



Full wwPDB X-ray Structure Validation Report

May 15, 2020 – 09:22 am BST

PDB ID : 6GEY
Title : Trypanosoma brucei PTR1 in complex with inhibitor 4g (F125)
Authors : Landi, G.; Pozzi, C.; Mangani, S.
Deposited on : 2018-04-27
Resolution : 1.56 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 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 : 2.11
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) : 2.11

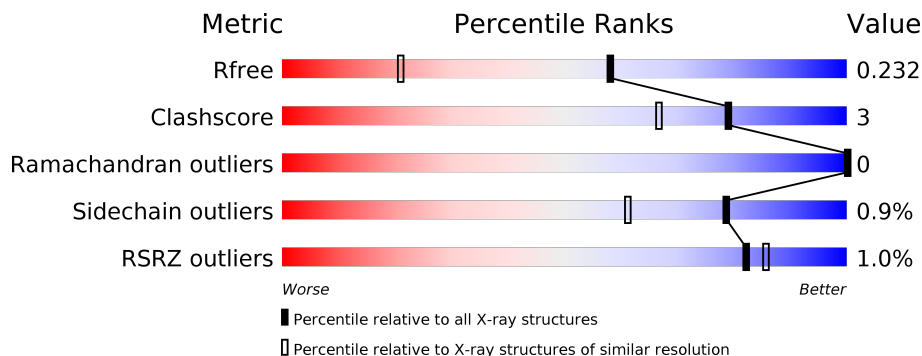
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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 on 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	288	 81% 6% 13%
1	B	288	 83% 13%
1	C	288	 79% 8% 13%
1	D	288	 81% 6% 13%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8539 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 Pteridine reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	252	1895	1195	333	356	11	0	8	0
1	B	252	1891	1191	328	360	12	0	7	0
1	C	251	1868	1174	327	356	11	0	6	0
1	D	250	1864	1178	324	350	12	0	9	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP O76290
A	-18	GLY	-	expression tag	UNP O76290
A	-17	SER	-	expression tag	UNP O76290
A	-16	SER	-	expression tag	UNP O76290
A	-15	HIS	-	expression tag	UNP O76290
A	-14	HIS	-	expression tag	UNP O76290
A	-13	HIS	-	expression tag	UNP O76290
A	-12	HIS	-	expression tag	UNP O76290
A	-11	HIS	-	expression tag	UNP O76290
A	-10	HIS	-	expression tag	UNP O76290
A	-9	SER	-	expression tag	UNP O76290
A	-8	SER	-	expression tag	UNP O76290
A	-7	GLY	-	expression tag	UNP O76290
A	-6	LEU	-	expression tag	UNP O76290
A	-5	VAL	-	expression tag	UNP O76290
A	-4	PRO	-	expression tag	UNP O76290
A	-3	ARG	-	expression tag	UNP O76290
A	-2	GLY	-	expression tag	UNP O76290
A	-1	SER	-	expression tag	UNP O76290
A	0	HIS	-	expression tag	UNP O76290
B	-19	MET	-	initiating methionine	UNP O76290

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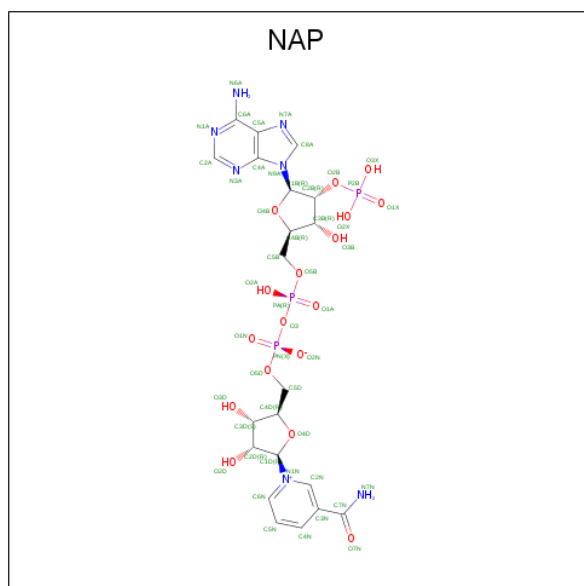
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP O76290
B	-17	SER	-	expression tag	UNP O76290
B	-16	SER	-	expression tag	UNP O76290
B	-15	HIS	-	expression tag	UNP O76290
B	-14	HIS	-	expression tag	UNP O76290
B	-13	HIS	-	expression tag	UNP O76290
B	-12	HIS	-	expression tag	UNP O76290
B	-11	HIS	-	expression tag	UNP O76290
B	-10	HIS	-	expression tag	UNP O76290
B	-9	SER	-	expression tag	UNP O76290
B	-8	SER	-	expression tag	UNP O76290
B	-7	GLY	-	expression tag	UNP O76290
B	-6	LEU	-	expression tag	UNP O76290
B	-5	VAL	-	expression tag	UNP O76290
B	-4	PRO	-	expression tag	UNP O76290
B	-3	ARG	-	expression tag	UNP O76290
B	-2	GLY	-	expression tag	UNP O76290
B	-1	SER	-	expression tag	UNP O76290
B	0	HIS	-	expression tag	UNP O76290
C	-19	MET	-	initiating methionine	UNP O76290
C	-18	GLY	-	expression tag	UNP O76290
C	-17	SER	-	expression tag	UNP O76290
C	-16	SER	-	expression tag	UNP O76290
C	-15	HIS	-	expression tag	UNP O76290
C	-14	HIS	-	expression tag	UNP O76290
C	-13	HIS	-	expression tag	UNP O76290
C	-12	HIS	-	expression tag	UNP O76290
C	-11	HIS	-	expression tag	UNP O76290
C	-10	HIS	-	expression tag	UNP O76290
C	-9	SER	-	expression tag	UNP O76290
C	-8	SER	-	expression tag	UNP O76290
C	-7	GLY	-	expression tag	UNP O76290
C	-6	LEU	-	expression tag	UNP O76290
C	-5	VAL	-	expression tag	UNP O76290
C	-4	PRO	-	expression tag	UNP O76290
C	-3	ARG	-	expression tag	UNP O76290
C	-2	GLY	-	expression tag	UNP O76290
C	-1	SER	-	expression tag	UNP O76290
C	0	HIS	-	expression tag	UNP O76290
D	-19	MET	-	initiating methionine	UNP O76290
D	-18	GLY	-	expression tag	UNP O76290
D	-17	SER	-	expression tag	UNP O76290

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP O76290
D	-15	HIS	-	expression tag	UNP O76290
D	-14	HIS	-	expression tag	UNP O76290
D	-13	HIS	-	expression tag	UNP O76290
D	-12	HIS	-	expression tag	UNP O76290
D	-11	HIS	-	expression tag	UNP O76290
D	-10	HIS	-	expression tag	UNP O76290
D	-9	SER	-	expression tag	UNP O76290
D	-8	SER	-	expression tag	UNP O76290
D	-7	GLY	-	expression tag	UNP O76290
D	-6	LEU	-	expression tag	UNP O76290
D	-5	VAL	-	expression tag	UNP O76290
D	-4	PRO	-	expression tag	UNP O76290
D	-3	ARG	-	expression tag	UNP O76290
D	-2	GLY	-	expression tag	UNP O76290
D	-1	SER	-	expression tag	UNP O76290
D	0	HIS	-	expression tag	UNP O76290

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



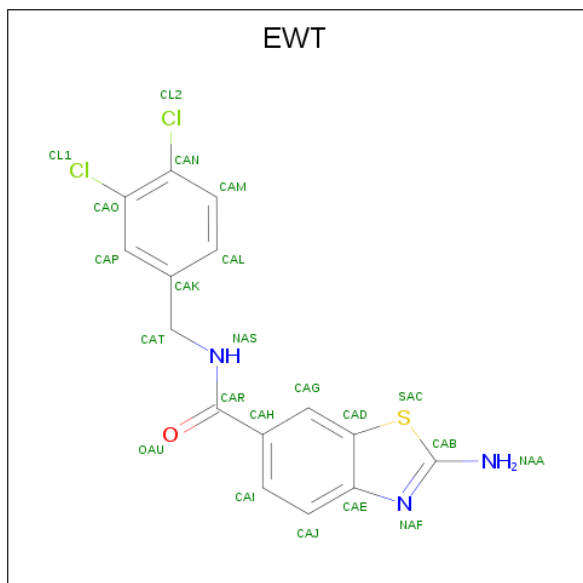
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
			Total	C	N	O			P	
2	A	1	Total	48	21	7	17	3	0	0
2	B	1	Total	48	21	7	17	3	0	0

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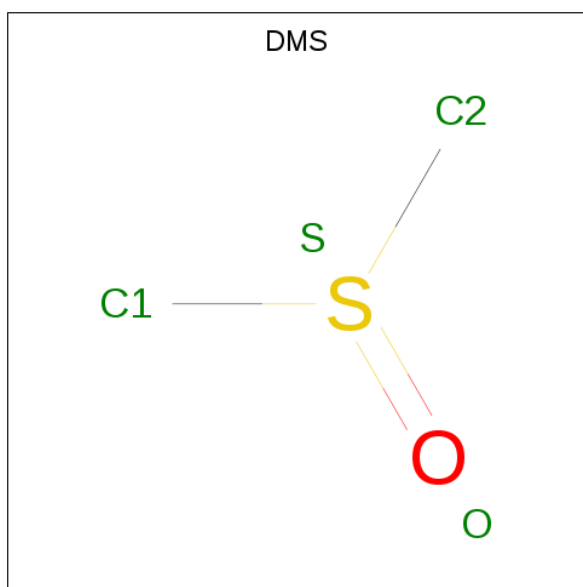
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 2-azanyl- {N}-[(3,4-dichlorophenyl)methyl]-1,3-benzothiazole-6-carboxamide (three-letter code: EWT) (formula: C₁₅H₁₁Cl₂N₃OS).



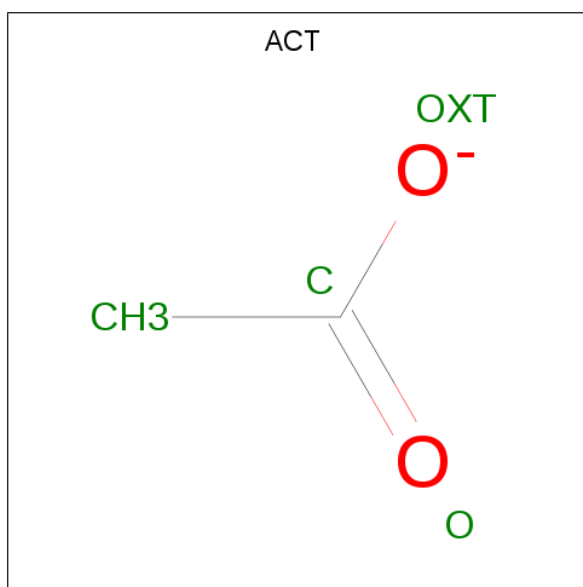
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	Cl	N	O	S	0	0
			22	15	2	3	1	1		
3	B	1	Total	C	Cl	N	O	S	0	0
			22	15	2	3	1	1		
3	C	1	Total	C	Cl	N	O	S	0	0
			22	15	2	3	1	1		
3	D	1	Total	C	Cl	N	O	S	0	0
			22	15	2	3	1	1		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	1
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	2	2		

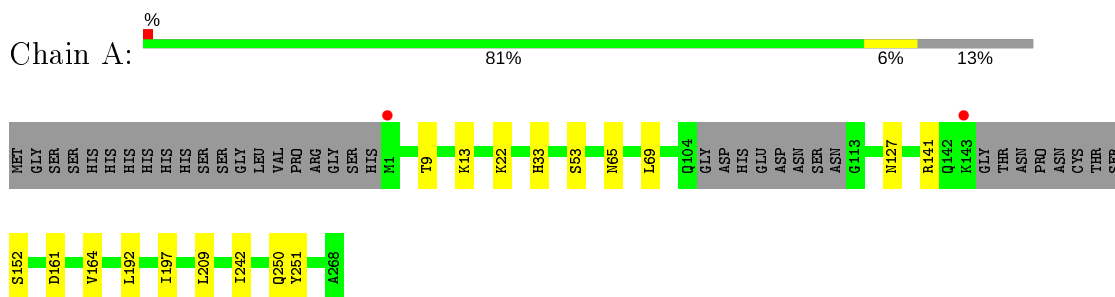
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	190	Total 192	O 192	0	2
6	B	201	Total 203	O 203	0	6
6	C	153	Total 153	O 153	0	1
6	D	177	Total 177	O 177	0	0

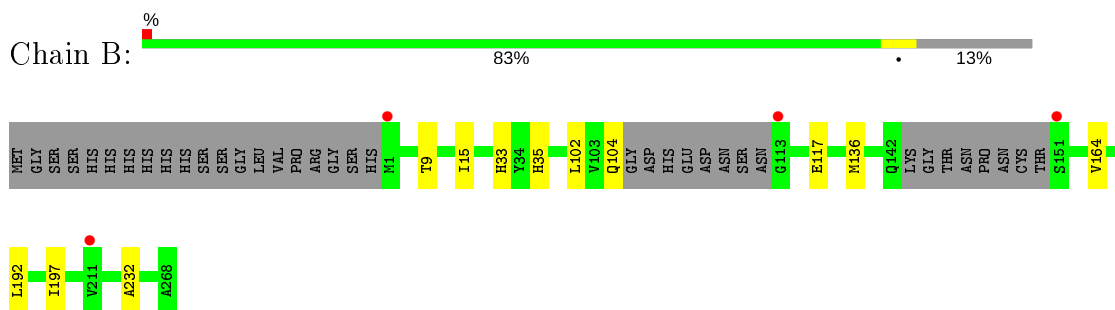
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

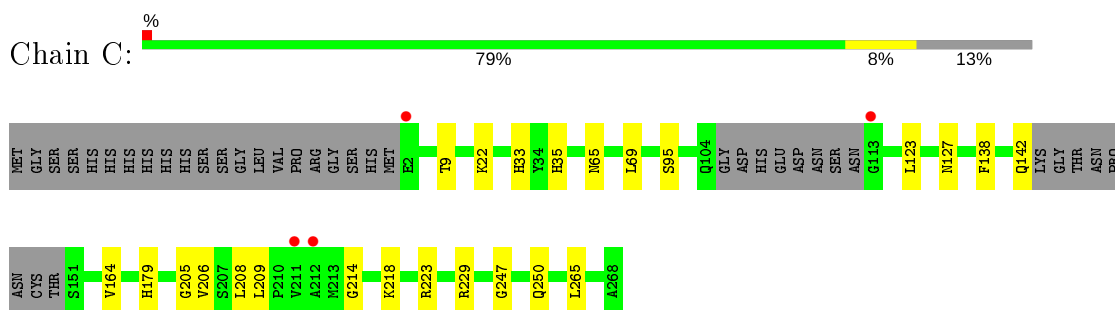
- Molecule 1: Pteridine reductase



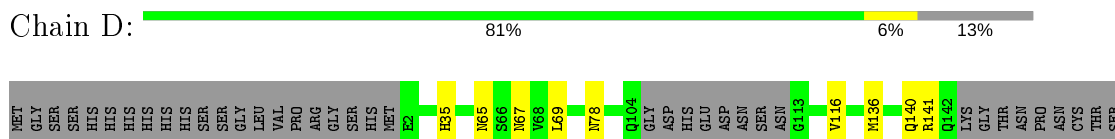
- Molecule 1: Pteridine reductase



- Molecule 1: Pteridine reductase



- Molecule 1: Pteridine reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.71Å 89.97Å 82.76Å 90.00° 115.55° 90.00°	Depositor
Resolution (Å)	67.41 – 1.56 67.41 – 1.56	Depositor EDS
% Data completeness (in resolution range)	89.6 (67.41-1.56) 89.6 (67.41-1.56)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 1.56Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.174 , 0.211 0.200 , 0.232	Depositor DCC
R_{free} test set	6300 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtrriage
Anisotropy	0.767	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8539	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.03 % 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 6.2192e-04. 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: ACT, NAP, DMS, EWT

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	0.97	0/1943	0.87	0/2636
1	B	1.04	0/1933	0.91	0/2626
1	C	1.02	0/1907	0.89	0/2593
1	D	1.00	0/1915	0.88	0/2602
All	All	1.01	0/7698	0.89	0/10457

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	1895	0	1928	11	0
1	B	1891	0	1896	10	0
1	C	1868	0	1860	16	0
1	D	1864	0	1883	13	0
2	A	48	0	25	0	0
2	B	48	0	25	2	0
2	C	48	0	25	3	0
2	D	48	0	25	1	0
3	A	22	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	22	0	0	0	0
3	C	22	0	0	0	0
3	D	22	0	0	1	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	D	4	0	6	0	0
5	C	4	0	3	0	0
6	A	192	0	0	3	0
6	B	203	0	0	0	0
6	C	153	0	0	1	0
6	D	177	0	0	1	0
All	All	8539	0	7688	43	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 3.

All (43) 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:D:152:SER:HB2	6:D:551:HOH:O	1.78	0.83
1:D:164:VAL:HG22	1:D:179:HIS:CD2	2.22	0.75
1:C:164:VAL:HG22	1:C:179:HIS:CD2	2.26	0.70
1:D:206[B]:VAL:HG21	1:D:209:LEU:HD21	1.80	0.64
1:B:104:GLN:H	1:D:140[B]:GLN:HE22	1.51	0.58
1:C:214:GLY:O	1:C:218:LYS:HG3	2.03	0.58
1:D:206[B]:VAL:CG2	1:D:209:LEU:HD21	2.38	0.54
1:A:22[A]:LYS:HG2	1:A:242:ILE:HG13	1.90	0.53
1:A:65:ASN:HA	1:A:69:LEU:HD22	1.91	0.52
1:C:206:VAL:HG23	1:C:209:LEU:HD13	1.93	0.49
1:B:136[B]:MET:HE1	1:D:116:VAL:HG21	1.95	0.49
1:A:9:THR:HA	1:A:33:HIS:HB3	1.94	0.48
1:D:78:ASN:OD1	1:D:141:ARG:NH1	2.42	0.48
1:B:15:ILE:HB	2:B:301:NAP:H51N	1.96	0.48
1:D:65:ASN:HA	1:D:69:LEU:HD22	1.95	0.47
1:C:9:THR:HA	1:C:33:HIS:HB3	1.97	0.47
1:B:9:THR:HA	1:B:33:HIS:HB3	1.97	0.46
1:A:127:ASN:HA	6:A:405:HOH:O	2.16	0.46
1:A:141:ARG:HG3	6:A:438:HOH:O	2.15	0.45
1:C:35:HIS:HB2	2:C:301:NAP:C2A	2.46	0.45
1:C:208:LEU:HD21	6:C:467:HOH:O	2.15	0.45
1:A:22[B]:LYS:HG3	6:A:505:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:LEU:O	1:D:136[B]:MET:HG3	2.16	0.45
1:D:221:TRP:NE1	3:D:302:EWT:CL1	2.87	0.44
1:B:35:HIS:HB2	2:B:301:NAP:C2A	2.46	0.44
1:C:95:SER:HB3	2:C:301:NAP:H3D	1.99	0.44
1:B:117:GLU:HG3	1:D:67:ASN:HA	1.99	0.43
1:C:265:LEU:HD11	1:D:254:GLY:HA3	2.01	0.43
1:D:35:HIS:HB2	2:D:301:NAP:C2A	2.49	0.42
1:A:161:ASP:HB3	1:A:164:VAL:HG13	2.00	0.42
1:C:65:ASN:HA	1:C:69:LEU:HD22	2.01	0.42
1:A:13[B]:LYS:HB3	1:A:13[B]:LYS:HE3	1.88	0.42
1:C:209:LEU:HG	1:C:218:LYS:HG2	2.02	0.42
1:C:247:GLY:HA2	1:C:250:GLN:HG3	2.02	0.42
1:A:192:LEU:HB3	1:A:197:ILE:HB	2.01	0.41
1:B:192:LEU:HB3	1:B:197:ILE:HB	2.03	0.41
1:A:251:TYR:CD2	1:B:232:ALA:HB2	2.55	0.41
1:C:123:LEU:O	1:C:127[B]:ASN:HB2	2.20	0.41
1:A:251:TYR:CE2	1:B:232:ALA:HB2	2.56	0.41
1:C:205:GLY:O	2:C:301:NAP:H4N	2.21	0.41
1:C:223:ARG:O	1:C:229:ARG:NH1	2.41	0.41
1:C:138:PHE:O	1:C:142:GLN:HG2	2.21	0.40
1:C:164:VAL:HG22	1:C:179:HIS:NE2	2.37	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	253/288 (88%)	244 (96%)	9 (4%)	0	100	100
1	B	253/288 (88%)	246 (97%)	7 (3%)	0	100	100
1	C	251/288 (87%)	242 (96%)	9 (4%)	0	100	100
1	D	252/288 (88%)	244 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1009/1152 (88%)	976 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	202/231 (87%)	198 (98%)	4 (2%)	55	26
1	B	199/231 (86%)	198 (100%)	1 (0%)	88	78
1	C	195/231 (84%)	194 (100%)	1 (0%)	88	78
1	D	197/231 (85%)	195 (99%)	2 (1%)	76	57
All	All	793/924 (86%)	785 (99%)	8 (1%)	78	57

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	SER
1	A	152	SER
1	A	209	LEU
1	A	250[A]	GLN
1	B	164	VAL
1	C	22	LYS
1	D	215[A]	GLU
1	D	215[B]	GLU

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

Mol	Chain	Res	Type
1	A	25	GLN
1	A	166	GLN
1	B	65	ASN
1	B	166	GLN

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Mol	Chain	Res	Type
1	B	250	GLN
1	D	67	ASN
1	D	127	ASN
1	D	140[B]	GLN
1	D	166	GLN
1	D	186	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	B	301	-	45,52,52	1.36	6 (13%)	56,80,80	1.49	10 (17%)
3	EWT	C	302	-	21,24,24	1.71	4 (19%)	29,34,34	1.94	8 (27%)
3	EWT	A	302	-	21,24,24	2.41	6 (28%)	29,34,34	1.86	8 (27%)
4	DMS	B	303	-	3,3,3	0.30	0	3,3,3	1.81	1 (33%)
3	EWT	D	302	-	21,24,24	1.83	6 (28%)	29,34,34	1.43	5 (17%)
4	DMS	D	303	-	3,3,3	0.41	0	3,3,3	1.56	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	C	301	-	45,52,52	1.23	4 (8%)	56,80,80	1.52	9 (16%)
5	ACT	C	303	-	1,3,3	1.36	0	0,3,3	0.00	-
2	NAP	A	301	-	45,52,52	1.64	12 (26%)	56,80,80	1.49	10 (17%)
2	NAP	D	301	-	45,52,52	1.47	7 (15%)	56,80,80	1.62	13 (23%)
4	DMS	A	303[A]	-	3,3,3	0.59	0	3,3,3	0.75	0
3	EWT	B	302	-	21,24,24	1.90	7 (33%)	29,34,34	1.32	5 (17%)

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	EWT	B	302	-	-	0/9/9/9	0/3/3/3
3	EWT	C	302	-	-	0/9/9/9	0/3/3/3
3	EWT	A	302	-	-	0/9/9/9	0/3/3/3
3	EWT	D	302	-	-	0/9/9/9	0/3/3/3
2	NAP	C	301	-	-	0/31/67/67	0/5/5/5
2	NAP	A	301	-	-	0/31/67/67	0/5/5/5
2	NAP	D	301	-	-	0/31/67/67	0/5/5/5
2	NAP	B	301	-	-	0/31/67/67	0/5/5/5

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	EWT	CAO-CL1	5.87	1.87	1.73
3	A	302	EWT	CAT-CAK	-4.68	1.41	1.51
3	A	302	EWT	CAH-CAR	-4.59	1.40	1.50
3	C	302	EWT	CAT-CAK	-4.33	1.42	1.51
2	B	301	NAP	C2A-N3A	4.21	1.38	1.32
3	D	302	EWT	CAH-CAR	-4.07	1.41	1.50
2	A	301	NAP	C2A-N3A	3.95	1.38	1.32
3	D	302	EWT	CAT-CAK	-3.89	1.43	1.51
3	A	302	EWT	CAJ-CAE	-3.75	1.35	1.41
3	B	302	EWT	CAT-CAK	-3.70	1.43	1.51
2	A	301	NAP	O4D-C1D	3.69	1.46	1.41
3	B	302	EWT	CAJ-CAE	-3.43	1.35	1.41
2	D	301	NAP	C2A-N3A	3.42	1.37	1.32
2	C	301	NAP	C5A-C4A	3.29	1.49	1.40
2	D	301	NAP	O4D-C1D	3.20	1.45	1.41
2	D	301	NAP	P2B-O2B	3.18	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAP	C5A-C4A	3.09	1.49	1.40
2	C	301	NAP	C2A-N3A	3.09	1.37	1.32
2	B	301	NAP	O4D-C1D	3.04	1.45	1.41
3	C	302	EWT	CAG-CAH	3.03	1.42	1.37
3	B	302	EWT	CAN-CL2	2.97	1.80	1.73
2	A	301	NAP	C7N-N7N	2.96	1.38	1.33
3	C	302	EWT	CAJ-CAE	-2.95	1.36	1.41
3	B	302	EWT	CAG-CAH	2.88	1.42	1.37
2	D	301	NAP	C7N-N7N	2.87	1.38	1.33
3	A	302	EWT	CAP-CAO	2.83	1.43	1.38
2	D	301	NAP	C4A-N3A	2.76	1.39	1.35
3	B	302	EWT	CAJ-CAI	2.76	1.42	1.36
2	A	301	NAP	C2N-N1N	2.75	1.38	1.35
2	D	301	NAP	C5A-C4A	2.72	1.48	1.40
3	D	302	EWT	CAI-CAH	2.72	1.44	1.39
2	B	301	NAP	C5A-C4A	2.70	1.48	1.40
2	A	301	NAP	C2A-N1A	2.67	1.38	1.33
3	D	302	EWT	CAG-CAH	2.57	1.41	1.37
2	A	301	NAP	P2B-O2B	2.55	1.64	1.59
2	B	301	NAP	C7N-N7N	2.53	1.37	1.33
2	C	301	NAP	C2N-N1N	2.48	1.38	1.35
3	B	302	EWT	CAH-CAR	-2.47	1.45	1.50
2	B	301	NAP	C2N-N1N	2.45	1.37	1.35
2	B	301	NAP	O4B-C4B	-2.45	1.39	1.45
2	A	301	NAP	C5N-C4N	2.43	1.44	1.38
3	A	302	EWT	CAP-CAK	2.38	1.43	1.39
2	C	301	NAP	C2A-N1A	2.37	1.38	1.33
2	D	301	NAP	C2A-N1A	2.36	1.38	1.33
3	D	302	EWT	CAJ-CAE	-2.35	1.37	1.41
3	C	302	EWT	CAH-CAR	-2.33	1.45	1.50
2	A	301	NAP	O4B-C1B	2.28	1.44	1.41
3	D	302	EWT	CAJ-CAI	2.21	1.41	1.36
3	B	302	EWT	CAI-CAH	2.14	1.43	1.39
2	A	301	NAP	C6A-C5A	2.10	1.51	1.43
2	A	301	NAP	C4A-N3A	2.07	1.38	1.35
2	A	301	NAP	C8A-N7A	2.06	1.38	1.34

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NAP	O7N-C7N-C3N	-5.55	112.99	119.63
2	A	301	NAP	C1B-N9A-C4A	-4.98	117.89	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
2	D	301	NAP	C1B-N9A-C4A	-4.83	118.16	126.64
3	C	302	EWT	CAP-CAO-CL1	4.69	126.07	118.49
3	C	302	EWT	CAE-CAD-SAC	-4.59	105.76	111.85
2	C	301	NAP	C1B-N9A-C4A	-4.50	118.73	126.64
2	B	301	NAP	C1B-N9A-C4A	-4.46	118.80	126.64
2	C	301	NAP	C3N-C7N-N7N	4.29	122.89	117.75
3	A	302	EWT	CAK-CAT-NAS	-4.09	104.28	113.05
3	A	302	EWT	CAP-CAO-CL1	3.77	124.57	118.49
3	A	302	EWT	CAJ-CAI-CAH	-3.71	116.60	120.79
2	B	301	NAP	C3N-C7N-N7N	3.47	121.91	117.75
3	C	302	EWT	CAG-CAD-SAC	3.37	131.84	125.10
2	A	301	NAP	O7N-C7N-C3N	-3.34	115.64	119.63
2	A	301	NAP	N3A-C2A-N1A	-3.30	123.52	128.68
3	C	302	EWT	CAI-CAH-CAG	-3.28	115.32	119.23
2	B	301	NAP	C2A-N1A-C6A	3.21	124.24	118.75
2	B	301	NAP	N3A-C2A-N1A	-3.18	123.71	128.68
2	D	301	NAP	N3A-C2A-N1A	-3.17	123.72	128.68
4	B	303	DMS	O-S-C1	3.14	122.56	106.54
3	A	302	EWT	CAD-CAE-NAF	2.99	115.00	108.04
2	B	301	NAP	O2A-PA-O1A	2.95	126.83	112.24
3	C	302	EWT	CAN-CAO-CL1	-2.94	113.66	120.85
3	D	302	EWT	OAU-CAR-NAS	-2.90	116.83	122.61
2	C	301	NAP	O2B-P2B-O1X	-2.89	98.25	109.39
2	C	301	NAP	C4A-C5A-N7A	-2.88	106.39	109.40
3	A	302	EWT	CAT-CAK-CAL	-2.83	115.04	120.91
2	D	301	NAP	C3N-C7N-N7N	2.83	121.15	117.75
3	B	302	EWT	CAE-CAD-SAC	-2.81	108.13	111.85
3	D	302	EWT	CAD-CAE-NAF	2.73	114.40	108.04
2	D	301	NAP	PN-O3-PA	-2.72	123.48	132.83
3	B	302	EWT	CAD-CAE-NAF	2.72	114.37	108.04
4	D	303	DMS	O-S-C1	2.64	120.03	106.54
3	A	302	EWT	CAT-CAK-CAP	2.62	126.31	120.64
3	C	302	EWT	CAM-CAN-CL2	2.61	123.65	118.41
3	D	302	EWT	CAE-CAD-SAC	-2.59	108.42	111.85
2	D	301	NAP	C2A-N1A-C6A	2.59	123.18	118.75
2	B	301	NAP	O4B-C4B-C3B	-2.58	100.00	105.11
2	A	301	NAP	O2A-PA-O1A	2.53	124.75	112.24
3	B	302	EWT	NAA-CAB-NAF	2.50	126.43	123.19
2	C	301	NAP	C2A-N1A-C6A	2.43	122.91	118.75
2	C	301	NAP	O4D-C1D-C2D	-2.43	103.38	106.93
2	B	301	NAP	O7N-C7N-C3N	-2.40	116.76	119.63
2	C	301	NAP	N3A-C2A-N1A	-2.37	124.97	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	EWT	CAE-CAD-SAC	-2.37	108.71	111.85
3	C	302	EWT	CAD-CAE-NAF	2.34	113.48	108.04
2	A	301	NAP	O2B-P2B-O1X	-2.32	100.42	109.39
3	A	302	EWT	CAG-CAD-SAC	2.32	129.75	125.10
2	B	301	NAP	N6A-C6A-N1A	2.32	123.40	118.57
2	A	301	NAP	O4B-C4B-C3B	-2.32	100.53	105.11
3	B	302	EWT	CAG-CAD-SAC	2.29	129.69	125.10
2	C	301	NAP	O7N-C7N-N7N	-2.29	119.32	122.58
2	A	301	NAP	PN-O3-PA	-2.27	125.03	132.83
2	D	301	NAP	O7N-C7N-N7N	2.27	125.80	122.58
2	C	301	NAP	O2D-C2D-C3D	2.20	118.95	111.82
3	B	302	EWT	CAJ-CAI-CAH	-2.20	118.30	120.79
3	D	302	EWT	CAP-CAO-CL1	2.18	122.00	118.49
2	D	301	NAP	C3D-C2D-C1D	2.16	104.23	100.98
2	A	301	NAP	N6A-C6A-N1A	2.14	123.02	118.57
2	A	301	NAP	C2A-N1A-C6A	2.10	122.35	118.75
3	D	302	EWT	CAG-CAD-SAC	2.09	129.29	125.10
2	B	301	NAP	O2D-C2D-C3D	2.09	118.59	111.82
2	B	301	NAP	PN-O3-PA	-2.09	125.66	132.83
2	D	301	NAP	O2X-P2B-O1X	2.08	118.83	110.68
2	D	301	NAP	C4A-C5A-N7A	-2.06	107.25	109.40
3	C	302	EWT	CAK-CAT-NAS	-2.06	108.64	113.05
2	A	301	NAP	C5N-C4N-C3N	-2.05	117.92	120.34
2	D	301	NAP	N6A-C6A-N1A	2.03	122.80	118.57
2	D	301	NAP	O4D-C1D-C2D	-2.03	103.96	106.93
2	D	301	NAP	O3X-P2B-O2X	2.00	115.29	107.64

There are no chirality outliers.

There are no torsion outliers.

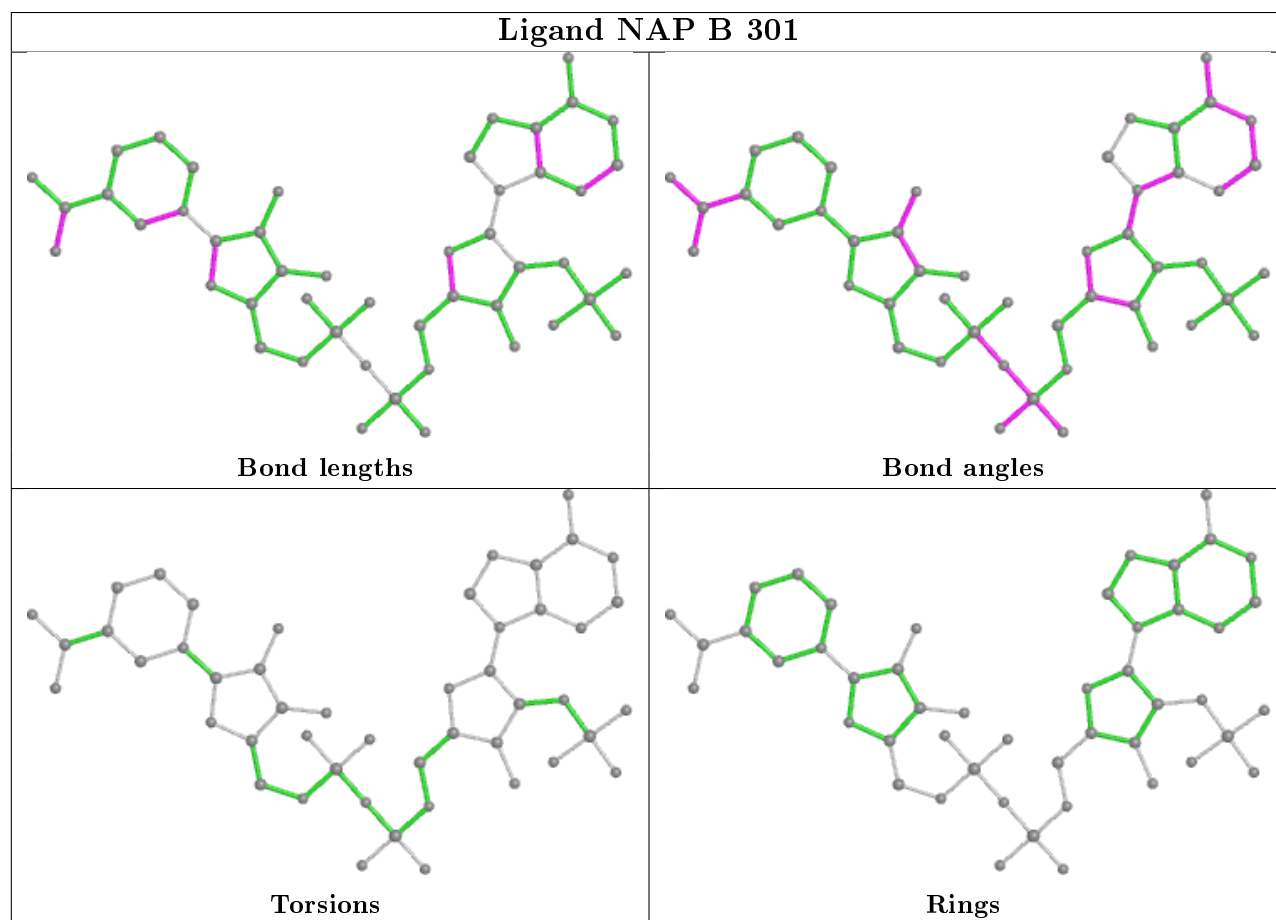
There are no ring outliers.

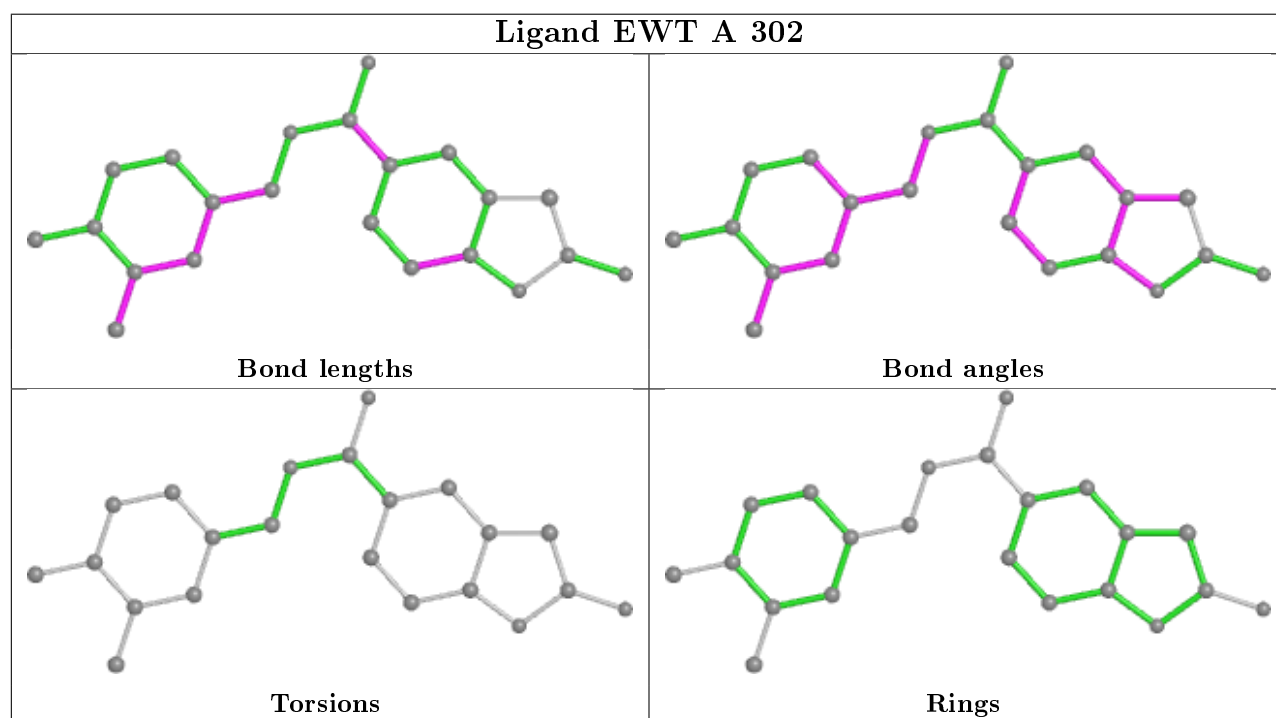
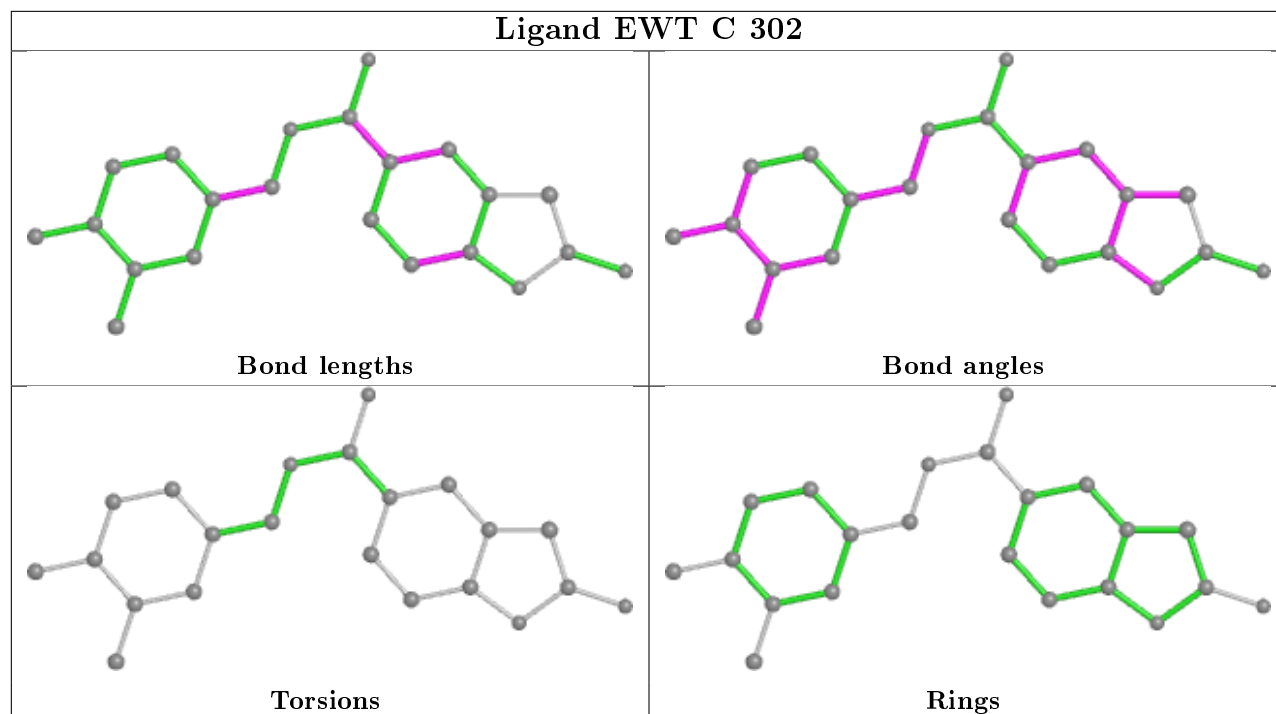
4 monomers are involved in 7 short contacts:

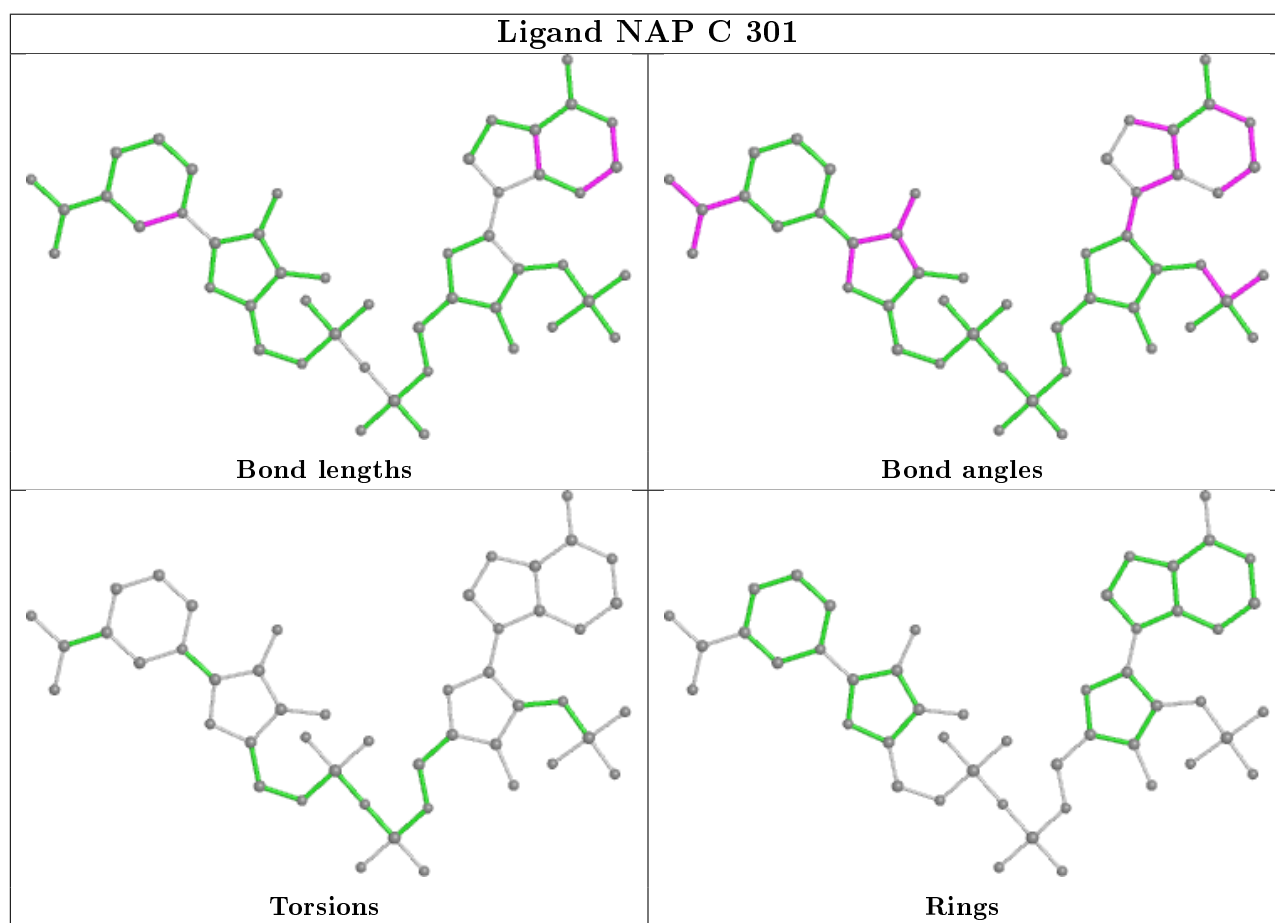
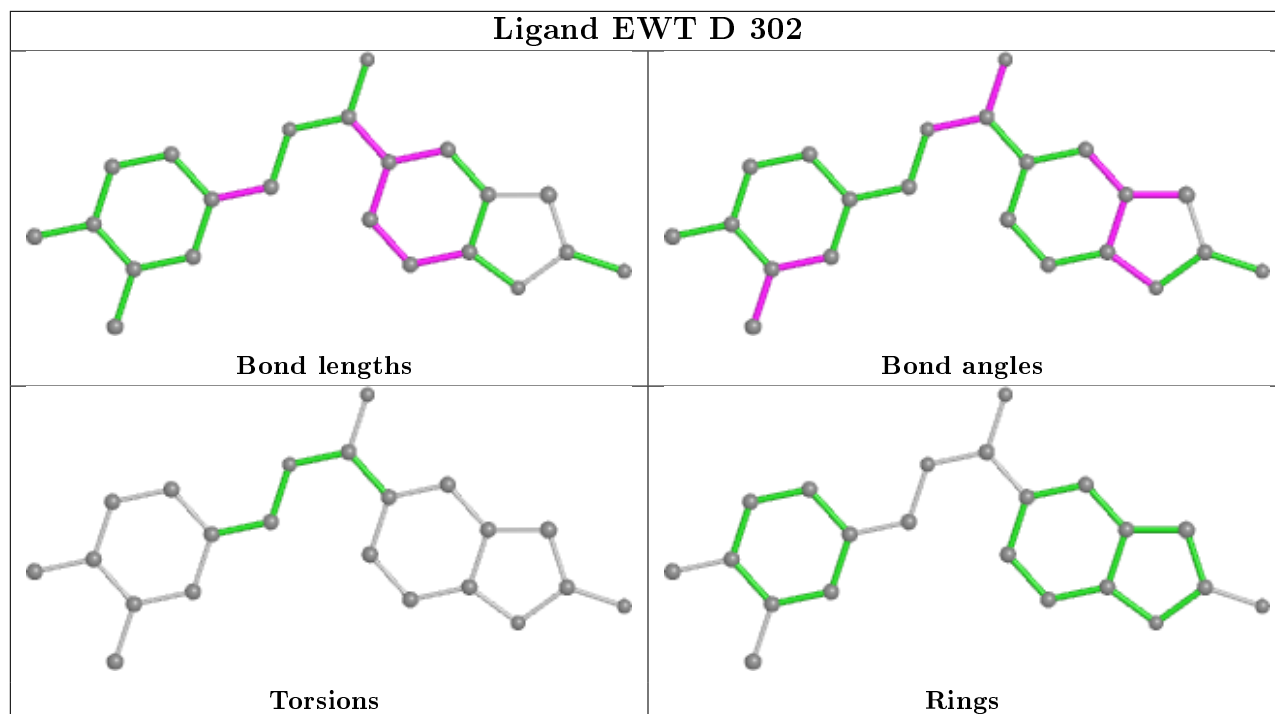
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	NAP	2	0
3	D	302	EWT	1	0
2	C	301	NAP	3	0
2	D	301	NAP	1	0

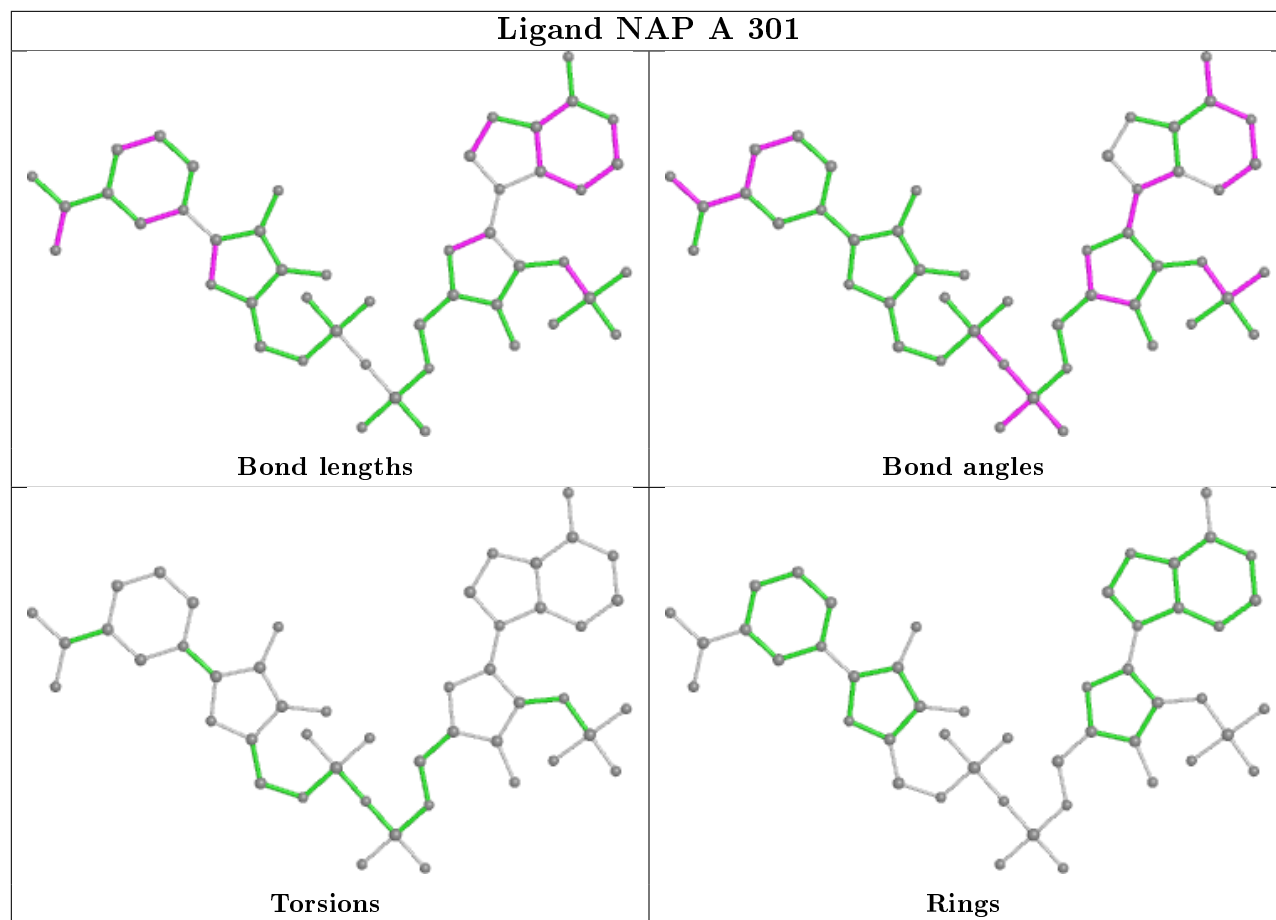
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

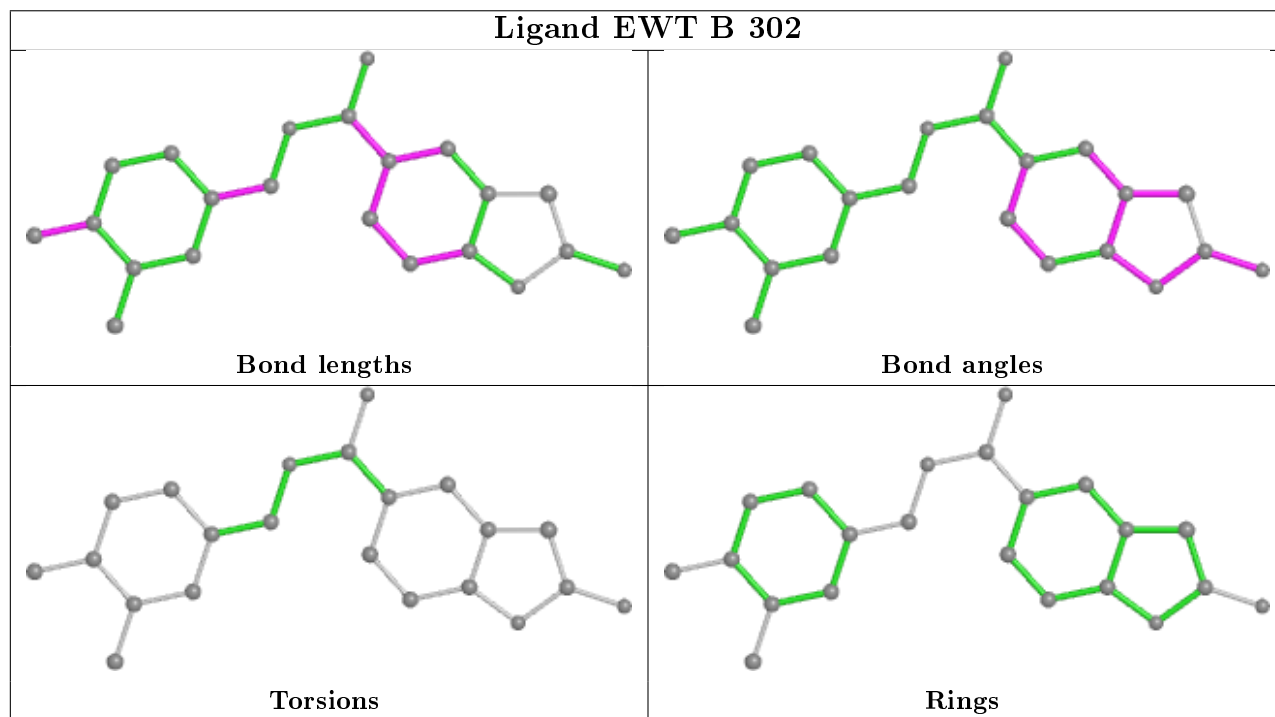
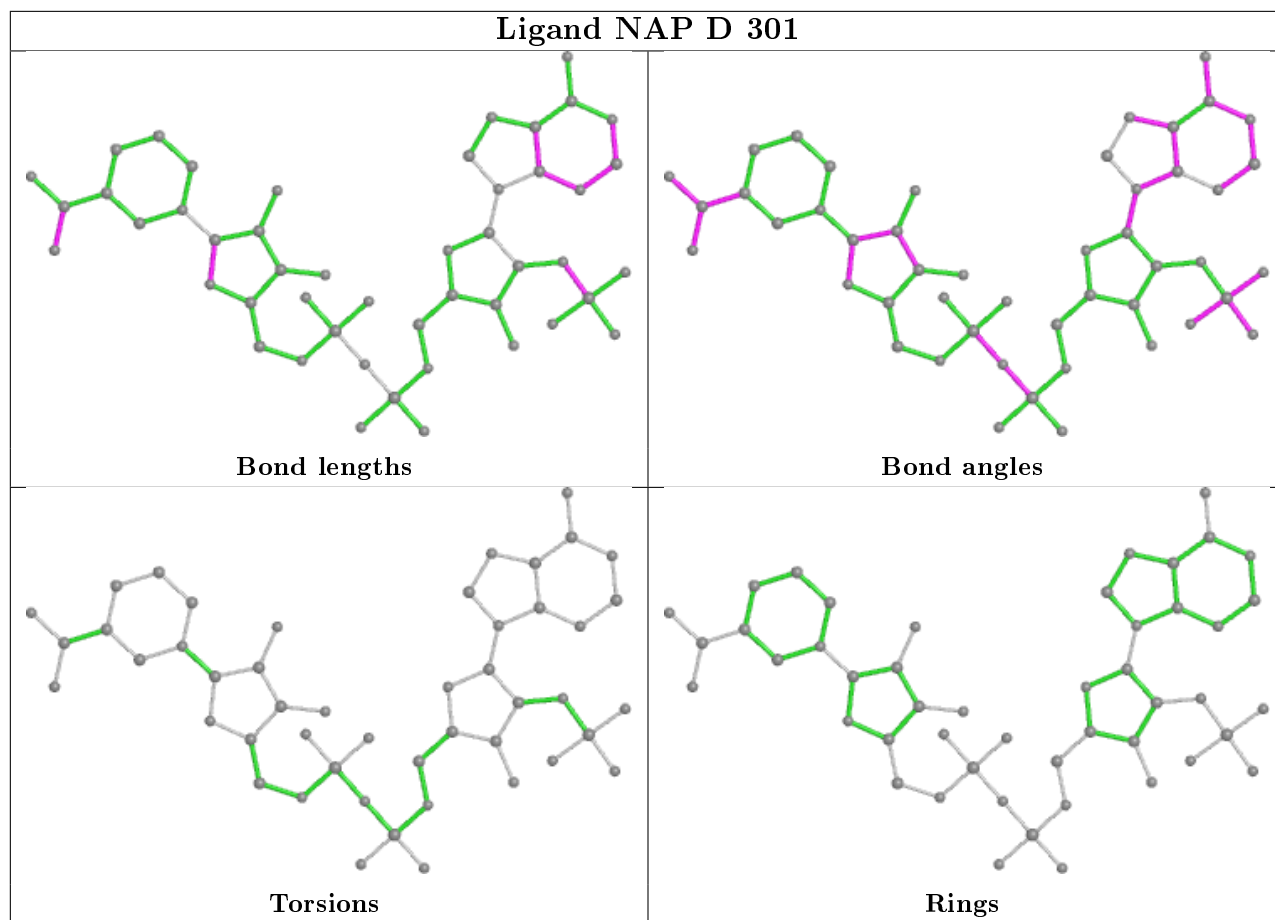
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	252/288 (87%)	-0.51	2 (0%) 86 89	12, 19, 38, 72	1 (0%)
1	B	252/288 (87%)	-0.58	4 (1%) 72 77	10, 17, 32, 72	0
1	C	251/288 (87%)	-0.45	4 (1%) 72 77	11, 20, 51, 63	2 (0%)
1	D	250/288 (86%)	-0.54	0 100 100	10, 19, 38, 55	2 (0%)
All	All	1005/1152 (87%)	-0.52	10 (0%) 82 86	10, 19, 39, 72	5 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	113	GLY	3.8
1	C	212	ALA	3.0
1	C	211	VAL	2.9
1	B	113	GLY	2.7
1	B	1	MET	2.4
1	A	143	LYS	2.4
1	B	151	SER	2.2
1	C	2	GLU	2.1
1	A	1	MET	2.1
1	B	211	VAL	2.1

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 carbohydrates in this entry.

6.4 Ligands

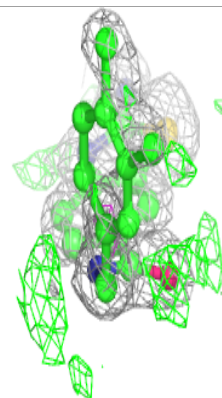
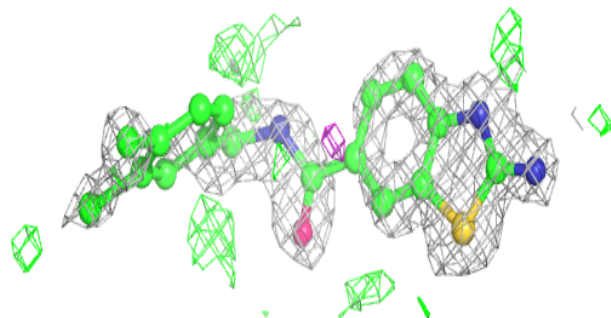
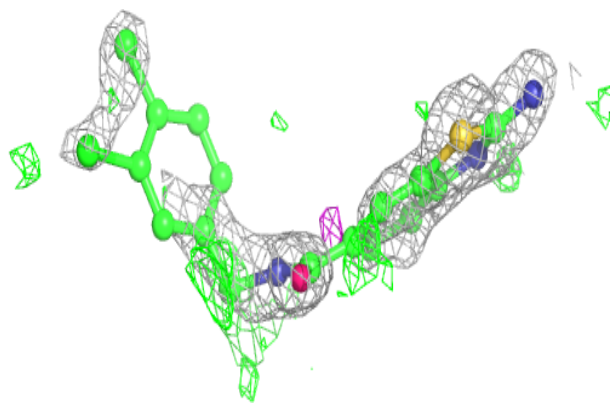
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EWT	C	302	22/22	0.89	0.17	24,32,36,42	22
4	DMS	B	303	4/4	0.89	0.17	19,22,23,28	4
4	DMS	D	303	4/4	0.91	0.14	36,39,41,57	0
2	NAP	C	301	48/48	0.92	0.11	16,21,28,30	48
3	EWT	B	302	22/22	0.94	0.12	22,33,61,68	0
4	DMS	A	303[A]	4/4	0.94	0.15	24,24,24,27	4
3	EWT	D	302	22/22	0.95	0.12	22,32,76,96	0
3	EWT	A	302	22/22	0.95	0.11	23,35,71,82	0
5	ACT	C	303	4/4	0.96	0.07	24,26,27,28	0
2	NAP	A	301	48/48	0.97	0.07	18,22,23,26	0
2	NAP	B	301	48/48	0.97	0.07	16,20,23,25	0
2	NAP	D	301	48/48	0.98	0.06	14,21,26,28	0

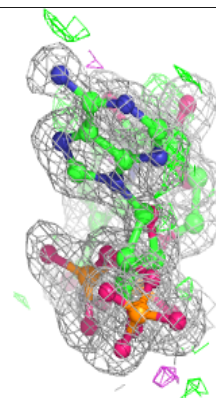
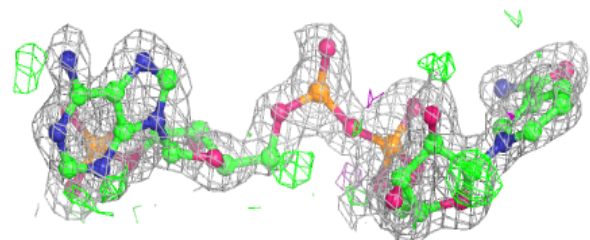
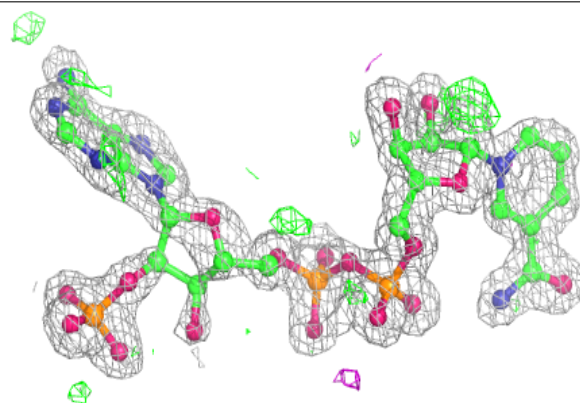
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EWT C 302:

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

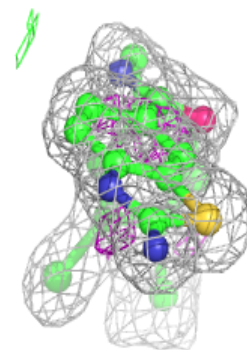
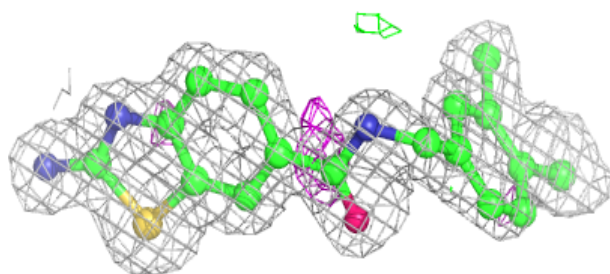
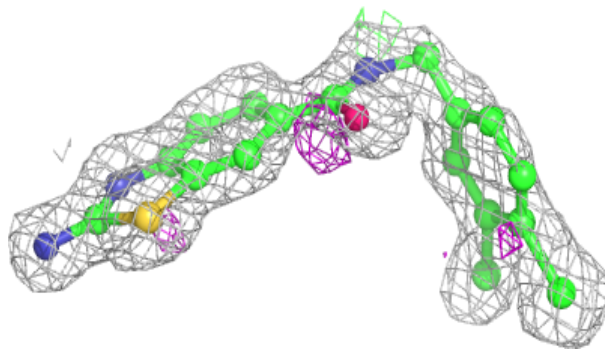
**Electron density around NAP C 301:**

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

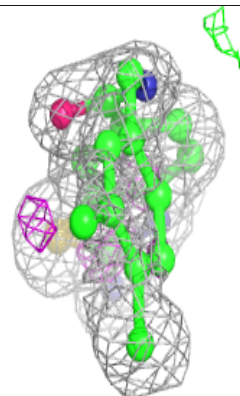
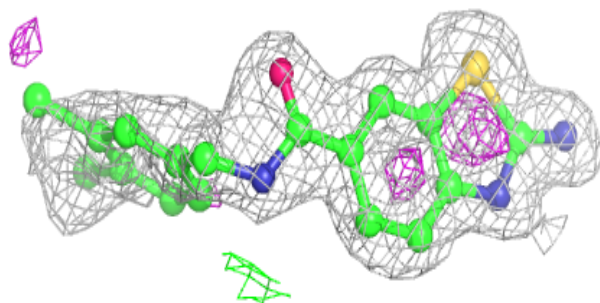
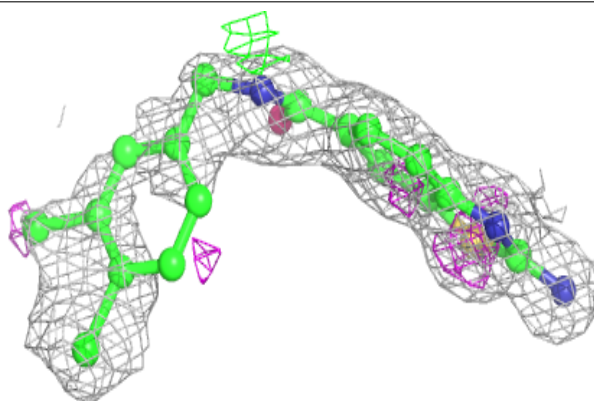


Electron density around EWT B 302:

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

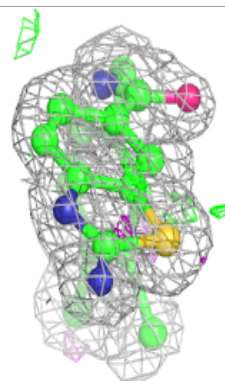
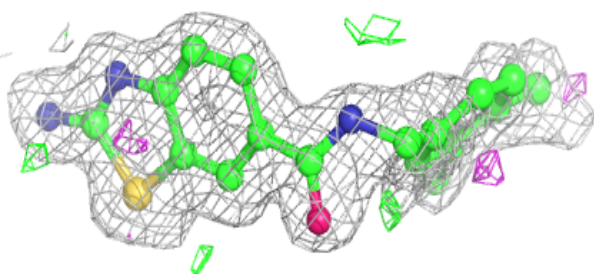
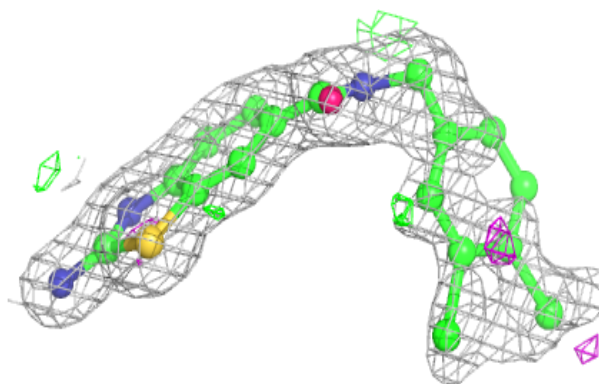
**Electron density around EWT D 302:**

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

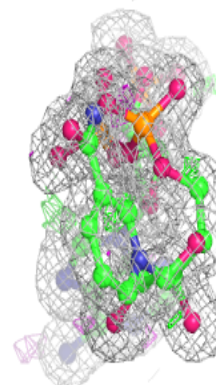
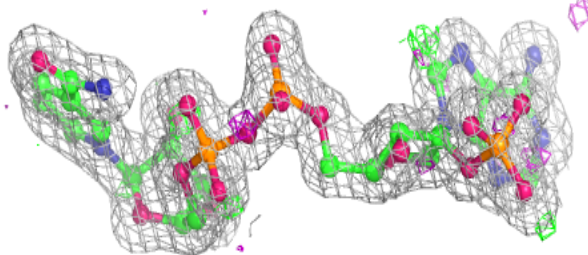
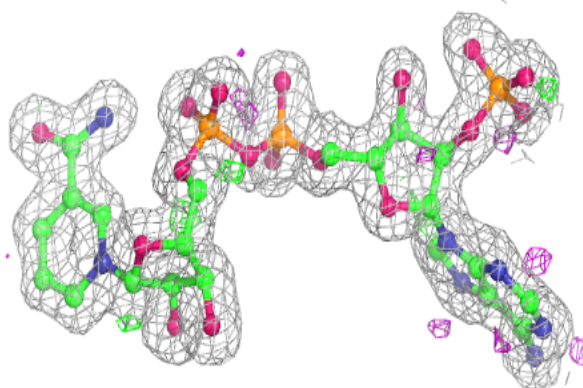


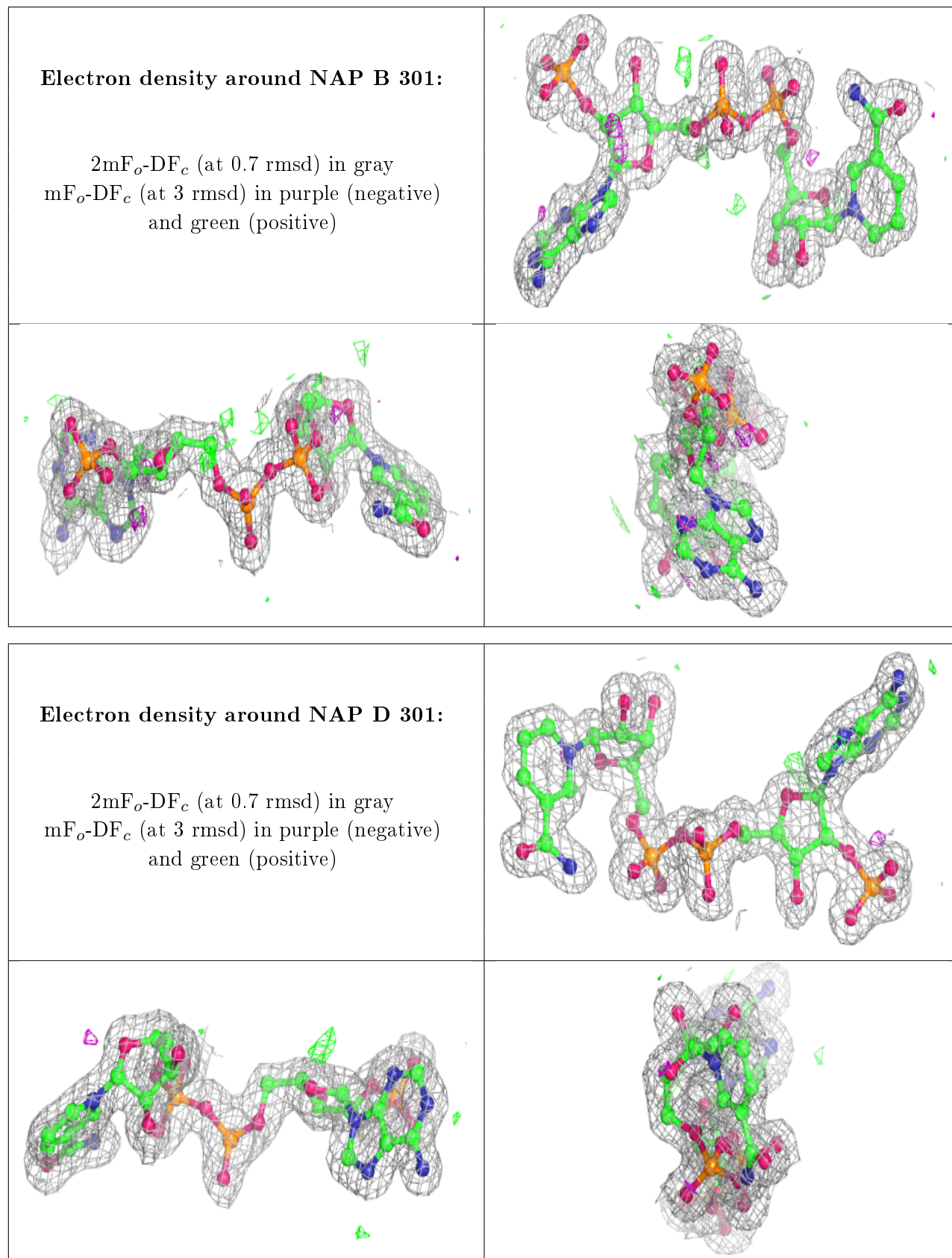
Electron density around EWT A 302:

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

**Electron density around NAP A 301:**

$2mF_o-DF_c$ (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.