



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:49 PM UTC

PDB ID : 5Z3M / pdb_00005z3m
Title : Crystal structure of Low Molecular Weight Phosphotyrosine phosphatase (VcLMWPTP-2) from *Vibrio cholerae*O395
Authors : Chatterjee, S.; Nath, S.; Sen, U.
Deposited on : 2018-01-08
Resolution : 2.60 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

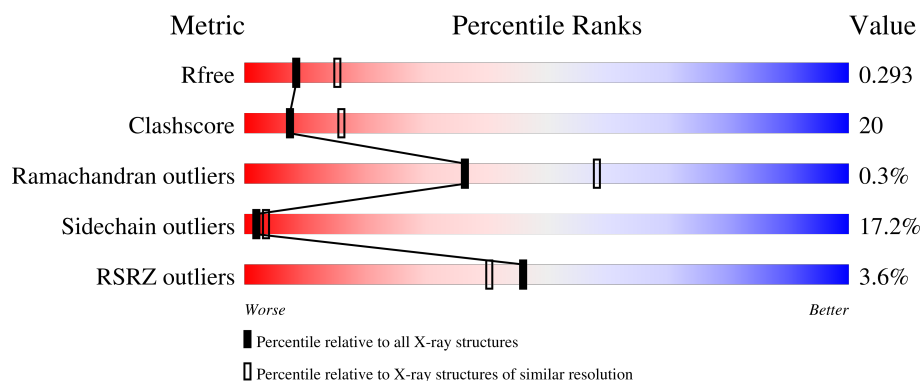
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 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 $\leq 5\%$. 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	166	51% 39% 8%
1	B	166	5% 42% 37% 11% 8%

2 Entry composition [i](#)

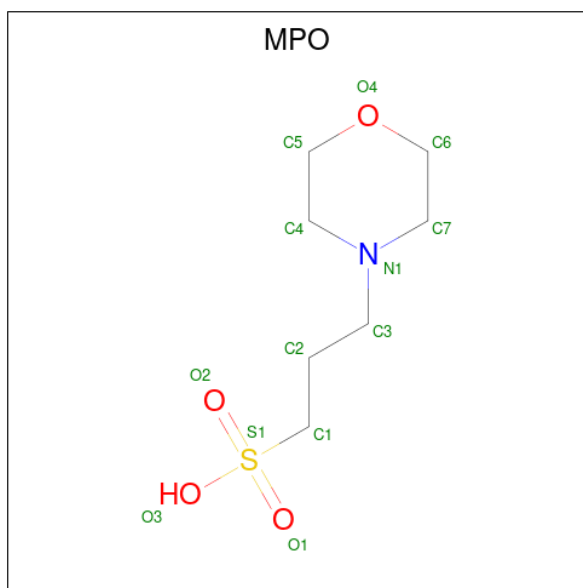
There are 5 unique types of molecules in this entry. The entry contains 2926 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphotyrosine protein phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1216	764	217	228	7			
1	B	152	Total	C	N	O	S	0	0	0
			1208	758	216	227	7			

- Molecule 2 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula: $C_7H_{15}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

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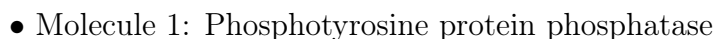
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	148	Total	O	0	0
			148	148		
5	B	108	Total	O	0	0
			108	108		

- Molecule 1: Phosphotyrosine protein phosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.91Å 51.87Å 83.90Å 90.00° 103.62° 90.00°	Depositor
Resolution (Å)	19.40 – 2.60 19.40 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.40-2.60) 98.5 (19.40-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.252 , 0.288 0.260 , 0.293	Depositor DCC
R_{free} test set	1035 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	1.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 74.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	2926	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 10.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MPO, 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	0.39	0/1236	0.82	0/1670
1	B	0.40	0/1228	0.87	3/1659 (0.2%)
All	All	0.39	0/2464	0.84	3/3329 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	VAL	N-CA-C	6.82	117.66	108.11
1	B	18	ARG	N-CA-C	6.00	117.62	111.14
1	B	91	ARG	N-CA-C	-5.20	106.79	113.23

There are no chirality outliers.

There are no planarity outliers.

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	1216	0	1228	48	0
1	B	1208	0	1217	60	0
2	A	13	0	15	3	0
2	B	13	0	15	1	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	132	0	176	7	0
4	B	78	0	104	3	0
5	A	148	0	0	5	0
5	B	108	0	0	2	0
All	All	2926	0	2755	110	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 20.

All (110) 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:B:15:ASN:ND2	1:B:41:SER:OG	1.98	0.95
1:A:15:ASN:ND2	1:A:41:SER:OG	2.00	0.95
1:B:12:CYS:HG	1:B:19:SER:HG	0.87	0.85
1:A:12:CYS:SG	1:A:19:SER:OG	2.41	0.79
1:B:111:LEU:O	1:B:114:SER:OG	2.02	0.78
1:B:15:ASN:HD21	1:B:41:SER:HG	1.30	0.77
1:A:10:VAL:HG13	1:A:89:MET:HE3	1.68	0.75
1:A:15:ASN:HD21	1:A:41:SER:HG	1.35	0.75
4:B:209:GOL:O3	5:B:301:HOH:O	2.05	0.74
1:A:18:ARG:HH12	1:A:93:ASN:HD21	1.38	0.72
1:B:28:ASP:OD1	1:B:32:GLN:NE2	2.24	0.71
1:B:126:PRO:HG3	1:B:137:THR:HG21	1.71	0.71
1:B:7:SER:HB3	1:B:83:HIS:HA	1.73	0.70
1:A:10:VAL:HG12	1:A:19:SER:HB3	1.76	0.67
4:A:223:GOL:O2	4:A:224:GOL:O1	2.13	0.66
1:A:112:PHE:HE2	1:A:141:ILE:HA	1.60	0.66
1:B:106:LYS:NZ	5:B:308:HOH:O	2.30	0.64
1:A:74:GLN:NE2	1:A:75:VAL:O	2.29	0.64
1:A:129:ARG:NH1	3:A:202:SO4:O1	2.30	0.63
1:B:145:ALA:HA	1:B:148:LEU:HD12	1.79	0.63
1:A:121:LYS:NZ	5:A:303:HOH:O	2.31	0.62
1:A:21:MET:HG2	1:A:60:LEU:HD11	1.82	0.62
1:B:40:ARG:HG3	1:B:83:HIS:HE1	1.66	0.61
1:A:73:GLN:NE2	5:A:307:HOH:O	2.25	0.61
1:A:119:GLN:NE2	5:A:314:HOH:O	2.33	0.61
1:B:12:CYS:HA	1:B:93:ASN:ND2	2.15	0.61
1:A:80:PHE:O	1:A:108:LYS:NZ	2.34	0.60
1:B:23:GLU:OE2	1:B:27:ARG:NH2	2.35	0.60
1:B:43:GLY:O	1:B:75:VAL:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:LEU:HB3	1:B:65:TYR:HB2	1.84	0.59
1:B:40:ARG:HG3	1:B:83:HIS:CE1	2.37	0.59
1:B:90:ASP:H	1:B:93:ASN:ND2	2.02	0.58
1:A:7:SER:OG	1:A:83:HIS:ND1	2.32	0.58
1:A:19:SER:HB2	1:A:41:SER:OG	2.03	0.58
4:A:204:GOL:O2	4:A:205:GOL:O2	2.20	0.57
1:B:80:PHE:O	1:B:108:LYS:NZ	2.36	0.57
1:B:18:ARG:HB3	1:B:89:MET:SD	2.45	0.56
1:A:88:ALA:HB3	1:A:111:LEU:HD23	1.88	0.55
4:A:207:GOL:H12	4:A:208:GOL:H2	1.88	0.55
1:A:13:THR:HG23	4:A:213:GOL:H32	1.88	0.54
1:A:15:ASN:ND2	1:A:41:SER:HG	1.97	0.54
1:B:44:THR:HA	1:B:75:VAL:HG12	1.89	0.54
1:B:154:GLU:O	1:B:156:GLY:N	2.41	0.54
1:A:14:GLY:HA3	2:A:201:MPO:H61	1.90	0.53
1:B:9:LEU:HB2	1:B:83:HIS:CD2	2.44	0.52
1:A:52:PRO:HB2	1:A:57:LEU:HD21	1.90	0.52
1:A:120:GLU:O	5:A:301:HOH:O	2.19	0.52
1:B:30:ILE:HD12	1:B:37:ILE:HD12	1.91	0.52
1:B:15:ASN:HB3	1:B:72:VAL:HG23	1.91	0.52
1:B:116:ALA:HB1	1:B:118:ARG:HG3	1.92	0.52
1:B:25:ILE:HD12	1:B:141:ILE:HG22	1.91	0.51
1:B:40:ARG:NH2	4:B:210:GOL:O1	2.44	0.51
1:B:49:LYS:O	4:B:204:GOL:H12	2.11	0.51
1:B:12:CYS:HB2	1:B:18:ARG:HH21	1.75	0.50
1:B:15:ASN:HD22	1:B:20:PRO:HD3	1.75	0.50
1:A:12:CYS:HA	1:A:93:ASN:ND2	2.26	0.50
1:A:32:GLN:O	4:A:207:GOL:H11	2.11	0.49
1:B:97:LEU:HB3	1:B:109:LEU:HD21	1.93	0.49
1:A:18:ARG:HG3	2:A:201:MPO:O2	2.12	0.49
1:B:18:ARG:NH1	1:B:125:ASP:OD1	2.46	0.48
1:B:68:MET:O	1:B:68:MET:HG3	2.14	0.48
1:B:17:CYS:O	1:B:21:MET:HG3	2.14	0.48
1:B:15:ASN:ND2	1:B:41:SER:HG	1.97	0.48
1:B:91:ARG:HG2	1:B:122:GLU:CD	2.38	0.48
1:A:18:ARG:HE	1:A:126:PRO:HD2	1.78	0.47
1:A:89:MET:HE2	1:A:112:PHE:HB2	1.95	0.47
1:B:15:ASN:HB2	1:B:43:GLY:N	2.28	0.47
1:A:51:MET:HE3	1:B:57:LEU:HD22	1.95	0.47
1:A:94:LEU:HD22	1:A:111:LEU:HG	1.96	0.47
1:A:54:ASP:O	1:A:58:GLN:HG3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LYS:NZ	1:B:146:VAL:HG22	2.29	0.46
1:B:104:GLU:H	1:B:104:GLU:HG3	1.43	0.46
1:A:58:GLN:O	1:A:61:GLN:HG2	2.16	0.46
1:A:65:TYR:O	1:A:67:PRO:HD3	2.16	0.46
1:A:15:ASN:HB2	1:A:43:GLY:N	2.29	0.46
1:A:17:CYS:O	1:A:21:MET:HG3	2.16	0.46
1:A:55:LYS:HA	1:A:58:GLN:NE2	2.31	0.45
1:B:74:GLN:CD	1:B:74:GLN:N	2.74	0.45
1:B:132:GLU:HA	1:B:135:GLN:HE21	1.80	0.45
1:A:152:TRP:HA	1:A:155:GLN:NE2	2.31	0.45
1:B:138:ALA:O	1:B:142:GLU:N	2.41	0.45
1:B:17:CYS:HB2	2:B:201:MPO:O3	2.17	0.45
1:A:28:ASP:O	1:A:32:GLN:HG2	2.16	0.45
1:A:57:LEU:HG	1:B:51:MET:HE3	1.98	0.45
1:B:28:ASP:O	1:B:32:GLN:HG3	2.17	0.45
1:B:74:GLN:CD	1:B:74:GLN:H	2.25	0.44
1:A:13:THR:HB	2:A:201:MPO:H22	1.99	0.44
1:B:90:ASP:HB2	1:B:93:ASN:CG	2.42	0.44
1:A:98:LEU:C	1:A:100:ILE:H	2.26	0.44
1:B:127:TYR:HA	1:B:128:ARG:HA	1.66	0.44
1:B:58:GLN:O	1:B:61:GLN:N	2.51	0.43
1:B:90:ASP:HB3	1:B:93:ASN:H	1.83	0.43
1:A:125:ASP:HA	1:A:126:PRO:HD2	1.83	0.43
1:B:54:ASP:O	1:B:57:LEU:N	2.52	0.42
1:A:18:ARG:NH1	1:A:93:ASN:HD21	2.11	0.42
1:B:90:ASP:H	1:B:93:ASN:HD22	1.66	0.42
1:B:28:ASP:O	1:B:31:ARG:HB3	2.19	0.42
1:B:111:LEU:HD23	1:B:111:LEU:HA	1.90	0.42
1:A:90:ASP:HA	1:A:122:GLU:HG2	2.01	0.42
4:A:204:GOL:O3	5:A:302:HOH:O	2.21	0.42
1:B:26:LEU:O	1:B:30:ILE:HG12	2.20	0.42
1:A:70:ASN:ND2	1:B:68:MET:HB2	2.35	0.42
1:B:116:ALA:O	1:B:121:LYS:NZ	2.53	0.41
1:A:29:LYS:HD3	4:A:210:GOL:H2	2.02	0.41
1:B:56:ALA:O	1:B:60:LEU:HD12	2.20	0.41
1:A:116:ALA:HB1	1:A:118:ARG:HD3	2.02	0.41
1:B:67:PRO:O	1:B:69:VAL:HG22	2.20	0.41
1:A:101:CYS:HA	1:A:102:PRO:HD2	1.83	0.41
1:B:9:LEU:HD11	1:B:42:ALA:HB3	2.02	0.40
1:A:10:VAL:HG11	1:A:22:ALA:HB3	2.04	0.40

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	151/166 (91%)	138 (91%)	12 (8%)	1 (1%)	18	38
1	B	150/166 (90%)	133 (89%)	17 (11%)	0	100	100
All	All	301/332 (91%)	271 (90%)	29 (10%)	1 (0%)	36	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	ASN

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	134/146 (92%)	117 (87%)	17 (13%)	4	9
1	B	133/146 (91%)	104 (78%)	29 (22%)	1	2
All	All	267/292 (91%)	221 (83%)	46 (17%)	2	3

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	9	LEU
1	A	19	SER
1	A	46	LYS
1	A	49	LYS

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Mol	Chain	Res	Type
1	A	68	MET
1	A	69	VAL
1	A	74	GLN
1	A	78	GLN
1	A	82	GLU
1	A	100	ILE
1	A	117	ASN
1	A	128	ARG
1	A	131	SER
1	A	146	VAL
1	A	153	GLN
1	A	155	GLN
1	B	6	LEU
1	B	7	SER
1	B	19	SER
1	B	29	LYS
1	B	31	ARG
1	B	33	LYS
1	B	38	GLN
1	B	39	VAL
1	B	41	SER
1	B	50	THR
1	B	60	LEU
1	B	68	MET
1	B	69	VAL
1	B	72	VAL
1	B	73	GLN
1	B	74	GLN
1	B	78	GLN
1	B	97	LEU
1	B	104	GLU
1	B	114	SER
1	B	118	ARG
1	B	122	GLU
1	B	125	ASP
1	B	128	ARG
1	B	131	SER
1	B	135	GLN
1	B	150	ASP
1	B	151	SER
1	B	153	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	36	ASN
1	A	58	GLN
1	A	61	GLN
1	A	70	ASN
1	A	73	GLN
1	A	93	ASN
1	A	155	GLN
1	B	15	ASN
1	B	77	GLN
1	B	83	HIS
1	B	93	ASN
1	B	135	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

39 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
4	GOL	B	204	-	5,5,5	0.36	0	5,5,5	0.38	0
4	GOL	B	208	-	5,5,5	0.35	0	5,5,5	0.36	0
4	GOL	A	206	-	5,5,5	0.37	0	5,5,5	0.34	0
4	GOL	A	216	-	5,5,5	0.38	0	5,5,5	0.30	0
4	GOL	A	207	-	5,5,5	0.35	0	5,5,5	0.37	0
4	GOL	A	220	-	5,5,5	0.37	0	5,5,5	0.34	0
4	GOL	A	215	-	5,5,5	0.37	0	5,5,5	0.27	0
4	GOL	B	207	-	5,5,5	0.37	0	5,5,5	0.27	0
4	GOL	B	215	-	5,5,5	0.36	0	5,5,5	0.39	0
4	GOL	A	212	-	5,5,5	0.35	0	5,5,5	0.35	0
4	GOL	A	209	-	5,5,5	0.35	0	5,5,5	0.38	0
4	GOL	A	222	-	5,5,5	0.31	0	5,5,5	0.33	0
4	GOL	B	212	-	5,5,5	0.37	0	5,5,5	0.30	0
4	GOL	A	223	-	5,5,5	0.34	0	5,5,5	0.45	0
4	GOL	B	206	-	5,5,5	0.37	0	5,5,5	0.33	0
4	GOL	B	213	-	5,5,5	0.39	0	5,5,5	0.30	0
4	GOL	A	210	-	5,5,5	0.37	0	5,5,5	0.39	0
4	GOL	A	218	-	5,5,5	0.38	0	5,5,5	0.30	0
4	GOL	A	219	-	5,5,5	0.37	0	5,5,5	0.28	0
2	MPO	B	201	-	13,13,13	1.31	2 (15%)	17,17,17	2.13	6 (35%)
4	GOL	A	214	-	5,5,5	0.38	0	5,5,5	0.26	0
4	GOL	A	204	-	5,5,5	0.38	0	5,5,5	0.35	0
4	GOL	A	213	-	5,5,5	0.38	0	5,5,5	0.21	0
4	GOL	A	205	-	5,5,5	0.40	0	5,5,5	0.58	0
4	GOL	A	208	-	5,5,5	0.36	0	5,5,5	0.31	0
4	GOL	B	209	-	5,5,5	0.42	0	5,5,5	0.35	0
4	GOL	A	221	-	5,5,5	0.38	0	5,5,5	0.32	0
3	SO4	B	202	-	4,4,4	0.23	0	6,6,6	0.06	0
4	GOL	B	203	-	5,5,5	0.38	0	5,5,5	0.32	0
4	GOL	A	203	-	5,5,5	0.37	0	5,5,5	0.27	0
3	SO4	A	202	-	4,4,4	0.24	0	6,6,6	0.08	0
4	GOL	A	217	-	5,5,5	0.36	0	5,5,5	0.37	0
4	GOL	B	211	-	5,5,5	0.37	0	5,5,5	0.30	0
4	GOL	A	211	-	5,5,5	0.37	0	5,5,5	0.28	0
4	GOL	B	214	-	5,5,5	0.29	0	5,5,5	0.34	0
2	MPO	A	201	-	13,13,13	1.25	2 (15%)	17,17,17	2.25	7 (41%)
4	GOL	B	210	-	5,5,5	0.37	0	5,5,5	0.31	0
4	GOL	B	205	-	5,5,5	0.32	0	5,5,5	0.57	0
4	GOL	A	224	-	5,5,5	0.32	0	5,5,5	0.38	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
4	GOL	B	204	-	-	2/4/4/4	-
4	GOL	B	208	-	-	2/4/4/4	-
4	GOL	A	206	-	-	2/4/4/4	-
4	GOL	A	216	-	-	2/4/4/4	-
4	GOL	A	207	-	-	2/4/4/4	-
4	GOL	A	220	-	-	2/4/4/4	-
4	GOL	A	215	-	-	4/4/4/4	-
4	GOL	B	207	-	-	2/4/4/4	-
4	GOL	B	215	-	-	4/4/4/4	-
4	GOL	A	212	-	-	2/4/4/4	-
4	GOL	A	209	-	-	4/4/4/4	-
4	GOL	A	222	-	-	4/4/4/4	-
4	GOL	B	212	-	-	0/4/4/4	-
4	GOL	A	223	-	-	4/4/4/4	-
4	GOL	B	206	-	-	2/4/4/4	-
4	GOL	B	213	-	-	0/4/4/4	-
4	GOL	A	210	-	-	2/4/4/4	-
4	GOL	A	218	-	-	2/4/4/4	-
4	GOL	A	219	-	-	2/4/4/4	-
2	MPO	B	201	-	-	3/7/15/15	0/1/1/1
4	GOL	A	214	-	-	4/4/4/4	-
4	GOL	A	204	-	-	2/4/4/4	-
4	GOL	A	213	-	-	2/4/4/4	-
4	GOL	A	205	-	-	2/4/4/4	-
4	GOL	A	208	-	-	2/4/4/4	-
4	GOL	B	209	-	-	4/4/4/4	-
4	GOL	A	221	-	-	2/4/4/4	-
4	GOL	B	203	-	-	4/4/4/4	-
4	GOL	A	203	-	-	1/4/4/4	-
4	GOL	A	217	-	-	4/4/4/4	-
4	GOL	B	211	-	-	4/4/4/4	-
4	GOL	A	211	-	-	2/4/4/4	-
4	GOL	B	214	-	-	2/4/4/4	-
2	MPO	A	201	-	-	4/7/15/15	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	210	-	-	2/4/4/4	-
4	GOL	B	205	-	-	2/4/4/4	-
4	GOL	A	224	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	MPO	O2-S1	2.88	1.53	1.45
2	A	201	MPO	O2-S1	2.72	1.52	1.45
2	B	201	MPO	O1-S1	2.52	1.52	1.45
2	A	201	MPO	O1-S1	2.49	1.52	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	MPO	C2-C1-S1	-5.32	105.10	113.25
2	A	201	MPO	O2-S1-O1	-4.11	100.45	113.82
2	B	201	MPO	C2-C1-S1	-4.04	107.05	113.25
2	B	201	MPO	O2-S1-O1	-4.03	100.71	113.82
2	B	201	MPO	C7-N1-C4	3.41	116.20	108.84
2	A	201	MPO	O2-S1-C1	3.34	111.78	106.73
2	B	201	MPO	O1-S1-C1	3.22	111.59	106.73
2	A	201	MPO	O3-S1-C1	3.06	111.98	106.00
2	A	201	MPO	C7-N1-C4	3.03	115.36	108.84
2	B	201	MPO	O3-S1-C1	2.93	111.73	106.00
2	A	201	MPO	C5-C4-N1	2.20	113.47	110.12
2	A	201	MPO	C6-C7-N1	2.14	113.38	110.12
2	B	201	MPO	C6-C7-N1	2.02	113.19	110.12

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201	MPO	C2-C1-S1-O1
4	A	204	GOL	C1-C2-C3-O3
4	A	205	GOL	O1-C1-C2-C3
4	A	206	GOL	O1-C1-C2-C3
4	A	207	GOL	C1-C2-C3-O3
4	A	208	GOL	O1-C1-C2-C3
4	A	209	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	209	GOL	C1-C2-C3-O3
4	A	212	GOL	C1-C2-C3-O3
4	A	213	GOL	O1-C1-C2-C3
4	A	214	GOL	O1-C1-C2-O2
4	A	214	GOL	O1-C1-C2-C3
4	A	214	GOL	C1-C2-C3-O3
4	A	214	GOL	O2-C2-C3-O3
4	A	215	GOL	O1-C1-C2-C3
4	A	217	GOL	O1-C1-C2-C3
4	A	217	GOL	C1-C2-C3-O3
4	A	217	GOL	O2-C2-C3-O3
4	A	218	GOL	O1-C1-C2-C3
4	A	219	GOL	O1-C1-C2-C3
4	A	220	GOL	O1-C1-C2-C3
4	A	221	GOL	O1-C1-C2-C3
4	A	222	GOL	O1-C1-C2-O2
4	A	222	GOL	C1-C2-C3-O3
4	A	223	GOL	O1-C1-C2-C3
4	A	223	GOL	C1-C2-C3-O3
4	A	224	GOL	C1-C2-C3-O3
4	A	224	GOL	O2-C2-C3-O3
4	B	203	GOL	O1-C1-C2-C3
4	B	203	GOL	C1-C2-C3-O3
4	B	203	GOL	O2-C2-C3-O3
4	B	204	GOL	O1-C1-C2-C3
4	B	206	GOL	O1-C1-C2-C3
4	B	207	GOL	O1-C1-C2-O2
4	B	207	GOL	O1-C1-C2-C3
4	B	208	GOL	O1-C1-C2-C3
4	B	209	GOL	C1-C2-C3-O3
4	B	211	GOL	O1-C1-C2-O2
4	B	211	GOL	O1-C1-C2-C3
4	B	214	GOL	C1-C2-C3-O3
4	B	214	GOL	O2-C2-C3-O3
4	B	215	GOL	O1-C1-C2-C3
2	A	201	MPO	C2-C3-N1-C7
2	A	201	MPO	C2-C1-S1-O3
2	B	201	MPO	C2-C1-S1-O3
4	A	205	GOL	O1-C1-C2-O2
4	A	218	GOL	O1-C1-C2-O2
4	B	211	GOL	O2-C2-C3-O3
4	A	210	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	211	GOL	O1-C1-C2-C3
4	A	215	GOL	C1-C2-C3-O3
4	A	216	GOL	O1-C1-C2-C3
4	A	222	GOL	O1-C1-C2-C3
4	B	205	GOL	O1-C1-C2-C3
4	B	209	GOL	O1-C1-C2-C3
4	B	210	GOL	O1-C1-C2-C3
4	B	211	GOL	C1-C2-C3-O3
4	B	215	GOL	C1-C2-C3-O3
4	A	204	GOL	O2-C2-C3-O3
4	A	207	GOL	O2-C2-C3-O3
4	A	209	GOL	O1-C1-C2-O2
4	A	209	GOL	O2-C2-C3-O3
4	A	213	GOL	O1-C1-C2-O2
4	A	216	GOL	O1-C1-C2-O2
4	A	219	GOL	O1-C1-C2-O2
4	A	220	GOL	O1-C1-C2-O2
4	A	221	GOL	O1-C1-C2-O2
4	A	223	GOL	O1-C1-C2-O2
4	B	203	GOL	O1-C1-C2-O2
4	B	208	GOL	O1-C1-C2-O2
4	B	209	GOL	O2-C2-C3-O3
4	B	210	GOL	O1-C1-C2-O2
4	B	215	GOL	O2-C2-C3-O3
4	A	206	GOL	O1-C1-C2-O2
4	A	208	GOL	O1-C1-C2-O2
4	A	215	GOL	O2-C2-C3-O3
4	A	217	GOL	O1-C1-C2-O2
4	B	206	GOL	O1-C1-C2-O2
4	B	209	GOL	O1-C1-C2-O2
4	B	215	GOL	O1-C1-C2-O2
2	A	201	MPO	C2-C1-S1-O1
2	A	201	MPO	C2-C1-S1-O2
2	B	201	MPO	C2-C1-S1-O2
4	A	212	GOL	O2-C2-C3-O3
4	A	215	GOL	O1-C1-C2-O2
4	A	222	GOL	O2-C2-C3-O3
4	A	223	GOL	O2-C2-C3-O3
4	B	204	GOL	O1-C1-C2-O2
4	A	203	GOL	O1-C1-C2-C3
4	A	210	GOL	O2-C2-C3-O3
4	A	211	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	205	GOL	O1-C1-C2-O2

There are no ring outliers.

14 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	204	GOL	1	0
4	A	207	GOL	2	0
4	A	223	GOL	1	0
4	A	210	GOL	1	0
2	B	201	MPO	1	0
4	A	204	GOL	2	0
4	A	213	GOL	1	0
4	A	205	GOL	1	0
4	A	208	GOL	1	0
4	B	209	GOL	1	0
3	A	202	SO4	1	0
2	A	201	MPO	3	0
4	B	210	GOL	1	0
4	A	224	GOL	1	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 [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	153/166 (92%)	0.35	2 (1%) 75 71	24, 38, 71, 93	0
1	B	152/166 (91%)	0.57	9 (5%) 28 23	23, 44, 77, 96	0
All	All	305/332 (91%)	0.45	11 (3%) 46 40	23, 40, 74, 96	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	GLY	3.3
1	B	129	ARG	2.5
1	A	152	TRP	2.5
1	B	36	ASN	2.4
1	B	73	GLN	2.3
1	B	5	GLY	2.3
1	B	123	VAL	2.2
1	B	150	ASP	2.1
1	B	127	TYR	2.1
1	B	126	PRO	2.0
1	B	153	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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
4	GOL	A	203	6/6	0.45	0.21	66,76,80,86	0
4	GOL	B	214	6/6	0.56	0.17	63,70,71,74	0
4	GOL	B	208	6/6	0.58	0.17	64,70,75,76	0
4	GOL	B	209	6/6	0.61	0.15	67,69,74,80	0
4	GOL	A	215	6/6	0.61	0.18	62,68,72,72	0
4	GOL	A	222	6/6	0.62	0.14	77,80,82,84	0
4	GOL	B	212	6/6	0.66	0.17	67,73,76,80	0
4	GOL	A	211	6/6	0.66	0.15	69,71,75,76	0
4	GOL	B	203	6/6	0.67	0.20	53,59,65,65	0
4	GOL	A	206	6/6	0.69	0.14	53,55,66,70	0
4	GOL	A	204	6/6	0.72	0.12	60,69,70,71	0
4	GOL	B	206	6/6	0.73	0.16	47,60,67,68	0
4	GOL	B	207	6/6	0.73	0.11	51,60,62,63	0
4	GOL	A	207	6/6	0.74	0.16	56,61,68,68	0
4	GOL	B	205	6/6	0.74	0.11	61,73,76,79	0
4	GOL	A	212	6/6	0.74	0.12	66,71,73,73	0
4	GOL	A	223	6/6	0.74	0.16	61,70,70,71	0
4	GOL	A	218	6/6	0.75	0.14	45,57,60,61	0
4	GOL	A	219	6/6	0.75	0.13	54,60,62,65	0
4	GOL	A	208	6/6	0.76	0.16	45,56,57,57	0
4	GOL	B	210	6/6	0.76	0.14	45,55,58,64	0
4	GOL	A	221	6/6	0.78	0.13	61,63,64,66	0
4	GOL	B	215	6/6	0.78	0.13	49,56,60,66	0
4	GOL	B	204	6/6	0.79	0.15	53,57,66,69	0
4	GOL	A	224	6/6	0.79	0.15	54,58,58,60	0
4	GOL	A	213	6/6	0.80	0.16	43,46,57,59	0
4	GOL	A	220	6/6	0.82	0.12	55,60,66,66	0
4	GOL	A	216	6/6	0.82	0.11	51,62,64,68	0
4	GOL	B	213	6/6	0.83	0.13	38,42,50,52	0
4	GOL	A	209	6/6	0.83	0.10	36,43,49,57	0
4	GOL	A	217	6/6	0.83	0.13	42,49,54,58	0
4	GOL	A	210	6/6	0.86	0.14	50,60,61,67	0
4	GOL	B	211	6/6	0.86	0.11	48,55,60,60	0
4	GOL	A	214	6/6	0.87	0.08	40,48,56,57	0
3	SO4	B	202	5/5	0.87	0.11	89,92,98,101	0
3	SO4	A	202	5/5	0.91	0.10	49,58,72,76	0
4	GOL	A	205	6/6	0.91	0.10	43,51,55,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MPO	B	201	13/13	0.95	0.11	25,44,47,52	0
2	MPO	A	201	13/13	0.95	0.10	7,29,37,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.