



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 04:26 AM BST

PDB ID : 4PL0  
Title : Crystal structure of the antibacterial peptide ABC transporter McjD in an outward occluded state  
Authors : Choudhury, H.G.; Beis, K.  
Deposited on : 2014-05-15  
Resolution : 2.70 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

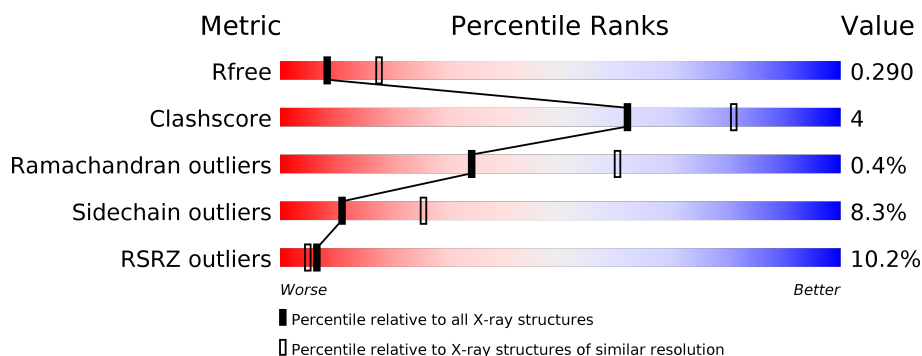
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 respectively. 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	580	<div> <div>12%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>..</div> </div> </div>
1	B	580	<div> <div>9%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>..</div> </div> </div>

## 2 Entry composition [i](#)

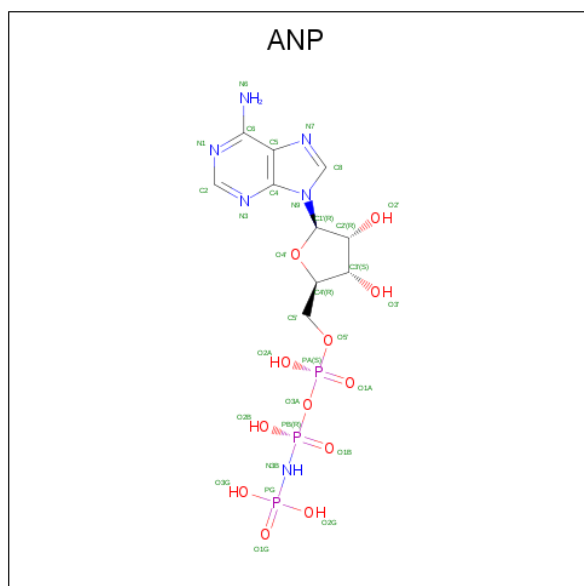
There are 4 unique types of molecules in this entry. The entry contains 9213 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Microcin-J25 export ATP-binding/permease protein McjD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	571	Total	C	N	O	S	0	0	0
			4527	2920	739	850	18			
1	B	576	Total	C	N	O	S	0	2	0
			4580	2954	750	858	18			

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).

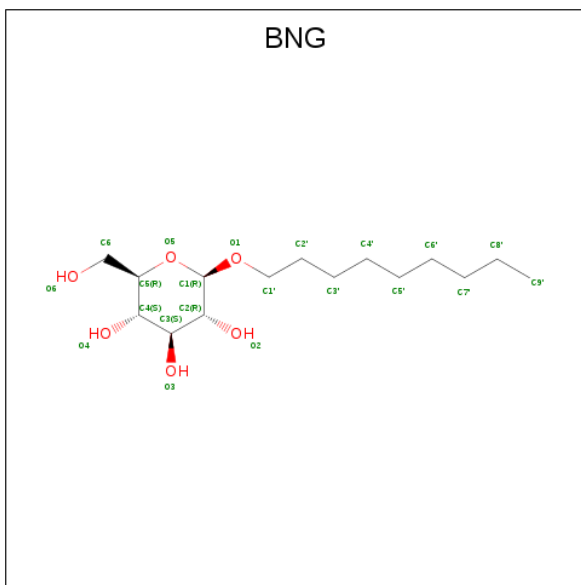


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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

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

- Molecule 4 is nonyl beta-D-glucopyranoside (three-letter code: BNG) (formula: C<sub>15</sub>H<sub>30</sub>O<sub>6</sub>).

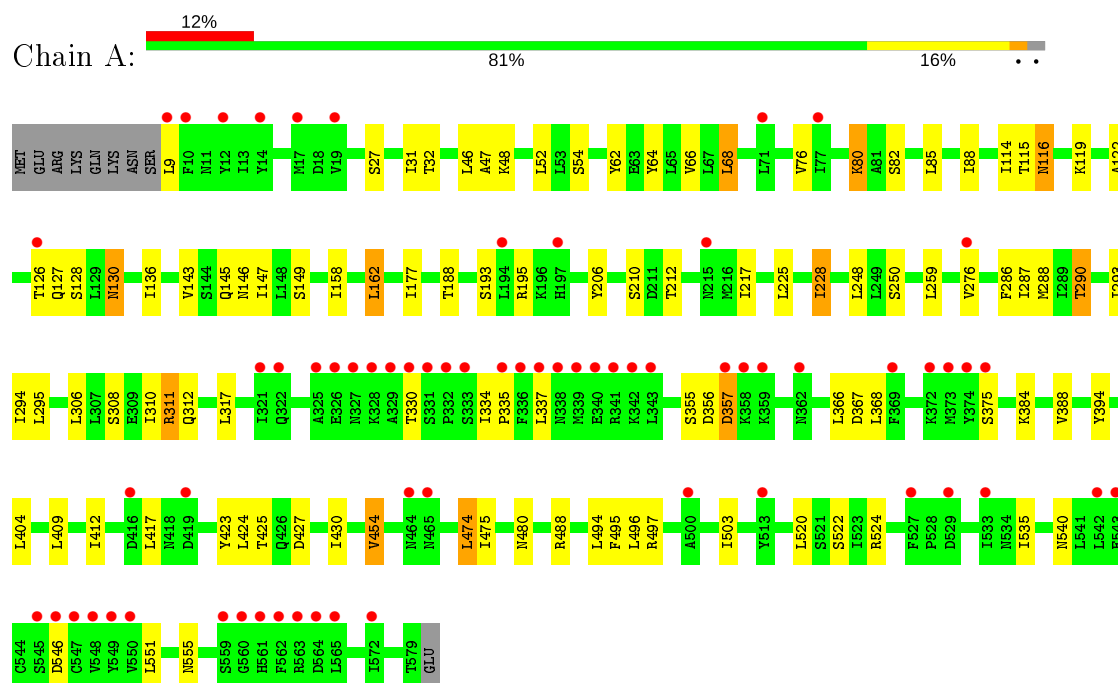


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 21 15 6	0	0
4	B	1	Total C O 21 15 6	0	0

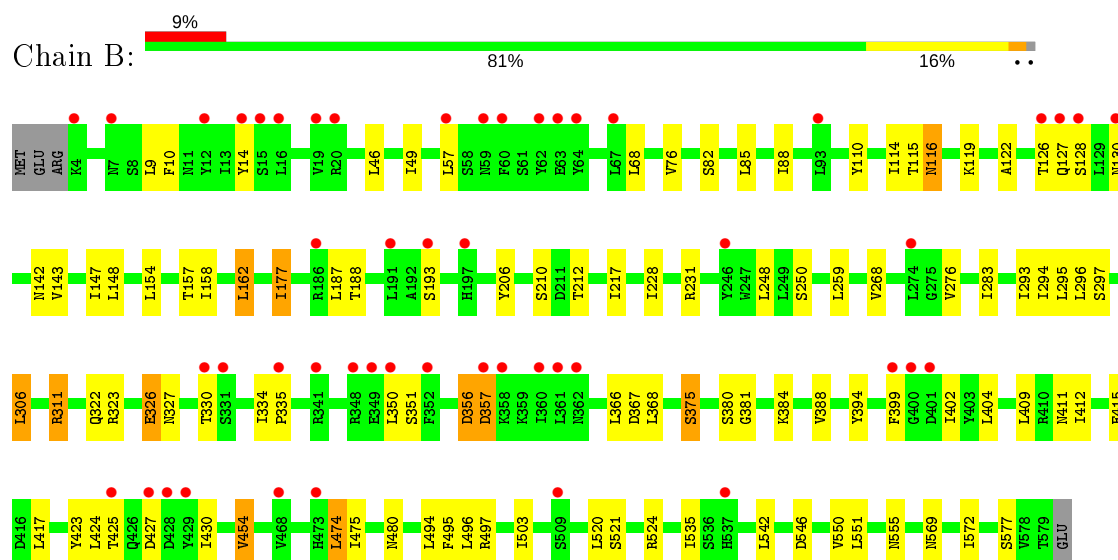
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Microcin-J25 export ATP-binding/permease protein McjD



- Molecule 1: Microcin-J25 export ATP-binding/permease protein McjD



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.83Å 107.92Å 232.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.96 – 2.70 48.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.96-2.70) 99.7 (48.96-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.247 , 0.266 0.267 , 0.290	Depositor DCC
$R_{free}$ test set	2891 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.1	Xtriage
Anisotropy	0.738	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 76.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9213	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% 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: BNG, MG, ANP

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	0.50	0/4603	0.64	1/6234 (0.0%)
1	B	0.50	0/4663	0.64	1/6313 (0.0%)
All	All	0.50	0/9266	0.64	2/12547 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	ASP	CB-CG-OD2	5.20	122.97	118.30
1	A	357	ASP	CB-CG-OD2	5.17	122.95	118.30

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	4527	0	4638	44	0
1	B	4580	0	4701	46	0
2	A	31	0	13	0	0
2	B	31	0	13	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	21	0	30	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	21	0	30	0	0
All	All	9213	0	9425	81	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 (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LYS:HB3	1:A:68:LEU:HD21	1.69	0.75
1:A:143:VAL:HA	1:A:147:ILE:HD12	1.73	0.71
1:B:143:VAL:HA	1:B:147:ILE:HD12	1.75	0.68
1:B:188:THR:HG23	1:B:311:ARG:HE	1.58	0.67
1:A:188:THR:HG23	1:A:308:SER:HA	1.78	0.64
1:A:32:THR:HG21	1:A:145:GLN:HA	1.81	0.62
1:B:454:VAL:HG22	1:B:495:PHE:HB2	1.81	0.62
1:A:454:VAL:HG22	1:A:495:PHE:HB2	1.83	0.61
1:B:212:THR:HG23	1:B:231:ARG:HH21	1.66	0.60
1:B:10:PHE:O	1:B:14:TYR:HD2	1.84	0.59
1:B:409:LEU:HA	1:B:412:ILE:HD12	1.85	0.58
1:A:409:LEU:HA	1:A:412:ILE:HD12	1.86	0.57
1:B:569:ASN:HD22	1:B:572:ILE:H	1.53	0.57
1:A:76:VAL:HG11	1:B:294:ILE:HG12	1.86	0.56
1:B:424:LEU:HD11	1:B:494:LEU:HD22	1.87	0.56
1:A:308:SER:O	1:A:312:GLN:HG2	2.06	0.56
1:B:366:LEU:HD23	1:B:368:LEU:HD11	1.87	0.56
1:A:158:ILE:O	1:A:162:LEU:HB2	2.06	0.56
1:B:384:LYS:HD2	1:B:535:ILE:HG23	1.87	0.56
1:B:351:SER:HB2	1:B:399:PHE:HB2	1.88	0.55
1:A:366:LEU:HD23	1:A:368:LEU:HD11	1.87	0.55
1:A:384:LYS:HD2	1:A:535:ILE:HG23	1.87	0.55
1:B:454:VAL:HG22	1:B:495:PHE:CB	2.36	0.55
1:A:475:ILE:HB	1:A:480:ASN:HB2	1.89	0.54
1:B:454:VAL:HG21	1:B:496:LEU:HG	1.90	0.54
1:B:475:ILE:HB	1:B:480:ASN:HB2	1.89	0.53
1:A:454:VAL:HG21	1:A:496:LEU:HG	1.91	0.52
1:A:430:ILE:HG21	1:A:474:LEU:HD22	1.90	0.52
1:A:188:THR:HG22	1:A:311:ARG:HG2	1.92	0.52
1:A:424:LEU:HD11	1:A:494:LEU:HD22	1.91	0.51
1:B:116:ASN:HA	1:B:119:LYS:HD3	1.92	0.51
1:A:27:SER:O	1:A:31:ILE:HD12	2.10	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:TYR:CE1	1:B:283:ILE:HD11	2.46	0.51
1:B:430:ILE:HG21	1:B:474:LEU:HD22	1.91	0.51
1:A:116:ASN:HA	1:A:119:LYS:HD3	1.92	0.51
1:B:217:ILE:H	1:B:217:ILE:HD12	1.76	0.50
1:A:217:ILE:HD12	1:A:217:ILE:H	1.75	0.50
1:A:454:VAL:HG22	1:A:495:PHE:CB	2.41	0.49
1:A:225:LEU:HB2	1:B:110:TYR:CZ	2.48	0.49
1:B:356:ASP:O	1:B:357:ASP:HB2	2.12	0.48
1:B:375:SER:HB3	1:B:542:LEU:HD23	1.95	0.48
1:A:136:ILE:HG13	1:A:317:LEU:HD21	1.96	0.48
1:A:334:ILE:HG12	1:A:337:LEU:HB2	1.96	0.48
1:A:294:ILE:HG12	1:B:76:VAL:HG11	1.96	0.48
1:A:290:THR:HA	1:A:293:ILE:HD12	1.95	0.48
1:A:210:SER:HB2	1:B:122:ALA:HB1	1.97	0.47
1:B:268:VAL:HG12	1:B:293:ILE:HD11	1.95	0.47
1:A:122:ALA:HB1	1:B:210:SER:HB2	1.97	0.47
1:A:32:THR:HG22	1:A:149:SER:HB2	1.96	0.47
1:A:286:PHE:O	1:A:290:THR:HG23	2.15	0.46
1:A:195:ARG:HD2	1:A:312:GLN:HB2	1.98	0.46
1:B:475:ILE:H	1:B:480:ASN:HD22	1.65	0.45
4:A:603:BNG:H4'1	1:B:46:LEU:HD11	1.97	0.45
1:B:322:GLN:O	1:B:326:GLU:HB2	2.16	0.45
1:A:80:LYS:HE3	1:B:297:SER:HB2	1.99	0.45
1:B:157:THR:HG21	1:B:296:LEU:HD21	1.98	0.45
1:B:154:LEU:HD22	1:B:177:ILE:HD13	1.99	0.45
1:A:146:ASN:O	1:A:306:LEU:HD22	2.16	0.44
1:A:388:VAL:HB	1:A:503:ILE:HD13	2.00	0.44
1:B:158:ILE:O	1:B:162:LEU:HB2	2.18	0.43
1:B:334:ILE:HG12	1:B:411:ASN:O	2.18	0.43
1:B:388:VAL:HB	1:B:503:ILE:HD13	2.00	0.43
1:B:142:ASN:OD1	1:B:306:LEU:HA	2.19	0.43
1:B:114:ILE:HD13	1:B:394:TYR:HA	2.01	0.43
1:A:212:THR:HG21	1:A:228:ILE:HG23	2.01	0.42
1:B:381:GLY:HA2	2:B:601:ANP:H3'	2.00	0.42
1:A:130:ASN:ND2	1:B:206:TYR:OH	2.53	0.42
1:B:49:ILE:HG13	1:B:68:LEU:HB3	2.01	0.42
1:A:114:ILE:HD13	1:A:394:TYR:HA	2.02	0.41
1:A:47:ALA:HB2	1:A:288:MET:HB2	2.03	0.41
1:A:409:LEU:HD22	1:A:417:LEU:HD11	2.02	0.41
1:B:350:LEU:HD22	1:B:402:ILE:HD11	2.01	0.41
1:B:550:VAL:HG11	1:B:569:ASN:HD21	1.85	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:GLN:HG2	1:A:206:TYR:CD2	2.56	0.41
1:A:228:ILE:HA	1:A:228:ILE:HD13	1.84	0.41
1:B:409:LEU:HD22	1:B:417:LEU:HD11	2.03	0.41
1:B:46:LEU:HA	1:B:46:LEU:HD12	1.89	0.41
1:A:355:SER:C	1:A:357:ASP:H	2.24	0.41
1:B:127:GLN:HG2	1:B:206:TYR:CD2	2.56	0.40
1:A:488:ARG:NH2	1:B:380:SER:HB3	2.36	0.40
1:A:52:LEU:HD21	1:A:64:TYR:CD2	2.56	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	569/580 (98%)	531 (93%)	36 (6%)	2 (0%)	34	60
1	B	576/580 (99%)	535 (93%)	38 (7%)	3 (0%)	29	54
All	All	1145/1160 (99%)	1066 (93%)	74 (6%)	5 (0%)	34	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	PRO
1	B	327	ASN
1	A	356	ASP
1	B	323	ARG
1	B	335	PRO

### 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	520/529 (98%)	476 (92%)	44 (8%)	10	24
1	B	527/529 (100%)	484 (92%)	43 (8%)	11	26
All	All	1047/1058 (99%)	960 (92%)	87 (8%)	11	25

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	46	LEU
1	A	54	SER
1	A	66	VAL
1	A	68	LEU
1	A	80	LYS
1	A	82	SER
1	A	85	LEU
1	A	88	ILE
1	A	115	THR
1	A	116	ASN
1	A	126	THR
1	A	128	SER
1	A	130	ASN
1	A	162	LEU
1	A	177	ILE
1	A	193	SER
1	A	228	ILE
1	A	248	LEU
1	A	250	SER
1	A	259	LEU
1	A	276	VAL
1	A	287	ILE
1	A	290	THR
1	A	295	LEU
1	A	310	ILE
1	A	311	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	330	THR
1	A	367	ASP
1	A	375	SER
1	A	404	LEU
1	A	423	TYR
1	A	425	THR
1	A	427	ASP
1	A	454	VAL
1	A	474	LEU
1	A	497	ARG
1	A	520	LEU
1	A	522	SER
1	A	524	ARG
1	A	540	ASN
1	A	546	ASP
1	A	551	LEU
1	A	555	ASN
1	B	9	LEU
1	B	57	LEU
1	B	82	SER
1	B	85	LEU
1	B	88	ILE
1	B	115	THR
1	B	116	ASN
1	B	126	THR
1	B	128	SER
1	B	130	ASN
1	B	148	LEU
1	B	162	LEU
1	B	177	ILE
1	B	187	LEU
1	B	193	SER
1	B	228	ILE
1	B	248	LEU
1	B	250	SER
1	B	259	LEU
1	B	276	VAL
1	B	295	LEU
1	B	306	LEU
1	B	311	ARG
1	B	326	GLU
1	B	330	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	356	ASP
1	B	367	ASP
1	B	375	SER
1	B	404	LEU
1	B	415	GLU
1	B	423	TYR
1	B	425	THR
1	B	427	ASP
1	B	454	VAL
1	B	474	LEU
1	B	497	ARG
1	B	520	LEU
1	B	521	SER
1	B	524	ARG
1	B	546	ASP
1	B	551	LEU
1	B	555	ASN
1	B	577	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	127	GLN
1	A	130	ASN
1	A	153	GLN
1	A	223	ASN
1	A	479	ASN
1	A	487	GLN
1	A	534	ASN
1	B	96	ASN
1	B	127	GLN
1	B	130	ASN
1	B	153	GLN
1	B	223	ASN
1	B	459	ASN
1	B	479	ASN
1	B	480	ASN
1	B	515	ASN
1	B	569	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	BNG	B	603	-	21,21,21	0.22	0	26,26,26	0.41	0
2	ANP	A	601	3	29,33,33	2.31	5 (17%)	31,52,52	2.05	6 (19%)
2	ANP	B	601	3	29,33,33	2.44	5 (17%)	31,52,52	2.12	6 (19%)
4	BNG	A	603	-	21,21,21	0.23	0	26,26,26	0.27	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
4	BNG	B	603	-	-	5/12/32/32	0/1/1/1
2	ANP	A	601	3	-	4/14/38/38	0/3/3/3
2	ANP	B	601	3	-	6/14/38/38	0/3/3/3
4	BNG	A	603	-	-	6/12/32/32	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ANP	PB-O1B	7.99	1.58	1.46
2	A	601	ANP	PB-O1B	7.74	1.58	1.46
2	B	601	ANP	PG-O1G	7.62	1.58	1.46
2	A	601	ANP	PG-O1G	7.33	1.57	1.46
2	B	601	ANP	PB-O3A	-4.29	1.53	1.59
2	A	601	ANP	PB-O3A	-3.75	1.54	1.59
2	A	601	ANP	PB-O2B	-3.25	1.48	1.56
2	B	601	ANP	PB-O2B	-3.22	1.48	1.56
2	B	601	ANP	PG-O3G	-2.97	1.48	1.56
2	A	601	ANP	PG-O3G	-2.34	1.50	1.56

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ANP	O2G-PG-O1G	-7.26	95.20	113.45
2	A	601	ANP	O2G-PG-O1G	-6.73	96.53	113.45
2	B	601	ANP	PA-O3A-PB	5.62	152.41	132.62
2	A	601	ANP	PA-O3A-PB	5.09	150.53	132.62
2	A	601	ANP	O3G-PG-O2G	4.05	118.44	107.64
2	B	601	ANP	O3G-PG-O2G	3.94	118.14	107.64
2	A	601	ANP	O1B-PB-N3B	-3.50	106.62	111.77
2	B	601	ANP	O1B-PB-N3B	-3.01	107.34	111.77
2	A	601	ANP	O2B-PB-O1B	2.62	115.41	109.92
2	B	601	ANP	C5-C6-N6	2.14	123.60	120.35
2	A	601	ANP	C5-C6-N6	2.07	123.50	120.35
2	B	601	ANP	O3G-PG-O1G	-2.06	108.27	113.45

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	ANP	PB-N3B-PG-O1G
2	B	601	ANP	PG-N3B-PB-O1B
2	B	601	ANP	PA-O3A-PB-O1B
2	B	601	ANP	C5'-O5'-PA-O1A
2	B	601	ANP	C5'-O5'-PA-O3A
2	A	601	ANP	PB-N3B-PG-O1G
2	A	601	ANP	PG-N3B-PB-O1B
2	A	601	ANP	PA-O3A-PB-O1B
4	B	603	BNG	C2'-C3'-C4'-C5'
4	A	603	BNG	C2-C1-O1-C1'

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	A	603	BNG	O5-C1-O1-C1'
4	A	603	BNG	C5'-C6'-C7'-C8'
4	A	603	BNG	C3'-C4'-C5'-C6'
4	B	603	BNG	O5-C5-C6-O6
4	A	603	BNG	C2'-C3'-C4'-C5'
4	B	603	BNG	C1'-C2'-C3'-C4'
4	B	603	BNG	C4'-C5'-C6'-C7'
2	B	601	ANP	PA-O3A-PB-O2B
2	A	601	ANP	PA-O3A-PB-O2B
4	B	603	BNG	O5-C1-O1-C1'
4	A	603	BNG	C4'-C5'-C6'-C7'

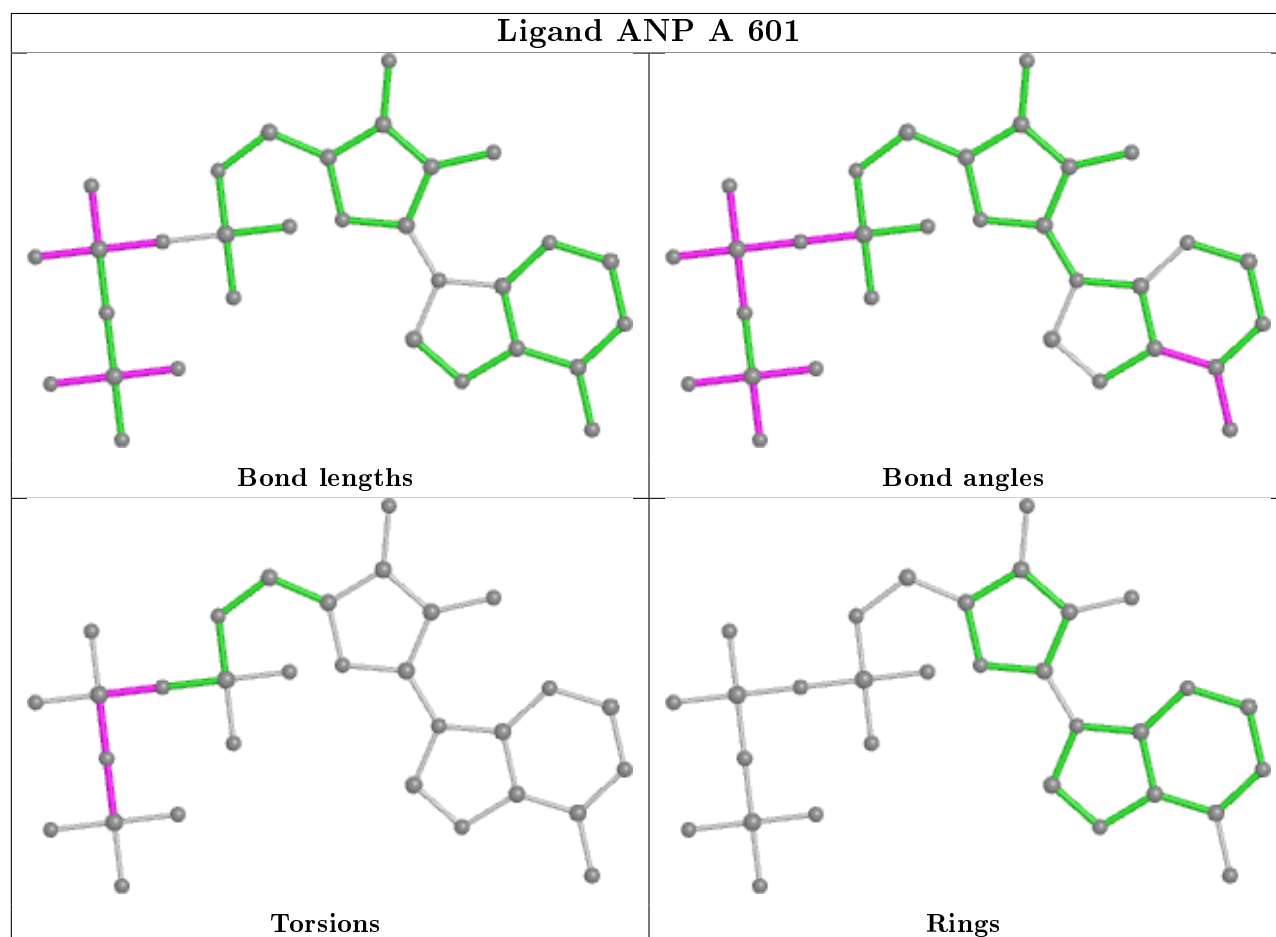
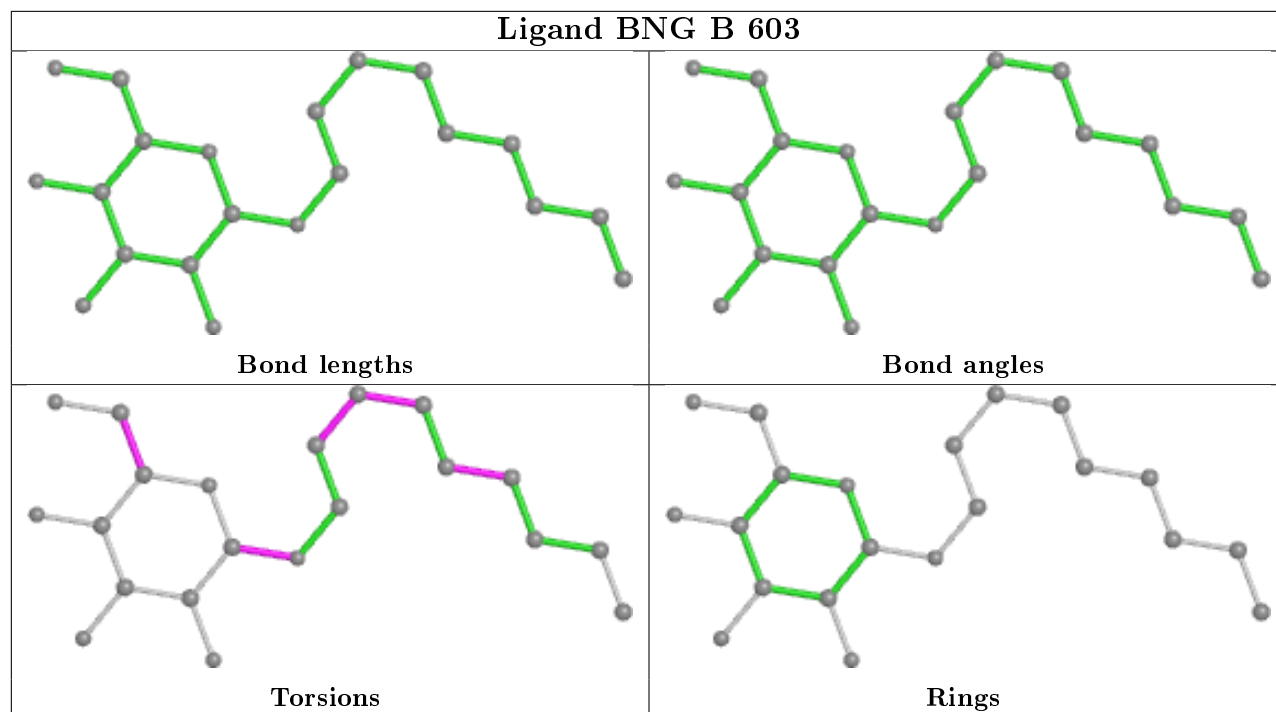
There are no ring outliers.

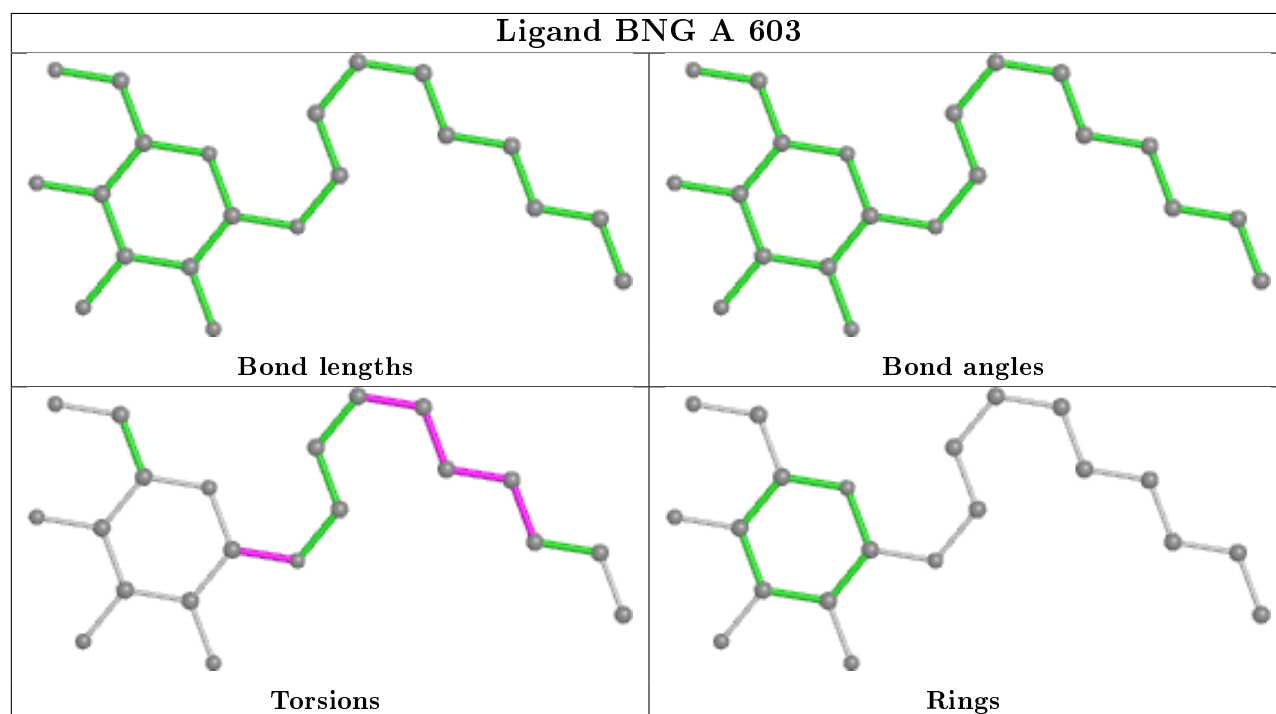
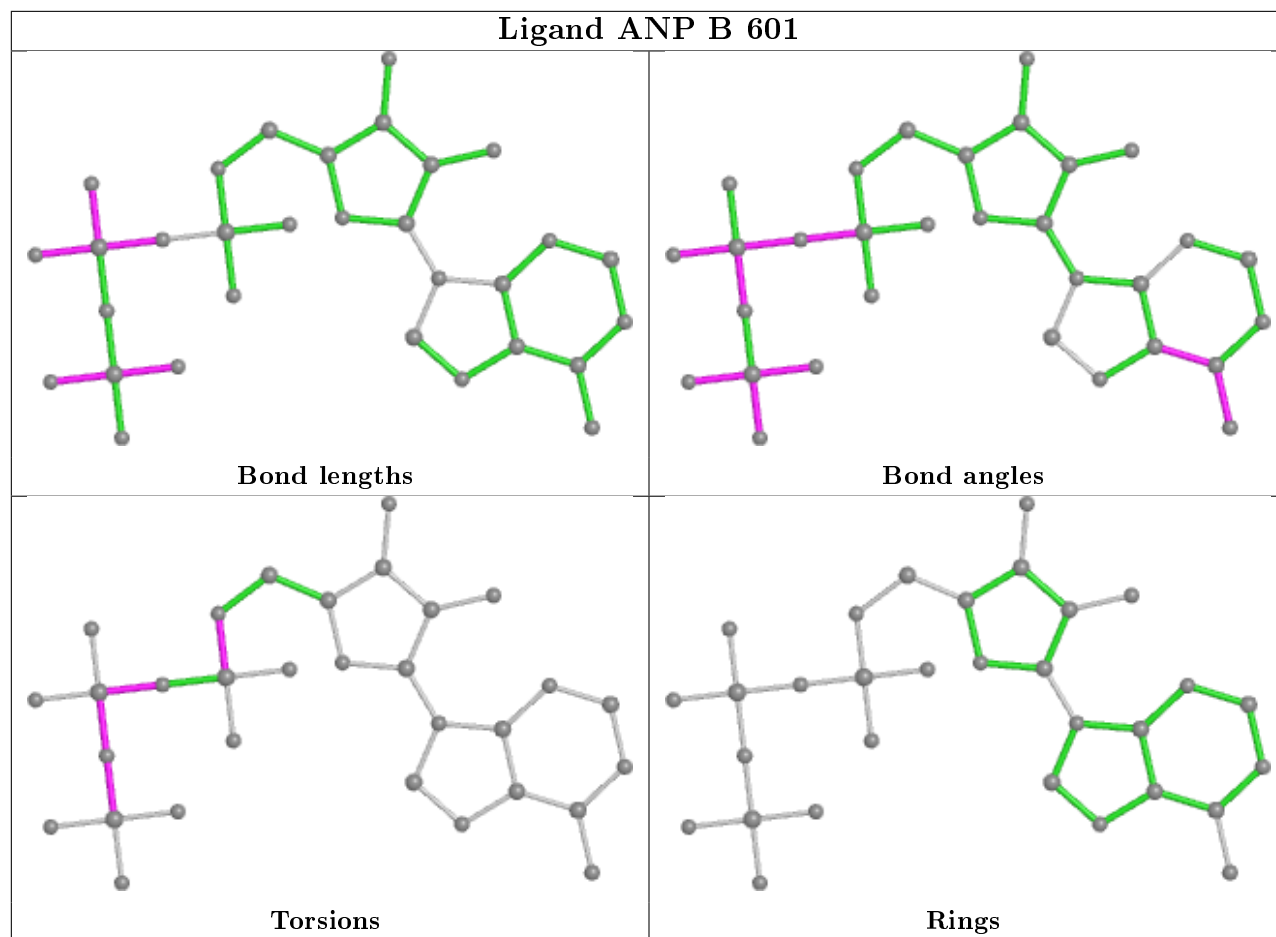
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	ANP	1	0
4	A	603	BNG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 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, 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	571/580 (98%)	0.62	67 (11%) 4 3	61, 95, 135, 202	0
1	B	576/580 (99%)	0.45	50 (8%) 10 8	63, 92, 134, 184	0
All	All	1147/1160 (98%)	0.53	117 (10%) 6 5	61, 94, 135, 202	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	336	PHE	18.2
1	A	329	ALA	11.4
1	A	328	LYS	10.0
1	A	335	PRO	9.9
1	A	341	ARG	9.5
1	A	327	ASN	9.1
1	A	330	THR	9.1
1	A	340	GLU	7.4
1	A	562	PHE	6.9
1	A	338	ASN	6.4
1	A	331	SER	5.5
1	A	326	GLU	5.1
1	A	339	MET	5.1
1	A	529	ASP	5.0
1	A	14	TYR	4.9
1	A	565	LEU	4.9
1	A	500	ALA	4.8
1	B	357	ASP	4.8
1	A	564	ASP	4.7
1	B	349	GLU	4.6
1	A	543	GLU	4.5
1	A	9	LEU	4.4
1	B	12	TYR	4.4
1	B	63	GLU	4.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	64	TYR	4.3
1	A	560	GLY	4.3
1	A	548	VAL	4.2
1	A	337	LEU	4.1
1	B	62	TYR	4.0
1	A	332	PRO	3.7
1	A	563	ARG	3.6
1	B	59	ASN	3.6
1	B	193	SER	3.6
1	B	350	LEU	3.5
1	A	374	TYR	3.5
1	B	19	VAL	3.5
1	A	549	TYR	3.5
1	B	16	LEU	3.5
1	A	333	SER	3.4
1	A	464	ASN	3.4
1	B	60	PHE	3.4
1	A	357	ASP	3.3
1	A	561	HIS	3.3
1	B	352	PHE	3.3
1	A	342	LYS	3.2
1	A	545	SER	3.1
1	B	473	HIS	3.1
1	A	17	MET	3.1
1	A	343	LEU	3.0
1	B	341	ARG	3.0
1	B	4	LYS	2.9
1	B	400	GLY	2.9
1	A	359	LYS	2.8
1	B	126	THR	2.8
1	A	547	CYS	2.8
1	B	191	LEU	2.8
1	B	20	ARG	2.8
1	B	331	SER	2.7
1	B	428	ASP	2.7
1	B	246	TYR	2.7
1	A	550	VAL	2.7
1	B	7	ASN	2.7
1	B	362	ASN	2.7
1	B	425	THR	2.7
1	B	127	GLN	2.7
1	A	362	ASN	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	419	ASP	2.6
1	B	14	TYR	2.6
1	B	335	PRO	2.6
1	B	427	ASP	2.6
1	A	12	TYR	2.6
1	A	542	LEU	2.6
1	A	533	ILE	2.6
1	B	15	SER	2.5
1	B	330	THR	2.5
1	A	197	HIS	2.5
1	B	401	ASP	2.5
1	B	274	LEU	2.5
1	A	19	VAL	2.5
1	A	77	ILE	2.5
1	A	572	ILE	2.5
1	A	10	PHE	2.5
1	B	537	HIS	2.4
1	B	130	ASN	2.4
1	A	375	SER	2.4
1	B	361	LEU	2.4
1	B	197	HIS	2.4
1	A	71	LEU	2.4
1	B	429	TYR	2.4
1	B	399	PHE	2.4
1	A	559	SER	2.4
1	A	527	PHE	2.4
1	A	215	ASN	2.3
1	A	276	VAL	2.3
1	B	93	LEU	2.3
1	A	322	GLN	2.3
1	B	360	ILE	2.3
1	B	468	VAL	2.3
1	B	348	ARG	2.3
1	A	369	PHE	2.2
1	A	358	LYS	2.2
1	A	372	LYS	2.2
1	A	373	MET	2.2
1	B	67	LEU	2.1
1	A	325	ALA	2.1
1	A	465	ASN	2.1
1	A	513	TYR	2.1
1	A	321	ILE	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	126	THR	2.1
1	A	546	ASP	2.1
1	B	57	LEU	2.1
1	B	128	SER	2.1
1	B	186	ARG	2.1
1	B	358	LYS	2.0
1	B	509	SER	2.0
1	A	194	LEU	2.0
1	A	416	ASP	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

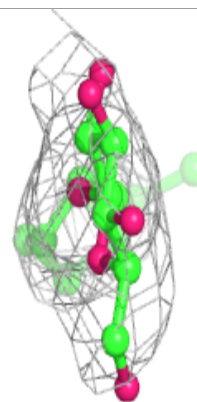
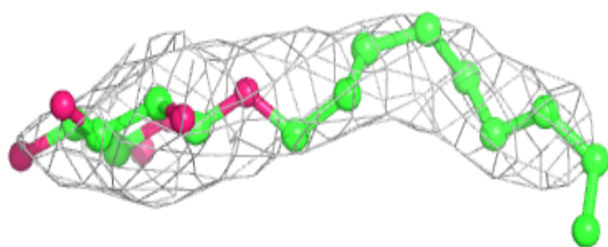
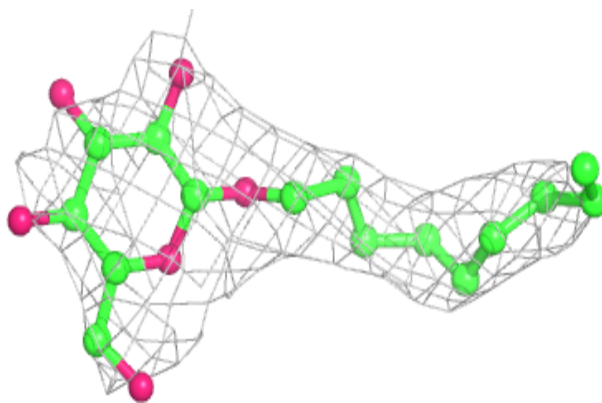
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BNG	A	603	21/21	0.85	0.26	92,123,129,129	0
4	BNG	B	603	21/21	0.90	0.27	96,111,120,124	0
3	MG	B	602	1/1	0.91	0.28	68,68,68,68	0
3	MG	A	602	1/1	0.94	0.24	69,69,69,69	0
2	ANP	B	601	31/31	0.95	0.15	81,88,94,94	0
2	ANP	A	601	31/31	0.96	0.15	91,103,107,109	0

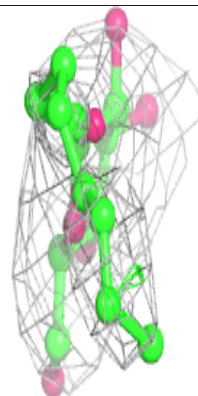
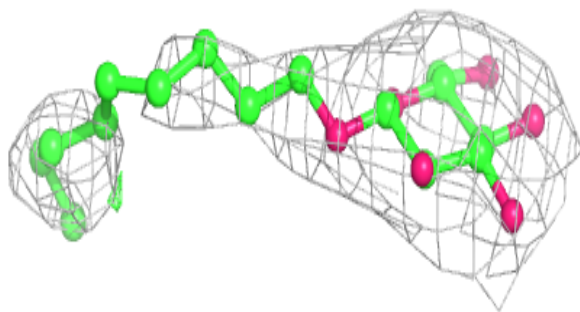
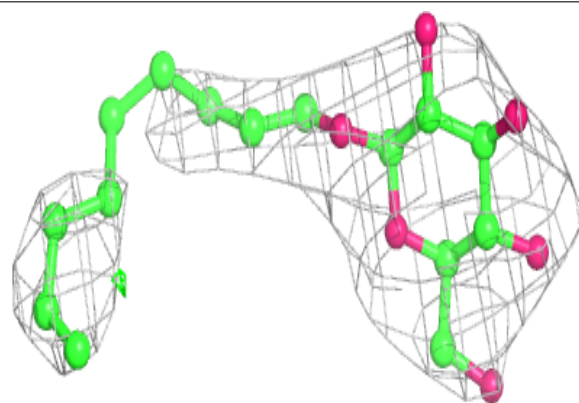
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around BNG A 603:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BNG B 603:**

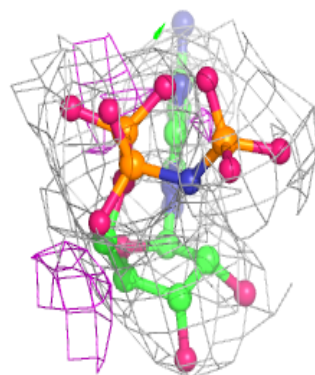
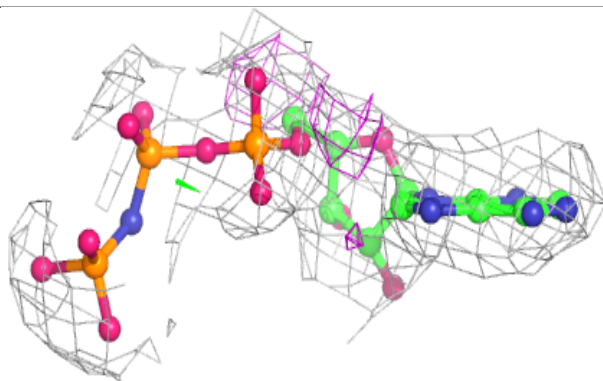
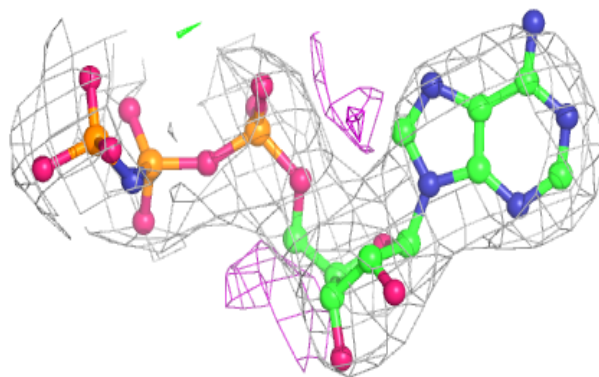
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



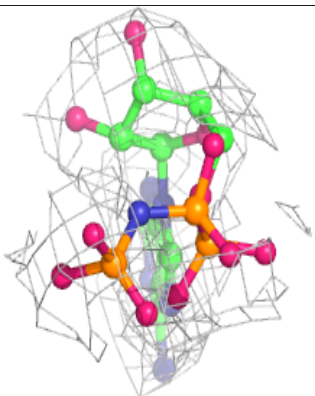
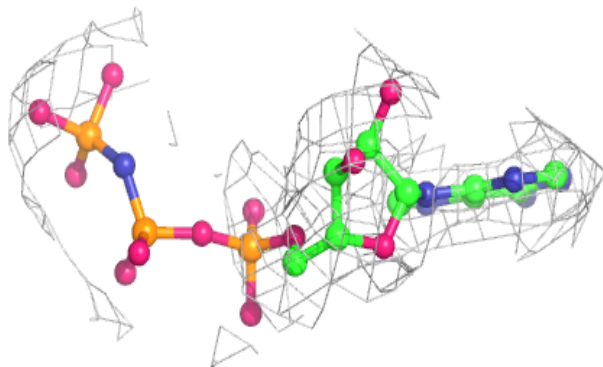
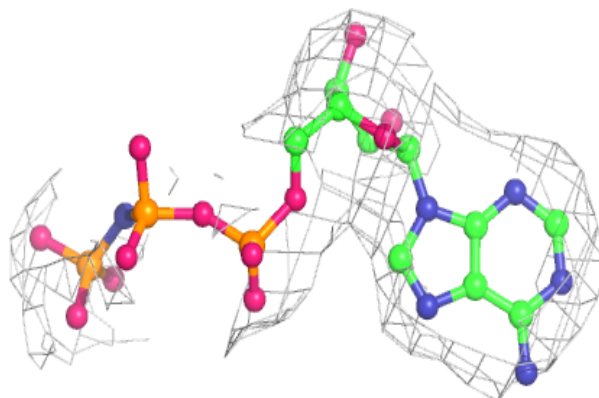


**Electron density around ANP B 601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ANP A 601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.