



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:31 am GMT

PDB ID : 1TLB
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

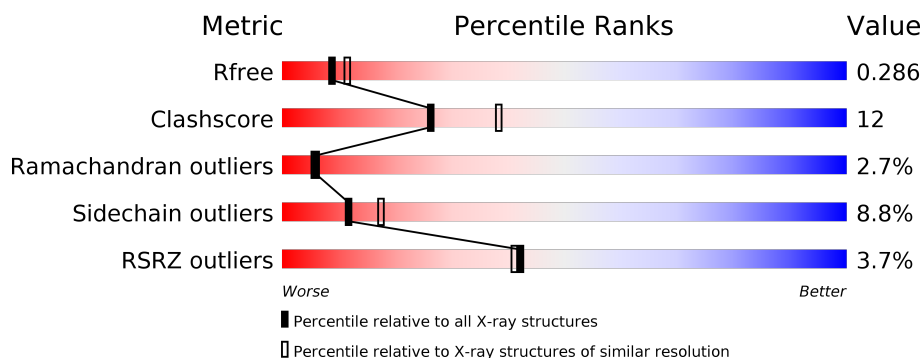
1 Overall quality at a glance

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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>23%</div> <div>6%</div> </div> </div>
1	D	326	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>29%</div> <div></div> </div> </div>
1	Q	326	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>6%</div> </div> </div>
1	S	326	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>5%</div> </div> </div>
1	U	326	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>29%</div> <div></div> </div> </div>
1	W	326	<div> <div>10%</div> <div> <div></div> <div>59%</div> <div>32%</div> <div>9%</div> </div> </div>

2 Entry composition [i](#)

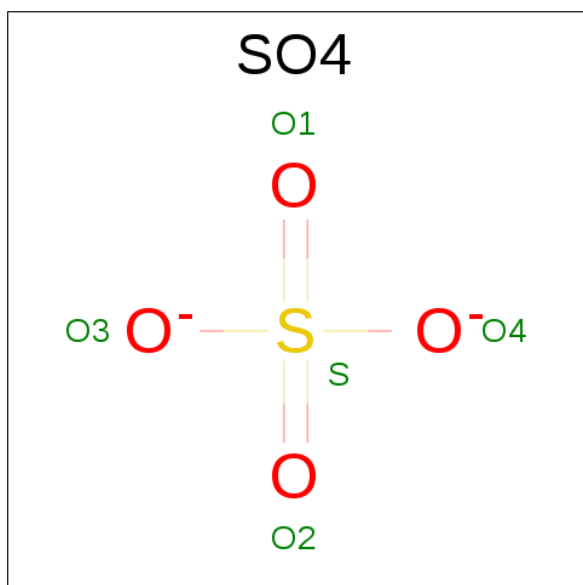
There are 3 unique types of molecules in this entry. The entry contains 16531 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: SO4) (formula: O₄S).



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

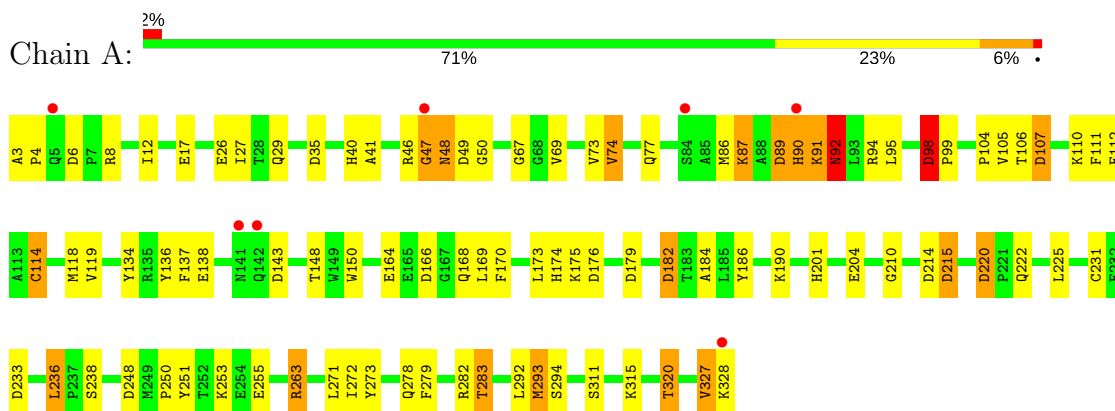
- Molecule 3 is water.

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		

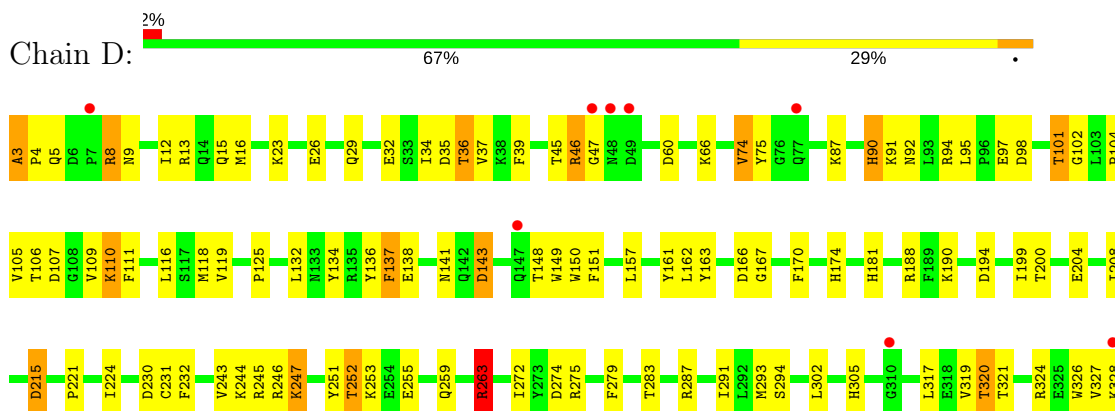
3 Residue-property plots

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

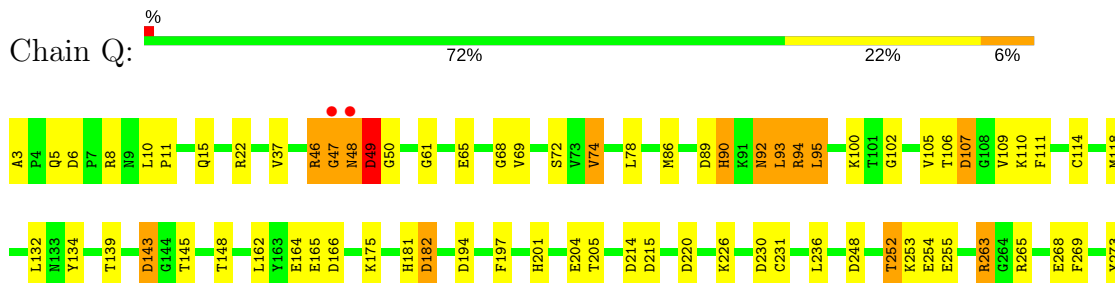
• Molecule 1: Coproporphyrinogen III oxidase



• Molecule 1: Coproporphyrinogen III oxidase

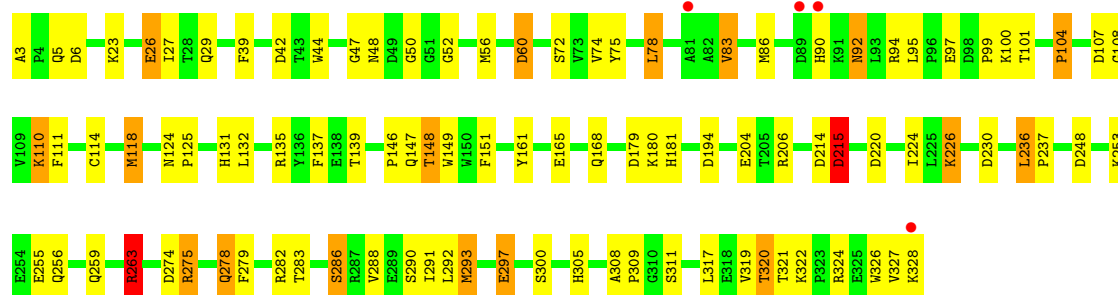


• Molecule 1: Coproporphyrinogen III oxidase

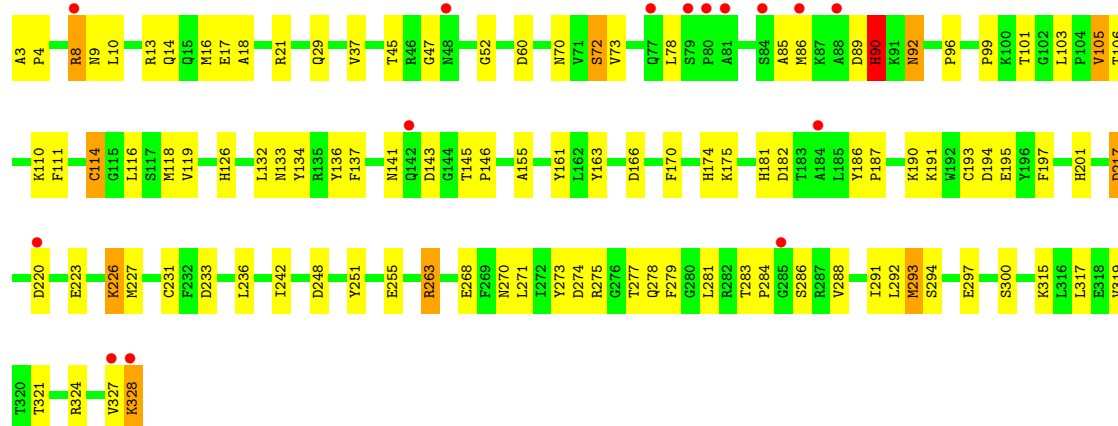




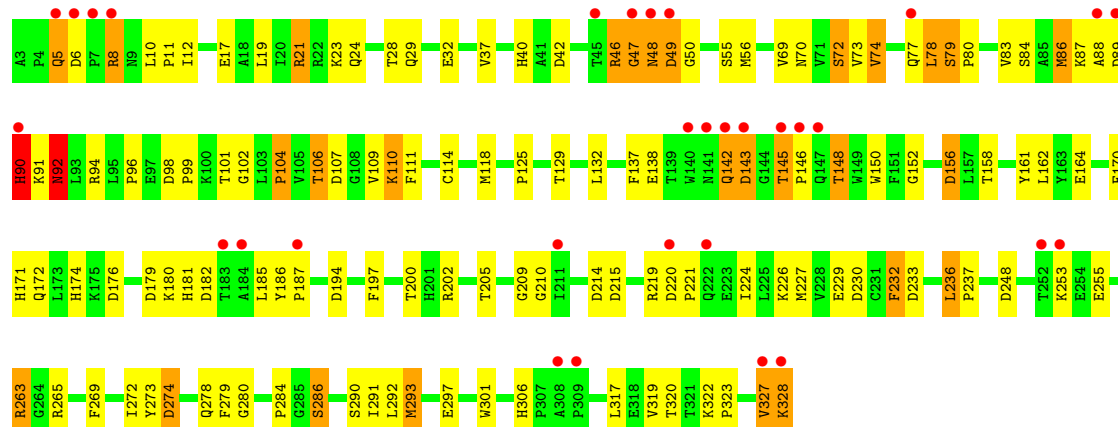
• Molecule 1: Coproporphyrinogen III oxidase



• Molecule 1: Coproporphyrinogen III oxidase



• Molecule 1: Coproporphyrinogen III oxidase



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 19.83 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.8 (158.11-2.40) 93.9 (19.83-2.40)	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 (5.29%)	DCC
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 , 46.8	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	0.93	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	1.09	1/2723 (0.0%)	1.24	20/3693 (0.5%)
1	D	1.01	3/2725 (0.1%)	1.14	15/3697 (0.4%)
1	Q	1.16	10/2725 (0.4%)	1.13	20/3697 (0.5%)
1	S	1.22	5/2723 (0.2%)	1.16	16/3694 (0.4%)
1	U	1.12	3/2725 (0.1%)	1.09	13/3697 (0.4%)
1	W	0.96	2/2725 (0.1%)	1.04	15/3697 (0.4%)
All	All	1.10	24/16346 (0.1%)	1.13	99/22175 (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 (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	110	LYS	C-N	-23.69	0.79	1.34
1	U	92	ASN	C-N	-23.66	0.79	1.34
1	D	90	HIS	C-N	-17.02	0.94	1.34
1	A	110	LYS	C-N	-14.84	0.99	1.34
1	U	110	LYS	C-N	-12.28	1.05	1.34
1	Q	110	LYS	C-N	-11.80	1.06	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	92	ASN	C-N	-10.01	1.11	1.34
1	D	110	LYS	C-N	8.97	1.54	1.34
1	Q	90	HIS	C-N	-8.81	1.13	1.34
1	W	92	ASN	C-N	-8.23	1.15	1.34
1	Q	65	GLU	CD-OE1	7.32	1.33	1.25
1	Q	92	ASN	C-N	-7.29	1.17	1.34
1	Q	48	ASN	CB-CG	6.23	1.65	1.51
1	Q	22	ARG	CZ-NH1	5.86	1.40	1.33
1	W	110	LYS	C-N	-5.71	1.21	1.34
1	S	92	ASN	C-N	-5.65	1.21	1.34
1	Q	319	VAL	CB-CG1	-5.49	1.41	1.52
1	U	315	LYS	CD-CE	5.41	1.64	1.51
1	Q	107	ASP	CB-CG	5.23	1.62	1.51
1	Q	165	GLU	CD-OE1	5.23	1.31	1.25
1	S	297	GLU	CG-CD	-5.17	1.44	1.51
1	S	322	LYS	CE-NZ	5.05	1.61	1.49
1	Q	69	VAL	CB-CG2	5.03	1.63	1.52
1	S	278	GLN	CG-CD	5.03	1.62	1.51

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	HIS	O-C-N	-26.18	80.81	122.70
1	D	90	HIS	O-C-N	-22.46	86.77	122.70
1	A	92	ASN	O-C-N	-17.91	94.04	122.70
1	D	90	HIS	CA-C-N	13.96	147.90	117.20
1	W	92	ASN	O-C-N	-13.95	100.38	122.70
1	U	110	LYS	C-N-CA	10.98	149.15	121.70
1	D	194	ASP	CB-CG-OD2	10.44	127.70	118.30
1	U	263	ARG	NE-CZ-NH2	-10.40	115.10	120.30
1	A	248	ASP	CB-CG-OD2	9.99	127.29	118.30
1	S	275	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	Q	92	ASN	O-C-N	-9.68	107.22	122.70
1	A	214	ASP	CB-CG-OD2	9.37	126.73	118.30
1	W	90	HIS	O-C-N	-9.31	107.80	122.70
1	Q	214	ASP	CB-CG-OD2	9.26	126.63	118.30
1	S	220	ASP	CB-CG-OD1	9.22	126.60	118.30
1	U	90	HIS	O-C-N	-9.07	108.19	122.70
1	S	194	ASP	CB-CG-OD2	8.77	126.19	118.30
1	U	263	ARG	NE-CZ-NH1	8.59	124.59	120.30
1	U	92	ASN	O-C-N	-8.49	109.11	122.70
1	D	90	HIS	C-N-CA	8.47	142.87	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	ASP	CB-CG-OD2	8.39	125.85	118.30
1	U	110	LYS	O-C-N	-8.38	109.29	122.70
1	S	215	ASP	CB-CG-OD2	8.32	125.78	118.30
1	S	214	ASP	CB-CG-OD2	8.28	125.75	118.30
1	A	110	LYS	C-N-CA	8.25	142.32	121.70
1	D	274	ASP	CB-CG-OD2	8.24	125.72	118.30
1	Q	194	ASP	CB-CG-OD2	8.20	125.68	118.30
1	A	89	ASP	CB-CG-OD2	8.14	125.63	118.30
1	D	166	ASP	CB-CG-OD2	7.69	125.22	118.30
1	D	194	ASP	CB-CG-OD1	-7.50	111.55	118.30
1	A	166	ASP	CB-CG-OD2	7.45	125.01	118.30
1	A	263	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	176	ASP	CB-CG-OD2	7.36	124.92	118.30
1	S	118	MET	CG-SD-CE	-7.34	88.46	100.20
1	D	275	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	U	60	ASP	CB-CG-OD2	7.07	124.66	118.30
1	S	275	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	Q	263	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	Q	143	ASP	CB-CG-OD2	6.68	124.31	118.30
1	U	233	ASP	CB-CG-OD2	6.64	124.28	118.30
1	Q	220	ASP	CB-CG-OD1	6.60	124.24	118.30
1	A	233	ASP	CB-CG-OD2	6.55	124.20	118.30
1	Q	46	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	S	60	ASP	CB-CG-OD2	6.53	124.17	118.30
1	D	46	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	W	143	ASP	CB-CG-OD2	6.35	124.02	118.30
1	W	194	ASP	CB-CG-OD2	6.29	123.96	118.30
1	S	248	ASP	CB-CG-OD2	6.28	123.95	118.30
1	S	110	LYS	C-N-CA	6.26	137.35	121.70
1	S	263	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	S	92	ASN	CA-C-N	-6.20	103.56	117.20
1	Q	89	ASP	CB-CG-OD2	6.15	123.84	118.30
1	A	35	ASP	CB-CG-OD2	6.13	123.82	118.30
1	S	135	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	U	182	ASP	CB-CG-OD2	6.10	123.79	118.30
1	W	274	ASP	CB-CG-OD2	6.09	123.78	118.30
1	W	220	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	107	ASP	CB-CG-OD2	6.07	123.77	118.30
1	D	46	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	A	182	ASP	CB-CG-OD2	6.05	123.74	118.30
1	U	8	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	D	98	ASP	CB-CG-OD2	6.04	123.74	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	ASP	CB-CG-OD2	6.03	123.72	118.30
1	D	263	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	Q	248	ASP	CB-CG-OD2	5.86	123.58	118.30
1	A	94	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	S	92	ASN	O-C-N	5.66	131.76	122.70
1	S	274	ASP	CB-CG-OD2	5.63	123.37	118.30
1	W	233	ASP	CB-CG-OD2	5.58	123.32	118.30
1	W	176	ASP	CB-CG-OD2	5.57	123.31	118.30
1	U	248	ASP	CB-CG-OD1	5.56	123.30	118.30
1	D	215	ASP	CB-CG-OD2	5.54	123.29	118.30
1	D	143	ASP	CB-CG-OD2	5.51	123.26	118.30
1	U	110	LYS	N-CA-C	5.51	125.88	111.00
1	D	60	ASP	CB-CG-OD2	5.47	123.22	118.30
1	Q	265	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	Q	46	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	W	49	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	236	LEU	CB-CG-CD1	5.36	120.10	111.00
1	Q	22	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	Q	8	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	47	GLY	N-CA-C	-5.33	99.77	113.10
1	Q	49	ASP	CB-CG-OD2	5.29	123.06	118.30
1	Q	265	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	U	217	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	179	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	98	ASP	CB-CG-OD2	5.21	122.98	118.30
1	W	21	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	W	89	ASP	CB-CG-OD2	5.17	122.95	118.30
1	W	46	ARG	CB-CA-C	5.15	120.70	110.40
1	Q	252	THR	OG1-CB-CG2	-5.14	98.19	110.00
1	W	102	GLY	N-CA-C	5.09	125.82	113.10
1	W	230	ASP	CB-CG-OD2	5.09	122.88	118.30
1	Q	166	ASP	CB-CG-OD2	5.04	122.83	118.30
1	S	179	ASP	CB-CG-OD2	5.04	122.83	118.30
1	Q	61	GLY	N-CA-C	-5.01	100.56	113.10
1	W	248	ASP	CB-CG-OD2	5.01	122.81	118.30
1	Q	110	LYS	C-N-CA	5.00	134.21	121.70
1	Q	182	ASP	CB-CG-OD2	5.00	122.80	118.30

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	Mainchain,Peptide
1	Q	86	MET	Peptide
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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2647	0	2547	52	0
1	D	2648	0	2550	54	0
1	Q	2648	0	2549	55	0
1	S	2647	0	2545	62	0
1	U	2648	0	2550	59	1
1	W	2648	0	2550	76	1
2	S	5	0	0	0	0
3	A	115	0	0	8	0
3	D	74	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	15291	343	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 (343) 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:CB	1:S:206:ARG:CD	2.46	0.92
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:HA	1:W:142:GLN:HE21	1.43	0.81
1:Q:303:TYR:CD1	1:S:293:MET:HE3	2.16	0.80
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:U:226:LYS:NZ	1:U:226:LYS:HA	2.01	0.75
1:S:293:MET:HE2	1:S:293:MET:HA	1.68	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:136:TYR:OH	1:A:138:GLU:OE2	2.07	0.70
1:S:168:GLN:HG2	1:S:326:TRP:O	1.90	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:A:3:ALA:HB1	1:A:4:PRO:HA	1.73	0.70
1:Q:48:ASN:CG	1:Q:50:GLY:H	1.95	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
1:Q:303:TYR:CD1	1:S:293:MET:HE1	2.28	0.68
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: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: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:D:118:MET:HE3	1:D:132:LEU:HB3	1.79	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:78:LEU:HD11	1:W:86:MET:SD	2.37	0.62
1:W:118:MET:HE2	1:W:132:LEU:HD13	1.81	0.62
1:Q:293:MET:HE1	3:Q:456:HOH:O	1.94	0.62
1:S:293:MET:HE2	3:S:704:HOH:O	1.99	0.62
1:S:305:HIS:HD2	3:S:754:HOH:O	1.83	0.62
1:U:226:LYS:HA	1:U:226:LYS:HZ3	1.65	0.61
1:S:5:GLN:O	1:S:6:ASP:C	2.37	0.61
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:317:LEU:HA	1:W:320:THR:HG22	1.82	0.61
1:W:55:SER:OG	1:W:70:ASN:ND2	2.33	0.61
1:S:131:HIS:NE2	3:S:717:HOH:O	2.31	0.60
1:A:201:HIS:ND1	1:A:273:TYR:OH	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:Q:303:TYR:HD1	1:S:293:MET:HE1	1.65	0.58
1:S:293:MET:HE2	1:S:293:MET:CA	2.34	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
1:S:148:THR:CG2	3:S:715:HOH:O	2.53	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:CA	1:W:142:GLN:HE21	2.15	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: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: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: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: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:SG	1:A:114:CYS:O	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:Q:143:ASP:OD1	1:Q:145:THR:OG1	2.16	0.53
1:S:39:PHE:HB3	1:S:56:MET:HE2	1.89	0.53
1:W:138:GLU:HG3	1:W:148:THR:O	2.08	0.53
1:W:79:SER:OG	1:W:80:PRO:HD2	2.07	0.53
1:S:151:PHE:CD1	1:S:224:ILE:HG21	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:328:LYS:C	3:U:431:HOH:O	2.46	0.53
1:W:73:VAL:HG22	1:W:114:CYS:HB2	1.90	0.53
1:W:125:PRO:O	3:W:337:HOH:O	2.19	0.52
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: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:Q:5:GLN:O	1:Q:6:ASP:C	2.48	0.52
1:W:10:LEU:N	1:W:11:PRO:CD	2.73	0.52
1:A:169:LEU:HD11	1:A:173:LEU:HD11	1.91	0.51
1:S:27:ILE:HG21	1:S:118:MET:HE1	1.93	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:S:27:ILE:HD13	1:S:118:MET:HE3	1.93	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:W:142:GLN:HA	1:W:142:GLN:NE2	2.20	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:186:TYR:CG	1:A:186:TYR:O	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:297:GLU:HA	1:W:301:TRP:O	2.13	0.49
1:U:271:LEU:HD22	1:W:272:ILE:HD11	1.95	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: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:87:LYS:HB2	1:A:215:ASP:OD1	2.14	0.48
1:D:252:THR:OG1	1:D:253:LYS:N	2.45	0.48
1:D:3:ALA:HB3	1:D:4:PRO:CA	2.40	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:W:5:GLN:O	1:W:6:ASP:C	2.52	0.48
1:W:72:SER:O	1:W:114:CYS:HA	2.14	0.48
1:D:15:GLN:O	1:D:16:MET:C	2.51	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: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:D:118:MET:HE2	1:D:132:LEU:HB3	1.95	0.47
1:D:199:ILE:O	1:D:200:THR:C	2.53	0.47
1:A:40:HIS:HB2	3:A:391:HOH:O	2.15	0.47
1:A:3:ALA:CB	1:A:4:PRO:CA	2.91	0.47
1:Q:201:HIS:HD2	1:Q:273:TYR:OH	1.98	0.47
1:W:274:ASP:O	1:W:278:GLN:NE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:6:ASP:HB2	3:Q:479:HOH:O	2.14	0.47
1:A:170:PHE:O	1:A:174:HIS:CD2	2.64	0.47
1:A:164:GLU:O	1:A:168:GLN:HG3	2.14	0.46
1:Q:252:THR:HG22	1:Q:255:GLU:CD	2.36	0.46
1:W:46:ARG:CB	1:W:47:GLY:CA	2.93	0.46
1:D:136:TYR:CE1	1:D:149:TRP:HB2	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:226:LYS:HA	1:U:226:LYS:CE	2.45	0.46
1:U:134:TYR:CZ	1:U:231:CYS:HB3	2.51	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:137:PHE:O	1:D:149:TRP:HA	2.17	0.45
1:D:66:LYS:NZ	3:D:398:HOH:O	2.48	0.45
1:U:293:MET:C	1:U:293:MET:SD	2.95	0.45
1:W:156:ASP:HA	1:W:209:GLY:O	2.16	0.45
1:W:24:GLN:O	1:W:28:THR:HG23	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:W:19:LEU:O	1:W:23:LYS:HG2	2.16	0.45
1:W:224:ILE:HG23	1:W:227:MET:HE2	1.98	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:S:293:MET:HA	1:S:293:MET:CE	2.30	0.45
1:U:155:ALA:HB3	1:U:174:HIS:CE1	2.52	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:190:LYS:NZ	1:U:194:ASP:OD1	2.34	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:116:LEU:C	1:D:116:LEU:HD23	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: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:D:231:CYS:O	1:D:232:PHE:C	2.56	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:Q:118:MET:HE3	1:Q:132:LEU:HB3	2.00	0.44
1:U:251:TYR:HA	1:U:255:GLU:OE1	2.17	0.44
1:U:201:HIS:HD2	1:U:273:TYR:OH	2.01	0.44
1:D:118:MET:HE2	1:D:132:LEU:HD22	2.00	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:Q:303:TYR:CE1	1:S:293:MET:HE3	2.53	0.43
1:U:283:THR:HA	1:U:284:PRO:HD3	1.76	0.43
1:U:119:VAL:HG21	1:U:294:SER:HB2	2.00	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: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:56:MET:HE1	1:U:18:ALA:HB1	2.00	0.43
1:A:293:MET:SD	1:A:293:MET:C	2.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:134:TYR:OH	1:U:231:CYS:HB3	2.18	0.42
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:Q:328:LYS:HZ2	1:Q:328:LYS:N	2.17	0.42
1:W:143:ASP:OD1	1:W:143:ASP:N	2.43	0.42
1:A:182:ASP:OD2	1:A:184:ALA:HB3	2.19	0.42
1:A:48:ASN:HA	3:A:356:HOH:O	2.18	0.42
1:A:175:LYS:CD	1:A:327:VAL:HG21	2.43	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:U:217:ASP:C	1:U:217:ASP:OD1	2.56	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:A:67:GLY:HA2	1:A:119:VAL:O	2.20	0.42
1:D:245:ARG:C	3:D:347:HOH:O	2.59	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:Q:315:LYS:NZ	3:Q:416:HOH:O	2.53	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:U:190:LYS:O	1:U:191:LYS:C	2.58	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:A:27:ILE:HD13	1:A:118:MET:HE1	2.02	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:D:134:TYR:OH	1:D:231:CYS:HB3	2.19	0.41
1:D:125:PRO:HD2	1:D:251:TYR:CD2	2.55	0.41
1:A:250:PRO:HB3	1:Q:309:PRO:HD2	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:181:HIS:HE1	1:S:226:LYS:HG3	1.85	0.41
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:118:MET:HE3	1:D:132:LEU:CB	2.50	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: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: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:S:27:ILE:HG21	1:S:118:MET:CE	2.51	0.40
1:U:9:ASN:O	1:U:10:LEU:C	2.60	0.40
1:D:190:LYS:HD3	1:D:190:LYS:C	2.42	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:202:ARG:HD2	1:W:265:ARG:CZ	2.51	0.40
1:W:200:THR:HB	1:W:273:TYR:OH	2.21	0.40
1:W:69:VAL:HA	1:W:118:MET:HB3	2.02	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

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	324/326 (99%)	298 (92%)	20 (6%)	6 (2%)	9	11
1	D	324/326 (99%)	299 (92%)	18 (6%)	7 (2%)	8	9
1	Q	324/326 (99%)	297 (92%)	17 (5%)	10 (3%)	5	4
1	S	324/326 (99%)	302 (93%)	15 (5%)	7 (2%)	8	9
1	U	324/326 (99%)	293 (90%)	25 (8%)	6 (2%)	9	11
1	W	324/326 (99%)	275 (85%)	32 (10%)	17 (5%)	2	1
All	All	1944/1956 (99%)	1764 (91%)	127 (6%)	53 (3%)	6	6

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

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Mol	Chain	Res	Type
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
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%)	257 (91%)	25 (9%)	11	17
1	D	282/282 (100%)	257 (91%)	25 (9%)	11	17
1	Q	282/282 (100%)	259 (92%)	23 (8%)	13	20
1	S	281/282 (100%)	256 (91%)	25 (9%)	11	17
1	U	282/282 (100%)	264 (94%)	18 (6%)	20	32
1	W	282/282 (100%)	249 (88%)	33 (12%)	6	8
All	All	1691/1692 (100%)	1542 (91%)	149 (9%)	12	17

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	29	GLN
1	A	49	ASP
1	A	74	VAL
1	A	77	GLN
1	A	87	LYS
1	A	91	LYS
1	A	92	ASN
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	215	ASP
1	A	236	LEU
1	A	253	LYS
1	A	263	ARG
1	A	283	THR
1	A	292	LEU
1	A	293	MET
1	A	320	THR
1	A	327	VAL
1	A	328	LYS
1	D	5	GLN
1	D	8	ARG
1	D	29	GLN
1	D	36	THR
1	D	37	VAL

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Mol	Chain	Res	Type
1	D	45	THR
1	D	74	VAL
1	D	94	ARG
1	D	101	THR
1	D	105	VAL
1	D	106	THR
1	D	109	VAL
1	D	110	LYS
1	D	137	PHE
1	D	148	THR
1	D	215	ASP
1	D	244	LYS
1	D	247	LYS
1	D	252	THR
1	D	263	ARG
1	D	293	MET
1	D	302	LEU
1	D	320	THR
1	D	327	VAL
1	D	328	LYS
1	Q	37	VAL
1	Q	74	VAL
1	Q	78	LEU
1	Q	94	ARG
1	Q	106	THR
1	Q	109	VAL
1	Q	111	PHE
1	Q	139	THR
1	Q	148	THR
1	Q	162	LEU
1	Q	164	GLU
1	Q	215	ASP
1	Q	226	LYS
1	Q	236	LEU
1	Q	253	LYS
1	Q	263	ARG
1	Q	282	ARG
1	Q	292	LEU
1	Q	293	MET
1	Q	315	LYS
1	Q	320	THR
1	Q	327	VAL

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Mol	Chain	Res	Type
1	Q	328	LYS
1	S	26	GLU
1	S	29	GLN
1	S	48	ASN
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	215	ASP
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	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	78	LEU
1	U	86	MET
1	U	103	LEU
1	U	105	VAL
1	U	111	PHE
1	U	114	CYS
1	U	137	PHE
1	U	226	LYS
1	U	236	LEU
1	U	263	ARG
1	U	286	SER
1	U	292	LEU

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Mol	Chain	Res	Type
1	U	293	MET
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	79	SER
1	W	87	LYS
1	W	91	LYS
1	W	92	ASN
1	W	98	ASP
1	W	106	THR
1	W	110	LYS
1	W	129	THR
1	W	142	GLN
1	W	145	THR
1	W	148	THR
1	W	156	ASP
1	W	162	LEU
1	W	164	GLU
1	W	219	ARG
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	293	MET
1	W	327	VAL
1	W	328	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	HIS
1	A	222	GLN
1	D	29	GLN

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	0.24	0	6,6,6	0.96	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	S	701	-	-	0/0/0/0	0/0/0/0

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

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%)	-0.18	7 (2%) 61 58	25, 39, 62, 72	0
1	D	306/326 (93%)	-0.02	8 (2%) 56 54	29, 48, 60, 69	0
1	Q	306/326 (93%)	-0.38	3 (0%) 82 80	22, 32, 55, 68	0
1	S	306/326 (93%)	-0.36	4 (1%) 77 75	23, 35, 49, 64	0
1	U	306/326 (93%)	0.09	15 (4%) 30 29	27, 46, 65, 84	0
1	W	306/326 (93%)	0.55	31 (10%) 8 7	36, 57, 80, 84	0
All	All	1836/1956 (93%)	-0.05	68 (3%) 42 41	22, 43, 67, 84	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	328	LYS	6.7
1	W	143	ASP	5.4
1	W	146	PRO	5.3
1	W	88	ALA	5.1
1	W	147	GLN	5.0
1	W	141	ASN	4.7
1	W	48	ASN	4.7
1	W	142	GLN	4.5
1	W	183	THR	4.3
1	U	79	SER	4.3
1	A	5	GLN	4.2
1	W	308	ALA	4.0
1	W	184	ALA	4.0
1	W	220	ASP	3.8
1	U	84	SER	3.7
1	W	49	ASP	3.6
1	U	48	ASN	3.5
1	W	89	ASP	3.5
1	U	327	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	W	187	PRO	3.3
1	U	86	MET	3.3
1	W	309	PRO	3.2
1	W	145	THR	3.2
1	Q	328	LYS	3.2
1	W	328	LYS	3.2
1	W	47	GLY	3.2
1	W	45	THR	3.2
1	W	140	TRP	3.1
1	A	328	LYS	3.0
1	A	142	GLN	2.9
1	Q	48	ASN	2.8
1	S	328	LYS	2.8
1	D	328	LYS	2.8
1	D	7	PRO	2.7
1	S	81	ALA	2.7
1	A	47	GLY	2.7
1	U	220	ASP	2.7
1	U	80	PRO	2.6
1	D	48	ASN	2.6
1	W	7	PRO	2.5
1	D	77	GLN	2.5
1	A	90	HIS	2.5
1	A	141	ASN	2.5
1	U	88	ALA	2.4
1	W	222	GLN	2.4
1	W	211	ILE	2.3
1	D	310	GLY	2.3
1	D	47	GLY	2.3
1	U	81	ALA	2.3
1	W	8	ARG	2.2
1	U	285	GLY	2.2
1	W	327	VAL	2.2
1	U	184	ALA	2.2
1	Q	47	GLY	2.2
1	W	252	THR	2.2
1	W	6	ASP	2.2
1	S	90	HIS	2.2
1	W	90	HIS	2.2
1	W	253	LYS	2.2
1	U	8	ARG	2.2
1	D	49	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	U	77	GLN	2.1
1	W	5	GLN	2.1
1	A	84	SER	2.1
1	U	142	GLN	2.1
1	D	147	GLN	2.1
1	S	89	ASP	2.0
1	W	77	GLN	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	S	701	5/5	0.97	0.09	-2.80	49,49,53,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.