Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 06:52 pm GMT

PDB ID	:	5EG1
Title	:	Antibacterial peptide ABC transporter McjD with a resolved lipid
Authors	:	Choudhury, H.G.; Beis, K.
Deposited on	:	2015-10-26
Resolution	:	3.42 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 (i)) were used in the production of this report:

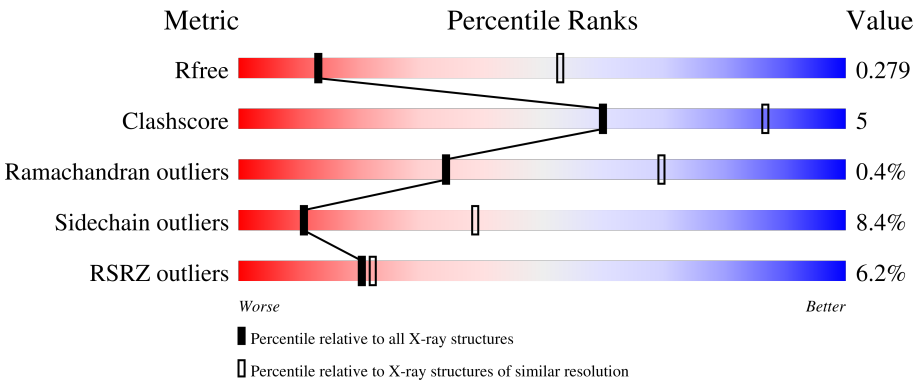
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 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	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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	A	580	7% 81% 16% • •
1	B	580	5% 81% 17% • •

2 Entry composition (i)

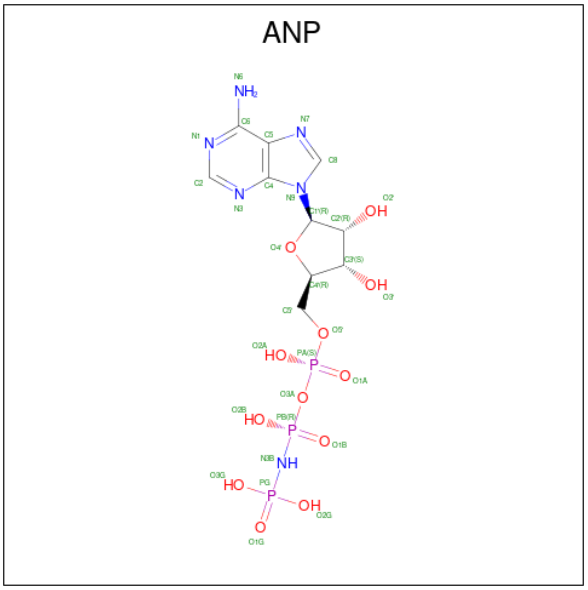
There are 4 unique types of molecules in this entry. The entry contains 9222 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	571	4527	2920	739	850	18	0	0	0
1	B	576	4580	2954	750	858	18	0	2	0

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

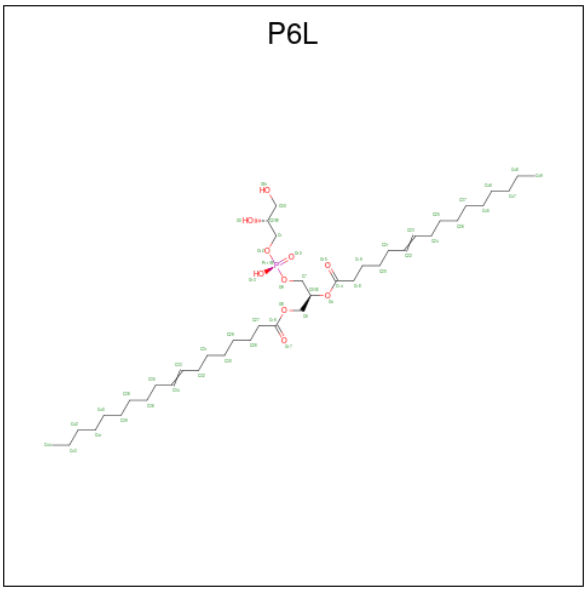


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	10	6	12	3	0	0
2	B	1	31	10	6	12	3	0	0

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

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

- Molecule 4 is (2S)-3-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-2-[(6E)-HEXADEC-6-ENOYLOXY]PROPYL (8E)-OCTADEC-8-ENOATE (three-letter code: P6L) (formula: $C_{40}H_{75}O_{10}P$).



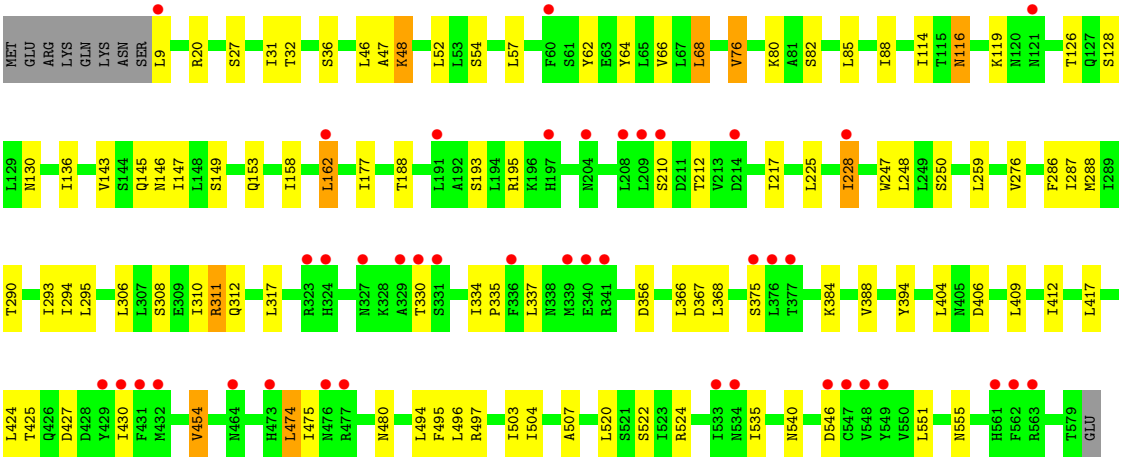
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
4	B	1	51	40	10	1	0	0

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.

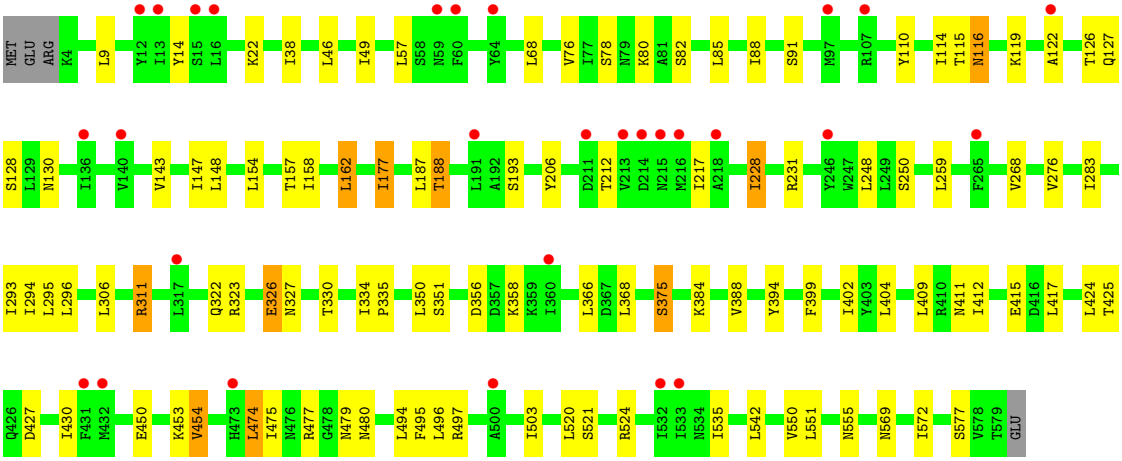
• Molecule 1: Microcin-J25 export ATP-binding/permease protein McjD

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.98Å 109.13Å 233.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.61 – 3.42 67.61 – 3.42	Depositor EDS
% Data completeness (in resolution range)	98.7 (67.61-3.42) 98.7 (67.61-3.42)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 3.41Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.254 , 0.272 0.262 , 0.279	Depositor DCC
R_{free} test set	1458 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	91.1	Xtriage
Anisotropy	1.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 73.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	9222	wwPDB-VP
Average B, all atoms (Å^2)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ANP, MG, P6L

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	0/6234
1	B	0.50	0/4663	0.64	0/6313
All	All	0.50	0/9266	0.64	0/12547

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	A	4527	0	4638	43	0
1	B	4580	0	4701	46	0
2	A	31	0	13	0	0
2	B	31	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	51	0	74	2	0
All	All	9222	0	9439	85	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 (85) 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:188:THR:HG22	1:B:311:ARG:HE	1.33	0.92
1:A:143:VAL:HA	1:A:147:ILE:HD12	1.76	0.67
1:B:143:VAL:HA	1:B:147:ILE:HD12	1.77	0.67
1:A:32:THR:HG21	1:A:145:GLN:HA	1.78	0.66
1:A:188:THR:HG23	1:A:308:SER:HA	1.78	0.64
1:B:454:VAL:HG22	1:B:495:PHE:HB2	1.81	0.62
1:B:212:THR:HG23	1:B:231:ARG:HH21	1.65	0.62
1:A:308:SER:O	1:A:312:GLN:HG2	2.01	0.60
1:B:351:SER:HB2	1:B:399:PHE:HB2	1.84	0.59
1:B:366:LEU:HD23	1:B:368:LEU:HD11	1.85	0.59
1:B:384:LYS:HD2	1:B:535:ILE:HG23	1.84	0.59
1:B:475:ILE:HB	1:B:480:ASN:HB2	1.85	0.59
1:A:454:VAL:HG22	1:A:495:PHE:HB2	1.84	0.58
1:A:475:ILE:HB	1:A:480:ASN:HB2	1.86	0.58
1:A:366:LEU:HD23	1:A:368:LEU:HD11	1.85	0.58
1:B:409:LEU:HA	1:B:412:ILE:HD12	1.86	0.57
1:A:76:VAL:HG11	1:B:294:ILE:HG12	1.87	0.56
1:B:454:VAL:HG21	1:B:496:LEU:HG	1.87	0.56
1:A:384:LYS:HD2	1:A:535:ILE:HG23	1.87	0.56
1:A:158:ILE:O	1:A:162:LEU:HB2	2.05	0.56
1:A:454:VAL:HG21	1:A:496:LEU:HG	1.87	0.56
1:A:409:LEU:HA	1:A:412:ILE:HD12	1.87	0.55
1:B:424:LEU:HD11	1:B:494:LEU:HD22	1.88	0.55
1:B:569:ASN:HD22	1:B:572:ILE:H	1.53	0.55
4:B:603:P6L:O15	4:B:603:P6L:H61	2.07	0.54
1:A:294:ILE:HG12	1:B:76:VAL:HG11	1.88	0.54
4:B:603:P6L:H362	4:B:603:P6L:H481	1.90	0.54
1:A:116:ASN:HA	1:A:119:LYS:HD3	1.90	0.53
1:A:217:ILE:HD12	1:A:217:ILE:H	1.73	0.53
1:B:454:VAL:HG22	1:B:495:PHE:CB	2.38	0.53
1:B:217:ILE:HD12	1:B:217:ILE:H	1.73	0.53
1:A:504:ILE:HG23	1:A:507:ALA:HB3	1.92	0.51
1:A:286:PHE:O	1:A:290:THR:HG23	2.10	0.51
1:A:27:SER:O	1:A:31:ILE:HD12	2.10	0.51
1:A:48:LYS:HB3	1:A:68:LEU:HD21	1.92	0.51
1:A:424:LEU:HD11	1:A:494:LEU:HD22	1.91	0.51
1:B:116:ASN:HA	1:B:119:LYS:HD3	1.93	0.51
1:B:430:ILE:HG21	1:B:474:LEU:HD22	1.93	0.51
1:A:430:ILE:HG21	1:A:474:LEU:HD22	1.93	0.50
1:A:454:VAL:HG22	1:A:495:PHE:CB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:THR:HG22	1:A:149:SER:HB2	1.93	0.50
1:A:195:ARG:HD2	1:A:312:GLN:HB2	1.93	0.50
1:A:188:THR:HG22	1:A:311:ARG:HG2	1.92	0.49
1:A:290:THR:HA	1:A:293:ILE:HD12	1.93	0.49
1:A:225:LEU:HB2	1:B:110:TYR:CZ	2.48	0.48
1:B:158:ILE:O	1:B:162:LEU:HB2	2.13	0.48
1:B:375:SER:HB3	1:B:542:LEU:HD23	1.93	0.48
1:A:334:ILE:HG12	1:A:337:LEU:HB2	1.95	0.48
1:A:136:ILE:HG13	1:A:317:LEU:HD21	1.98	0.45
1:B:268:VAL:HG12	1:B:293:ILE:HD11	1.98	0.45
1:A:62:TYR:CE1	1:B:283:ILE:HD11	2.51	0.45
1:A:52:LEU:HD21	1:A:64:TYR:CD2	2.51	0.45
1:B:154:LEU:HD22	1:B:177:ILE:HD13	1.99	0.45
1:B:114:ILE:HD13	1:B:394:TYR:HA	2.00	0.44
1:A:146:ASN:O	1:A:306:LEU:HD22	2.18	0.44
1:A:247:TRP:HE1	1:B:91:SER:HG	1.66	0.44
1:A:388:VAL:HB	1:A:503:ILE:HD13	2.00	0.44
1:B:38:ILE:HG21	1:B:78:SER:OG	2.18	0.44
1:A:48:LYS:HD2	1:A:48:LYS:HA	1.85	0.44
1:B:127:GLN:HG2	1:B:206:TYR:CD2	2.53	0.44
1:A:114:ILE:HD13	1:A:394:TYR:HA	2.00	0.43
1:B:158:ILE:HG22	1:B:162:LEU:HD22	2.00	0.43
1:A:47:ALA:HB2	1:A:288:MET:HB2	2.00	0.43
1:B:322:GLN:O	1:B:326:GLU:HB2	2.18	0.43
1:B:350:LEU:HD22	1:B:402:ILE:HD11	2.00	0.43
1:B:14:TYR:CE1	1:B:22:LYS:HD3	2.54	0.42
1:B:334:ILE:HG12	1:B:411:ASN:O	2.18	0.42
1:A:36:SER:HB2	1:A:153:GLN:HG3	2.01	0.42
1:B:409:LEU:HD22	1:B:417:LEU:HD11	2.01	0.42
1:A:158:ILE:HG22	1:A:162:LEU:HD22	2.02	0.42
1:B:388:VAL:HB	1:B:503:ILE:HD13	2.01	0.41
1:B:157:THR:HG21	1:B:296:LEU:HD21	2.02	0.41
1:B:450:GLU:HA	1:B:453:LYS:HE3	2.03	0.41
1:A:409:LEU:HD22	1:A:417:LEU:HD11	2.01	0.41
1:B:46:LEU:HD12	1:B:46:LEU:HA	1.86	0.41
1:B:409:LEU:HD23	1:B:412:ILE:HD12	2.01	0.41
1:B:228:ILE:HD13	1:B:228:ILE:HA	1.87	0.41
1:A:212:THR:HG21	1:A:228:ILE:HG23	2.03	0.41
1:B:550:VAL:HG11	1:B:569:ASN:HD21	1.86	0.41
1:B:49:ILE:HG13	1:B:68:LEU:HB3	2.02	0.41
1:A:57:LEU:HB3	1:A:62:TYR:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:SER:HB2	1:B:122:ALA:HB1	2.03	0.40
1:B:212:THR:HG22	1:B:228:ILE:HD12	2.03	0.40
1:B:475:ILE:H	1:B:480:ASN:HD22	1.70	0.40
1:B:477:ARG:HB2	1:B:479:ASN:HD21	1.87	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	Percentiles	
1	A	569/580 (98%)	530 (93%)	37 (6%)	2 (0%)	34	69
1	B	576/580 (99%)	534 (93%)	39 (7%)	3 (0%)	29	65
All	All	1145/1160 (99%)	1064 (93%)	76 (7%)	5 (0%)	34	69

All (5) Ramachandran outliers are listed below:

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

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	Percentiles	
1	A	520/529 (98%)	475 (91%)	45 (9%)	10	38
1	B	527/529 (100%)	484 (92%)	43 (8%)	11	40
All	All	1047/1058 (99%)	959 (92%)	88 (8%)	11	39

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	20	ARG
1	A	46	LEU
1	A	48	LYS
1	A	54	SER
1	A	66	VAL
1	A	68	LEU
1	A	76	VAL
1	A	80	LYS
1	A	82	SER
1	A	85	LEU
1	A	88	ILE
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	295	LEU
1	A	310	ILE
1	A	311	ARG
1	A	330	THR
1	A	367	ASP
1	A	375	SER
1	A	404	LEU
1	A	406	ASP
1	A	425	THR
1	A	427	ASP

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Mol	Chain	Res	Type
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	80	LYS
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	188	THR
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
1	B	356	ASP
1	B	358	LYS
1	B	375	SER
1	B	404	LEU
1	B	415	GLU

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Mol	Chain	Res	Type
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	551	LEU
1	B	555	ASN
1	B	577	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	A	153	GLN
1	A	223	ASN
1	A	443	ASN
1	A	479	ASN
1	A	487	GLN
1	A	534	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	534	ASN
1	B	569	ASN

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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	601	3	29,33,33	1.04	1 (3%)	31,52,52	1.69	4 (12%)
4	P6L	B	603	-	50,50,50	0.33	0	53,56,56	0.72	3 (5%)
2	ANP	B	601	3	29,33,33	1.09	1 (3%)	31,52,52	1.78	4 (12%)

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	601	3	-	5/14/38/38	0/3/3/3
4	P6L	B	603	-	-	29/55/55/55	-
2	ANP	B	601	3	-	5/14/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ANP	PB-O3A	-4.73	1.53	1.59
2	A	601	ANP	PB-O3A	-4.34	1.53	1.59

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	ANP	PB-O3A-PA	7.65	159.57	132.62
2	A	601	ANP	PB-O3A-PA	7.24	158.12	132.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	ANP	O2B-PB-O1B	2.87	115.94	109.92
4	B	603	P6L	O4-C5-C6	2.80	118.53	108.40
2	A	601	ANP	O1G-PG-N3B	2.76	115.84	111.77
2	B	601	ANP	O1G-PG-N3B	2.74	115.80	111.77
2	B	601	ANP	O2B-PB-O1B	2.53	115.22	109.92
2	A	601	ANP	C5-C6-N6	2.13	123.59	120.35
4	B	603	P6L	C5-O4-C14	2.08	122.91	117.79
4	B	603	P6L	C7-C5-C6	2.02	116.56	111.79
2	B	601	ANP	C5-C6-N6	2.01	123.41	120.35

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ANP	PB-N3B-PG-O1G
2	A	601	ANP	PG-N3B-PB-O1B
2	A	601	ANP	PA-O3A-PB-O1B
2	A	601	ANP	PA-O3A-PB-O2B
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	PA-O3A-PB-O2B
4	B	603	P6L	C7-O9-P11-O12
4	B	603	P6L	C1-O12-P11-O9
4	B	603	P6L	C6-C5-O4-C14
4	B	603	P6L	C39-C40-C41-C42
4	B	603	P6L	C24-C25-C26-C37
4	B	603	P6L	C16-C27-C28-C29
4	B	603	P6L	C18-C14-O4-C5
4	B	603	P6L	O15-C14-O4-C5
4	B	603	P6L	C25-C26-C37-C45
4	B	603	P6L	C37-C45-C46-C47
4	B	603	P6L	C27-C28-C29-C30
4	B	603	P6L	C23-C24-C25-C26
4	B	603	P6L	C18-C19-C20-C21
4	B	603	P6L	C28-C29-C30-C31
4	B	603	P6L	O4-C5-C6-O8
4	B	603	P6L	C7-C5-C6-O8
4	B	603	P6L	C7-O9-P11-O13
4	B	603	P6L	C1-O12-P11-O13
4	B	603	P6L	C29-C30-C31-C32
4	B	603	P6L	C5-C7-O9-P11

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Mol	Chain	Res	Type	Atoms
4	B	603	P6L	C36-C38-C39-C40
4	B	603	P6L	C6-C5-C7-O9
4	B	603	P6L	C19-C20-C21-C22
4	B	603	P6L	C38-C39-C40-C41
4	B	603	P6L	O4-C14-C18-C19
4	B	603	P6L	C31-C32-C33-C34
4	B	603	P6L	C33-C34-C35-C36
4	B	603	P6L	O15-C14-C18-C19
2	A	601	ANP	C5'-O5'-PA-O1A
2	B	601	ANP	C5'-O5'-PA-O1A
4	B	603	P6L	C22-C23-C24-C25

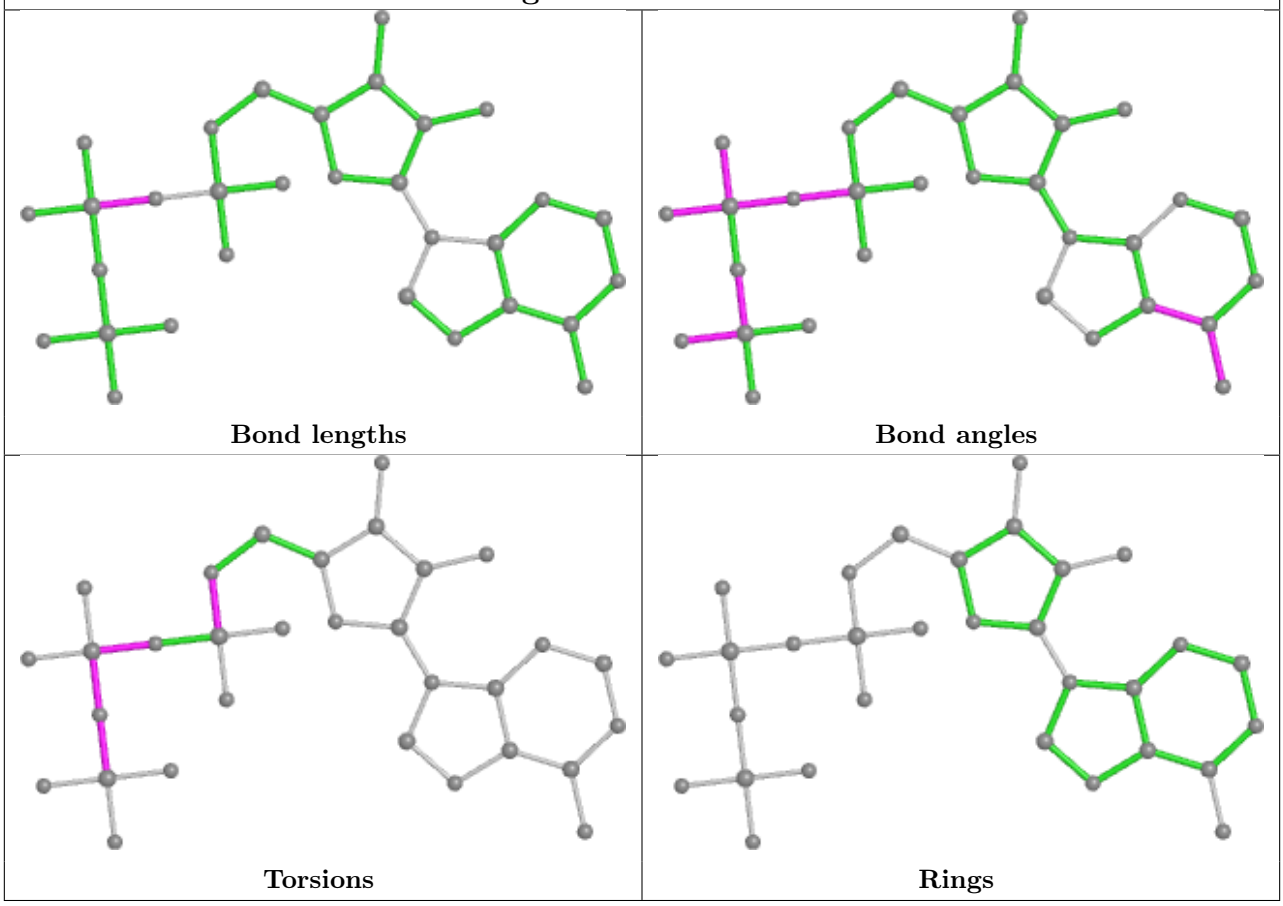
There are no ring outliers.

1 monomer is involved in 2 short contacts:

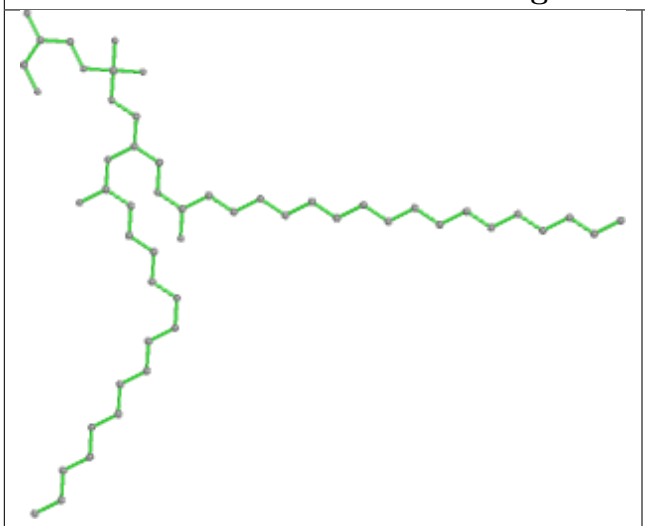
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	603	P6L	2	0

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 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.

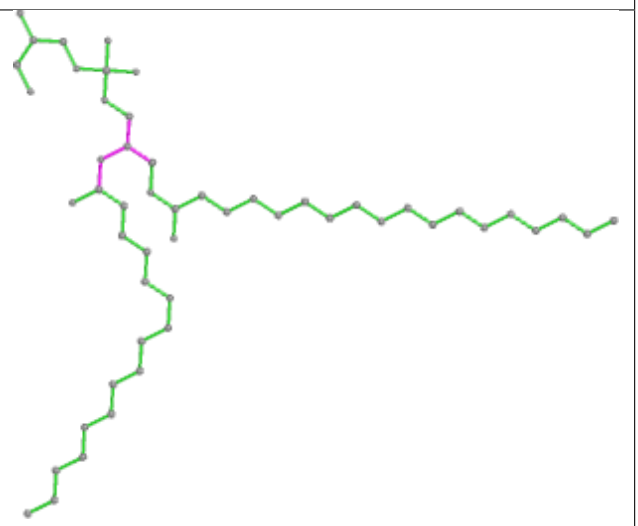
Ligand ANP A 601



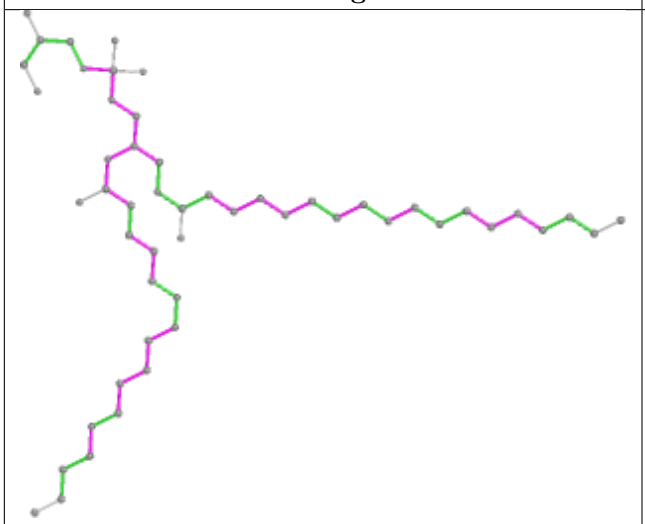
Ligand P6L B 603



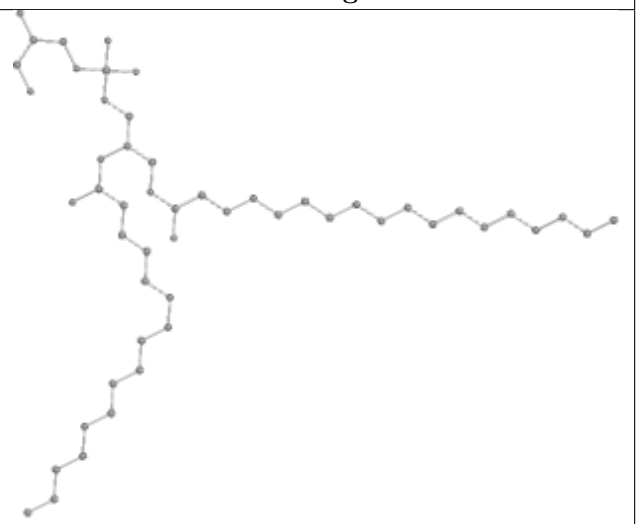
Bond lengths



Bond angles

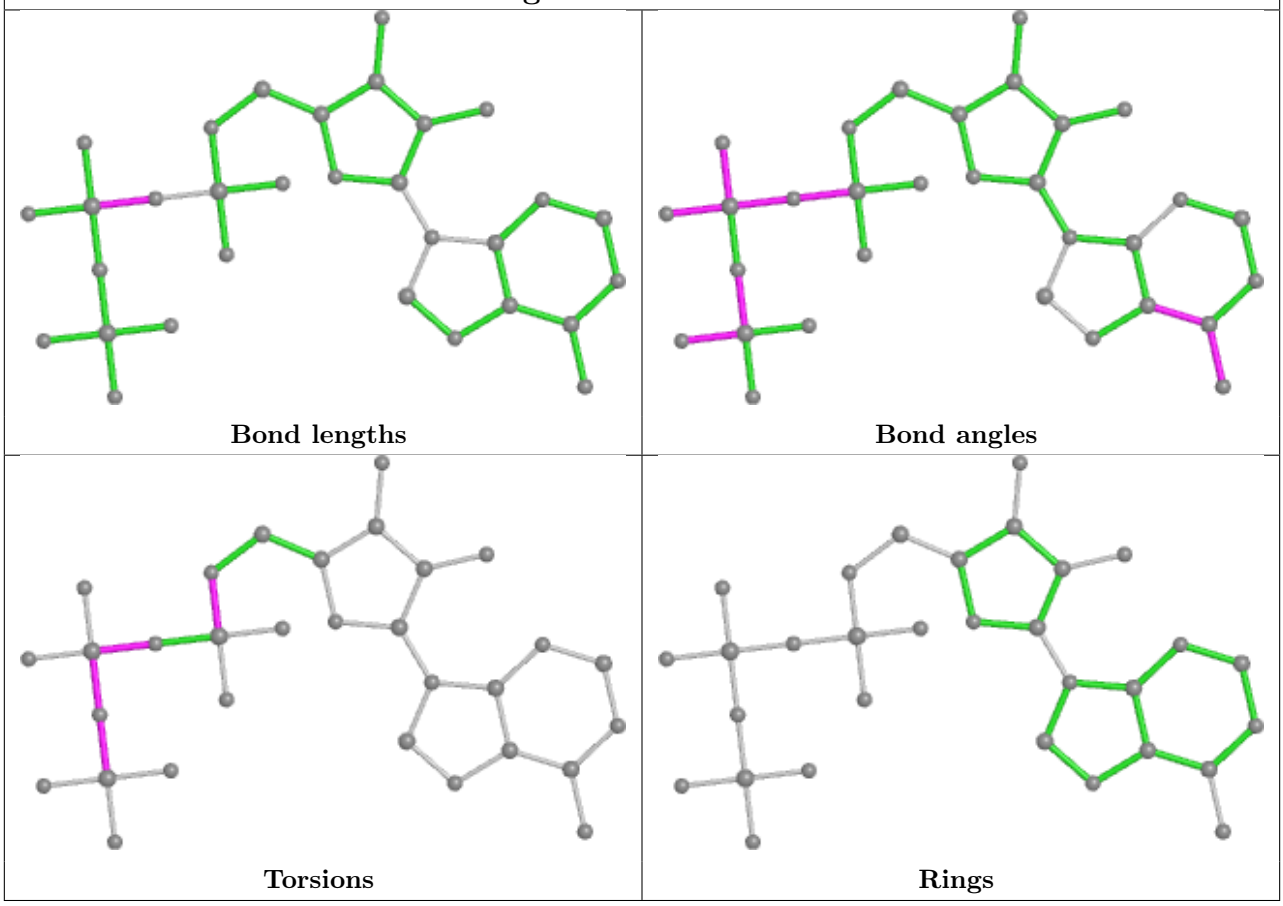


Torsions



Rings

Ligand ANP B 601



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, 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	571/580 (98%)	0.53	42 (7%)	14	17	85, 123, 168, 229	0
1	B	576/580 (99%)	0.39	29 (5%)	28	29	89, 118, 162, 211	0
All	All	1147/1160 (98%)	0.46	71 (6%)	20	22	85, 120, 165, 229	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	431	PHE	5.4
1	B	16	LEU	5.1
1	B	59	ASN	5.0
1	A	476	ASN	5.0
1	B	246	TYR	4.8
1	B	215	ASN	4.8
1	A	562	PHE	4.6
1	A	341	ARG	4.3
1	A	432	MET	4.2
1	B	12	TYR	4.0
1	A	330	THR	3.9
1	B	432	MET	3.7
1	A	430	ILE	3.6
1	A	340	GLU	3.6
1	B	214	ASP	3.6
1	A	464	ASN	3.5
1	B	431	PHE	3.5
1	A	327	ASN	3.4
1	A	329	ALA	3.3
1	B	60	PHE	3.3
1	B	360	ILE	3.2
1	A	339	MET	3.1
1	B	211	ASP	3.1
1	A	9	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	532	ILE	2.9
1	A	204	ASN	2.7
1	B	13	ILE	2.7
1	B	191	LEU	2.7
1	B	473	HIS	2.7
1	A	546	ASP	2.6
1	A	375	SER	2.6
1	A	336	PHE	2.6
1	A	548	VAL	2.6
1	A	549	TYR	2.6
1	B	97	MET	2.5
1	A	191	LEU	2.5
1	B	216	MET	2.5
1	B	213	VAL	2.5
1	A	533	ILE	2.4
1	B	218	ALA	2.4
1	A	561	HIS	2.4
1	A	197	HIS	2.4
1	A	210	SER	2.4
1	A	534	ASN	2.3
1	A	323	ARG	2.3
1	A	331	SER	2.3
1	A	376	LEU	2.3
1	A	60	PHE	2.3
1	B	500	ALA	2.3
1	A	208	LEU	2.2
1	B	533	ILE	2.2
1	B	15	SER	2.2
1	A	377	THR	2.2
1	A	547	CYS	2.2
1	A	121	ASN	2.2
1	A	477	ARG	2.2
1	A	429	TYR	2.1
1	B	140	VAL	2.1
1	B	317	LEU	2.1
1	A	214	ASP	2.1
1	A	563	ARG	2.1
1	A	228	ILE	2.1
1	A	324	HIS	2.1
1	B	107	ARG	2.1
1	A	473	HIS	2.1
1	B	64	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	265	PHE	2.0
1	B	122	ALA	2.0
1	A	209	LEU	2.0
1	B	136	ILE	2.0
1	A	162	LEU	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)

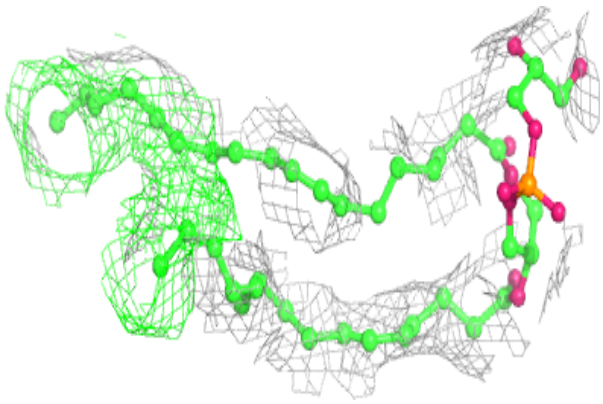
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

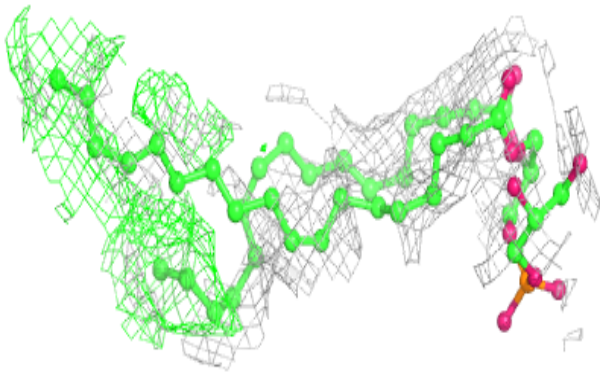
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	P6L	B	603	51/51	0.38	0.25	146,183,214,217	0
3	MG	B	602	1/1	0.85	0.24	91,91,91,91	0
3	MG	A	602	1/1	0.89	0.29	84,84,84,84	0
2	ANP	B	601	31/31	0.91	0.20	113,120,129,130	0
2	ANP	A	601	31/31	0.95	0.22	118,128,142,143	0

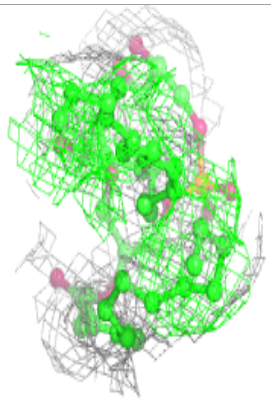
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P6L 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)

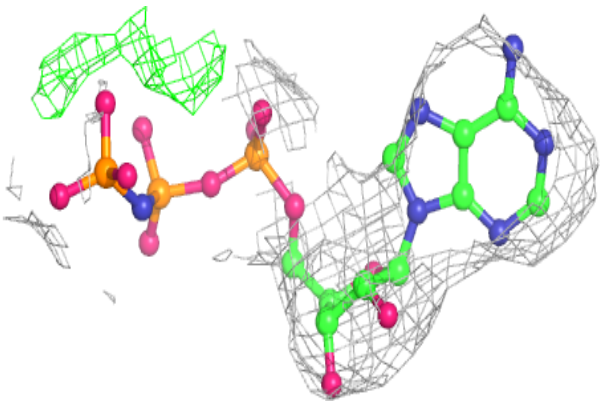


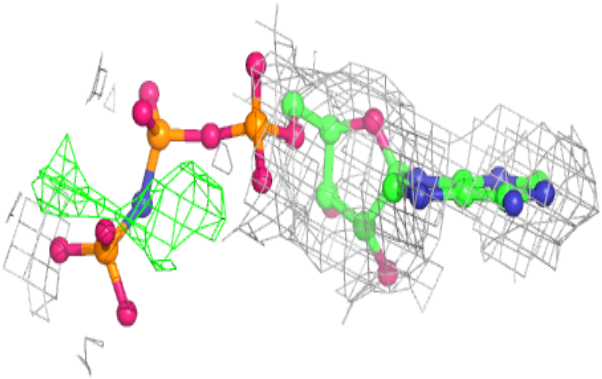


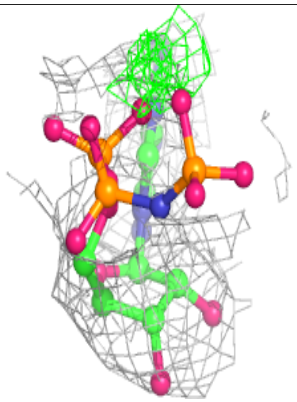


Electron density around ANP B 601:

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

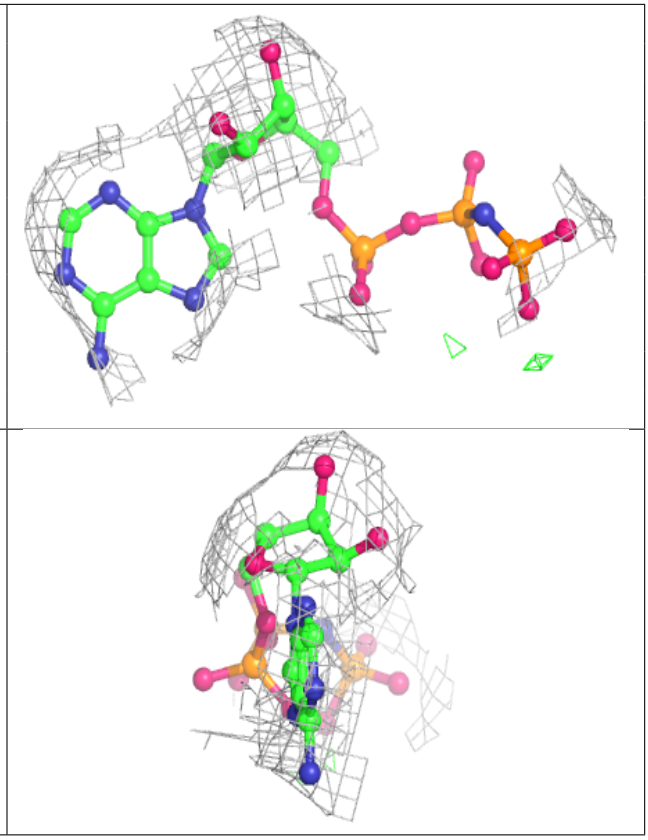






Electron density around ANP A 601:

$2mF_o$-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.