



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 01:41 am BST

PDB ID : 6EYP  
Title : X-ray structure of the unliganded uridine phosphorylase from *Vibrio cholerae* at 1.22Å  
Authors : Prokofev, I.I.; Balaev, V.V.; Gabdoulkhakov, A.G.; Betzel, C.; Lashkov, A.A.  
Deposited on : 2017-11-13  
Resolution : 1.22 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

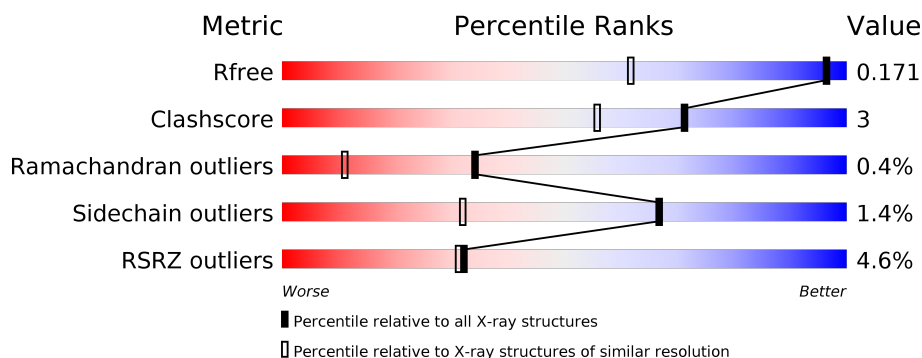
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.22 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	1232 (1.24-1.20)
Clashscore	141614	1294 (1.24-1.20)
Ramachandran outliers	138981	1251 (1.24-1.20)
Sidechain outliers	138945	1250 (1.24-1.20)
RSRZ outliers	127900	1209 (1.24-1.20)

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	253	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>..</div> </div> </div>
1	B	253	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>.</div> </div> </div>
1	C	253	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>8%</div> <div>.</div> </div> </div>
1	D	253	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>.</div> </div> </div>
1	E	253	<div> <div>5%</div> <div> <div></div> <div>92%</div> <div>7%</div> <div>..</div> </div> </div>
1	F	253	<div> <div>6%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>

## 2 Entry composition [i](#)

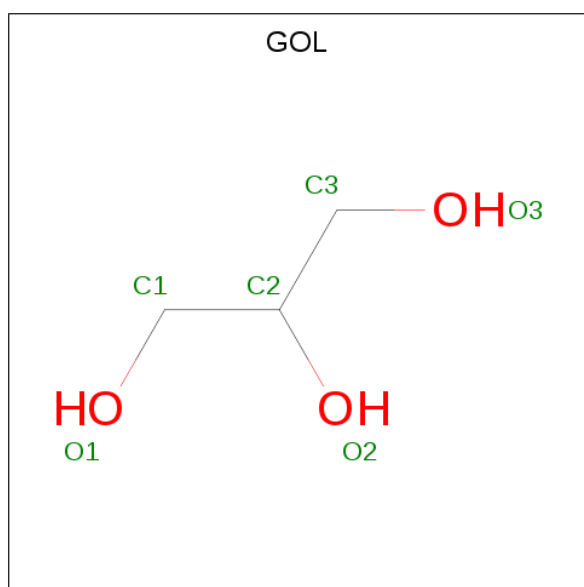
There are 5 unique types of molecules in this entry. The entry contains 14636 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	251	Total	C	N	O	S	0	24	0
			2073	1293	368	396	16			
1	B	252	Total	C	N	O	S	0	22	0
			2073	1290	369	397	17			
1	C	251	Total	C	N	O	S	0	25	0
			2085	1299	370	398	18			
1	D	251	Total	C	N	O	S	0	28	0
			2141	1334	383	405	19			
1	E	251	Total	C	N	O	S	0	29	0
			2104	1315	372	399	18			
1	F	252	Total	C	N	O	S	0	32	0
			2143	1336	385	404	18			

- Molecule 2 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
2	A	1	Total C O 12 6 6	0	1
2	B	1	Total C O 12 6 6	0	1
2	C	1	Total C O 12 6 6	0	1
2	D	1	Total C O 12 6 6	0	1
2	D	1	Total C O 18 9 9	0	1
2	E	1	Total C O 12 6 6	0	1
2	F	1	Total C O 12 6 6	0	1
2	F	1	Total C O 12 6 6	0	1

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0
3	E	1	Total Na 1 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Mg 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	323	Total O 328 328	0	7
5	B	303	Total O 307 307	0	5
5	C	321	Total O 326 326	0	5

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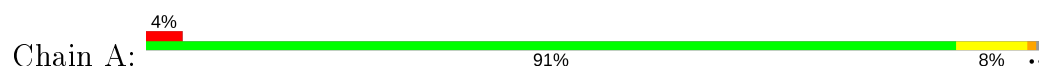
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	349	Total 356	O 356	0	6
5	E	295	Total 298	O 298	0	3
5	F	293	Total 296	O 296	0	4

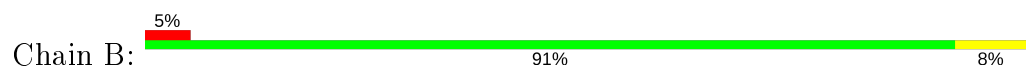
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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



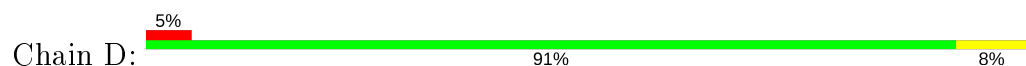
- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase



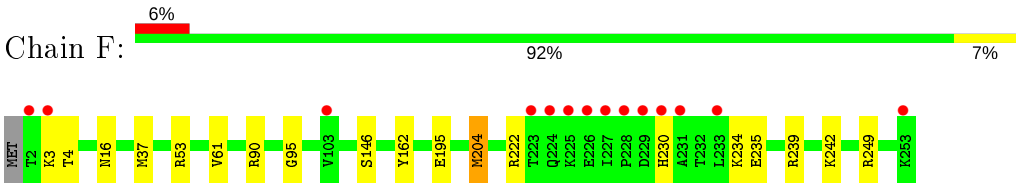
- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.94Å 92.94Å 140.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.48 – 1.22 46.47 – 1.22	Depositor EDS
% Data completeness (in resolution range)	99.7 (26.48-1.22) 99.7 (46.47-1.22)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.05 (at 1.22Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.138 , 0.170 0.139 , 0.171	Depositor DCC
$R_{free}$ test set	4195 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	9.7	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 66.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.000 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	14636	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4038e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, MG, NA

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	0.62	0/2119	0.83	6/2858 (0.2%)
1	B	0.67	0/2108	0.79	1/2849 (0.0%)
1	C	0.66	0/2119	0.82	2/2861 (0.1%)
1	D	0.65	0/2178	0.84	5/2934 (0.2%)
1	E	0.64	0/2157	0.83	4/2910 (0.1%)
1	F	0.64	0/2193	0.79	2/2957 (0.1%)
All	All	0.64	0/12874	0.82	20/17369 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ARG	NE-CZ-NH2	-8.17	116.21	120.30
1	C	89	LEU	CB-CG-CD1	6.92	122.77	111.00
1	E	204[A]	MET	CG-SD-CE	-6.76	89.38	100.20
1	E	204[B]	MET	CG-SD-CE	-6.76	89.38	100.20
1	C	178	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	222	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	222	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	A	222	ARG	CG-CD-NE	6.26	124.94	111.80
1	A	86	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	F	204[A]	MET	CG-SD-CE	-5.70	91.08	100.20
1	F	204[B]	MET	CG-SD-CE	-5.70	91.08	100.20
1	D	89	LEU	CB-CG-CD1	5.44	120.25	111.00
1	E	53[A]	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	E	53[B]	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	D	252[A]	LEU	C-N-CA	5.27	134.88	121.70
1	D	252[B]	LEU	C-N-CA	5.27	134.88	121.70
1	B	188	ASP	CB-CG-OD1	5.21	122.98	118.30
1	A	89	LEU	CB-CG-CD1	5.20	119.84	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	253[A]	LYS	N-CA-CB	5.05	119.69	110.60
1	D	253[B]	LYS	N-CA-CB	5.05	119.69	110.60

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	2073	0	2088	20	0
1	B	2073	0	2070	14	0
1	C	2085	0	2089	13	0
1	D	2141	0	2155	15	0
1	E	2104	0	2129	16	0
1	F	2143	0	2164	14	0
2	A	12	0	16	0	0
2	B	12	0	16	0	0
2	C	12	0	16	0	0
2	D	30	0	40	2	0
2	E	12	0	16	0	0
2	F	24	0	32	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	C	1	0	0	0	0
5	A	328	0	0	6	0
5	B	307	0	0	6	0
5	C	326	0	0	4	0
5	D	356	0	0	6	0
5	E	298	0	0	6	0
5	F	296	0	0	8	0
All	All	14636	0	12831	89	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 3.

All (89) 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)
2:D:302[B]:GOL:H11	1:E:126[B]:GLU:OE2	1.59	1.02
1:B:214[A]:CYS:SG	5:B:535:HOH:O	2.21	0.97
1:B:177[A]:ARG:NH2	5:B:401[A]:HOH:O	1.89	0.83
2:D:302[B]:GOL:C1	1:E:126[B]:GLU:OE2	2.27	0.83
1:A:15:LEU:HG	1:A:62[B]:VAL:HG11	1.59	0.83
1:E:95[A]:GLY:O	5:E:401:HOH:O	1.96	0.83
1:E:106[A]:MET:SD	5:E:608:HOH:O	2.40	0.80
1:D:239[B]:ARG:HH21	1:D:239[B]:ARG:HG3	1.47	0.79
1:A:16[B]:ASN:HB2	1:A:53:ARG:HD2	1.65	0.76
1:A:240[A]:SER:OG	5:A:401:HOH:O	2.06	0.73
1:D:95[B]:GLY:O	5:D:401:HOH:O	2.08	0.72
1:B:2:THR:O	5:B:402:HOH:O	2.09	0.69
1:C:95:GLY:O	5:C:401:HOH:O	2.10	0.69
1:F:95[B]:GLY:O	5:F:401:HOH:O	2.10	0.68
1:A:225:LYS:NZ	5:A:402:HOH:O	2.18	0.67
1:B:29[B]:ARG:HD3	5:B:588:HOH:O	1.95	0.66
1:F:3:LYS:O	5:F:402:HOH:O	2.14	0.64
1:E:53[B]:ARG:NH1	5:E:404:HOH:O	2.29	0.63
1:D:225:LYS:NZ	5:D:405:HOH:O	2.32	0.63
1:F:16[A]:ASN:HB2	1:F:53[A]:ARG:HD2	1.81	0.62
1:A:16[A]:ASN:HB3	1:A:53:ARG:HD2	1.82	0.62
1:B:16[A]:ASN:HB2	1:B:53[A]:ARG:HD2	1.82	0.61
1:C:53[B]:ARG:NH2	5:C:402:HOH:O	2.33	0.61
1:C:16[A]:ASN:HB2	1:C:53[A]:ARG:HD2	1.82	0.60
1:D:53[B]:ARG:NH2	5:D:406:HOH:O	2.36	0.59
1:B:232:THR:O	1:B:236:THR:N	2.27	0.58
1:B:12[A]:GLU:HG3	5:B:546:HOH:O	2.04	0.57
1:F:242[B]:LYS:HE3	5:F:516:HOH:O	2.04	0.57
1:C:238:ALA:O	1:C:242[A]:LYS:HG2	2.05	0.57
1:E:224:GLN:HB3	1:E:226:GLU:OE1	2.05	0.56
1:F:234:LYS:HE2	5:F:438:HOH:O	2.05	0.56
1:B:214[A]:CYS:SG	5:B:564:HOH:O	2.58	0.56
1:B:26:ASP:HB3	1:B:29[A]:ARG:HG3	1.85	0.56
1:A:226:GLU:H	1:A:226:GLU:CD	2.08	0.55
1:A:224:GLN:HB3	1:A:226:GLU:OE2	2.06	0.55
1:A:106[B]:MET:CE	1:A:239[B]:ARG:HD2	2.37	0.54
1:C:246[A]:GLU:OE1	1:C:249[A]:ARG:NH1	2.35	0.54
1:D:242[B]:LYS:N	1:D:242[B]:LYS:HD3	2.22	0.54
1:E:174[B]:ARG:NH1	5:E:402:HOH:O	2.04	0.53
1:B:57:ASP:OD2	1:B:249[B]:ARG:HG3	2.09	0.52
1:F:146:SER:O	1:F:239[B]:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:ASP:OD2	1:E:249[B]:ARG:HG3	2.11	0.51
1:A:185[A]:GLU:HG3	5:A:529:HOH:O	2.09	0.50
1:A:174[A]:ARG:HD2	5:C:422:HOH:O	2.11	0.50
1:C:174[A]:ARG:HD2	5:E:552:HOH:O	2.12	0.50
5:A:529:HOH:O	1:E:174[A]:ARG:HD2	2.12	0.49
1:F:249[B]:ARG:NH2	5:F:406:HOH:O	2.42	0.49
1:F:146:SER:O	1:F:239[A]:ARG:NH2	2.47	0.48
1:B:74:SER:HA	1:B:204[A]:MET:HE1	1.95	0.48
1:C:57:ASP:OD2	1:C:249[B]:ARG:HG3	2.14	0.48
1:D:122:PHE:CE1	1:D:204[A]:MET:HG3	2.48	0.48
1:D:239[B]:ARG:NH2	1:D:239[B]:ARG:HG3	2.25	0.47
1:D:253[A]:LYS:HE2	1:D:253[A]:LYS:HB2	1.65	0.47
1:A:106[B]:MET:HE1	1:A:239[B]:ARG:HD2	1.95	0.47
1:A:204[B]:MET:HB3	1:A:204[B]:MET:HE3	1.80	0.46
1:D:239[A]:ARG:HD2	5:D:513:HOH:O	2.16	0.46
1:F:235[A]:GLU:HG3	5:F:438:HOH:O	2.15	0.46
1:F:242[B]:LYS:HG3	5:F:516:HOH:O	2.15	0.46
1:E:21:ALA:HB2	1:E:62[B]:VAL:HG13	1.98	0.45
1:B:157:SER:HB3	1:B:199:ALA:HB2	1.97	0.45
1:A:106[A]:MET:SD	1:A:239[A]:ARG:HD2	2.57	0.45
1:A:46:HIS:HD2	5:A:418:HOH:O	2.00	0.45
1:A:177:ARG:NE	1:C:185[A]:GLU:OE1	2.49	0.44
1:E:157:SER:HB3	1:E:199:ALA:HB2	1.99	0.44
1:F:146:SER:HB2	1:F:239[B]:ARG:HD2	2.00	0.43
1:C:188:ASP:HB2	5:C:422:HOH:O	2.18	0.43
1:A:217:GLY:HA3	5:A:401:HOH:O	2.19	0.43
1:D:157:SER:HB3	1:D:199:ALA:HB2	2.00	0.43
1:E:46[B]:HIS:HE1	5:E:491:HOH:O	2.02	0.43
1:E:242[A]:LYS:HB2	1:E:242[A]:LYS:HE3	1.76	0.43
1:D:21:ALA:HA	1:D:62[B]:VAL:O	2.18	0.43
1:D:37:MET:SD	1:D:61[B]:VAL:HG21	2.58	0.43
1:F:222[B]:ARG:HB2	5:F:410[B]:HOH:O	2.19	0.43
1:A:174[B]:ARG:HD3	1:C:188:ASP:HB3	2.01	0.42
1:F:37:MET:SD	1:F:61[B]:VAL:HG21	2.58	0.42
1:B:21:ALA:HA	1:B:62[B]:VAL:O	2.20	0.42
1:D:46[A]:HIS:ND1	5:D:407:HOH:O	2.36	0.42
1:D:204[A]:MET:HB3	1:D:204[A]:MET:HE3	1.81	0.42
1:F:204[B]:MET:HE3	1:F:204[B]:MET:HB3	1.88	0.42
1:A:174[B]:ARG:CD	1:C:188:ASP:HB3	2.50	0.42
1:A:122:PHE:CE1	1:A:204[B]:MET:HG3	2.55	0.42
1:B:239[B]:ARG:HH21	1:B:239[B]:ARG:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204[B]:MET:HE3	1:E:204[B]:MET:HB3	1.87	0.41
1:C:157:SER:HB3	1:C:199:ALA:HB2	2.02	0.40
1:D:234:LYS:NZ	5:D:417:HOH:O	2.53	0.40
1:A:106[B]:MET:HE3	1:A:239[B]:ARG:HD2	2.00	0.40
1:C:74:SER:HA	1:C:204[A]:MET:HE1	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	273/253 (108%)	268 (98%)	4 (2%)	1 (0%)	34	11
1	B	272/253 (108%)	268 (98%)	3 (1%)	1 (0%)	34	11
1	C	274/253 (108%)	271 (99%)	2 (1%)	1 (0%)	34	11
1	D	279/253 (110%)	275 (99%)	3 (1%)	1 (0%)	34	11
1	E	278/253 (110%)	273 (98%)	4 (1%)	1 (0%)	34	11
1	F	282/253 (112%)	278 (99%)	3 (1%)	1 (0%)	34	11
All	All	1658/1518 (109%)	1633 (98%)	19 (1%)	6 (0%)	34	11

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	TYR
1	B	162	TYR
1	C	162	TYR
1	D	162	TYR
1	E	162	TYR
1	F	162	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	224/203 (110%)	222 (99%)	2 (1%)	78	50
1	B	224/203 (110%)	219 (98%)	5 (2%)	52	14
1	C	225/203 (111%)	224 (100%)	1 (0%)	91	76
1	D	231/203 (114%)	223 (96%)	8 (4%)	36	5
1	E	229/203 (113%)	226 (99%)	3 (1%)	69	34
1	F	232/203 (114%)	227 (98%)	5 (2%)	52	14
All	All	1365/1218 (112%)	1341 (98%)	24 (2%)	67	22

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	GLU
1	A	222	ARG
1	B	29[A]	ARG
1	B	29[B]	ARG
1	B	195	GLU
1	B	239[A]	ARG
1	B	239[B]	ARG
1	C	195	GLU
1	D	3	LYS
1	D	90[A]	ARG
1	D	90[B]	ARG
1	D	195	GLU
1	D	204[A]	MET
1	D	204[B]	MET
1	D	253[A]	LYS
1	D	253[B]	LYS
1	E	90[A]	ARG
1	E	90[B]	ARG
1	E	195	GLU
1	F	4	THR
1	F	90[A]	ARG
1	F	90[B]	ARG

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Mol	Chain	Res	Type
1	F	195	GLU
1	F	230	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	144	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 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	GOL	D	302[B]	-	5,5,5	0.34	0	5,5,5	0.94	0
2	GOL	D	301[B]	-	5,5,5	0.57	0	5,5,5	0.53	0
2	GOL	A	301[B]	-	5,5,5	0.53	0	5,5,5	0.42	0
2	GOL	D	302[C]	-	5,5,5	0.50	0	5,5,5	0.40	0
2	GOL	D	301[A]	-	5,5,5	0.45	0	5,5,5	0.50	0
2	GOL	B	301[A]	-	5,5,5	0.34	0	5,5,5	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	E	301[A]	-	5,5,5	0.34	0	5,5,5	0.69	0
2	GOL	C	301[A]	-	5,5,5	0.37	0	5,5,5	0.75	0
2	GOL	A	301[A]	-	5,5,5	0.39	0	5,5,5	0.71	0
2	GOL	C	301[B]	-	5,5,5	0.50	0	5,5,5	0.55	0
2	GOL	F	301[A]	-	5,5,5	0.35	0	5,5,5	0.64	0
2	GOL	B	301[B]	-	5,5,5	0.47	0	5,5,5	0.75	0
2	GOL	F	301[B]	-	5,5,5	0.29	0	5,5,5	1.14	1 (20%)
2	GOL	F	302[B]	-	5,5,5	0.53	0	5,5,5	0.81	0
2	GOL	D	302[A]	-	5,5,5	0.42	0	5,5,5	0.52	0
2	GOL	E	301[B]	-	5,5,5	0.49	0	5,5,5	0.42	0
2	GOL	F	302[A]	-	5,5,5	0.50	0	5,5,5	0.44	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	GOL	D	302[B]	-	-	0/4/4/4	-
2	GOL	D	301[B]	-	-	0/4/4/4	-
2	GOL	A	301[B]	-	-	1/4/4/4	-
2	GOL	D	302[C]	-	-	0/4/4/4	-
2	GOL	D	301[A]	-	-	2/4/4/4	-
2	GOL	B	301[A]	-	-	2/4/4/4	-
2	GOL	E	301[A]	-	-	2/4/4/4	-
2	GOL	C	301[A]	-	-	2/4/4/4	-
2	GOL	A	301[A]	-	-	2/4/4/4	-
2	GOL	C	301[B]	-	-	0/4/4/4	-
2	GOL	F	301[A]	-	-	1/4/4/4	-
2	GOL	B	301[B]	-	-	1/4/4/4	-
2	GOL	F	301[B]	-	-	0/4/4/4	-
2	GOL	F	302[B]	-	-	4/4/4/4	-
2	GOL	D	302[A]	-	-	4/4/4/4	-
2	GOL	E	301[B]	-	-	1/4/4/4	-
2	GOL	F	302[A]	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	F	301[B]	GOL	C3-C2-C1	-2.12	103.45	111.70

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301[A]	GOL	O1-C1-C2-C3
2	B	301[A]	GOL	O1-C1-C2-C3
2	E	301[A]	GOL	O1-C1-C2-C3
2	A	301[A]	GOL	C1-C2-C3-O3
2	F	302[B]	GOL	O1-C1-C2-C3
2	D	302[A]	GOL	C1-C2-C3-O3
2	F	302[B]	GOL	O1-C1-C2-O2
2	F	301[A]	GOL	O1-C1-C2-C3
2	D	302[A]	GOL	O1-C1-C2-C3
2	B	301[A]	GOL	O1-C1-C2-O2
2	A	301[A]	GOL	O2-C2-C3-O3
2	D	302[A]	GOL	O1-C1-C2-O2
2	D	302[A]	GOL	O2-C2-C3-O3
2	D	301[A]	GOL	O1-C1-C2-O2
2	C	301[A]	GOL	O2-C2-C3-O3
2	E	301[A]	GOL	O1-C1-C2-O2
2	F	302[B]	GOL	O2-C2-C3-O3
2	B	301[B]	GOL	C1-C2-C3-O3
2	C	301[A]	GOL	C1-C2-C3-O3
2	F	302[B]	GOL	C1-C2-C3-O3
2	A	301[B]	GOL	O1-C1-C2-C3
2	E	301[B]	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	302[B]	GOL	2	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	251/253 (99%)	0.22	10 (3%)	38 37	8, 13, 25, 54	0
1	B	252/253 (99%)	0.25	12 (4%)	30 29	7, 12, 26, 75	1 (0%)
1	C	251/253 (99%)	0.10	9 (3%)	42 40	7, 12, 24, 42	1 (0%)
1	D	251/253 (99%)	0.15	12 (4%)	30 29	7, 12, 24, 39	0
1	E	251/253 (99%)	0.20	12 (4%)	30 29	8, 13, 31, 56	3 (1%)
1	F	252/253 (99%)	0.31	14 (5%)	24 22	9, 15, 34, 66	1 (0%)
All	All	1508/1518 (99%)	0.21	69 (4%)	32 31	7, 13, 28, 75	6 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	ILE	12.1
1	B	231	ALA	9.6
1	F	2	THR	9.1
1	C	227	ILE	8.9
1	B	2	THR	8.6
1	E	227	ILE	8.5
1	B	230	HIS	8.3
1	B	232	THR	7.4
1	F	227	ILE	7.2
1	F	228	PRO	7.0
1	E	226	GLU	6.8
1	C	230	HIS	5.5
1	F	233	LEU	5.3
1	B	233	LEU	5.3
1	E	225[A]	LYS	5.3
1	D	225	LYS	5.2
1	A	226	GLU	5.1
1	A	225	LYS	5.0
1	C	4	THR	5.0

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Mol	Chain	Res	Type	RSRZ
1	F	226[A]	GLU	4.8
1	E	4[A]	THR	4.6
1	F	230	HIS	4.5
1	C	253	LYS	4.3
1	F	225[A]	LYS	4.2
1	B	229	ASP	4.2
1	F	229	ASP	4.2
1	C	228	PRO	4.1
1	D	229	ASP	4.1
1	D	230	HIS	4.0
1	C	231	ALA	4.0
1	B	3	LYS	3.9
1	A	232	THR	3.9
1	E	233	LEU	3.8
1	B	227	ILE	3.7
1	A	228	PRO	3.7
1	D	226[A]	GLU	3.6
1	A	231	ALA	3.5
1	A	230	HIS	3.5
1	E	3	LYS	3.4
1	D	228	PRO	3.4
1	F	231	ALA	3.4
1	C	3	LYS	3.3
1	B	228	PRO	3.3
1	D	224	GLN	3.3
1	F	3	LYS	3.1
1	D	227	ILE	3.1
1	B	234	LYS	3.1
1	D	231	ALA	2.9
1	E	231	ALA	2.9
1	E	232	THR	2.8
1	E	253	LYS	2.8
1	F	224	GLN	2.8
1	A	3	LYS	2.7
1	D	239[A]	ARG	2.6
1	D	3	LYS	2.6
1	A	233	LEU	2.6
1	B	236	THR	2.5
1	B	253	LYS	2.5
1	D	253[A]	LYS	2.5
1	D	252[A]	LEU	2.4
1	E	234	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	229	ASP	2.3
1	E	229	ASP	2.3
1	F	103	VAL	2.2
1	C	225	LYS	2.2
1	F	253	LYS	2.1
1	F	223	THR	2.1
1	E	228	PRO	2.1
1	C	16[A]	ASN	2.0

## 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
2	GOL	D	302[B]	6/6	0.71	0.24	11,18,20,21	6
2	GOL	D	302[C]	6/6	0.71	0.24	11,12,13,15	6
2	GOL	D	302[A]	6/6	0.71	0.24	21,23,24,24	6
2	GOL	B	301[B]	6/6	0.88	0.12	9,13,18,22	6
2	GOL	F	302[B]	6/6	0.88	0.14	25,27,29,31	6
2	GOL	B	301[A]	6/6	0.88	0.12	11,14,18,20	6
2	GOL	F	302[A]	6/6	0.88	0.14	12,14,15,16	6
2	GOL	C	301[A]	6/6	0.89	0.14	10,14,16,16	6
2	GOL	C	301[B]	6/6	0.89	0.14	10,13,16,19	6
2	GOL	F	301[A]	6/6	0.90	0.15	14,19,20,22	6
2	GOL	A	301[B]	6/6	0.90	0.13	11,12,13,14	6
2	GOL	F	301[B]	6/6	0.90	0.15	11,14,17,20	6
2	GOL	D	301[B]	6/6	0.90	0.14	10,17,20,21	6
2	GOL	A	301[A]	6/6	0.90	0.13	10,19,21,23	6
2	GOL	D	301[A]	6/6	0.90	0.14	14,16,16,16	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	E	301[B]	6/6	0.91	0.12	11,16,20,22	6
2	GOL	E	301[A]	6/6	0.91	0.12	15,19,19,20	6
3	NA	C	302	1/1	1.00	0.10	9,9,9,9	1
3	NA	A	302	1/1	1.00	0.12	9,9,9,9	1
4	MG	C	303	1/1	1.00	0.07	11,11,11,11	1
3	NA	E	302	1/1	1.00	0.05	14,14,14,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.