



wwPDB X-ray Structure Validation Summary Report i

Feb 26, 2014 – 04:58 PM GMT

PDB ID : 4G3M
Title : Complex Structure of Bacillus subtilis RibG: The Deamination Process in Riboflavin Biosynthesis
Authors : Chen, S.C.; Shen, C.Y.; Yen, T.M.; Yu, H.C.; Chang, T.H.; Lai, W.L.; Liaw, S.H.
Deposited on : 2012-07-15
Resolution : 2.56 Å(reported)

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We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

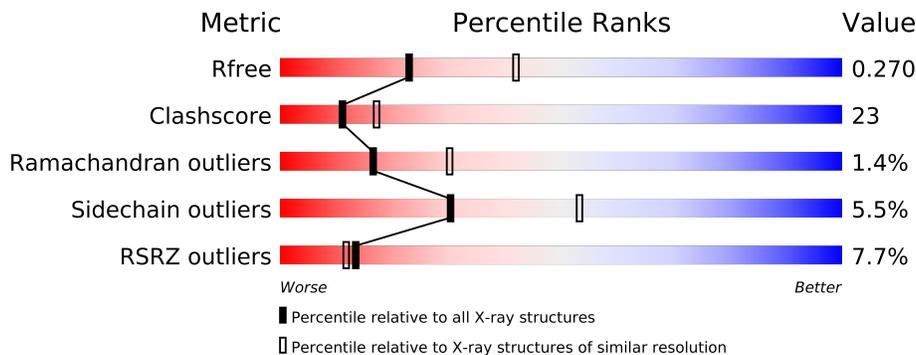
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.56 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}	66092	2347 (2.60-2.52)
Clashscore	79885	2876 (2.60-2.52)
Ramachandran outliers	78287	2826 (2.60-2.52)
Sidechain outliers	78261	2826 (2.60-2.52)
RSRZ outliers	66119	2347 (2.60-2.52)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	373	
1	B	373	
1	C	373	
1	D	373	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 11519 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Riboflavin biosynthesis protein RibD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	361	2756	1749	472	520	15	0	0	0
1	B	361	2751	1745	471	520	15	0	0	0
1	C	361	2751	1745	471	520	15	0	0	0
1	D	361	2751	1745	471	520	15	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP P17618
A	-10	ARG	-	EXPRESSION TAG	UNP P17618
A	-9	GLY	-	EXPRESSION TAG	UNP P17618
A	-8	SER	-	EXPRESSION TAG	UNP P17618
A	-7	HIS	-	EXPRESSION TAG	UNP P17618
A	-6	HIS	-	EXPRESSION TAG	UNP P17618
A	-5	HIS	-	EXPRESSION TAG	UNP P17618
A	-4	HIS	-	EXPRESSION TAG	UNP P17618
A	-3	HIS	-	EXPRESSION TAG	UNP P17618
A	-2	HIS	-	EXPRESSION TAG	UNP P17618
A	-1	GLY	-	EXPRESSION TAG	UNP P17618
A	0	SER	-	EXPRESSION TAG	UNP P17618
B	-11	MET	-	EXPRESSION TAG	UNP P17618
B	-10	ARG	-	EXPRESSION TAG	UNP P17618
B	-9	GLY	-	EXPRESSION TAG	UNP P17618
B	-8	SER	-	EXPRESSION TAG	UNP P17618
B	-7	HIS	-	EXPRESSION TAG	UNP P17618
B	-6	HIS	-	EXPRESSION TAG	UNP P17618
B	-5	HIS	-	EXPRESSION TAG	UNP P17618
B	-4	HIS	-	EXPRESSION TAG	UNP P17618
B	-3	HIS	-	EXPRESSION TAG	UNP P17618

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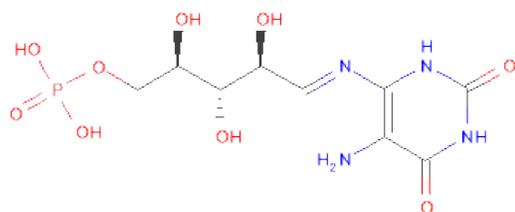
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	EXPRESSION TAG	UNP P17618
B	-1	GLY	-	EXPRESSION TAG	UNP P17618
B	0	SER	-	EXPRESSION TAG	UNP P17618
C	-11	MET	-	EXPRESSION TAG	UNP P17618
C	-10	ARG	-	EXPRESSION TAG	UNP P17618
C	-9	GLY	-	EXPRESSION TAG	UNP P17618
C	-8	SER	-	EXPRESSION TAG	UNP P17618
C	-7	HIS	-	EXPRESSION TAG	UNP P17618
C	-6	HIS	-	EXPRESSION TAG	UNP P17618
C	-5	HIS	-	EXPRESSION TAG	UNP P17618
C	-4	HIS	-	EXPRESSION TAG	UNP P17618
C	-3	HIS	-	EXPRESSION TAG	UNP P17618
C	-2	HIS	-	EXPRESSION TAG	UNP P17618
C	-1	GLY	-	EXPRESSION TAG	UNP P17618
C	0	SER	-	EXPRESSION TAG	UNP P17618
D	-11	MET	-	EXPRESSION TAG	UNP P17618
D	-10	ARG	-	EXPRESSION TAG	UNP P17618
D	-9	GLY	-	EXPRESSION TAG	UNP P17618
D	-8	SER	-	EXPRESSION TAG	UNP P17618
D	-7	HIS	-	EXPRESSION TAG	UNP P17618
D	-6	HIS	-	EXPRESSION TAG	UNP P17618
D	-5	HIS	-	EXPRESSION TAG	UNP P17618
D	-4	HIS	-	EXPRESSION TAG	UNP P17618
D	-3	HIS	-	EXPRESSION TAG	UNP P17618
D	-2	HIS	-	EXPRESSION TAG	UNP P17618
D	-1	GLY	-	EXPRESSION TAG	UNP P17618
D	0	SER	-	EXPRESSION TAG	UNP P17618

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

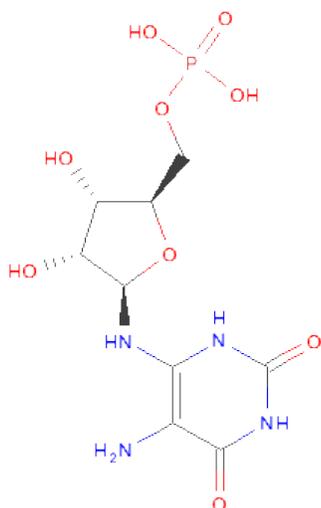
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is [(2R,3S,4S,5E)-5-[[5-AZANYL-2,4-BIS(OXIDANYLIDENE)-1H-PYRIMIDIN-6-YL]IMINO]-2,3,4-TRIS(OXIDANYL)PENTYL]DIHYDROGEN PHOSPHATE (three-letter code: AI9) (formula: C₉H₁₅N₄O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total 23	9	4	9	1	0	0
3	B	1	Total 23	9	4	9	1	0	0
3	C	1	Total 23	9	4	9	1	0	0
3	D	1	Total 23	9	4	9	1	0	0

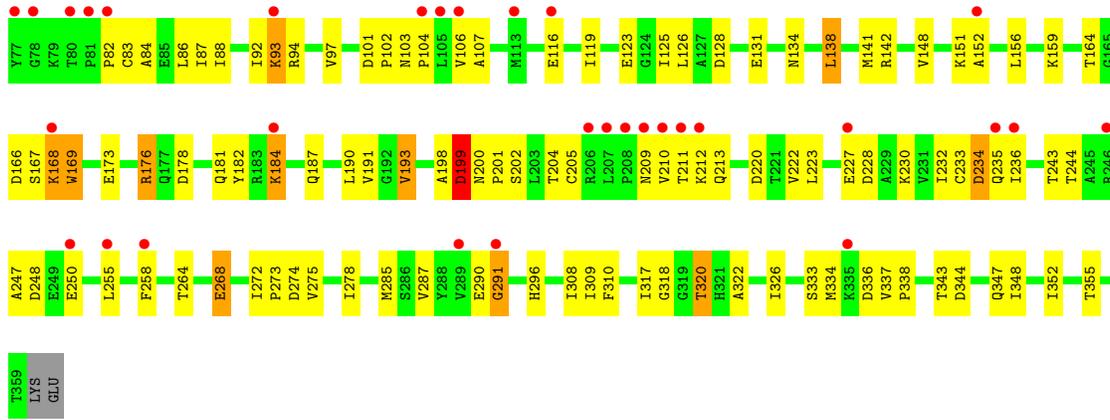
- Molecule 4 is N-(5-AMINO-2,6-DIOXO-1,2,3,6-TETRAHYDROPYRIMIDIN-4-YL)-5-O-PHOSPHONO-BETA-D-RIBOFURANOSYLAMINE (three-letter code: AOF) (formula: $C_9H_{15}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			23	9	4	9	1		
4	C	1	Total	C	N	O	P	0	0
			23	9	4	9	1		
4	D	1	Total	C	N	O	P	0	0
			23	9	4	9	1		

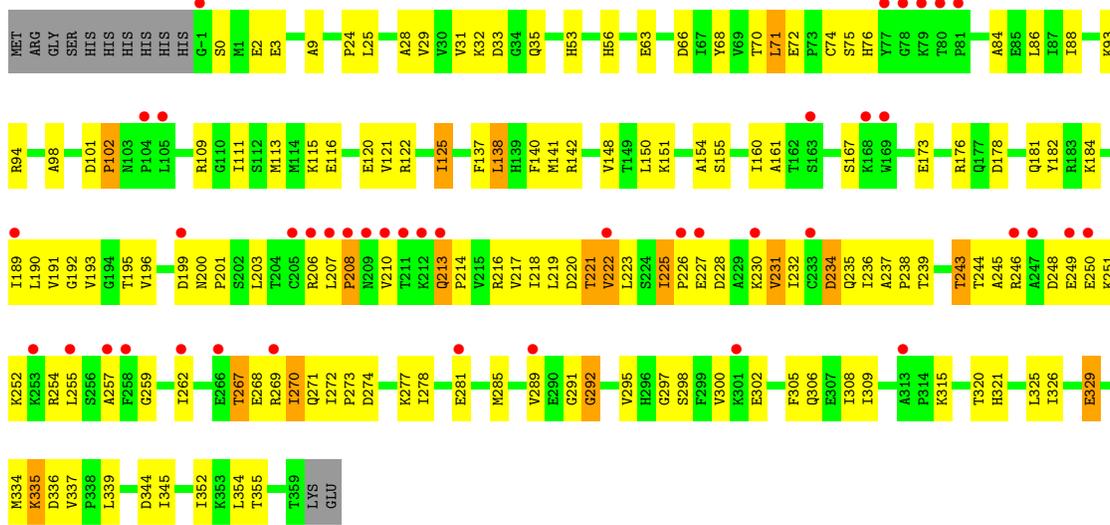
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	115	Total	O	0	0
			115	115		
5	B	70	Total	O	0	0
			70	70		
5	C	86	Total	O	0	0
			86	86		
5	D	74	Total	O	0	0
			74	74		



• Molecule 1: Riboflavin biosynthesis protein RibD

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.01Å 109.19Å 189.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.72 – 2.56 29.72 – 2.56	Depositor EDS
% Data completeness (in resolution range)	94.7 (29.72-2.56) 95.1 (29.72-2.56)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 2.57Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.222 , 0.270 0.223 , 0.270	Depositor DCC
R_{free} test set	5745 reflections (10.18%)	DCC
Wilson B-factor (Å ²)	56.2	Xtrriage
Anisotropy	0.085	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.8	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Outliers	0 of 58652 reflections	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11519	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: AOF, ZN, AI9

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	0.40	0/2807	0.64	0/3797
1	B	0.36	0/2802	0.60	0/3791
1	C	0.35	0/2802	0.59	0/3791
1	D	0.36	0/2802	0.59	0/3791
All	All	0.37	0/11213	0.61	0/15170

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2756	0	2800	89	0
1	B	2751	0	2790	125	0
1	C	2751	0	2790	132	0
1	D	2751	0	2790	184	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	23	0	15	1	0
3	B	23	0	15	2	0
3	C	23	0	15	0	0
3	D	23	0	15	0	0
4	B	23	0	15	0	0
4	C	23	0	15	1	0
4	D	23	0	15	0	0
5	A	115	0	0	5	0
5	B	70	0	0	4	0
5	C	86	0	0	4	0
5	D	74	0	0	6	0
All	All	11519	0	11275	506	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

The worst 5 of 506 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:213:GLN:CG	1:D:237:ALA:HB2	1.52	1.39
1:C:230:LYS:O	1:C:234:ASP:HB2	1.29	1.27
1:D:213:GLN:HB3	1:D:237:ALA:CB	1.76	1.15
1:D:213:GLN:CB	1:D:237:ALA:HB2	1.76	1.15
1:D:213:GLN:HB3	1:D:237:ALA:HB1	1.31	1.12

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	359/373 (96%)	341 (95%)	17 (5%)	1 (0%)	50 74
1	B	359/373 (96%)	320 (89%)	32 (9%)	7 (2%)	12 21
1	C	359/373 (96%)	330 (92%)	25 (7%)	4 (1%)	21 39
1	D	359/373 (96%)	322 (90%)	29 (8%)	8 (2%)	10 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1436/1492 (96%)	1313 (91%)	103 (7%)	20 (1%)	16 30

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	168	LYS
1	C	291	GLY
1	D	222	VAL
1	D	231	VAL
1	D	267	THR

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	295/305 (97%)	280 (95%)	15 (5%)	33 57
1	B	294/305 (96%)	279 (95%)	15 (5%)	33 57
1	C	294/305 (96%)	274 (93%)	20 (7%)	22 40
1	D	294/305 (96%)	279 (95%)	15 (5%)	33 57
All	All	1177/1220 (96%)	1112 (94%)	65 (6%)	30 53

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	355	THR
1	C	116	GLU
1	D	221	THR
1	C	14	LYS
1	C	71	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	235	GLN
1	C	23	ASN

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Mol	Chain	Res	Type
1	D	306	GLN
1	B	271	GLN
1	B	341	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	AI9	A	402	-	23,23,23	2.08	7 (30%)	28,33,33	1.62	5 (17%)
4	AOF	B	402	2	24,24,24	1.65	4 (16%)	32,36,36	2.89	16 (50%)
3	AI9	B	403	-	23,23,23	2.25	7 (30%)	28,33,33	1.58	5 (17%)
4	AOF	C	402	2	24,24,24	1.69	5 (20%)	32,36,36	2.78	15 (46%)
3	AI9	C	403	-	23,23,23	2.12	7 (30%)	28,33,33	1.50	5 (17%)
4	AOF	D	402	2	24,24,24	1.55	5 (20%)	32,36,36	3.04	17 (53%)
3	AI9	D	403	-	23,23,23	2.25	6 (26%)	28,33,33	1.58	5 (17%)

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	AI9	A	402	-	-	0/18/19/19	0/1/1/1
4	AOF	B	402	2	-	0/10/26/26	0/2/2/2
3	AI9	B	403	-	-	0/18/19/19	0/1/1/1
4	AOF	C	402	2	-	0/10/26/26	0/2/2/2
3	AI9	C	403	-	-	0/18/19/19	0/1/1/1
4	AOF	D	402	2	-	0/10/26/26	0/2/2/2
3	AI9	D	403	-	-	0/18/19/19	0/1/1/1

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	AI9	O2-C2	5.43	1.34	1.23
3	D	403	AI9	O2-C2	4.98	1.33	1.23
3	D	403	AI9	O4-C4	4.84	1.34	1.24
3	C	403	AI9	O2-C2	4.75	1.33	1.23
3	A	402	AI9	O2-C2	4.69	1.33	1.23

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	402	AOF	O4'-C1'-N1'	-8.69	101.44	109.91
4	C	402	AOF	O4'-C1'-N1'	-7.64	102.46	109.91
4	D	402	AOF	C6-N1'-C1'	6.97	131.30	123.15
4	B	402	AOF	C6-N1'-C1'	6.90	131.22	123.15
4	B	402	AOF	O4'-C1'-N1'	-6.44	103.63	109.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 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	361/373 (96%)	0.09	11 (3%) 48 48	33, 49, 64, 78	0
1	B	361/373 (96%)	0.34	23 (6%) 19 17	40, 58, 73, 85	0
1	C	361/373 (96%)	0.52	36 (9%) 8 6	42, 60, 77, 84	0
1	D	361/373 (96%)	0.55	42 (11%) 5 4	37, 61, 82, 87	0
All	All	1444/1492 (96%)	0.37	112 (7%) 13 11	33, 56, 77, 87	0

The worst 5 of 112 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	169	TRP	8.0
1	B	-1	GLY	6.5
1	C	105	LEU	6.5
1	B	208	PRO	6.4
1	B	169	TRP	6.0

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ZN	A	401	1/1	0.16	0.92	39,39,39,39	0
3	AI9	C	403	23/23	0.20	0.31	62,73,80,81	0
4	AOF	D	402	23/23	0.23	0.07	71,73,76,77	0
3	AI9	B	403	23/23	0.20	0.06	70,78,81,83	0
3	AI9	D	403	23/23	0.19	-0.13	75,77,81,81	0
3	AI9	A	402	23/23	0.14	-0.26	52,60,62,63	0
4	AOF	B	402	23/23	0.17	-0.55	63,66,69,72	0
4	AOF	C	402	23/23	0.16	-0.72	67,72,74,74	0
2	ZN	D	401	1/1	0.05	-1.14	53,53,53,53	0
2	ZN	B	401	1/1	0.14	-1.42	63,63,63,63	0
2	ZN	C	401	1/1	0.08	-1.67	69,69,69,69	0

6.5 Other polymers

There are no such residues in this entry.