



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:14 PM UTC

PDB ID : 1TLB / pdb_00001tlb
Title : Yeast coproporphyrinogen oxidase
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Deposited on : 2004-06-09
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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

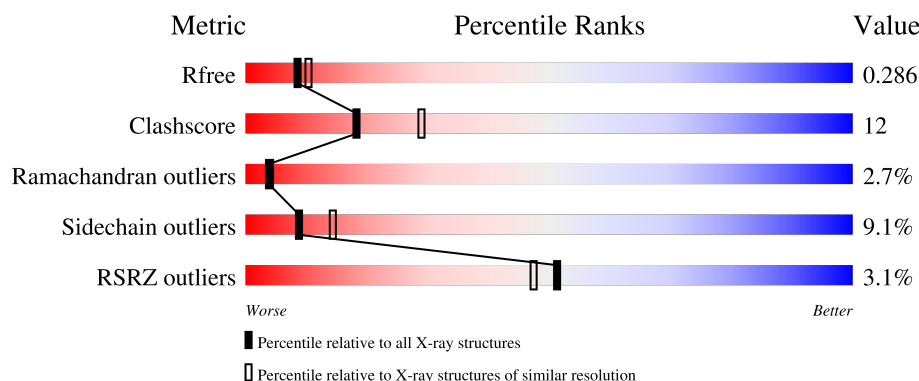
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	326	2% 71% 23% 6%
1	D	326	% 65% 31% 5%
1	Q	326	% 71% 23% 6%
1	S	326	68% 24% 7%
1	U	326	4% 66% 30%

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Mol	Chain	Length	Quality of chain
1	W	326	10% 57% 34% 8%

2 Entry composition [i](#)

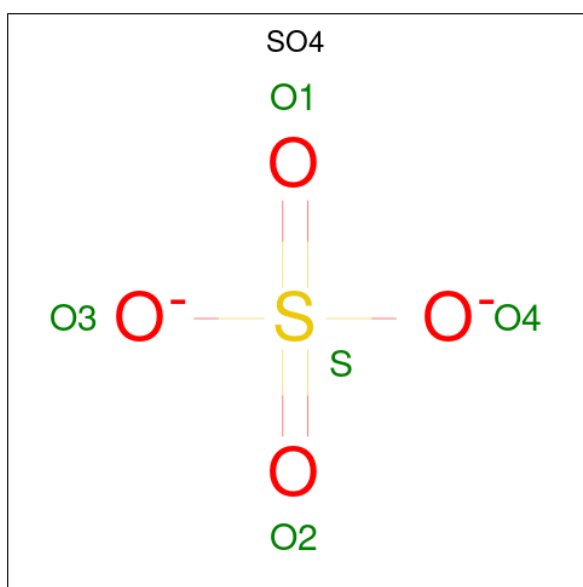
There are 3 unique types of molecules in this entry. The entry contains 16531 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Coproporphyrinogen III oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	152	0	0
			2647	1682	465	490	10			
1	D	326	Total	C	N	O	S	152	0	0
			2648	1683	465	490	10			
1	Q	326	Total	C	N	O	S	152	0	0
			2648	1683	465	490	10			
1	S	326	Total	C	N	O	S	152	0	0
			2647	1682	465	490	10			
1	U	326	Total	C	N	O	S	152	0	0
			2648	1683	465	490	10			
1	W	326	Total	C	N	O	S	152	0	0
			2648	1683	465	490	10			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

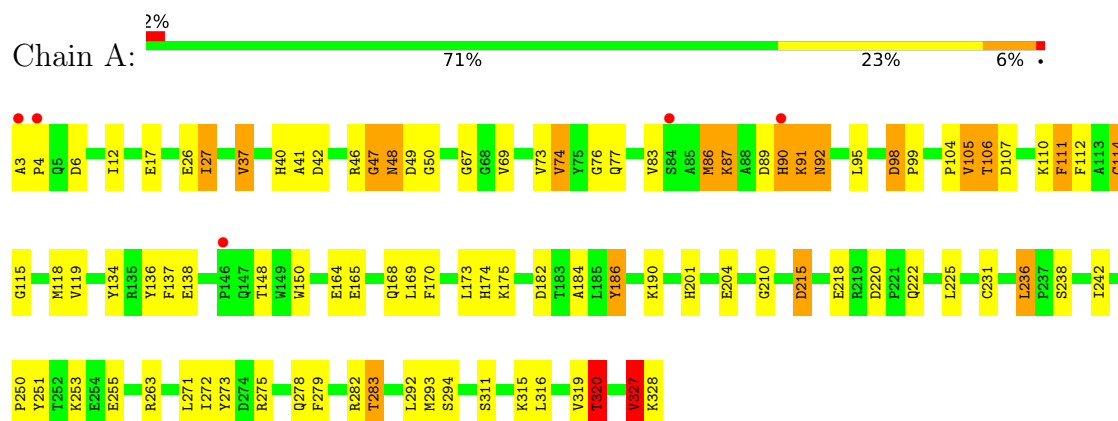
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	115	Total	O	0	0
			115	115		
3	D	74	Total	O	0	0
			74	74		
3	Q	151	Total	O	0	0
			151	151		
3	S	140	Total	O	0	0
			140	140		
3	U	103	Total	O	0	0
			103	103		
3	W	57	Total	O	0	0
			57	57		

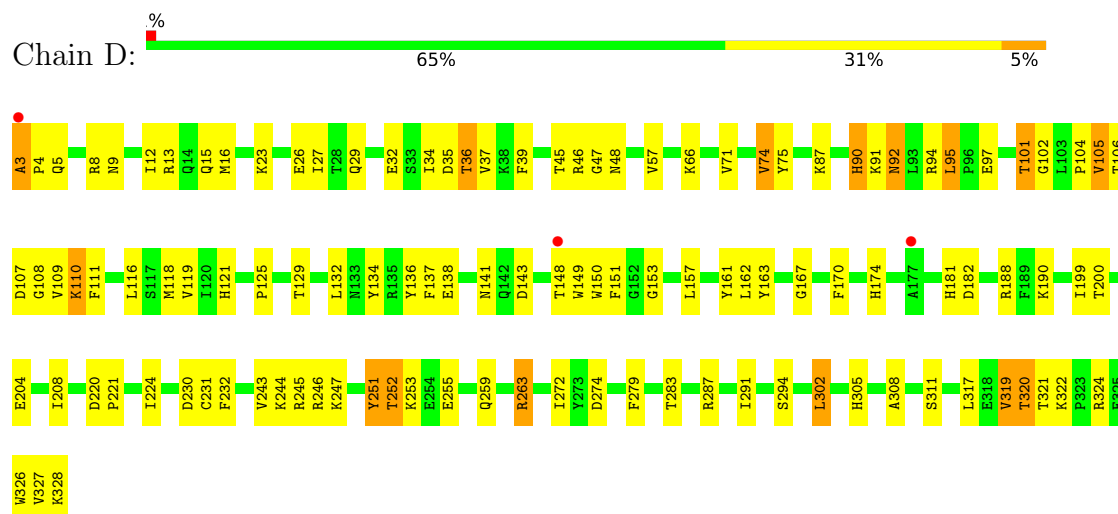
3 Residue-property plots [i](#)

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.

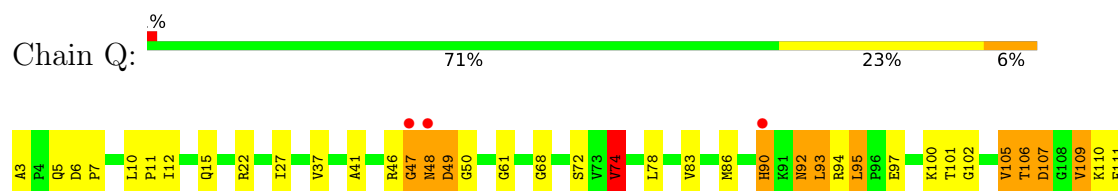
• Molecule 1: Coproporphyrinogen III oxidase

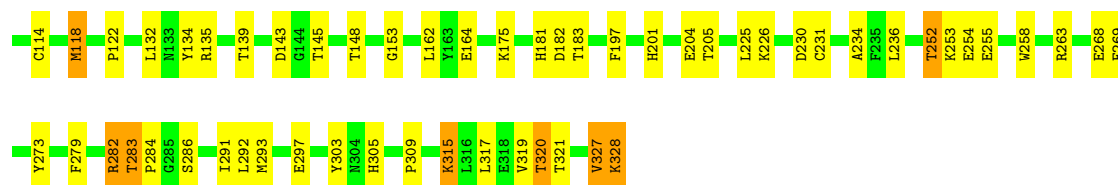


• Molecule 1: Coproporphyrinogen III oxidase



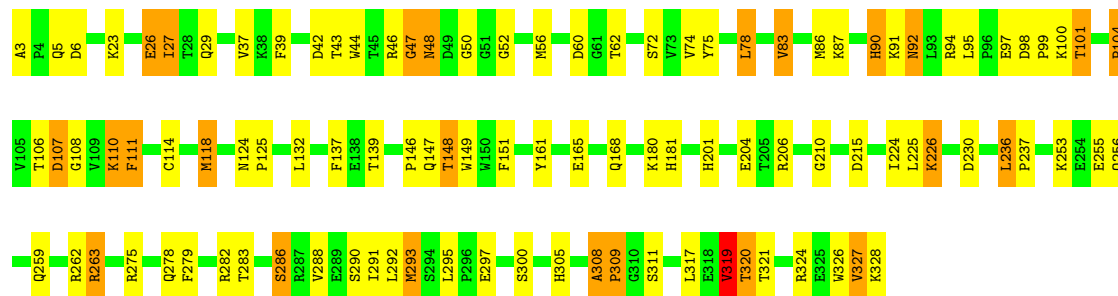
• Molecule 1: Coproporphyrinogen III oxidase





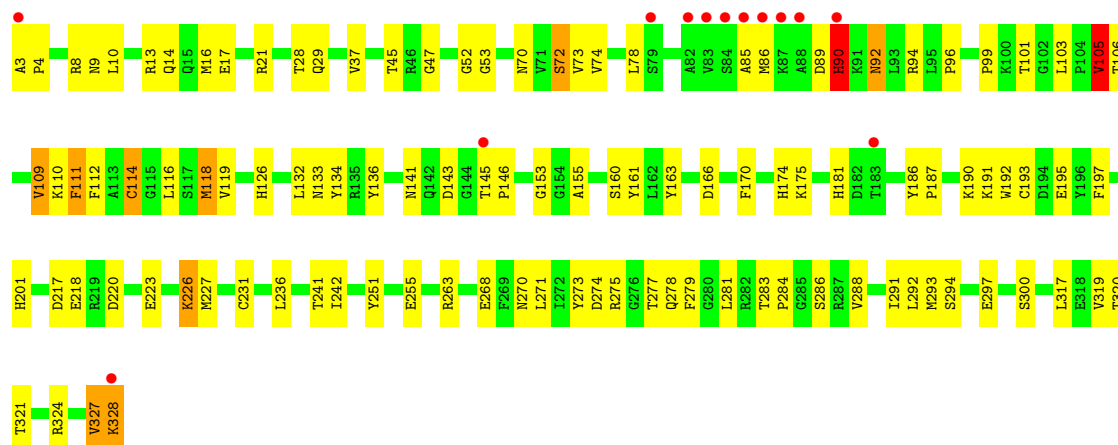
• Molecule 1: Coproporphyrinogen III oxidase

Chain S: 68% 24% 7%



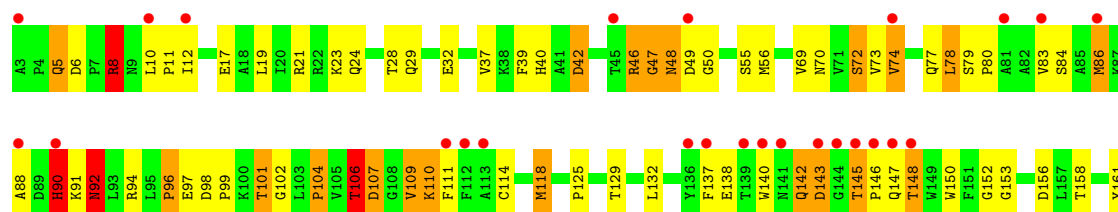
• Molecule 1: Coproporphyrinogen III oxidase

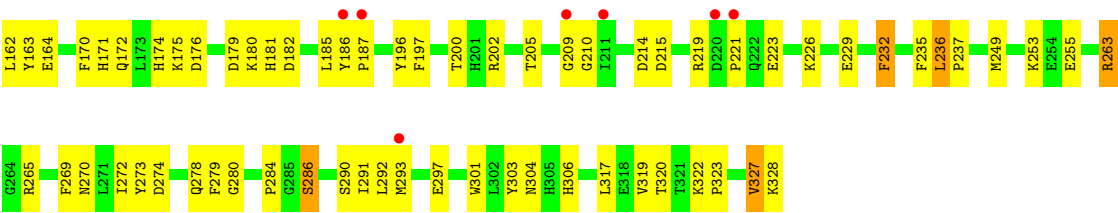
Chain U: 4% 66% 30%



• Molecule 1: Coproporphyrinogen III oxidase

Chain W: 10% 57% 34% 8%





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	232.77Å 65.24Å 166.07Å 90.00° 107.85° 90.00°	Depositor
Resolution (Å)	158.11 – 2.40 158.08 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.8 (158.11-2.40) 93.7 (158.08-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.85 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.208 , 0.282 0.214 , 0.286	Depositor DCC
R_{free} test set	4402 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.714	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16531	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.37	8/2723 (0.3%)	1.43	23/3693 (0.6%)
1	D	1.32	6/2725 (0.2%)	1.35	15/3697 (0.4%)
1	Q	1.44	14/2725 (0.5%)	1.25	15/3697 (0.4%)
1	S	1.57	13/2723 (0.5%)	1.32	16/3694 (0.4%)
1	U	1.49	10/2725 (0.4%)	1.34	12/3697 (0.3%)
1	W	1.20	9/2725 (0.3%)	1.21	12/3697 (0.3%)
All	All	1.41	60/16346 (0.4%)	1.32	93/22175 (0.4%)

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	A	0	6
1	D	0	4
1	Q	0	7
1	S	0	4
1	U	0	2
1	W	0	3
All	All	0	26

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	92	ASN	C-N	-37.16	0.79	1.33
1	S	110	LYS	C-N	-35.75	0.79	1.33
1	D	90	HIS	C-N	-27.71	0.94	1.33
1	A	110	LYS	C-N	-24.57	0.99	1.33
1	U	110	LYS	C-N	-20.26	1.05	1.33
1	Q	110	LYS	C-N	-19.46	1.06	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	92	ASN	C-N	-16.19	1.11	1.33
1	D	110	LYS	C-N	15.00	1.54	1.33
1	W	92	ASN	C-N	-13.26	1.15	1.33
1	Q	90	HIS	C-N	-13.22	1.13	1.33
1	Q	92	ASN	C-N	-11.72	1.17	1.33
1	S	92	ASN	C-N	-9.03	1.21	1.33
1	W	110	LYS	C-N	-8.89	1.21	1.33
1	Q	107	ASP	N-CA	7.59	1.55	1.46
1	S	90	HIS	C-N	-7.52	1.22	1.33
1	S	107	ASP	N-CA	7.30	1.55	1.46
1	U	109	VAL	N-CA	7.26	1.55	1.46
1	Q	106	THR	CA-C	7.20	1.61	1.52
1	W	96	PRO	CA-C	7.19	1.62	1.52
1	S	101	THR	CA-CB	7.14	1.65	1.53
1	A	105	VAL	CA-CB	7.10	1.64	1.54
1	U	109	VAL	CA-C	7.04	1.61	1.52
1	Q	41	ALA	CA-CB	-6.96	1.43	1.53
1	S	327	VAL	CA-C	6.67	1.60	1.52
1	U	320	THR	CA-CB	6.55	1.64	1.53
1	A	327	VAL	CA-C	6.54	1.58	1.52
1	U	110	LYS	CA-C	6.41	1.60	1.52
1	W	90	HIS	C-N	-6.41	1.24	1.33
1	A	90	HIS	C-N	-6.32	1.24	1.33
1	Q	234	ALA	CA-CB	-6.27	1.42	1.53
1	W	107	ASP	N-CA	6.13	1.54	1.46
1	A	105	VAL	CA-C	6.13	1.60	1.52
1	A	106	THR	N-CA	6.09	1.53	1.45
1	U	105	VAL	CA-CB	6.04	1.62	1.54
1	A	236	LEU	N-CA	5.96	1.51	1.46
1	U	241	THR	CA-CB	5.96	1.62	1.53
1	S	309	PRO	C-O	5.88	1.31	1.24
1	S	295	LEU	CA-C	-5.82	1.47	1.53
1	Q	109	VAL	CA-C	5.78	1.59	1.52
1	S	27	ILE	C-O	-5.68	1.17	1.24
1	S	106	THR	N-CA	5.67	1.52	1.46
1	Q	22	ARG	CZ-NH1	5.66	1.40	1.32
1	S	262	ARG	C-O	-5.51	1.17	1.24
1	D	105	VAL	N-CA	5.49	1.53	1.46
1	U	28	THR	C-O	-5.47	1.17	1.24
1	Q	107	ASP	CA-C	5.44	1.60	1.52
1	W	106	THR	CA-C	5.41	1.60	1.52
1	D	121	HIS	C-O	-5.41	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	201	HIS	N-CA	5.40	1.53	1.46
1	Q	48	ASN	CB-CG	5.33	1.65	1.52
1	A	92	ASN	C-N	-5.29	1.27	1.32
1	Q	258	TRP	C-O	-5.22	1.17	1.24
1	W	101	THR	CA-C	5.17	1.59	1.52
1	U	192	TRP	CA-C	5.11	1.59	1.52
1	W	97	GLU	CA-CB	5.06	1.59	1.52
1	Q	122	PRO	CA-C	-5.04	1.46	1.52
1	W	42	ASP	N-CA	-5.02	1.40	1.46
1	Q	105	VAL	CA-C	5.01	1.59	1.52
1	S	106	THR	CA-C	5.01	1.59	1.52
1	D	302	LEU	CA-C	-5.01	1.46	1.52

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	90	HIS	O-C-N	-31.98	86.77	123.22
1	A	90	HIS	O-C-N	-30.14	80.81	122.41
1	A	92	ASN	O-C-N	-21.81	94.04	122.39
1	W	92	ASN	O-C-N	-16.70	100.38	122.59
1	U	110	LYS	CA-C-N	16.28	149.15	122.29
1	U	110	LYS	C-N-CA	16.28	149.15	122.29
1	U	110	LYS	O-C-N	-12.42	109.29	123.33
1	A	110	LYS	CA-C-N	12.14	142.32	122.29
1	A	110	LYS	C-N-CA	12.14	142.32	122.29
1	D	90	HIS	CA-C-N	11.17	142.87	121.54
1	D	90	HIS	C-N-CA	11.17	142.87	121.54
1	Q	92	ASN	O-C-N	-11.04	107.22	122.46
1	U	90	HIS	O-C-N	-10.82	108.19	122.59
1	U	110	LYS	N-CA-C	10.76	125.88	108.99
1	W	90	HIS	O-C-N	-9.50	107.80	123.00
1	S	110	LYS	CA-C-N	9.44	137.35	122.62
1	S	110	LYS	C-N-CA	9.44	137.35	122.62
1	S	48	ASN	N-CA-C	9.20	123.47	110.50
1	A	42	ASP	N-CA-C	8.73	123.90	109.06
1	D	108	GLY	O-C-N	8.63	128.75	122.62
1	U	92	ASN	O-C-N	-8.31	109.11	122.41
1	S	92	ASN	O-C-N	7.85	131.76	122.34
1	Q	61	GLY	N-CA-C	-7.81	100.56	112.51
1	S	111	PHE	N-CA-C	7.52	121.38	109.50
1	D	48	ASN	N-CA-C	7.45	121.03	110.23
1	Q	110	LYS	CA-C-N	7.22	134.21	122.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	110	LYS	C-N-CA	7.22	134.21	122.29
1	Q	225	LEU	N-CA-C	6.94	118.85	111.28
1	S	46	ARG	N-CA-C	6.84	119.58	111.71
1	A	110	LYS	O-C-N	-6.70	114.70	123.21
1	Q	83	VAL	N-CA-C	6.70	116.85	110.42
1	A	27	ILE	N-CA-C	6.64	117.43	110.72
1	W	153	GLY	N-CA-C	6.48	119.37	110.56
1	S	91	LYS	N-CA-C	-6.28	105.48	113.02
1	A	218	GLU	N-CA-C	6.26	119.85	112.72
1	Q	12	ILE	N-CA-C	6.25	116.99	110.62
1	D	27	ILE	N-CA-C	6.21	116.88	110.36
1	Q	97	GLU	N-CA-C	-6.20	100.47	109.59
1	S	319	VAL	N-CA-CB	-6.16	102.70	112.07
1	U	111	PHE	N-CA-C	6.13	118.74	109.23
1	D	251	TYR	N-CA-C	6.11	118.70	109.23
1	W	110	LYS	N-CA-C	6.10	118.61	108.13
1	U	53	GLY	N-CA-C	6.01	119.28	110.80
1	Q	135	ARG	N-CA-C	5.93	117.86	108.79
1	S	308	ALA	CA-C-N	5.85	125.99	119.32
1	S	308	ALA	C-N-CA	5.85	125.99	119.32
1	D	153	GLY	N-CA-C	5.85	118.75	110.74
1	Q	90	HIS	O-C-N	-5.82	114.85	122.59
1	U	153	GLY	N-CA-C	5.77	117.77	110.38
1	A	83	VAL	N-CA-C	5.75	117.17	110.62
1	W	8	ARG	N-CA-C	5.75	117.41	111.03
1	D	220	ASP	CB-CA-C	5.71	117.67	109.11
1	A	37	VAL	CB-CA-C	5.68	119.79	110.69
1	A	47	GLY	N-CA-C	-5.66	99.77	113.18
1	S	118	MET	CG-SD-CE	-5.65	88.46	100.90
1	Q	153	GLY	N-CA-C	5.61	118.66	110.63
1	D	110	LYS	CA-C-N	-5.61	113.79	122.59
1	D	110	LYS	C-N-CA	-5.61	113.79	122.59
1	A	242	ILE	N-CA-C	5.61	116.25	110.36
1	Q	252	THR	OG1-CB-CG2	-5.56	98.19	109.30
1	A	86	MET	CB-CA-C	-5.52	101.63	110.79
1	A	76	GLY	N-CA-C	5.50	117.46	110.20
1	W	270	ASN	N-CA-C	5.50	118.20	111.82
1	W	96	PRO	N-CA-C	5.49	123.79	112.47
1	S	98	ASP	N-CA-C	5.48	118.17	109.40
1	U	160	SER	N-CA-C	-5.45	106.31	113.12
1	S	107	ASP	N-CA-C	5.42	122.33	110.80
1	D	274	ASP	N-CA-C	5.41	116.94	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	110	LYS	N-CA-C	5.34	118.10	109.40
1	W	102	GLY	N-CA-C	5.33	125.82	113.18
1	D	108	GLY	CA-C-N	5.29	129.45	122.51
1	D	108	GLY	C-N-CA	5.29	129.45	122.51
1	A	115	GLY	N-CA-C	5.28	120.90	111.03
1	U	118	MET	N-CA-C	5.25	117.99	109.06
1	Q	111	PHE	N-CA-C	5.19	117.27	109.23
1	W	46	ARG	CB-CA-C	5.17	120.70	110.42
1	A	316	LEU	N-CA-C	-5.16	105.56	111.14
1	S	210	GLY	N-CA-C	-5.14	101.00	113.18
1	W	196	TYR	N-CA-C	5.14	116.88	111.28
1	A	275	ARG	N-CA-C	5.11	116.93	111.36
1	A	111	PHE	N-CA-C	5.10	117.14	109.23
1	A	92	ASN	CA-C-N	5.09	128.58	123.13
1	A	92	ASN	C-N-CA	5.09	128.58	123.13
1	A	186	TYR	N-CA-C	5.09	121.05	109.81
1	S	47	GLY	CA-C-N	-5.08	112.96	120.94
1	S	47	GLY	C-N-CA	-5.08	112.96	120.94
1	U	327	VAL	N-CA-C	5.08	116.22	108.80
1	W	110	LYS	CA-C-N	5.07	131.32	122.81
1	W	110	LYS	C-N-CA	5.07	131.32	122.81
1	Q	7	PRO	N-CA-C	5.05	120.25	114.03
1	A	320	THR	N-CA-CB	-5.03	102.79	110.33
1	Q	74	VAL	CB-CA-C	5.01	118.71	110.69
1	A	319	VAL	CA-C-O	5.00	125.02	119.42

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	41	ALA	Peptide
1	A	47	GLY	Peptide
1	A	48	ASN	Peptide
1	A	90	HIS	Mainchain
1	A	92	ASN	Mainchain
1	A	99	PRO	Peptide
1	D	102	GLY	Peptide
1	D	3	ALA	Peptide
1	D	47	GLY	Peptide
1	D	90	HIS	Mainchain
1	Q	47	GLY	Peptide,Mainchain
1	Q	86	MET	Peptide

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Mol	Chain	Res	Type	Group
1	Q	90	HIS	Mainchain
1	Q	92	ASN	Mainchain
1	Q	93	LEU	Peptide
1	Q	95	LEU	Peptide
1	S	104	PRO	Peptide
1	S	47	GLY	Peptide
1	S	90	HIS	Mainchain
1	S	92	ASN	Mainchain
1	U	90	HIS	Mainchain
1	U	92	ASN	Mainchain
1	W	104	PRO	Peptide
1	W	90	HIS	Mainchain
1	W	92	ASN	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	2647	0	2547	52	0
1	D	2648	0	2550	54	0
1	Q	2648	0	2550	57	0
1	S	2647	0	2545	63	0
1	U	2648	0	2550	60	1
1	W	2648	0	2552	83	1
2	S	5	0	0	0	0
3	A	115	0	0	8	0
3	D	74	0	0	4	0
3	Q	151	0	0	8	0
3	S	140	0	0	11	1
3	U	103	0	0	8	1
3	W	57	0	0	10	0
All	All	16531	0	15294	354	2

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 12.

All (354) 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:Q:279:PHE:O	1:Q:283:THR:HG23	1.62	0.98
1:S:204:GLU:HB2	1:S:320:THR:HG23	1.42	0.97
1:Q:3:ALA:N	3:Q:407:HOH:O	1.99	0.94
1:A:204:GLU:HB2	1:A:320:THR:HG23	1.51	0.93
1:S:206:ARG:CD	1:S:206:ARG:CB	2.46	0.92
1:Q:303:TYR:CD1	1:S:293:MET:HE3	2.06	0.90
1:D:181:HIS:NE2	1:D:230:ASP:OD1	2.07	0.87
1:A:220:ASP:OD1	1:A:222:GLN:HB2	1.76	0.84
1:Q:48:ASN:HB3	1:Q:49:ASP:HA	1.61	0.82
1:S:42:ASP:OD2	1:U:14:GLN:NE2	2.11	0.82
1:U:279:PHE:O	1:U:283:THR:HG23	1.79	0.81
1:Q:204:GLU:HB2	1:Q:320:THR:HG23	1.61	0.81
1:Q:282:ARG:NH1	3:Q:465:HOH:O	2.13	0.81
1:W:142:GLN:HE21	1:W:142:GLN:HA	1.43	0.81
1:D:3:ALA:HB3	1:D:4:PRO:HA	1.63	0.80
1:Q:303:TYR:CD1	1:S:293:MET:CE	2.63	0.80
1:W:280:GLY:O	3:W:364:HOH:O	2.01	0.78
1:A:3:ALA:N	3:A:415:HOH:O	2.16	0.78
1:Q:252:THR:HG23	1:Q:255:GLU:H	1.48	0.76
1:W:274:ASP:O	1:W:278:GLN:HG2	1.84	0.76
1:S:27:ILE:HD13	1:S:118:MET:HE1	1.67	0.76
1:U:226:LYS:NZ	1:U:226:LYS:HA	2.01	0.75
1:D:287:ARG:O	1:D:291:ILE:HD12	1.87	0.75
1:U:319:VAL:HG13	1:U:324:ARG:HG2	1.68	0.74
1:Q:293:MET:CE	3:Q:456:HOH:O	2.35	0.74
1:D:204:GLU:HB2	1:D:320:THR:HG23	1.68	0.74
1:Q:48:ASN:CG	1:Q:50:GLY:H	1.95	0.74
1:W:48:ASN:O	1:W:50:GLY:N	2.21	0.74
1:W:46:ARG:HH11	1:W:74:VAL:HG22	1.53	0.73
1:S:279:PHE:O	1:S:283:THR:HG23	1.88	0.73
1:D:204:GLU:HB2	1:D:320:THR:CG2	2.20	0.72
1:U:288:VAL:HA	1:U:291:ILE:HD12	1.72	0.71
1:A:175:LYS:HD3	1:A:327:VAL:HG21	1.71	0.71
1:S:168:GLN:HG2	1:S:326:TRP:O	1.90	0.70
1:S:293:MET:HE2	1:S:293:MET:HA	1.72	0.70
1:U:220:ASP:O	1:U:223:GLU:HB2	1.91	0.70
1:U:73:VAL:HG22	1:U:114:CYS:HB2	1.72	0.70
1:S:27:ILE:HG21	1:S:118:MET:HE1	1.73	0.70
1:A:3:ALA:HB1	1:A:4:PRO:HA	1.73	0.70
1:W:163:TYR:OH	1:W:249:MET:HE1	1.92	0.69
1:S:146:PRO:O	3:S:727:HOH:O	2.09	0.69
1:A:170:PHE:O	1:A:174:HIS:HD2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:195:GLU:OE2	3:U:383:HOH:O	2.12	0.68
1:D:118:MET:CE	1:D:132:LEU:HB3	2.23	0.67
1:A:136:TYR:OH	1:A:138:GLU:OE2	2.07	0.67
1:W:90:HIS:HA	3:W:384:HOH:O	1.93	0.67
1:A:3:ALA:CB	1:A:4:PRO:HA	2.25	0.66
1:S:139:THR:OG1	1:S:147:GLN:NE2	2.28	0.66
1:U:277:THR:O	1:U:281:LEU:HG	1.95	0.66
1:S:5:GLN:O	1:S:6:ASP:C	2.37	0.66
1:Q:201:HIS:HE1	1:Q:268:GLU:OE1	1.77	0.66
1:S:139:THR:CB	1:S:147:GLN:HE21	2.08	0.65
1:Q:252:THR:OG1	1:Q:254:GLU:OE1	2.12	0.65
1:W:28:THR:O	1:W:32:GLU:HG3	1.96	0.65
1:Q:303:TYR:HD1	1:S:293:MET:CE	2.07	0.65
1:W:181:HIS:NE2	3:W:365:HOH:O	2.30	0.64
1:W:180:LYS:HB2	3:W:365:HOH:O	1.97	0.63
1:A:282:ARG:CZ	3:A:442:HOH:O	2.46	0.63
1:W:118:MET:HE2	1:W:132:LEU:HD13	1.81	0.63
1:W:78:LEU:HD11	1:W:86:MET:SD	2.37	0.62
1:S:305:HIS:HD2	3:S:754:HOH:O	1.83	0.62
1:Q:48:ASN:HB3	1:Q:49:ASP:CA	2.31	0.61
1:S:319:VAL:HG22	1:S:324:ARG:HG2	1.82	0.61
1:W:327:VAL:HG13	1:W:328:LYS:N	2.16	0.61
1:W:55:SER:OG	1:W:70:ASN:ND2	2.33	0.61
1:W:317:LEU:HA	1:W:320:THR:HG22	1.82	0.61
1:A:201:HIS:ND1	1:A:273:TYR:OH	2.32	0.60
1:W:47:GLY:HA3	1:W:48:ASN:O	2.01	0.60
1:U:141:ASN:OD1	1:U:146:PRO:O	2.20	0.60
1:U:226:LYS:HA	1:U:226:LYS:HZ3	1.66	0.60
1:Q:143:ASP:OD1	1:Q:145:THR:OG1	2.16	0.59
1:A:186:TYR:O	1:A:190:LYS:HB2	2.03	0.59
1:S:286:SER:HB3	1:S:291:ILE:HD11	1.85	0.59
1:W:118:MET:HE1	1:W:235:PHE:CZ	2.38	0.59
1:S:293:MET:HE2	1:S:293:MET:CA	2.33	0.59
1:S:293:MET:CE	1:S:293:MET:HA	2.30	0.58
1:A:173:LEU:HD12	1:A:238:SER:HB3	1.84	0.58
1:W:172:GLN:OE1	1:W:327:VAL:HG22	2.03	0.58
1:A:282:ARG:NE	3:A:442:HOH:O	2.36	0.58
1:W:46:ARG:HB3	1:W:47:GLY:HA2	1.85	0.58
1:W:161:TYR:OH	1:W:255:GLU:HA	2.04	0.57
1:A:46:ARG:HD2	1:A:74:VAL:HG22	1.87	0.57
1:Q:48:ASN:HA	1:Q:50:GLY:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:293:MET:HE2	3:S:704:HOH:O	2.05	0.57
1:S:148:THR:CG2	3:S:715:HOH:O	2.53	0.57
1:Q:303:TYR:CD1	1:S:293:MET:HE1	2.39	0.57
1:U:143:ASP:OD2	1:U:145:THR:N	2.27	0.57
1:Q:297:GLU:O	1:S:300:SER:HA	2.05	0.57
1:W:142:GLN:HE21	1:W:142:GLN:CA	2.15	0.57
1:D:118:MET:HE2	1:D:132:LEU:HB3	1.86	0.57
1:A:119:VAL:HG21	1:A:294:SER:HB2	1.87	0.56
1:D:151:PHE:CD1	1:D:224:ILE:HG21	2.39	0.56
1:D:279:PHE:O	1:D:283:THR:HG23	2.05	0.56
1:Q:5:GLN:O	1:Q:6:ASP:C	2.48	0.56
1:U:328:LYS:C	3:U:431:HOH:O	2.46	0.56
1:Q:305:HIS:HD2	3:Q:425:HOH:O	1.87	0.56
1:Q:48:ASN:HA	1:Q:50:GLY:H	1.71	0.56
1:S:39:PHE:HB3	1:S:56:MET:HE2	1.88	0.56
1:W:171:HIS:CE1	1:W:210:GLY:HA2	2.41	0.55
1:A:134:TYR:OH	1:A:231:CYS:HB3	2.06	0.55
1:Q:27:ILE:HD13	1:Q:118:MET:HE1	1.89	0.55
1:A:69:VAL:HG22	1:A:118:MET:HG3	1.87	0.55
1:D:119:VAL:HG21	1:D:294:SER:HB2	1.89	0.55
1:Q:293:MET:HE3	3:Q:456:HOH:O	2.05	0.55
1:A:3:ALA:N	3:A:341:HOH:O	2.39	0.55
1:Q:11:PRO:O	1:Q:15:GLN:HG3	2.07	0.55
1:W:118:MET:CE	1:W:132:LEU:HD13	2.37	0.54
1:A:114:CYS:O	1:A:114:CYS:SG	2.65	0.54
1:W:182:ASP:HB3	1:W:185:LEU:HG	1.90	0.54
1:W:286:SER:HB3	1:W:291:ILE:HD11	1.89	0.54
1:A:3:ALA:HB1	1:A:4:PRO:CA	2.37	0.54
1:W:73:VAL:HG13	1:W:114:CYS:HB3	1.90	0.54
1:W:306:HIS:CE1	3:W:347:HOH:O	2.61	0.54
1:W:197:PHE:HA	1:W:269:PHE:CE1	2.44	0.54
1:W:138:GLU:HG3	1:W:148:THR:O	2.08	0.53
1:Q:293:MET:HE1	3:Q:456:HOH:O	2.05	0.53
1:W:79:SER:OG	1:W:80:PRO:HD2	2.07	0.53
1:D:118:MET:HE3	1:D:132:LEU:HB3	1.89	0.53
1:S:151:PHE:CD1	1:S:224:ILE:HG21	2.43	0.53
1:W:73:VAL:HG22	1:W:114:CYS:HB2	1.90	0.53
1:D:15:GLN:O	1:D:16:MET:C	2.51	0.52
1:W:5:GLN:O	1:W:6:ASP:C	2.52	0.52
1:S:87:LYS:NZ	3:S:769:HOH:O	2.34	0.52
1:W:125:PRO:O	3:W:337:HOH:O	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:46:ARG:HD3	1:Q:50:GLY:O	2.09	0.52
1:W:317:LEU:HA	1:W:320:THR:CG2	2.38	0.52
1:A:26:GLU:OE1	3:A:433:HOH:O	2.18	0.52
1:U:193:CYS:HB3	3:U:355:HOH:O	2.10	0.52
1:W:263:ARG:CG	1:W:263:ARG:HH11	2.22	0.52
1:D:199:ILE:O	1:D:200:THR:C	2.53	0.52
1:S:86:MET:HG2	1:S:279:PHE:CE1	2.45	0.52
1:U:17:GLU:HB2	3:U:410:HOH:O	2.09	0.52
1:W:181:HIS:CD2	3:W:365:HOH:O	2.62	0.52
1:A:251:TYR:HA	1:A:255:GLU:OE1	2.10	0.52
1:D:243:VAL:O	1:D:247:LYS:HB3	2.09	0.52
1:W:10:LEU:N	1:W:11:PRO:CD	2.73	0.52
1:Q:252:THR:HG22	1:Q:255:GLU:CD	2.36	0.51
1:A:169:LEU:HD11	1:A:173:LEU:HD11	1.91	0.51
1:S:308:ALA:O	1:S:311:SER:OG	2.20	0.51
1:A:278:GLN:HG2	1:A:282:ARG:NH2	2.26	0.51
1:Q:303:TYR:HD1	1:S:293:MET:HE1	1.73	0.51
1:U:72:SER:O	1:U:114:CYS:HA	2.10	0.51
1:Q:48:ASN:CB	1:Q:49:ASP:HA	2.38	0.51
1:S:278:GLN:HB3	1:S:282:ARG:CZ	2.41	0.51
1:Q:72:SER:O	1:Q:114:CYS:HA	2.11	0.51
1:S:317:LEU:O	1:S:321:THR:OG1	2.23	0.51
1:S:290:SER:O	1:S:293:MET:HB2	2.10	0.51
1:S:204:GLU:OE1	1:S:320:THR:HG21	2.11	0.51
1:U:186:TYR:HB3	1:U:187:PRO:CD	2.41	0.50
1:W:205:THR:O	1:W:320:THR:OG1	2.29	0.50
1:D:170:PHE:O	1:D:174:HIS:HD2	1.94	0.50
1:U:181:HIS:NE2	1:U:227:MET:HA	2.27	0.50
1:S:259:GLN:HG2	1:S:263:ARG:HD2	1.93	0.50
1:W:17:GLU:O	1:W:21:ARG:HG3	2.11	0.50
1:S:3:ALA:N	3:S:728:HOH:O	2.45	0.50
1:U:293:MET:SD	1:U:293:MET:C	2.95	0.50
1:Q:317:LEU:HA	1:Q:320:THR:HG22	1.93	0.50
1:U:3:ALA:N	3:U:342:HOH:O	2.43	0.50
1:S:60:ASP:HB3	3:S:816:HOH:O	2.11	0.50
1:U:70:ASN:O	1:U:116:LEU:HA	2.11	0.50
1:Q:10:LEU:HB3	1:Q:11:PRO:HD3	1.93	0.50
1:S:293:MET:CE	3:S:704:HOH:O	2.59	0.50
1:A:279:PHE:O	1:A:283:THR:HG22	2.12	0.50
1:W:284:PRO:HG2	3:W:368:HOH:O	2.12	0.50
1:D:157:LEU:HD23	1:D:208:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:TYR:O	1:A:186:TYR:CG	2.64	0.49
1:D:204:GLU:OE1	1:D:320:THR:HG21	2.12	0.49
1:Q:252:THR:HG23	1:Q:255:GLU:N	2.23	0.49
1:A:17:GLU:HG3	1:A:73:VAL:HG21	1.95	0.49
1:U:271:LEU:HD22	1:W:272:ILE:HD11	1.95	0.49
1:U:297:GLU:HA	1:W:301:TRP:O	2.13	0.49
1:W:118:MET:HE3	1:W:132:LEU:HB3	1.93	0.49
1:D:116:LEU:C	1:D:116:LEU:HD23	2.38	0.49
1:D:167:GLY:HA3	1:D:326:TRP:CE3	2.47	0.49
1:Q:201:HIS:CE1	1:Q:268:GLU:OE1	2.62	0.49
1:U:116:LEU:O	1:U:133:ASN:HA	2.13	0.49
1:A:46:ARG:HD3	1:A:50:GLY:O	2.12	0.48
1:D:231:CYS:O	1:D:232:PHE:C	2.56	0.48
1:Q:197:PHE:HA	1:Q:269:PHE:CE1	2.48	0.48
1:W:170:PHE:O	1:W:174:HIS:HD2	1.96	0.48
1:A:27:ILE:HD13	1:A:118:MET:HE1	1.95	0.48
1:A:87:LYS:HB2	1:A:215:ASP:OD1	2.14	0.48
1:D:3:ALA:HB3	1:D:4:PRO:CA	2.40	0.48
1:D:252:THR:OG1	1:D:253:LYS:N	2.45	0.48
1:W:290:SER:O	1:W:293:MET:HG3	2.13	0.48
1:U:170:PHE:O	1:U:174:HIS:HD2	1.96	0.48
1:A:87:LYS:HD3	1:A:89:ASP:O	2.14	0.48
1:S:204:GLU:CB	1:S:320:THR:HG23	2.30	0.48
1:U:118:MET:CE	1:U:132:LEU:HD13	2.44	0.48
1:D:12:ILE:HG13	1:D:221:PRO:HB2	1.94	0.48
1:D:141:ASN:HB2	1:D:143:ASP:OD2	2.12	0.48
1:D:305:HIS:HD2	3:D:343:HOH:O	1.96	0.48
1:S:27:ILE:CD1	1:S:118:MET:HE1	2.40	0.48
1:W:72:SER:O	1:W:114:CYS:HA	2.14	0.48
1:Q:303:TYR:CE1	1:S:293:MET:HE3	2.47	0.48
1:Q:328:LYS:NZ	1:Q:328:LYS:N	2.61	0.48
1:S:78:LEU:CD1	1:S:83:VAL:HG22	2.43	0.48
1:A:271:LEU:HD22	1:D:272:ILE:HD11	1.94	0.47
1:D:149:TRP:CZ2	1:D:221:PRO:HD3	2.50	0.47
1:A:293:MET:SD	1:A:293:MET:C	2.97	0.47
1:Q:46:ARG:HD2	1:Q:74:VAL:HG22	1.95	0.47
1:W:142:GLN:CA	1:W:142:GLN:NE2	2.78	0.47
1:A:3:ALA:CB	1:A:4:PRO:CA	2.91	0.47
1:A:40:HIS:HB2	3:A:391:HOH:O	2.15	0.47
1:Q:118:MET:HE3	1:Q:132:LEU:HB3	1.95	0.47
1:Q:201:HIS:HD2	1:Q:273:TYR:OH	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:274:ASP:O	1:W:278:GLN:NE2	2.47	0.47
1:Q:6:ASP:HB2	3:Q:479:HOH:O	2.14	0.47
1:U:217:ASP:C	1:U:217:ASP:OD1	2.56	0.47
1:A:170:PHE:O	1:A:174:HIS:CD2	2.64	0.47
1:D:245:ARG:C	3:D:347:HOH:O	2.59	0.46
1:A:164:GLU:O	1:A:168:GLN:HG3	2.14	0.46
1:W:46:ARG:CB	1:W:47:GLY:CA	2.93	0.46
1:U:190:LYS:O	1:U:191:LYS:C	2.58	0.46
1:D:136:TYR:CE1	1:D:149:TRP:HB2	2.51	0.46
1:W:163:TYR:CZ	1:W:249:MET:HE1	2.51	0.46
1:D:319:VAL:HG22	1:D:324:ARG:HG2	1.96	0.46
1:A:86:MET:HG2	1:A:279:PHE:CE1	2.51	0.46
1:S:23:LYS:HA	1:S:26:GLU:HG2	1.97	0.46
1:D:161:TYR:OH	1:D:255:GLU:HA	2.15	0.46
1:U:134:TYR:CZ	1:U:231:CYS:HB3	2.51	0.46
1:U:226:LYS:HA	1:U:226:LYS:CE	2.45	0.46
1:W:10:LEU:N	1:W:11:PRO:HD2	2.31	0.46
1:W:284:PRO:CG	3:W:368:HOH:O	2.64	0.46
1:U:201:HIS:HE1	1:U:268:GLU:OE1	1.99	0.46
1:D:66:LYS:NZ	3:D:398:HOH:O	2.48	0.45
1:D:137:PHE:O	1:D:149:TRP:HA	2.17	0.45
1:U:118:MET:HE3	1:U:132:LEU:HD13	1.97	0.45
1:W:24:GLN:O	1:W:28:THR:HG23	2.16	0.45
1:W:156:ASP:HA	1:W:209:GLY:O	2.16	0.45
1:Q:315:LYS:HG3	3:Q:414:HOH:O	2.15	0.45
1:W:86:MET:HG2	1:W:279:PHE:CE1	2.51	0.45
1:Q:286:SER:HB3	1:Q:291:ILE:HD11	1.99	0.45
1:S:118:MET:HG2	1:S:132:LEU:HB3	1.98	0.45
1:U:9:ASN:O	1:U:10:LEU:C	2.60	0.45
1:W:19:LEU:O	1:W:23:LYS:HG2	2.16	0.45
1:D:190:LYS:HD3	1:D:190:LYS:C	2.42	0.45
1:S:50:GLY:HA2	1:S:75:TYR:O	2.17	0.45
1:U:45:THR:HA	1:U:52:GLY:HA3	1.99	0.45
1:U:85:ALA:HB1	1:U:275:ARG:O	2.17	0.45
1:U:89:ASP:HB2	3:U:373:HOH:O	2.16	0.45
1:U:155:ALA:HB3	1:U:174:HIS:CE1	2.52	0.45
1:W:46:ARG:CB	1:W:47:GLY:HA2	2.46	0.45
1:D:75:TYR:HA	1:D:111:PHE:O	2.16	0.45
1:U:126:HIS:ND1	1:U:163:TYR:OH	2.48	0.45
1:W:78:LEU:CD2	1:W:83:VAL:HG22	2.47	0.45
1:U:17:GLU:O	1:U:21:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:327:VAL:HG22	1:U:328:LYS:N	2.32	0.45
1:W:229:GLU:O	1:W:232:PHE:HB2	2.16	0.45
1:D:162:LEU:HD11	1:D:326:TRP:HH2	1.83	0.44
1:S:308:ALA:HA	1:S:309:PRO:HD3	1.86	0.44
1:D:46:ARG:HD2	1:D:74:VAL:HG22	1.97	0.44
1:Q:46:ARG:NH2	1:Q:284:PRO:O	2.43	0.44
1:U:4:PRO:O	1:U:13:ARG:NH1	2.38	0.44
1:D:35:ASP:OD1	1:D:36:THR:N	2.46	0.44
1:S:275:ARG:HD2	3:S:762:HOH:O	2.18	0.44
1:U:166:ASP:OD2	1:U:242:ILE:HG23	2.18	0.44
1:U:175:LYS:HD3	1:U:327:VAL:HG21	2.00	0.44
1:W:140:TRP:C	1:W:147:GLN:HB2	2.42	0.44
1:D:317:LEU:O	1:D:321:THR:HG23	2.16	0.44
1:Q:181:HIS:NE2	1:Q:230:ASP:OD1	2.39	0.44
1:U:143:ASP:OD2	1:U:145:THR:CB	2.66	0.44
1:A:137:PHE:HB2	1:A:150:TRP:CE2	2.53	0.44
1:A:169:LEU:CD1	1:A:173:LEU:HD11	2.47	0.44
1:S:215:ASP:N	1:S:215:ASP:OD1	2.49	0.44
1:W:137:PHE:HB3	1:W:150:TRP:CH2	2.53	0.44
1:U:201:HIS:HD2	1:U:273:TYR:OH	2.01	0.44
1:U:251:TYR:HA	1:U:255:GLU:OE1	2.17	0.44
1:Q:317:LEU:O	1:Q:321:THR:HG23	2.18	0.44
1:W:145:THR:HB	1:W:146:PRO:HD2	2.00	0.44
1:U:119:VAL:HG21	1:U:294:SER:HB2	2.00	0.43
1:U:283:THR:HA	1:U:284:PRO:HD3	1.76	0.43
1:W:152:GLY:HA2	1:W:214:ASP:HA	1.99	0.43
1:W:236:LEU:N	1:W:237:PRO:CD	2.81	0.43
1:Q:68:GLY:HA3	1:Q:293:MET:SD	2.59	0.43
1:A:190:LYS:HA	1:A:210:GLY:O	2.18	0.43
1:Q:134:TYR:OH	1:Q:231:CYS:HB3	2.19	0.43
1:Q:283:THR:HA	1:Q:284:PRO:HD3	1.73	0.43
1:U:197:PHE:HB2	3:U:344:HOH:O	2.17	0.43
1:D:46:ARG:CD	1:D:74:VAL:HG22	2.49	0.43
1:W:12:ILE:CD1	1:W:221:PRO:HB2	2.49	0.43
1:D:182:ASP:OD2	1:D:182:ASP:C	2.59	0.43
1:W:39:PHE:HB3	1:W:56:MET:HE2	2.01	0.43
1:Q:46:ARG:CD	1:Q:74:VAL:HG22	2.49	0.43
1:S:181:HIS:NE2	1:S:230:ASP:OD1	2.51	0.43
1:S:161:TYR:OH	1:S:255:GLU:HA	2.19	0.43
1:D:32:GLU:OE2	1:D:39:PHE:N	2.47	0.42
1:U:134:TYR:OH	1:U:231:CYS:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:ARG:O	3:D:372:HOH:O	2.21	0.42
1:Q:175:LYS:HD2	1:Q:327:VAL:HG21	2.00	0.42
1:A:272:ILE:O	1:A:278:GLN:NE2	2.51	0.42
1:D:23:LYS:HA	1:D:26:GLU:HG2	1.99	0.42
1:D:308:ALA:O	1:D:311:SER:OG	2.28	0.42
1:Q:328:LYS:N	1:Q:328:LYS:HZ2	2.17	0.42
1:W:143:ASP:OD1	1:W:143:ASP:N	2.43	0.42
1:A:48:ASN:HA	3:A:356:HOH:O	2.18	0.42
1:A:182:ASP:OD2	1:A:184:ALA:HB3	2.19	0.42
1:A:175:LYS:CD	1:A:327:VAL:HG21	2.43	0.42
1:S:43:THR:OG1	1:U:17:GLU:OE2	2.28	0.42
1:S:139:THR:OG1	1:S:147:GLN:HG3	2.19	0.42
1:W:78:LEU:CD1	1:W:86:MET:SD	3.06	0.42
1:A:17:GLU:HG3	1:A:73:VAL:CG2	2.49	0.42
1:D:259:GLN:O	1:D:263:ARG:HD3	2.20	0.42
1:Q:201:HIS:O	1:S:288:VAL:HG21	2.19	0.42
1:W:175:LYS:O	1:W:176:ASP:C	2.63	0.42
1:A:67:GLY:HA2	1:A:119:VAL:O	2.20	0.42
1:W:322:LYS:HA	1:W:323:PRO:HD2	1.88	0.42
1:A:311:SER:O	1:A:315:LYS:HG3	2.19	0.42
1:D:163:TYR:HB3	1:D:246:ARG:NH2	2.35	0.42
1:Q:197:PHE:O	1:Q:205:THR:HA	2.20	0.42
1:U:317:LEU:O	1:U:321:THR:HG23	2.19	0.42
1:D:136:TYR:CZ	1:D:149:TRP:HB2	2.54	0.41
1:S:72:SER:O	1:S:114:CYS:HA	2.19	0.41
1:U:16:MET:HG2	1:U:136:TYR:HB2	2.02	0.41
1:S:44:TRP:CZ3	1:S:52:GLY:HA2	2.56	0.41
1:U:270:ASN:HA	1:U:274:ASP:HB3	2.02	0.41
1:W:88:ALA:HB3	1:W:215:ASP:OD2	2.21	0.41
1:Q:252:THR:HG22	1:Q:255:GLU:CG	2.50	0.41
1:U:17:GLU:HG3	1:U:73:VAL:HG21	2.02	0.41
1:W:40:HIS:O	1:W:56:MET:HA	2.21	0.41
1:A:250:PRO:HB3	1:Q:309:PRO:HD2	2.03	0.41
1:D:125:PRO:HD2	1:D:251:TYR:CD2	2.55	0.41
1:D:134:TYR:OH	1:D:231:CYS:HB3	2.19	0.41
1:S:118:MET:HE3	1:S:132:LEU:HD22	2.01	0.41
1:W:73:VAL:HG22	1:W:114:CYS:CB	2.50	0.41
1:D:204:GLU:HB2	1:D:320:THR:HG22	2.01	0.41
1:S:180:LYS:NZ	3:S:771:HOH:O	2.53	0.41
1:S:181:HIS:HE1	1:S:226:LYS:HG3	1.85	0.41
1:U:112:PHE:CD1	1:U:112:PHE:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:319:VAL:O	1:W:319:VAL:HG12	2.20	0.41
1:A:12:ILE:HD13	1:A:225:LEU:HD12	2.02	0.41
1:U:161:TYR:OH	1:U:255:GLU:HA	2.20	0.41
1:W:78:LEU:HD12	1:W:111:PHE:CG	2.56	0.41
1:D:87:LYS:CG	1:D:150:TRP:CZ2	3.03	0.41
1:S:124:ASN:HA	1:S:125:PRO:HD3	1.91	0.41
1:W:269:PHE:CD2	1:W:269:PHE:C	2.99	0.41
1:A:17:GLU:CG	1:A:73:VAL:HG21	2.51	0.41
1:S:236:LEU:N	1:S:237:PRO:CD	2.84	0.41
1:U:186:TYR:CB	1:U:187:PRO:CD	2.99	0.41
1:U:278:GLN:HG3	3:U:336:HOH:O	2.21	0.41
1:W:186:TYR:HB3	1:W:187:PRO:HD3	2.03	0.41
1:W:303:TYR:O	1:W:304:ASN:C	2.64	0.41
1:S:305:HIS:CD2	3:S:754:HOH:O	2.67	0.41
1:A:282:ARG:NH1	3:A:382:HOH:O	2.50	0.40
1:Q:327:VAL:C	1:Q:328:LYS:HZ1	2.29	0.40
1:W:158:THR:CG2	3:W:377:HOH:O	2.68	0.40
1:D:8:ARG:HD2	1:D:9:ASN:ND2	2.35	0.40
1:U:300:SER:HB3	1:W:297:GLU:O	2.20	0.40
1:S:137:PHE:O	1:S:149:TRP:HA	2.22	0.40
1:W:69:VAL:HA	1:W:118:MET:HB3	2.02	0.40
1:W:200:THR:HB	1:W:273:TYR:OH	2.21	0.40
1:W:202:ARG:HD2	1:W:265:ARG:CZ	2.51	0.40
1:D:13:ARG:HD3	1:D:138:GLU:OE2	2.21	0.40
1:S:278:GLN:HB3	1:S:282:ARG:NH2	2.37	0.40

All (2) 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)
3:S:727:HOH:O	3:U:372:HOH:O[4_555]	1.49	0.71
1:U:101:THR:O	1:W:8:ARG:NH2[2_555]	2.06	0.14

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	324/326 (99%)	298 (92%)	20 (6%)	6 (2%)	6	8
1	D	324/326 (99%)	299 (92%)	18 (6%)	7 (2%)	5	6
1	Q	324/326 (99%)	297 (92%)	17 (5%)	10 (3%)	3	3
1	S	324/326 (99%)	302 (93%)	15 (5%)	7 (2%)	5	6
1	U	324/326 (99%)	293 (90%)	25 (8%)	6 (2%)	6	8
1	W	324/326 (99%)	275 (85%)	32 (10%)	17 (5%)	1	1
All	All	1944/1956 (99%)	1764 (91%)	127 (6%)	53 (3%)	4	4

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	LYS
1	A	105	VAL
1	D	95	LEU
1	D	97	GLU
1	D	101	THR
1	Q	105	VAL
1	Q	107	ASP
1	S	94	ARG
1	S	99	PRO
1	S	107	ASP
1	U	90	HIS
1	U	105	VAL
1	W	49	ASP
1	W	96	PRO
1	W	104	PRO
1	W	106	THR
1	W	107	ASP
1	A	98	ASP
1	D	91	LYS
1	D	107	ASP
1	Q	47	GLY
1	Q	49	ASP
1	Q	94	ARG
1	Q	100	LYS
1	S	83	VAL
1	S	104	PRO
1	U	99	PRO

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Mol	Chain	Res	Type
1	U	106	THR
1	W	48	ASN
1	Q	93	LEU
1	Q	95	LEU
1	Q	102	GLY
1	U	47	GLY
1	W	47	GLY
1	W	84	SER
1	W	86	MET
1	W	90	HIS
1	W	101	THR
1	A	107	ASP
1	Q	182	ASP
1	W	94	ARG
1	W	232	PHE
1	D	34	ILE
1	W	92	ASN
1	W	179	ASP
1	D	104	PRO
1	S	95	LEU
1	A	104	PRO
1	U	96	PRO
1	A	6	ASP
1	S	108	GLY
1	W	109	VAL
1	W	99	PRO

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	282/282 (100%)	259 (92%)	23 (8%)	10	18
1	D	282/282 (100%)	255 (90%)	27 (10%)	8	12
1	Q	282/282 (100%)	258 (92%)	24 (8%)	10	16
1	S	281/282 (100%)	253 (90%)	28 (10%)	7	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	282/282 (100%)	262 (93%)	20 (7%)	13	23
1	W	282/282 (100%)	250 (89%)	32 (11%)	5	8
All	All	1691/1692 (100%)	1537 (91%)	154 (9%)	9	14

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	A	49	ASP
1	A	74	VAL
1	A	77	GLN
1	A	87	LYS
1	A	91	LYS
1	A	95	LEU
1	A	98	ASP
1	A	106	THR
1	A	111	PHE
1	A	112	PHE
1	A	114	CYS
1	A	148	THR
1	A	165	GLU
1	A	215	ASP
1	A	236	LEU
1	A	253	LYS
1	A	263	ARG
1	A	283	THR
1	A	292	LEU
1	A	320	THR
1	A	327	VAL
1	A	328	LYS
1	D	5	GLN
1	D	29	GLN
1	D	36	THR
1	D	37	VAL
1	D	45	THR
1	D	57	VAL
1	D	71	VAL
1	D	74	VAL
1	D	92	ASN
1	D	94	ARG
1	D	95	LEU

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Mol	Chain	Res	Type
1	D	101	THR
1	D	105	VAL
1	D	106	THR
1	D	109	VAL
1	D	110	LYS
1	D	129	THR
1	D	148	THR
1	D	244	LYS
1	D	252	THR
1	D	263	ARG
1	D	302	LEU
1	D	319	VAL
1	D	320	THR
1	D	322	LYS
1	D	327	VAL
1	D	328	LYS
1	Q	37	VAL
1	Q	74	VAL
1	Q	78	LEU
1	Q	101	THR
1	Q	106	THR
1	Q	109	VAL
1	Q	118	MET
1	Q	139	THR
1	Q	148	THR
1	Q	162	LEU
1	Q	164	GLU
1	Q	183	THR
1	Q	226	LYS
1	Q	236	LEU
1	Q	253	LYS
1	Q	263	ARG
1	Q	282	ARG
1	Q	283	THR
1	Q	292	LEU
1	Q	315	LYS
1	Q	319	VAL
1	Q	320	THR
1	Q	327	VAL
1	Q	328	LYS
1	S	26	GLU
1	S	29	GLN

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Mol	Chain	Res	Type
1	S	37	VAL
1	S	48	ASN
1	S	62	THR
1	S	74	VAL
1	S	78	LEU
1	S	97	GLU
1	S	100	LYS
1	S	101	THR
1	S	110	LYS
1	S	111	PHE
1	S	148	THR
1	S	165	GLU
1	S	225	LEU
1	S	226	LYS
1	S	236	LEU
1	S	253	LYS
1	S	256	GLN
1	S	263	ARG
1	S	286	SER
1	S	292	LEU
1	S	293	MET
1	S	297	GLU
1	S	319	VAL
1	S	320	THR
1	S	327	VAL
1	S	328	LYS
1	U	8	ARG
1	U	29	GLN
1	U	37	VAL
1	U	72	SER
1	U	74	VAL
1	U	78	LEU
1	U	86	MET
1	U	94	ARG
1	U	103	LEU
1	U	105	VAL
1	U	109	VAL
1	U	111	PHE
1	U	114	CYS
1	U	218	GLU
1	U	226	LYS
1	U	236	LEU

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Mol	Chain	Res	Type
1	U	263	ARG
1	U	286	SER
1	U	292	LEU
1	U	328	LYS
1	W	5	GLN
1	W	8	ARG
1	W	29	GLN
1	W	37	VAL
1	W	42	ASP
1	W	72	SER
1	W	74	VAL
1	W	77	GLN
1	W	78	LEU
1	W	91	LYS
1	W	92	ASN
1	W	98	ASP
1	W	106	THR
1	W	109	VAL
1	W	110	LYS
1	W	118	MET
1	W	129	THR
1	W	142	GLN
1	W	143	ASP
1	W	145	THR
1	W	148	THR
1	W	162	LEU
1	W	164	GLU
1	W	219	ARG
1	W	223	GLU
1	W	226	LYS
1	W	236	LEU
1	W	253	LYS
1	W	263	ARG
1	W	286	SER
1	W	292	LEU
1	W	327	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	GLN
1	A	174	HIS

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Mol	Chain	Res	Type
1	A	222	GLN
1	A	278	GLN
1	D	29	GLN
1	D	141	ASN
1	D	147	GLN
1	D	174	HIS
1	D	270	ASN
1	D	278	GLN
1	D	305	HIS
1	Q	168	GLN
1	Q	201	HIS
1	S	141	ASN
1	S	147	GLN
1	S	256	GLN
1	S	305	HIS
1	U	15	GLN
1	U	29	GLN
1	U	40	HIS
1	U	168	GLN
1	U	174	HIS
1	U	201	HIS
1	U	278	GLN
1	W	70	ASN
1	W	142	GLN
1	W	174	HIS
1	W	222	GLN

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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	S	701	-	4,4,4	0.29	0	6,6,6	1.00	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	Q	3
1	D	2
1	U	2
1	W	1
1	A	1
1	S	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Q	92:ASN	C	93:LEU	N	1.17
1	W	92:ASN	C	93:LEU	N	1.15
1	Q	90:HIS	C	91:LYS	N	1.13
1	D	92:ASN	C	93:LEU	N	1.11
1	Q	110:LYS	C	111:PHE	N	1.06
1	U	110:LYS	C	111:PHE	N	1.05
1	A	110:LYS	C	111:PHE	N	0.99
1	D	90:HIS	C	91:LYS	N	0.94
1	S	110:LYS	C	111:PHE	N	0.79
1	U	92:ASN	C	93:LEU	N	0.79

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	306/326 (93%)	-0.02	5 (1%) 70 66	25, 39, 62, 72	0
1	D	306/326 (93%)	0.24	3 (0%) 79 76	29, 48, 60, 69	0
1	Q	306/326 (93%)	-0.29	3 (0%) 79 76	22, 32, 55, 68	0
1	S	306/326 (93%)	-0.30	0 100 100	23, 35, 49, 64	0
1	U	306/326 (93%)	0.32	13 (4%) 40 36	27, 46, 65, 84	0
1	W	306/326 (93%)	0.76	32 (10%) 11 8	36, 57, 80, 84	0
All	All	1836/1956 (93%)	0.12	56 (3%) 51 47	22, 43, 67, 84	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	146	PRO	3.8
1	U	83	VAL	3.8
1	W	3	ALA	3.8
1	W	45	THR	3.6
1	W	141	ASN	3.5
1	U	86	MET	3.4
1	Q	48	ASN	3.4
1	W	221	PRO	3.1
1	U	84	SER	3.1
1	W	144	GLY	3.1
1	D	3	ALA	3.0
1	U	328	LYS	3.0
1	W	49	ASP	2.9
1	W	111	PHE	2.9
1	W	140	TRP	2.9
1	W	139	THR	2.9
1	W	83	VAL	2.8
1	A	146	PRO	2.8
1	W	187	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	W	10	LEU	2.7
1	U	145	THR	2.7
1	W	112	PHE	2.7
1	U	90	HIS	2.7
1	Q	90	HIS	2.5
1	D	177	ALA	2.5
1	U	88	ALA	2.5
1	Q	47	GLY	2.5
1	W	147	GLN	2.4
1	W	136	TYR	2.4
1	W	81	ALA	2.4
1	U	183	THR	2.3
1	W	113	ALA	2.3
1	W	186	TYR	2.3
1	A	3	ALA	2.3
1	W	88	ALA	2.3
1	W	145	THR	2.3
1	W	211	ILE	2.3
1	W	220	ASP	2.3
1	W	74	VAL	2.3
1	A	84	SER	2.2
1	A	4	PRO	2.2
1	U	85	ALA	2.2
1	W	148	THR	2.2
1	W	137	PHE	2.2
1	U	82	ALA	2.2
1	U	3	ALA	2.1
1	W	293	MET	2.1
1	U	79	SER	2.1
1	D	148	THR	2.1
1	W	209	GLY	2.1
1	A	90	HIS	2.1
1	W	90	HIS	2.1
1	W	12	ILE	2.1
1	U	87	LYS	2.1
1	W	143	ASP	2.1
1	W	86	MET	2.1

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

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	SO4	S	701	5/5	0.96	0.08	49,49,53,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.