



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:33 AM UTC

PDB ID : 1Y3T / pdb_00001y3t
Title : Crystal structure of YxaG, a dioxygenase from *Bacillus subtilis*
Authors : Gopal, B.; Madan, L.L.; Betz, S.F.; Kossiakoff, A.A.
Deposited on : 2004-11-26
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

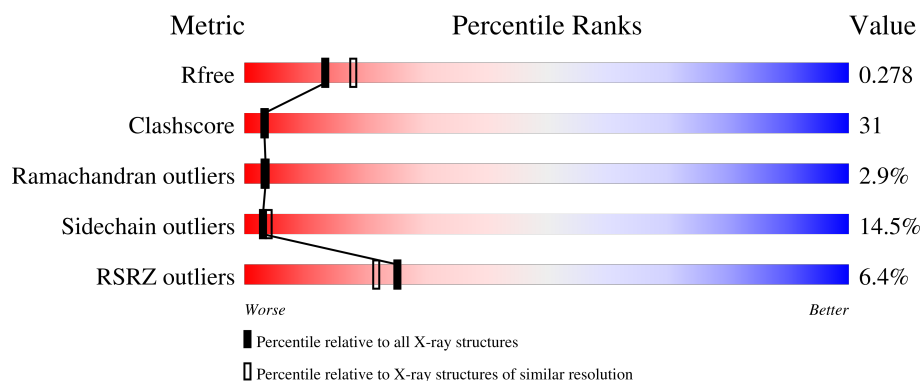
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	337	6% 37% 37% 16% 8% .
1	B	337	7% 39% 38% 12% 9% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5508 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 Hypothetical protein yxaG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	65	0	0
			2570	1630	444	485	11			
1	B	330	Total	C	N	O	S	61	0	0
			2571	1630	444	486	11			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		
2	B	2	Total	Fe	0	0
			2	2		

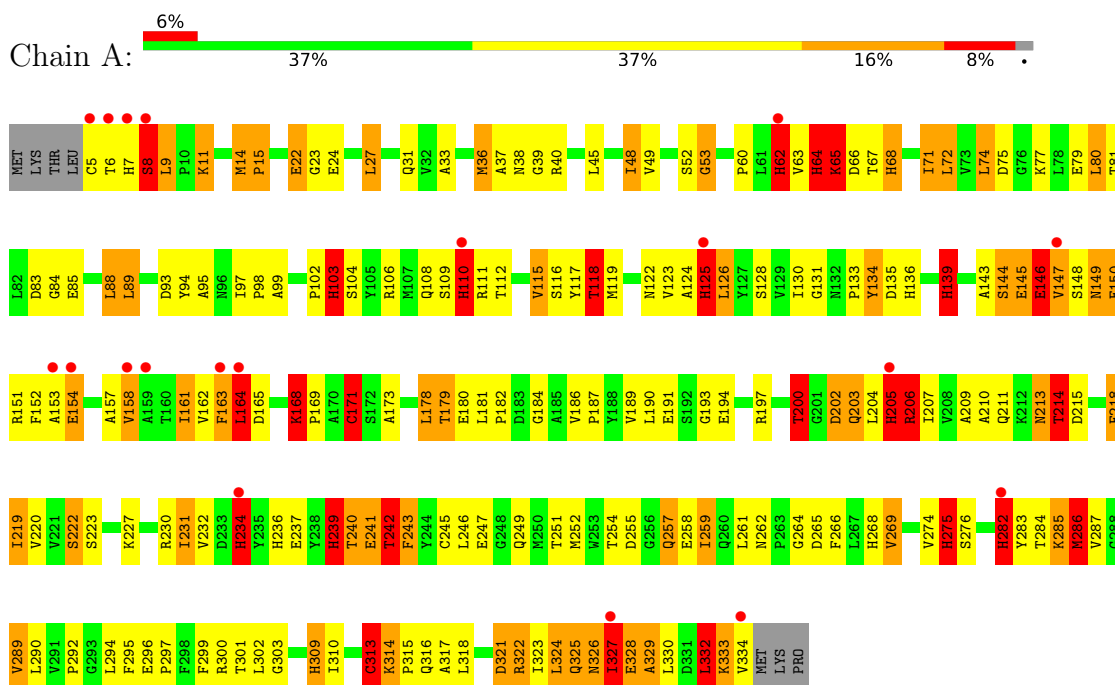
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	182	Total	O	0	0
			182	182		
3	B	181	Total	O	0	0
			181	181		

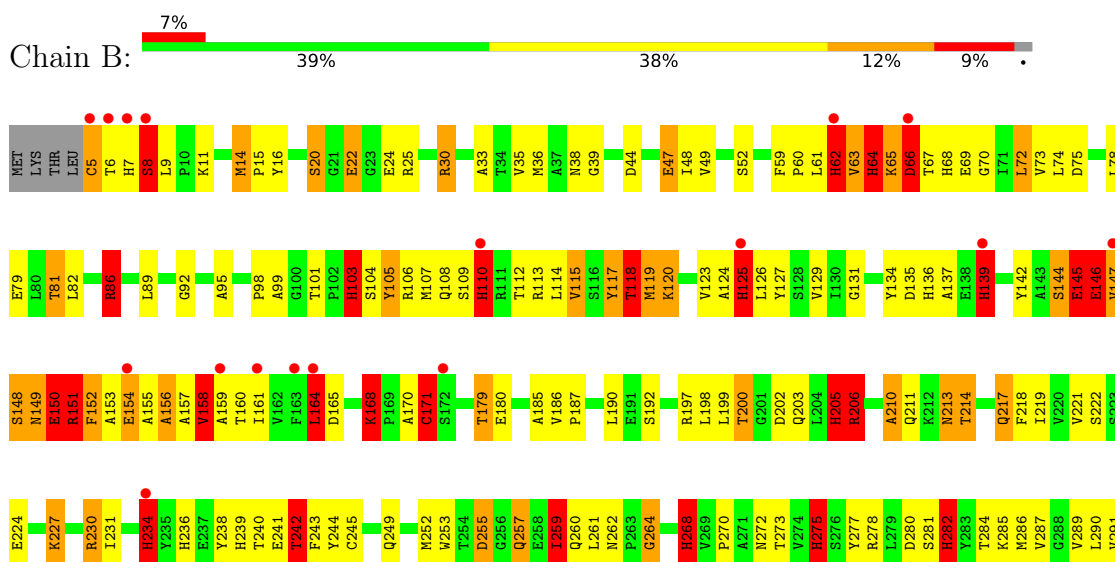
3 Residue-property plots

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

• Molecule 1: Hypothetical protein yxaG



• Molecule 1: Hypothetical protein yxaG





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.42Å 128.43Å 51.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.29 – 2.40 90.81 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.5 (91.29-2.40) 97.6 (90.81-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.217 , 0.277 0.221 , 0.278	Depositor DCC
R_{free} test set	1696 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5508	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	2.91	188/2635 (7.1%)	1.99	72/3576 (2.0%)
1	B	3.11	177/2636 (6.7%)	2.04	93/3578 (2.6%)
All	All	3.01	365/5271 (6.9%)	2.01	165/7154 (2.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	17
1	B	0	19
All	All	0	36

All (365) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	LEU	C-N	-47.50	0.67	1.33
1	B	8	SER	CA-C	42.37	2.09	1.52
1	A	164	LEU	C-N	-30.02	0.91	1.33
1	B	171	CYS	C-N	-27.79	0.94	1.33
1	A	110	HIS	CE1-NE2	25.12	1.57	1.32
1	B	149	ASN	C-N	-22.56	1.02	1.33
1	A	8	SER	CA-C	20.48	1.80	1.52
1	A	171	CYS	C-N	-20.48	1.03	1.33
1	B	8	SER	C-N	-20.16	0.91	1.33
1	B	8	SER	CA-CB	-19.41	1.20	1.53
1	A	8	SER	C-N	-19.37	0.93	1.33
1	A	152	PHE	C-N	-15.64	1.14	1.33
1	A	110	HIS	ND1-CE1	14.79	1.47	1.32
1	B	309	HIS	CA-CB	14.16	1.75	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	327	ILE	CA-C	12.56	1.68	1.52
1	A	275	HIS	CA-CB	-12.34	1.32	1.53
1	B	327	ILE	N-CA	11.75	1.61	1.46
1	A	328	GLU	CD-OE1	11.56	1.47	1.25
1	B	35	VAL	N-CA	-11.45	1.33	1.46
1	A	171	CYS	CA-CB	-11.33	1.34	1.53
1	A	205	HIS	CA-CB	10.55	1.68	1.53
1	A	289	VAL	CA-CB	-10.52	1.42	1.54
1	B	147	VAL	CB-CG1	10.45	1.87	1.52
1	B	147	VAL	CA-C	10.43	1.66	1.52
1	A	327	ILE	N-CA	10.42	1.60	1.46
1	B	79	GLU	CA-C	-10.41	1.39	1.52
1	A	103	HIS	CA-CB	-10.41	1.36	1.53
1	B	95	ALA	CA-CB	-10.37	1.37	1.53
1	B	151	ARG	N-CA	10.29	1.60	1.46
1	A	286	MET	SD-CE	10.19	2.05	1.79
1	B	33	ALA	CA-CB	10.06	1.67	1.53
1	A	143	ALA	CA-CB	-9.87	1.38	1.53
1	B	245	CYS	C-O	-9.83	1.12	1.24
1	A	328	GLU	N-CA	-9.80	1.34	1.46
1	B	62	HIS	CA-CB	-9.59	1.37	1.53
1	B	230	ARG	C-O	-9.54	1.12	1.23
1	A	24	GLU	C-O	9.46	1.35	1.24
1	A	153	ALA	CA-CB	9.41	1.68	1.53
1	B	243	PHE	C-O	-9.37	1.13	1.24
1	B	67	THR	C-O	-9.19	1.13	1.24
1	A	231	ILE	CA-CB	9.06	1.66	1.54
1	A	149	ASN	C-N	-8.99	1.22	1.33
1	A	103	HIS	C-O	-8.97	1.12	1.23
1	B	268	HIS	CA-CB	-8.97	1.39	1.53
1	A	64	HIS	CA-CB	8.96	1.65	1.53
1	A	151	ARG	N-CA	8.94	1.58	1.46
1	B	327	ILE	CA-C	8.88	1.64	1.52
1	B	277	TYR	C-O	-8.70	1.13	1.23
1	A	173	ALA	C-O	-8.67	1.13	1.24
1	B	328	GLU	CD-OE1	8.60	1.41	1.25
1	B	161	ILE	CA-CB	8.58	1.64	1.54
1	A	79	GLU	CA-CB	-8.55	1.41	1.53
1	A	182	PRO	CA-C	-8.46	1.42	1.52
1	B	312	PRO	CA-C	-8.45	1.44	1.52
1	B	110	HIS	CA-CB	8.37	1.67	1.53
1	B	275	HIS	CB-CG	-8.34	1.38	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	152	PHE	C-O	-8.31	1.13	1.24
1	A	232	VAL	C-O	8.29	1.34	1.24
1	A	147	VAL	CA-C	8.26	1.63	1.52
1	B	203	GLN	C-O	-8.23	1.13	1.24
1	B	151	ARG	CA-CB	-8.20	1.42	1.52
1	B	6	THR	C-O	8.20	1.34	1.23
1	A	139	HIS	CE1-NE2	-8.18	1.24	1.32
1	B	35	VAL	CA-CB	8.18	1.63	1.54
1	B	14	MET	N-CA	-8.17	1.38	1.46
1	B	261	LEU	C-O	-8.17	1.14	1.24
1	B	139	HIS	CA-C	8.16	1.62	1.53
1	B	262	ASN	C-O	-8.16	1.17	1.24
1	B	82	LEU	CA-C	-8.07	1.43	1.52
1	A	265	ASP	CG-OD2	8.05	1.40	1.25
1	A	258	GLU	C-O	-8.05	1.14	1.24
1	B	221	VAL	C-O	-8.04	1.15	1.24
1	B	15	PRO	C-O	8.01	1.32	1.23
1	B	238	TYR	C-O	-7.87	1.13	1.24
1	A	118	THR	CB-CG2	-7.83	1.26	1.52
1	A	65	LYS	CD-CE	7.81	1.75	1.52
1	B	327	ILE	CA-CB	7.80	1.64	1.54
1	A	115	VAL	N-CA	-7.77	1.37	1.46
1	A	209	ALA	CA-C	-7.75	1.43	1.52
1	A	6	THR	C-O	7.74	1.33	1.23
1	A	65	LYS	CG-CD	7.72	1.75	1.52
1	A	268	HIS	CA-C	7.68	1.62	1.52
1	A	202	ASP	C-O	-7.68	1.13	1.23
1	A	285	LYS	CA-C	-7.64	1.43	1.52
1	A	74	LEU	C-O	-7.62	1.13	1.23
1	A	163	PHE	C-O	-7.58	1.15	1.24
1	A	124	ALA	C-O	7.57	1.33	1.24
1	A	282	HIS	CA-CB	7.57	1.66	1.53
1	B	234	HIS	CA-CB	-7.56	1.41	1.53
1	B	202	ASP	C-O	-7.55	1.13	1.23
1	B	221	VAL	CA-CB	-7.49	1.44	1.54
1	B	154	GLU	CD-OE2	7.45	1.39	1.25
1	A	40	ARG	N-CA	-7.45	1.37	1.46
1	B	66	ASP	CG-OD2	7.43	1.39	1.25
1	A	190	LEU	CA-C	7.38	1.61	1.52
1	A	324	LEU	C-O	7.37	1.32	1.24
1	B	156	ALA	C-O	-7.36	1.14	1.24
1	A	283	TYR	C-O	-7.30	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	300	ARG	N-CA	7.29	1.55	1.46
1	A	81	THR	CA-CB	-7.27	1.43	1.53
1	B	110	HIS	CG-ND1	7.24	1.46	1.38
1	A	326	ASN	C-O	7.17	1.33	1.24
1	A	191	GLU	N-CA	-7.17	1.37	1.46
1	B	115	VAL	CA-CB	7.14	1.64	1.54
1	A	112	THR	C-O	7.13	1.32	1.24
1	B	101	THR	CA-C	7.12	1.61	1.52
1	A	266	PHE	C-O	7.12	1.32	1.23
1	B	286	MET	N-CA	-7.11	1.36	1.45
1	A	68	HIS	CA-C	7.05	1.62	1.52
1	B	39	GLY	C-O	-7.04	1.14	1.23
1	A	151	ARG	CA-C	7.02	1.61	1.53
1	B	301	THR	C-O	-7.01	1.15	1.24
1	A	240	THR	CA-CB	-6.99	1.43	1.53
1	B	117	TYR	CA-C	6.96	1.61	1.52
1	A	209	ALA	C-O	-6.95	1.15	1.23
1	A	213	ASN	N-CA	-6.92	1.36	1.46
1	A	158	VAL	CB-CG2	-6.88	1.29	1.52
1	A	330	LEU	N-CA	-6.88	1.38	1.46
1	B	328	GLU	N-CA	-6.88	1.37	1.46
1	B	151	ARG	C-O	-6.88	1.12	1.23
1	B	309	HIS	CE1-NE2	6.88	1.39	1.32
1	A	49	VAL	C-O	-6.84	1.16	1.24
1	A	106	ARG	CA-C	6.83	1.60	1.52
1	B	118	THR	CB-CG2	-6.82	1.30	1.52
1	A	110	HIS	CA-CB	-6.78	1.42	1.53
1	A	144	SER	CA-C	6.77	1.60	1.53
1	A	62	HIS	CB-CG	-6.76	1.40	1.50
1	B	186	VAL	C-O	-6.76	1.17	1.24
1	A	245	CYS	CA-CB	-6.72	1.43	1.53
1	B	144	SER	CB-OG	6.72	1.55	1.42
1	A	109	SER	CA-C	-6.70	1.44	1.52
1	A	321	ASP	CA-C	-6.69	1.44	1.52
1	B	309	HIS	CG-ND1	6.66	1.45	1.38
1	B	48	ILE	C-O	6.64	1.30	1.24
1	B	33	ALA	C-O	6.59	1.31	1.24
1	B	109	SER	CA-C	-6.58	1.45	1.52
1	B	154	GLU	CD-OE1	6.58	1.37	1.25
1	B	294	LEU	C-O	-6.58	1.16	1.24
1	B	151	ARG	CA-C	6.57	1.61	1.53
1	A	108	GLN	CA-C	6.56	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	GLU	CG-CD	6.53	1.68	1.52
1	A	243	PHE	N-CA	-6.52	1.38	1.46
1	B	213	ASN	CA-C	6.50	1.61	1.52
1	A	257	GLN	C-O	-6.48	1.16	1.23
1	A	193	GLY	C-O	-6.46	1.14	1.24
1	B	326	ASN	C-O	6.41	1.33	1.23
1	B	199	LEU	C-O	-6.40	1.16	1.24
1	B	296	GLU	CA-C	6.39	1.59	1.52
1	A	276	SER	CB-OG	-6.38	1.29	1.42
1	A	151	ARG	C-N	-6.38	1.24	1.33
1	A	200	THR	CB-CG2	-6.36	1.31	1.52
1	B	227	LYS	N-CA	6.36	1.54	1.46
1	B	198	LEU	CA-C	-6.35	1.45	1.52
1	B	78	LEU	C-O	-6.34	1.16	1.24
1	A	116	SER	CA-C	6.33	1.60	1.52
1	B	259	ILE	N-CA	6.32	1.53	1.46
1	A	130	ILE	C-O	-6.31	1.15	1.24
1	B	281	SER	N-CA	6.27	1.53	1.45
1	A	75	ASP	CA-C	6.25	1.60	1.52
1	A	45	LEU	C-O	-6.24	1.16	1.24
1	A	322	ARG	C-O	-6.24	1.16	1.24
1	B	217	GLN	CD-OE1	-6.24	1.11	1.23
1	A	60	PRO	C-O	6.23	1.30	1.23
1	B	139	HIS	CA-CB	6.22	1.64	1.53
1	B	79	GLU	C-O	-6.21	1.16	1.24
1	A	123	VAL	CA-CB	6.21	1.62	1.54
1	A	219	ILE	N-CA	6.19	1.52	1.46
1	A	71	ILE	CG1-CD1	6.19	1.75	1.51
1	A	75	ASP	C-O	6.17	1.31	1.23
1	B	62	HIS	ND1-CE1	6.16	1.38	1.32
1	A	161	ILE	CB-CG2	-6.14	1.32	1.52
1	B	287	VAL	N-CA	-6.12	1.39	1.46
1	B	309	HIS	CD2-NE2	6.12	1.44	1.37
1	B	328	GLU	CD-OE2	6.12	1.36	1.25
1	A	286	MET	C-O	-6.11	1.16	1.23
1	B	326	ASN	CG-ND2	6.11	1.46	1.33
1	B	278	ARG	C-O	6.11	1.31	1.23
1	B	60	PRO	C-O	6.10	1.30	1.23
1	A	299	PHE	C-O	6.10	1.31	1.24
1	A	234	HIS	CA-CB	6.09	1.64	1.53
1	A	283	TYR	CA-CB	6.08	1.63	1.53
1	A	234	HIS	CB-CG	-6.07	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	260	GLN	N-CA	-6.06	1.38	1.46
1	A	48	ILE	N-CA	-6.06	1.39	1.46
1	A	309	HIS	CA-CB	-6.04	1.44	1.53
1	A	123	VAL	N-CA	6.04	1.53	1.46
1	B	110	HIS	CA-C	-6.04	1.44	1.52
1	B	139	HIS	ND1-CE1	6.00	1.38	1.32
1	B	103	HIS	CA-CB	5.99	1.63	1.53
1	B	6	THR	CA-C	5.99	1.60	1.52
1	A	150	GLU	C-O	-5.98	1.16	1.24
1	A	134	TYR	N-CA	5.98	1.53	1.46
1	A	178	LEU	CA-C	5.98	1.60	1.52
1	B	155	ALA	C-O	-5.98	1.16	1.24
1	A	112	THR	CA-CB	5.97	1.62	1.53
1	A	268	HIS	N-CA	-5.97	1.38	1.46
1	B	106	ARG	NE-CZ	5.96	1.39	1.33
1	A	94	TYR	C-O	-5.96	1.16	1.24
1	A	64	HIS	CG-ND1	-5.95	1.31	1.38
1	A	274	VAL	C-O	-5.95	1.16	1.24
1	A	14	MET	C-O	-5.95	1.16	1.24
1	A	203	GLN	N-CA	-5.95	1.38	1.46
1	B	206	ARG	C-O	5.95	1.30	1.24
1	A	139	HIS	CG-CD2	-5.92	1.29	1.35
1	A	301	THR	C-O	-5.91	1.17	1.24
1	B	131	GLY	C-O	-5.90	1.16	1.23
1	A	72	LEU	CA-C	-5.90	1.45	1.52
1	A	151	ARG	C-O	-5.89	1.16	1.23
1	A	62	HIS	CA-C	5.89	1.59	1.52
1	B	52	SER	CB-OG	-5.89	1.30	1.42
1	B	112	THR	CA-C	-5.89	1.45	1.52
1	B	47	GLU	CD-OE1	5.87	1.36	1.25
1	A	158	VAL	CA-C	-5.87	1.45	1.52
1	A	287	VAL	C-O	-5.86	1.17	1.24
1	B	213	ASN	CA-CB	-5.86	1.43	1.53
1	A	147	VAL	CB-CG1	5.85	1.71	1.52
1	A	275	HIS	N-CA	-5.83	1.38	1.46
1	B	311	PHE	C-O	-5.83	1.16	1.23
1	B	105	TYR	C-O	-5.82	1.16	1.23
1	B	73	VAL	C-O	-5.82	1.16	1.24
1	A	65	LYS	CE-NZ	5.82	1.66	1.49
1	B	78	LEU	CA-CB	-5.82	1.44	1.53
1	A	286	MET	CA-C	-5.79	1.45	1.52
1	A	181	LEU	CA-C	5.79	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	THR	CA-CB	-5.78	1.45	1.53
1	A	220	VAL	CA-C	-5.78	1.45	1.52
1	A	207	ILE	C-O	-5.78	1.17	1.23
1	A	135	ASP	CA-C	-5.76	1.44	1.52
1	B	205	HIS	CA-CB	-5.75	1.43	1.53
1	A	33	ALA	CA-CB	5.75	1.61	1.53
1	A	218	PHE	C-O	5.74	1.30	1.23
1	A	289	VAL	C-O	5.73	1.30	1.24
1	A	323	ILE	C-O	5.73	1.30	1.24
1	A	249	GLN	CA-C	-5.73	1.45	1.52
1	B	244	TYR	N-CA	-5.72	1.39	1.46
1	B	124	ALA	C-N	-5.72	1.26	1.33
1	A	11	LYS	CA-C	-5.71	1.44	1.52
1	A	220	VAL	N-CA	-5.69	1.39	1.46
1	B	150	GLU	C-O	-5.69	1.16	1.24
1	B	154	GLU	CG-CD	5.69	1.66	1.52
1	B	221	VAL	CA-C	-5.68	1.45	1.52
1	A	173	ALA	CA-CB	-5.67	1.45	1.53
1	B	298	PHE	CA-C	-5.67	1.45	1.52
1	B	92	GLY	CA-C	5.66	1.59	1.51
1	A	332	LEU	CB-CG	-5.65	1.42	1.53
1	A	95	ALA	CA-CB	-5.64	1.45	1.53
1	A	241	GLU	CA-CB	-5.64	1.40	1.53
1	B	137	ALA	C-O	-5.63	1.17	1.24
1	B	302	LEU	C-O	-5.63	1.17	1.24
1	A	262	ASN	CA-C	5.62	1.61	1.52
1	A	194	GLU	N-CA	-5.59	1.38	1.45
1	B	146	GLU	CG-CD	5.59	1.66	1.52
1	B	63	VAL	CB-CG2	-5.59	1.34	1.52
1	A	149	ASN	C-O	5.58	1.31	1.24
1	B	192	SER	CA-CB	5.58	1.62	1.53
1	B	148	SER	C-N	-5.58	1.25	1.33
1	A	37	ALA	N-CA	-5.58	1.39	1.46
1	B	139	HIS	C-N	5.58	1.40	1.33
1	B	108	GLN	CB-CG	5.57	1.69	1.52
1	A	206	ARG	CA-CB	-5.57	1.45	1.53
1	B	281	SER	CB-OG	-5.56	1.31	1.42
1	A	247	GLU	CD-OE1	5.56	1.35	1.25
1	B	159	ALA	CA-CB	5.56	1.63	1.53
1	B	72	LEU	N-CA	-5.54	1.39	1.46
1	A	38	ASN	C-O	5.53	1.31	1.24
1	A	133	PRO	C-O	-5.53	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	GLU	N-CA	-5.52	1.39	1.46
1	B	107	MET	SD-CE	5.51	1.93	1.79
1	B	70	GLY	C-O	-5.49	1.17	1.23
1	B	114	LEU	C-O	-5.49	1.17	1.23
1	A	80	LEU	CA-C	5.49	1.59	1.52
1	A	83	ASP	C-O	-5.49	1.16	1.23
1	B	147	VAL	N-CA	-5.49	1.39	1.46
1	B	185	ALA	CA-C	5.48	1.60	1.52
1	B	144	SER	C-O	5.47	1.29	1.23
1	B	307	GLU	CD-OE2	5.47	1.35	1.25
1	A	163	PHE	CG-CD1	5.46	1.50	1.38
1	B	309	HIS	ND1-CE1	5.46	1.38	1.32
1	A	328	GLU	CG-CD	-5.46	1.38	1.52
1	A	27	LEU	CG-CD2	5.46	1.70	1.52
1	A	53	GLY	CA-C	-5.46	1.45	1.51
1	A	230	ARG	C-O	-5.45	1.17	1.23
1	B	156	ALA	CA-CB	5.45	1.62	1.53
1	B	255	ASP	N-CA	5.45	1.53	1.46
1	B	325	GLN	N-CA	5.45	1.53	1.46
1	A	52	SER	N-CA	-5.45	1.38	1.45
1	A	269	VAL	C-O	5.44	1.31	1.24
1	A	303	GLY	N-CA	-5.44	1.39	1.44
1	A	71	ILE	C-O	5.43	1.29	1.24
1	A	189	VAL	CB-CG2	5.42	1.70	1.52
1	B	49	VAL	C-O	-5.42	1.18	1.24
1	A	22	GLU	CA-C	5.42	1.60	1.53
1	A	123	VAL	CB-CG1	5.42	1.70	1.52
1	B	160	THR	N-CA	-5.42	1.39	1.46
1	B	309	HIS	N-CA	5.40	1.53	1.45
1	B	305	PRO	CA-CB	-5.39	1.46	1.53
1	A	9	LEU	N-CA	5.34	1.53	1.46
1	B	142	TYR	C-O	-5.34	1.17	1.23
1	B	272	ASN	N-CA	5.32	1.53	1.46
1	B	22	GLU	C-O	5.30	1.30	1.23
1	A	327	ILE	CG1-CD1	5.29	1.72	1.51
1	A	31	GLN	CA-CB	-5.28	1.44	1.53
1	B	273	THR	CA-CB	-5.28	1.45	1.53
1	B	5	CYS	CA-C	5.27	1.64	1.52
1	B	16	TYR	CA-C	-5.27	1.46	1.52
1	B	103	HIS	C-O	5.27	1.30	1.23
1	A	289	VAL	CA-C	5.27	1.58	1.52
1	B	268	HIS	C-O	-5.27	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	52	SER	C-N	-5.26	1.28	1.33
1	A	111	ARG	CZ-NH2	5.25	1.40	1.33
1	B	242	THR	C-O	-5.25	1.17	1.23
1	A	88	LEU	CA-C	5.23	1.59	1.53
1	B	139	HIS	CG-CD2	-5.22	1.30	1.35
1	A	222	SER	CB-OG	5.22	1.52	1.42
1	A	103	HIS	N-CA	-5.22	1.39	1.46
1	B	304	ASP	C-O	-5.22	1.17	1.24
1	B	120	LYS	CA-C	-5.21	1.46	1.53
1	A	284	THR	N-CA	-5.20	1.39	1.46
1	B	261	LEU	CG-CD2	-5.20	1.35	1.52
1	A	302	LEU	CA-C	5.20	1.59	1.52
1	B	313	CYS	C-O	-5.20	1.18	1.24
1	B	86	ARG	NE-CZ	5.19	1.38	1.33
1	B	137	ALA	CA-C	-5.18	1.46	1.52
1	A	108	GLN	CB-CG	5.18	1.68	1.52
1	A	39	GLY	CA-C	5.17	1.58	1.52
1	A	60	PRO	N-CA	5.17	1.53	1.47
1	B	119	MET	CG-SD	5.17	1.93	1.80
1	A	67	THR	CA-CB	-5.15	1.45	1.53
1	B	210	ALA	CA-CB	5.13	1.61	1.53
1	B	20	SER	C-O	5.13	1.30	1.24
1	A	237	GLU	C-O	-5.12	1.17	1.24
1	A	126	LEU	CA-CB	-5.12	1.45	1.53
1	B	44	ASP	CG-OD1	5.12	1.35	1.25
1	B	312	PRO	C-O	-5.12	1.17	1.23
1	B	60	PRO	CA-C	5.12	1.59	1.52
1	A	282	HIS	ND1-CE1	5.12	1.37	1.32
1	B	67	THR	CA-CB	-5.11	1.45	1.53
1	A	242	THR	C-O	-5.10	1.17	1.23
1	A	300	ARG	N-CA	5.10	1.52	1.46
1	A	111	ARG	CZ-NH1	5.09	1.39	1.32
1	A	111	ARG	C-O	-5.09	1.17	1.23
1	B	285	LYS	N-CA	-5.09	1.39	1.46
1	B	123	VAL	CA-CB	5.09	1.61	1.54
1	B	135	ASP	C-O	-5.08	1.17	1.24
1	A	125	HIS	C-O	5.08	1.30	1.24
1	A	5	CYS	CA-C	5.08	1.63	1.52
1	A	287	VAL	CA-C	5.08	1.58	1.52
1	B	145	GLU	C-O	5.07	1.30	1.24
1	B	334	VAL	CA-CB	5.07	1.68	1.54
1	A	264	GLY	C-N	-5.06	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	THR	CB-OG1	5.06	1.51	1.43
1	B	190	LEU	N-CA	-5.06	1.40	1.46
1	A	223	SER	CA-C	-5.06	1.46	1.52
1	A	184	GLY	C-O	5.06	1.29	1.23
1	A	85	GLU	C-O	-5.06	1.17	1.23
1	A	52	SER	C-O	-5.05	1.17	1.23
1	A	181	LEU	C-O	-5.05	1.17	1.24
1	B	157	ALA	C-O	-5.04	1.17	1.23
1	B	72	LEU	C-O	-5.03	1.18	1.24
1	A	246	LEU	C-N	-5.02	1.27	1.33
1	B	278	ARG	CZ-NH1	-5.02	1.25	1.32
1	B	64	HIS	N-CA	-5.01	1.40	1.46
1	A	261	LEU	CG-CD2	-5.01	1.36	1.52
1	B	30	ARG	C-O	-5.01	1.17	1.24
1	B	117	TYR	CG-CD2	-5.01	1.28	1.39

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	LEU	O-C-N	-20.92	94.77	122.59
1	B	8	SER	CA-C-N	15.64	159.97	121.80
1	B	8	SER	C-N-CA	15.64	159.97	121.80
1	B	8	SER	O-C-N	-14.86	102.83	122.59
1	A	110	HIS	ND1-CE1-NE2	-14.63	93.77	108.40
1	A	151	ARG	O-C-N	-14.00	105.80	122.46
1	A	8	SER	CA-C-N	11.61	150.13	121.80
1	A	8	SER	C-N-CA	11.61	150.13	121.80
1	A	327	ILE	CA-C-O	11.55	130.50	120.22
1	B	327	ILE	N-CA-C	11.45	124.72	107.77
1	B	8	SER	CA-CB-OG	-11.43	88.23	111.10
1	A	214	THR	OG1-CB-CG2	-11.29	86.72	109.30
1	B	139	HIS	N-CA-C	-11.28	95.50	109.83
1	B	309	HIS	CA-CB-CG	-10.82	102.98	113.80
1	A	152	PHE	CA-C-N	10.66	134.94	120.54
1	A	152	PHE	C-N-CA	10.66	134.94	120.54
1	B	147	VAL	O-C-N	10.07	135.16	122.57
1	B	103	HIS	CA-CB-CG	-9.84	103.96	113.80
1	A	151	ARG	CA-C-O	-9.71	111.21	122.37
1	B	151	ARG	N-CA-C	9.48	125.47	111.81
1	B	139	HIS	ND1-CE1-NE2	-9.14	99.26	108.40
1	B	268	HIS	CA-CB-CG	9.01	122.81	113.80
1	B	147	VAL	CA-C-N	8.89	138.52	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	VAL	C-N-CA	8.89	138.52	121.54
1	B	214	THR	OG1-CB-CG2	-8.80	91.69	109.30
1	A	151	ARG	N-CA-C	8.60	123.52	108.56
1	B	62	HIS	N-CA-C	8.59	121.20	108.14
1	B	164	LEU	O-C-N	-8.53	111.25	122.59
1	B	63	VAL	CA-C-N	-8.49	111.02	122.99
1	B	63	VAL	C-N-CA	-8.49	111.02	122.99
1	B	110	HIS	CA-CB-CG	-8.47	105.33	113.80
1	A	151	ARG	CA-CB-CG	-8.28	97.55	114.10
1	A	327	ILE	N-CA-C	8.25	121.45	107.18
1	B	8	SER	CB-CA-C	-8.15	94.19	110.42
1	B	64	HIS	CA-CB-CG	8.11	121.91	113.80
1	B	139	HIS	CA-CB-CG	-8.10	105.70	113.80
1	A	8	SER	O-C-N	-8.07	111.85	122.59
1	B	151	ARG	CB-CA-C	8.05	121.89	111.50
1	A	103	HIS	N-CA-C	8.05	120.75	108.52
1	B	179	THR	N-CA-CB	-8.03	100.22	110.90
1	A	239	HIS	N-CA-C	8.03	121.27	109.07
1	B	205	HIS	CA-CB-CG	8.01	121.81	113.80
1	B	110	HIS	CG-ND1-CE1	-7.96	95.77	109.30
1	B	8	SER	N-CA-C	-7.95	93.87	110.80
1	B	328	GLU	CB-CG-CD	-7.89	99.18	112.60
1	A	275	HIS	N-CA-CB	-7.88	99.58	111.56
1	B	275	HIS	CA-CB-CG	-7.82	105.98	113.80
1	B	293	GLY	O-C-N	-7.67	112.73	122.70
1	B	139	HIS	CB-CA-C	7.60	121.35	109.42
1	B	328	GLU	OE1-CD-OE2	-7.55	104.78	122.90
1	A	205	HIS	CA-CB-CG	-7.55	106.25	113.80
1	B	62	HIS	CA-CB-CG	7.54	121.34	113.80
1	A	234	HIS	CA-CB-CG	-7.51	106.29	113.80
1	B	293	GLY	CA-C-O	-7.50	107.52	120.57
1	A	275	HIS	N-CA-C	7.48	119.94	108.42
1	B	151	ARG	CA-CB-CG	-7.38	99.33	114.10
1	A	147	VAL	CA-C-N	7.30	135.49	121.54
1	A	147	VAL	C-N-CA	7.30	135.49	121.54
1	A	147	VAL	O-C-N	7.16	131.52	122.57
1	B	149	ASN	CA-C-N	7.14	135.32	121.18
1	B	149	ASN	C-N-CA	7.14	135.32	121.18
1	A	84	GLY	N-CA-C	7.12	124.80	115.47
1	B	291	VAL	CA-C-O	-7.05	116.28	119.94
1	A	36	MET	CG-SD-CE	-6.96	85.59	100.90
1	B	326	ASN	N-CA-C	6.94	119.69	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	CYS	O-C-N	-6.94	113.36	122.59
1	A	64	HIS	CA-CB-CG	-6.92	106.89	113.80
1	B	103	HIS	CB-CA-C	6.79	122.58	110.16
1	B	147	VAL	CA-C-O	-6.79	112.30	120.78
1	B	309	HIS	N-CA-CB	6.76	120.87	110.80
1	A	275	HIS	CA-CB-CG	6.69	120.49	113.80
1	B	294	LEU	N-CA-C	-6.66	104.73	114.39
1	A	242	THR	N-CA-CB	-6.56	99.12	111.00
1	B	242	THR	N-CA-CB	-6.56	99.43	111.37
1	A	158	VAL	CB-CA-C	-6.55	100.54	111.29
1	B	8	SER	CA-C-O	6.46	129.75	120.51
1	A	31	GLN	N-CA-C	6.45	119.82	110.28
1	B	309	HIS	ND1-CE1-NE2	-6.40	102.00	108.40
1	B	315	PRO	CA-C-O	-6.40	113.73	121.03
1	B	101	THR	O-C-N	-6.39	115.45	121.20
1	A	309	HIS	CA-CB-CG	6.39	120.19	113.80
1	A	103	HIS	CA-CB-CG	6.33	120.13	113.80
1	B	101	THR	CA-C-O	6.29	125.34	119.24
1	B	152	PHE	N-CA-C	6.22	124.05	110.80
1	A	164	LEU	CA-C-N	6.21	133.39	121.54
1	A	164	LEU	C-N-CA	6.21	133.39	121.54
1	A	146	GLU	N-CA-C	6.20	124.01	110.80
1	B	171	CYS	N-CA-C	6.12	123.84	110.80
1	B	168	LYS	N-CA-C	6.12	123.33	109.81
1	A	171	CYS	N-CA-C	6.12	123.82	110.80
1	B	148	SER	O-C-N	-6.11	114.46	122.59
1	A	328	GLU	N-CA-CB	-6.08	100.12	111.13
1	B	264	GLY	CA-C-O	-6.07	112.27	119.07
1	B	187	PRO	CA-C-O	-6.03	114.46	121.34
1	B	171	CYS	CA-C-N	6.03	130.12	121.50
1	B	171	CYS	C-N-CA	6.03	130.12	121.50
1	B	170	ALA	N-CA-C	-6.00	104.86	111.82
1	A	168	LYS	N-CA-C	5.99	123.06	109.81
1	B	150	GLU	N-CA-CB	5.99	120.86	110.39
1	B	120	LYS	CB-CA-C	-5.98	108.68	115.79
1	A	103	HIS	N-CA-CB	-5.97	101.75	111.24
1	B	150	GLU	N-CA-C	-5.95	105.87	113.01
1	A	62	HIS	CA-CB-CG	-5.95	107.86	113.80
1	A	15	PRO	CA-C-O	-5.92	114.59	121.34
1	B	161	ILE	CB-CA-C	5.90	118.23	110.91
1	A	122	ASN	N-CA-C	5.89	120.89	111.81
1	B	144	SER	N-CA-CB	-5.88	102.54	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	293	GLY	N-CA-C	-5.86	99.30	113.18
1	B	148	SER	CA-C-N	-5.84	110.38	121.54
1	B	148	SER	C-N-CA	-5.84	110.38	121.54
1	A	151	ARG	N-CA-CB	-5.82	102.72	110.57
1	B	25	ARG	N-CA-C	5.80	118.69	109.24
1	A	314	LYS	N-CA-CB	-5.74	102.88	110.17
1	B	282	HIS	N-CA-CB	5.68	119.98	110.32
1	A	325	GLN	N-CA-C	5.67	119.71	112.34
1	A	328	GLU	CA-CB-CG	-5.66	102.77	114.10
1	B	161	ILE	CA-CB-CG1	5.66	120.02	110.40
1	A	282	HIS	N-CA-CB	5.66	119.94	110.32
1	A	8	SER	CB-CA-C	-5.64	99.19	110.42
1	B	86	ARG	NE-CZ-NH2	5.63	124.27	119.20
1	B	63	VAL	CG1-CB-CG2	-5.62	98.45	110.80
1	B	275	HIS	CB-CG-ND1	-5.61	114.29	122.70
1	B	158	VAL	CB-CA-C	-5.57	102.16	111.29
1	B	147	VAL	CA-CB-CG1	5.53	119.80	110.40
1	A	313	CYS	CA-C-N	5.50	129.00	121.74
1	A	313	CYS	C-N-CA	5.50	129.00	121.74
1	A	64	HIS	N-CA-CB	5.49	119.17	110.55
1	A	64	HIS	CB-CA-C	5.49	119.19	110.19
1	B	234	HIS	N-CA-CB	-5.49	102.36	111.57
1	B	309	HIS	N-CA-C	-5.47	105.40	113.61
1	B	245	CYS	O-C-N	-5.42	116.13	122.96
1	A	154	GLU	CB-CG-CD	5.36	121.72	112.60
1	A	251	THR	OG1-CB-CG2	-5.36	98.57	109.30
1	A	242	THR	CA-CB-CG2	5.36	119.61	110.50
1	A	144	SER	CA-C-N	-5.34	111.33	121.54
1	A	144	SER	C-N-CA	-5.34	111.33	121.54
1	A	15	PRO	CB-CA-C	-5.33	104.58	111.46
1	A	23	GLY	N-CA-C	-5.32	104.55	111.52
1	B	305	PRO	N-CD-CG	-5.31	95.23	103.20
1	B	157	ALA	N-CA-C	5.30	117.25	109.24
1	A	151	ARG	CA-C-N	5.28	131.21	121.70
1	A	151	ARG	C-N-CA	5.28	131.21	121.70
1	A	9	LEU	CA-C-N	5.26	125.55	119.92
1	A	9	LEU	C-N-CA	5.26	125.55	119.92
1	A	151	ARG	CG-CD-NE	5.26	123.56	112.00
1	A	128	SER	CA-C-N	-5.24	113.25	120.74
1	A	128	SER	C-N-CA	-5.24	113.25	120.74
1	B	332	LEU	CD1-CG-CD2	5.21	122.26	110.80
1	B	147	VAL	N-CA-C	5.20	120.15	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	327	ILE	CA-C-O	5.19	125.52	120.27
1	B	110	HIS	CB-CG-ND1	-5.19	114.92	122.70
1	A	254	THR	O-C-N	5.18	129.91	123.28
1	B	146	GLU	CA-CB-CG	5.18	124.45	114.10
1	A	131	GLY	O-C-N	-5.16	119.10	123.59
1	B	62	HIS	N-CA-CB	-5.14	102.93	111.57
1	B	125	HIS	CA-CB-CG	5.11	118.91	113.80
1	B	145	GLU	N-CA-C	5.10	121.66	110.80
1	B	314	LYS	N-CA-CB	-5.09	102.58	110.01
1	A	234	HIS	CB-CG-ND1	-5.08	115.08	122.70
1	B	103	HIS	O-C-N	-5.07	117.80	123.48
1	A	326	ASN	N-CA-C	5.06	121.57	110.80
1	B	129	VAL	N-CA-C	5.06	115.28	110.53
1	A	83	ASP	CB-CA-C	-5.03	104.34	112.09
1	A	207	ILE	N-CA-C	-5.03	99.88	107.73
1	B	328	GLU	CG-CD-OE2	5.02	129.95	118.40

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	HIS	Sidechain
1	A	110	HIS	Sidechain
1	A	145	GLU	Peptide
1	A	146	GLU	Peptide
1	A	150	GLU	Mainchain,Peptide
1	A	164	LEU	Mainchain
1	A	169	PRO	Peptide
1	A	171	CYS	Peptide
1	A	205	HIS	Sidechain
1	A	234	HIS	Sidechain
1	A	239	HIS	Sidechain
1	A	275	HIS	Sidechain
1	A	282	HIS	Sidechain
1	A	327	ILE	Peptide
1	A	62	HIS	Sidechain
1	A	64	HIS	Sidechain
1	B	103	HIS	Sidechain
1	B	110	HIS	Sidechain
1	B	125	HIS	Sidechain
1	B	139	HIS	Sidechain
1	B	145	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	B	146	GLU	Peptide
1	B	150	GLU	Mainchain,Peptide
1	B	151	ARG	Peptide
1	B	164	LEU	Mainchain
1	B	171	CYS	Peptide
1	B	205	HIS	Sidechain
1	B	268	HIS	Sidechain
1	B	275	HIS	Sidechain
1	B	293	GLY	Mainchain
1	B	309	HIS	Sidechain
1	B	327	ILE	Peptide
1	B	62	HIS	Sidechain
1	B	8	SER	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2570	0	2480	168	0
1	B	2571	0	2480	155	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	182	0	0	30	0
3	B	181	0	0	33	0
All	All	5508	0	4960	302	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 31.

All (302) 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:A:71:ILE:CD1	1:A:71:ILE:CG1	1.75	1.61
1:B:309:HIS:CB	1:B:309:HIS:CA	1.75	1.59
1:A:65:LYS:CE	1:A:65:LYS:CD	1.75	1.59
1:A:65:LYS:CD	1:A:65:LYS:CG	1.75	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:VAL:CB	1:B:147:VAL:CG1	1.87	1.50
1:A:286:MET:SD	1:A:286:MET:CE	2.05	1.44
1:B:145:GLU:O	1:B:146:GLU:CG	1.65	1.43
1:A:310:ILE:HG21	1:B:139:HIS:CE1	1.54	1.43
1:B:197:ARG:CZ	1:B:309:HIS:HE1	1.32	1.41
1:A:110:HIS:CE1	1:B:309:HIS:CG	2.11	1.39
1:B:329:ALA:HB1	3:B:575:HOH:O	1.28	1.33
1:B:146:GLU:HB3	3:B:435:HOH:O	1.33	1.29
1:B:197:ARG:CZ	1:B:309:HIS:CE1	2.22	1.22
1:A:310:ILE:CG2	1:B:139:HIS:HE1	1.51	1.21
1:B:5:CYS:SG	3:B:553:HOH:O	2.01	1.18
1:B:156:ALA:HB3	3:B:486:HOH:O	1.42	1.15
1:A:147:VAL:C	3:A:515:HOH:O	1.88	1.13
1:B:146:GLU:CB	3:B:435:HOH:O	1.90	1.13
1:B:146:GLU:OE2	3:B:425:HOH:O	1.62	1.12
1:B:145:GLU:C	1:B:146:GLU:HG2	1.74	1.12
1:A:227:LYS:HE3	1:A:282:HIS:CE1	1.84	1.10
1:B:150:GLU:OE2	3:B:510:HOH:O	1.69	1.10
1:A:125:HIS:HE1	1:A:157:ALA:HB2	1.07	1.09
1:A:313:CYS:HB2	3:A:414:HOH:O	1.52	1.09
1:A:110:HIS:HE1	1:B:309:HIS:ND1	1.51	1.07
1:A:329:ALA:HB1	3:A:583:HOH:O	0.92	1.07
1:A:97:ILE:HG21	1:A:103:HIS:ND1	1.70	1.06
1:A:239:HIS:CE1	1:A:295:PHE:HB2	1.90	1.06
1:A:110:HIS:CE1	1:B:309:HIS:ND1	2.23	1.05
1:A:269:VAL:HG11	1:A:275:HIS:ND1	1.73	1.02
1:B:146:GLU:O	3:B:461:HOH:O	1.78	1.02
1:A:62:HIS:CE1	1:A:64:HIS:HE1	1.78	1.01
1:A:97:ILE:HG21	1:A:103:HIS:CE1	1.94	1.01
1:B:241:GLU:OE1	3:B:572:HOH:O	1.79	1.01
1:A:125:HIS:CE1	1:A:157:ALA:HB2	1.96	1.00
1:A:146:GLU:CB	3:A:549:HOH:O	2.09	0.99
1:B:146:GLU:OE1	3:B:425:HOH:O	1.80	0.99
1:A:333:LYS:HD2	1:A:333:LYS:C	1.87	0.98
1:A:214:THR:HG21	1:A:218:PHE:O	1.63	0.98
1:A:210:ALA:H	1:A:213:ASN:HD22	1.05	0.97
1:A:146:GLU:HB3	3:A:549:HOH:O	1.65	0.97
1:A:68:HIS:HD2	1:A:99:ALA:H	1.14	0.95
1:A:146:GLU:OE1	3:A:480:HOH:O	1.86	0.94
1:A:62:HIS:NE2	1:A:64:HIS:CE1	2.35	0.94
1:B:309:HIS:CA	1:B:309:HIS:CG	2.51	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LYS:CE	1:A:282:HIS:CE1	2.51	0.93
1:A:146:GLU:CD	3:A:480:HOH:O	2.11	0.92
1:B:197:ARG:NH2	1:B:309:HIS:CE1	2.37	0.91
1:A:234:HIS:HE1	1:A:275:HIS:CD2	1.89	0.91
1:A:227:LYS:CE	1:A:282:HIS:HE1	1.83	0.90
1:A:242:THR:HG22	1:A:289:VAL:H	1.37	0.90
1:B:145:GLU:O	1:B:146:GLU:HG2	0.72	0.89
1:A:269:VAL:HG11	1:A:275:HIS:CE1	2.08	0.88
1:A:227:LYS:HE3	1:A:282:HIS:HE1	1.35	0.88
1:B:333:LYS:HD2	1:B:333:LYS:C	1.98	0.88
1:B:197:ARG:NE	1:B:309:HIS:CE1	2.42	0.87
1:A:269:VAL:HG11	1:A:275:HIS:HD1	1.41	0.85
1:B:327:ILE:HA	3:B:577:HOH:O	1.76	0.85
1:A:326:ASN:O	3:A:424:HOH:O	1.95	0.84
1:B:197:ARG:NH2	1:B:309:HIS:HE1	1.72	0.84
1:A:8:SER:CA	1:A:9:LEU:N	2.42	0.82
1:A:97:ILE:HG21	1:A:103:HIS:HD1	1.38	0.82
1:B:59:PHE:CE2	1:B:62:HIS:CE1	2.67	0.82
1:B:327:ILE:CG1	3:B:577:HOH:O	2.27	0.82
1:A:146:GLU:HB2	3:A:549:HOH:O	1.75	0.82
1:B:147:VAL:O	3:B:569:HOH:O	1.97	0.81
1:A:62:HIS:CE1	1:A:64:HIS:CE1	2.68	0.80
1:A:62:HIS:NE2	1:A:64:HIS:HE1	1.78	0.80
1:B:234:HIS:CD2	1:B:275:HIS:HE1	2.00	0.80
1:A:328:GLU:OE1	3:A:571:HOH:O	2.00	0.80
1:B:146:GLU:CD	3:B:425:HOH:O	2.03	0.80
1:A:97:ILE:HD13	1:A:103:HIS:CE1	2.17	0.79
1:B:68:HIS:HD2	1:B:99:ALA:H	1.30	0.79
1:A:110:HIS:CE1	1:B:309:HIS:CB	2.65	0.78
1:A:227:LYS:NZ	1:A:282:HIS:HE1	1.82	0.78
1:A:139:HIS:C	1:A:139:HIS:CD2	2.62	0.78
1:B:65:LYS:H	1:B:158:VAL:HG12	1.48	0.78
1:B:309:HIS:CB	1:B:309:HIS:HA	2.10	0.78
1:B:214:THR:HG21	1:B:218:PHE:O	1.84	0.78
1:B:68:HIS:CD2	1:B:99:ALA:H	2.03	0.77
1:A:313:CYS:SG	1:B:136:HIS:CD2	2.78	0.76
1:B:242:THR:HG22	1:B:289:VAL:H	1.48	0.76
1:B:321:ASP:O	1:B:325:GLN:HG3	1.86	0.76
1:B:125:HIS:CD2	3:B:456:HOH:O	2.39	0.76
1:A:200:THR:HB	1:A:205:HIS:NE2	2.01	0.75
1:B:200:THR:HG22	1:B:200:THR:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:PHE:HE2	1:B:62:HIS:CE1	2.03	0.75
1:A:239:HIS:CE1	1:A:295:PHE:CB	2.69	0.75
1:A:333:LYS:HB2	3:A:403:HOH:O	1.85	0.75
1:B:234:HIS:NE2	1:B:236:HIS:CE1	2.55	0.75
1:A:147:VAL:O	3:A:430:HOH:O	2.02	0.75
1:A:241:GLU:OE1	3:A:512:HOH:O	2.03	0.74
1:B:59:PHE:CE2	1:B:62:HIS:HE1	2.04	0.74
1:A:252:MET:HB2	1:A:259:ILE:HD11	1.68	0.74
1:B:252:MET:HB2	1:B:259:ILE:HD11	1.68	0.73
1:A:200:THR:O	1:A:200:THR:HG22	1.89	0.73
1:A:310:ILE:CG2	1:B:139:HIS:CE1	2.42	0.72
1:B:24:GLU:OE2	3:B:503:HOH:O	2.07	0.71
1:A:74:LEU:HD11	1:A:115:VAL:HG23	1.72	0.71
1:B:146:GLU:CB	1:B:147:VAL:HG23	2.21	0.70
1:A:139:HIS:HD2	1:A:139:HIS:O	1.74	0.70
1:B:210:ALA:H	1:B:213:ASN:HD22	1.38	0.70
1:A:146:GLU:OE2	3:A:480:HOH:O	2.08	0.69
1:A:234:HIS:CE1	1:A:275:HIS:CD2	2.75	0.69
1:A:97:ILE:CG2	1:A:103:HIS:HD1	2.05	0.69
1:A:242:THR:HG22	1:A:289:VAL:N	2.07	0.69
1:B:147:VAL:CG1	1:B:147:VAL:CG2	2.70	0.68
1:B:145:GLU:C	1:B:146:GLU:CG	2.45	0.68
1:A:162:VAL:O	3:A:412:HOH:O	2.11	0.67
1:A:310:ILE:HG21	1:B:139:HIS:HE1	0.62	0.67
1:B:200:THR:O	1:B:200:THR:CG2	2.41	0.67
1:A:139:HIS:CD2	1:B:310:ILE:HG21	2.30	0.66
1:A:329:ALA:CB	3:A:583:HOH:O	1.76	0.66
1:A:269:VAL:CG1	1:A:275:HIS:HD1	2.08	0.66
1:B:327:ILE:HG12	3:B:577:HOH:O	1.94	0.66
1:B:30:ARG:HG2	1:B:139:HIS:HD2	1.60	0.65
1:B:7:HIS:CD2	1:B:22:GLU:OE2	2.50	0.65
1:A:139:HIS:C	1:A:139:HIS:HD2	2.04	0.65
1:A:231:ILE:HG23	3:A:503:HOH:O	1.97	0.64
1:A:243:PHE:CE1	1:A:252:MET:HE1	2.32	0.64
1:A:318:LEU:HD12	3:A:543:HOH:O	1.96	0.64
1:B:86:ARG:HD3	3:B:472:HOH:O	1.96	0.64
1:A:118:THR:HG23	3:A:417:HOH:O	1.97	0.63
1:A:242:THR:CG2	1:A:289:VAL:H	2.09	0.63
1:B:206:ARG:NH1	1:B:222:SER:O	2.31	0.63
1:B:20:SER:HB2	1:B:264:GLY:HA3	1.78	0.63
1:B:205:HIS:CE1	1:B:299:PHE:CE2	2.86	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:LYS:NZ	3:B:539:HOH:O	2.30	0.63
1:B:65:LYS:H	1:B:158:VAL:CG1	2.11	0.63
1:A:219:ILE:HD11	1:A:290:LEU:HD12	1.81	0.62
1:A:252:MET:HB2	1:A:259:ILE:CD1	2.29	0.62
1:A:333:LYS:C	1:A:333:LYS:CD	2.69	0.62
1:B:146:GLU:HB2	3:B:435:HOH:O	1.76	0.62
1:B:62:HIS:CD2	1:B:103:HIS:HE1	2.18	0.62
1:A:146:GLU:CB	1:A:147:VAL:HG23	2.29	0.62
1:B:68:HIS:HD2	1:B:98:PRO:HA	1.65	0.62
1:B:252:MET:HB2	1:B:259:ILE:CD1	2.29	0.62
1:B:327:ILE:HG13	3:B:577:HOH:O	1.93	0.62
1:B:333:LYS:HB2	3:B:419:HOH:O	1.99	0.61
1:A:118:THR:CG2	3:A:417:HOH:O	2.48	0.61
1:B:234:HIS:CD2	1:B:275:HIS:CE1	2.86	0.61
1:B:242:THR:HG23	3:B:438:HOH:O	1.99	0.61
1:B:333:LYS:C	1:B:333:LYS:CD	2.73	0.60
1:B:309:HIS:CB	1:B:309:HIS:C	2.67	0.60
1:B:282:HIS:HD2	3:B:417:HOH:O	1.84	0.60
1:A:110:HIS:CE1	1:B:309:HIS:HB3	2.37	0.60
1:A:110:HIS:CG	1:B:309:HIS:HB3	2.37	0.60
1:B:74:LEU:HD11	1:B:115:VAL:HG23	1.84	0.60
1:B:219:ILE:HD11	1:B:290:LEU:HD12	1.83	0.60
1:B:206:ARG:HD3	1:B:206:ARG:N	2.17	0.60
1:A:65:LYS:H	1:A:158:VAL:HG12	1.67	0.59
1:A:242:THR:HG21	1:A:289:VAL:HB	1.83	0.59
1:A:36:MET:CE	3:A:454:HOH:O	2.50	0.59
1:A:110:HIS:ND1	1:B:309:HIS:HB3	2.18	0.59
1:B:66:ASP:H	1:B:158:VAL:HG11	1.68	0.59
1:B:126:LEU:C	1:B:126:LEU:HD12	2.27	0.59
1:A:227:LYS:NZ	1:A:282:HIS:CE1	2.67	0.59
1:A:309:HIS:ND1	1:B:110:HIS:CD2	2.70	0.59
1:B:103:HIS:HD1	1:B:103:HIS:N	2.00	0.59
1:A:234:HIS:HE2	1:A:236:HIS:CE1	2.19	0.58
1:A:259:ILE:HD12	1:A:259:ILE:O	2.03	0.58
1:B:103:HIS:N	1:B:103:HIS:ND1	2.48	0.58
1:B:118:THR:HB	3:B:468:HOH:O	2.02	0.58
1:B:146:GLU:HB2	1:B:147:VAL:CG2	2.33	0.58
1:B:146:GLU:C	1:B:147:VAL:HG23	2.28	0.58
1:A:65:LYS:CE	1:A:65:LYS:CG	2.81	0.58
1:B:68:HIS:CD2	1:B:98:PRO:HA	2.38	0.58
1:B:146:GLU:HB2	1:B:147:VAL:HG23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:MET:CE	1:A:286:MET:CG	2.81	0.58
1:A:321:ASP:O	1:A:325:GLN:HG3	2.02	0.58
1:B:125:HIS:HB3	3:B:502:HOH:O	2.03	0.58
1:A:66:ASP:H	1:A:158:VAL:HG11	1.69	0.58
1:B:66:ASP:O	1:B:120:LYS:NZ	2.32	0.58
1:A:110:HIS:NE2	1:B:309:HIS:CG	2.72	0.57
1:B:236:HIS:CG	1:B:239:HIS:CE1	2.91	0.57
1:A:333:LYS:HD2	1:A:333:LYS:O	2.04	0.57
1:A:119:MET:HE3	1:A:218:PHE:CD2	2.40	0.56
1:A:146:GLU:HB2	1:A:147:VAL:HG23	1.86	0.56
1:B:64:HIS:NE2	1:B:69:GLU:OE1	2.33	0.56
1:B:146:GLU:C	1:B:147:VAL:CG2	2.78	0.56
1:A:14:MET:HB2	1:A:15:PRO:HD2	1.85	0.56
1:A:62:HIS:CE1	1:A:103:HIS:CD2	2.92	0.56
1:B:146:GLU:CA	1:B:147:VAL:HG23	2.36	0.56
1:B:68:HIS:HD2	1:B:99:ALA:N	2.02	0.56
1:A:68:HIS:HE1	1:A:215:ASP:OD2	1.89	0.56
1:B:259:ILE:HD12	1:B:259:ILE:O	2.06	0.56
1:A:309:HIS:CE1	1:B:110:HIS:NE2	2.74	0.55
1:A:68:HIS:CD2	1:A:99:ALA:H	2.07	0.55
1:A:313:CYS:CB	3:A:414:HOH:O	2.31	0.55
1:B:81:THR:O	1:B:103:HIS:HA	2.05	0.55
1:A:210:ALA:H	1:A:213:ASN:ND2	1.89	0.55
1:B:38:ASN:HA	1:B:47:GLU:HG2	1.89	0.55
1:B:205:HIS:CE1	1:B:299:PHE:HE2	2.23	0.55
1:B:211:GLN:NE2	1:B:293:GLY:O	2.40	0.55
1:A:36:MET:HE1	3:A:454:HOH:O	2.06	0.55
1:A:64:HIS:ND1	1:A:64:HIS:N	2.50	0.55
1:A:200:THR:O	1:A:200:THR:CG2	2.54	0.55
1:B:65:LYS:N	1:B:158:VAL:HG12	2.21	0.54
1:B:234:HIS:CD2	1:B:234:HIS:C	2.85	0.54
1:A:102:PRO:O	1:A:103:HIS:HB3	2.06	0.54
1:B:86:ARG:CD	3:B:472:HOH:O	2.54	0.54
1:B:205:HIS:CE1	1:B:299:PHE:CD2	2.96	0.54
1:A:206:ARG:NH1	1:A:222:SER:O	2.41	0.54
1:A:36:MET:HE3	3:A:406:HOH:O	2.07	0.53
1:A:243:PHE:CZ	1:A:252:MET:HE1	2.43	0.53
1:B:333:LYS:HD2	1:B:333:LYS:O	2.07	0.53
1:A:62:HIS:ND1	1:A:62:HIS:C	2.63	0.53
1:B:8:SER:CA	1:B:9:LEU:N	2.72	0.53
1:A:68:HIS:CD2	1:A:98:PRO:HA	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ASN:O	3:B:577:HOH:O	2.18	0.52
1:A:239:HIS:NE2	1:A:295:PHE:HB2	2.23	0.52
1:A:27:LEU:HD22	1:A:134:TYR:CE1	2.45	0.52
1:A:97:ILE:CD1	1:A:103:HIS:CE1	2.91	0.51
1:A:110:HIS:HD2	3:A:488:HOH:O	1.93	0.51
1:A:292:PRO:O	3:A:423:HOH:O	2.19	0.51
1:B:61:LEU:O	1:B:62:HIS:HB3	2.10	0.51
1:A:333:LYS:HD2	1:A:334:VAL:N	2.25	0.51
1:A:7:HIS:CD2	1:A:22:GLU:OE2	2.64	0.50
1:A:68:HIS:HD2	1:A:99:ALA:N	1.97	0.50
1:A:242:THR:HG22	1:A:289:VAL:O	2.11	0.50
1:A:65:LYS:CD	1:A:65:LYS:CB	2.82	0.50
1:A:239:HIS:HE1	1:A:295:PHE:CB	2.20	0.50
1:A:234:HIS:ND1	1:A:234:HIS:C	2.70	0.50
1:B:211:GLN:HA	1:B:214:THR:HG22	1.93	0.50
1:A:227:LYS:HE3	1:A:282:HIS:ND1	2.22	0.49
1:B:65:LYS:N	1:B:158:VAL:CG1	2.75	0.49
1:A:74:LEU:HD11	1:A:115:VAL:CG2	2.42	0.49
1:A:77:LYS:HB3	1:A:88:LEU:HD11	1.93	0.49
1:B:14:MET:O	1:B:268:HIS:CD2	2.66	0.49
1:B:309:HIS:CG	1:B:309:HIS:HA	2.41	0.49
1:B:118:THR:HG23	3:B:566:HOH:O	2.12	0.48
1:A:71:ILE:CD1	1:A:71:ILE:CB	2.81	0.48
1:B:253:TRP:O	1:B:275:HIS:HA	2.13	0.48
1:B:253:TRP:HA	1:B:257:GLN:O	2.13	0.48
1:A:197:ARG:HB3	1:A:204:LEU:HD11	1.95	0.48
1:A:126:LEU:C	1:A:126:LEU:HD12	2.39	0.48
1:A:146:GLU:CA	1:A:147:VAL:HG23	2.44	0.47
1:A:146:GLU:HB2	1:A:147:VAL:CG2	2.44	0.47
1:B:242:THR:HG22	1:B:289:VAL:N	2.22	0.47
1:A:65:LYS:N	1:A:158:VAL:HG12	2.29	0.47
1:B:268:HIS:CD2	1:B:270:PRO:HD3	2.50	0.47
1:A:332:LEU:HD13	1:A:333:LYS:N	2.29	0.47
1:B:110:HIS:N	1:B:110:HIS:ND1	2.63	0.46
1:B:119:MET:HE3	1:B:218:PHE:CD2	2.51	0.46
1:A:296:GLU:N	1:A:297:PRO:HD2	2.31	0.46
1:A:48:ILE:HG12	1:A:117:TYR:HD2	1.81	0.46
1:A:7:HIS:HD2	1:A:22:GLU:OE2	1.99	0.46
1:A:161:ILE:HG21	3:A:576:HOH:O	2.15	0.46
1:A:285:LYS:NZ	3:A:558:HOH:O	2.45	0.46
1:B:139:HIS:CE1	1:B:139:HIS:O	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ILE:HD13	1:B:139:HIS:ND1	2.31	0.45
1:B:59:PHE:HB2	1:B:105:TYR:CZ	2.51	0.45
1:A:211:GLN:HA	1:A:214:THR:HG22	1.98	0.45
1:A:227:LYS:HD2	1:A:282:HIS:ND1	2.31	0.45
1:B:117:TYR:OH	3:B:550:HOH:O	2.21	0.45
1:A:210:ALA:O	1:A:214:THR:HG22	2.15	0.45
1:A:53:GLY:HA2	1:A:139:HIS:ND1	2.32	0.45
1:A:234:HIS:NE2	1:A:236:HIS:CE1	2.85	0.45
1:B:20:SER:HB2	1:B:264:GLY:CA	2.47	0.45
1:B:200:THR:HB	1:B:205:HIS:NE2	2.31	0.45
1:A:282:HIS:HB3	3:A:562:HOH:O	2.16	0.44
1:B:329:ALA:CB	3:B:575:HOH:O	2.15	0.44
1:A:327:ILE:C	1:A:328:GLU:HG3	2.42	0.44
1:B:275:HIS:ND1	1:B:275:HIS:N	2.63	0.44
1:B:62:HIS:CD2	1:B:103:HIS:CE1	3.03	0.43
1:B:151:ARG:HA	1:B:153:ALA:H	1.82	0.43
1:A:74:LEU:CD1	1:A:115:VAL:HG23	2.44	0.43
1:A:186:VAL:HB	1:A:187:PRO:HD2	2.00	0.43
1:A:234:HIS:HE1	1:A:275:HIS:NE2	2.15	0.43
1:A:66:ASP:H	1:A:158:VAL:CG1	2.32	0.43
1:B:217:GLN:O	1:B:292:PRO:HA	2.19	0.43
1:B:75:ASP:OD2	1:B:113:ARG:HD3	2.19	0.42
1:A:89:LEU:HB3	1:A:93:ASP:HB2	2.00	0.42
1:B:275:HIS:N	1:B:275:HIS:HD1	2.17	0.42
1:A:80:LEU:HD12	1:A:104:SER:O	2.20	0.42
1:B:126:LEU:HD12	1:B:127:TYR:N	2.34	0.42
1:A:202:ASP:HB3	1:A:315:PRO:HB3	2.01	0.42
1:B:234:HIS:NE2	1:B:236:HIS:HE1	2.13	0.42
1:A:62:HIS:HE1	1:A:103:HIS:CD2	2.36	0.42
1:A:110:HIS:CD2	1:B:309:HIS:CB	3.03	0.42
1:A:146:GLU:C	1:A:147:VAL:HG23	2.45	0.42
1:B:105:TYR:CD1	1:B:105:TYR:C	2.97	0.42
1:B:134:TYR:CE2	1:B:136:HIS:HB2	2.54	0.42
1:A:309:HIS:CE1	1:B:110:HIS:HE2	2.38	0.41
1:B:61:LEU:HA	1:B:104:SER:HB3	2.01	0.41
1:B:36:MET:HE3	3:B:412:HOH:O	2.19	0.41
1:B:242:THR:HG21	1:B:289:VAL:HB	2.01	0.41
1:A:178:LEU:HG	1:A:179:THR:N	2.35	0.41
1:A:275:HIS:CD2	1:A:275:HIS:C	2.99	0.41
1:B:64:HIS:HB3	1:B:158:VAL:O	2.20	0.41
1:A:97:ILE:CG2	1:A:103:HIS:ND1	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:HIS:CD2	1:B:313:CYS:SG	3.14	0.41
1:B:158:VAL:HG22	3:B:409:HOH:O	2.20	0.41
1:A:242:THR:CG2	1:A:289:VAL:HB	2.47	0.41
1:A:294:LEU:C	1:A:294:LEU:HD12	2.46	0.41
1:B:224:GLU:HA	1:B:284:THR:O	2.21	0.41
1:A:110:HIS:CG	1:B:309:HIS:CB	3.03	0.41
1:B:145:GLU:O	1:B:146:GLU:CD	2.56	0.41
1:B:249:GLN:O	1:B:280:ASP:HB2	2.21	0.41
1:A:317:ALA:HA	3:A:543:HOH:O	2.22	0.40
1:A:200:THR:CB	1:A:205:HIS:NE2	2.79	0.40
1:A:203:GLN:HB3	1:A:205:HIS:HE1	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	328/337 (97%)	299 (91%)	19 (6%)	10 (3%)	3	3
1	B	328/337 (97%)	304 (93%)	15 (5%)	9 (3%)	4	4
All	All	656/674 (97%)	603 (92%)	34 (5%)	19 (3%)	3	3

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	146	GLU
1	A	148	SER
1	A	149	ASN
1	A	168	LYS
1	A	171	CYS
1	B	146	GLU

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Mol	Chain	Res	Type
1	B	148	SER
1	B	149	ASN
1	B	165	ASP
1	B	168	LYS
1	B	171	CYS
1	B	152	PHE
1	B	255	ASP
1	A	165	ASP
1	A	329	ALA
1	A	145	GLU
1	A	255	ASP
1	B	164	LEU

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	273/285 (96%)	235 (86%)	38 (14%)	3	4
1	B	273/285 (96%)	232 (85%)	41 (15%)	3	3
All	All	546/570 (96%)	467 (86%)	79 (14%)	3	4

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	11	LYS
1	A	62	HIS
1	A	63	VAL
1	A	64	HIS
1	A	65	LYS
1	A	72	LEU
1	A	89	LEU
1	A	103	HIS
1	A	118	THR
1	A	125	HIS

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Mol	Chain	Res	Type
1	A	139	HIS
1	A	144	SER
1	A	146	GLU
1	A	154	GLU
1	A	163	PHE
1	A	164	LEU
1	A	168	LYS
1	A	179	THR
1	A	180	GLU
1	A	200	THR
1	A	206	ARG
1	A	214	THR
1	A	234	HIS
1	A	240	THR
1	A	242	THR
1	A	257	GLN
1	A	259	ILE
1	A	275	HIS
1	A	282	HIS
1	A	286	MET
1	A	313	CYS
1	A	314	LYS
1	A	316	GLN
1	A	322	ARG
1	A	324	LEU
1	A	332	LEU
1	A	333	LYS
1	B	8	SER
1	B	11	LYS
1	B	62	HIS
1	B	63	VAL
1	B	64	HIS
1	B	65	LYS
1	B	66	ASP
1	B	72	LEU
1	B	86	ARG
1	B	89	LEU
1	B	118	THR
1	B	125	HIS
1	B	139	HIS
1	B	144	SER
1	B	146	GLU

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Mol	Chain	Res	Type
1	B	151	ARG
1	B	154	GLU
1	B	158	VAL
1	B	164	LEU
1	B	168	LYS
1	B	179	THR
1	B	180	GLU
1	B	200	THR
1	B	205	HIS
1	B	206	ARG
1	B	230	ARG
1	B	231	ILE
1	B	234	HIS
1	B	240	THR
1	B	242	THR
1	B	257	GLN
1	B	259	ILE
1	B	268	HIS
1	B	282	HIS
1	B	313	CYS
1	B	314	LYS
1	B	322	ARG
1	B	324	LEU
1	B	332	LEU
1	B	333	LYS
1	B	334	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	64	HIS
1	A	68	HIS
1	A	110	HIS
1	A	122	ASN
1	A	125	HIS
1	A	132	ASN
1	A	136	HIS
1	A	211	GLN
1	A	213	ASN
1	A	268	HIS
1	A	282	HIS

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Mol	Chain	Res	Type
1	A	325	GLN
1	B	7	HIS
1	B	62	HIS
1	B	68	HIS
1	B	122	ASN
1	B	125	HIS
1	B	132	ASN
1	B	136	HIS
1	B	139	HIS
1	B	211	GLN
1	B	213	ASN
1	B	268	HIS
1	B	272	ASN
1	B	282	HIS
1	B	309	HIS

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 ⓘ

Of 4 ligands modelled in this entry, 4 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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4
1	B	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	152:PHE	C	153:ALA	N	1.14
1	A	171:CYS	C	172:SER	N	1.03
1	B	149:ASN	C	150:GLU	N	1.02
1	B	171:CYS	C	172:SER	N	0.94
1	A	8:SER	C	9:LEU	N	0.93
1	A	164:LEU	C	165:ASP	N	0.91
1	B	8:SER	C	9:LEU	N	0.91
1	B	164:LEU	C	165:ASP	N	0.67

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	320/337 (94%)	-0.04	19 (5%) 28 24	26, 38, 64, 88	1 (0%)
1	B	321/337 (95%)	0.01	22 (6%) 23 19	25, 38, 64, 89	1 (0%)
All	All	641/674 (95%)	-0.02	41 (6%) 25 22	25, 38, 64, 89	2 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	8	SER	8.5
1	A	8	SER	5.6
1	B	147	VAL	5.0
1	B	164	LEU	5.0
1	A	327	ILE	3.7
1	A	6	THR	3.6
1	A	334	VAL	3.6
1	A	164	LEU	3.2
1	B	328	GLU	3.2
1	B	327	ILE	3.2
1	B	5	CYS	3.1
1	B	6	THR	3.0
1	A	154	GLU	3.0
1	B	139	HIS	3.0
1	B	7	HIS	2.9
1	B	159	ALA	2.7
1	A	5	CYS	2.7
1	A	159	ALA	2.7
1	B	293	GLY	2.7
1	B	172	SER	2.6
1	A	163	PHE	2.6
1	A	62	HIS	2.6
1	B	125	HIS	2.5
1	B	234	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	334	VAL	2.4
1	A	153	ALA	2.4
1	A	125	HIS	2.4
1	B	309	HIS	2.4
1	A	234	HIS	2.2
1	A	147	VAL	2.2
1	A	110	HIS	2.1
1	A	7	HIS	2.1
1	A	158	VAL	2.1
1	B	161	ILE	2.1
1	B	154	GLU	2.1
1	A	282	HIS	2.1
1	B	66	ASP	2.1
1	B	62	HIS	2.1
1	B	110	HIS	2.1
1	B	163	PHE	2.0
1	A	205	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FE	A	401	1/1	0.98	0.07	51,51,51,51	0
2	FE	B	402	1/1	0.98	0.08	43,43,43,43	0
2	FE	B	401	1/1	0.99	0.06	50,50,50,50	0
2	FE	A	402	1/1	0.99	0.08	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.