

Full wwPDB X-ray Structure Validation Report (i)

Mar 3, 2024 – 01:13 AM EST

PDB ID	:	6AWH
Title	:	Staphylococcus aureus Type II pantothenate kinase in complex with ATP and
		pantothenate analog Deoxy-MeO-N5Pan
Authors	:	Chen, Y.; Antoshchenko, T.; Strauss, E.; Barnard, L.; Huang, Y.H.
Deposited on	:	2017-09-05
Resolution	:	1.90 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

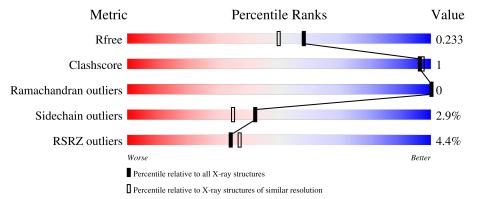
Xtriage (Phenix) EDS buster-report Percentile statistics Refmac CCP4 Ideal geometry (proteins) Ideal geometry (DNA, RNA)	:::::::::::::::::::::::::::::::::::::::	20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove) Engh & Huber (2001) Parkinson et al. (1996)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		Parkinson et al. (1996) 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.90 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 >=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 <=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	А	266	2% 9 5%	5%
1	В	266	2% 94%	6% •
1	С	266	3% 96%	•
1	D	266	96%	•••



6AWH

2 Entry composition (i)

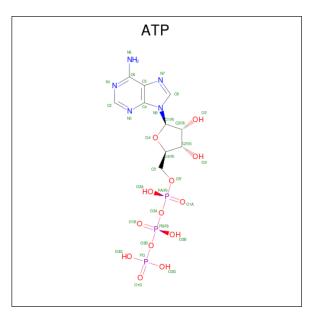
There are 5 unique types of molecules in this entry. The entry contains 8978 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	1 A	266	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	Ο	Ο
	Π	200	2041	1292	350	393	6	0	0	0
1	В	264	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
	D	204	2024	1283	347	388	6	0	0	
1	С	265	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	U	200	2032	1287	349	390	6	0	0	
1	1 D	264	Total	С	Ν	0	S	0	1	0
			2034	1289	350	389	6	0	1	

• Molecule 1 is a protein called Type II pantothenate kinase.

• Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
9	2 A	1	Total	С	Ν	Ο	Р	0	0
		1	31	10	5	13	3	0	0
0	2 B	1	Total	С	Ν	Ο	Р	0	0
		1	31	10	5	13	3	0	U

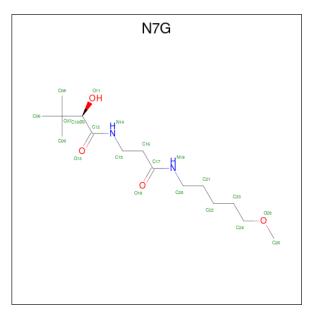


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
0	2 C	1	Total	С	Ν	Ο	Р	0	0
		1	31	10	5	13	3	0	0
0	2 D	1	Total	С	Ν	Ο	Р	0	0
		1	31	10	5	13	3	0	U

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Mg 1 1	0	0
3	В	1	Total Mg 1 1	0	0
3	С	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

• Molecule 4 is (2R)-2-hydroxy-N-{3-[(5-methoxypentyl)amino]-3-oxopropyl}-3,3-dimethylbu tanamide (three-letter code: N7G) (formula: $C_{15}H_{30}N_2O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	В	1	Total 21				0	0
4	В	1	Total 21	C 15		0 4	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C N O 21 15 2 4	0	0
4	D	1	Total C N O 21 15 2 4	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	153	Total O 153 153	0	0
5	В	177	Total O 177 177	0	0
5	С	164	Total O 164 164	0	0
5	D	141	Total O 141 141	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: Type II pantothenate kinase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	56.78Å 136.67Å 141.39Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.27 - 1.90	Depositor
Resolution (A)	44.56 - 1.90	EDS
% Data completeness	99.2 (98.27-1.90)	Depositor
(in resolution range)	99.2(44.56-1.90)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.32 (at 1.89 Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.195 , 0.226	Depositor
n, n _{free}	0.203 , 0.233	DCC
R_{free} test set	4363 reflections (5.01%)	wwPDB-VP
Wilson B-factor $(Å^2)$	23.0	Xtriage
Anisotropy	0.628	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36, 39.8	EDS
L-test for $twinning^2$	$< L > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8978	wwPDB-VP
Average B, all atoms $(Å^2)$	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 44.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6168e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities estimated from amplitudes.

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: MG, ATP, N7G $\,$

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.60	0/2076	0.74	0/2813	
1	В	0.61	0/2058	0.73	0/2787	
1	С	0.59	0/2067	0.72	0/2801	
1	D	0.57	0/2069	0.71	0/2802	
All	All	0.59	0/8270	0.73	0/11203	

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 (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	А	2041	0	2027	6	0
1	В	2024	0	2014	6	0
1	С	2032	0	2021	4	0
1	D	2034	0	2020	2	0
2	А	31	0	12	0	0
2	В	31	0	12	0	0
2	С	31	0	12	0	0
2	D	31	0	12	0	0
3	А	1	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	1	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
4	В	42	0	0	0	0
4	D	42	0	0	0	0
5	А	153	0	0	0	0
5	В	177	0	0	1	0
5	С	164	0	0	2	0
5	D	141	0	0	0	0
All	All	8978	0	8130	16	0

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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 1.

All (16) 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:C:227:PHE:HB2	5:C:401:HOH:O	1.86	0.74
1:A:182:HIS:HB3	1:A:185:ALA:HB3	1.73	0.69
1:A:132:SER:O	1:A:133:GLN:HG2	2.07	0.53
1:A:159:ILE:HG22	1:B:52:GLY:HA3	1.93	0.51
1:B:2:LYS:HG2	1:B:46:LYS:HB3	1.95	0.49
1:D:148:ASP:OD1	1:D:150:ASN:HB2	2.13	0.49
1:C:34:GLN:O	1:C:37:GLU:HG3	2.14	0.47
1:C:125:GLN:NE2	5:C:404:HOH:O	2.48	0.46
1:B:44:ILE:HG21	1:B:47:LEU:HB2	1.98	0.45
1:B:228:HIS:HE1	5:B:493:HOH:O	1.98	0.45
1:B:19:ASP:HB2	1:B:21:GLN:N	2.32	0.44
1:C:161:LYS:HE2	1:D:53:ASN:OD1	2.18	0.44
1:A:134:ILE:HD11	1:A:143:MET:SD	2.60	0.42
1:A:132:SER:C	1:A:133:GLN:HG2	2.41	0.41
1:A:134:ILE:CD1	1:A:143:MET:SD	3.09	0.41
1:B:77:GLY:HA3	1:B:257:SER:O	2.21	0.40

There are no symmetry-related clashes.



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	Perce	ntiles
1	А	264/266~(99%)	259~(98%)	5(2%)	0	100	100
1	В	260/266~(98%)	257~(99%)	3~(1%)	0	100	100
1	С	263/266~(99%)	259~(98%)	4 (2%)	0	100	100
1	D	261/266~(98%)	257~(98%)	4(2%)	0	100	100
All	All	1048/1064~(98%)	1032 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	Percei	ntiles
1	А	216/216~(100%)	208~(96%)	8 (4%)	34	25
1	В	214/216~(99%)	209~(98%)	5(2%)	50	45
1	С	215/216~(100%)	210~(98%)	5(2%)	50	45
1	D	215/216~(100%)	208~(97%)	7 (3%)	38	29
All	All	860/864~(100%)	835~(97%)	25 (3%)	42	35

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	30	LYS
1	А	43	GLN



Mol	Chain	Res	Type
1	А	46	LYS
1	А	62	ASN
1	А	109	GLN
1	А	133	GLN
1	А	178	HIS
1	А	186	ASP
1	В	25	LYS
1	В	27	GLU
1	В	109	GLN
1	В	178	HIS
1	В	243	LEU
1	C C C C C D	1	MET
1	С	3	VAL
1	С	37	GLU
1	С	178	HIS
1	С	209	ILE
1	D	19	ASP
1	D	21	GLN
1	D	109	GLN
1	D	150	ASN
1	D	178	HIS
1	D	218	GLU
1	D	243	LEU

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Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	62	ASN
1	А	76	GLN
1	А	125	GLN
1	А	133	GLN
1	А	146	HIS
1	А	228	HIS
1	В	109	GLN
1	В	133	GLN
1	В	146	HIS
1	В	228	HIS
1	С	41	GLN
1	С	42	GLN
1	С	125	GLN
1	D	146	HIS



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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	Tuno	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
N101	Type	Ullalli	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	ATP	В	301	3	26,33,33	1.00	1 (3%)	$31,\!52,\!52$	1.21	3 (9%)
2	ATP	D	301	3	26,33,33	0.98	2 (7%)	$31,\!52,\!52$	1.26	4 (12%)
4	N7G	В	302	-	19,20,20	0.70	1 (5%)	24,25,25	1.28	2 (8%)
4	N7G	D	303	-	19,20,20	0.91	1 (5%)	24,25,25	0.94	1 (4%)
2	ATP	С	301	3	26,33,33	0.90	1 (3%)	31,52,52	1.23	3 (9%)
4	N7G	В	303	-	19,20,20	1.14	2 (10%)	$24,\!25,\!25$	0.73	0
2	ATP	А	301	3	26,33,33	0.93	3 (11%)	31,52,52	1.36	4 (12%)
4	N7G	D	302	-	19,20,20	1.18	1 (5%)	$24,\!25,\!25$	0.94	1 (4%)

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	ATP	В	301	3	-	2/18/38/38	0/3/3/3
2	ATP	D	301	3	-	3/18/38/38	0/3/3/3
4	N7G	В	302	-	-	2/24/24/24	-
4	N7G	D	303	-	-	2/24/24/24	-
2	ATP	С	301	3	-	1/18/38/38	0/3/3/3
4	N7G	В	303	-	-	2/24/24/24	-
2	ATP	А	301	3	-	1/18/38/38	0/3/3/3
4	N7G	D	302	-	-	2/24/24/24	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
4	D	302	N7G	C07-C10	4.18	1.58	1.55
4	В	303	N7G	C07-C10	3.14	1.57	1.55
4	D	303	N7G	C07-C10	2.78	1.57	1.55
2	В	301	ATP	C5-C4	2.72	1.48	1.40
2	D	301	ATP	C5-C4	2.60	1.47	1.40
4	В	303	N7G	O11-C10	2.56	1.47	1.42
2	С	301	ATP	C2-N3	2.21	1.35	1.32
2	А	301	ATP	C5-N7	-2.16	1.31	1.39
4	В	302	N7G	O11-C10	2.14	1.46	1.42
2	D	301	ATP	C2-N3	2.12	1.35	1.32
2	А	301	ATP	O4'-C1'	2.08	1.44	1.41
2	А	301	ATP	C5-C4	2.07	1.46	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	301	ATP	N3-C2-N1	-4.59	121.50	128.68
2	С	301	ATP	N3-C2-N1	-3.79	122.75	128.68
2	D	301	ATP	N3-C2-N1	-3.72	122.87	128.68
2	В	301	ATP	N3-C2-N1	-3.32	123.49	128.68
4	В	302	N7G	C15-C16-C17	-3.20	107.03	112.36
4	В	302	N7G	C20-N19-C17	-3.07	117.14	122.84
4	D	302	N7G	C20-N19-C17	-2.79	117.65	122.84
2	А	301	ATP	O3G-PG-O2G	2.77	118.23	107.64
2	С	301	ATP	N6-C6-N1	2.48	123.72	118.57
2	D	301	ATP	O3G-PG-O2G	2.35	116.61	107.64
2	В	301	ATP	N6-C6-N1	2.24	123.22	118.57
2	С	301	ATP	O2G-PG-O1G	2.19	119.26	110.68
2	А	301	ATP	C2-N1-C6	2.18	122.49	118.75
2	В	301	ATP	C2-N1-C6	2.14	122.41	118.75



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	301	ATP	N6-C6-N1	2.13	123.00	118.57
2	D	301	ATP	C2-N1-C6	2.12	122.38	118.75
4	D	303	N7G	C23-C22-C21	-2.03	104.12	114.42
2	D	301	ATP	O2B-PB-O1B	2.03	122.26	112.24

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There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
4	В	303	N7G	N19-C20-C21-C22
4	D	303	N7G	C22-C23-C24-O25
4	В	302	N7G	C22-C23-C24-O25
4	D	302	N7G	C20-C21-C22-C23
4	В	303	N7G	C22-C23-C24-O25
2	В	301	ATP	PG-O3B-PB-O2B
2	А	301	ATP	PG-O3B-PB-O2B
2	В	301	ATP	PG-O3B-PB-O1B
2	С	301	ATP	PG-O3B-PB-O1B
2	D	301	ATP	PG-O3B-PB-O1B
4	В	302	N7G	C20-C21-C22-C23
2	D	301	ATP	PB-O3B-PG-O3G
2	D	301	ATP	PB-O3A-PA-O1A
4	D	303	N7G	C20-C21-C22-C23
4	D	302	N7G	C21-C22-C23-C24

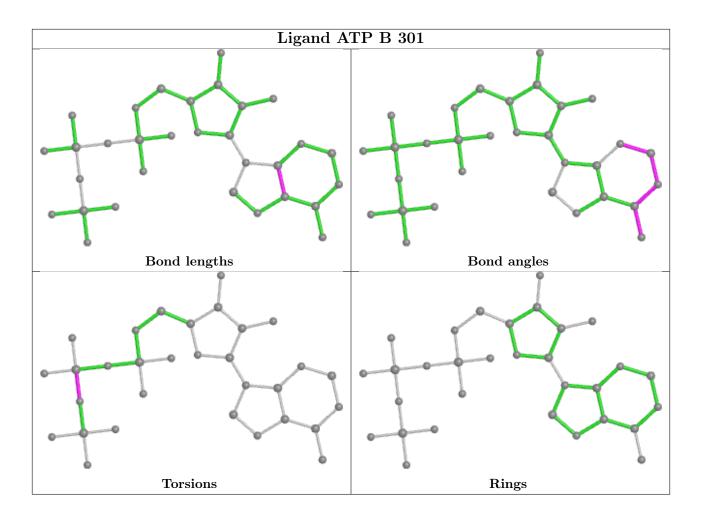
All (15) torsion outliers are listed below:

There are no ring outliers.

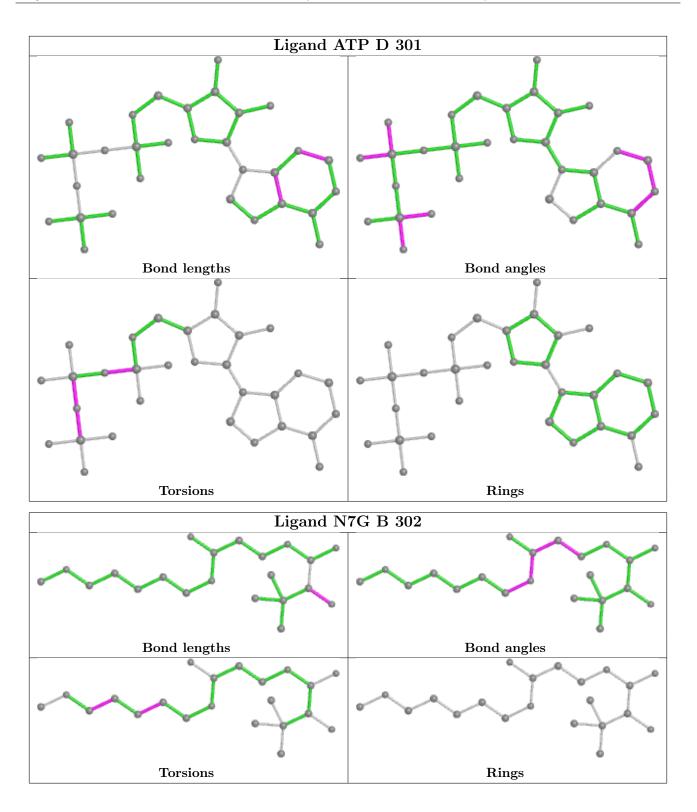
No monomer is involved in short contacts.

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 then 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.

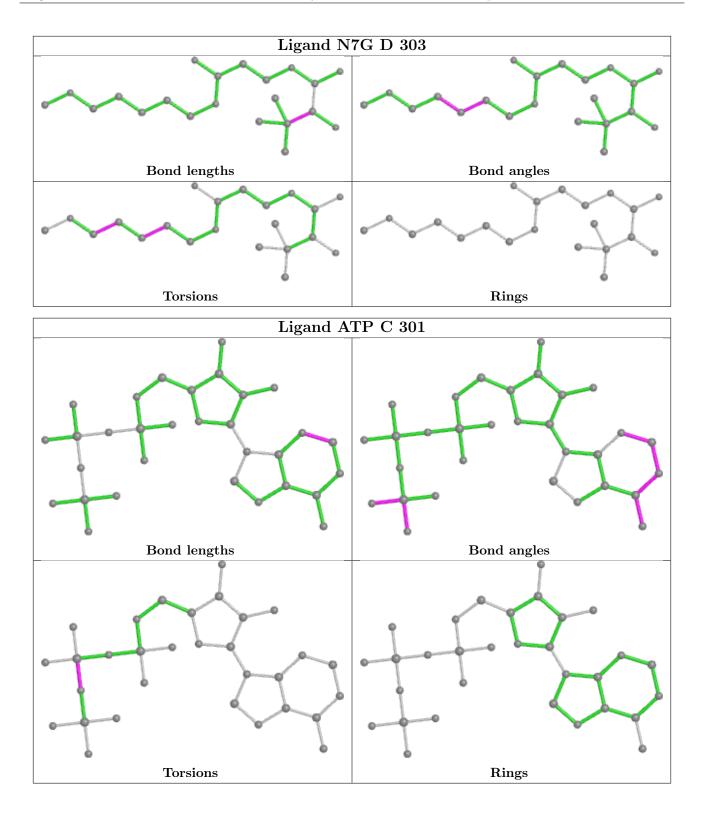




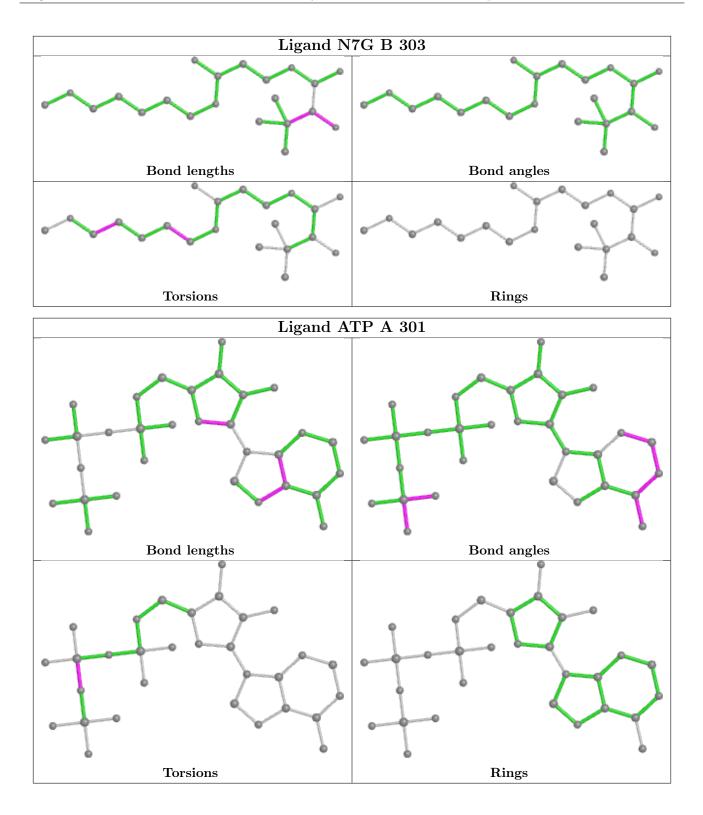




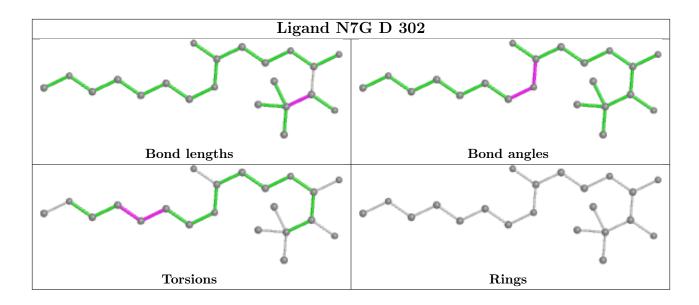












5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	266/266~(100%)	0.00	6 (2%) 60 63	16, 25, 49, 75	0
1	В	264/266~(99%)	-0.03	5 (1%) 66 69	16, 23, 46, 71	0
1	С	265/266~(99%)	0.12	8 (3%) 50 53	16, 26, 47, 60	0
1	D	264/266~(99%)	0.40	28 (10%) 6 7	16, 27, 64, 86	0
All	All	1059/1064~(99%)	0.12	47 (4%) 34 37	16, 25, 53, 86	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	41	GLN	5.1
1	D	43	GLN	4.5
1	D	36	VAL	4.2
1	D	61	ILE	4.0
1	D	62	ASN	4.0
1	D	33	ASP	3.9
1	D	38	TRP	3.7
1	D	64	PRO	3.7
1	D	264	TYR	3.6
1	D	59	GLU	3.3
1	В	19	ASP	3.3
1	D	40	ASN	3.2
1	А	43	GLN	3.1
1	С	41	GLN	3.0
1	А	184	ASP	3.0
1	D	54	ALA	3.0
1	С	162	ASP	2.9
1	D	58	ALA	2.9
1	А	266	GLU	2.8
1	D	37	GLU	2.8
1	В	184	ASP	2.8



Mol	Chain	Res	Type	RSRZ
1	А	185	ALA	2.8
1	D	65	ALA	2.8
1	D	184	ASP	2.7
1	D	63	ILE	2.7
1	С	161	LYS	2.7
1	В	186	ASP	2.7
1	В	21	GLN	2.6
1	D	60	ASN	2.5
1	D	44	ILE	2.5
1	D	42	GLN	2.5
1	D	39	LEU	2.5
1	А	88	ASP	2.5
1	С	20	ASN	2.5
1	С	163	THR	2.4
1	А	59	GLU	2.4
1	С	37	GLU	2.4
1	D	46	LYS	2.4
1	D	56	VAL	2.3
1	D	57	ILE	2.3
1	С	146	HIS	2.3
1	В	162	ASP	2.3
1	С	19	ASP	2.2
1	D	55	GLY	2.2
1	D	2	LYS	2.2
1	D	35	VAL	2.1
1	D	45	GLU	2.0

Continued from previous page...

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.

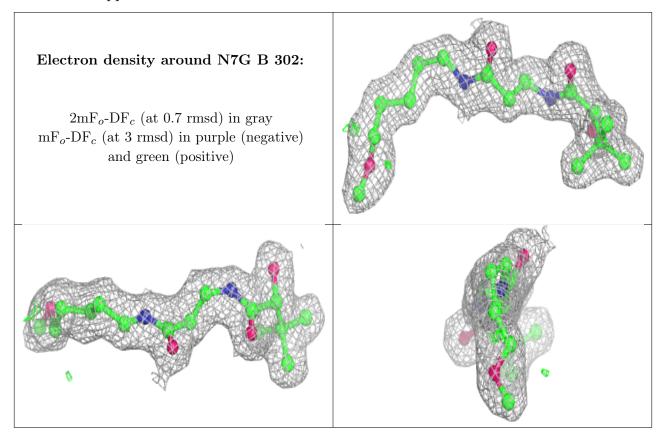
6.4 Ligands (i)

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^{th} 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.

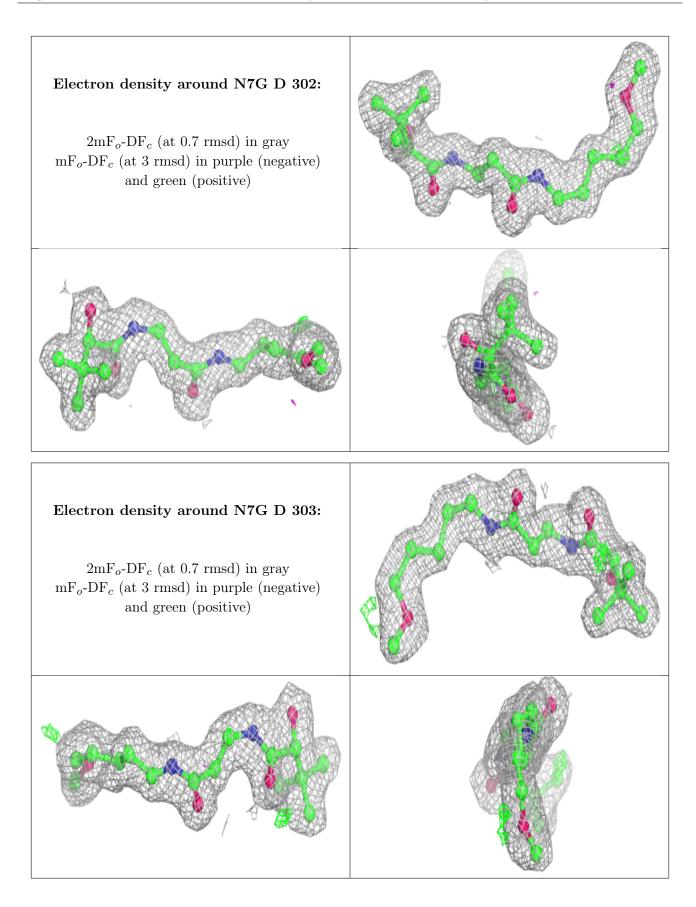


Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	В	304	1/1	0.96	0.06	23,23,23,23	0
4	N7G	В	302	21/21	0.96	0.10	19,20,29,29	0
4	N7G	D	302	21/21	0.96	0.14	17,19,21,22	0
4	N7G	D	303	21/21	0.96	0.10	21,23,26,28	0
4	N7G	В	303	21/21	0.97	0.12	16,18,19,20	0
3	MG	D	304	1/1	0.97	0.08	32,32,32,32	0
2	ATP	D	301	31/31	0.97	0.08	22,25,31,32	1
2	ATP	А	301	31/31	0.98	0.08	16,19,22,23	0
3	MG	А	302	1/1	0.98	0.07	$19,\!19,\!19,\!19$	0
2	ATP	В	301	31/31	0.98	0.07	18,22,27,29	1
2	ATP	С	301	31/31	0.98	0.08	16,19,23,26	0
3	MG	С	302	1/1	0.99	0.05	$19,\!19,\!19,\!19$	0

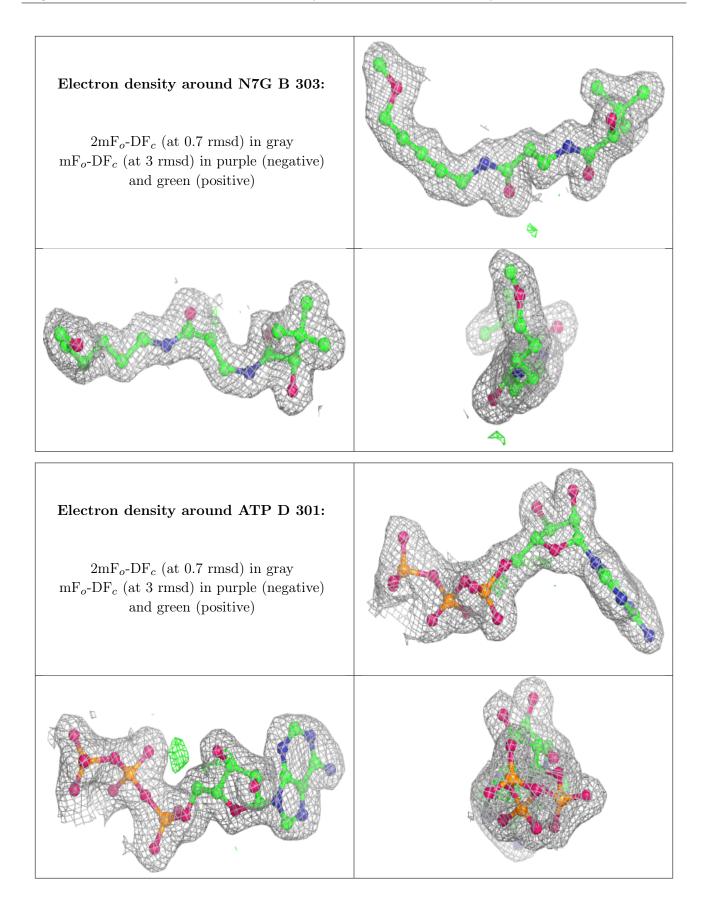
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



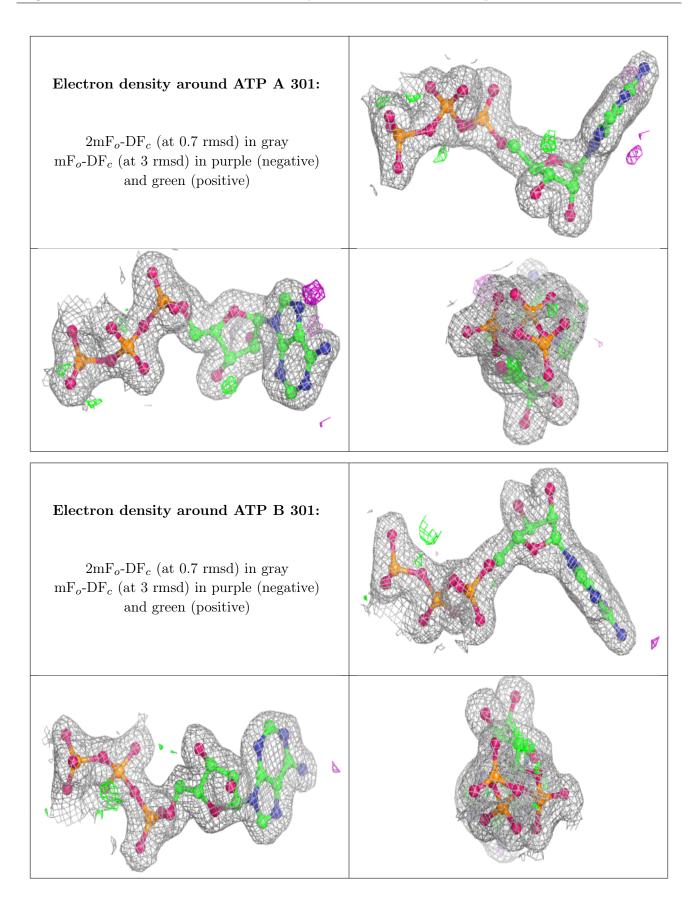




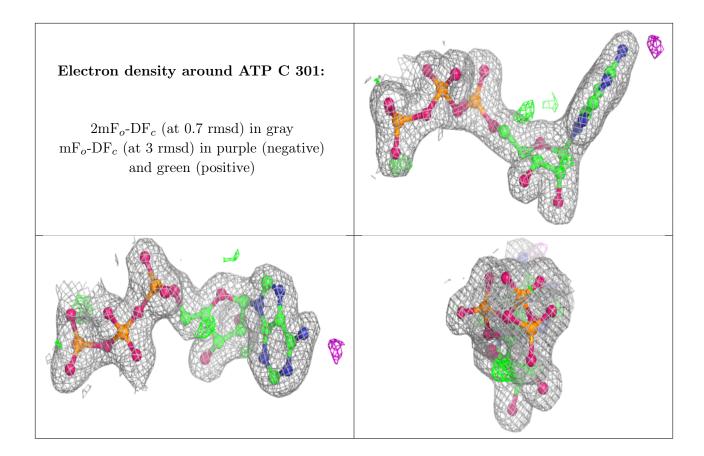












6.5 Other polymers (i)

There are no such residues in this entry.

