



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:11 pm BST

PDB ID : 6RZQ
Title : Plasmodium falciparum Hsp70-x chaperone nucleotide binding domain - ANP-PnP bound state
Authors : Vakonakis, I.; Day, J.
Deposited on : 2019-06-13
Resolution : 1.81 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

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 : 2.11
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) : 2.11

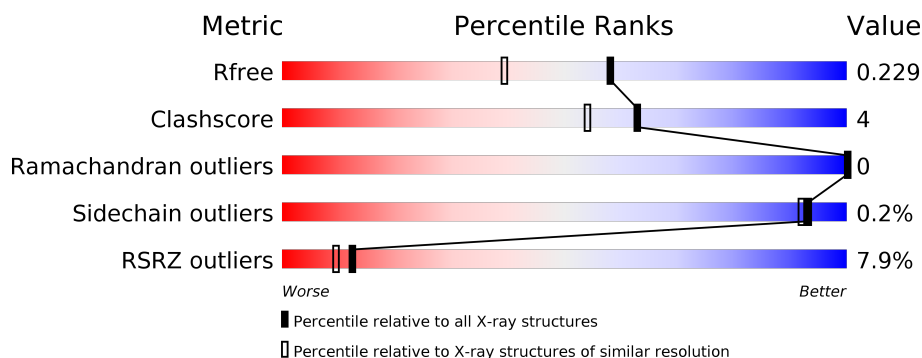
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	393	
1	B	393	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6336 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 Heat shock protein 70.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	4	0
			2935	1839	504	578	14			
1	B	379	Total	C	N	O	S	0	3	0
			2932	1841	506	573	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLY	-	expression tag	UNP K7NTP5
A	28	PRO	-	expression tag	UNP K7NTP5
B	27	GLY	-	expression tag	UNP K7NTP5
B	28	PRO	-	expression tag	UNP K7NTP5

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

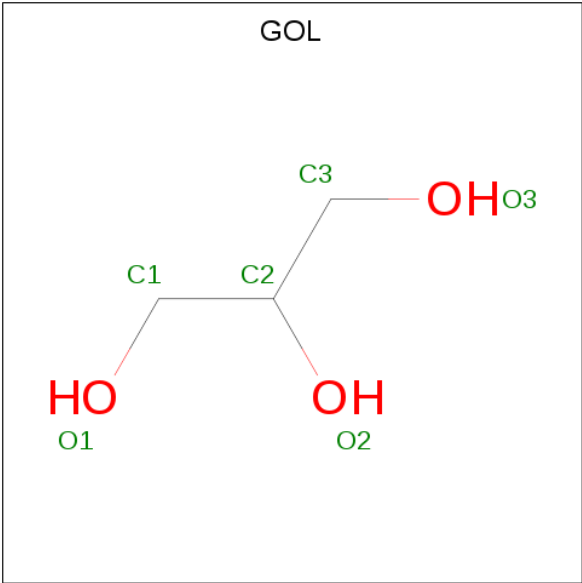
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

Continued on next page...

Continued from previous page...

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

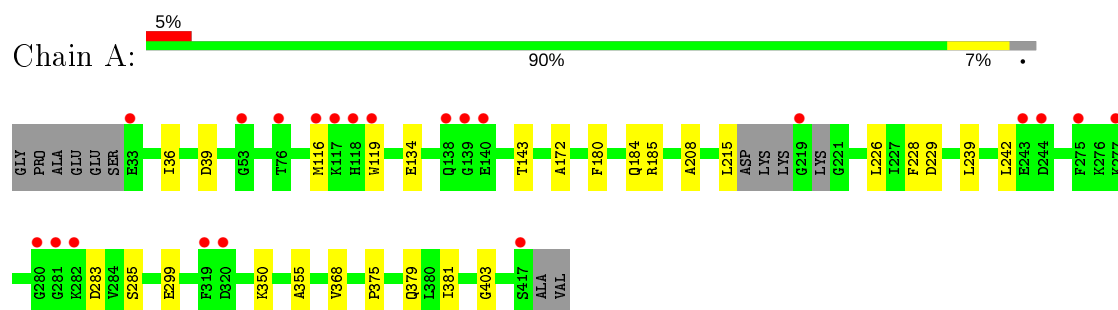
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	211	Total 211	O 211	0	0
5	B	146	Total 146	O 146	0	0

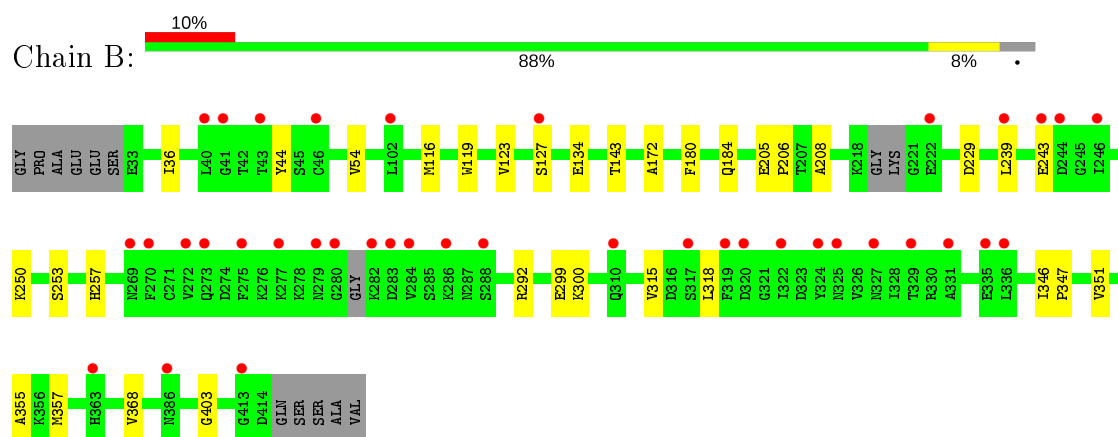
3 Residue-property plots [i](#)

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: Heat shock protein 70



- Molecule 1: Heat shock protein 70



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.29Å 102.71Å 103.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.47 – 1.81 37.44 – 1.81	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.47-1.81) 99.8 (37.44-1.81)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.192 , 0.224 0.200 , 0.229	Depositor DCC
R_{free} test set	3923 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.628	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6336	wwPDB-VP
Average B, all atoms (Å ²)	54.0	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, MG, ANP, CSX

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	0.71	0/2972	0.80	0/4002
1	B	0.68	0/2973	0.79	0/4002
All	All	0.70	0/5945	0.79	0/8004

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	2935	0	2954	24	1
1	B	2932	0	2963	25	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	13	1	0
3	B	31	0	13	1	0
4	A	30	0	40	6	0
4	B	18	0	24	4	0
5	A	211	0	0	6	0
5	B	146	0	0	7	0
All	All	6336	0	6007	52	1

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 (52) 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:299[A]:GLU:OE1	4:B:505:GOL:H11	1.67	0.94
1:B:299[A]:GLU:OE1	4:B:505:GOL:C1	2.28	0.81
1:A:379:GLN:OE1	4:A:503:GOL:O2	1.99	0.79
1:B:116:MET:HE2	5:B:723:HOH:O	1.84	0.76
1:A:215:LEU:O	1:A:242:LEU:CD2	2.38	0.72
3:A:502:ANP:O1B	5:A:601:HOH:O	2.08	0.71
4:B:505:GOL:O2	5:B:601:HOH:O	2.07	0.71
1:A:215:LEU:O	1:A:242:LEU:HD23	1.92	0.70
1:A:299[B]:GLU:OE1	5:A:602:HOH:O	2.10	0.69
3:B:502:ANP:O1B	5:B:602:HOH:O	2.11	0.67
1:B:239[A]:LEU:HD23	1:B:355:ALA:CB	2.28	0.64
1:B:116:MET:HA	1:B:119:TRP:CE3	2.38	0.58
1:B:253:SER:OG	1:B:351:VAL:HG13	2.03	0.58
1:A:185:ARG:CZ	1:B:54:VAL:HG21	2.34	0.57
1:A:134:GLU:HG2	1:A:143:THR:HG22	1.87	0.56
1:A:185:ARG:NE	1:B:54:VAL:HG21	2.23	0.53
1:A:116[B]:MET:HA	1:A:119:TRP:CE3	2.45	0.52
1:A:116[A]:MET:HA	1:A:119:TRP:CE3	2.45	0.52
1:B:346:ILE:HB	1:B:347:PRO:HD3	1.91	0.52
4:A:506:GOL:H12	5:A:701:HOH:O	2.09	0.51
1:A:283:ASP:OD1	1:A:285:SER:OG	2.23	0.51
1:A:39:ASP:OD2	5:A:601:HOH:O	2.19	0.50
1:A:239:LEU:HD23	1:A:355:ALA:CB	2.41	0.50
1:B:257:HIS:HD2	5:B:738:HOH:O	1.94	0.49
1:A:375:PRO:CB	4:A:503:GOL:H31	2.43	0.48
1:B:243:GLU:OE2	1:B:250:LYS:HE3	2.14	0.48
1:B:44:TYR:O	5:B:602:HOH:O	2.20	0.47
1:A:299[A]:GLU:OE2	4:A:505:GOL:O2	2.33	0.47
4:A:506:GOL:C1	5:A:701:HOH:O	2.62	0.46
1:B:292:ARG:NH1	5:B:606:HOH:O	2.40	0.46
1:B:299[A]:GLU:OE2	4:B:504:GOL:O2	2.33	0.46
1:A:229:ASP:HA	1:A:368:VAL:O	2.17	0.45
1:B:180:PHE:CD2	1:B:184:GLN:HB3	2.50	0.45
1:B:239[A]:LEU:HD21	1:B:357:MET:SD	2.57	0.45
1:A:36:ILE:O	1:A:172:ALA:HA	2.15	0.45
1:B:300:LYS:HG3	5:B:636:HOH:O	2.17	0.44
1:B:315:VAL:HG11	1:B:318:LEU:HD13	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:GLU:HG2	1:B:143:THR:HG22	1.99	0.44
1:A:228:PHE:CE1	1:A:381:ILE:HD11	2.52	0.44
1:B:229:ASP:HA	1:B:368:VAL:O	2.18	0.43
1:A:215:LEU:C	1:A:242:LEU:CD2	2.87	0.43
1:A:180:PHE:CD2	1:A:184:GLN:HB3	2.54	0.43
1:B:208:ALA:O	1:B:403:GLY:HA3	2.19	0.42
1:A:350:LYS:HD3	5:A:678:HOH:O	2.19	0.42
1:A:239:LEU:HD23	1:A:355:ALA:HB2	2.02	0.41
1:B:116:MET:HE3	1:B:123:VAL:HB	2.03	0.41
1:A:208:ALA:O	1:A:403:GLY:HA3	2.20	0.41
1:A:375:PRO:HB2	4:A:503:GOL:H31	2.02	0.41
1:B:36:ILE:O	1:B:172:ALA:HA	2.20	0.41
1:B:205:GLU:N	1:B:206:PRO:HD2	2.35	0.40
1:B:239[A]:LEU:HD23	1:B:355:ALA:HB1	2.02	0.40
1:A:228:PHE:CZ	1:A:381:ILE:HD11	2.57	0.40

All (1) 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:379:GLN:NE2	1:B:127:SER:OG[3_655]	2.08	0.12

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	378/393 (96%)	373 (99%)	5 (1%)	0	100	100
1	B	375/393 (95%)	368 (98%)	7 (2%)	0	100	100
All	All	753/786 (96%)	741 (98%)	12 (2%)	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	320/326 (98%)	319 (100%)	1 (0%)	92	91
1	B	320/326 (98%)	320 (100%)	0	100	100
All	All	640/652 (98%)	639 (100%)	1 (0%)	93	92

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

Mol	Chain	Res	Type
1	A	226	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	223	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	CSX	A	391[B]	-	3,6,7	1.03	0	1,6,8	1.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSX	A	391[A]	-	3,6,7	1.03	0	1,6,8	2.67	1 (100%)
1	CSX	B	391	1	3,6,7	1.16	0	1,6,8	2.94	1 (100%)

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
1	CSX	A	391[B]	-	-	0/1/5/7	-
1	CSX	A	391[A]	-	-	0/1/5/7	-
1	CSX	B	391	1	-	0/1/5/7	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	391	CSX	CA-CB-SG	-2.94	106.94	113.36
1	A	391[A]	CSX	CA-CB-SG	-2.67	107.52	113.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 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	$\# Z > 2$
3	ANP	B	502	2	29,33,33	1.41	4 (13%)	31,52,52	1.70	7 (22%)
3	ANP	A	502	2	29,33,33	1.37	5 (17%)	31,52,52	1.70	2 (6%)
4	GOL	A	506	-	5,5,5	0.13	0	5,5,5	0.56	0
4	GOL	B	503	-	5,5,5	0.15	0	5,5,5	0.46	0
4	GOL	B	504	-	5,5,5	0.21	0	5,5,5	0.48	0
4	GOL	A	503	-	5,5,5	0.14	0	5,5,5	0.33	0
4	GOL	A	507	-	5,5,5	0.15	0	5,5,5	0.40	0
4	GOL	B	505	-	5,5,5	0.15	0	5,5,5	0.51	0
4	GOL	A	504	-	5,5,5	0.06	0	5,5,5	0.22	0
4	GOL	A	505	-	5,5,5	0.19	0	5,5,5	0.47	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
3	ANP	B	502	2	-	3/14/38/38	0/3/3/3
3	ANP	A	502	2	-	1/14/38/38	0/3/3/3
4	GOL	A	506	-	-	2/4/4/4	-
4	GOL	B	503	-	-	4/4/4/4	-
4	GOL	B	504	-	-	2/4/4/4	-
4	GOL	A	503	-	-	2/4/4/4	-
4	GOL	A	507	-	-	3/4/4/4	-
4	GOL	B	505	-	-	2/4/4/4	-
4	GOL	A	504	-	-	0/4/4/4	-
4	GOL	A	505	-	-	2/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	ANP	PB-O1B	4.26	1.52	1.46
3	A	502	ANP	PB-O1B	3.71	1.52	1.46
3	B	502	ANP	PG-O1G	3.63	1.51	1.46
3	A	502	ANP	PG-O1G	3.04	1.51	1.46
3	A	502	ANP	PB-O2B	-2.86	1.49	1.56
3	B	502	ANP	PG-O2G	-2.64	1.49	1.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	ANP	PB-O2B	-2.50	1.50	1.56
3	A	502	ANP	PB-O3A	2.30	1.62	1.59
3	A	502	ANP	PG-O2G	-2.06	1.51	1.56

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	ANP	O1G-PG-N3B	-7.59	100.60	111.77
3	B	502	ANP	O1B-PB-N3B	-5.22	104.08	111.77
3	B	502	ANP	O2B-PB-O1B	3.96	118.22	109.92
3	B	502	ANP	O1G-PG-N3B	-3.47	106.66	111.77
3	A	502	ANP	O2B-PB-O1B	2.70	115.59	109.92
3	B	502	ANP	O3A-PB-N3B	-2.41	99.91	106.59
3	B	502	ANP	O2G-PG-O1G	-2.20	107.92	113.45
3	B	502	ANP	C5-C6-N6	2.16	123.64	120.35
3	B	502	ANP	O4'-C1'-C2'	-2.15	103.79	106.93

There are no chirality outliers.

All (21) torsion outliers are listed below:

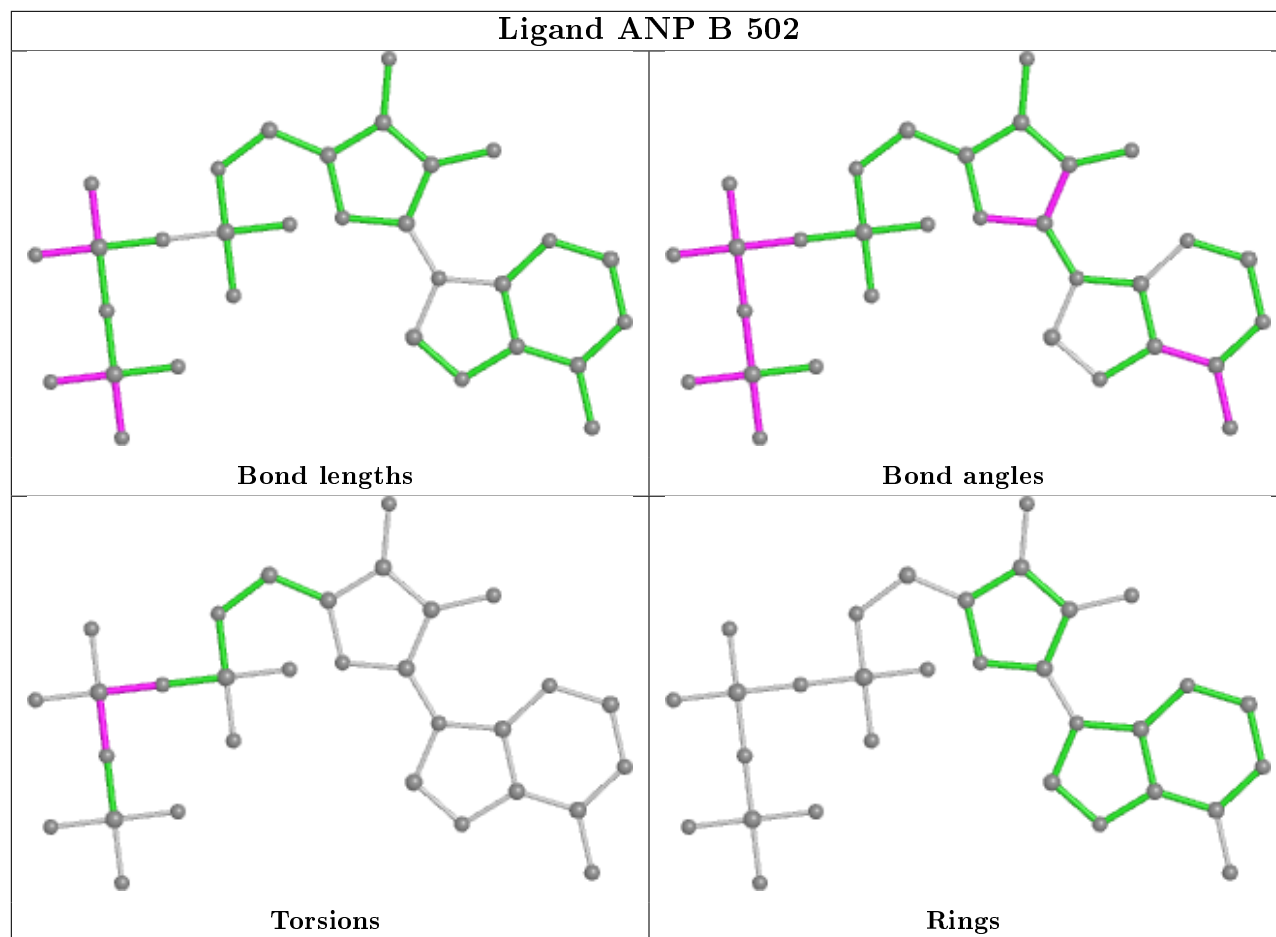
Mol	Chain	Res	Type	Atoms
3	B	502	ANP	PG-N3B-PB-O1B
3	B	502	ANP	PA-O3A-PB-O1B
3	B	502	ANP	PA-O3A-PB-O2B
3	A	502	ANP	PG-N3B-PB-O1B
4	A	507	GOL	C1-C2-C3-O3
4	A	507	GOL	O2-C2-C3-O3
4	B	503	GOL	C1-C2-C3-O3
4	B	504	GOL	O1-C1-C2-C3
4	A	503	GOL	C1-C2-C3-O3
4	B	505	GOL	C1-C2-C3-O3
4	A	505	GOL	C1-C2-C3-O3
4	A	506	GOL	O2-C2-C3-O3
4	A	506	GOL	C1-C2-C3-O3
4	B	503	GOL	O1-C1-C2-C3
4	A	503	GOL	O2-C2-C3-O3
4	B	505	GOL	O2-C2-C3-O3
4	A	505	GOL	O2-C2-C3-O3
4	B	503	GOL	O2-C2-C3-O3
4	B	504	GOL	O1-C1-C2-O2
4	B	503	GOL	O1-C1-C2-O2
4	A	507	GOL	O1-C1-C2-O2

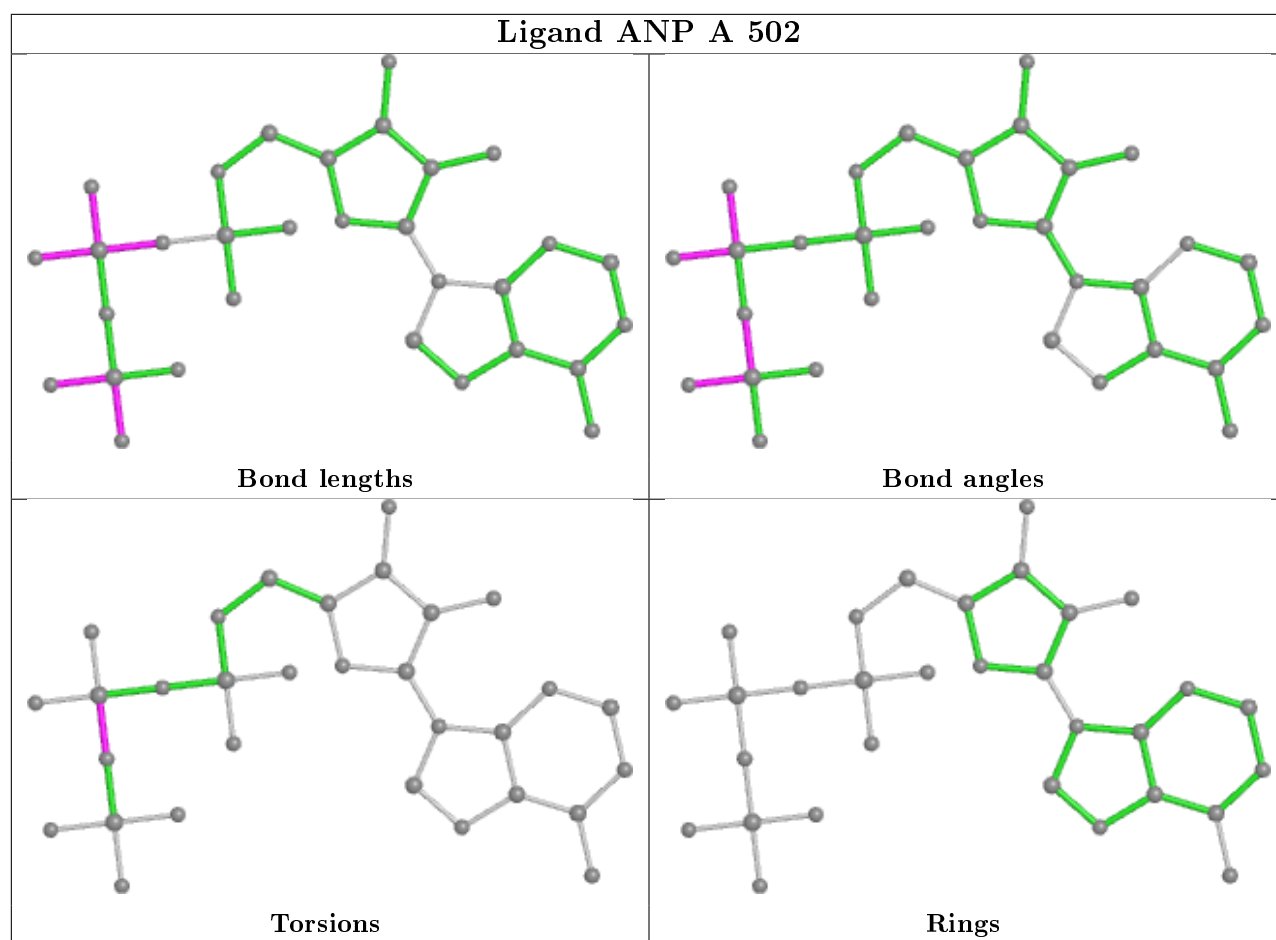
There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	ANP	1	0
3	A	502	ANP	1	0
4	A	506	GOL	2	0
4	B	504	GOL	1	0
4	A	503	GOL	3	0
4	B	505	GOL	3	0
4	A	505	GOL	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 [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	380/393 (96%)	0.20	21 (5%) 25 20	31, 46, 73, 98	0
1	B	378/393 (96%)	0.53	39 (10%) 6 5	34, 56, 91, 117	0
All	All	758/786 (96%)	0.36	60 (7%) 12 9	31, 50, 87, 117	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	244	ASP	6.0
1	B	286	LYS	4.7
1	B	324	TYR	4.6
1	B	319	PHE	4.5
1	B	275	PHE	4.4
1	A	280	GLY	4.4
1	B	320	ASP	4.4
1	B	246	ILE	3.9
1	A	417	SER	3.6
1	B	277	LYS	3.6
1	B	243	GLU	3.6
1	B	284	VAL	3.5
1	A	320	ASP	3.4
1	B	322	ILE	3.4
1	B	283	ASP	3.3
1	A	139	GLY	3.2
1	B	269	ASN	3.1
1	A	281	GLY	3.1
1	B	222	GLU	3.1
1	B	335	GLU	3.0
1	B	40	LEU	3.0
1	B	279	ASN	3.0
1	B	329	THR	2.9
1	B	273	GLN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	219	GLY	2.8
1	B	310	GLN	2.8
1	A	33	GLU	2.8
1	A	140	GLU	2.8
1	A	243	GLU	2.8
1	A	76	THR	2.7
1	B	282	LYS	2.6
1	A	244	ASP	2.6
1	A	277	LYS	2.6
1	B	413	GLY	2.5
1	A	118	HIS	2.5
1	B	270	PHE	2.4
1	B	325	ASN	2.4
1	B	327	ASN	2.4
1	B	127	SER	2.4
1	A	117	LYS	2.4
1	A	282	LYS	2.4
1	B	317	SER	2.3
1	B	331	ALA	2.3
1	B	336	LEU	2.3
1	A	53	GLY	2.3
1	B	280	GLY	2.3
1	B	239[A]	LEU	2.3
1	B	288	SER	2.3
1	A	119	TRP	2.2
1	B	41	GLY	2.2
1	B	43	THR	2.2
1	B	386	ASN	2.2
1	A	138	GLN	2.2
1	B	102	LEU	2.1
1	B	363	HIS	2.1
1	A	116[A]	MET	2.1
1	A	319	PHE	2.1
1	A	275	PHE	2.0
1	B	272	VAL	2.0
1	B	46	CYS	2.0

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

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, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	CSX	A	391[B]	7/8	0.94	0.14	33,38,42,43	4
1	CSX	A	391[A]	7/8	0.94	0.14	38,39,42,48	4
1	CSX	B	391	7/8	0.96	0.08	52,54,64,65	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

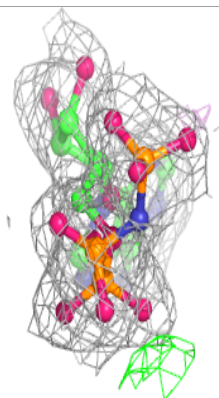
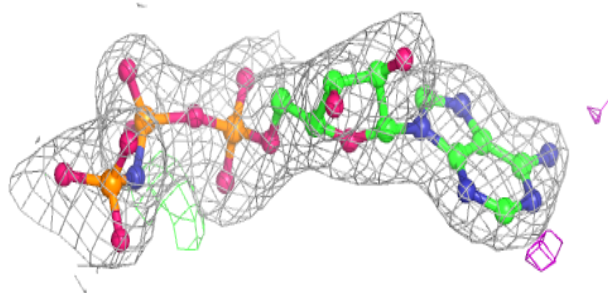
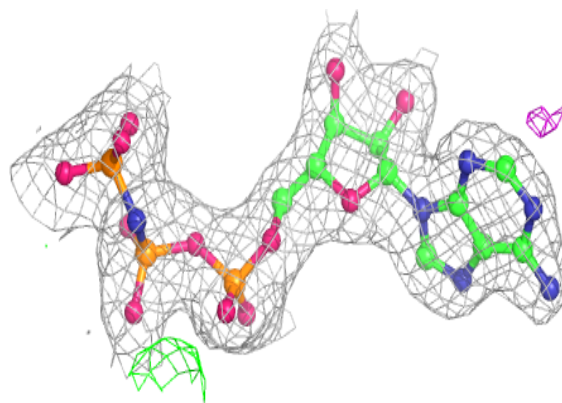
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	503	6/6	0.69	0.38	81,88,99,104	0
4	GOL	B	505	6/6	0.70	0.23	78,87,90,99	0
4	GOL	A	507	6/6	0.75	0.20	58,69,75,79	0
4	GOL	B	504	6/6	0.85	0.22	52,73,78,79	0
4	GOL	A	506	6/6	0.88	0.17	58,70,71,85	0
4	GOL	B	503	6/6	0.89	0.18	69,75,79,82	0
4	GOL	A	504	6/6	0.91	0.28	74,81,88,90	0
4	GOL	A	505	6/6	0.92	0.16	39,59,70,73	0
2	MG	B	501	1/1	0.95	0.41	58,58,58,58	0
2	MG	A	501	1/1	0.97	0.29	47,47,47,47	0
3	ANP	B	502	31/31	0.98	0.13	39,46,56,59	0
3	ANP	A	502	31/31	0.99	0.11	31,34,37,42	0

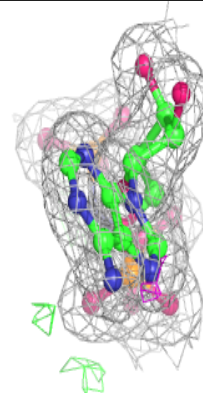
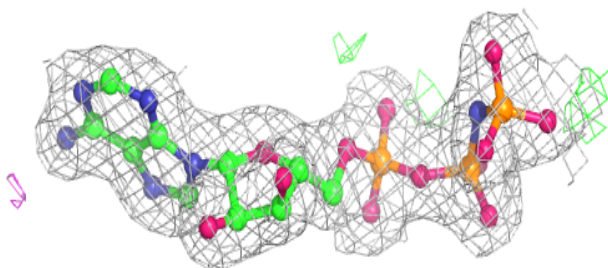
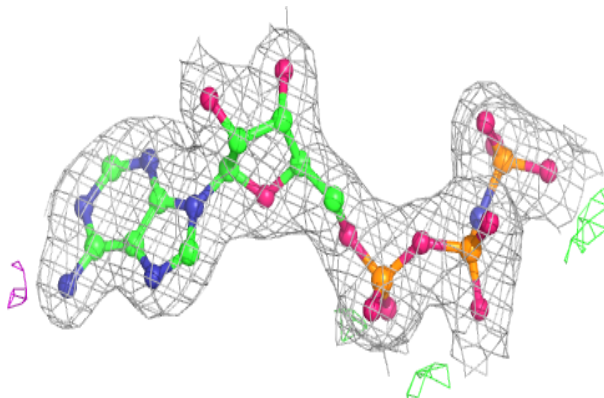
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP B 502:

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

**Electron density around ANP A 502:**

$2mF_o-DF_c$ (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.