD-NE	-6.51	1.35	1.46
1	O	141	ARG	CD-NE	-6.51	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	24	GLY	C-O	6.40	1.33	1.23
1	O	24	GLY	C-O	6.36	1.33	1.23
1	G	24	GLY	C-O	6.35	1.33	1.23
1	Y	132	SER	N-CA	6.34	1.59	1.46
1	Y	24	GLY	C-O	6.34	1.33	1.23
1	Y	55	CYS	CB-SG	6.33	1.93	1.82
1	O	55	CYS	CB-SG	6.32	1.93	1.82
1	O	132	SER	N-CA	6.31	1.58	1.46
1	G	132	SER	N-CA	6.31	1.58	1.46
1	B	55	CYS	CB-SG	6.30	1.93	1.82
1	B	132	SER	N-CA	6.30	1.58	1.46
1	G	55	CYS	CB-SG	6.29	1.93	1.82
1	O	32	SER	CB-OG	6.26	1.50	1.42
1	B	32	SER	CB-OG	6.23	1.50	1.42
1	G	32	SER	CB-OG	6.22	1.50	1.42
1	G	13	PRO	CA-CB	6.21	1.66	1.53
1	Y	32	SER	CB-OG	6.20	1.50	1.42
1	B	13	PRO	CA-CB	6.20	1.66	1.53
1	Y	13	PRO	CA-CB	6.19	1.66	1.53
1	B	76	GLU	CD-OE2	-6.19	1.18	1.25
1	O	13	PRO	CA-CB	6.18	1.66	1.53
1	O	76	GLU	CD-OE2	-6.15	1.18	1.25
1	G	76	GLU	CD-OE2	-6.14	1.18	1.25
1	Y	128	GLY	C-O	6.10	1.33	1.23
1	Y	76	GLU	CD-OE2	-6.08	1.19	1.25
1	O	128	GLY	C-O	6.08	1.33	1.23
1	B	128	GLY	C-O	6.06	1.33	1.23
1	G	128	GLY	C-O	6.05	1.33	1.23
1	O	76	GLU	N-CA	5.55	1.57	1.46
1	B	76	GLU	N-CA	5.55	1.57	1.46
1	Y	76	GLU	N-CA	5.54	1.57	1.46
1	G	111	ILE	C-N	5.54	1.43	1.33
1	Y	2	THR	CA-CB	5.54	1.67	1.53
1	G	76	GLU	N-CA	5.53	1.57	1.46
1	O	2	THR	CA-CB	5.52	1.67	1.53
1	O	111	ILE	C-N	5.52	1.43	1.33
1	B	2	THR	CA-CB	5.51	1.67	1.53
1	Y	111	ILE	C-N	5.50	1.43	1.33
1	G	2	THR	CA-CB	5.50	1.67	1.53
1	B	111	ILE	C-N	5.49	1.43	1.33
1	B	113	ARG	CG-CD	5.48	1.65	1.51
1	Y	113	ARG	CG-CD	5.47	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	113	ARG	CG-CD	5.45	1.65	1.51
1	G	113	ARG	CG-CD	5.43	1.65	1.51
1	G	119	GLU	CB-CG	5.34	1.62	1.52
1	O	119	GLU	CB-CG	5.34	1.62	1.52
1	B	119	GLU	CB-CG	5.34	1.62	1.52
1	Y	119	GLU	CB-CG	5.33	1.62	1.52
1	B	147	ILE	CB-CG1	5.33	1.69	1.54
1	O	147	ILE	CB-CG1	5.30	1.68	1.54
1	O	135	THR	CB-OG1	5.29	1.53	1.43
1	Y	147	ILE	CB-CG1	5.29	1.68	1.54
1	G	147	ILE	CB-CG1	5.29	1.68	1.54
1	G	145	GLY	CA-C	-5.29	1.43	1.51
1	B	83	GLY	N-CA	-5.28	1.38	1.46
1	B	135	THR	CB-OG1	5.28	1.53	1.43
1	O	83	GLY	N-CA	-5.28	1.38	1.46
1	Y	83	GLY	N-CA	-5.28	1.38	1.46
1	Y	135	THR	CB-OG1	5.28	1.53	1.43
1	G	135	THR	CB-OG1	5.28	1.53	1.43
1	B	145	GLY	CA-C	-5.27	1.43	1.51
1	G	113	ARG	CZ-NH1	-5.25	1.26	1.33
1	G	83	GLY	N-CA	-5.25	1.38	1.46
1	O	145	GLY	CA-C	-5.24	1.43	1.51
1	O	113	ARG	CZ-NH1	-5.24	1.26	1.33
1	Y	145	GLY	CA-C	-5.23	1.43	1.51
1	Y	113	ARG	CZ-NH1	-5.22	1.26	1.33
1	B	113	ARG	CZ-NH1	-5.22	1.26	1.33
1	G	63	ASN	C-O	-5.21	1.13	1.23
1	O	63	ASN	C-O	-5.20	1.13	1.23
1	Y	63	ASN	C-O	-5.19	1.13	1.23
1	Y	56	THR	C-N	-5.18	1.22	1.34
1	B	63	ASN	C-O	-5.18	1.13	1.23
1	B	56	THR	C-N	-5.17	1.22	1.34
1	B	105	SER	CB-OG	5.17	1.49	1.42
1	O	56	THR	C-N	-5.16	1.22	1.34
1	G	56	THR	C-N	-5.16	1.22	1.34
1	Y	105	SER	CB-OG	5.15	1.49	1.42
1	G	105	SER	CB-OG	5.15	1.49	1.42
1	O	105	SER	CB-OG	5.14	1.49	1.42
1	O	41	HIS	CA-CB	5.06	1.65	1.53
1	B	41	HIS	CA-CB	5.06	1.65	1.53
1	Y	41	HIS	CA-CB	5.05	1.65	1.53
1	G	41	HIS	CA-CB	5.04	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	85	VAL	C-O	5.03	1.32	1.23
1	B	31	GLY	N-CA	5.03	1.53	1.46
1	Y	85	VAL	C-O	5.02	1.32	1.23
1	O	85	VAL	C-O	5.02	1.32	1.23
1	Y	45	VAL	N-CA	5.01	1.56	1.46
1	B	45	VAL	N-CA	5.01	1.56	1.46
1	O	45	VAL	N-CA	5.00	1.56	1.46

All (852) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	113	ARG	NE-CZ-NH1	40.56	140.58	120.30
1	G	113	ARG	NE-CZ-NH1	40.55	140.57	120.30
1	B	113	ARG	NE-CZ-NH1	40.53	140.56	120.30
1	Y	113	ARG	NE-CZ-NH1	40.51	140.56	120.30
1	B	141	ARG	NE-CZ-NH1	24.89	132.75	120.30
1	Y	141	ARG	NE-CZ-NH1	24.87	132.74	120.30
1	O	141	ARG	NE-CZ-NH1	24.84	132.72	120.30
1	G	141	ARG	NE-CZ-NH1	24.72	132.66	120.30
1	Y	25	ASP	CB-CG-OD1	22.06	138.15	118.30
1	O	25	ASP	CB-CG-OD1	22.05	138.14	118.30
1	G	25	ASP	CB-CG-OD1	22.05	138.14	118.30
1	B	25	ASP	CB-CG-OD1	22.04	138.14	118.30
1	B	99	ASP	CB-CG-OD2	18.83	135.25	118.30
1	Y	99	ASP	CB-CG-OD2	18.81	135.22	118.30
1	O	99	ASP	CB-CG-OD2	18.80	135.22	118.30
1	G	99	ASP	CB-CG-OD2	18.80	135.22	118.30
1	G	151	LYS	CB-CA-C	-18.54	73.33	110.40
1	B	151	LYS	CB-CA-C	-18.53	73.34	110.40
1	O	151	LYS	CB-CA-C	-18.53	73.35	110.40
1	Y	151	LYS	CB-CA-C	-18.52	73.36	110.40
1	Y	77	ARG	NE-CZ-NH1	17.61	129.11	120.30
1	G	77	ARG	NE-CZ-NH1	17.59	129.10	120.30
1	O	77	ARG	NE-CZ-NH1	17.56	129.08	120.30
1	B	77	ARG	NE-CZ-NH1	17.51	129.05	120.30
1	B	113	ARG	NE-CZ-NH2	-17.21	111.70	120.30
1	O	113	ARG	NE-CZ-NH2	-17.20	111.70	120.30
1	Y	113	ARG	NE-CZ-NH2	-17.18	111.71	120.30
1	G	113	ARG	NE-CZ-NH2	-17.18	111.71	120.30
1	G	9	LYS	CB-CG-CD	15.34	151.49	111.60
1	O	9	LYS	CB-CG-CD	15.34	151.47	111.60
1	Y	9	LYS	CB-CG-CD	15.33	151.45	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	9	LYS	CB-CG-CD	15.31	151.41	111.60
1	Y	141	ARG	CD-NE-CZ	15.20	144.88	123.60
1	O	141	ARG	CD-NE-CZ	15.20	144.88	123.60
1	B	141	ARG	CD-NE-CZ	15.19	144.87	123.60
1	G	141	ARG	CD-NE-CZ	15.17	144.83	123.60
1	B	107	GLU	OE1-CD-OE2	14.93	141.21	123.30
1	O	107	GLU	OE1-CD-OE2	14.87	141.15	123.30
1	G	107	GLU	OE1-CD-OE2	14.84	141.11	123.30
1	Y	107	GLU	OE1-CD-OE2	14.82	141.09	123.30
1	G	62	PHE	C-N-CA	14.77	158.62	121.70
1	O	62	PHE	C-N-CA	14.74	158.56	121.70
1	Y	62	PHE	C-N-CA	14.74	158.55	121.70
1	B	62	PHE	C-N-CA	14.73	158.53	121.70
1	Y	74	ASP	CB-CG-OD2	14.34	131.21	118.30
1	G	74	ASP	CB-CG-OD2	14.33	131.20	118.30
1	O	74	ASP	CB-CG-OD2	14.30	131.17	118.30
1	B	74	ASP	CB-CG-OD2	14.26	131.14	118.30
1	Y	81	ASP	CB-CG-OD1	13.73	130.65	118.30
1	O	81	ASP	CB-CG-OD1	13.69	130.62	118.30
1	G	81	ASP	CB-CG-OD1	13.69	130.62	118.30
1	B	81	ASP	CB-CG-OD1	13.67	130.61	118.30
1	Y	3	LYS	CD-CE-NZ	13.13	141.91	111.70
1	B	3	LYS	CD-CE-NZ	13.13	141.89	111.70
1	O	3	LYS	CD-CE-NZ	13.12	141.88	111.70
1	G	3	LYS	CD-CE-NZ	13.11	141.85	111.70
1	Y	122	ASP	CB-CG-OD1	12.88	129.89	118.30
1	O	122	ASP	CB-CG-OD1	12.85	129.86	118.30
1	B	122	ASP	CB-CG-OD1	12.84	129.85	118.30
1	G	122	ASP	CB-CG-OD1	12.79	129.81	118.30
1	B	96	ASP	CB-CG-OD2	11.87	128.98	118.30
1	G	96	ASP	CB-CG-OD2	11.86	128.97	118.30
1	O	96	ASP	CB-CG-OD2	11.82	128.94	118.30
1	O	105	SER	N-CA-CB	11.79	128.19	110.50
1	G	105	SER	N-CA-CB	11.79	128.19	110.50
1	Y	105	SER	N-CA-CB	11.78	128.18	110.50
1	Y	96	ASP	CB-CG-OD2	11.78	128.90	118.30
1	B	105	SER	N-CA-CB	11.77	128.16	110.50
1	B	141	ARG	NE-CZ-NH2	-11.74	114.43	120.30
1	O	141	ARG	NE-CZ-NH2	-11.71	114.44	120.30
1	Y	141	ARG	NE-CZ-NH2	-11.69	114.46	120.30
1	G	141	ARG	NE-CZ-NH2	-11.63	114.49	120.30
1	Y	151	LYS	CA-C-O	11.59	144.43	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	151	LYS	CA-C-O	11.57	144.40	120.10
1	B	151	LYS	CA-C-O	11.56	144.39	120.10
1	G	151	LYS	CA-C-O	11.56	144.37	120.10
1	B	11	ASP	CB-CG-OD1	11.37	128.53	118.30
1	G	11	ASP	CB-CG-OD1	11.37	128.53	118.30
1	O	11	ASP	CB-CG-OD1	11.32	128.49	118.30
1	Y	11	ASP	CB-CG-OD1	11.30	128.47	118.30
1	O	50	ASP	CB-CG-OD2	11.21	128.39	118.30
1	Y	50	ASP	CB-CG-OD2	11.20	128.38	118.30
1	B	50	ASP	CB-CG-OD2	11.16	128.35	118.30
1	G	50	ASP	CB-CG-OD2	11.15	128.34	118.30
1	Y	75	GLU	N-CA-CB	10.72	129.90	110.60
1	B	75	GLU	N-CA-CB	10.72	129.89	110.60
1	B	11	ASP	CB-CG-OD2	-10.71	108.66	118.30
1	O	75	GLU	N-CA-CB	10.71	129.87	110.60
1	G	75	GLU	N-CA-CB	10.70	129.86	110.60
1	O	11	ASP	CB-CG-OD2	-10.67	108.69	118.30
1	Y	11	ASP	CB-CG-OD2	-10.67	108.70	118.30
1	G	11	ASP	CB-CG-OD2	-10.67	108.70	118.30
1	G	113	ARG	NH1-CZ-NH2	-10.67	107.67	119.40
1	O	113	ARG	NH1-CZ-NH2	-10.66	107.67	119.40
1	B	113	ARG	NH1-CZ-NH2	-10.65	107.69	119.40
1	Y	113	ARG	NH1-CZ-NH2	-10.65	107.69	119.40
1	G	36	LEU	CA-CB-CG	10.53	139.52	115.30
1	O	36	LEU	CA-CB-CG	10.52	139.49	115.30
1	Y	36	LEU	CA-CB-CG	10.51	139.46	115.30
1	B	36	LEU	CA-CB-CG	10.51	139.47	115.30
1	G	103	SER	N-CA-CB	-10.35	94.97	110.50
1	O	103	SER	N-CA-CB	-10.34	94.99	110.50
1	Y	103	SER	N-CA-CB	-10.34	94.99	110.50
1	B	3	LYS	CB-CG-CD	10.34	138.48	111.60
1	B	103	SER	N-CA-CB	-10.34	94.99	110.50
1	G	3	LYS	CB-CG-CD	10.32	138.43	111.60
1	O	3	LYS	CB-CG-CD	10.32	138.42	111.60
1	Y	3	LYS	CB-CG-CD	10.30	138.39	111.60
1	B	3	LYS	CA-CB-CG	10.31	136.07	113.40
1	G	3	LYS	CA-CB-CG	10.30	136.06	113.40
1	O	3	LYS	CA-CB-CG	10.29	136.04	113.40
1	Y	3	LYS	CA-CB-CG	10.28	136.01	113.40
1	B	76	GLU	CG-CD-OE1	-10.04	98.21	118.30
1	G	76	GLU	CG-CD-OE1	-10.03	98.23	118.30
1	B	20	PHE	CB-CG-CD1	10.03	127.82	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	76	GLU	CG-CD-OE1	-10.03	98.25	118.30
1	Y	76	GLU	CG-CD-OE1	-10.01	98.28	118.30
1	B	11	ASP	CA-CB-CG	9.99	135.37	113.40
1	O	20	PHE	CB-CG-CD1	9.98	127.79	120.80
1	O	11	ASP	CA-CB-CG	9.97	135.34	113.40
1	G	11	ASP	CA-CB-CG	9.97	135.34	113.40
1	Y	20	PHE	CB-CG-CD1	9.97	127.78	120.80
1	G	20	PHE	CB-CG-CD1	9.96	127.78	120.80
1	Y	11	ASP	CA-CB-CG	9.96	135.32	113.40
1	B	123	ASP	CB-CG-OD1	9.90	127.21	118.30
1	O	123	ASP	CB-CG-OD1	9.90	127.21	118.30
1	G	123	ASP	CB-CG-OD1	9.89	127.20	118.30
1	Y	123	ASP	CB-CG-OD1	9.88	127.19	118.30
1	B	86	THR	CA-C-N	9.57	138.25	117.20
1	G	86	THR	CA-C-N	9.55	138.21	117.20
1	O	86	THR	CA-C-N	9.54	138.19	117.20
1	Y	86	THR	CA-C-N	9.53	138.16	117.20
1	O	73	LYS	CB-CA-C	-9.46	91.48	110.40
1	G	73	LYS	CB-CA-C	-9.46	91.48	110.40
1	B	73	LYS	CB-CA-C	-9.45	91.50	110.40
1	Y	73	LYS	CB-CA-C	-9.44	91.52	110.40
1	B	20	PHE	CB-CG-CD2	-9.32	114.28	120.80
1	G	20	PHE	CB-CG-CD2	-9.30	114.29	120.80
1	O	20	PHE	CB-CG-CD2	-9.28	114.31	120.80
1	Y	20	PHE	CB-CG-CD2	-9.23	114.34	120.80
1	B	88	ASP	CB-CG-OD1	9.18	126.57	118.30
1	B	58	ALA	N-CA-CB	9.16	122.93	110.10
1	G	88	ASP	CB-CG-OD1	9.16	126.54	118.30
1	Y	88	ASP	CB-CG-OD1	9.15	126.53	118.30
1	O	58	ALA	N-CA-CB	9.13	122.88	110.10
1	O	88	ASP	CB-CG-OD1	9.12	126.51	118.30
1	Y	58	ALA	N-CA-CB	9.12	122.86	110.10
1	G	58	ALA	N-CA-CB	9.11	122.86	110.10
1	Y	25	ASP	OD1-CG-OD2	-9.08	106.05	123.30
1	O	25	ASP	OD1-CG-OD2	-9.06	106.08	123.30
1	B	28	VAL	CA-CB-CG2	-9.06	97.30	110.90
1	O	28	VAL	CA-CB-CG2	-9.06	97.31	110.90
1	G	25	ASP	OD1-CG-OD2	-9.06	106.08	123.30
1	Y	28	VAL	CA-CB-CG2	-9.06	97.31	110.90
1	B	25	ASP	OD1-CG-OD2	-9.05	106.10	123.30
1	G	28	VAL	CA-CB-CG2	-9.04	97.35	110.90
1	G	51	ASN	O-C-N	-8.99	108.31	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	51	ASN	O-C-N	-8.99	108.32	122.70
1	B	51	ASN	O-C-N	-8.99	108.32	122.70
1	O	51	ASN	O-C-N	-8.98	108.33	122.70
1	B	88	ASP	CB-CG-OD2	-8.83	110.36	118.30
1	Y	88	ASP	CB-CG-OD2	-8.79	110.39	118.30
1	G	88	ASP	CB-CG-OD2	-8.79	110.39	118.30
1	O	88	ASP	CB-CG-OD2	-8.78	110.39	118.30
1	G	151	LYS	N-CA-C	8.77	134.68	111.00
1	O	151	LYS	N-CA-C	8.77	134.67	111.00
1	B	151	LYS	N-CA-C	8.77	134.67	111.00
1	Y	151	LYS	N-CA-C	8.75	134.63	111.00
1	B	126	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	Y	126	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	O	126	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	G	126	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	G	46	HIS	O-C-N	8.61	136.48	122.70
1	B	46	HIS	O-C-N	8.61	136.48	122.70
1	Y	46	HIS	O-C-N	8.61	136.48	122.70
1	O	46	HIS	O-C-N	8.61	136.47	122.70
1	G	127	GLY	CA-C-O	-8.60	105.11	120.60
1	O	127	GLY	CA-C-O	-8.57	105.17	120.60
1	B	127	GLY	CA-C-O	-8.56	105.19	120.60
1	Y	127	GLY	CA-C-O	-8.55	105.21	120.60
1	O	123	ASP	CB-CG-OD2	-8.54	110.62	118.30
1	B	123	ASP	CB-CG-OD2	-8.54	110.62	118.30
1	G	123	ASP	CB-CG-OD2	-8.52	110.63	118.30
1	G	51	ASN	CB-CG-OD1	8.51	138.61	121.60
1	Y	123	ASP	CB-CG-OD2	-8.50	110.65	118.30
1	O	51	ASN	CB-CG-OD1	8.49	138.59	121.60
1	Y	14	VAL	CG1-CB-CG2	-8.49	97.32	110.90
1	Y	51	ASN	CB-CG-OD1	8.48	138.57	121.60
1	G	14	VAL	CG1-CB-CG2	-8.48	97.32	110.90
1	B	51	ASN	CB-CG-OD1	8.48	138.57	121.60
1	B	14	VAL	CG1-CB-CG2	-8.48	97.34	110.90
1	O	14	VAL	CG1-CB-CG2	-8.47	97.34	110.90
1	G	62	PHE	O-C-N	-8.44	109.20	122.70
1	Y	62	PHE	O-C-N	-8.43	109.21	122.70
1	B	62	PHE	O-C-N	-8.42	109.23	122.70
1	O	62	PHE	O-C-N	-8.42	109.23	122.70
1	O	14	VAL	O-C-N	8.28	135.94	122.70
1	B	14	VAL	O-C-N	8.27	135.93	122.70
1	G	14	VAL	O-C-N	8.25	135.89	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	14	VAL	O-C-N	8.24	135.89	122.70
1	B	27	VAL	CA-C-O	-8.24	102.80	120.10
1	Y	27	VAL	CA-C-O	-8.23	102.81	120.10
1	O	27	VAL	CA-C-O	-8.22	102.83	120.10
1	G	27	VAL	CA-C-O	-8.22	102.83	120.10
1	Y	9	LYS	N-CA-CB	8.22	125.40	110.60
1	G	9	LYS	N-CA-CB	8.22	125.39	110.60
1	O	9	LYS	N-CA-CB	8.22	125.39	110.60
1	B	9	LYS	N-CA-CB	8.21	125.38	110.60
1	G	140	SER	CA-CB-OG	-8.15	89.20	111.20
1	O	140	SER	CA-CB-OG	-8.14	89.22	111.20
1	B	1	ALA	CB-CA-C	8.14	122.31	110.10
1	O	97	ILE	CA-C-N	8.14	135.10	117.20
1	Y	97	ILE	CA-C-N	8.14	135.10	117.20
1	G	97	ILE	CA-C-N	8.14	135.10	117.20
1	B	140	SER	CA-CB-OG	-8.14	89.23	111.20
1	Y	140	SER	CA-CB-OG	-8.13	89.24	111.20
1	O	1	ALA	CB-CA-C	8.13	122.29	110.10
1	O	47	GLN	CA-C-O	-8.13	103.03	120.10
1	Y	47	GLN	CA-C-O	-8.13	103.03	120.10
1	B	97	ILE	CA-C-N	8.13	135.08	117.20
1	B	47	GLN	CA-C-O	-8.12	103.04	120.10
1	G	47	GLN	CA-C-O	-8.11	103.07	120.10
1	G	1	ALA	CB-CA-C	8.11	122.26	110.10
1	Y	1	ALA	CB-CA-C	8.11	122.26	110.10
1	Y	75	GLU	O-C-N	8.07	135.62	122.70
1	Y	115	MET	CA-CB-CG	8.06	127.01	113.30
1	B	75	GLU	O-C-N	8.05	135.58	122.70
1	O	75	GLU	O-C-N	8.04	135.57	122.70
1	O	115	MET	CA-CB-CG	8.04	126.97	113.30
1	G	115	MET	CA-CB-CG	8.04	126.96	113.30
1	B	115	MET	CA-CB-CG	8.04	126.97	113.30
1	G	37	THR	C-N-CA	8.02	141.75	121.70
1	G	75	GLU	O-C-N	8.01	135.52	122.70
1	O	37	THR	C-N-CA	8.01	141.72	121.70
1	Y	37	THR	C-N-CA	8.01	141.72	121.70
1	B	37	THR	C-N-CA	7.99	141.68	121.70
1	B	15	GLN	CA-CB-CG	7.90	130.79	113.40
1	Y	15	GLN	CA-CB-CG	7.90	130.78	113.40
1	B	96	ASP	O-C-N	-7.90	110.06	122.70
1	O	96	ASP	O-C-N	-7.90	110.06	122.70
1	Y	96	ASP	O-C-N	-7.89	110.08	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	15	GLN	CA-CB-CG	7.89	130.75	113.40
1	G	96	ASP	O-C-N	-7.88	110.09	122.70
1	O	15	GLN	CA-CB-CG	7.88	130.74	113.40
1	G	32	SER	CA-CB-OG	-7.87	89.95	111.20
1	O	32	SER	CA-CB-OG	-7.87	89.96	111.20
1	G	74	ASP	OD1-CG-OD2	-7.86	108.36	123.30
1	Y	74	ASP	OD1-CG-OD2	-7.86	108.37	123.30
1	B	32	SER	CA-CB-OG	-7.86	89.98	111.20
1	Y	32	SER	CA-CB-OG	-7.85	90.00	111.20
1	O	38	GLU	CA-CB-CG	7.85	130.67	113.40
1	O	74	ASP	OD1-CG-OD2	-7.84	108.41	123.30
1	Y	38	GLU	CA-CB-CG	7.84	130.64	113.40
1	B	38	GLU	CA-CB-CG	7.83	130.63	113.40
1	B	74	ASP	OD1-CG-OD2	-7.83	108.42	123.30
1	G	38	GLU	CA-CB-CG	7.83	130.63	113.40
1	O	104	LEU	CB-CA-C	7.78	124.97	110.20
1	Y	104	LEU	CB-CA-C	7.77	124.96	110.20
1	B	104	LEU	CB-CA-C	7.76	124.95	110.20
1	G	104	LEU	CB-CA-C	7.76	124.95	110.20
1	Y	45	VAL	CB-CA-C	7.73	126.08	111.40
1	O	45	VAL	CB-CA-C	7.72	126.08	111.40
1	G	45	VAL	CB-CA-C	7.72	126.07	111.40
1	B	45	VAL	CB-CA-C	7.72	126.07	111.40
1	G	149	ILE	O-C-N	-7.65	110.46	122.70
1	O	130	GLU	CB-CA-C	-7.64	95.12	110.40
1	G	130	GLU	CB-CA-C	-7.63	95.13	110.40
1	Y	130	GLU	CB-CA-C	-7.63	95.14	110.40
1	O	149	ILE	O-C-N	-7.62	110.50	122.70
1	B	21	GLU	OE1-CD-OE2	7.61	132.43	123.30
1	B	130	GLU	CB-CA-C	-7.61	95.19	110.40
1	Y	149	ILE	O-C-N	-7.60	110.53	122.70
1	B	149	ILE	O-C-N	-7.60	110.55	122.70
1	O	21	GLU	OE1-CD-OE2	7.58	132.39	123.30
1	G	21	GLU	OE1-CD-OE2	7.57	132.39	123.30
1	Y	21	GLU	OE1-CD-OE2	7.57	132.38	123.30
1	O	86	THR	CA-CB-CG2	7.44	122.82	112.40
1	Y	86	THR	CA-CB-CG2	7.43	122.81	112.40
1	G	86	THR	CA-CB-CG2	7.43	122.81	112.40
1	Y	63	ASN	N-CA-CB	-7.43	97.23	110.60
1	B	86	THR	CA-CB-CG2	7.43	122.80	112.40
1	O	63	ASN	N-CA-CB	-7.42	97.25	110.60
1	G	63	ASN	N-CA-CB	-7.41	97.27	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	ASN	N-CA-CB	-7.40	97.28	110.60
1	B	96	ASP	CB-CG-OD1	-7.33	111.70	118.30
1	G	96	ASP	CB-CG-OD1	-7.31	111.72	118.30
1	O	96	ASP	CB-CG-OD1	-7.29	111.74	118.30
1	G	24	GLY	C-N-CA	7.27	139.88	121.70
1	O	24	GLY	C-N-CA	7.26	139.85	121.70
1	B	24	GLY	C-N-CA	7.25	139.84	121.70
1	Y	24	GLY	C-N-CA	7.25	139.83	121.70
1	Y	96	ASP	CB-CG-OD1	-7.24	111.78	118.30
1	B	107	GLU	CG-CD-OE2	-7.24	103.83	118.30
1	G	94	ILE	CA-C-O	-7.23	104.92	120.10
1	O	107	GLU	CG-CD-OE2	-7.22	103.85	118.30
1	O	94	ILE	CA-C-O	-7.21	104.95	120.10
1	Y	94	ILE	CA-C-O	-7.21	104.96	120.10
1	Y	107	GLU	CG-CD-OE2	-7.21	103.88	118.30
1	G	107	GLU	CG-CD-OE2	-7.21	103.88	118.30
1	B	94	ILE	CA-C-O	-7.21	104.96	120.10
1	B	86	THR	CA-C-O	-7.20	104.97	120.10
1	B	130	GLU	CA-CB-CG	7.20	129.24	113.40
1	G	86	THR	CA-C-O	-7.19	105.00	120.10
1	O	86	THR	CA-C-O	-7.19	105.00	120.10
1	Y	86	THR	CA-C-O	-7.19	105.01	120.10
1	Y	130	GLU	CA-CB-CG	7.18	129.20	113.40
1	B	118	HIS	CG-ND1-CE1	7.17	118.25	108.20
1	O	130	GLU	CA-CB-CG	7.17	129.17	113.40
1	G	130	GLU	CA-CB-CG	7.17	129.17	113.40
1	O	118	HIS	CG-ND1-CE1	7.16	118.23	108.20
1	Y	118	HIS	CG-ND1-CE1	7.16	118.22	108.20
1	B	150	ALA	O-C-N	7.15	134.14	122.70
1	Y	56	THR	CA-CB-CG2	7.15	122.41	112.40
1	G	56	THR	CA-CB-CG2	7.15	122.41	112.40
1	O	56	THR	CA-CB-CG2	7.14	122.40	112.40
1	B	56	THR	CA-CB-CG2	7.14	122.40	112.40
1	B	93	ALA	N-CA-CB	7.14	120.09	110.10
1	G	41	HIS	CA-C-O	-7.14	105.11	120.10
1	G	93	ALA	N-CA-CB	7.14	120.09	110.10
1	G	118	HIS	CG-ND1-CE1	7.13	118.19	108.20
1	Y	41	HIS	CA-C-O	-7.13	105.12	120.10
1	O	93	ALA	N-CA-CB	7.12	120.07	110.10
1	Y	150	ALA	O-C-N	7.12	134.10	122.70
1	G	150	ALA	O-C-N	7.12	134.10	122.70
1	Y	93	ALA	N-CA-CB	7.12	120.06	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	37	THR	N-CA-CB	-7.11	96.79	110.30
1	O	41	HIS	CA-C-O	-7.11	105.17	120.10
1	G	94	ILE	O-C-N	7.11	134.08	122.70
1	B	94	ILE	O-C-N	7.11	134.07	122.70
1	O	150	ALA	O-C-N	7.11	134.07	122.70
1	B	41	HIS	CA-C-O	-7.11	105.18	120.10
1	O	37	THR	N-CA-CB	-7.09	96.82	110.30
1	O	94	ILE	O-C-N	7.09	134.04	122.70
1	B	37	THR	N-CA-CB	-7.08	96.85	110.30
1	G	37	THR	N-CA-CB	-7.07	96.86	110.30
1	Y	94	ILE	O-C-N	7.07	134.01	122.70
1	O	73	LYS	N-CA-CB	7.03	123.26	110.60
1	G	62	PHE	CB-CG-CD2	7.03	125.72	120.80
1	G	73	LYS	N-CA-CB	7.02	123.24	110.60
1	B	73	LYS	N-CA-CB	7.02	123.24	110.60
1	Y	73	LYS	N-CA-CB	7.01	123.23	110.60
1	B	62	PHE	CB-CG-CD2	6.99	125.70	120.80
1	O	62	PHE	CB-CG-CD2	6.99	125.69	120.80
1	G	76	GLU	CG-CD-OE2	6.98	132.26	118.30
1	Y	62	PHE	CB-CG-CD2	6.98	125.68	120.80
1	Y	76	GLU	CG-CD-OE2	6.97	132.25	118.30
1	G	137	ASN	OD1-CG-ND2	6.97	137.93	121.90
1	O	76	GLU	CG-CD-OE2	6.96	132.23	118.30
1	B	76	GLU	CG-CD-OE2	6.96	132.22	118.30
1	O	137	ASN	OD1-CG-ND2	6.96	137.90	121.90
1	B	137	ASN	OD1-CG-ND2	6.96	137.90	121.90
1	Y	106	GLY	CA-C-O	6.95	133.11	120.60
1	Y	137	ASN	OD1-CG-ND2	6.94	137.87	121.90
1	O	106	GLY	CA-C-O	6.93	133.07	120.60
1	B	106	GLY	CA-C-O	6.93	133.07	120.60
1	G	106	GLY	CA-C-O	6.92	133.06	120.60
1	O	110	ILE	CA-CB-CG2	6.92	124.74	110.90
1	B	110	ILE	CA-CB-CG2	6.92	124.73	110.90
1	B	13	PRO	CB-CA-C	-6.91	94.72	112.00
1	G	110	ILE	CA-CB-CG2	6.91	124.72	110.90
1	G	13	PRO	CB-CA-C	-6.91	94.73	112.00
1	Y	110	ILE	CA-CB-CG2	6.91	124.71	110.90
1	O	13	PRO	CB-CA-C	-6.90	94.74	112.00
1	Y	13	PRO	CB-CA-C	-6.89	94.77	112.00
1	B	126	ARG	CD-NE-CZ	-6.87	113.98	123.60
1	O	126	ARG	CD-NE-CZ	-6.86	114.00	123.60
1	Y	126	ARG	CD-NE-CZ	-6.85	114.01	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	23	LYS	CA-C-N	-6.85	102.51	116.20
1	G	45	VAL	CA-CB-CG2	6.84	121.17	110.90
1	Y	23	LYS	CA-C-N	-6.84	102.52	116.20
1	B	98	VAL	CA-C-O	-6.84	105.74	120.10
1	O	23	LYS	CA-C-N	-6.84	102.53	116.20
1	Y	98	VAL	CA-C-O	-6.83	105.75	120.10
1	O	45	VAL	CA-CB-CG2	6.83	121.15	110.90
1	Y	36	LEU	CA-C-O	6.83	134.44	120.10
1	G	98	VAL	CA-C-O	-6.83	105.76	120.10
1	B	23	LYS	CA-C-N	-6.83	102.54	116.20
1	G	126	ARG	CD-NE-CZ	-6.83	114.04	123.60
1	B	36	LEU	CA-C-O	6.83	134.44	120.10
1	O	98	VAL	CA-C-O	-6.82	105.78	120.10
1	O	50	ASP	OD1-CG-OD2	-6.82	110.35	123.30
1	G	6	ALA	O-C-N	-6.82	111.79	122.70
1	B	45	VAL	CA-CB-CG2	6.82	121.13	110.90
1	O	36	LEU	CA-C-O	6.81	134.41	120.10
1	Y	6	ALA	O-C-N	-6.81	111.80	122.70
1	Y	45	VAL	CA-CB-CG2	6.81	121.12	110.90
1	G	36	LEU	CA-C-O	6.81	134.41	120.10
1	Y	50	ASP	OD1-CG-OD2	-6.81	110.36	123.30
1	B	50	ASP	OD1-CG-OD2	-6.80	110.37	123.30
1	O	6	ALA	O-C-N	-6.79	111.84	122.70
1	G	50	ASP	OD1-CG-OD2	-6.79	110.40	123.30
1	O	92	VAL	O-C-N	6.78	133.55	122.70
1	B	92	VAL	O-C-N	6.78	133.55	122.70
1	B	6	ALA	O-C-N	-6.77	111.87	122.70
1	Y	92	VAL	O-C-N	6.77	133.53	122.70
1	G	92	VAL	O-C-N	6.76	133.52	122.70
1	B	8	LEU	CB-CG-CD2	-6.75	99.52	111.00
1	G	126	ARG	CB-CG-CD	6.73	129.09	111.60
1	Y	126	ARG	CB-CG-CD	6.72	129.08	111.60
1	O	126	ARG	CB-CG-CD	6.72	129.07	111.60
1	B	126	ARG	CB-CG-CD	6.72	129.07	111.60
1	G	151	LYS	CG-CD-CE	6.71	132.04	111.90
1	O	8	LEU	CB-CG-CD2	-6.71	99.59	111.00
1	Y	22	ALA	C-N-CA	6.71	138.47	121.70
1	Y	8	LEU	CB-CG-CD2	-6.71	99.60	111.00
1	O	22	ALA	C-N-CA	6.71	138.46	121.70
1	O	151	LYS	CG-CD-CE	6.71	132.02	111.90
1	B	22	ALA	C-N-CA	6.70	138.45	121.70
1	G	22	ALA	C-N-CA	6.70	138.44	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	151	LYS	CG-CD-CE	6.69	131.98	111.90
1	B	151	LYS	CG-CD-CE	6.69	131.97	111.90
1	G	8	LEU	CB-CG-CD2	-6.68	99.64	111.00
1	B	36	LEU	CA-C-N	-6.68	102.51	117.20
1	O	36	LEU	CA-C-N	-6.67	102.52	117.20
1	Y	36	LEU	CA-C-N	-6.67	102.53	117.20
1	G	36	LEU	CA-C-N	-6.66	102.55	117.20
1	G	87	ALA	N-CA-CB	6.65	119.41	110.10
1	B	87	ALA	N-CA-CB	6.65	119.40	110.10
1	B	73	LYS	CA-C-O	-6.63	106.18	120.10
1	O	73	LYS	CA-C-O	-6.63	106.18	120.10
1	Y	73	LYS	CA-C-O	-6.62	106.19	120.10
1	G	73	LYS	CA-C-O	-6.62	106.19	120.10
1	O	87	ALA	N-CA-CB	6.61	119.36	110.10
1	B	44	HIS	CB-CA-C	-6.61	97.19	110.40
1	G	6	ALA	CB-CA-C	6.60	120.01	110.10
1	B	6	ALA	CB-CA-C	6.60	120.00	110.10
1	O	44	HIS	CB-CA-C	-6.59	97.21	110.40
1	Y	44	HIS	CB-CA-C	-6.59	97.21	110.40
1	Y	6	ALA	CB-CA-C	6.59	119.99	110.10
1	Y	87	ALA	N-CA-CB	6.59	119.33	110.10
1	B	13	PRO	O-C-N	-6.59	112.16	122.70
1	O	6	ALA	CB-CA-C	6.59	119.98	110.10
1	G	44	HIS	CB-CA-C	-6.58	97.23	110.40
1	O	13	PRO	O-C-N	-6.57	112.19	122.70
1	G	13	PRO	O-C-N	-6.55	112.21	122.70
1	Y	13	PRO	O-C-N	-6.55	112.22	122.70
1	Y	40	ASP	O-C-N	6.54	133.16	122.70
1	Y	23	LYS	N-CA-CB	6.53	122.36	110.60
1	O	23	LYS	N-CA-CB	6.52	122.34	110.60
1	B	23	LYS	N-CA-CB	6.52	122.33	110.60
1	G	70	GLY	C-N-CA	6.51	135.97	122.30
1	B	40	ASP	O-C-N	6.51	133.11	122.70
1	Y	126	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	O	70	GLY	C-N-CA	6.50	135.96	122.30
1	G	23	LYS	N-CA-CB	6.49	122.29	110.60
1	O	40	ASP	O-C-N	6.49	133.08	122.70
1	B	70	GLY	C-N-CA	6.49	135.92	122.30
1	Y	70	GLY	C-N-CA	6.48	135.91	122.30
1	B	126	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	G	40	ASP	O-C-N	6.46	133.04	122.70
1	O	126	ARG	NE-CZ-NH2	-6.46	117.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	39	GLY	O-C-N	6.45	133.02	122.70
1	B	77	ARG	NH1-CZ-NH2	-6.45	112.31	119.40
1	O	39	GLY	O-C-N	6.44	133.00	122.70
1	G	39	GLY	O-C-N	6.43	133.00	122.70
1	Y	77	ARG	NH1-CZ-NH2	-6.43	112.33	119.40
1	B	39	GLY	O-C-N	6.43	132.99	122.70
1	O	77	ARG	NH1-CZ-NH2	-6.43	112.33	119.40
1	B	38	GLU	CG-CD-OE1	6.42	131.14	118.30
1	G	126	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	G	77	ARG	NH1-CZ-NH2	-6.41	112.35	119.40
1	Y	38	GLU	CG-CD-OE1	6.40	131.10	118.30
1	G	38	GLU	CG-CD-OE1	6.40	131.10	118.30
1	O	38	GLU	CG-CD-OE1	6.40	131.09	118.30
1	B	99	ASP	OD1-CG-OD2	-6.37	111.19	123.30
1	O	99	ASP	OD1-CG-OD2	-6.37	111.20	123.30
1	Y	99	ASP	OD1-CG-OD2	-6.35	111.23	123.30
1	G	79	VAL	C-N-CA	-6.35	108.97	122.30
1	B	40	ASP	CB-CG-OD2	6.34	124.01	118.30
1	G	99	ASP	OD1-CG-OD2	-6.34	111.25	123.30
1	O	79	VAL	C-N-CA	-6.33	109.01	122.30
1	B	79	VAL	C-N-CA	-6.32	109.02	122.30
1	Y	79	VAL	C-N-CA	-6.32	109.03	122.30
1	G	40	ASP	CB-CG-OD2	6.30	123.97	118.30
1	O	40	ASP	CB-CG-OD2	6.29	123.96	118.30
1	Y	40	ASP	CB-CG-OD2	6.29	123.96	118.30
1	Y	110	ILE	O-C-N	-6.28	112.65	122.70
1	Y	94	ILE	N-CA-CB	6.28	125.24	110.80
1	G	110	ILE	O-C-N	-6.28	112.66	122.70
1	G	94	ILE	N-CA-CB	6.27	125.23	110.80
1	O	110	ILE	O-C-N	-6.27	112.67	122.70
1	O	94	ILE	N-CA-CB	6.26	125.21	110.80
1	B	94	ILE	N-CA-CB	6.25	125.17	110.80
1	B	137	ASN	CB-CG-OD1	-6.25	109.11	121.60
1	B	110	ILE	O-C-N	-6.24	112.72	122.70
1	G	137	ASN	CB-CG-OD1	-6.23	109.13	121.60
1	Y	137	ASN	CB-CG-OD1	-6.23	109.14	121.60
1	O	137	ASN	CB-CG-OD1	-6.22	109.15	121.60
1	B	10	GLY	O-C-N	6.18	132.59	122.70
1	Y	32	SER	C-N-CA	6.17	137.14	121.70
1	O	10	GLY	O-C-N	6.17	132.58	122.70
1	G	96	ASP	CA-C-N	6.17	130.78	117.20
1	O	52	THR	C-N-CA	6.17	137.12	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	98	VAL	N-CA-C	-6.17	94.35	111.00
1	B	98	VAL	N-CA-C	-6.17	94.35	111.00
1	O	96	ASP	CA-C-N	6.16	130.76	117.20
1	Y	98	VAL	N-CA-C	-6.16	94.36	111.00
1	B	96	ASP	CA-C-N	6.16	130.76	117.20
1	B	52	THR	C-N-CA	6.16	137.10	121.70
1	Y	10	GLY	O-C-N	6.16	132.56	122.70
1	Y	52	THR	C-N-CA	6.16	137.09	121.70
1	O	32	SER	C-N-CA	6.15	137.08	121.70
1	G	52	THR	C-N-CA	6.15	137.07	121.70
1	Y	96	ASP	CA-C-N	6.15	130.72	117.20
1	G	10	GLY	O-C-N	6.15	132.54	122.70
1	G	98	VAL	N-CA-C	-6.14	94.41	111.00
1	B	32	SER	C-N-CA	6.14	137.06	121.70
1	G	32	SER	C-N-CA	6.14	137.05	121.70
1	Y	139	GLY	C-N-CA	6.09	136.94	121.70
1	B	5	VAL	O-C-N	6.09	132.44	122.70
1	O	5	VAL	O-C-N	6.09	132.44	122.70
1	B	139	GLY	C-N-CA	6.08	136.90	121.70
1	O	139	GLY	C-N-CA	6.08	136.89	121.70
1	Y	5	VAL	O-C-N	6.08	132.42	122.70
1	Y	90	ASN	CB-CG-ND2	6.08	131.28	116.70
1	B	75	GLU	CB-CA-C	-6.07	98.25	110.40
1	O	90	ASN	CB-CG-ND2	6.07	131.27	116.70
1	B	90	ASN	CB-CG-ND2	6.07	131.27	116.70
1	G	5	VAL	O-C-N	6.07	132.41	122.70
1	G	75	GLU	CB-CA-C	-6.07	98.26	110.40
1	O	75	GLU	CB-CA-C	-6.07	98.27	110.40
1	Y	75	GLU	CB-CA-C	-6.07	98.27	110.40
1	G	139	GLY	C-N-CA	6.06	136.85	121.70
1	G	3	LYS	C-N-CA	6.06	136.85	121.70
1	G	90	ASN	CB-CG-ND2	6.06	131.24	116.70
1	Y	3	LYS	C-N-CA	6.05	136.84	121.70
1	B	3	LYS	C-N-CA	6.05	136.83	121.70
1	O	3	LYS	C-N-CA	6.05	136.82	121.70
1	Y	3	LYS	CG-CD-CE	6.04	130.01	111.90
1	B	122	ASP	OD1-CG-OD2	-6.04	111.83	123.30
1	O	66	SER	C-N-CA	6.03	136.76	121.70
1	O	122	ASP	OD1-CG-OD2	-6.03	111.85	123.30
1	Y	66	SER	C-N-CA	6.03	136.76	121.70
1	Y	122	ASP	OD1-CG-OD2	-6.03	111.85	123.30
1	O	3	LYS	CG-CD-CE	6.02	129.97	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	3	LYS	CG-CD-CE	6.02	129.97	111.90
1	B	66	SER	C-N-CA	6.02	136.75	121.70
1	B	84	ASN	C-N-CA	6.02	136.76	121.70
1	Y	81	ASP	OD1-CG-OD2	-6.02	111.86	123.30
1	B	3	LYS	CB-CA-C	6.02	122.44	110.40
1	G	66	SER	C-N-CA	6.02	136.74	121.70
1	Y	3	LYS	CB-CA-C	6.01	122.43	110.40
1	G	3	LYS	CB-CA-C	6.01	122.43	110.40
1	G	81	ASP	OD1-CG-OD2	-6.01	111.87	123.30
1	O	3	LYS	CB-CA-C	6.01	122.42	110.40
1	O	84	ASN	C-N-CA	6.01	136.73	121.70
1	O	81	ASP	OD1-CG-OD2	-6.01	111.88	123.30
1	Y	84	ASN	C-N-CA	6.01	136.72	121.70
1	G	84	ASN	C-N-CA	6.01	136.72	121.70
1	G	122	ASP	OD1-CG-OD2	-6.01	111.88	123.30
1	B	3	LYS	CG-CD-CE	6.00	129.92	111.90
1	Y	141	ARG	NH1-CZ-NH2	-6.00	112.80	119.40
1	G	57	SER	CA-C-N	6.00	130.40	117.20
1	G	132	SER	CB-CA-C	6.00	121.49	110.10
1	B	81	ASP	OD1-CG-OD2	-5.99	111.92	123.30
1	B	141	ARG	NH1-CZ-NH2	-5.99	112.82	119.40
1	O	132	SER	CB-CA-C	5.98	121.47	110.10
1	Y	132	SER	CB-CA-C	5.98	121.46	110.10
1	O	141	ARG	NH1-CZ-NH2	-5.97	112.83	119.40
1	G	105	SER	CB-CA-C	-5.97	98.75	110.10
1	O	57	SER	CA-C-N	5.97	130.34	117.20
1	B	132	SER	CB-CA-C	5.97	121.44	110.10
1	Y	57	SER	CA-C-N	5.97	130.33	117.20
1	B	57	SER	CA-C-N	5.97	130.33	117.20
1	O	105	SER	CB-CA-C	-5.97	98.77	110.10
1	Y	105	SER	CB-CA-C	-5.97	98.76	110.10
1	G	141	ARG	NH1-CZ-NH2	-5.96	112.85	119.40
1	G	130	GLU	N-CA-CB	5.95	121.32	110.60
1	B	105	SER	CB-CA-C	-5.95	98.80	110.10
1	O	130	GLU	N-CA-CB	5.94	121.29	110.60
1	B	130	GLU	N-CA-CB	5.93	121.28	110.60
1	Y	130	GLU	N-CA-CB	5.92	121.26	110.60
1	Y	96	ASP	CA-CB-CG	-5.89	100.44	113.40
1	O	51	ASN	CB-CA-C	5.89	122.17	110.40
1	G	51	ASN	CB-CA-C	5.88	122.17	110.40
1	G	96	ASP	CA-CB-CG	-5.88	100.46	113.40
1	O	96	ASP	CA-CB-CG	-5.88	100.47	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	51	ASN	CB-CA-C	5.87	122.14	110.40
1	B	51	ASN	CB-CA-C	5.87	122.14	110.40
1	B	96	ASP	CA-CB-CG	-5.87	100.50	113.40
1	O	47	GLN	N-CA-CB	-5.86	100.05	110.60
1	Y	47	GLN	N-CA-CB	-5.85	100.07	110.60
1	G	47	GLN	N-CA-CB	-5.84	100.08	110.60
1	B	8	LEU	CB-CG-CD1	5.84	120.93	111.00
1	B	47	GLN	N-CA-CB	-5.84	100.09	110.60
1	G	8	LEU	CB-CG-CD1	5.83	120.92	111.00
1	O	8	LEU	CB-CG-CD1	5.83	120.92	111.00
1	Y	8	LEU	CB-CG-CD1	5.83	120.91	111.00
1	B	45	VAL	N-CA-C	-5.82	95.30	111.00
1	G	45	VAL	N-CA-C	-5.81	95.31	111.00
1	O	45	VAL	N-CA-C	-5.81	95.32	111.00
1	Y	45	VAL	N-CA-C	-5.81	95.32	111.00
1	G	86	THR	C-N-CA	5.79	136.18	121.70
1	G	97	ILE	CA-C-O	-5.79	107.94	120.10
1	B	86	THR	C-N-CA	5.79	136.17	121.70
1	Y	97	ILE	CA-C-O	-5.79	107.95	120.10
1	O	76	GLU	CB-CG-CD	-5.78	98.60	114.20
1	Y	76	GLU	CB-CG-CD	-5.78	98.60	114.20
1	G	118	HIS	CA-C-O	5.77	132.22	120.10
1	O	97	ILE	CA-C-O	-5.77	107.98	120.10
1	G	76	GLU	CB-CG-CD	-5.77	98.62	114.20
1	B	76	GLU	CB-CG-CD	-5.77	98.61	114.20
1	O	86	THR	C-N-CA	5.77	136.13	121.70
1	O	118	HIS	CA-C-O	5.77	132.21	120.10
1	Y	142	LEU	N-CA-CB	-5.77	98.86	110.40
1	B	97	ILE	CA-C-O	-5.76	108.00	120.10
1	B	118	HIS	CA-C-O	5.76	132.20	120.10
1	Y	118	HIS	CA-C-O	5.76	132.19	120.10
1	Y	86	THR	C-N-CA	5.76	136.09	121.70
1	B	70	GLY	O-C-N	-5.75	113.42	123.20
1	O	70	GLY	O-C-N	-5.75	113.43	123.20
1	O	142	LEU	N-CA-CB	-5.75	98.90	110.40
1	Y	70	GLY	O-C-N	-5.75	113.43	123.20
1	G	142	LEU	N-CA-CB	-5.75	98.91	110.40
1	G	70	GLY	O-C-N	-5.74	113.44	123.20
1	B	142	LEU	N-CA-CB	-5.74	98.93	110.40
1	O	147	ILE	CA-CB-CG2	5.71	122.32	110.90
1	B	147	ILE	CA-CB-CG2	5.71	122.32	110.90
1	Y	147	ILE	CA-CB-CG2	5.71	122.31	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	86	THR	OG1-CB-CG2	-5.70	96.88	110.00
1	G	147	ILE	CA-CB-CG2	5.70	122.31	110.90
1	Y	86	THR	OG1-CB-CG2	-5.70	96.89	110.00
1	B	117	VAL	CB-CA-C	5.69	122.22	111.40
1	O	117	VAL	CB-CA-C	5.69	122.21	111.40
1	B	57	SER	N-CA-CB	-5.69	101.96	110.50
1	O	86	THR	OG1-CB-CG2	-5.69	96.92	110.00
1	B	86	THR	OG1-CB-CG2	-5.68	96.92	110.00
1	G	57	SER	N-CA-CB	-5.68	101.98	110.50
1	Y	117	VAL	CB-CA-C	5.68	122.18	111.40
1	O	57	SER	N-CA-CB	-5.67	101.99	110.50
1	B	51	ASN	C-N-CA	5.67	135.88	121.70
1	Y	57	SER	N-CA-CB	-5.67	102.00	110.50
1	G	117	VAL	CB-CA-C	5.67	122.17	111.40
1	O	51	ASN	C-N-CA	5.67	135.87	121.70
1	G	51	ASN	C-N-CA	5.67	135.87	121.70
1	G	141	ARG	CA-CB-CG	5.67	125.87	113.40
1	Y	142	LEU	O-C-N	5.66	131.76	122.70
1	Y	51	ASN	C-N-CA	5.65	135.82	121.70
1	O	141	ARG	CA-CB-CG	5.65	125.82	113.40
1	B	141	ARG	CA-CB-CG	5.64	125.82	113.40
1	G	19	HIS	CA-CB-CG	-5.64	104.01	113.60
1	B	16	GLY	O-C-N	5.64	131.73	122.70
1	O	16	GLY	O-C-N	5.64	131.72	122.70
1	O	142	LEU	O-C-N	5.64	131.72	122.70
1	Y	141	ARG	CA-CB-CG	5.64	125.81	113.40
1	Y	16	GLY	O-C-N	5.64	131.72	122.70
1	G	16	GLY	O-C-N	5.63	131.72	122.70
1	B	142	LEU	O-C-N	5.63	131.72	122.70
1	O	19	HIS	CA-CB-CG	-5.63	104.03	113.60
1	B	19	HIS	CA-CB-CG	-5.63	104.03	113.60
1	Y	19	HIS	CA-CB-CG	-5.62	104.04	113.60
1	O	109	SER	N-CA-CB	-5.62	102.07	110.50
1	G	142	LEU	O-C-N	5.62	131.69	122.70
1	G	53	GLN	CA-CB-CG	-5.61	101.05	113.40
1	G	109	SER	N-CA-CB	-5.61	102.08	110.50
1	Y	109	SER	N-CA-CB	-5.61	102.09	110.50
1	B	109	SER	N-CA-CB	-5.60	102.10	110.50
1	O	53	GLN	CA-CB-CG	-5.60	101.08	113.40
1	B	53	GLN	CA-CB-CG	-5.59	101.09	113.40
1	Y	53	GLN	CA-CB-CG	-5.59	101.10	113.40
1	Y	84	ASN	OD1-CG-ND2	-5.58	109.07	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	96	ASP	N-CA-CB	-5.57	100.57	110.60
1	O	84	ASN	OD1-CG-ND2	-5.56	109.12	121.90
1	B	36	LEU	CB-CA-C	5.55	120.74	110.20
1	O	96	ASP	N-CA-CB	-5.54	100.62	110.60
1	G	84	ASN	OD1-CG-ND2	-5.54	109.15	121.90
1	Y	36	LEU	CB-CA-C	5.53	120.71	110.20
1	B	84	ASN	OD1-CG-ND2	-5.53	109.18	121.90
1	B	96	ASP	N-CA-CB	-5.53	100.64	110.60
1	O	36	LEU	CB-CA-C	5.53	120.70	110.20
1	G	96	ASP	N-CA-CB	-5.53	100.65	110.60
1	G	36	LEU	CB-CA-C	5.53	120.70	110.20
1	B	109	SER	O-C-N	-5.52	113.87	122.70
1	G	109	SER	O-C-N	-5.52	113.87	122.70
1	B	48	PHE	C-N-CA	-5.52	110.72	122.30
1	G	48	PHE	C-N-CA	-5.51	110.73	122.30
1	Y	109	SER	O-C-N	-5.51	113.89	122.70
1	Y	113	ARG	CD-NE-CZ	5.51	131.31	123.60
1	G	62	PHE	CA-C-N	5.51	129.31	117.20
1	O	48	PHE	C-N-CA	-5.50	110.74	122.30
1	O	113	ARG	CD-NE-CZ	5.50	131.30	123.60
1	O	109	SER	O-C-N	-5.50	113.90	122.70
1	Y	48	PHE	C-N-CA	-5.50	110.76	122.30
1	Y	37	THR	O-C-N	-5.49	113.92	122.70
1	G	113	ARG	CD-NE-CZ	5.48	131.28	123.60
1	B	62	PHE	CA-C-N	5.48	129.26	117.20
1	B	104	LEU	CA-CB-CG	5.48	127.91	115.30
1	O	113	ARG	CB-CG-CD	-5.48	97.36	111.60
1	O	62	PHE	CA-C-N	5.48	129.25	117.20
1	Y	113	ARG	CB-CG-CD	-5.48	97.36	111.60
1	B	113	ARG	CD-NE-CZ	5.48	131.27	123.60
1	O	37	THR	O-C-N	-5.47	113.94	122.70
1	Y	62	PHE	CA-C-N	5.47	129.25	117.20
1	O	104	LEU	CA-CB-CG	5.47	127.89	115.30
1	B	113	ARG	CB-CG-CD	-5.47	97.37	111.60
1	Y	104	LEU	CA-CB-CG	5.47	127.88	115.30
1	G	113	ARG	CB-CG-CD	-5.47	97.39	111.60
1	B	37	THR	O-C-N	-5.47	113.95	122.70
1	G	104	LEU	CA-CB-CG	5.46	127.86	115.30
1	Y	120	LYS	CA-C-O	5.45	131.55	120.10
1	G	37	THR	O-C-N	-5.45	113.98	122.70
1	G	120	LYS	CA-C-O	5.45	131.54	120.10
1	Y	61	HIS	N-CA-CB	5.44	120.40	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	120	LYS	CA-C-O	5.44	131.53	120.10
1	B	120	LYS	CA-C-O	5.43	131.50	120.10
1	B	133	THR	CA-CB-CG2	-5.42	104.81	112.40
1	O	61	HIS	N-CA-CB	5.41	120.34	110.60
1	B	61	HIS	N-CA-CB	5.41	120.34	110.60
1	G	61	HIS	N-CA-CB	5.41	120.34	110.60
1	O	133	THR	CA-CB-CG2	-5.40	104.83	112.40
1	G	133	THR	CA-CB-CG2	-5.40	104.84	112.40
1	Y	133	THR	CA-CB-CG2	-5.39	104.86	112.40
1	B	5	VAL	CA-C-O	-5.38	108.79	120.10
1	G	89	LYS	O-C-N	5.38	131.31	122.70
1	O	5	VAL	CA-C-O	-5.37	108.81	120.10
1	Y	5	VAL	CA-C-O	-5.37	108.83	120.10
1	B	89	LYS	O-C-N	5.37	131.29	122.70
1	O	89	LYS	O-C-N	5.36	131.28	122.70
1	B	78	HIS	CA-C-O	-5.36	108.84	120.10
1	O	78	HIS	CA-C-O	-5.36	108.84	120.10
1	G	5	VAL	CA-C-O	-5.36	108.84	120.10
1	G	78	HIS	CA-C-O	-5.36	108.85	120.10
1	Y	78	HIS	CA-C-O	-5.35	108.86	120.10
1	B	21	GLU	C-N-CA	5.34	135.06	121.70
1	Y	89	LYS	O-C-N	5.33	131.24	122.70
1	O	48	PHE	CB-CG-CD2	5.33	124.53	120.80
1	Y	21	GLU	C-N-CA	5.33	135.03	121.70
1	O	21	GLU	C-N-CA	5.33	135.02	121.70
1	G	99	ASP	CB-CG-OD1	-5.33	113.50	118.30
1	B	48	PHE	CB-CG-CD2	5.33	124.53	120.80
1	G	21	GLU	C-N-CA	5.32	135.00	121.70
1	Y	99	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	O	108	TYR	CD1-CE1-CZ	-5.30	115.03	119.80
1	Y	143	ALA	CA-C-N	5.29	128.83	117.20
1	B	99	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	B	108	TYR	CD1-CE1-CZ	-5.28	115.04	119.80
1	O	143	ALA	CA-C-N	5.28	128.82	117.20
1	G	48	PHE	CB-CG-CD2	5.28	124.50	120.80
1	Y	108	TYR	CD1-CE1-CZ	-5.28	115.05	119.80
1	O	99	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	G	108	TYR	CD1-CE1-CZ	-5.27	115.06	119.80
1	Y	103	SER	O-C-N	-5.27	114.27	122.70
1	G	143	ALA	CA-C-N	5.27	128.79	117.20
1	B	143	ALA	CA-C-N	5.26	128.78	117.20
1	Y	48	PHE	CB-CG-CD2	5.25	124.48	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	103	SER	O-C-N	-5.24	114.32	122.70
1	G	103	SER	O-C-N	-5.24	114.32	122.70
1	G	8	LEU	CA-CB-CG	5.23	127.33	115.30
1	Y	22	ALA	CA-C-N	5.22	128.69	117.20
1	O	8	LEU	CA-CB-CG	5.22	127.30	115.30
1	B	76	GLU	OE1-CD-OE2	5.22	129.56	123.30
1	G	51	ASN	OD1-CG-ND2	-5.22	109.90	121.90
1	G	149	ILE	CA-CB-CG2	5.21	121.33	110.90
1	Y	8	LEU	CA-CB-CG	5.21	127.29	115.30
1	B	103	SER	O-C-N	-5.21	114.36	122.70
1	B	149	ILE	CA-CB-CG2	5.21	121.32	110.90
1	O	22	ALA	CA-C-N	5.20	128.64	117.20
1	O	149	ILE	CA-CB-CG2	5.20	121.30	110.90
1	B	8	LEU	CA-CB-CG	5.20	127.26	115.30
1	Y	51	ASN	OD1-CG-ND2	-5.20	109.95	121.90
1	Y	150	ALA	CB-CA-C	-5.20	102.31	110.10
1	Y	149	ILE	CA-CB-CG2	5.19	121.28	110.90
1	G	22	ALA	CA-C-N	5.19	128.62	117.20
1	O	51	ASN	OD1-CG-ND2	-5.19	109.97	121.90
1	G	100	PRO	N-CA-CB	-5.19	96.89	102.60
1	O	76	GLU	OE1-CD-OE2	5.18	129.52	123.30
1	B	22	ALA	CA-C-N	5.18	128.60	117.20
1	O	150	ALA	CB-CA-C	-5.18	102.33	110.10
1	G	150	ALA	CB-CA-C	-5.18	102.33	110.10
1	B	51	ASN	OD1-CG-ND2	-5.18	109.98	121.90
1	B	9	LYS	CB-CA-C	-5.18	100.04	110.40
1	B	150	ALA	CB-CA-C	-5.18	102.33	110.10
1	B	100	PRO	N-CA-CB	-5.17	96.91	102.60
1	G	76	GLU	OE1-CD-OE2	5.17	129.50	123.30
1	Y	125	GLY	CA-C-O	-5.17	111.30	120.60
1	G	47	GLN	N-CA-C	5.16	124.94	111.00
1	O	125	GLY	CA-C-O	-5.16	111.31	120.60
1	B	47	GLN	N-CA-C	5.16	124.94	111.00
1	B	125	GLY	CA-C-O	-5.16	111.31	120.60
1	O	47	GLN	N-CA-C	5.16	124.93	111.00
1	Y	100	PRO	N-CA-CB	-5.16	96.93	102.60
1	Y	9	LYS	CB-CA-C	-5.15	100.09	110.40
1	G	125	GLY	CA-C-O	-5.15	111.33	120.60
1	B	117	VAL	CA-CB-CG1	5.15	118.63	110.90
1	B	131	GLU	CB-CG-CD	-5.15	100.29	114.20
1	O	9	LYS	CB-CA-C	-5.15	100.10	110.40
1	O	100	PRO	N-CA-CB	-5.15	96.94	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	76	GLU	OE1-CD-OE2	5.15	129.48	123.30
1	Y	117	VAL	CA-CB-CG1	5.15	118.62	110.90
1	G	28	VAL	CA-CB-CG1	5.14	118.62	110.90
1	Y	131	GLU	CB-CG-CD	-5.14	100.32	114.20
1	G	117	VAL	CA-CB-CG1	5.14	118.61	110.90
1	Y	47	GLN	N-CA-C	5.14	124.88	111.00
1	G	9	LYS	CB-CA-C	-5.14	100.12	110.40
1	O	28	VAL	CA-CB-CG1	5.14	118.60	110.90
1	O	131	GLU	CB-CG-CD	-5.13	100.33	114.20
1	G	57	SER	CA-CB-OG	-5.13	97.34	111.20
1	B	57	SER	CA-CB-OG	-5.13	97.35	111.20
1	O	57	SER	CA-CB-OG	-5.13	97.35	111.20
1	O	117	VAL	CA-CB-CG1	5.13	118.59	110.90
1	G	131	GLU	CB-CG-CD	-5.12	100.37	114.20
1	Y	57	SER	CA-CB-OG	-5.12	97.38	111.20
1	Y	28	VAL	CA-CB-CG1	5.11	118.57	110.90
1	G	58	ALA	CB-CA-C	-5.11	102.44	110.10
1	O	58	ALA	CB-CA-C	-5.11	102.44	110.10
1	B	28	VAL	CA-CB-CG1	5.11	118.56	110.90
1	G	144	CYS	CA-CB-SG	-5.10	104.82	114.00
1	B	58	ALA	CB-CA-C	-5.10	102.45	110.10
1	Y	58	ALA	CB-CA-C	-5.09	102.46	110.10
1	O	144	CYS	CA-CB-SG	-5.09	104.84	114.00
1	G	103	SER	CA-C-N	5.09	128.39	117.20
1	Y	103	SER	CA-C-N	5.08	128.38	117.20
1	B	144	CYS	CA-CB-SG	-5.08	104.86	114.00
1	O	103	SER	CA-C-N	5.07	128.36	117.20
1	Y	144	CYS	CA-CB-SG	-5.07	104.87	114.00
1	B	103	SER	CA-C-N	5.07	128.36	117.20
1	G	52	THR	N-CA-CB	5.07	119.93	110.30
1	G	56	THR	N-CA-CB	5.07	119.93	110.30
1	B	52	THR	N-CA-CB	5.07	119.93	110.30
1	G	57	SER	O-C-N	-5.07	114.60	122.70
1	B	56	THR	N-CA-CB	5.07	119.93	110.30
1	Y	56	THR	N-CA-CB	5.06	119.92	110.30
1	B	57	SER	O-C-N	-5.06	114.60	122.70
1	O	52	THR	N-CA-CB	5.06	119.91	110.30
1	O	56	THR	N-CA-CB	5.06	119.91	110.30
1	O	80	GLY	N-CA-C	5.05	125.73	113.10
1	B	80	GLY	N-CA-C	5.05	125.73	113.10
1	O	53	GLN	CB-CA-C	-5.04	100.31	110.40
1	G	80	GLY	N-CA-C	5.04	125.71	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	57	SER	O-C-N	-5.04	114.63	122.70
1	Y	52	THR	N-CA-CB	5.04	119.88	110.30
1	Y	151	LYS	N-CA-CB	-5.04	101.53	110.60
1	G	53	GLN	CB-CA-C	-5.04	100.32	110.40
1	Y	80	GLY	N-CA-C	5.04	125.69	113.10
1	G	151	LYS	N-CA-CB	-5.03	101.54	110.60
1	Y	53	GLN	CB-CA-C	-5.03	100.34	110.40
1	Y	57	SER	O-C-N	-5.03	114.65	122.70
1	G	26	THR	CA-CB-CG2	5.03	119.44	112.40
1	O	151	LYS	N-CA-CB	-5.03	101.55	110.60
1	G	48	PHE	CG-CD2-CE2	5.03	126.33	120.80
1	B	53	GLN	CB-CA-C	-5.03	100.34	110.40
1	Y	26	THR	CA-CB-CG2	5.02	119.43	112.40
1	O	48	PHE	CG-CD2-CE2	5.02	126.32	120.80
1	B	54	GLY	C-N-CA	5.02	134.25	121.70
1	O	26	THR	CA-CB-CG2	5.02	119.43	112.40
1	B	151	LYS	N-CA-CB	-5.02	101.57	110.60
1	B	48	PHE	CG-CD2-CE2	5.01	126.32	120.80
1	Y	54	GLY	C-N-CA	5.01	134.22	121.70
1	G	54	GLY	C-N-CA	5.01	134.22	121.70
1	B	26	THR	CA-CB-CG2	5.01	119.41	112.40
1	O	54	GLY	C-N-CA	5.01	134.21	121.70
1	O	20	PHE	CA-CB-CG	5.00	125.90	113.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1094	0	1058	58	131
1	G	1094	0	1058	60	87
1	O	1094	0	1057	59	210
1	Y	1094	0	1057	62	49
2	B	1	0	0	0	0
2	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
All	All	4384	0	4230	238	265

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (238) 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:B:51:ASN:ND2	1:B:146:VAL:HG23	1.89	0.88
1:G:51:ASN:ND2	1:G:146:VAL:HG23	1.89	0.88
1:O:51:ASN:ND2	1:O:146:VAL:HG23	1.89	0.88
1:Y:51:ASN:ND2	1:Y:146:VAL:HG23	1.89	0.87
1:B:45:VAL:HG12	1:B:115:MET:HE1	1.60	0.83
1:O:45:VAL:HG12	1:O:115:MET:HE1	1.65	0.79
1:B:45:VAL:HG12	1:B:115:MET:CE	2.15	0.77
1:G:45:VAL:HG12	1:G:115:MET:CE	2.15	0.77
1:O:45:VAL:HG12	1:O:115:MET:CE	2.15	0.77
1:Y:45:VAL:HG12	1:Y:115:MET:CE	2.15	0.76
1:B:0:ACE:O	1:B:1:ALA:HB2	1.87	0.75
1:B:45:VAL:CG1	1:B:115:MET:HE1	2.18	0.74
1:Y:0:ACE:O	1:Y:1:ALA:HB2	1.87	0.73
1:O:0:ACE:O	1:O:1:ALA:HB2	1.87	0.73
1:G:0:ACE:O	1:G:1:ALA:HB2	1.87	0.73
1:B:47:GLN:HE21	1:B:60:PRO:HG2	1.54	0.72
1:G:47:GLN:HE21	1:G:60:PRO:HG2	1.54	0.72
1:Y:47:GLN:HE21	1:Y:60:PRO:HG2	1.54	0.71
1:O:47:GLN:HE21	1:O:60:PRO:HG2	1.54	0.70
1:O:45:VAL:CG1	1:O:115:MET:HE1	2.22	0.69
1:Y:45:VAL:HG12	1:Y:115:MET:HE1	1.75	0.67
1:G:33:ILE:CG2	1:G:36:LEU:HD22	2.25	0.66
1:B:33:ILE:CG2	1:B:36:LEU:HD22	2.25	0.66
1:Y:33:ILE:CG2	1:Y:36:LEU:HD22	2.25	0.66
1:O:33:ILE:CG2	1:O:36:LEU:HD22	2.25	0.65
1:G:45:VAL:HG12	1:G:115:MET:HE2	1.79	0.65
1:G:45:VAL:CG1	1:G:115:MET:CE	2.76	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:LYS:HZ2	1:G:10:GLY:H	1.44	0.63
1:O:74:ASP:OD2	1:O:126:ARG:NH2	2.32	0.63
1:Y:45:VAL:CG1	1:Y:115:MET:CE	2.76	0.63
1:B:74:ASP:OD2	1:B:126:ARG:NH2	2.32	0.63
1:G:74:ASP:OD2	1:G:126:ARG:NH2	2.32	0.63
1:Y:74:ASP:OD2	1:Y:126:ARG:NH2	2.32	0.62
1:O:45:VAL:CG1	1:O:115:MET:CE	2.76	0.62
1:O:50:ASP:OD1	1:O:52:THR:OG1	2.16	0.61
1:B:51:ASN:HD21	1:B:146:VAL:HG23	1.65	0.61
1:O:51:ASN:HD21	1:O:146:VAL:HG23	1.65	0.61
1:B:45:VAL:CG1	1:B:115:MET:CE	2.76	0.61
1:Y:51:ASN:HD21	1:Y:146:VAL:HG23	1.65	0.61
1:G:45:VAL:HG12	1:G:115:MET:HE1	1.82	0.61
1:G:50:ASP:OD1	1:G:52:THR:OG1	2.16	0.61
1:O:1:ALA:HB3	1:O:111:ILE:CD1	2.31	0.61
1:G:37:THR:HG22	1:G:41:HIS:CE1	2.36	0.61
1:B:9:LYS:HZ2	1:B:10:GLY:H	1.49	0.60
1:Y:115:MET:HE3	1:Y:147:ILE:HD11	1.83	0.60
1:Y:1:ALA:HB3	1:Y:111:ILE:CD1	2.31	0.60
1:G:115:MET:HE3	1:G:147:ILE:HD11	1.81	0.60
1:B:1:ALA:HB3	1:B:111:ILE:CD1	2.31	0.60
1:Y:45:VAL:CG1	1:Y:115:MET:HE1	2.31	0.60
1:B:37:THR:HG22	1:B:41:HIS:CE1	2.36	0.60
1:G:1:ALA:HB3	1:G:111:ILE:CD1	2.31	0.60
1:O:37:THR:HG22	1:O:41:HIS:CE1	2.37	0.59
1:G:45:VAL:CG1	1:G:115:MET:HE2	2.33	0.59
1:G:51:ASN:HD21	1:G:146:VAL:HG23	1.65	0.59
1:O:9:LYS:HZ2	1:O:10:GLY:H	1.49	0.59
1:Y:37:THR:HG22	1:Y:41:HIS:CE1	2.36	0.59
1:B:50:ASP:OD1	1:B:52:THR:OG1	2.16	0.58
1:Y:45:VAL:HB	1:Y:115:MET:HE2	1.85	0.58
1:Y:50:ASP:OD1	1:Y:52:THR:OG1	2.16	0.58
1:Y:45:VAL:HG12	1:Y:115:MET:HE2	1.85	0.57
1:O:45:VAL:HB	1:O:115:MET:HE2	1.86	0.57
1:G:45:VAL:HB	1:G:115:MET:HE2	1.86	0.57
1:G:4:ALA:HB2	1:G:111:ILE:HD11	1.87	0.56
1:B:4:ALA:HB2	1:B:111:ILE:HD11	1.87	0.56
1:B:73:LYS:N	1:B:73:LYS:HD3	2.19	0.56
1:Y:4:ALA:HB2	1:Y:111:ILE:HD11	1.87	0.56
1:G:45:VAL:CB	1:G:115:MET:HE2	2.36	0.55
1:G:73:LYS:N	1:G:73:LYS:HD3	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:VAL:HB	1:B:115:MET:HE2	1.87	0.55
1:G:129:ASN:OD1	1:G:132:SER:N	2.39	0.55
1:G:45:VAL:CG1	1:G:115:MET:HE1	2.36	0.55
1:Y:114:THR:CG2	1:Y:144:CYS:HB2	2.37	0.55
1:Y:129:ASN:OD1	1:Y:132:SER:N	2.39	0.55
1:G:114:THR:CG2	1:G:144:CYS:HB2	2.37	0.55
1:O:4:ALA:HB2	1:O:111:ILE:HD11	1.87	0.55
1:O:115:MET:HE3	1:O:147:ILE:HD11	1.88	0.55
1:Y:73:LYS:HD3	1:Y:73:LYS:N	2.19	0.55
1:B:114:THR:CG2	1:B:144:CYS:HB2	2.37	0.54
1:O:73:LYS:HD3	1:O:73:LYS:N	2.19	0.54
1:O:114:THR:CG2	1:O:144:CYS:HB2	2.37	0.54
1:Y:45:VAL:CG1	1:Y:115:MET:HE2	2.38	0.54
1:B:74:ASP:CG	1:B:126:ARG:HH22	2.12	0.53
1:Y:74:ASP:CG	1:Y:126:ARG:HH22	2.12	0.53
1:Y:34:THR:HG22	1:Y:92:VAL:HG22	1.91	0.53
1:O:74:ASP:CG	1:O:126:ARG:HH22	2.12	0.53
1:G:46:HIS:CD2	1:G:116:VAL:HG13	2.44	0.53
1:B:118:HIS:CE1	1:B:141:ARG:HG2	2.44	0.53
1:G:118:HIS:CE1	1:G:141:ARG:HG2	2.44	0.53
1:G:34:THR:HG22	1:G:92:VAL:HG22	1.91	0.53
1:B:46:HIS:CD2	1:B:116:VAL:HG13	2.44	0.53
1:O:118:HIS:CE1	1:O:141:ARG:HG2	2.44	0.53
1:Y:46:HIS:CD2	1:Y:116:VAL:HG13	2.44	0.53
1:B:34:THR:HG22	1:B:92:VAL:HG22	1.91	0.52
1:Y:9:LYS:HZ2	1:Y:10:GLY:H	1.57	0.52
1:B:115:MET:HE3	1:B:147:ILE:HD11	1.91	0.52
1:O:46:HIS:CD2	1:O:116:VAL:HG13	2.44	0.52
1:Y:45:VAL:CB	1:Y:115:MET:HE2	2.38	0.52
1:O:34:THR:HG22	1:O:92:VAL:HG22	1.91	0.52
1:G:74:ASP:CG	1:G:126:ARG:HH22	2.12	0.52
1:O:129:ASN:OD1	1:O:132:SER:N	2.39	0.52
1:G:33:ILE:CD1	1:G:117:VAL:HG21	2.40	0.52
1:Y:118:HIS:CE1	1:Y:141:ARG:HG2	2.44	0.52
1:G:150:ALA:HB1	1:G:151:LYS:HD2	1.93	0.51
1:Y:150:ALA:HB1	1:Y:151:LYS:HD2	1.93	0.51
1:O:150:ALA:HB1	1:O:151:LYS:HD2	1.93	0.51
1:B:129:ASN:OD1	1:B:132:SER:N	2.39	0.51
1:B:3:LYS:HD2	1:B:151:LYS:HD3	1.93	0.51
1:B:33:ILE:HG22	1:B:36:LEU:HD22	1.92	0.51
1:G:3:LYS:HD2	1:G:151:LYS:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ILE:CD1	1:B:117:VAL:HG21	2.40	0.51
1:O:33:ILE:CD1	1:O:117:VAL:HG21	2.40	0.51
1:O:3:LYS:HD2	1:O:151:LYS:HD3	1.93	0.51
1:O:51:ASN:ND2	1:O:146:VAL:CG2	2.70	0.51
1:Y:33:ILE:CD1	1:Y:117:VAL:HG21	2.40	0.50
1:B:49:GLY:HA3	1:B:112:GLY:O	2.12	0.50
1:B:150:ALA:HB1	1:B:151:LYS:HD2	1.93	0.50
1:O:33:ILE:HG22	1:O:36:LEU:HD22	1.92	0.50
1:O:123:ASP:OD1	1:O:132:SER:OG	2.24	0.50
1:Y:33:ILE:HG22	1:Y:36:LEU:HD22	1.92	0.50
1:G:51:ASN:ND2	1:G:146:VAL:CG2	2.70	0.50
1:G:49:GLY:HA3	1:G:112:GLY:O	2.12	0.50
1:Y:49:GLY:HA3	1:Y:112:GLY:O	2.12	0.49
1:Y:51:ASN:ND2	1:Y:146:VAL:CG2	2.70	0.49
1:O:49:GLY:HA3	1:O:112:GLY:O	2.12	0.49
1:G:33:ILE:HG22	1:G:36:LEU:HD22	1.93	0.49
1:O:33:ILE:HG21	1:O:36:LEU:HD22	1.95	0.49
1:Y:3:LYS:HD2	1:Y:151:LYS:HD3	1.93	0.49
1:G:40:ASP:HB2	1:G:121:PRO:HB3	1.96	0.48
1:Y:33:ILE:HG21	1:Y:36:LEU:HD22	1.95	0.48
1:O:45:VAL:CB	1:O:115:MET:HE2	2.43	0.48
1:O:9:LYS:HD3	1:O:10:GLY:O	2.14	0.48
1:Y:9:LYS:HD3	1:Y:10:GLY:O	2.14	0.48
1:B:9:LYS:HD3	1:B:10:GLY:O	2.14	0.47
1:O:40:ASP:HB2	1:O:121:PRO:HB3	1.96	0.47
1:B:33:ILE:HG21	1:B:36:LEU:HD22	1.95	0.47
1:O:75:GLU:O	1:O:75:GLU:HG2	2.15	0.47
1:B:75:GLU:O	1:B:75:GLU:HG2	2.15	0.47
1:G:75:GLU:O	1:G:75:GLU:HG2	2.15	0.47
1:B:51:ASN:ND2	1:B:146:VAL:CG2	2.70	0.47
1:B:40:ASP:HB2	1:B:121:PRO:HB3	1.96	0.47
1:G:9:LYS:HD3	1:G:10:GLY:O	2.14	0.47
1:G:4:ALA:HA	1:G:148:GLY:O	2.15	0.47
1:O:4:ALA:HA	1:O:148:GLY:O	2.15	0.46
1:Y:40:ASP:HB2	1:Y:121:PRO:HB3	1.96	0.46
1:Y:9:LYS:NZ	1:Y:14:VAL:O	2.46	0.46
1:G:33:ILE:HG21	1:G:36:LEU:HD22	1.95	0.46
1:Y:4:ALA:HA	1:Y:148:GLY:O	2.15	0.46
1:B:4:ALA:HA	1:B:148:GLY:O	2.16	0.46
1:B:150:ALA:CB	1:B:151:LYS:HD2	2.46	0.46
1:Y:75:GLU:O	1:Y:75:GLU:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:9:LYS:NZ	1:O:14:VAL:O	2.46	0.46
1:Y:89:LYS:HD2	1:Y:89:LYS:H	1.81	0.46
1:B:89:LYS:H	1:B:89:LYS:HD2	1.81	0.45
1:O:45:VAL:HG12	1:O:115:MET:HE2	1.96	0.45
1:G:150:ALA:CB	1:G:151:LYS:HD2	2.46	0.45
1:O:89:LYS:H	1:O:89:LYS:HD2	1.81	0.45
1:B:51:ASN:HD22	1:B:146:VAL:HG23	1.78	0.45
1:Y:123:ASP:OD1	1:Y:132:SER:OG	2.24	0.45
1:B:45:VAL:CB	1:B:115:MET:HE2	2.46	0.45
1:B:14:VAL:HG21	1:B:142:LEU:HD13	1.99	0.45
1:G:14:VAL:HG21	1:G:142:LEU:HD13	1.99	0.45
1:G:111:ILE:HD13	1:G:149:ILE:HG12	1.99	0.45
1:Y:150:ALA:CB	1:Y:151:LYS:HD2	2.46	0.45
1:G:89:LYS:H	1:G:89:LYS:HD2	1.81	0.44
1:O:45:VAL:HA	1:O:114:THR:O	2.18	0.44
1:O:150:ALA:CB	1:O:151:LYS:HD2	2.46	0.44
1:B:123:ASP:OD1	1:B:132:SER:OG	2.24	0.44
1:B:111:ILE:HD13	1:B:149:ILE:HG12	1.99	0.44
1:B:45:VAL:HA	1:B:114:THR:O	2.17	0.44
1:G:74:ASP:OD1	1:G:126:ARG:NH2	2.51	0.44
1:Y:14:VAL:HG21	1:Y:142:LEU:HD13	1.99	0.44
1:O:74:ASP:OD1	1:O:126:ARG:NH2	2.51	0.43
1:Y:45:VAL:HA	1:Y:114:THR:O	2.17	0.43
1:Y:51:ASN:HD22	1:Y:146:VAL:HG23	1.78	0.43
1:B:74:ASP:OD1	1:B:126:ARG:NH2	2.51	0.43
1:O:103:SER:OG	1:O:105:SER:O	2.31	0.43
1:O:111:ILE:HD13	1:O:149:ILE:HG12	1.99	0.43
1:Y:103:SER:O	1:Y:109:SER:HA	2.19	0.43
1:O:45:VAL:CG1	1:O:115:MET:HE2	2.47	0.43
1:G:45:VAL:HA	1:G:114:THR:O	2.18	0.43
1:Y:134:LYS:HB3	1:Y:134:LYS:HE2	1.59	0.43
1:G:123:ASP:OD1	1:G:132:SER:OG	2.24	0.43
1:Y:111:ILE:HD13	1:Y:149:ILE:HG12	1.99	0.43
1:O:14:VAL:HG21	1:O:142:LEU:HD13	1.99	0.43
1:Y:74:ASP:OD1	1:Y:126:ARG:NH2	2.51	0.43
1:G:9:LYS:HE2	1:G:15:GLN:OE1	2.19	0.43
1:B:9:LYS:HE2	1:B:15:GLN:OE1	2.19	0.43
1:G:9:LYS:NZ	1:G:14:VAL:O	2.46	0.43
1:O:103:SER:O	1:O:109:SER:HA	2.19	0.43
1:G:115:MET:O	1:G:144:CYS:HA	2.19	0.42
1:B:103:SER:O	1:B:109:SER:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:MET:O	1:B:144:CYS:HA	2.19	0.42
1:B:114:THR:HG22	1:B:144:CYS:HB2	2.01	0.42
1:G:103:SER:O	1:G:109:SER:HA	2.19	0.42
1:O:51:ASN:HD22	1:O:146:VAL:HG23	1.78	0.42
1:Y:115:MET:O	1:Y:144:CYS:HA	2.19	0.42
1:O:9:LYS:HE2	1:O:15:GLN:OE1	2.19	0.42
1:O:114:THR:HG22	1:O:144:CYS:HB2	2.01	0.42
1:Y:9:LYS:HE2	1:Y:15:GLN:OE1	2.19	0.42
1:G:33:ILE:HD12	1:G:117:VAL:HG21	2.02	0.41
1:G:114:THR:HG22	1:G:144:CYS:HB2	2.01	0.41
1:G:51:ASN:HD22	1:G:146:VAL:HG23	1.78	0.41
1:B:108:TYR:N	1:B:108:TYR:CD1	2.89	0.41
1:O:115:MET:O	1:O:144:CYS:HA	2.19	0.41
1:Y:114:THR:HG22	1:Y:144:CYS:HB2	2.01	0.41
1:Y:15:GLN:O	1:Y:33:ILE:HA	2.21	0.41
1:Y:45:VAL:HG21	1:Y:110:ILE:CG2	2.51	0.41
1:G:28:VAL:HG22	1:G:98:VAL:HG22	2.03	0.41
1:O:150:ALA:HB1	1:O:151:LYS:HE3	2.03	0.41
1:Y:59:GLY:HA3	1:Y:60:PRO:HD2	1.87	0.41
1:B:9:LYS:NZ	1:B:14:VAL:O	2.46	0.41
1:G:15:GLN:O	1:G:33:ILE:HA	2.21	0.41
1:O:45:VAL:HG21	1:O:110:ILE:CG2	2.51	0.41
1:Y:108:TYR:CD1	1:Y:108:TYR:N	2.89	0.41
1:Y:28:VAL:HG22	1:Y:98:VAL:HG22	2.03	0.41
1:B:45:VAL:HG21	1:B:110:ILE:CG2	2.51	0.41
1:G:59:GLY:HA3	1:G:60:PRO:HD2	1.87	0.41
1:G:5:VAL:HG11	1:B:52:THR:HG23	2.02	0.41
1:O:33:ILE:HD12	1:O:117:VAL:HG21	2.02	0.41
1:B:15:GLN:O	1:B:33:ILE:HA	2.21	0.41
1:G:3:LYS:HA	1:G:20:PHE:O	2.21	0.41
1:Y:3:LYS:HA	1:Y:20:PHE:O	2.21	0.41
1:B:3:LYS:HA	1:B:20:PHE:O	2.21	0.41
1:Y:33:ILE:HD12	1:Y:117:VAL:HG21	2.02	0.41
1:Y:47:GLN:NE2	1:Y:60:PRO:HG2	2.30	0.41
1:B:134:LYS:HB3	1:B:134:LYS:HE2	1.59	0.40
1:B:150:ALA:HB1	1:B:151:LYS:HE3	2.03	0.40
1:O:123:ASP:O	1:O:124:LEU:HB2	2.21	0.40
1:B:123:ASP:O	1:B:124:LEU:HB2	2.21	0.40
1:B:45:VAL:CG1	1:B:115:MET:HE2	2.51	0.40
1:O:3:LYS:HA	1:O:20:PHE:O	2.21	0.40
1:G:108:TYR:CD1	1:G:108:TYR:N	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:123:ASP:O	1:G:124:LEU:HB2	2.21	0.40
1:G:45:VAL:HG21	1:G:110:ILE:CG2	2.51	0.40
1:O:37:THR:HG22	1:O:41:HIS:HE1	1.84	0.40
1:Y:150:ALA:HB1	1:Y:151:LYS:HE3	2.03	0.40
1:Y:149:ILE:HG21	1:Y:149:ILE:HD13	1.88	0.40
1:O:28:VAL:HG22	1:O:98:VAL:HG22	2.03	0.40

All (265) 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:Y:13:PRO:CD	1:Y:90:ASN:N[2_455]	0.22	1.98
1:O:98:VAL:O	1:G:23:LYS:CE[2_555]	0.46	1.74
1:O:64:PRO:C	1:B:101:LEU:C[1_554]	0.47	1.73
1:O:26:THR:OG1	1:G:26:THR:OG1[2_555]	0.51	1.69
1:O:62:PHE:CZ	1:B:25:ASP:O[1_554]	0.53	1.67
1:Y:37:THR:CB	1:Y:37:THR:OG1[2_455]	0.55	1.65
1:O:113:ARG:CD	1:B:25:ASP:OD1[1_554]	0.55	1.65
1:Y:25:ASP:OD1	1:Y:25:ASP:OD1[2_454]	0.59	1.61
1:O:25:ASP:CB	1:G:25:ASP:CA[2_555]	0.61	1.59
1:Y:13:PRO:CB	1:Y:90:ASN:C[2_455]	0.67	1.53
1:O:66:SER:N	1:B:101:LEU:CG[1_554]	0.77	1.43
1:O:65:LEU:CD1	1:B:108:TYR:CB[1_554]	0.79	1.41
1:O:109:SER:O	1:B:24:GLY:C[1_554]	0.82	1.38
1:O:108:TYR:CZ	1:B:103:SER:OG[1_554]	0.85	1.35
1:O:62:PHE:CZ	1:B:25:ASP:C[1_554]	0.86	1.34
1:O:106:GLY:C	1:B:22:ALA:CB[1_554]	0.87	1.33
1:G:107:GLU:CB	1:G:107:GLU:CB[2_556]	0.88	1.32
1:Y:13:PRO:CG	1:Y:90:ASN:C[2_455]	0.91	1.29
1:O:65:LEU:N	1:B:101:LEU:O[1_554]	0.91	1.29
1:O:23:LYS:CE	1:G:98:VAL:O[2_555]	0.92	1.28
1:G:107:GLU:OE2	1:G:108:TYR:CE1[2_556]	0.92	1.28
1:O:108:TYR:CE2	1:B:103:SER:OG[1_554]	0.93	1.27
1:Y:37:THR:CB	1:Y:37:THR:CB[2_455]	0.93	1.27
1:O:23:LYS:CD	1:G:98:VAL:O[2_555]	0.95	1.25
1:O:108:TYR:CZ	1:B:103:SER:CB[1_554]	0.95	1.25
1:O:23:LYS:O	1:G:26:THR:CB[2_555]	0.97	1.23
1:O:107:GLU:OE1	1:B:104:LEU:N[1_554]	1.00	1.20
1:O:23:LYS:O	1:G:26:THR:CG2[2_555]	1.00	1.20
1:Y:13:PRO:CB	1:Y:90:ASN:O[2_455]	1.01	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:100:PRO:CB	1:G:24:GLY:N[2_555]	1.02	1.18
1:Y:13:PRO:CG	1:Y:91:GLY:N[2_455]	1.03	1.17
1:O:64:PRO:C	1:B:101:LEU:CA[1_554]	1.04	1.16
1:O:25:ASP:CB	1:G:25:ASP:CB[2_555]	1.04	1.16
1:Y:38:GLU:OE1	1:Y:142:LEU:CD2[2_455]	1.04	1.16
1:O:107:GLU:N	1:B:22:ALA:CB[1_554]	1.06	1.14
1:Y:13:PRO:N	1:Y:90:ASN:CA[2_455]	1.09	1.11
1:Y:37:THR:OG1	1:Y:37:THR:CG2[2_455]	1.09	1.11
1:O:108:TYR:CE1	1:B:103:SER:CA[1_554]	1.14	1.06
1:O:67:LYS:CA	1:B:65:LEU:CD1[1_554]	1.14	1.06
1:O:25:ASP:CG	1:G:25:ASP:CA[2_555]	1.14	1.06
1:O:66:SER:CA	1:B:101:LEU:CD2[1_554]	1.17	1.03
1:O:65:LEU:CD1	1:B:108:TYR:CG[1_554]	1.18	1.02
1:O:64:PRO:O	1:B:101:LEU:C[1_554]	1.18	1.02
1:Y:13:PRO:CA	1:Y:90:ASN:CA[2_455]	1.18	1.02
1:O:25:ASP:CG	1:G:25:ASP:C[2_555]	1.21	0.99
1:O:98:VAL:O	1:G:23:LYS:NZ[2_555]	1.22	0.98
1:O:62:PHE:CE1	1:B:25:ASP:O[1_554]	1.23	0.97
1:O:89:LYS:CG	1:Y:129:ASN:ND2[4_445]	1.24	0.96
1:O:108:TYR:CE1	1:B:103:SER:CB[1_554]	1.25	0.95
1:O:23:LYS:NZ	1:G:98:VAL:N[2_555]	1.26	0.94
1:O:107:GLU:OE1	1:B:103:SER:C[1_554]	1.26	0.94
1:O:113:ARG:NE	1:B:25:ASP:OD1[1_554]	1.27	0.93
1:O:113:ARG:CD	1:B:25:ASP:CG[1_554]	1.28	0.92
1:O:64:PRO:O	1:B:102:ILE:N[1_554]	1.28	0.92
1:O:113:ARG:NE	1:B:25:ASP:CG[1_554]	1.28	0.92
1:Y:13:PRO:CD	1:Y:90:ASN:CA[2_455]	1.29	0.91
1:O:26:THR:CB	1:G:26:THR:OG1[2_555]	1.29	0.91
1:O:26:THR:CG2	1:G:23:LYS:O[2_555]	1.30	0.90
1:O:65:LEU:O	1:B:79:VAL:CG2[1_554]	1.30	0.90
1:O:25:ASP:CA	1:G:25:ASP:CG[2_555]	1.30	0.90
1:O:24:GLY:N	1:G:100:PRO:CB[2_555]	1.30	0.90
1:O:66:SER:CB	1:B:101:LEU:CD2[1_554]	1.31	0.89
1:Y:12:GLY:O	1:Y:90:ASN:ND2[2_455]	1.33	0.87
1:O:64:PRO:CA	1:B:101:LEU:CA[1_554]	1.33	0.87
1:O:66:SER:N	1:B:101:LEU:CD2[1_554]	1.34	0.86
1:O:109:SER:O	1:B:25:ASP:N[1_554]	1.36	0.84
1:Y:11:ASP:OD2	1:Y:89:LYS:NZ[2_455]	1.36	0.84
1:Y:13:PRO:CD	1:Y:89:LYS:C[2_455]	1.39	0.81
1:O:25:ASP:CA	1:G:25:ASP:CB[2_555]	1.41	0.79
1:Y:13:PRO:CG	1:Y:90:ASN:CA[2_455]	1.42	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:65:LEU:N	1:B:101:LEU:C[1_554]	1.42	0.78
1:O:64:PRO:C	1:B:101:LEU:O[1_554]	1.43	0.77
1:Y:13:PRO:CB	1:Y:90:ASN:CA[2_455]	1.44	0.76
1:O:109:SER:N	1:B:24:GLY:O[1_554]	1.44	0.76
1:O:98:VAL:C	1:G:23:LYS:CE[2_555]	1.44	0.76
1:O:98:VAL:CG1	1:G:28:VAL:CG2[2_555]	1.45	0.75
1:O:23:LYS:C	1:G:26:THR:CG2[2_555]	1.46	0.74
1:Y:12:GLY:CA	1:Y:89:LYS:CG[2_455]	1.47	0.73
1:Y:13:PRO:CA	1:Y:90:ASN:CB[2_455]	1.49	0.71
1:O:98:VAL:O	1:G:23:LYS:CD[2_555]	1.49	0.71
1:O:64:PRO:CA	1:B:101:LEU:N[1_554]	1.50	0.70
1:O:108:TYR:CE2	1:B:105:SER:O[1_554]	1.51	0.69
1:G:64:PRO:O	1:G:65:LEU:CD2[2_556]	1.51	0.69
1:O:98:VAL:N	1:G:23:LYS:NZ[2_555]	1.51	0.69
1:O:65:LEU:CG	1:B:108:TYR:CB[1_554]	1.52	0.68
1:O:26:THR:CB	1:G:23:LYS:O[2_555]	1.53	0.67
1:O:108:TYR:CE1	1:B:103:SER:OG[1_554]	1.53	0.67
1:G:107:GLU:OE2	1:G:108:TYR:CD1[2_556]	1.53	0.67
1:O:76:GLU:CD	1:B:65:LEU:CD2[1_554]	1.54	0.66
1:O:108:TYR:CD2	1:B:103:SER:OG[1_554]	1.54	0.66
1:O:65:LEU:C	1:B:101:LEU:CG[1_554]	1.54	0.66
1:O:66:SER:N	1:B:101:LEU:CD1[1_554]	1.55	0.65
1:O:76:GLU:OE2	1:B:65:LEU:CD2[1_554]	1.55	0.65
1:O:108:TYR:OH	1:B:103:SER:CB[1_554]	1.56	0.64
1:O:98:VAL:CG2	1:G:28:VAL:CG1[2_555]	1.56	0.64
1:O:25:ASP:OD1	1:G:25:ASP:O[2_555]	1.56	0.64
1:O:24:GLY:CA	1:G:100:PRO:CA[2_555]	1.57	0.63
1:Y:13:PRO:N	1:Y:90:ASN:N[2_455]	1.58	0.62
1:G:107:GLU:CD	1:G:108:TYR:CD1[2_556]	1.58	0.62
1:O:24:GLY:CA	1:G:100:PRO:CB[2_555]	1.59	0.61
1:O:64:PRO:N	1:B:100:PRO:O[1_554]	1.59	0.61
1:O:26:THR:OG1	1:G:26:THR:CB[2_555]	1.59	0.61
1:Y:37:THR:CA	1:Y:37:THR:OG1[2_455]	1.59	0.61
1:O:109:SER:O	1:B:24:GLY:CA[1_554]	1.60	0.60
1:Y:12:GLY:N	1:Y:89:LYS:CG[2_455]	1.60	0.60
1:Y:12:GLY:C	1:Y:90:ASN:CG[2_455]	1.61	0.59
1:O:64:PRO:C	1:B:102:ILE:N[1_554]	1.62	0.58
1:O:25:ASP:OD1	1:G:25:ASP:C[2_555]	1.63	0.57
1:O:113:ARG:CG	1:B:25:ASP:OD1[1_554]	1.64	0.56
1:O:76:GLU:OE2	1:B:65:LEU:CB[1_554]	1.64	0.56
1:O:64:PRO:CA	1:B:101:LEU:C[1_554]	1.64	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:62:PHE:CE2	1:B:25:ASP:CA[1_554]	1.64	0.56
1:O:25:ASP:CB	1:G:25:ASP:C[2_555]	1.64	0.56
1:O:62:PHE:CE2	1:B:25:ASP:O[1_554]	1.66	0.54
1:Y:13:PRO:CG	1:Y:90:ASN:N[2_455]	1.66	0.54
1:O:75:GLU:O	1:B:107:GLU:OE2[1_554]	1.67	0.53
1:O:62:PHE:CD2	1:B:25:ASP:CB[1_554]	1.67	0.53
1:O:28:VAL:CG2	1:G:98:VAL:CG2[2_555]	1.67	0.53
1:O:107:GLU:O	1:B:26:THR:O[1_554]	1.67	0.53
1:O:25:ASP:OD2	1:G:24:GLY:O[2_555]	1.69	0.51
1:O:106:GLY:CA	1:B:22:ALA:CB[1_554]	1.69	0.51
1:Y:13:PRO:N	1:Y:90:ASN:CB[2_455]	1.70	0.50
1:O:66:SER:OG	1:B:101:LEU:CD2[1_554]	1.70	0.50
1:O:100:PRO:CA	1:G:24:GLY:N[2_555]	1.70	0.50
1:O:26:THR:CG2	1:G:23:LYS:C[2_555]	1.70	0.50
1:O:62:PHE:CE1	1:B:25:ASP:C[1_554]	1.71	0.49
1:O:24:GLY:N	1:G:100:PRO:CA[2_555]	1.71	0.49
1:O:25:ASP:CA	1:G:25:ASP:OD2[2_555]	1.71	0.49
1:Y:25:ASP:CG	1:Y:25:ASP:OD1[2_454]	1.72	0.48
1:O:67:LYS:CE	1:B:64:PRO:CG[1_554]	1.74	0.46
1:O:64:PRO:O	1:B:101:LEU:CA[1_554]	1.75	0.45
1:O:23:LYS:CE	1:G:98:VAL:C[2_555]	1.75	0.45
1:O:67:LYS:CB	1:B:65:LEU:CD1[1_554]	1.75	0.45
1:Y:12:GLY:C	1:Y:90:ASN:OD1[2_455]	1.76	0.44
1:O:25:ASP:OD2	1:G:25:ASP:CA[2_555]	1.76	0.44
1:O:107:GLU:CG	1:B:27:VAL:CG2[1_554]	1.78	0.42
1:O:23:LYS:CG	1:G:98:VAL:O[2_555]	1.78	0.42
1:O:113:ARG:NH2	1:B:26:THR:N[1_554]	1.78	0.42
1:O:107:GLU:CD	1:B:103:SER:C[1_554]	1.79	0.41
1:O:64:PRO:CB	1:B:102:ILE:O[1_554]	1.80	0.40
1:Y:37:THR:OG1	1:Y:37:THR:OG1[2_455]	1.80	0.40
1:O:109:SER:C	1:B:24:GLY:C[1_554]	1.80	0.40
1:O:23:LYS:CE	1:G:98:VAL:N[2_555]	1.81	0.39
1:Y:13:PRO:N	1:Y:90:ASN:CG[2_455]	1.81	0.39
1:O:89:LYS:CD	1:Y:129:ASN:ND2[4_445]	1.81	0.39
1:O:107:GLU:OE1	1:B:104:LEU:CA[1_554]	1.82	0.38
1:O:107:GLU:OE1	1:B:103:SER:O[1_554]	1.82	0.38
1:O:26:THR:CA	1:G:23:LYS:O[2_555]	1.82	0.38
1:O:109:SER:O	1:B:24:GLY:O[1_554]	1.82	0.38
1:O:68:LYS:CD	1:B:67:LYS:NZ[1_554]	1.82	0.38
1:O:67:LYS:CD	1:B:108:TYR:CZ[1_554]	1.83	0.37
1:O:25:ASP:CG	1:G:25:ASP:O[2_555]	1.84	0.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:64:PRO:CA	1:B:100:PRO:C[1_554]	1.84	0.36
1:O:106:GLY:O	1:B:22:ALA:CB[1_554]	1.85	0.35
1:O:77:ARG:O	1:B:108:TYR:OH[1_554]	1.85	0.35
1:O:65:LEU:CD2	1:B:108:TYR:CB[1_554]	1.85	0.35
1:O:62:PHE:CZ	1:B:25:ASP:CA[1_554]	1.86	0.34
1:O:25:ASP:O	1:G:25:ASP:OD1[2_555]	1.86	0.34
1:O:109:SER:CA	1:B:24:GLY:O[1_554]	1.86	0.34
1:O:25:ASP:OD2	1:G:25:ASP:N[2_555]	1.86	0.34
1:Y:13:PRO:CB	1:Y:91:GLY:N[2_455]	1.87	0.33
1:O:25:ASP:CB	1:G:25:ASP:N[2_555]	1.87	0.33
1:O:62:PHE:CE2	1:B:25:ASP:C[1_554]	1.88	0.32
1:Y:12:GLY:O	1:Y:90:ASN:CG[2_455]	1.88	0.32
1:O:25:ASP:CA	1:G:25:ASP:CA[2_555]	1.90	0.30
1:O:108:TYR:CD1	1:B:103:SER:OG[1_554]	1.90	0.30
1:O:65:LEU:N	1:B:101:LEU:CA[1_554]	1.90	0.30
1:O:76:GLU:OE2	1:B:65:LEU:CG[1_554]	1.91	0.29
1:O:65:LEU:CB	1:B:108:TYR:CD2[1_554]	1.92	0.28
1:O:64:PRO:CA	1:B:100:PRO:O[1_554]	1.92	0.28
1:O:65:LEU:CA	1:B:101:LEU:O[1_554]	1.92	0.28
1:Y:37:THR:CA	1:Y:37:THR:CB[2_455]	1.92	0.28
1:O:89:LYS:CG	1:Y:129:ASN:CG[4_445]	1.93	0.27
1:O:98:VAL:C	1:G:23:LYS:NZ[2_555]	1.94	0.26
1:O:75:GLU:O	1:B:107:GLU:CD[1_554]	1.95	0.25
1:O:25:ASP:N	1:G:25:ASP:C[2_555]	1.95	0.25
1:Y:12:GLY:CA	1:Y:90:ASN:OD1[2_455]	1.96	0.24
1:O:67:LYS:CD	1:B:108:TYR:CE1[1_554]	1.97	0.23
1:O:109:SER:C	1:B:24:GLY:O[1_554]	1.97	0.23
1:O:65:LEU:CD2	1:B:108:TYR:O[1_554]	1.98	0.22
1:O:25:ASP:CA	1:G:25:ASP:C[2_555]	1.98	0.22
1:O:25:ASP:N	1:G:25:ASP:O[2_555]	1.98	0.22
1:O:28:VAL:CG2	1:G:98:VAL:CG1[2_555]	1.98	0.22
1:Y:130:GLU:OE1	1:B:53:GLN:CD[4_455]	1.98	0.22
1:O:108:TYR:CG	1:B:103:SER:OG[1_554]	1.98	0.22
1:Y:12:GLY:C	1:Y:90:ASN:ND2[2_455]	1.98	0.22
1:O:25:ASP:OD2	1:G:24:GLY:C[2_555]	1.99	0.21
1:O:62:PHE:CE2	1:B:25:ASP:CB[1_554]	1.99	0.21
1:O:65:LEU:CD1	1:B:108:TYR:CD2[1_554]	1.99	0.21
1:Y:12:GLY:N	1:Y:89:LYS:CD[2_455]	1.99	0.21
1:O:63:ASN:O	1:B:101:LEU:CD1[1_554]	1.99	0.21
1:O:62:PHE:CZ	1:B:26:THR:N[1_554]	2.00	0.20
1:O:25:ASP:C	1:G:25:ASP:CG[2_555]	2.00	0.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:107:GLU:C	1:G:107:GLU:OE1[2_556]	2.00	0.20
1:O:107:GLU:CD	1:B:104:LEU:N[1_554]	2.00	0.20
1:O:108:TYR:CE1	1:B:103:SER:C[1_554]	2.01	0.19
1:O:25:ASP:O	1:G:25:ASP:N[2_555]	2.01	0.19
1:G:107:GLU:CA	1:G:107:GLU:CB[2_556]	2.01	0.19
1:O:68:LYS:CE	1:B:67:LYS:CE[1_554]	2.01	0.19
1:O:28:VAL:CB	1:G:98:VAL:CG2[2_555]	2.02	0.18
1:O:98:VAL:CA	1:G:23:LYS:NZ[2_555]	2.03	0.17
1:Y:130:GLU:OE1	1:B:53:GLN:NE2[4_455]	2.04	0.16
1:O:63:ASN:O	1:B:101:LEU:CA[1_554]	2.04	0.16
1:O:64:PRO:N	1:B:101:LEU:CA[1_554]	2.05	0.15
1:O:23:LYS:CD	1:G:98:VAL:C[2_555]	2.05	0.15
1:O:66:SER:CA	1:B:101:LEU:CG[1_554]	2.05	0.15
1:O:64:PRO:O	1:B:101:LEU:CB[1_554]	2.05	0.15
1:O:107:GLU:N	1:B:22:ALA:CA[1_554]	2.05	0.15
1:O:26:THR:CA	1:G:26:THR:OG1[2_555]	2.05	0.15
1:O:108:TYR:CZ	1:B:103:SER:CA[1_554]	2.05	0.15
1:O:100:PRO:CB	1:G:23:LYS:C[2_555]	2.05	0.15
1:O:62:PHE:CD1	1:B:25:ASP:OD2[1_554]	2.06	0.14
1:O:23:LYS:O	1:G:26:THR:CA[2_555]	2.06	0.14
1:O:113:ARG:CZ	1:B:25:ASP:OD1[1_554]	2.06	0.14
1:O:62:PHE:CG	1:B:25:ASP:CB[1_554]	2.06	0.14
1:O:24:GLY:N	1:G:100:PRO:N[2_555]	2.06	0.14
1:Y:38:GLU:CD	1:Y:142:LEU:CD2[2_455]	2.06	0.14
1:O:108:TYR:CD2	1:B:105:SER:O[1_554]	2.07	0.13
1:G:107:GLU:CB	1:G:107:GLU:CG[2_556]	2.07	0.13
1:O:113:ARG:NE	1:B:25:ASP:CB[1_554]	2.07	0.13
1:O:63:ASN:OD1	1:B:101:LEU:CD1[1_554]	2.07	0.13
1:O:23:LYS:CG	1:G:98:VAL:C[2_555]	2.07	0.13
1:O:65:LEU:CG	1:B:108:TYR:CG[1_554]	2.07	0.13
1:O:68:LYS:CD	1:B:67:LYS:CE[1_554]	2.08	0.12
1:O:28:VAL:CG1	1:G:98:VAL:CG2[2_555]	2.08	0.12
1:O:107:GLU:OE2	1:B:103:SER:N[1_554]	2.08	0.12
1:Y:11:ASP:C	1:Y:89:LYS:CD[2_455]	2.08	0.12
1:O:108:TYR:CE2	1:B:103:SER:CB[1_554]	2.08	0.12
1:O:23:LYS:CB	1:G:98:VAL:C[2_555]	2.09	0.11
1:Y:13:PRO:N	1:Y:89:LYS:C[2_455]	2.09	0.11
1:O:100:PRO:O	1:G:24:GLY:CA[2_555]	2.09	0.11
1:O:68:LYS:NZ	1:B:67:LYS:CE[1_554]	2.09	0.11
1:O:67:LYS:CD	1:B:108:TYR:OH[1_554]	2.10	0.10
1:O:75:GLU:CG	1:B:107:GLU:OE2[1_554]	2.10	0.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:13:PRO:CA	1:Y:90:ASN:C[2_455]	2.10	0.10
1:O:65:LEU:CD1	1:B:108:TYR:CA[1_554]	2.10	0.10
1:O:113:ARG:CZ	1:B:25:ASP:CG[1_554]	2.10	0.10
1:O:23:LYS:NZ	1:G:97:ILE:C[2_555]	2.11	0.09
1:O:100:PRO:CB	1:G:24:GLY:CA[2_555]	2.11	0.09
1:O:64:PRO:CD	1:B:100:PRO:O[1_554]	2.11	0.09
1:O:64:PRO:C	1:B:101:LEU:CB[1_554]	2.11	0.09
1:O:25:ASP:N	1:G:25:ASP:OD2[2_555]	2.11	0.09
1:G:107:GLU:CG	1:G:107:GLU:OE1[2_556]	2.12	0.08
1:O:66:SER:OG	1:B:77:ARG:NE[1_554]	2.12	0.08
1:O:25:ASP:CG	1:G:25:ASP:N[2_555]	2.13	0.07
1:G:107:GLU:O	1:G:107:GLU:OE1[2_556]	2.13	0.07
1:O:25:ASP:C	1:G:25:ASP:OD1[2_555]	2.13	0.07
1:O:106:GLY:C	1:B:22:ALA:CA[1_554]	2.13	0.07
1:O:28:VAL:CG2	1:G:98:VAL:CB[2_555]	2.15	0.05
1:Y:13:PRO:CG	1:Y:90:ASN:O[2_455]	2.15	0.05
1:O:107:GLU:OE2	1:B:27:VAL:CG2[1_554]	2.16	0.04
1:O:64:PRO:C	1:B:101:LEU:N[1_554]	2.16	0.04
1:O:107:GLU:OE2	1:B:103:SER:CA[1_554]	2.17	0.03
1:O:89:LYS:CE	1:Y:129:ASN:ND2[4_445]	2.17	0.03
1:O:65:LEU:CG	1:B:108:TYR:CD2[1_554]	2.17	0.03
1:Y:13:PRO:CD	1:Y:90:ASN:C[2_455]	2.18	0.02
1:O:25:ASP:OD2	1:G:25:ASP:C[2_555]	2.18	0.02
1:O:25:ASP:CG	1:G:26:THR:N[2_555]	2.18	0.02
1:O:67:LYS:CG	1:B:65:LEU:CD1[1_554]	2.18	0.02
1:O:25:ASP:C	1:G:25:ASP:N[2_555]	2.18	0.02
1:O:66:SER:OG	1:B:77:ARG:CD[1_554]	2.19	0.01
1:Y:38:GLU:OE1	1:Y:142:LEU:CG[2_455]	2.19	0.01
1:O:23:LYS:CG	1:G:98:VAL:CG1[2_555]	2.19	0.01
1:O:23:LYS:CB	1:G:99:ASP:N[2_555]	2.19	0.01
1:O:66:SER:N	1:B:101:LEU:CB[1_554]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	150/152 (99%)	146 (97%)	4 (3%)	0	100	100
1	G	150/152 (99%)	146 (97%)	4 (3%)	0	100	100
1	O	150/152 (99%)	146 (97%)	4 (3%)	0	100	100
1	Y	150/152 (99%)	146 (97%)	4 (3%)	0	100	100
All	All	600/608 (99%)	584 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	116/116 (100%)	104 (90%)	12 (10%)	7	4
1	G	116/116 (100%)	104 (90%)	12 (10%)	7	4
1	O	116/116 (100%)	104 (90%)	12 (10%)	7	4
1	Y	116/116 (100%)	104 (90%)	12 (10%)	7	4
All	All	464/464 (100%)	416 (90%)	48 (10%)	7	4

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	2	THR
1	O	9	LYS
1	O	11	ASP
1	O	37	THR
1	O	73	LYS
1	O	76	GLU
1	O	89	LYS
1	O	100	PRO
1	O	105	SER
1	O	120	LYS
1	O	134	LYS
1	O	151	LYS
1	Y	2	THR

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Mol	Chain	Res	Type
1	Y	9	LYS
1	Y	11	ASP
1	Y	37	THR
1	Y	73	LYS
1	Y	76	GLU
1	Y	89	LYS
1	Y	100	PRO
1	Y	105	SER
1	Y	120	LYS
1	Y	134	LYS
1	Y	151	LYS
1	G	2	THR
1	G	9	LYS
1	G	11	ASP
1	G	37	THR
1	G	73	LYS
1	G	76	GLU
1	G	89	LYS
1	G	100	PRO
1	G	105	SER
1	G	120	LYS
1	G	134	LYS
1	G	151	LYS
1	B	2	THR
1	B	9	LYS
1	B	11	ASP
1	B	37	THR
1	B	73	LYS
1	B	76	GLU
1	B	89	LYS
1	B	100	PRO
1	B	105	SER
1	B	120	LYS
1	B	134	LYS
1	B	151	LYS

Some 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	47	GLN
1	O	51	ASN

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Mol	Chain	Res	Type
1	O	53	GLN
1	Y	19	HIS
1	Y	47	GLN
1	Y	51	ASN
1	Y	53	GLN
1	G	19	HIS
1	G	47	GLN
1	G	51	ASN
1	G	53	GLN
1	B	19	HIS
1	B	47	GLN
1	B	51	ASN
1	B	53	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.