Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 08:42 PM EDT

PDB ID	:	6P1D
Title	:	Crystal structure of EGFR with mutant-selective dihydrodibenzodiazepinone allosteric inhibitor
Authors	:	Heppner, D.E.; Eck, M.J.
Deposited on	:	2019-05-19
Resolution	:	2.40 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:

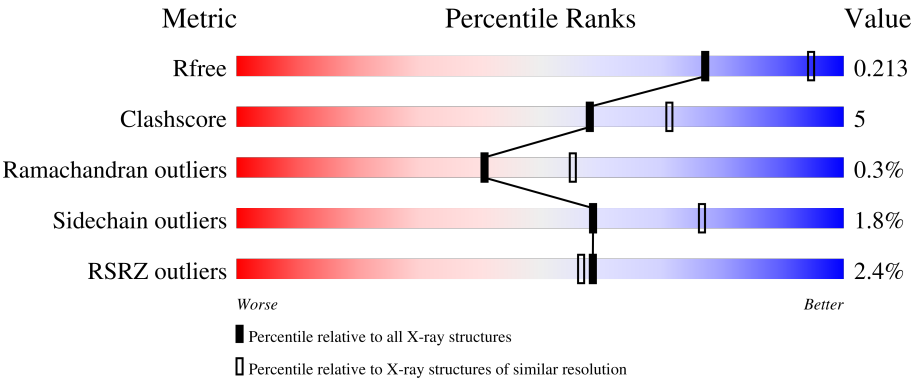
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	327	83% 11% 6%
1	B	327	2% 78% 13% 8%
1	C	327	78% 10% 11%
1	D	327	4% 76% 14% 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10222 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.

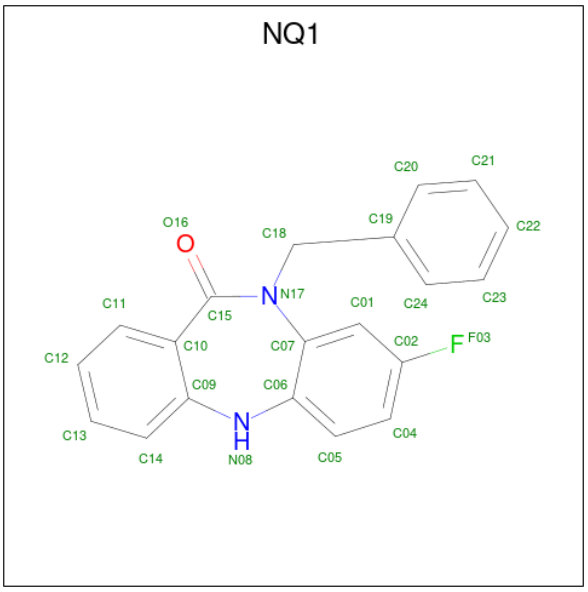
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	295	Total	C	N	O	S	0	0	0
			2380	1530	404	427	19			
1	A	309	Total	C	N	O	S	0	3	0
			2519	1616	428	455	20			
1	B	300	Total	C	N	O	S	0	2	0
			2427	1558	412	438	19			
1	C	292	Total	C	N	O	S	0	1	0
			2353	1515	399	421	18			

There are 8 discrepancies between the modelled and reference sequences:

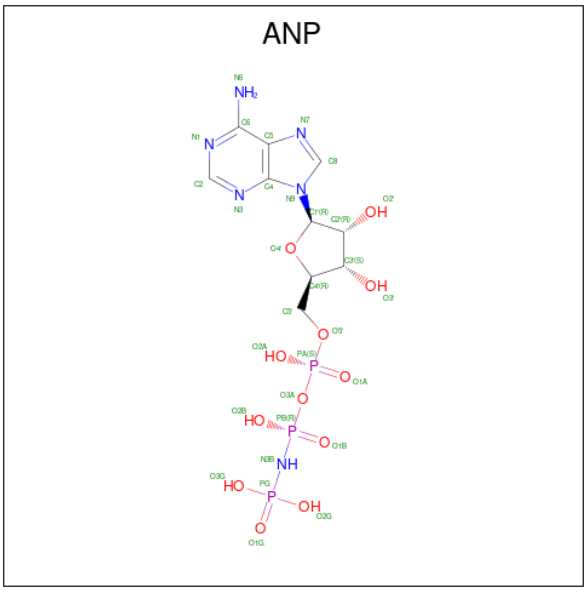
Chain	Residue	Modelled	Actual	Comment	Reference
D	790	MET	THR	conflict	UNP P00533
D	948	ARG	VAL	conflict	UNP P00533
A	790	MET	THR	conflict	UNP P00533
A	948	ARG	VAL	conflict	UNP P00533
B	790	MET	THR	conflict	UNP P00533
B	948	ARG	VAL	conflict	UNP P00533
C	790	MET	THR	conflict	UNP P00533
C	948	ARG	VAL	conflict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

- Molecule 2 is 10-benzyl-8-fluoro-5,10-dihydro-11H-dibenzo[b,e][1,4]diazepin-11-one (three-letter code: NQ1) (formula: $C_{20}H_{15}FN_2O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	F	N	O	0	0
			24	20	1	2	1		
2	B	1	Total	C	F	N	O	0	0
			24	20	1	2	1		
2	C	1	Total	C	F	N	O	0	0
			24	20	1	2	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		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

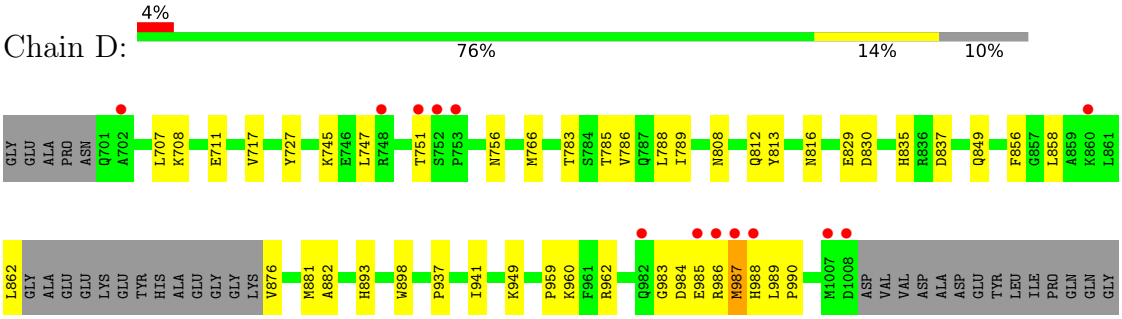
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	82	Total	O	0	0
			82	82		
5	A	108	Total	O	0	0
			108	108		
5	B	84	Total	O	0	0
			84	84		
5	C	69	Total	O	0	0
			69	69		

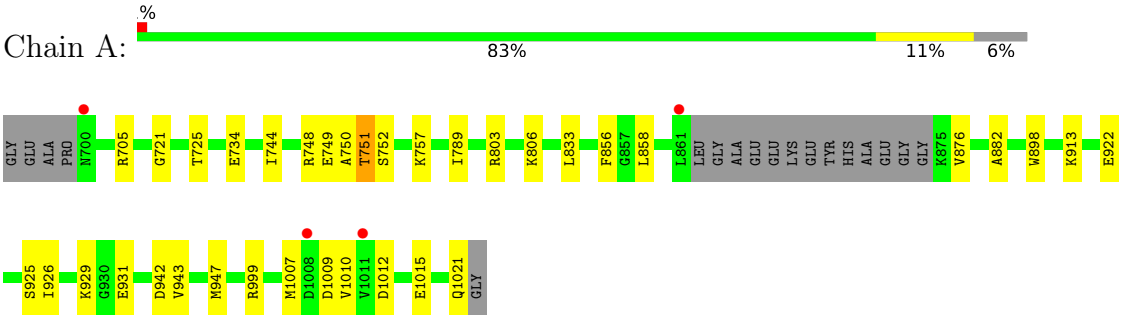
3 Residue-property plots (i)

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.

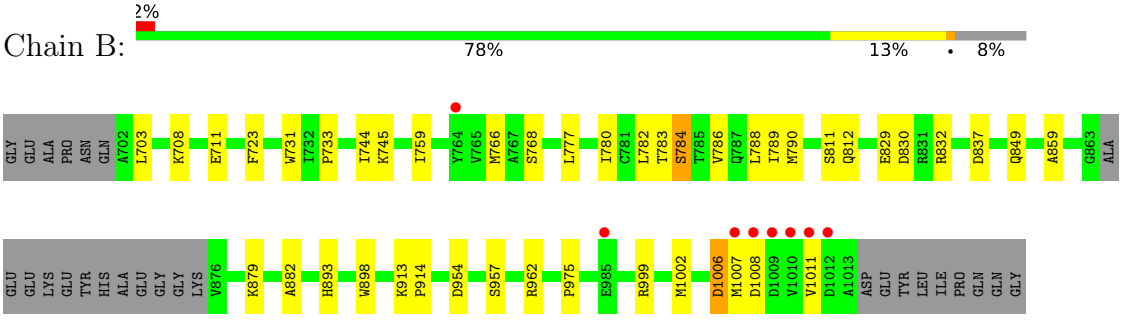
• Molecule 1: Epidermal growth factor receptor



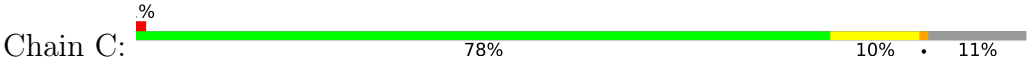
• Molecule 1: Epidermal growth factor receptor

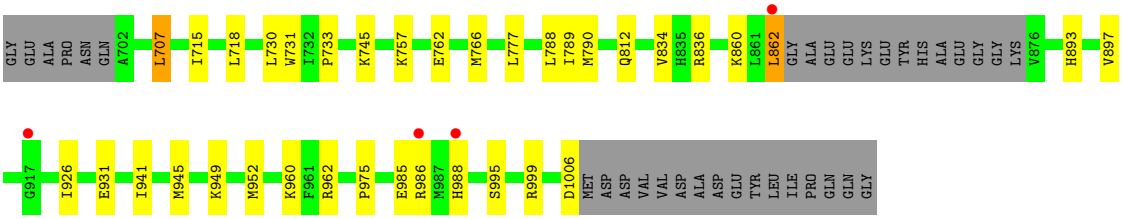


• Molecule 1: Epidermal growth factor receptor



• Molecule 1: Epidermal growth factor receptor




GLY GLU ALA PRO ASN GLN A702 L707 I715 L718 L730 W731 I732 P733 K745 K757 E762 M766 L777 L788 I789 M790 Q812 V834 H835 R836 K860 L861 L862 GLY ALA GLU GLU LYS GLU TYR HIS ALA GLU GLY GLY LYS V876 H893 V897
G917 I926 E931 I941 M945 K949 M952 K960 F961 R962 P975 E985 R986 M987 H988 S995 R999 D1006 MET ASP ASP 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	71.95Å 101.81Å 86.51Å 90.00° 101.04° 90.00°	Depositor
Resolution (Å)	65.17 – 2.40 65.21 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (65.17-2.40) 96.5 (65.21-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.195 , 0.213 0.195 , 0.213	Depositor DCC
R_{free} test set	2336 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10222	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 8.08% 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: NQ1, MG, ANP

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	0.30	0/2576	0.49	0/3482
1	B	0.28	0/2482	0.50	0/3356
1	C	0.25	0/2408	0.42	0/3258
1	D	0.31	0/2432	0.50	0/3288
All	All	0.28	0/9898	0.48	0/13384

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	2519	0	2566	18	0
1	B	2427	0	2474	27	0
1	C	2353	0	2400	25	0
1	D	2380	0	2430	30	0
2	B	24	0	0	3	0
2	C	24	0	0	2	0
2	D	24	0	0	4	0
3	A	31	0	13	0	0
3	B	31	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	31	0	13	0	0
3	D	31	0	13	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	108	0	0	2	0
5	B	84	0	0	2	0
5	C	69	0	0	3	0
5	D	82	0	0	4	0
All	All	10222	0	9922	95	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 (95) 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:A:749:GLU:HB2	1:B:832:ARG:HG3	1.70	0.71
1:D:962:ARG:NH2	1:C:718:LEU:O	2.27	0.67
1:B:766:MET:HG3	2:B:1102:NQ1:C14	2.25	0.65
1:D:812:GLN:NE2	1:D:816:ASN:OD1	2.32	0.63
1:D:941:ILE:HD11	1:A:922:GLU:HG2	1.81	0.62
1:A:806:LYS:HE2	5:A:1258:HOH:O	2.02	0.59
1:A:926:ILE:HG23	1:A:931:GLU:HB2	1.84	0.59
1:A:1012:ASP:HB2	1:A:1015:GLU:HG3	1.84	0.59
1:B:812:GLN:HG2	1:B:975:PRO:HG3	1.85	0.59
1:A:748:ARG:NH1	1:A:750:ALA:HA	2.16	0.59
1:C:707:LEU:HD13	1:C:789:ILE:HD13	1.86	0.58
1:D:989:LEU:HG	1:D:990:PRO:HD2	1.86	0.57
1:B:777:LEU:HD11	1:B:788:LEU:HB3	1.86	0.57
1:D:766:MET:HG3	2:D:1101:NQ1:C14	2.35	0.57
1:C:834:VAL:HG12	1:C:836:ARG:HG3	1.87	0.56
1:D:830:ASP:CB	5:D:1202:HOH:O	2.53	0.56
1:B:708:LYS:O	1:B:711:GLU:HG2	2.05	0.56
1:B:837:ASP:OD2	3:B:1101:ANP:O2G	2.26	0.53
1:A:913:LYS:HB3	5:A:1222:HOH:O	2.08	0.53
1:B:849:GLN:NE2	5:B:1209:HOH:O	2.41	0.53
1:C:731:TRP:CZ3	1:C:733:PRO:HG3	2.44	0.52
1:A:925:SER:O	1:A:929:LYS:HG2	2.10	0.52
1:A:803:ARG:O	1:A:806:LYS:HE3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:913:LYS:HB3	5:B:1269:HOH:O	2.11	0.49
1:D:813:TYR:OH	1:D:990:PRO:HD3	2.12	0.49
1:D:751:THR:OG1	1:D:756:ASN:OD1	2.28	0.49
1:D:876:VAL:HG13	1:D:881:MET:SD	2.54	0.48
1:D:708:LYS:O	1:D:711:GLU:HG2	2.13	0.48
1:D:788:LEU:HD13	2:D:1101:NQ1:C11	2.43	0.48
1:C:745:LYS:HB2	2:C:1101:NQ1:C23	2.44	0.48
1:D:830:ASP:HB3	5:D:1202:HOH:O	2.13	0.48
1:D:837:ASP:OD2	3:D:1102:ANP:O2G	2.32	0.47
1:C:949:LYS:O	1:C:952:MET:HG2	2.14	0.47
1:D:813:TYR:HE2	1:D:988:HIS:O	1.96	0.47
1:A:833:LEU:HB3	1:A:856:PHE:CE1	2.48	0.47
1:B:780:ILE:HD11	1:B:782:LEU:HD21	1.95	0.47
1:D:788:LEU:C	1:D:789:ILE:HD12	2.35	0.47
1:C:941:ILE:O	1:C:945:MET:HG2	2.15	0.47
1:D:747:LEU:HD12	1:D:786:VAL:HB	1.95	0.47
1:C:715:ILE:HG13	1:C:730:LEU:HG	1.97	0.47
1:B:703:LEU:HD13	1:B:768:SER:HA	1.97	0.46
1:C:926:ILE:HG23	1:C:931:GLU:HB3	1.96	0.46
1:C:995:SER:O	1:C:999:ARG:HG3	2.15	0.46
1:D:983:GLY:O	1:D:986:ARG:HG2	2.15	0.46
1:C:960:LYS:HA	5:C:1221:HOH:O	2.16	0.46
1:D:835:HIS:CD2	1:D:856:PHE:HB3	2.51	0.46
1:C:757:LYS:HA	1:C:757:LYS:HD3	1.73	0.46
1:C:986:ARG:NE	1:C:986:ARG:HA	2.31	0.46
1:D:783:THR:OG1	1:D:785:THR:O	2.32	0.46
1:A:943:VAL:HG12	1:A:947:MET:HE2	1.97	0.46
1:D:849:GLN:NE2	1:D:990:PRO:HG3	2.31	0.46
1:D:937:PRO:HD2	5:D:1245:HOH:O	2.15	0.45
1:D:949:LYS:HG2	1:D:959:PRO:HD3	1.98	0.45
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.51	0.45
1:B:744:ILE:HG12	1:B:789:ILE:CD1	2.47	0.45
1:D:717:VAL:HG22	1:D:727:TYR:CE2	2.53	0.44
1:C:999:ARG:HD2	1:C:1006:ASP:C	2.37	0.44
1:B:1006:ASP:O	1:B:1008:ASP:N	2.50	0.44
1:C:777:LEU:HD11	1:C:788:LEU:HB3	1.98	0.44
1:C:985:GLU:HB2	5:C:1244:HOH:O	2.17	0.44
1:D:882:ALA:HA	1:D:898:TRP:CD2	2.52	0.44
1:A:751:THR:HG23	1:A:752:SER:H	1.82	0.44
1:B:811:SER:OG	1:B:975:PRO:HB2	2.17	0.44
1:B:744:ILE:HG12	1:B:789:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:GLY:O	1:B:962:ARG:NH1	2.52	0.43
1:D:829:GLU:HA	1:D:893:HIS:CE1	2.54	0.43
1:B:829:GLU:HA	1:B:893:HIS:CE1	2.53	0.43
1:A:744:ILE:HG12	1:A:789:ILE:HD12	2.00	0.43
1:C:962:ARG:HG3	5:C:1236:HOH:O	2.19	0.43
1:B:759:ILE:HD13	1:B:786:VAL:HG21	2.01	0.43
1:C:862:LEU:HD13	1:C:862:LEU:HA	1.92	0.43
1:A:999:ARG:NH1	1:A:1007:MET:HG2	2.34	0.42
1:B:882:ALA:HA	1:B:898:TRP:CD2	2.53	0.42
1:C:812:GLN:NE2	1:C:975:PRO:HG3	2.34	0.42
1:C:762:GLU:O	1:C:766:MET:HG2	2.18	0.42
1:D:984:ASP:HA	1:D:987:MET:HG3	2.02	0.42
1:B:783:THR:OG1	1:B:784:SER:N	2.52	0.42
1:B:731:TRP:CH2	1:B:733:PRO:HG3	2.55	0.42
1:B:745:LYS:HB2	2:B:1102:NQ1:C23	2.50	0.42
1:C:893:HIS:O	1:C:897:VAL:HG23	2.19	0.42
1:B:879:LYS:HD3	1:B:914:PRO:O	2.19	0.42
1:C:790:MET:HG2	2:C:1101:NQ1:C22	2.50	0.41
1:B:954:ASP:OD2	1:B:957:SER:HB2	2.19	0.41
1:A:858:LEU:HD23	1:A:858:LEU:HA	1.82	0.41
1:C:945:MET:O	1:C:949:LYS:HG2	2.19	0.41
1:D:745:LYS:HD3	2:D:1101:NQ1:O16	2.20	0.41
1:B:999:ARG:HD2	1:B:1006:ASP:HA	2.02	0.41
1:C:788:LEU:C	1:C:789:ILE:HD12	2.41	0.41
1:D:960:LYS:HE2	5:D:1228:HOH:O	2.20	0.41
1:B:723:PHE:CE1	1:B:859:ALA:HA	2.55	0.41
1:C:960:LYS:HE3	1:C:960:LYS:HB3	1.91	0.41
1:D:858:LEU:HD13	2:D:1101:NQ1:C11	2.51	0.41
1:D:987:MET:H	1:D:987:MET:HG2	1.65	0.41
1:A:725:THR:OG1	1:B:830:ASP:OD2	2.25	0.40
1:B:790:MET:HG2	2:B:1102:NQ1:C22	2.52	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	308/327 (94%)	301 (98%)	7 (2%)	0	100 100
1	B	298/327 (91%)	286 (96%)	9 (3%)	3 (1%)	15 23
1	C	289/327 (88%)	286 (99%)	3 (1%)	0	100 100
1	D	291/327 (89%)	285 (98%)	5 (2%)	1 (0%)	41 55
All	All	1186/1308 (91%)	1158 (98%)	24 (2%)	4 (0%)	41 55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	784	SER
1	B	1007	MET
1	B	1006	ASP
1	D	808	ASN

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	280/287 (98%)	271 (97%)	9 (3%)	39 59
1	B	269/287 (94%)	267 (99%)	2 (1%)	84 92
1	C	260/287 (91%)	256 (98%)	4 (2%)	65 80
1	D	264/287 (92%)	260 (98%)	4 (2%)	65 80
All	All	1073/1148 (94%)	1054 (98%)	19 (2%)	59 76

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	707	LEU
1	D	862	LEU
1	D	985	GLU
1	D	987	MET

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Mol	Chain	Res	Type
1	A	705	ARG
1	A	734	GLU
1	A	751	THR
1	A	757	LYS
1	A	876	VAL
1	A	942	ASP
1	A	1009	ASP
1	A	1010	VAL
1	A	1021	GLN
1	B	1002	MET
1	B	1011	VAL
1	C	707	LEU
1	C	860	LYS
1	C	862	LEU
1	C	988	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	849	GLN
1	B	849	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 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	C	1102	4	29,33,33	1.09	4 (13%)	31,52,52	1.03	3 (9%)
3	ANP	A	1101	4	29,33,33	1.10	4 (13%)	31,52,52	0.99	3 (9%)
2	NQ1	D	1101	-	27,27,27	2.51	7 (25%)	37,38,38	1.36	5 (13%)
2	NQ1	C	1101	-	27,27,27	2.52	8 (29%)	37,38,38	1.43	6 (16%)
2	NQ1	B	1102	-	27,27,27	2.50	8 (29%)	37,38,38	1.59	7 (18%)
3	ANP	B	1101	4	29,33,33	1.09	4 (13%)	31,52,52	0.94	3 (9%)
3	ANP	D	1102	4	29,33,33	1.08	4 (13%)	31,52,52	0.95	2 (6%)

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	C	1102	4	-	5/14/38/38	0/3/3/3
3	ANP	A	1101	4	-	4/14/38/38	0/3/3/3
2	NQ1	D	1101	-	-	2/4/4/4	0/4/4/4
2	NQ1	C	1101	-	-	2/4/4/4	0/4/4/4
2	NQ1	B	1102	-	-	1/4/4/4	0/4/4/4
3	ANP	B	1101	4	-	4/14/38/38	0/3/3/3
3	ANP	D	1102	4	-	4/14/38/38	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	NQ1	C15-N17	6.71	1.45	1.37
2	C	1101	NQ1	C15-N17	6.69	1.45	1.37
2	B	1102	NQ1	C15-N17	6.56	1.45	1.37
2	B	1102	NQ1	C06-N08	5.47	1.48	1.41
2	B	1102	NQ1	C09-N08	5.31	1.48	1.41
2	C	1101	NQ1	C09-N08	5.15	1.47	1.41
2	C	1101	NQ1	C06-N08	5.13	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	NQ1	C06-N08	5.10	1.47	1.41
2	D	1101	NQ1	C09-N08	5.08	1.47	1.41
2	C	1101	NQ1	C07-N17	4.86	1.48	1.43
2	D	1101	NQ1	C07-N17	4.80	1.47	1.43
2	B	1102	NQ1	C07-N17	4.21	1.47	1.43
2	D	1101	NQ1	C10-C15	3.46	1.55	1.50
2	C	1101	NQ1	C10-C15	3.44	1.55	1.50
2	B	1102	NQ1	C06-C07	-3.15	1.37	1.40
2	B	1102	NQ1	C10-C15	3.14	1.55	1.50
2	C	1101	NQ1	C06-C07	-3.00	1.37	1.40
2	D	1101	NQ1	C06-C07	-3.00	1.37	1.40
3	A	1101	ANP	PG-N3B	2.68	1.70	1.63
2	D	1101	NQ1	C10-C09	-2.60	1.37	1.41
2	B	1102	NQ1	C10-C09	-2.59	1.37	1.41
3	D	1102	ANP	PG-N3B	2.58	1.70	1.63
3	B	1101	ANP	PG-N3B	2.57	1.70	1.63
3	C	1102	ANP	PG-N3B	2.56	1.70	1.63
2	C	1101	NQ1	C10-C09	-2.47	1.37	1.41
3	B	1101	ANP	PG-O1G	2.46	1.50	1.46
3	D	1102	ANP	PG-O1G	2.46	1.50	1.46
3	C	1102	ANP	PG-O1G	2.42	1.50	1.46
3	A	1101	ANP	PG-O1G	2.39	1.49	1.46
3	C	1102	ANP	PB-O1B	2.34	1.49	1.46
3	B	1101	ANP	PB-O3A	-2.22	1.56	1.59
3	A	1101	ANP	PB-O1B	2.21	1.49	1.46
3	D	1102	ANP	PB-O1B	2.21	1.49	1.46
3	B	1101	ANP	PB-O1B	2.18	1.49	1.46
3	A	1101	ANP	PB-O3A	-2.15	1.56	1.59
3	D	1102	ANP	PB-O3A	-2.13	1.56	1.59
3	C	1102	ANP	PB-O3A	-2.12	1.56	1.59
2	B	1102	NQ1	O16-C15	-2.11	1.18	1.22
2	C	1101	NQ1	C04-C02	2.01	1.41	1.37

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1101	NQ1	C07-N17-C15	4.21	129.45	124.96
2	D	1101	NQ1	C07-N17-C15	4.01	129.24	124.96
2	B	1102	NQ1	C07-N17-C15	4.00	129.23	124.96
2	B	1102	NQ1	C19-C18-N17	3.98	120.11	113.39
2	B	1102	NQ1	C18-N17-C07	-3.76	114.31	118.28
2	D	1101	NQ1	C18-N17-C07	-3.36	114.73	118.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1101	NQ1	C18-N17-C07	-2.88	115.23	118.28
3	A	1101	ANP	PB-O3A-PA	-2.88	122.48	132.62
2	C	1101	NQ1	C19-C18-N17	2.72	117.98	113.39
3	B	1101	ANP	PB-O3A-PA	-2.71	123.06	132.62
3	D	1102	ANP	PB-O3A-PA	-2.61	123.41	132.62
3	C	1102	ANP	O1G-PG-N3B	-2.50	108.09	111.77
2	C	1101	NQ1	C05-C06-C07	2.43	121.89	118.83
3	D	1102	ANP	C5-C6-N6	2.35	123.92	120.35
2	B	1102	NQ1	C04-C02-C01	-2.34	120.25	123.29
2	B	1102	NQ1	C10-C15-N17	2.32	123.11	119.63
3	C	1102	ANP	PB-O3A-PA	-2.32	124.45	132.62
3	C	1102	ANP	C5-C6-N6	2.31	123.86	120.35
3	A	1101	ANP	C5-C6-N6	2.30	123.85	120.35
2	B	1102	NQ1	C05-C04-C02	2.28	120.72	118.36
2	D	1101	NQ1	C05-C06-C07	2.25	121.67	118.83
3	B	1101	ANP	C5-C6-N6	2.22	123.73	120.35
2	C	1101	NQ1	O16-C15-N17	-2.20	118.77	121.01
2	D	1101	NQ1	C04-C02-C01	-2.17	120.47	123.29
2	B	1102	NQ1	C18-C19-C24	-2.15	116.72	120.77
3	A	1101	ANP	O2G-PG-O1G	-2.05	108.30	113.45
2	D	1101	NQ1	C05-C04-C02	2.05	120.48	118.36
2	C	1101	NQ1	C04-C02-C01	-2.02	120.66	123.29
3	B	1101	ANP	O3G-PG-O1G	-2.01	108.39	113.45

There are no chirality outliers.

All (22) 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	1101	ANP	PG-N3B-PB-O1B
3	A	1101	ANP	PA-O3A-PB-O1B
3	A	1101	ANP	PA-O3A-PB-O2B
3	B	1101	ANP	PG-N3B-PB-O1B
3	B	1101	ANP	PA-O3A-PB-O1B
3	B	1101	ANP	PA-O3A-PB-O2B
3	C	1102	ANP	PB-N3B-PG-O1G
3	C	1102	ANP	PG-N3B-PB-O1B
3	C	1102	ANP	PG-N3B-PB-O3A
3	C	1102	ANP	PA-O3A-PB-O1B
3	C	1102	ANP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
3	D	1102	ANP	PG-N3B-PB-O3A
3	A	1101	ANP	PG-N3B-PB-O3A
3	B	1101	ANP	PG-N3B-PB-O3A
2	C	1101	NQ1	N17-C18-C19-C20
2	D	1101	NQ1	N17-C18-C19-C24
2	C	1101	NQ1	N17-C18-C19-C24
2	D	1101	NQ1	N17-C18-C19-C20
2	B	1102	NQ1	N17-C18-C19-C20

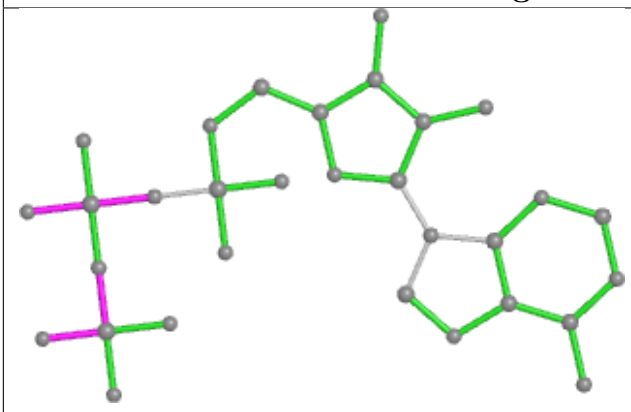
There are no ring outliers.

5 monomers are involved in 11 short contacts:

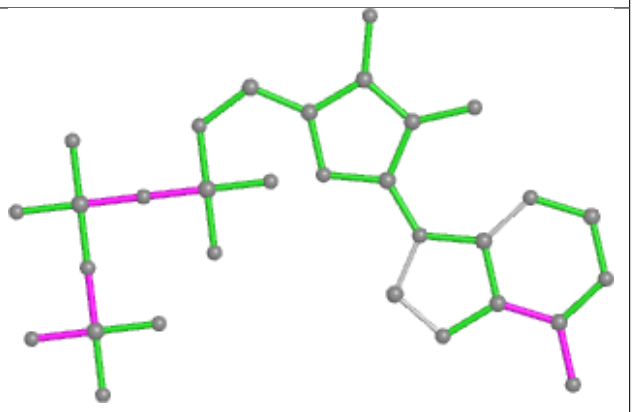
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1101	NQ1	4	0
2	C	1101	NQ1	2	0
2	B	1102	NQ1	3	0
3	B	1101	ANP	1	0
3	D	1102	ANP	1	0

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 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.

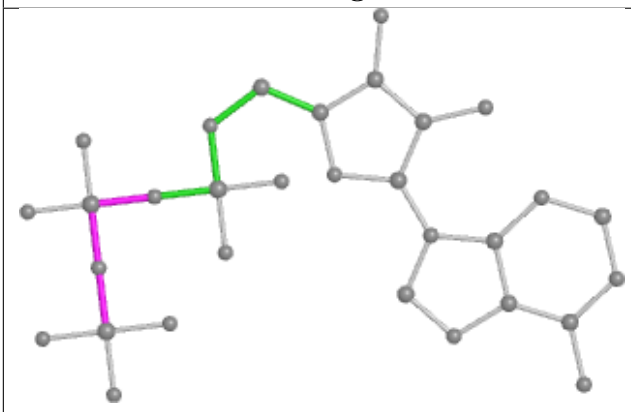
Ligand ANP C 1102



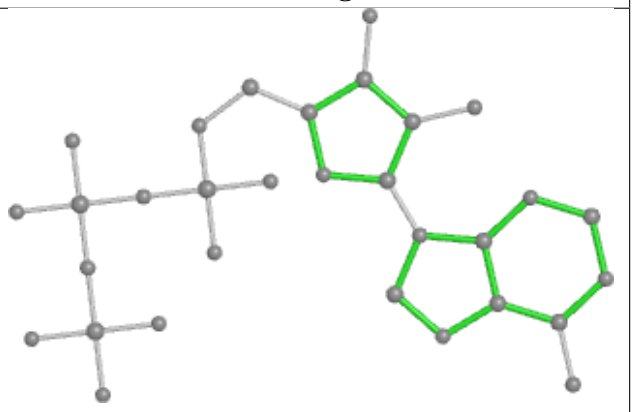
Bond lengths



Bond angles

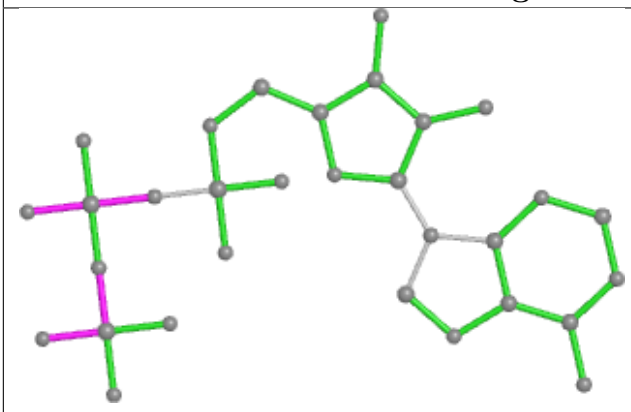


Torsions



Rings

Ligand ANP A 1101



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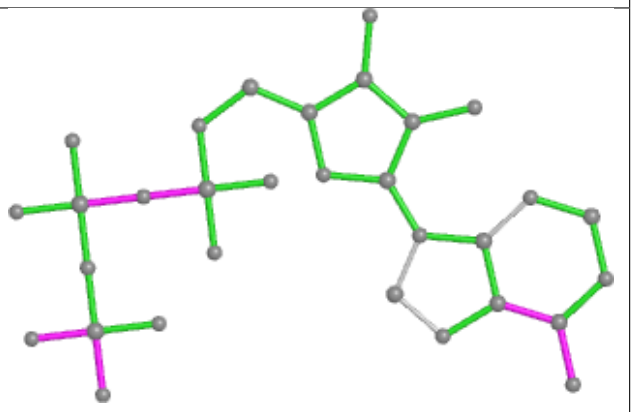

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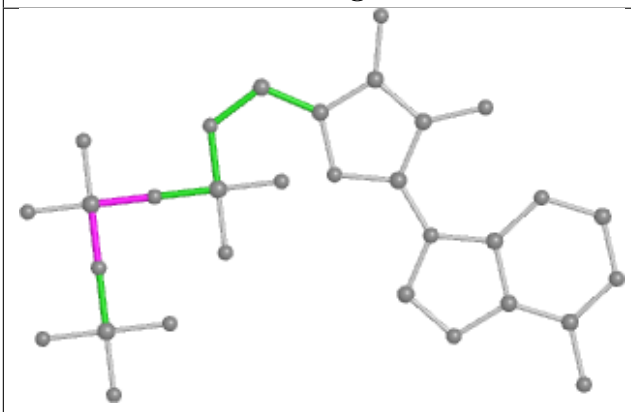

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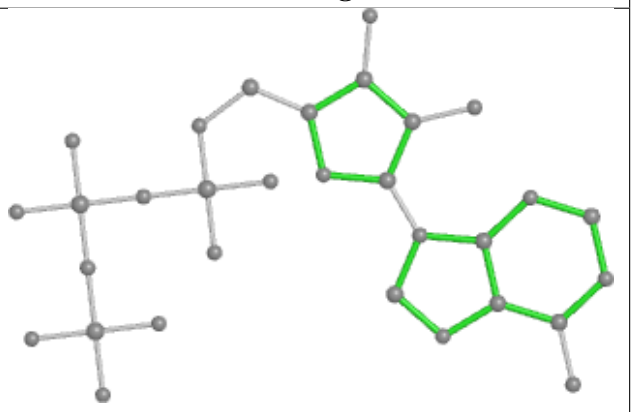
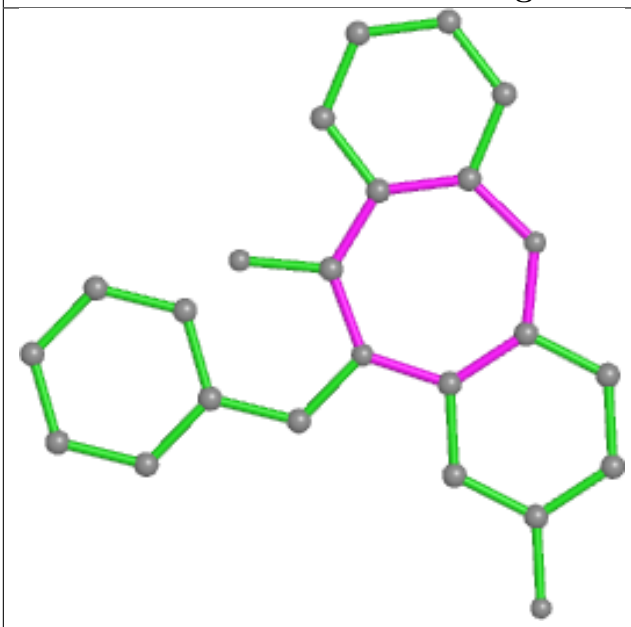


Rings

Ligand NQ1 D 1101



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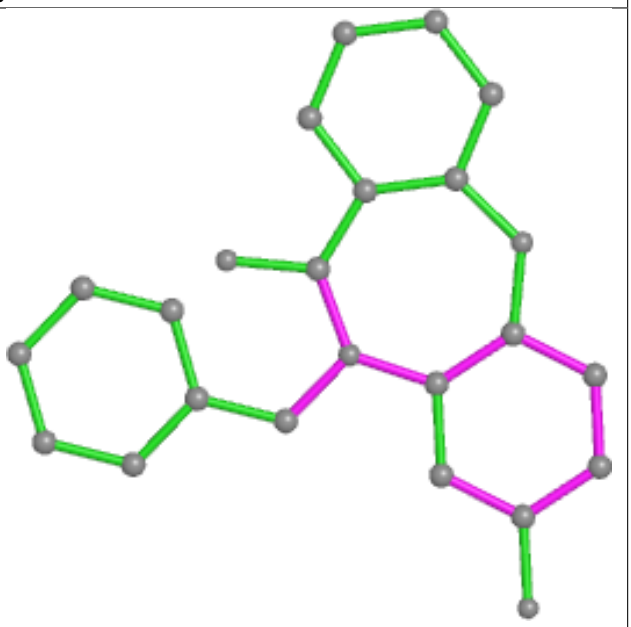

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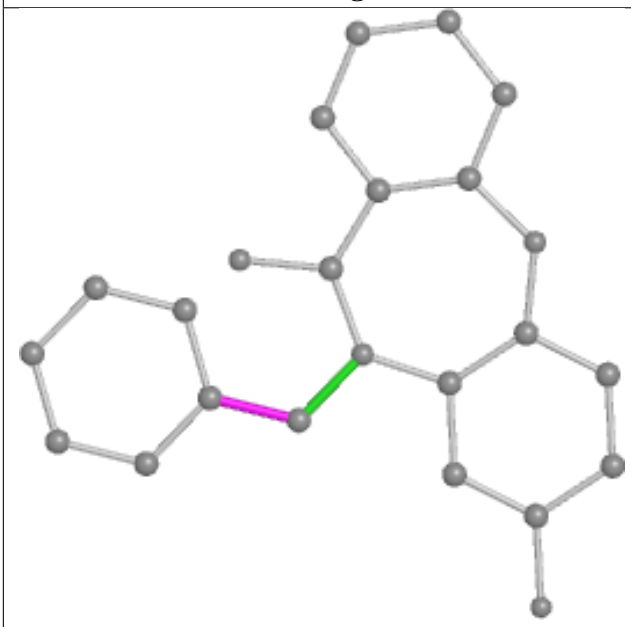

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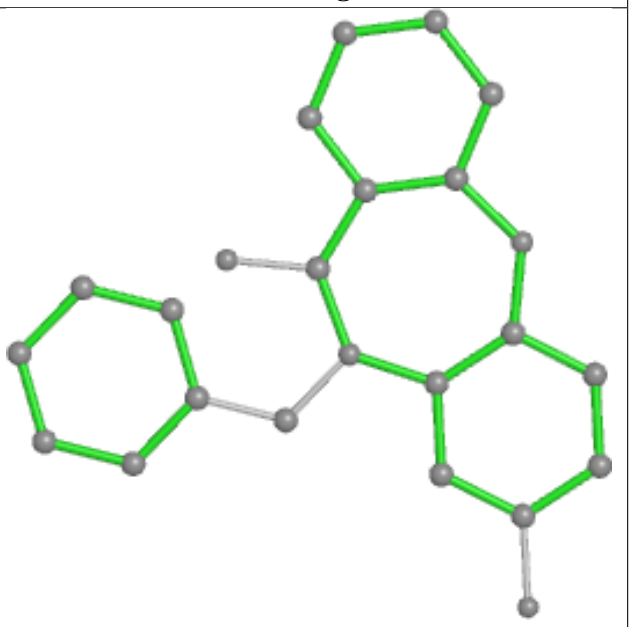
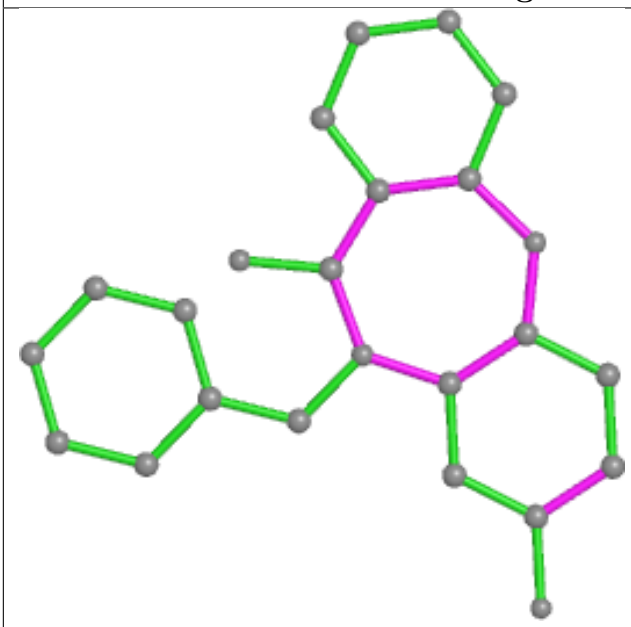


Rings

Ligand NQ1 C 1101



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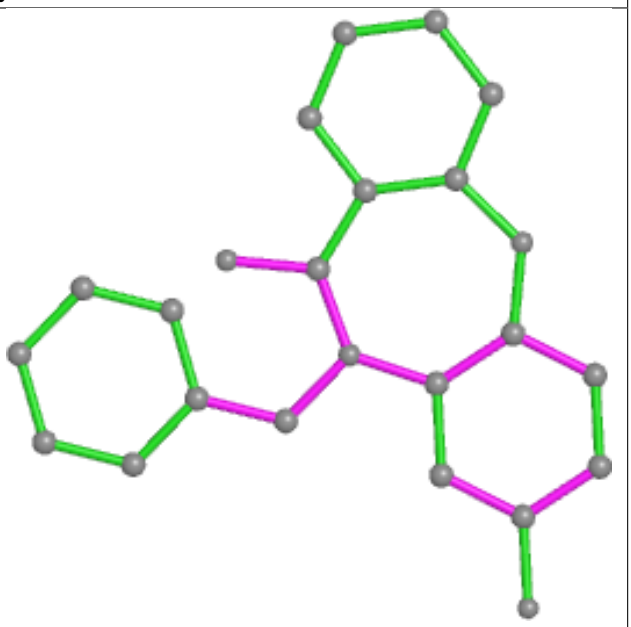
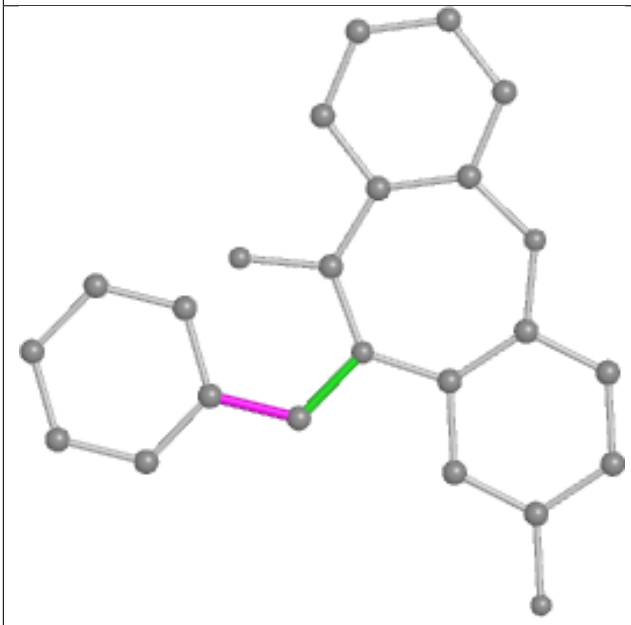


Bond angles



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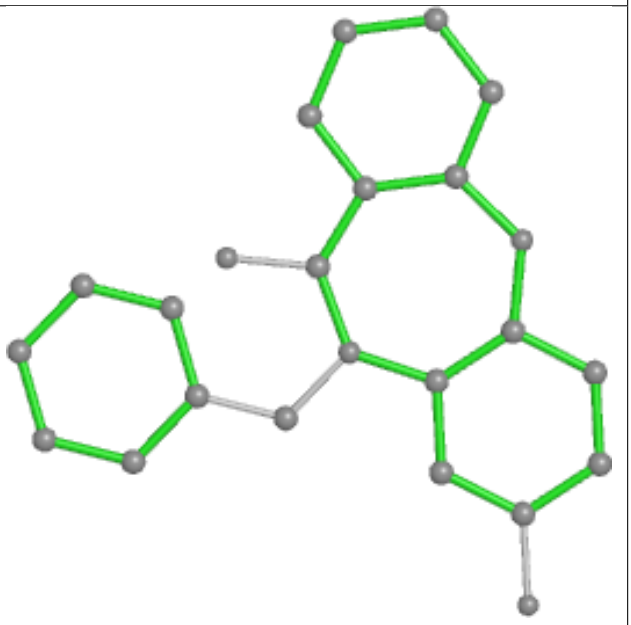
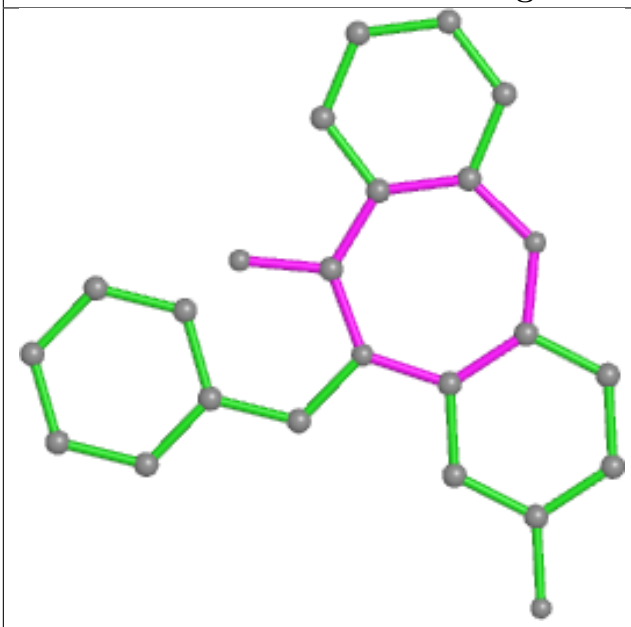
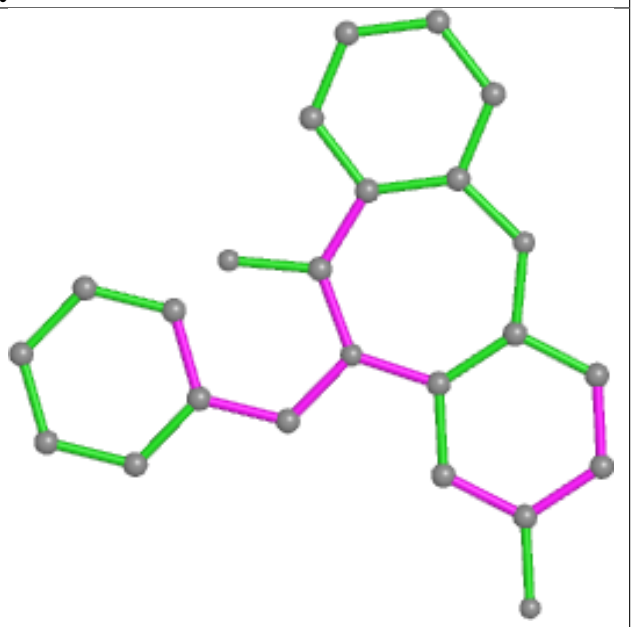


Rings

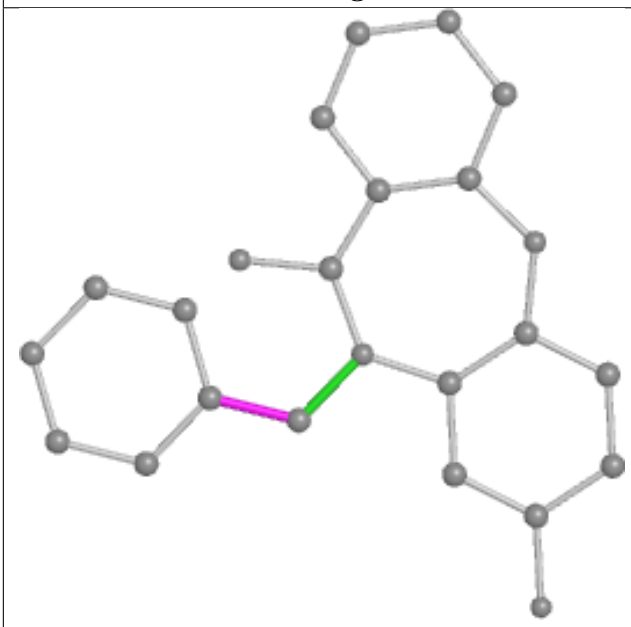
Ligand NQ1 B 1102



Bond lengths



Bond angles



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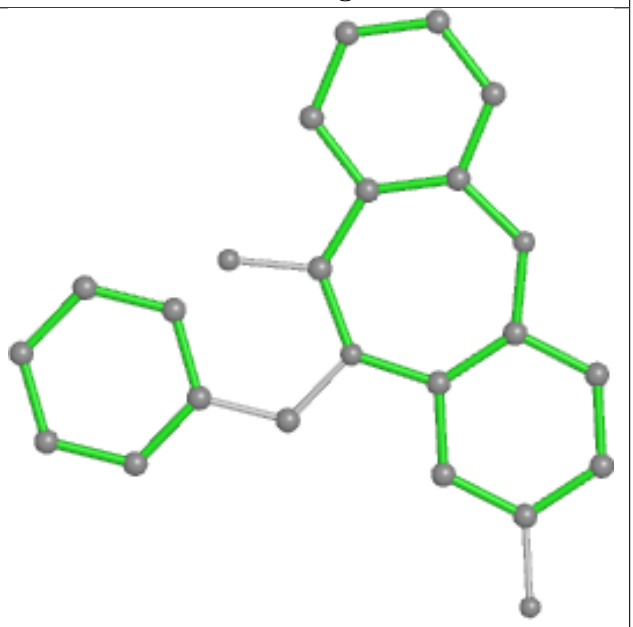
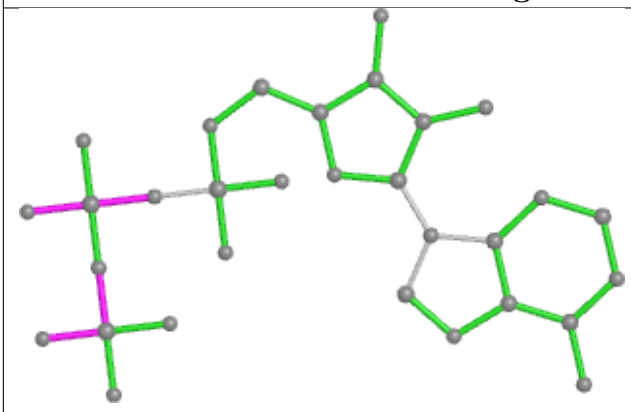
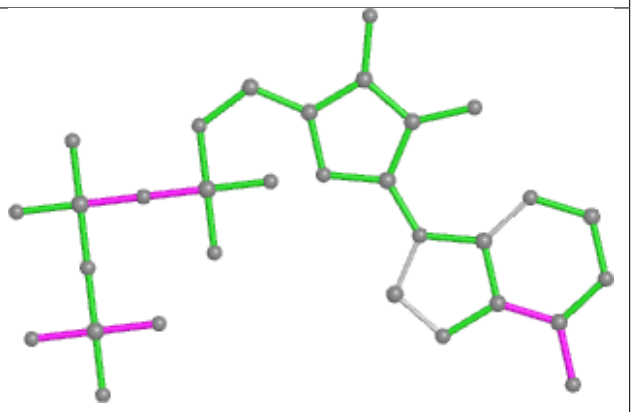


Rings

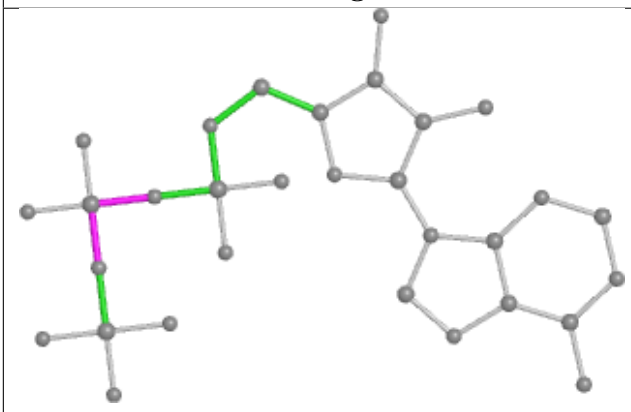
Ligand ANP B 1101



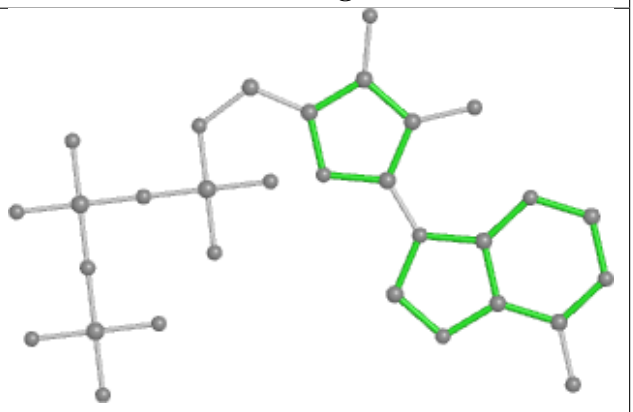
Bond lengths



Bond angles

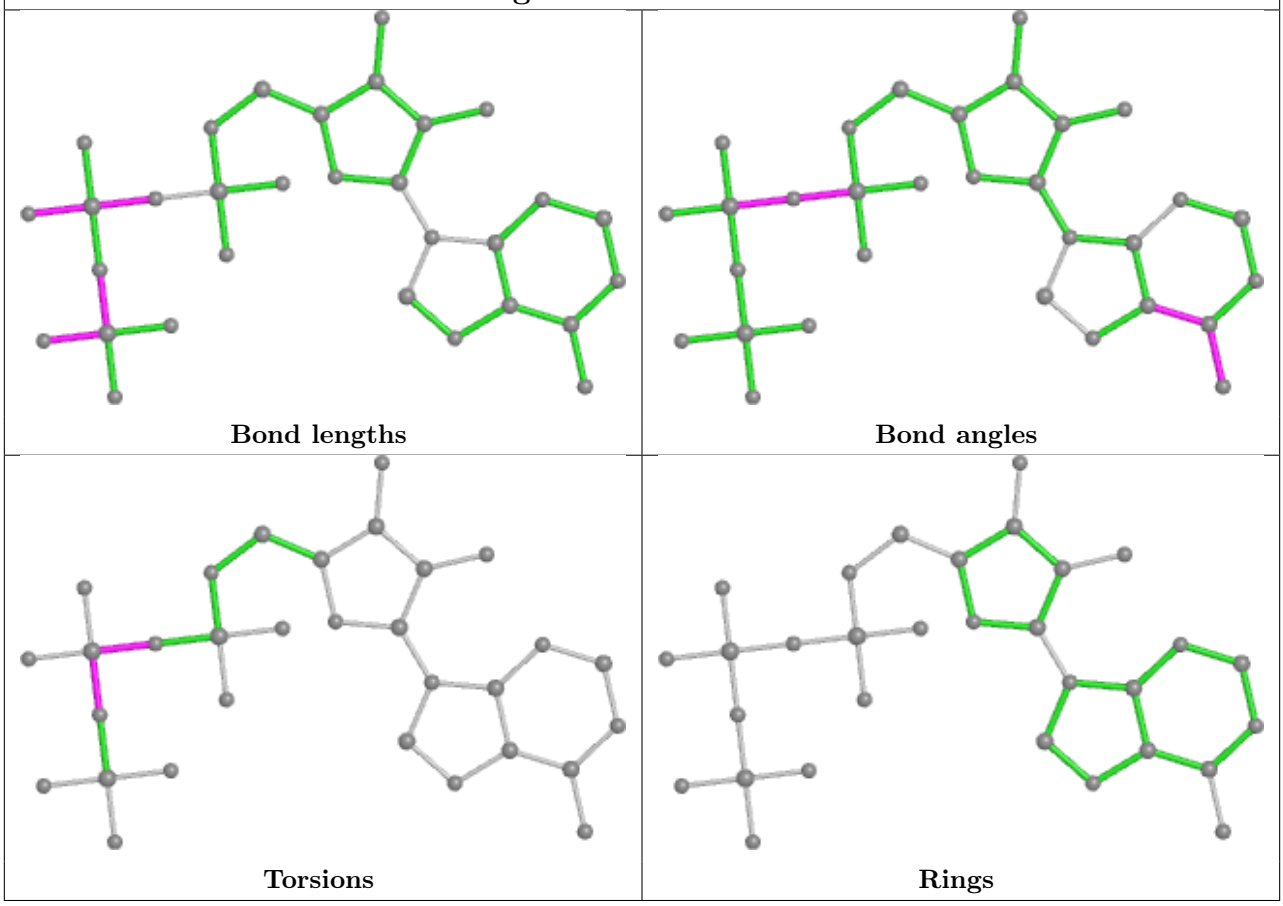


Torsions



Rings

Ligand ANP D 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	309/327 (94%)	-0.09	4 (1%)	77	75	20, 30, 53, 85	0
1	B	300/327 (91%)	-0.03	8 (2%)	54	52	18, 34, 54, 124	0
1	C	292/327 (89%)	-0.02	4 (1%)	75	73	20, 35, 56, 80	0
1	D	295/327 (90%)	-0.01	13 (4%)	34	33	19, 33, 63, 88	0
All	All	1196/1308 (91%)	-0.04	29 (2%)	59	57	18, 33, 57, 124	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1009	ASP	8.5
1	B	1010	VAL	6.2
1	A	1008	ASP	5.3
1	B	1008	ASP	5.2
1	B	1007	MET	5.0
1	A	1011	VAL	4.8
1	A	861	LEU	4.2
1	C	986	ARG	3.6
1	C	917	GLY	3.5
1	C	988	HIS	3.3
1	D	988	HIS	3.2
1	D	753	PRO	3.2
1	D	1007	MET	3.1
1	C	862	LEU	3.0
1	D	752	SER	2.9
1	D	860	LYS	2.8
1	A	700	ASN	2.7
1	B	1011	VAL	2.7
1	D	748	ARG	2.7
1	D	702	ALA	2.7
1	B	985	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	751	THR	2.5
1	D	987	MET	2.5
1	D	1008	ASP	2.4
1	D	986	ARG	2.3
1	D	985	GLU	2.2
1	B	1012	ASP	2.2
1	B	764	TYR	2.2
1	D	982	GLN	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)

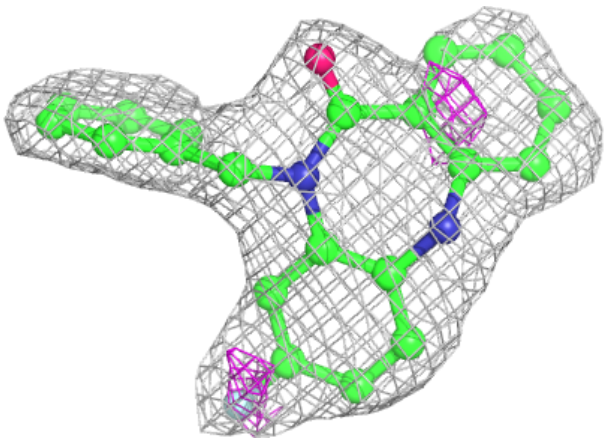
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

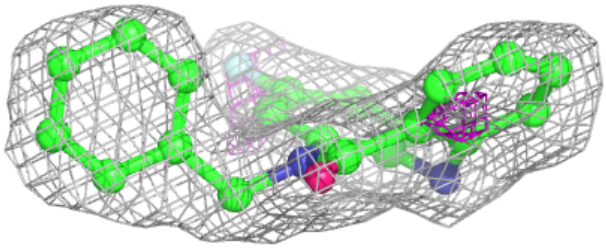
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	C	1103	1/1	0.89	0.11	30,30,30,30	0
4	MG	A	1102	1/1	0.90	0.08	28,28,28,28	0
2	NQ1	D	1101	24/24	0.92	0.23	27,31,39,41	0
2	NQ1	B	1102	24/24	0.92	0.26	29,34,44,45	0
4	MG	D	1103	1/1	0.94	0.07	21,21,21,21	0
2	NQ1	C	1101	24/24	0.95	0.17	23,29,38,39	0
3	ANP	C	1102	31/31	0.96	0.13	25,32,37,41	0
4	MG	B	1103	1/1	0.96	0.06	29,29,29,29	0
3	ANP	A	1101	31/31	0.96	0.12	24,28,35,37	0
3	ANP	B	1101	31/31	0.97	0.14	19,29,36,41	0
3	ANP	D	1102	31/31	0.97	0.14	19,25,32,35	0

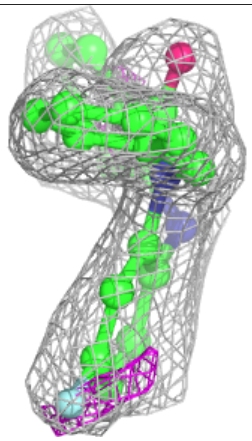
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NQ1 D 1101:

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

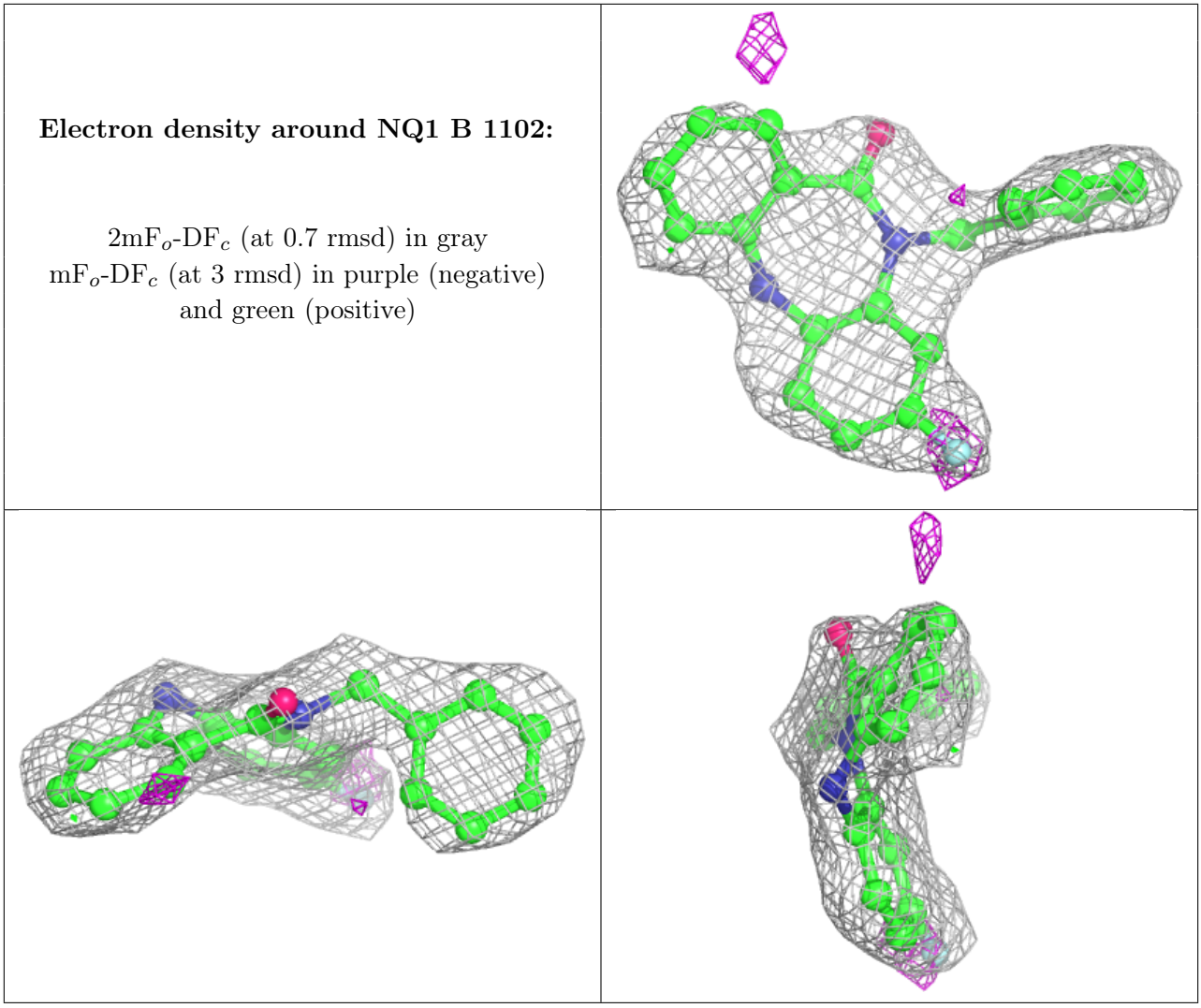






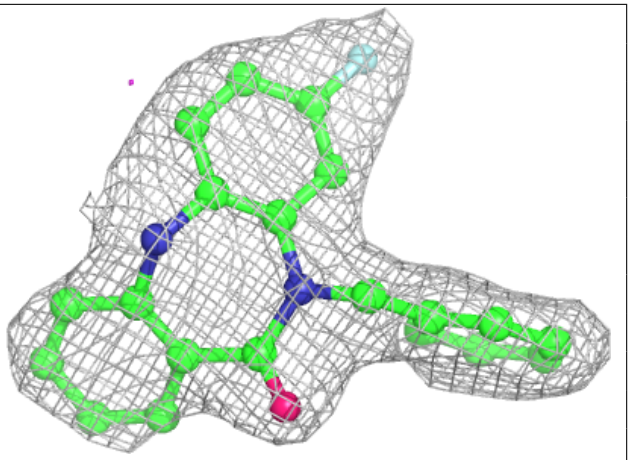
Electron density around NQ1 B 1102:

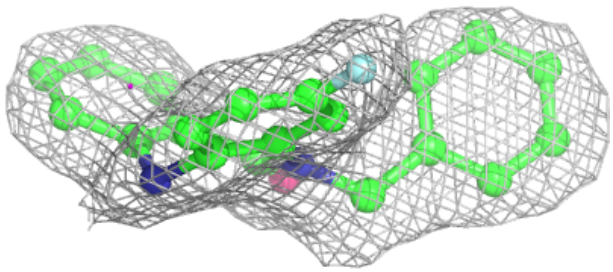
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

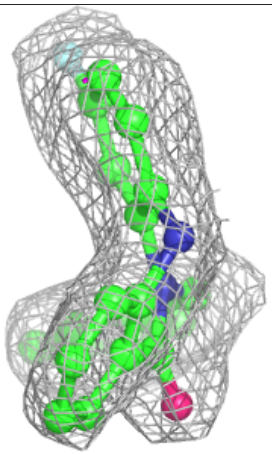


Electron density around NQ1 C 1101:

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

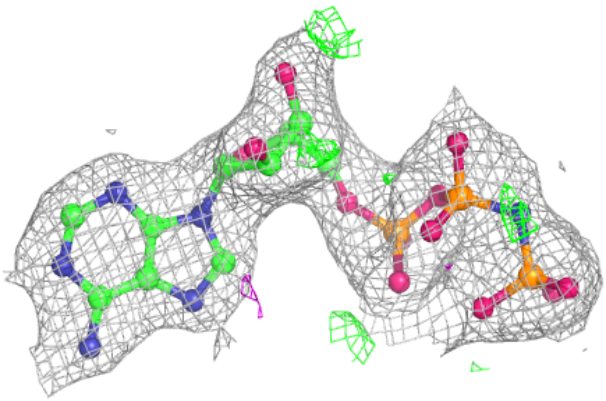


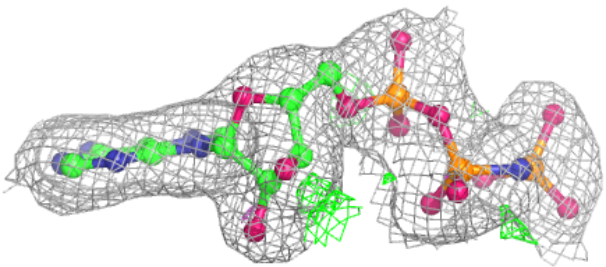


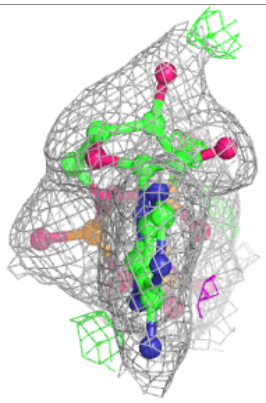


Electron density around ANP C 1102:

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

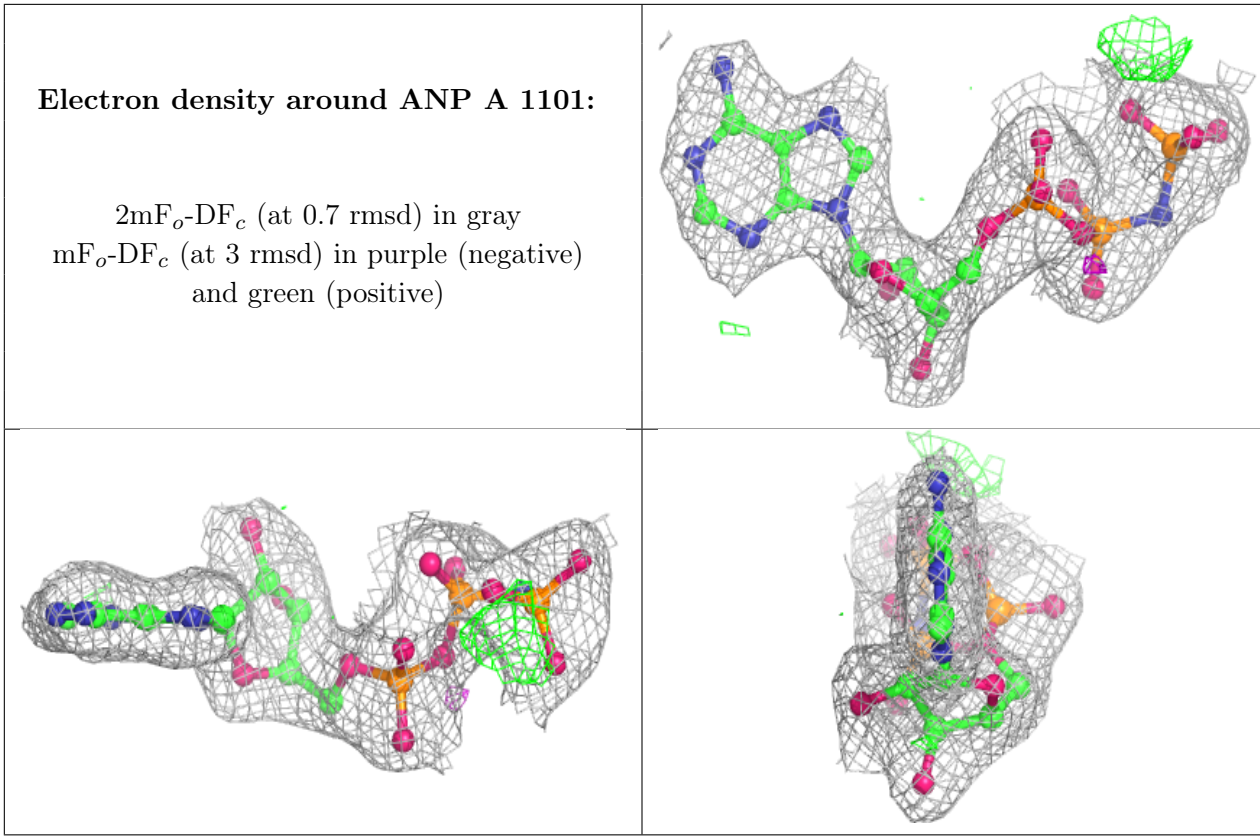






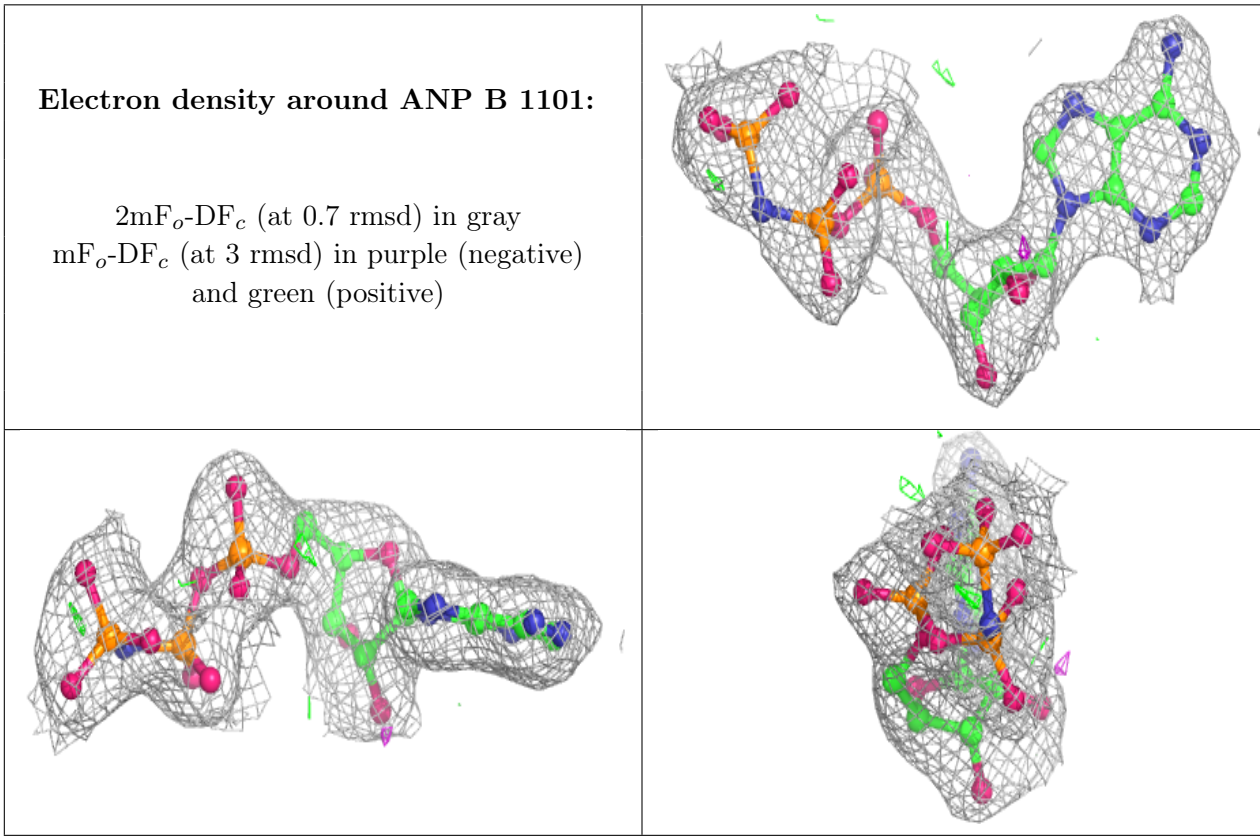
Electron density around ANP A 1101:

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



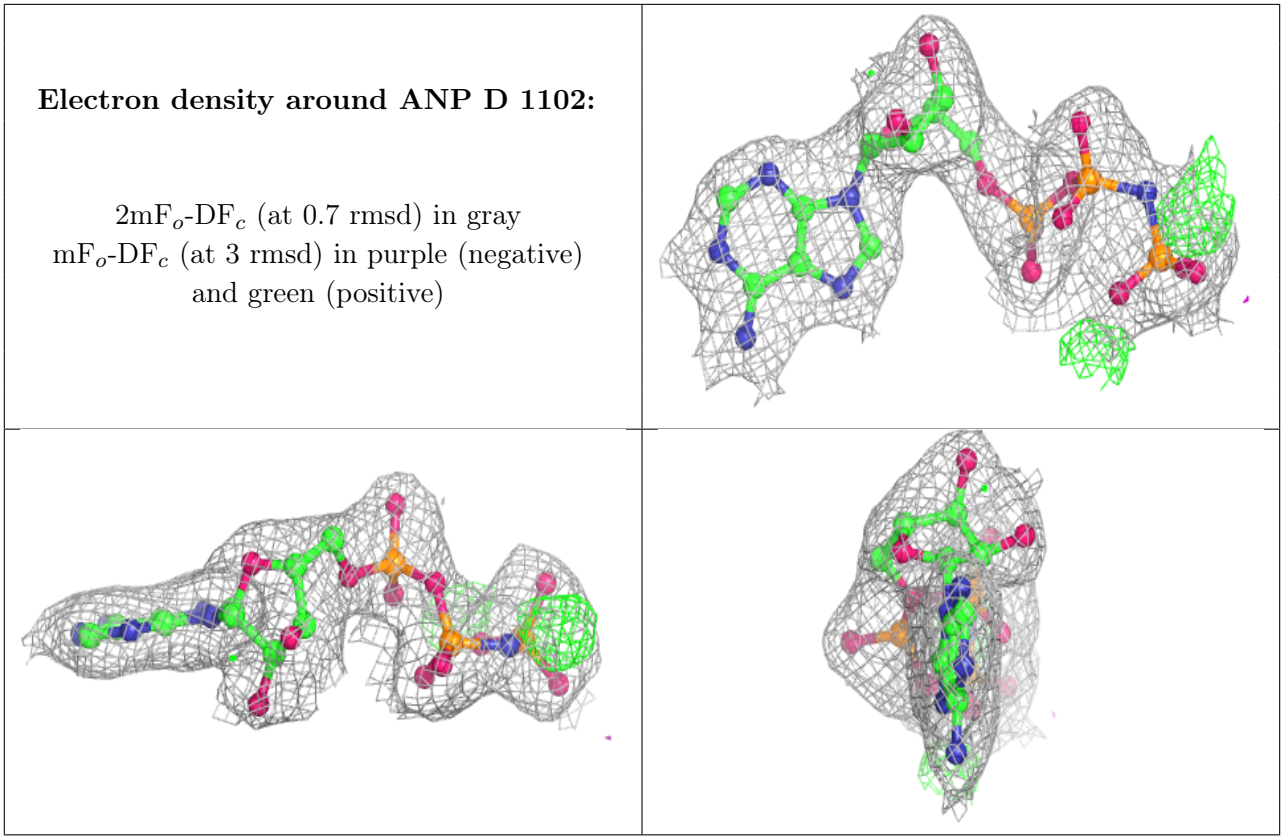
Electron density around ANP B 1101:

$2mF_o$-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.