



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:13 PM GMT

PDB ID : 4R2X  
Title : Unique conformation of uridine and asymmetry of the hexameric molecule revealed in the high-resolution structures of *Shewanella oneidensis* uridine phosphorylase in the free form and in complex with uridine  
Authors : Safonova, T.N.; Mordkovich, N.N.; Manuvera, V.A.; Veiko, V.P.; Popov, V.O.; Polyakov, K.M.  
Deposited on : 2014-08-13  
Resolution : 0.93 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

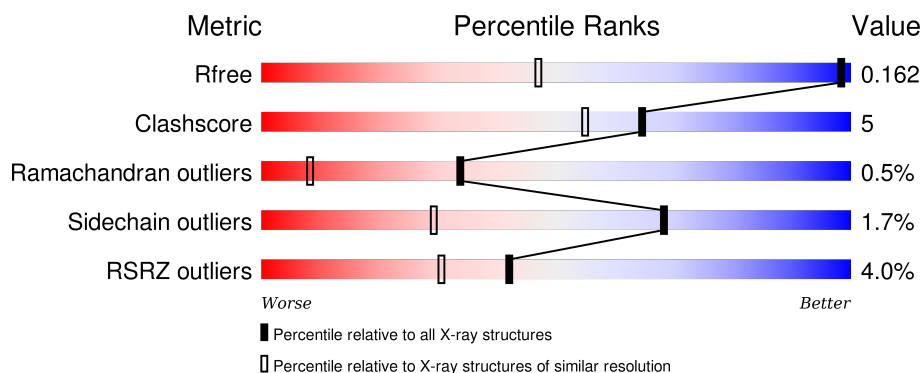
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 0.93 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))
$R_{free}$	91344	1341 (1.10-0.78)
Clashscore	102246	1063 (1.08-0.80)
Ramachandran outliers	100387	1355 (1.10-0.78)
Sidechain outliers	100360	1354 (1.10-0.78)
RSRZ outliers	91569	1346 (1.10-0.78)

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. 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>4%</div> <div>90%</div> <div>5%</div> <div>.</div> </div>
1	B	252	<div> <div>5%</div> <div>86%</div> <div>8%</div> <div>5%</div> <div>.</div> </div>
1	C	252	<div> <div>2%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	D	252	<div> <div>3%</div> <div>94%</div> <div>5%</div> <div>.</div> </div>
1	E	252	<div> <div>7%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	252	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	304[B]	-	-	X	-
2	SO4	E	301[A]	-	-	X	-
2	SO4	E	303[A]	-	-	X	-
4	GOL	A	303[A]	-	-	-	X
4	GOL	A	303[B]	-	-	-	X
4	GOL	A	304	-	-	-	X
4	GOL	A	305	-	-	-	X
4	GOL	B	305[A]	-	-	-	X
4	GOL	B	305[B]	-	-	-	X
4	GOL	C	303[A]	-	-	-	X
4	GOL	C	303[B]	-	-	-	X
4	GOL	C	304	-	-	-	X
4	GOL	C	305	-	-	-	X
4	GOL	C	306	-	-	-	X
4	GOL	D	304	-	-	-	X
4	GOL	D	305	-	-	-	X
4	GOL	E	305	-	-	X	X
4	GOL	F	303[A]	-	-	-	X
4	GOL	F	303[B]	-	-	-	X
4	GOL	F	305[A]	-	-	-	X
4	GOL	F	305[B]	-	-	-	X

## 2 Entry composition [i](#)

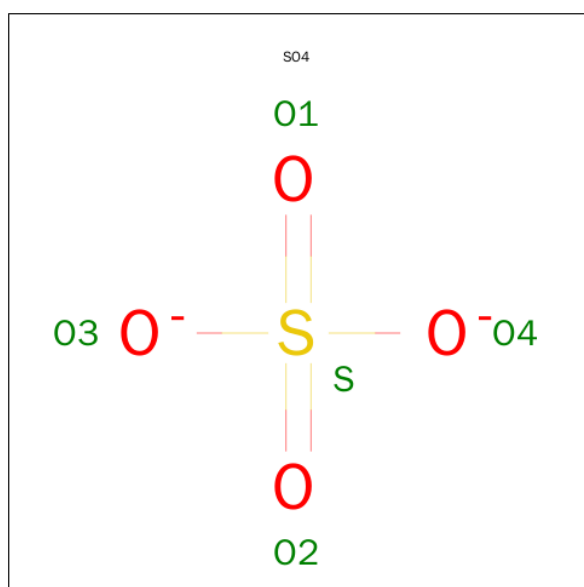
There are 5 unique types of molecules in this entry. The entry contains 23087 atoms, of which 10718 are hydrogens and 0 are deuteriums.

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	C	247	Total	C	H	N	O	S	0	9	0
			3682	1175	1810	320	361	16			
1	D	249	Total	C	H	N	O	S	0	8	0
			3659	1171	1789	319	364	16			
1	E	241	Total	C	H	N	O	S	0	15	0
			3601	1157	1754	321	354	15			
1	F	242	Total	C	H	N	O	S	0	5	0
			3551	1143	1734	310	349	15			
1	A	241	Total	C	H	N	O	S	0	8	0
			3560	1146	1738	314	347	15			
1	B	240	Total	C	H	N	O	S	0	18	0
			3631	1161	1775	325	355	15			

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



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	0	1
			12	3	5	4		
4	C	1	Total	C	H	O	0	0
			12	3	6	3		
4	C	1	Total	C	H	O	0	0
			12	3	6	3		
4	C	1	Total	C	O		0	0
			6	3	3			
4	D	1	Total	C	H	O	0	0
			12	3	6	3		
4	D	1	Total	C	H	O	0	0
			12	3	6	3		
4	D	1	Total	C	H	O	0	0
			12	3	6	3		
4	E	1	Total	C	H	O	0	0
			12	3	6	3		
4	E	1	Total	C	H	O	0	0
			12	3	6	3		
4	E	1	Total	C	H	O	0	0
			12	3	6	3		
4	F	1	Total	C	H	O	0	1
			24	6	12	6		
4	F	1	Total	C	H	O	0	0
			12	3	6	3		
4	F	1	Total	C	H	O	0	1
			14	3	7	4		
4	A	1	Total	C	H	O	0	1
			9	3	2	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			12	3	6	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			12	3	6	3		
4	B	1	Total	C	H	O	0	0
			12	3	6	3		
4	B	1	Total	C	H	O	0	1
			24	6	12	6		

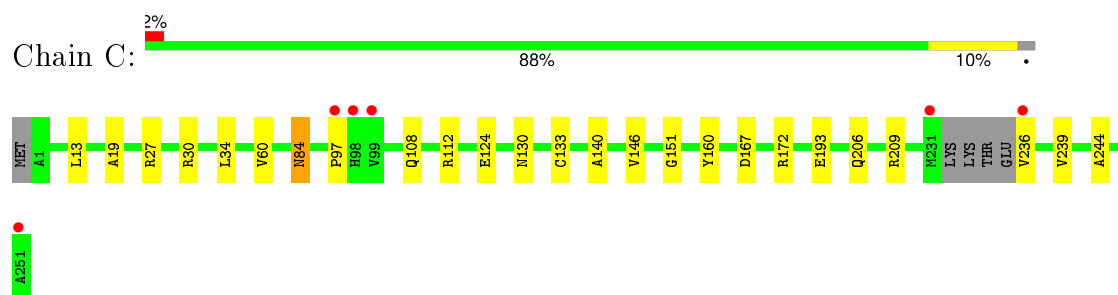
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	199	Total	O	0	0
			199	199		
5	D	210	Total	O	0	0
			210	210		
5	E	162	Total	O	0	0
			162	162		
5	F	175	Total	O	0	0
			175	175		
5	A	184	Total	O	0	0
			184	184		
5	B	162	Total	O	0	0
			162	162		

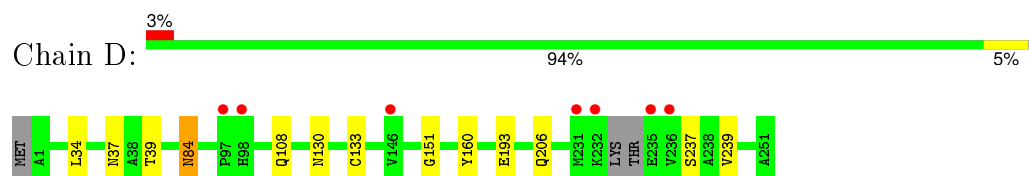
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

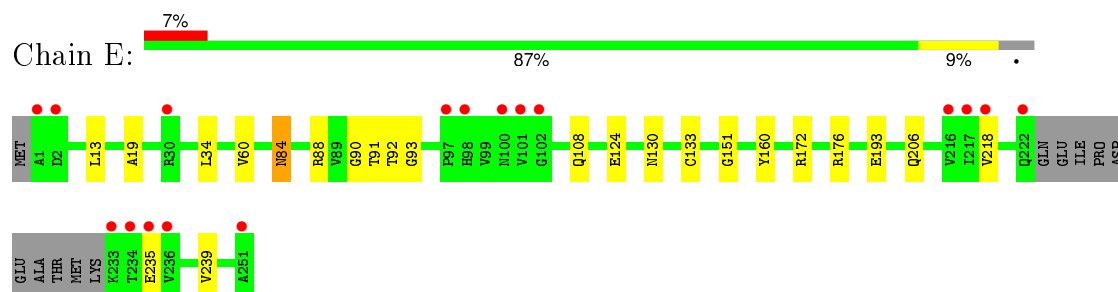
- Molecule 1: uridine phosphorylase



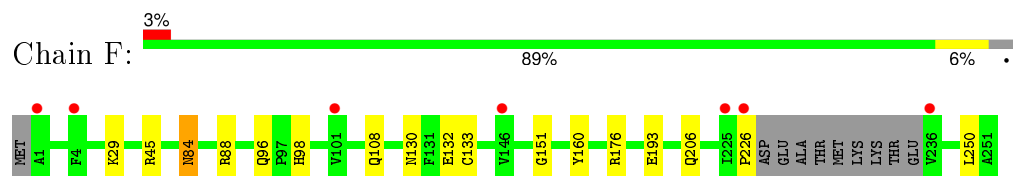
- Molecule 1: uridine phosphorylase



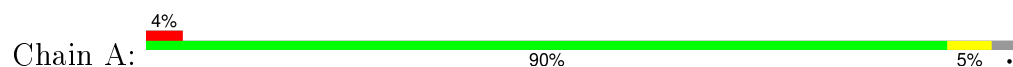
- Molecule 1: uridine phosphorylase

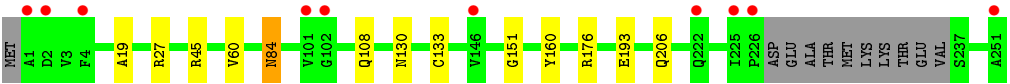


- Molecule 1: uridine phosphorylase

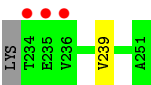
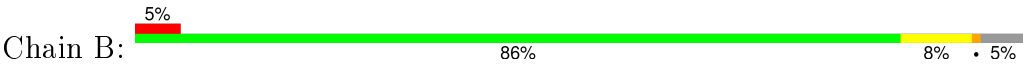


- Molecule 1: uridine phosphorylase





● Molecule 1: uridine phosphorylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.54Å 95.93Å 91.61Å 90.00° 120.00° 90.00°	Depositor
Resolution (Å)	29.66 – 0.93 29.66 – 0.93	Depositor EDS
% Data completeness (in resolution range)	95.9 (29.66-0.93) 95.8 (29.66-0.93)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.87	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 0.93Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.149 , 0.164 0.157 , 0.162	Depositor DCC
$R_{free}$ test set	43996 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	6.8	Xtriage
Anisotropy	0.742	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.45 , 44.3	EDS
Estimated twinning fraction	0.802 for H, K, L 0.100 for -H-L, K, H 0.098 for L, K, -H-L 0.198 for l,k,-h-l 0.198 for -h-l,k,h 0.048 for h,-k,-h-l 0.047 for l,-k,h 0.047 for -h-l,-k,l	Xtriage
Reported twinning fraction	0.802 for H, K, L 0.100 for -H-L, K, H 0.098 for L, K, -H-L	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 883283 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	23087	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, SO4, CL

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	0.75	0/1893	0.86	2/2573 (0.1%)
1	B	0.66	0/1934	0.83	6/2627 (0.2%)
1	C	0.77	0/1945	0.87	2/2643 (0.1%)
1	D	0.76	0/1941	0.84	0/2638
1	E	0.65	0/1932	0.80	2/2624 (0.1%)
1	F	0.71	0/1873	0.82	1/2545 (0.0%)
All	All	0.72	0/11518	0.84	13/15650 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	88	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	B	112	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	E	176	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	B	124[A]	GLU	CG-CD-OE2	-6.00	106.30	118.30
1	B	124[B]	GLU	CG-CD-OE2	-6.00	106.30	118.30
1	A	176	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	C	112	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	C	209	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	27	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	124[A]	GLU	CA-CB-CG	5.25	124.94	113.40
1	B	124[B]	GLU	CA-CB-CG	5.25	124.94	113.40
1	E	172	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	112	ARG	NE-CZ-NH2	-5.02	117.79	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	1822	1738	1819	10	0
1	B	1856	1775	1838	22	0
1	C	1872	1810	1861	26	0
1	D	1870	1789	1841	10	0
1	E	1847	1754	1837	25	0
1	F	1817	1734	1803	11	0
2	A	5	0	0	0	0
2	B	20	0	0	3	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	20	0	0	7	0
2	F	5	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
4	A	19	16	22	0	0
4	B	24	24	32	2	0
4	C	25	17	30	3	0
4	D	18	18	24	0	0
4	E	18	18	24	7	0
4	F	25	25	30	4	0
5	A	184	0	0	2	0
5	B	162	0	0	4	0
5	C	199	0	0	7	0
5	D	210	0	0	4	0
5	E	162	0	0	20	0
5	F	175	0	0	1	0
All	All	12369	10718	11161	115	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 5.

All (115) 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)
4:E:305:GOL:H12	5:E:550:HOH:O	1.18	1.27
2:E:303[A]:SO4:O3	5:E:554:HOH:O	1.58	1.21
1:E:92[A]:THR:HA	5:E:536:HOH:O	1.42	1.17
2:E:301[A]:SO4:S	5:E:519:HOH:O	1.98	1.17
1:E:88[A]:ARG:NH2	5:E:554:HOH:O	1.70	1.13
1:C:167[B]:ASP:OD2	5:C:592:HOH:O	1.76	1.01
4:E:305:GOL:H32	5:E:550:HOH:O	1.73	0.87
4:E:305:GOL:C1	5:E:550:HOH:O	1.89	0.86
1:E:90[A]:GLY:HA3	5:E:554:HOH:O	1.81	0.80
1:B:218[B]:VAL:HG22	1:B:219[B]:ASN:H	1.46	0.78
1:E:91[A]:THR:O	5:E:536:HOH:O	2.02	0.77
1:D:237:SER:HB2	5:D:533:HOH:O	1.85	0.76
2:E:301[A]:SO4:O1	5:E:519:HOH:O	1.89	0.74
1:F:108[A]:GLN:HE21	1:F:151:GLY:HA2	1.53	0.74
1:E:88[A]:ARG:CZ	5:E:554:HOH:O	2.22	0.73
1:C:97:PRO:O	5:C:583:HOH:O	2.07	0.73
1:C:206[A]:GLN:NE2	5:C:599:HOH:O	2.21	0.72
1:A:108[B]:GLN:HE21	1:A:151:GLY:HA2	1.52	0.72
1:C:34:LEU:CD1	1:C:239[A]:VAL:HG12	2.22	0.70
1:F:130:ASN:HD22	1:F:133:CYS:H	1.40	0.70
4:E:305:GOL:H31	1:B:124[B]:GLU:OE1	1.93	0.69
1:B:27:ARG:NH2	2:B:304[B]:SO4:O1	2.23	0.69
1:C:124[B]:GLU:OE1	4:F:303[B]:GOL:H12	1.94	0.68
2:E:303[A]:SO4:O4	5:E:562:HOH:O	0.68	0.67
1:E:130:ASN:HD22	1:E:133:CYS:H	1.43	0.67
1:B:130:ASN:HD22	1:B:133:CYS:H	1.43	0.66
1:C:130:ASN:HD22	1:C:133:CYS:H	1.43	0.65
1:C:108[B]:GLN:HE21	1:C:151:GLY:HA2	1.61	0.65
1:E:88[A]:ARG:NH1	5:E:554:HOH:O	2.29	0.65
1:D:130:ASN:HD22	1:D:133:CYS:H	1.46	0.64
1:B:218[B]:VAL:HG22	1:B:219[B]:ASN:N	2.13	0.63
1:E:91[B]:THR:HG21	1:E:235:GLU:OE2	1.98	0.63
1:E:108[B]:GLN:HE21	1:E:151:GLY:HA2	1.62	0.63
1:D:108[A]:GLN:HE21	1:D:151:GLY:HA2	1.65	0.61
1:A:130:ASN:HD22	1:A:133:CYS:H	1.47	0.61
1:E:19:ALA:HB2	1:E:60[B]:VAL:HG23	1.82	0.60
1:F:226:PRO:HB3	5:F:542:HOH:O	2.01	0.60
1:F:176:ARG:HG3	4:F:303[A]:GOL:H12	1.83	0.60
1:D:108[B]:GLN:HG3	5:D:582:HOH:O	2.02	0.59
1:B:108[B]:GLN:HG3	5:B:514:HOH:O	2.02	0.59
1:C:13:LEU:HG	1:C:60[B]:VAL:HG21	1.83	0.59
1:E:93[B]:GLY:HA2	1:E:218:VAL:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91[B]:THR:HG21	1:E:235:GLU:CD	2.24	0.57
1:B:218[A]:VAL:HG23	5:B:559:HOH:O	2.04	0.57
1:C:34:LEU:HD11	1:C:239[A]:VAL:HG12	1.87	0.56
1:B:108[A]:GLN:HE21	1:B:151:GLY:HA2	1.70	0.56
1:E:90[A]:GLY:HA2	5:E:561:HOH:O	2.07	0.55
1:E:84:ASN:C	1:E:84:ASN:HD22	2.10	0.55
1:C:108[A]:GLN:NE2	5:C:518:HOH:O	2.39	0.55
1:C:244:ALA:HB1	4:C:306:GOL:H11	1.88	0.55
1:E:124[B]:GLU:OE2	4:B:305[B]:GOL:H12	2.08	0.54
1:B:84:ASN:C	1:B:84:ASN:HD22	2.11	0.54
1:A:108[A]:GLN:HG3	5:A:531:HOH:O	2.07	0.54
1:D:37:ASN:O	1:D:39:THR:HG23	2.07	0.54
1:C:13:LEU:HG	1:C:60[B]:VAL:CG2	2.37	0.53
4:E:305:GOL:C2	5:E:550:HOH:O	2.38	0.53
1:F:176:ARG:CG	4:F:303[A]:GOL:H12	2.38	0.53
1:D:39:THR:HG23	5:D:609:HOH:O	2.08	0.52
1:A:84:ASN:HD22	1:A:84:ASN:C	2.13	0.51
1:E:108[A]:GLN:NE2	5:E:501:HOH:O	2.42	0.51
1:B:108[B]:GLN:NE2	5:B:514:HOH:O	2.43	0.51
1:A:19:ALA:HB2	1:A:60[B]:VAL:HG13	1.92	0.51
1:E:34:LEU:HD12	1:E:239[A]:VAL:HG12	1.92	0.51
2:E:301[A]:SO4:O3	5:E:519:HOH:O	2.14	0.50
1:E:19:ALA:CB	1:E:60[B]:VAL:HG23	2.40	0.50
1:C:84:ASN:HD22	1:C:84:ASN:C	2.15	0.50
1:D:84:ASN:C	1:D:84:ASN:HD22	2.14	0.50
1:E:34:LEU:CD1	1:E:239[A]:VAL:HG12	2.42	0.50
4:E:302:GOL:H11	2:E:303[A]:SO4:O3	2.12	0.50
1:C:140:ALA:O	4:C:306:GOL:H31	2.12	0.50
1:C:206[B]:GLN:NE2	5:C:427:HOH:O	2.44	0.50
1:B:217[A]:ILE:HG13	1:B:218[A]:VAL:HG13	1.95	0.49
1:E:108[A]:GLN:HG3	5:E:501:HOH:O	2.12	0.49
1:B:34:LEU:CD1	1:B:239:VAL:HG12	2.43	0.49
1:E:88[A]:ARG:NH1	5:E:561:HOH:O	2.41	0.48
1:C:108[A]:GLN:HG3	5:C:518:HOH:O	2.13	0.48
1:F:84:ASN:C	1:F:84:ASN:HD22	2.16	0.48
1:C:146:VAL:HG21	1:C:236:VAL:HB	1.95	0.48
1:A:45:ARG:NH2	2:B:304[B]:SO4:O1	2.46	0.47
1:C:124[B]:GLU:OE1	4:F:303[B]:GOL:C1	2.60	0.47
1:B:220:ARG:HG2	5:B:559:HOH:O	2.14	0.47
1:B:34:LEU:HD12	1:B:239:VAL:HG12	1.96	0.47
4:B:303:GOL:H11	2:B:304[A]:SO4:O3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:LEU:CD1	1:C:239[A]:VAL:CG1	2.93	0.46
1:B:130:ASN:HD21	1:B:132:GLU:HB3	1.81	0.46
1:C:172[B]:ARG:NH1	5:C:537:HOH:O	2.40	0.45
1:D:39:THR:CG2	5:D:609:HOH:O	2.65	0.45
1:F:130:ASN:ND2	1:F:133:CYS:H	2.11	0.45
1:C:34:LEU:HD12	1:C:239[A]:VAL:HG12	1.99	0.45
1:D:34:LEU:CD1	1:D:239[A]:VAL:HG12	2.47	0.44
2:E:303[B]:SO4:O1	1:F:45:ARG:NH2	2.48	0.44
1:B:90[B]:GLY:O	1:B:214[B]:ALA:HA	2.17	0.44
1:B:31:ILE:HG12	1:B:239:VAL:HG13	2.00	0.43
1:C:130:ASN:ND2	1:C:133:CYS:H	2.14	0.43
1:F:130:ASN:HD21	1:F:132:GLU:HB3	1.83	0.43
1:E:108[A]:GLN:CG	5:E:501:HOH:O	2.66	0.43
4:E:305:GOL:C3	1:B:124[B]:GLU:OE1	2.65	0.42
1:F:96:GLN:HB3	1:F:98:HIS:CE1	2.54	0.42
1:A:19:ALA:CB	1:A:60[B]:VAL:HG13	2.49	0.42
1:B:217[A]:ILE:O	1:B:218[A]:VAL:CG1	2.67	0.42
1:A:130:ASN:ND2	1:A:133:CYS:H	2.16	0.42
1:C:34:LEU:HD12	1:C:239[A]:VAL:CG1	2.50	0.41
1:E:130:ASN:ND2	1:E:133:CYS:H	2.14	0.41
1:E:13:LEU:HG	1:E:60[B]:VAL:CG1	2.51	0.41
1:C:140:ALA:O	4:C:306:GOL:C3	2.69	0.41
1:A:108[A]:GLN:CG	5:A:531:HOH:O	2.68	0.41
1:B:217[A]:ILE:C	1:B:218[A]:VAL:HG13	2.40	0.41
1:B:218[B]:VAL:CG2	1:B:219[B]:ASN:H	2.26	0.41

There are no symmetry-related clashes.

## 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	245/252 (97%)	242 (99%)	2 (1%)	1 (0%)	39 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	254/252 (101%)	248 (98%)	3 (1%)	3 (1%)	16	1
1	C	252/252 (100%)	248 (98%)	3 (1%)	1 (0%)	39	12
1	D	253/252 (100%)	249 (98%)	3 (1%)	1 (0%)	39	12
1	E	252/252 (100%)	248 (98%)	3 (1%)	1 (0%)	39	12
1	F	243/252 (96%)	240 (99%)	2 (1%)	1 (0%)	39	12
All	All	1499/1512 (99%)	1475 (98%)	16 (1%)	8 (0%)	34	8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	160	TYR
1	F	160	TYR
1	B	160	TYR
1	C	160	TYR
1	D	160	TYR
1	A	160	TYR
1	B	218[A]	VAL
1	B	218[B]	VAL

### 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	196/198 (99%)	194 (99%)	2 (1%)	82	51
1	B	197/198 (100%)	191 (97%)	6 (3%)	48	10
1	C	202/198 (102%)	198 (98%)	4 (2%)	63	23
1	D	200/198 (101%)	198 (99%)	2 (1%)	82	51
1	E	199/198 (100%)	197 (99%)	2 (1%)	82	51
1	F	194/198 (98%)	190 (98%)	4 (2%)	61	20
All	All	1188/1188 (100%)	1168 (98%)	20 (2%)	68	29

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	27	ARG
1	C	30	ARG
1	C	84	ASN
1	C	193	GLU
1	D	84	ASN
1	D	193	GLU
1	E	84	ASN
1	E	193	GLU
1	F	29	LYS
1	F	84	ASN
1	F	193	GLU
1	F	250	LEU
1	A	84	ASN
1	A	193	GLU
1	B	29	LYS
1	B	30	ARG
1	B	84	ASN
1	B	124[A]	GLU
1	B	124[B]	GLU
1	B	193	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	84	ASN
1	C	130	ASN
1	C	222	GLN
1	D	84	ASN
1	D	130	ASN
1	D	206	GLN
1	E	84	ASN
1	E	130	ASN
1	F	84	ASN
1	F	130	ASN
1	F	222	GLN
1	A	84	ASN
1	A	98	HIS
1	A	130	ASN
1	B	84	ASN
1	B	98	HIS
1	B	130	ASN
1	B	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 ⓘ

Of 40 ligands modelled in this entry, 4 are monoatomic - leaving 36 for Mogul analysis.

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	A	301	-	4,4,4	0.76	0	6,6,6	0.29	0
4	GOL	A	303[A]	-	5,5,5	0.41	0	5,5,5	0.55	0
4	GOL	A	303[B]	-	5,5,5	0.37	0	5,5,5	0.86	0
4	GOL	A	304	-	5,5,5	0.24	0	5,5,5	0.50	0
4	GOL	A	305	-	5,5,5	0.25	0	5,5,5	0.41	0
2	SO4	B	301[A]	-	4,4,4	0.64	0	6,6,6	0.35	0
2	SO4	B	301[B]	-	4,4,4	0.26	0	6,6,6	0.73	0
4	GOL	B	302	-	5,5,5	0.31	0	5,5,5	0.34	0
4	GOL	B	303	-	5,5,5	0.29	0	5,5,5	0.35	0
2	SO4	B	304[A]	-	4,4,4	0.68	0	6,6,6	0.40	0
2	SO4	B	304[B]	-	4,4,4	0.24	0	6,6,6	0.47	0
4	GOL	B	305[A]	-	5,5,5	0.34	0	5,5,5	1.33	1 (20%)
4	GOL	B	305[B]	-	5,5,5	0.32	0	5,5,5	0.84	0
2	SO4	C	301	-	4,4,4	0.62	0	6,6,6	0.32	0
4	GOL	C	303[A]	-	5,5,5	0.38	0	5,5,5	0.67	0
4	GOL	C	303[B]	-	5,5,5	0.40	0	5,5,5	0.52	0
4	GOL	C	304	-	5,5,5	0.43	0	5,5,5	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	C	305	-	5,5,5	0.32	0	5,5,5	0.54	0
4	GOL	C	306	-	5,5,5	0.53	0	5,5,5	1.11	0
2	SO4	D	301	-	4,4,4	0.83	0	6,6,6	0.26	0
4	GOL	D	303	-	5,5,5	0.29	0	5,5,5	0.69	0
4	GOL	D	304	-	5,5,5	0.30	0	5,5,5	0.30	0
4	GOL	D	305	-	5,5,5	0.49	0	5,5,5	0.56	0
2	SO4	E	301[A]	-	4,4,4	0.35	0	6,6,6	0.56	0
2	SO4	E	301[B]	-	4,4,4	0.27	0	6,6,6	0.28	0
4	GOL	E	302	-	5,5,5	0.20	0	5,5,5	0.46	0
2	SO4	E	303[A]	-	4,4,4	0.57	0	6,6,6	0.29	0
2	SO4	E	303[B]	-	4,4,4	0.25	0	6,6,6	0.25	0
4	GOL	E	304	-	5,5,5	0.33	0	5,5,5	0.19	0
4	GOL	E	305	-	5,5,5	0.12	0	5,5,5	0.65	0
2	SO4	F	301	-	4,4,4	0.29	0	6,6,6	0.39	0
4	GOL	F	303[A]	-	5,5,5	0.20	0	5,5,5	0.77	0
4	GOL	F	303[B]	-	5,5,5	0.27	0	5,5,5	0.48	0
4	GOL	F	304	-	5,5,5	0.40	0	5,5,5	0.43	0
4	GOL	F	305[A]	-	5,5,5	0.47	0	5,5,5	0.51	0
4	GOL	F	305[B]	-	5,5,5	0.49	0	5,5,5	0.62	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	A	301	-	-	0/0/0/0	0/0/0/0
4	GOL	A	303[A]	-	-	0/4/4/4	0/0/0/0
4	GOL	A	303[B]	-	-	0/4/4/4	0/0/0/0
4	GOL	A	304	-	-	0/4/4/4	0/0/0/0
4	GOL	A	305	-	-	0/4/4/4	0/0/0/0
2	SO4	B	301[A]	-	-	0/0/0/0	0/0/0/0
2	SO4	B	301[B]	-	-	0/0/0/0	0/0/0/0
4	GOL	B	302	-	-	0/4/4/4	0/0/0/0
4	GOL	B	303	-	-	0/4/4/4	0/0/0/0
2	SO4	B	304[A]	-	-	0/0/0/0	0/0/0/0
2	SO4	B	304[B]	-	-	0/0/0/0	0/0/0/0
4	GOL	B	305[A]	-	-	0/4/4/4	0/0/0/0
4	GOL	B	305[B]	-	-	0/4/4/4	0/0/0/0
2	SO4	C	301	-	-	0/0/0/0	0/0/0/0
4	GOL	C	303[A]	-	-	0/4/4/4	0/0/0/0
4	GOL	C	303[B]	-	-	0/4/4/4	0/0/0/0
4	GOL	C	304	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	305	-	-	0/4/4/4	0/0/0/0
4	GOL	C	306	-	-	0/4/4/4	0/0/0/0
2	SO4	D	301	-	-	0/0/0/0	0/0/0/0
4	GOL	D	303	-	-	0/4/4/4	0/0/0/0
4	GOL	D	304	-	-	0/4/4/4	0/0/0/0
4	GOL	D	305	-	-	0/4/4/4	0/0/0/0
2	SO4	E	301[A]	-	-	0/0/0/0	0/0/0/0
2	SO4	E	301[B]	-	-	0/0/0/0	0/0/0/0
4	GOL	E	302	-	-	0/4/4/4	0/0/0/0
2	SO4	E	303[A]	-	-	0/0/0/0	0/0/0/0
2	SO4	E	303[B]	-	-	0/0/0/0	0/0/0/0
4	GOL	E	304	-	-	0/4/4/4	0/0/0/0
4	GOL	E	305	-	-	0/4/4/4	0/0/0/0
2	SO4	F	301	-	-	0/0/0/0	0/0/0/0
4	GOL	F	303[A]	-	-	0/4/4/4	0/0/0/0
4	GOL	F	303[B]	-	-	0/4/4/4	0/0/0/0
4	GOL	F	304	-	-	0/4/4/4	0/0/0/0
4	GOL	F	305[A]	-	-	0/4/4/4	0/0/0/0
4	GOL	F	305[B]	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	305[A]	GOL	O3-C3-C2	2.10	120.36	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	303	GOL	1	0
2	B	304[A]	SO4	1	0
2	B	304[B]	SO4	2	0
4	B	305[B]	GOL	1	0
4	C	306	GOL	3	0
2	E	301[A]	SO4	3	0
4	E	302	GOL	1	0
2	E	303[A]	SO4	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	303[B]	SO4	1	0
4	E	305	GOL	6	0
4	F	303[A]	GOL	2	0
4	F	303[B]	GOL	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	241/252 (95%)	-0.04	10 (4%) 41 30	4, 7, 17, 20	1 (0%)
1	B	240/252 (95%)	0.09	12 (5%) 32 24	5, 9, 20, 28	1 (0%)
1	C	247/252 (98%)	-0.15	6 (2%) 62 49	4, 7, 15, 28	0
1	D	249/252 (98%)	-0.12	7 (2%) 56 44	4, 7, 16, 35	0
1	E	241/252 (95%)	0.11	17 (7%) 19 15	5, 8, 21, 28	1 (0%)
1	F	242/252 (96%)	-0.07	7 (2%) 55 43	4, 8, 18, 41	1 (0%)
All	All	1460/1512 (96%)	-0.03	59 (4%) 42 30	4, 8, 18, 41	4 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	236	VAL	7.9
1	E	236	VAL	6.2
1	F	236	VAL	6.0
1	E	234	THR	5.9
1	B	101	VAL	5.5
1	A	1	ALA	5.3
1	D	232	LYS	5.2
1	C	236	VAL	5.2
1	B	234	THR	5.2
1	E	217	ILE	5.1
1	B	102	GLY	4.9
1	A	226	PRO	4.8
1	A	101	VAL	4.6
1	E	101	VAL	4.6
1	B	236	VAL	4.6
1	B	100	ASN	4.2
1	A	225	ILE	3.9
1	F	1	ALA	3.8
1	B	98	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	233	LYS	3.8
1	F	146	VAL	3.6
1	E	1	ALA	3.5
1	B	222	GLN	3.4
1	E	235	GLU	3.3
1	E	102	GLY	3.3
1	B	1	ALA	3.3
1	E	218	VAL	3.2
1	E	100	ASN	3.2
1	E	98	HIS	3.1
1	A	4	PHE	3.1
1	C	99	VAL	3.1
1	F	101	VAL	3.1
1	D	146	VAL	3.0
1	C	231	MET	3.0
1	A	222	GLN	2.9
1	B	217[A]	ILE	2.8
1	E	2	ASP	2.8
1	F	225	ILE	2.8
1	F	226	PRO	2.8
1	B	218[A]	VAL	2.8
1	E	97	PRO	2.7
1	D	231	MET	2.6
1	E	30	ARG	2.6
1	E	251	ALA	2.5
1	D	98	HIS	2.5
1	C	98	HIS	2.5
1	B	104	VAL	2.5
1	A	102	GLY	2.4
1	C	251	ALA	2.3
1	D	235	GLU	2.3
1	E	222	GLN	2.3
1	B	235	GLU	2.2
1	A	146	VAL	2.2
1	A	251	ALA	2.2
1	F	4	PHE	2.2
1	D	97	PRO	2.1
1	A	2	ASP	2.1
1	C	97	PRO	2.1
1	E	216	VAL	2.1

## 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	C	305	6/6	0.93	0.17	11.36	7,16,19,20	0
4	GOL	A	305	6/6	0.92	0.13	8.08	5,10,12,14	14
4	GOL	B	305[A]	6/6	0.89	0.16	7.83	6,8,10,11	12
4	GOL	F	305[A]	6/6	0.92	0.12	7.37	4,7,10,12	2
4	GOL	F	303[A]	6/6	0.89	0.16	7.32	6,14,20,21	12
4	GOL	F	303[B]	6/6	0.89	0.16	7.32	4,4,6,11	12
4	GOL	B	305[B]	6/6	0.89	0.16	7.32	7,8,11,12	12
4	GOL	C	303[A]	6/6	0.95	0.11	6.58	3,7,8,10	2
4	GOL	C	303[B]	6/6	0.95	0.11	5.82	3,5,7,8	2
4	GOL	D	304	6/6	0.95	0.13	3.90	6,12,14,16	0
4	GOL	A	303[A]	6/6	0.94	0.10	3.79	3,8,10,10	1
4	GOL	A	304	6/6	0.95	0.10	3.68	7,8,10,11	0
4	GOL	C	304	6/6	0.95	0.11	3.32	7,9,10,11	0
4	GOL	F	305[B]	6/6	0.92	0.12	2.98	4,5,9,10	2
4	GOL	C	306	6/6	0.82	0.23	2.79	19,20,22,24	0
4	GOL	A	303[B]	6/6	0.94	0.10	2.63	3,8,10,10	1
4	GOL	D	305	6/6	0.97	0.10	2.57	6,8,9,10	0
4	GOL	E	305	6/6	0.95	0.10	2.17	5,6,8,10	12
4	GOL	F	304	6/6	0.95	0.09	1.96	6,9,10,10	0
4	GOL	D	303	6/6	0.97	0.10	1.92	3,6,7,8	0
4	GOL	E	304	6/6	0.96	0.08	1.00	7,8,10,10	0
4	GOL	E	302	6/6	0.93	0.10	0.57	5,10,12,12	12
3	CL	F	302	1/1	1.00	0.08	0.50	9,9,9,9	0
2	SO4	B	304[A]	5/5	0.95	0.11	0.50	9,9,11,11	5
2	SO4	E	303[A]	5/5	0.96	0.10	0.29	6,9,9,11	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	B	302	6/6	0.98	0.06	0.11	7,7,10,10	0
2	SO4	B	304[B]	5/5	0.95	0.11	0.09	9,10,10,11	5
2	SO4	E	303[B]	5/5	0.96	0.10	0.04	11,12,15,16	5
4	GOL	B	303	6/6	0.95	0.08	-0.23	5,9,11,12	12
3	CL	A	302	1/1	1.00	0.07	-0.47	10,10,10,10	0
2	SO4	D	301	5/5	0.99	0.05	-0.50	6,6,6,7	0
2	SO4	A	301	5/5	0.99	0.05	-1.07	7,7,8,9	0
2	SO4	C	301	5/5	0.99	0.04	-1.43	6,6,6,7	0
2	SO4	F	301	5/5	0.99	0.04	-1.53	7,7,7,8	0
3	CL	D	302	1/1	0.99	0.04	-2.16	7,7,7,7	0
3	CL	C	302	1/1	1.00	0.03	-3.08	7,7,7,7	0
2	SO4	E	301[A]	5/5	0.98	0.07	-	11,12,14,16	5
2	SO4	E	301[B]	5/5	0.98	0.07	-	8,11,11,12	5
2	SO4	B	301[B]	5/5	0.95	0.10	-	6,7,8,9	5
2	SO4	B	301[A]	5/5	0.95	0.10	-	11,13,14,15	5

## 6.5 Other polymers ⓘ

There are no such residues in this entry.