



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:52 PM GMT

PDB ID : 4OOC
Title : Dehydratase domain of the polyketide PpsC from Mycobacterium tuberculosis
Authors : Faille, A.; Mourey, L.; Pedelacq, J.D.
Deposited on : 2014-01-31
Resolution : 2.70 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-20026982
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-20026982

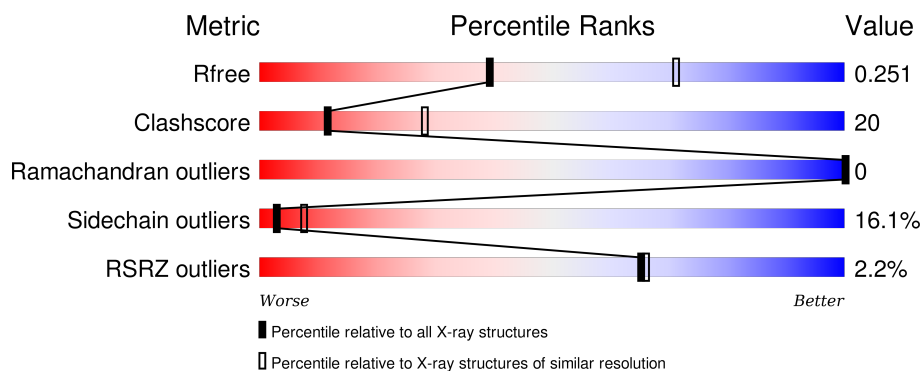
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	325	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1988 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 Phthiocerol synthesis polyketide synthase type I PpsC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			1978	1237	350	384	7			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	900	MET	-	EXPRESSION TAG	UNP P96202
A	901	GLY	-	EXPRESSION TAG	UNP P96202
A	902	SER	-	EXPRESSION TAG	UNP P96202
A	903	SER	-	EXPRESSION TAG	UNP P96202
A	904	HIS	-	EXPRESSION TAG	UNP P96202
A	905	HIS	-	EXPRESSION TAG	UNP P96202
A	906	HIS	-	EXPRESSION TAG	UNP P96202
A	907	HIS	-	EXPRESSION TAG	UNP P96202
A	908	HIS	-	EXPRESSION TAG	UNP P96202
A	909	HIS	-	EXPRESSION TAG	UNP P96202
A	910	SER	-	EXPRESSION TAG	UNP P96202
A	911	SER	-	EXPRESSION TAG	UNP P96202
A	912	GLY	-	EXPRESSION TAG	UNP P96202
A	913	LEU	-	EXPRESSION TAG	UNP P96202
A	914	VAL	-	EXPRESSION TAG	UNP P96202
A	915	PRO	-	EXPRESSION TAG	UNP P96202
A	916	ARG	-	EXPRESSION TAG	UNP P96202
A	917	GLY	-	EXPRESSION TAG	UNP P96202
A	918	SER	-	EXPRESSION TAG	UNP P96202
A	919	HIS	-	EXPRESSION TAG	UNP P96202
A	920	MET	-	EXPRESSION TAG	UNP P96202
A	1223	GLY	-	EXPRESSION TAG	UNP P96202
A	1224	SER	-	EXPRESSION TAG	UNP P96202

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

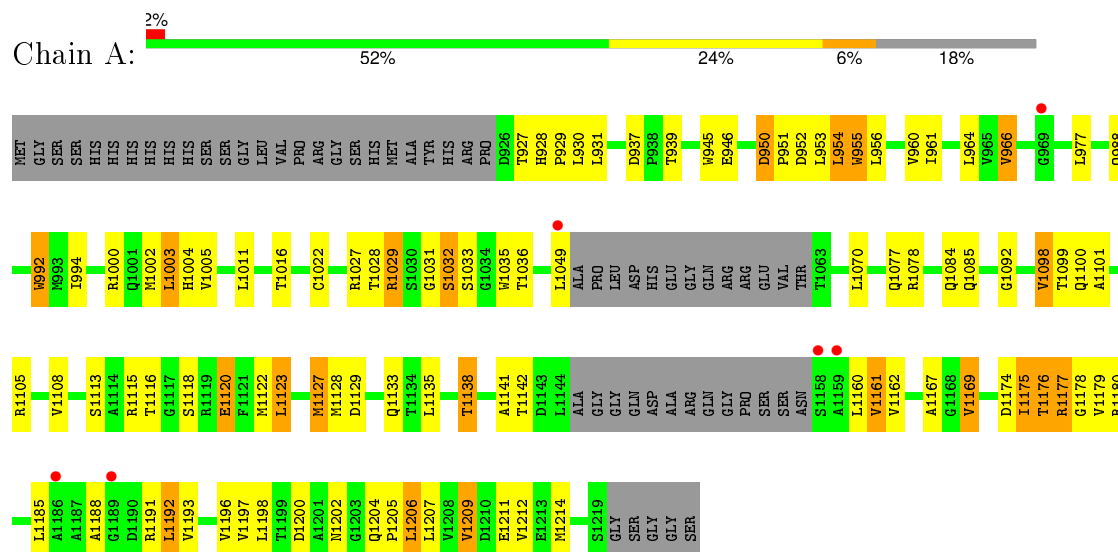


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		

- Molecule 1: Phthiocerol synthesis polyketide synthase type I PpsC



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	89.51Å 89.51Å 159.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.38 – 2.70 36.38 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (36.38-2.70) 99.8 (36.38-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.208 , 0.251 0.207 , 0.251	Depositor DCC
R_{free} test set	939 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	86.6	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 18424 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1988	wwPDB-VP
Average B, all atoms (Å ²)	90.0	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PO4

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	0.61	2/2010 (0.1%)	0.80	2/2751 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	955	TRP	CD2-CE2	5.74	1.48	1.41
1	A	992	TRP	CD2-CE2	5.21	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	955	TRP	CB-CA-C	-5.92	98.56	110.40
1	A	1032	SER	CB-CA-C	5.76	121.05	110.10

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	1978	0	1951	80	0
2	A	5	0	0	0	0
3	A	5	0	0	0	0
All	All	1988	0	1951	80	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 (80) 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:955:TRP:HE3	1:A:955:TRP:O	1.32	1.09
1:A:955:TRP:O	1:A:955:TRP:CE3	2.08	1.06
1:A:1127:MET:HG2	1:A:1175:ILE:HG13	1.43	1.01
1:A:1070:LEU:HD11	1:A:1098:VAL:HG23	1.52	0.90
1:A:1138:THR:HG21	1:A:1185:LEU:HB3	1.56	0.87
1:A:1070:LEU:HD11	1:A:1098:VAL:CG2	2.03	0.86
1:A:1099:THR:HG22	1:A:1101:ALA:H	1.40	0.86
1:A:1192:LEU:HD13	1:A:1214:MET:HB2	1.57	0.85
1:A:1032:SER:O	1:A:1033:SER:HB2	1.79	0.82
1:A:1123:LEU:O	1:A:1123:LEU:HD12	1.81	0.81
1:A:1200:ASP:HB2	1:A:1204:GLN:H	1.52	0.75
1:A:994:ILE:HB	1:A:1169:VAL:HG13	1.71	0.72
1:A:1070:LEU:CD1	1:A:1098:VAL:HG23	2.19	0.71
1:A:946:GLU:OE1	1:A:1029:ARG:NH1	2.24	0.70
1:A:1003:LEU:HD13	1:A:1028:THR:HG21	1.75	0.68
1:A:1138:THR:HG22	1:A:1141:ALA:H	1.59	0.67
1:A:937:ASP:OD1	1:A:939:THR:HG22	1.95	0.66
1:A:1105:ARG:HD2	1:A:1180:ARG:NH2	2.12	0.65
1:A:1105:ARG:HD2	1:A:1180:ARG:HH21	1.62	0.65
1:A:1175:ILE:O	1:A:1178:GLY:N	2.23	0.64
1:A:1129:ASP:O	1:A:1133:GLN:HG3	1.99	0.62
1:A:1070:LEU:CD1	1:A:1098:VAL:CG2	2.77	0.61
1:A:1099:THR:HG22	1:A:1100:GLN:N	2.16	0.61
1:A:964:LEU:HD22	1:A:1004:HIS:CE1	2.36	0.60
1:A:1078:ARG:NH1	1:A:1142:THR:HG22	2.17	0.59
1:A:1123:LEU:C	1:A:1123:LEU:HD12	2.23	0.59
1:A:1127:MET:CG	1:A:1175:ILE:HG13	2.27	0.59
1:A:1099:THR:HG22	1:A:1101:ALA:N	2.14	0.59
1:A:960:VAL:HG22	1:A:1085:GLN:HB3	1.85	0.58
1:A:1092:GLY:O	1:A:1108:VAL:HA	2.06	0.56
1:A:1135:LEU:O	1:A:1138:THR:HB	2.06	0.55
1:A:1200:ASP:HB2	1:A:1204:GLN:N	2.21	0.55
1:A:1174:ASP:HB3	1:A:1176:THR:HG23	1.88	0.55
1:A:955:TRP:CD2	1:A:955:TRP:O	2.60	0.54
1:A:1078:ARG:HH12	1:A:1142:THR:HG22	1.72	0.54
1:A:1174:ASP:HB3	1:A:1176:THR:CG2	2.38	0.53
1:A:1200:ASP:HB3	1:A:1202:ASN:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027:ARG:HD3	1:A:1035:TRP:HB3	1.90	0.53
1:A:1200:ASP:OD2	1:A:1204:GLN:HB2	2.09	0.53
1:A:977:LEU:HD22	1:A:992:TRP:HB2	1.91	0.52
1:A:937:ASP:CG	1:A:939:THR:HG22	2.29	0.52
1:A:951:PRO:HG3	1:A:1005:VAL:O	2.09	0.52
1:A:1191:ARG:HG3	1:A:1191:ARG:O	2.11	0.51
1:A:1167:ALA:HB3	1:A:1211:GLU:HB3	1.93	0.51
1:A:953:LEU:HG	1:A:954:LEU:CD2	2.42	0.50
1:A:1084:GLN:HB2	1:A:1160:LEU:HD22	1.94	0.49
1:A:929:PRO:HD3	1:A:1120:GLU:HG3	1.95	0.48
1:A:1160:LEU:HD13	1:A:1162:VAL:HG13	1.95	0.47
1:A:1188:ALA:O	1:A:1191:ARG:O	2.33	0.47
1:A:1161:VAL:HG23	1:A:1214:MET:CE	2.46	0.46
1:A:955:TRP:C	1:A:955:TRP:CE3	2.84	0.46
1:A:950:ASP:HB3	1:A:952:ASP:OD2	2.16	0.46
1:A:1049:LEU:HD21	1:A:1205:PRO:HG2	1.98	0.46
1:A:1192:LEU:CD1	1:A:1214:MET:HB2	2.38	0.46
1:A:946:GLU:CD	1:A:1029:ARG:NH1	2.69	0.46
1:A:1115:ARG:O	1:A:1118:SER:CB	2.63	0.46
1:A:1029:ARG:HB2	1:A:1035:TRP:CD1	2.51	0.45
1:A:1128:MET:HG3	1:A:1207:LEU:HD21	1.98	0.45
1:A:1099:THR:CG2	1:A:1100:GLN:N	2.79	0.45
1:A:1032:SER:O	1:A:1033:SER:CB	2.55	0.44
1:A:966:VAL:HG21	1:A:1002:MET:HE3	1.99	0.44
1:A:1138:THR:O	1:A:1138:THR:HG22	2.17	0.44
1:A:1016:THR:O	1:A:1022:CYS:HB2	2.18	0.44
1:A:1175:ILE:HG12	1:A:1176:THR:N	2.32	0.43
1:A:1206:LEU:HA	1:A:1206:LEU:HD12	1.86	0.43
1:A:1175:ILE:C	1:A:1177:ARG:N	2.72	0.43
1:A:953:LEU:HG	1:A:954:LEU:HD22	2.00	0.43
1:A:1174:ASP:O	1:A:1175:ILE:C	2.57	0.42
1:A:1200:ASP:HB3	1:A:1202:ASN:N	2.34	0.42
1:A:961:ILE:HD12	1:A:1002:MET:HE3	2.02	0.42
1:A:1011:LEU:HD12	1:A:1027:ARG:O	2.20	0.42
1:A:928:HIS:HB3	1:A:931:LEU:HB3	2.01	0.42
1:A:1209:VAL:HG22	1:A:1212:VAL:HG23	2.02	0.42
1:A:1175:ILE:O	1:A:1176:THR:C	2.57	0.42
1:A:1105:ARG:CD	1:A:1180:ARG:NH2	2.81	0.42
1:A:1127:MET:HA	1:A:1127:MET:CE	2.50	0.41
1:A:1161:VAL:CG2	1:A:1214:MET:HE3	2.51	0.41
1:A:1029:ARG:NE	1:A:1031:GLY:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1120:GLU:HG2	1:A:1120:GLU:H	1.63	0.41
1:A:1175:ILE:HB	1:A:1198:LEU:CD2	2.51	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	262/325 (81%)	250 (95%)	12 (5%)	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	205/254 (81%)	172 (84%)	33 (16%)	3	7

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	927	THR
1	A	930	LEU
1	A	945	TRP
1	A	950	ASP

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Mol	Chain	Res	Type
1	A	954	LEU
1	A	956	LEU
1	A	966	VAL
1	A	988	GLN
1	A	1000	ARG
1	A	1003	LEU
1	A	1029	ARG
1	A	1036	THR
1	A	1077	GLN
1	A	1098	VAL
1	A	1113	SER
1	A	1116	THR
1	A	1120	GLU
1	A	1122	MET
1	A	1123	LEU
1	A	1127	MET
1	A	1138	THR
1	A	1161	VAL
1	A	1169	VAL
1	A	1175	ILE
1	A	1176	THR
1	A	1177	ARG
1	A	1179	VAL
1	A	1192	LEU
1	A	1193	VAL
1	A	1196	VAL
1	A	1197	VAL
1	A	1206	LEU
1	A	1209	VAL

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	1004	HIS
1	A	1038	HIS
1	A	1077	GLN

5.3.3 RNA ⓘ

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](#)

1 ligand is 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	PO4	A	1301	-	4,4,4	0.50	0	6,6,6	0.24	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	PO4	A	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 [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	268/325 (82%)	-0.07	6 (2%) 65 66	65, 85, 125, 146	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1159	ALA	3.4
1	A	1158	SER	2.7
1	A	1049	LEU	2.3
1	A	1186	ALA	2.2
1	A	969	GLY	2.1
1	A	1189	GLY	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	PO4	A	1301	5/5	0.92	0.32	1.51	134,135,140,147	0

6.5 Other polymers [i](#)

There are no such residues in this entry.