Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2021 – 01:10 pm GMT

PDB ID	:	7Q4H
Title	:	A thermostable lipase from Thermoanaerobacter thermohydrosulfuricus in complex with PMSF
Deposited on	:	2021-10-30
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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 (i) symbol.

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

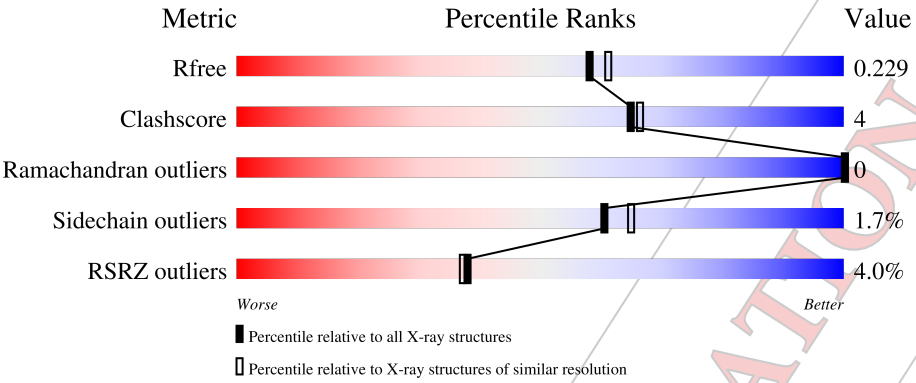
MolProbity	:	4.02b-467
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	259	6% 90% 10%
2	B	259	2% 89% 10%

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
4	GOL	A	303	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4326 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 Hydrolase_4 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	259	2048	1317	333	386	12	0	1	0

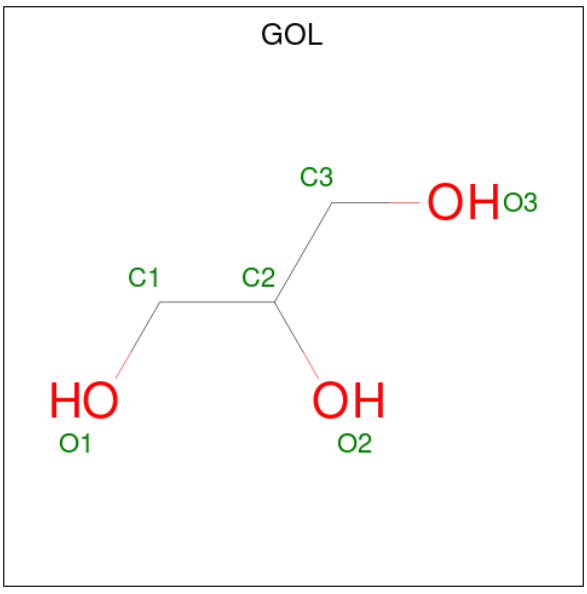
- Molecule 2 is a protein called Hydrolase_4 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	259	2071	1332	335	392	12	0	1	0

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

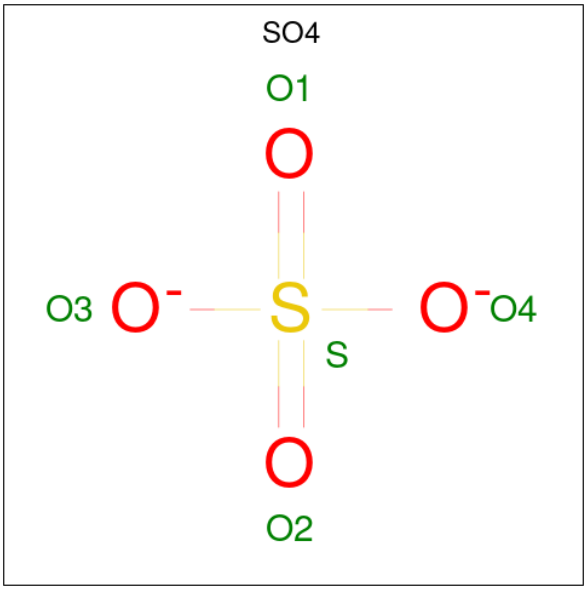
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	A	1	1	1	0	0

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



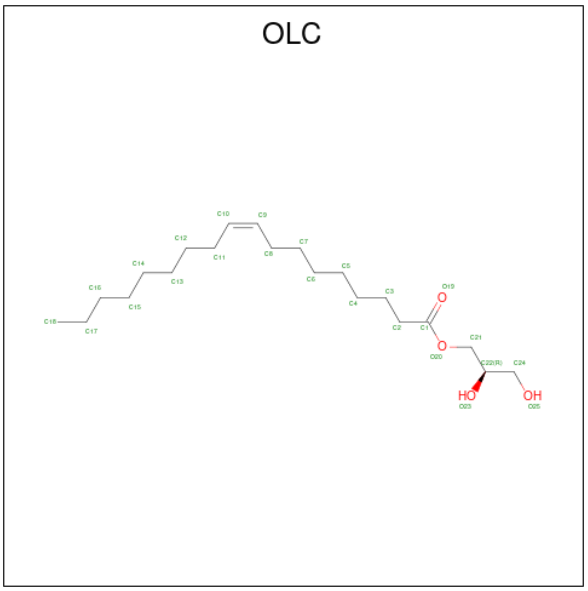
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 12 6 6	0	1
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 25 21 4	0	0

- Molecule 7 is water.

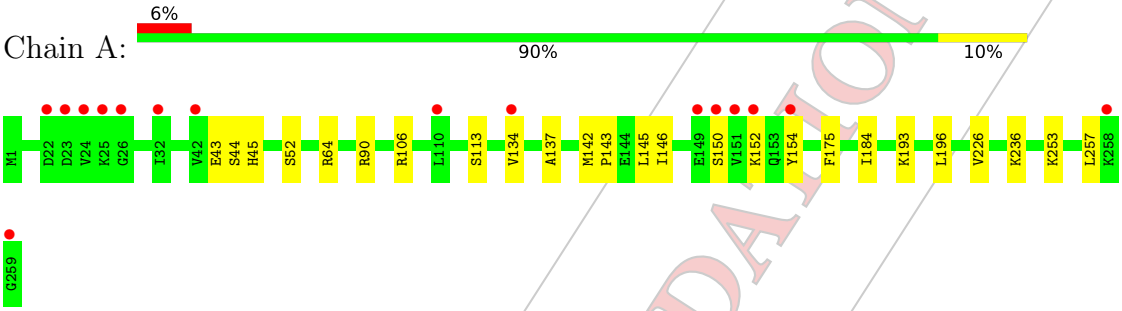
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	72	Total O 72 72	0	0
7	B	64	Total O 64 64	0	0

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.

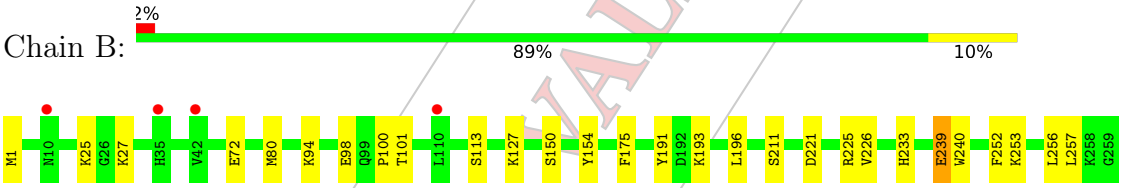
• Molecule 1: Hydrolase_4 domain-containing protein

Chain A:



• Molecule 2: Hydrolase_4 domain-containing protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	84.81Å 84.81Å 157.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 2.00 29.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.98-2.00) 98.2 (29.98-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.184 , 0.228 0.188 , 0.229	Depositor DCC
R_{free} test set	1219 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å^2)	37.4	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4326	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: MLY, MLZ, CL, SO4, SEB, GOL, OLC

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	0.28	0/2014	0.48	0/2705
2	B	0.27	0/2015	0.45	0/2705
All	All	0.28	0/4029	0.47	0/5410

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	2048	0	2023	17	0
2	B	2071	0	2061	15	0
3	A	1	0	0	0	0
4	A	24	0	32	6	0
4	B	6	0	8	0	0
5	A	10	0	0	0	0
5	B	5	0	0	0	0
6	B	25	0	40	3	0
7	A	72	0	0	1	0
7	B	64	0	0	1	0
All	All	4326	0	4164	34	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 4.

All (34) 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:B:150:SER:HA	2:B:154:TYR:HB2	1.52	0.89
6:B:301:OLC:H16	6:B:301:OLC:H12A	1.72	0.71
2:B:94:LYS:NZ	2:B:98:GLU:OE2	2.22	0.66
1:A:45:HIS:H	4:A:303:GOL:C1	2.10	0.65
1:A:236:MLY:HH22	4:A:303:GOL:H32	1.78	0.63
1:A:45:HIS:H	4:A:303:GOL:H11	1.64	0.63
2:B:113:SEB:OD2	2:B:233:HIS:NE2	2.31	0.63
1:A:44:SER:HA	4:A:303:GOL:H12	1.81	0.63
1:A:90:ARG:NH2	7:A:405:HOH:O	2.38	0.57
2:B:196:LEU:HD11	2:B:226:VAL:HG23	1.87	0.56
2:B:127:LYS:O	2:B:193:LYS:NZ	2.38	0.56
2:B:80:MET:HE1	2:B:175:PHE:HE2	1.71	0.54
1:A:196:LEU:HD11	1:A:226:VAL:HG23	1.91	0.53
1:A:253:MLZ:HG3	1:A:257:LEU:HD12	1.91	0.53
1:A:43:GLU:OE1	4:A:302[A]:GOL:H31	2.10	0.52
1:A:142:MET:HA	1:A:145:LEU:HD12	1.91	0.52
2:B:239[A]:GLU:HG2	2:B:240:TRP:N	2.23	0.51
2:B:253:MLY:HG3	2:B:257:LEU:HD12	1.95	0.48
1:A:150:SER:HA	1:A:154:TYR:CD2	2.49	0.48
2:B:113:SEB:HI1	6:B:301:OLC:H12A	1.94	0.48
2:B:27:MLZ:HD3	2:B:100:PRO:O	2.16	0.46
2:B:252:PHE:O	2:B:256:LEU:HB2	2.16	0.46
1:A:193:MLY:HD3	1:A:193:MLY:HH23	1.60	0.45
1:A:146:ILE:HD13	1:A:175:PHE:HE1	1.84	0.43
6:B:301:OLC:H2	6:B:301:OLC:H21	1.74	0.43
1:A:134:VAL:HG22	1:A:196:LEU:HB3	2.00	0.43
1:A:64:ARG:NH2	2:B:72:GLU:OE2	2.52	0.43
2:B:211:SER:OG	2:B:225:ARG:NH1	2.50	0.42
4:A:303:GOL:H31	7:B:431:HOH:O	2.18	0.42
2:B:191:TYR:CZ	2:B:193:LYS:HB2	2.54	0.42
2:B:25:MLZ:HD3	2:B:25:MLZ:HA	1.64	0.42
1:A:236:MLY:HH23	1:A:236:MLY:HD2	1.80	0.41
1:A:113:SEB:HA	1:A:137:ALA:O	2.21	0.41
1:A:143:PRO:HD3	1:A:184:ILE:HD12	2.03	0.41

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	252/259 (97%)	245 (97%)	7 (3%)	0	100	100
2	B	250/259 (96%)	243 (97%)	7 (3%)	0	100	100
All	All	502/518 (97%)	488 (97%)	14 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	209/216 (97%)	206 (99%)	3 (1%)	67	72
2	B	212/214 (99%)	207 (98%)	5 (2%)	49	51
All	All	421/430 (98%)	413 (98%)	8 (2%)	60	61

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	SER
1	A	106	ARG
1	A	152	LYS
2	B	1	MET
2	B	101	THR
2	B	221	ASP
2	B	239[A]	GLU
2	B	239[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

14 non-standard protein/DNA/RNA residues are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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	253/259 (97%)	0.02	16 (6%) 20 19	26, 42, 85, 138	0
2	B	251/259 (96%)	0.00	4 (1%) 72 70	25, 46, 79, 104	0
All	All	504/518 (97%)	0.01	20 (3%) 38 37	25, 44, 80, 138	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	151	VAL	5.7
1	A	150	SER	4.4
1	A	23	ASP	3.9
1	A	259	GLY	3.9
2	B	42	VAL	3.7
1	A	154	TYR	3.3
1	A	149	GLU	2.8
1	A	110	LEU	2.8
2	B	110	LEU	2.6
1	A	24	VAL	2.6
1	A	42	VAL	2.5
1	A	22	ASP	2.5
1	A	32	ILE	2.4
1	A	152	LYS	2.4
2	B	35	HIS	2.4
1	A	25	LYS	2.3
2	B	10	ASN	2.3
1	A	258	LYS	2.2
1	A	26	GLY	2.2
1	A	134	VAL	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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
2	MLZ	B	25	10/11	0.79	0.23	60,78,82,85	0
2	MLZ	B	27	10/11	0.88	0.14	70,73,78,79	0
2	SEB	B	113	16/17	0.90	0.17	34,64,81,90	0
2	MLY	B	131	11/12	0.90	0.14	55,60,89,90	0
1	SEB	A	113	16/17	0.91	0.14	30,60,67,73	0
1	MLY	A	193	11/12	0.92	0.12	50,54,66,67	0
1	MLY	A	236	11/12	0.92	0.12	36,42,66,70	0
2	MLY	B	194	11/12	0.93	0.14	50,61,72,73	0
2	MLY	B	253	11/12	0.93	0.18	49,55,62,64	0
1	MLZ	A	253	10/11	0.94	0.12	46,53,59,61	0
2	MLZ	B	236	10/11	0.95	0.11	26,36,58,60	0
1	MLZ	A	189	10/11	0.95	0.13	46,59,74,74	0
2	MLY	B	3	11/12	0.96	0.12	30,35,48,51	0
1	MLZ	A	12	10/11	0.98	0.10	31,39,48,55	0

6.3 Carbohydrates (i)

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
6	OLC	B	301	25/25	0.77	0.24	50,68,92,93	0
4	GOL	A	304	6/6	0.85	0.20	74,79,81,82	0
4	GOL	A	302[A]	6/6	0.87	0.23	45,54,56,61	6
4	GOL	A	302[B]	6/6	0.87	0.23	28,54,55,61	6
4	GOL	B	302	6/6	0.90	0.29	43,52,58,63	0
4	GOL	A	303	6/6	0.91	0.15	46,52,59,69	0
5	SO4	A	305	5/5	0.92	0.24	85,86,87,89	5
5	SO4	B	303	5/5	0.93	0.15	46,48,68,69	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	A	306	5/5	0.95	0.18	92,95,96,98	0
3	CL	A	301	1/1	1.00	0.13	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.