Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 11:22 AM JST

PDB ID	:	5Z3M
Title	:	Crystal structure of Low Molecular Weight Phosphotyrosine phosphatase (VcLMWPTP-2) from Vibrio choleraeO395
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:

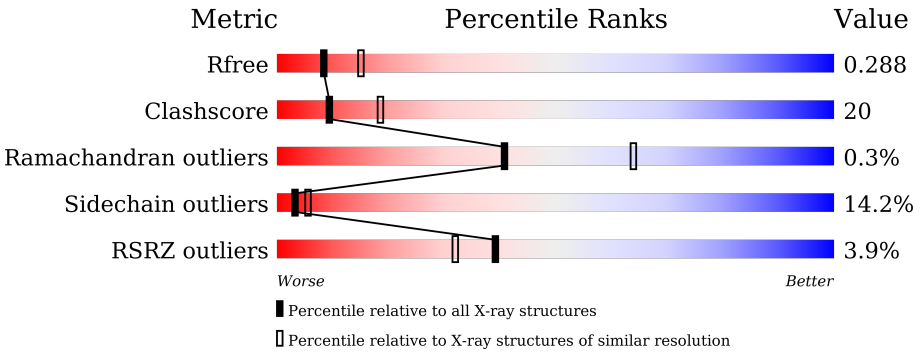
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 <=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	3% 53% 37% · 8%
1	B	166	4% 45% 37% 10% 8%

2 Entry composition

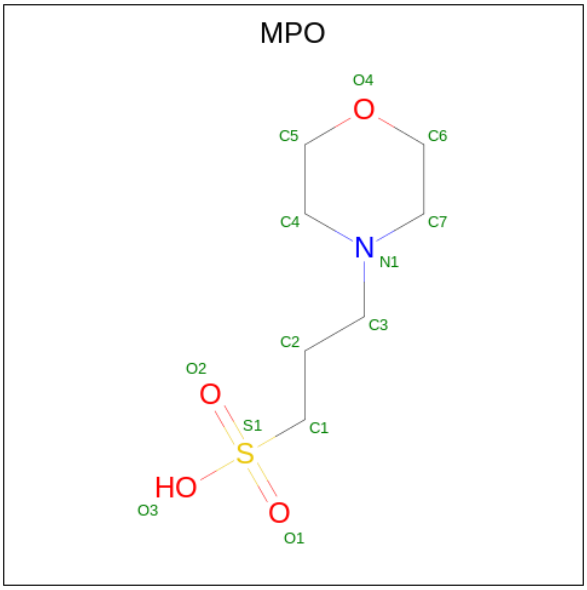
There are 5 unique types of molecules in this entry. The entry contains 2926 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

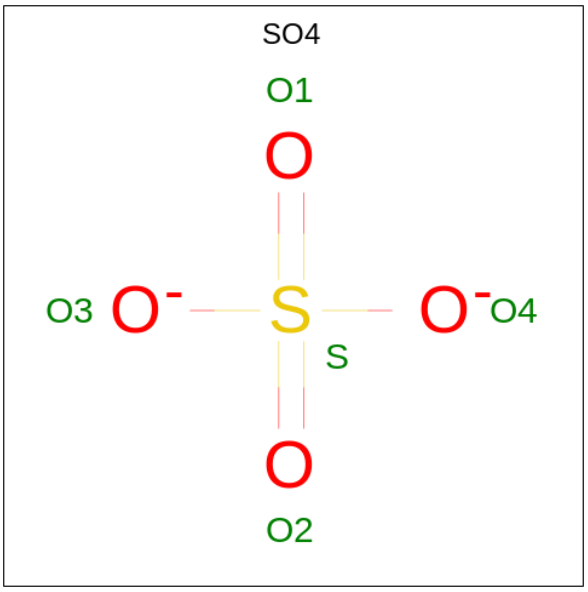
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1216	764	217	228	7			
1	B	152	Total	C	N	O	S	0	0	0
			1208	758	216	227	7			

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



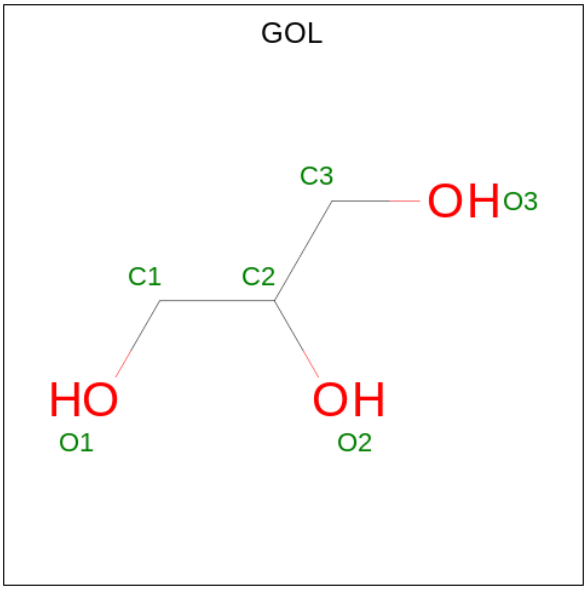
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 5 is water.

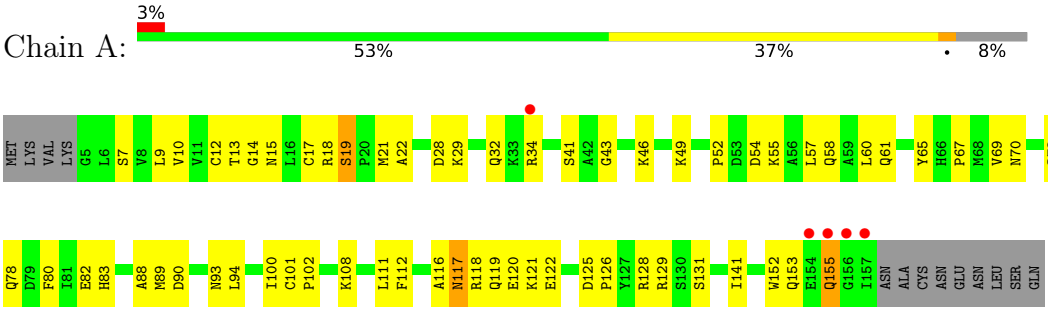
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	148	Total O 148 148	0	0
5	B	108	Total O 108 108	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

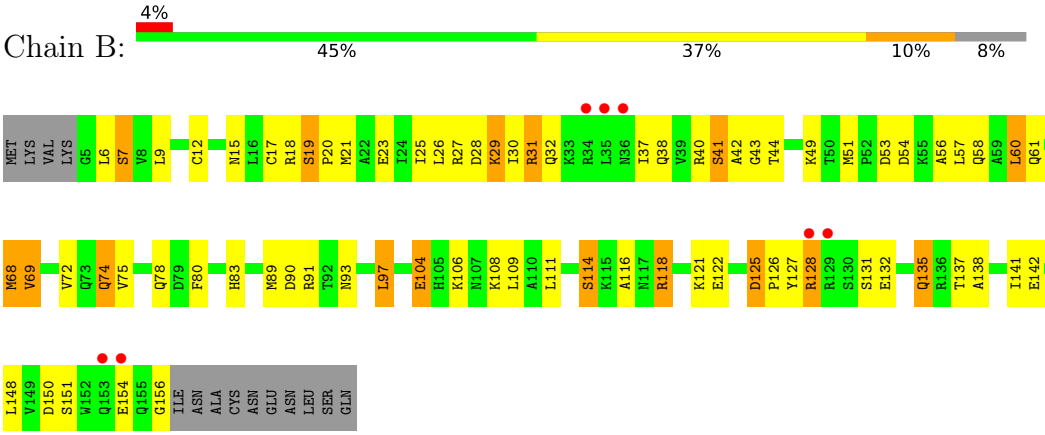
• Molecule 1: Phosphotyrosine protein phosphatase

Chain A:



• Molecule 1: Phosphotyrosine protein phosphatase

Chain B:



4 Data and refinement statistics (i)

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 42.96 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.40-2.60) 98.9 (42.96-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.88 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.252 , 0.288 0.257 , 0.288	Depositor DCC
R_{free} test set	1035 reflections (5.02%)	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)	0.33 , 75.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPO, GOL, 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	0.29	0/1236	0.52	0/1670
1	B	0.30	0/1228	0.55	0/1659
All	All	0.30	0/2464	0.53	0/3329

There are no bond length outliers.

There are no bond angle outliers.

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	1216	0	1228	46	0
1	B	1208	0	1217	58	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
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	107	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 (107) 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	1.24	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: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:15:ASN:HD21	1:B:41:SER:HG	1.34	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:A:89:MET:HE2	1:A:112:PHE:HB2	1.77	0.65
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: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
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:A:10:VAL:HG13	1:A:89:MET:HE3	1.84	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:80:PHE:O	1:A:108:LYS:NZ	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:15:ASN:ND2	1:B:41:SER:HG	1.97	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:A:18:ARG:HE	1:A:126:PRO:HD2	1.78	0.47
1:B:15:ASN:HB2	1:B:43:GLY:N	2.28	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
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:12:CYS:SG	1:B:19:SER:OG	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:28:ASP:O	1:B:32:GLN:HG3	2.17	0.45
1:A:13:THR:HB	2:A:201:MPO:H22	1.99	0.44
1:B:91:ARG:HG2	1:B:122:GLU:CD	2.38	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:57:LEU:HG	1:B:51:MET:HE3	2.00	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:B:106:LYS:NZ	5:B:308:HOH:O	2.30	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:B:74:GLN:CD	1:B:74:GLN:N	2.74	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 (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	151/166 (91%)	138 (91%)	12 (8%)	1 (1%)	22 43
1	B	150/166 (90%)	133 (89%)	17 (11%)	0	100 100
All	All	301/332 (91%)	271 (90%)	29 (10%)	1 (0%)	41 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	134/146 (92%)	119 (89%)	15 (11%)	6 10
1	B	133/146 (91%)	110 (83%)	23 (17%)	2 3
All	All	267/292 (91%)	229 (86%)	38 (14%)	3 5

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	19	SER
1	A	34	ARG
1	A	46	LYS
1	A	49	LYS
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	153	GLN
1	A	155	GLN

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Mol	Chain	Res	Type
1	B	6	LEU
1	B	7	SER
1	B	19	SER
1	B	29	LYS
1	B	31	ARG
1	B	38	GLN
1	B	41	SER
1	B	53	ASP
1	B	60	LEU
1	B	68	MET
1	B	69	VAL
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	125	ASP
1	B	128	ARG
1	B	131	SER
1	B	135	GLN
1	B	150	ASP
1	B	151	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	58	GLN
1	A	61	GLN
1	A	70	ASN
1	A	73	GLN
1	A	74	GLN
1	A	93	ASN
1	A	155	GLN
1	B	15	ASN
1	B	83	HIS
1	B	93	ASN
1	B	135	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 monosaccharides in this entry.

5.6 Ligand geometry

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	A	219	-	5,5,5	0.37	0	5,5,5	0.25	0
4	GOL	A	210	-	5,5,5	0.37	0	5,5,5	0.35	0
4	GOL	B	212	-	5,5,5	0.37	0	5,5,5	0.27	0
4	GOL	A	213	-	5,5,5	0.37	0	5,5,5	0.19	0
4	GOL	A	221	-	5,5,5	0.38	0	5,5,5	0.29	0
4	GOL	A	214	-	5,5,5	0.37	0	5,5,5	0.23	0
4	GOL	B	210	-	5,5,5	0.37	0	5,5,5	0.27	0
4	GOL	B	203	-	5,5,5	0.38	0	5,5,5	0.28	0
4	GOL	A	215	-	5,5,5	0.37	0	5,5,5	0.24	0
4	GOL	A	216	-	5,5,5	0.37	0	5,5,5	0.26	0
4	GOL	B	208	-	5,5,5	0.34	0	5,5,5	0.33	0
4	GOL	A	222	-	5,5,5	0.31	0	5,5,5	0.30	0
4	GOL	A	205	-	5,5,5	0.39	0	5,5,5	0.53	0
4	GOL	A	203	-	5,5,5	0.37	0	5,5,5	0.24	0
4	GOL	B	213	-	5,5,5	0.38	0	5,5,5	0.26	0
4	GOL	A	223	-	5,5,5	0.33	0	5,5,5	0.41	0
4	GOL	B	215	-	5,5,5	0.35	0	5,5,5	0.36	0
4	GOL	B	211	-	5,5,5	0.37	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	A	224	-	5,5,5	0.31	0	5,5,5	0.34	0
4	GOL	A	220	-	5,5,5	0.36	0	5,5,5	0.30	0
4	GOL	A	208	-	5,5,5	0.35	0	5,5,5	0.27	0
4	GOL	B	209	-	5,5,5	0.42	0	5,5,5	0.32	0
3	SO4	A	202	-	4,4,4	0.14	0	6,6,6	0.05	0
4	GOL	A	207	-	5,5,5	0.35	0	5,5,5	0.34	0
4	GOL	B	205	-	5,5,5	0.32	0	5,5,5	0.54	0
2	MPO	B	201	-	13,13,13	1.27	2 (15%)	17,17,17	2.24	6 (35%)
4	GOL	A	204	-	5,5,5	0.37	0	5,5,5	0.31	0
2	MPO	A	201	-	13,13,13	1.22	2 (15%)	17,17,17	2.36	7 (41%)
4	GOL	A	218	-	5,5,5	0.38	0	5,5,5	0.27	0
4	GOL	A	217	-	5,5,5	0.36	0	5,5,5	0.34	0
4	GOL	B	214	-	5,5,5	0.29	0	5,5,5	0.30	0
4	GOL	A	211	-	5,5,5	0.37	0	5,5,5	0.25	0
4	GOL	A	209	-	5,5,5	0.34	0	5,5,5	0.35	0
4	GOL	B	204	-	5,5,5	0.35	0	5,5,5	0.34	0
4	GOL	A	212	-	5,5,5	0.35	0	5,5,5	0.33	0
3	SO4	B	202	-	4,4,4	0.14	0	6,6,6	0.05	0
4	GOL	B	207	-	5,5,5	0.36	0	5,5,5	0.23	0
4	GOL	B	206	-	5,5,5	0.37	0	5,5,5	0.30	0
4	GOL	A	206	-	5,5,5	0.37	0	5,5,5	0.30	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	A	219	-	-	2/4/4/4	-
4	GOL	A	210	-	-	3/4/4/4	-
4	GOL	B	212	-	-	0/4/4/4	-
4	GOL	A	213	-	-	2/4/4/4	-
4	GOL	A	221	-	-	2/4/4/4	-
4	GOL	A	214	-	-	4/4/4/4	-
4	GOL	B	210	-	-	2/4/4/4	-
4	GOL	B	203	-	-	4/4/4/4	-
4	GOL	A	215	-	-	4/4/4/4	-
4	GOL	A	216	-	-	2/4/4/4	-
4	GOL	B	208	-	-	2/4/4/4	-
4	GOL	A	222	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	205	-	-	2/4/4/4	-
4	GOL	A	203	-	-	1/4/4/4	-
4	GOL	B	213	-	-	0/4/4/4	-
4	GOL	A	223	-	-	4/4/4/4	-
4	GOL	B	215	-	-	4/4/4/4	-
4	GOL	B	211	-	-	4/4/4/4	-
4	GOL	A	224	-	-	2/4/4/4	-
4	GOL	A	220	-	-	2/4/4/4	-
4	GOL	A	208	-	-	2/4/4/4	-
4	GOL	B	209	-	-	4/4/4/4	-
4	GOL	A	207	-	-	2/4/4/4	-
4	GOL	B	205	-	-	2/4/4/4	-
2	MPO	B	201	-	-	3/7/15/15	0/1/1/1
4	GOL	A	204	-	-	2/4/4/4	-
2	MPO	A	201	-	-	5/7/15/15	0/1/1/1
4	GOL	A	218	-	-	2/4/4/4	-
4	GOL	A	217	-	-	4/4/4/4	-
4	GOL	B	214	-	-	2/4/4/4	-
4	GOL	A	211	-	-	2/4/4/4	-
4	GOL	A	209	-	-	4/4/4/4	-
4	GOL	B	204	-	-	2/4/4/4	-
4	GOL	A	212	-	-	2/4/4/4	-
4	GOL	B	207	-	-	2/4/4/4	-
4	GOL	B	206	-	-	2/4/4/4	-
4	GOL	A	206	-	-	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	2.79	1.53	1.45
2	A	201	MPO	O2-S1	2.63	1.52	1.45
2	B	201	MPO	O1-S1	2.44	1.52	1.45
2	A	201	MPO	O1-S1	2.41	1.52	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	MPO	C2-C1-S1	-5.32	105.10	113.25
2	B	201	MPO	C2-C1-S1	-4.04	107.05	113.25
2	A	201	MPO	O2-S1-C1	4.04	111.78	106.92
2	A	201	MPO	O2-S1-O1	-3.90	100.45	113.95
2	B	201	MPO	O1-S1-C1	3.88	111.59	106.92
2	A	201	MPO	O3-S1-C1	3.84	111.98	105.77
2	B	201	MPO	O2-S1-O1	-3.82	100.71	113.95
2	B	201	MPO	O3-S1-C1	3.69	111.73	105.77
2	B	201	MPO	C7-N1-C4	3.27	116.20	108.83
2	A	201	MPO	C7-N1-C4	2.90	115.36	108.83
2	A	201	MPO	C5-C4-N1	2.22	113.47	110.10
2	A	201	MPO	C6-C7-N1	2.16	113.38	110.10
2	B	201	MPO	C6-C7-N1	2.03	113.19	110.10

There are no chirality outliers.

All (94) 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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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	203	GOL	O1-C1-C2-C3
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	210	GOL	C1-C2-C3-O3
4	A	210	GOL	O2-C2-C3-O3
4	A	211	GOL	O1-C1-C2-O2
4	B	205	GOL	O1-C1-C2-O2
2	A	201	MPO	C1-C2-C3-N1

There are no ring outliers.

14 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	210	GOL	1	0
4	A	213	GOL	1	0
4	B	210	GOL	1	0
4	A	205	GOL	1	0
4	A	223	GOL	1	0
4	A	224	GOL	1	0
4	A	208	GOL	1	0
4	B	209	GOL	1	0
3	A	202	SO4	1	0
4	A	207	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	MPO	1	0
4	A	204	GOL	2	0
2	A	201	MPO	3	0
4	B	204	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

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^{th} 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%)	0.07	5 (3%) 46 39	24, 38, 71, 93	0
1	B	152/166 (91%)	0.12	7 (4%) 32 26	23, 44, 77, 96	0
All	All	305/332 (91%)	0.10	12 (3%) 39 32	23, 40, 74, 96	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	GLY	4.5
1	A	155	GLN	3.4
1	A	154	GLU	2.9
1	A	157	ILE	2.7
1	A	34	ARG	2.7
1	B	128	ARG	2.6
1	B	154	GLU	2.5
1	B	36	ASN	2.5
1	B	35	LEU	2.5
1	B	153	GLN	2.4
1	B	129	ARG	2.3
1	B	34	ARG	2.2

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	B	214	6/6	0.52	0.26	63,70,71,74	0
4	GOL	A	207	6/6	0.55	0.19	56,61,68,68	0
4	GOL	B	203	6/6	0.61	0.24	53,59,65,65	0
4	GOL	A	211	6/6	0.64	0.28	69,71,75,76	0
4	GOL	B	206	6/6	0.69	0.21	47,60,67,68	0
4	GOL	A	222	6/6	0.70	0.27	77,80,82,84	0
4	GOL	B	208	6/6	0.71	0.23	64,70,75,76	0
4	GOL	A	223	6/6	0.71	0.24	61,70,70,71	0
4	GOL	A	219	6/6	0.73	0.21	54,60,62,65	0
4	GOL	A	212	6/6	0.74	0.22	66,71,73,73	0
4	GOL	B	207	6/6	0.74	0.21	51,60,62,63	0
4	GOL	A	203	6/6	0.76	0.28	66,76,80,86	0
4	GOL	A	218	6/6	0.76	0.22	45,57,60,61	0
4	GOL	B	212	6/6	0.77	0.24	67,73,76,80	0
4	GOL	A	220	6/6	0.77	0.23	55,60,66,66	0
4	GOL	A	216	6/6	0.78	0.21	51,62,64,68	0
4	GOL	A	215	6/6	0.78	0.25	62,68,72,72	0
4	GOL	A	221	6/6	0.79	0.36	61,63,64,66	0
4	GOL	B	215	6/6	0.79	0.29	49,56,60,66	0
4	GOL	A	213	6/6	0.80	0.26	43,46,57,59	0
4	GOL	A	209	6/6	0.80	0.21	36,43,49,57	0
4	GOL	A	210	6/6	0.81	0.24	50,60,61,67	0
4	GOL	B	204	6/6	0.81	0.22	53,57,66,69	0
4	GOL	B	213	6/6	0.82	0.26	38,42,50,52	0
4	GOL	B	209	6/6	0.82	0.21	67,69,74,80	0
4	GOL	A	204	6/6	0.82	0.28	60,69,70,71	0
4	GOL	A	206	6/6	0.83	0.25	53,55,66,70	0
4	GOL	B	205	6/6	0.83	0.14	61,73,76,79	0
4	GOL	A	224	6/6	0.84	0.34	54,58,58,60	0
4	GOL	A	208	6/6	0.85	0.33	45,56,57,57	0
4	GOL	A	217	6/6	0.85	0.30	42,49,54,58	0
4	GOL	B	210	6/6	0.87	0.14	45,55,58,64	0
4	GOL	B	211	6/6	0.88	0.21	48,55,60,60	0
4	GOL	A	214	6/6	0.89	0.12	40,48,56,57	0
3	SO4	B	202	5/5	0.92	0.23	89,92,98,101	0
4	GOL	A	205	6/6	0.94	0.13	43,51,55,59	0
2	MPO	B	201	13/13	0.94	0.24	25,44,47,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MPO	A	201	13/13	0.94	0.21	7,29,37,50	0
3	SO4	A	202	5/5	0.96	0.13	49,58,72,76	0

6.5 Other polymers (i)

There are no such residues in this entry.