



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:56 AM UTC

PDB ID : 1L4B / pdb_00001l4b
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

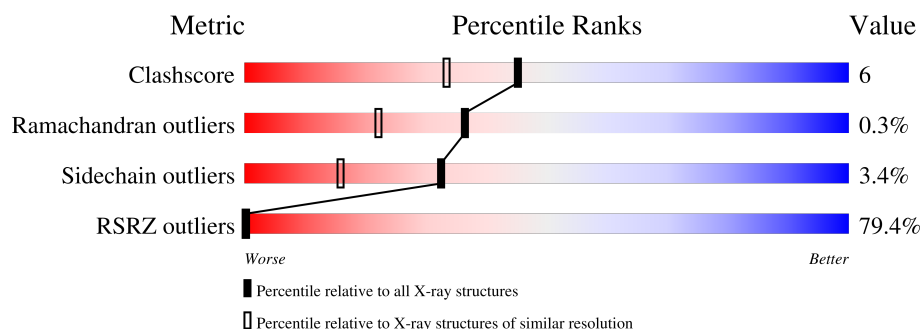
1 Overall quality at a glance

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	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 of 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 $\leq 5\%$. 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	76% 79% 16% ..

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 (CCD ID: PO4) (formula: O_4P).



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

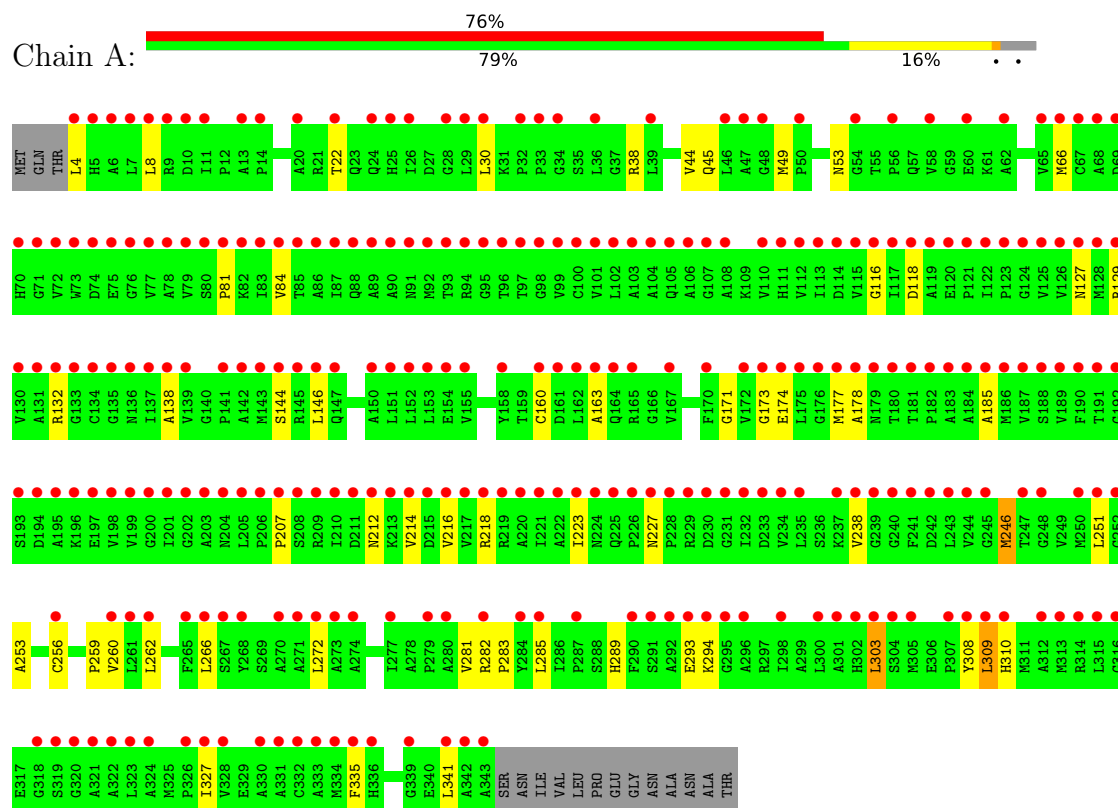
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total 121	O 121	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 56.32 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (500.00-1.70) 88.4 (56.32-1.70)	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.	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.3	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 [i](#)

5.1 Standard geometry [i](#)

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	0.54	2/2400 (0.1%)	0.91	6/3275 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	246	MET	SD-CE	-5.42	1.66	1.79
1	A	66	MET	SD-CE	-5.39	1.66	1.79

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	PRO	N-CA-CB	5.91	109.78	103.39
1	A	227	ASN	CA-C-N	5.73	126.11	119.47
1	A	227	ASN	C-N-CA	5.73	126.11	119.47
1	A	294	LYS	N-CA-C	5.51	117.72	111.11
1	A	171	GLY	N-CA-C	-5.31	102.72	111.38
1	A	53	ASN	N-CA-C	5.09	118.61	111.74

There are no chirality outliers.

There are no planarity outliers.

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	2362	0	2354	28	1
2	A	5	0	0	0	0
3	A	121	0	0	3	0
All	All	2488	0	2354	28	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 (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: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:173:GLY:C	1:A:246:MET:HE3	2.41	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:45:GLN:HG2	1:A:49:MET:HE3	2.00	0.43
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%)	36 22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	GLY

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	232/263 (88%)	224 (97%)	8 (3%)	32 16

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	285	LEU
1	A	303	LEU
1	A	309	LEU

Sometimes 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
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 oligosaccharides 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	1.56	0	6,6,6	0.52	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 ⓘ

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%)	3.41	270 (79%) 0 0	10, 19, 46, 77	0

All (270) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	PRO	11.4
1	A	4	LEU	10.8
1	A	146	LEU	9.3
1	A	73	TRP	8.7
1	A	341	LEU	8.6
1	A	79	VAL	8.6
1	A	343	ALA	8.5
1	A	78	ALA	8.0
1	A	210	ILE	7.6
1	A	342	ALA	7.0
1	A	83	ILE	6.7
1	A	172	VAL	6.7
1	A	77	VAL	6.7
1	A	214	VAL	6.6
1	A	222	ALA	6.6
1	A	82	LYS	6.6
1	A	203	ALA	6.5
1	A	30	LEU	6.4
1	A	164	GLN	6.3
1	A	205	LEU	6.3
1	A	216	VAL	6.2
1	A	131	ALA	6.1
1	A	80	SER	6.0
1	A	7	LEU	5.9
1	A	199	VAL	5.9
1	A	195	ALA	5.9
1	A	137	ILE	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	75	GLU	5.8
1	A	76	GLY	5.8
1	A	117	ILE	5.8
1	A	314	ARG	5.8
1	A	163	ALA	5.8
1	A	265	PHE	5.8
1	A	133	GLY	5.7
1	A	303	LEU	5.7
1	A	84	VAL	5.7
1	A	6	ALA	5.6
1	A	213	LYS	5.5
1	A	179	ASN	5.5
1	A	204	ASN	5.4
1	A	241	PHE	5.3
1	A	139	VAL	5.3
1	A	178	ALA	5.3
1	A	113	ILE	5.2
1	A	221	ILE	5.2
1	A	101	VAL	5.1
1	A	90	ALA	5.1
1	A	67	CYS	5.1
1	A	81	PRO	5.1
1	A	87	ILE	5.1
1	A	201	ILE	5.0
1	A	220	ALA	5.0
1	A	209	ARG	5.0
1	A	218	ARG	5.0
1	A	187	VAL	4.9
1	A	240	GLY	4.9
1	A	243	LEU	4.9
1	A	238	VAL	4.9
1	A	142	ALA	4.9
1	A	184	ALA	4.8
1	A	22	THR	4.8
1	A	228	PRO	4.7
1	A	202	GLY	4.7
1	A	339	GLY	4.7
1	A	232	ILE	4.7
1	A	9	ARG	4.7
1	A	89	ALA	4.7
1	A	119	ALA	4.7
1	A	122	ILE	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	34	GLY	4.7
1	A	125	VAL	4.6
1	A	182	PRO	4.6
1	A	124	GLY	4.6
1	A	295	GLY	4.6
1	A	8	LEU	4.5
1	A	315	LEU	4.5
1	A	223	ILE	4.5
1	A	206	PRO	4.5
1	A	72	VAL	4.4
1	A	13	ALA	4.3
1	A	190	PHE	4.3
1	A	234	VAL	4.3
1	A	102	LEU	4.3
1	A	158	TYR	4.2
1	A	217	VAL	4.2
1	A	69	ASP	4.2
1	A	212	ASN	4.2
1	A	28	GLY	4.1
1	A	260	VAL	4.1
1	A	68	ALA	4.1
1	A	296	ALA	4.1
1	A	175	LEU	4.1
1	A	266	LEU	4.1
1	A	227	ASN	4.0
1	A	5	HIS	4.0
1	A	198	VAL	4.0
1	A	138	ALA	4.0
1	A	160	CYS	4.0
1	A	85	THR	3.9
1	A	193	SER	3.9
1	A	292	ALA	3.9
1	A	126	VAL	3.9
1	A	313	MET	3.9
1	A	191	THR	3.9
1	A	185	ALA	3.9
1	A	99	VAL	3.9
1	A	298	ILE	3.9
1	A	70	HIS	3.9
1	A	93	THR	3.8
1	A	92	MET	3.8
1	A	302	HIS	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	277	ILE	3.8
1	A	29	LEU	3.8
1	A	36	LEU	3.8
1	A	150	ALA	3.8
1	A	177	MET	3.8
1	A	208	SER	3.7
1	A	39	LEU	3.7
1	A	262	LEU	3.7
1	A	211	ASP	3.7
1	A	180	THR	3.6
1	A	225	GLN	3.6
1	A	128	MET	3.6
1	A	33	PRO	3.6
1	A	321	ALA	3.6
1	A	167	VAL	3.6
1	A	300	LEU	3.6
1	A	200	GLY	3.5
1	A	290	PHE	3.5
1	A	280	ALA	3.5
1	A	132	ARG	3.5
1	A	268	TYR	3.5
1	A	116	GLY	3.5
1	A	130	VAL	3.5
1	A	291	SER	3.5
1	A	318	GLY	3.5
1	A	293	GLU	3.4
1	A	151	LEU	3.4
1	A	86	ALA	3.4
1	A	143	MET	3.4
1	A	98	GLY	3.4
1	A	127	ASN	3.4
1	A	154	GLU	3.3
1	A	194	ASP	3.3
1	A	310	HIS	3.3
1	A	95	GLY	3.3
1	A	272	LEU	3.3
1	A	141	PRO	3.3
1	A	144	SER	3.3
1	A	294	LYS	3.3
1	A	74	ASP	3.3
1	A	189	VAL	3.3
1	A	244	VAL	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	312	ALA	3.3
1	A	324	ALA	3.3
1	A	71	GLY	3.3
1	A	32	PRO	3.3
1	A	251	LEU	3.3
1	A	331	ALA	3.3
1	A	181	THR	3.2
1	A	60	GLU	3.2
1	A	155	VAL	3.2
1	A	118	ASP	3.2
1	A	152	LEU	3.2
1	A	235	LEU	3.2
1	A	237	LYS	3.2
1	A	106	ALA	3.2
1	A	176	GLY	3.2
1	A	219	ARG	3.2
1	A	121	PRO	3.2
1	A	197	GLU	3.2
1	A	327	ILE	3.1
1	A	110	VAL	3.1
1	A	94	ARG	3.1
1	A	319	SER	3.1
1	A	129	ARG	3.1
1	A	50	PRO	3.0
1	A	58	VAL	3.0
1	A	66	MET	3.0
1	A	309	LEU	3.0
1	A	224	ASN	3.0
1	A	103	ALA	3.0
1	A	134	CYS	3.0
1	A	186	MET	3.0
1	A	252	GLY	3.0
1	A	112	VAL	3.0
1	A	242	ASP	3.0
1	A	274	ALA	3.0
1	A	91	ASN	3.0
1	A	215	ASP	2.9
1	A	165	ARG	2.9
1	A	188	SER	2.9
1	A	308	TYR	2.9
1	A	153	LEU	2.9
1	A	192	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	196	LYS	2.9
1	A	96	THR	2.9
1	A	301	ALA	2.8
1	A	135	GLY	2.8
1	A	88	GLN	2.8
1	A	162	LEU	2.8
1	A	323	LEU	2.8
1	A	256	CYS	2.8
1	A	111	HIS	2.8
1	A	183	ALA	2.8
1	A	136	ASN	2.8
1	A	24	GLN	2.8
1	A	174	GLU	2.8
1	A	316	GLY	2.8
1	A	65	VAL	2.7
1	A	328	VAL	2.7
1	A	26	ILE	2.7
1	A	97	THR	2.7
1	A	230	ASP	2.7
1	A	100	CYS	2.7
1	A	247	THR	2.7
1	A	56	PRO	2.7
1	A	261	LEU	2.7
1	A	47	ALA	2.7
1	A	322	ALA	2.7
1	A	229	ARG	2.6
1	A	307	PRO	2.6
1	A	46	LEU	2.6
1	A	332	CYS	2.6
1	A	273	ALA	2.6
1	A	279	PRO	2.6
1	A	173	GLY	2.6
1	A	267	SER	2.6
1	A	123	PRO	2.6
1	A	239	GLY	2.6
1	A	334	MET	2.6
1	A	10	ASP	2.5
1	A	147	GLN	2.5
1	A	115	VAL	2.5
1	A	104	ALA	2.5
1	A	333	ALA	2.5
1	A	54	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	120	GLU	2.5
1	A	285	LEU	2.5
1	A	161	ASP	2.5
1	A	25	HIS	2.5
1	A	48	GLY	2.4
1	A	20	ALA	2.4
1	A	145	ARG	2.4
1	A	336	HIS	2.4
1	A	226	PRO	2.4
1	A	271	ALA	2.4
1	A	231	GLY	2.3
1	A	233	ASP	2.3
1	A	14	PRO	2.3
1	A	287	PRO	2.3
1	A	250	MET	2.3
1	A	107	GLY	2.3
1	A	245	GLY	2.3
1	A	320	GLY	2.3
1	A	335	PHE	2.2
1	A	326	PRO	2.2
1	A	270	ALA	2.2
1	A	62	ALA	2.2
1	A	305	MET	2.2
1	A	105	GLN	2.2
1	A	11	ILE	2.2
1	A	114	ASP	2.1
1	A	170	PHE	2.1
1	A	108	ALA	2.1
1	A	248	GLY	2.1
1	A	304	SER	2.1
1	A	330	ALA	2.0
1	A	282	ARG	2.0
1	A	284	TYR	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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	A	998	5/5	0.78	0.16	21,22,23,24	0

6.5 Other polymers

There are no such residues in this entry.