Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 04:27 am BST

PDB ID	:	5K6A
Title	:	Trypanosoma brucei Pteridine reductase 1 (PTR1) in complex with compound 1
Authors	:	Landi, G.; Pozzi, C.; Di Pisa, F.; Dello lacono, L.; Mangani, S.
Deposited on	:	2016-05-24
Resolution	:	1.70 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:

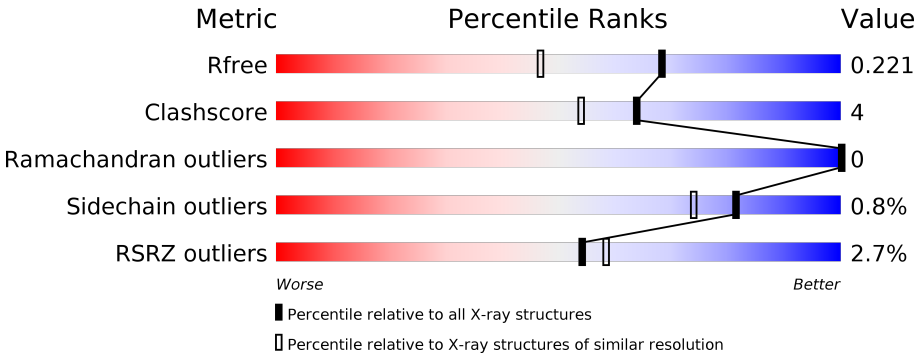
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	% 77% 9% • 14%
1	B	288	% 78% 8% 14%
1	D	288	3% 81% 5% 14%
2	C	288	3% 72% 10% 17%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8396 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
1	A	248	Total	C	N	O	S	0	5	0
			1853	1166	324	351	12			
1	B	247	Total	C	N	O	S	0	8	0
			1868	1175	326	355	12			
1	D	248	Total	C	N	O	S	0	8	0
			1853	1172	321	348	12			

There are 60 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
B	-18	GLY	-	expression tag	UNP O76290
B	-17	SER	-	expression tag	UNP O76290

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Chain	Residue	Modelled	Actual	Comment	Reference
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
D	-19	MET	-	initiating methionine	UNP O76290
D	-18	GLY	-	expression tag	UNP O76290
D	-17	SER	-	expression tag	UNP O76290
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

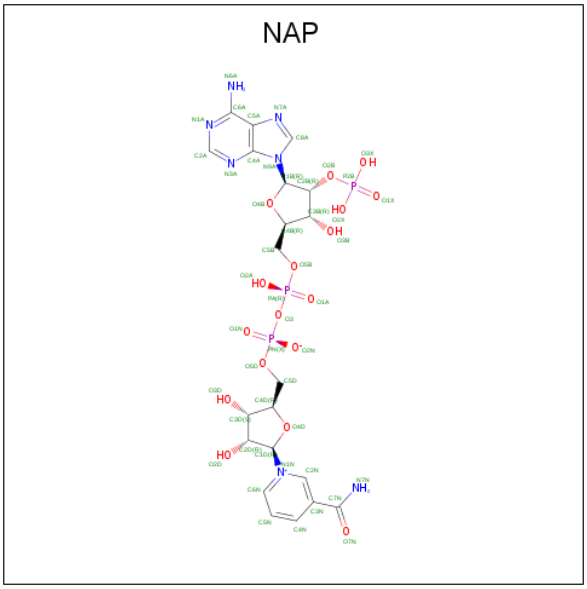
- Molecule 2 is a protein called Pteridine reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	238	Total	C	N	O	S	0	7	0
			1771	1116	305	339	11			

There are 20 discrepancies between the modelled and reference sequences:

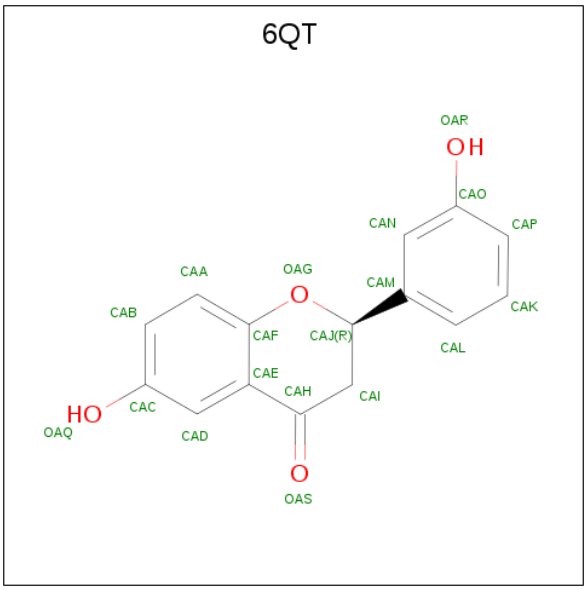
Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	initiating methionine	UNP O76290
C	-18	GLY	-	expression tag	UNP O76290
C	-17	SER	-	expression tag	UNP O76290
C	-16	SER	-	expression tag	UNP O76290
C	-15	HIS	-	expression tag	UNP O76290
C	-14	HIS	-	expression tag	UNP O76290
C	-13	HIS	-	expression 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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



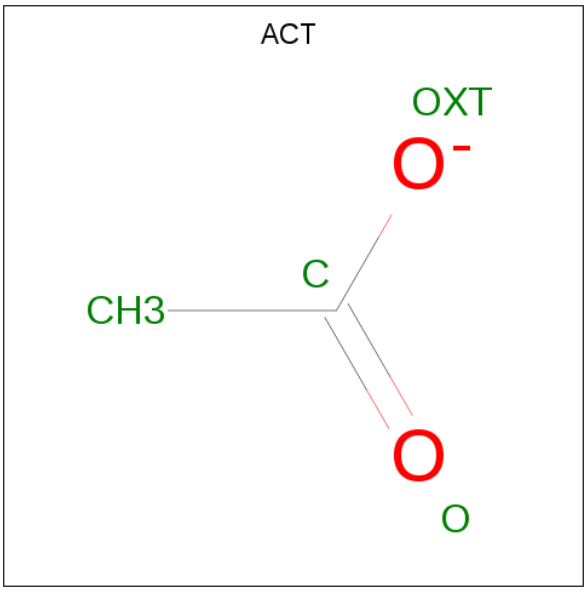
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 48 21 7 17 3	0	0
3	B	1	Total C N O P 48 21 7 17 3	0	0
3	C	1	Total C N O P 48 21 7 17 3	0	0
3	D	1	Total C N O P 48 21 7 17 3	0	0

- Molecule 4 is (2 {R})-2-(3-hydroxyphenyl)-6-oxidanyl-2,3-dihydrochromen-4-one (three-letter code: 6QT) (formula: $C_{15}H_{12}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 19 15 4	0	0
4	B	1	Total C O 19 15 4	0	0
4	C	1	Total C O 19 15 4	0	0
4	D	1	Total C O 19 15 4	0	0

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



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

- Molecule 6 is water.

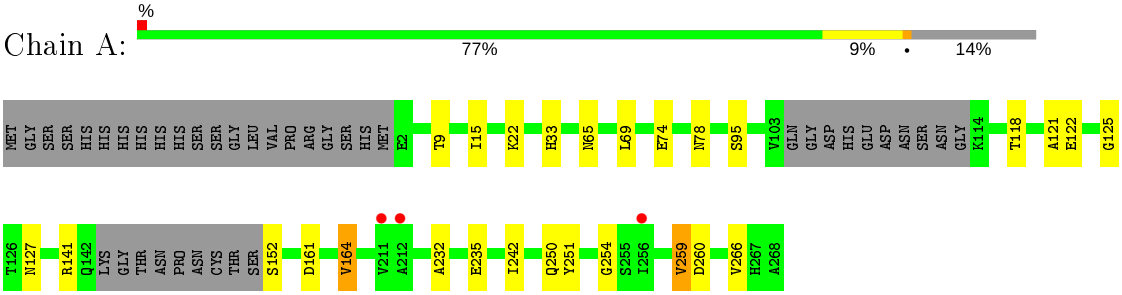
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	208	Total O 209 209	0	1
6	B	212	Total O 212 212	0	0
6	C	174	Total O 175 175	0	2
6	D	179	Total O 179 179	0	2

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.

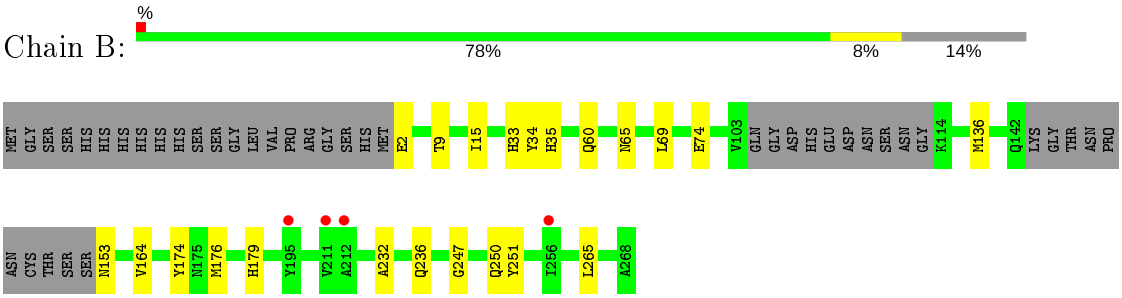
- Molecule 1: Pteridine reductase

Chain A:



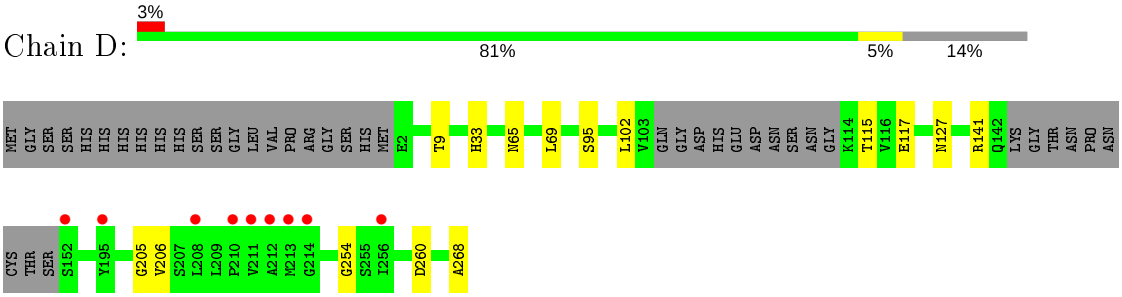
- Molecule 1: Pteridine reductase

Chain B:



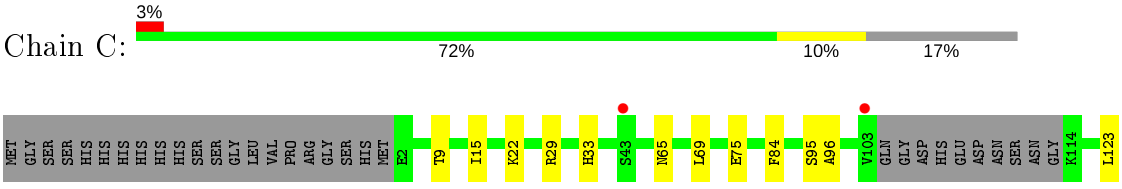
- Molecule 1: Pteridine reductase

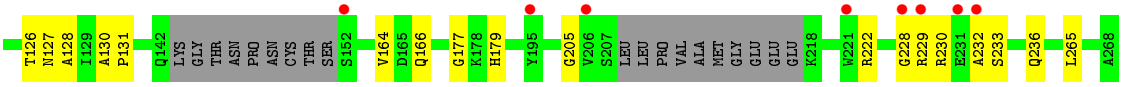
Chain D:



- Molecule 2: Pteridine reductase

Chain C:




T126
N127
A128
I129
A130
P131
Q142
LYS
GLY
THR
ASN
PRO
ASN
CYS
THR
SER
S152
V164
D165
Q166
G177
K178
H179
Y195
G205
V206
S207
LEU
LEU
PRO
VAL
ALA
MET
GLY
GLU
GLU
GLU
K218
W221
R222
G228
R229
R230
E231
A232
S233
Q236
L265
A268

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.72Å 89.89Å 82.68Å 90.00° 115.75° 90.00°	Depositor
Resolution (Å)	74.47 – 1.70 41.72 – 1.70	Depositor EDS
% Data completeness (in resolution range)	92.7 (74.47-1.70) 92.7 (41.72-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.180 , 0.220 0.180 , 0.221	Depositor DCC
R_{free} test set	4859 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	15.9	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8396	wwPDB-VP
Average B, all atoms (Å^2)	18.0	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 33.20 % 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 8.3038e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OCS, NAP, CSX, 6QT, ACT

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	0.90	1/1884 (0.1%)	0.89	3/2558 (0.1%)
1	B	0.87	0/1905	0.89	0/2585
1	D	0.81	0/1893	0.82	0/2571
2	C	0.83	0/1799	0.85	0/2444
All	All	0.85	1/7481 (0.0%)	0.86	3/10158 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	259	VAL	C-N	15.72	1.70	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	259	VAL	O-C-N	7.97	135.45	122.70
1	A	259	VAL	C-N-CA	-7.85	102.07	121.70
1	A	259	VAL	CA-C-N	-5.91	104.19	117.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1853	0	1864	22	0
1	B	1868	0	1879	18	0
1	D	1853	0	1871	10	0
2	C	1771	0	1768	21	0
3	A	48	0	25	1	0
3	B	48	0	25	2	0
3	C	48	0	25	4	0
3	D	48	0	25	0	0
4	A	19	0	0	0	0
4	B	19	0	0	0	0
4	C	19	0	0	0	0
4	D	19	0	0	0	0
5	A	4	0	3	0	0
5	C	4	0	3	0	0
6	A	209	0	0	1	0
6	B	212	0	0	5	0
6	C	175	0	0	4	0
6	D	179	0	0	1	0
All	All	8396	0	7488	63	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 4.

All (63) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:VAL:C	1:A:260:ASP:N	1.70	1.44
1:A:259:VAL:C	1:A:260:ASP:CA	2.46	0.82
1:D:95[B]:SER:HB2	1:D:127:ASN:HD21	1.45	0.81
1:A:259:VAL:CA	1:A:260:ASP:N	2.56	0.67
1:A:259:VAL:C	1:A:260:ASP:HA	2.20	0.61
2:C:96:ALA:H	2:C:127[B]:ASN:HD21	1.46	0.61
2:C:232:ALA:HA	2:C:236:GLN:OE1	2.01	0.61
1:D:95[B]:SER:HB2	1:D:127:ASN:ND2	2.14	0.61
2:C:95[B]:SER:OG	3:C:301:NAP:H3D	2.02	0.60
2:C:177:GLY:HA3	6:C:404:HOH:O	2.04	0.58
1:A:78:ASN:OD1	1:A:141:ARG:NH1	2.35	0.58
1:D:141:ARG:HG2	6:D:516:HOH:O	2.04	0.57
1:A:250:GLN:HG2	6:B:462:HOH:O	2.05	0.57
2:C:128:ALA:C	2:C:131:PRO:HD2	2.26	0.55
1:A:161:ASP:O	1:A:164:VAL:HG22	2.07	0.55
2:C:65:ASN:HA	2:C:69:LEU:HD22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ILE:HB	3:B:301:NAP:H51N	1.88	0.54
2:C:75:GLU:OE1	6:C:401:HOH:O	2.18	0.54
1:D:65:ASN:HA	1:D:69:LEU:HD22	1.90	0.54
1:A:74:GLU:HG3	6:A:452:HOH:O	2.07	0.54
2:C:9:THR:HA	2:C:33:HIS:HB3	1.90	0.54
1:B:2:GLU:N	6:B:401:HOH:O	2.41	0.53
2:C:123:LEU:O	2:C:127[A]:ASN:HB2	2.09	0.53
1:A:95[B]:SER:HB2	1:A:127:ASN:HD21	1.74	0.52
1:A:22:LYS:HG2	1:A:242:ILE:HG13	1.91	0.52
1:A:250:GLN:CD	1:B:236:GLN:HE21	2.12	0.52
1:B:9:THR:HA	1:B:33:HIS:HB3	1.92	0.52
2:C:228:GLY:HA3	2:C:230:ARG:NH1	2.24	0.52
1:D:205:GLY:HA3	1:D:260:ASP:HB2	1.91	0.52
1:A:65:ASN:HA	1:A:69:LEU:HD22	1.90	0.52
1:D:9:THR:HA	1:D:33:HIS:HB3	1.93	0.51
1:B:164:VAL:HG22	1:B:179:HIS:CD2	2.46	0.51
2:C:164:VAL:HG22	2:C:179:HIS:CD2	2.47	0.49
1:A:22:LYS:HE3	1:A:235:GLU:HG3	1.94	0.49
1:B:65:ASN:HA	1:B:69:LEU:HD22	1.95	0.49
1:A:266:VAL:HB	1:D:268:ALA:HB2	1.95	0.48
2:C:95[B]:SER:OG	3:C:301:NAP:C3D	2.61	0.48
1:B:247:GLY:HA2	1:B:250:GLN:HG3	1.97	0.47
2:C:205:GLY:O	3:C:301:NAP:H4N	2.15	0.47
2:C:265:LEU:HD11	1:D:254:GLY:HA3	1.96	0.47
2:C:15:ILE:HB	3:C:301:NAP:H51N	1.98	0.46
2:C:126:THR:OG1	2:C:127[B]:ASN:ND2	2.50	0.45
1:A:232:ALA:HB2	1:B:251:TYR:CE2	2.52	0.45
1:A:251:TYR:CE2	1:B:232:ALA:HB2	2.52	0.45
2:C:233:SER:N	6:C:409:HOH:O	2.50	0.44
1:A:9:THR:HA	1:A:33:HIS:HB3	1.99	0.44
1:A:254:GLY:HA3	1:B:265:LEU:HD11	1.99	0.43
1:A:15:ILE:HB	3:A:301:NAP:H51N	2.01	0.43
1:B:34:TYR:CZ	1:B:60:GLN:HB2	2.54	0.42
1:A:121:ALA:O	1:A:125:GLY:HA3	2.20	0.42
1:A:118:THR:O	1:A:122:GLU:HG3	2.20	0.42
1:B:35:HIS:HB2	3:B:301:NAP:C2A	2.49	0.42
1:A:251:TYR:CD2	1:B:232:ALA:HB2	2.55	0.42
1:B:153:ASN:N	6:B:412:HOH:O	2.53	0.42
1:B:136[A]:MET:CE	6:B:602:HOH:O	2.67	0.41
1:B:174:TYR:HA	6:B:414:HOH:O	2.19	0.41
1:D:115:THR:OG1	1:D:117[B]:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:29:ARG:HD2	2:C:84:PHE:CD1	2.56	0.41
2:C:130:ALA:N	2:C:131:PRO:CD	2.84	0.41
1:B:136[B]:MET:HE2	1:D:102:LEU:HA	2.03	0.41
2:C:222:ARG:O	2:C:229:ARG:HA	2.21	0.40
2:C:232:ALA:C	6:C:409:HOH:O	2.60	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	246/288 (85%)	238 (97%)	8 (3%)	0	100	100
1	B	248/288 (86%)	241 (97%)	7 (3%)	0	100	100
1	D	249/288 (86%)	241 (97%)	8 (3%)	0	100	100
2	C	235/288 (82%)	228 (97%)	7 (3%)	0	100	100
All	All	978/1152 (85%)	948 (97%)	30 (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	195/230 (85%)	193 (99%)	2 (1%)	76	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	197/230 (86%)	196 (100%)	1 (0%)	88 83
1	D	194/230 (84%)	193 (100%)	1 (0%)	88 83
2	C	185/229 (81%)	183 (99%)	2 (1%)	73 63
All	All	771/919 (84%)	765 (99%)	6 (1%)	81 74

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	SER
1	A	164	VAL
1	B	74	GLU
2	C	22	LYS
2	C	166	GLN
1	D	206	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
1	A	250	GLN
1	B	236	GLN
1	D	127	ASN
1	D	166	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)

5 non-standard protein/DNA/RNA residues 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	OCS	C	59	2	7,8,9	1.80	3 (42%)	6,11,13	2.20	3 (50%)
2	CSX	C	168	2	3,6,7	0.43	0	1,6,8	0.25	0
1	CSX	D	168	1	3,6,7	0.64	0	1,6,8	1.18	0
1	CSX	A	168	1	3,6,7	0.37	0	1,6,8	1.22	0
1	CSX	B	168	1	3,6,7	0.87	0	1,6,8	0.72	0

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
2	OCS	C	59	2	-	1/4/7/9	-
2	CSX	C	168	2	-	0/1/5/7	-
1	CSX	D	168	1	-	0/1/5/7	-
1	CSX	A	168	1	-	0/1/5/7	-
1	CSX	B	168	1	-	0/1/5/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	59	OCS	OD3-SG	2.89	1.53	1.45
2	C	59	OCS	O-C	2.35	1.29	1.19
2	C	59	OCS	CB-SG	-2.14	1.69	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	59	OCS	OD3-SG-CB	2.94	110.44	106.94
2	C	59	OCS	OD2-SG-CB	2.79	110.19	105.74
2	C	59	OCS	OD2-SG-OD3	-2.65	104.79	111.27

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	59	OCS	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

10 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	$\#\|Z\| > 2$
4	6QT	C	302	-	21,21,21	1.96	3 (14%)	30,30,30	1.20	4 (13%)
4	6QT	A	302	-	21,21,21	2.03	8 (38%)	30,30,30	1.18	1 (3%)
3	NAP	C	301	-	45,52,52	1.13	4 (8%)	56,80,80	1.48	10 (17%)
5	ACT	C	303	-	1,3,3	1.43	0	0,3,3	0.00	-
3	NAP	A	301	-	45,52,52	1.33	7 (15%)	56,80,80	1.33	7 (12%)
4	6QT	B	302	-	21,21,21	2.18	6 (28%)	30,30,30	1.44	6 (20%)
3	NAP	D	301	-	45,52,52	1.43	8 (17%)	56,80,80	1.63	10 (17%)
4	6QT	D	302	-	21,21,21	2.21	6 (28%)	30,30,30	1.07	1 (3%)
3	NAP	B	301	-	45,52,52	1.21	5 (11%)	56,80,80	1.44	7 (12%)
5	ACT	A	303	-	1,3,3	2.19	1 (100%)	0,3,3	0.00	-

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
4	6QT	C	302	-	-	0/4/16/16	0/3/3/3
4	6QT	A	302	-	-	0/4/16/16	0/3/3/3
3	NAP	C	301	-	-	2/31/67/67	0/5/5/5
3	NAP	A	301	-	-	0/31/67/67	0/5/5/5
4	6QT	B	302	-	-	0/4/16/16	0/3/3/3
3	NAP	D	301	-	-	0/31/67/67	0/5/5/5
4	6QT	D	302	-	-	0/4/16/16	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	B	301	-	-	0/31/67/67	0/5/5/5

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	302	6QT	CAM-CAJ	-5.61	1.41	1.51
4	D	302	6QT	CAM-CAJ	-5.57	1.41	1.51
4	B	302	6QT	CAI-CAH	-5.00	1.42	1.50
4	D	302	6QT	CAI-CAH	-4.93	1.42	1.50
4	C	302	6QT	CAI-CAH	-4.89	1.42	1.50
4	C	302	6QT	CAM-CAJ	-4.88	1.43	1.51
4	A	302	6QT	CAM-CAJ	-4.79	1.43	1.51
3	A	301	NAP	C2N-N1N	3.88	1.39	1.35
4	C	302	6QT	CAE-CAH	-3.81	1.42	1.48
3	D	301	NAP	O4D-C1D	3.76	1.46	1.41
4	D	302	6QT	CAE-CAH	-3.47	1.43	1.48
4	A	302	6QT	CAI-CAH	-3.42	1.44	1.50
3	D	301	NAP	C2A-N3A	3.28	1.37	1.32
4	A	302	6QT	CAE-CAH	-3.25	1.43	1.48
3	A	301	NAP	C2A-N3A	3.25	1.37	1.32
3	D	301	NAP	C7N-N7N	3.17	1.39	1.33
3	B	301	NAP	C5A-C4A	3.13	1.49	1.40
3	C	301	NAP	C5A-C4A	3.10	1.49	1.40
3	C	301	NAP	O4D-C1D	3.10	1.45	1.41
3	B	301	NAP	C4A-N3A	3.07	1.39	1.35
4	B	302	6QT	CAE-CAH	-2.94	1.44	1.48
3	B	301	NAP	C2A-N3A	2.90	1.36	1.32
3	D	301	NAP	C5A-C4A	2.88	1.48	1.40
3	D	301	NAP	P2B-O2B	2.75	1.64	1.59
4	B	302	6QT	CAN-CAM	2.74	1.43	1.39
4	B	302	6QT	OAG-CAJ	2.71	1.50	1.44
3	A	301	NAP	C5A-C4A	2.68	1.48	1.40
4	A	302	6QT	CAD-CAE	2.53	1.43	1.39
4	D	302	6QT	OAG-CAJ	2.52	1.50	1.44
3	D	301	NAP	C4N-C3N	2.47	1.43	1.39
3	C	301	NAP	C2N-N1N	2.40	1.37	1.35
3	A	301	NAP	O4D-C1D	2.40	1.44	1.41
4	A	302	6QT	CAN-CAM	2.38	1.42	1.39
3	B	301	NAP	C7N-N7N	2.35	1.37	1.33
4	A	302	6QT	CAN-CAO	2.28	1.42	1.39
3	C	301	NAP	C2A-N3A	2.26	1.35	1.32
4	A	302	6QT	OAS-CAH	2.24	1.25	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	NAP	O2D-C2D	2.22	1.48	1.43
3	D	301	NAP	C6A-C5A	2.21	1.51	1.43
3	A	301	NAP	C8A-N7A	2.20	1.38	1.34
5	A	303	ACT	CH3-C	2.19	1.51	1.48
3	A	301	NAP	P2B-O2B	2.16	1.63	1.59
3	B	301	NAP	C2N-N1N	2.16	1.37	1.35
4	D	302	6QT	OAS-CAH	2.10	1.25	1.22
3	A	301	NAP	C4A-N3A	2.09	1.38	1.35
4	B	302	6QT	CAN-CAO	2.09	1.42	1.39
4	D	302	6QT	CAL-CAM	2.08	1.42	1.39
4	A	302	6QT	CAD-CAC	2.03	1.42	1.39

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	301	NAP	O7N-C7N-C3N	-6.02	112.43	119.63
3	D	301	NAP	N3A-C2A-N1A	-4.69	121.35	128.68
3	B	301	NAP	O7N-C7N-C3N	-4.09	114.74	119.63
3	A	301	NAP	N3A-C2A-N1A	-4.06	122.33	128.68
3	C	301	NAP	C3N-C7N-N7N	3.97	122.52	117.75
3	A	301	NAP	C1B-N9A-C4A	-3.63	120.26	126.64
3	B	301	NAP	C2A-N1A-C6A	3.63	124.97	118.75
3	B	301	NAP	N3A-C2A-N1A	-3.51	123.20	128.68
3	C	301	NAP	O2B-P2B-O1X	-3.39	96.31	109.39
4	B	302	6QT	OAG-CAF-CAE	-3.21	118.41	122.09
4	A	302	6QT	CAI-CAH-CAE	3.20	121.32	116.63
3	A	301	NAP	N6A-C6A-N1A	3.15	125.11	118.57
3	D	301	NAP	C3N-C7N-N7N	3.15	121.53	117.75
3	C	301	NAP	C1B-N9A-C4A	-3.00	121.37	126.64
3	C	301	NAP	N3A-C2A-N1A	-2.99	124.01	128.68
4	C	302	6QT	CAI-CAH-CAE	2.89	120.87	116.63
3	D	301	NAP	C1B-N9A-C4A	-2.88	121.58	126.64
4	B	302	6QT	CAI-CAH-CAE	2.85	120.81	116.63
3	C	301	NAP	O7N-C7N-N7N	-2.84	118.55	122.58
4	C	302	6QT	OAG-CAF-CAE	-2.82	118.86	122.09
4	B	302	6QT	CAF-CAE-CAH	2.69	121.40	119.85
3	D	301	NAP	C2D-C3D-C4D	2.65	107.78	102.64
3	D	301	NAP	C2A-N1A-C6A	2.61	123.23	118.75
4	D	302	6QT	OAG-CAF-CAE	-2.61	119.09	122.09
3	C	301	NAP	C2A-N1A-C6A	2.53	123.07	118.75
3	A	301	NAP	C2A-N1A-C6A	2.52	123.06	118.75
3	A	301	NAP	C5A-C6A-N6A	-2.46	116.62	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	301	NAP	O2B-P2B-O1X	-2.45	99.92	109.39
3	D	301	NAP	O7N-C7N-N7N	2.44	126.04	122.58
4	B	302	6QT	OAS-CAH-CAI	-2.42	117.38	120.79
4	C	302	6QT	CAO-CAN-CAM	2.35	122.13	120.11
3	C	301	NAP	C4A-C5A-N7A	-2.35	106.95	109.40
3	B	301	NAP	O3X-P2B-O2X	2.35	116.60	107.64
3	D	301	NAP	PN-O3-PA	-2.30	124.95	132.83
3	A	301	NAP	O2X-P2B-O1X	2.26	119.54	110.68
3	D	301	NAP	O2N-PN-O1N	2.26	123.40	112.24
3	C	301	NAP	O2N-PN-O1N	2.22	123.22	112.24
4	B	302	6QT	OAG-CAJ-CAM	2.17	111.59	107.66
3	B	301	NAP	C1B-N9A-C4A	-2.12	122.91	126.64
3	D	301	NAP	C4A-C5A-N7A	-2.10	107.21	109.40
4	C	302	6QT	OAS-CAH-CAI	-2.09	117.84	120.79
3	C	301	NAP	PN-O3-PA	-2.09	125.65	132.83
3	C	301	NAP	O3X-P2B-O1X	2.08	118.83	110.68
4	B	302	6QT	CAA-CAF-CAE	2.05	123.70	119.90
3	B	301	NAP	N6A-C6A-N1A	2.05	122.82	118.57
3	A	301	NAP	C5N-C4N-C3N	-2.01	117.97	120.34

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	301	NAP	O4D-C4D-C5D-O5D
3	C	301	NAP	C5B-O5B-PA-O1A

There are no ring outliers.

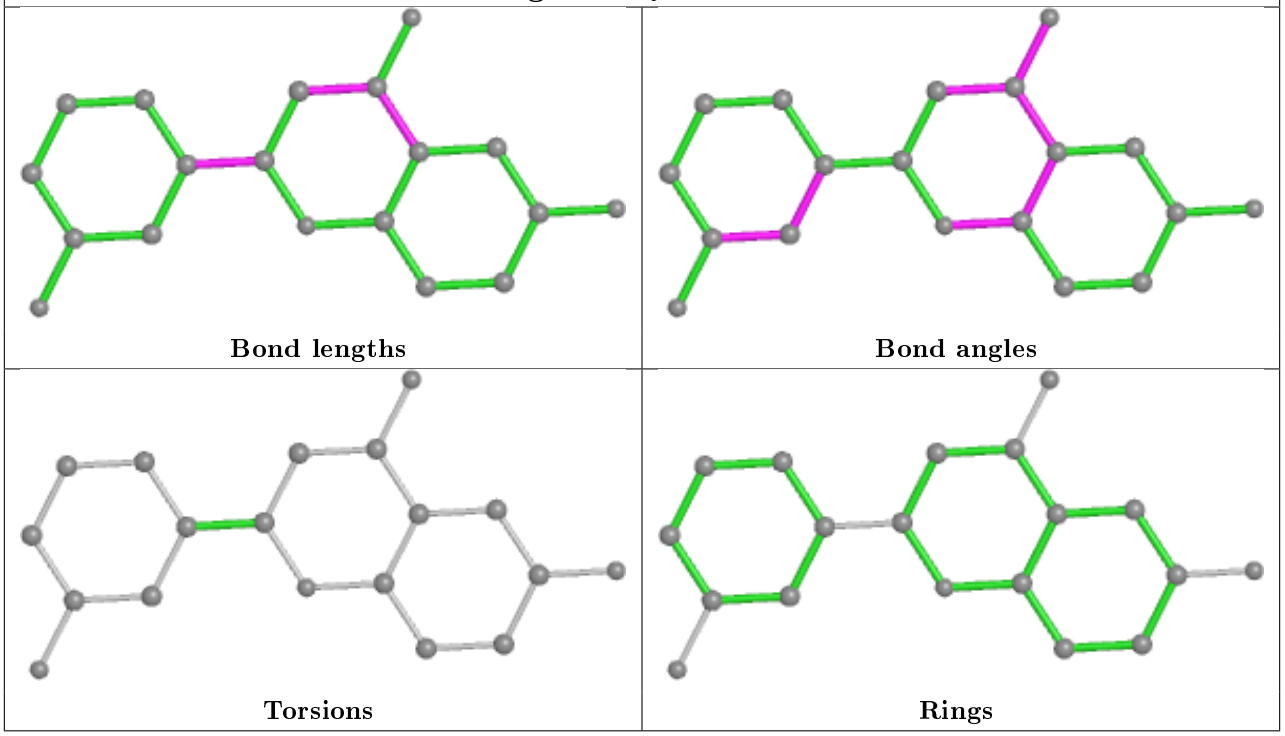
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	NAP	4	0
3	A	301	NAP	1	0
3	B	301	NAP	2	0

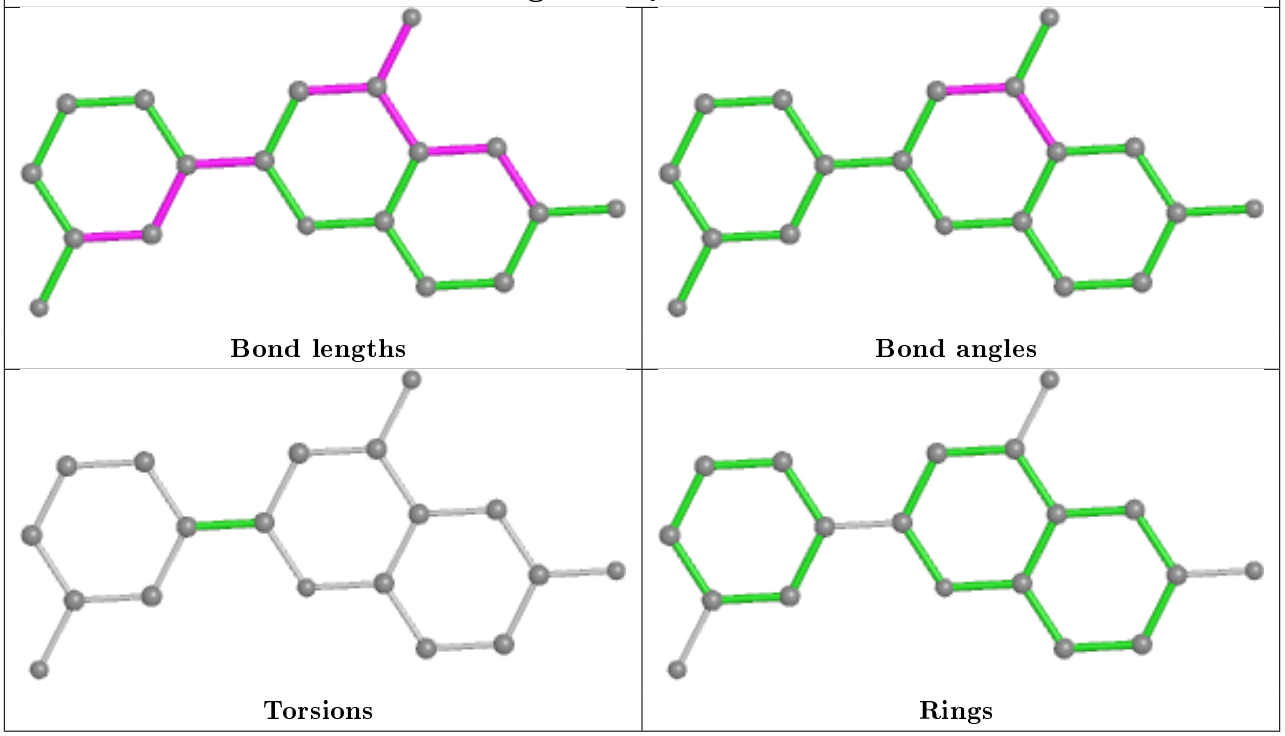
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

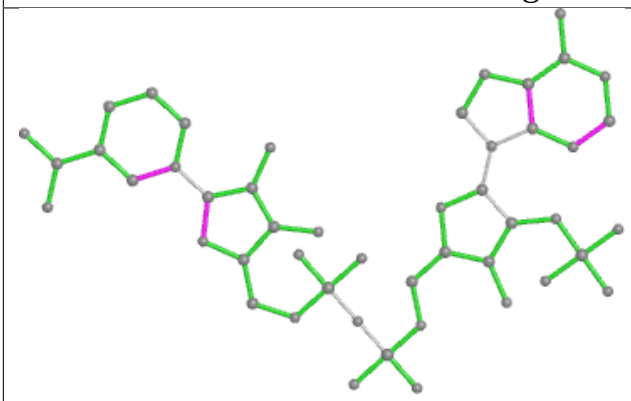
Ligand 6QT C 302



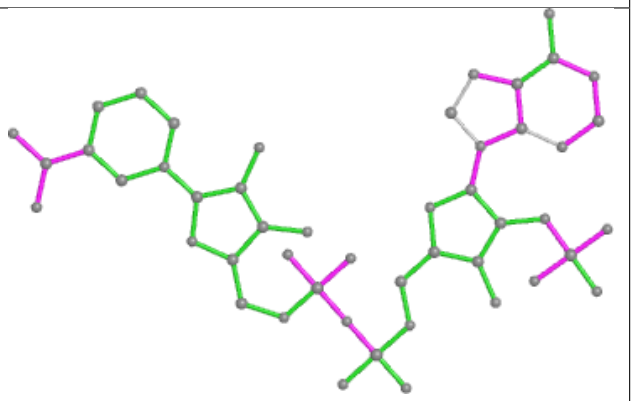
Ligand 6QT A 302



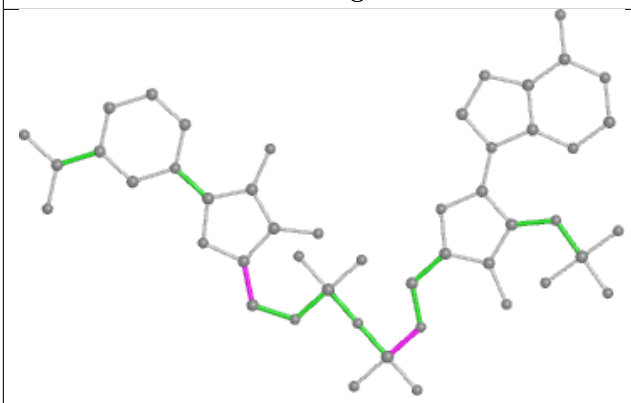
Ligand NAP C 301



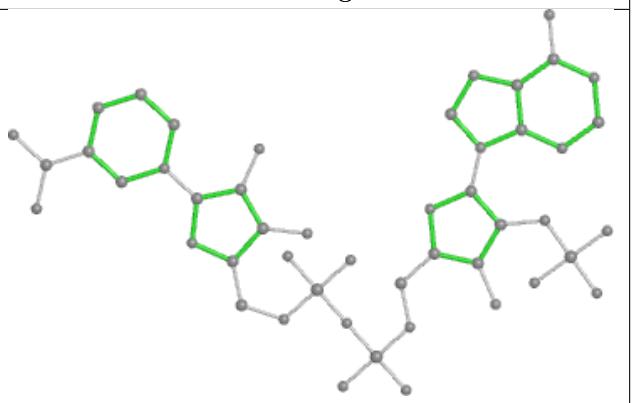
Bond lengths



Bond angles

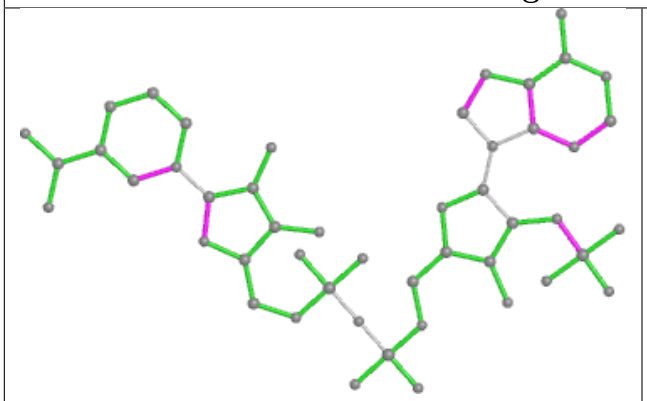


Torsions

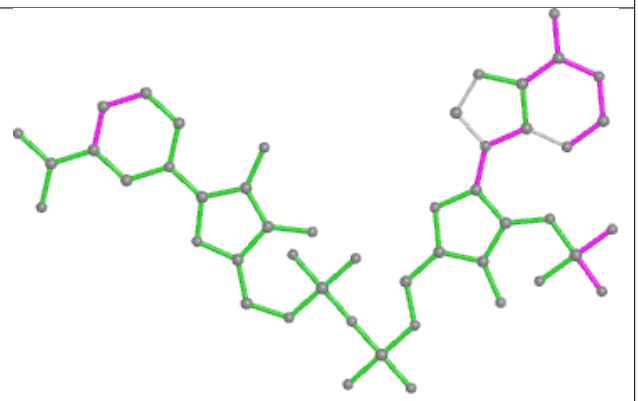


Rings

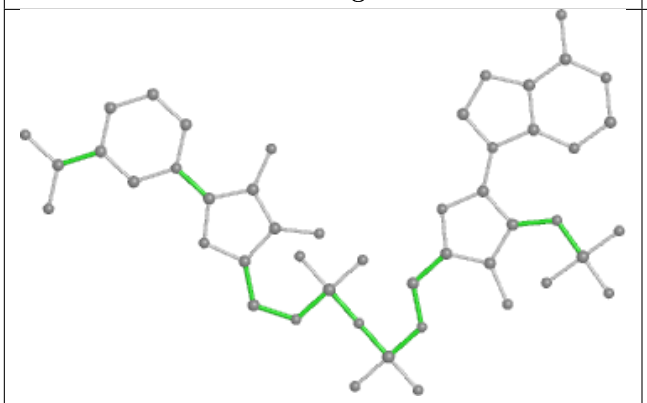
Ligand NAP A 301



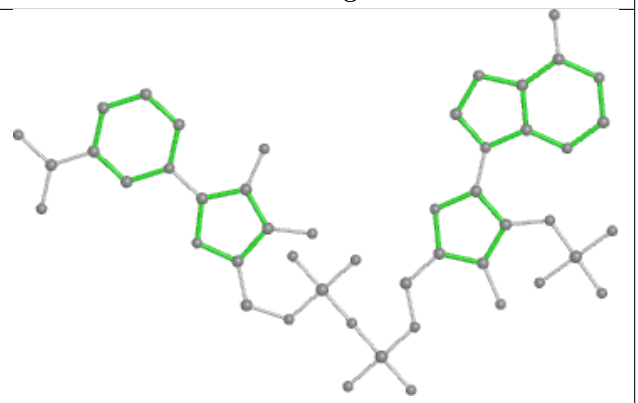
Bond lengths



Bond angles

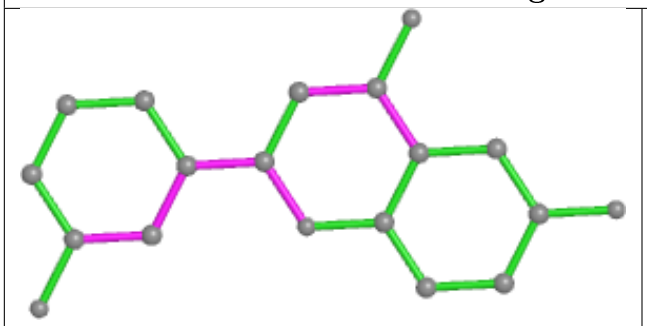


Torsions

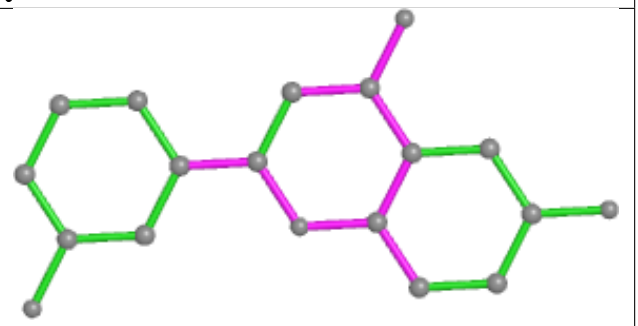


Rings

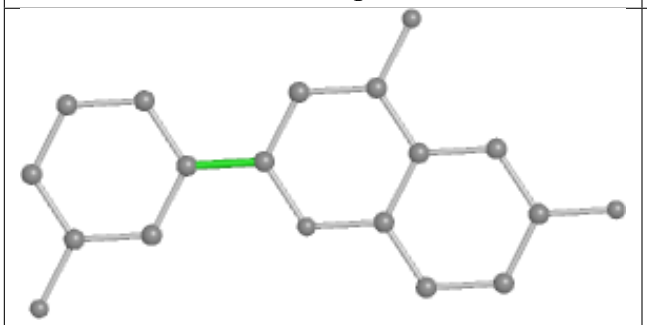
Ligand 6QT B 302



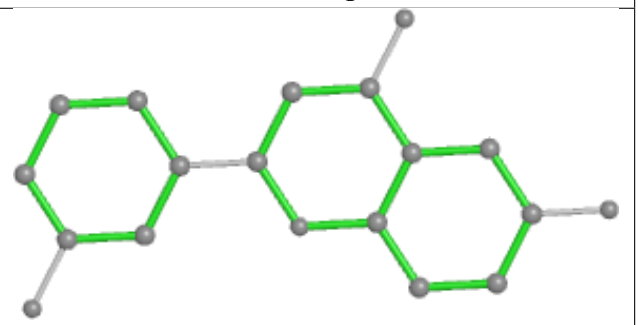
Bond lengths



Bond angles

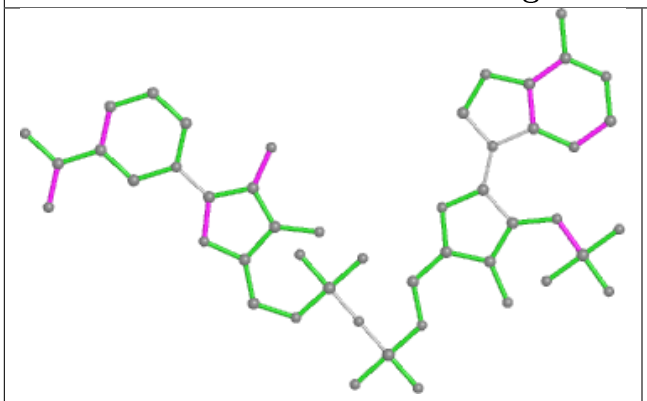


Torsions

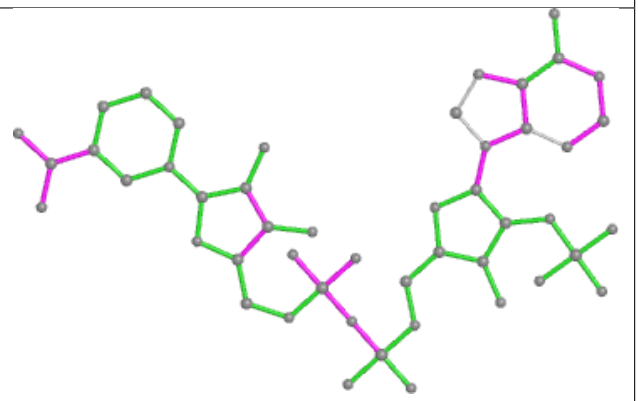


Rings

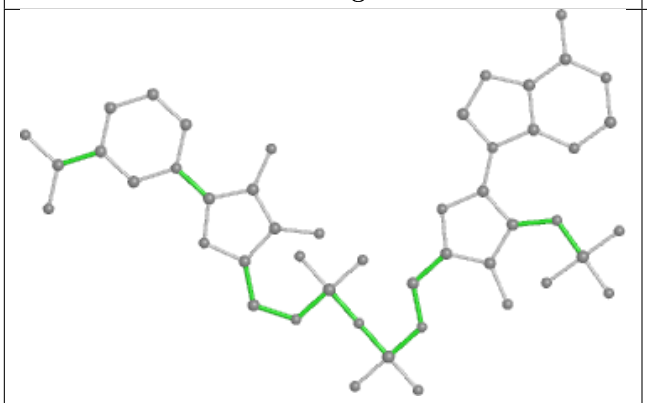
Ligand NAP D 301



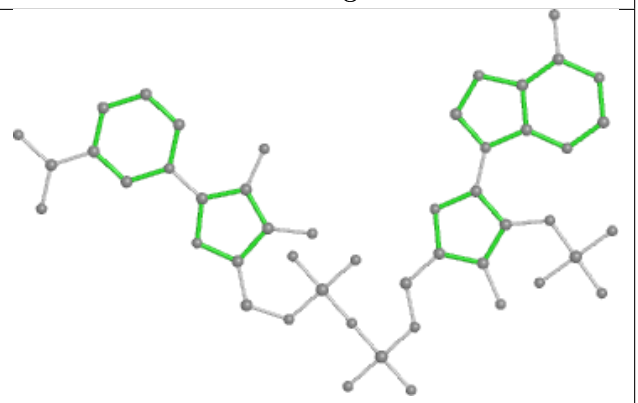
Bond lengths



Bond angles

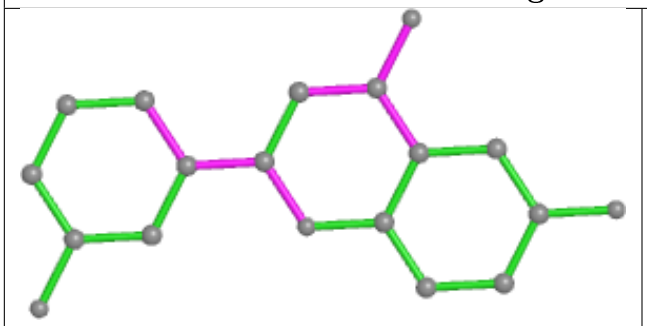


Torsions

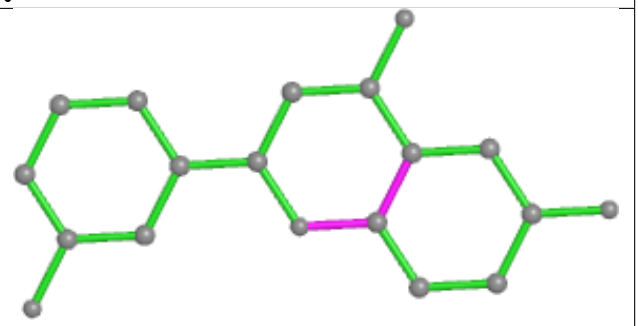


Rings

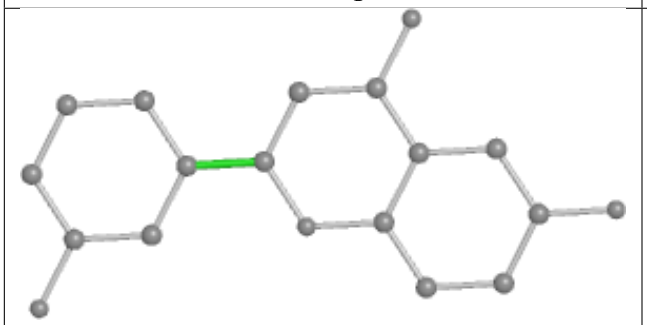
Ligand 6QT D 302



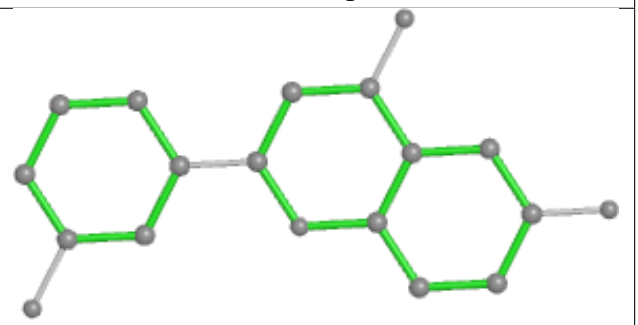
Bond lengths



Bond angles

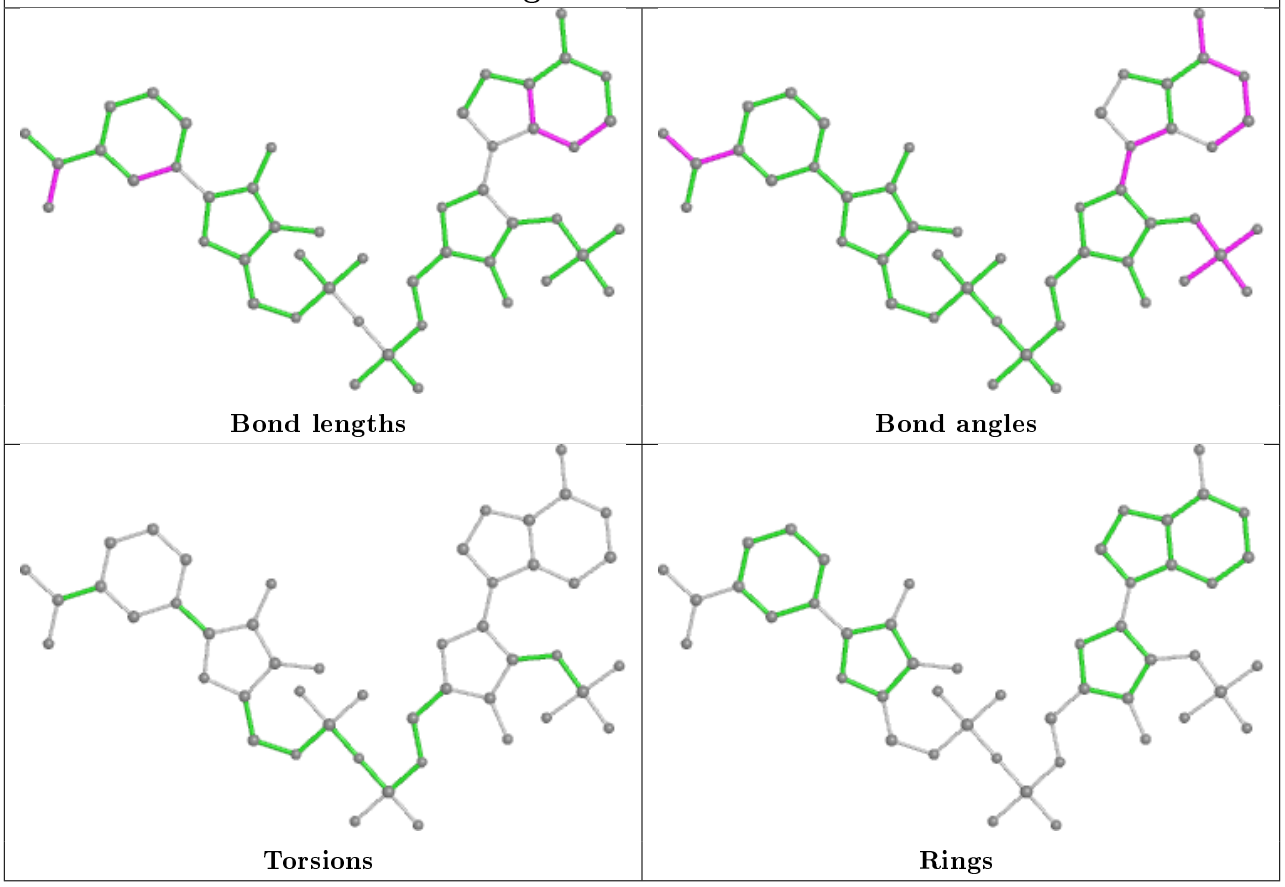


Torsions



Rings

Ligand NAP B 301



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	259:VAL	C	260:ASP	N	1.70

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	247/288 (85%)	-0.02	3 (1%)	79	82	8, 16, 28, 38	12 (4%)
1	B	246/288 (85%)	-0.06	4 (1%)	72	76	7, 14, 26, 40	10 (4%)
1	D	247/288 (85%)	0.05	9 (3%)	42	47	8, 16, 32, 47	7 (2%)
2	C	236/288 (81%)	0.05	10 (4%)	36	40	8, 17, 33, 43	7 (2%)
All	All	976/1152 (84%)	0.01	26 (2%)	54	58	7, 16, 30, 47	36 (3%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	211	VAL	5.3
1	B	212	ALA	5.2
1	B	211	VAL	4.9
1	A	212	ALA	4.8
2	C	221	TRP	3.9
1	D	212	ALA	3.6
2	C	152	SER	3.3
1	A	211	VAL	3.0
2	C	232	ALA	2.9
2	C	229	ARG	2.7
2	C	103	VAL	2.6
2	C	206	VAL	2.5
1	B	256	ILE	2.4
2	C	231	GLU	2.3
1	B	195	TYR	2.3
2	C	228	GLY	2.2
1	D	213	MET	2.2
1	D	210	PRO	2.1
1	D	195	TYR	2.1
1	A	256	ILE	2.1
1	D	256	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	43	SER	2.1
1	D	214	GLY	2.1
2	C	195	TYR	2.0
1	D	152	SER	2.0
1	D	208	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSX	D	168	7/8	0.94	0.07	20,22,36,42	0
2	CSX	C	168	7/8	0.95	0.07	19,21,29,36	2
1	CSX	A	168	7/8	0.95	0.07	20,23,40,49	0
1	CSX	B	168	7/8	0.95	0.07	18,20,29,33	2
2	OCS	C	59	9/10	0.98	0.08	14,17,24,28	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	6QT	C	302	19/19	0.79	0.17	23,27,30,30	19
3	NAP	C	301	48/48	0.86	0.15	15,20,25,26	48
4	6QT	D	302	19/19	0.91	0.16	23,26,35,36	0
4	6QT	B	302	19/19	0.94	0.10	19,22,32,32	0
4	6QT	A	302	19/19	0.94	0.11	23,24,34,35	0
3	NAP	D	301	48/48	0.95	0.11	14,19,23,26	0
3	NAP	A	301	48/48	0.96	0.08	14,18,20,23	0
3	NAP	B	301	48/48	0.96	0.09	11,17,19,21	0

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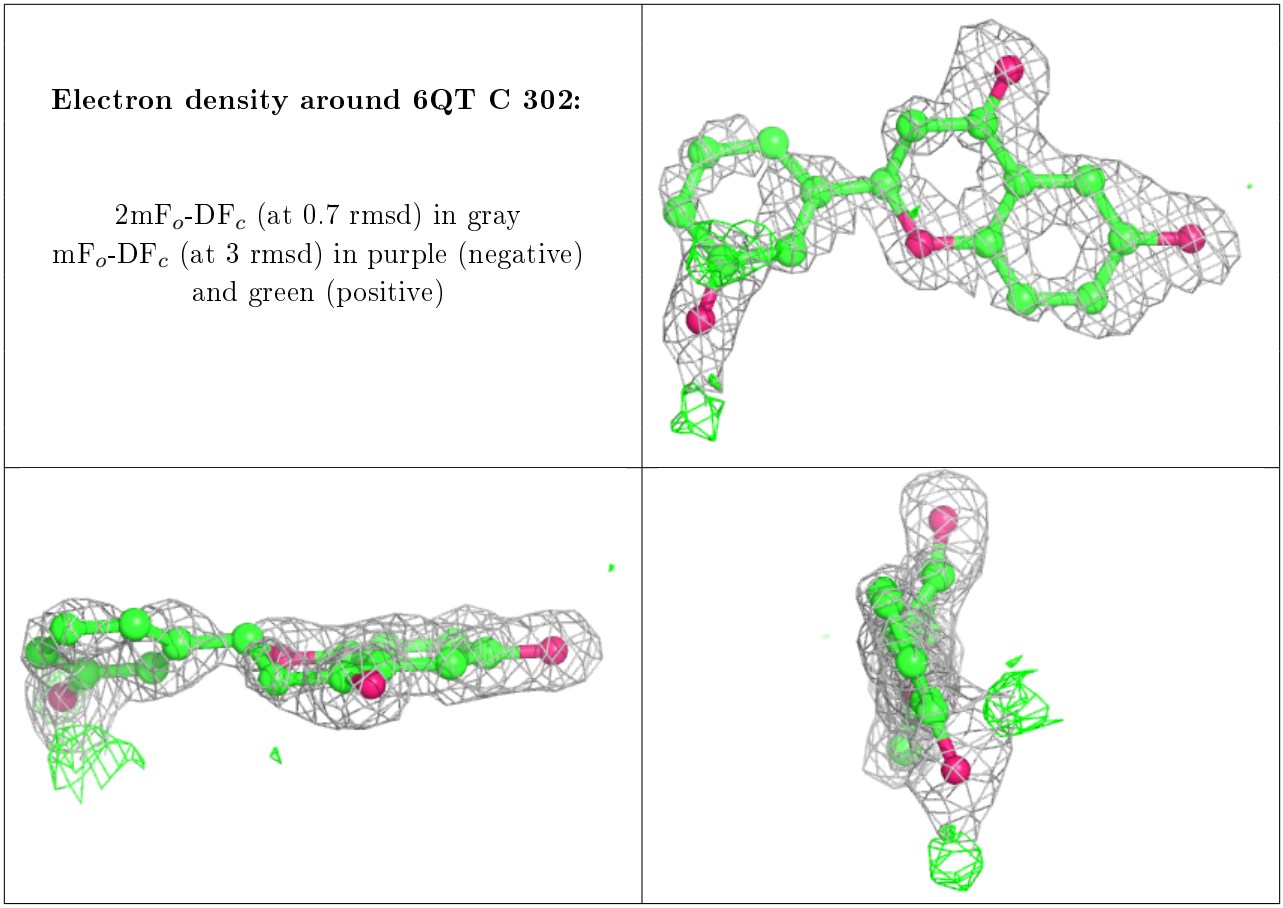
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ACT	C	303	4/4	0.97	0.06	21,22,22,23	0
5	ACT	A	303	4/4	0.97	0.11	23,23,23,24	0

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.

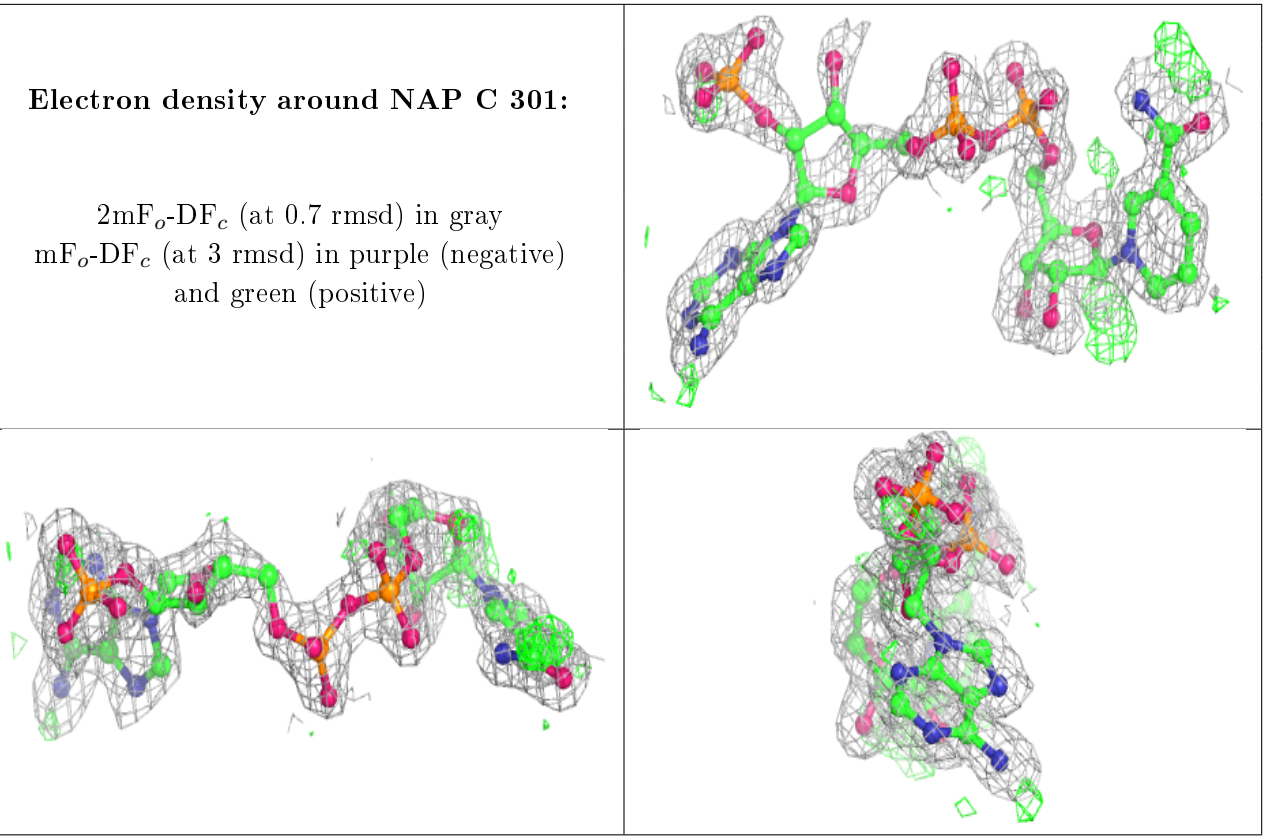
Electron density around 6QT C 302:

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



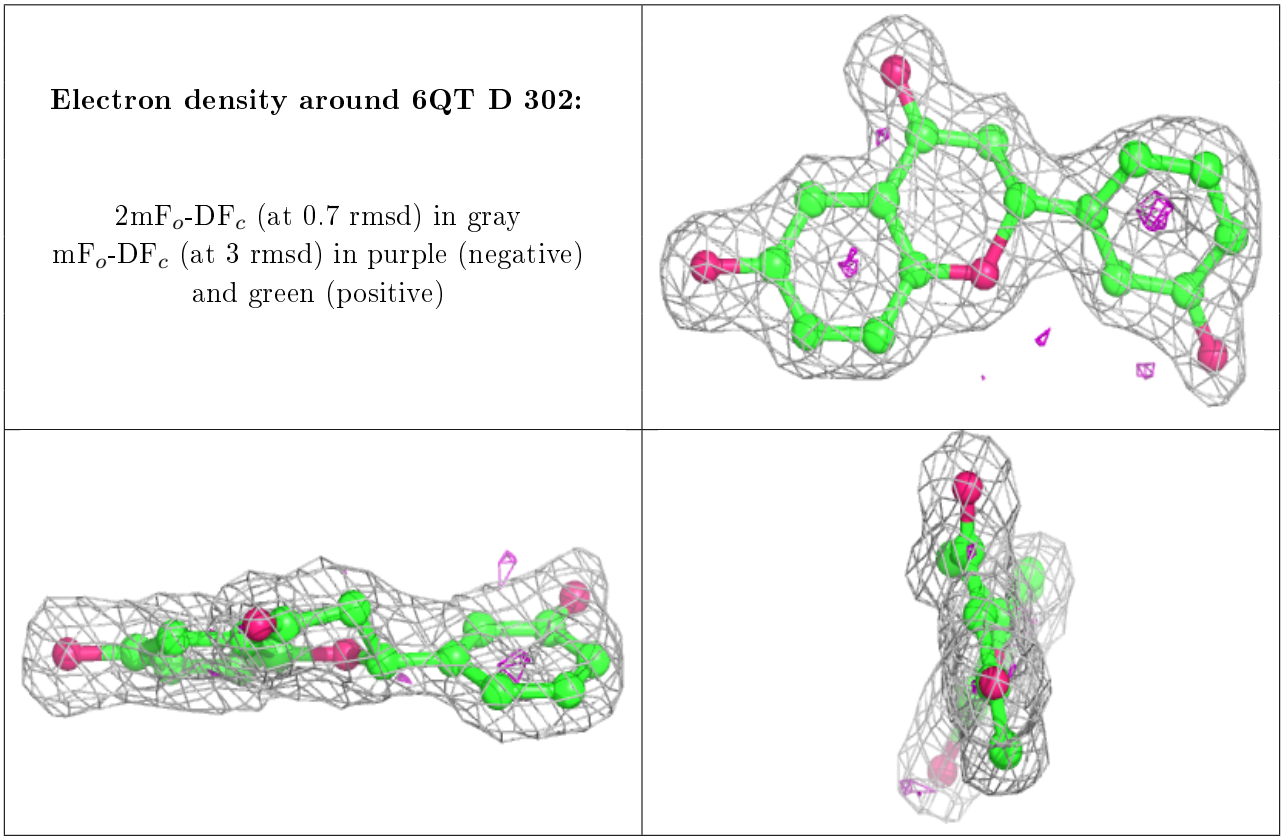
Electron density around NAP C 301:

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



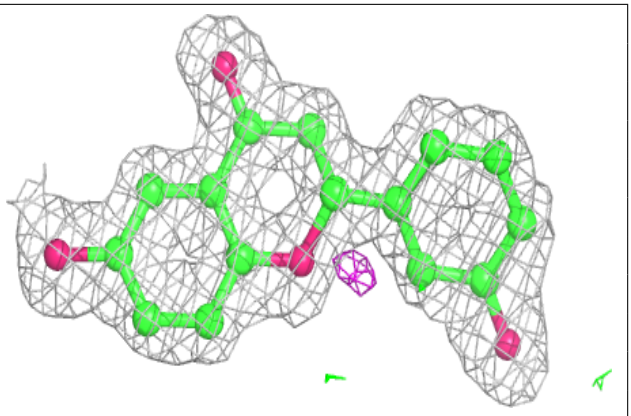
Electron density around 6QT D 302:

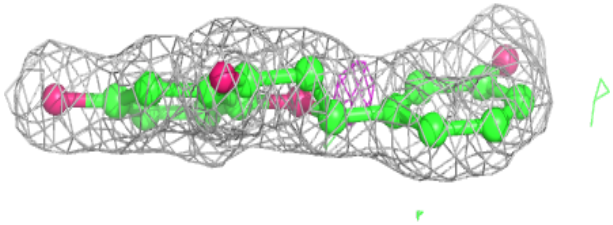
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

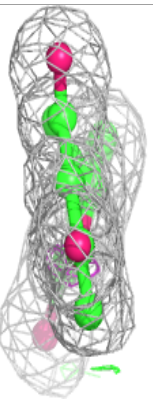


Electron density around 6QT B 302:

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

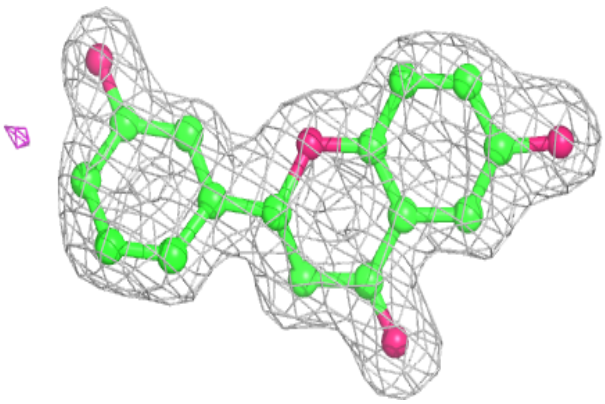


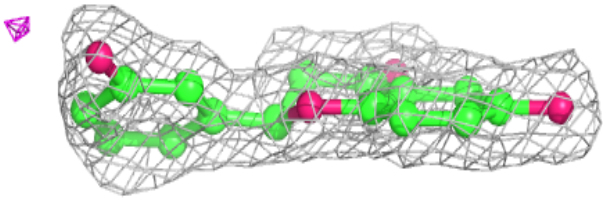


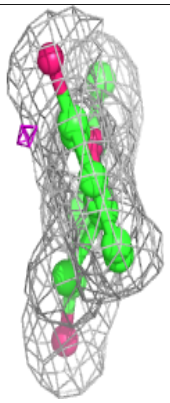


Electron density around 6QT A 302:

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

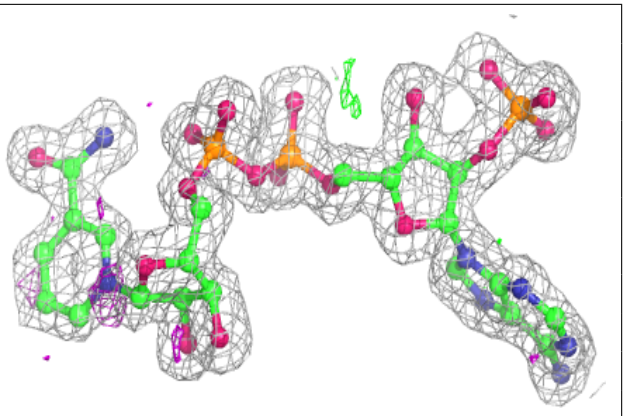


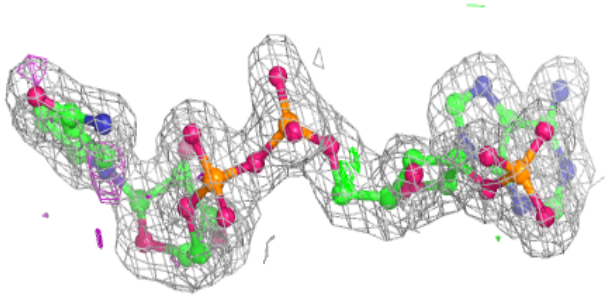


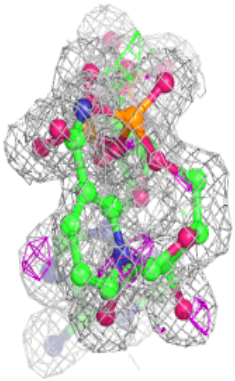


Electron density around NAP D 301:

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

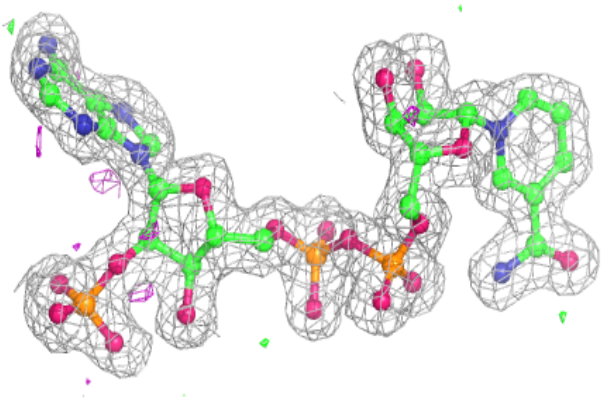


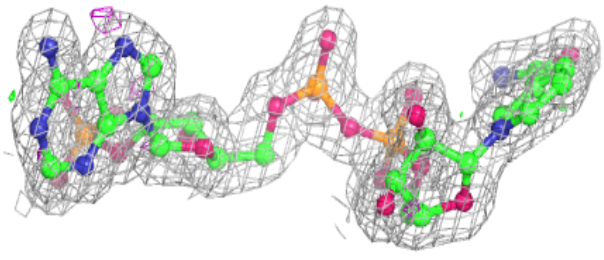


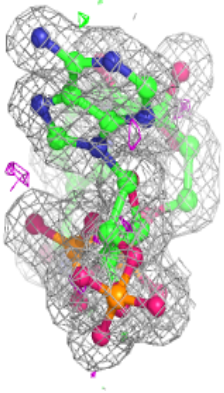


Electron density around NAP A 301:

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

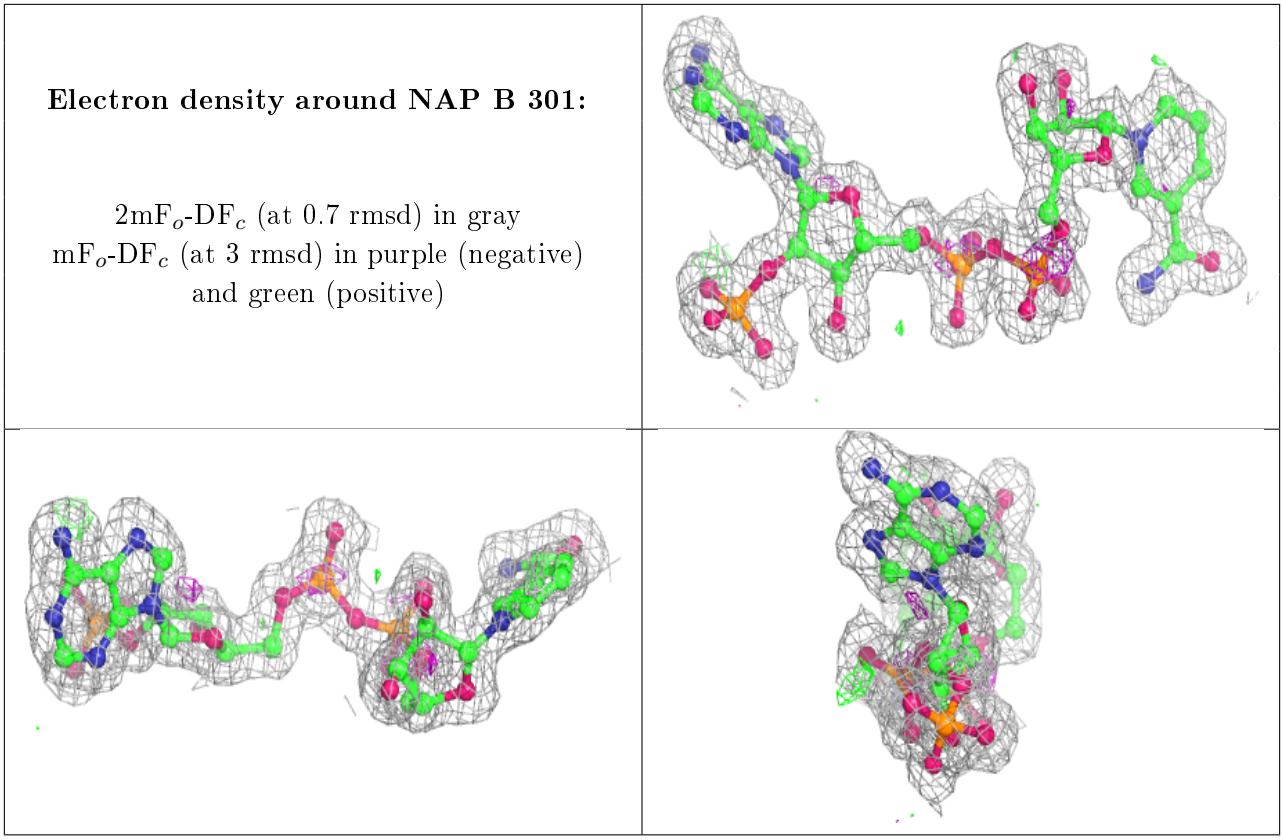






Electron density around NAP B 301:

$2mF_o$-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.