



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2025 – 06:08 PM EDT

PDB ID : 9BQ7 / pdb\_00009bq7  
Title : Human Topoisomerase 2 Alpha ATPase domain bound to BNS22 and non-hydrolyzable ATP analog AMPPNP  
Authors : Cong, A.T.Q.; Austin, C.A.; Kubes, J.; Karabanovich, G.; Melnikova, I.; Lencova, O.; Kollarova, P.; Piskackova, H.B.; Kerestes, V.; Applova, L.; Arrouye, L.; Alvey, J.A.; Paluncic, J.; Witter, T.L.; Jirkovska, A.; Kunes, J.; Sterbova, P.; Sterba, M.; Simunek, T.; Roh, J.; Schellenberg, M.J.  
Deposited on : 2024-05-09  
Resolution : 2.05 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

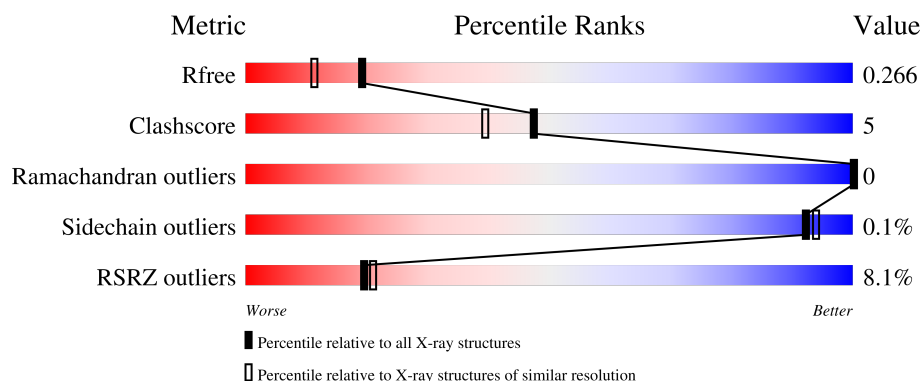
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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))
$R_{free}$	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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 of 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	399	<div> <div>3%</div> <div>86%</div> <div>11%</div> <div>•</div> </div>
1	B	399	<div> <div>12%</div> <div>80%</div> <div>16%</div> <div>•</div> </div>

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6575 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.

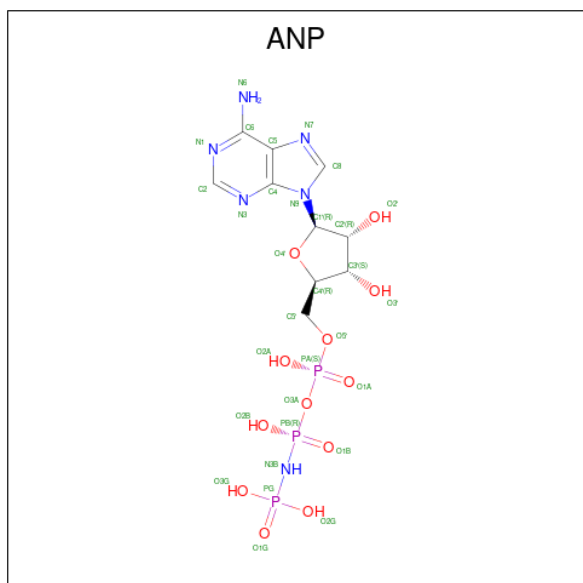
- Molecule 1 is a protein called DNA topoisomerase 2-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	1	0
			3078	1959	522	578	19			
1	B	385	Total	C	N	O	S	0	0	0
			3072	1955	521	577	19			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	SER	-	expression tag	UNP P11388
A	27	ASN	-	expression tag	UNP P11388
A	28	ALA	-	expression tag	UNP P11388
B	26	SER	-	expression tag	UNP P11388
B	27	ASN	-	expression tag	UNP P11388
B	28	ALA	-	expression tag	UNP P11388

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).

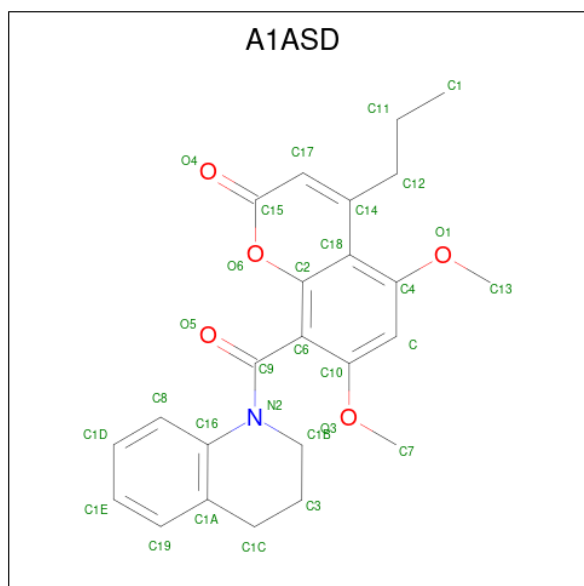


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is 8-(3,4-dihydroquinoline-1(2H)-carbonyl)-5,7-dimethoxy-4-propyl-2H-1-benzopyran-2-one (CCD ID: A1ASD) (formula: C<sub>24</sub>H<sub>25</sub>NO<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

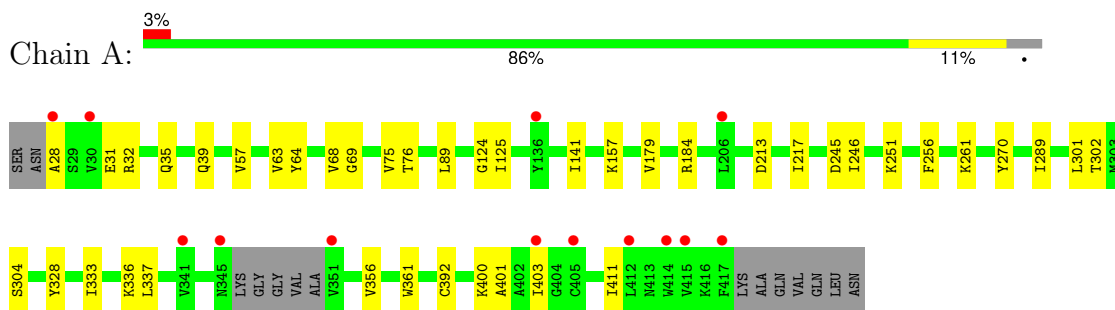
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	189	Total O 189 189	0	0
7	B	104	Total O 104 104	0	0

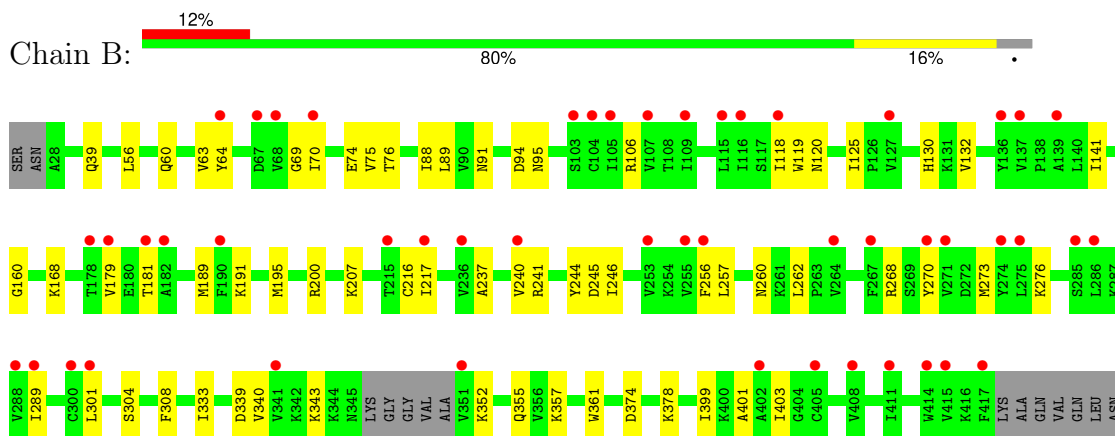
### 3 Residue-property plots [i](#)

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: DNA topoisomerase 2-alpha



- Molecule 1: DNA topoisomerase 2-alpha



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.93Å 92.85Å 126.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.00 – 2.05 47.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.00-2.05) 99.7 (47.00-2.05)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.225 , 0.263 0.227 , 0.266	Depositor DCC
$R_{free}$ test set	50590 reflections (3.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.8	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 66.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6575	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, ANP, GOL, A1ASD, 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	0.13	0/3138	0.34	0/4230
1	B	0.12	0/3129	0.32	0/4218
All	All	0.12	0/6267	0.33	0/8448

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-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 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	3078	0	3087	27	0
1	B	3072	0	3079	42	0
2	A	31	0	13	1	0
2	B	31	0	13	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	30	0	0	0	0
4	B	30	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	1	0
6	B	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	189	0	0	2	0
7	B	104	0	0	1	0
All	All	6575	0	6200	68	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 5.

All (68) 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:B:304:SER:HB2	1:B:361:TRP:HB2	1.65	0.78
1:B:340:VAL:HG21	1:B:403:ILE:HD12	1.73	0.69
1:B:195:MET:HE2	1:B:200:ARG:HG3	1.73	0.69
1:B:240:VAL:HG22	1:B:257:LEU:HD21	1.77	0.67
1:A:301:LEU:HD22	1:A:333:ILE:HD13	1.79	0.64
1:B:125:ILE:HD13	1:B:141:ILE:HD11	1.80	0.63
1:B:352:LYS:HB2	1:B:355:GLN:HG3	1.81	0.63
1:A:31:GLU:N	1:A:31:GLU:OE1	2.31	0.63
1:B:268:ARG:NH1	7:B:1004:HOH:O	2.35	0.60
1:A:28:ALA:HA	1:A:32:ARG:HH21	1.66	0.59
1:B:301:LEU:HD22	1:B:333:ILE:HD13	1.84	0.59
1:A:125:ILE:HD13	1:A:141:ILE:HD11	1.86	0.58
1:B:91:ASN:HB3	2:B:901:ANP:N7	2.19	0.57
1:B:119:TRP:HD1	1:B:216:CYS:HB2	1.69	0.57
1:B:168:LYS:NZ	2:B:901:ANP:O2A	2.36	0.57
1:A:289:ILE:HD12	1:A:401:ALA:HB1	1.85	0.56
1:B:89:LEU:HG	1:B:246:ILE:HG13	1.86	0.56
1:B:245:ASP:OD2	1:B:270:TYR:OH	2.20	0.56
1:B:399:ILE:O	1:B:403:ILE:HG12	2.06	0.56
1:B:60:GLN:HA	1:B:74:GLU:HA	1.87	0.55
1:B:289:ILE:HD12	1:B:401:ALA:HB1	1.90	0.54
1:B:378:LYS:NZ	2:B:901:ANP:O2G	2.28	0.53
1:B:70:ILE:HD12	1:B:273:MET:HB3	1.91	0.53
1:A:32:ARG:O	1:A:35[A]:GLN:NE2	2.43	0.52
1:A:39:GLN:HG2	1:B:39:GLN:NE2	2.25	0.52
1:B:106:ARG:HA	1:B:256:PHE:HB2	1.91	0.52
1:A:245:ASP:OD2	1:A:270:TYR:OH	2.21	0.50
1:A:304:SER:HB2	1:A:361:TRP:HB2	1.94	0.48
1:A:57:VAL:O	1:A:76:THR:HA	2.14	0.47
1:A:184:ARG:N	1:A:213:ASP:OD2	2.44	0.47
1:B:257:LEU:HD23	6:B:903:GOL:H2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:HG	1:A:246:ILE:HG13	1.97	0.47
1:B:63:VAL:HG11	1:B:75:VAL:HG11	1.96	0.47
1:A:124:GLY:H	1:A:213:ASP:HB3	1.80	0.47
1:A:63:VAL:HG11	1:A:75:VAL:HG11	1.97	0.46
1:B:64:TYR:HA	1:B:69:GLY:O	2.15	0.46
1:A:179:VAL:HG22	1:A:217:ILE:HD12	1.97	0.46
1:B:95:ASN:HD22	1:B:120:ASN:HD21	1.64	0.45
1:B:130:HIS:CE1	1:B:132:VAL:HB	2.51	0.45
1:A:39:GLN:HG2	1:B:39:GLN:HE21	1.81	0.45
1:B:125:ILE:HB	1:B:181:THR:HG21	1.99	0.45
1:B:241:ARG:NH2	1:B:245:ASP:OD1	2.38	0.45
2:A:901:ANP:O2B	2:A:901:ANP:O3'	2.32	0.45
1:B:63:VAL:HB	1:B:237:ALA:HB1	1.98	0.45
1:A:256:PHE:CZ	1:A:261:LYS:HD3	2.52	0.44
1:B:179:VAL:HG22	1:B:217:ILE:HD12	1.99	0.44
1:A:400:LYS:O	1:A:403:ILE:HG13	2.18	0.43
1:B:88:ILE:HB	1:B:118:ILE:HD12	1.99	0.43
1:B:189:MET:HE3	1:B:207:LYS:HB2	2.01	0.43
1:A:328:TYR:HE2	1:A:392:CYS:HB3	1.83	0.43
1:B:374:ASP:HB2	5:B:905:CL:CL	2.55	0.43
1:A:28:ALA:HA	1:A:32:ARG:NH2	2.32	0.43
1:B:308:PHE:CD1	1:B:357:LYS:HG2	2.52	0.43
1:B:339:ASP:O	1:B:343:LYS:HG2	2.18	0.43
1:B:56:LEU:HD22	1:B:76:THR:HG22	2.01	0.42
1:B:257:LEU:N	1:B:260:ASN:O	2.46	0.42
1:A:251:LYS:HE3	7:A:1155:HOH:O	2.18	0.42
1:B:95:ASN:HD22	1:B:120:ASN:ND2	2.18	0.41
1:A:157:LYS:NZ	7:A:1014:HOH:O	2.53	0.41
1:A:302:THR:HG23	1:A:361:TRP:HB3	2.03	0.41
1:A:64:TYR:CE2	1:A:69:GLY:HA2	2.56	0.41
1:A:337:LEU:HD23	1:A:403:ILE:HG22	2.03	0.41
1:A:336:LYS:HD3	1:A:336:LYS:HA	1.83	0.40
1:B:276:LYS:HB2	1:B:276:LYS:HE3	1.86	0.40
1:B:179:VAL:O	1:B:191:LYS:HA	2.21	0.40
1:A:356:VAL:HG22	1:A:411:ILE:HD13	2.03	0.40
1:B:244:TYR:CZ	1:B:262:LEU:HD22	2.57	0.40
1:B:94:ASP:CG	1:B:160:GLY:H	2.29	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	382/399 (96%)	374 (98%)	8 (2%)	0	100	100
1	B	381/399 (96%)	367 (96%)	14 (4%)	0	100	100
All	All	763/798 (96%)	741 (97%)	22 (3%)	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	343/356 (96%)	342 (100%)	1 (0%)	91	92
1	B	342/356 (96%)	342 (100%)	0	100	100
All	All	685/712 (96%)	684 (100%)	1 (0%)	92	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	150	ASN

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Mol	Chain	Res	Type
1	A	284	ASN
1	B	39	GLN
1	B	120	ASN
1	B	163	ASN
1	B	309	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	ANP	A	901	3	29,33,33	1.11	3 (10%)	31,52,52	0.82	2 (6%)
4	A1ASD	A	903	-	33,33,33	0.59	0	42,47,47	1.30	6 (14%)
6	GOL	B	903	-	5,5,5	0.93	0	5,5,5	1.07	0
2	ANP	B	901	3	29,33,33	1.12	4 (13%)	31,52,52	0.78	1 (3%)
4	A1ASD	B	904	-	33,33,33	0.60	0	42,47,47	1.27	6 (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
2	ANP	A	901	3	-	5/14/38/38	0/3/3/3
4	A1ASD	A	903	-	-	1/15/25/25	0/4/4/4
6	GOL	B	903	-	-	0/4/4/4	-
2	ANP	B	901	3	-	5/14/38/38	0/3/3/3
4	A1ASD	B	904	-	-	2/15/25/25	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	ANP	PG-N3B	2.58	1.70	1.63
2	B	901	ANP	PG-N3B	2.53	1.70	1.63
2	A	901	ANP	PB-O1B	2.49	1.50	1.46
2	B	901	ANP	PG-O1G	2.44	1.49	1.46
2	B	901	ANP	PB-O1B	2.37	1.49	1.46
2	A	901	ANP	PG-O1G	2.29	1.49	1.46
2	B	901	ANP	PB-O3A	-2.22	1.56	1.59

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	904	A1ASD	C12-C14-C18	4.25	126.12	119.02
4	A	903	A1ASD	C12-C14-C18	4.02	125.74	119.02
4	A	903	A1ASD	C18-C2-C6	2.96	125.26	120.95
4	B	904	A1ASD	C18-C2-C6	2.90	125.18	120.95
4	A	903	A1ASD	C6-C9-N2	2.46	120.12	117.55
4	B	904	A1ASD	C6-C9-N2	2.42	120.08	117.55
4	A	903	A1ASD	O6-C2-C6	-2.41	113.05	116.02
2	B	901	ANP	C5-C6-N6	2.29	123.80	120.31
2	A	901	ANP	C5-C6-N6	2.28	123.78	120.31
4	B	904	A1ASD	O6-C2-C6	-2.26	113.24	116.02
4	B	904	A1ASD	C12-C14-C17	-2.21	115.10	121.61
4	A	903	A1ASD	C12-C14-C17	-2.20	115.12	121.61
4	B	904	A1ASD	O1-C4-C	-2.08	120.49	124.08
4	A	903	A1ASD	O1-C4-C	-2.08	120.49	124.08
2	A	901	ANP	O2G-PG-O1G	-2.05	108.31	113.45

There are no chirality outliers.

All (13) torsion outliers are listed below:

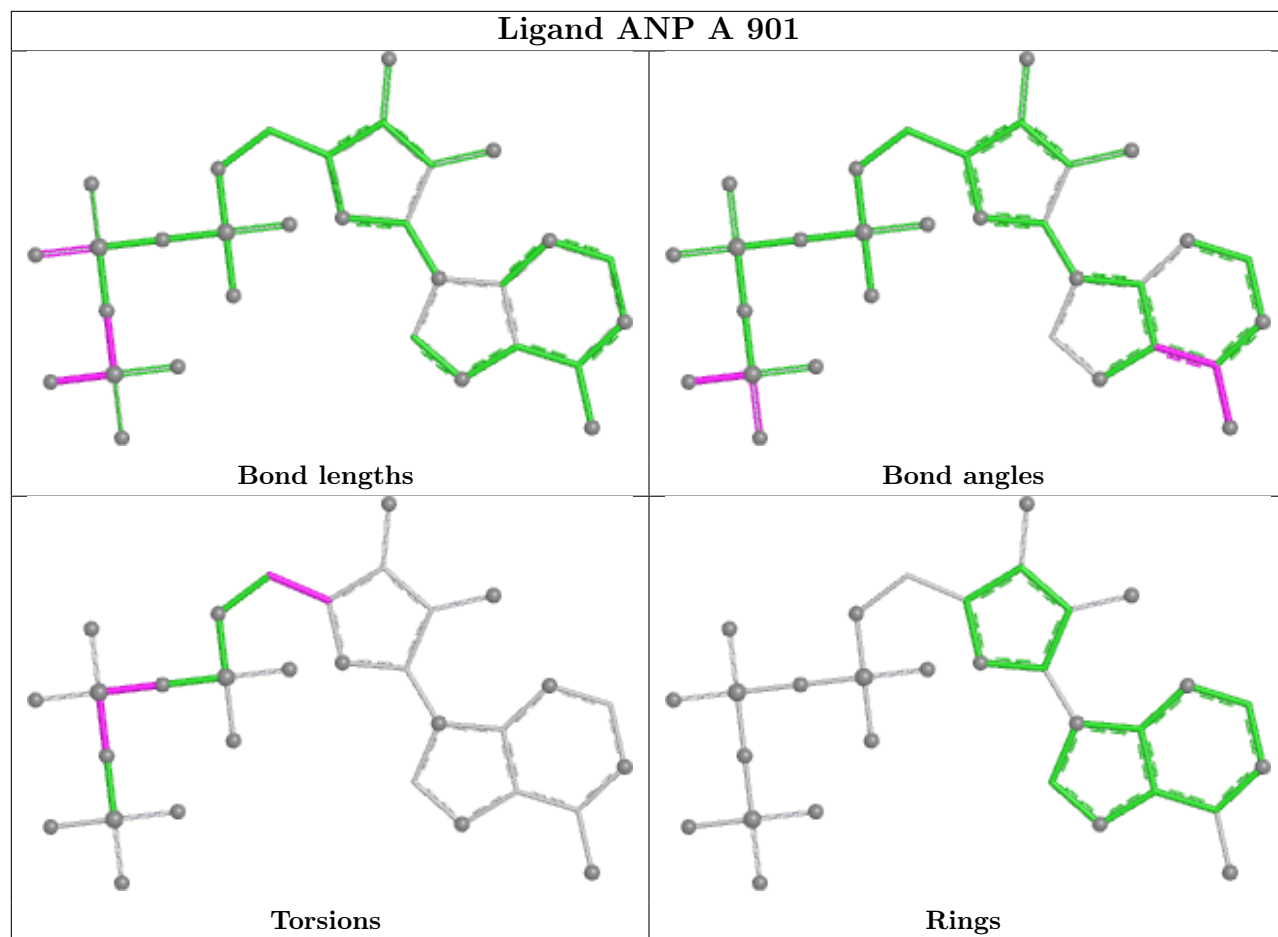
Mol	Chain	Res	Type	Atoms
2	A	901	ANP	PG-N3B-PB-O1B
2	A	901	ANP	PA-O3A-PB-O2B
2	B	901	ANP	PG-N3B-PB-O1B
2	B	901	ANP	PA-O3A-PB-O2B
4	B	904	A1ASD	C1-C11-C12-C14
4	A	903	A1ASD	C11-C12-C14-C18
4	B	904	A1ASD	C11-C12-C14-C18
2	A	901	ANP	C3'-C4'-C5'-O5'
2	B	901	ANP	C3'-C4'-C5'-O5'
2	A	901	ANP	O4'-C4'-C5'-O5'
2	B	901	ANP	O4'-C4'-C5'-O5'
2	A	901	ANP	PA-O3A-PB-O1B
2	B	901	ANP	PA-O3A-PB-O1B

There are no ring outliers.

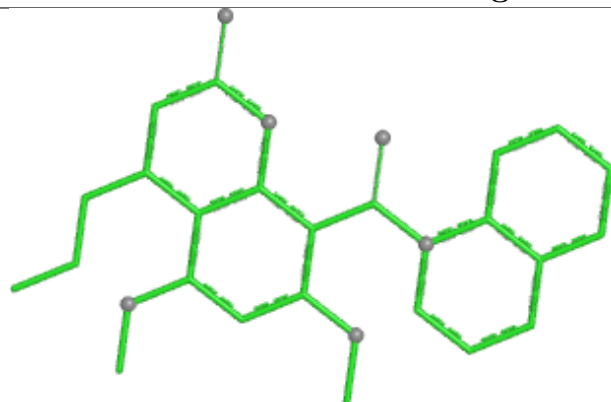
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	ANP	1	0
6	B	903	GOL	1	0
2	B	901	ANP	3	0

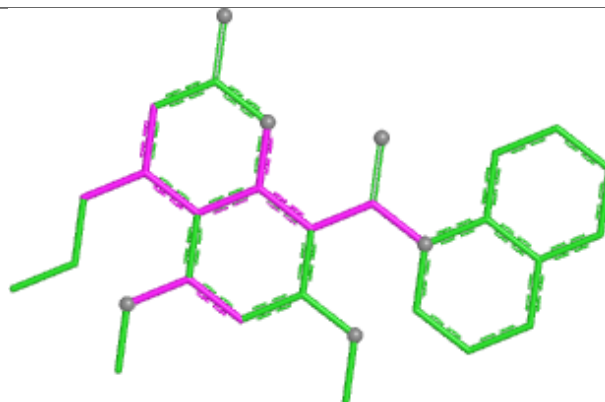
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



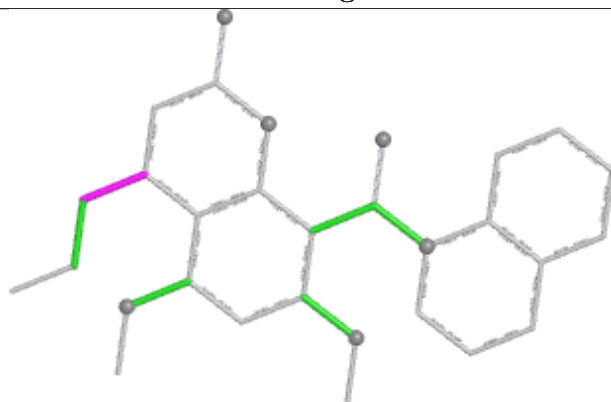
## Ligand A1ASD A 903



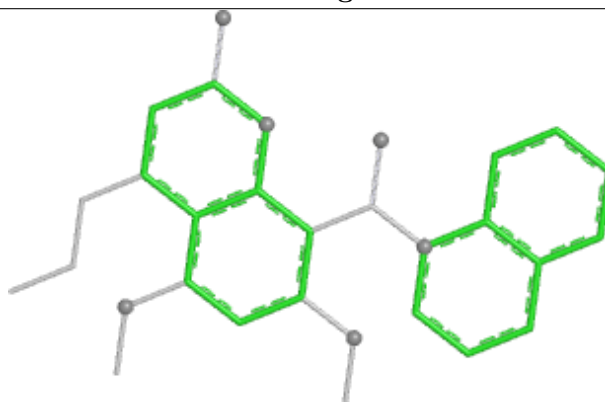
Bond lengths



Bond angles

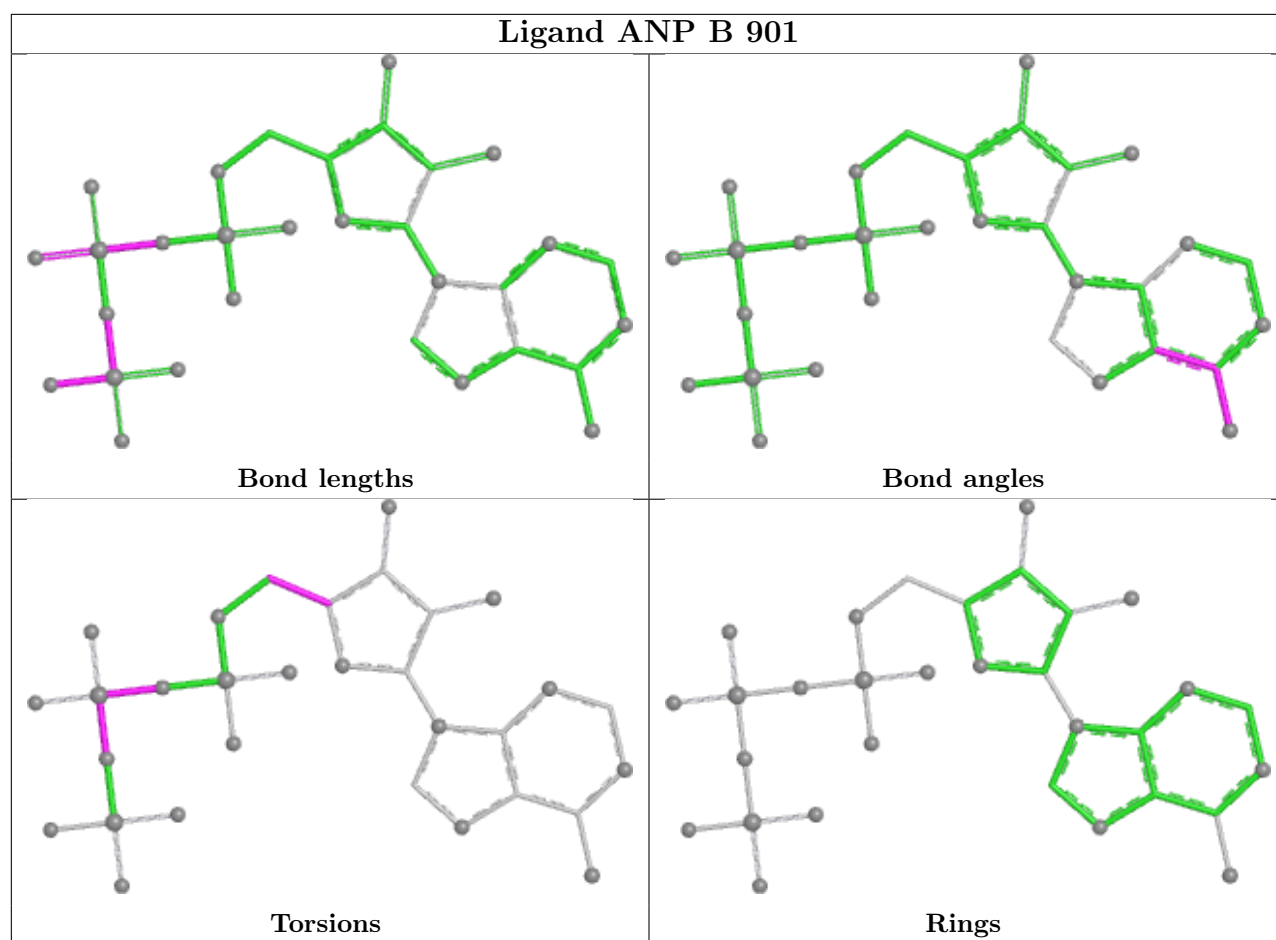


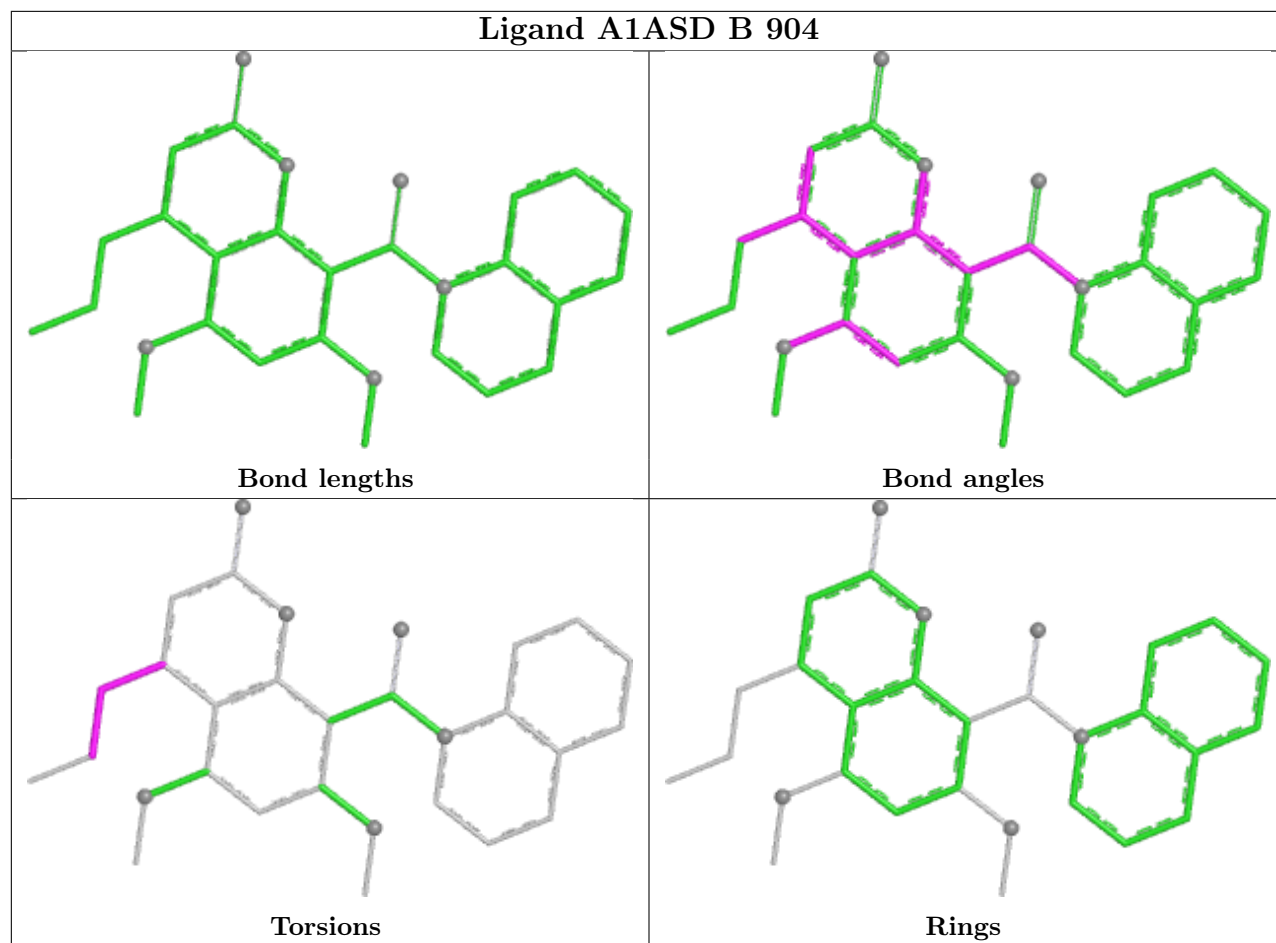
Torsions



Rings







## 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	385/399 (96%)	0.31	13 (3%)	48 50	27, 62, 129, 184	1 (0%)
1	B	385/399 (96%)	0.98	49 (12%)	9 9	35, 91, 156, 208	0
All	All	770/798 (96%)	0.64	62 (8%)	19 21	27, 76, 144, 208	1 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	417	PHE	3.4
1	A	28	ALA	3.4
1	B	402	ALA	3.4
1	A	30	VAL	3.3
1	B	270	TYR	3.3
1	A	414	TRP	3.2
1	B	127	VAL	3.1
1	B	70	ILE	3.1
1	B	253	VAL	3.0
1	A	417	PHE	3.0
1	B	415	VAL	2.9
1	B	105	ILE	2.9
1	B	405	CYS	2.9
1	A	415	VAL	2.8
1	B	109	ILE	2.8
1	B	136	TYR	2.8
1	B	255	VAL	2.8
1	A	341	VAL	2.7
1	B	217	ILE	2.7
1	B	240	VAL	2.7
1	B	301	LEU	2.6
1	B	179	VAL	2.6
1	B	181	THR	2.6
1	B	104	CYS	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	275	LEU	2.6
1	B	64	TYR	2.6
1	B	300	CYS	2.6
1	B	107	VAL	2.5
1	B	182	ALA	2.5
1	B	256	PHE	2.4
1	B	103	SER	2.4
1	A	405	CYS	2.4
1	B	286	LEU	2.3
1	A	351	VAL	2.3
1	B	341	VAL	2.3
1	B	264	VAL	2.3
1	B	190	PHE	2.3
1	B	274	TYR	2.3
1	B	215	THR	2.3
1	B	236	VAL	2.3
1	B	408	VAL	2.3
1	B	67	ASP	2.2
1	A	206	LEU	2.2
1	B	411	ILE	2.2
1	B	115	LEU	2.2
1	B	289	ILE	2.2
1	B	137	VAL	2.2
1	B	118	ILE	2.1
1	A	403	ILE	2.1
1	B	178	THR	2.1
1	B	68	VAL	2.1
1	B	267	PHE	2.1
1	B	271	VAL	2.1
1	A	412	LEU	2.1
1	B	285	SER	2.1
1	A	345	ASN	2.0
1	A	136	TYR	2.0
1	B	116	ILE	2.0
1	B	139	ALA	2.0
1	B	414	TRP	2.0
1	B	288	VAL	2.0
1	B	351	VAL	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 oligosaccharides in this entry.

## 6.4 Ligands ⓘ

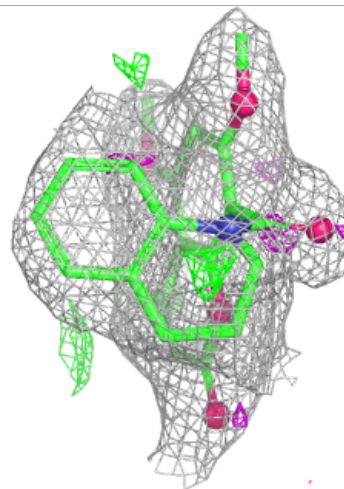
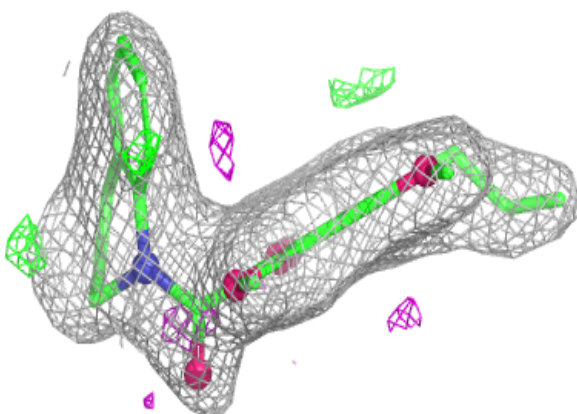
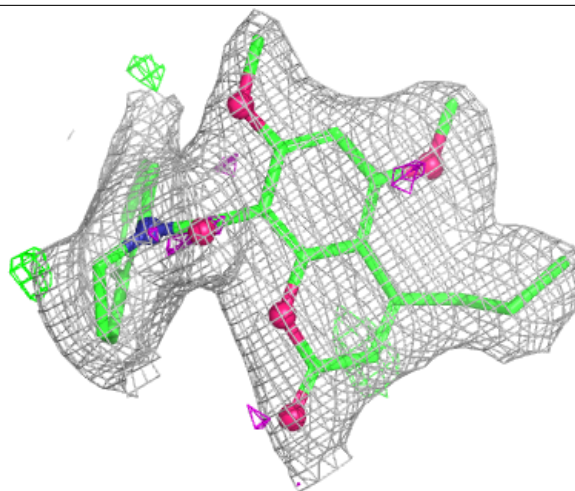
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
6	GOL	B	903	6/6	0.78	0.17	98,104,104,104	0
4	A1ASD	B	904	30/30	0.90	0.11	39,57,65,68	0
4	A1ASD	A	903	30/30	0.95	0.08	29,35,47,50	0
2	ANP	B	901	31/31	0.96	0.09	48,58,70,72	0
5	CL	B	905	1/1	0.98	0.13	46,46,46,46	0
2	ANP	A	901	31/31	0.98	0.06	30,45,49,52	0
3	MG	B	902	1/1	0.99	0.06	34,34,34,34	0
5	CL	A	904	1/1	0.99	0.11	37,37,37,37	0
3	MG	A	902	1/1	1.00	0.05	33,33,33,33	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.

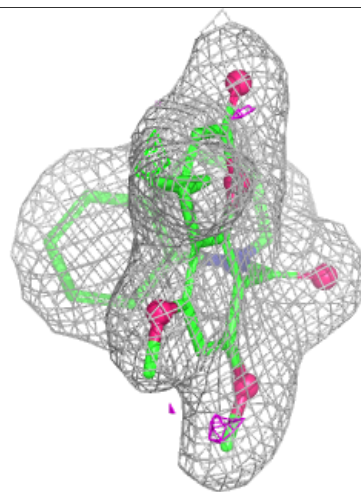
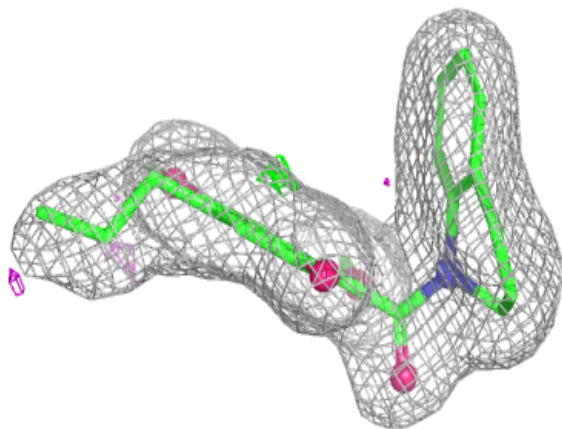
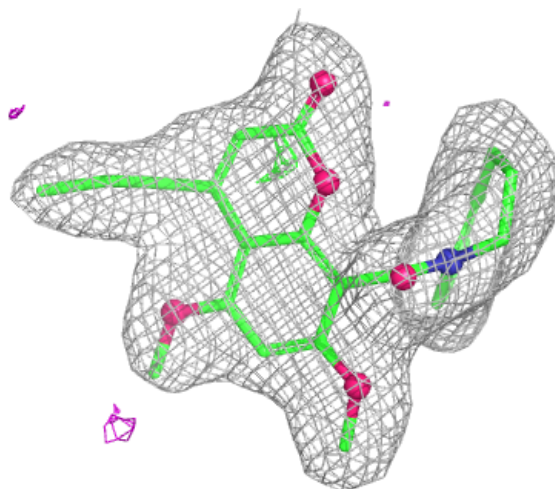
**Electron density around A1ASD B 904:**

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



**Electron density around A1ASD A 903:**

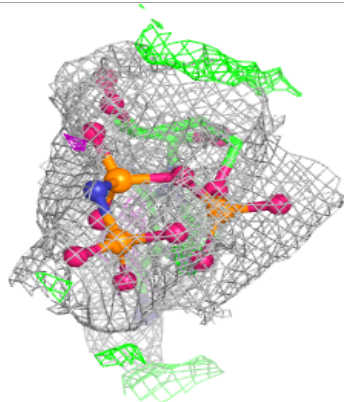
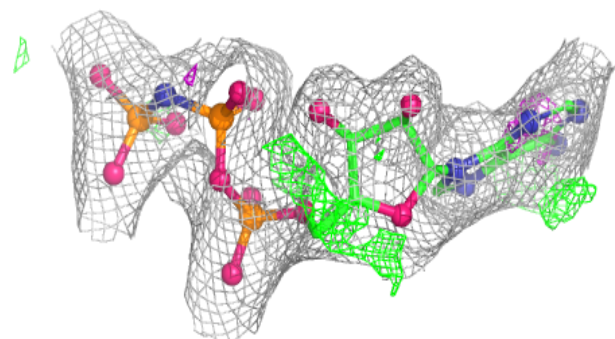
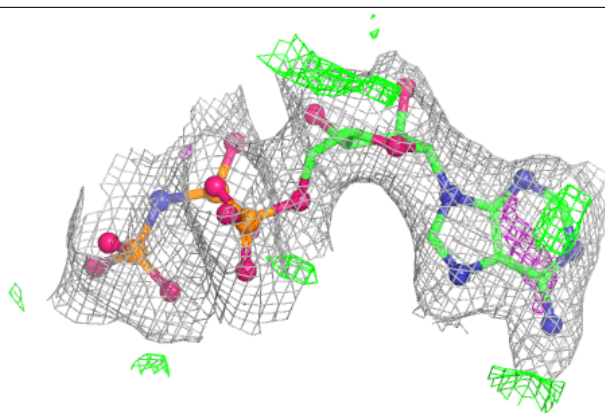
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



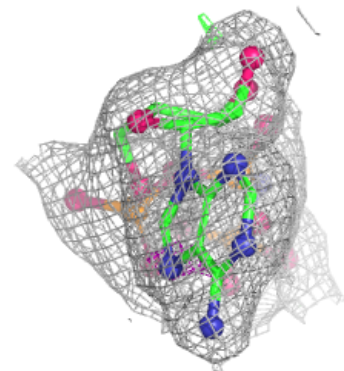
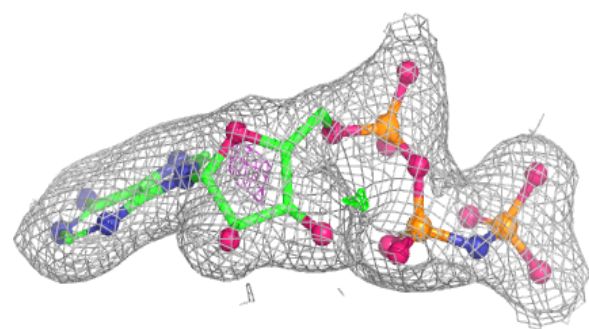
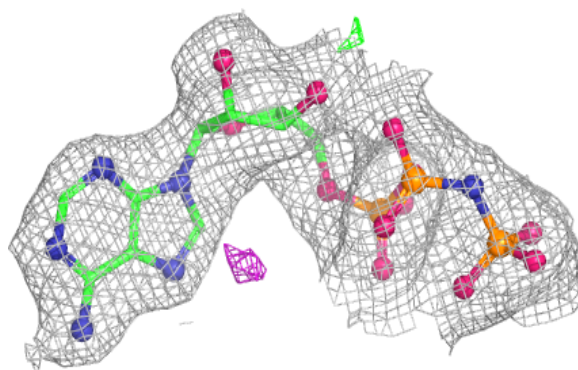


**Electron density around ANP B 901:**

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

**Electron density around ANP A 901:**

$2mF_o-DF_c$  (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.