



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 5, 2017 – 02:41 PM EST

PDB ID : 5T3E
Title : Crystal structure of a nonribosomal peptide synthetase heterocyclization domain.
Authors : Bloudoff, K.; Schmeing, T.M.
Deposited on : 2016-08-25
Resolution : 2.30 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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) : rb-20028442

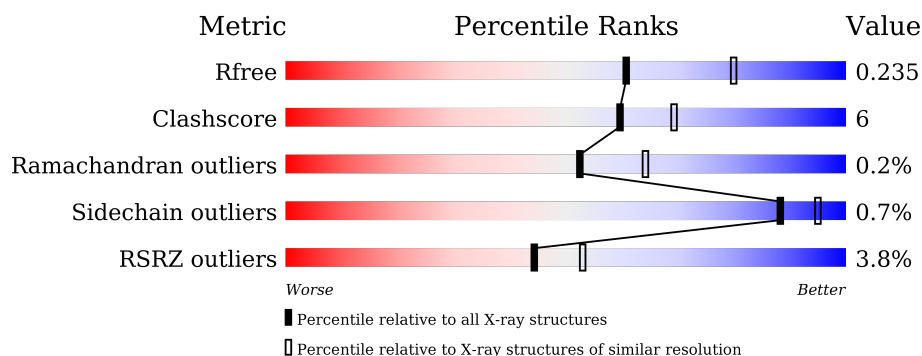
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 $\leq 5\%$. 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	445	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	445	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7230 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.

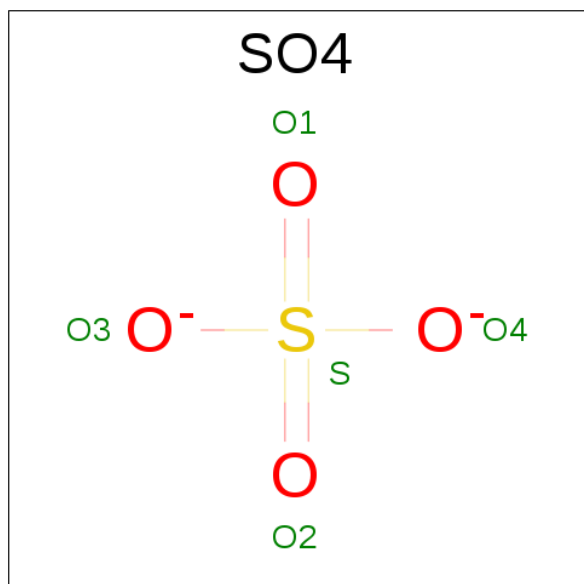
- Molecule 1 is a protein called Bacillamide synthetase heterocyclization domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3516	2262	579	657	18			
1	B	430	Total	C	N	O	S	0	0	0
			3487	2244	574	652	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	843	GLY	-	expression tag	UNP A0A0N0Y601
B	843	GLY	-	expression tag	UNP A0A0N0Y601

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	132	Total	O	0	0
			132	132		
3	B	85	Total	O	0	0
			85	85		

- Molecule 1: Bacillamide synthetase heterocyclization domain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.69Å 124.94Å 68.92Å 90.00° 95.66° 90.00°	Depositor
Resolution (Å)	39.89 – 2.30 39.89 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.89-2.30) 93.9 (39.89-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.201 , 0.237 0.197 , 0.235	Depositor DCC
R_{free} test set	2475 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7230	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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

5.1 Standard geometry

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	0.30	0/3607	0.49	1/4905 (0.0%)
1	B	0.32	1/3578 (0.0%)	0.54	2/4869 (0.0%)
All	All	0.31	1/7185 (0.0%)	0.51	3/9774 (0.0%)

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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1268	GLU	CD-OE2	-6.19	1.18	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1137	LEU	CB-CG-CD1	7.17	123.19	111.00
1	B	1162	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	1085	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1185	MET	Peptide

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	3516	0	3421	32	0
1	B	3487	0	3379	47	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	132	0	0	3	0
3	B	85	0	0	0	0
All	All	7230	0	6800	79	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 6.

All (79) 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:1180:THR:HG22	1:A:1190:VAL:HG21	1.56	0.86
1:B:1109:ARG:HH12	1:B:1146:GLN:H	1.23	0.85
1:A:1006:GLN:NE2	1:A:1007:LEU:O	2.16	0.77
1:B:1048:PRO:HB3	1:B:1111:LEU:HD22	1.67	0.75
1:A:1089:THR:HG23	1:A:1092:ALA:H	1.55	0.72
1:B:1048:PRO:HG2	1:B:1193:ILE:HG13	1.74	0.70
1:A:1048:PRO:HG2	1:A:1193:ILE:HG13	1.73	0.69
1:B:1109:ARG:HH22	1:B:1146:GLN:HB2	1.58	0.69
1:B:1114:ASN:OD1	1:B:1137:LEU:HD23	1.94	0.67
1:B:1162:LEU:O	1:B:1166:GLU:HG3	1.95	0.66
1:B:1040:LYS:O	1:B:1044:PHE:HB2	1.97	0.65
1:B:1139:LEU:HD11	1:B:1176:ILE:HG13	1.79	0.64
1:B:1248:ASP:HB3	1:B:1251:VAL:HG12	1.78	0.64
1:A:1021:TYR:HA	1:A:1024:MET:HE2	1.80	0.63
1:B:1045:PRO:HB3	1:B:1110:ARG:HB3	1.80	0.63
1:A:1074:ASP:OD1	1:A:1078:LYS:NZ	2.31	0.63
1:A:983:LEU:HD23	1:A:984:MET:HG2	1.81	0.62
1:B:1161:LEU:O	1:B:1165:LEU:HD22	2.00	0.60
1:B:1036:TYR:O	1:B:1039:ASN:OD1	2.21	0.57
1:B:1071:ILE:HB	1:B:1236:LEU:HB3	1.87	0.57
1:B:1108:GLN:NE2	1:B:1110:ARG:O	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:859:TYR:CG	1:A:874:PRO:HG3	2.43	0.54
1:A:960:LEU:HB2	1:A:983:LEU:HD13	1.90	0.53
1:A:1023:ASP:OD2	1:A:1026:ARG:NH2	2.39	0.53
1:A:983:LEU:HD23	1:A:984:MET:CG	2.39	0.52
1:B:1158:GLN:O	1:B:1162:LEU:HD13	2.10	0.52
1:A:1051:LEU:HD23	1:A:1051:LEU:H	1.73	0.51
1:A:1176:ILE:O	1:A:1180:THR:HG23	2.11	0.51
1:B:1156:GLN:CD	1:B:1156:GLN:H	2.13	0.51
1:B:1253:GLU:O	1:B:1257:THR:HG23	2.10	0.51
1:B:1192:PRO:HB2	1:B:1224:TYR:H	1.76	0.51
1:B:1152:THR:O	1:B:1156:GLN:NE2	2.44	0.51
1:A:879:GLU:HB3	1:A:974:LEU:HD11	1.94	0.50
1:B:1153:LYS:O	1:B:1157:THR:HG23	2.12	0.50
1:B:1190:VAL:HG12	1:B:1191:MET:HG2	1.93	0.50
1:B:884:LEU:HD11	1:B:1210:ILE:HA	1.92	0.49
1:B:874:PRO:HG2	1:B:981:ALA:HB3	1.94	0.49
1:A:904:ARG:NH2	3:A:1409:HOH:O	2.46	0.49
1:B:1109:ARG:NH1	1:B:1145:ASP:HA	2.28	0.49
1:B:1088:VAL:HG11	1:B:1154:VAL:HG12	1.95	0.48
1:B:984:MET:HB2	1:B:988:SER:HB2	1.95	0.48
1:A:942:ARG:NH1	3:A:1405:HOH:O	2.42	0.48
1:A:1192:PRO:HB2	1:A:1224:TYR:H	1.78	0.48
1:B:1113:ILE:HB	1:B:1140:LEU:HB2	1.95	0.47
1:B:872:ILE:O	1:B:872:ILE:HD12	2.14	0.47
1:A:1113:ILE:HD12	1:A:1142:MET:SD	2.55	0.46
1:A:859:TYR:CD1	1:A:874:PRO:HG3	2.51	0.46
1:A:949:ILE:HD13	1:A:1217:HIS:CG	2.50	0.46
1:B:1109:ARG:HH12	1:B:1146:GLN:N	2.04	0.46
1:B:1139:LEU:HD12	1:B:1175:PHE:CD2	2.52	0.45
1:A:1151:PHE:O	1:A:1155:GLU:HG3	2.17	0.44
1:A:1180:THR:OG1	1:A:1181:ARG:N	2.51	0.44
1:B:1105:TRP:CZ3	1:B:1251:VAL:HG23	2.51	0.44
1:B:1127:VAL:HG13	1:B:1128:GLU:HG2	2.00	0.43
1:B:847:SER:OG	1:B:847:SER:O	2.33	0.43
1:A:1023:ASP:HA	1:A:1026:ARG:NH2	2.33	0.43
1:B:1045:PRO:CB	1:B:1110:ARG:HB3	2.47	0.43
1:B:1153:LYS:HA	1:B:1156:GLN:OE1	2.18	0.43
1:A:879:GLU:O	1:A:1213:LEU:HD12	2.18	0.43
1:B:859:TYR:CD1	1:B:874:PRO:HG3	2.54	0.43
1:A:1071:ILE:HB	1:A:1236:LEU:HB3	2.01	0.42
1:A:1209:GLU:OE1	3:A:1401:HOH:O	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:937:GLN:O	1:B:941:LEU:HG	2.19	0.42
1:B:1165:LEU:HA	1:B:1168:ARG:HG3	2.01	0.42
1:B:1078:LYS:HD2	1:B:1267:VAL:HG13	2.02	0.42
1:B:933:PRO:HG2	1:B:936:LYS:HD3	2.02	0.42
1:A:1066:SER:OG	1:A:1241:ASN:OD1	2.36	0.42
1:A:1196:THR:HB	1:A:1228:VAL:HG22	2.01	0.41
1:A:984:MET:HE2	1:A:984:MET:HB2	1.82	0.41
1:B:1039:ASN:OD1	1:B:1040:LYS:HG2	2.21	0.41
1:B:1114:ASN:HB3	1:B:1194:VAL:HG22	2.02	0.41
1:A:960:LEU:HB2	1:A:983:LEU:CD1	2.50	0.41
1:B:859:TYR:CG	1:B:874:PRO:HG3	2.56	0.41
1:A:881:GLU:OE1	1:A:1214:ARG:NH1	2.53	0.41
1:B:958:TRP:CE2	1:B:959:PRO:HB3	2.56	0.41
1:B:1165:LEU:O	1:B:1168:ARG:HD3	2.20	0.41
1:B:1242:TYR:CD1	1:B:1252:MET:HG2	2.55	0.41
1:A:1177:ARG:HA	1:A:1180:THR:HG23	2.03	0.40
1:B:1246:LEU:HD12	1:B:1246:LEU:HA	1.97	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	430/445 (97%)	419 (97%)	9 (2%)	2 (0%)	34	41
1	B	428/445 (96%)	418 (98%)	10 (2%)	0	100	100
All	All	858/890 (96%)	837 (98%)	19 (2%)	2 (0%)	52	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1186	ARG

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Mol	Chain	Res	Type
1	A	1145	ASP

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	384/400 (96%)	379 (99%)	5 (1%)	76	87
1	B	379/400 (95%)	379 (100%)	0	100	100
All	All	763/800 (95%)	758 (99%)	5 (1%)	88	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	947	ARG
1	A	1006	GLN
1	A	1026	ARG
1	A	1039	ASN
1	A	1051	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	898	GLN
1	A	1039	ASN
1	A	1129	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 [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	1301	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	B	1301	-	4,4,4	0.24	0	6,6,6	0.07	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	1301	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1301	-	-	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 ⓘ

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, 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	432/445 (97%)	0.12	11 (2%) 61 70	35, 55, 84, 100	0
1	B	430/445 (96%)	0.42	22 (5%) 32 41	43, 64, 96, 117	0
All	All	862/890 (96%)	0.27	33 (3%) 44 53	35, 59, 93, 117	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1041	LEU	3.6
1	B	1272	ILE	3.5
1	B	1203	GLY	3.5
1	A	1026	ARG	3.4
1	B	1204	ALA	3.4
1	B	1051	LEU	3.2
1	B	1268	GLU	3.1
1	A	1202	ALA	3.1
1	A	1203	GLY	3.1
1	B	1033	ALA	3.0
1	B	1037	TRP	3.0
1	B	1035	ALA	2.7
1	A	1028	THR	2.7
1	B	1175	PHE	2.6
1	B	1042	PRO	2.6
1	B	1201	GLY	2.5
1	B	1038	THR	2.4
1	A	952	VAL	2.4
1	A	1184	GLN	2.4
1	A	1204	ALA	2.3
1	B	1274	PRO	2.3
1	A	1039	ASN	2.3
1	B	1181	ARG	2.3
1	B	1179	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	953	PHE	2.2
1	B	960	LEU	2.2
1	A	960	LEU	2.1
1	B	1269	GLN	2.1
1	B	1170	TYR	2.1
1	B	1027	GLY	2.1
1	B	955	LEU	2.1
1	A	1277	ILE	2.1
1	B	1273	ASN	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 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(\AA^2)	Q<0.9
2	SO4	A	1301	5/5	0.98	0.12	-	68,70,86,94	0
2	SO4	B	1301	5/5	0.97	0.18	-	78,83,90,102	0

6.5 Other polymers [i](#)

There are no such residues in this entry.