



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:38 PM GMT

PDB ID : 4A1O
Title : CRYSTAL STRUCTURE OF MYCOBACTERIUM TUBERCULOSIS PURH
COMPLEXED WITH AICAR AND A NOVEL NUCLEOTIDE CFAIR, AT
2.48 Å RESOLUTION.
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Deposited on : 2011-09-17
Resolution : 2.48 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 (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

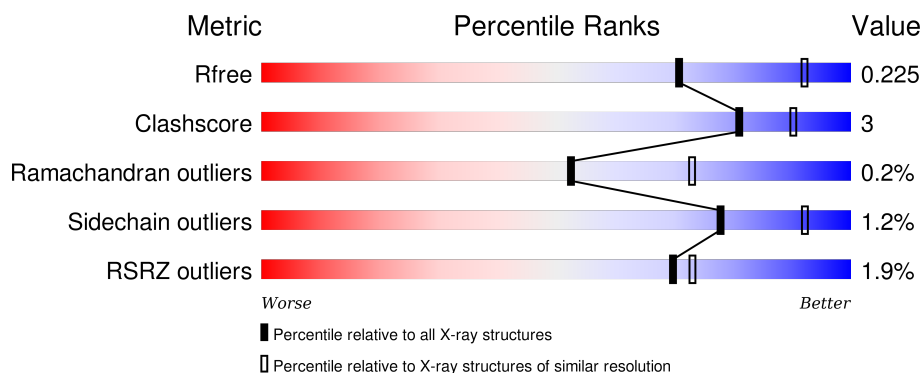
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (2.50-2.46)

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	523	 2% 90% 8%
1	B	523	 0% 91% 7%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8032 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.

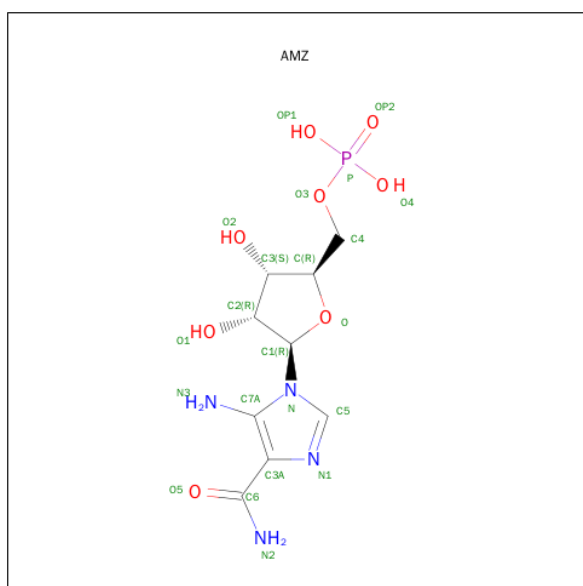
- Molecule 1 is a protein called BIFUNCTIONAL PURINE BIOSYNTHESIS PROTEIN PURH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	1	0
			3832	2407	688	725	12			
1	B	517	Total	C	N	O	S	0	1	0
			3844	2417	689	726	12			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	K	0	0
			1	1		
2	A	1	Total	K	0	0
			1	1		

- Molecule 3 is AMINOIMIDAZOLE 4-CARBOXAMIDE RIBONUCLEOTIDE (three-letter code: AMZ) (formula: $C_9H_{15}N_4O_8P$).



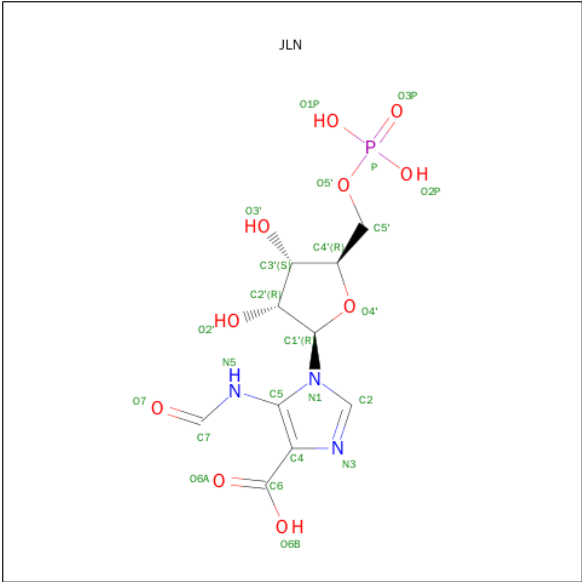
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			22	9	4	8	1		
3	B	1	Total	C	N	O	P	0	0
			22	9	4	8	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 5 is 5-(FORMYLAMINO)-1-(5-O-PHOSPHONO-BETA-D-RIBOFURANOSYL)-1H-IMIDAZOLE-4-CARBOXYLIC ACID (three-letter code: JLN) (formula: C₁₀H₁₄N₃O₁₀P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			24	10	3	10	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	142	Total	O	0	0
			142	142		
6	B	129	Total	O	0	0
			129	129		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.26Å 107.88Å 130.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.84 – 2.48 43.84 – 2.48	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.84-2.48) 99.2 (43.84-2.48)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.33 (at 2.48Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.182 , 0.227 0.177 , 0.225	Depositor DCC
R_{free} test set	1914 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.6	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	1 of 38215 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8032	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: K, AMZ, PO4, JLN

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	0.50	0/3914	0.65	0/5338
1	B	0.51	0/3927	0.64	0/5358
All	All	0.50	0/7841	0.65	0/10696

There are no bond length outliers.

There are no bond angle outliers.

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	3832	0	3773	29	0
1	B	3844	0	3793	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	22	0	13	0	0
3	B	22	0	13	0	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
5	A	24	0	9	3	0
6	A	142	0	0	0	0
6	B	129	0	0	0	0
All	All	8032	0	7601	50	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 (50) 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:179:SER:HA	1:B:196:MET:HE3	1.51	0.91
1:A:189:ASP:OD2	1:B:189:ASP:OD2	2.05	0.74
1:A:182:PHE:HB2	1:B:196:MET:CE	2.17	0.73
1:A:182:PHE:HB2	1:B:196:MET:HE1	1.69	0.73
1:B:60:LEU:O	1:B:77:ARG:HD2	1.98	0.63
1:A:98:LEU:HD11	1:B:66:VAL:HG11	1.81	0.61
1:A:179:SER:HA	1:B:196:MET:CE	2.29	0.59
1:B:138:VAL:HG12	1:B:185:ILE:HD11	1.85	0.58
1:B:14:LEU:HD21	1:B:137:MET:CE	2.35	0.56
1:B:77:ARG:HG3	1:B:100:ILE:HG12	1.87	0.55
1:A:18:TYR:CD2	1:A:112:PRO:HD3	2.41	0.55
1:B:479:LEU:HD21	1:B:506:ALA:HB2	1.89	0.54
1:A:479:LEU:HD21	1:A:506:ALA:HB2	1.88	0.54
1:A:182:PHE:HB2	1:B:196:MET:HE2	1.91	0.52
1:A:108:VAL:O	1:A:152:THR:HA	2.09	0.52
1:A:133:GLY:HA3	5:A:1528:JLN:C6	2.41	0.51
1:B:369:GLY:HA2	1:B:387:GLN:CD	2.31	0.50
1:B:108:VAL:O	1:B:152:THR:HA	2.11	0.49
1:B:217:TRP:HB3	1:B:236:TYR:HB3	1.95	0.49
1:A:464:GLY:HA2	1:A:488:THR:HG23	1.94	0.49
1:B:273:ASP:O	1:B:419:ARG:NH1	2.42	0.48
1:B:14:LEU:HD21	1:B:137:MET:HE1	1.96	0.47
1:B:30:LEU:HD23	1:B:164:LEU:HD11	1.97	0.47
1:A:297:VAL:HG21	1:A:322:GLU:O	2.16	0.46
1:A:95:LEU:HB3	1:A:100:ILE:O	2.15	0.46
1:B:139:ARG:HG2	1:B:185:ILE:HD13	1.97	0.46
1:A:267:ALA:HB2	1:A:282:ILE:HG13	1.98	0.46
1:B:14:LEU:HD21	1:B:137:MET:HE2	1.97	0.46
1:A:217:TRP:HB3	1:A:236:TYR:HB3	1.97	0.45
1:A:197:GLN:NE2	1:A:212:TRP:O	2.48	0.45
1:A:138:VAL:CG1	1:A:185:ILE:HD11	2.47	0.45
1:A:131:ASP:OD1	5:A:1528:JLN:N5	2.50	0.45
1:B:471:ALA:HB2	1:B:521:PHE:CE1	2.52	0.45
1:B:297:VAL:HG21	1:B:322:GLU:O	2.16	0.45
1:A:82:LEU:HD22	1:A:106:VAL:HG21	2.00	0.44
1:A:267:ALA:HA	1:A:282:ILE:HG13	2.00	0.43
1:B:138:VAL:CG1	1:B:185:ILE:HD11	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PRO:HA	1:A:157:TYR:CE1	2.53	0.43
1:A:7:ARG:HA	1:A:169:PHE:O	2.17	0.43
1:B:154:PRO:HA	1:B:157:TYR:CE1	2.54	0.43
1:B:7:ARG:HA	1:B:169:PHE:O	2.19	0.42
1:B:139:ARG:CG	1:B:185:ILE:HD13	2.49	0.42
1:A:38:ILE:HG13	1:A:55:THR:HB	2.02	0.42
1:A:471:ALA:HB2	1:A:521:PHE:CE1	2.54	0.42
1:A:325:VAL:O	1:A:329:GLU:HG3	2.20	0.42
1:B:197:GLN:OE1	1:B:212:TRP:O	2.38	0.41
1:A:133:GLY:HA3	5:A:1528:JLN:C4	2.50	0.41
1:A:267:ALA:CA	1:A:282:ILE:HG13	2.51	0.41
1:B:82:LEU:HD22	1:B:106:VAL:HG21	2.02	0.41
1:A:223:LEU:HD11	1:B:381:LEU:HD22	2.02	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	513/523 (98%)	500 (98%)	11 (2%)	2 (0%)	39	59
1	B	516/523 (99%)	506 (98%)	10 (2%)	0	100	100
All	All	1029/1046 (98%)	1006 (98%)	21 (2%)	2 (0%)	52	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	GLY
1	A	70	ARG

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	383/389 (98%)	378 (99%)	5 (1%)	76	91
1	B	385/389 (99%)	380 (99%)	5 (1%)	76	91
All	All	768/778 (99%)	758 (99%)	10 (1%)	78	91

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	297	VAL
1	A	310	LEU
1	A	359	ARG
1	A	421[A]	CYS
1	A	421[B]	CYS
1	B	171	LEU
1	B	269	ARG
1	B	297	VAL
1	B	359	ARG
1	B	479	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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
3	AMZ	A	1525	-	18,23,23	2.90	7 (38%)	20,35,35	2.14	8 (40%)
4	PO4	A	1526	-	4,4,4	1.65	0	6,6,6	0.28	0
4	PO4	A	1527	-	4,4,4	1.79	1 (25%)	6,6,6	0.32	0
5	JLN	A	1528	-	17,25,25	3.72	8 (47%)	19,37,37	3.46	8 (42%)
3	AMZ	B	1525	-	18,23,23	2.33	5 (27%)	20,35,35	1.51	3 (15%)
4	PO4	B	1526	-	4,4,4	1.44	0	6,6,6	0.29	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
3	AMZ	A	1525	-	-	0/6/30/30	0/2/2/2
4	PO4	A	1526	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1527	-	-	0/0/0/0	0/0/0/0
5	JLN	A	1528	-	-	0/7/33/33	0/2/2/2
3	AMZ	B	1525	-	-	0/6/30/30	0/2/2/2
4	PO4	B	1526	-	-	0/0/0/0	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1528	JLN	O2'-C2'	-6.44	1.27	1.43
5	A	1528	JLN	C2-N3	-5.51	1.24	1.35
5	A	1528	JLN	C7-N5	-5.00	1.27	1.34
5	A	1528	JLN	P-O1P	-3.39	1.42	1.54
5	A	1528	JLN	O3'-C3'	-3.20	1.35	1.43
3	A	1525	AMZ	C3A-C7A	-2.27	1.41	1.44
4	A	1527	PO4	P-O2	2.28	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1525	AMZ	C3-C	2.41	1.59	1.53
3	B	1525	AMZ	O1-C2	2.62	1.49	1.43
5	A	1528	JLN	C3'-C4'	2.69	1.60	1.53
3	A	1525	AMZ	O1-C2	2.75	1.49	1.43
5	A	1528	JLN	C3'-C2'	3.47	1.62	1.53
3	A	1525	AMZ	C6-N2	3.56	1.40	1.33
3	A	1525	AMZ	C3-C	3.97	1.63	1.53
3	A	1525	AMZ	C7A-N3	4.00	1.43	1.33
3	B	1525	AMZ	C7A-N3	4.06	1.43	1.33
3	B	1525	AMZ	O5-C6	4.15	1.33	1.24
3	A	1525	AMZ	O5-C6	5.88	1.36	1.24
3	B	1525	AMZ	O-C1	6.67	1.49	1.41
3	A	1525	AMZ	O-C1	6.76	1.49	1.41
5	A	1528	JLN	O4'-C1'	9.71	1.53	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1528	JLN	O7-C7-N5	-8.43	115.42	125.84
3	A	1525	AMZ	O2-C3-C2	-5.03	95.46	111.83
5	A	1528	JLN	O3'-C3'-C4'	-4.36	97.96	111.05
5	A	1528	JLN	O1P-P-O5'	-4.21	94.45	106.56
3	B	1525	AMZ	O2-C3-C2	-4.10	98.48	111.83
5	A	1528	JLN	C5'-C4'-C3'	-3.55	101.13	115.21
3	A	1525	AMZ	C3A-C6-N2	-3.09	110.62	115.90
3	A	1525	AMZ	O2-C3-C	-2.92	102.29	111.05
3	B	1525	AMZ	C3A-C6-N2	-2.67	111.32	115.90
3	A	1525	AMZ	C2-C3-C	-2.46	97.56	102.61
5	A	1528	JLN	O2P-P-O3P	-2.09	103.85	110.58
3	A	1525	AMZ	O4-P-O3	-2.03	100.72	106.56
3	B	1525	AMZ	C2-C1-N	2.23	118.12	114.17
3	A	1525	AMZ	O1-C2-C3	2.28	119.24	111.83
3	A	1525	AMZ	O4-P-OP2	2.90	119.92	110.58
3	A	1525	AMZ	O5-C6-N2	2.93	126.72	122.59
5	A	1528	JLN	O5'-P-O3P	4.19	117.80	107.14
5	A	1528	JLN	C2'-C1'-N1	5.82	124.50	114.17
5	A	1528	JLN	O2P-P-O1P	6.50	132.13	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1528	JLN	3	0

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	516/523 (98%)	-0.05	13 (2%) 61 64	32, 49, 74, 88	17 (3%)
1	B	517/523 (98%)	-0.12	7 (1%) 78 80	31, 49, 72, 90	20 (3%)
All	All	1033/1046 (98%)	-0.09	20 (1%) 70 73	31, 49, 73, 90	37 (3%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	HIS	6.1
1	A	205	PRO	5.8
1	B	242	TRP	4.9
1	A	115	GLN	4.3
1	A	117	VAL	4.2
1	A	207	ALA	3.5
1	A	116	THR	3.5
1	A	119	SER	3.3
1	A	112	PRO	3.1
1	A	242	TRP	3.1
1	A	206	VAL	2.8
1	B	91	HIS	2.8
1	A	368	ALA	2.7
1	B	98	LEU	2.3
1	B	94	ALA	2.3
1	B	158	HIS	2.3
1	B	88	LYS	2.1
1	A	121	ALA	2.1
1	A	505	ALA	2.1
1	B	155	LEU	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(\AA^2)	Q<0.9
4	PO4	A	1526	5/5	0.91	0.23	1.88	106,111,112,113	0
4	PO4	A	1527	5/5	0.98	0.16	0.64	67,68,74,74	0
4	PO4	B	1526	5/5	0.86	0.18	0.58	113,118,119,120	0
3	AMZ	B	1525	22/22	0.98	0.14	0.13	34,41,45,51	0
3	AMZ	A	1525	22/22	0.98	0.13	-0.23	31,34,37,51	0
5	JLN	A	1528	24/24	0.95	0.10	-1.25	44,52,65,72	0
2	K	B	1524	1/1	1.00	0.10	-1.71	34,34,34,34	0
2	K	A	1524	1/1	0.99	0.09	-2.02	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.