



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:45 PM UTC

PDB ID : 5JDC / pdb_00005jdc
Title : Trypanosoma brucei PTR1 in complex with inhibitor NP-13 (Hesperetin)
Authors : Mangani, S.; Pozzi, C.; Di Pisa, F.; Landi, G.; Dello Iacono, L.
Deposited on : 2016-04-16
Resolution : 1.78 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

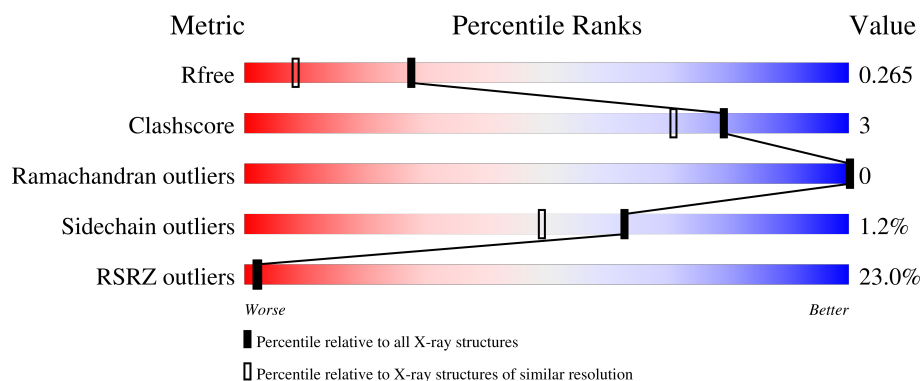
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	288	21% 80% 6% 14%
1	B	288	10% 80% 5% 15%
1	D	288	25% 78% 8% 14%
2	C	288	22% 74% 9% 17%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7836 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	249	Total	C	N	O	S	0	0	0
			1845	1161	326	347	11			
1	B	246	Total	C	N	O	S	0	3	0
			1838	1156	320	350	12			
1	D	248	Total	C	N	O	S	0	2	0
			1831	1152	325	343	11			

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

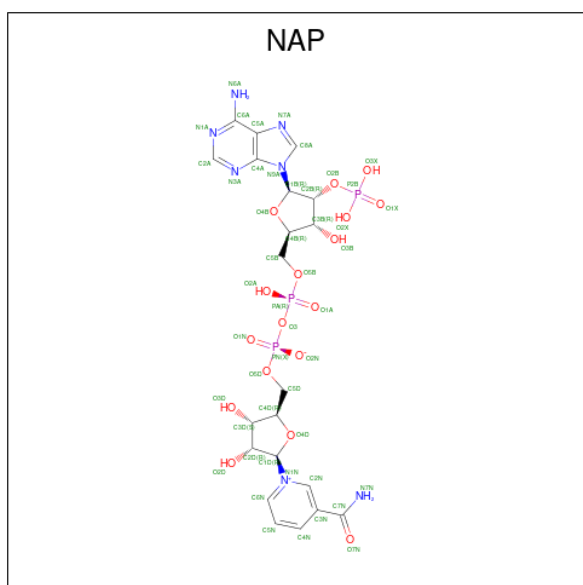
- Molecule 2 is a protein called Pteridine reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	239	Total	C	N	O	S	0	0	0
			1771	1114	313	334	10			

There are 20 discrepancies between the modelled and reference sequences:

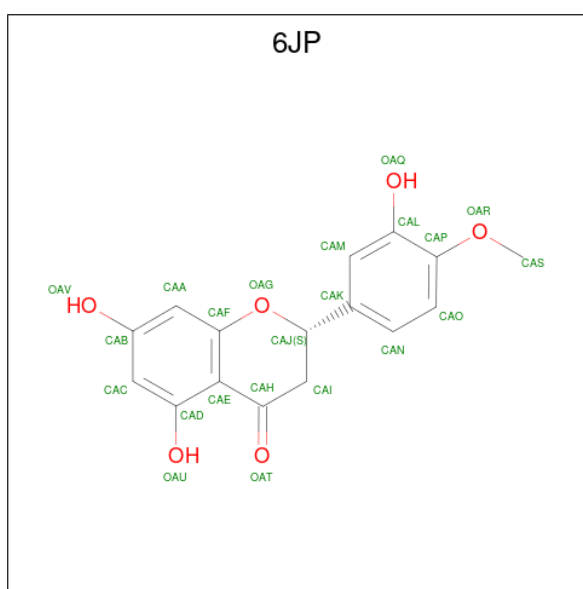
Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	initiating methionine	UNP O76290
C	-18	GLY	-	expression tag	UNP O76290
C	-17	SER	-	expression tag	UNP O76290
C	-16	SER	-	expression tag	UNP O76290
C	-15	HIS	-	expression tag	UNP O76290
C	-14	HIS	-	expression tag	UNP O76290
C	-13	HIS	-	expression 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 (CCD ID: 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	
3	B	1	Total	C	N	O	P	
			48	21	7	17	3	
3	C	1	Total	C	N	O	P	
			48	21	7	17	3	
3	D	1	Total	C	N	O	P	
			48	21	7	17	3	

- Molecule 4 is (2S)-5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-2,3-dihydro-4H-1-benzopyran-4-one (CCD ID: 6JP) (formula: C₁₆H₁₄O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O		
			22	16	6	0	0
4	B	1	Total	C	O		
			22	16	6	0	0
4	C	1	Total	C	O		
			22	16	6	0	0
4	D	1	Total	C	O		
			22	16	6	0	0

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

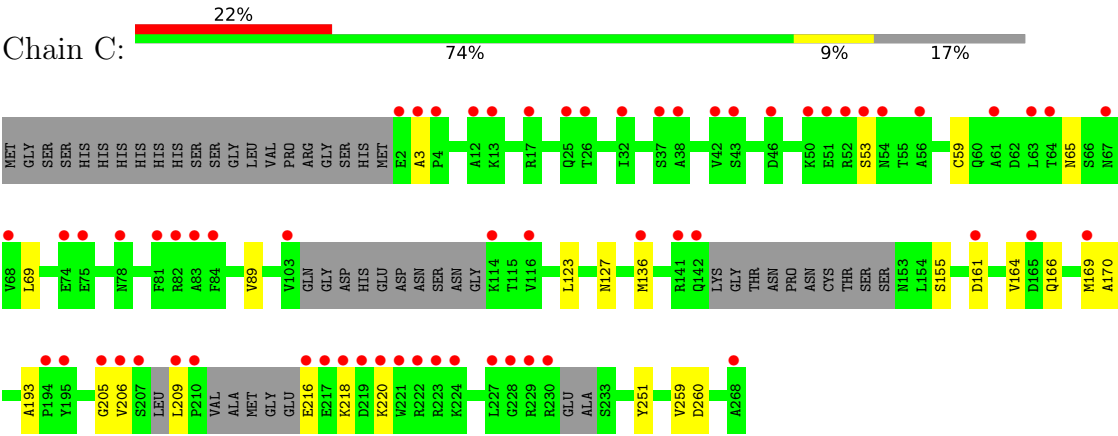


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	66	Total 66	O 66	0	0
7	B	86	Total 86	O 86	0	0
7	C	54	Total 54	O 54	0	0
7	D	51	Total 51	O 51	0	0

● Molecule 2: 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	74.84Å 90.04Å 82.94Å 90.00° 115.78° 90.00°	Depositor
Resolution (Å)	53.68 – 1.78 53.68 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.1 (53.68-1.78) 99.1 (53.68-1.78)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.208 , 0.241 (Not available) , 0.265	Depositor DCC
R_{free} test set	4615 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	14.5	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7836	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 38.38 % 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 3.7194e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OCS, 6JP, GOL, NAP, CSX, 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	1.18	1/1864 (0.1%)	1.10	2/2528 (0.1%)
1	B	1.35	3/1855 (0.2%)	1.11	4/2516 (0.2%)
1	D	1.19	1/1856 (0.1%)	1.13	5/2520 (0.2%)
2	C	1.22	2/1777 (0.1%)	1.11	4/2408 (0.2%)
All	All	1.24	7/7352 (0.1%)	1.11	15/9972 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	259	VAL	C-N	22.85	1.64	1.33
1	B	193	ALA	C-O	-6.00	1.19	1.24
1	B	204	PRO	CA-C	-5.78	1.45	1.52
1	D	205	GLY	C-N	-5.61	1.26	1.33
2	C	193	ALA	C-O	-5.48	1.19	1.24
1	A	100	THR	C-O	5.31	1.30	1.24
2	C	260	ASP	C-N	-5.05	1.26	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	206	VAL	CA-C-O	8.90	129.91	120.48
2	C	259	VAL	O-C-N	6.42	130.60	122.57
2	C	205	GLY	N-CA-C	-6.35	104.43	110.21
1	D	251	TYR	CA-C-O	6.28	126.59	119.18
1	D	205	GLY	O-C-N	-6.13	114.73	122.70
1	D	30	VAL	N-CA-C	5.62	116.22	108.12
1	A	251	TYR	O-C-N	-5.55	115.67	122.34
1	A	250	GLN	N-CA-C	5.47	118.16	111.82
1	D	250	GLN	N-CA-C	5.45	119.67	113.19
1	B	259	VAL	CA-C-N	-5.44	113.99	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	VAL	C-N-CA	-5.44	113.99	122.37
1	B	250	GLN	N-CA-C	5.41	119.36	112.87
2	C	3	ALA	CA-C-N	-5.28	115.14	120.21
2	C	3	ALA	C-N-CA	-5.28	115.14	120.21
1	B	206	VAL	CB-CA-C	5.04	117.89	110.98

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	1845	0	1867	13	0
1	B	1838	0	1846	9	0
1	D	1831	0	1846	11	0
2	C	1771	0	1776	10	0
3	A	48	0	25	0	0
3	B	48	0	25	0	0
3	C	48	0	25	0	0
3	D	48	0	25	1	0
4	A	22	0	0	1	0
4	B	22	0	0	3	0
4	C	22	0	0	0	0
4	D	22	0	0	0	0
5	A	4	0	3	1	0
5	C	4	0	3	0	0
6	C	6	0	8	0	0
7	A	66	0	0	1	0
7	B	86	0	0	1	0
7	C	54	0	0	0	0
7	D	51	0	0	0	0
All	All	7836	0	7449	40	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 (40) 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:168[A]:CSX:HG	4:B:302:6JP:CAS	1.81	0.94
2:C:161:ASP:HB3	2:C:164:VAL:HG13	1.76	0.67
1:A:141:ARG:HG2	7:A:465:HOH:O	1.95	0.66
1:A:193:ALA:HB3	1:A:194:PRO:HD3	1.82	0.60
1:A:251:TYR:CE2	1:B:232:ALA:HB2	2.37	0.59
1:A:65:ASN:HA	1:A:69:LEU:HD22	1.88	0.56
2:C:209:LEU:HD13	2:C:218:LYS:HG3	1.88	0.56
1:A:168:CSX:HG	4:A:302:6JP:CAP	2.19	0.55
1:B:128:ALA:C	1:B:131:PRO:HD2	2.32	0.54
2:C:209:LEU:HD13	2:C:218:LYS:CG	2.38	0.54
1:A:128:ALA:C	1:A:131:PRO:HD2	2.33	0.53
2:C:65:ASN:HA	2:C:69:LEU:HD22	1.91	0.52
1:D:205:GLY:HA3	1:D:260:ASP:HB2	1.92	0.51
1:B:168[A]:CSX:SG	4:B:302:6JP:CAS	2.94	0.51
1:A:17:ARG:HD3	5:A:303:ACT:H3	1.93	0.50
2:C:251:TYR:CE2	1:D:232:ALA:HB2	2.47	0.49
1:D:69:LEU:N	1:D:70:PRO:HD2	2.27	0.49
1:A:251:TYR:CD2	1:B:232:ALA:HB2	2.48	0.48
1:A:193:ALA:N	1:A:194:PRO:CD	2.76	0.48
1:D:69:LEU:N	1:D:70:PRO:CD	2.77	0.47
1:B:172:SER:O	1:B:176:MET:HG3	2.15	0.46
1:D:164:VAL:HG22	1:D:179:HIS:CD2	2.52	0.44
2:C:123:LEU:O	2:C:127:ASN:HB2	2.17	0.44
1:D:205:GLY:O	3:D:301:NAP:H4N	2.16	0.44
1:A:102:LEU:O	2:C:136:MET:HG3	2.17	0.44
1:D:210:PRO:HG2	1:D:213:MET:HE3	2.00	0.43
2:C:169:MET:O	2:C:170:ALA:HB3	2.19	0.43
4:B:302:6JP:OAT	4:B:302:6JP:OAU	2.37	0.42
2:C:89:VAL:HA	2:C:155:SER:O	2.19	0.42
1:A:29:ARG:HG2	1:A:55:THR:HG22	2.01	0.42
1:B:9:THR:HA	1:B:33:HIS:HB3	2.02	0.42
2:C:206:VAL:O	2:C:206:VAL:HG23	2.19	0.41
1:D:9:THR:HA	1:D:33:HIS:HB3	2.02	0.41
1:D:123:LEU:O	1:D:127:ASN:HB2	2.19	0.41
1:B:26:THR:HG22	1:B:26:THR:O	2.21	0.41
1:A:26:THR:O	1:A:26:THR:HG22	2.21	0.41
1:D:32:ILE:HD13	1:D:44:LEU:HD23	2.03	0.41
1:B:67:ASN:HB2	7:B:461:HOH:O	2.20	0.41
1:A:193:ALA:N	1:A:194:PRO:HD2	2.36	0.40
1:D:222:ARG:HD3	1:D:231:GLU:OE2	2.21	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	242/288 (84%)	234 (97%)	8 (3%)	0	100	100
1	B	239/288 (83%)	233 (98%)	6 (2%)	0	100	100
1	D	243/288 (84%)	234 (96%)	9 (4%)	0	100	100
2	C	225/288 (78%)	218 (97%)	7 (3%)	0	100	100
All	All	949/1152 (82%)	919 (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	193/230 (84%)	191 (99%)	2 (1%)	68	55
1	B	192/230 (84%)	191 (100%)	1 (0%)	81	73
1	D	191/230 (83%)	189 (99%)	2 (1%)	68	55
2	C	184/229 (80%)	180 (98%)	4 (2%)	45	26
All	All	760/919 (83%)	751 (99%)	9 (1%)	63	49

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	HIS
1	A	209	LEU
1	B	179	HIS
2	C	53	SER
2	C	166	GLN
2	C	216	GLU
2	C	220	LYS
1	D	47	GLU
1	D	169	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	127	ASN
1	A	175	ASN
1	A	186	GLN
1	B	92	ASN
1	B	175	ASN
1	B	236	GLN
2	C	54	ASN
2	C	92	ASN
2	C	140	GLN
1	D	65	ASN
1	D	92	ASN
1	D	140	GLN
1	D	179	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 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	$\# Z > 2$
1	CSX	B	168[B]	1	3,6,7	1.38	0	1,6,8	3.37	1 (100%)
2	CSX	C	168	2	3,6,7	0.48	0	1,6,8	1.16	0
1	CSX	A	168	1	3,6,7	0.54	0	1,6,8	1.10	0
1	CSX	B	168[A]	1	3,6,7	0.87	0	1,6,8	0.17	0
2	OCS	C	59	2	6,8,9	2.45	2 (33%)	7,11,13	1.71	2 (28%)
1	CSX	D	168	1	3,6,7	0.58	0	1,6,8	1.06	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
1	CSX	B	168[B]	1	-	2/2/5/7	-
2	CSX	C	168	2	-	0/2/5/7	-
1	CSX	A	168	1	-	0/2/5/7	-
1	CSX	B	168[A]	1	-	0/2/5/7	-
2	OCS	C	59	2	-	1/4/7/9	-
1	CSX	D	168	1	-	0/2/5/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	59	OCS	OD3-SG	5.00	1.59	1.45
2	C	59	OCS	CB-CA	-2.97	1.51	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168[B]	CSX	CA-CB-SG	3.37	121.10	113.17
2	C	59	OCS	OD3-SG-CB	3.09	111.38	106.76
2	C	59	OCS	CA-CB-SG	-2.20	110.34	113.61

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	168[B]	CSX	N-CA-CB-SG

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Mol	Chain	Res	Type	Atoms
1	B	168[B]	CSX	C-CA-CB-SG
2	C	59	OCS	N-CA-CB-SG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	168	CSX	1	0
1	B	168[A]	CSX	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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
3	NAP	A	301	-	50,52,52	1.41	9 (18%)	71,80,80	1.64	14 (19%)
4	6JP	D	302	-	24,24,24	1.99	6 (25%)	35,35,35	1.53	6 (17%)
5	ACT	C	303	-	3,3,3	0.89	0	3,3,3	0.28	0
3	NAP	C	301	-	50,52,52	1.59	7 (14%)	71,80,80	1.73	17 (23%)
4	6JP	C	302	-	24,24,24	1.69	3 (12%)	35,35,35	1.73	7 (20%)
5	ACT	A	303	-	3,3,3	1.28	0	3,3,3	1.10	0
3	NAP	D	301	-	50,52,52	1.56	9 (18%)	71,80,80	1.87	18 (25%)
4	6JP	A	302	-	24,24,24	1.86	3 (12%)	35,35,35	1.65	6 (17%)
3	NAP	B	301	-	50,52,52	1.53	7 (14%)	71,80,80	1.92	18 (25%)
4	6JP	B	302	-	24,24,24	1.87	6 (25%)	35,35,35	2.18	9 (25%)
6	GOL	C	304	-	5,5,5	0.78	0	5,5,5	0.80	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
3	NAP	A	301	-	-	0/35/67/67	0/5/5/5
4	6JP	D	302	-	-	2/6/18/18	0/3/3/3
3	NAP	C	301	-	-	1/35/67/67	0/5/5/5
4	6JP	C	302	-	-	2/6/18/18	0/3/3/3
3	NAP	D	301	-	-	2/35/67/67	0/5/5/5
4	6JP	A	302	-	-	2/6/18/18	0/3/3/3
3	NAP	B	301	-	-	0/35/67/67	0/5/5/5
4	6JP	B	302	-	-	3/6/18/18	0/3/3/3
6	GOL	C	304	-	-	0/4/4/4	-

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	302	6JP	CAK-CAJ	-5.54	1.42	1.51
3	C	301	NAP	C5A-C4A	5.28	1.48	1.39
4	D	302	6JP	CAI-CAH	-4.93	1.41	1.50
3	C	301	NAP	PN-O3	4.93	1.64	1.59
4	B	302	6JP	CAI-CAH	-4.78	1.41	1.50
4	B	302	6JP	CAK-CAJ	-4.69	1.43	1.51
4	D	302	6JP	CAK-CAJ	-4.68	1.43	1.51
4	C	302	6JP	CAK-CAJ	-4.63	1.43	1.51
3	B	301	NAP	C5A-C4A	4.46	1.47	1.39
3	A	301	NAP	C5A-C4A	4.34	1.46	1.39
4	A	302	6JP	CAI-CAH	-4.31	1.42	1.50
3	D	301	NAP	PA-O3	4.26	1.64	1.59
4	C	302	6JP	CAI-CAH	-4.12	1.43	1.50
3	B	301	NAP	PN-O3	3.97	1.63	1.59
3	C	301	NAP	PA-O3	3.93	1.63	1.59
3	D	301	NAP	P2B-O2B	3.87	1.66	1.59
3	A	301	NAP	P2B-O2B	3.84	1.66	1.59
3	D	301	NAP	O4D-C1D	3.82	1.45	1.40
3	D	301	NAP	C5A-C4A	3.58	1.45	1.39
3	B	301	NAP	C5A-C6A	3.56	1.50	1.41
3	B	301	NAP	P2B-O2B	3.50	1.65	1.59
3	B	301	NAP	PA-O3	3.38	1.63	1.59
3	D	301	NAP	PN-O3	3.22	1.63	1.59
3	D	301	NAP	C7N-N7N	3.07	1.38	1.33
3	D	301	NAP	C8A-N7A	2.96	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	NAP	PN-O3	2.92	1.62	1.59
4	D	302	6JP	CAM-CAK	2.88	1.43	1.39
3	D	301	NAP	C4A-N9A	-2.84	1.31	1.37
3	C	301	NAP	P2B-O2B	2.83	1.64	1.59
4	C	302	6JP	CAN-CAK	2.73	1.43	1.39
3	C	301	NAP	C5A-C6A	2.73	1.48	1.41
3	A	301	NAP	C8A-N7A	2.73	1.36	1.31
3	B	301	NAP	C2N-N1N	2.72	1.38	1.35
3	A	301	NAP	C4A-N9A	-2.71	1.32	1.37
4	B	302	6JP	OAG-CAF	-2.62	1.34	1.38
3	A	301	NAP	C2N-N1N	2.51	1.37	1.35
3	C	301	NAP	C4A-N9A	-2.37	1.32	1.37
4	D	302	6JP	CAC-CAD	2.26	1.42	1.38
3	B	301	NAP	C4A-N9A	-2.24	1.33	1.37
3	A	301	NAP	PA-O2A	-2.24	1.44	1.55
3	A	301	NAP	C5A-C6A	2.20	1.47	1.41
3	A	301	NAP	O7N-C7N	2.18	1.28	1.24
4	B	302	6JP	CAE-CAH	-2.16	1.41	1.46
4	A	302	6JP	CAM-CAK	2.15	1.42	1.39
4	B	302	6JP	CAM-CAK	2.14	1.42	1.39
3	D	301	NAP	C5A-C6A	2.13	1.46	1.41
3	C	301	NAP	C8A-N7A	2.12	1.35	1.31
4	B	302	6JP	CAL-CAP	2.10	1.44	1.40
4	D	302	6JP	CAA-CAF	2.09	1.42	1.38
4	D	302	6JP	CAE-CAH	-2.06	1.41	1.46

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	302	6JP	OAR-CAP-CAL	6.16	123.78	114.55
4	C	302	6JP	CAS-OAR-CAP	5.68	125.84	117.51
3	D	301	NAP	C4A-N9A-C8A	5.17	111.16	105.74
3	B	301	NAP	C3N-C7N-N7N	5.00	123.89	117.74
4	B	302	6JP	CAS-OAR-CAP	4.68	124.38	117.51
3	C	301	NAP	C3N-C7N-N7N	4.68	123.50	117.74
3	D	301	NAP	N3A-C2A-N1A	-4.66	121.53	128.58
3	B	301	NAP	C2B-C1B-N9A	-4.47	106.40	113.75
4	B	302	6JP	OAR-CAP-CAO	-4.40	116.89	124.30
4	D	302	6JP	CAS-OAR-CAP	4.36	123.91	117.51
3	D	301	NAP	C4A-N9A-C1B	-4.36	116.44	126.63
3	A	301	NAP	O4B-C1B-N9A	4.30	116.34	108.09
4	A	302	6JP	OAG-CAF-CAE	-4.23	117.39	121.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	301	NAP	C2B-C1B-N9A	-4.22	106.80	113.75
3	D	301	NAP	N9A-C8A-N7A	-4.21	107.97	113.94
3	C	301	NAP	N3A-C2A-N1A	-4.13	122.33	128.58
3	B	301	NAP	C4A-N9A-C8A	4.06	110.01	105.74
3	B	301	NAP	C5A-C4A-N3A	-4.04	121.15	126.72
4	B	302	6JP	OAG-CAF-CAE	-3.99	117.63	121.64
4	C	302	6JP	OAR-CAP-CAL	3.96	120.49	114.55
3	A	301	NAP	C4A-N9A-C8A	3.91	109.85	105.74
3	C	301	NAP	C5A-C4A-N3A	-3.82	121.46	126.72
4	A	302	6JP	CAS-OAR-CAP	3.79	123.08	117.51
3	B	301	NAP	O4B-C1B-N9A	3.79	115.36	108.09
3	C	301	NAP	C2A-N1A-C6A	3.75	124.89	118.73
3	D	301	NAP	C6A-C5A-N7A	3.73	139.28	132.09
3	A	301	NAP	C5A-C4A-N3A	-3.72	121.60	126.72
3	B	301	NAP	C4A-C5A-N7A	-3.69	106.36	110.58
3	B	301	NAP	N3A-C2A-N1A	-3.65	123.06	128.58
3	B	301	NAP	C6A-C5A-N7A	3.61	139.06	132.09
3	A	301	NAP	C2B-C1B-N9A	-3.60	107.83	113.75
4	D	302	6JP	OAG-CAF-CAE	-3.60	118.03	121.64
3	A	301	NAP	N3A-C2A-N1A	-3.48	123.31	128.58
3	A	301	NAP	C4A-N9A-C1B	-3.48	118.50	126.63
3	B	301	NAP	C2A-N3A-C4A	3.46	120.28	111.83
3	D	301	NAP	O4B-C1B-N9A	3.42	114.66	108.09
3	B	301	NAP	N3A-C4A-N9A	3.41	132.97	127.17
4	B	302	6JP	OAU-CAD-CAE	-3.40	114.86	121.14
3	A	301	NAP	N3A-C4A-N9A	3.33	132.83	127.17
3	C	301	NAP	C4A-N9A-C8A	3.27	109.17	105.74
3	C	301	NAP	C4A-C5A-N7A	-3.26	106.86	110.58
4	A	302	6JP	CAF-OAG-CAJ	3.25	121.22	115.54
3	D	301	NAP	C4A-C5A-N7A	-3.22	106.89	110.58
3	C	301	NAP	N3A-C4A-N9A	3.22	132.64	127.17
3	C	301	NAP	O4B-C1B-N9A	3.12	114.08	108.09
3	B	301	NAP	O7N-C7N-C3N	-3.11	115.80	119.60
3	D	301	NAP	C2A-N1A-C6A	3.09	123.80	118.73
3	C	301	NAP	C2A-N3A-C4A	3.04	119.27	111.83
3	A	301	NAP	C2A-N3A-C4A	3.04	119.25	111.83
3	B	301	NAP	O2A-PA-O1A	3.00	126.39	112.44
3	C	301	NAP	P2B-O2B-C2B	3.00	131.44	123.43
4	D	302	6JP	CAD-CAC-CAB	2.99	122.44	119.67
3	B	301	NAP	O2B-P2B-O1X	-2.98	98.70	109.33
3	D	301	NAP	C2A-N3A-C4A	2.95	119.04	111.83
3	D	301	NAP	C5A-N7A-C8A	2.86	107.94	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	302	6JP	CAI-CAH-CAE	2.76	121.75	116.77
4	B	302	6JP	CAF-CAE-CAH	2.67	122.89	120.29
3	A	301	NAP	N9A-C8A-N7A	-2.64	110.20	113.94
3	D	301	NAP	C5A-C4A-N3A	-2.63	123.10	126.72
3	B	301	NAP	N9A-C8A-N7A	-2.58	110.27	113.94
3	C	301	NAP	C6A-C5A-N7A	2.57	137.04	132.09
4	C	302	6JP	OAR-CAP-CAO	-2.55	120.00	124.30
3	B	301	NAP	O3X-P2B-O2X	2.55	117.37	107.80
3	D	301	NAP	C6A-C5A-C4A	-2.54	113.71	117.18
4	A	302	6JP	CAI-CAH-CAE	2.54	121.35	116.77
4	C	302	6JP	OAG-CAF-CAE	-2.53	119.10	121.64
3	C	301	NAP	C5A-N7A-C8A	2.52	107.41	103.45
3	B	301	NAP	C5A-N7A-C8A	2.51	107.40	103.45
3	A	301	NAP	O7N-C7N-C3N	-2.51	116.53	119.60
3	B	301	NAP	C4A-N9A-C1B	-2.48	120.84	126.63
4	B	302	6JP	CAF-OAG-CAJ	2.41	119.75	115.54
3	C	301	NAP	C4A-N9A-C1B	-2.40	121.02	126.63
3	A	301	NAP	C6A-C5A-N7A	2.40	136.72	132.09
3	D	301	NAP	O4B-C1B-C2B	2.39	110.71	106.59
4	C	302	6JP	CAD-CAC-CAB	2.33	121.82	119.67
3	A	301	NAP	C4D-O4D-C1D	2.32	112.05	109.92
3	C	301	NAP	N9A-C8A-N7A	-2.32	110.65	113.94
3	D	301	NAP	C1B-N9A-C8A	2.32	132.24	127.09
4	C	302	6JP	CAJ-CAI-CAH	-2.28	105.47	112.25
4	A	302	6JP	OAU-CAD-CAE	-2.27	116.94	121.14
4	D	302	6JP	CAF-OAG-CAJ	2.26	119.50	115.54
4	A	302	6JP	CAJ-CAI-CAH	-2.25	105.55	112.25
4	D	302	6JP	OAT-CAH-CAE	-2.24	119.02	122.49
3	C	301	NAP	O7N-C7N-N7N	-2.23	119.39	122.62
4	B	302	6JP	CAJ-CAI-CAH	-2.22	105.64	112.25
3	D	301	NAP	N3A-C4A-N9A	2.21	130.93	127.17
4	B	302	6JP	CAD-CAC-CAB	2.17	121.67	119.67
3	A	301	NAP	O3X-P2B-O2X	2.15	115.86	107.80
3	A	301	NAP	O2B-P2B-O1X	-2.15	101.68	109.33
3	B	301	NAP	O5B-PA-O1A	2.13	117.37	108.94
3	D	301	NAP	O2X-P2B-O1X	2.11	119.06	110.83
3	C	301	NAP	O7N-C7N-C3N	-2.09	117.04	119.60
3	C	301	NAP	O2N-PN-O1N	2.07	122.06	112.44
4	C	302	6JP	CAD-CAE-CAH	2.06	123.64	120.92
3	D	301	NAP	O7N-C7N-C3N	-2.06	117.08	119.60

There are no chirality outliers.

All (12) torsion outliers are listed below:

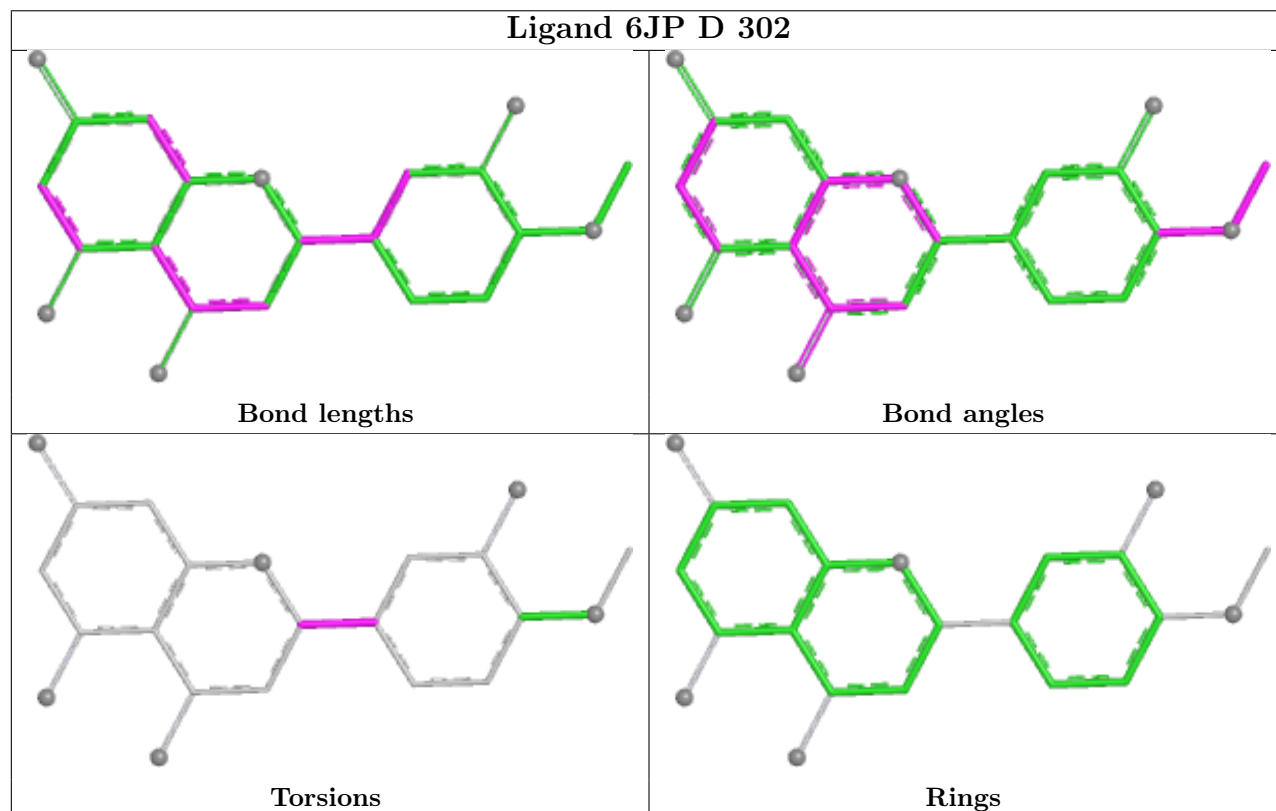
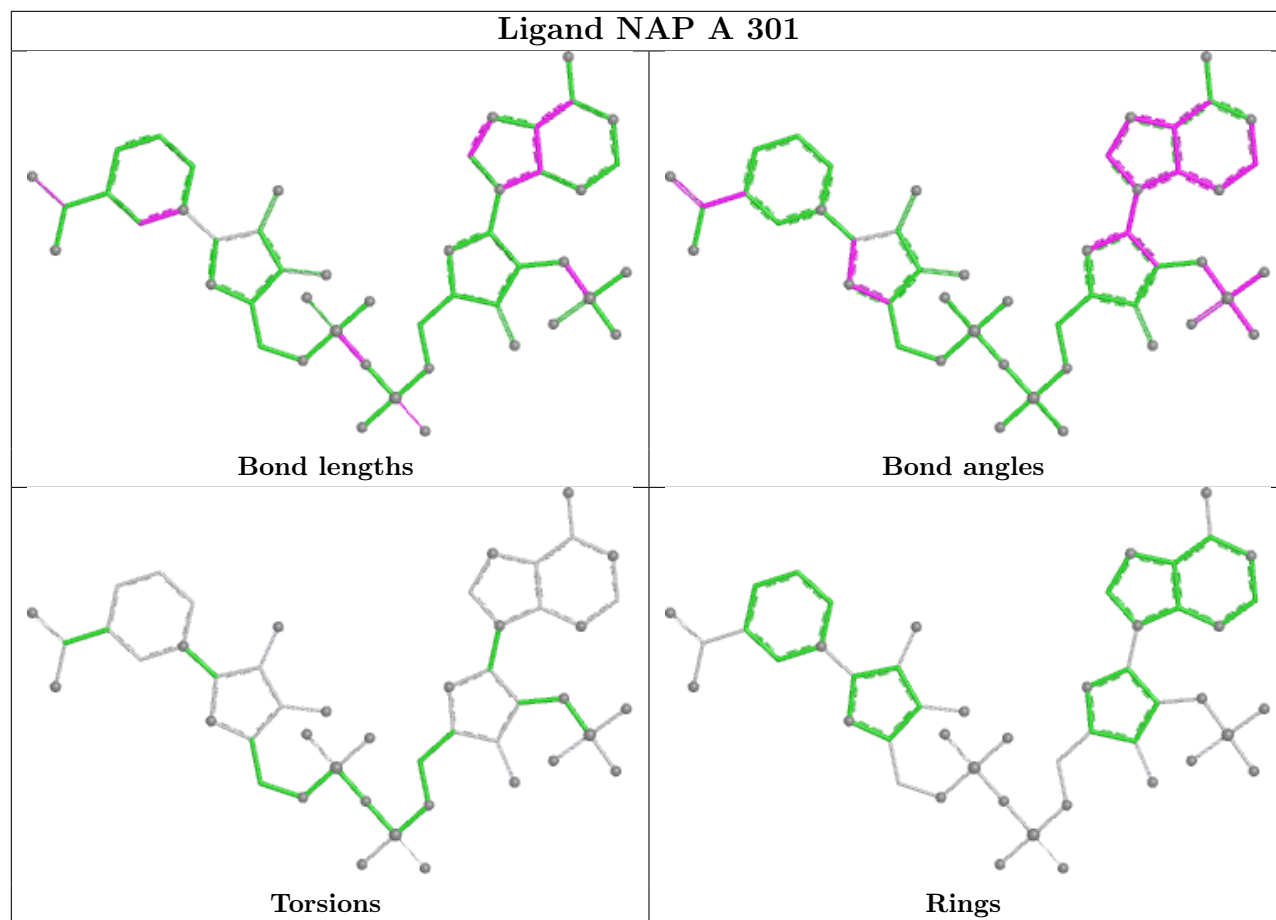
Mol	Chain	Res	Type	Atoms
4	B	302	6JP	CAO-CAP-OAR-CAS
4	B	302	6JP	CAL-CAP-OAR-CAS
3	D	301	NAP	C5B-O5B-PA-O1A
3	C	301	NAP	C2B-O2B-P2B-O2X
4	C	302	6JP	CAI-CAJ-CAK-CAN
3	D	301	NAP	O4D-C1D-N1N-C6N
4	C	302	6JP	CAI-CAJ-CAK-CAM
4	A	302	6JP	CAI-CAJ-CAK-CAM
4	A	302	6JP	CAI-CAJ-CAK-CAN
4	D	302	6JP	CAI-CAJ-CAK-CAM
4	D	302	6JP	CAI-CAJ-CAK-CAN
4	B	302	6JP	CAI-CAJ-CAK-CAM

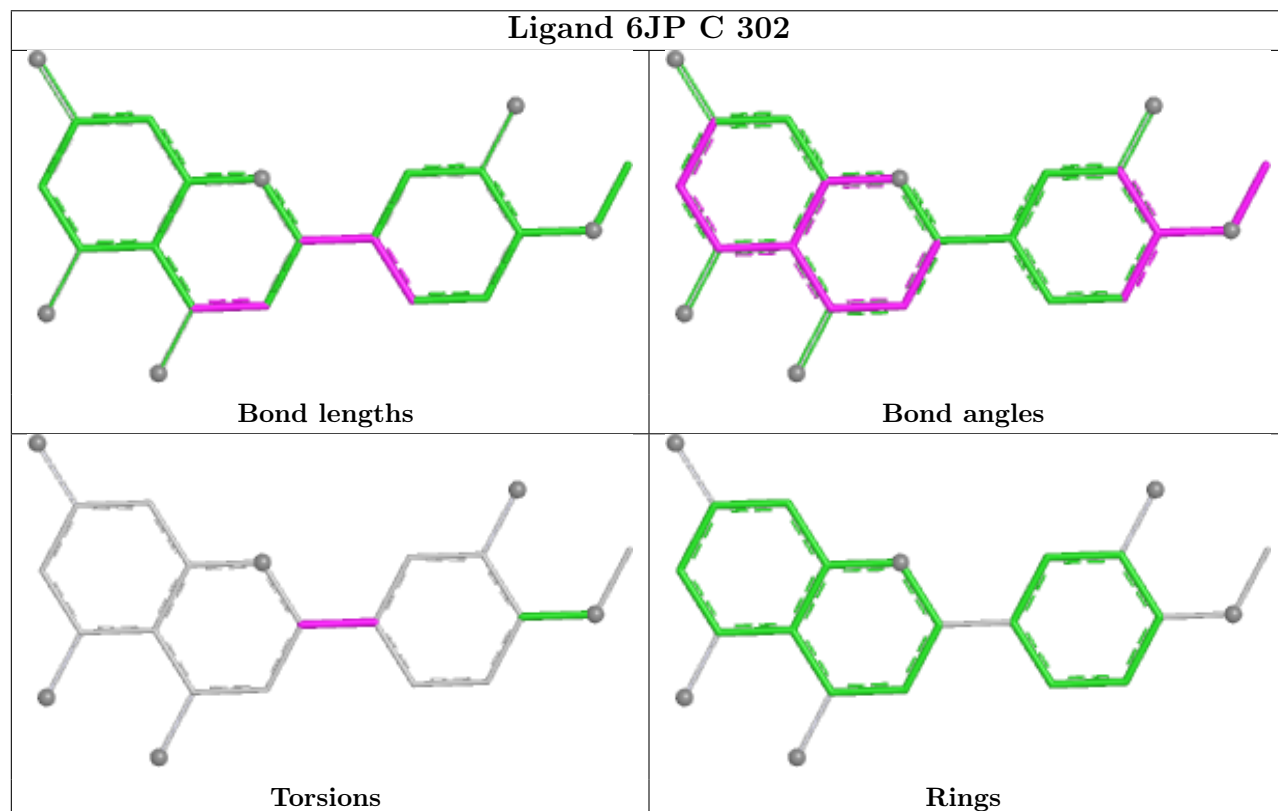
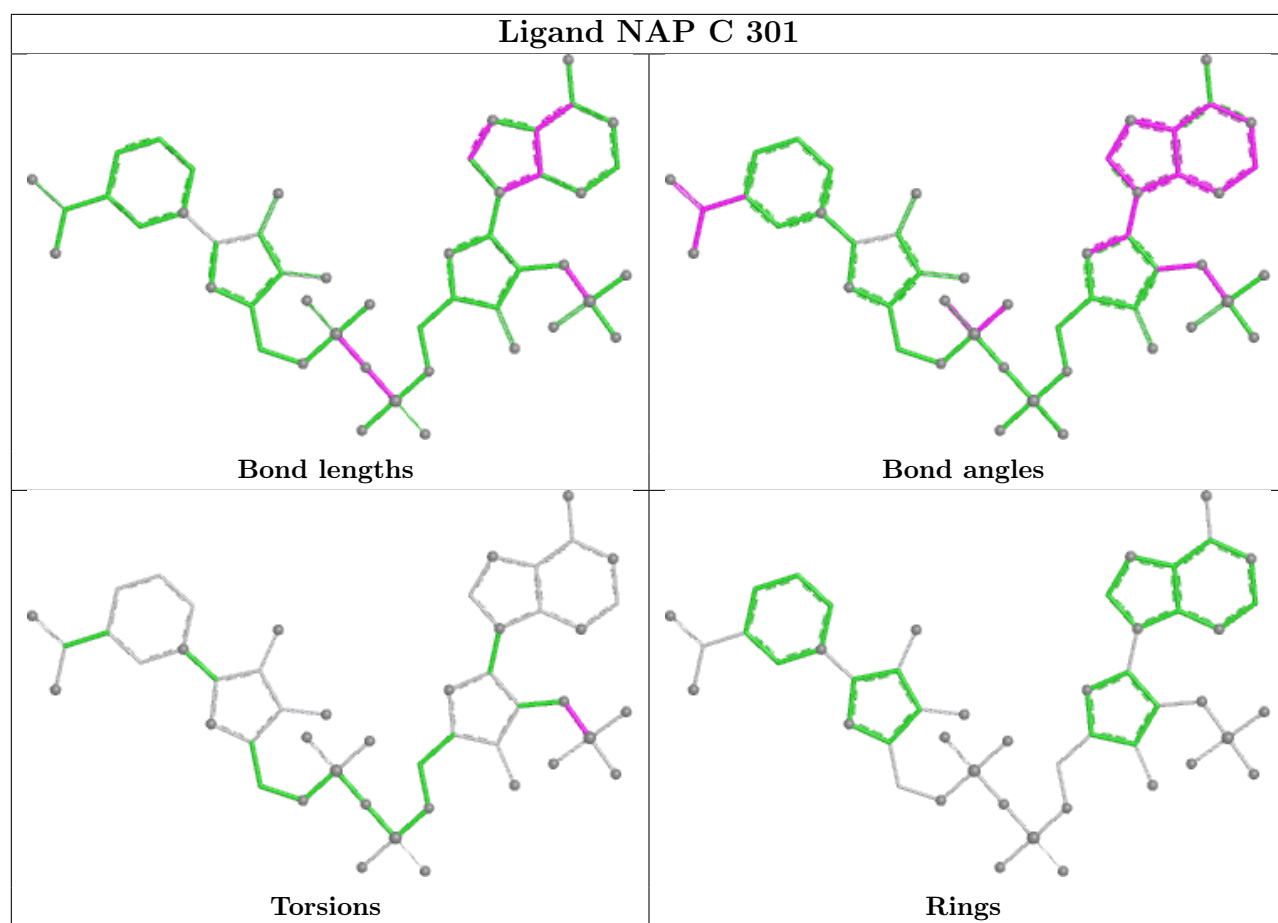
There are no ring outliers.

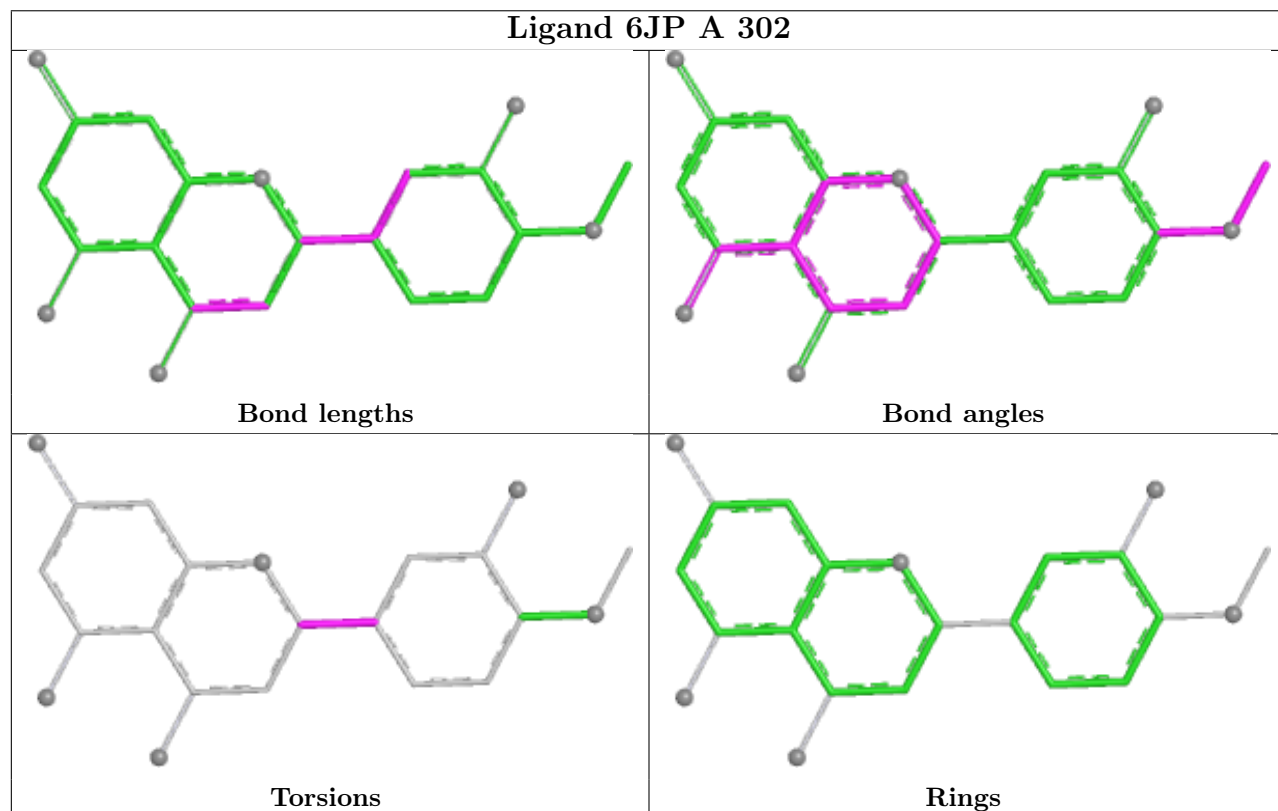
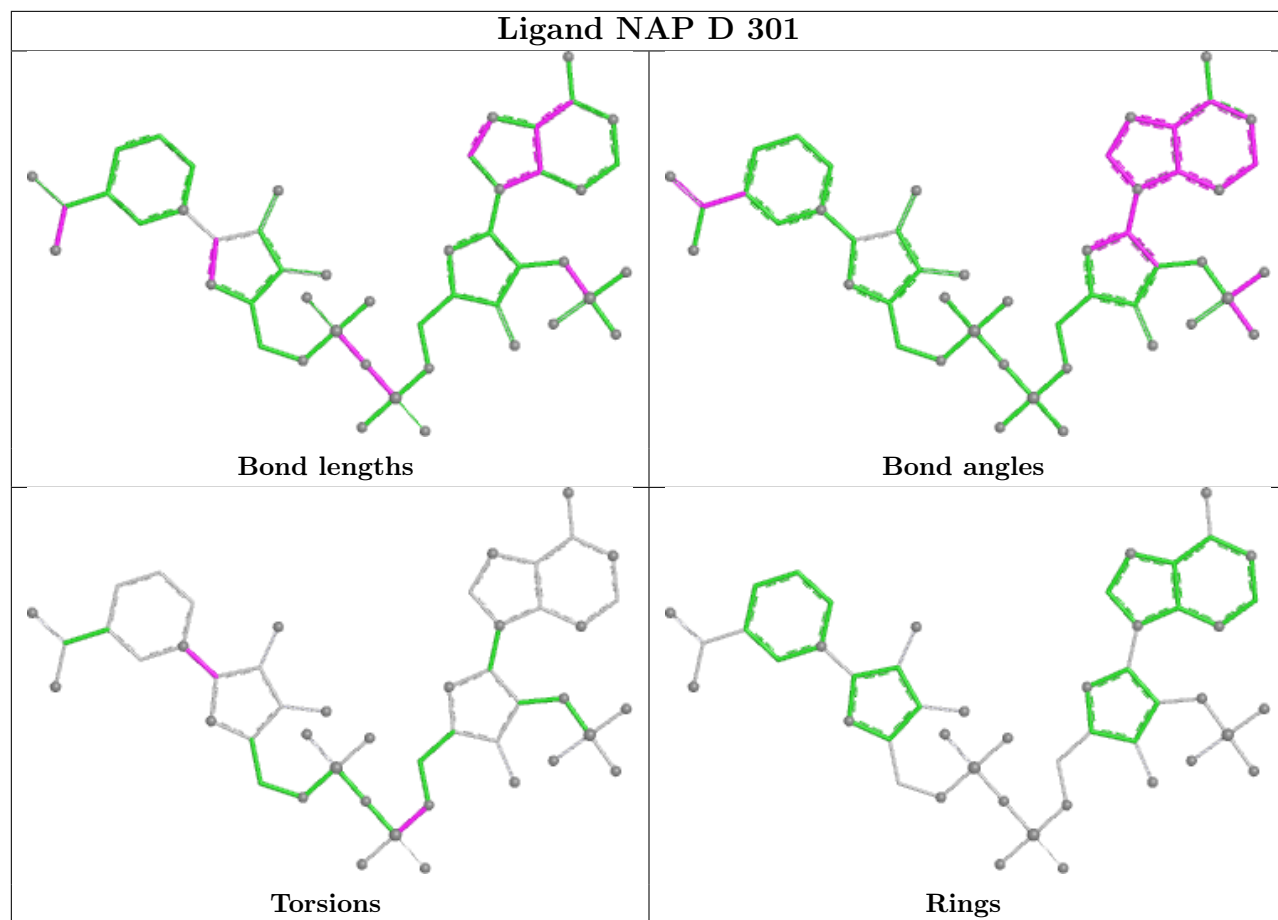
4 monomers are involved in 6 short contacts:

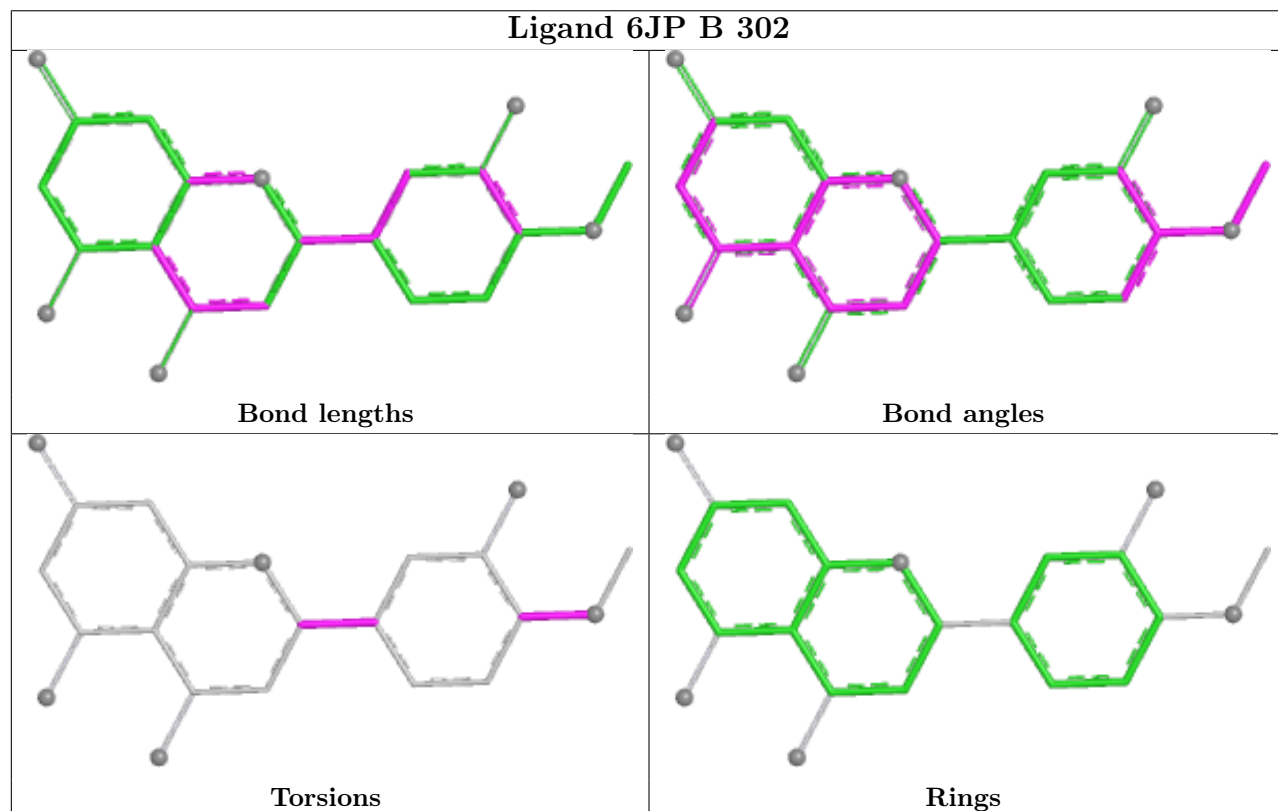
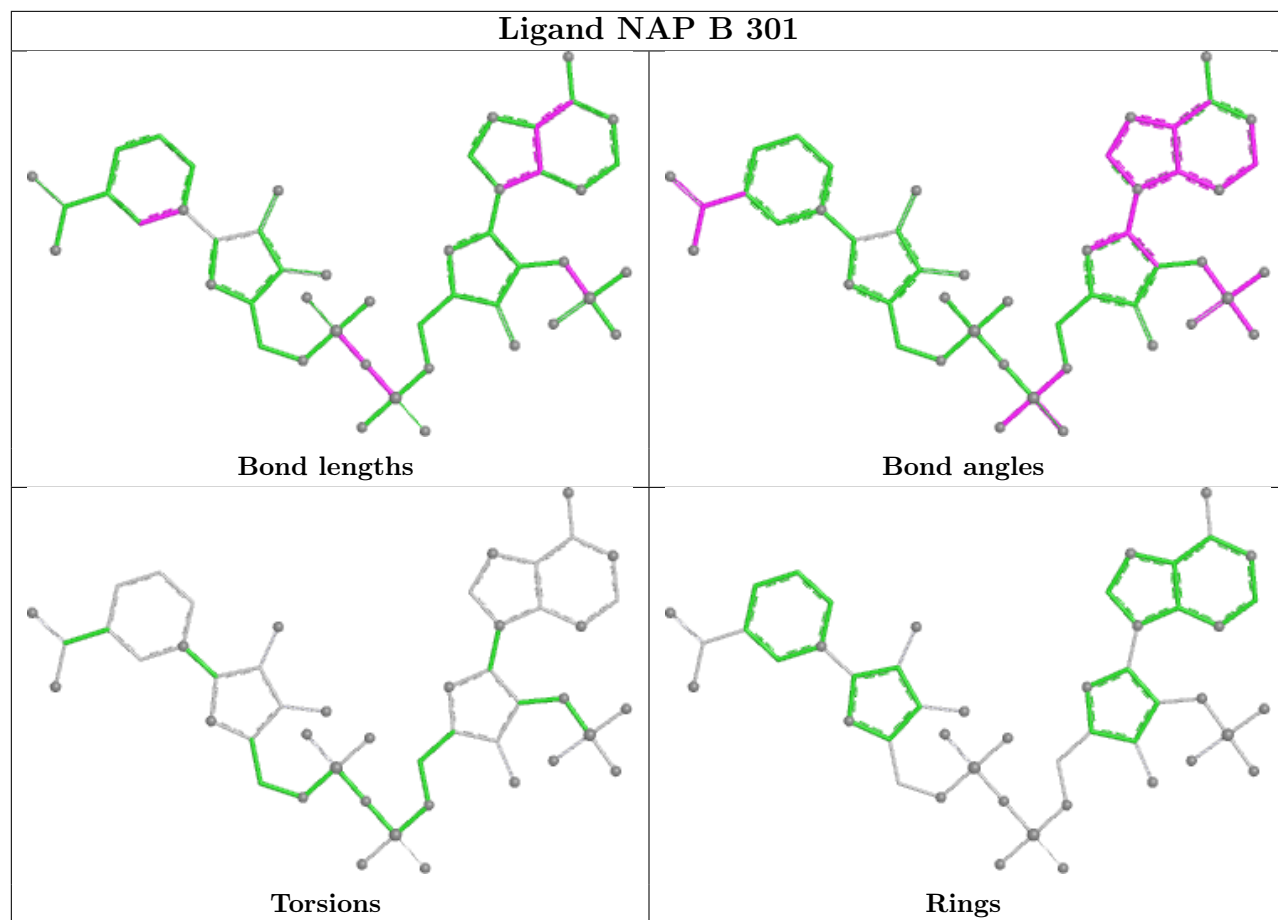
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	303	ACT	1	0
3	D	301	NAP	1	0
4	A	302	6JP	1	0
4	B	302	6JP	3	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	259:VAL	C	260:ASP	N	1.64

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	248/288 (86%)	1.42	61 (24%)	2 2	10, 19, 38, 51	0
1	B	245/288 (85%)	1.07	30 (12%)	8 9	9, 16, 33, 43	2 (0%)
1	D	247/288 (85%)	1.55	72 (29%)	1 1	9, 19, 40, 55	2 (0%)
2	C	237/288 (82%)	1.54	62 (26%)	1 1	10, 19, 42, 63	0
All	All	977/1152 (84%)	1.39	225 (23%)	2 2	9, 19, 38, 63	4 (0%)

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	209	LEU	8.7
1	D	211	VAL	8.6
2	C	206	VAL	7.7
2	C	221	TRP	7.3
2	C	220	LYS	6.7
1	B	212	ALA	6.5
1	A	212	ALA	6.1
1	A	211	VAL	6.0
2	C	210	PRO	5.8
1	D	212	ALA	5.8
2	C	216	GLU	5.6
1	D	208	LEU	5.3
2	C	207	SER	5.3
1	D	210	PRO	5.2
2	C	218	LYS	5.0
1	D	214	GLY	5.0
1	A	152	SER	4.9
1	B	208	LEU	4.7
1	A	221	TRP	4.7
1	D	152	SER	4.7
1	B	103	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	103	VAL	4.6
2	C	229	ARG	4.6
1	A	113	GLY	4.6
1	A	50	LYS	4.6
1	B	221	TRP	4.5
2	C	195	TYR	4.4
1	D	103	VAL	4.4
2	C	219	ASP	4.3
2	C	2	GLU	4.2
2	C	103	VAL	4.1
2	C	46	ASP	4.0
1	D	221	TRP	4.0
1	B	195	TYR	4.0
1	D	13	LYS	4.0
1	A	195	TYR	3.9
1	D	195	TYR	3.9
1	D	220	LYS	3.9
1	A	214	GLY	3.9
2	C	217	GLU	3.9
2	C	228	GLY	3.8
1	D	209	LEU	3.8
1	A	141	ARG	3.7
1	B	210	PRO	3.7
1	D	116	VAL	3.7
1	D	222	ARG	3.6
2	C	169	MET	3.6
1	D	223	ARG	3.6
1	D	3	ALA	3.5
1	A	206	VAL	3.5
1	D	216	GLU	3.5
2	C	141	ARG	3.5
1	A	56	ALA	3.5
2	C	230	ARG	3.5
1	B	116	VAL	3.4
1	D	40	ALA	3.4
2	C	67	ASN	3.4
1	A	39	GLU	3.4
1	A	32	ILE	3.4
1	D	230	ARG	3.4
1	B	2	GLU	3.3
2	C	222	ARG	3.3
1	D	48	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	C	42	VAL	3.3
1	D	251	TYR	3.2
1	D	68	VAL	3.2
1	D	2	GLU	3.2
1	D	57	VAL	3.2
1	D	206	VAL	3.2
1	B	82	ARG	3.2
1	D	51	GLU	3.2
1	A	48	LEU	3.2
1	A	58	VAL	3.2
1	A	2	GLU	3.2
1	B	68	VAL	3.1
1	D	169	MET	3.1
1	D	213	MET	3.1
1	D	26	THR	3.1
1	D	12	ALA	3.1
2	C	83	ALA	3.1
1	A	217	GLU	3.1
1	D	47	GLU	3.0
1	D	42	VAL	3.0
1	A	40	ALA	3.0
1	A	46	ASP	3.0
1	D	53[A]	SER	3.0
1	A	169	MET	3.0
1	B	230	ARG	3.0
1	B	206	VAL	3.0
1	A	53	SER	3.0
1	A	42	VAL	2.9
2	C	3	ALA	2.9
1	D	215	GLU	2.9
1	A	57	VAL	2.9
1	A	54	ASN	2.9
2	C	54	ASN	2.9
1	A	68	VAL	2.9
1	A	260	ASP	2.9
1	D	218	LYS	2.9
2	C	53	SER	2.9
1	D	45	ALA	2.8
1	A	51	GLU	2.8
2	C	136	MET	2.8
1	A	85	GLY	2.8
2	C	268	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	46	ASP	2.8
2	C	223	ARG	2.8
1	B	67	ASN	2.8
1	B	141	ARG	2.7
1	D	260	ASP	2.7
1	A	153	ASN	2.7
1	D	268	ALA	2.7
1	B	190	LEU	2.7
2	C	82	ARG	2.6
1	B	217	GLU	2.6
1	D	140	GLN	2.6
1	B	220	LYS	2.6
2	C	32	ILE	2.6
2	C	75	GLU	2.6
1	D	43	SER	2.6
2	C	43	SER	2.6
1	A	13	LYS	2.6
1	D	224	LYS	2.6
2	C	224	LYS	2.6
1	B	118	THR	2.6
1	D	118	THR	2.6
2	C	165	ASP	2.6
1	D	4	PRO	2.6
1	A	67	ASN	2.6
1	A	194	PRO	2.6
1	A	3	ALA	2.5
1	A	45	ALA	2.5
1	D	219	ASP	2.5
1	A	114	LYS	2.5
1	A	52	ARG	2.5
2	C	51	GLU	2.5
1	A	84	PHE	2.5
1	D	80	CYS	2.5
2	C	38	ALA	2.5
2	C	61	ALA	2.5
1	D	97	PHE	2.5
1	D	190	LEU	2.5
2	C	4	PRO	2.5
1	A	220	LYS	2.5
2	C	50	LYS	2.5
1	A	216	GLU	2.5
1	A	223	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	74	GLU	2.4
1	B	216	GLU	2.4
1	D	81	PHE	2.4
1	D	207	SER	2.4
2	C	161	ASP	2.4
2	C	84	PHE	2.4
1	A	83	ALA	2.4
2	C	142	GLN	2.4
1	D	21	VAL	2.4
1	D	141	ARG	2.4
2	C	227	LEU	2.4
1	D	83	ALA	2.4
2	C	56	ALA	2.4
1	A	115	THR	2.4
1	D	58	VAL	2.4
2	C	205	GLY	2.3
1	A	44	LEU	2.3
1	A	55	THR	2.3
1	A	34	TYR	2.3
1	A	30	VAL	2.3
2	C	25	GLN	2.3
1	D	229	ARG	2.3
1	B	114	LYS	2.3
1	D	56	ALA	2.3
1	A	208	LEU	2.3
1	D	250	GLN	2.3
1	B	53	SER	2.3
2	C	37	SER	2.3
1	D	52	ARG	2.3
2	C	68	VAL	2.3
1	B	219	ASP	2.3
2	C	194	PRO	2.3
1	A	117	GLU	2.2
1	B	250	GLN	2.2
1	A	38	ALA	2.2
1	B	268	ALA	2.2
1	A	79	SER	2.2
1	B	209	LEU	2.2
2	C	63	LEU	2.2
2	C	78	ASN	2.2
2	C	116	VAL	2.2
1	B	169	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	180	ALA	2.2
1	D	87	CYS	2.2
1	B	75	GLU	2.2
1	A	209	LEU	2.2
1	D	44	LEU	2.2
1	A	82	ARG	2.2
2	C	81	PHE	2.2
1	D	31	VAL	2.1
1	A	193	ALA	2.1
1	D	170	ALA	2.1
2	C	13	LYS	2.1
1	D	142	GLN	2.1
1	D	77	ILE	2.1
2	C	52	ARG	2.1
1	A	116	VAL	2.1
1	D	232	ALA	2.1
1	A	59	CYS	2.1
2	C	114	LYS	2.1
2	C	17	ARG	2.1
1	D	32	ILE	2.1
1	D	34	TYR	2.1
2	C	12	ALA	2.1
1	D	36	ASN	2.1
2	C	74	GLU	2.1
2	C	26	THR	2.1
2	C	64	THR	2.1
1	D	50	LYS	2.1
1	A	49	ASN	2.0
1	D	41	ALA	2.0
1	D	61	ALA	2.0
1	B	260	ASP	2.0
1	A	26	THR	2.0
1	B	115	THR	2.0
1	A	81	PHE	2.0
1	A	41	ALA	2.0
1	A	35	HIS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CSX	C	168	7/8	0.84	0.14	22,26,41,50	0
1	CSX	A	168	7/8	0.87	0.12	23,28,54,55	0
1	CSX	D	168	7/8	0.87	0.13	23,28,50,54	0
1	CSX	B	168[A]	7/8	0.92	0.12	18,21,22,25	7
1	CSX	B	168[B]	7/8	0.92	0.12	20,23,27,30	7
2	OCS	C	59	9/10	0.93	0.09	16,19,24,24	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

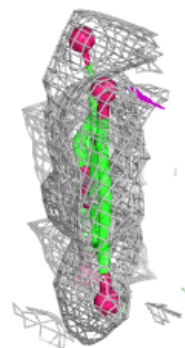
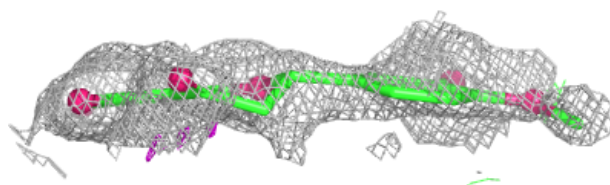
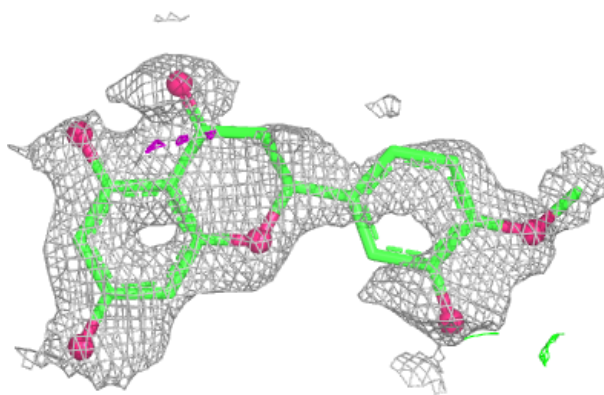
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	6JP	C	302	22/22	0.65	0.24	47,55,64,81	0
4	6JP	D	302	22/22	0.68	0.20	37,44,48,49	0
6	GOL	C	304	6/6	0.72	0.25	29,39,40,44	0
4	6JP	B	302	22/22	0.73	0.22	36,42,58,64	0
4	6JP	A	302	22/22	0.77	0.17	27,35,44,50	0
5	ACT	A	303	4/4	0.81	0.19	22,23,24,34	0
3	NAP	C	301	48/48	0.81	0.15	21,33,45,55	0
5	ACT	C	303	4/4	0.87	0.13	26,27,30,31	0
3	NAP	D	301	48/48	0.88	0.12	17,26,36,41	0
3	NAP	B	301	48/48	0.91	0.10	15,20,31,33	0
3	NAP	A	301	48/48	0.91	0.10	16,21,33,37	0

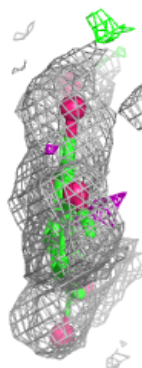
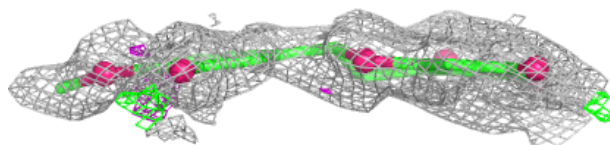
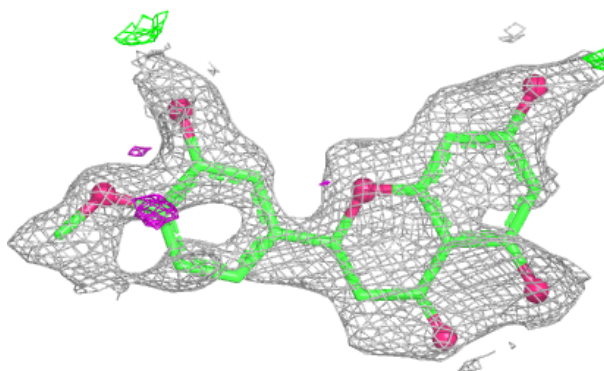
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6JP 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)

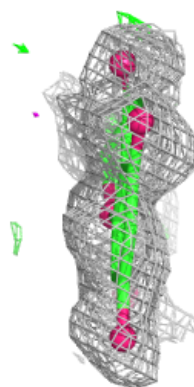
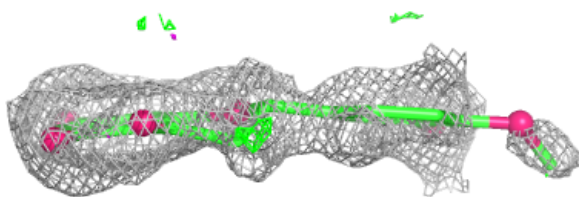
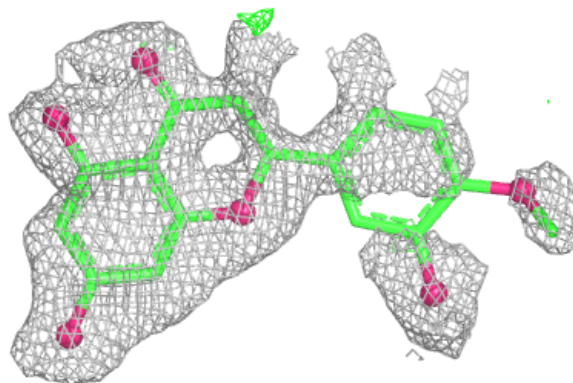
**Electron density around 6JP D 302:**

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

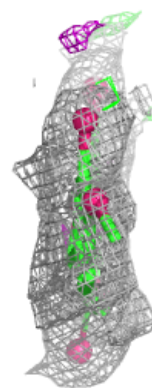
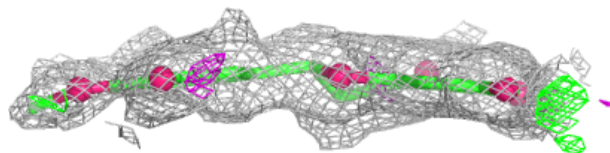
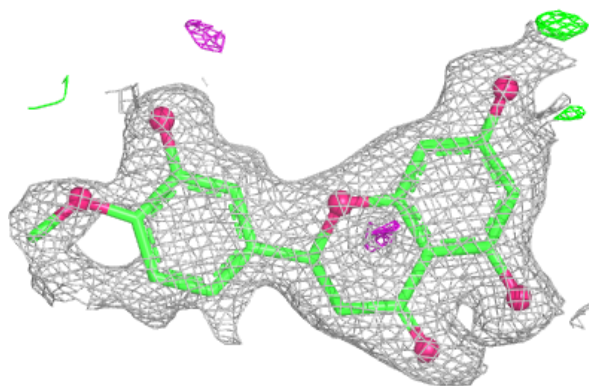


Electron density around 6JP B 302:

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

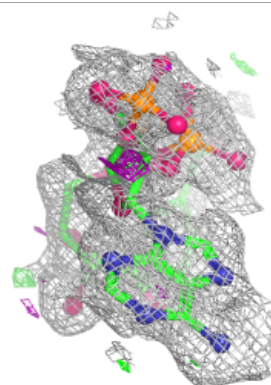
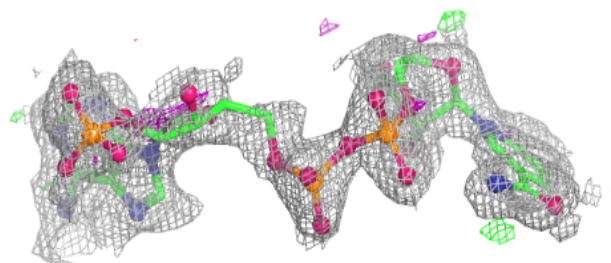
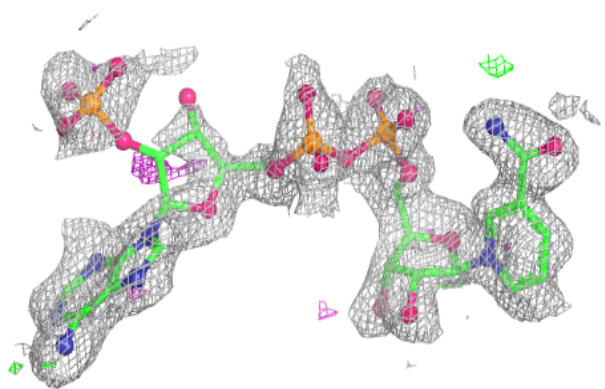
**Electron density around 6JP A 302:**

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

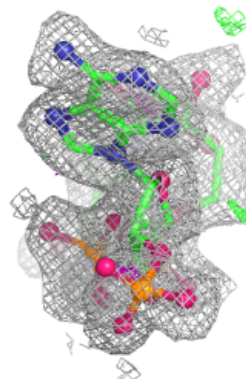
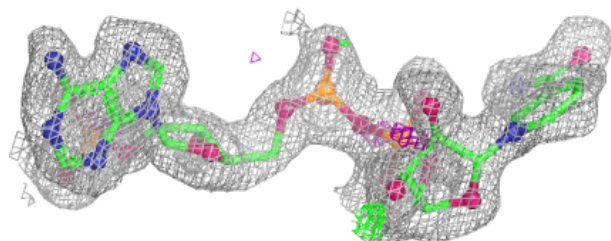
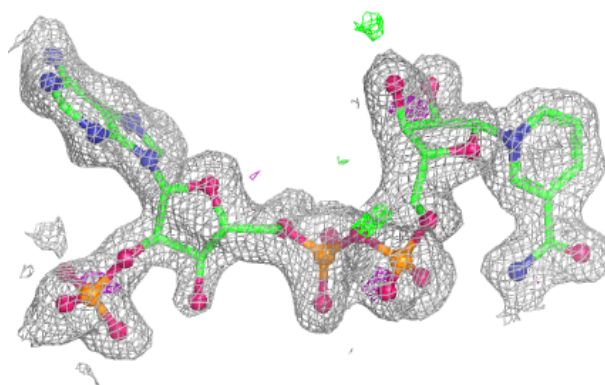


Electron density around NAP C 301:

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

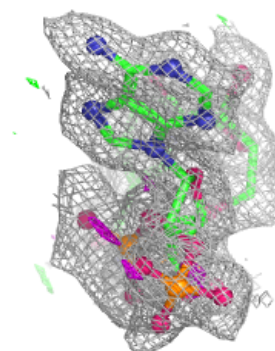
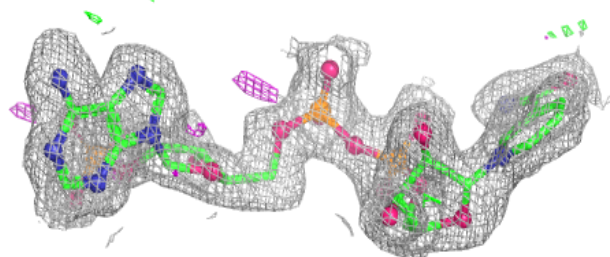
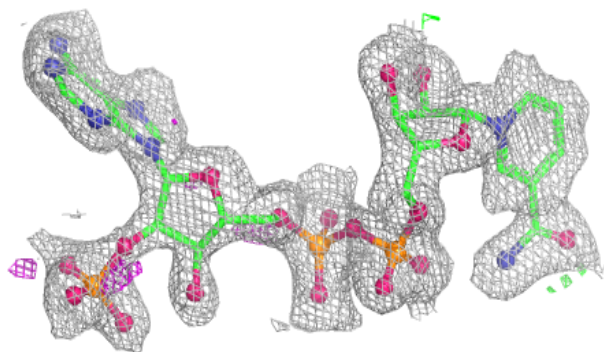
**Electron density around NAP D 301:**

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

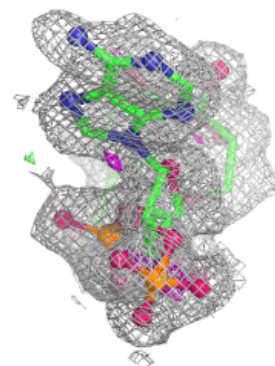
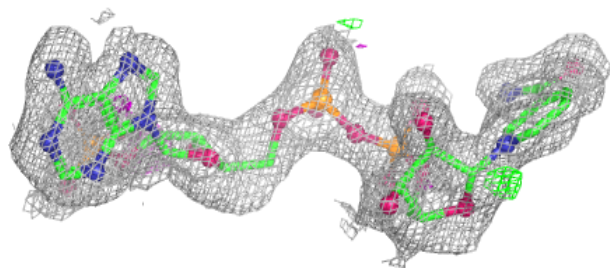
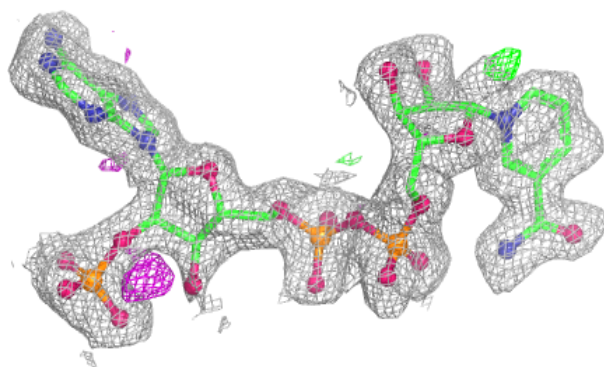


Electron density around NAP B 301:

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

**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 ⓘ

There are no such residues in this entry.