



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 9, 2016 – 12:13 PM EDT

PDB ID : 5IQC  
Title : Aminoglycoside Phosphotransferase (2'')-Ia (CTD of AAC(6')-Ie/APH(2'')-Ia)  
in complex with GMPPNP, Magnesium, and Gentamicin C1  
Authors : Caldwell, S.J.; Berghuis, A.M.  
Deposited on : 2016-03-10  
Resolution : 2.30 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027674  
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) : rb-20027674

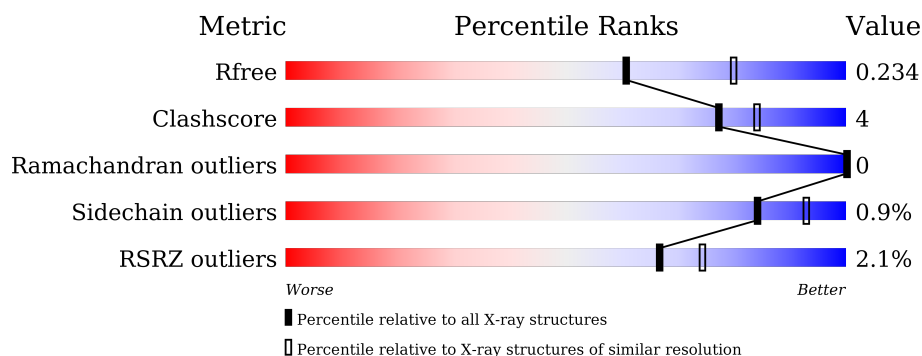
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>91%</span> <span>6% ..</span> </div> </div>
1	B	305	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 1%, green 95%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>2%</span> <span>89%</span> <span>9% .</span> </div> </div>
1	C	305	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 97%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>90%</span> <span>8% .</span> </div> </div>
1	D	305	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 5%, yellow 1%, green 89%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>5%</span> <span>87%</span> <span>8% 5%</span> </div> </div>

## 2 Entry composition [i](#)

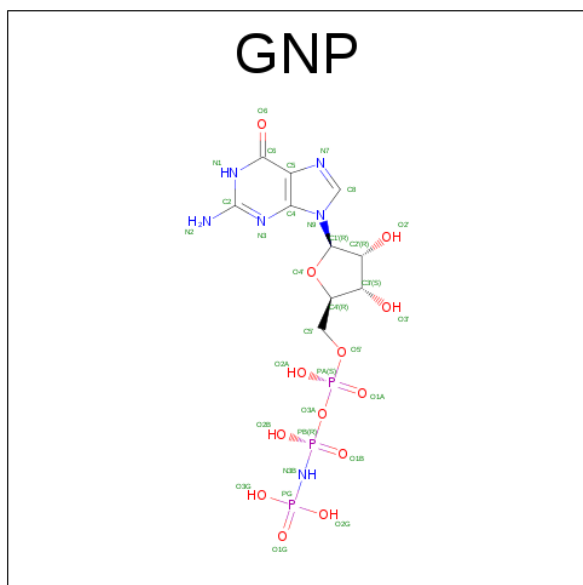
There are 7 unique types of molecules in this entry. The entry contains 10898 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	301	Total	C	N	O	S	0	0	0
			2466	1569	383	504	10			
1	B	299	Total	C	N	O	S	0	4	0
			2486	1588	380	507	11			
1	C	297	Total	C	N	O	S	0	3	0
			2458	1568	382	498	10			
1	D	290	Total	C	N	O	S	0	1	0
			2407	1539	374	484	10			

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



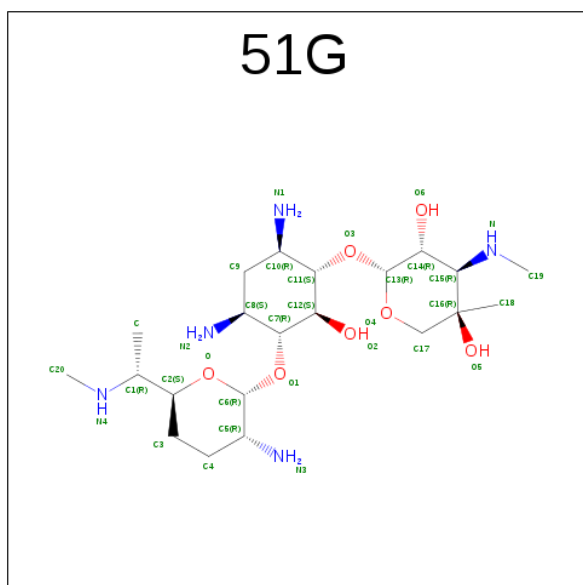
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			41	10	7	19	5		
2	B	1	Total	C	N	O	P	0	1
			41	10	7	19	5		

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 3 is gentamicin C1 (three-letter code: 51G) (formula:  $C_{21}H_{43}N_5O_7$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			33	21	5	7		
3	B	1	Total	C	N	O	0	0
			33	21	5	7		
3	C	1	Total	C	N	O	0	0
			33	21	5	7		
3	D	1	Total	C	N	O	0	1
			45	28	6	11		

- 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...*

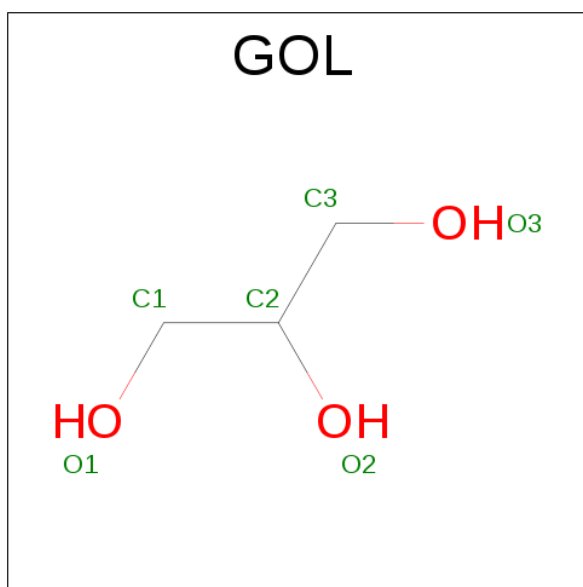
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	3	Total	Mg	0	0
			3	3		

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

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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	190	Total	O	0	0
			190	190		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	246	Total 246	O 246	0	0
7	C	193	Total 193	O 193	0	0
7	D	129	Total 129	O 129	0	0

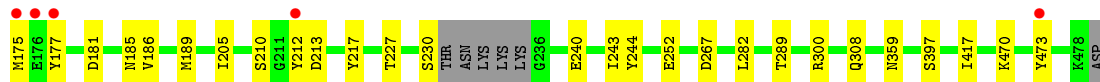
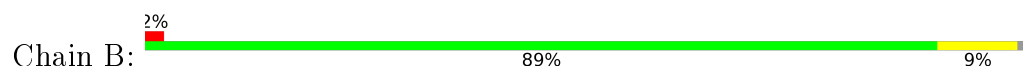
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

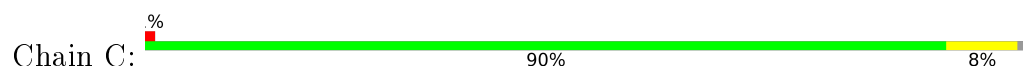
- Molecule 1: Bifunctional AAC/APH



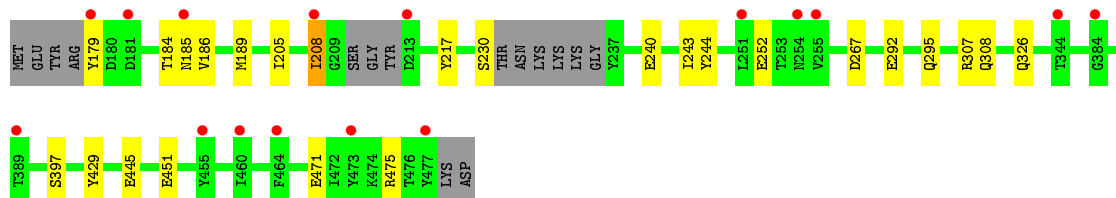
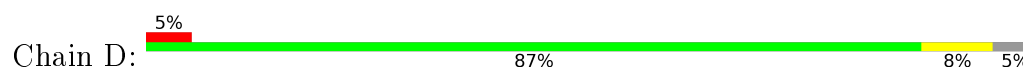
- Molecule 1: Bifunctional AAC/APH



- Molecule 1: Bifunctional AAC/APH



- Molecule 1: Bifunctional AAC/APH



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.78 Å 98.89 Å 93.86 Å 90.00° 105.51° 90.00°	Depositor
Resolution (Å)	90.44 – 2.30 55.54 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.2 (90.44-2.30) 96.2 (55.54-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.179 , 0.229 0.186 , 0.234	Depositor DCC
$R_{free}$ test set	3446 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.4	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10898	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MG, GNP, 51G, 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	0.66	0/2510	0.76	0/3388
1	B	0.68	0/2543	0.74	1/3431 (0.0%)
1	C	0.67	0/2511	0.75	0/3386
1	D	0.60	0/2452	0.70	0/3306
All	All	0.65	0/10016	0.74	1/13511 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	300	ARG	NE-CZ-NH1	5.45	123.03	120.30

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	2466	0	2350	18	0
1	B	2486	0	2375	20	0
1	C	2458	0	2367	20	0
1	D	2407	0	2318	17	0
2	A	41	0	2	1	0
2	B	41	0	2	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	41	0	2	1	0
2	D	32	0	13	0	0
3	A	33	0	0	0	0
3	B	33	0	0	1	0
3	C	33	0	0	0	0
3	D	45	0	0	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	3	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	0	0
6	B	6	0	8	0	0
6	D	6	0	8	0	0
7	A	190	0	0	3	0
7	B	246	0	0	8	0
7	C	193	0	0	8	0
7	D	129	0	0	3	0
All	All	10898	0	9445	73	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 4.

All (73) 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:B:500[B]:GNP:O2B	7:B:901:HOH:O	1.75	1.01
1:D:451:GLU:OE1	3:D:600[A]:51G:O5	1.90	0.90
1:B:289:THR:HG22	7:B:1371:HOH:O	1.73	0.88
1:D:208:ILE:HD11	7:D:1142:HOH:O	1.75	0.86
2:B:500[B]:GNP:O2G	7:B:1299:HOH:O	1.94	0.86
1:A:448:TYR:HH	1:B:175:MET:N	1.76	0.83
1:A:448:TYR:OH	1:B:175:MET:N	2.16	0.79
2:A:500[B]:GNP:O1B	7:A:901:HOH:O	2.08	0.72
1:B:359:ASN:OD1	7:B:1050:HOH:O	2.10	0.70
1:C:185[B]:ASN:ND2	1:D:184:THR:OG1	2.25	0.70
1:C:475:ARG:NE	7:C:1194:HOH:O	2.21	0.68
2:B:500[B]:GNP:O1G	7:B:909:HOH:O	0.65	0.64
1:C:185[A]:ASN:OD1	1:C:217:TYR:OH	2.19	0.60
1:A:180:ASP:HB2	1:B:181:ASP:OD2	2.02	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:600:51G:O6	3:B:600:51G:C19	2.50	0.59
1:B:230:SER:OG	1:B:267:ASP:O	2.22	0.57
1:B:289:THR:HA	7:B:1371:HOH:O	2.05	0.56
1:C:297:LEU:HD21	1:C:387:ARG:NE	2.20	0.56
2:C:500[A]:GNP:O1B	7:C:909:HOH:O	2.05	0.56
1:D:230:SER:CB	1:D:267:ASP:O	2.54	0.56
1:C:463:GLU:HB3	7:C:1001:HOH:O	2.04	0.55
1:D:185:ASN:OD1	1:D:217:TYR:OH	2.24	0.55
1:A:445:GLU:OE2	1:A:475:ARG:NH2	2.41	0.53
1:B:210:SER:HA	7:B:1206:HOH:O	2.08	0.53
1:B:185:ASN:OD1	1:B:217:TYR:OH	2.23	0.52
1:A:182:ASN:ND2	1:B:213:ASP:HA	2.25	0.52
1:D:307[A]:ARG:NH1	1:D:429:TYR:O	2.43	0.52
1:A:180:ASP:OD2	1:A:184:THR:OG1	2.11	0.51
1:C:478:LYS:NZ	7:C:1272:HOH:O	2.44	0.51
1:D:208:ILE:CD1	7:D:1142:HOH:O	2.47	0.50
1:A:319:GLU:HG2	1:C:264:TYR:CD1	2.46	0.50
1:C:185[A]:ASN:ND2	1:D:179:TYR:OH	2.42	0.50
1:B:243:ILE:HD13	1:B:397:SER:HB2	1.94	0.49
1:A:243:ILE:HD13	1:A:397:SER:HB2	1.94	0.49
1:D:292:GLU:HA	1:D:295:GLN:HE21	1.77	0.49
1:A:228:LYS:CE	1:A:231:THR:HG21	2.43	0.49
1:D:445:GLU:OE2	1:D:475:ARG:NH2	2.43	0.48
1:A:254:ASN:HB2	7:A:1095:HOH:O	2.14	0.47
1:C:186:VAL:HG13	1:C:205:ILE:HG23	1.97	0.47
1:A:180:ASP:OD1	1:A:181:ASP:N	2.47	0.47
1:B:186:VAL:HG13	1:B:205:ILE:HG23	1.97	0.47
1:D:326:GLN:NE2	7:D:1013:HOH:O	2.48	0.46
1:D:186:VAL:HG13	1:D:205:ILE:HG23	1.97	0.46
2:B:500[B]:GNP:PG	7:B:911:HOH:O	2.74	0.45
1:A:319:GLU:HG2	1:C:264:TYR:CE1	2.51	0.45
1:C:386:ASN:ND2	7:C:1147:HOH:O	2.49	0.45
1:D:240:GLU:HG2	1:D:244:TYR:CE2	2.52	0.45
1:C:298:LEU:HA	7:C:1268:HOH:O	2.17	0.45
1:D:189:MET:HG2	1:D:217:TYR:CE1	2.52	0.45
1:C:228:LYS:HE2	7:C:1098:HOH:O	2.16	0.44
1:C:189:MET:HG2	1:C:217:TYR:CE1	2.53	0.44
1:D:243:ILE:HD13	1:D:397:SER:HB2	1.99	0.43
1:A:212:TYR:HA	1:B:177:TYR:CE2	2.53	0.43
1:B:240:GLU:HG2	1:B:244:TYR:CE2	2.52	0.43
1:B:189:MET:HG2	1:B:217:TYR:CE1	2.52	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ASP:HB2	7:A:1008:HOH:O	2.19	0.43
1:A:212:TYR:HA	1:B:177:TYR:CD2	2.54	0.42
1:C:240:GLU:HG2	1:C:244:TYR:CE2	2.54	0.42
1:C:212:TYR:CD1	1:C:212:TYR:O	2.73	0.42
1:D:252:GLU:O	1:D:308:GLN:NE2	2.43	0.42
1:A:240:GLU:HG2	1:A:244:TYR:CE2	2.55	0.41
1:D:471:GLU:OE2	1:D:475:ARG:NH1	2.53	0.41
1:C:275:LYS:NZ	7:C:1190:HOH:O	2.53	0.41
1:C:252:GLU:O	1:C:308:GLN:NE2	2.43	0.41
1:A:189:MET:HG2	1:A:217:TYR:CE1	2.55	0.41
1:B:470:LYS:O	1:B:473:TYR:HB3	2.20	0.41
1:A:182:ASN:HB3	1:A:184:THR:OG1	2.21	0.41
1:B:189:MET:SD	1:B:227:THR:HG21	2.61	0.41
1:C:282:LEU:HD21	1:C:417:ILE:HD11	2.03	0.41
1:B:282:LEU:HD21	1:B:417:ILE:HD11	2.03	0.40
1:B:252:GLU:O	1:B:308:GLN:NE2	2.43	0.40
1:C:471:GLU:OE2	1:C:475:ARG:NH1	2.55	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	299/305 (98%)	288 (96%)	11 (4%)	0	100	100
1	B	299/305 (98%)	289 (97%)	10 (3%)	0	100	100
1	C	298/305 (98%)	288 (97%)	10 (3%)	0	100	100
1	D	285/305 (93%)	275 (96%)	10 (4%)	0	100	100
All	All	1181/1220 (97%)	1140 (96%)	41 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	272/281 (97%)	266 (98%)	6 (2%)	60	77
1	B	276/281 (98%)	275 (100%)	1 (0%)	93	97
1	C	273/281 (97%)	271 (99%)	2 (1%)	88	95
1	D	267/281 (95%)	266 (100%)	1 (0%)	93	97
All	All	1088/1124 (97%)	1078 (99%)	10 (1%)	84	93

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

Mol	Chain	Res	Type
1	A	181	ASP
1	A	231	THR
1	A	319	GLU
1	A	356	GLU
1	A	467	ASN
1	A	479	ASP
1	B	212	TYR
1	C	213	ASP
1	C	478	LYS
1	D	208	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	185	ASN
1	A	341	ASN
1	A	359	ASN
1	C	327	ASN
1	C	341	ASN
1	D	295	GLN
1	D	296	ASN
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 26 ligands modelled in this entry, 12 are monoatomic - leaving 14 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[A]	4	29,34,34	2.28	6 (20%)	28,54,54	1.56	4 (14%)
2	GNP	A	500[B]	4	29,34,34	2.26	6 (20%)	28,54,54	1.45	2 (7%)
3	51G	A	600	-	31,35,35	0.82	1 (3%)	35,52,52	1.27	2 (5%)
2	GNP	B	500[A]	4	29,34,34	4.44	12 (41%)	28,54,54	1.69	4 (14%)
2	GNP	B	500[B]	4	29,34,34	3.81	10 (34%)	28,54,54	1.65	3 (10%)
3	51G	B	600	-	31,35,35	0.76	1 (3%)	35,52,52	1.05	2 (5%)
6	GOL	B	804	-	5,5,5	0.54	0	5,5,5	0.44	0
2	GNP	C	500[A]	4	29,34,34	2.10	7 (24%)	28,54,54	1.64	4 (14%)
2	GNP	C	500[B]	4	29,34,34	2.31	8 (27%)	28,54,54	1.63	3 (10%)
3	51G	C	600	-	31,35,35	0.69	1 (3%)	35,52,52	1.04	1 (2%)
2	GNP	D	500	4	29,34,34	4.89	11 (37%)	28,54,54	1.71	5 (17%)
3	51G	D	600[A]	-	31,35,35	0.82	1 (3%)	35,52,52	1.76	3 (8%)
3	51G	D	600[B]	-	31,35,35	0.82	1 (3%)	35,52,52	1.12	1 (2%)
6	GOL	D	804	-	5,5,5	0.59	0	5,5,5	0.62	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
2	GNP	A	500[A]	4	-	0/16/38/38	0/3/3/3
2	GNP	A	500[B]	4	-	1/16/38/38	0/3/3/3
3	51G	A	600	-	-	0/15/69/69	0/3/3/3
2	GNP	B	500[A]	4	-	1/16/38/38	0/3/3/3
2	GNP	B	500[B]	4	-	0/16/38/38	0/3/3/3
3	51G	B	600	-	-	0/15/69/69	0/3/3/3
6	GOL	B	804	-	-	0/4/4/4	0/0/0/0
2	GNP	C	500[A]	4	-	0/16/38/38	0/3/3/3
2	GNP	C	500[B]	4	-	0/16/38/38	0/3/3/3
3	51G	C	600	-	-	0/15/69/69	0/3/3/3
2	GNP	D	500	4	-	0/16/38/38	0/3/3/3
3	51G	D	600[A]	-	-	0/15/69/69	0/3/3/3
3	51G	D	600[B]	-	-	0/15/69/69	0/3/3/3
6	GOL	D	804	-	-	0/4/4/4	0/0/0/0

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500[B]	GNP	C4-N9	-8.74	1.36	1.47
2	A	500[A]	GNP	C4-N9	-8.74	1.36	1.47
2	C	500[A]	GNP	C4-N9	-7.54	1.37	1.47
2	C	500[B]	GNP	C4-N9	-7.54	1.37	1.47
2	D	500	GNP	C4-N9	-7.49	1.37	1.47
2	B	500[A]	GNP	C4-N9	-7.07	1.38	1.47
2	B	500[B]	GNP	C4-N9	-7.07	1.38	1.47
2	C	500[B]	GNP	PB-O3A	-5.42	1.52	1.59
2	A	500[B]	GNP	C5-C6	-5.40	1.43	1.53
2	A	500[A]	GNP	C5-C6	-5.40	1.43	1.53
2	D	500	GNP	C5-C6	-5.24	1.43	1.53
2	C	500[A]	GNP	C5-C6	-4.74	1.44	1.53
2	C	500[B]	GNP	C5-C6	-4.74	1.44	1.53
2	B	500[A]	GNP	PB-O3A	-4.37	1.53	1.59
2	D	500	GNP	PB-O2B	-4.24	1.45	1.56
2	B	500[A]	GNP	PB-O2B	-4.21	1.45	1.56
2	B	500[B]	GNP	PG-O2G	-4.16	1.45	1.56
2	B	500[B]	GNP	PB-O2B	-4.11	1.45	1.56
2	B	500[A]	GNP	PG-O2G	-3.92	1.46	1.56
2	D	500	GNP	PG-O3G	-3.88	1.46	1.56
2	B	500[A]	GNP	C5-C6	-3.47	1.46	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500[B]	GNP	C5-C6	-3.47	1.46	1.53
2	B	500[A]	GNP	C8-N9	-3.13	1.37	1.47
2	B	500[B]	GNP	C8-N9	-3.13	1.37	1.47
2	C	500[A]	GNP	C8-N9	-2.87	1.37	1.47
2	C	500[B]	GNP	C8-N9	-2.87	1.37	1.47
2	A	500[B]	GNP	C8-N9	-2.85	1.38	1.47
2	A	500[A]	GNP	C8-N9	-2.85	1.38	1.47
2	D	500	GNP	C8-N9	-2.60	1.38	1.47
2	D	500	GNP	C2-N3	-2.43	1.33	1.43
2	C	500[A]	GNP	C2-N3	-2.38	1.33	1.43
2	C	500[B]	GNP	C2-N3	-2.38	1.33	1.43
2	A	500[B]	GNP	C2-N3	-2.32	1.33	1.43
2	A	500[A]	GNP	C2-N3	-2.32	1.33	1.43
2	C	500[A]	GNP	PA-O5'	-2.29	1.49	1.59
2	C	500[B]	GNP	PA-O5'	-2.29	1.49	1.59
2	B	500[A]	GNP	C2-N3	-2.24	1.34	1.43
2	B	500[B]	GNP	C2-N3	-2.24	1.34	1.43
2	A	500[B]	GNP	C1'-N9	2.14	1.46	1.42
2	A	500[A]	GNP	C1'-N9	2.14	1.46	1.42
2	B	500[A]	GNP	PG-O3G	2.16	1.62	1.56
2	B	500[A]	GNP	C6-N1	2.43	1.37	1.33
2	B	500[B]	GNP	C6-N1	2.43	1.37	1.33
2	B	500[A]	GNP	C1'-N9	2.48	1.46	1.42
2	B	500[B]	GNP	C1'-N9	2.48	1.46	1.42
2	C	500[A]	GNP	C6-N1	2.73	1.37	1.33
2	C	500[B]	GNP	C6-N1	2.73	1.37	1.33
2	D	500	GNP	C1'-N9	3.03	1.47	1.42
2	C	500[A]	GNP	C1'-N9	3.26	1.48	1.42
2	C	500[B]	GNP	C1'-N9	3.26	1.48	1.42
2	A	500[B]	GNP	C6-N1	3.48	1.39	1.33
2	A	500[A]	GNP	C6-N1	3.48	1.39	1.33
2	D	500	GNP	C6-N1	3.49	1.39	1.33
3	C	600	51G	C2-C1	3.68	1.58	1.52
2	D	500	GNP	PG-O2G	3.89	1.67	1.56
3	B	600	51G	C2-C1	4.06	1.58	1.52
3	A	600	51G	C2-C1	4.20	1.58	1.52
3	D	600[A]	51G	C2-C1	4.41	1.59	1.52
3	D	600[B]	51G	C2-C1	4.41	1.59	1.52
2	B	500[B]	GNP	PG-O1G	11.24	1.58	1.46
2	B	500[B]	GNP	PB-O1B	12.71	1.59	1.46
2	B	500[A]	GNP	PG-O1G	13.22	1.60	1.46
2	D	500	GNP	PB-O1B	14.75	1.62	1.46

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500[A]	GNP	PB-O1B	15.60	1.62	1.46
2	D	500	GNP	PG-O1G	17.43	1.64	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	600[B]	51G	C14-C15-N	-4.01	100.26	111.30
2	B	500[A]	GNP	O6-C6-N1	-3.56	118.13	122.80
2	B	500[B]	GNP	O6-C6-N1	-3.56	118.13	122.80
2	D	500	GNP	O2B-PB-O1B	-3.44	103.25	110.02
2	D	500	GNP	O3G-PG-O1G	-3.39	104.66	113.58
3	D	600[A]	51G	O3-C11-C10	-3.24	101.07	108.92
2	C	500[A]	GNP	O6-C6-N1	-2.72	119.22	122.80
2	C	500[B]	GNP	O6-C6-N1	-2.72	119.22	122.80
2	A	500[A]	GNP	O3G-PG-O1G	-2.53	106.93	113.58
3	B	600	51G	O3-C11-C12	-2.41	100.89	107.18
2	C	500[A]	GNP	O2G-PG-O1G	-2.30	107.51	113.58
2	D	500	GNP	O2G-PG-O1G	-2.22	107.72	113.58
3	D	600[A]	51G	C13-C14-C15	-2.10	105.75	109.44
3	A	600	51G	O1-C7-C8	-2.09	103.85	108.92
2	A	500[A]	GNP	O2G-PG-O1G	-2.09	108.09	113.58
2	B	500[A]	GNP	O3A-PB-N3B	2.12	111.90	106.07
3	B	600	51G	C17-O4-C13	2.71	115.07	111.22
2	A	500[B]	GNP	O6-C6-C5	3.88	127.11	119.69
2	A	500[A]	GNP	O6-C6-C5	3.88	127.11	119.69
2	D	500	GNP	O6-C6-C5	3.92	127.19	119.69
2	C	500[A]	GNP	O6-C6-C5	4.80	128.87	119.69
2	C	500[B]	GNP	O6-C6-C5	4.80	128.87	119.69
3	C	600	51G	C17-O4-C13	4.93	118.22	111.22
2	B	500[A]	GNP	C4-C5-N7	5.00	110.47	102.67
2	B	500[B]	GNP	C4-C5-N7	5.00	110.47	102.67
2	D	500	GNP	C4-C5-N7	5.03	110.51	102.67
2	A	500[B]	GNP	C4-C5-N7	5.06	110.57	102.67
2	A	500[A]	GNP	C4-C5-N7	5.06	110.57	102.67
2	C	500[A]	GNP	C4-C5-N7	5.13	110.68	102.67
2	C	500[B]	GNP	C4-C5-N7	5.13	110.68	102.67
2	B	500[A]	GNP	O6-C6-C5	5.31	129.84	119.69
2	B	500[B]	GNP	O6-C6-C5	5.31	129.84	119.69
3	A	600	51G	C17-O4-C13	5.61	119.20	111.22
3	D	600[A]	51G	O3-C13-O4	8.41	127.61	109.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500[B]	GNP	O1G-PG-N3B-PB
2	B	500[A]	GNP	O1G-PG-N3B-PB

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500[B]	GNP	1	0
2	B	500[B]	GNP	4	0
3	B	600	51G	1	0
2	C	500[A]	GNP	1	0
3	D	600[A]	51G	2	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, 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	301/305 (98%)	-0.04	2 (0%) 89 92	39, 55, 79, 114	0
1	B	299/305 (98%)	-0.07	5 (1%) 73 79	29, 46, 81, 109	0
1	C	297/305 (97%)	0.01	2 (0%) 89 92	28, 53, 80, 106	0
1	D	290/305 (95%)	0.29	16 (5%) 29 37	44, 64, 97, 134	0
All	All	1187/1220 (97%)	0.04	25 (2%) 67 74	28, 55, 87, 134	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	179	TYR	5.6
1	C	185[A]	ASN	4.9
1	D	477	TYR	4.7
1	D	455	TYR	4.5
1	D	473	TYR	4.2
1	D	255	VAL	3.8
1	A	179	TYR	3.7
1	D	251	LEU	3.4
1	B	177	TYR	3.3
1	B	176	GLU	2.9
1	D	464	PHE	2.8
1	D	389	THR	2.8
1	D	208	ILE	2.6
1	D	185	ASN	2.4
1	D	181	ASP	2.4
1	D	460	ILE	2.4
1	D	254	ASN	2.4
1	D	213	ASP	2.3
1	C	212	TYR	2.3
1	A	182	ASN	2.2
1	D	384	GLY	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	344	THR	2.1
1	B	212	TYR	2.1
1	B	473	TYR	2.1
1	B	175	MET	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	51G	D	600[B]	33/33	0.95	0.16	1.57	47,58,75,79	12
6	GOL	D	804	6/6	0.90	0.18	1.11	68,76,82,84	0
3	51G	D	600[A]	33/33	0.95	0.16	0.90	47,51,73,79	12
3	51G	B	600	33/33	0.96	0.13	0.65	40,50,86,92	0
2	GNP	A	500[A]	32/32	0.98	0.14	0.54	39,45,50,52	9
2	GNP	A	500[B]	32/32	0.98	0.14	0.37	37,44,50,52	9
2	GNP	B	500[A]	32/32	0.98	0.11	-0.38	34,41,58,62	9
6	GOL	B	804	6/6	0.92	0.12	-0.39	62,70,72,76	0
3	51G	A	600	33/33	0.95	0.12	-0.50	49,56,64,68	0
2	GNP	B	500[B]	32/32	0.98	0.11	-0.72	34,38,41,43	9
3	51G	C	600	33/33	0.94	0.11	-1.03	64,82,92,94	0
2	GNP	D	500	32/32	0.97	0.10	-1.14	48,54,61,61	0
2	GNP	C	500[B]	32/32	0.97	0.10	-1.47	44,49,53,55	9
2	GNP	C	500[A]	32/32	0.97	0.10	-1.74	46,52,57,61	9
4	MG	C	702	1/1	0.99	0.09	-2.81	54,54,54,54	0
4	MG	B	702	1/1	0.94	0.09	-4.15	52,52,52,52	0
4	MG	A	702	1/1	0.95	0.07	-5.15	51,51,51,51	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	B	700	1/1	0.99	0.12	-	29,29,29,29	0
4	MG	C	800	1/1	0.95	0.10	-	64,64,64,64	0
4	MG	A	700	1/1	0.98	0.16	-	30,30,30,30	0
5	CL	C	802	1/1	0.98	0.09	-	50,50,50,50	0
5	CL	A	802	1/1	0.86	0.09	-	75,75,75,75	0
5	CL	B	801	1/1	0.83	0.15	-	84,84,84,84	0
4	MG	D	700	1/1	0.99	0.09	-	38,38,38,38	0
4	MG	C	700	1/1	0.99	0.10	-	37,37,37,37	0
4	MG	D	702	1/1	0.95	0.04	-	67,67,67,67	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.