



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:23 PM UTC

PDB ID : 8GB4 / pdb_00008gb4
Title : EGFR(T790M/V948R) kinase in complex with benzimidazole allosteric inhibitor
Authors : Beyett, T.S.; Eck, M.J.
Deposited on : 2023-02-24
Resolution : 2.59 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

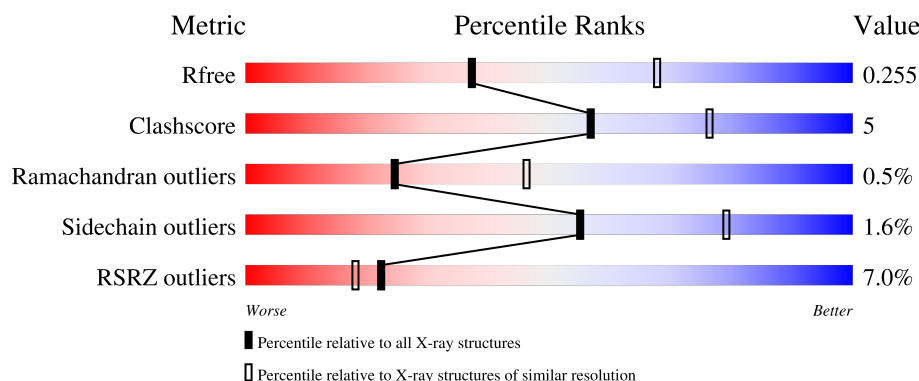
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	331	 4% 82% 7% 12%
1	B	331	 6% 73% 14% 12%
1	C	331	 9% 74% 14% 10%
1	D	331	 6% 79% 8% 12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9858 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	A	292	Total	C	N	O	S	0	1	0
			2360	1516	401	423	20			
1	B	290	Total	C	N	O	S	0	1	0
			2348	1508	399	421	20			
1	C	297	Total	C	N	O	S	0	1	0
			2398	1538	406	434	20			
1	D	291	Total	C	N	O	S	0	1	0
			2353	1511	400	422	20			

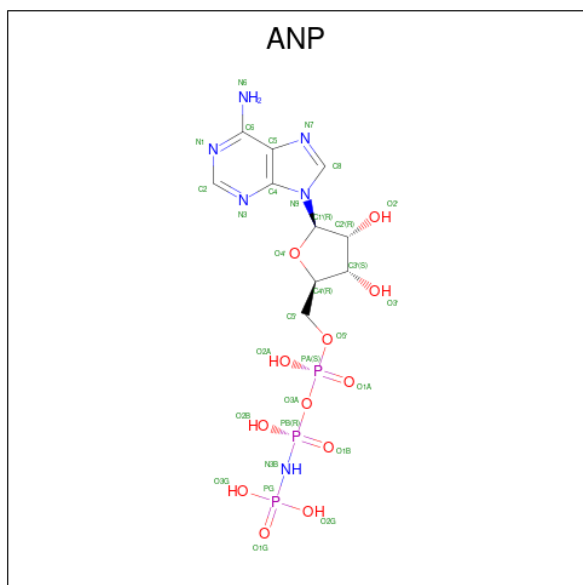
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	692	GLY	-	expression tag	UNP P00533
A	693	SER	-	expression tag	UNP P00533
A	694	THR	-	expression tag	UNP P00533
A	790	MET	THR	engineered mutation	UNP P00533
A	948	ARG	VAL	engineered mutation	UNP P00533
B	692	GLY	-	expression tag	UNP P00533
B	693	SER	-	expression tag	UNP P00533
B	694	THR	-	expression tag	UNP P00533
B	790	MET	THR	engineered mutation	UNP P00533
B	948	ARG	VAL	engineered mutation	UNP P00533
C	692	GLY	-	expression tag	UNP P00533
C	693	SER	-	expression tag	UNP P00533
C	694	THR	-	expression tag	UNP P00533
C	790	MET	THR	engineered mutation	UNP P00533
C	948	ARG	VAL	engineered mutation	UNP P00533
D	692	GLY	-	expression tag	UNP P00533
D	693	SER	-	expression tag	UNP P00533
D	694	THR	-	expression tag	UNP P00533
D	790	MET	THR	engineered mutation	UNP P00533
D	948	ARG	VAL	engineered mutation	UNP P00533

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

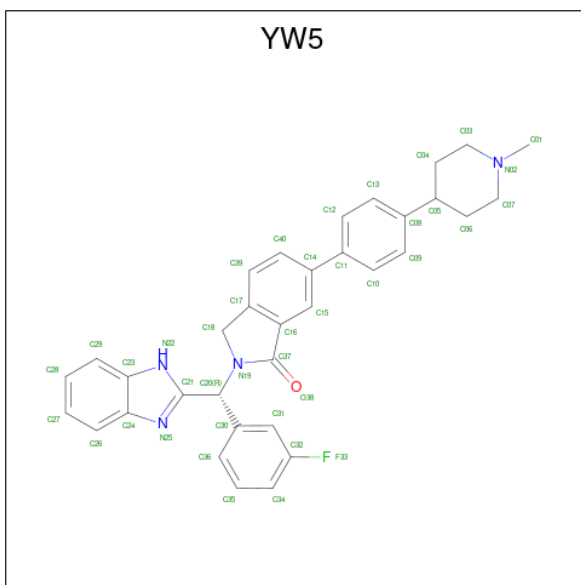
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

- Molecule 4 is 2-[(R)-(1H-benzimidazol-2-yl)(3-fluorophenyl)methyl]-6-[4-(1-methylpiperidin-4-yl)phenyl]-2,3-dihydro-1H-isoindol-1-one (CCD ID: YW5) (formula: C₃₄H₃₁FN₄O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 40	C 34	F 1	N 4	O 1	0	0
4	B	1	Total 40	C 34	F 1	N 4	O 1	0	0
4	C	1	Total 40	C 34	F 1	N 4	O 1	0	0
4	D	1	Total 40	C 34	F 1	N 4	O 1	0	0

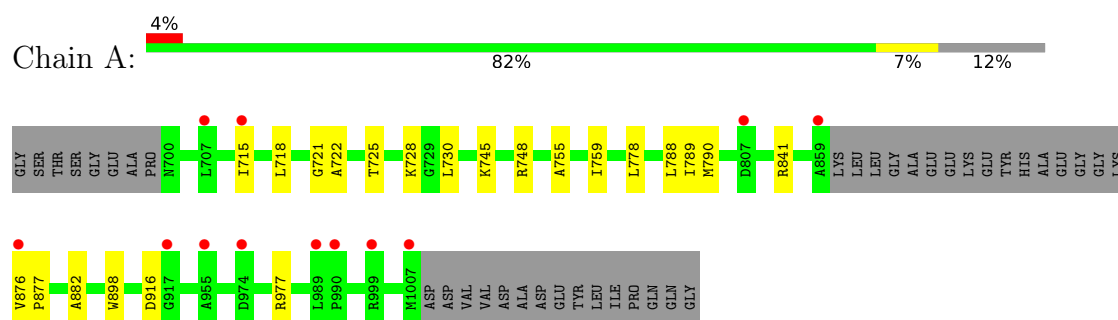
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	22	Total O 22 22	0	0
5	B	36	Total O 36 36	0	0
5	C	22	Total O 22 22	0	0
5	D	31	Total O 31 31	0	0

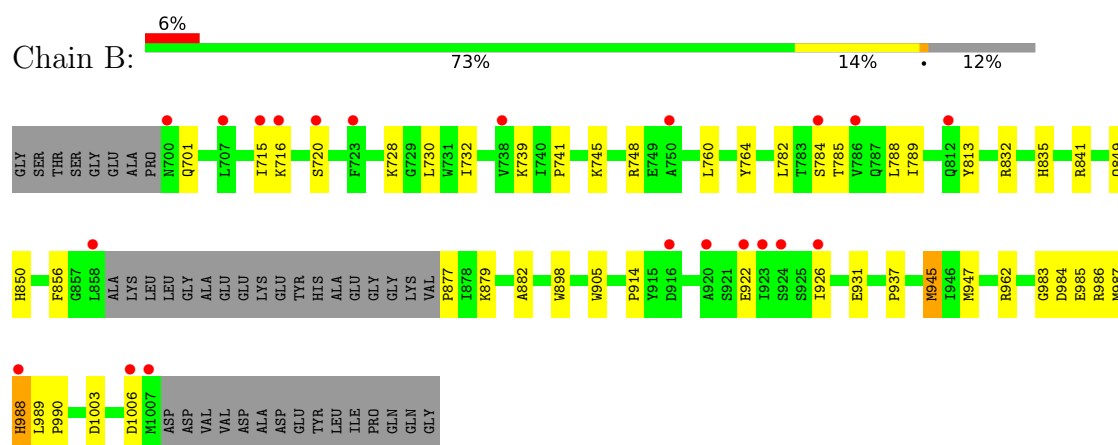
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

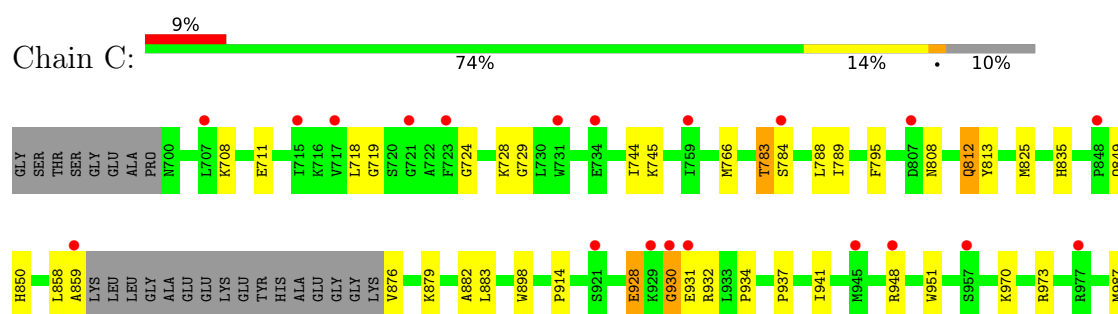
• Molecule 1: Epidermal growth factor receptor

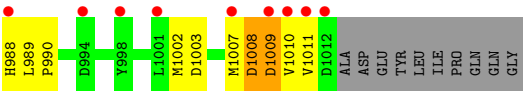


• Molecule 1: Epidermal growth factor receptor

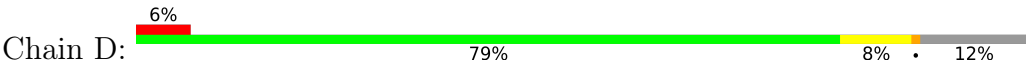


• Molecule 1: Epidermal growth factor receptor





● Molecule 1: Epidermal growth factor receptor



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.45Å 73.45Å 118.42Å 90.00° 118.45° 90.00°	Depositor
Resolution (Å)	104.11 – 2.59 104.11 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.2 (104.11-2.59) 97.2 (104.11-2.60)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
R, R_{free}	0.229 , 0.254 0.229 , 0.255	Depositor DCC
R_{free} test set	1925 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9858	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8339e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MG, ANP, YW5

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	0.16	0/2415	0.37	0/3265
1	B	0.24	0/2403	0.44	0/3247
1	C	0.22	0/2453	0.45	0/3318
1	D	0.18	0/2408	0.39	0/3254
All	All	0.20	0/9679	0.41	0/13084

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2360	0	2406	11	0
1	B	2348	0	2393	34	0
1	C	2398	0	2436	35	0
1	D	2353	0	2398	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	13	0	0
3	C	31	0	13	1	0
3	D	31	0	13	0	0
4	A	40	0	0	1	0
4	B	40	0	0	1	0
4	C	40	0	0	0	0
4	D	40	0	0	2	0
5	A	22	0	0	0	0
5	B	36	0	0	2	0
5	C	22	0	0	1	0
5	D	31	0	0	0	0
All	All	9858	0	9685	90	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 (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:989:LEU:HG	1:B:990:PRO:HD2	1.44	0.99
1:C:849:GLN:HG2	1:C:990:PRO:HG3	1.60	0.84
1:C:988:HIS:ND1	1:C:989:LEU:O	2.19	0.76
1:B:720:SER:OG	1:B:748:ARG:NH2	2.22	0.73
1:A:722:ALA:HA	1:A:748:ARG:HH21	1.56	0.70
1:B:760:LEU:HD11	1:B:782:LEU:HD11	1.75	0.69
1:B:849:GLN:HG2	1:B:990:PRO:HG3	1.74	0.68
1:B:849:GLN:NE2	5:B:1204:HOH:O	2.28	0.66
1:B:931:GLU:HG3	1:D:977:ARG:NH1	2.14	0.63
1:B:813:TYR:OH	1:B:990:PRO:HD3	2.02	0.59
1:B:984:ASP:HA	1:B:987:MET:HG3	1.83	0.59
1:C:808:ASN:HA	1:C:987:MET:HE2	1.85	0.58
1:D:836:ARG:HD3	1:D:859:ALA:HB2	1.86	0.58
1:D:941:ILE:HG13	1:D:945:MET:HE3	1.88	0.56
1:D:841:ARG:HH22	1:D:877:PRO:HB3	1.72	0.54
1:D:974:ASP:OD2	1:D:977:ARG:NE	2.42	0.53
1:A:916:ASP:HB3	1:C:941:ILE:HG21	1.91	0.52
1:C:1008:ASP:O	1:C:1009:ASP:C	2.52	0.52
1:C:724:GLY:C	1:D:832:ARG:HH22	2.17	0.52
1:B:715:ILE:HG13	1:B:730:LEU:HG	1.93	0.51
1:C:813:TYR:OH	1:C:990:PRO:HD3	2.11	0.51
1:D:922:GLU:O	1:D:926:ILE:HG23	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:719:GLY:HA3	3:C:1102:ANP:H4'	1.93	0.49
1:C:825:MET:HE1	1:C:835:HIS:HB2	1.94	0.49
1:B:987:MET:O	1:B:988:HIS:HB2	2.11	0.49
1:D:749:GLU:HG2	1:D:750:ALA:O	2.13	0.49
1:B:945:MET:SD	1:C:937:PRO:HD3	2.53	0.49
1:B:841:ARG:HH22	1:B:877:PRO:HB3	1.78	0.48
1:C:931:GLU:OE1	1:C:948:ARG:NH2	2.46	0.48
1:A:755:ALA:O	1:A:759:ILE:HG13	2.15	0.46
1:A:725:THR:OG1	1:B:832:ARG:NH1	2.48	0.46
1:B:732:ILE:HG13	1:B:739:LYS:HD3	1.97	0.46
1:B:962:ARG:NH2	5:B:1201:HOH:O	2.23	0.46
1:B:931:GLU:HG3	1:D:977:ARG:HH12	1.78	0.46
1:B:985:GLU:HG2	1:B:986:ARG:N	2.30	0.46
1:D:708:LYS:O	1:D:711:GLU:HG2	2.16	0.45
1:B:879:LYS:HD3	1:B:914:PRO:O	2.17	0.45
1:C:708:LYS:O	1:C:711:GLU:HG2	2.17	0.45
1:C:729:GLY:HA3	1:C:744:ILE:HD11	1.99	0.45
1:B:788:LEU:C	1:B:789:ILE:HD12	2.42	0.45
1:B:882:ALA:HA	1:B:898:TRP:CD2	2.52	0.45
1:D:745:LYS:HE2	4:D:1103:YW5:N25	2.32	0.45
1:C:788:LEU:C	1:C:789:ILE:HD12	2.42	0.45
1:D:782:LEU:HA	1:D:786:VAL:HG22	1.99	0.45
1:B:983:GLY:O	1:B:987:MET:HG2	2.17	0.45
1:B:945:MET:HE2	1:C:934:PRO:HG2	1.98	0.44
1:C:718:LEU:HD21	1:C:728:LYS:HB2	1.98	0.44
1:C:879:LYS:HD3	1:C:914:PRO:O	2.17	0.44
1:C:931:GLU:OE1	1:C:932:ARG:HG2	2.16	0.44
1:D:715:ILE:HG13	1:D:730:LEU:HG	2.00	0.44
1:A:788:LEU:C	1:A:789:ILE:HD12	2.42	0.44
1:C:930:GLY:O	1:C:931:GLU:HG2	2.18	0.44
1:C:1007:MET:O	1:C:1008:ASP:C	2.60	0.44
1:B:835:HIS:CD2	1:B:856:PHE:HB3	2.52	0.44
1:B:813:TYR:CE2	1:B:989:LEU:HD12	2.53	0.44
1:B:905:TRP:HD1	1:B:947:MET:HE1	1.83	0.44
1:D:788:LEU:C	1:D:789:ILE:HD12	2.42	0.44
1:B:850:HIS:ND1	1:B:1003:ASP:OD2	2.50	0.43
1:B:945:MET:CE	1:C:934:PRO:HG2	2.48	0.43
1:A:841:ARG:HH22	1:A:877:PRO:HB3	1.84	0.43
1:B:922:GLU:O	1:B:926:ILE:HG23	2.18	0.43
1:B:937:PRO:HD3	1:D:945:MET:HE2	1.99	0.43
1:B:989:LEU:CG	1:B:990:PRO:HD2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:795:PHE:CE2	1:C:1002:MET:HE1	2.54	0.43
1:C:970:LYS:HE2	1:C:970:LYS:HB3	1.85	0.43
1:C:766:MET:HE1	1:C:858:LEU:HD23	2.00	0.42
1:A:715:ILE:HG13	1:A:730:LEU:HG	2.01	0.42
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.54	0.42
1:C:932:ARG:HB3	1:C:951:TRP:CE3	2.54	0.42
1:D:970:LYS:HE2	1:D:970:LYS:HB3	1.86	0.42
1:C:729:GLY:HA3	1:C:744:ILE:CD1	2.50	0.42
1:C:989:LEU:HB3	1:C:990:PRO:HD2	2.01	0.42
1:C:812:GLN:HB3	1:C:989:LEU:HG	2.01	0.41
1:C:882:ALA:HA	1:C:898:TRP:CD2	2.55	0.41
1:A:718:LEU:HD21	1:A:728:LYS:HB2	2.01	0.41
1:B:730:LEU:HD23	1:B:741:PRO:HA	2.03	0.41
1:B:745:LYS:HE2	4:B:1103:YW5:N25	2.35	0.41
1:C:858:LEU:HB2	1:C:859:ALA:H	1.64	0.41
1:B:716:LYS:O	1:B:728:LYS:N	2.45	0.41
1:B:701:GLN:HG3	1:B:764:TYR:CE1	2.56	0.41
1:C:850:HIS:ND1	1:C:1003:ASP:OD2	2.42	0.41
1:D:731:TRP:CZ3	1:D:733:PRO:HG3	2.56	0.41
1:C:783:THR:OG1	1:C:784:SER:N	2.54	0.41
1:D:744:ILE:HG12	1:D:789:ILE:HG13	2.02	0.41
1:A:778:LEU:HG	1:A:790:MET:HA	2.03	0.41
1:C:973:ARG:NH2	5:C:1208:HOH:O	2.54	0.41
1:A:759:ILE:HG12	4:A:1103:YW5:C09	2.51	0.40
1:C:849:GLN:HB3	1:C:1011:VAL:HG11	2.02	0.40
1:D:759:ILE:HG12	4:D:1103:YW5:C09	2.52	0.40
1:C:883:LEU:HD21	1:C:928:GLU:HG3	2.03	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	289/331 (87%)	281 (97%)	7 (2%)	1 (0%)	36	58
1	B	287/331 (87%)	276 (96%)	8 (3%)	3 (1%)	12	28
1	C	294/331 (89%)	279 (95%)	13 (4%)	2 (1%)	18	38
1	D	288/331 (87%)	280 (97%)	8 (3%)	0	100	100
All	All	1158/1324 (88%)	1116 (96%)	36 (3%)	6 (0%)	24	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1006	ASP
1	C	930	GLY
1	B	988	HIS
1	C	1009	ASP
1	A	721	GLY
1	B	784	SER

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	262/290 (90%)	259 (99%)	3 (1%)	65	84
1	B	261/290 (90%)	259 (99%)	2 (1%)	73	88
1	C	267/290 (92%)	260 (97%)	7 (3%)	40	68
1	D	261/290 (90%)	256 (98%)	5 (2%)	50	75
All	All	1051/1160 (91%)	1034 (98%)	17 (2%)	55	79

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	745	LYS
1	A	876	VAL
1	A	977	ARG
1	B	785	THR
1	B	945	MET

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Mol	Chain	Res	Type
1	C	745	LYS
1	C	783	THR
1	C	812	GLN
1	C	876	VAL
1	C	928	GLU
1	C	1008	ASP
1	C	1010	VAL
1	D	754	LYS
1	D	783	THR
1	D	786	VAL
1	D	858	LEU
1	D	945	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	791	GLN
1	A	849	GLN
1	A	988	HIS
1	B	812	GLN
1	B	816	ASN
1	C	756	ASN
1	C	791	GLN
1	C	849	GLN
1	C	982	GLN
1	D	988	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ANP	A	1102	2	33,33,33	1.06	5 (15%)	45,52,52	0.88	2 (4%)
4	YW5	A	1103	-	46,46,46	3.18	23 (50%)	63,67,67	3.20	21 (33%)
4	YW5	C	1103	-	46,46,46	3.16	23 (50%)	63,67,67	3.22	21 (33%)
3	ANP	D	1102	2	33,33,33	1.05	5 (15%)	45,52,52	0.88	2 (4%)
3	ANP	B	1102	2	33,33,33	1.07	5 (15%)	45,52,52	0.86	2 (4%)
3	ANP	C	1102	2	33,33,33	1.04	5 (15%)	45,52,52	0.91	3 (6%)
4	YW5	B	1103	-	46,46,46	3.21	23 (50%)	63,67,67	3.13	20 (31%)
4	YW5	D	1103	-	46,46,46	3.26	22 (47%)	63,67,67	3.29	24 (38%)

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	A	1102	2	-	3/18/38/38	0/3/3/3
4	YW5	A	1103	-	-	0/18/42/42	0/7/7/7
4	YW5	C	1103	-	-	4/18/42/42	0/7/7/7
3	ANP	D	1102	2	-	2/18/38/38	0/3/3/3
3	ANP	B	1102	2	-	8/18/38/38	0/3/3/3
3	ANP	C	1102	2	-	2/18/38/38	0/3/3/3
4	YW5	B	1103	-	-	2/18/42/42	0/7/7/7
4	YW5	D	1103	-	-	0/18/42/42	0/7/7/7

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1103	YW5	C30-C20	8.64	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1103	YW5	C30-C20	8.48	1.63	1.52
4	D	1103	YW5	C30-C20	8.33	1.62	1.52
4	C	1103	YW5	C21-N25	8.22	1.43	1.32
4	D	1103	YW5	C21-N25	7.93	1.43	1.32
4	B	1103	YW5	C21-N25	7.92	1.43	1.32
4	A	1103	YW5	C21-N25	7.88	1.43	1.32
4	C	1103	YW5	C30-C20	7.60	1.61	1.52
4	D	1103	YW5	C18-C17	7.19	1.59	1.50
4	C	1103	YW5	C18-C17	6.30	1.58	1.50
4	B	1103	YW5	C37-N19	6.10	1.42	1.36
4	A	1103	YW5	C18-C17	6.06	1.58	1.50
4	D	1103	YW5	C20-N19	6.03	1.53	1.46
4	B	1103	YW5	C18-C17	5.94	1.58	1.50
4	C	1103	YW5	C20-N19	5.68	1.53	1.46
4	D	1103	YW5	C18-N19	5.62	1.53	1.47
4	A	1103	YW5	C37-N19	5.55	1.41	1.36
4	A	1103	YW5	C16-C37	5.54	1.57	1.48
4	C	1103	YW5	C20-C21	5.51	1.62	1.51
4	D	1103	YW5	C37-N19	5.36	1.41	1.36
4	A	1103	YW5	C20-N19	5.34	1.53	1.46
4	C	1103	YW5	C37-N19	5.29	1.41	1.36
4	D	1103	YW5	C16-C37	5.28	1.57	1.48
4	B	1103	YW5	C20-C21	5.23	1.62	1.51
4	B	1103	YW5	C20-N19	5.15	1.52	1.46
4	B	1103	YW5	C16-C37	4.98	1.56	1.48
4	C	1103	YW5	C14-C11	4.97	1.60	1.49
4	D	1103	YW5	C14-C11	4.89	1.60	1.49
4	A	1103	YW5	C18-N19	4.80	1.52	1.47
4	B	1103	YW5	C18-N19	4.76	1.52	1.47
4	D	1103	YW5	C20-C21	4.67	1.60	1.51
4	A	1103	YW5	C14-C11	4.55	1.59	1.49
4	A	1103	YW5	C20-C21	4.51	1.60	1.51
4	C	1103	YW5	C18-N19	4.51	1.52	1.47
4	B	1103	YW5	C14-C11	4.49	1.59	1.49
4	C	1103	YW5	C16-C37	4.19	1.55	1.48
4	B	1103	YW5	C23-N22	4.03	1.46	1.38
4	D	1103	YW5	C23-N22	3.96	1.45	1.38
4	A	1103	YW5	C23-N22	3.93	1.45	1.38
4	B	1103	YW5	C08-C05	3.88	1.59	1.52
4	C	1103	YW5	C23-N22	3.86	1.45	1.38
4	C	1103	YW5	C29-C23	3.38	1.45	1.39
4	A	1103	YW5	C08-C05	3.23	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1103	YW5	C29-C23	3.12	1.44	1.39
4	D	1103	YW5	C13-C12	3.11	1.43	1.38
4	C	1103	YW5	C08-C05	3.00	1.58	1.52
4	B	1103	YW5	C29-C23	2.98	1.44	1.39
4	A	1103	YW5	C29-C23	2.90	1.44	1.39
3	C	1102	ANP	PB-O1B	2.87	1.50	1.46
4	C	1103	YW5	C28-C27	2.87	1.44	1.38
4	D	1103	YW5	C28-C27	2.84	1.44	1.38
4	A	1103	YW5	C28-C27	2.83	1.44	1.38
4	D	1103	YW5	C40-C39	2.75	1.43	1.38
3	D	1102	ANP	PB-O1B	2.74	1.50	1.46
4	B	1103	YW5	C28-C27	2.74	1.44	1.38
3	A	1102	ANP	PB-O1B	2.74	1.50	1.46
3	B	1102	ANP	PB-O1B	2.72	1.50	1.46
4	C	1103	YW5	C40-C39	2.69	1.43	1.38
4	D	1103	YW5	C40-C14	2.65	1.44	1.39
4	B	1103	YW5	C07-N02	2.64	1.52	1.46
3	B	1102	ANP	PG-O1G	2.61	1.50	1.46
3	B	1102	ANP	PG-O3G	-2.61	1.49	1.56
3	D	1102	ANP	PG-O3G	-2.60	1.49	1.56
4	A	1103	YW5	C36-C30	2.59	1.43	1.39
4	B	1103	YW5	C36-C30	2.58	1.43	1.39
3	A	1102	ANP	PG-O1G	2.58	1.50	1.46
4	A	1103	YW5	C40-C39	2.57	1.43	1.38
3	C	1102	ANP	PG-O1G	2.57	1.50	1.46
4	B	1103	YW5	C03-N02	2.56	1.52	1.46
3	A	1102	ANP	PB-O2B	-2.56	1.50	1.56
4	B	1103	YW5	C26-C24	2.54	1.44	1.40
3	D	1102	ANP	PG-O2G	-2.53	1.50	1.56
4	C	1103	YW5	C40-C14	2.51	1.44	1.39
4	C	1103	YW5	C26-C24	2.50	1.43	1.40
4	D	1103	YW5	C26-C24	2.50	1.43	1.40
4	D	1103	YW5	C36-C30	2.49	1.43	1.39
3	D	1102	ANP	PB-O2B	-2.48	1.50	1.56
3	B	1102	ANP	PB-O2B	-2.47	1.50	1.56
3	A	1102	ANP	PG-O3G	-2.47	1.50	1.56
4	B	1103	YW5	C40-C14	2.45	1.44	1.39
4	D	1103	YW5	C39-C17	2.45	1.43	1.39
4	A	1103	YW5	C07-N02	2.45	1.52	1.46
3	A	1102	ANP	PG-O2G	-2.44	1.50	1.56
3	B	1102	ANP	PG-O2G	-2.43	1.50	1.56
3	C	1102	ANP	PB-O2B	-2.43	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1103	YW5	C03-N02	2.41	1.52	1.46
4	A	1103	YW5	C03-N02	2.39	1.52	1.46
4	C	1103	YW5	C36-C30	2.38	1.42	1.39
4	C	1103	YW5	C13-C12	2.37	1.42	1.38
4	C	1103	YW5	C07-N02	2.35	1.52	1.46
4	C	1103	YW5	C03-N02	2.34	1.52	1.46
4	A	1103	YW5	C40-C14	2.34	1.44	1.39
4	B	1103	YW5	C10-C09	2.33	1.42	1.38
4	A	1103	YW5	C26-C24	2.33	1.43	1.40
3	D	1102	ANP	PG-O1G	2.30	1.49	1.46
4	B	1103	YW5	C04-C05	2.29	1.59	1.53
4	A	1103	YW5	C39-C17	2.29	1.43	1.39
4	C	1103	YW5	C24-N25	2.28	1.44	1.39
3	C	1102	ANP	PG-O2G	-2.28	1.50	1.56
4	B	1103	YW5	C31-C32	2.27	1.41	1.37
4	C	1103	YW5	C31-C32	2.26	1.41	1.37
3	C	1102	ANP	PG-O3G	-2.26	1.50	1.56
4	B	1103	YW5	C40-C39	2.21	1.42	1.38
4	A	1103	YW5	C04-C05	2.19	1.58	1.53
4	A	1103	YW5	C10-C09	2.19	1.42	1.38
4	D	1103	YW5	C07-N02	2.17	1.51	1.46
4	A	1103	YW5	C31-C32	2.11	1.41	1.37
4	D	1103	YW5	C31-C32	2.11	1.41	1.37
4	B	1103	YW5	C15-C16	2.11	1.43	1.39
4	C	1103	YW5	C10-C09	2.05	1.42	1.38
4	D	1103	YW5	C12-C11	2.04	1.43	1.39

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1103	YW5	C18-N19-C37	-16.31	106.28	113.15
4	A	1103	YW5	C18-N19-C37	-16.29	106.28	113.15
4	D	1103	YW5	C18-N19-C37	-16.17	106.33	113.15
4	B	1103	YW5	C18-N19-C37	-16.12	106.36	113.15
4	A	1103	YW5	C17-C18-N19	9.05	107.12	102.31
4	C	1103	YW5	C16-C37-N19	8.57	111.87	106.42
4	B	1103	YW5	C17-C18-N19	8.50	106.83	102.31
4	D	1103	YW5	C16-C37-N19	8.34	111.72	106.42
4	D	1103	YW5	C17-C18-N19	8.11	106.62	102.31
4	B	1103	YW5	C16-C37-N19	7.80	111.38	106.42
4	C	1103	YW5	C17-C18-N19	7.79	106.45	102.31
4	A	1103	YW5	C16-C37-N19	7.61	111.26	106.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1103	YW5	C07-C06-C05	6.95	119.14	111.00
4	C	1103	YW5	C07-C06-C05	6.29	118.37	111.00
4	A	1103	YW5	C07-C06-C05	5.74	117.72	111.00
4	C	1103	YW5	C03-C04-C05	5.44	117.36	111.00
4	D	1103	YW5	C03-C04-C05	5.29	117.19	111.00
4	A	1103	YW5	C03-C04-C05	5.01	116.86	111.00
4	B	1103	YW5	C07-C06-C05	4.95	116.79	111.00
4	D	1103	YW5	C06-C05-C08	-4.55	101.91	112.67
4	D	1103	YW5	O38-C37-N19	-4.33	121.90	125.34
4	B	1103	YW5	C04-C03-N02	-4.26	105.70	111.20
4	A	1103	YW5	O38-C37-N19	-4.20	122.00	125.34
3	D	1102	ANP	O2B-PB-O1B	4.14	118.75	109.87
4	B	1103	YW5	C06-C07-N02	-4.11	105.89	111.20
4	B	1103	YW5	C03-C04-C05	4.09	115.78	111.00
3	C	1102	ANP	O2B-PB-O1B	4.07	118.61	109.87
4	A	1103	YW5	C04-C03-N02	-4.04	105.99	111.20
3	A	1102	ANP	O2B-PB-O1B	4.00	118.46	109.87
4	C	1103	YW5	O38-C37-N19	-3.99	122.17	125.34
4	C	1103	YW5	C04-C03-N02	-3.96	106.09	111.20
3	B	1102	ANP	O2B-PB-O1B	3.92	118.27	109.87
4	B	1103	YW5	C17-C16-C37	-3.92	106.81	108.94
4	C	1103	YW5	C17-C16-C37	-3.78	106.89	108.94
4	B	1103	YW5	O38-C37-N19	-3.77	122.35	125.34
4	C	1103	YW5	C06-C07-N02	-3.74	106.37	111.20
4	D	1103	YW5	C01-N02-C07	-3.71	103.57	110.63
4	A	1103	YW5	C17-C16-C37	-3.63	106.97	108.94
4	A	1103	YW5	C06-C07-N02	-3.62	106.53	111.20
4	D	1103	YW5	C04-C03-N02	-3.48	106.71	111.20
4	A	1103	YW5	C18-N19-C20	-3.45	120.62	123.84
4	D	1103	YW5	C17-C16-C37	-3.30	107.15	108.94
4	D	1103	YW5	C06-C07-N02	-3.30	106.95	111.20
4	B	1103	YW5	C18-N19-C20	-3.26	120.81	123.84
4	D	1103	YW5	C01-N02-C03	-3.22	104.50	110.63
4	C	1103	YW5	C40-C14-C15	-3.02	114.07	118.23
4	D	1103	YW5	C40-C14-C15	-2.98	114.13	118.23
4	A	1103	YW5	C40-C14-C15	-2.83	114.33	118.23
4	D	1103	YW5	C23-C24-N25	-2.75	105.65	109.42
4	A	1103	YW5	C01-N02-C07	-2.74	105.41	110.63
4	C	1103	YW5	C18-N19-C20	-2.73	121.30	123.84
4	B	1103	YW5	C23-C24-N25	-2.72	105.69	109.42
4	A	1103	YW5	C23-C24-N25	-2.72	105.70	109.42
4	C	1103	YW5	C01-N02-C07	-2.72	105.46	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1103	YW5	C40-C14-C15	-2.72	114.49	118.23
4	C	1103	YW5	C01-N02-C03	-2.65	105.58	110.63
4	C	1103	YW5	C23-C24-N25	-2.65	105.80	109.42
4	B	1103	YW5	C15-C14-C11	2.56	125.13	120.84
4	A	1103	YW5	C01-N02-C03	-2.55	105.78	110.63
4	C	1103	YW5	C06-C05-C08	-2.52	106.71	112.67
4	D	1103	YW5	C18-C17-C16	-2.49	108.17	109.73
4	D	1103	YW5	C29-C23-C24	-2.49	119.37	122.10
4	A	1103	YW5	C29-C23-C24	-2.46	119.40	122.10
4	B	1103	YW5	C29-C23-C24	-2.45	119.41	122.10
3	D	1102	ANP	O2G-PG-O1G	-2.40	107.42	113.45
3	A	1102	ANP	O2G-PG-O1G	-2.37	107.51	113.45
4	A	1103	YW5	C15-C16-C37	2.33	133.39	129.39
4	C	1103	YW5	C29-C23-C24	-2.32	119.56	122.10
4	B	1103	YW5	C10-C11-C14	2.31	125.25	121.25
4	C	1103	YW5	C39-C17-C16	-2.29	118.28	120.28
4	D	1103	YW5	C18-C17-C39	2.25	133.52	128.70
4	D	1103	YW5	C39-C17-C16	-2.24	118.32	120.28
4	B	1103	YW5	C04-C05-C08	2.21	117.90	112.67
4	B	1103	YW5	C15-C16-C37	2.20	133.17	129.39
4	A	1103	YW5	C18-C17-C16	-2.20	108.35	109.73
4	D	1103	YW5	C24-C23-N22	2.20	108.35	105.71
4	A	1103	YW5	C24-C23-N22	2.19	108.34	105.71
3	B	1102	ANP	O2G-PG-O1G	-2.13	108.10	113.45
4	B	1103	YW5	C24-C23-N22	2.13	108.27	105.71
4	A	1103	YW5	C30-C31-C32	2.13	121.04	118.74
4	D	1103	YW5	C30-C31-C32	2.13	121.04	118.74
3	C	1102	ANP	O2G-PG-O1G	-2.12	108.14	113.45
4	C	1103	YW5	C18-C17-C39	2.11	133.22	128.70
3	C	1102	ANP	O3G-PG-O1G	-2.10	108.17	113.45
4	C	1103	YW5	C26-C24-N25	2.10	134.16	128.21
4	D	1103	YW5	C16-C15-C14	2.07	124.67	120.82
4	A	1103	YW5	C16-C15-C14	2.05	124.63	120.82
4	B	1103	YW5	C26-C24-N25	2.04	134.01	128.21
4	C	1103	YW5	C24-C23-N22	2.03	108.15	105.71
4	D	1103	YW5	C26-C24-N25	2.03	133.97	128.21
4	A	1103	YW5	C18-C17-C39	2.02	133.02	128.70
4	D	1103	YW5	C13-C08-C09	-2.02	115.80	118.30
4	B	1103	YW5	C01-N02-C07	-2.01	106.80	110.63
4	C	1103	YW5	C13-C08-C09	-2.01	115.82	118.30
4	D	1103	YW5	C30-C20-N19	2.00	114.35	112.07

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102	ANP	PB-N3B-PG-O1G
3	B	1102	ANP	PB-N3B-PG-O1G
3	D	1102	ANP	C5'-O5'-PA-O1A
3	B	1102	ANP	O4'-C4'-C5'-O5'
3	B	1102	ANP	C3'-C4'-C5'-O5'
3	C	1102	ANP	PB-O3A-PA-O1A
4	B	1103	YW5	C04-C05-C08-C13
4	C	1103	YW5	C10-C11-C14-C15
3	B	1102	ANP	C5'-O5'-PA-O1A
3	B	1102	ANP	C5'-O5'-PA-O2A
3	B	1102	ANP	C5'-O5'-PA-O3A
4	C	1103	YW5	C10-C11-C14-C40
4	B	1103	YW5	C04-C05-C08-C09
4	C	1103	YW5	C12-C11-C14-C15
3	A	1102	ANP	PB-O3A-PA-O1A
3	C	1102	ANP	PB-O3A-PA-O2A
3	B	1102	ANP	PB-O3A-PA-O1A
3	D	1102	ANP	PB-O3A-PA-O1A
3	B	1102	ANP	PB-O3A-PA-O2A
4	C	1103	YW5	C12-C11-C14-C40
3	A	1102	ANP	PA-O3A-PB-O1B

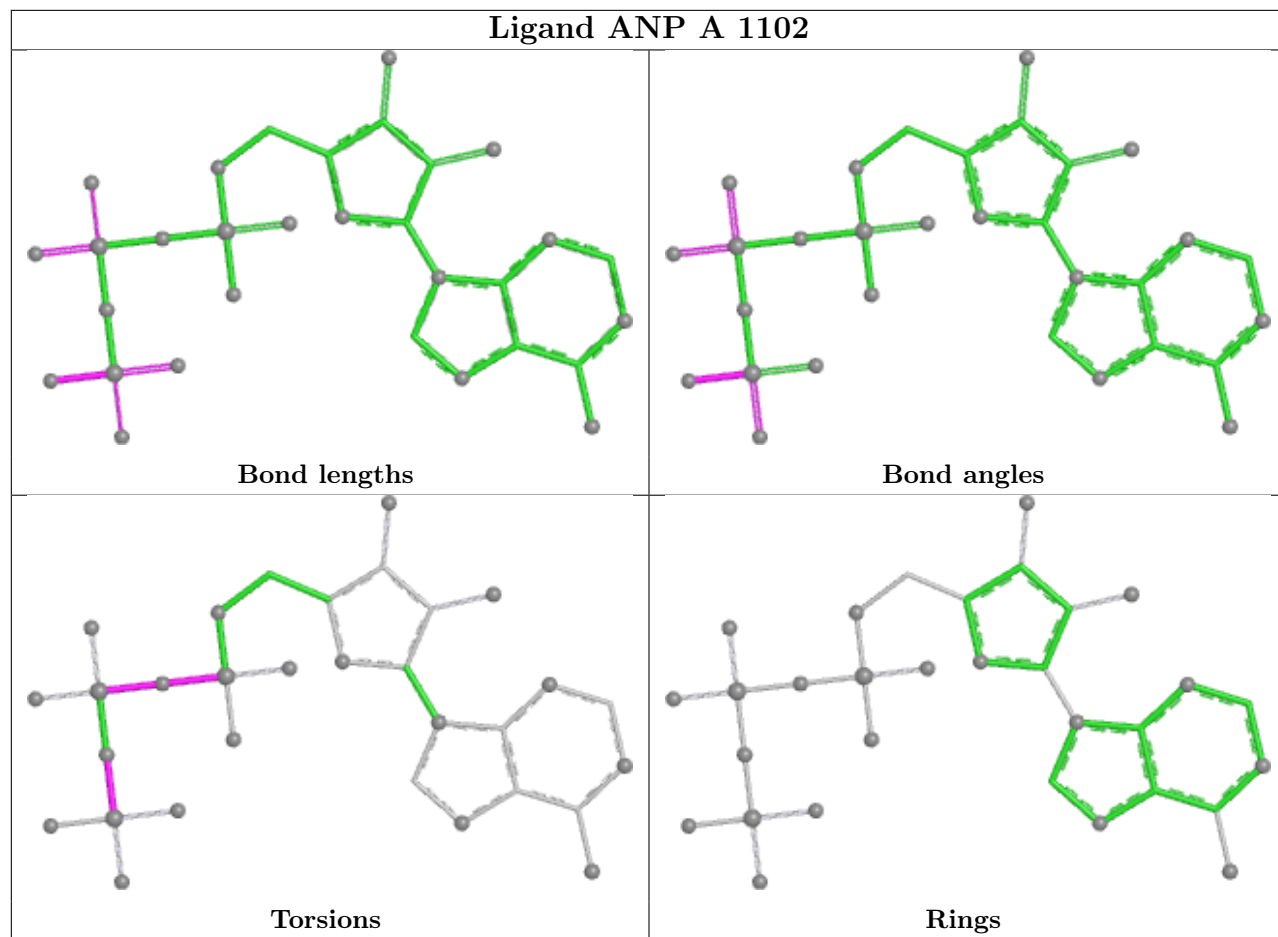
There are no ring outliers.

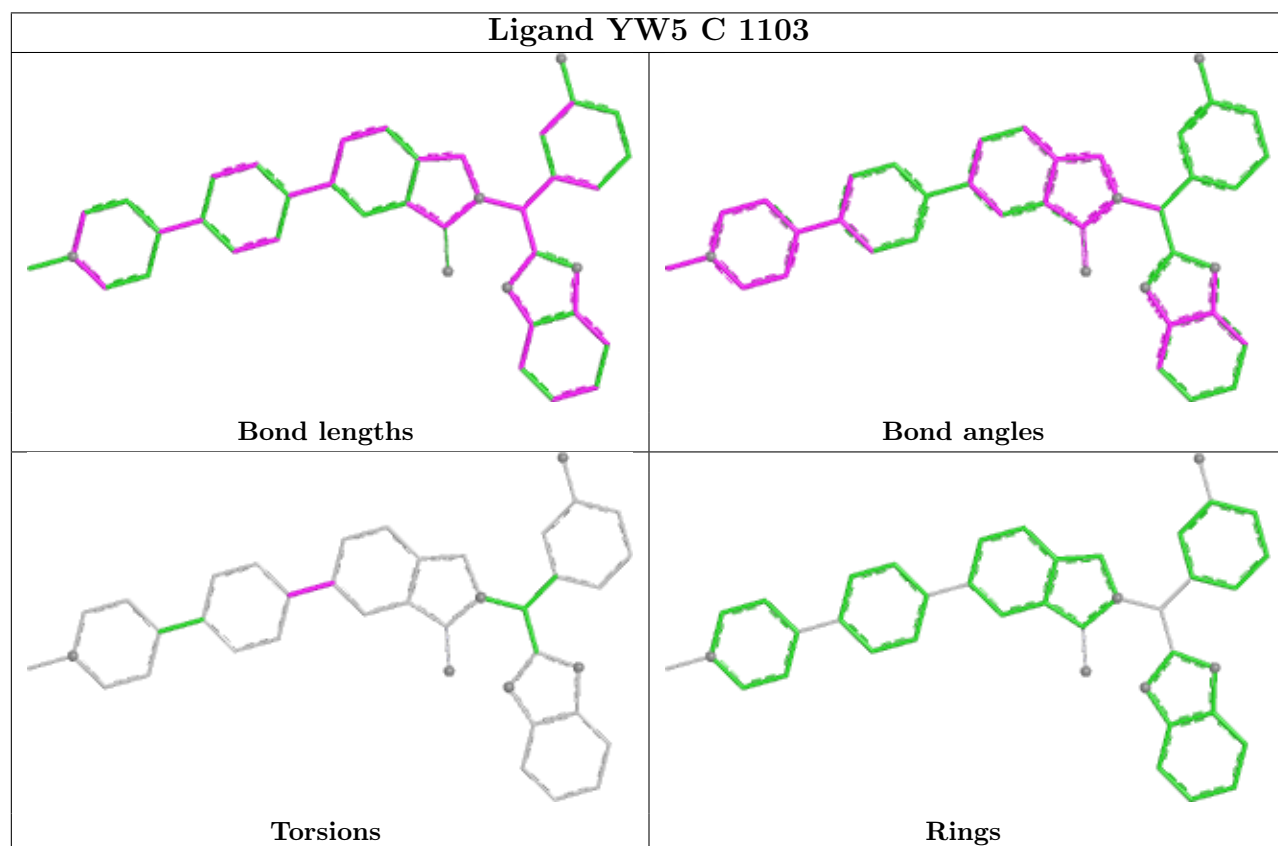
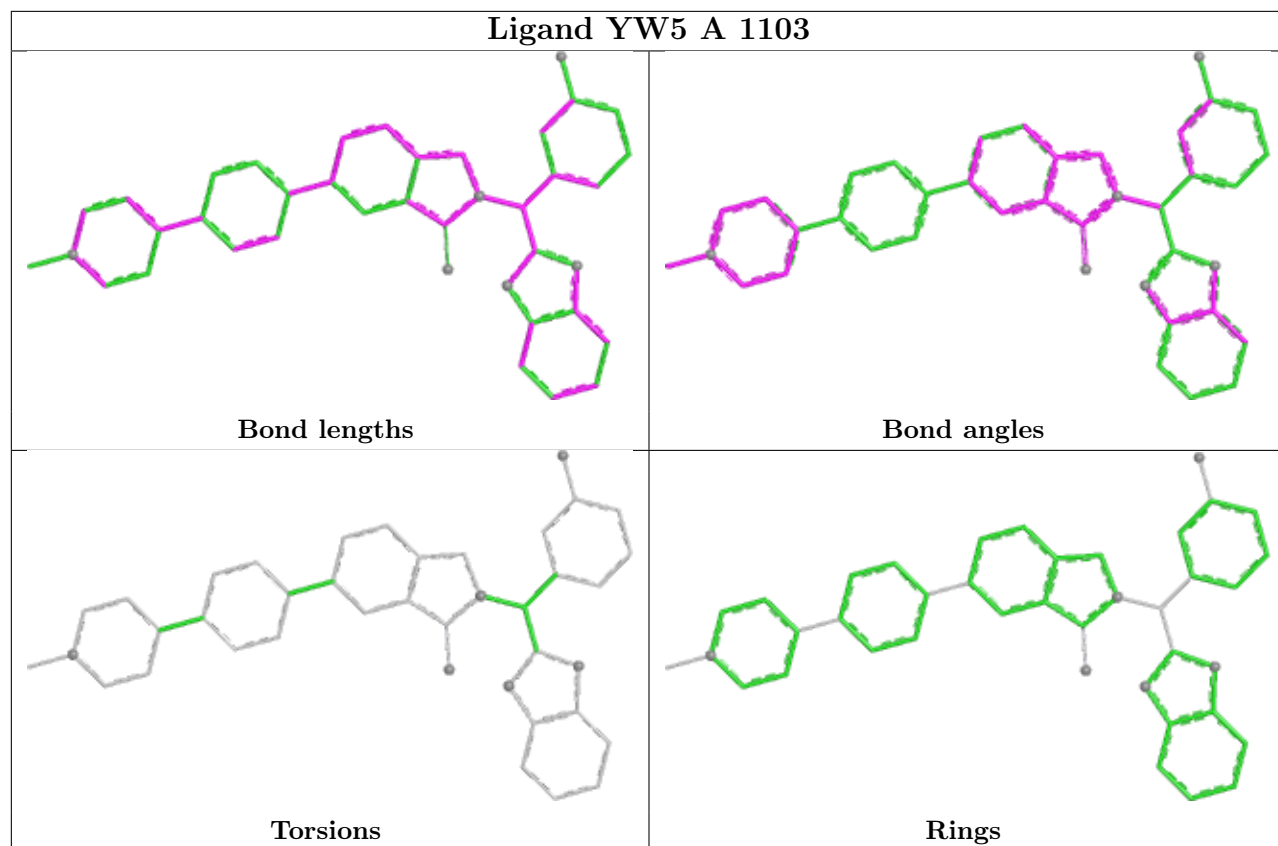
4 monomers are involved in 5 short contacts:

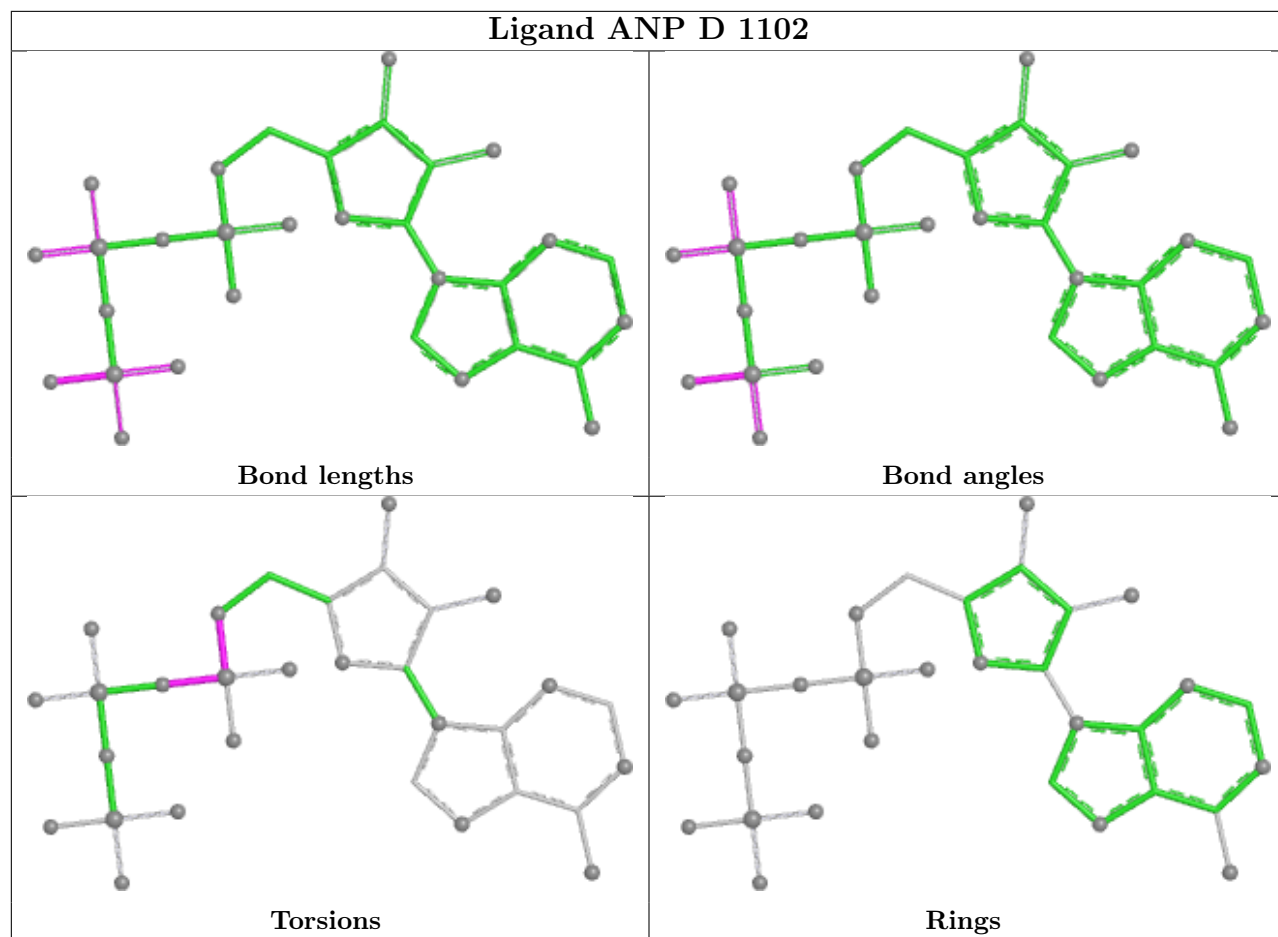
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1103	YW5	1	0
3	C	1102	ANP	1	0
4	B	1103	YW5	1	0
4	D	1103	YW5	2	0

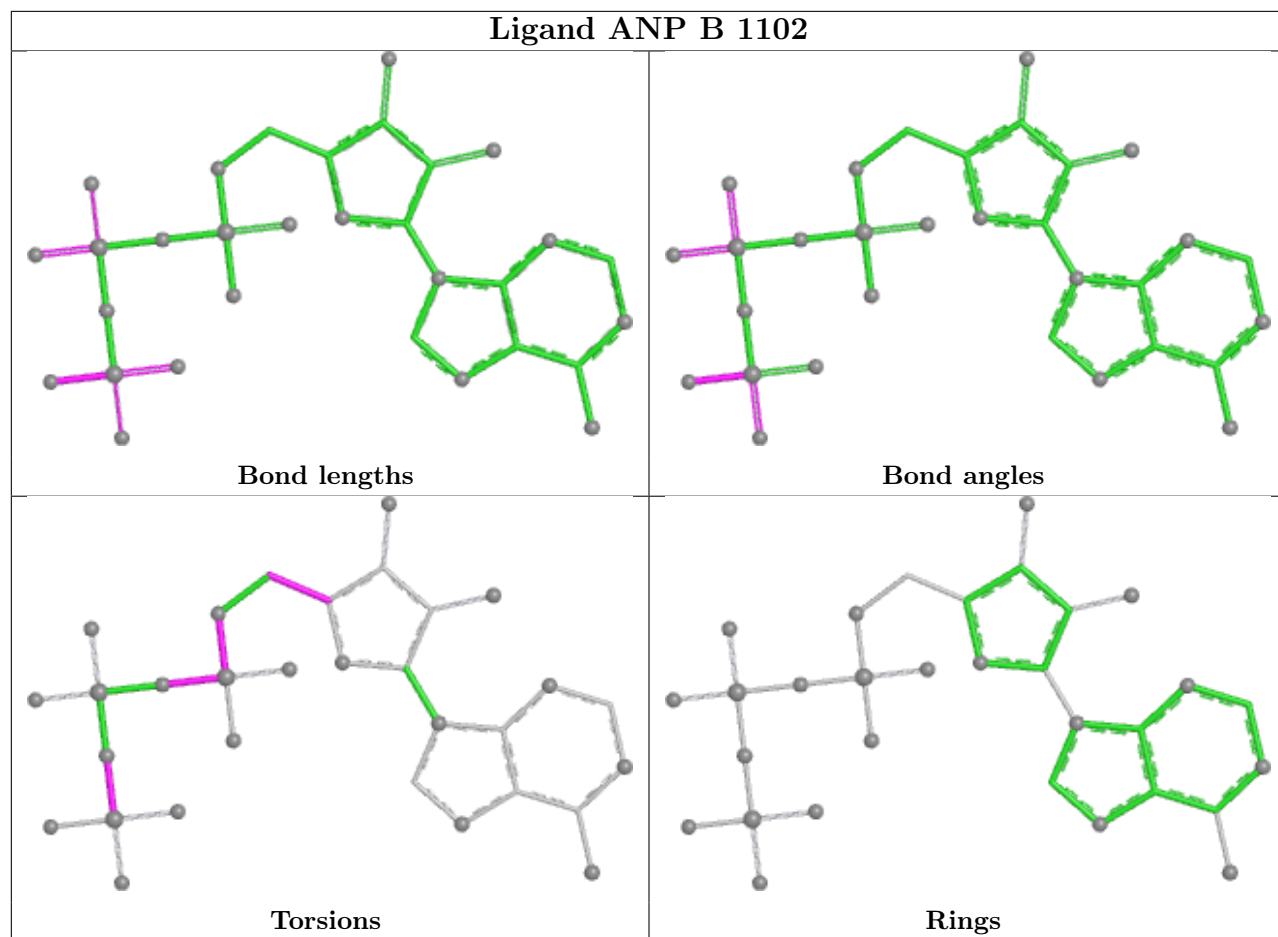
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

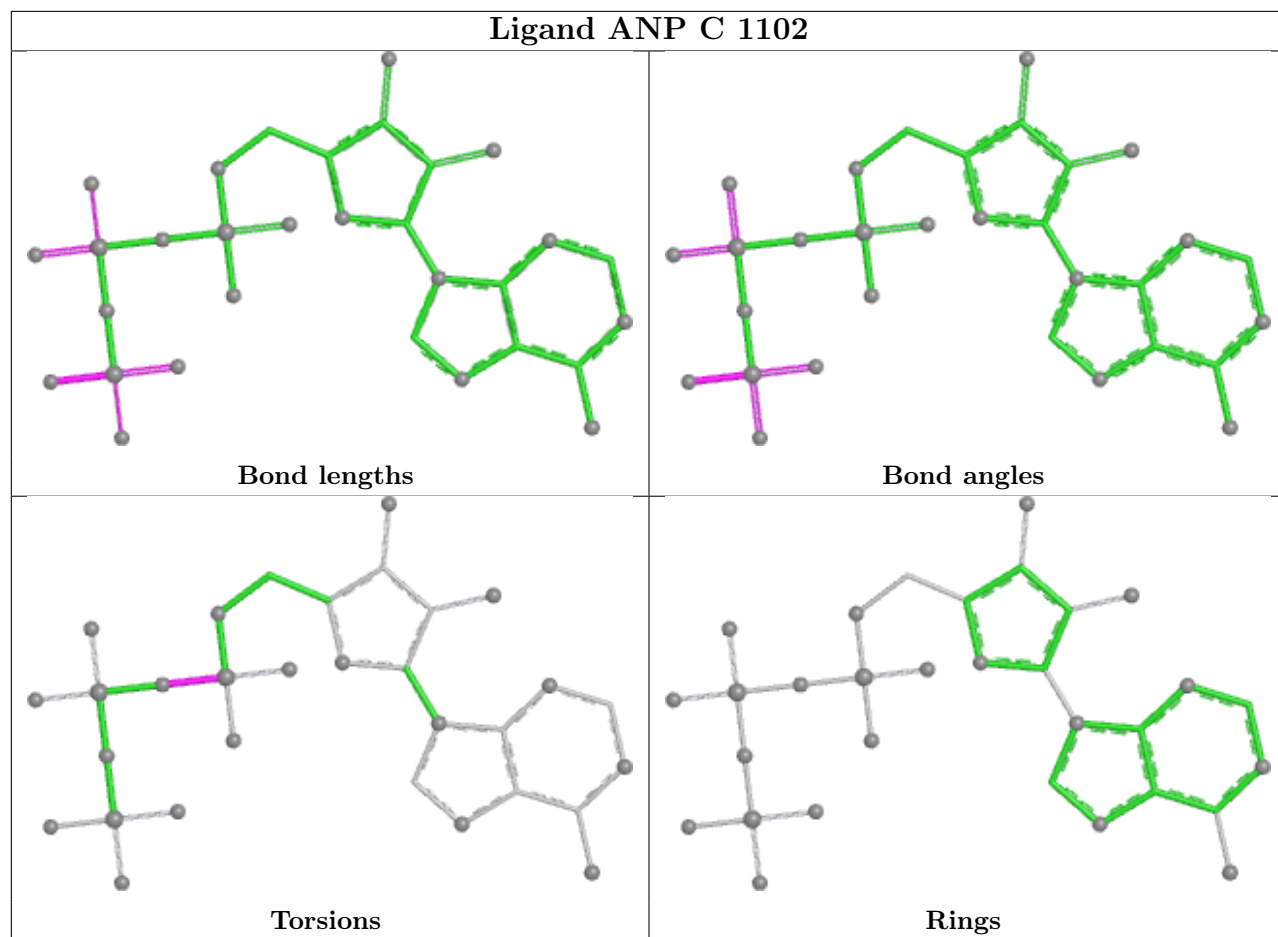




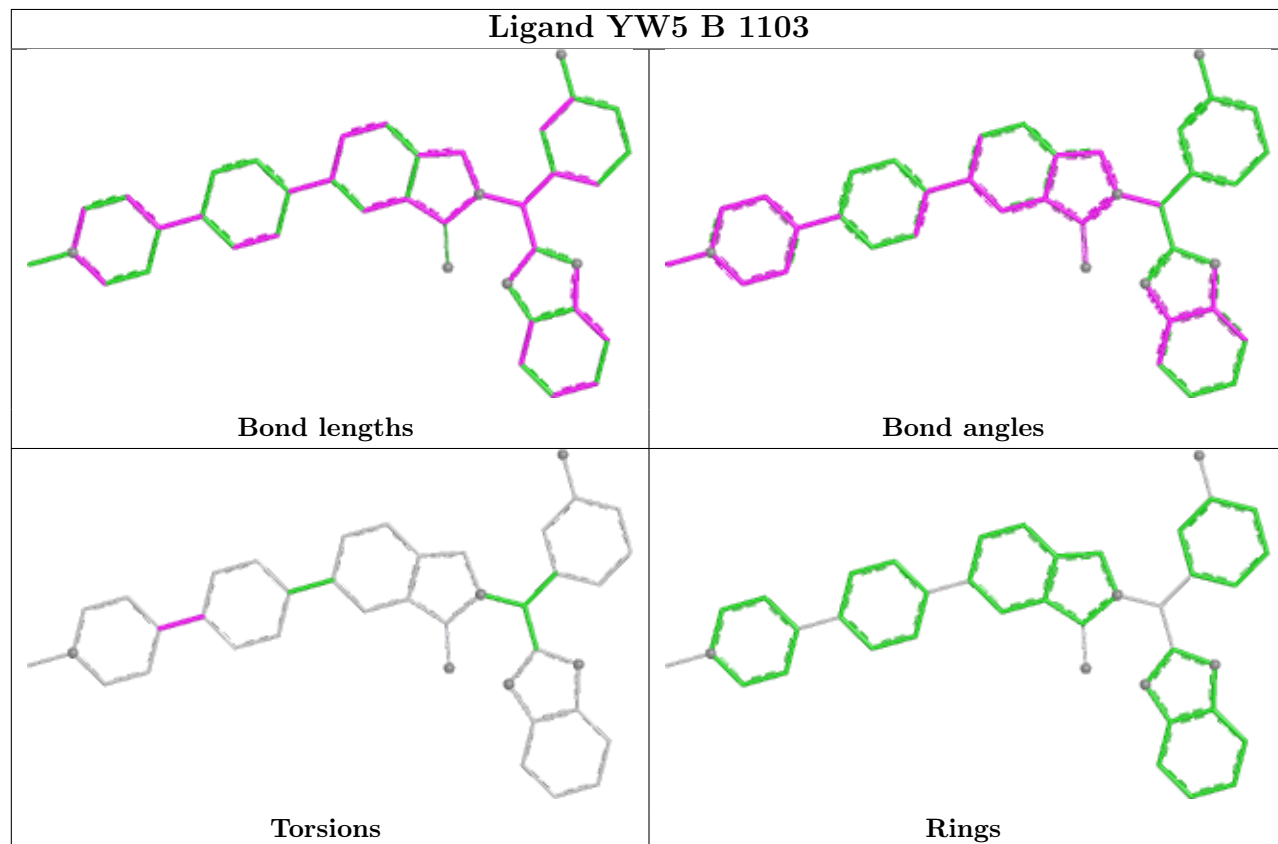


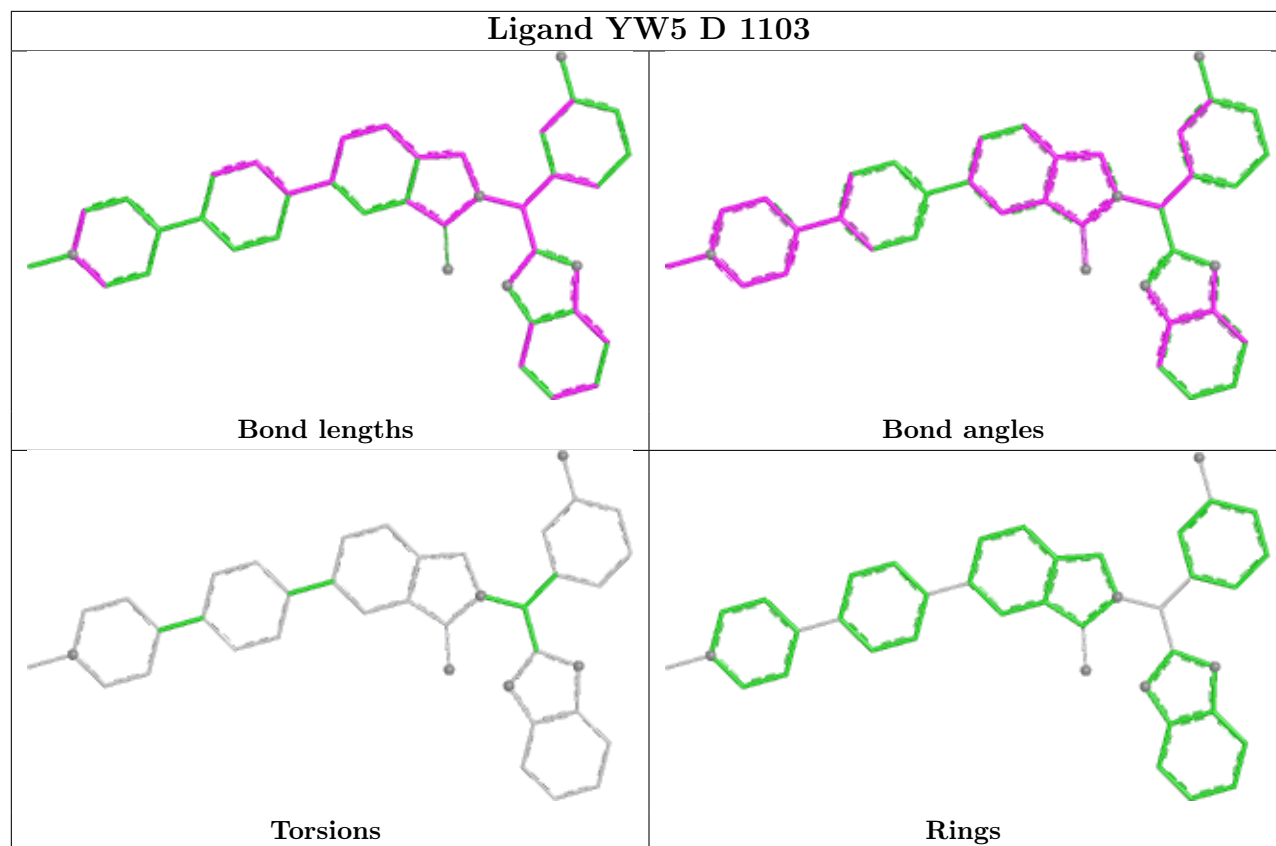


Ligand ANP C 1102



Ligand YW5 B 1103





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	292/331 (88%)	0.60	12 (4%)	41 36	31, 52, 78, 96	1 (0%)
1	B	290/331 (87%)	0.61	21 (7%)	21 17	25, 50, 78, 89	1 (0%)
1	C	297/331 (89%)	0.90	29 (9%)	13 10	30, 57, 87, 107	1 (0%)
1	D	291/331 (87%)	0.66	20 (6%)	23 18	26, 51, 86, 104	1 (0%)
All	All	1170/1324 (88%)	0.69	82 (7%)	22 18	25, 54, 83, 107	4 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	859	ALA	3.9
1	A	974	ASP	3.8
1	C	1011	VAL	3.7
1	D	720	SER	3.5
1	B	1007	MET	3.5
1	D	989	LEU	3.4
1	D	945	MET	3.3
1	C	1009	ASP	3.2
1	C	931	GLU	3.2
1	B	858	LEU	3.0
1	C	717	VAL	2.9
1	C	994	ASP	2.9
1	C	988	HIS	2.9
1	A	955	ALA	2.9
1	B	988	HIS	2.8
1	C	929	LYS	2.8
1	B	700	ASN	2.8
1	A	989	LEU	2.8
1	D	1007	MET	2.8
1	C	977	ARG	2.8
1	C	998	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	784	SER	2.7
1	D	997	PHE	2.7
1	B	715	ILE	2.7
1	C	848	PRO	2.7
1	D	990	PRO	2.6
1	C	721	GLY	2.6
1	D	716	LYS	2.6
1	C	759	ILE	2.5
1	B	786	VAL	2.5
1	D	994	ASP	2.5
1	A	1007	MET	2.5
1	D	917	GLY	2.5
1	C	715	ILE	2.5
1	B	738	VAL	2.5
1	B	926	ILE	2.4
1	C	948	ARG	2.4
1	A	707	LEU	2.4
1	A	999	ARG	2.4
1	C	1010	VAL	2.4
1	B	920	ALA	2.4
1	C	807	ASP	2.3
1	D	931	GLU	2.3
1	B	784	SER	2.3
1	C	930	GLY	2.3
1	D	1006	ASP	2.3
1	C	957	SER	2.3
1	A	876	VAL	2.3
1	D	786	VAL	2.3
1	D	859	ALA	2.2
1	B	707	LEU	2.2
1	C	707	LEU	2.2
1	C	945	MET	2.2
1	B	720	SER	2.2
1	D	706	ILE	2.2
1	D	922	GLU	2.2
1	B	723	PHE	2.2
1	D	918	ILE	2.2
1	A	807	ASP	2.2
1	B	916	ASP	2.2
1	A	990	PRO	2.2
1	B	1006	ASP	2.1
1	D	717	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	1007	MET	2.1
1	A	859	ALA	2.1
1	D	755	ALA	2.1
1	C	1001	LEU	2.1
1	D	993	THR	2.1
1	C	734	GLU	2.1
1	A	715	ILE	2.1
1	B	923	ILE	2.1
1	B	924	SER	2.1
1	B	812	GLN	2.0
1	B	750	ALA	2.0
1	D	1001	LEU	2.0
1	C	1012	ASP	2.0
1	C	723	PHE	2.0
1	A	917	GLY	2.0
1	B	716	LYS	2.0
1	B	922	GLU	2.0
1	C	731	TRP	2.0
1	C	921	SER	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(Å ²)	Q<0.9
4	YW5	B	1103	40/40	0.86	0.17	41,54,87,89	0
4	YW5	C	1103	40/40	0.88	0.15	41,52,69,71	0
4	YW5	D	1103	40/40	0.89	0.15	37,47,84,87	0
2	MG	A	1101	1/1	0.91	0.08	48,48,48,48	0

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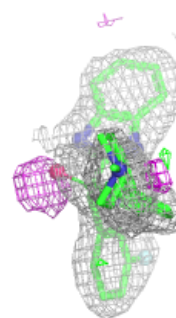
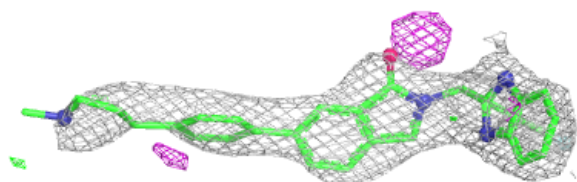
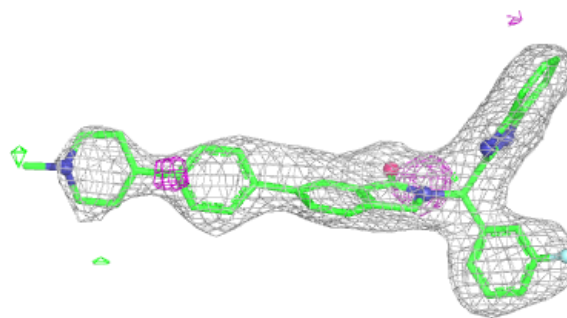
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	1101	1/1	0.92	0.10	44,44,44,44	0
3	ANP	C	1102	31/31	0.92	0.09	42,52,64,70	0
4	YW5	A	1103	40/40	0.92	0.13	36,45,72,75	0
3	ANP	A	1102	31/31	0.94	0.08	33,46,51,53	0
3	ANP	D	1102	31/31	0.95	0.08	36,44,50,57	0
3	ANP	B	1102	31/31	0.96	0.07	35,41,47,48	0
2	MG	C	1101	1/1	0.97	0.05	51,51,51,51	0
2	MG	D	1101	1/1	0.97	0.04	42,42,42,42	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.

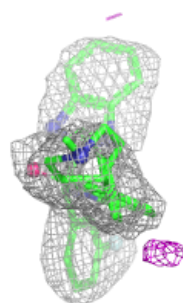
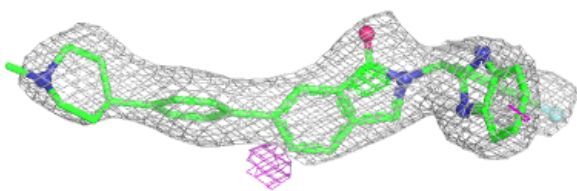
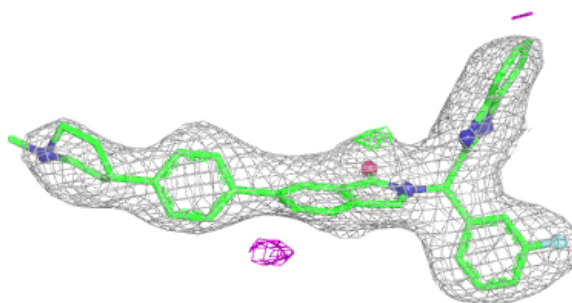
Electron density around YW5 B 1103:

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

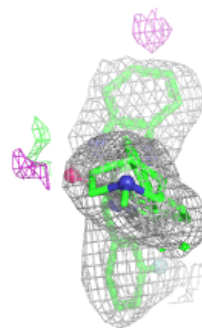
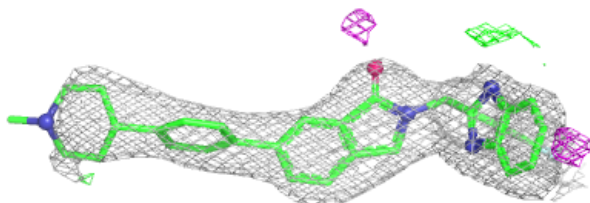
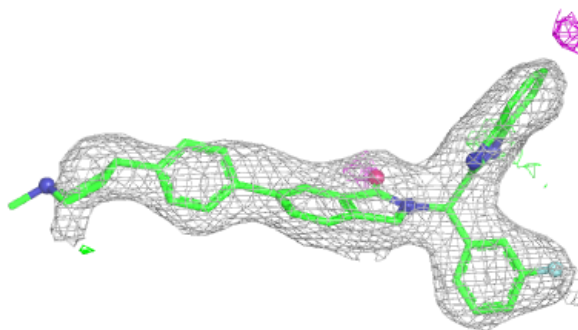


Electron density around YW5 C 1103:

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

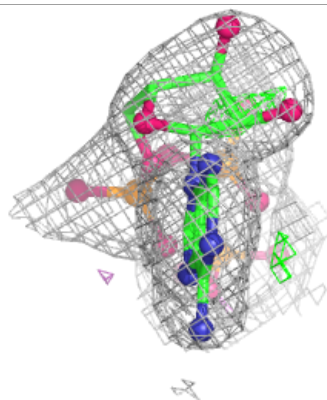
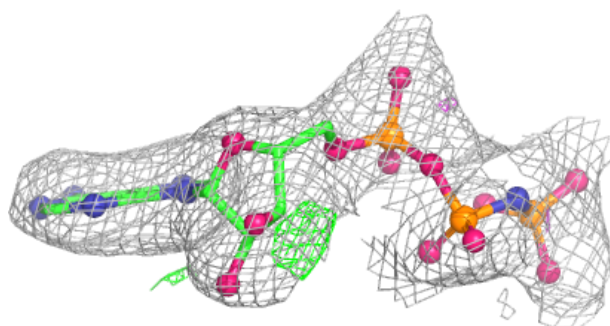
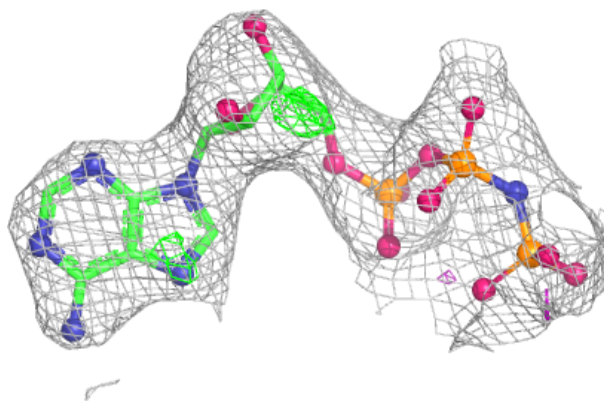
**Electron density around YW5 D 1103:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

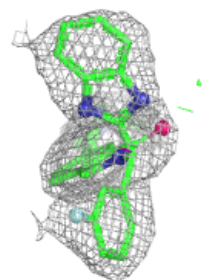
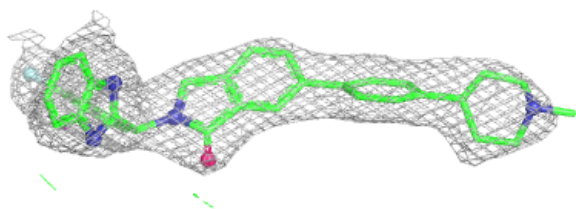
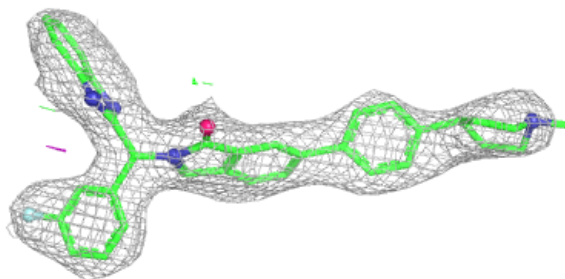


Electron density around ANP C 1102:

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

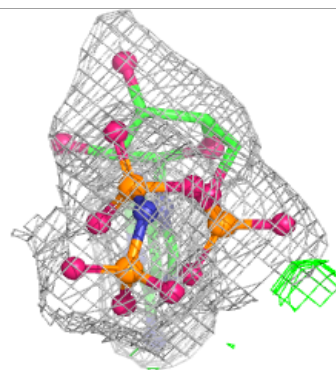
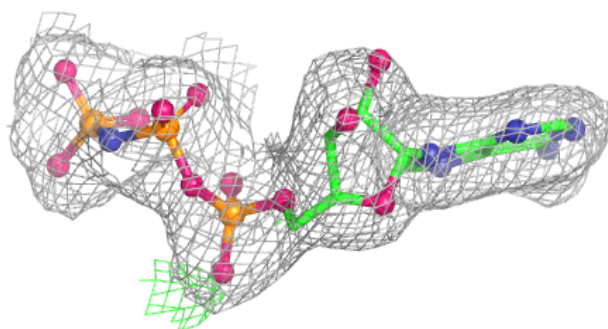
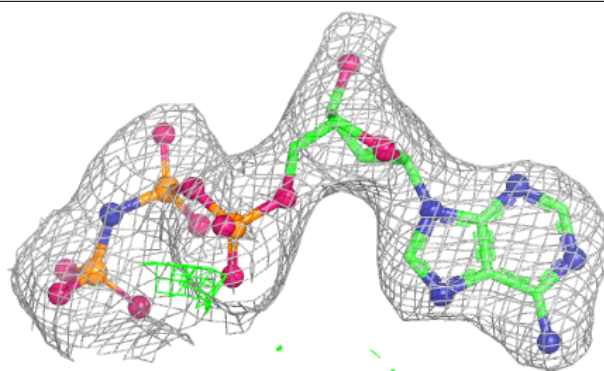
**Electron density around YW5 A 1103:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

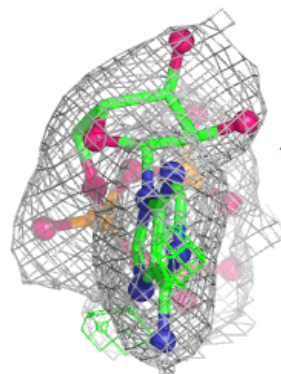
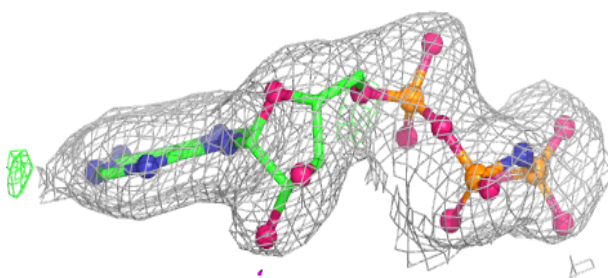
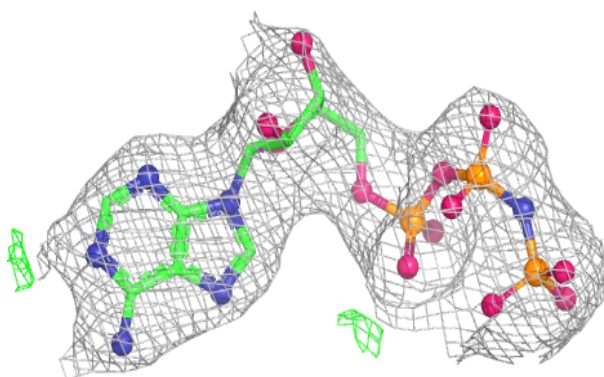


Electron density around ANP A 1102:

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and green (positive)

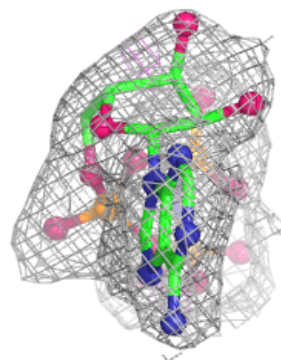
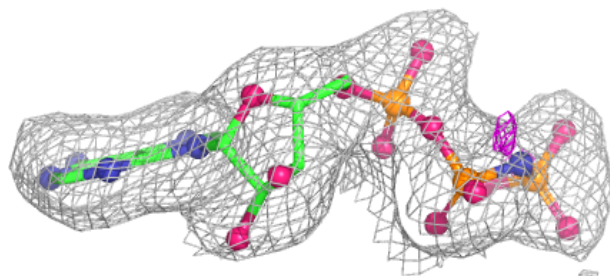
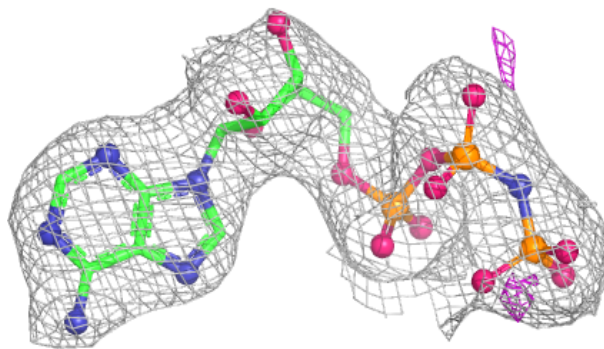
**Electron density around ANP D 1102:**

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.