Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2014 – 03:30 PM GMT

PDB ID : 3BH6
Title : Crystal structure of the RP2-Arl3 complex bound to GppNHp
Authors : Veltel, S.; Gasper, R.; Wittinghofer, A.
Deposited on : 2007-11-28
Resolution : 2.60 Å(reported)

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

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	trunk22714
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)	:	trunk22714

1   Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Rfree		0.270
Clashscore		10
Ramachandran outliers		0.2%
Sidechain outliers		10.3%
RSRZ outliers		2.7%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution
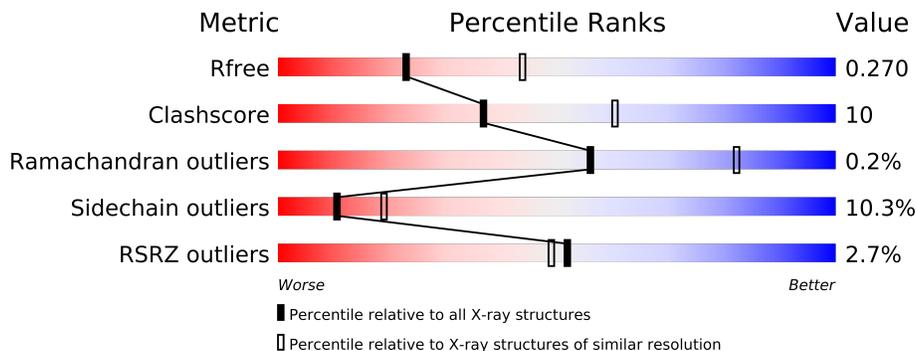
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. 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	164	
2	B	352	

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 3825 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 ADP-ribosylation factor-like protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	0	0
			1277	809	219	245	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	GLY	-	EXPRESSION TAG	UNP Q9WUL7
A	15	GLY	-	EXPRESSION TAG	UNP Q9WUL7
A	16	SER	-	EXPRESSION TAG	UNP Q9WUL7
A	71	LEU	GLN	ENGINEERED	UNP Q9WUL7

- Molecule 2 is a protein called Protein XRP2.

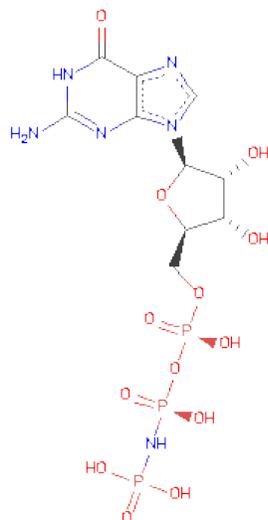| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	314	Total	C	N	O	S	0	1	0
			2467	1569	408	471	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	EXPRESSION TAG	UNP O75695
B	0	SER	-	EXPRESSION TAG	UNP O75695

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHOSPHOAMINOPHOSPHONICACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 32	C 10	N 6	O 13	P 3	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total 11	O 11	0	0
5	B	37	Total 37	O 37	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
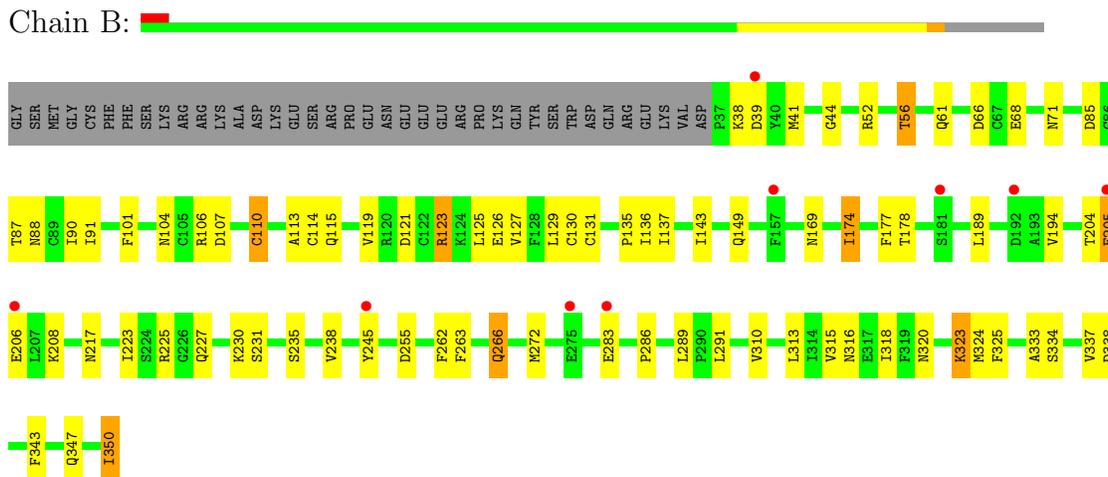
• Molecule 1: ADP-ribosylation factor-like protein 3

Chain A:
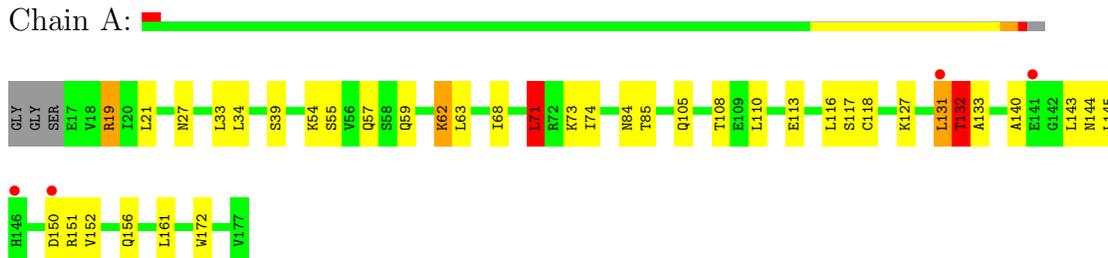
• Molecule 2: Protein XRP2

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.86Å 78.49Å 98.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.81 – 2.60 19.71 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.81-2.60) 99.9 (19.71-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.215 , 0.271 0.219 , 0.270	Depositor DCC
R_{free} test set	1812 reflections (11.11%)	DCC
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 15.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	0 of 18116 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3825	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, 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	0.60	0/1298	0.66	1/1758 (0.1%)
2	B	0.66	0/2518	0.64	2/3408 (0.1%)
All	All	0.64	0/3816	0.65	3/5166 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	LEU	CA-CB-CG	5.92	128.93	115.30
2	B	205	GLU	CB-CA-C	-5.75	98.89	110.40
2	B	205	GLU	N-CA-C	5.24	125.14	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	1277	0	1281	29	0
2	B	2467	0	2415	55	0
3	A	1	0	0	0	0
4	A	32	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	11	0	0	1	0
5	B	37	0	0	2	0
All	All	3825	0	3709	76	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 10.

All (76) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:323:LYS:HD3	2:B:323:LYS:H	1.10	1.13
1:A:132:THR:HG23	2:B:61:GLN:NE2	1.66	1.09
1:A:132:THR:HG23	2:B:61:GLN:HE21	1.18	1.05
1:A:132:THR:CG2	2:B:61:GLN:NE2	2.24	0.99
2:B:323:LYS:HD3	2:B:323:LYS:N	1.88	0.88
2:B:174:ILE:N	2:B:174:ILE:HD13	1.92	0.84
2:B:323:LYS:H	2:B:323:LYS:CD	1.90	0.83
1:A:131:LEU:HG	1:A:132:THR:N	1.93	0.82
1:A:131:LEU:HG	1:A:132:THR:H	1.50	0.75
1:A:71:LEU:HD12	1:A:74:ILE:HG12	1.71	0.72
2:B:106:ARG:HD3	2:B:123:ARG:NH2	2.04	0.70
2:B:286:PRO:HA	2:B:289:LEU:HD12	1.76	0.67
2:B:135:PRO:HB2	2:B:174:ILE:HD12	1.77	0.66
2:B:149:GLN:HG3	2:B:223:ILE:HD11	1.81	0.63
2:B:131:CYS:H	2:B:169:ASN:HD22	1.46	0.62
2:B:130:CYS:HA	2:B:169:ASN:ND2	2.16	0.61
1:A:150:ASP:HB3	5:A:179:HOH:O	2.01	0.61
2:B:174:ILE:CD1	2:B:174:ILE:N	2.62	0.60
2:B:88:ASN:HA	2:B:107:ASP:O	2.01	0.60
1:A:34:LEU:HD11	1:A:54:LYS:HB2	1.84	0.59
2:B:131:CYS:H	2:B:169:ASN:ND2	2.03	0.56
2:B:52:ARG:HD2	2:B:56:THR:HG23	1.86	0.56
1:A:132:THR:OG1	2:B:61:GLN:NE2	2.38	0.55
2:B:104:ASN:HA	2:B:121:ASP:O	2.07	0.55
1:A:27:ASN:H	4:A:1:GNP:HNB3	1.55	0.55
2:B:125:LEU:HB2	2:B:143:ILE:HG23	1.89	0.55
2:B:291:LEU:HD11	2:B:323:LYS:HG3	1.90	0.54
2:B:106:ARG:HD3	2:B:123:ARG:HH21	1.74	0.53
1:A:152:VAL:HG12	1:A:172:TRP:HZ2	1.74	0.53
1:A:127:LYS:HG2	4:A:1:GNP:C6	2.42	0.50
2:B:316:ASN:O	2:B:320:ASN:ND2	2.45	0.49
1:A:116:LEU:O	1:A:151:ARG:NH2	2.45	0.49
1:A:152:VAL:HG12	1:A:172:TRP:CZ2	2.47	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:131:LEU:C	1:A:133:ALA:H	2.16	0.49
2:B:266:GLN:HG3	5:B:357:HOH:O	2.12	0.49
2:B:238:VAL:HA	2:B:325:PHE:O	2.14	0.48
1:A:62:LYS:HE3	1:A:62:LYS:H	1.77	0.48
2:B:350:ILE:H	2:B:350:ILE:HD12	1.78	0.48
1:A:117:SER:O	1:A:118:CYS:HB2	2.15	0.47
2:B:41:MET:HB2	5:B:374:HOH:O	2.13	0.47
1:A:143:LEU:O	1:A:144:ASN:C	2.51	0.47
2:B:333:ALA:O	2:B:337:VAL:HG23	2.14	0.46
1:A:131:LEU:HD23	2:B:61:GLN:HB3	1.96	0.46
1:A:132:THR:CB	2:B:61:GLN:NE2	2.78	0.46
1:A:21:LEU:HD11	1:A:68:ILE:HD13	1.97	0.46
2:B:85:ASP:HA	2:B:104:ASN:O	2.15	0.46
2:B:91:ILE:O	2:B:110:CYS:HA	2.15	0.46
2:B:113:ALA:HA	2:B:130:CYS:O	2.16	0.45
2:B:315:VAL:HG22	2:B:324:MET:HE1	1.98	0.45
2:B:68:GLU:HG3	2:B:87:THR:HB	1.97	0.45
2:B:136:ILE:CG1	2:B:177:PHE:HE1	2.30	0.45
2:B:114:CYS:O	2:B:131:CYS:HA	2.17	0.45
2:B:315:VAL:HG22	2:B:324:MET:CE	2.48	0.44
1:A:19:ARG:HD2	1:A:85:THR:HA	1.98	0.44
2:B:52:ARG:CD	2:B:56:THR:HG23	2.46	0.44
2:B:71:ASN:HD22	2:B:90:ILE:HB	1.82	0.44
2:B:119:VAL:HB	2:B:137:ILE:HG22	2.00	0.44
2:B:205:GLU:O	2:B:206:GLU:C	2.54	0.44
1:A:21:LEU:CD1	1:A:68:ILE:CD1	2.96	0.43
2:B:126:GLU:HG2	2:B:189:LEU:HD21	1.99	0.43
2:B:225:ARG:HD2	2:B:263:PHE:HB3	2.00	0.43
2:B:127:VAL:HG12	2:B:129:LEU:HB2	2.00	0.42
1:A:110:LEU:O	1:A:113:GLU:HB2	2.19	0.42
1:A:140:ALA:O	1:A:145:LEU:HG	2.19	0.42
2:B:174:ILE:HD13	2:B:174:ILE:H	1.78	0.42
2:B:44:GLY:HA2	2:B:66:ASP:O	2.20	0.42
1:A:131:LEU:HG	1:A:132:THR:CG2	2.50	0.42
1:A:73:LYS:HD3	2:B:178:THR:HG22	2.01	0.41
2:B:262:PHE:HE1	2:B:310:VAL:HG11	1.85	0.41
2:B:315:VAL:CG2	2:B:324:MET:HE2	2.51	0.41
2:B:52:ARG:HD3	2:B:56:THR:HG21	2.02	0.41
2:B:52:ARG:HB3	2:B:56:THR:CG2	2.51	0.41
2:B:52:ARG:CD	2:B:56:THR:CG2	2.98	0.41
1:A:55:SER:HA	1:A:63:LEU:O	2.22	0.40
1:A:132:THR:HG21	2:B:61:GLN:NE2	2.25	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:136:ILE:HG13	2:B:177:PHE:HE1	1.85	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	159/164 (97%)	152 (96%)	6 (4%)	1 (1%)	33	63
2	B	312/352 (89%)	299 (96%)	13 (4%)	0	100	100
All	All	471/516 (91%)	451 (96%)	19 (4%)	1 (0%)	56	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	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	141/142 (99%)	127 (90%)	14 (10%)	11	21
2	B	276/311 (89%)	247 (90%)	29 (10%)	10	18
All	All	417/453 (92%)	374 (90%)	43 (10%)	10	19

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	33	LEU
1	A	39	SER
1	A	57	GLN
1	A	59	GLN
1	A	62	LYS
1	A	71	LEU
1	A	84	ASN
1	A	105	GLN
1	A	108	THR
1	A	131	LEU
1	A	132	THR
1	A	156	GLN
1	A	161	LEU
2	B	38	LYS
2	B	39	ASP
2	B	56	THR
2	B	101	PHE
2	B	110	CYS
2	B	115	GLN
2	B	123	ARG
2	B	174	ILE
2	B	194	VAL
2	B	204	THR
2	B	208	LYS
2	B	217	ASN
2	B	227	GLN
2	B	230	LYS
2	B	231	SER
2	B	235	SER
2	B	245	TYR
2	B	255	ASP
2	B	266	GLN
2	B	272	MET
2	B	283	GLU
2	B	313	LEU
2	B	318	ILE
2	B	323	LYS
2	B	334	SER
2	B	338	ASP
2	B	343	PHE
2	B	347	GLN
2	B	350	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	44	HIS
1	A	156	GLN
2	B	61	GLN
2	B	69	ASN
2	B	71	ASN
2	B	115	GLN
2	B	169	ASN
2	B	196	GLN
2	B	303	ASN

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	#$|Z| > 2$
4	GNP	A	1	3	34,34,34	2.32	8 (23%)	48,54,54	4.41	7 (14%)

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
4	GNP	A	1	3	-	1/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	GNP	PB-N3B	-6.81	1.58	1.64
4	A	1	GNP	PG-N3B	-5.77	1.59	1.64
4	A	1	GNP	PG-O1G	5.27	1.52	1.46
4	A	1	GNP	PB-O3A	-4.81	1.53	1.59
4	A	1	GNP	PA-O3A	-3.57	1.53	1.59
4	A	1	GNP	PB-O2B	-3.11	1.48	1.56
4	A	1	GNP	C6-N1	2.39	1.40	1.36
4	A	1	GNP	PG-O2G	-2.11	1.50	1.56

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	GNP	C6-C5-N7	-28.09	130.36	134.14
4	A	1	GNP	C6-N1-C2	7.87	124.64	120.20
4	A	1	GNP	O1G-PG-N3B	-3.46	106.60	111.83
4	A	1	GNP	PB-N3B-PG	-3.14	124.80	130.07
4	A	1	GNP	C2-N3-C4	-2.84	111.89	115.30
4	A	1	GNP	O2B-PB-O1B	2.62	115.43	109.90
4	A	1	GNP	O3G-PG-O2G	2.13	113.80	107.69

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	GNP	O1B-PB-N3B-PG

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 ⓘ

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	161/164 (98%)	-0.06	4 (2%)	54	52	20, 35, 50, 54	0
2	B	314/352 (89%)	-0.06	9 (2%)	49	46	18, 35, 49, 58	1 (0%)
All	All	475/516 (92%)	-0.06	13 (2%)	52	49	18, 35, 50, 58	1 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	245	TYR	3.2
2	B	192	ASP	2.8
2	B	205	GLU	2.6
2	B	39	ASP	2.5
2	B	181	SER	2.4
1	A	150	ASP	2.2
1	A	146	HIS	2.2
2	B	275	GLU	2.2
2	B	206	GLU	2.1
1	A	141	GLU	2.1
2	B	157	PHE	2.0
1	A	131	LEU	2.0
2	B	283	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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
4	GNP	A	1	32/32	0.13	-0.54	23,30,32,32	0
3	MG	A	2	1/1	0.09	-1.28	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.