Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:45 am BST

PDB ID	:	6NLR
Title	:	Crystal structure of the putative histidinol phosphatase hisK from Listeria monocytogenes with trinuclear metals determined by PIXE revealing sulphate ion in active site. Based on PIXE analysis and original date from 3DCP
Authors	:	Snell, E.H.; Garman, E.F.; Lowe, E.D.
Deposited on	:	2019-01-09
Resolution	:	2.10 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 following versions of software and data (see references ①) were used in the production of this report:

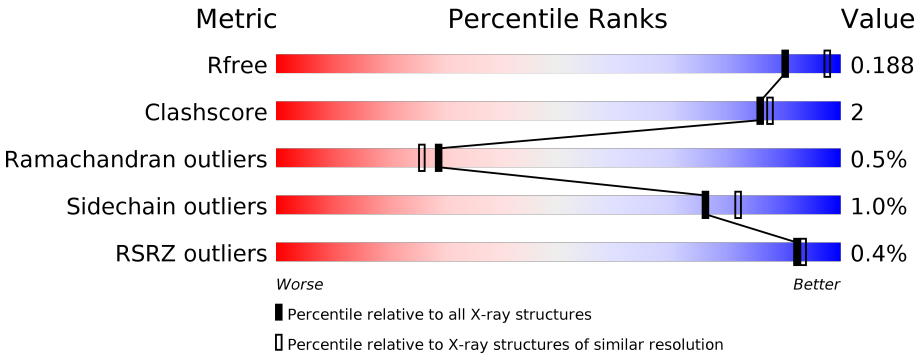
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 >=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	283	92% 6% •
1	B	283	% 91% 5% • •
1	C	283	91% 5% • •

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7194 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 Histidinol-phosphatase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	Se	0	1	0
			2236	1430	358	436	4	8			
1	B	273	Total	C	N	O	S	Se	0	1	0
			2202	1409	354	427	4	8			
1	C	274	Total	C	N	O	S	Se	0	0	0
			2201	1408	353	428	4	8			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	134	ILE	LEU	conflict	UNP A0A3A6YEN9
A	276	LEU	-	expression tag	UNP A0A3A6YEN9
A	277	GLU	-	expression tag	UNP A0A3A6YEN9
A	278	HIS	-	expression tag	UNP A0A3A6YEN9
A	279	HIS	-	expression tag	UNP A0A3A6YEN9
A	280	HIS	-	expression tag	UNP A0A3A6YEN9
A	281	HIS	-	expression tag	UNP A0A3A6YEN9
A	282	HIS	-	expression tag	UNP A0A3A6YEN9
A	283	HIS	-	expression tag	UNP A0A3A6YEN9
B	134	ILE	LEU	conflict	UNP A0A3A6YEN9
B	276	LEU	-	expression tag	UNP A0A3A6YEN9
B	277	GLU	-	expression tag	UNP A0A3A6YEN9
B	278	HIS	-	expression tag	UNP A0A3A6YEN9
B	279	HIS	-	expression tag	UNP A0A3A6YEN9
B	280	HIS	-	expression tag	UNP A0A3A6YEN9
B	281	HIS	-	expression tag	UNP A0A3A6YEN9
B	282	HIS	-	expression tag	UNP A0A3A6YEN9
B	283	HIS	-	expression tag	UNP A0A3A6YEN9
C	134	ILE	LEU	conflict	UNP A0A3A6YEN9
C	276	LEU	-	expression tag	UNP A0A3A6YEN9
C	277	GLU	-	expression tag	UNP A0A3A6YEN9
C	278	HIS	-	expression tag	UNP A0A3A6YEN9
C	279	HIS	-	expression tag	UNP A0A3A6YEN9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	280	HIS	-	expression tag	UNP A0A3A6YEN9
C	281	HIS	-	expression tag	UNP A0A3A6YEN9
C	282	HIS	-	expression tag	UNP A0A3A6YEN9
C	283	HIS	-	expression tag	UNP A0A3A6YEN9

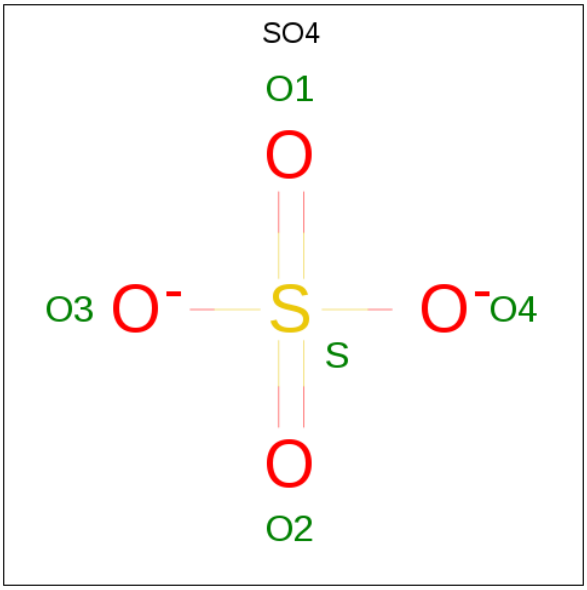
- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mn 2 2	0	0
2	C	1	Total Mn 1 1	0	0

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Co 1 1	0	0
3	A	1	Total Co 1 1	0	0
3	C	1	Total Co 1 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Fe 2 2	0	0
5	C	1	Total Fe 1 1	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Ca 1 1	0	0
6	C	1	Total Ca 1 1	0	0

- Molecule 7 is water.

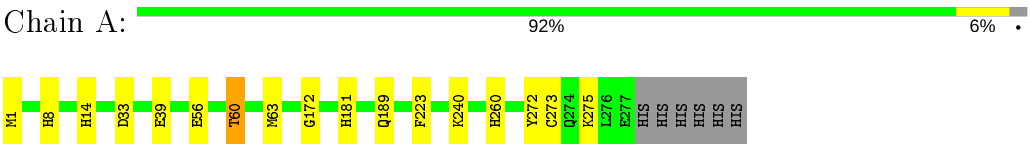
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	193	Total O 193 193	0	0
7	B	152	Total O 152 152	0	0
7	C	184	Total O 184 184	0	0

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.

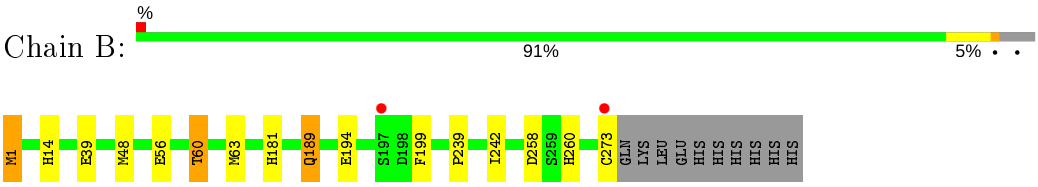
- Molecule 1: Histidinol-phosphatase

Chain A:



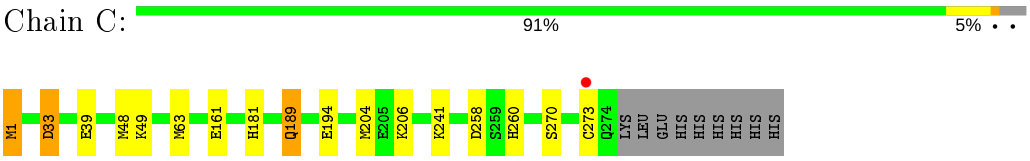
- Molecule 1: Histidinol-phosphatase

Chain B:



- Molecule 1: Histidinol-phosphatase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α, β, γ	191.28Å 191.28Å 48.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.60 – 2.10 41.56 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (41.60-2.10) 98.5 (41.56-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0241	Depositor
R, R_{free}	0.155 , 0.186 0.156 , 0.188	Depositor DCC
R_{free} test set	2868 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	26.5	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7194	wwPDB-VP
Average B, all atoms (Å^2)	33.0	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 30.59 % 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 1.2743e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: CA, MN, CO, FE, 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	0.71	0/2283	0.80	1/3063 (0.0%)
1	B	0.65	0/2250	0.76	2/3020 (0.1%)
1	C	0.68	0/2248	0.77	2/3017 (0.1%)
All	All	0.68	0/6781	0.78	5/9100 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1	MSE	CG-SE-CE	8.54	117.68	98.90
1	A	1	MSE	CG-SE-CE	6.54	113.29	98.90
1	B	1	MSE	CG-SE-CE	6.44	113.08	98.90
1	B	48	MSE	CG-SE-CE	5.54	111.08	98.90
1	C	48	MSE	CG-SE-CE	5.36	110.69	98.90

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	2236	0	2130	10	0
1	B	2202	0	2093	10	0
1	C	2201	0	2095	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	C	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	193	0	0	1	0
7	B	152	0	0	3	0
7	C	184	0	0	0	0
All	All	7194	0	6318	28	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 2.

All (28) 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:A:14:HIS:HB3	1:A:60:THR:HG23	1.54	0.89
1:B:14:HIS:HB3	1:B:60:THR:HG23	1.57	0.85
1:A:56:GLU:O	1:A:60:THR:HB	1.92	0.70
1:B:56:GLU:O	1:B:60:THR:HB	1.91	0.69
1:A:273:CYS:SG	7:A:575:HOH:O	2.50	0.68
1:A:172:GLY:HA2	1:C:49:LYS:HG2	1.82	0.60
1:A:14:HIS:HD2	1:A:60:THR:O	1.88	0.56
1:B:199:PHE:HE2	1:B:242:ILE:HD11	1.72	0.55
1:B:273:CYS:SG	7:B:550:HOH:O	2.58	0.55
1:B:239:PRO:HD2	1:B:242:ILE:HD13	1.88	0.54
1:C:204:MSE:SE	1:C:241:LYS:HE3	2.61	0.50
1:A:240:LYS:HD3	1:A:275:LYS:HG3	1.93	0.49
1:C:258:ASP:O	1:C:260:HIS:HD2	1.99	0.46
1:C:189:GLN:HG2	1:C:194:GLU:O	2.17	0.44
1:A:223:PHE:CE1	1:A:272:TYR:HA	2.52	0.44
1:B:258:ASP:O	1:B:260:HIS:HD2	2.00	0.44
1:A:39:GLU:HG3	1:A:63:MSE:HE2	2.00	0.43
7:B:407:HOH:O	1:C:270:SER:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MSE:HB2	1:C:33:ASP:OD2	2.19	0.42
1:C:39:GLU:CG	1:C:63:MSE:HE2	2.50	0.42
1:A:14:HIS:HB3	1:A:60:THR:CG2	2.39	0.42
1:C:161:GLU:OE1	1:C:206:LYS:NZ	2.46	0.42
1:C:39:GLU:HG3	1:C:63:MSE:HE2	2.00	0.42
1:B:39:GLU:HG3	1:B:63:MSE:HE2	2.01	0.41
1:A:8:HIS:CD2	1:A:260:HIS:CE1	3.08	0.41
1:B:189:GLN:HG2	1:B:194:GLU:O	2.21	0.41
1:B:199:PHE:CE2	1:B:242:ILE:HD11	2.54	0.40
1:B:1:MSE:HB2	7:B:520:HOH:O	2.21	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	276/283 (98%)	268 (97%)	7 (2%)	1 (0%)	34	32
1	B	272/283 (96%)	264 (97%)	7 (3%)	1 (0%)	34	32
1	C	272/283 (96%)	264 (97%)	6 (2%)	2 (1%)	22	18
All	All	820/849 (97%)	796 (97%)	20 (2%)	4 (0%)	29	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	HIS
1	C	181	HIS
1	B	181	HIS
1	C	273	CYS

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	241/238 (101%)	238 (99%)	3 (1%)	71 77
1	B	237/238 (100%)	235 (99%)	2 (1%)	81 86
1	C	237/238 (100%)	235 (99%)	2 (1%)	81 86
All	All	715/714 (100%)	708 (99%)	7 (1%)	76 82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	60	THR
1	A	189	GLN
1	B	60	THR
1	B	189	GLN
1	C	33	ASP
1	C	189	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	109	ASN
1	A	128	GLN
1	A	147	GLN
1	B	109	ASN
1	B	128	GLN
1	B	165	GLN
1	B	260	HIS
1	C	147	GLN
1	C	260	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 11 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
4	SO4	C	305	3,2,5	4,4,4	0.27	0	6,6,6	0.09	0
4	SO4	B	305	3,5	4,4,4	0.27	0	6,6,6	0.08	0
4	SO4	A	304	3,2	4,4,4	0.26	0	6,6,6	0.13	0

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

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	269/283 (95%)	-0.65	0 100 100	20, 29, 44, 75	0
1	B	265/283 (93%)	-0.52	2 (0%) 86 88	23, 34, 57, 79	0
1	C	266/283 (93%)	-0.61	1 (0%) 92 93	19, 30, 45, 84	0
All	All	800/849 (94%)	-0.59	3 (0%) 92 93	19, 31, 50, 84	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	273	CYS	3.9
1	B	197	SER	2.4
1	C	273	CYS	2.1

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^{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	CA	C	304	1/1	0.95	0.46	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CA	B	304	1/1	0.96	0.40	76,76,76,76	0
5	FE	B	302	1/1	0.98	0.05	35,35,35,35	0
4	SO4	C	305	5/5	0.98	0.07	35,42,48,55	0
4	SO4	B	305	5/5	0.98	0.08	39,39,48,55	0
4	SO4	A	304	5/5	0.98	0.06	36,36,49,56	0
3	CO	B	301	1/1	0.99	0.08	24,24,24,24	0
2	MN	A	301	1/1	0.99	0.06	27,27,27,27	1
2	MN	C	301	1/1	0.99	0.05	28,28,28,28	1
3	CO	A	303	1/1	1.00	0.08	22,22,22,22	0
2	MN	A	302	1/1	1.00	0.09	16,16,16,16	1
5	FE	C	303	1/1	1.00	0.10	23,23,23,23	0
5	FE	B	303	1/1	1.00	0.05	27,27,27,27	0
3	CO	C	302	1/1	1.00	0.08	22,22,22,22	0

6.5 Other polymers

There are no such residues in this entry.