Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:01 PM GMT

PDB ID	:	4E3E
Title	:	CRYSTAL STRUCTURE OF putative MaoC domain protein dehydratase from Chloroflexus aurantiacus J-10-fl
Authors	:	Malashkevich, V.N.; Bhosle, R.; Toro, R.; Hillerich, B.; Gizzi, A.; Garforth, S.; Kar, A.; Chan, M.K.; Lafluer, J.; Patel, H.; Matikainen, B.; Chamala, S.; Lim, S.; Celikgil, A.; Villegas, G.; Evans, B.; Zenchek, W.; Love, J.; Fiser, A.; Khafizov, K.; Seidel, R.; Bonanno, J.B.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on	:	2012-03-09
Resolution	:	1.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

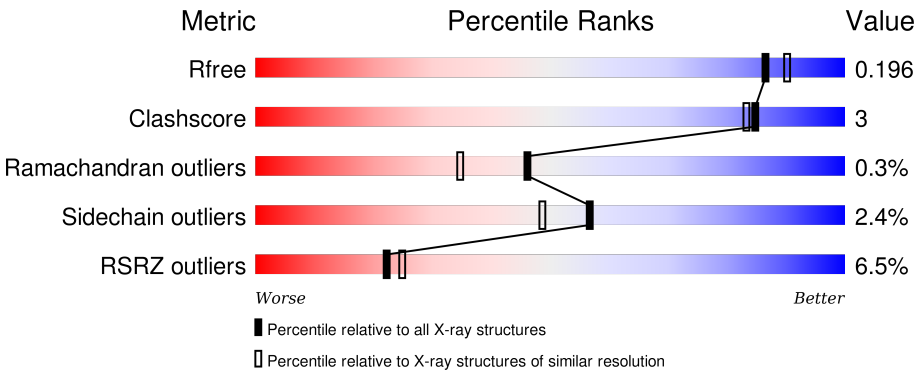
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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. 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	352	7% 93% 6% •
1	B	352	6% 92% 7% •

2 Entry composition (i)

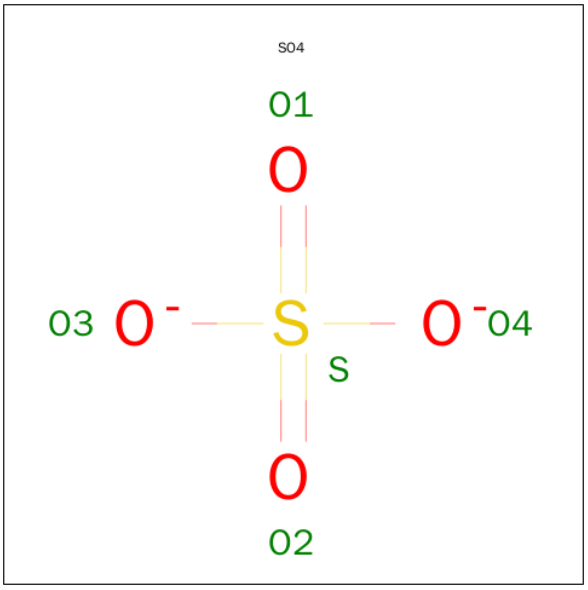
There are 3 unique types of molecules in this entry. The entry contains 5973 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MaoC domain protein dehydratase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	351	2735	1733	484	513	1	4	0	1	0
1	B	351	2748	1743	487	513	1	4	0	3	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

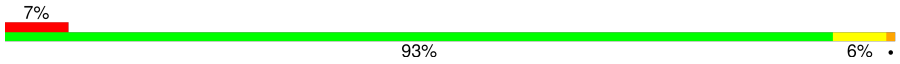
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	244	244	244	0	0
			Total	O		
3	B	236	236	236	0	0

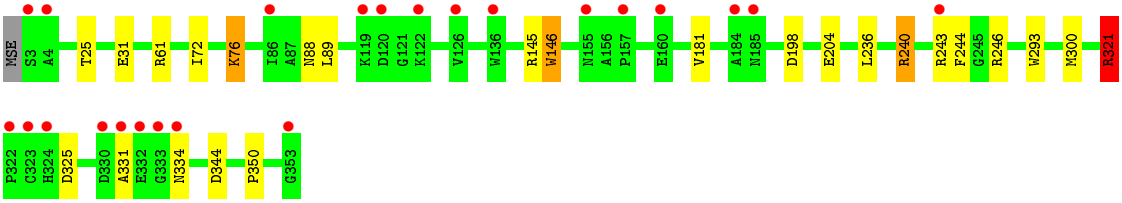
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: MaoC domain protein dehydratase

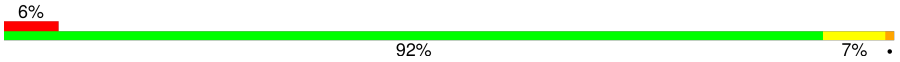
Chain A:

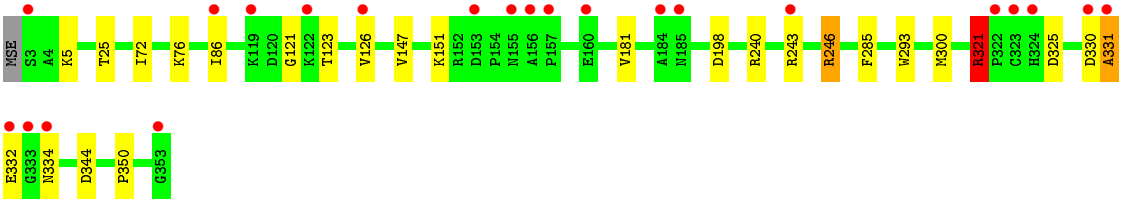




- Molecule 1: MaoC domain protein dehydratase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	133.44Å 133.44Å 170.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.41 – 1.90 19.26 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.41-1.90) 99.9 (19.26-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.141 , 0.188 0.152 , 0.196	Depositor DCC
R_{free} test set	4475 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 57.3	EDS
Estimated twinning fraction	0.015 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.000 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.002 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l 0.000 for -h,2/3*h+1/3*k-2/3*l,-2/3*h-4/3*k-1/3*l 0.000 for 1/3*h+2/3*k+2/3*l,-k,4/3*h+2/3*k-1/3*l 0.014 for -1/3*h-2/3*k-2/3*l,-2/3*h-1/3*k+2/3*l,-2/3*h+2/3*k-1/3*l 0.488 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 89192 reflections	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	5973	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.62	2/2801 (0.1%)	0.64	2/3815 (0.1%)
1	B	0.63	1/2820 (0.0%)	0.67	2/3840 (0.1%)
All	All	0.62	3/5621 (0.1%)	0.65	4/7655 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	293	TRP	CD2-CE2	5.47	1.48	1.41
1	A	146	TRP	CD2-CE2	5.42	1.47	1.41
1	A	293	TRP	CD2-CE2	5.05	1.47	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	344	ASP	CB-CG-OD1	6.86	124.47	118.30
1	A	344	ASP	CB-CG-OD1	6.10	123.79	118.30
1	B	5	LYS	CD-CE-NZ	-5.52	99.01	111.70
1	A	76	LYS	CD-CE-NZ	-5.31	99.48	111.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	331	ALA	Peptide

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	2735	0	2680	10	0
1	B	2748	0	2704	22	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	244	0	0	0	0
3	B	236	0	0	2	0
All	All	5973	0	5384	32	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 (32) 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:321[B]:ARG:NH2	1:B:321[B]:ARG:HG3	1.55	1.08
1:B:321[B]:ARG:HH21	1:B:321[B]:ARG:CG	1.62	1.07
1:B:321[A]:ARG:CG	1:B:321[A]:ARG:HH21	1.68	1.06
1:B:321[A]:ARG:HG3	1:B:321[A]:ARG:NH2	1.63	0.99
1:B:321[A]:ARG:HH21	1:B:321[A]:ARG:HG3	0.81	0.94
1:B:331:ALA:HB3	1:B:334:ASN:HB2	1.50	0.93
1:B:321[B]:ARG:HH21	1:B:321[B]:ARG:HG3	0.73	0.83
1:B:321[A]:ARG:CG	1:B:321[A]:ARG:NH2	2.36	0.67
1:B:243:ARG:HG3	3:B:660:HOH:O	1.96	0.65
1:A:236:LEU:O	1:A:240:ARG:HB3	1.98	0.63
1:B:331:ALA:O	1:B:334:ASN:N	2.30	0.63
1:B:330:ASP:O	1:B:331:ALA:C	2.39	0.60
1:B:331:ALA:CB	1:B:334:ASN:HB2	2.29	0.60
1:B:86:ILE:HD12	1:B:123:THR:HG21	1.86	0.56
1:B:121:GLY:O	1:B:151:LYS:HE2	2.10	0.52
1:B:321[B]:ARG:CG	1:B:321[B]:ARG:NH2	2.33	0.51
1:A:72:ILE:O	1:A:76:LYS:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ASP:O	1:B:332:GLU:OE2	2.30	0.50
1:B:126:VAL:HG13	1:B:147:VAL:HG12	1.97	0.46
1:B:240:ARG:NH1	3:B:830:HOH:O	2.48	0.45
1:B:181:VAL:HG11	1:B:350:PRO:HB3	1.99	0.45
1:B:86:ILE:CD1	1:B:123:THR:HG21	2.46	0.45
1:B:246:ARG:HG3	1:B:285:PHE:CD1	2.51	0.45
1:A:181:VAL:HG11	1:A:350:PRO:HB3	1.99	0.45
1:B:72:ILE:O	1:B:76:LYS:HG2	2.17	0.44
1:A:31:GLU:OE2	1:A:61:ARG:NH1	2.49	0.43
1:A:88:ASN:OD1	1:A:145:ARG:HD2	2.20	0.42
1:A:89:LEU:HB2	1:A:146:TRP:CD1	2.55	0.42
1:A:331:ALA:O	1:A:334:ASN:N	2.45	0.42
1:A:243:ARG:HG3	1:A:244:PHE:N	2.36	0.41
1:A:321[A]:ARG:HE	1:A:321[A]:ARG:HB2	1.45	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	350/352 (99%)	339 (97%)	9 (3%)	2 (1%)	30	17
1	B	352/352 (100%)	341 (97%)	9 (3%)	2 (1%)	30	17
All	All	702/704 (100%)	680 (97%)	18 (3%)	4 (1%)	46	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	321[A]	ARG
1	B	321[B]	ARG
1	A	321[A]	ARG
1	A	321[B]	ARG

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	291/286 (102%)	282 (97%)	9 (3%)	47	37
1	B	293/286 (102%)	286 (98%)	7 (2%)	57	49
All	All	584/572 (102%)	568 (97%)	16 (3%)	57	43

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	THR
1	A	198	ASP
1	A	204	GLU
1	A	240	ARG
1	A	246	ARG
1	A	300	MSE
1	A	321[A]	ARG
1	A	321[B]	ARG
1	A	325	ASP
1	B	25	THR
1	B	198	ASP
1	B	246	ARG
1	B	300	MSE
1	B	321[A]	ARG
1	B	321[B]	ARG
1	B	325	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	268	ASN
1	A	276	ASN
1	B	118	ASN
1	B	276	ASN

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)

2 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	$\#\|Z\| > 2$
2	SO4	A	500	-	4,4,4	0.39	0	6,6,6	0.26	0
2	SO4	B	500	-	4,4,4	0.41	0	6,6,6	0.22	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	SO4	A	500	-	-	0/0/0/0	0/0/0/0
2	SO4	B	500	-	-	0/0/0/0	0/0/0/0

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 (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	347/352 (98%)	0.05	23 (6%)	22	24	21, 30, 60, 98	0
1	B	347/352 (98%)	0.03	22 (6%)	23	26	22, 30, 60, 101	0
All	All	694/704 (98%)	0.04	45 (6%)	22	25	21, 30, 60, 101	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	CYS	11.0
1	B	323	CYS	10.0
1	A	330	ASP	9.5
1	A	324	HIS	8.1
1	B	324	HIS	7.3
1	B	331	ALA	7.1
1	B	330	ASP	6.9
1	A	331	ALA	6.2
1	B	184	ALA	6.0
1	B	3	SER	5.8
1	A	184	ALA	5.7
1	A	322	PRO	5.3
1	A	3	SER	5.1
1	B	243	ARG	4.9
1	B	353	GLY	4.5
1	B	322	PRO	4.4
1	A	332	GLU	4.3
1	B	332	GLU	4.2
1	A	243	ARG	4.1
1	A	155	ASN	3.9
1	A	353	GLY	3.9
1	B	334	ASN	3.8
1	A	185	ASN	3.7
1	A	86	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	155	ASN	3.6
1	A	119	LYS	3.4
1	B	119	LYS	3.3
1	B	185	ASN	3.2
1	B	160	GLU	3.1
1	A	333	GLY	3.1
1	B	157	PRO	3.0
1	A	157	PRO	3.0
1	A	334	ASN	2.9
1	B	126	VAL	2.8
1	A	160	GLU	2.8
1	B	86	ILE	2.8
1	B	333	GLY	2.7
1	A	126	VAL	2.6
1	A	122	LYS	2.6
1	B	122	LYS	2.3
1	A	136	TRP	2.2
1	B	153	ASP	2.2
1	B	156	ALA	2.2
1	A	120	ASP	2.1
1	A	4	ALA	2.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	A	500	5/5	0.78	0.17	-	45,46,50,55	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	B	500	5/5	0.73	0.20	-	46,46,51,55	5

6.5 Other polymers (i)

There are no such residues in this entry.