Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 09:14 PM EDT

PDB ID	:	1TLB
Title	:	Yeast coproporphyrinogen oxidase
Authors	:	Phillip, J.D.; Whitby, F.G.; Warby, C.A.; Labbe, P.; Yang, C.; Pflugrath, J.W.; Ferrara, J.D.; Robinson, H.; Kushner, J.P.; Hill, C.P.
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 (i) 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 (i)) were used in the production of this report:

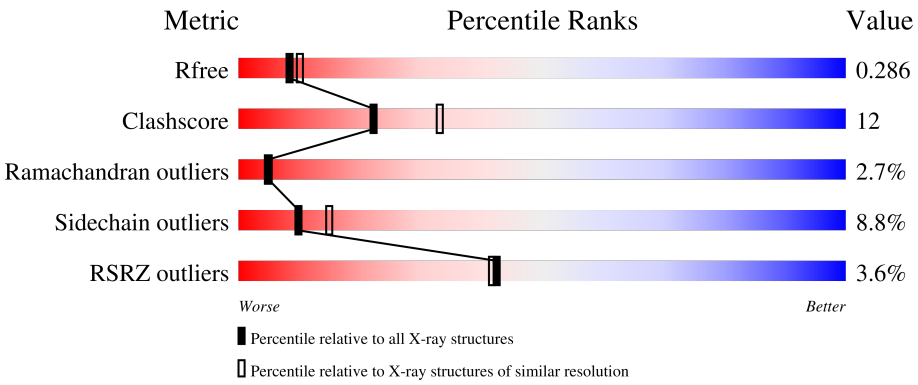
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 <=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	2%, 67%, 29% •
1	Q	326	%, 72%, 22%, 6%
1	S	326	%, 70%, 25%, 5% •
1	U	326	5%, 67%, 29% •

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Mol	Chain	Length	Quality of chain
1	W	326	9% 59% 32% 9%

2 Entry composition (i)

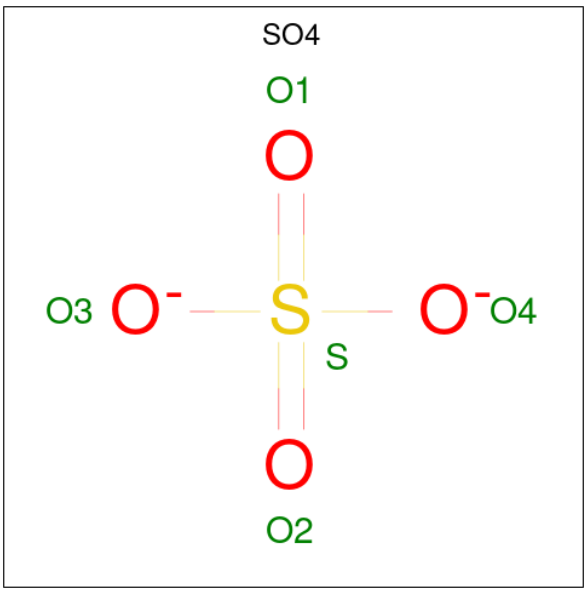
There are 3 unique types of molecules in this entry. The entry contains 16531 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	326	2647	1682	465	490	10	152	0	0
1	D	326	2648	1683	465	490	10	152	0	0
1	Q	326	2648	1683	465	490	10	152	0	0
1	S	326	2647	1682	465	490	10	152	0	0
1	U	326	2648	1683	465	490	10	152	0	0
1	W	326	2648	1683	465	490	10	152	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

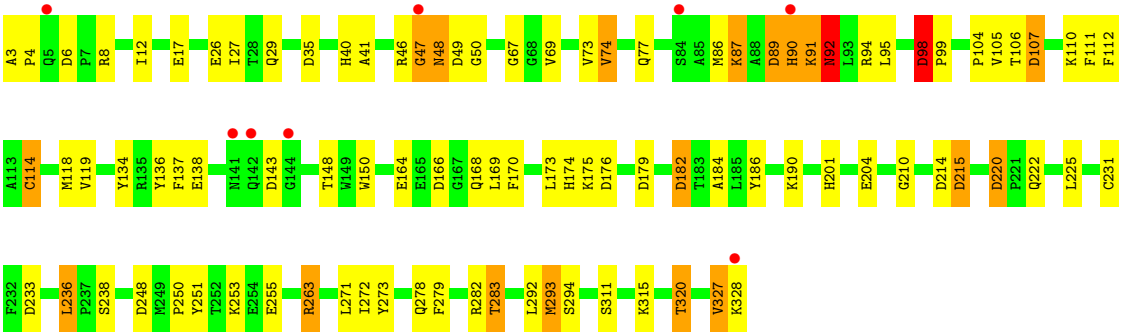
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	115	115	115	0	0
			Total	O		
3	D	74	74	74	0	0
			Total	O		
3	Q	151	151	151	0	0
			Total	O		
3	S	140	140	140	0	0
			Total	O		
3	U	103	103	103	0	0
			Total	O		
3	W	57	57	57	0	0

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.

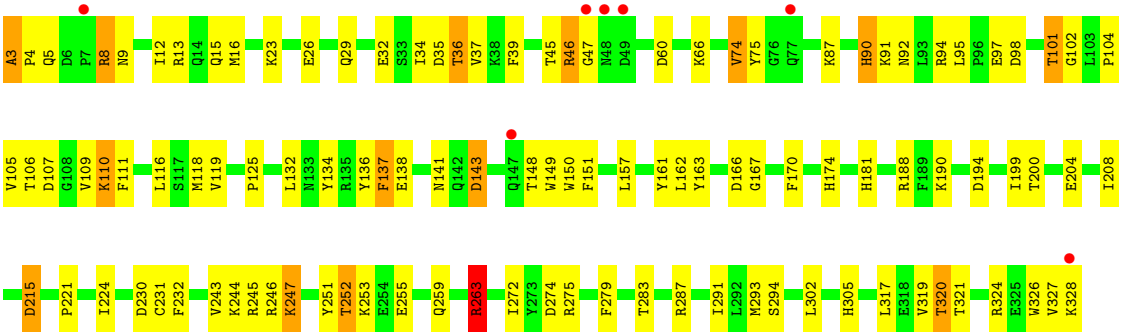
• Molecule 1: Coproporphyrinogen III oxidase

Chain A:



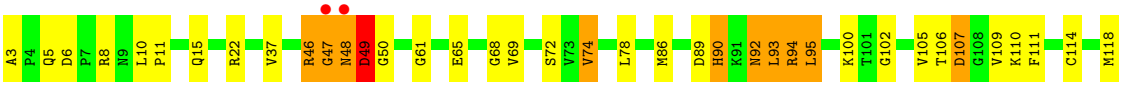
• Molecule 1: Coproporphyrinogen III oxidase

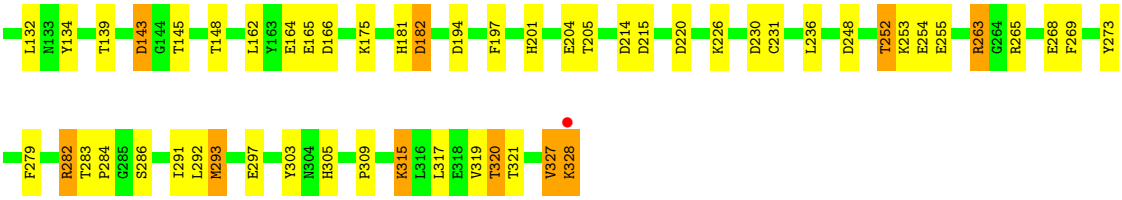
Chain D:



• Molecule 1: Coproporphyrinogen III oxidase

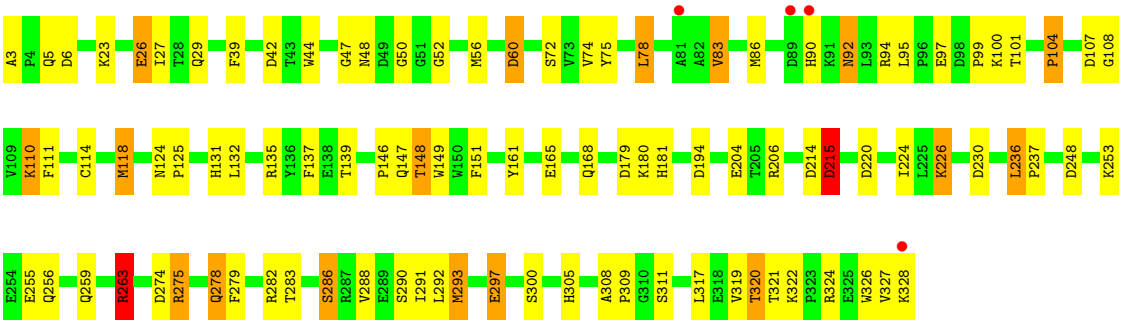
Chain Q:





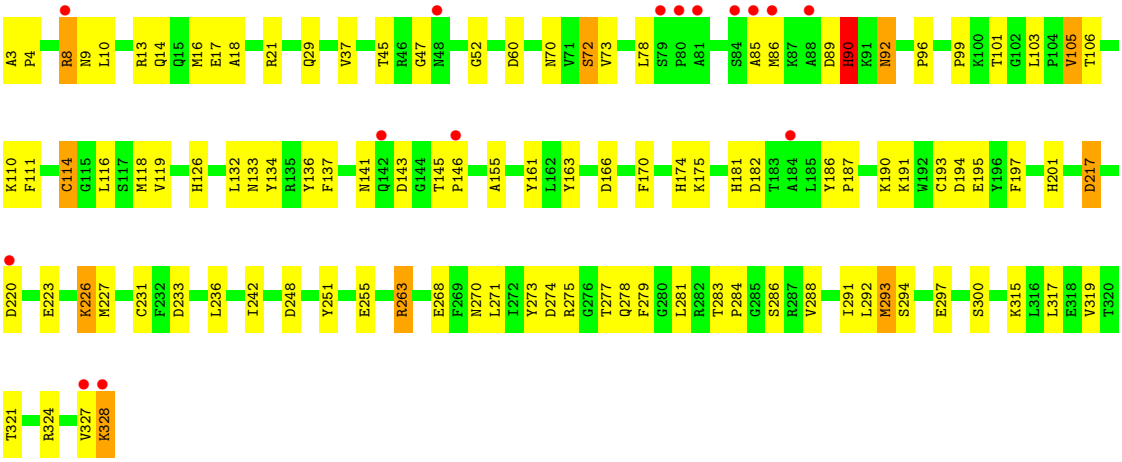
• Molecule 1: Coproporphyrinogen III oxidase

Chain S:



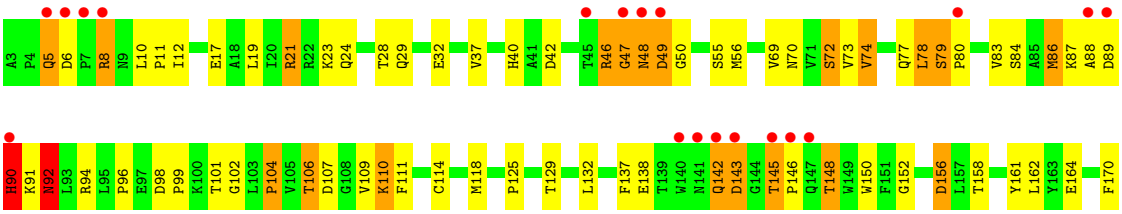
• Molecule 1: Coproporphyrinogen III oxidase

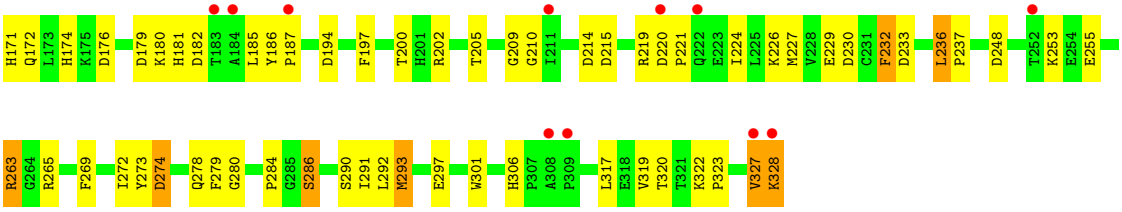
Chain U:



• Molecule 1: Coproporphyrinogen III oxidase

Chain W:




H171 Q172 L173 H174 K175 D176 D179 K180 H181 D182 T183 A184 L185 Y186 P187 D194 F197 T200 H201 R202 T205 G209 G210 I211 D214 D215 R219 D220 P221 Q222 E223 I224 L225 K226 M227 V228 E229 D230 C231 F232 D233 L236 P237 D248 T252 K253 E254 E255
R263 G264 R265 F269 I272 Y273 D274 Q278 F279 G280 P284 G285 S286 S290 I291 L292 M293 E297 W301 H306 P307 A308 P309 L317 E318 V319 T320 T321 K322 P323 V327 K328

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.02%)	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 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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	Peptide,Mainchain
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:CD	1:S:206:ARG:CB	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:HE21	1:W:142:GLN:HA	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: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: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:HE21	1:W:142:GLN:CA	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: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: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: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: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: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: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: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: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: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:293:MET:SD	1:U:293:MET:C	2.95	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: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:CE	1:S:293:MET:HA	2.30	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
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:35:ASP:OD1	1:D:36:THR:N	2.46	0.44
1:D:116:LEU:C	1:D:116:LEU:HD23	2.38	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: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: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: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:Q:46:ARG:CD	1:Q:74:VAL:HG22	2.49	0.43
1:S:56:MET:HE1	1:U:18:ALA:HB1	2.00	0.43
1:S:181:HIS:NE2	1:S:230:ASP:OD1	2.51	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: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: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: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: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:87:LYS:CG	1:D:150:TRP:CZ2	3.03	0.41
1:D:118:MET:HE3	1:D:132:LEU:CB	2.50	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:C	1:D:190:LYS:HD3	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: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%)	8 10
1	D	324/326 (99%)	299 (92%)	18 (6%)	7 (2%)	6 7
1	Q	324/326 (99%)	297 (92%)	17 (5%)	10 (3%)	4 3
1	S	324/326 (99%)	302 (93%)	15 (5%)	7 (2%)	6 7
1	U	324/326 (99%)	293 (90%)	25 (8%)	6 (2%)	8 10
1	W	324/326 (99%)	275 (85%)	32 (10%)	17 (5%)	2 1
All	All	1944/1956 (99%)	1764 (91%)	127 (6%)	53 (3%)	5 5

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	282/282 (100%)	257 (91%)	25 (9%)	9 14
1	D	282/282 (100%)	257 (91%)	25 (9%)	9 14
1	Q	282/282 (100%)	259 (92%)	23 (8%)	11 17
1	S	281/282 (100%)	256 (91%)	25 (9%)	9 14
1	U	282/282 (100%)	264 (94%)	18 (6%)	17 28
1	W	282/282 (100%)	249 (88%)	33 (12%)	5 7
All	All	1691/1692 (100%)	1542 (91%)	149 (9%)	10 15

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

Sometimes 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 monosaccharides 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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.16	8 (2%)	56	54	25, 39, 62, 72	0
1	D	306/326 (93%)	-0.01	7 (2%)	60	58	29, 48, 60, 69	0
1	Q	306/326 (93%)	-0.37	3 (0%)	82	80	22, 32, 55, 68	0
1	S	306/326 (93%)	-0.34	4 (1%)	77	75	23, 35, 49, 64	0
1	U	306/326 (93%)	0.11	15 (4%)	29	28	27, 46, 65, 84	0
1	W	306/326 (93%)	0.58	30 (9%)	7	7	36, 57, 80, 84	0
All	All	1836/1956 (93%)	-0.03	67 (3%)	42	42	22, 43, 67, 84	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	328	LYS	6.6
1	W	146	PRO	5.8
1	W	143	ASP	5.6
1	W	88	ALA	5.5
1	W	147	GLN	5.1
1	W	183	THR	4.7
1	W	141	ASN	4.6
1	U	79	SER	4.6
1	W	48	ASN	4.5
1	W	308	ALA	4.3
1	W	142	GLN	4.1
1	U	84	SER	4.0
1	A	5	GLN	4.0
1	W	184	ALA	4.0
1	W	220	ASP	3.8
1	W	89	ASP	3.7
1	W	145	THR	3.7
1	U	48	ASN	3.6
1	W	187	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	U	327	VAL	3.5
1	W	328	LYS	3.4
1	W	49	ASP	3.3
1	Q	328	LYS	3.3
1	W	45	THR	3.2
1	U	86	MET	3.2
1	W	140	TRP	3.1
1	W	47	GLY	3.1
1	W	309	PRO	3.0
1	D	328	LYS	3.0
1	A	328	LYS	3.0
1	A	47	GLY	2.9
1	D	7	PRO	2.9
1	D	48	ASN	2.8
1	Q	48	ASN	2.8
1	A	142	GLN	2.8
1	S	81	ALA	2.8
1	S	328	LYS	2.8
1	U	80	PRO	2.7
1	U	88	ALA	2.6
1	D	77	GLN	2.6
1	D	49	ASP	2.6
1	W	222	GLN	2.6
1	W	7	PRO	2.5
1	U	220	ASP	2.5
1	W	6	ASP	2.5
1	A	90	HIS	2.5
1	W	211	ILE	2.4
1	U	81	ALA	2.4
1	S	90	HIS	2.4
1	W	8	ARG	2.4
1	A	141	ASN	2.4
1	W	327	VAL	2.3
1	W	90	HIS	2.3
1	U	85	ALA	2.3
1	Q	47	GLY	2.2
1	U	8	ARG	2.2
1	A	144	GLY	2.2
1	D	47	GLY	2.2
1	D	147	GLN	2.1
1	W	5	GLN	2.1
1	U	184	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	W	252	THR	2.1
1	U	142	GLN	2.1
1	A	84	SER	2.1
1	S	89	ASP	2.1
1	U	146	PRO	2.0
1	W	80	PRO	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 monosaccharides 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(Å^2)	Q<0.9
2	SO4	S	701	5/5	0.97	0.10	49,49,53,54	0

6.5 Other polymers (i)

There are no such residues in this entry.