



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:18 am BST

PDB ID : 4R2W  
Title : X-ray structure of uridine phosphorylase from *Shewanella oneidensis* MR-1 in complex with uridine at 1.6 Å resolution  
Authors : Safonova, T.N.; Mordkovich, N.N.; Manuvera, V.A.; Veiko, V.P.; Popov, V.O.; Polyakov, K.P.  
Deposited on : 2014-08-13  
Resolution : 1.60 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

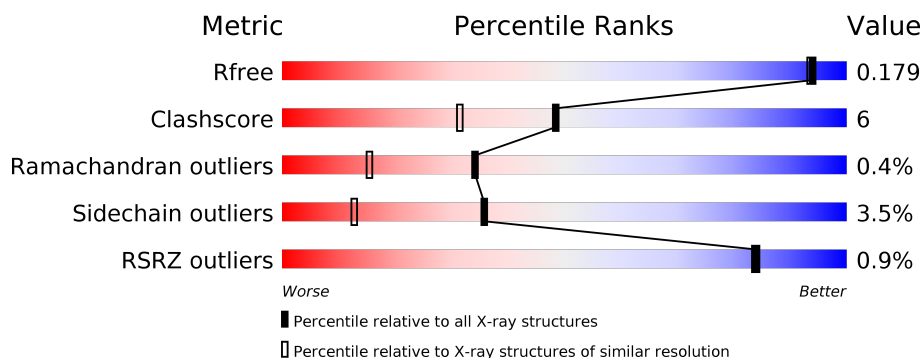
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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  $\geq 3$ , 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	252	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>• •</div> </div> </div>
1	B	252	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>• 5%</div> </div> </div>
1	C	252	<div> <div></div> <div> <div>89%</div> <div>8%</div> <div>• •</div> </div> </div>
1	D	252	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div>•</div> </div> </div>
1	E	252	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>• •</div> </div> </div>
1	F	252	<div> <div></div> <div> <div>85%</div> <div>11%</div> <div>• •</div> </div> </div>

## 2 Entry composition [i](#)

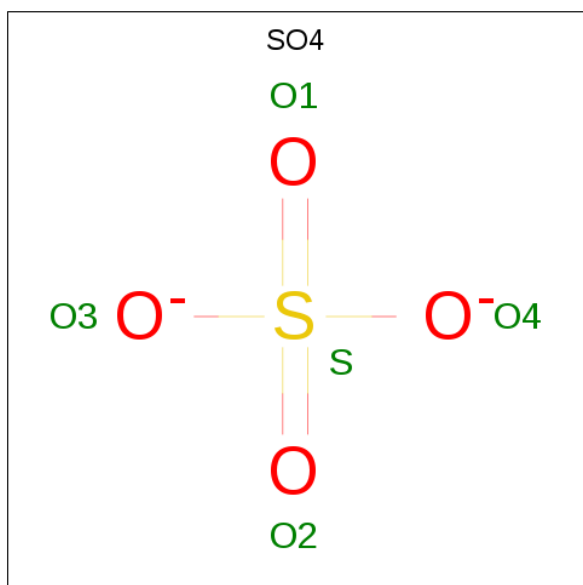
There are 5 unique types of molecules in this entry. The entry contains 11552 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uridine phosphorylase.

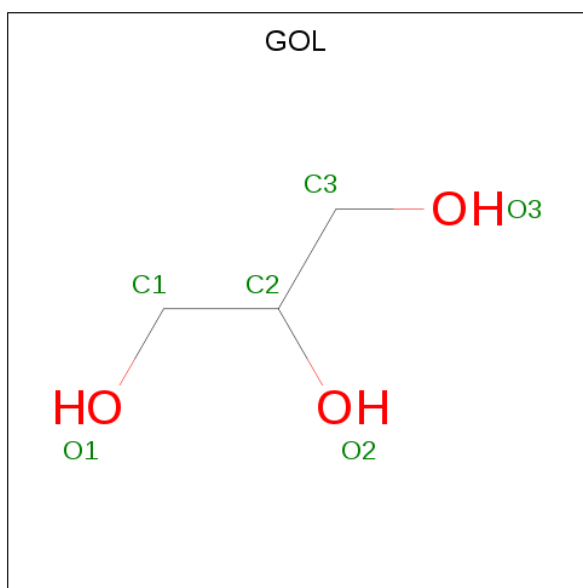
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	3	0
			1812	1138	314	347	13			
1	B	239	Total	C	N	O	S	0	3	0
			1784	1120	311	340	13			
1	C	248	Total	C	N	O	S	0	4	0
			1853	1162	319	358	14			
1	D	251	Total	C	N	O	S	0	2	0
			1873	1174	322	363	14			
1	E	241	Total	C	N	O	S	0	0	0
			1780	1119	307	341	13			
1	F	242	Total	C	N	O	S	0	4	0
			1798	1129	311	344	14			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 10 8 2	0	1
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



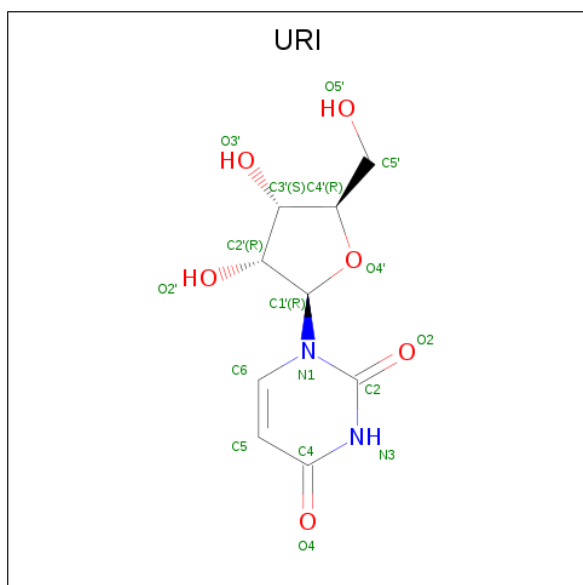
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is URIDINE (three-letter code: URI) (formula:  $C_9H_{12}N_2O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	F	1	Total	C	N	O	0	0
			17	9	2	6		

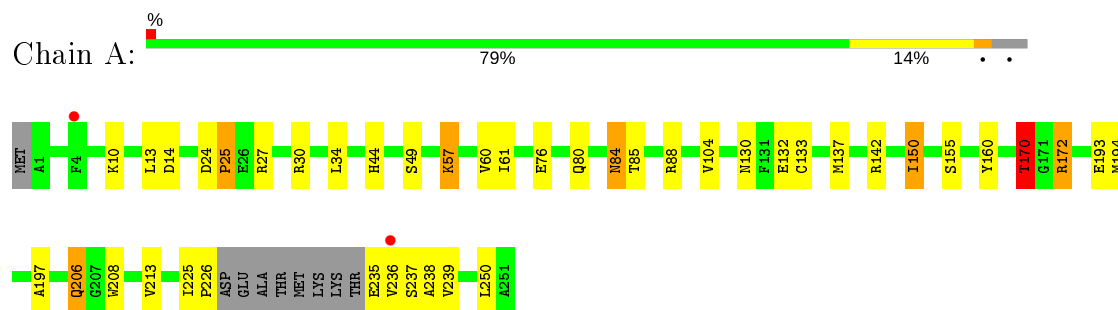
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	96	Total	O	0	0
			96	96		
5	B	77	Total	O	0	0
			77	77		
5	C	116	Total	O	0	0
			116	116		
5	D	107	Total	O	0	0
			107	107		
5	E	76	Total	O	0	0
			76	76		
5	F	82	Total	O	0	0
			82	82		

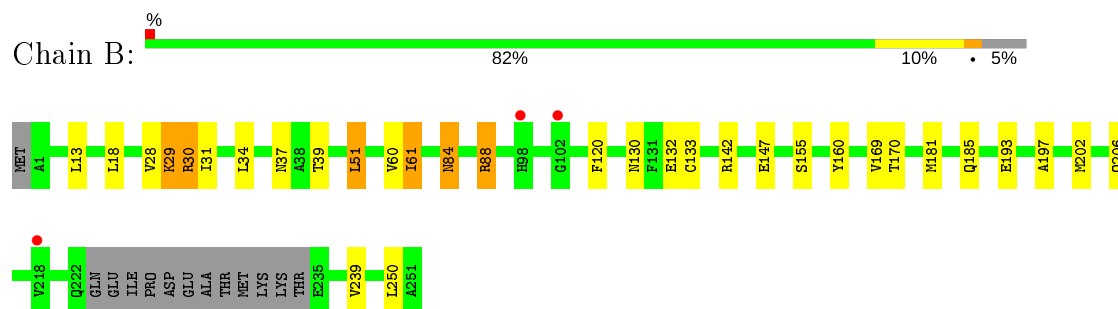
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

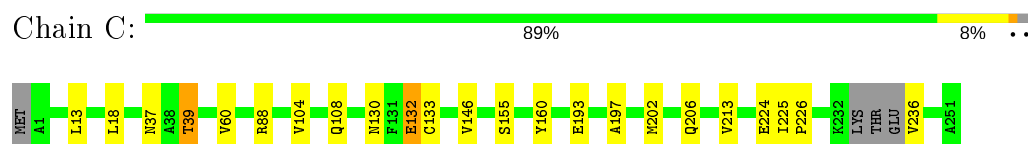
- Molecule 1: Uridine phosphorylase



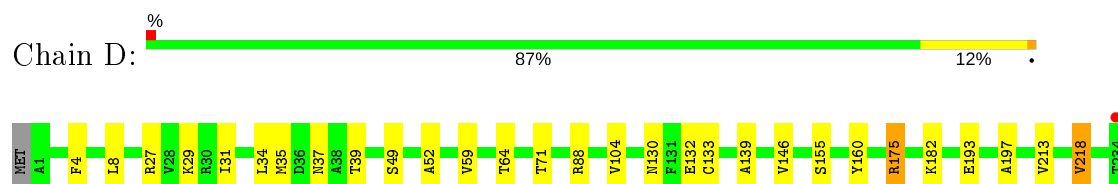
- Molecule 1: Uridine phosphorylase

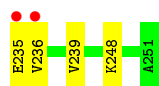


- Molecule 1: Uridine phosphorylase

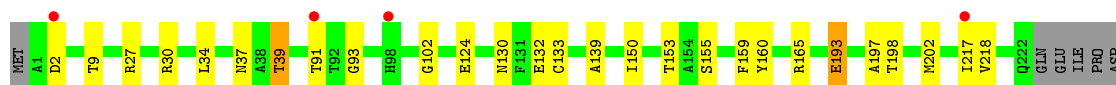
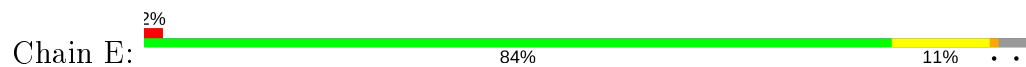


- Molecule 1: Uridine phosphorylase

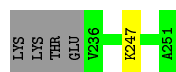
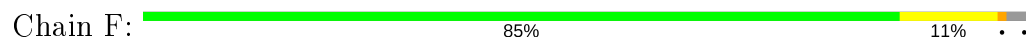




- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.92Å 96.48Å 91.93Å 90.00° 120.01° 90.00°	Depositor
Resolution (Å)	19.49 – 1.60 19.49 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.6 (19.49-1.60) 95.2 (19.49-1.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 1.51Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.177 , 0.192 0.179 , 0.179	Depositor DCC
$R_{free}$ test set	10270 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.1	Xtriage
Anisotropy	0.962	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 34.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.357 for -h-l,k,h 0.357 for l,k,-h-l 0.107 for l,-k,h 0.106 for h,-k,-h-l 0.104 for -h-l,-k,l	Xtriage
Reported twinning fraction	0.523 for H, K, L 0.318 for -H-L, K, H 0.159 for L, K, -H-L	Depositor
Outliers	0 of 208882 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11552	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, URI, 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	0.87	0/1861	1.00	3/2533 (0.1%)
1	B	0.84	0/1830	0.97	4/2487 (0.2%)
1	C	0.91	0/1905	0.97	1/2592 (0.0%)
1	D	0.93	0/1919	0.99	4/2608 (0.2%)
1	E	0.85	1/1811 (0.1%)	0.92	0/2464
1	F	0.91	2/1855 (0.1%)	0.94	1/2521 (0.0%)
All	All	0.89	3/11181 (0.0%)	0.97	13/15205 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	124	GLU	CD-OE1	-6.60	1.18	1.25
1	F	124	GLU	CD-OE1	-5.95	1.19	1.25
1	F	192	TYR	CG-CD2	5.14	1.45	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	MET	CG-SD-CE	-10.27	83.77	100.20
1	D	27	ARG	NE-CZ-NH2	-8.29	116.15	120.30
1	C	88	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	D	27	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	F	220	ARG	NE-CZ-NH1	-7.61	116.50	120.30
1	D	218	VAL	CB-CA-C	-7.47	97.20	111.40
1	B	88[A]	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	B	88[B]	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	B	88[A]	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	B	88[B]	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	A	170	THR	OG1-CB-CG2	5.74	123.20	110.00
1	A	170	THR	N-CA-CB	-5.58	99.70	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	88	ARG	NE-CZ-NH2	-5.39	117.61	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	1812	0	1794	40	0
1	B	1784	0	1771	29	0
1	C	1853	0	1836	20	0
1	D	1873	0	1860	18	0
1	E	1780	0	1764	22	0
1	F	1798	0	1775	12	0
2	A	15	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	10	0	0	0	0
3	A	6	0	8	1	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	12	0	16	0	0
3	F	6	0	8	0	0
4	F	17	0	12	2	0
5	A	96	0	0	2	0
5	B	77	0	0	1	0
5	C	116	0	0	1	0
5	D	107	0	0	0	0
5	E	76	0	0	0	0
5	F	82	0	0	0	0
All	All	11552	0	10860	132	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (132) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172[A]:ARG:CG	1:A:172[A]:ARG:HH11	1.41	1.29
1:A:172[A]:ARG:HG2	1:A:172[A]:ARG:HH11	1.04	1.10
1:C:236:VAL:N	5:C:448:HOH:O	1.95	0.98
1:B:130:ASN:HD21	1:B:132:GLU:HG3	1.28	0.97
1:A:172[A]:ARG:CG	1:A:172[A]:ARG:NH1	2.16	0.94
1:B:28:VAL:HG13	1:B:61:ILE:HG12	1.49	0.94
1:A:206:GLN:HG3	1:B:170:THR:HG21	1.48	0.92
1:A:172[A]:ARG:HH11	1:A:172[A]:ARG:HG3	1.30	0.91
1:A:172[A]:ARG:HG2	1:A:172[A]:ARG:NH1	1.80	0.88
1:E:27:ARG:HG2	1:E:30:ARG:NH2	1.89	0.87
1:D:175:ARG:HH11	1:D:175:ARG:HG3	1.45	0.82
1:A:206:GLN:HG3	1:B:170:THR:CG2	2.09	0.81
1:C:13:LEU:HG	1:C:60:VAL:HG21	1.62	0.81
1:A:172[A]:ARG:NH1	1:A:172[A]:ARG:HG3	1.92	0.78
1:A:170:THR:HG21	1:B:206:GLN:NE2	1.99	0.78
1:F:155[B]:SER:OG	1:F:197:ALA:HB2	1.85	0.75
1:D:35:MET:SD	1:D:59:VAL:HG21	2.26	0.75
1:E:91:THR:HB	1:E:217:ILE:HG13	1.69	0.74
1:E:102:GLY:HA2	1:E:234:THR:HG21	1.69	0.72
1:A:34:LEU:CD1	1:A:239:VAL:HG12	2.20	0.71
1:B:29:LYS:HD2	1:B:30:ARG:N	2.06	0.71
1:D:175:ARG:HG3	1:D:175:ARG:NH1	2.06	0.70
1:E:102:GLY:HA2	1:E:234:THR:CG2	2.21	0.70
1:A:170:THR:HG21	1:B:206:GLN:HE22	1.57	0.69
1:C:13:LEU:HG	1:C:60:VAL:CG2	2.22	0.68
1:E:130:ASN:HD22	1:E:133:CYS:H	1.41	0.68
1:B:51:LEU:HD23	1:B:60:VAL:HG22	1.76	0.66
1:F:35:MET:SD	1:F:59:VAL:HG21	2.34	0.66
1:F:130:ASN:HD22	1:F:133:CYS:H	1.45	0.64
1:B:130:ASN:ND2	1:B:132:GLU:HG3	2.09	0.64
1:B:31:ILE:HB	1:B:61:ILE:CD1	2.29	0.61
1:C:104:VAL:HG11	1:C:213:VAL:CG2	2.31	0.61
1:E:34:LEU:CD1	1:E:239:VAL:HG12	2.31	0.60
1:A:34:LEU:CD1	1:A:239:VAL:CG1	2.80	0.60
1:E:27:ARG:HG2	1:E:30:ARG:HH21	1.65	0.59
1:E:139:ALA:HB3	1:E:248:LYS:HE3	1.84	0.59
1:C:104:VAL:CG1	1:C:213:VAL:CG2	2.80	0.58
1:D:37:ASN:O	1:D:39:THR:HG23	2.05	0.57
1:B:155:SER:HB3	1:B:197:ALA:HB2	1.87	0.57
1:D:175:ARG:HH11	1:D:175:ARG:CG	2.16	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:ASN:HD22	1:D:133:CYS:H	1.54	0.56
1:B:84:ASN:C	1:B:84:ASN:HD22	2.09	0.55
1:E:130:ASN:HD21	1:E:132:GLU:HB3	1.71	0.55
1:A:84:ASN:HD22	1:A:84:ASN:C	2.10	0.55
1:F:202:MET:O	1:F:206:GLN:HG3	2.07	0.55
1:B:31:ILE:HB	1:B:61:ILE:HD13	1.88	0.54
1:B:130:ASN:HD22	1:B:133:CYS:H	1.54	0.54
1:A:104:VAL:HG13	1:A:213:VAL:CG2	2.37	0.54
1:F:55:ASP:OD2	1:F:247[A]:LYS:HE3	2.08	0.54
1:A:235:GLU:N	1:A:238:ALA:HB3	2.23	0.54
1:E:37:ASN:O	1:E:39:THR:CG2	2.56	0.53
1:A:155:SER:HB3	1:A:197:ALA:HB2	1.91	0.53
1:B:142:ARG:NE	1:B:147:GLU:OE2	2.38	0.53
1:B:13:LEU:HD23	1:B:60:VAL:HG21	1.89	0.52
1:A:150:ILE:C	1:A:150:ILE:HD12	2.30	0.52
1:A:225[A]:ILE:HD11	5:A:475:HOH:O	2.09	0.52
1:A:34:LEU:HD11	1:A:239:VAL:CG1	2.40	0.52
1:B:37:ASN:O	1:B:39:THR:HG23	2.09	0.52
1:C:225:ILE:HG23	1:C:226:PRO:HD2	1.91	0.52
1:A:130:ASN:HD21	1:A:132:GLU:HB3	1.75	0.51
1:B:181:MET:O	1:B:185:GLN:HG3	2.10	0.51
1:B:13:LEU:CD2	1:B:60:VAL:HG21	2.41	0.51
1:A:57:LYS:HD2	1:A:250:LEU:O	2.12	0.50
1:E:159:PHE:O	1:E:165:ARG:NH1	2.43	0.50
1:C:37:ASN:O	1:C:39[B]:THR:HG23	2.12	0.50
1:A:170:THR:HG23	1:A:172[A]:ARG:HB3	1.93	0.49
1:A:34:LEU:HD11	1:A:239:VAL:HG12	1.94	0.49
1:E:27:ARG:CG	1:E:30:ARG:HH21	2.25	0.49
1:F:193:GLU:HA	4:F:301:URI:O2	2.12	0.49
1:D:130:ASN:HD21	1:D:132:GLU:HB3	1.78	0.49
1:D:139:ALA:C	1:D:248[A]:LYS:NZ	2.66	0.49
1:A:172[A]:ARG:NH1	1:B:206:GLN:OE1	2.45	0.48
1:C:146:VAL:HG21	1:C:236:VAL:HB	1.96	0.48
1:B:34:LEU:CD1	1:B:239:VAL:HG12	2.43	0.48
1:A:130:ASN:HD22	1:A:133:CYS:H	1.62	0.47
1:A:235:GLU:HA	1:A:236:VAL:HA	1.58	0.47
1:C:104:VAL:CG1	1:C:213:VAL:HG22	2.44	0.47
1:D:139:ALA:C	1:D:248[A]:LYS:HZ2	2.17	0.47
1:C:130:ASN:HD22	1:C:133:CYS:H	1.61	0.47
1:A:13:LEU:HG	1:A:60:VAL:HG21	1.96	0.47
1:E:93:GLY:HA2	1:E:218:VAL:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:LEU:C	1:C:18:LEU:HD23	2.36	0.46
1:A:172[A]:ARG:NH2	1:B:120:PHE:O	2.49	0.46
1:C:202:MET:O	1:C:206:GLN:HG2	2.14	0.46
4:F:301:URI:H2'	4:F:301:URI:O2	2.15	0.46
1:A:76:GLU:O	1:A:80:GLN:HG3	2.16	0.46
1:C:37:ASN:O	1:C:39[A]:THR:HG22	2.15	0.45
1:B:202:MET:O	1:B:206:GLN:HG2	2.16	0.45
1:D:146:VAL:HG21	1:D:236:VAL:HG13	1.99	0.45
1:E:37:ASN:O	1:E:39:THR:HG22	2.16	0.45
1:E:155:SER:HB3	1:E:197:ALA:HB2	1.99	0.44
1:A:206:GLN:HG2	1:A:208:TRP:CH2	2.53	0.44
1:C:13:LEU:CG	1:C:60:VAL:HG21	2.39	0.44
1:A:170:THR:CG2	1:B:206:GLN:NE2	2.77	0.44
1:D:8:LEU:HD21	1:D:49[A]:SER:OG	2.18	0.44
1:D:64:THR:HB	1:D:71:THR:HA	1.99	0.44
1:A:49:SER:HA	1:A:61:ILE:O	2.18	0.44
1:E:37:ASN:O	1:E:39:THR:HG23	2.18	0.43
1:B:18:LEU:C	1:B:18:LEU:HD23	2.38	0.43
1:D:31:ILE:HG12	1:D:239:VAL:HG13	2.00	0.43
1:C:155:SER:HB3	1:C:197:ALA:HB2	2.00	0.43
1:E:153:THR:HG21	1:E:193:GLU:HG3	1.99	0.43
1:A:44:HIS:HE1	5:A:417:HOH:O	2.01	0.43
1:C:130:ASN:HD21	1:C:132:GLU:CG	2.30	0.43
1:D:155:SER:HB3	1:D:197:ALA:HB2	2.01	0.43
1:F:164:GLU:HG2	1:F:166:TYR:CE2	2.54	0.43
1:D:34:LEU:HD23	1:D:34:LEU:HA	1.81	0.42
1:B:130:ASN:HD21	1:B:132:GLU:CG	2.15	0.42
1:F:8:LEU:HD21	1:F:49:SER:OG	2.19	0.42
1:A:84:ASN:ND2	1:A:85:THR:OG1	2.53	0.42
1:E:217:ILE:O	1:E:217:ILE:HG22	2.19	0.42
1:E:91:THR:HB	1:E:217:ILE:CG1	2.45	0.42
1:A:80:GLN:HG2	1:B:169:VAL:HG12	2.01	0.42
1:A:194:MET:SD	3:A:303:GOL:H11	2.60	0.41
1:E:198:THR:O	1:E:202:MET:HG2	2.20	0.41
1:F:155[A]:SER:HB3	1:F:197:ALA:HB2	2.01	0.41
1:B:88[B]:ARG:NE	5:B:511:HOH:O	2.08	0.41
1:D:52:ALA:O	1:D:59:VAL:HG22	2.21	0.41
1:E:34:LEU:HD12	1:E:239:VAL:HG12	2.03	0.41
1:F:121:ALA:HB2	1:F:205:THR:HG21	2.02	0.41
1:B:29:LYS:HD2	1:B:30:ARG:CA	2.51	0.41
1:E:2:ASP:OD1	1:E:9:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:225:ILE:HA	1:F:226:PRO:HD3	1.71	0.41
1:A:24:ASP:HB3	1:A:27:ARG:HG3	2.03	0.40
1:C:108:GLN:NE2	1:F:129:ALA:O	2.54	0.40
1:D:104:VAL:CG1	1:D:213:VAL:CG2	3.00	0.40
1:A:24:ASP:HA	1:A:25:PRO:HD2	2.00	0.40
1:C:132:GLU:H	1:C:132:GLU:HG3	1.55	0.40
1:A:10:LYS:HB2	1:A:10:LYS:HE2	1.72	0.40
1:C:104:VAL:CG1	1:C:213:VAL:HG23	2.51	0.40
1:C:225:ILE:HD13	1:D:4:PHE:HB2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/252 (96%)	237 (98%)	4 (2%)	1 (0%)	34	15
1	B	238/252 (94%)	234 (98%)	3 (1%)	1 (0%)	34	15
1	C	248/252 (98%)	245 (99%)	2 (1%)	1 (0%)	34	15
1	D	251/252 (100%)	246 (98%)	4 (2%)	1 (0%)	34	15
1	E	237/252 (94%)	231 (98%)	5 (2%)	1 (0%)	34	15
1	F	242/252 (96%)	236 (98%)	5 (2%)	1 (0%)	34	15
All	All	1458/1512 (96%)	1429 (98%)	23 (2%)	6 (0%)	34	15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	160	TYR
1	A	160	TYR
1	C	160	TYR

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Mol	Chain	Res	Type
1	F	160	TYR
1	D	160	TYR
1	E	160	TYR

### 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	191/198 (96%)	176 (92%)	15 (8%)	12	2
1	B	187/198 (94%)	180 (96%)	7 (4%)	34	11
1	C	196/198 (99%)	190 (97%)	6 (3%)	40	15
1	D	199/198 (100%)	193 (97%)	6 (3%)	41	16
1	E	185/198 (93%)	182 (98%)	3 (2%)	62	41
1	F	190/198 (96%)	183 (96%)	7 (4%)	34	11
All	All	1148/1188 (97%)	1104 (96%)	44 (4%)	36	10

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14[A]	ASP
1	A	14[B]	ASP
1	A	25	PRO
1	A	30	ARG
1	A	57	LYS
1	A	84	ASN
1	A	88	ARG
1	A	142	ARG
1	A	150	ILE
1	A	170	THR
1	A	172[A]	ARG
1	A	172[B]	ARG
1	A	193	GLU
1	A	206	GLN
1	A	237	SER

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Mol	Chain	Res	Type
1	B	29	LYS
1	B	30	ARG
1	B	51	LEU
1	B	61	ILE
1	B	84	ASN
1	B	193	GLU
1	B	250	LEU
1	C	39[A]	THR
1	C	39[B]	THR
1	C	132	GLU
1	C	193	GLU
1	C	224[A]	GLU
1	C	224[B]	GLU
1	D	29	LYS
1	D	175	ARG
1	D	182	LYS
1	D	193	GLU
1	D	218	VAL
1	D	235	GLU
1	E	39	THR
1	E	150	ILE
1	E	193	GLU
1	F	51	LEU
1	F	104	VAL
1	F	108	GLN
1	F	124	GLU
1	F	142	ARG
1	F	167	ASP
1	F	193	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	84	ASN
1	A	130	ASN
1	B	84	ASN
1	B	108	GLN
1	B	130	ASN
1	C	130	ASN
1	D	130	ASN
1	E	130	ASN

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Mol	Chain	Res	Type
1	F	130	ASN
1	F	206	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

16 ligands are 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	C	301	-	4,4,4	0.48	0	6,6,6	0.38	0
2	SO4	D	301	-	4,4,4	0.49	0	6,6,6	0.88	0
3	GOL	A	303	-	5,5,5	0.31	0	5,5,5	1.14	0
2	SO4	A	302	-	4,4,4	0.53	0	6,6,6	0.28	0
2	SO4	A	301[B]	-	4,4,4	0.29	0	6,6,6	0.18	0
3	GOL	D	302	-	5,5,5	0.44	0	5,5,5	0.73	0
3	GOL	B	302	-	5,5,5	0.71	0	5,5,5	0.54	0
2	SO4	F	303	-	4,4,4	0.71	0	6,6,6	0.39	0
3	GOL	D	303	-	5,5,5	0.43	0	5,5,5	0.57	0
2	SO4	F	302	-	4,4,4	0.44	0	6,6,6	0.91	0
4	URI	F	301	-	14,18,18	1.21	1 (7%)	14,26,26	1.70	3 (21%)
2	SO4	A	301[A]	-	4,4,4	0.31	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	C	302	-	5,5,5	0.88	0	5,5,5	1.22	0
3	GOL	F	304	-	5,5,5	0.57	0	5,5,5	0.38	0
2	SO4	B	301	-	4,4,4	0.31	0	6,6,6	0.87	0
2	SO4	E	301	-	4,4,4	0.42	0	6,6,6	0.32	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
3	GOL	A	303	-	-	4/4/4/4	-
3	GOL	D	302	-	-	4/4/4/4	-
3	GOL	B	302	-	-	0/4/4/4	-
4	URI	F	301	-	-	1/4/22/22	0/2/2/2
3	GOL	C	302	-	-	4/4/4/4	-
3	GOL	F	304	-	-	0/4/4/4	-
3	GOL	D	303	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	301	URI	C2-N3	-3.05	1.32	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	301	URI	C3'-C2'-C1'	3.80	106.70	100.98
4	F	301	URI	O2'-C2'-C3'	-2.53	103.63	111.82
4	F	301	URI	C2'-C3'-C4'	2.11	106.73	102.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	GOL	C1-C2-C3-O3
3	D	302	GOL	O1-C1-C2-C3
3	D	302	GOL	C1-C2-C3-O3
4	F	301	URI	C2'-C1'-N1-C6
3	C	302	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	C	302	GOL	C1-C2-C3-O3
3	C	302	GOL	O2-C2-C3-O3
3	D	302	GOL	O2-C2-C3-O3
3	A	303	GOL	O1-C1-C2-C3
3	A	303	GOL	O2-C2-C3-O3
3	A	303	GOL	O1-C1-C2-O2
3	C	302	GOL	O1-C1-C2-O2
3	D	302	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	303	GOL	1	0
4	F	301	URI	2	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	243/252 (96%)	-0.32	2 (0%) 86 86	11, 15, 26, 34	0
1	B	239/252 (94%)	-0.20	3 (1%) 77 77	10, 16, 31, 39	0
1	C	248/252 (98%)	-0.36	0 100 100	10, 15, 25, 35	0
1	D	251/252 (99%)	-0.28	3 (1%) 79 78	11, 15, 28, 52	0
1	E	241/252 (95%)	-0.29	4 (1%) 70 69	12, 16, 29, 36	0
1	F	242/252 (96%)	-0.35	1 (0%) 92 92	11, 16, 25, 32	0
All	All	1464/1512 (96%)	-0.30	13 (0%) 84 84	10, 16, 28, 52	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	236	VAL	5.8
1	A	4	PHE	4.2
1	D	236	VAL	3.6
1	B	102	GLY	3.4
1	D	235	GLU	3.4
1	B	98	HIS	3.2
1	E	217	ILE	3.1
1	E	2	ASP	3.0
1	B	218	VAL	2.8
1	E	98	HIS	2.5
1	D	234	THR	2.5
1	E	91	THR	2.5
1	F	4	PHE	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 ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	URI	F	301	17/17	0.84	0.14	14,27,31,32	0
3	GOL	D	303	6/6	0.86	0.15	18,22,23,24	0
3	GOL	D	302	6/6	0.89	0.11	20,20,22,24	0
3	GOL	B	302	6/6	0.89	0.10	20,21,22,22	0
2	SO4	E	301	5/5	0.89	0.11	13,13,14,14	5
3	GOL	A	303	6/6	0.90	0.12	21,22,24,28	0
2	SO4	A	301[A]	5/5	0.92	0.13	19,21,22,23	5
2	SO4	A	301[B]	5/5	0.92	0.13	16,17,18,18	5
3	GOL	F	304	6/6	0.93	0.11	20,22,23,23	0
3	GOL	C	302	6/6	0.94	0.11	15,17,17,18	0
2	SO4	F	302	5/5	0.95	0.09	27,29,30,32	0
2	SO4	B	301	5/5	0.95	0.11	12,13,13,14	5
2	SO4	D	301	5/5	0.95	0.09	13,13,13,15	0
2	SO4	C	301	5/5	0.98	0.06	12,13,14,14	0
2	SO4	A	302	5/5	0.99	0.05	14,16,16,17	0
2	SO4	F	303	5/5	0.99	0.04	14,14,15,17	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.