



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:40 am GMT

PDB ID : 1L4B
Title : Crystal Structure of CobT in apo state
Authors : Cheong, C.-G.; Escalante-Semerena, J.; Rayment, I.
Deposited on : 2002-03-04
Resolution : 1.70 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

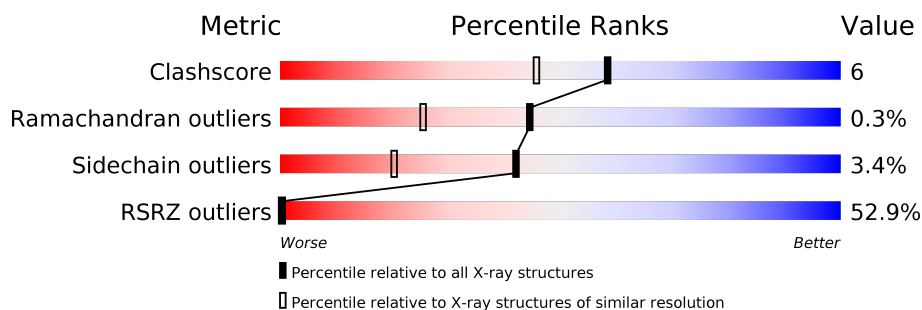
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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))
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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	356	<div> <div>51%</div> <div>81%</div> <div>14%</div> <div>..</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2488 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.

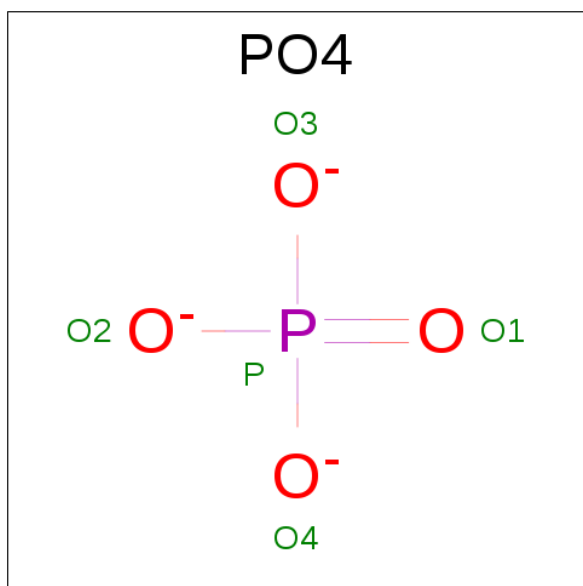
- Molecule 1 is a protein called Nicotinate-nucleotide--dimethylbenzimidazole phosphoribosyl transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	340	2362	1487	411	441	23	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	THR	ALA	CONFLICT	UNP Q05603

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



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

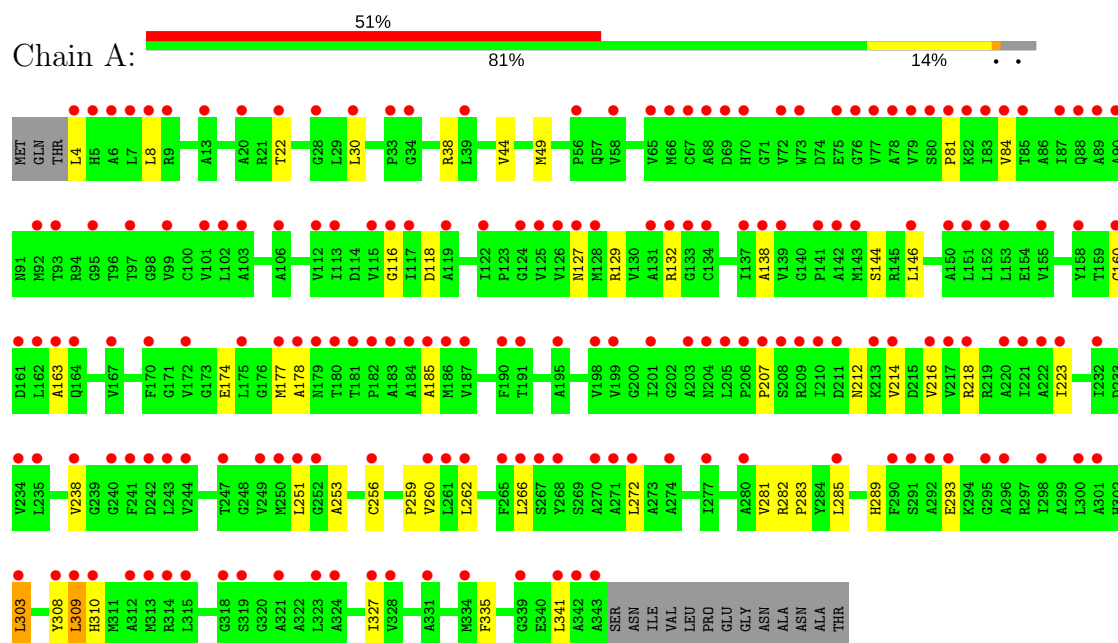
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total 121	O 121	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: Nicotinate-nucleotide--dimethylbenzimidazole phosphoribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	72.10Å 90.20Å 47.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	500.00 – 1.70 27.36 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (500.00-1.70) 88.1 (27.36-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.03 (at 1.70Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.191 , 0.218 0.345 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	2488	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.91% 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: 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	0.39	0/2400	0.63	1/3275 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	207	PRO	N-CA-CB	5.40	109.78	103.30

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	2362	0	2354	26	1
2	A	5	0	0	0	0
3	A	121	0	0	3	0
All	All	2488	0	2354	26	1

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 (26) 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:127:ASN:OD1	1:A:129:ARG:HG2	1.91	0.70
1:A:30:LEU:HD12	1:A:341:LEU:HD23	1.72	0.70
1:A:22:THR:HG23	1:A:335:PHE:CE1	2.33	0.64
1:A:293:GLU:HG3	3:A:541:HOH:O	1.97	0.62
1:A:272:LEU:HD23	1:A:303:LEU:HD13	1.83	0.61
1:A:251:LEU:HD23	1:A:281:VAL:HG21	1.83	0.60
1:A:310:HIS:HE1	3:A:461:HOH:O	1.85	0.60
1:A:289:HIS:HD2	3:A:457:HOH:O	1.87	0.57
1:A:81:PRO:HG2	1:A:84:VAL:HG23	1.89	0.54
1:A:309:LEU:HD11	1:A:327:ILE:HD11	1.90	0.53
1:A:238:VAL:HG12	1:A:238:VAL:O	2.09	0.52
1:A:185:ALA:HB1	1:A:238:VAL:HG11	1.91	0.52
1:A:282:ARG:HB3	1:A:283:PRO:HD3	1.93	0.51
1:A:212:ASN:O	1:A:216:VAL:HG23	2.09	0.51
1:A:22:THR:HG23	1:A:335:PHE:HE1	1.77	0.48
1:A:177:MET:O	1:A:178:ALA:HB3	2.14	0.48
1:A:144:SER:OG	1:A:146:LEU:HG	2.15	0.46
1:A:253:ALA:CB	1:A:260:VAL:CG2	2.96	0.44
1:A:118:ASP:OD2	1:A:132:ARG:HD3	2.18	0.44
1:A:253:ALA:HB3	1:A:260:VAL:CG2	2.48	0.43
1:A:49:MET:SD	1:A:259:PRO:HB3	2.58	0.43
1:A:214:VAL:HG12	1:A:218:ARG:NH1	2.35	0.42
1:A:138:ALA:O	1:A:223:ILE:HD12	2.19	0.41
1:A:160:CYS:O	1:A:163:ALA:HB3	2.21	0.41
1:A:22:THR:HG21	1:A:44:VAL:HA	2.03	0.41
1:A:4:LEU:O	1:A:8:LEU:HG	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:TYR:O	1:A:310:HIS:N[2_665]	2.13	0.07

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	338/356 (95%)	328 (97%)	9 (3%)	1 (0%)	44 25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	GLY

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	232/263 (88%)	224 (97%)	8 (3%)	42 20

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

Mol	Chain	Res	Type
1	A	38	ARG
1	A	174	GLU
1	A	256	CYS
1	A	262	LEU
1	A	266	LEU
1	A	285	LEU
1	A	303	LEU
1	A	309	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	57	GLN
1	A	276	GLN
1	A	289	HIS
1	A	310	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	337	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](#)

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	998	-	4,4,4	1.23	0	6,6,6	0.44	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	998	-	-	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

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	340/356 (95%)	2.29	180 (52%) 0 0	10, 19, 46, 77	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	PRO	8.3
1	A	78	ALA	7.6
1	A	146	LEU	6.8
1	A	79	VAL	6.1
1	A	4	LEU	5.9
1	A	172	VAL	5.4
1	A	87	ILE	5.3
1	A	203	ALA	5.3
1	A	77	VAL	5.2
1	A	67	CYS	5.1
1	A	210	ILE	5.1
1	A	137	ILE	5.0
1	A	6	ALA	5.0
1	A	184	ALA	4.9
1	A	30	LEU	4.9
1	A	214	VAL	4.8
1	A	216	VAL	4.8
1	A	341	LEU	4.8
1	A	243	LEU	4.7
1	A	241	PHE	4.7
1	A	222	ALA	4.6
1	A	142	ALA	4.5
1	A	99	VAL	4.5
1	A	113	ILE	4.5
1	A	265	PHE	4.4
1	A	73	TRP	4.4
1	A	187	VAL	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	7	LEU	4.4
1	A	163	ALA	4.4
1	A	201	ILE	4.3
1	A	179	ASN	4.1
1	A	205	LEU	4.1
1	A	117	ILE	4.1
1	A	34	GLY	4.1
1	A	199	VAL	4.0
1	A	266	LEU	4.0
1	A	206	PRO	3.9
1	A	90	ALA	3.9
1	A	131	ALA	3.9
1	A	125	VAL	3.8
1	A	213	LYS	3.8
1	A	160	CYS	3.8
1	A	182	PRO	3.7
1	A	76	GLY	3.7
1	A	221	ILE	3.7
1	A	220	ALA	3.6
1	A	343	ALA	3.6
1	A	128	MET	3.6
1	A	240	GLY	3.6
1	A	83	ILE	3.6
1	A	139	VAL	3.5
1	A	238	VAL	3.5
1	A	89	ALA	3.5
1	A	301	ALA	3.4
1	A	177	MET	3.4
1	A	122	ILE	3.4
1	A	164	GLN	3.4
1	A	101	VAL	3.3
1	A	244	VAL	3.3
1	A	300	LEU	3.3
1	A	72	VAL	3.3
1	A	92	MET	3.3
1	A	68	ALA	3.3
1	A	185	ALA	3.3
1	A	314	ARG	3.3
1	A	190	PHE	3.2
1	A	315	LEU	3.2
1	A	119	ALA	3.2
1	A	204	ASN	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	321	ALA	3.2
1	A	260	VAL	3.2
1	A	262	LEU	3.2
1	A	133	GLY	3.2
1	A	195	ALA	3.1
1	A	58	VAL	3.1
1	A	81	PRO	3.1
1	A	153	LEU	3.1
1	A	178	ALA	3.1
1	A	13	ALA	3.0
1	A	134	CYS	3.0
1	A	274	ALA	3.0
1	A	292	ALA	3.0
1	A	102	LEU	3.0
1	A	143	MET	3.0
1	A	80	SER	3.0
1	A	186	MET	2.9
1	A	303	LEU	2.9
1	A	66	MET	2.9
1	A	268	TYR	2.9
1	A	28	GLY	2.9
1	A	85	THR	2.9
1	A	175	LEU	2.9
1	A	75	GLU	2.9
1	A	218	ARG	2.8
1	A	9	ARG	2.8
1	A	232	ILE	2.8
1	A	296	ALA	2.8
1	A	342	ALA	2.8
1	A	152	LEU	2.8
1	A	217	VAL	2.8
1	A	211	ASP	2.8
1	A	112	VAL	2.8
1	A	151	LEU	2.8
1	A	261	LEU	2.8
1	A	256	CYS	2.8
1	A	39	LEU	2.8
1	A	252	GLY	2.8
1	A	312	ALA	2.8
1	A	158	TYR	2.7
1	A	180	THR	2.7
1	A	20	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	318	GLY	2.7
1	A	270	ALA	2.7
1	A	339	GLY	2.7
1	A	126	VAL	2.7
1	A	93	THR	2.7
1	A	97	THR	2.7
1	A	103	ALA	2.6
1	A	84	VAL	2.6
1	A	70	HIS	2.6
1	A	272	LEU	2.6
1	A	251	LEU	2.6
1	A	323	LEU	2.6
1	A	181	THR	2.6
1	A	223	ILE	2.6
1	A	115	VAL	2.6
1	A	150	ALA	2.6
1	A	22	THR	2.5
1	A	293	GLU	2.5
1	A	138	ALA	2.5
1	A	8	LEU	2.5
1	A	308	TYR	2.5
1	A	191	THR	2.5
1	A	124	GLY	2.5
1	A	234	VAL	2.5
1	A	208	SER	2.5
1	A	141	PRO	2.5
1	A	291	SER	2.5
1	A	5	HIS	2.4
1	A	56	PRO	2.4
1	A	324	ALA	2.4
1	A	95	GLY	2.4
1	A	250	MET	2.4
1	A	167	VAL	2.4
1	A	309	LEU	2.4
1	A	69	ASP	2.4
1	A	116	GLY	2.4
1	A	247	THR	2.4
1	A	33	PRO	2.3
1	A	155	VAL	2.3
1	A	267	SER	2.3
1	A	285	LEU	2.3
1	A	209	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	198	VAL	2.3
1	A	295	GLY	2.3
1	A	82	LYS	2.2
1	A	319	SER	2.2
1	A	106	ALA	2.2
1	A	65	VAL	2.2
1	A	328	VAL	2.2
1	A	298	ILE	2.2
1	A	183	ALA	2.2
1	A	249	VAL	2.2
1	A	271	ALA	2.2
1	A	127	ASN	2.1
1	A	310	HIS	2.1
1	A	132	ARG	2.1
1	A	162	LEU	2.1
1	A	313	MET	2.1
1	A	170	PHE	2.1
1	A	280	ALA	2.1
1	A	334	MET	2.1
1	A	161	ASP	2.1
1	A	290	PHE	2.1
1	A	331	ALA	2.1
1	A	242	ASP	2.1
1	A	88	GLN	2.0
1	A	277	ILE	2.0
1	A	327	ILE	2.0
1	A	235	LEU	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	998	5/5	0.77	0.18	-1.27	21,22,23,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.