



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:10 AM UTC

PDB ID : 8FV3 / pdb_00008fv3
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

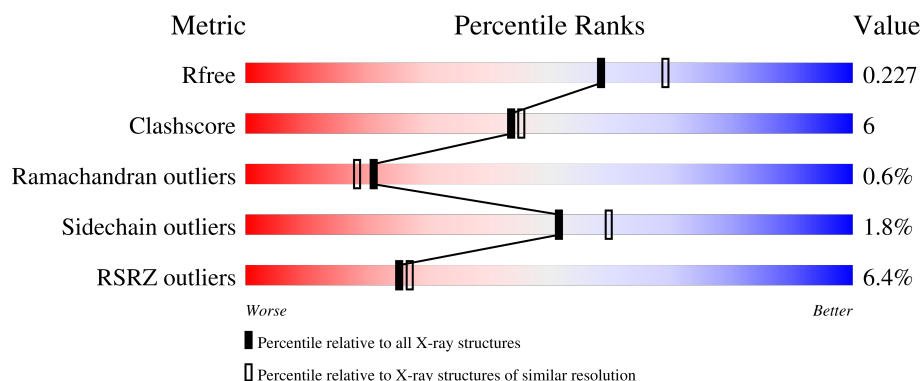
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	328	5% 78% 13% 9%
1	B	328	5% 83% 10% 6%
1	C	328	7% 73% 15% 11%
1	D	328	7% 73% 16% 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:

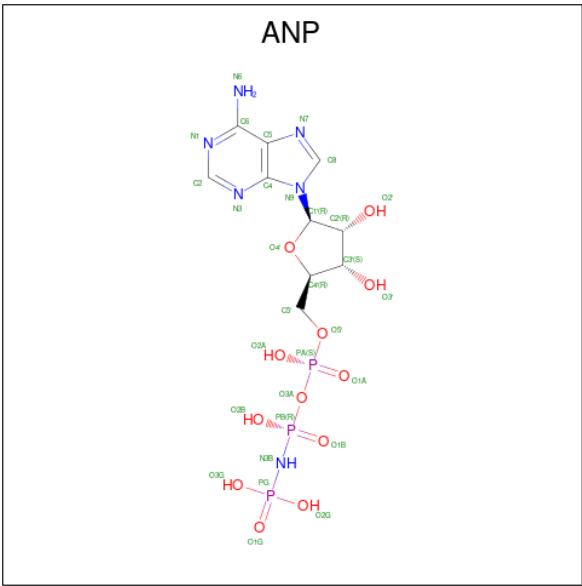
Chain	Residue	Modelled	Actual	Comment	Reference
D	790	MET	THR	engineered mutation	UNP P00533
D	948	ARG	VAL	engineered mutation	UNP P00533
A	790	MET	THR	engineered mutation	UNP P00533
A	948	ARG	VAL	engineered mutation	UNP P00533
B	790	MET	THR	engineered mutation	UNP P00533
B	948	ARG	VAL	engineered mutation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

- Molecule 2 is MAGNESIUM ION (CCD ID: 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		

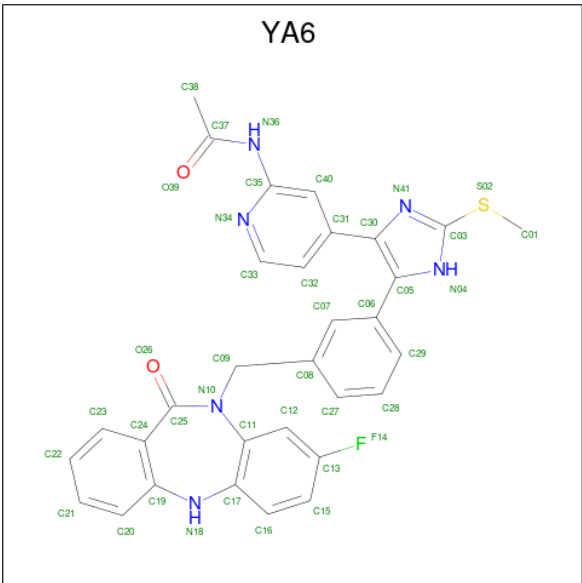
- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID:

ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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-(methylsulfonyl)-1H-imidazol-4-yl]pyridin-2-yl}acetamide (CCD ID: YA6) (formula: C₃₁H₂₅FN₆O₂S) (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		

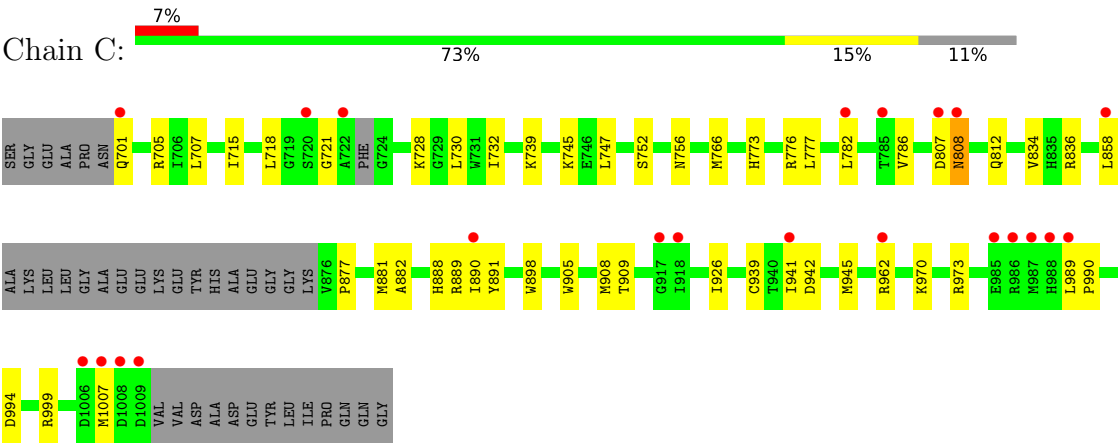
- Molecule 5 is water.

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		

- Molecule 1: Epidermal growth factor receptor



● Molecule 1: Epidermal growth factor receptor



4 Data and refinement statistics

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 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (65.80-2.10) 95.8 (65.80-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.190 , 0.226 0.190 , 0.227	Depositor DCC
R_{free} test set	1999 reflections (2.71%)	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 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, MG, YA6

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	0.36	0/2408	0.51	0/3265
1	B	0.45	0/2479	0.59	0/3356
1	C	0.39	0/2355	0.55	0/3191
1	D	0.39	0/2386	0.58	1/3228 (0.0%)
All	All	0.40	0/9628	0.56	1/13040 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	989	LEU	N-CA-C	-6.78	102.17	110.31

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	2359	0	2351	31	0
1	B	2428	0	2414	27	0
1	C	2305	0	2311	31	0
1	D	2337	0	2345	32	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
3	A	31	0	13	1	0
3	B	31	0	13	0	0
3	D	31	0	13	0	0
4	C	41	0	0	0	0
5	A	75	0	0	4	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	116	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 6.

All (116) 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:C:766:MET:HE2	1:C:777:LEU:HD22	1.64	0.79
1:D:893:HIS:HD2	5:D:1270:HOH:O	1.69	0.75
1:C:701:GLN:C	5:C:1203:HOH:O	2.29	0.75
1:A:913[B]:LYS:HE2	1:A:914:PRO:HD2	1.69	0.74
1:B:793:MET:HE1	1:B:852:LYS:HD3	1.72	0.72
1:B:960:LYS:HZ2	1:B:961:PHE:H	1.39	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:A:790:MET:HE2	3:A:1102:ANP:HN61	1.60	0.66
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:D:986:ARG:O	1:D:987:MET:C	2.48	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:ALA:HA	1:A:766:MET:HE2	1.87	0.56
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:C:941:ILE:HD11	1:C:945:MET:HE3	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
1:D:999:ARG:HD2	5:D:1205:HOH:O	2.09	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:B:944:TYR:HD1	1:B:947:MET:HE2	1.74	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:751:THR:C	1:D:753:PRO:HD3	2.36	0.50
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:B:944:TYR:CD1	1:B:947:MET:HE2	2.48	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:A:968:PHE:HA	1:A:971:MET:HE3	1.95	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:999:ARG:NH1	1:C:1007:MET:HE3	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:810:GLY:HA2	1:D:987:MET:HG3	1.98	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
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:A:967:GLU:HG3	1:A:971:MET:HE2	1.99	0.44
1:C:990:PRO:HB2	1:C:994:ASP:HB2	2.00	0.44
1:D:985:GLU:H	1:D:985:GLU:CD	2.25	0.44
1:A:832:ARG:NH1	1:B:748:ARG:HA	2.33	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:A:1002:MET:HE2	1:A:1002:MET:HB3	1.71	0.43
1:D:705:ARG:NH1	1:D:707:LEU:HD13	2.34	0.43
1:D:905:TRP:HD1	1:D:947:MET:HE1	1.84	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:952:MET:HE3	1:A:957:SER:HB3	2.01	0.42
1:A:944:TYR:O	1:A:948:ARG:HG2	2.20	0.42
1:A:879:LYS:NZ	5:A:1209:HOH:O	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:882:ALA:HA	1:C:898:TRP:CD2	2.55	0.41
1:B:745:LYS:HB2	1:B:790:MET:HE1	2.03	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	36	36
1	B	299/328 (91%)	290 (97%)	7 (2%)	2 (1%)	18	15
1	C	285/328 (87%)	273 (96%)	11 (4%)	1 (0%)	30	28
1	D	290/328 (88%)	279 (96%)	8 (3%)	3 (1%)	12	9
All	All	1166/1312 (89%)	1124 (96%)	35 (3%)	7 (1%)	21	18

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

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Mol	Chain	Res	Type
1	D	749	GLU
1	B	1013	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	252/288 (88%)	250 (99%)	2 (1%)	73	81
1	B	259/288 (90%)	255 (98%)	4 (2%)	57	65
1	C	251/288 (87%)	245 (98%)	6 (2%)	43	49
1	D	250/288 (87%)	244 (98%)	6 (2%)	43	49
All	All	1012/1152 (88%)	994 (98%)	18 (2%)	51	60

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	701	GLN
1	D	708	LYS
1	D	716	LYS
1	D	762	GLU
1	D	783	THR
1	D	860	LYS
1	A	809	ILE
1	A	1010	VAL
1	B	762	GLU
1	B	960	LYS
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	926	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	787	GLN
1	D	893	HIS
1	D	894	GLN
1	A	773	HIS
1	A	826	ASN
1	A	893	HIS
1	A	976	GLN
1	B	701	GLN
1	B	773	HIS
1	B	805	HIS
1	B	808	ASN
1	B	888	HIS
1	C	808	ASN
1	C	812	GLN
1	C	816	ASN
1	C	826	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 oligosaccharides 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	D	1102	2	33,33,33	1.07	4 (12%)	45,52,52	0.68	1 (2%)
4	YA6	C	1101	-	46,46,46	2.50	17 (36%)	63,66,66	1.94	18 (28%)
3	ANP	B	1102	2	33,33,33	1.96	12 (36%)	45,52,52	2.01	13 (28%)
3	ANP	A	1102	2	33,33,33	1.88	11 (33%)	45,52,52	1.97	12 (26%)

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

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1101	YA6	C25-N10	7.14	1.45	1.36
4	C	1101	YA6	C37-N36	5.76	1.46	1.36
4	C	1101	YA6	C17-N18	4.75	1.47	1.41
4	C	1101	YA6	C30-N41	-4.73	1.30	1.38
4	C	1101	YA6	C06-C05	4.42	1.54	1.47
4	C	1101	YA6	C19-N18	4.39	1.46	1.41
3	B	1102	ANP	C5-C4	4.35	1.46	1.39
3	B	1102	ANP	PG-N3B	4.25	1.74	1.63
3	A	1102	ANP	C5-C4	4.25	1.46	1.39
3	B	1102	ANP	PB-N3B	4.22	1.74	1.63
4	C	1101	YA6	C31-C30	4.12	1.54	1.48
4	C	1101	YA6	C03-S02	4.06	1.81	1.75
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	C05-N04	-3.40	1.31	1.37
4	C	1101	YA6	C11-N10	3.18	1.46	1.43
4	C	1101	YA6	C24-C25	3.17	1.54	1.50
3	B	1102	ANP	PG-O1G	3.17	1.51	1.46
3	A	1102	ANP	PB-O1B	3.09	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1102	ANP	PG-O1G	3.06	1.50	1.46
3	D	1102	ANP	PA-O3A	2.89	1.62	1.59
3	B	1102	ANP	PB-O1B	2.86	1.50	1.46
4	C	1101	YA6	C35-N36	2.74	1.46	1.40
3	A	1102	ANP	PB-O2B	-2.70	1.49	1.56
4	C	1101	YA6	C17-C11	-2.64	1.37	1.40
3	A	1102	ANP	PG-O2G	-2.64	1.49	1.56
3	D	1102	ANP	PG-N3B	2.63	1.70	1.63
3	A	1102	ANP	C5-C6	2.59	1.48	1.41
3	A	1102	ANP	C5-N7	-2.58	1.34	1.39
3	A	1102	ANP	PG-O3G	-2.55	1.50	1.56
3	B	1102	ANP	C5-C6	2.52	1.48	1.41
3	B	1102	ANP	C5-N7	-2.51	1.34	1.39
3	B	1102	ANP	PG-O3G	-2.47	1.50	1.56
3	B	1102	ANP	PG-O2G	-2.44	1.50	1.56
3	B	1102	ANP	PB-O2B	-2.44	1.50	1.56
3	D	1102	ANP	PB-O1B	2.41	1.49	1.46
3	A	1102	ANP	PG-O1G	2.29	1.49	1.46
4	C	1101	YA6	O26-C25	-2.27	1.17	1.22
4	C	1101	YA6	O39-C37	-2.25	1.18	1.23
4	C	1101	YA6	C24-C19	-2.21	1.37	1.41
3	A	1102	ANP	C4-N9	-2.19	1.33	1.37
3	B	1102	ANP	C4-N9	-2.17	1.33	1.37
4	C	1101	YA6	C15-C13	2.08	1.41	1.37
3	B	1102	ANP	C8-N7	2.01	1.35	1.31

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1101	YA6	C09-N10-C11	-5.80	111.91	118.13
3	A	1102	ANP	C5-C4-N3	-5.73	118.83	126.72
3	B	1102	ANP	C5-C4-N3	-5.61	118.99	126.72
4	C	1101	YA6	C11-N10-C25	5.58	130.56	124.75
3	B	1102	ANP	O1G-PG-N3B	-4.77	104.75	111.77
3	A	1102	ANP	N3-C4-N9	4.57	134.93	127.17
3	B	1102	ANP	N3-C4-N9	4.56	134.92	127.17
4	C	1101	YA6	C08-C09-N10	4.54	120.85	113.46
3	A	1102	ANP	O2B-PB-O1B	4.29	119.06	109.87
4	C	1101	YA6	C01-S02-C03	4.27	109.19	102.27
3	B	1102	ANP	O2B-PB-O1B	4.13	118.74	109.87
3	A	1102	ANP	C2-N3-C4	3.61	120.64	111.83
3	B	1102	ANP	C2-N3-C4	3.57	120.55	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1102	ANP	C4-C5-N7	-3.57	106.50	110.58
3	A	1102	ANP	C4-C5-N7	-3.50	106.58	110.58
4	C	1101	YA6	C33-N34-C35	3.28	121.90	117.21
3	A	1102	ANP	O1G-PG-N3B	-3.28	106.95	111.77
3	B	1102	ANP	C4-N9-C8	3.10	108.99	105.74
3	B	1102	ANP	N3-C2-N1	-3.08	123.92	128.58
3	A	1102	ANP	N3-C2-N1	-3.03	123.99	128.58
3	A	1102	ANP	C4-N9-C8	2.84	108.72	105.74
4	C	1101	YA6	S02-C03-N04	2.71	125.53	119.66
3	B	1102	ANP	C5-N7-C8	2.68	107.66	103.45
4	C	1101	YA6	C24-C25-N10	2.61	123.34	119.69
3	A	1102	ANP	C5-N7-C8	2.60	107.54	103.45
4	C	1101	YA6	C35-N36-C37	-2.50	125.60	128.16
4	C	1101	YA6	C38-C37-N36	2.44	118.61	114.95
4	C	1101	YA6	C20-C19-N18	-2.41	114.63	118.94
4	C	1101	YA6	C40-C35-N34	-2.40	119.77	122.92
4	C	1101	YA6	C15-C13-C12	-2.34	120.15	123.23
4	C	1101	YA6	C32-C33-N34	-2.29	121.17	123.97
3	B	1102	ANP	N9-C8-N7	-2.24	110.76	113.94
4	C	1101	YA6	C20-C19-C24	2.23	122.28	119.37
3	B	1102	ANP	C6-C5-N7	2.21	136.35	132.09
4	C	1101	YA6	C16-C15-C13	2.20	120.64	118.38
3	A	1102	ANP	O2G-PG-O3G	2.18	113.45	107.59
3	D	1102	ANP	O2G-PG-O1G	-2.14	108.08	113.45
3	A	1102	ANP	N9-C8-N7	-2.12	110.93	113.94
3	A	1102	ANP	C6-C5-N7	2.11	136.16	132.09
4	C	1101	YA6	C09-C08-C27	-2.09	116.90	120.75
4	C	1101	YA6	C31-C30-N41	2.08	122.61	119.53
3	B	1102	ANP	O2G-PG-O3G	2.08	113.17	107.59
4	C	1101	YA6	O26-C25-N10	-2.05	119.15	121.09
3	B	1102	ANP	C2'-C3'-C4'	2.00	106.47	102.61

There are no chirality outliers.

All (12) 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-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

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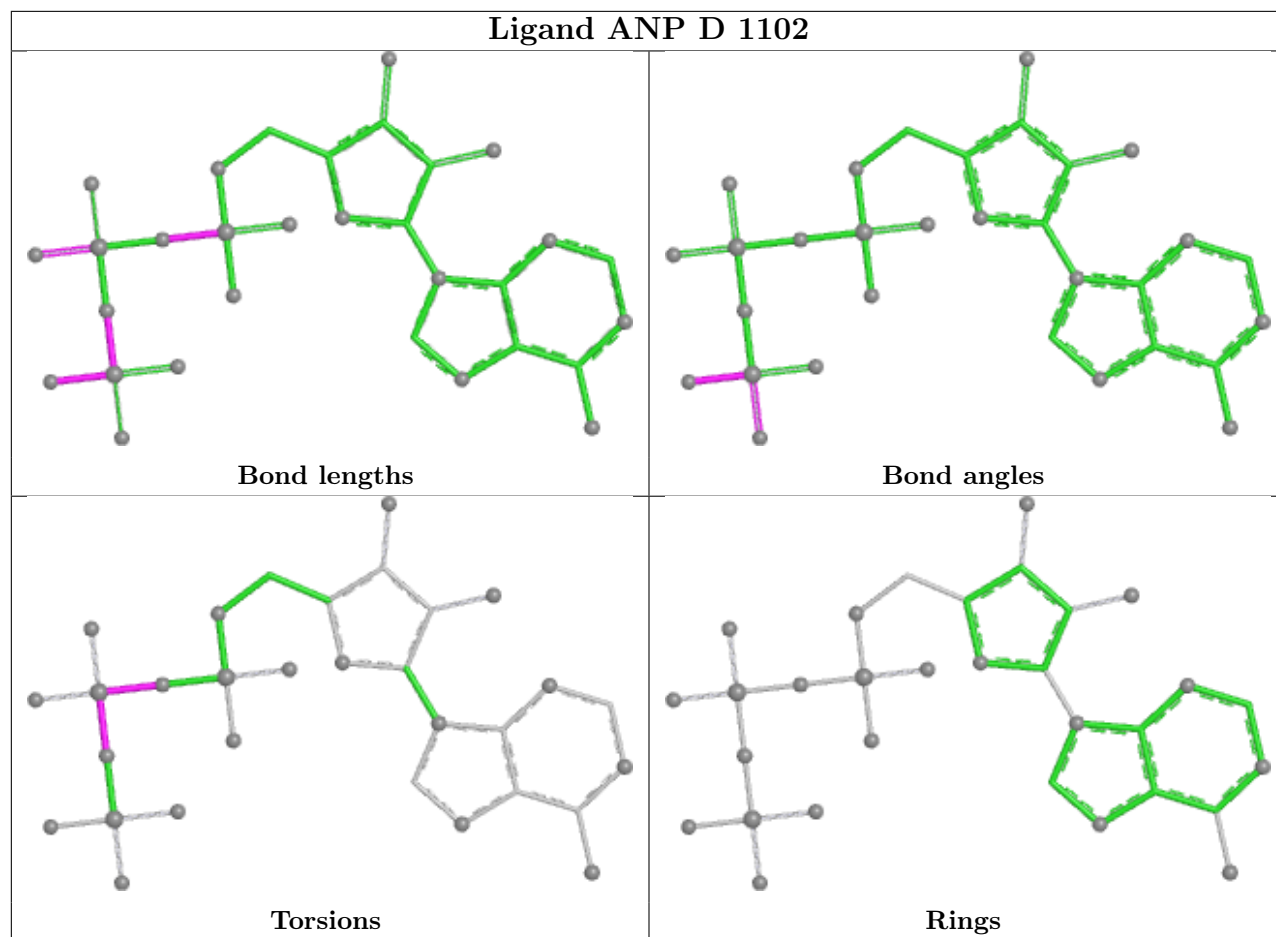
Mol	Chain	Res	Type	Atoms
3	B	1102	ANP	PG-N3B-PB-O1B
3	B	1102	ANP	PA-O3A-PB-O2B
3	A	1102	ANP	O4'-C4'-C5'-O5'
3	A	1102	ANP	C3'-C4'-C5'-O5'
3	D	1102	ANP	PA-O3A-PB-O1B
3	B	1102	ANP	PA-O3A-PB-O1B

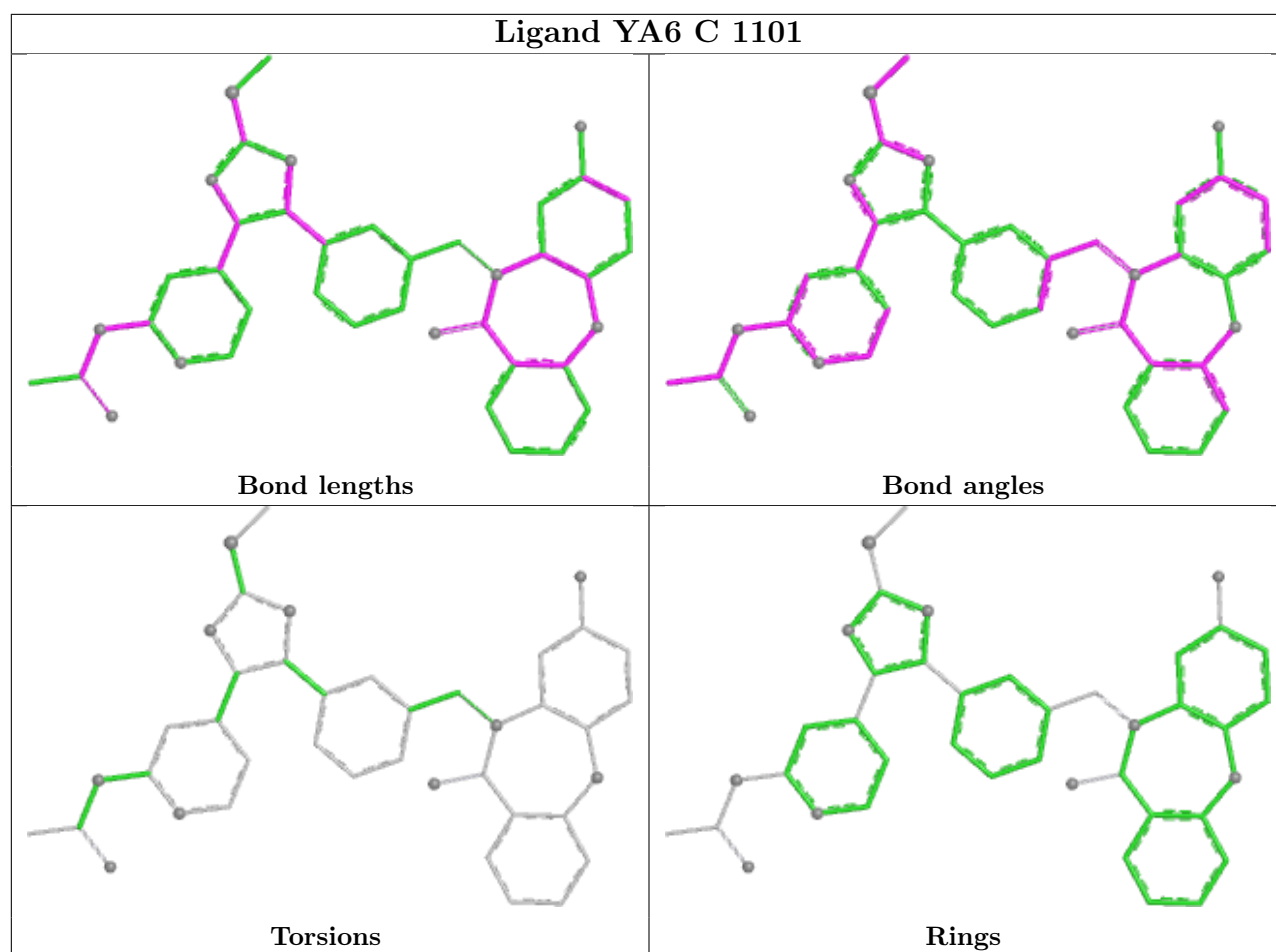
There are no ring outliers.

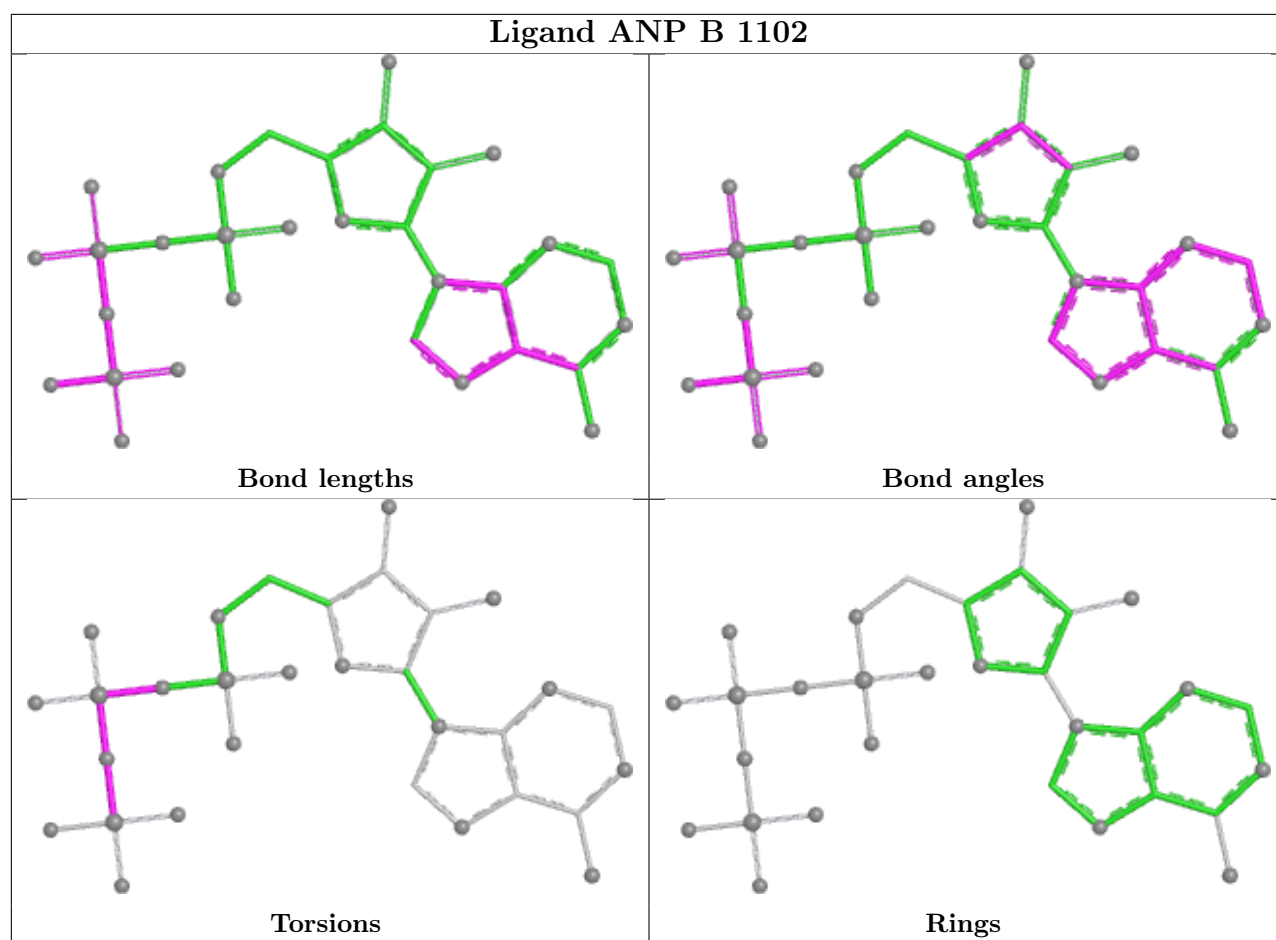
1 monomer is involved in 1 short contact:

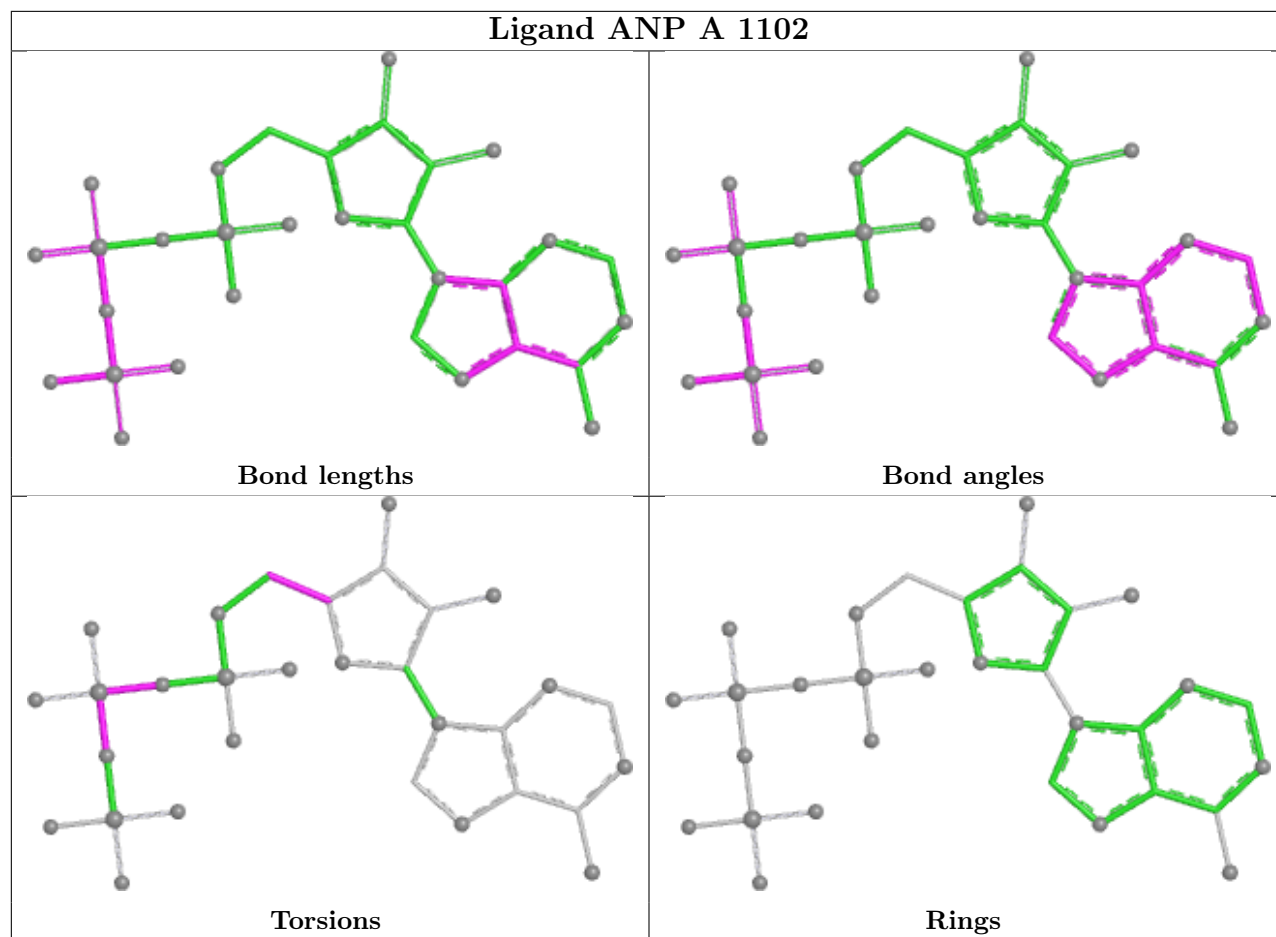
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102	ANP	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	299/328 (91%)	0.43	15 (5%) 34 36	17, 37, 60, 78	1 (0%)
1	B	307/328 (93%)	0.20	16 (5%) 33 35	17, 30, 52, 79	0
1	C	291/328 (88%)	0.48	22 (7%) 20 21	22, 37, 63, 92	0
1	D	295/328 (89%)	0.34	23 (7%) 19 20	13, 32, 60, 82	1 (0%)
All	All	1192/1312 (90%)	0.36	76 (6%) 25 27	13, 34, 60, 92	2 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1010	VAL	5.2
1	B	751	THR	4.3
1	C	722	ALA	4.3
1	A	750	ALA	4.2
1	A	753	PRO	3.7
1	D	989	LEU	3.5
1	B	723	PHE	3.5
1	D	751	THR	3.5
1	D	988	HIS	3.4
1	C	1009	ASP	3.3
1	C	917	GLY	3.2
1	A	1013	ALA	3.2
1	D	1006	ASP	3.2
1	D	1008	ASP	3.2
1	C	1008	ASP	3.1
1	C	989	LEU	3.1
1	A	1010	VAL	3.0
1	A	861	LEU	3.0
1	C	988	HIS	3.0
1	A	1007	MET	2.9
1	D	1007	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	750	ALA	2.9
1	B	1013	ALA	2.9
1	C	782	LEU	2.8
1	D	753	PRO	2.8
1	B	749	GLU	2.8
1	C	1006	ASP	2.8
1	C	808	ASN	2.8
1	A	1012	ASP	2.8
1	A	862	LEU	2.8
1	A	701	GLN	2.7
1	D	875	LYS	2.7
1	B	750	ALA	2.7
1	D	749	GLU	2.7
1	B	1008	ASP	2.7
1	D	859	ALA	2.6
1	B	990	PRO	2.6
1	A	807	ASP	2.6
1	C	1007	MET	2.6
1	D	986	ARG	2.6
1	C	701	GLN	2.6
1	B	988	HIS	2.6
1	A	808	ASN	2.6
1	D	783	THR	2.6
1	D	876	VAL	2.6
1	B	752	SER	2.5
1	C	720	SER	2.5
1	C	918	ILE	2.4
1	D	785	THR	2.4
1	C	985	GLU	2.4
1	C	986	ARG	2.4
1	D	995	SER	2.4
1	D	782	LEU	2.3
1	D	990	PRO	2.3
1	B	753	PRO	2.3
1	C	941	ILE	2.3
1	A	1009	ASP	2.3
1	C	987	MET	2.3
1	B	1012	ASP	2.3
1	C	890	ILE	2.2
1	C	962	ARG	2.2
1	D	862	LEU	2.2
1	B	782	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	861	LEU	2.2
1	C	858	LEU	2.2
1	D	760	LEU	2.2
1	B	862	LEU	2.1
1	B	1015	GLU	2.1
1	A	860	LYS	2.1
1	B	785	THR	2.1
1	A	857	GLY	2.1
1	D	808	ASN	2.0
1	C	807	ASP	2.0
1	D	748	ARG	2.0
1	C	785	THR	2.0
1	A	1014	ASP	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 oligosaccharides 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.

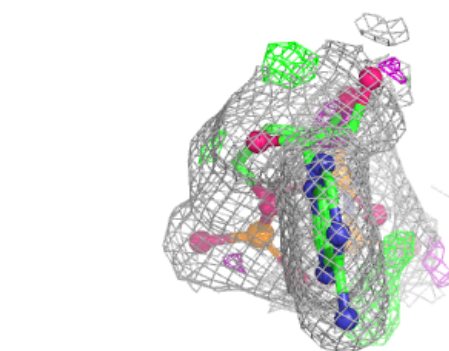
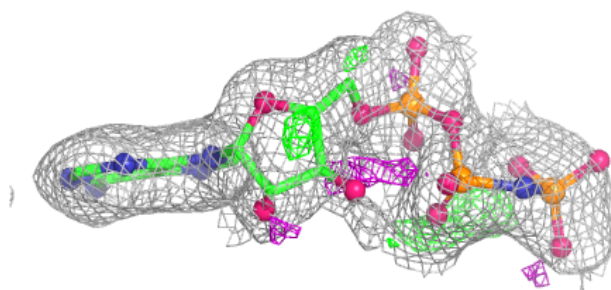
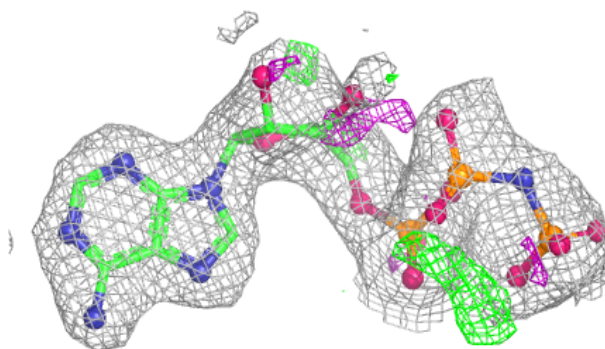
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ANP	A	1102	31/31	0.91	0.10	29,38,46,58	0
3	ANP	B	1102	31/31	0.91	0.09	32,40,49,53	0
2	MG	A	1101	1/1	0.93	0.09	35,35,35,35	0
4	YA6	C	1101	41/41	0.93	0.09	26,32,40,48	0
3	ANP	D	1102	31/31	0.94	0.07	24,33,40,41	0
2	MG	B	1101	1/1	0.96	0.05	32,32,32,32	0
2	MG	D	1101	1/1	0.97	0.04	33,33,33,33	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

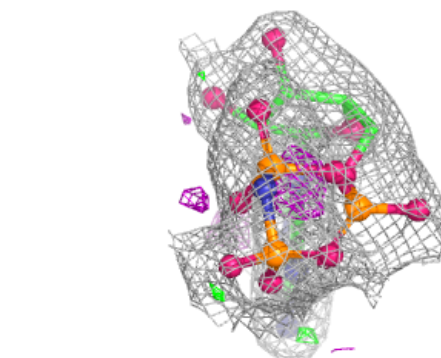
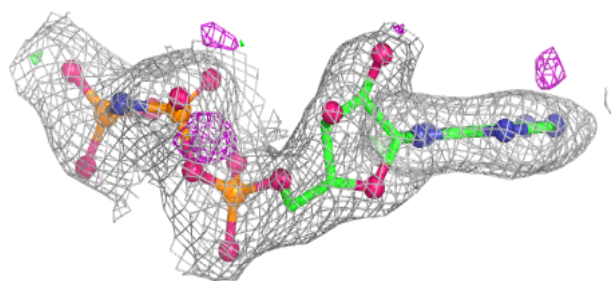
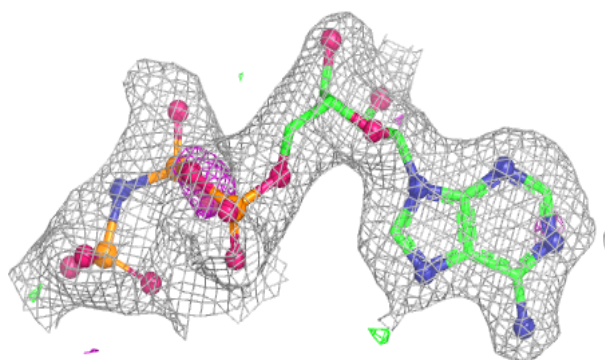
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

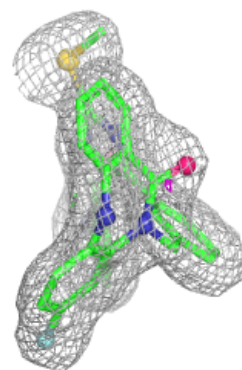
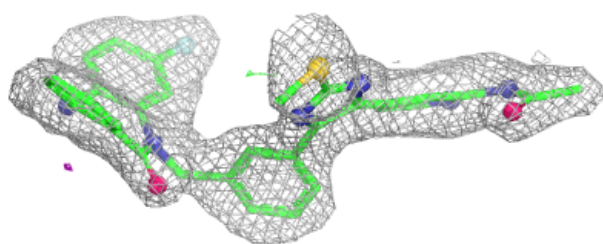
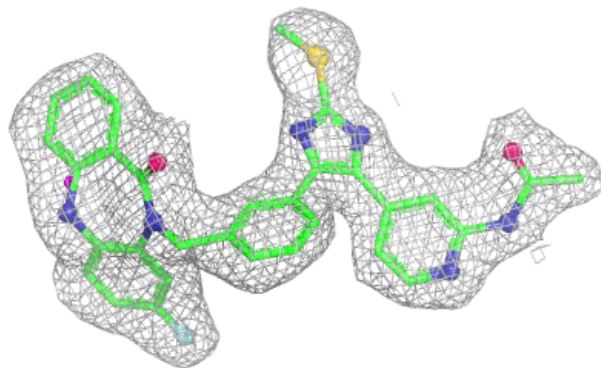
**Electron density around ANP B 1102:**

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

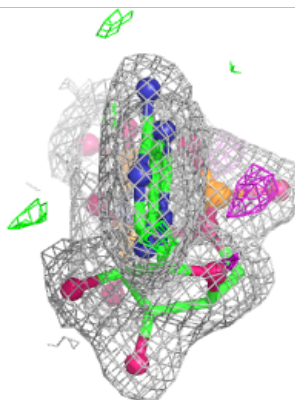
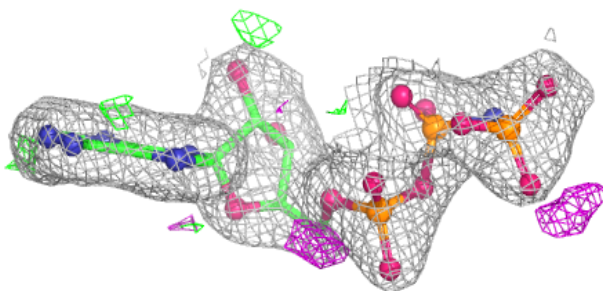
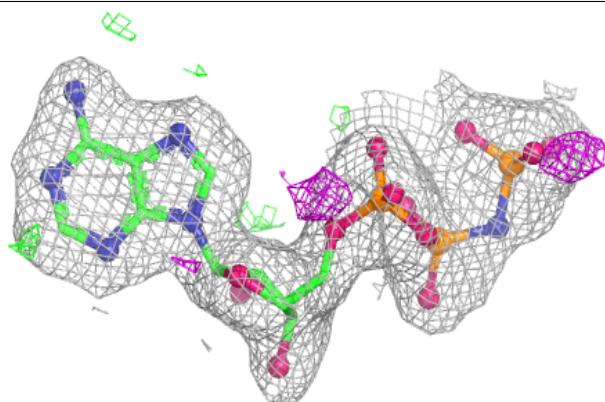


Electron density around YA6 C 1101:

$2mF_o-DF_c$ (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.