



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 07:47 am GMT

PDB ID : 3LM8
Title : Crystal Structure of Thiamine pyrophosphokinase from *Bacillus subtilis*, Northeast Structural Genomics Consortium Target SR677
Authors : Kuzin, A.; Abashidze, M.; Seetharaman, J.; Mao, M.; Xiao, R.; Foote, E.L.; Ciccocanti, C.; Wang, H.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2010-01-29
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

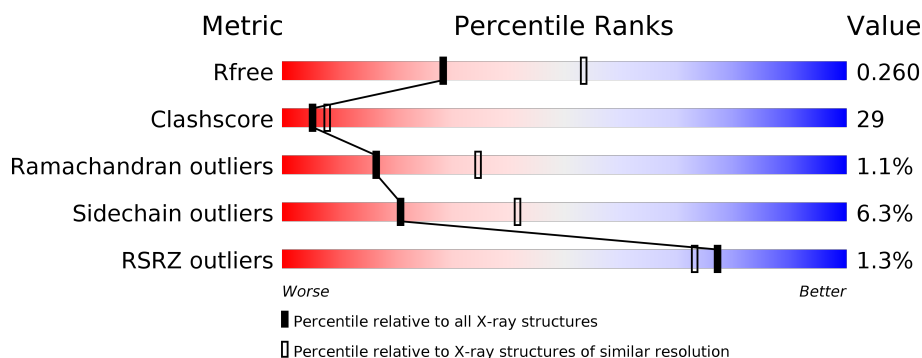
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	222	<div> <div>%</div> <div> <div>46%</div> <div>47%</div> <div>• •</div> </div> </div>
1	B	222	<div> <div>48%</div> <div>40%</div> <div>8%</div> <div>•</div> </div>
1	C	222	<div> <div>2%</div> <div>50%</div> <div>42%</div> <div>• •</div> </div>
1	D	222	<div> <div>%</div> <div>50%</div> <div>43%</div> <div>• 5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	VIB	D	223	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6941 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 Thiamine pyrophosphokinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	Se	0	0	0
			1701	1091	285	321	2	2			
1	B	214	Total	C	N	O	S	Se	0	0	0
			1701	1091	285	321	2	2			
1	C	213	Total	C	N	O	S	Se	0	0	0
			1692	1086	284	318	2	2			
1	D	212	Total	C	N	O	S	Se	0	0	0
			1683	1080	282	317	2	2			

There are 36 discrepancies between the modelled and reference sequences:

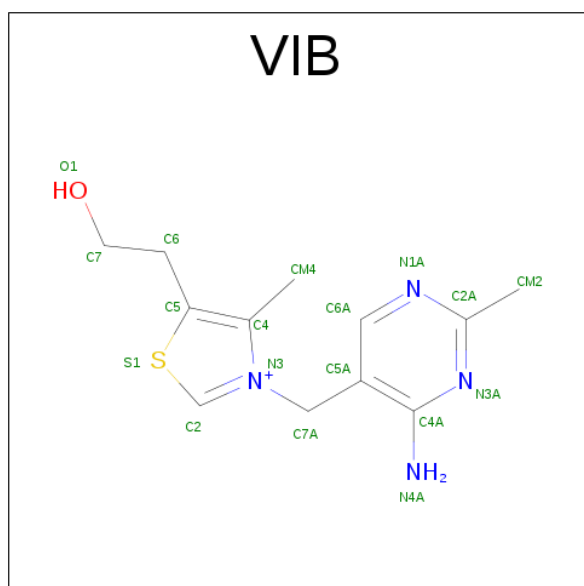
Chain	Residue	Modelled	Actual	Comment	Reference
A	203	VAL	ALA	engineered	UNP O34664
A	215	LEU	-	expression tag	UNP O34664
A	216	GLU	-	expression tag	UNP O34664
A	217	HIS	-	expression tag	UNP O34664
A	218	HIS	-	expression tag	UNP O34664
A	219	HIS	-	expression tag	UNP O34664
A	220	HIS	-	expression tag	UNP O34664
A	221	HIS	-	expression tag	UNP O34664
A	222	HIS	-	expression tag	UNP O34664
B	203	VAL	ALA	engineered	UNP O34664
B	215	LEU	-	expression tag	UNP O34664
B	216	GLU	-	expression tag	UNP O34664
B	217	HIS	-	expression tag	UNP O34664
B	218	HIS	-	expression tag	UNP O34664
B	219	HIS	-	expression tag	UNP O34664
B	220	HIS	-	expression tag	UNP O34664
B	221	HIS	-	expression tag	UNP O34664
B	222	HIS	-	expression tag	UNP O34664
C	203	VAL	ALA	engineered	UNP O34664
C	215	LEU	-	expression tag	UNP O34664
C	216	GLU	-	expression tag	UNP O34664

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Chain	Residue	Modelled	Actual	Comment	Reference
C	217	HIS	-	expression tag	UNP O34664
C	218	HIS	-	expression tag	UNP O34664
C	219	HIS	-	expression tag	UNP O34664
C	220	HIS	-	expression tag	UNP O34664
C	221	HIS	-	expression tag	UNP O34664
C	222	HIS	-	expression tag	UNP O34664
D	203	VAL	ALA	engineered	UNP O34664
D	215	LEU	-	expression tag	UNP O34664
D	216	GLU	-	expression tag	UNP O34664
D	217	HIS	-	expression tag	UNP O34664
D	218	HIS	-	expression tag	UNP O34664
D	219	HIS	-	expression tag	UNP O34664
D	220	HIS	-	expression tag	UNP O34664
D	221	HIS	-	expression tag	UNP O34664
D	222	HIS	-	expression tag	UNP O34664

- Molecule 2 is 3-(4-AMINO-2-METHYL-PYRIMIDIN-5-YLMETHYL)-5-(2-HYDROXY-ETHYL)-4-METHYL-THIAZOL-3-IUM (three-letter code: VIB) (formula: C₁₂H₁₇N₄OS).



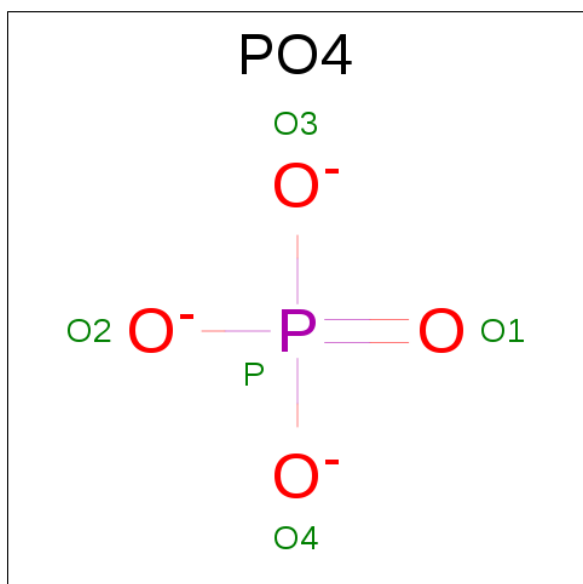
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			18	12	4	1	1		
2	B	1	Total	C	N	O	S	0	0
			18	12	4	1	1		
2	C	1	Total	C	N	O	S	0	0
			18	12	4	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	S	0	0
			18	12	4	1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

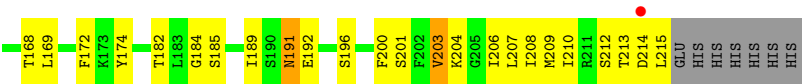
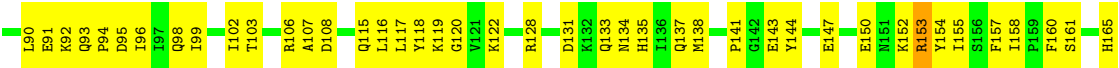
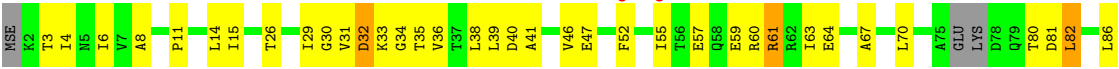
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Mg	0	0
			3	3		
4	A	2	Total	Mg	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total 20	O 20	0	0
5	B	13	Total 13	O 13	0	0
5	C	21	Total 21	O 21	0	0
5	D	13	Total 13	O 13	0	0



● Molecule 1: Thiamine pyrophosphokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.94Å 62.15Å 84.16Å 82.89° 82.02° 87.61°	Depositor
Resolution (Å)	20.00 – 2.60 41.38 – 2.56	Depositor EDS
% Data completeness (in resolution range)	82.4 (20.00-2.60) 89.2 (41.38-2.56)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.54Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.213 , 0.253 0.230 , 0.260	Depositor DCC
R_{free} test set	1346 reflections (4.81%)	DCC
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6941	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.69% 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: VIB, PO4, MG

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	0.37	0/1734	0.64	0/2346
1	B	0.96	20/1734 (1.2%)	0.76	1/2346 (0.0%)
1	C	0.38	0/1724	0.65	0/2331
1	D	0.37	0/1715	0.63	0/2320
All	All	0.58	20/6907 (0.3%)	0.67	1/9343 (0.0%)

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	163	ASP	C-O	-12.21	1.00	1.23
1	B	166	GLU	C-O	-10.88	1.02	1.23
1	B	167	LEU	C-O	-8.98	1.06	1.23
1	B	164	ILE	C-O	-7.97	1.08	1.23
1	B	166	GLU	CD-OE1	-7.91	1.17	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	ASP	CB-CG-OD2	9.20	126.58	118.30

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	1701	0	1708	107	0
1	B	1701	0	1708	99	0
1	C	1692	0	1701	107	0
1	D	1683	0	1688	99	0
2	A	18	0	17	2	0
2	B	18	0	17	3	0
2	C	18	0	17	2	0
2	D	18	0	17	1	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
4	A	2	0	0	0	0
4	B	3	0	0	0	0
5	A	20	0	0	0	0
5	B	13	0	0	0	0
5	C	21	0	0	0	0
5	D	13	0	0	0	0
All	All	6941	0	6873	397	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 29.

The worst 5 of 397 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:B:77:LYS:HD3	1:B:77:LYS:H	1.08	1.18
1:A:113:ASN:HA	1:A:116:LEU:HD23	1.40	1.03
1:A:46:VAL:HG23	1:A:47:GLU:HG2	1.47	0.95
1:A:6:ILE:HG12	1:A:29:ILE:HD11	1.48	0.94
1:C:160:PHE:HB3	1:C:206:ILE:HD13	1.53	0.91

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	212/222 (96%)	199 (94%)	12 (6%)	1 (0%)	32	58
1	B	212/222 (96%)	193 (91%)	15 (7%)	4 (2%)	9	18
1	C	209/222 (94%)	190 (91%)	18 (9%)	1 (0%)	32	58
1	D	208/222 (94%)	193 (93%)	12 (6%)	3 (1%)	13	26
All	All	841/888 (95%)	775 (92%)	57 (7%)	9 (1%)	17	35

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	105	GLY
1	B	132	LYS
1	A	77	LYS
1	B	160	PHE
1	D	92	LYS

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	187/192 (97%)	177 (95%)	10 (5%)	26	50
1	B	187/192 (97%)	170 (91%)	17 (9%)	11	21
1	C	186/192 (97%)	176 (95%)	10 (5%)	26	49
1	D	185/192 (96%)	175 (95%)	10 (5%)	26	49
All	All	745/768 (97%)	698 (94%)	47 (6%)	21	42

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	138	MSE
1	B	199	THR
1	D	153	ARG

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Mol	Chain	Res	Type
1	B	164	ILE
1	C	17	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	134	ASN
1	B	191	ASN
1	D	137	GLN
1	B	151	ASN
1	B	178	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](#)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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	$\# Z > 2$
2	VIB	A	223	-	14,19,19	1.96	1 (7%)	18,26,26	2.06	7 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	A	224	-	4,4,4	1.28	0	6,6,6	0.40	0
2	VIB	B	223	-	14,19,19	1.99	1 (7%)	18,26,26	2.05	8 (44%)
3	PO4	B	224	-	4,4,4	1.31	0	6,6,6	0.40	0
3	PO4	B	225	-	4,4,4	1.30	0	6,6,6	0.39	0
2	VIB	C	223	-	14,19,19	1.95	1 (7%)	18,26,26	2.15	7 (38%)
3	PO4	C	224	-	4,4,4	1.30	0	6,6,6	0.38	0
2	VIB	D	223	-	14,19,19	1.92	1 (7%)	18,26,26	2.01	6 (33%)

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	VIB	A	223	-	-	0/6/7/7	0/2/2/2
3	PO4	A	224	-	-	0/0/0/0	0/0/0/0
2	VIB	B	223	-	-	0/6/7/7	0/2/2/2
3	PO4	B	224	-	-	0/0/0/0	0/0/0/0
3	PO4	B	225	-	-	0/0/0/0	0/0/0/0
2	VIB	C	223	-	-	0/6/7/7	0/2/2/2
3	PO4	C	224	-	-	0/0/0/0	0/0/0/0
2	VIB	D	223	-	-	0/6/7/7	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	223	VIB	C4-N3	-6.69	1.33	1.39
2	A	223	VIB	C4-N3	-6.57	1.34	1.39
2	C	223	VIB	C4-N3	-6.56	1.34	1.39
2	D	223	VIB	C4-N3	-6.42	1.34	1.39

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	223	VIB	N1A-C2A-N3A	-3.16	120.13	125.59
2	A	223	VIB	N1A-C2A-N3A	-3.04	120.32	125.59
2	B	223	VIB	N1A-C2A-N3A	-3.02	120.36	125.59
2	C	223	VIB	N1A-C2A-N3A	-2.96	120.46	125.59
2	D	223	VIB	CM4-C4-C5	-2.87	121.75	127.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	223	VIB	2	0
2	B	223	VIB	3	0
2	C	223	VIB	2	0
2	D	223	VIB	1	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 [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	212/222 (95%)	0.02	2 (0%) 84 81	16, 34, 64, 95	0
1	B	212/222 (95%)	-0.03	1 (0%) 90 89	16, 36, 63, 74	0
1	C	211/222 (95%)	0.13	5 (2%) 59 52	16, 35, 66, 98	0
1	D	210/222 (94%)	0.09	3 (1%) 75 71	16, 36, 72, 100	0
All	All	845/888 (95%)	0.05	11 (1%) 77 73	16, 35, 65, 100	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	52	PHE	3.1
1	A	77	LYS	2.9
1	C	214	ASP	2.7
1	B	63	ILE	2.6
1	D	55	ILE	2.2

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(Å ²)	Q<0.9
2	VIB	D	223	18/18	0.90	0.27	2.34	12,36,52,58	0
4	MG	B	228	1/1	0.83	0.26	1.52	40,40,40,40	0
3	PO4	B	225	5/5	0.90	0.25	0.77	81,82,85,87	0
2	VIB	A	223	18/18	0.93	0.19	0.68	14,32,72,72	0
2	VIB	B	223	18/18	0.90	0.21	0.36	18,37,78,81	0
3	PO4	B	224	5/5	0.93	0.21	0.22	70,72,75,79	0
3	PO4	A	224	5/5	0.89	0.19	-0.01	63,68,86,89	0
2	VIB	C	223	18/18	0.94	0.18	-0.36	5,28,53,57	0
4	MG	B	227	1/1	0.87	0.16	-0.59	40,40,40,40	0
3	PO4	C	224	5/5	0.95	0.14	-2.30	63,68,73,80	0
4	MG	A	226	1/1	0.78	0.27	-	43,43,43,43	0
4	MG	B	226	1/1	0.80	0.25	-	46,46,46,46	0
4	MG	A	225	1/1	0.91	0.33	-	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.