



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2017 – 01:16 PM EDT

PDB ID : 5IQD  
Title : Aminoglycoside Phosphotransferase (2'')-Ia (CTD of AAC(6')-Ie/APH(2'')-Ia)  
in complex with GMPPNP, Magnesium, and Ribostamycin  
Authors : Caldwell, S.J.; Berghuis, A.M.  
Deposited on : unknown  
Resolution : 2.20 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](mailto: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 : rb-20029824  
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) : rb-20029824

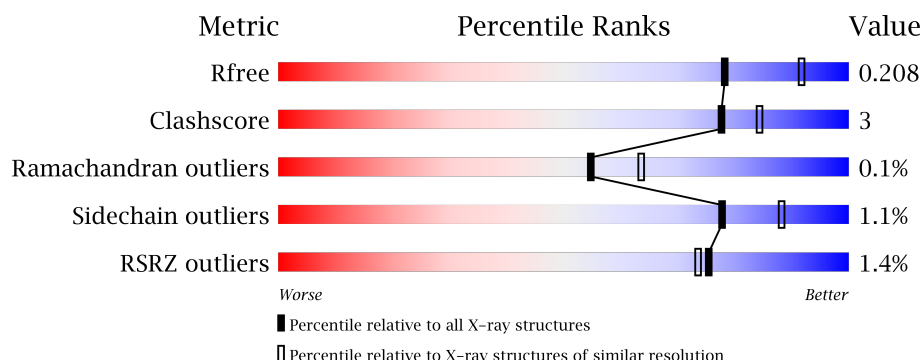
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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  $\geq 3$ , 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	305	<div> <div>0.1%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>.</div> </div> </div>
1	B	305	<div> <div></div> <div> <div>89%</div> <div>9%</div> <div>..</div> </div> </div>
1	C	305	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>.</div> </div> </div>
1	D	305	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>..</div> </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
3	RIO	A	600	-	-	-	X
3	RIO	C	600	-	-	-	X
3	RIO	D	600	-	-	-	X

## 2 Entry composition [i](#)

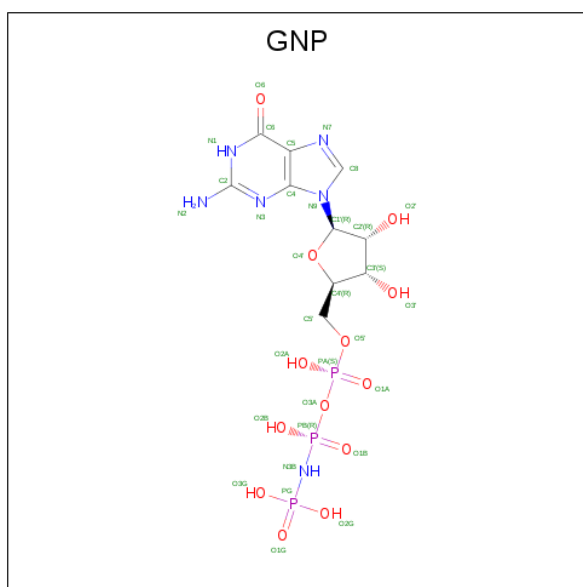
There are 6 unique types of molecules in this entry. The entry contains 11182 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 AAC/APH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	4	0
			2447	1559	381	496	11			
1	B	299	Total	C	N	O	S	0	3	0
			2478	1581	382	504	11			
1	C	292	Total	C	N	O	S	0	3	0
			2425	1548	377	489	11			
1	D	297	Total	C	N	O	S	0	3	0
			2453	1566	383	493	11			

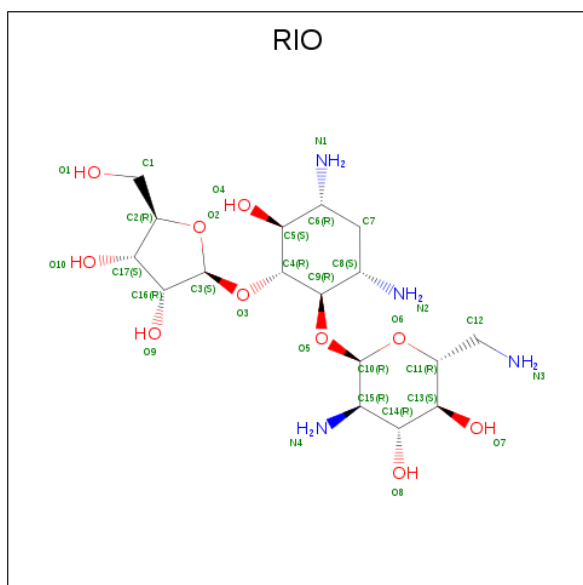
- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula:  $C_{10}H_{17}N_6O_{13}P_3$ ).



Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
2	D	1	Total	C	N	O	P	0	1
			41	10	7	19	5		

- Molecule 3 is RIBOSTAMYCIN (three-letter code: RIO) (formula:  $C_{17}H_{34}N_4O_{10}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			31	17	4	10		
3	B	1	Total	C	N	O	0	0
			31	17	4	10		
3	C	1	Total	C	N	O	0	0
			31	17	4	10		
3	D	1	Total	C	N	O	0	0
			31	17	4	10		

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

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

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total 2	Mg 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Cl 1	0	0
5	A	1	Total 1	Cl 1	0	0
5	C	1	Total 1	Cl 1	0	0


- Molecule 6 is water.

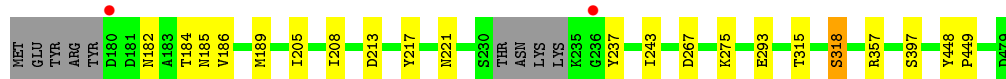
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	279	Total 279	O 279	0	0
6	B	325	Total 325	O 325	0	0
6	C	275	Total 275	O 275	0	0
6	D	219	Total 219	O 219	0	0

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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: Bifunctional AAC/APH

Chain A: 




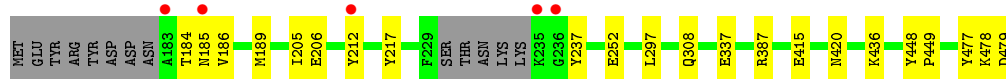
- Molecule 1: Bifunctional AAC/APH

Chain B: 




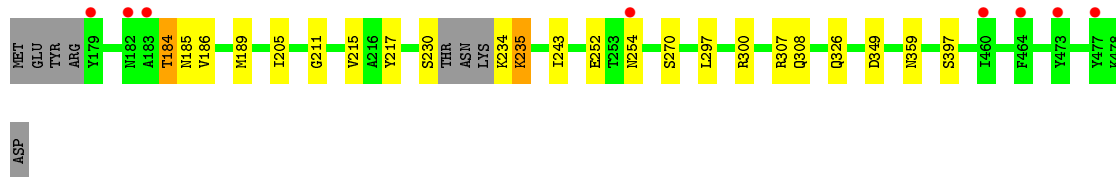
- Molecule 1: Bifunctional AAC/APH

Chain C: 



- Molecule 1: Bifunctional AAC/APH

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.22Å 99.67Å 93.40Å 90.00° 104.90° 90.00°	Depositor
Resolution (Å)	90.26 – 2.20 55.93 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (90.26-2.20) 100.0 (55.93-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.162 , 0.202 0.170 , 0.208	Depositor DCC
$R_{free}$ test set	4078 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.5	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11182	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: RIO, GNP, MG, CL

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	0.88	0/2498	0.85	2/3369 (0.1%)
1	B	0.86	0/2528	0.82	1/3410 (0.0%)
1	C	0.84	1/2474 (0.0%)	0.84	0/3335
1	D	0.75	0/2502	0.80	0/3373
All	All	0.83	1/10002 (0.0%)	0.83	3/13487 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	477	TYR	CG-CD1	-5.45	1.32	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	B	301	ASP	CB-CG-OD1	5.05	122.84	118.30
1	A	208	ILE	CB-CA-C	-5.03	101.53	111.60

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	2447	0	2346	13	1
1	B	2478	0	2373	18	1
1	C	2425	0	2334	22	0
1	D	2453	0	2361	21	0
2	A	32	0	13	0	0
2	B	41	0	2	0	0
2	C	32	0	13	0	0
2	D	41	0	2	2	0
3	A	31	0	34	0	0
3	B	31	0	34	0	0
3	C	31	0	34	1	0
3	D	31	0	34	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	1	0
6	A	279	0	0	4	0
6	B	325	0	0	6	1
6	C	275	0	0	8	3
6	D	219	0	0	9	0
All	All	11182	0	9580	67	3

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 (67) 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)
2:D:500[B]:GNP:O2G	6:D:1299:HOH:O	1.77	1.00
5:C:802:CL:CL	6:C:1107:HOH:O	2.29	0.86
1:D:359:ASN:OD1	6:D:1050:HOH:O	1.99	0.80
1:C:184:THR:HG21	1:D:215:VAL:HG21	1.61	0.80
1:C:237:TYR:HA	6:C:1384:HOH:O	1.80	0.79
1:B:349[A]:ASP:OD1	6:B:1135:HOH:O	2.07	0.71
1:D:211:GLY:HA3	6:D:1091:HOH:O	1.89	0.70
1:C:185:ASN:OD1	1:D:184:THR:OG1	2.09	0.70
2:D:500[B]:GNP:O2B	6:D:901:HOH:O	2.10	0.69
1:A:185:ASN:ND2	1:B:179:TYR:OH	2.26	0.68
1:D:185:ASN:ND2	1:D:217:TYR:OH	2.28	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:LYS:NZ	6:B:1272:HOH:O	2.29	0.65
1:C:184:THR:CG2	1:D:215:VAL:HG21	2.27	0.65
1:D:270:SER:OG	6:D:1212:HOH:O	2.15	0.65
1:B:463:GLU:OE1	6:B:1001:HOH:O	2.14	0.65
1:B:298:LEU:HA	6:B:1268:HOH:O	2.00	0.62
1:D:307[A]:ARG:NH2	6:D:1005:HOH:O	2.32	0.62
1:A:243:ILE:HD13	1:A:397:SER:HB2	1.83	0.59
1:C:237:TYR:CA	6:C:1384:HOH:O	2.45	0.58
1:D:254:ASN:HB2	6:D:1500:HOH:O	2.04	0.57
1:B:467:ASN:ND2	6:B:1434:HOH:O	2.38	0.56
1:B:243:ILE:HD13	1:B:397:SER:HB2	1.89	0.55
1:C:436:LYS:NZ	6:C:1113:HOH:O	2.39	0.55
1:C:186:VAL:HG13	1:C:205:ILE:HG23	1.87	0.55
1:D:186:VAL:HG13	1:D:205:ILE:HG23	1.89	0.55
1:D:326:GLN:NE2	6:D:1013:HOH:O	2.33	0.54
1:B:186:VAL:HG13	1:B:205:ILE:HG23	1.89	0.54
1:A:186:VAL:HG13	1:A:205:ILE:HG23	1.90	0.53
1:B:252:GLU:O	1:B:308:GLN:NE2	2.34	0.52
1:C:252:GLU:O	1:C:308:GLN:NE2	2.31	0.52
1:D:349:ASP:OD1	6:D:1171:HOH:O	2.19	0.52
1:A:182:ASN:HA	1:B:181:ASP:OD1	2.10	0.52
1:B:189:MET:HG2	1:B:217:TYR:CE1	2.44	0.52
1:D:243:ILE:HD13	1:D:397[A]:SER:HB2	1.92	0.51
1:A:184:THR:HG21	1:B:215:VAL:HG21	1.91	0.51
1:C:184:THR:CG2	1:D:185:ASN:OD1	2.59	0.50
1:D:252:GLU:O	1:D:308:GLN:NE2	2.36	0.50
1:C:189:MET:HG2	1:C:217:TYR:CE1	2.47	0.49
1:D:189:MET:HG2	1:D:217:TYR:CE1	2.47	0.49
1:B:474:LYS:NZ	6:B:1216:HOH:O	2.32	0.48
1:C:186:VAL:CG1	1:C:205:ILE:HG23	2.44	0.47
1:B:230:SER:O	1:B:231:THR:HB	2.14	0.47
1:A:221[B]:ASN:ND2	6:A:1199:HOH:O	2.39	0.46
1:A:448:TYR:HB3	1:A:449:PRO:HD3	1.98	0.46
1:A:189:MET:HG2	1:A:217:TYR:CE1	2.50	0.46
6:A:1217:HOH:O	1:B:479:ASP:N	2.44	0.46
1:C:448:TYR:HB3	1:C:449:PRO:HD3	1.97	0.46
1:A:315:THR:O	1:A:318:SER:OG	2.33	0.45
1:B:186:VAL:CG1	1:B:205:ILE:HG23	2.47	0.45
1:D:297:LEU:HD23	1:D:300:ARG:HH11	1.81	0.45
1:A:186:VAL:CG1	1:A:205:ILE:HG23	2.47	0.44
1:C:337:GLU:HG2	6:C:1341:HOH:O	2.17	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:VAL:CG1	1:D:205:ILE:HG23	2.47	0.43
1:C:478:LYS:O	1:C:479:ASP:CB	2.67	0.43
1:C:420:ASN:ND2	6:C:1031:HOH:O	2.51	0.43
1:C:308:GLN:HB2	6:C:1191:HOH:O	2.19	0.43
1:A:184:THR:CG2	1:B:185:ASN:ND2	2.82	0.42
1:C:415:GLU:OE1	3:C:600:RIO:N2	2.52	0.42
1:A:275:LYS:NZ	6:A:1190:HOH:O	2.51	0.42
1:C:297:LEU:HD23	1:C:387:ARG:HD3	2.02	0.42
1:B:234:LYS:O	1:B:235:LYS:HB2	2.20	0.41
1:D:234:LYS:O	1:D:235:LYS:HB2	2.20	0.41
1:C:184:THR:HG22	1:D:185:ASN:OD1	2.21	0.41
1:C:206:GLU:HB3	6:C:1328:HOH:O	2.21	0.41
1:C:478:LYS:O	1:C:479:ASP:HB2	2.21	0.41
1:A:237:TYR:HA	6:A:1384:HOH:O	2.22	0.40
1:C:184:THR:HB	1:D:185:ASN:OD1	2.21	0.40

All (3) 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:293:GLU:OE1	6:C:1080:HOH:O[2_747]	2.11	0.09
6:B:1391:HOH:O	6:C:1240:HOH:O[2_746]	2.13	0.07
1:B:288:SER:O	6:C:1219:HOH:O[2_646]	2.18	0.02

## 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	296/305 (97%)	285 (96%)	11 (4%)	0	100	100
1	B	298/305 (98%)	286 (96%)	12 (4%)	0	100	100
1	C	291/305 (95%)	280 (96%)	11 (4%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	296/305 (97%)	285 (96%)	10 (3%)	1 (0%)	44	49
All	All	1181/1220 (97%)	1136 (96%)	44 (4%)	1 (0%)	55	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	235	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	271/281 (96%)	268 (99%)	3 (1%)	78	88
1	B	275/281 (98%)	269 (98%)	6 (2%)	57	70
1	C	269/281 (96%)	268 (100%)	1 (0%)	93	97
1	D	271/281 (96%)	269 (99%)	2 (1%)	87	93
All	All	1086/1124 (97%)	1074 (99%)	12 (1%)	78	88

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	ASP
1	A	267	ASP
1	A	318	SER
1	B	182	ASN
1	B	184	THR
1	B	230	SER
1	B	285	GLU
1	B	463	GLU
1	B	470	LYS
1	C	212	TYR
1	D	184	THR
1	D	230	SER

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	341	ASN
1	A	431	ASN
1	A	467	ASN
1	B	467	ASN
1	C	327	ASN
1	C	341	ASN
1	C	420	ASN
1	D	296	ASN
1	D	326	GLN
1	D	420	ASN

### 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 21 ligands modelled in this entry, 11 are monoatomic - leaving 10 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	GNP	A	500	4	27,34,34	2.77	7 (25%)	26,54,54	1.70	7 (26%)
3	RIO	A	600	-	33,33,33	0.49	0	44,49,49	1.08	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GNP	B	500[A]	4	27,34,34	2.00	5 (18%)	26,54,54	1.19	3 (11%)
2	GNP	B	500[B]	4	27,34,34	1.99	4 (14%)	26,54,54	1.39	3 (11%)
3	RIO	B	600	-	33,33,33	0.44	0	44,49,49	1.18	3 (6%)
2	GNP	C	500	4	27,34,34	2.42	6 (22%)	26,54,54	1.33	3 (11%)
3	RIO	C	600	-	33,33,33	0.44	0	44,49,49	1.04	2 (4%)
2	GNP	D	500[A]	4	27,34,34	2.32	5 (18%)	26,54,54	1.43	4 (15%)
2	GNP	D	500[B]	4	27,34,34	2.32	6 (22%)	26,54,54	1.09	1 (3%)
3	RIO	D	600	-	33,33,33	0.37	0	44,49,49	1.11	4 (9%)

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	GNP	A	500	4	-	0/16/38/38	0/3/3/3
3	RIO	A	600	-	-	0/12/68/68	0/3/3/3
2	GNP	B	500[A]	4	-	0/16/38/38	0/3/3/3
2	GNP	B	500[B]	4	-	0/16/38/38	0/3/3/3
3	RIO	B	600	-	-	0/12/68/68	0/3/3/3
2	GNP	C	500	4	-	0/16/38/38	0/3/3/3
3	RIO	C	600	-	-	0/12/68/68	0/3/3/3
2	GNP	D	500[A]	4	-	1/16/38/38	0/3/3/3
2	GNP	D	500[B]	4	-	0/16/38/38	0/3/3/3
3	RIO	D	600	-	-	0/12/68/68	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	GNP	C4-N9	-8.38	1.36	1.47
2	D	500[A]	GNP	C4-N9	-7.92	1.37	1.47
2	D	500[B]	GNP	C4-N9	-7.92	1.37	1.47
2	C	500	GNP	C4-N9	-7.55	1.37	1.47
2	B	500[A]	GNP	C4-N9	-7.55	1.37	1.47
2	B	500[B]	GNP	C4-N9	-7.55	1.37	1.47
2	C	500	GNP	C5-C6	-6.93	1.40	1.53
2	A	500	GNP	C5-C6	-6.80	1.40	1.53
2	D	500[A]	GNP	C5-C6	-6.00	1.42	1.53
2	D	500[B]	GNP	C5-C6	-6.00	1.42	1.53
2	C	500	GNP	PB-O3A	-4.99	1.53	1.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	GNP	PB-O3A	-3.84	1.54	1.59
2	B	500[A]	GNP	C5-C6	-3.79	1.46	1.53
2	B	500[B]	GNP	C5-C6	-3.79	1.46	1.53
2	D	500[A]	GNP	C8-N9	-3.35	1.36	1.46
2	D	500[B]	GNP	C8-N9	-3.35	1.36	1.46
2	B	500[A]	GNP	C8-N9	-3.27	1.36	1.46
2	B	500[B]	GNP	C8-N9	-3.27	1.36	1.46
2	A	500	GNP	C8-N9	-3.03	1.37	1.46
2	C	500	GNP	C8-N9	-2.80	1.38	1.46
2	C	500	GNP	PG-O2G	2.12	1.62	1.56
2	B	500[A]	GNP	PB-O2B	2.16	1.62	1.56
2	C	500	GNP	C6-N1	2.23	1.37	1.33
2	D	500[B]	GNP	PB-O2B	2.25	1.62	1.56
2	D	500[A]	GNP	PB-O3A	2.59	1.62	1.59
2	D	500[B]	GNP	PB-O3A	2.72	1.62	1.59
2	B	500[A]	GNP	C6-N1	2.87	1.38	1.33
2	B	500[B]	GNP	C6-N1	2.87	1.38	1.33
2	A	500	GNP	C6-N1	2.99	1.38	1.33
2	D	500[A]	GNP	C6-N1	3.26	1.38	1.33
2	D	500[B]	GNP	C6-N1	3.26	1.38	1.33
2	A	500	GNP	PG-O2G	4.49	1.69	1.56
2	A	500	GNP	PB-O2B	5.19	1.71	1.56

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500[B]	GNP	O1G-PG-N3B	-5.05	104.23	111.79
3	B	600	RIO	O3-C3-O2	-4.23	106.85	111.43
2	A	500	GNP	O1G-PG-N3B	-3.47	106.60	111.79
2	A	500	GNP	O2G-PG-O1G	-3.31	105.00	113.41
2	C	500	GNP	O1G-PG-N3B	-3.02	107.27	111.79
2	A	500	GNP	O2'-C2'-C1'	-2.98	99.90	109.96
3	D	600	RIO	C4-C9-C8	-2.84	105.70	111.28
3	A	600	RIO	C3-O3-C4	-2.36	112.24	118.00
2	B	500[A]	GNP	O2B-PB-O1B	-2.36	104.97	109.87
2	C	500	GNP	O6-C6-N1	-2.30	119.64	122.70
3	B	600	RIO	C4-C9-C8	-2.19	106.99	111.28
3	A	600	RIO	C4-C9-C8	-2.16	107.05	111.28
2	D	500[A]	GNP	O3G-PG-O2G	-2.11	101.78	107.69
2	B	500[A]	GNP	O2'-C2'-C1'	-2.04	103.07	109.96
2	B	500[B]	GNP	O2'-C2'-C1'	-2.04	103.07	109.96
2	A	500	GNP	O3'-C3'-C2'	-2.02	105.36	111.83

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	C	600	RIO	C5-C6-N1	2.00	114.84	110.92
3	D	600	RIO	O5-C9-C4	2.07	112.82	107.50
3	D	600	RIO	O5-C10-O6	2.10	115.78	110.70
3	D	600	RIO	C10-O5-C9	2.10	123.12	118.00
2	A	500	GNP	PA-O3A-PB	2.21	140.17	132.38
3	A	600	RIO	O3-C3-O2	2.22	113.83	111.43
2	D	500[A]	GNP	O3A-PB-N3B	2.63	113.89	106.59
3	B	600	RIO	O3-C4-C9	2.71	114.46	107.50
2	A	500	GNP	O3G-PG-O2G	2.92	115.88	107.69
2	B	500[A]	GNP	O6-C6-C5	3.16	125.73	119.69
2	B	500[B]	GNP	O6-C6-C5	3.16	125.73	119.69
3	C	600	RIO	O3-C4-C9	3.22	115.79	107.50
2	A	500	GNP	O6-C6-C5	3.70	126.76	119.69
2	D	500[A]	GNP	O1G-PG-N3B	3.75	117.40	111.79
2	D	500[A]	GNP	O6-C6-C5	3.97	127.28	119.69
2	D	500[B]	GNP	O6-C6-C5	3.97	127.28	119.69
2	C	500	GNP	O6-C6-C5	4.36	128.03	119.69

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	500[A]	GNP	O1B-PB-N3B-PG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	600	RIO	1	0
2	D	500[B]	GNP	2	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	296/305 (97%)	-0.26	2 (0%) 87 86	27, 41, 64, 121	0
1	B	299/305 (98%)	-0.33	1 (0%) 93 93	26, 41, 72, 103	0
1	C	292/305 (95%)	-0.23	5 (1%) 70 68	24, 42, 73, 96	0
1	D	297/305 (97%)	-0.06	8 (2%) 55 52	33, 50, 91, 126	0
All	All	1184/1220 (97%)	-0.22	16 (1%) 75 73	24, 43, 77, 126	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	179	TYR	5.9
1	D	473	TYR	4.4
1	A	180	ASP	3.8
1	A	236	GLY	3.8
1	B	179	TYR	3.4
1	D	254	ASN	3.0
1	D	464	PHE	2.9
1	D	460	ILE	2.6
1	C	185	ASN	2.5
1	C	212	TYR	2.3
1	D	182	ASN	2.2
1	C	235	LYS	2.2
1	C	236	GLY	2.2
1	D	477	TYR	2.1
1	C	183	ALA	2.1
1	D	183	ALA	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	RIO	A	600	31/31	0.92	0.17	5.26	41,49,56,59	0
3	RIO	D	600	31/31	0.94	0.19	4.15	46,50,60,65	0
3	RIO	C	600	31/31	0.82	0.21	3.13	64,70,80,88	0
2	GNP	A	500	32/32	0.98	0.12	0.37	29,34,38,40	0
3	RIO	B	600	31/31	0.96	0.12	0.02	35,38,46,47	0
2	GNP	B	500[A]	32/32	0.98	0.10	-0.37	29,34,37,40	9
2	GNP	D	500[A]	32/32	0.98	0.10	-0.50	34,39,45,48	9
2	GNP	D	500[B]	32/32	0.98	0.10	-0.55	34,39,41,42	9
2	GNP	B	500[B]	32/32	0.98	0.10	-0.61	29,34,37,40	9
2	GNP	C	500	32/32	0.98	0.09	-1.13	35,39,43,44	0
4	MG	B	702	1/1	0.98	0.06	-2.13	36,36,36,36	0
4	MG	D	702	1/1	0.99	0.04	-4.22	43,43,43,43	0
4	MG	A	702	1/1	0.99	0.06	-4.27	37,37,37,37	0
4	MG	C	702	1/1	0.98	0.04	-5.09	38,38,38,38	0
4	MG	A	700	1/1	0.94	0.09	-	35,35,35,35	0
4	MG	D	700	1/1	0.99	0.09	-	31,31,31,31	0
5	CL	B	802	1/1	0.94	0.10	-	72,72,72,72	0
4	MG	C	700	1/1	0.98	0.07	-	34,34,34,34	0
4	MG	B	700	1/1	0.99	0.07	-	30,30,30,30	0
5	CL	A	802	1/1	0.94	0.13	-	62,62,62,62	0
5	CL	C	802	1/1	0.95	0.08	-	63,63,63,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.