Full wwPDB X-ray Structure Validation Report ⓘ

Jan 9, 2024 – 02:25 PM EST

PDB ID	:	8FV3
Title	:	EGFR(T790M/V948R) in complex with compound 1 (LN4503)
Authors	:	Ogboo, B.C.; Heppner, D.E.
Deposited on	:	2023-01-18
Resolution	:	2.10 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

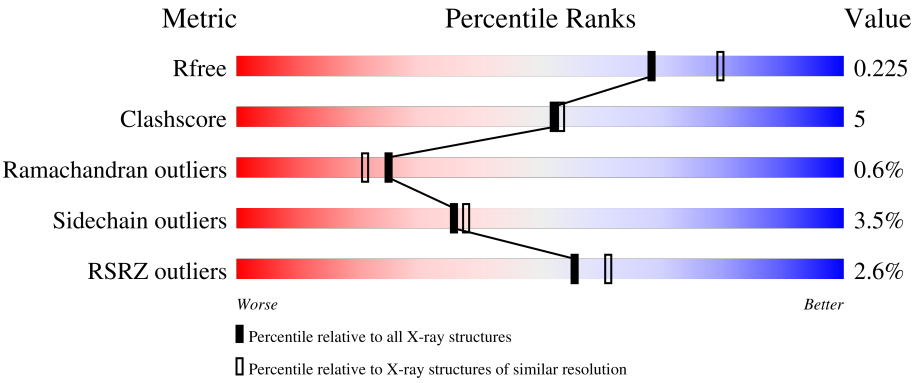
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	328	2% 78% 13% 9%
1	B	328	2% 83% 10% • 6%
1	C	328	4% 73% 15% • 11%
1	D	328	2% 74% 14% • 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9901 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	295	Total	C	N	O	S	0	1	0
			2337	1501	399	418	19			
1	A	299	Total	C	N	O	S	0	1	0
			2359	1518	400	423	18			
1	B	307	Total	C	N	O	S	0	0	0
			2428	1559	414	436	19			
1	C	291	Total	C	N	O	S	0	0	0
			2305	1481	389	416	19			

There are 8 discrepancies between the modelled and reference sequences:

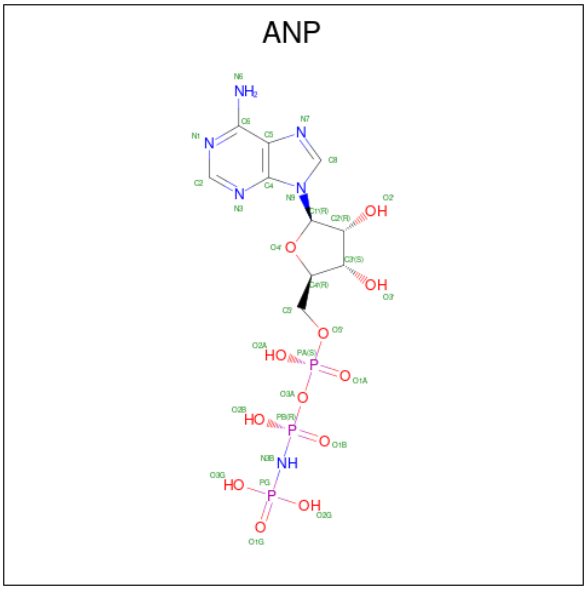
Chain	Residue	Modelled	Actual	Comment	Reference
D	790	MET	THR	engineered mutation	UNP P00533
D	948	ARG	VAL	engineered mutation	UNP P00533
A	790	MET	THR	engineered mutation	UNP P00533
A	948	ARG	VAL	engineered mutation	UNP P00533
B	790	MET	THR	engineered mutation	UNP P00533
B	948	ARG	VAL	engineered mutation	UNP P00533
C	790	MET	THR	engineered mutation	UNP P00533
C	948	ARG	VAL	engineered mutation	UNP P00533

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

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

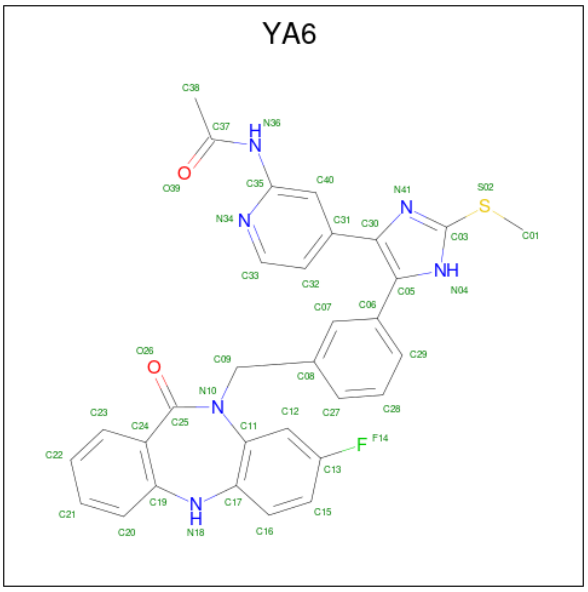
- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter

code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
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 N-{(4P)-4-[(4P)-5-{3-[(8-fluoro-11-oxo-5,11-dihydro-10H-dibenzo[b,e][1,4] diazepin-10-yl)methyl]phenyl}-2-(methylsulfanyl)-1H-imidazol-4-yl]pyridin-2-yl}acetam ide (three-letter code: YA6) (formula: $C_{31}H_{25}FN_6O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	C	1	Total	C	F	N	O	S	0	0
			41	31	1	6	2	1		

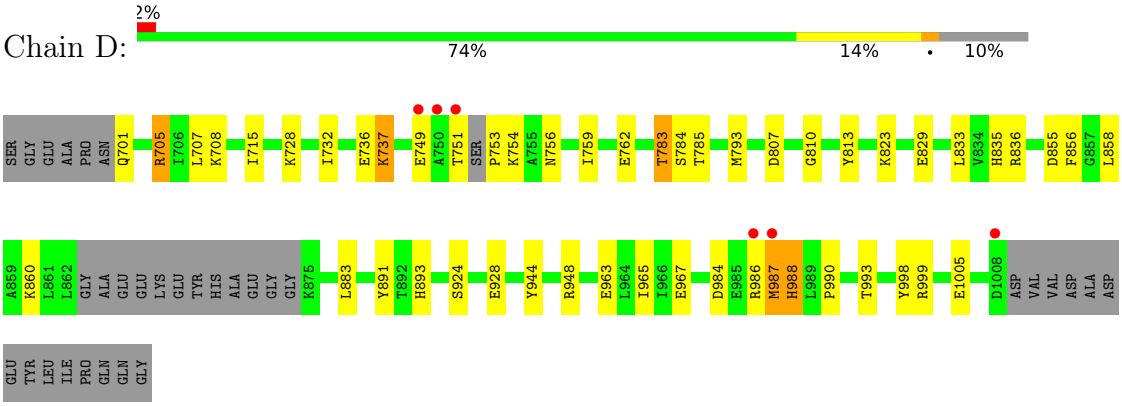
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	85	Total	O	0	0
			85	85		
5	A	75	Total	O	0	0
			75	75		
5	B	112	Total	O	0	0
			112	112		
5	C	63	Total	O	0	0
			63	63		

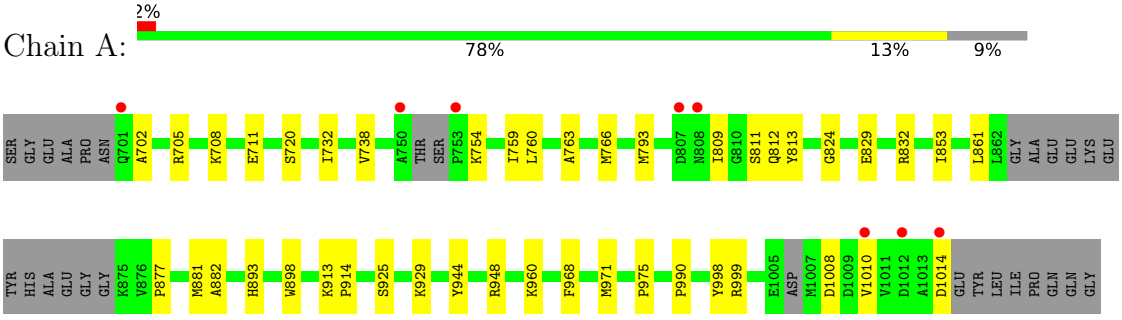
3 Residue-property plots (i)

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.

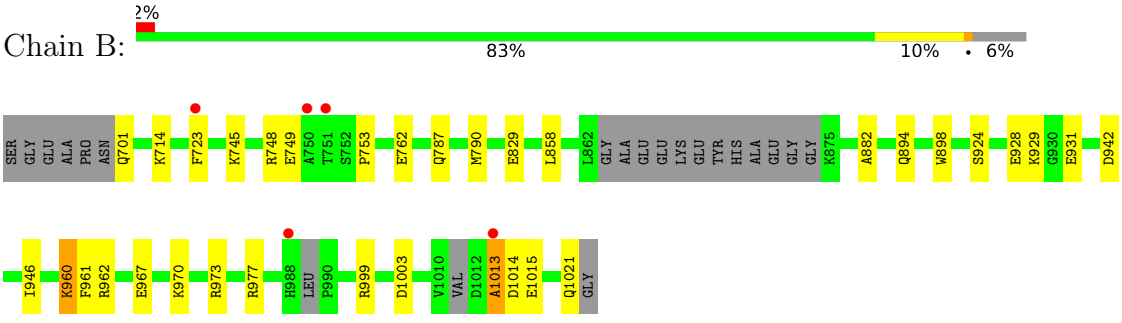
• Molecule 1: Epidermal growth factor receptor



• Molecule 1: Epidermal growth factor receptor

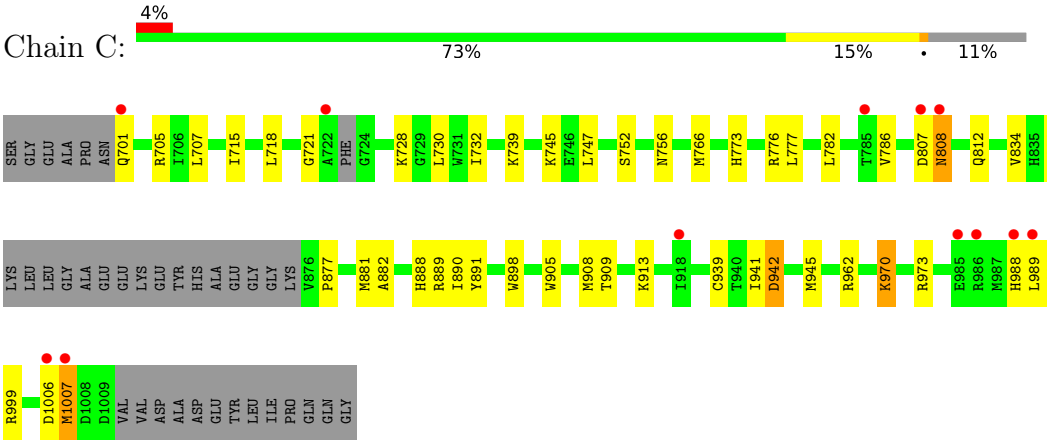


• Molecule 1: Epidermal growth factor receptor



• Molecule 1: Epidermal growth factor receptor

Chain C:


4%
73%
15%
11%
SER GLY GLU ALA PRO ASN Q701 R705 I706 L707 I715 L718 G721 A722 PHE G724 K728 G729 L730 W731 I732 K739 K745 E746 L747 S752 N756 M766 H773 R776 L777 L782 T785 V786 D807 N808 Q812 V834 H835 R836 L858 ALA
LYS LEU LEU GLY ALA GLU GLU LYS GLU TYR HIS ALA GLU GLY GLY LYS V876 P877 M881 A882 H888 R889 I890 Y891 W898 W905 M908 T909 K913 I918 C939 T940 I941 D942 M945 R962 K970 R973 E985 R986 M987 H988 L989 P990 D994
R999 D1006 M1007 D1008 D1009 VAL VAL ASP ALA ASP GLU TYR LEU ILE PRO GLN GLN GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.37Å 103.22Å 87.14Å 90.00° 101.48° 90.00°	Depositor
Resolution (Å)	65.80 – 2.10 65.80 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.3 (65.80-2.10) 95.2 (65.80-2.09)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.190 , 0.226 0.189 , 0.225	Depositor DCC
R_{free} test set	1999 reflections (2.72%)	wwPDB-VP
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9901	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.27% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, YA6, 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	0.40	0/2408	0.58	0/3265
1	B	0.44	0/2479	0.61	0/3356
1	C	0.41	0/2355	0.60	0/3191
1	D	0.42	0/2386	0.61	0/3228
All	All	0.42	0/9628	0.60	0/13040

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	2359	0	2351	26	0
1	B	2428	0	2414	23	0
1	C	2305	0	2311	30	0
1	D	2337	0	2345	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	13	0	0
3	B	31	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	31	0	13	0	0
4	C	41	0	0	0	0
5	A	75	0	0	3	0
5	B	112	0	0	1	0
5	C	63	0	0	6	0
5	D	85	0	0	4	0
All	All	9901	0	9460	104	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 (104) 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:812:GLN:HG2	1:C:989:LEU:HG	1.58	0.85
1:D:893:HIS:HD2	5:D:1270:HOH:O	1.69	0.75
1:A:913[B]:LYS:HE2	1:A:914:PRO:HD2	1.69	0.74
1:B:960:LYS:HZ2	1:B:961:PHE:H	1.38	0.70
1:C:701:GLN:C	5:C:1203:HOH:O	2.29	0.69
1:C:701:GLN:N	5:C:1203:HOH:O	2.26	0.68
1:C:773:HIS:HD2	5:C:1234:HOH:O	1.75	0.68
1:D:833:LEU:HD13	1:D:856:PHE:CZ	2.31	0.66
1:B:970:LYS:HE2	1:B:973:ARG:HH11	1.62	0.65
1:A:832:ARG:NH2	1:B:749:GLU:H	1.95	0.64
1:A:832:ARG:HH22	1:B:749:GLU:H	1.44	0.63
1:D:715:ILE:HD11	1:D:728:LYS:HD3	1.82	0.61
1:B:701:GLN:NE2	5:B:1201:HOH:O	2.21	0.61
1:A:732:ILE:HD12	1:A:738:VAL:O	2.01	0.61
1:A:944:TYR:CZ	1:A:948:ARG:HD3	2.37	0.60
1:D:924:SER:O	1:D:928:GLU:HG3	2.02	0.59
1:C:701:GLN:CA	5:C:1203:HOH:O	2.51	0.59
1:C:962:ARG:HG2	5:C:1226:HOH:O	2.03	0.59
1:A:893:HIS:HD2	5:A:1238:HOH:O	1.87	0.57
1:C:888:HIS:HB2	1:C:890:ILE:HD12	1.85	0.57
1:D:783:THR:OG1	1:D:784:SER:N	2.38	0.56
1:B:714:LYS:NZ	1:B:787:GLN:OE1	2.35	0.54
1:D:835:HIS:O	1:D:836:ARG:HB2	2.07	0.54
1:D:756:ASN:HA	1:D:759:ILE:HD12	1.89	0.54
1:B:745:LYS:HE2	1:B:858:LEU:HD21	1.90	0.54
1:B:970:LYS:HA	1:B:973:ARG:NH1	2.22	0.53
1:A:763:ALA:HA	1:A:766:MET:CE	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:999:ARG:HD2	5:D:1205:HOH:O	2.09	0.53
1:D:986:ARG:O	1:D:987:MET:C	2.48	0.53
1:B:970:LYS:HE2	1:B:973:ARG:NH1	2.24	0.53
1:D:984:ASP:HA	1:D:987:MET:HG2	1.91	0.52
1:A:829:GLU:HG3	1:A:893:HIS:CG	2.45	0.52
1:B:723:PHE:CD2	1:B:858:LEU:HD23	2.45	0.52
1:D:993:THR:OG1	1:A:702:ALA:HA	2.11	0.51
1:D:807:ASP:HB2	5:D:1249:HOH:O	2.12	0.50
1:B:829:GLU:OE2	1:B:960:LYS:HE3	2.12	0.50
1:C:705:ARG:HD3	1:C:707:LEU:HG	1.94	0.49
1:C:877:PRO:O	1:C:881:MET:HG3	2.12	0.49
1:C:721:GLY:HA3	5:C:1240:HOH:O	2.12	0.49
1:B:999:ARG:HD2	1:B:1003:ASP:O	2.12	0.49
1:B:946:ILE:HD13	1:B:967:GLU:HG2	1.95	0.49
1:D:732:ILE:HD11	1:D:736:GLU:O	2.13	0.48
1:C:705:ARG:HH11	1:C:705:ARG:HG3	1.78	0.48
1:C:908:MET:HG3	1:C:939:CYS:SG	2.53	0.48
1:D:793:MET:HG3	5:D:1212:HOH:O	2.13	0.48
1:B:929:LYS:O	1:B:929:LYS:HD3	2.13	0.48
1:C:747:LEU:HD12	1:C:786:VAL:HB	1.95	0.48
1:C:836:ARG:HD2	1:C:891:TYR:CG	2.48	0.48
1:C:834:VAL:HG12	1:C:836:ARG:HG2	1.96	0.47
1:B:894:GLN:OE1	1:B:960:LYS:HE2	2.13	0.47
1:B:924:SER:O	1:B:928:GLU:HG3	2.15	0.47
1:C:766:MET:HE1	1:C:777:LEU:HD22	1.96	0.47
1:D:833:LEU:HB3	1:D:856:PHE:CE1	2.49	0.47
1:A:925:SER:O	1:A:929:LYS:HG3	2.15	0.47
1:A:824:GLY:HA3	1:A:853:ILE:HD12	1.97	0.47
1:A:813:TYR:OH	1:A:990:PRO:HD3	2.15	0.47
1:B:1013:ALA:O	1:B:1014:ASP:HB2	2.14	0.46
1:D:813:TYR:OH	1:D:990:PRO:HG3	2.15	0.46
1:D:963:GLU:O	1:D:967:GLU:HG3	2.16	0.46
1:B:929:LYS:HD2	1:B:931:GLU:CG	2.46	0.46
1:A:708:LYS:O	1:A:711:GLU:HG2	2.16	0.46
1:A:759:ILE:HG23	1:A:861:LEU:HD11	1.98	0.46
1:A:763:ALA:HA	1:A:766:MET:HE2	1.97	0.46
1:D:810:GLY:HA2	1:D:987:MET:HG3	1.98	0.45
1:D:751:THR:C	1:D:753:PRO:HD3	2.36	0.45
1:C:718:LEU:HD21	1:C:728:LYS:HB2	1.99	0.45
1:C:756:ASN:HB3	1:C:782:LEU:HD22	1.99	0.45
1:C:999:ARG:HH22	1:C:1007:MET:HG2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:829:GLU:HG3	1:D:893:HIS:CG	2.52	0.45
1:D:813:TYR:HE2	1:D:988:HIS:O	2.00	0.45
1:D:944:TYR:CZ	1:D:948:ARG:HD3	2.51	0.45
1:B:882:ALA:HA	1:B:898:TRP:CD2	2.52	0.45
1:B:929:LYS:HD2	1:B:931:GLU:HG3	1.97	0.45
1:C:970:LYS:HA	1:C:973:ARG:NH1	2.31	0.45
1:A:960:LYS:HD2	5:A:1202:HOH:O	2.15	0.45
1:D:883:LEU:HD21	1:D:928:GLU:HG2	1.98	0.44
1:C:889:ARG:HD3	1:C:889:ARG:HA	1.87	0.44
1:A:877:PRO:O	1:A:881:MET:HG3	2.17	0.44
1:A:811:SER:OG	1:A:975:PRO:HB2	2.17	0.44
1:C:732:ILE:HD12	1:C:739:LYS:HG2	2.00	0.44
1:C:990:PRO:HB2	1:C:994:ASP:HB2	2.00	0.44
1:A:832:ARG:NH1	1:B:748:ARG:HA	2.33	0.43
1:C:766:MET:CE	1:C:777:LEU:HD22	2.48	0.43
1:A:832:ARG:HH12	1:B:748:ARG:HA	1.83	0.43
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.52	0.43
1:D:705:ARG:NH1	1:D:707:LEU:HD13	2.34	0.43
1:D:855:ASP:HA	1:D:858:LEU:HD13	2.00	0.43
1:A:760:LEU:HD12	1:A:760:LEU:HA	1.85	0.43
1:D:836:ARG:HG2	1:D:891:TYR:CD2	2.54	0.43
1:C:715:ILE:HG13	1:C:730:LEU:HG	2.01	0.42
1:A:812:GLN:HG2	1:A:975:PRO:HG3	2.00	0.42
1:D:737:LYS:HB3	1:D:737:LYS:HE3	1.84	0.42
1:D:754:LYS:HB3	1:D:754:LYS:HE2	1.76	0.42
1:A:944:TYR:O	1:A:948:ARG:HG2	2.20	0.42
1:A:968:PHE:CD1	1:A:971:MET:HE3	2.55	0.41
1:C:882:ALA:HA	1:C:898:TRP:CD2	2.55	0.41
1:B:942:ASP:O	1:B:946:ILE:HG13	2.20	0.41
1:C:941:ILE:O	1:C:945:MET:HG2	2.21	0.41
1:D:823:LYS:HA	1:D:965:ILE:HD11	2.04	0.40
1:C:942:ASP:OD1	1:C:942:ASP:N	2.54	0.40
1:C:745:LYS:HB2	1:C:745:LYS:HE3	1.82	0.40
1:D:783:THR:HG23	1:D:785:THR:O	2.21	0.40
1:A:793:MET:HE1	5:A:1203:HOH:O	2.21	0.40
1:C:905:TRP:O	1:C:909:THR:HG23	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	Percentiles	
1	A	292/328 (89%)	282 (97%)	9 (3%)	1 (0%)	41	41
1	B	299/328 (91%)	290 (97%)	7 (2%)	2 (1%)	22	18
1	C	285/328 (87%)	273 (96%)	11 (4%)	1 (0%)	34	32
1	D	290/328 (88%)	279 (96%)	8 (3%)	3 (1%)	15	11
All	All	1166/1312 (89%)	1124 (96%)	35 (3%)	7 (1%)	25	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	808	ASN
1	D	987	MET
1	A	1008	ASP
1	D	988	HIS
1	B	753	PRO
1	D	749	GLU
1	B	1013	ALA

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	252/288 (88%)	244 (97%)	8 (3%)	39	41
1	B	259/288 (90%)	252 (97%)	7 (3%)	44	48
1	C	251/288 (87%)	240 (96%)	11 (4%)	28	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	250/288 (87%)	241 (96%)	9 (4%)	35 36
All	All	1012/1152 (88%)	977 (96%)	35 (4%)	36 38

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	701	GLN
1	D	705	ARG
1	D	708	LYS
1	D	737	LYS
1	D	762	GLU
1	D	783	THR
1	D	860	LYS
1	D	998	TYR
1	D	1005	GLU
1	A	705	ARG
1	A	720	SER
1	A	754	LYS
1	A	809	ILE
1	A	998	TYR
1	A	999	ARG
1	A	1010	VAL
1	A	1014	ASP
1	B	762	GLU
1	B	790	MET
1	B	960	LYS
1	B	962	ARG
1	B	977	ARG
1	B	1015	GLU
1	B	1021	GLN
1	C	752	SER
1	C	776	ARG
1	C	807	ASP
1	C	808	ASN
1	C	858	LEU
1	C	913	LYS
1	C	942	ASP
1	C	970	LYS
1	C	988	HIS
1	C	1006	ASP
1	C	1007	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	893	HIS
1	D	894	GLN
1	A	893	HIS
1	A	976	GLN
1	B	701	GLN
1	C	812	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ANP	B	1102	2	29,33,33	1.78	8 (27%)	31,52,52	1.70	6 (19%)
3	ANP	D	1102	2	29,33,33	1.10	3 (10%)	31,52,52	1.02	3 (9%)
4	YA6	C	1101	-	44,46,46	2.59	18 (40%)	56,66,66	2.27	17 (30%)
3	ANP	A	1102	2	29,33,33	1.71	8 (27%)	31,52,52	1.64	7 (22%)

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	1102	2	-	4/14/38/38	0/3/3/3
3	ANP	D	1102	2	-	3/14/38/38	0/3/3/3
4	YA6	C	1101	-	-	1/16/18/18	0/6/6/6
3	ANP	A	1102	2	-	5/14/38/38	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1101	YA6	C03-S02	7.04	1.81	1.75
4	C	1101	YA6	C25-N10	6.32	1.45	1.37
4	C	1101	YA6	C37-N36	5.79	1.46	1.36
4	C	1101	YA6	C17-N18	4.72	1.47	1.41
4	C	1101	YA6	C06-C05	4.67	1.54	1.49
4	C	1101	YA6	C31-C30	4.54	1.54	1.49
4	C	1101	YA6	C19-N18	4.36	1.46	1.41
3	B	1102	ANP	PG-N3B	4.25	1.74	1.63
3	B	1102	ANP	PB-N3B	4.22	1.74	1.63
3	A	1102	ANP	PG-N3B	3.98	1.73	1.63
3	A	1102	ANP	PB-N3B	3.87	1.73	1.63
4	C	1101	YA6	C11-N10	3.22	1.46	1.43
3	B	1102	ANP	PG-O1G	3.04	1.51	1.46
4	C	1101	YA6	C24-C25	3.01	1.54	1.50
3	A	1102	ANP	PB-O1B	2.97	1.50	1.46
3	D	1102	ANP	PG-O1G	2.94	1.50	1.46
4	C	1101	YA6	C35-N36	2.79	1.46	1.40
3	B	1102	ANP	PB-O1B	2.75	1.50	1.46
4	C	1101	YA6	C30-N41	-2.65	1.30	1.37
3	A	1102	ANP	PB-O2B	-2.64	1.49	1.56
3	D	1102	ANP	PG-N3B	2.63	1.70	1.63
4	C	1101	YA6	C17-C11	-2.59	1.37	1.40
3	A	1102	ANP	PG-O2G	-2.58	1.49	1.56
3	A	1102	ANP	PG-O3G	-2.50	1.50	1.56
4	C	1101	YA6	C30-C05	-2.48	1.38	1.44
3	B	1102	ANP	PG-O3G	-2.42	1.50	1.56
3	B	1102	ANP	PG-O2G	-2.39	1.50	1.56
3	B	1102	ANP	PB-O2B	-2.39	1.50	1.56
4	C	1101	YA6	O26-C25	-2.38	1.17	1.22
3	D	1102	ANP	PB-O1B	2.32	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1101	YA6	C05-N04	-2.30	1.31	1.37
3	B	1102	ANP	C5-C4	2.23	1.46	1.40
4	C	1101	YA6	O39-C37	-2.22	1.18	1.23
3	A	1102	ANP	PG-O1G	2.21	1.49	1.46
4	C	1101	YA6	C24-C19	-2.20	1.37	1.41
3	A	1102	ANP	C5-C4	2.17	1.46	1.40
4	C	1101	YA6	C15-C13	2.11	1.41	1.37

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1101	YA6	C01-S02-C03	9.28	109.19	102.27
4	C	1101	YA6	C09-N10-C11	-6.03	111.91	118.28
4	C	1101	YA6	C11-N10-C25	5.24	130.56	124.96
3	B	1102	ANP	O1G-PG-N3B	-4.77	104.75	111.77
4	C	1101	YA6	C08-C09-N10	4.42	120.85	113.39
3	A	1102	ANP	O2B-PB-O1B	4.36	119.06	109.92
3	B	1102	ANP	O2B-PB-O1B	4.20	118.74	109.92
4	C	1101	YA6	C33-N34-C35	3.30	121.90	117.22
3	A	1102	ANP	O1G-PG-N3B	-3.28	106.95	111.77
3	B	1102	ANP	N3-C2-N1	-3.04	123.92	128.68
3	A	1102	ANP	N3-C2-N1	-3.00	123.99	128.68
3	A	1102	ANP	C3'-C2'-C1'	2.83	105.25	100.98
3	B	1102	ANP	C4-C5-N7	-2.78	106.50	109.40
3	A	1102	ANP	C4-C5-N7	-2.70	106.58	109.40
3	A	1102	ANP	PB-O3A-PA	-2.59	123.50	132.62
4	C	1101	YA6	C24-C25-N10	2.48	123.34	119.63
4	C	1101	YA6	C38-C37-N36	2.48	118.61	114.98
4	C	1101	YA6	C35-N36-C37	-2.47	125.60	128.16
4	C	1101	YA6	C05-C30-N41	-2.46	107.11	113.76
4	C	1101	YA6	C15-C13-C12	-2.42	120.15	123.29
4	C	1101	YA6	C20-C19-N18	-2.41	114.63	119.00
3	B	1102	ANP	PB-O3A-PA	-2.37	124.28	132.62
4	C	1101	YA6	C30-C05-N04	-2.26	107.66	113.76
4	C	1101	YA6	C32-C33-N34	-2.25	121.17	123.96
3	D	1102	ANP	C5-C6-N6	2.23	123.75	120.35
4	C	1101	YA6	C20-C19-C24	2.20	122.28	119.38
4	C	1101	YA6	C16-C15-C13	2.20	120.64	118.36
3	A	1102	ANP	O2G-PG-O3G	2.18	113.45	107.64
3	D	1102	ANP	PB-O3A-PA	-2.16	125.03	132.62
4	C	1101	YA6	C40-C35-N34	-2.14	119.77	122.75
3	D	1102	ANP	O2G-PG-O1G	-2.14	108.08	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1102	ANP	O2G-PG-O3G	2.08	113.17	107.64
4	C	1101	YA6	C09-C08-C27	-2.06	116.90	120.77

There are no chirality outliers.

All (13) torsion outliers are listed below:

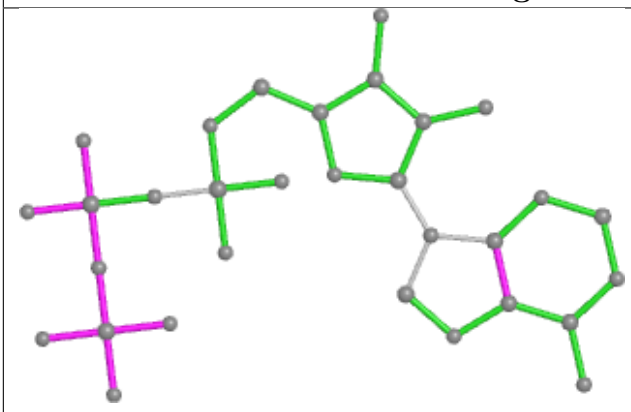
Mol	Chain	Res	Type	Atoms
3	D	1102	ANP	PG-N3B-PB-O1B
3	D	1102	ANP	PA-O3A-PB-O1B
3	D	1102	ANP	PA-O3A-PB-O2B
3	A	1102	ANP	PG-N3B-PB-O1B
3	A	1102	ANP	PA-O3A-PB-O1B
3	A	1102	ANP	PA-O3A-PB-O2B
3	B	1102	ANP	PB-N3B-PG-O1G
3	B	1102	ANP	PG-N3B-PB-O1B
3	B	1102	ANP	PA-O3A-PB-O1B
3	B	1102	ANP	PA-O3A-PB-O2B
3	A	1102	ANP	O4'-C4'-C5'-O5'
3	A	1102	ANP	C3'-C4'-C5'-O5'
4	C	1101	YA6	N04-C05-C06-C29

There are no ring outliers.

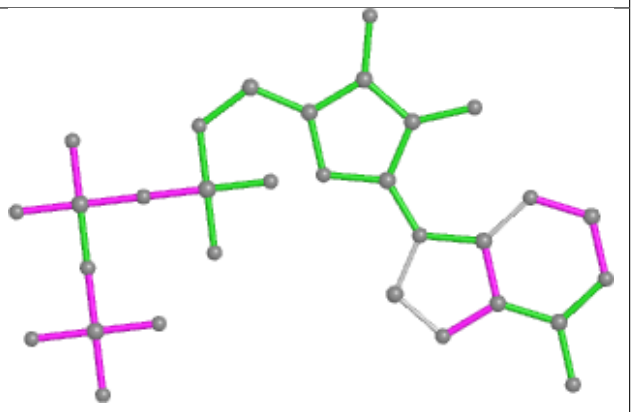
No monomer is involved in short contacts.

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.

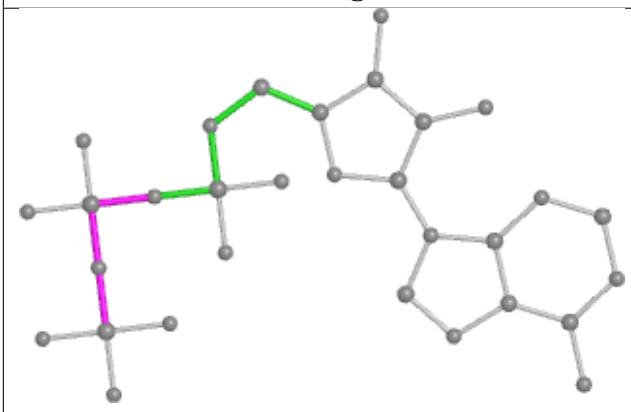
Ligand ANP B 1102



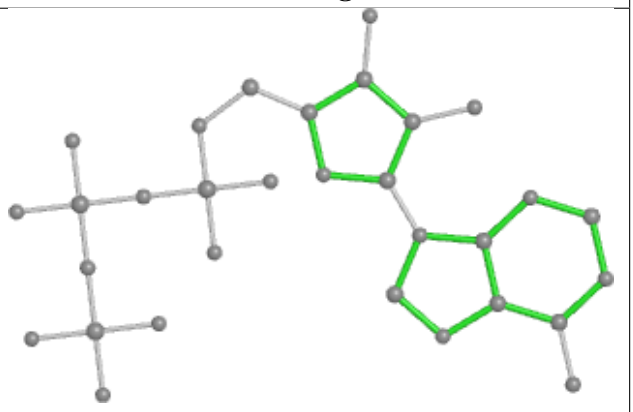
Bond lengths



Bond angles

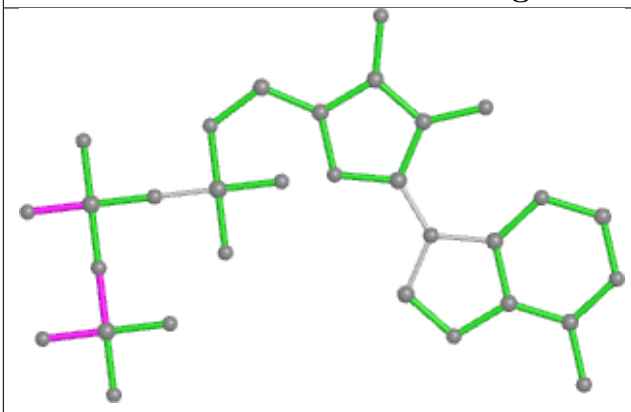


Torsions



Rings

Ligand ANP D 1102



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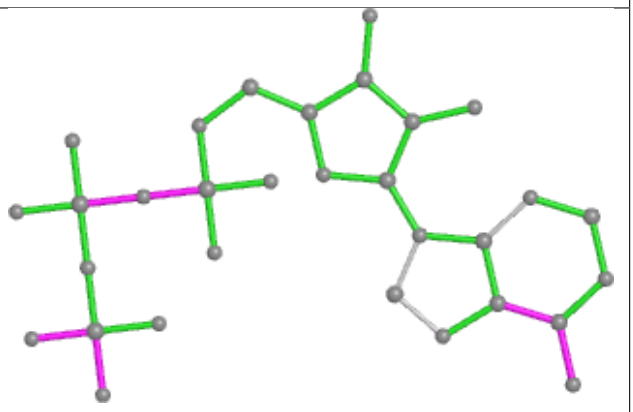
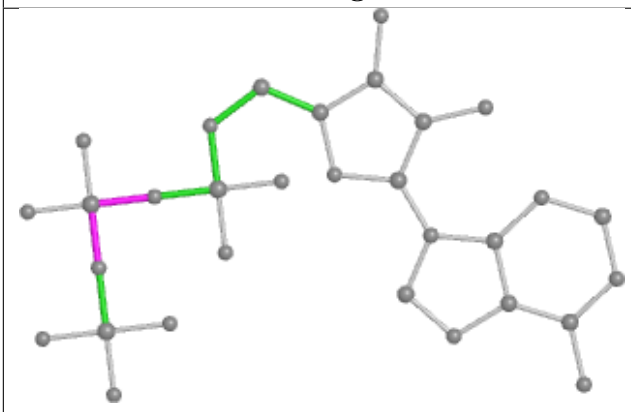
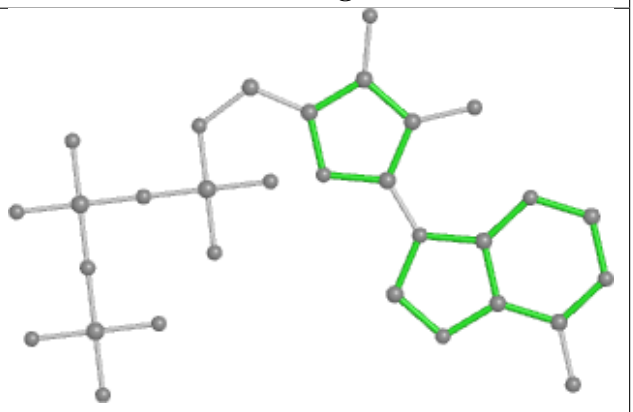


Bond angles

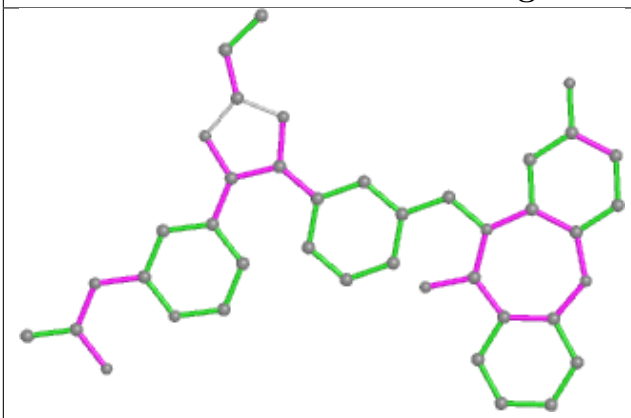


Torsions

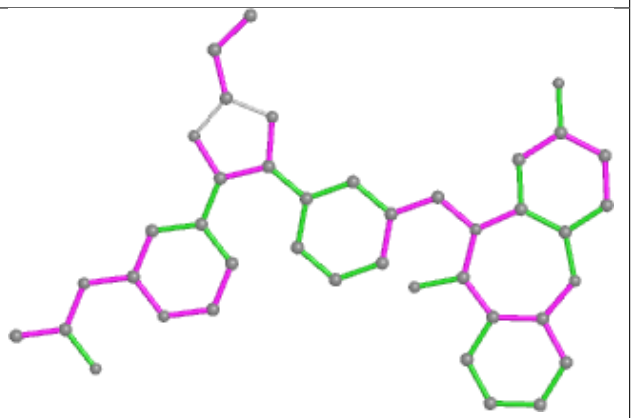


Rings

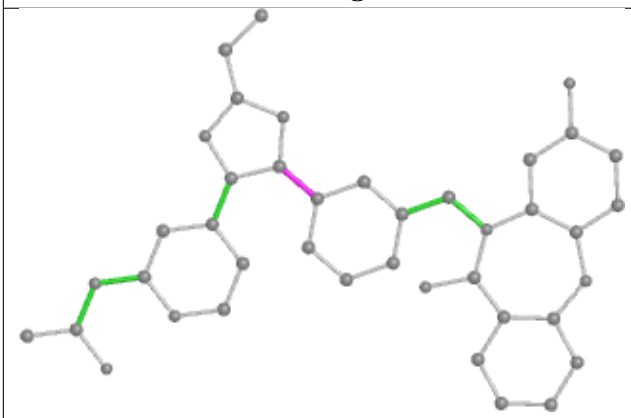
Ligand YA6 C 1101



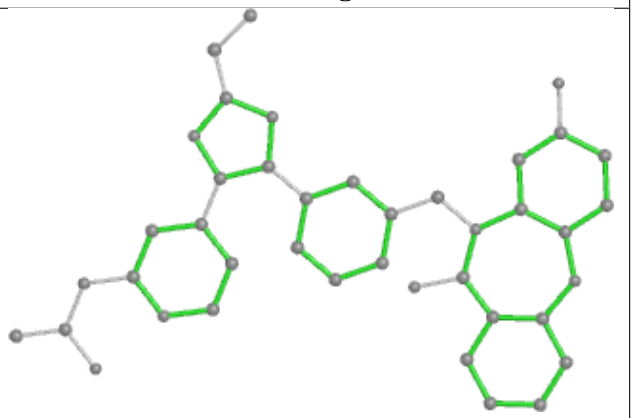
Bond lengths



Bond angles

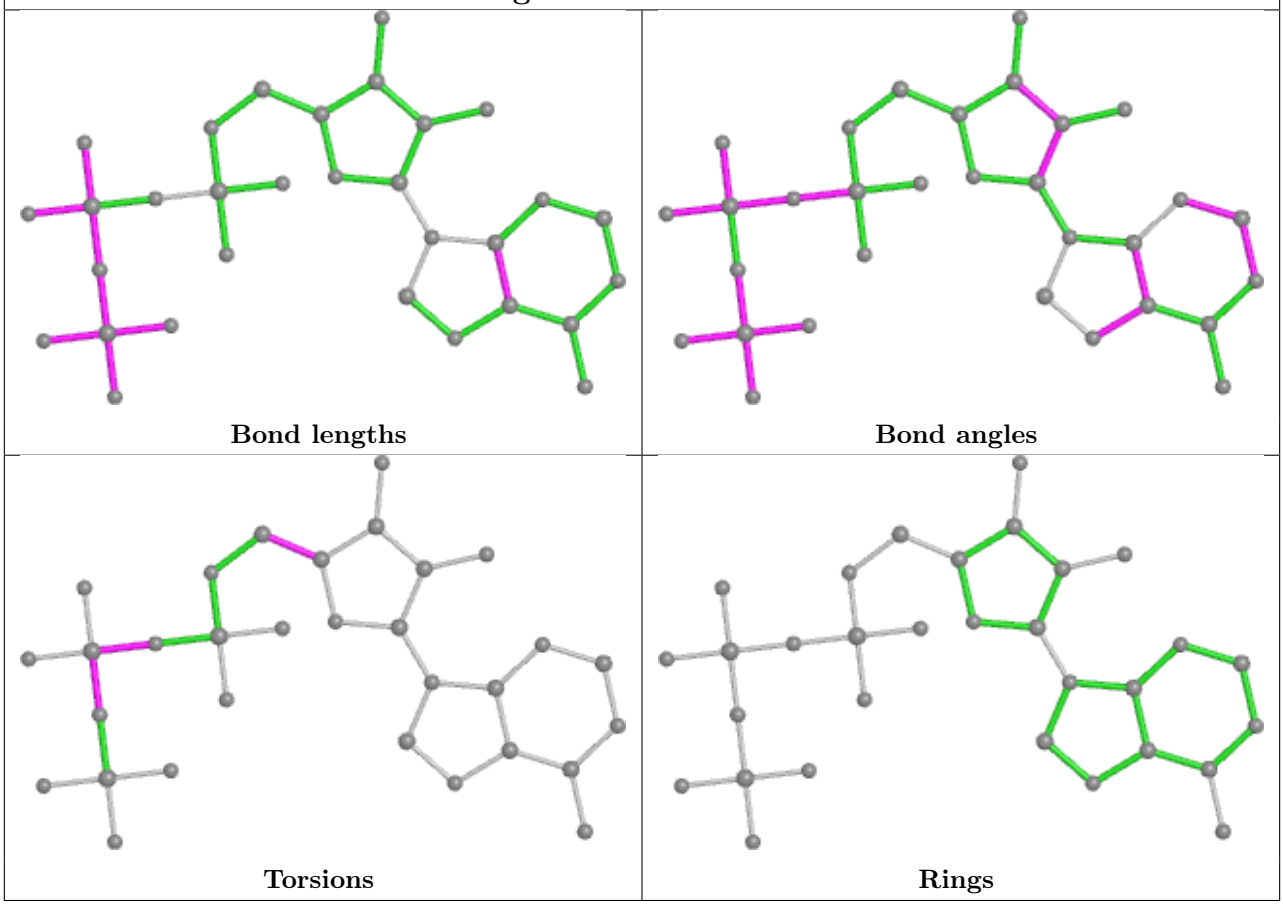


Torsions



Rings

Ligand ANP A 1102



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^{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	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	299/328 (91%)	0.08	8 (2%) 54 60	19, 37, 60, 78	0
1	B	307/328 (93%)	-0.01	5 (1%) 72 75	17, 30, 52, 79	0
1	C	291/328 (88%)	0.09	12 (4%) 37 43	22, 37, 63, 92	0
1	D	295/328 (89%)	0.08	6 (2%) 65 69	17, 32, 60, 82	0
All	All	1192/1312 (90%)	0.06	31 (2%) 56 61	17, 34, 60, 92	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	750	ALA	4.7
1	C	988	HIS	4.0
1	C	986	ARG	4.0
1	A	701	GLN	3.9
1	D	986	ARG	3.6
1	D	750	ALA	3.5
1	B	751	THR	3.2
1	A	1012	ASP	3.2
1	D	987	MET	3.1
1	A	1014	ASP	3.0
1	C	1007	MET	2.9
1	A	750	ALA	2.8
1	C	918	ILE	2.8
1	C	1006	ASP	2.6
1	C	701	GLN	2.6
1	C	807	ASP	2.6
1	B	723	PHE	2.4
1	C	808	ASN	2.3
1	C	985	GLU	2.3
1	C	722	ALA	2.2
1	D	1008	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	749	GLU	2.2
1	B	988	HIS	2.2
1	D	751	THR	2.2
1	A	807	ASP	2.1
1	A	1010	VAL	2.1
1	B	1013	ALA	2.1
1	A	808	ASN	2.1
1	C	989	LEU	2.1
1	C	785	THR	2.0
1	A	753	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

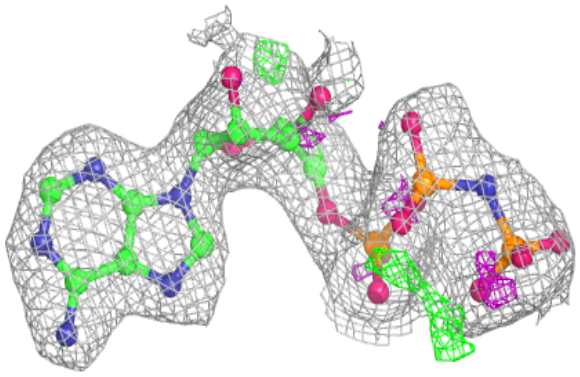
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

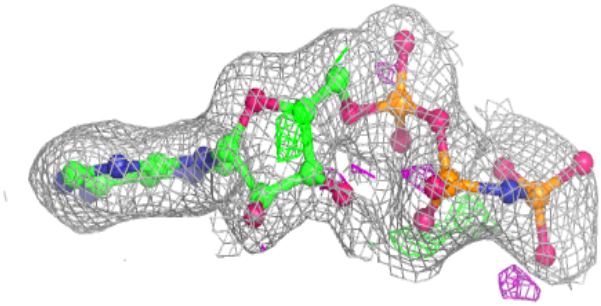
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	A	1101	1/1	0.73	0.12	35,35,35,35	0
2	MG	D	1101	1/1	0.86	0.06	33,33,33,33	0
2	MG	B	1101	1/1	0.90	0.07	32,32,32,32	0
3	ANP	A	1102	31/31	0.92	0.13	29,38,46,58	0
3	ANP	B	1102	31/31	0.93	0.13	32,40,49,53	0
4	YA6	C	1101	41/41	0.93	0.14	26,32,40,48	0
3	ANP	D	1102	31/31	0.95	0.12	24,33,40,41	0

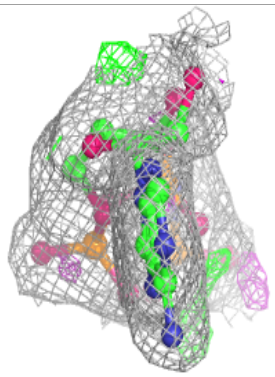
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP A 1102:

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

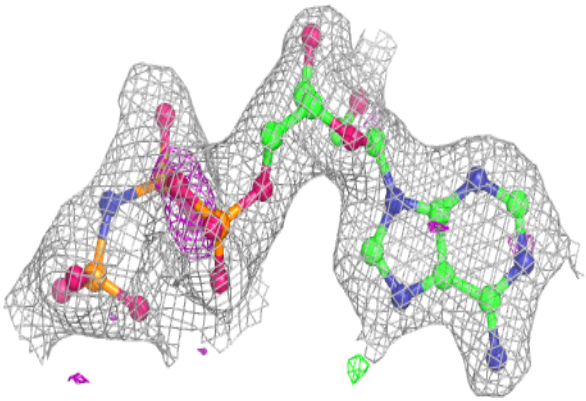


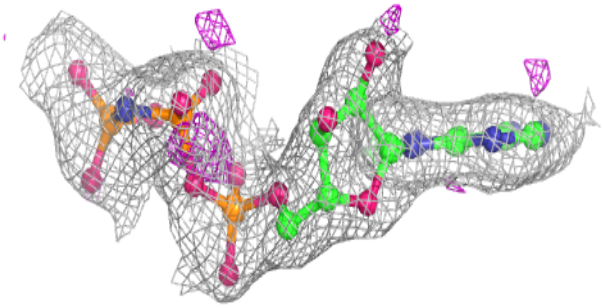


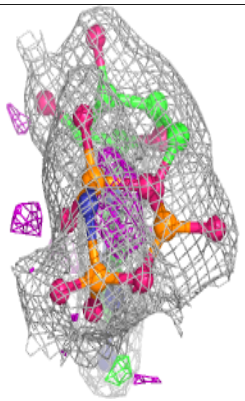


Electron density around ANP B 1102:

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

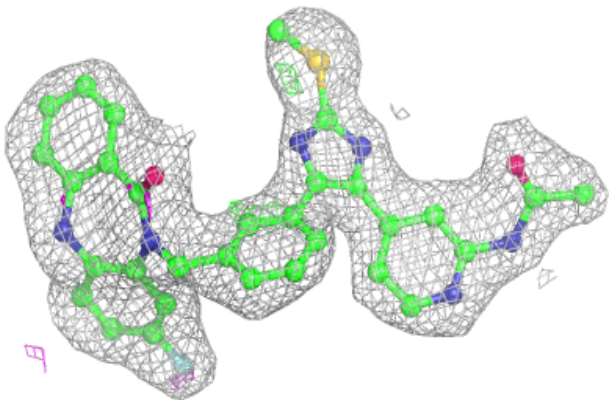


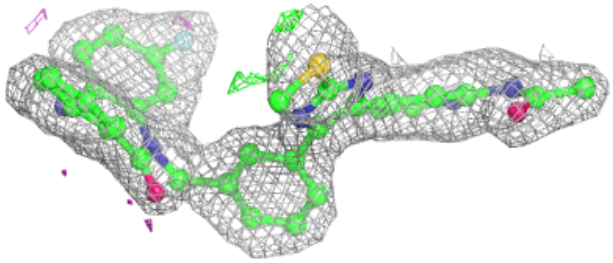


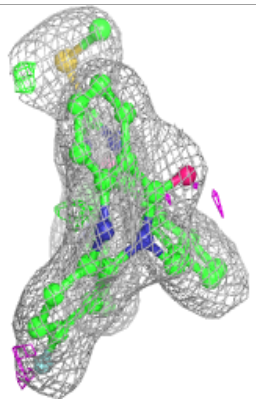


Electron density around YA6 C 1101:

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

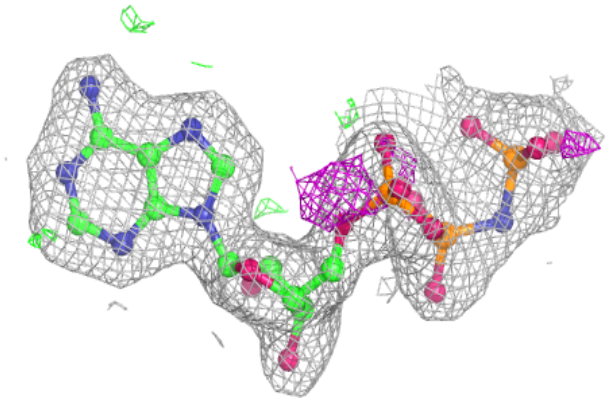


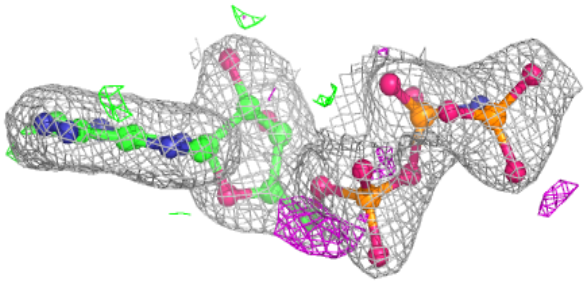


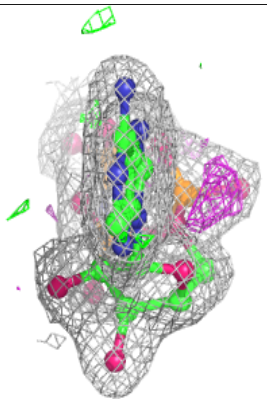


Electron density around ANP D 1102:

$2mF_o$-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.