



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:36 PM UTC

PDB ID : 1SOS / pdb_00001sos
Title : ATOMIC STRUCTURES OF WILD-TYPE AND THERMOSTABLE MUTANT RECOMBINANT HUMAN CU, ZN SUPEROXIDE DISMUTASE
Authors : Parge, H.E.; Hallewell, R.A.; Tainer, J.A.
Deposited on : 1992-02-11
Resolution : 2.50 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	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

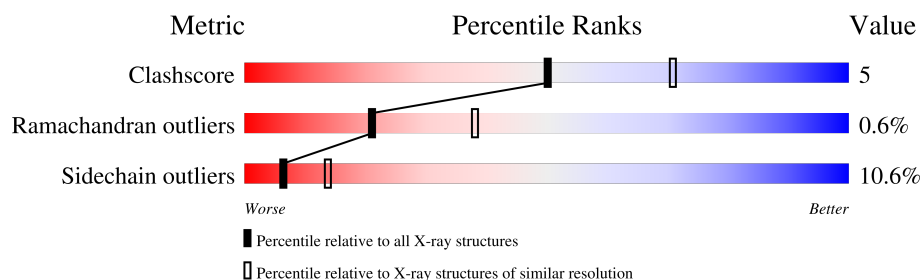
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	A	154	70% 22% 8%
1	B	154	62% 36% ..
1	C	154	66% 30% ..
1	D	154	64% 32% ..
1	E	154	54% 36% 8% .
1	F	154	62% 32% 5% .
1	G	154	64% 29% 5% .
1	H	154	62% 30% 8% .

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Mol	Chain	Length	Quality of chain
1	I	154	62%31%6%•
1	J	154	66%26%7%•

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11649 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 SUPEROXIDE DISMUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	154	Total	C	N	O	S	0	0	0
			1112	681	203	226	2			
1	F	154	Total	C	N	O	S	0	0	0
			1112	681	203	226	2			
1	B	154	Total	C	N	O	S	0	0	0
			1112	681	203	226	2			
1	G	154	Total	C	N	O	S	0	0	0
			1112	681	203	226	2			
1	C	154	Total	C	N	O	S	0	0	0
			1112	681	203	226	2			
1	H	154	Total	C	N	O	S	0	0	0
			1112	681	203	226	2			
1	D	154	Total	C	N	O	S	0	0	0
			1112	681	203	226	2			
1	I	154	Total	C	N	O	S	0	0	0
			1112	681	203	226	2			
1	E	154	Total	C	N	O	S	0	0	0
			1112	681	203	226	2			
1	J	154	Total	C	N	O	S	0	0	0
			1112	681	203	226	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	F	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		

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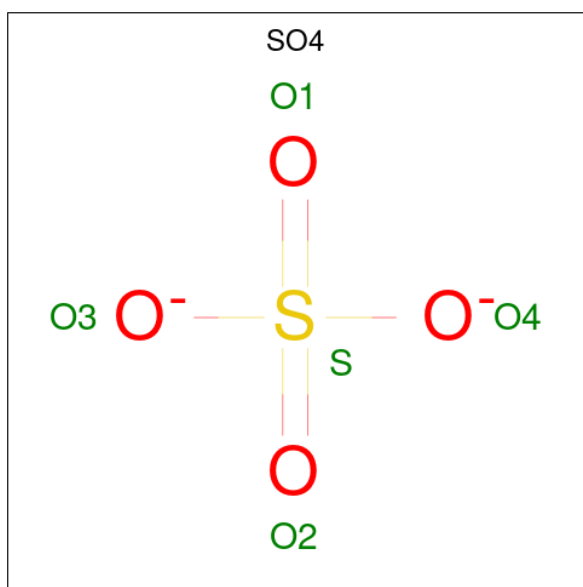
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total 1	Cu 1	0	0
2	H	1	Total 1	Cu 1	0	0
2	D	1	Total 1	Cu 1	0	0
2	I	1	Total 1	Cu 1	0	0
2	E	1	Total 1	Cu 1	0	0
2	J	1	Total 1	Cu 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0
3	F	1	Total 1	Zn 1	0	0
3	B	1	Total 1	Zn 1	0	0
3	G	1	Total 1	Zn 1	0	0
3	C	1	Total 1	Zn 1	0	0
3	H	1	Total 1	Zn 1	0	0
3	D	1	Total 1	Zn 1	0	0
3	I	1	Total 1	Zn 1	0	0
3	E	1	Total 1	Zn 1	0	0
3	J	1	Total 1	Zn 1	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

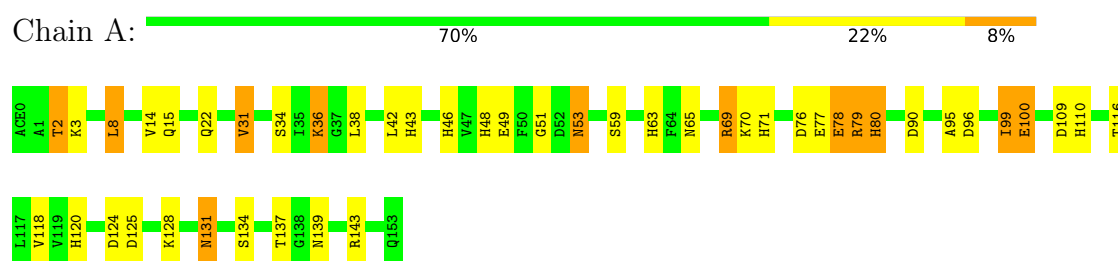
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total	O	0	0
			56	56		
5	F	52	Total	O	0	0
			52	52		
5	B	54	Total	O	0	0
			54	54		
5	G	63	Total	O	0	0
			63	63		
5	C	43	Total	O	0	0
			43	43		
5	H	63	Total	O	0	0
			63	63		
5	D	43	Total	O	0	0
			43	43		
5	I	46	Total	O	0	0
			46	46		
5	E	39	Total	O	0	0
			39	39		
5	J	40	Total	O	0	0
			40	40		

3 Residue-property plots

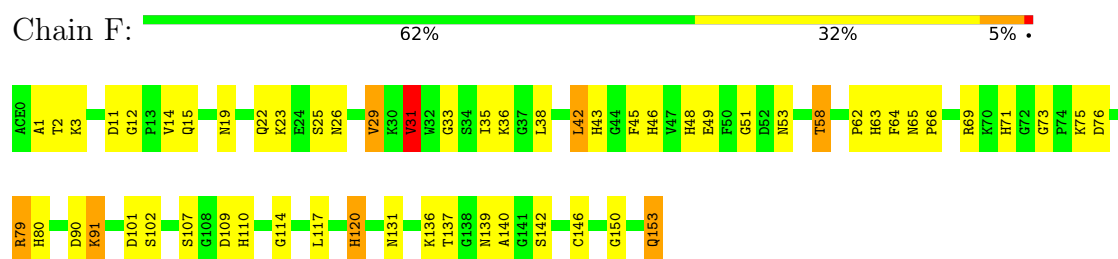
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

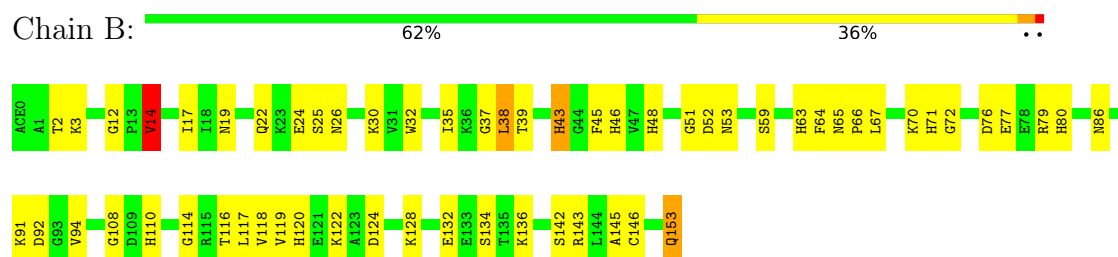
• Molecule 1: SUPEROXIDE DISMUTASE



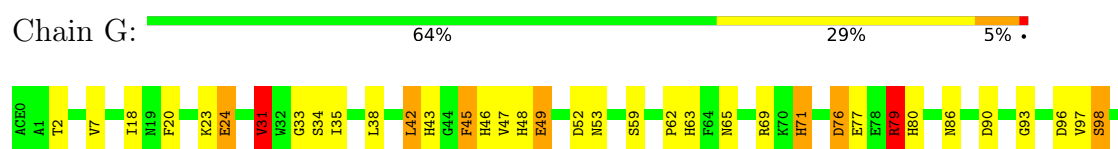
• Molecule 1: SUPEROXIDE DISMUTASE



• Molecule 1: SUPEROXIDE DISMUTASE



• Molecule 1: SUPEROXIDE DISMUTASE





• Molecule 1: SUPEROXIDE DISMUTASE

Chain C: 66% 30%



• Molecule 1: SUPEROXIDE DISMUTASE

Chain H: 62% 30% 8%



• Molecule 1: SUPEROXIDE DISMUTASE

Chain D: 64% 32%



• Molecule 1: SUPEROXIDE DISMUTASE

Chain I: 62% 31% 6%



• Molecule 1: SUPEROXIDE DISMUTASE

Chain E: 54% 36% 8%





● Molecule 1: SUPEROXIDE DISMUTASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	205.20Å 167.00Å 145.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.202 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11649	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.33	10/1128 (0.9%)	1.95	32/1521 (2.1%)
1	B	1.34	13/1128 (1.2%)	2.06	41/1521 (2.7%)
1	C	1.37	15/1128 (1.3%)	2.03	41/1521 (2.7%)
1	D	1.28	15/1128 (1.3%)	1.99	33/1521 (2.2%)
1	E	1.17	12/1128 (1.1%)	2.06	47/1521 (3.1%)
1	F	1.42	14/1128 (1.2%)	2.09	38/1521 (2.5%)
1	G	1.40	12/1128 (1.1%)	2.03	36/1521 (2.4%)
1	H	1.38	15/1128 (1.3%)	2.04	36/1521 (2.4%)
1	I	1.34	14/1128 (1.2%)	2.05	43/1521 (2.8%)
1	J	1.31	18/1128 (1.6%)	1.99	23/1521 (1.5%)
All	All	1.34	138/11280 (1.2%)	2.03	370/15210 (2.4%)

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	D	0	1

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	31	VAL	CA-CB	10.24	1.66	1.54
1	D	71	HIS	CD2-NE2	-8.74	1.28	1.37
1	J	29	VAL	CA-CB	8.59	1.65	1.54
1	C	71	HIS	CD2-NE2	-8.44	1.28	1.37
1	B	71	HIS	CD2-NE2	-8.38	1.28	1.37
1	G	43	HIS	CD2-NE2	-8.07	1.28	1.37
1	B	46	HIS	CD2-NE2	-7.96	1.29	1.37
1	G	48	HIS	CG-ND1	-7.94	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	14	VAL	CA-CB	7.91	1.64	1.54
1	F	48	HIS	CG-ND1	-7.81	1.29	1.38
1	C	80	HIS	CD2-NE2	-7.78	1.29	1.37
1	J	80	HIS	CD2-NE2	-7.75	1.29	1.37
1	I	120	HIS	CD2-NE2	-7.74	1.29	1.37
1	D	80	HIS	CD2-NE2	-7.61	1.29	1.37
1	I	46	HIS	CD2-NE2	-7.59	1.29	1.37
1	J	120	HIS	CG-ND1	-7.45	1.30	1.38
1	J	31	VAL	CA-CB	7.40	1.63	1.54
1	A	80	HIS	CD2-NE2	-7.34	1.29	1.37
1	H	110	HIS	CD2-NE2	-7.30	1.29	1.37
1	G	71	HIS	CD2-NE2	-7.25	1.29	1.37
1	G	110	HIS	CD2-NE2	-7.25	1.29	1.37
1	F	80	HIS	CD2-NE2	-7.25	1.29	1.37
1	H	71	HIS	CD2-NE2	-7.23	1.29	1.37
1	I	71	HIS	CD2-NE2	-7.23	1.29	1.37
1	A	48	HIS	CD2-NE2	-7.23	1.29	1.37
1	C	48	HIS	CG-ND1	-7.19	1.30	1.38
1	C	43	HIS	CD2-NE2	-7.18	1.29	1.37
1	G	63	HIS	CD2-NE2	-7.16	1.29	1.37
1	F	110	HIS	CD2-NE2	-7.13	1.30	1.37
1	D	71	HIS	CG-ND1	-7.12	1.30	1.38
1	B	46	HIS	CG-ND1	-7.11	1.30	1.38
1	B	48	HIS	CG-ND1	-7.09	1.30	1.38
1	E	71	HIS	CD2-NE2	-7.07	1.30	1.37
1	H	71	HIS	CG-ND1	-7.00	1.30	1.38
1	H	80	HIS	CD2-NE2	-6.96	1.30	1.37
1	F	48	HIS	CD2-NE2	-6.95	1.30	1.37
1	E	31	VAL	CA-CB	6.93	1.62	1.54
1	D	43	HIS	CD2-NE2	-6.92	1.30	1.37
1	I	80	HIS	CG-ND1	-6.91	1.30	1.38
1	C	120	HIS	CG-ND1	-6.90	1.30	1.38
1	H	29	VAL	CA-CB	6.89	1.62	1.54
1	J	103	VAL	CA-CB	6.88	1.63	1.54
1	F	71	HIS	CD2-NE2	-6.85	1.30	1.37
1	G	46	HIS	CD2-NE2	-6.79	1.30	1.37
1	E	80	HIS	CD2-NE2	-6.79	1.30	1.37
1	F	120	HIS	CD2-NE2	-6.78	1.30	1.37
1	A	43	HIS	CD2-NE2	-6.73	1.30	1.37
1	H	14	VAL	CA-CB	6.71	1.62	1.54
1	C	120	HIS	CD2-NE2	-6.71	1.30	1.37
1	B	63	HIS	CD2-NE2	-6.69	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	120	HIS	CD2-NE2	-6.66	1.30	1.37
1	D	46	HIS	CD2-NE2	-6.65	1.30	1.37
1	G	80	HIS	CD2-NE2	-6.64	1.30	1.37
1	E	120	HIS	CG-ND1	-6.63	1.30	1.38
1	F	46	HIS	CD2-NE2	-6.60	1.30	1.37
1	G	120	HIS	CD2-NE2	-6.60	1.30	1.37
1	I	110	HIS	CD2-NE2	-6.60	1.30	1.37
1	A	120	HIS	CD2-NE2	-6.59	1.30	1.37
1	I	29	VAL	CA-CB	6.59	1.62	1.54
1	J	71	HIS	CD2-NE2	-6.59	1.30	1.37
1	I	80	HIS	CD2-NE2	-6.59	1.30	1.37
1	A	48	HIS	CG-ND1	-6.58	1.31	1.38
1	B	43	HIS	CD2-NE2	-6.54	1.30	1.37
1	A	71	HIS	CD2-NE2	-6.54	1.30	1.37
1	E	110	HIS	CD2-NE2	-6.53	1.30	1.37
1	C	46	HIS	CD2-NE2	-6.53	1.30	1.37
1	I	43	HIS	CD2-NE2	-6.50	1.30	1.37
1	J	43	HIS	CD2-NE2	-6.42	1.30	1.37
1	A	110	HIS	CD2-NE2	-6.41	1.30	1.37
1	J	48	HIS	CD2-NE2	-6.40	1.30	1.37
1	I	48	HIS	CD2-NE2	-6.37	1.30	1.37
1	G	71	HIS	CG-ND1	-6.33	1.31	1.38
1	H	46	HIS	CD2-NE2	-6.30	1.30	1.37
1	F	120	HIS	CG-ND1	-6.27	1.31	1.38
1	D	48	HIS	CD2-NE2	-6.24	1.30	1.37
1	H	43	HIS	CD2-NE2	-6.24	1.30	1.37
1	J	110	HIS	CD2-NE2	-6.22	1.31	1.37
1	A	80	HIS	CG-ND1	-6.21	1.31	1.38
1	C	80	HIS	CG-ND1	-6.17	1.31	1.38
1	A	71	HIS	CG-ND1	-6.13	1.31	1.38
1	G	120	HIS	CG-ND1	-6.13	1.31	1.38
1	A	46	HIS	CD2-NE2	-6.07	1.31	1.37
1	D	110	HIS	CD2-NE2	-6.06	1.31	1.37
1	E	120	HIS	CD2-NE2	-6.02	1.31	1.37
1	D	104	ILE	CA-CB	6.00	1.60	1.54
1	J	46	HIS	CD2-NE2	-5.98	1.31	1.37
1	C	110	HIS	CD2-NE2	-5.94	1.31	1.37
1	D	80	HIS	CG-ND1	-5.91	1.31	1.38
1	J	63	HIS	CD2-NE2	-5.88	1.31	1.37
1	C	31	VAL	CA-CB	5.88	1.61	1.54
1	I	63	HIS	CD2-NE2	-5.86	1.31	1.37
1	H	48	HIS	CD2-NE2	-5.85	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	71	HIS	CG-ND1	-5.84	1.31	1.38
1	H	63	HIS	CD2-NE2	-5.84	1.31	1.37
1	F	63	HIS	CG-ND1	-5.83	1.31	1.38
1	H	121	GLU	CA-CB	-5.83	1.44	1.53
1	B	110	HIS	CD2-NE2	-5.79	1.31	1.37
1	J	48	HIS	CG-ND1	-5.76	1.31	1.38
1	I	63	HIS	CG-ND1	-5.72	1.31	1.38
1	C	113	ILE	CA-CB	5.68	1.60	1.54
1	F	63	HIS	CD2-NE2	-5.66	1.31	1.37
1	B	80	HIS	CG-ND1	-5.66	1.32	1.38
1	E	46	HIS	CD2-NE2	-5.63	1.31	1.37
1	C	71	HIS	CG-ND1	-5.58	1.32	1.38
1	J	80	HIS	CG-ND1	-5.57	1.32	1.38
1	C	48	HIS	CD2-NE2	-5.56	1.31	1.37
1	D	31	VAL	CA-CB	5.54	1.61	1.54
1	B	120	HIS	CD2-NE2	-5.54	1.31	1.37
1	J	151	ILE	CA-CB	-5.53	1.48	1.54
1	H	120	HIS	CD2-NE2	-5.53	1.31	1.37
1	F	31	VAL	CA-CB	5.50	1.61	1.54
1	B	48	HIS	CD2-NE2	-5.50	1.31	1.37
1	D	48	HIS	CG-ND1	-5.49	1.32	1.38
1	D	63	HIS	CD2-NE2	-5.49	1.31	1.37
1	H	117	LEU	CA-CB	-5.48	1.45	1.53
1	E	48	HIS	CG-ND1	-5.47	1.32	1.38
1	D	120	HIS	CG-ND1	-5.46	1.32	1.38
1	C	137	THR	CA-CB	-5.46	1.46	1.54
1	J	120	HIS	CD2-NE2	-5.43	1.31	1.37
1	J	148	VAL	CA-CB	5.38	1.60	1.54
1	F	43	HIS	CD2-NE2	-5.35	1.31	1.37
1	B	80	HIS	CD2-NE2	-5.34	1.31	1.37
1	J	43	HIS	CG-ND1	-5.32	1.32	1.38
1	F	71	HIS	CG-ND1	-5.31	1.32	1.38
1	H	48	HIS	CG-ND1	-5.27	1.32	1.38
1	F	29	VAL	CA-CB	5.26	1.61	1.54
1	E	96	ASP	CA-CB	-5.26	1.46	1.53
1	D	46	HIS	CG-ND1	-5.25	1.32	1.38
1	E	48	HIS	CD2-NE2	-5.22	1.32	1.37
1	E	43	HIS	CD2-NE2	-5.21	1.32	1.37
1	I	48	HIS	CG-ND1	-5.17	1.32	1.38
1	J	134	SER	CA-CB	-5.17	1.45	1.53
1	C	63	HIS	CD2-NE2	-5.16	1.32	1.37
1	I	120	HIS	CG-ND1	-5.14	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	53	ASN	CA-CB	5.13	1.60	1.53
1	G	48	HIS	CD2-NE2	-5.11	1.32	1.37
1	H	63	HIS	CG-ND1	-5.11	1.32	1.38
1	E	80	HIS	CG-ND1	-5.06	1.32	1.38

All (370) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	49	GLU	N-CA-C	12.09	124.46	111.28
1	B	26	ASN	CA-CB-CG	11.27	123.87	112.60
1	C	83	ASP	CA-CB-CG	11.07	123.67	112.60
1	F	131	ASN	CA-CB-CG	11.03	123.63	112.60
1	F	80	HIS	CA-CB-CG	11.03	124.83	113.80
1	E	53	ASN	OD1-CG-ND2	-10.75	111.85	122.60
1	E	53	ASN	CB-CG-ND2	10.56	132.24	116.40
1	F	90	ASP	CA-CB-CG	10.50	123.10	112.60
1	C	90	ASP	CA-CB-CG	10.24	122.84	112.60
1	A	100	GLU	N-CA-C	-10.11	92.36	109.24
1	G	53	ASN	OD1-CG-ND2	-10.03	112.57	122.60
1	E	49	GLU	N-CA-C	9.92	122.09	111.28
1	E	45	PHE	CA-CB-CG	9.64	123.44	113.80
1	A	49	GLU	N-CA-C	9.55	121.77	111.36
1	I	49	GLU	N-CA-C	9.53	121.66	111.28
1	G	76	ASP	CA-CB-CG	9.37	121.97	112.60
1	B	53	ASN	OD1-CG-ND2	-9.29	113.31	122.60
1	I	125	ASP	CA-CB-CG	9.12	121.72	112.60
1	D	49	GLU	N-CA-C	8.80	120.64	111.14
1	J	52	ASP	CA-CB-CG	8.78	121.38	112.60
1	I	65	ASN	CA-CB-CG	8.76	121.36	112.60
1	G	139	ASN	OD1-CG-ND2	-8.74	113.86	122.60
1	G	124	ASP	CA-CB-CG	8.65	121.25	112.60
1	D	125	ASP	CA-CB-CG	8.52	121.12	112.60
1	D	131	ASN	CA-CB-CG	8.52	121.12	112.60
1	C	131	ASN	CA-CB-CG	8.50	121.10	112.60
1	A	131	ASN	CA-CB-CG	8.40	121.00	112.60
1	I	80	HIS	CA-CB-CG	8.36	122.16	113.80
1	B	22	GLN	OE1-CD-NE2	-8.34	114.26	122.60
1	H	131	ASN	CA-CB-CG	8.31	120.92	112.60
1	A	76	ASP	CA-CB-CG	8.27	120.87	112.60
1	J	92	ASP	CA-CB-CG	8.27	120.87	112.60
1	A	90	ASP	CA-CB-CG	8.24	120.84	112.60
1	G	125	ASP	CA-CB-CG	8.18	120.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	124	ASP	CA-CB-CG	8.04	120.64	112.60
1	H	109	ASP	CA-CB-CG	8.03	120.63	112.60
1	E	77	GLU	N-CA-C	-7.99	101.86	111.69
1	F	45	PHE	CA-CB-CG	7.97	121.77	113.80
1	H	125	ASP	CA-CB-CG	7.93	120.53	112.60
1	B	43	HIS	CB-CG-CD2	-7.85	120.99	131.20
1	H	44	GLY	CA-C-O	-7.84	114.51	121.41
1	J	12	GLY	CA-C-N	7.79	127.45	119.82
1	J	12	GLY	C-N-CA	7.79	127.45	119.82
1	J	46	HIS	CA-CB-CG	7.79	121.58	113.80
1	H	53	ASN	CA-CB-CG	-7.76	104.84	112.60
1	I	131	ASN	CA-CB-CG	7.74	120.34	112.60
1	B	52	ASP	CA-CB-CG	7.67	120.27	112.60
1	D	43	HIS	CB-CG-CD2	-7.67	121.23	131.20
1	H	2	THR	CA-CB-OG1	-7.64	98.14	109.60
1	I	120	HIS	CB-CG-CD2	-7.62	121.30	131.20
1	H	49	GLU	N-CA-C	7.60	120.45	111.71
1	H	80	HIS	CA-CB-CG	7.54	121.34	113.80
1	I	124	ASP	CA-CB-CG	7.50	120.09	112.60
1	B	63	HIS	ND1-CE1-NE2	7.46	115.86	108.40
1	D	100	GLU	N-CA-C	-7.45	95.50	108.69
1	I	63	HIS	CE1-NE2-CD2	-7.45	101.55	109.00
1	F	11	ASP	CA-CB-CG	7.44	120.04	112.60
1	B	63	HIS	CB-CG-CD2	-7.39	121.60	131.20
1	H	2	THR	N-CA-C	-7.37	104.53	113.97
1	F	49	GLU	N-CA-C	7.36	118.95	111.07
1	A	69	ARG	CB-CG-CD	-7.35	94.39	111.30
1	C	139	ASN	OD1-CG-ND2	-7.33	115.27	122.60
1	D	63	HIS	ND1-CE1-NE2	7.28	115.68	108.40
1	D	120	HIS	CB-CG-CD2	-7.25	121.77	131.20
1	C	88	THR	CA-CB-OG1	-7.24	98.74	109.60
1	B	110	HIS	N-CA-C	-7.23	102.72	112.26
1	C	26	ASN	CA-CB-CG	7.22	119.83	112.60
1	E	71	HIS	CB-CG-CD2	-7.19	121.85	131.20
1	C	50	PHE	CA-CB-CG	-7.19	106.61	113.80
1	F	63	HIS	ND1-CE1-NE2	7.17	115.57	108.40
1	I	30	LYS	CA-CB-CG	7.15	128.40	114.10
1	H	63	HIS	ND1-CE1-NE2	7.12	115.52	108.40
1	F	139	ASN	OD1-CG-ND2	-7.11	115.49	122.60
1	C	49	GLU	N-CA-C	7.09	119.01	111.28
1	G	133	GLU	N-CA-CB	-7.07	99.32	110.28
1	B	70	LYS	CA-CB-CG	-7.06	99.99	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	63	HIS	CE1-NE2-CD2	-7.04	101.96	109.00
1	F	25	SER	N-CA-C	7.03	121.30	112.87
1	E	63	HIS	ND1-CE1-NE2	7.02	115.42	108.40
1	E	52	ASP	CA-CB-CG	7.00	119.61	112.60
1	E	148	VAL	N-CA-C	-6.99	98.30	108.71
1	B	65	ASN	O-C-N	-6.97	115.10	121.37
1	D	52	ASP	CA-CB-CG	6.95	119.55	112.60
1	H	19	ASN	OD1-CG-ND2	-6.94	115.66	122.60
1	I	37	GLY	N-CA-C	-6.94	105.75	115.32
1	B	19	ASN	CA-CB-CG	-6.88	105.72	112.60
1	G	90	ASP	CA-CB-CG	6.88	119.48	112.60
1	I	63	HIS	ND1-CE1-NE2	6.88	115.28	108.40
1	E	76	ASP	CA-CB-CG	6.87	119.47	112.60
1	G	109	ASP	CA-CB-CG	6.85	119.45	112.60
1	I	139	ASN	OD1-CG-ND2	-6.85	115.75	122.60
1	C	125	ASP	CA-CB-CG	6.83	119.43	112.60
1	E	76	ASP	N-CA-C	-6.79	98.86	109.72
1	E	100	GLU	CA-CB-CG	-6.79	100.53	114.10
1	B	2	THR	CA-CB-OG1	-6.78	99.43	109.60
1	H	120	HIS	CB-CG-CD2	-6.77	122.40	131.20
1	D	104	ILE	N-CA-C	-6.77	102.56	110.21
1	G	107	SER	CA-CB-OG	6.76	124.62	111.10
1	G	98	SER	O-C-N	-6.74	115.38	123.27
1	H	86	ASN	OD1-CG-ND2	-6.73	115.87	122.60
1	I	41	GLY	CA-C-N	6.72	130.26	120.71
1	I	41	GLY	C-N-CA	6.72	130.26	120.71
1	I	32	TRP	CG-CD2-CE3	6.69	140.59	133.90
1	G	49	GLU	N-CA-C	6.68	118.56	111.28
1	D	143	ARG	N-CA-C	-6.67	98.33	108.67
1	C	35	ILE	O-C-N	-6.63	116.02	123.18
1	D	63	HIS	CE1-NE2-CD2	-6.62	102.38	109.00
1	E	125	ASP	CA-CB-CG	6.62	119.22	112.60
1	H	90	ASP	CA-CB-CG	6.60	119.20	112.60
1	B	63	HIS	CE1-NE2-CD2	-6.58	102.42	109.00
1	A	63	HIS	CB-CG-CD2	-6.58	122.65	131.20
1	H	32	TRP	CG-CD2-CE3	6.56	140.46	133.90
1	H	139	ASN	CA-CB-CG	6.55	119.15	112.60
1	G	79	ARG	CB-CG-CD	-6.55	96.24	111.30
1	J	90	ASP	CA-CB-CG	6.53	119.13	112.60
1	C	121	GLU	N-CA-C	6.51	119.38	111.82
1	A	36	LYS	CB-CG-CD	-6.51	96.32	111.30
1	C	43	HIS	CB-CG-CD2	-6.51	122.74	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	139	ASN	CB-CG-ND2	6.50	126.15	116.40
1	I	120	HIS	CB-CG-ND1	6.50	132.45	122.70
1	E	80	HIS	CA-CB-CG	6.50	120.30	113.80
1	C	43	HIS	CB-CG-ND1	6.49	132.44	122.70
1	C	79	ARG	CB-CG-CD	-6.49	96.38	111.30
1	D	65	ASN	O-C-N	-6.48	115.98	121.23
1	G	45	PHE	O-C-N	-6.42	115.04	123.13
1	E	35	ILE	N-CA-C	-6.42	98.90	108.46
1	A	120	HIS	CB-CG-CD2	-6.39	122.90	131.20
1	D	50	PHE	CA-CB-CG	-6.36	107.44	113.80
1	D	47	VAL	N-CA-C	-6.34	98.60	107.80
1	A	109	ASP	CA-CB-CG	6.32	118.92	112.60
1	A	99	ILE	N-CA-C	-6.31	99.11	108.45
1	F	48	HIS	CE1-NE2-CD2	-6.30	102.70	109.00
1	E	86	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	D	25	SER	N-CA-C	6.29	124.19	110.80
1	C	12	GLY	CA-C-N	6.29	125.91	119.56
1	C	12	GLY	C-N-CA	6.29	125.91	119.56
1	F	46	HIS	CB-CG-CD2	-6.28	123.03	131.20
1	D	121	GLU	O-C-N	6.28	128.54	122.07
1	J	139	ASN	OD1-CG-ND2	-6.28	116.32	122.60
1	E	90	ASP	CA-CB-CG	6.28	118.88	112.60
1	D	106	LEU	N-CA-C	-6.27	104.79	112.88
1	F	12	GLY	CA-C-N	6.26	125.83	119.19
1	F	12	GLY	C-N-CA	6.26	125.83	119.19
1	I	112	ILE	N-CA-C	-6.24	106.66	112.83
1	A	63	HIS	ND1-CE1-NE2	6.23	114.63	108.40
1	I	63	HIS	CB-CG-CD2	-6.23	123.10	131.20
1	C	13	PRO	N-CA-C	6.23	121.65	113.86
1	I	105	SER	CA-CB-OG	-6.22	98.65	111.10
1	C	22	GLN	OE1-CD-NE2	-6.21	116.39	122.60
1	B	120	HIS	CB-CG-CD2	-6.21	123.12	131.20
1	H	153	GLN	OE1-CD-NE2	-6.20	116.40	122.60
1	H	63	HIS	CE1-NE2-CD2	-6.19	102.81	109.00
1	J	79	ARG	NE-CZ-NH1	6.18	127.68	121.50
1	G	47	VAL	N-CA-C	-6.17	99.54	108.17
1	C	79	ARG	NE-CZ-NH1	6.16	127.66	121.50
1	G	80	HIS	CA-CB-CG	6.16	119.96	113.80
1	I	46	HIS	CB-CG-CD2	-6.15	123.21	131.20
1	G	86	ASN	CB-CG-ND2	6.14	125.61	116.40
1	B	12	GLY	CA-C-N	6.14	125.84	119.64
1	B	12	GLY	C-N-CA	6.14	125.84	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	92	ASP	CA-CB-CG	6.13	118.73	112.60
1	I	12	GLY	CA-C-N	6.13	125.75	119.56
1	I	12	GLY	C-N-CA	6.13	125.75	119.56
1	I	139	ASN	CA-CB-CG	6.10	118.70	112.60
1	B	35	ILE	N-CA-C	-6.09	98.70	107.78
1	G	131	ASN	CA-CB-CG	6.08	118.68	112.60
1	G	53	ASN	CB-CG-ND2	6.07	125.51	116.40
1	G	46	HIS	CB-CG-CD2	-6.07	123.31	131.20
1	D	37	GLY	N-CA-C	-6.06	106.88	115.43
1	I	131	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	G	43	HIS	CB-CG-CD2	-6.04	123.35	131.20
1	C	53	ASN	CA-CB-CG	6.03	118.63	112.60
1	E	2	THR	N-CA-C	-6.03	105.58	113.12
1	C	26	ASN	OD1-CG-ND2	-6.02	116.58	122.60
1	C	63	HIS	ND1-CE1-NE2	6.02	114.42	108.40
1	A	63	HIS	CE1-NE2-CD2	-6.02	102.98	109.00
1	H	99	ILE	N-CA-C	-6.02	99.82	108.42
1	A	128	LYS	N-CA-C	-6.01	106.20	112.93
1	F	11	ASP	N-CA-C	-6.01	101.24	109.71
1	F	63	HIS	CB-CG-CD2	-6.00	123.40	131.20
1	E	124	ASP	CA-CB-CG	6.00	118.59	112.60
1	I	119	VAL	N-CA-C	-5.99	99.78	108.17
1	B	43	HIS	CA-C-N	5.98	125.78	120.10
1	B	43	HIS	C-N-CA	5.98	125.78	120.10
1	F	150	GLY	O-C-N	-5.97	118.41	123.60
1	J	53	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	A	80	HIS	N-CA-C	-5.96	101.18	110.42
1	D	90	ASP	CA-CB-CG	5.96	118.56	112.60
1	D	131	ASN	OD1-CG-ND2	-5.94	116.66	122.60
1	E	46	HIS	CB-CG-CD2	-5.94	123.48	131.20
1	H	32	TRP	CB-CG-CD1	-5.89	118.06	126.90
1	H	2	THR	CA-CB-CG2	5.88	120.49	110.50
1	G	77	GLU	CA-CB-CG	5.87	125.85	114.10
1	G	35	ILE	N-CA-C	-5.87	99.71	108.46
1	E	26	ASN	OD1-CG-ND2	-5.87	116.73	122.60
1	C	120	HIS	CB-CG-CD2	-5.85	123.59	131.20
1	E	106	LEU	N-CA-C	-5.85	105.98	113.23
1	G	139	ASN	CB-CG-ND2	5.84	125.17	116.40
1	H	45	PHE	CA-CB-CG	5.84	119.64	113.80
1	I	53	ASN	OD1-CG-ND2	-5.84	116.76	122.60
1	D	126	LEU	N-CA-CB	-5.83	103.59	112.28
1	I	120	HIS	N-CA-C	5.83	119.59	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	ILE	N-CA-C	-5.83	99.15	107.77
1	C	15	GLN	OE1-CD-NE2	-5.82	116.78	122.60
1	G	86	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	J	143	ARG	N-CA-C	-5.81	99.73	108.96
1	E	63	HIS	CB-CG-CD2	-5.79	123.68	131.20
1	A	53	ASN	CA-CB-CG	-5.78	106.82	112.60
1	D	35	ILE	N-CA-C	-5.78	100.16	108.48
1	F	120	HIS	CB-CG-CD2	-5.77	123.70	131.20
1	E	76	ASP	O-C-N	-5.77	115.69	123.19
1	J	121	GLU	O-C-N	5.77	128.01	122.07
1	F	53	ASN	CB-CG-ND2	5.76	125.04	116.40
1	F	53	ASN	OD1-CG-ND2	-5.75	116.85	122.60
1	C	65	ASN	CA-CB-CG	5.75	118.35	112.60
1	A	8	LEU	O-C-N	-5.74	116.53	123.13
1	G	63	HIS	CB-CG-CD2	-5.74	123.74	131.20
1	J	131	ASN	CA-CB-CG	5.73	118.33	112.60
1	E	103	VAL	CG1-CB-CG2	-5.69	98.27	110.80
1	F	22	GLN	OE1-CD-NE2	-5.69	116.91	122.60
1	E	109	ASP	CA-C-O	5.69	126.56	120.70
1	B	65	ASN	N-CA-CB	-5.69	102.85	111.21
1	E	73	GLY	O-C-N	-5.67	116.09	121.77
1	B	71	HIS	CB-CG-CD2	-5.67	123.83	131.20
1	E	25	SER	N-CA-C	5.67	122.88	110.80
1	B	38	LEU	N-CA-CB	-5.67	101.39	110.63
1	H	77	GLU	N-CA-C	-5.67	104.72	111.69
1	A	124	ASP	CA-CB-CG	5.67	118.27	112.60
1	I	19	ASN	CB-CG-ND2	5.66	124.89	116.40
1	G	52	ASP	CA-CB-CG	5.65	118.25	112.60
1	E	153	GLN	OE1-CD-NE2	-5.65	116.95	122.60
1	I	32	TRP	CB-CG-CD1	-5.65	118.43	126.90
1	E	63	HIS	CE1-NE2-CD2	-5.65	103.35	109.00
1	I	26	ASN	N-CA-C	-5.64	106.99	112.97
1	C	135	THR	CA-C-O	5.63	125.93	119.35
1	J	45	PHE	N-CA-C	-5.63	99.11	108.34
1	I	43	HIS	CB-CG-CD2	-5.61	123.90	131.20
1	E	107	SER	CA-CB-OG	5.61	122.33	111.10
1	B	124	ASP	CA-CB-CG	5.60	118.20	112.60
1	G	42	LEU	O-C-N	5.59	129.65	123.16
1	B	32	TRP	CG-CD2-CE3	5.59	139.49	133.90
1	D	71	HIS	CB-CG-CD2	-5.59	123.93	131.20
1	D	69	ARG	NE-CZ-NH2	-5.58	114.18	119.20
1	I	100	GLU	N-CA-C	-5.57	99.34	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	50	PHE	CA-CB-CG	-5.55	108.25	113.80
1	E	69	ARG	N-CA-C	-5.54	100.99	109.41
1	B	108	GLY	O-C-N	-5.53	117.49	122.86
1	J	25	SER	N-CA-C	5.53	122.58	110.80
1	F	33	GLY	O-C-N	-5.53	117.96	124.15
1	H	43	HIS	CB-CG-CD2	-5.51	124.03	131.20
1	J	54	THR	N-CA-CB	-5.51	101.64	110.19
1	G	65	ASN	O-C-N	-5.51	116.57	121.20
1	H	96	ASP	CA-CB-CG	-5.51	107.09	112.60
1	A	2	THR	N-CA-C	-5.48	105.72	112.90
1	A	125	ASP	CA-CB-CG	5.48	118.08	112.60
1	C	22	GLN	CG-CD-NE2	5.46	124.59	116.40
1	F	3	LYS	N-CA-C	5.46	118.34	109.06
1	I	13	PRO	N-CA-C	5.46	120.68	113.86
1	J	54	THR	CA-CB-OG1	-5.45	101.42	109.60
1	I	109	ASP	CA-CB-CG	5.44	118.04	112.60
1	F	109	ASP	CA-CB-CG	5.43	118.03	112.60
1	B	22	GLN	CG-CD-NE2	5.43	124.55	116.40
1	G	136	LYS	N-CA-C	-5.43	104.84	112.12
1	A	137	THR	CA-C-O	5.43	124.79	118.77
1	G	24	GLU	N-CA-C	-5.42	100.56	109.40
1	I	132	GLU	CA-CB-CG	-5.42	103.27	114.10
1	C	63	HIS	CE1-NE2-CD2	-5.41	103.59	109.00
1	H	14	VAL	CA-C-O	5.41	126.36	120.57
1	E	12	GLY	CA-C-N	5.40	125.05	119.05
1	E	12	GLY	C-N-CA	5.40	125.05	119.05
1	B	32	TRP	CB-CG-CD1	-5.40	118.80	126.90
1	D	35	ILE	O-C-N	-5.40	117.35	123.18
1	H	79	ARG	NE-CZ-NH1	5.39	126.89	121.50
1	H	48	HIS	CB-CG-ND1	5.39	130.78	122.70
1	J	109	ASP	CA-CB-CG	5.38	117.98	112.60
1	J	94	VAL	O-C-N	-5.38	117.23	122.93
1	E	69	ARG	CG-CD-NE	-5.38	100.17	112.00
1	H	63	HIS	CB-CG-CD2	-5.38	124.21	131.20
1	E	119	VAL	N-CA-C	-5.38	100.64	108.17
1	A	131	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	I	79	ARG	CA-CB-CG	5.37	124.84	114.10
1	C	65	ASN	N-CA-CB	-5.37	104.43	111.09
1	A	139	ASN	CB-CG-ND2	5.37	124.45	116.40
1	G	2	THR	CA-CB-OG1	-5.37	101.55	109.60
1	D	63	HIS	CB-CG-CD2	-5.36	124.24	131.20
1	C	35	ILE	N-CA-C	-5.35	100.78	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	HIS	CB-CG-CD2	-5.34	124.25	131.20
1	D	133	GLU	N-CA-C	5.33	117.51	111.11
1	B	72	GLY	N-CA-C	-5.33	103.46	111.19
1	D	43	HIS	CB-CG-ND1	5.31	130.67	122.70
1	D	139	ASN	N-CA-C	5.31	118.76	111.54
1	C	3	LYS	CG-CD-CE	-5.30	99.10	111.30
1	F	110	HIS	CB-CG-CD2	-5.28	124.33	131.20
1	J	72	GLY	O-C-N	-5.28	117.31	123.44
1	H	124	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	22	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	H	39	THR	N-CA-C	-5.27	103.43	110.55
1	F	48	HIS	ND1-CE1-NE2	5.27	113.67	108.40
1	F	73	GLY	CA-C-N	5.27	125.58	119.47
1	F	73	GLY	C-N-CA	5.27	125.58	119.47
1	B	77	GLU	N-CA-C	-5.27	104.97	111.40
1	C	150	GLY	CA-C-O	-5.27	115.71	121.77
1	F	22	GLN	CA-C-O	5.26	125.82	120.24
1	E	139	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	G	120	HIS	CB-CG-CD2	-5.26	124.36	131.20
1	F	120	HIS	CB-CG-ND1	5.25	130.58	122.70
1	I	53	ASN	CB-CG-ND2	5.25	124.28	116.40
1	B	53	ASN	CB-CG-ND2	5.24	124.26	116.40
1	E	11	ASP	CA-CB-CG	5.24	117.84	112.60
1	E	43	HIS	CB-CG-CD2	-5.24	124.39	131.20
1	G	143	ARG	O-C-N	-5.24	116.03	122.68
1	B	45	PHE	CA-CB-CG	5.23	119.03	113.80
1	C	9	LYS	CA-CB-CG	-5.22	103.66	114.10
1	A	65	ASN	CA-CB-CG	5.22	117.82	112.60
1	F	101	ASP	CA-CB-CG	-5.21	107.39	112.60
1	A	139	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	B	80	HIS	CA-CB-CG	5.21	119.01	113.80
1	C	46	HIS	CA-CB-CG	5.20	119.00	113.80
1	H	86	ASN	CB-CG-ND2	5.19	124.18	116.40
1	C	15	GLN	CG-CD-NE2	5.18	124.17	116.40
1	D	119	VAL	N-CA-C	-5.17	100.97	108.36
1	I	88	THR	N-CA-C	5.17	116.95	108.52
1	A	8	LEU	N-CA-CB	-5.17	101.49	110.17
1	I	128	LYS	CB-CG-CD	-5.16	99.42	111.30
1	B	76	ASP	N-CA-C	-5.16	102.83	110.46
1	E	46	HIS	CB-CG-ND1	5.16	130.43	122.70
1	C	63	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	F	153	GLN	OE1-CD-NE2	-5.13	117.47	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	126	LEU	N-CA-C	5.13	118.83	112.47
1	I	83	ASP	N-CA-C	5.13	117.02	107.99
1	B	153	GLN	CA-CB-CG	5.12	124.35	114.10
1	D	43	HIS	CA-CB-CG	-5.12	108.67	113.80
1	B	86	ASN	CA-CB-CG	5.12	117.72	112.60
1	A	71	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	F	23	LYS	CB-CG-CD	-5.12	99.53	111.30
1	C	11	ASP	N-CA-C	5.11	119.50	113.16
1	F	137	THR	CA-C-O	5.10	124.44	118.77
1	F	26	ASN	CB-CG-ND2	5.10	124.05	116.40
1	E	28	PRO	N-CA-C	5.10	119.21	111.15
1	A	15	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	I	48	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	B	142	SER	CA-CB-OG	-5.09	100.93	111.10
1	D	123	ALA	N-CA-C	5.09	117.61	110.23
1	J	124	ASP	N-CA-C	-5.08	101.68	109.76
1	C	55	ALA	N-CA-C	-5.07	104.27	110.61
1	F	42	LEU	N-CA-C	5.07	117.82	109.76
1	B	37	GLY	CA-C-O	5.07	124.89	119.06
1	G	96	ASP	CA-C-O	-5.06	114.62	120.49
1	H	153	GLN	CG-CD-NE2	5.06	123.99	116.40
1	B	43	HIS	CB-CG-ND1	5.06	130.29	122.70
1	G	69	ARG	CA-CB-CG	-5.06	103.98	114.10
1	E	71	HIS	O-C-N	5.06	128.98	123.01
1	F	65	ASN	N-CA-C	5.05	116.04	108.76
1	J	142	SER	N-CA-C	5.05	116.81	110.24
1	J	38	LEU	O-C-N	-5.05	117.32	123.03
1	I	73	GLY	CA-C-N	5.04	126.14	119.84
1	I	73	GLY	C-N-CA	5.04	126.14	119.84
1	A	120	HIS	CB-CG-ND1	5.04	130.26	122.70
1	E	32	TRP	O-C-N	-5.04	115.79	122.74
1	B	30	LYS	O-C-N	-5.04	117.15	123.04
1	E	32	TRP	CB-CG-CD1	-5.03	119.36	126.90
1	C	11	ASP	CA-CB-CG	-5.02	107.58	112.60
1	E	73	GLY	CA-C-N	5.02	124.68	119.56
1	E	73	GLY	C-N-CA	5.02	124.68	119.56
1	B	38	LEU	CB-CA-C	5.01	117.97	109.50
1	H	59	SER	N-CA-C	5.01	119.15	113.19
1	A	78	GLU	CB-CG-CD	5.01	121.12	112.60
1	H	52	ASP	CA-CB-CG	5.00	117.61	112.60
1	F	35	ILE	N-CA-C	-5.00	101.28	108.48
1	G	96	ASP	N-CA-C	-5.00	101.60	109.25

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	12	GLY	Peptide

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	A	1112	0	1077	9	0
1	B	1112	0	1077	11	0
1	C	1112	0	1077	9	0
1	D	1112	0	1077	11	0
1	E	1112	0	1077	18	0
1	F	1112	0	1077	9	0
1	G	1112	0	1077	11	0
1	H	1112	0	1077	15	0
1	I	1112	0	1077	16	0
1	J	1112	0	1077	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	1	0	0	0	0
4	F	5	0	0	0	0
4	I	5	0	0	0	0
5	A	56	0	0	0	0
5	B	54	0	0	1	0
5	C	43	0	0	1	0
5	D	43	0	0	1	0
5	E	39	0	0	0	0
5	F	52	0	0	1	0
5	G	63	0	0	0	0
5	H	63	0	0	1	0
5	I	46	0	0	1	0
5	J	40	0	0	1	0
All	All	11649	0	10770	117	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (117) 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:119:VAL:HG12	1:B:145:ALA:HB3	1.71	0.72
1:J:0:ACE:H1	1:J:107:SER:HA	1.70	0.72
1:E:70:LYS:HD2	1:E:135:THR:HB	1.72	0.71
1:I:14:VAL:HG22	1:I:145:ALA:HB2	1.73	0.70
1:I:31:VAL:HG13	1:I:99:ILE:HB	1.74	0.69
1:C:43:HIS:HD2	1:C:120:HIS:O	1.77	0.67
1:A:118:VAL:HG11	1:A:143:ARG:HG2	1.76	0.67
1:D:31:VAL:HG13	1:D:99:ILE:HB	1.79	0.65
1:B:132:GLU:HG2	1:B:136:LYS:HE2	1.79	0.64
1:H:14:VAL:HG11	1:H:144:LEU:HB3	1.81	0.61
1:C:50:PHE:CE1	1:H:153:GLN:HB3	2.37	0.60
1:E:119:VAL:HG12	1:E:145:ALA:HB3	1.82	0.59
1:C:14:VAL:HG21	1:C:144:LEU:HD13	1.84	0.59
1:A:79:ARG:HD3	1:A:80:HIS:O	2.05	0.56
1:F:76:ASP:O	1:F:79:ARG:HG2	2.06	0.56
1:G:121:GLU:HA	1:G:144:LEU:HD11	1.88	0.55
1:D:39:THR:O	1:D:43:HIS:HE1	1.89	0.55
1:F:14:VAL:HA	1:F:36:LYS:O	2.06	0.55
1:I:65:ASN:HB2	1:I:80:HIS:HB3	1.89	0.55
1:E:8:LEU:HD11	1:E:117:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ARG:HD3	1:A:78:GLU:HA	1.90	0.54
1:J:112:ILE:HA	1:J:115:ARG:HD2	1.90	0.54
1:A:31:VAL:HG13	1:A:99:ILE:HB	1.90	0.53
1:C:81:VAL:HG13	1:C:103:VAL:HG12	1.91	0.53
1:J:43:HIS:HE1	5:J:175:HOH:O	1.93	0.52
1:E:118:VAL:HG22	1:E:146:CYS:HB3	1.93	0.51
1:B:67:LEU:HD12	5:B:175:HOH:O	2.10	0.51
1:C:50:PHE:CZ	1:H:153:GLN:HB3	2.45	0.51
1:I:73:GLY:HA3	1:I:126:LEU:HD22	1.92	0.51
1:F:64:PHE:CE1	1:F:66:PRO:HD3	2.46	0.50
1:A:14:VAL:HA	1:A:36:LYS:O	2.12	0.50
1:C:73:GLY:HA2	1:C:126:LEU:HD22	1.94	0.50
1:I:133:GLU:HA	1:I:136:LYS:HE3	1.94	0.50
1:F:58:THR:HG22	5:F:389:HOH:O	2.11	0.49
1:A:131:ASN:O	1:A:134:SER:HB3	2.12	0.49
1:G:105:SER:O	1:G:111:SER:HA	2.12	0.49
1:D:17:ILE:HD13	1:I:54:THR:HG22	1.94	0.49
1:J:49:GLU:O	1:J:115:ARG:NH1	2.45	0.48
1:J:84:LEU:HD11	1:J:104:ILE:HG21	1.96	0.48
1:H:73:GLY:HA2	1:H:126:LEU:HD22	1.95	0.48
1:D:112:ILE:HD12	1:D:149:ILE:HD13	1.95	0.48
1:H:20:PHE:CD1	1:H:31:VAL:HB	2.48	0.48
1:E:81:VAL:HG13	1:E:103:VAL:HG12	1.95	0.48
1:C:91:LYS:HG3	5:C:165:HOH:O	2.13	0.47
1:I:73:GLY:CA	1:I:126:LEU:HD22	2.44	0.47
1:G:20:PHE:CD2	1:G:31:VAL:HB	2.49	0.47
1:I:116:THR:CG2	1:I:146:CYS:HB2	2.45	0.47
1:G:38:LEU:O	1:G:93:GLY:HA2	2.14	0.47
1:G:45:PHE:CZ	1:G:117:LEU:HD21	2.50	0.47
1:B:43:HIS:HA	1:B:122:LYS:O	2.15	0.46
1:E:120:HIS:HB3	1:E:140:ALA:O	2.14	0.46
1:C:31:VAL:HG13	1:C:99:ILE:HB	1.98	0.46
1:G:76:ASP:O	1:G:79:ARG:HG2	2.15	0.46
1:J:52:ASP:HB3	1:J:59:SER:O	2.16	0.46
1:I:108:GLY:O	1:I:111:SER:HB2	2.15	0.46
1:B:51:GLY:HA3	1:B:114:GLY:O	2.16	0.46
1:E:2:THR:O	1:E:21:GLU:HA	2.16	0.46
1:H:120:HIS:HB3	1:H:140:ALA:O	2.16	0.45
1:H:51:GLY:HA2	1:H:116:THR:OG1	2.17	0.45
1:H:64:PHE:CZ	1:H:66:PRO:HG3	2.52	0.45
1:E:71:HIS:CD2	1:E:138:GLY:HA3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLY:HA2	1:A:116:THR:OG1	2.16	0.45
1:H:90:ASP:HB2	5:H:206:HOH:O	2.17	0.45
1:I:36:LYS:HA	1:I:93:GLY:O	2.16	0.45
1:J:92:ASP:O	1:J:94:VAL:HG23	2.17	0.44
1:I:79:ARG:HD3	1:I:80:HIS:O	2.18	0.44
1:B:14:VAL:HG22	1:B:145:ALA:HB2	2.00	0.44
1:I:71:HIS:HB2	1:I:80:HIS:CE1	2.52	0.44
1:J:116:THR:CG2	1:J:146:CYS:HB2	2.47	0.44
1:I:21:GLU:O	1:I:29:VAL:HA	2.18	0.44
1:G:20:PHE:CE2	1:G:31:VAL:HB	2.53	0.44
1:A:69:ARG:HH11	1:A:69:ARG:HG2	1.82	0.44
1:D:40:GLU:HG3	1:D:90:ASP:C	2.42	0.44
1:D:89:ALA:HA	1:D:94:VAL:O	2.18	0.43
1:F:19:ASN:O	1:F:31:VAL:HA	2.17	0.43
1:E:116:THR:CG2	1:E:146:CYS:HB2	2.48	0.43
1:J:71:HIS:HB3	1:J:135:THR:HA	1.99	0.43
1:E:113:ILE:HG21	1:E:151:ILE:HG13	2.00	0.43
1:G:71:HIS:HB3	1:G:135:THR:HA	2.00	0.43
1:C:121:GLU:HG3	1:C:144:LEU:HD21	2.01	0.43
1:F:117:LEU:O	1:F:146:CYS:HA	2.17	0.43
1:B:117:LEU:O	1:B:146:CYS:HA	2.18	0.43
1:I:117:LEU:O	1:I:146:CYS:HA	2.19	0.43
1:D:103:VAL:HG13	5:D:176:HOH:O	2.19	0.43
1:I:10:GLY:HA3	1:I:144:LEU:O	2.19	0.43
1:B:116:THR:CG2	1:B:146:CYS:HB2	2.49	0.42
1:D:14:VAL:HA	1:D:36:LYS:O	2.19	0.42
1:G:49:GLU:HG2	1:G:115:ARG:NH1	2.35	0.42
1:H:1:ALA:HB2	1:H:151:ILE:HG23	2.01	0.42
1:E:7:VAL:O	1:E:147:GLY:HA3	2.19	0.42
1:A:34:SER:HA	1:A:95:ALA:O	2.19	0.42
1:D:20:PHE:CD1	1:D:31:VAL:HB	2.55	0.42
1:H:8:LEU:O	1:H:15:GLN:HA	2.20	0.42
1:E:139:ASN:HD22	1:E:139:ASN:N	2.18	0.42
1:F:91:LYS:N	1:F:91:LYS:HD3	2.35	0.42
1:G:18:ILE:HD13	1:G:33:GLY:HA3	2.02	0.42
1:E:118:VAL:HG11	1:E:143:ARG:HG2	2.00	0.42
1:H:125:ASP:O	1:H:127:GLY:N	2.53	0.41
1:J:8:LEU:O	1:J:15:GLN:HA	2.20	0.41
1:B:64:PHE:CE1	1:B:66:PRO:HD3	2.55	0.41
1:E:12:GLY:HA3	1:E:13:PRO:HD3	1.84	0.41
1:F:120:HIS:HB3	1:F:140:ALA:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:VAL:HG11	1:B:143:ARG:HG2	2.02	0.41
1:H:19:ASN:O	1:H:31:VAL:HA	2.21	0.41
1:I:65:ASN:HA	5:I:378:HOH:O	2.19	0.41
1:D:22:GLN:HB2	1:D:29:VAL:HG22	2.03	0.41
1:E:80:HIS:HE1	1:E:136:LYS:O	2.03	0.41
1:B:92:ASP:O	1:B:94:VAL:HG23	2.20	0.41
1:H:64:PHE:CE1	1:H:66:PRO:HG3	2.55	0.41
1:E:4:ALA:HA	1:E:152:ALA:H	1.86	0.41
1:J:67:LEU:HB2	1:J:69:ARG:HG2	2.03	0.41
1:H:14:VAL:HA	1:H:36:LYS:O	2.22	0.41
1:E:30:LYS:HE3	1:E:32:TRP:CE3	2.56	0.40
1:F:51:GLY:HA3	1:F:114:GLY:O	2.21	0.40
1:E:91:LYS:H	1:E:91:LYS:HG2	1.70	0.40
1:G:122:LYS:HB2	1:G:122:LYS:HE3	1.94	0.40
1:D:80:HIS:HE1	1:D:136:LYS:O	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	152/154 (99%)	146 (96%)	6 (4%)	0	100	100
1	B	152/154 (99%)	140 (92%)	12 (8%)	0	100	100
1	C	152/154 (99%)	146 (96%)	6 (4%)	0	100	100
1	D	152/154 (99%)	141 (93%)	10 (7%)	1 (1%)	18	34
1	E	152/154 (99%)	139 (91%)	11 (7%)	2 (1%)	9	18
1	F	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	18	34
1	G	152/154 (99%)	146 (96%)	6 (4%)	0	100	100
1	H	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	18	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	152/154 (99%)	144 (95%)	8 (5%)	0	100	100
1	J	152/154 (99%)	138 (91%)	10 (7%)	4 (3%)	4	7
All	All	1520/1540 (99%)	1430 (94%)	81 (5%)	9 (1%)	21	38

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	126	LEU
1	D	25	SER
1	J	24	GLU
1	J	25	SER
1	J	93	GLY
1	F	1	ALA
1	E	25	SER
1	E	103	VAL
1	J	103	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	A	117/117 (100%)	104 (89%)	13 (11%)	6	12
1	B	117/117 (100%)	105 (90%)	12 (10%)	7	14
1	C	117/117 (100%)	107 (92%)	10 (8%)	10	22
1	D	117/117 (100%)	108 (92%)	9 (8%)	12	25
1	E	117/117 (100%)	103 (88%)	14 (12%)	5	10
1	F	117/117 (100%)	100 (86%)	17 (14%)	3	6
1	G	117/117 (100%)	105 (90%)	12 (10%)	7	14
1	H	117/117 (100%)	102 (87%)	15 (13%)	4	9
1	I	117/117 (100%)	105 (90%)	12 (10%)	7	14
1	J	117/117 (100%)	107 (92%)	10 (8%)	10	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1170/1170 (100%)	1046 (89%)	124 (11%)	6 14

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	3	LYS
1	A	8	LEU
1	A	31	VAL
1	A	38	LEU
1	A	42	LEU
1	A	53	ASN
1	A	59	SER
1	A	70	LYS
1	A	77	GLU
1	A	79	ARG
1	A	96	ASP
1	A	100	GLU
1	F	2	THR
1	F	15	GLN
1	F	29	VAL
1	F	31	VAL
1	F	38	LEU
1	F	42	LEU
1	F	58	THR
1	F	62	PRO
1	F	69	ARG
1	F	75	LYS
1	F	79	ARG
1	F	91	LYS
1	F	102	SER
1	F	107	SER
1	F	136	LYS
1	F	142	SER
1	F	153	GLN
1	B	3	LYS
1	B	14	VAL
1	B	24	GLU
1	B	25	SER
1	B	38	LEU
1	B	39	THR
1	B	59	SER

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Mol	Chain	Res	Type
1	B	79	ARG
1	B	91	LYS
1	B	128	LYS
1	B	134	SER
1	B	153	GLN
1	G	7	VAL
1	G	23	LYS
1	G	24	GLU
1	G	31	VAL
1	G	34	SER
1	G	42	LEU
1	G	59	SER
1	G	62	PRO
1	G	79	ARG
1	G	97	VAL
1	G	98	SER
1	G	107	SER
1	C	8	LEU
1	C	31	VAL
1	C	38	LEU
1	C	42	LEU
1	C	59	SER
1	C	79	ARG
1	C	102	SER
1	C	107	SER
1	C	133	GLU
1	C	142	SER
1	H	14	VAL
1	H	25	SER
1	H	29	VAL
1	H	31	VAL
1	H	38	LEU
1	H	42	LEU
1	H	53	ASN
1	H	59	SER
1	H	67	LEU
1	H	68	SER
1	H	69	ARG
1	H	77	GLU
1	H	79	ARG
1	H	107	SER
1	H	113	ILE

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Mol	Chain	Res	Type
1	D	30	LYS
1	D	31	VAL
1	D	38	LEU
1	D	42	LEU
1	D	53	ASN
1	D	79	ARG
1	D	91	LYS
1	D	107	SER
1	D	153	GLN
1	I	11	ASP
1	I	14	VAL
1	I	15	GLN
1	I	29	VAL
1	I	31	VAL
1	I	36	LYS
1	I	42	LEU
1	I	59	SER
1	I	79	ARG
1	I	102	SER
1	I	111	SER
1	I	131	ASN
1	E	23	LYS
1	E	31	VAL
1	E	34	SER
1	E	38	LEU
1	E	53	ASN
1	E	58	THR
1	E	59	SER
1	E	62	PRO
1	E	75	LYS
1	E	77	GLU
1	E	102	SER
1	E	107	SER
1	E	109	ASP
1	E	139	ASN
1	J	25	SER
1	J	29	VAL
1	J	31	VAL
1	J	36	LYS
1	J	54	THR
1	J	59	SER
1	J	62	PRO

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Mol	Chain	Res	Type
1	J	79	ARG
1	J	96	ASP
1	J	103	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	F	15	GLN
1	F	153	GLN
1	B	139	ASN
1	G	26	ASN
1	G	110	HIS
1	C	15	GLN
1	C	43	HIS
1	H	153	GLN
1	D	43	HIS
1	I	110	HIS
1	I	131	ASN
1	I	139	ASN
1	E	19	ASN
1	E	26	ASN
1	E	153	GLN
1	J	139	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 20 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	F	356	-	4,4,4	0.35	0	6,6,6	0.27	0
4	SO4	I	357	-	4,4,4	0.36	0	6,6,6	0.21	0

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

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.