



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:07 PM UTC

PDB ID : 8RHU / pdb_00008rhu
Title : Crystal Structure of Trypanosoma brucei PTR1 in complex with the cofactor and inhibitor P25
Authors : Pozzi, C.; Mangani, S.; Landi, G.
Deposited on : 2023-12-17
Resolution : 1.71 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

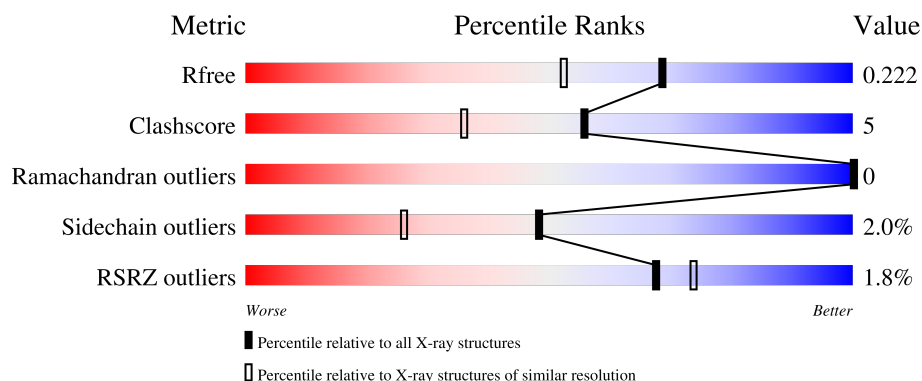
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	289	0% 77% 9% 14%
1	B	289	2% 76% 10% 13%
1	C	289	0% 78% 7% 14%
1	D	289	2% 75% 11% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACT	C	303	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8310 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	3	0
			1862	1170	330	351	11			
1	B	250	Total	C	N	O	S	0	9	0
			1908	1201	334	362	11			
1	C	249	Total	C	N	O	S	0	7	0
			1878	1182	329	356	11			
1	D	249	Total	C	N	O	S	0	5	0
			1856	1171	324	350	11			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP O76290
A	-19	GLY	-	expression tag	UNP O76290
A	-18	SER	-	expression tag	UNP O76290
A	-17	SER	-	expression tag	UNP O76290
A	-16	HIS	-	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	SER	-	expression tag	UNP O76290
A	-9	SER	-	expression tag	UNP O76290
A	-8	GLY	-	expression tag	UNP O76290
A	-7	LEU	-	expression tag	UNP O76290
A	-6	VAL	-	expression tag	UNP O76290
A	-5	PRO	-	expression tag	UNP O76290
A	-4	ARG	-	expression tag	UNP O76290
A	-3	GLY	-	expression tag	UNP O76290
A	-2	SER	-	expression tag	UNP O76290
A	-1	HIS	-	expression tag	UNP O76290
A	0	MET	-	expression tag	UNP O76290

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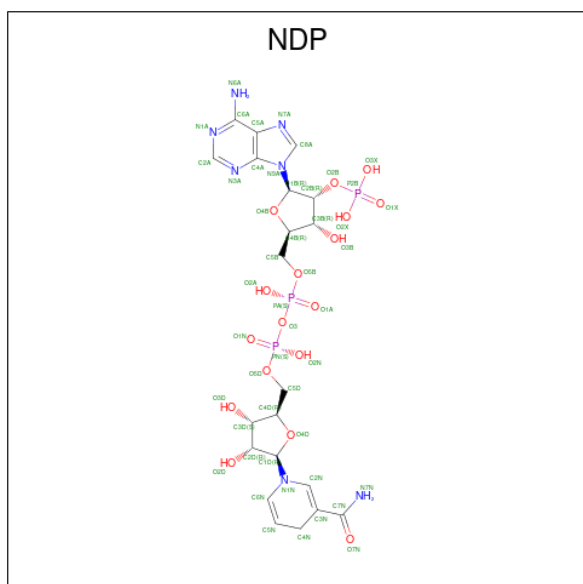
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	initiating methionine	UNP O76290
B	-19	GLY	-	expression tag	UNP O76290
B	-18	SER	-	expression tag	UNP O76290
B	-17	SER	-	expression tag	UNP O76290
B	-16	HIS	-	expression tag	UNP O76290
B	-15	HIS	-	expression tag	UNP O76290
B	-14	HIS	-	expression 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	SER	-	expression tag	UNP O76290
B	-9	SER	-	expression tag	UNP O76290
B	-8	GLY	-	expression tag	UNP O76290
B	-7	LEU	-	expression tag	UNP O76290
B	-6	VAL	-	expression tag	UNP O76290
B	-5	PRO	-	expression tag	UNP O76290
B	-4	ARG	-	expression tag	UNP O76290
B	-3	GLY	-	expression tag	UNP O76290
B	-2	SER	-	expression tag	UNP O76290
B	-1	HIS	-	expression tag	UNP O76290
B	0	MET	-	expression tag	UNP O76290
C	-20	MET	-	initiating methionine	UNP O76290
C	-19	GLY	-	expression tag	UNP O76290
C	-18	SER	-	expression tag	UNP O76290
C	-17	SER	-	expression tag	UNP O76290
C	-16	HIS	-	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	SER	-	expression tag	UNP O76290
C	-9	SER	-	expression tag	UNP O76290
C	-8	GLY	-	expression tag	UNP O76290
C	-7	LEU	-	expression tag	UNP O76290
C	-6	VAL	-	expression tag	UNP O76290
C	-5	PRO	-	expression tag	UNP O76290
C	-4	ARG	-	expression tag	UNP O76290
C	-3	GLY	-	expression tag	UNP O76290
C	-2	SER	-	expression tag	UNP O76290
C	-1	HIS	-	expression tag	UNP O76290
C	0	MET	-	expression tag	UNP O76290

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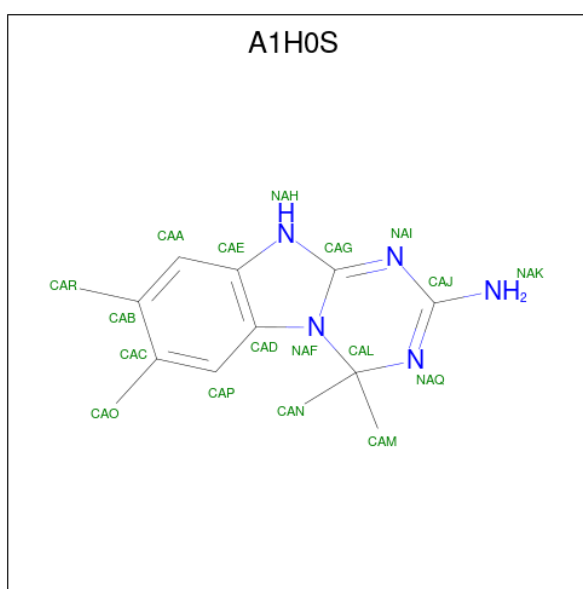
Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	initiating methionine	UNP O76290
D	-19	GLY	-	expression tag	UNP O76290
D	-18	SER	-	expression tag	UNP O76290
D	-17	SER	-	expression tag	UNP O76290
D	-16	HIS	-	expression tag	UNP O76290
D	-15	HIS	-	expression tag	UNP O76290
D	-14	HIS	-	expression 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	SER	-	expression tag	UNP O76290
D	-9	SER	-	expression tag	UNP O76290
D	-8	GLY	-	expression tag	UNP O76290
D	-7	LEU	-	expression tag	UNP O76290
D	-6	VAL	-	expression tag	UNP O76290
D	-5	PRO	-	expression tag	UNP O76290
D	-4	ARG	-	expression tag	UNP O76290
D	-3	GLY	-	expression tag	UNP O76290
D	-2	SER	-	expression tag	UNP O76290
D	-1	HIS	-	expression tag	UNP O76290
D	0	MET	-	expression tag	UNP O76290

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



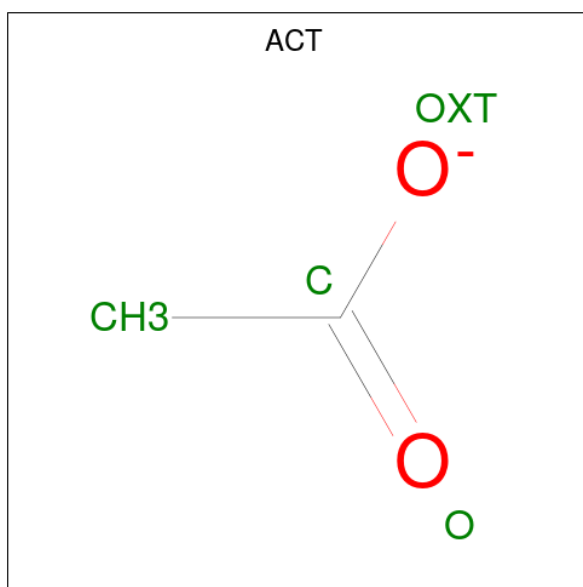
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 4,4,7,8-tetramethyl-10 {H}-[1,3,5]triazino[1,2-a]benzimidazol-2-amine (CCD ID: A1H0S) (formula: C₁₃H₁₇N₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			18	13	5		
3	C	1	Total	C	N	0	0
			18	13	5		
3	D	1	Total	C	N	0	0
			18	13	5		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	135	Total	O	0	2
			136	136		
5	B	146	Total	O	0	3
			148	148		
5	C	137	Total	O	0	3
			138	138		
5	D	122	Total	O	0	1
			122	122		

- 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	74.03Å 89.65Å 84.17Å 90.00° 115.88° 90.00°	Depositor
Resolution (Å)	75.72 – 1.71 75.72 – 1.71	Depositor EDS
% Data completeness (in resolution range)	99.4 (75.72-1.71) 99.4 (75.72-1.71)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.185 , 0.221 0.185 , 0.222	Depositor DCC
R_{free} test set	5331 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8310	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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 21.92 % 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 6.3450e-03. 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: ACT, CSX, NDP, A1H0S

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	0.66	0/1890	1.14	2/2564 (0.1%)
1	B	0.69	2/1954 (0.1%)	1.12	1/2648 (0.0%)
1	C	0.65	0/1918	1.13	1/2603 (0.0%)
1	D	0.67	2/1887 (0.1%)	1.18	5/2561 (0.2%)
All	All	0.67	4/7649 (0.1%)	1.14	9/10376 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	219[A]	ASP	C-O	5.61	1.31	1.24
1	D	219[B]	ASP	C-O	5.61	1.31	1.24
1	B	230[A]	ARG	C-O	5.46	1.30	1.23
1	B	230[B]	ARG	C-O	5.46	1.30	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	98	TYR	N-CA-CB	8.23	119.00	111.27
1	D	219[A]	ASP	CA-C-O	8.10	129.25	120.10
1	D	219[B]	ASP	CA-C-O	8.10	129.25	120.10
1	B	216	GLU	CB-CG-CD	6.67	123.95	112.60
1	C	78	ASN	CA-CB-CG	-5.61	106.99	112.60
1	D	126	THR	CA-CB-OG1	-5.50	101.36	109.60
1	D	258	LYS	CB-CA-C	-5.22	100.71	109.53
1	A	173	LEU	N-CA-CB	5.12	117.50	110.07
1	A	13	LYS	CB-CG-CD	5.07	122.95	111.30

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	1862	0	1883	17	0
1	B	1908	0	1938	22	0
1	C	1878	0	1885	20	0
1	D	1856	0	1865	20	0
2	A	48	0	26	2	0
2	B	48	0	26	1	0
2	C	48	0	26	2	0
2	D	48	0	26	3	0
3	A	18	0	0	1	0
3	C	18	0	0	1	0
3	D	18	0	0	1	0
4	A	8	0	6	0	0
4	B	4	0	3	0	0
4	C	4	0	3	3	0
5	A	136	0	0	2	0
5	B	148	0	0	0	0
5	C	138	0	0	2	0
5	D	122	0	0	2	0
All	All	8310	0	7687	73	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (73) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:VAL:H	4:C:303:ACT:H2	1.19	1.05
1:A:136:MET:O	1:A:140:GLN:HG2	1.80	0.81
1:B:43:SER:O	1:B:47[A]:GLU:HG3	1.81	0.80
1:C:58:VAL:N	4:C:303:ACT:H2	1.98	0.77
1:C:58:VAL:H	4:C:303:ACT:CH3	2.00	0.72
1:A:22:LYS:HG2	1:A:242:ILE:HG13	1.72	0.71
2:C:301:NDP:H41N	3:C:302:A1H0S:CAE	2.21	0.71
1:A:236:GLN:HE21	1:B:250[A]:GLN:HG3	1.65	0.59
1:C:2:GLU:OE1	1:C:29:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:VAL:HG22	5:A:482:HOH:O	2.05	0.57
1:C:9:THR:HA	1:C:33:HIS:HB3	1.90	0.54
1:C:74[B]:GLU:HA	1:C:74[B]:GLU:OE1	2.07	0.54
1:B:161:ASP:HB3	1:B:164:VAL:HG13	1.90	0.54
1:D:206[A]:VAL:HG21	1:D:209:LEU:HD21	1.88	0.54
2:D:301:NDP:H41N	3:D:302:A1H0S:CAE	2.38	0.54
5:A:470:HOH:O	1:B:250[A]:GLN:HG2	2.07	0.53
1:C:82[B]:ARG:HH12	1:C:141:ARG:NH2	2.07	0.53
1:A:236:GLN:NE2	1:B:250[A]:GLN:HG3	2.24	0.52
1:C:72:SER:O	1:C:75[A]:GLU:HG2	2.11	0.51
2:A:301:NDP:H41N	3:A:302:A1H0S:CAE	2.41	0.51
1:B:205:GLY:O	2:B:301:NDP:H42N	2.10	0.50
1:A:98:TYR:HB2	1:A:99:PRO:HD2	1.92	0.50
1:C:116:VAL:HG23	5:C:464:HOH:O	2.12	0.49
1:A:114:LYS:HE2	1:A:122:GLU:OE1	2.13	0.49
1:D:9:THR:HA	1:D:33:HIS:HB3	1.94	0.49
1:B:34:TYR:CZ	1:B:60[B]:GLN:HB2	2.48	0.49
1:D:160:CYS:HB3	5:D:481:HOH:O	2.12	0.48
1:B:247:GLY:HA2	1:B:250[B]:GLN:HG3	1.95	0.48
1:D:65:ASN:HA	1:D:69:LEU:HD22	1.95	0.48
1:A:232:ALA:HB2	1:B:251:TYR:CE2	2.49	0.47
1:D:205:GLY:O	2:D:301:NDP:H42N	2.14	0.47
1:C:82[B]:ARG:NH1	1:C:141:ARG:NH2	2.63	0.47
1:D:138:PHE:O	1:D:142:GLN:HG2	2.14	0.47
1:D:225:VAL:O	1:D:229:ARG:HD3	2.14	0.46
1:B:206[B]:VAL:CG2	1:B:209:LEU:HD21	2.46	0.46
1:C:232:ALA:HB2	1:D:251:TYR:CE2	2.51	0.46
1:D:35:HIS:HB2	2:D:301:NDP:C2A	2.46	0.46
1:D:98:TYR:HB2	1:D:99:PRO:HD2	1.96	0.46
1:A:251:TYR:CE2	1:B:232:ALA:HB2	2.51	0.46
1:A:102:LEU:O	1:C:136:MET:HG3	2.15	0.45
1:A:9:THR:HA	1:A:33:HIS:HB3	1.98	0.45
1:D:193:ALA:HB3	1:D:194:PRO:HD3	2.00	0.44
1:B:17:ARG:HG3	1:B:44:LEU:HD22	1.99	0.44
1:B:193:ALA:N	1:B:194:PRO:CD	2.81	0.44
1:C:35:HIS:HB2	2:C:301:NDP:C2A	2.48	0.44
1:B:225:VAL:O	1:B:229:ARG:HD3	2.17	0.44
1:B:9:THR:HA	1:B:33:HIS:HB3	1.99	0.43
1:B:206[B]:VAL:HG13	1:B:231:GLU:HA	2.01	0.43
1:C:250:GLN:NE2	1:D:236:GLN:HE21	2.17	0.43
1:A:128:ALA:C	1:A:131:PRO:HD2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:PHE:CE2	1:B:136:MET:HE1	2.53	0.43
1:B:98:TYR:HB2	1:B:99:PRO:HD2	2.00	0.43
1:D:207:SER:O	1:D:208:LEU:C	2.61	0.43
1:C:82[B]:ARG:HD3	1:C:82[B]:ARG:HA	1.68	0.43
1:C:208:LEU:HA	5:C:409:HOH:O	2.18	0.43
1:C:232:ALA:HB2	1:D:251:TYR:CD2	2.54	0.43
1:B:132:PHE:CE2	1:B:136:MET:CE	3.02	0.43
1:C:207:SER:O	1:C:208:LEU:C	2.61	0.42
1:A:193:ALA:N	1:A:194:PRO:CD	2.81	0.42
1:B:136:MET:HE2	1:B:136:MET:HB2	1.91	0.42
1:A:35:HIS:HB2	2:A:301:NDP:C2A	2.50	0.41
1:C:22:LYS:CE	1:C:235:GLU:HG3	2.50	0.41
1:D:69:LEU:N	1:D:70:PRO:CD	2.83	0.41
1:A:65:ASN:HA	1:A:69:LEU:HD22	2.01	0.41
1:D:214:GLY:HA3	5:D:489:HOH:O	2.21	0.41
1:D:206[A]:VAL:CG2	1:D:209:LEU:HD21	2.49	0.41
1:D:78:ASN:OD1	1:D:141:ARG:NH1	2.54	0.41
1:B:230[A]:ARG:HE	1:B:230[A]:ARG:HB3	1.64	0.41
1:C:130:ALA:HB3	1:C:131:PRO:HD3	2.02	0.41
1:A:236:GLN:HE21	1:B:250[A]:GLN:CG	2.34	0.41
1:D:193:ALA:N	1:D:194:PRO:CD	2.84	0.41

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	245/289 (85%)	236 (96%)	9 (4%)	0	100	100
1	B	252/289 (87%)	242 (96%)	10 (4%)	0	100	100
1	C	249/289 (86%)	240 (96%)	9 (4%)	0	100	100
1	D	246/289 (85%)	236 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	992/1156 (86%)	954 (96%)	38 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	196/231 (85%)	192 (98%)	4 (2%)	48	26
1	B	203/231 (88%)	198 (98%)	5 (2%)	42	18
1	C	196/231 (85%)	190 (97%)	6 (3%)	35	12
1	D	192/231 (83%)	190 (99%)	2 (1%)	68	53
All	All	787/924 (85%)	770 (98%)	17 (2%)	48	23

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

Mol	Chain	Res	Type
1	A	140	GLN
1	A	166	GLN
1	A	209	LEU
1	A	211	VAL
1	B	43	SER
1	B	51[A]	GLU
1	B	51[B]	GLU
1	B	131	PRO
1	B	166	GLN
1	C	2	GLU
1	C	74[A]	GLU
1	C	74[B]	GLU
1	C	78	ASN
1	C	166	GLN
1	C	250	GLN
1	D	117	GLU
1	D	166	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	92	ASN
1	A	140	GLN
1	A	236	GLN
1	A	250	GLN
1	B	92	ASN
1	B	119	GLN
1	B	127	ASN
1	B	140	GLN
1	B	236	GLN
1	C	92	ASN
1	C	127	ASN
1	C	186	GLN
1	C	250	GLN
1	D	92	ASN
1	D	140	GLN
1	D	250	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	C	168	1	3,6,7	0.65	0	1,6,8	2.96	1 (100%)
1	CSX	A	168	1	3,6,7	0.77	0	1,6,8	0.31	0
1	CSX	B	168	1	3,6,7	0.72	0	1,6,8	0.79	0
1	CSX	D	168	1	3,6,7	0.65	0	1,6,8	3.29	1 (100%)

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	C	168	1	-	0/2/5/7	-
1	CSX	A	168	1	-	0/2/5/7	-
1	CSX	B	168	1	-	0/2/5/7	-
1	CSX	D	168	1	-	0/2/5/7	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	168	CSX	CA-CB-SG	-3.29	105.44	113.17
1	C	168	CSX	CA-CB-SG	-2.96	106.20	113.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
2	NDP	B	301	-	51,52,52	0.88	3 (5%)	71,80,80	0.94	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACT	A	303	-	3,3,3	1.33	0	3,3,3	0.76	0
2	NDP	A	301	-	51,52,52	0.75	1 (1%)	71,80,80	0.95	6 (8%)
4	ACT	C	303	-	3,3,3	2.03	2 (66%)	3,3,3	0.37	0
4	ACT	B	302	-	3,3,3	1.32	0	3,3,3	0.65	0
2	NDP	C	301	-	51,52,52	0.71	1 (1%)	71,80,80	0.99	3 (4%)
4	ACT	A	304	-	3,3,3	0.91	0	3,3,3	0.59	0
3	A1H0S	C	302	-	17,20,20	2.43	7 (41%)	23,32,32	2.28	5 (21%)
3	A1H0S	D	302	-	17,20,20	2.75	9 (52%)	23,32,32	2.35	5 (21%)
3	A1H0S	A	302	-	17,20,20	2.70	9 (52%)	23,32,32	2.97	5 (21%)
2	NDP	D	301	-	51,52,52	0.64	1 (1%)	71,80,80	0.93	1 (1%)

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	NDP	B	301	-	-	1/34/77/77	0/5/5/5
2	NDP	A	301	-	-	1/34/77/77	0/5/5/5
2	NDP	C	301	-	-	2/34/77/77	0/5/5/5
3	A1H0S	C	302	-	-	-	0/3/3/3
3	A1H0S	D	302	-	-	-	0/3/3/3
3	A1H0S	A	302	-	-	-	0/3/3/3
2	NDP	D	301	-	-	1/34/77/77	0/5/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	A1H0S	CAR-CAB	-5.85	1.40	1.51
3	D	302	A1H0S	CAR-CAB	-5.73	1.40	1.51
3	A	302	A1H0S	CAO-CAC	-5.36	1.41	1.51
3	D	302	A1H0S	CAO-CAC	-5.33	1.41	1.51
3	C	302	A1H0S	CAR-CAB	-4.96	1.41	1.51
3	C	302	A1H0S	CAO-CAC	-4.59	1.42	1.51
3	C	302	A1H0S	CAG-NAI	3.61	1.41	1.32
3	D	302	A1H0S	CAJ-NAQ	3.44	1.43	1.34
2	B	301	NDP	P2B-O2B	3.43	1.65	1.59
3	A	302	A1H0S	CAJ-NAQ	3.36	1.43	1.34
2	C	301	NDP	P2B-O2B	3.28	1.65	1.59
3	C	302	A1H0S	CAD-NAF	-3.18	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	A1H0S	CAD-NAF	-3.14	1.36	1.41
3	D	302	A1H0S	CAD-NAF	-3.14	1.36	1.41
3	D	302	A1H0S	CAE-CAD	-3.06	1.35	1.40
3	D	302	A1H0S	CAA-CAE	-2.92	1.34	1.39
3	A	302	A1H0S	CAP-CAD	-2.87	1.35	1.39
2	B	301	NDP	PA-O3	2.75	1.62	1.59
2	B	301	NDP	PN-O3	2.70	1.62	1.59
4	C	303	ACT	OXT-C	-2.70	1.18	1.30
2	D	301	NDP	P2B-O2B	2.67	1.64	1.59
3	D	302	A1H0S	CAG-NAI	2.61	1.38	1.32
3	A	302	A1H0S	CAJ-NAI	2.59	1.41	1.36
3	D	302	A1H0S	CAE-NAH	-2.57	1.34	1.38
3	C	302	A1H0S	CAJ-NAQ	2.51	1.41	1.34
2	A	301	NDP	P2B-O2B	2.44	1.63	1.59
3	A	302	A1H0S	CAA-CAE	-2.43	1.35	1.39
3	D	302	A1H0S	CAP-CAD	-2.32	1.35	1.39
3	A	302	A1H0S	CAE-CAD	-2.25	1.36	1.40
3	C	302	A1H0S	CAE-CAD	-2.21	1.36	1.40
4	C	303	ACT	O-C	2.21	1.31	1.22
3	A	302	A1H0S	CAE-NAH	-2.08	1.35	1.38
3	C	302	A1H0S	CAA-CAB	2.00	1.42	1.39

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	A1H0S	CAM-CAL-NAF	11.14	118.58	110.24
3	D	302	A1H0S	CAM-CAL-NAF	7.13	115.58	110.24
3	C	302	A1H0S	CAM-CAL-NAF	5.78	114.56	110.24
3	A	302	A1H0S	CAN-CAL-CAM	-5.48	101.59	110.68
3	C	302	A1H0S	CAN-CAL-CAM	-5.37	101.78	110.68
3	D	302	A1H0S	CAN-CAL-CAM	-5.23	102.00	110.68
3	C	302	A1H0S	NAI-CAJ-NAQ	-4.63	118.84	126.48
3	A	302	A1H0S	CAP-CAD-CAE	-3.91	118.36	121.55
2	D	301	NDP	O4B-C1B-N9A	3.45	114.72	108.09
3	D	302	A1H0S	CAP-CAD-CAE	-3.37	118.81	121.55
3	A	302	A1H0S	NAI-CAJ-NAQ	-3.37	120.92	126.48
3	C	302	A1H0S	NAK-CAJ-NAI	3.19	121.64	116.57
2	C	301	NDP	C2B-C1B-N9A	-3.11	108.63	113.75
3	D	302	A1H0S	NAI-CAJ-NAQ	-3.10	121.37	126.48
2	B	301	NDP	O4B-C1B-N9A	2.87	113.59	108.09
2	C	301	NDP	O2B-P2B-O1X	-2.81	99.32	109.33
2	C	301	NDP	O4B-C1B-N9A	2.76	113.39	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	A1H0S	NAK-CAJ-NAQ	2.66	121.21	117.09
3	C	302	A1H0S	CAP-CAD-CAE	-2.65	119.39	121.55
2	A	301	NDP	O4B-C4B-C3B	-2.54	100.11	105.15
2	A	301	NDP	O4B-C1B-N9A	2.46	112.82	108.09
2	B	301	NDP	C2B-C1B-N9A	-2.38	109.84	113.75
2	B	301	NDP	O3-PA-O1A	-2.31	103.75	110.70
2	A	301	NDP	O2B-P2B-O1X	-2.29	101.18	109.33
2	A	301	NDP	C2B-C1B-N9A	-2.27	110.02	113.75
3	A	302	A1H0S	NAK-CAJ-NAQ	2.18	120.46	117.09
2	B	301	NDP	O2D-C2D-C3D	2.06	118.43	111.82
2	A	301	NDP	C6N-N1N-C2N	2.04	121.50	119.32
2	A	301	NDP	C4B-O4B-C1B	-2.00	105.04	109.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NDP	O4D-C1D-N1N-C6N
2	C	301	NDP	O4D-C1D-N1N-C6N
2	D	301	NDP	O4D-C1D-N1N-C6N
2	B	301	NDP	O4D-C1D-N1N-C6N
2	C	301	NDP	C3B-C2B-O2B-P2B

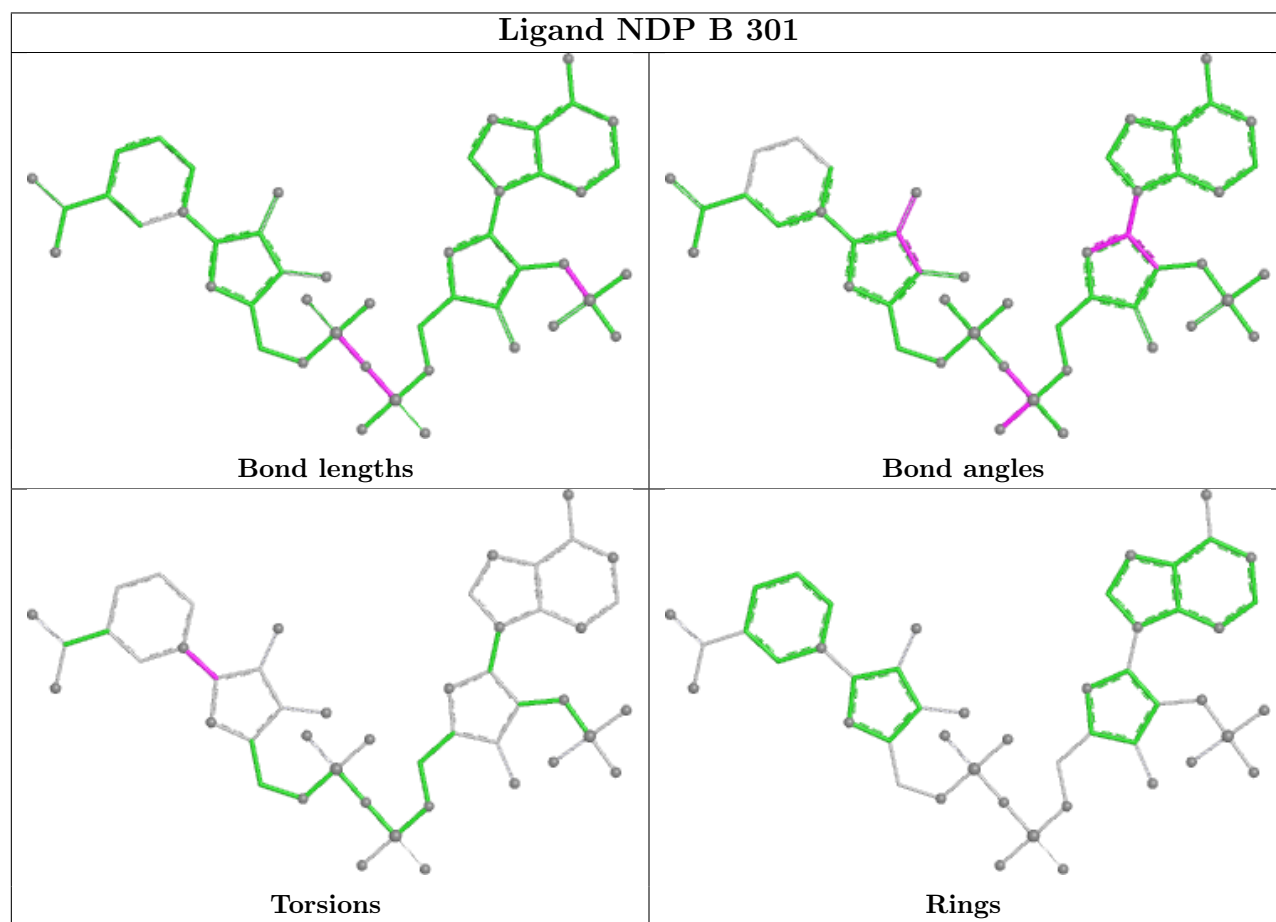
There are no ring outliers.

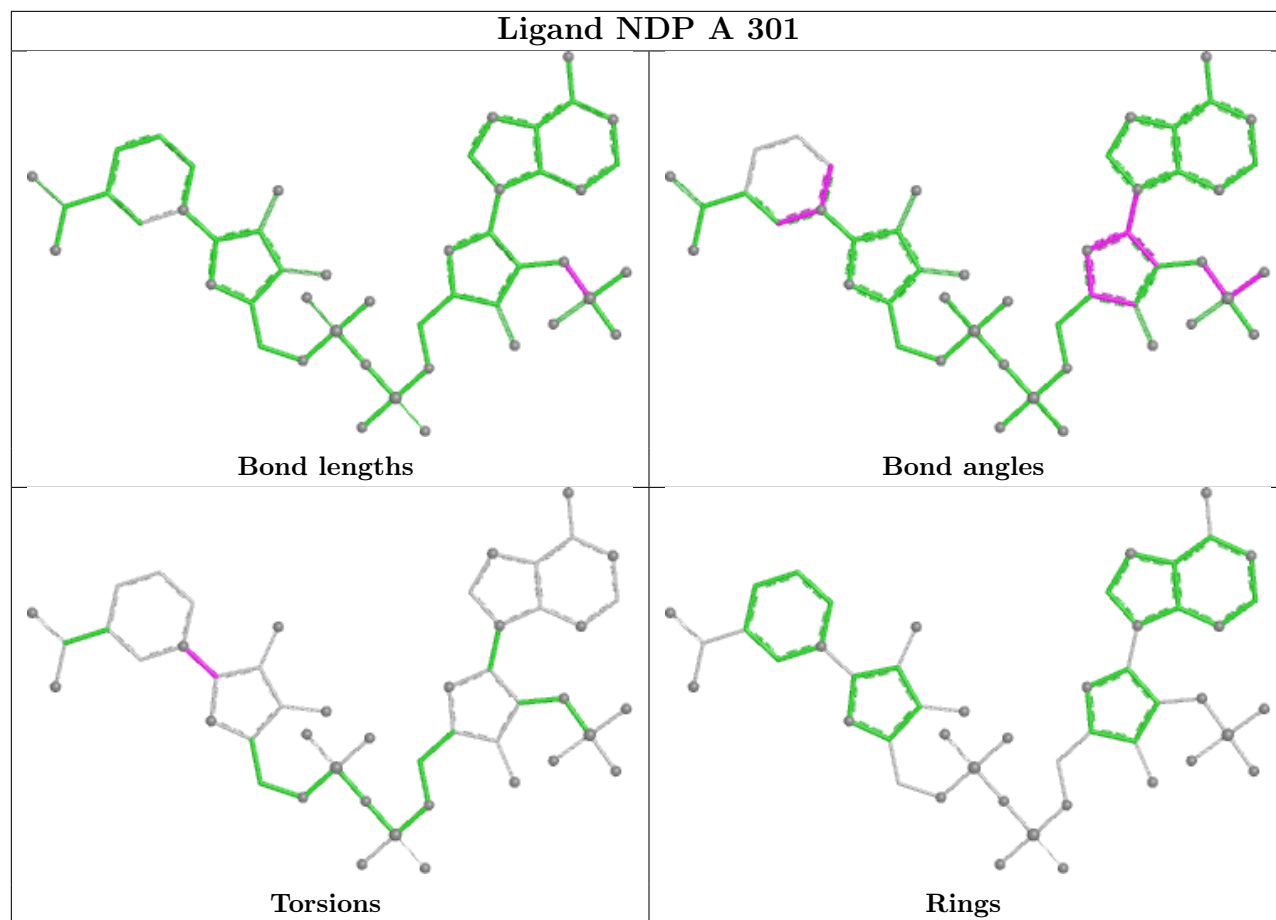
8 monomers are involved in 11 short contacts:

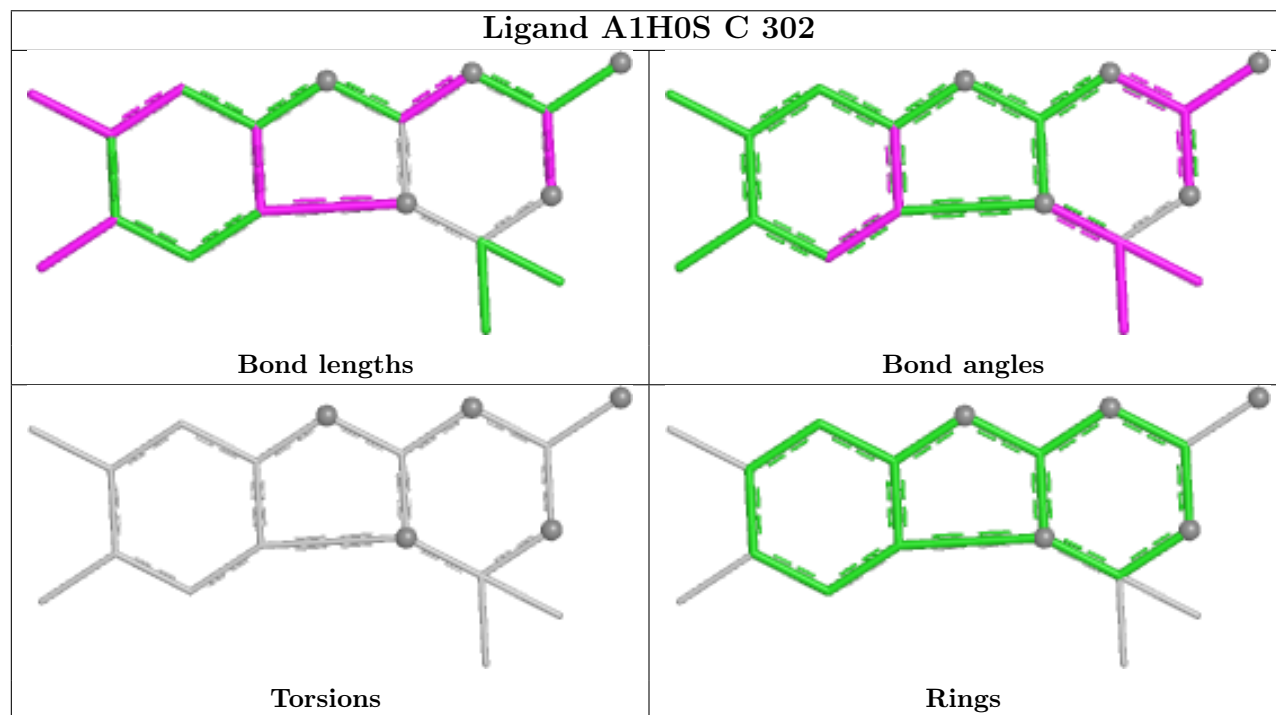
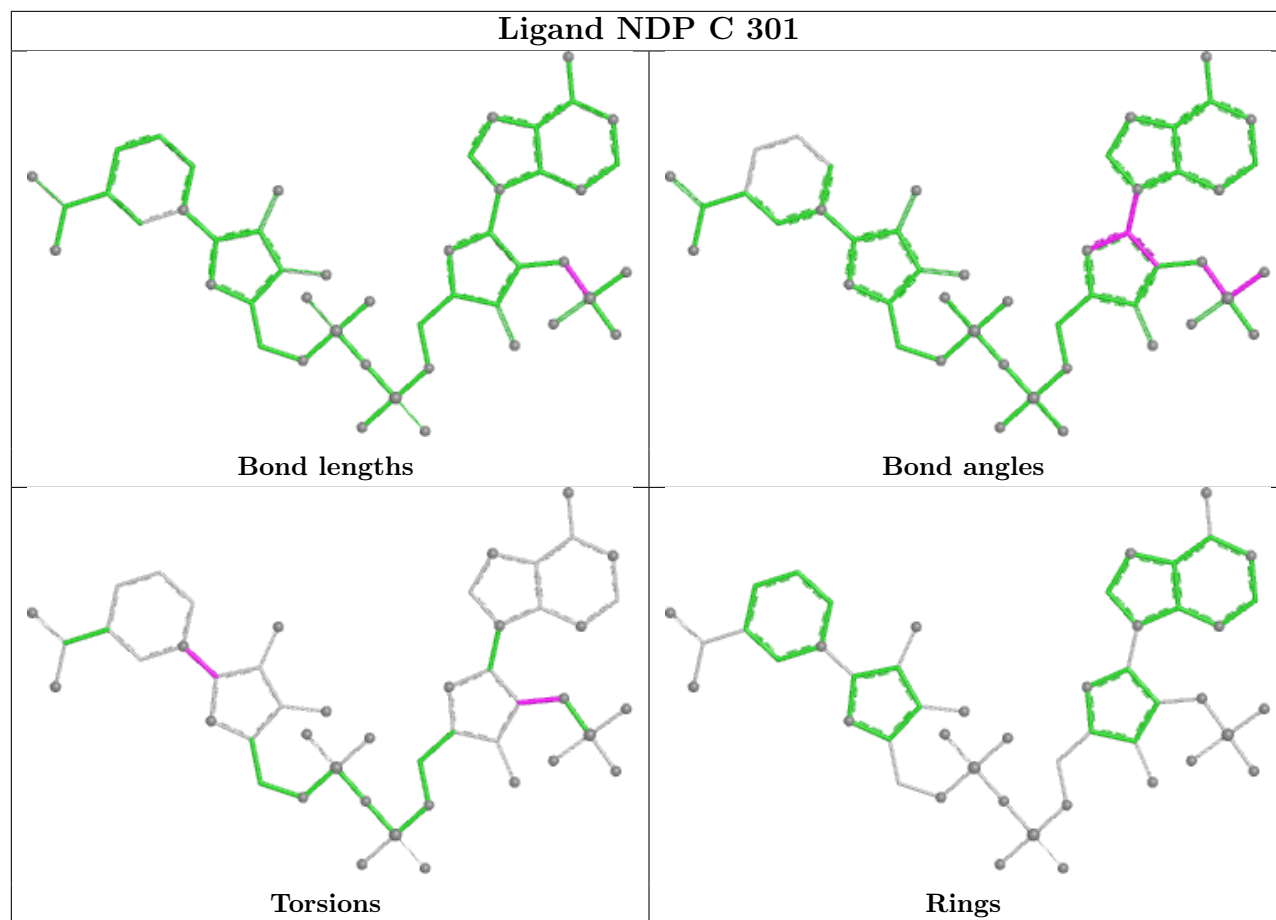
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	NDP	1	0
2	A	301	NDP	2	0
4	C	303	ACT	3	0
2	C	301	NDP	2	0
3	C	302	A1H0S	1	0
3	D	302	A1H0S	1	0
3	A	302	A1H0S	1	0
2	D	301	NDP	3	0

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

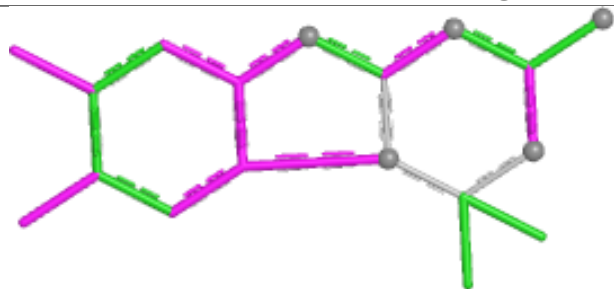
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



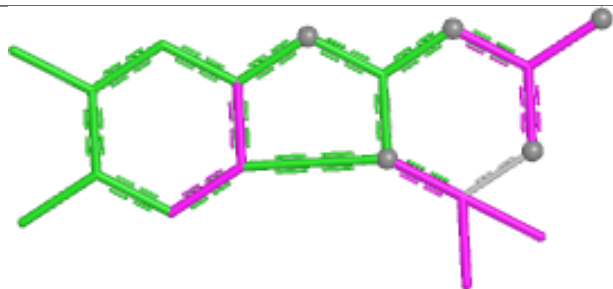




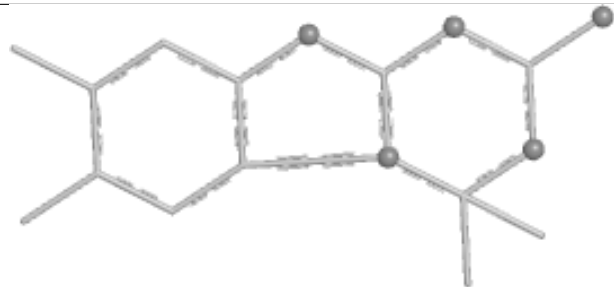
Ligand A1H0S D 302



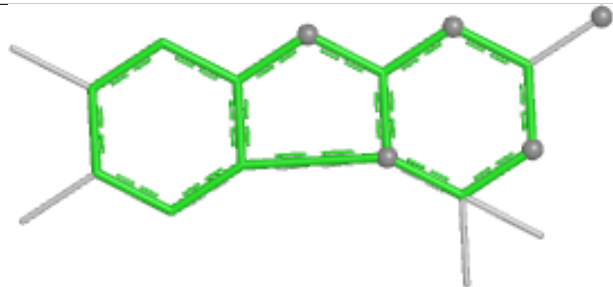
Bond lengths



Bond angles

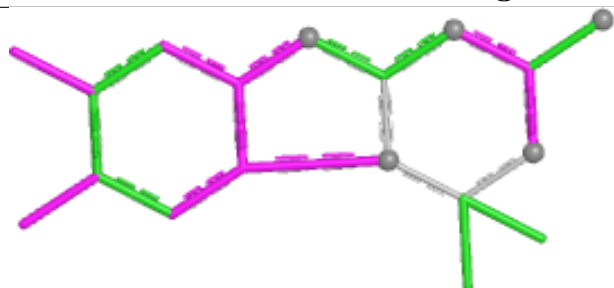


Torsions

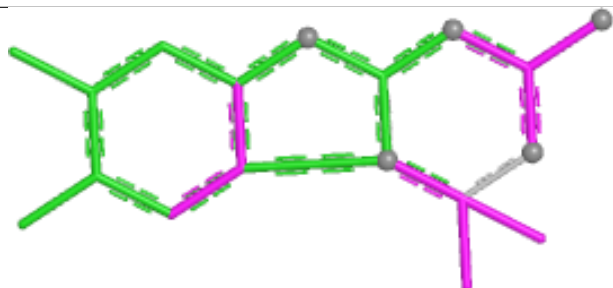


Rings

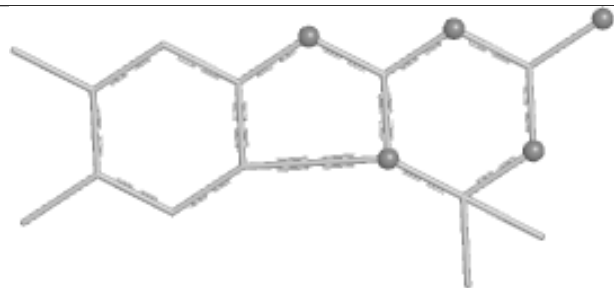
Ligand A1H0S A 302



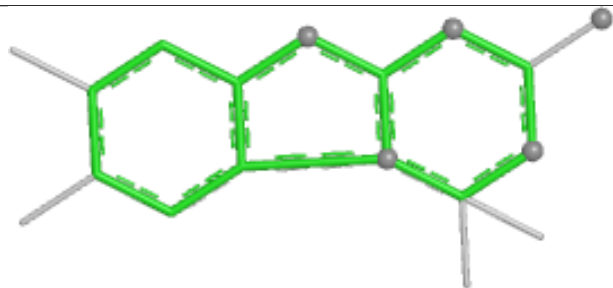
Bond lengths



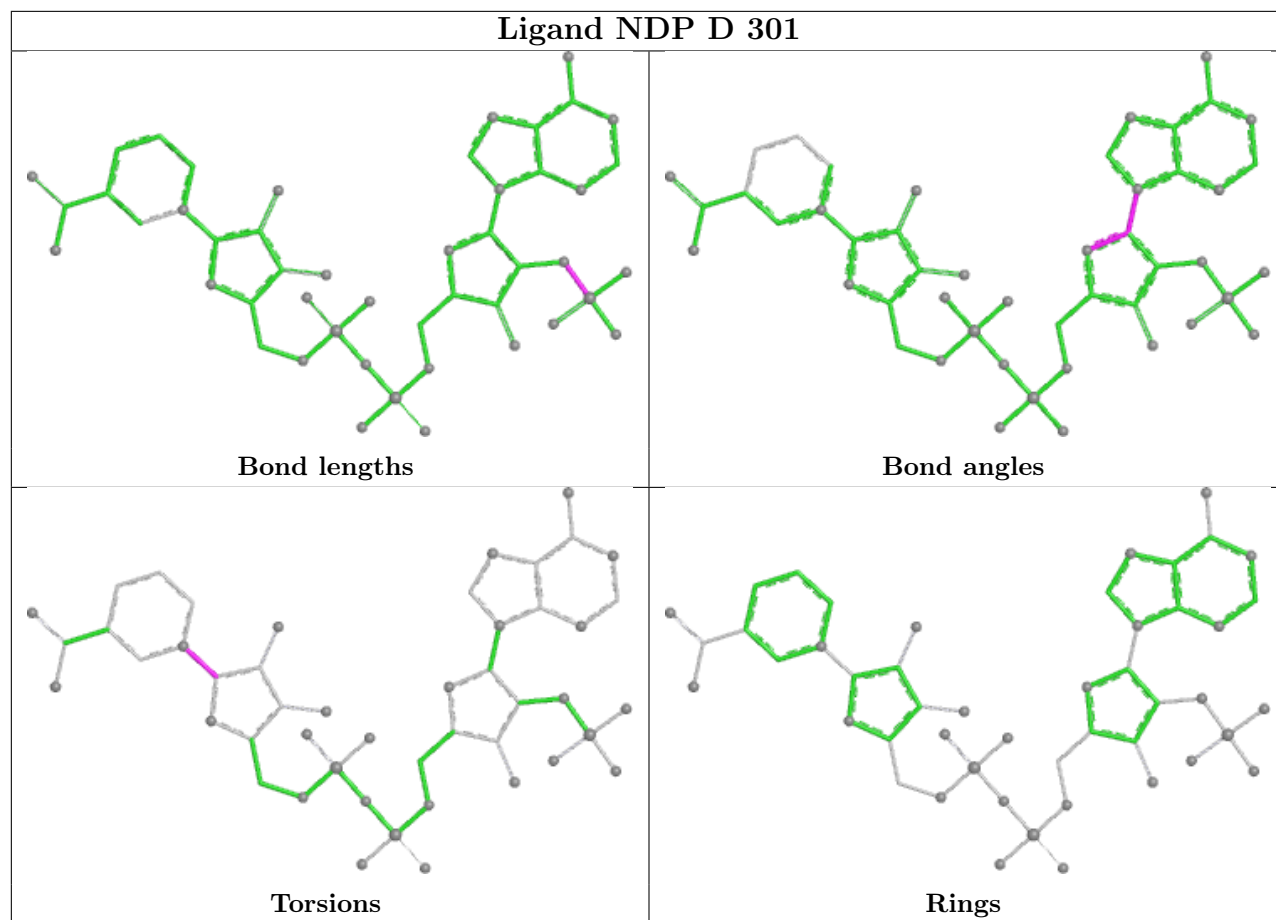
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	248/289 (85%)	-0.09	3 (1%) 76 81	13, 26, 42, 65	12 (4%)
1	B	249/289 (86%)	-0.09	6 (2%) 59 67	15, 25, 42, 64	17 (6%)
1	C	248/289 (85%)	-0.05	4 (1%) 70 76	13, 25, 44, 60	21 (8%)
1	D	248/289 (85%)	0.04	5 (2%) 65 72	13, 27, 47, 79	20 (8%)
All	All	993/1156 (85%)	-0.05	18 (1%) 67 74	13, 26, 43, 79	70 (7%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	104	GLN	4.6
1	D	211	VAL	3.7
1	B	152	SER	3.4
1	B	211	VAL	3.1
1	B	143	LYS	2.9
1	A	195	TYR	2.8
1	C	2	GLU	2.7
1	D	213	MET	2.6
1	D	103	VAL	2.5
1	B	2	GLU	2.5
1	D	152	SER	2.5
1	C	211	VAL	2.4
1	A	103	VAL	2.3
1	B	103	VAL	2.3
1	B	208	LEU	2.2
1	A	113	GLY	2.1
1	D	212	ALA	2.0
1	C	152	SER	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, 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
1	CSX	A	168	7/8	0.95	0.07	26,29,49,51	0
1	CSX	B	168	7/8	0.96	0.07	25,29,45,49	0
1	CSX	D	168	7/8	0.96	0.06	27,31,39,48	0
1	CSX	C	168	7/8	0.98	0.05	24,28,41,44	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

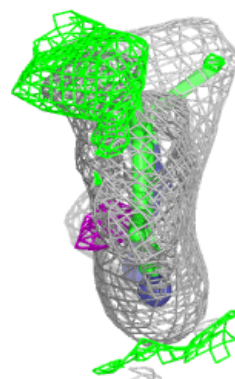
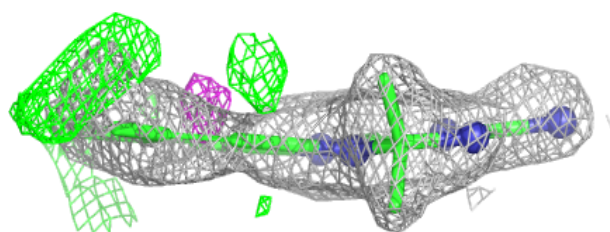
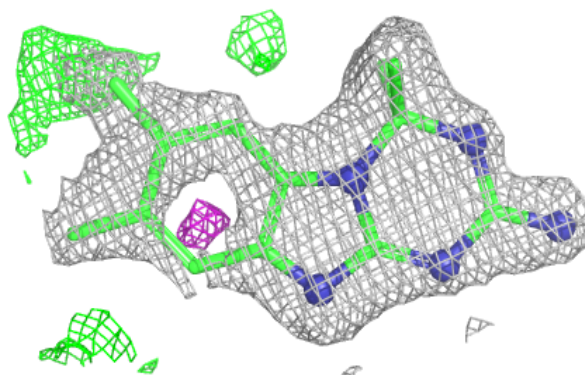
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	A1H0S	C	302	18/18	0.79	0.17	38,41,53,54	18
3	A1H0S	D	302	18/18	0.84	0.15	37,44,52,53	18
3	A1H0S	A	302	18/18	0.88	0.12	33,41,51,52	0
4	ACT	C	303	4/4	0.90	0.13	21,24,29,31	4
4	ACT	B	302	4/4	0.91	0.14	22,27,34,34	4
4	ACT	A	304	4/4	0.91	0.17	21,24,32,34	4
4	ACT	A	303	4/4	0.93	0.09	23,23,23,30	4
2	NDP	B	301	48/48	0.95	0.07	23,27,32,34	48
2	NDP	C	301	48/48	0.96	0.07	22,27,31,33	0
2	NDP	A	301	48/48	0.96	0.06	21,25,29,32	0
2	NDP	D	301	48/48	0.97	0.06	21,28,35,40	0

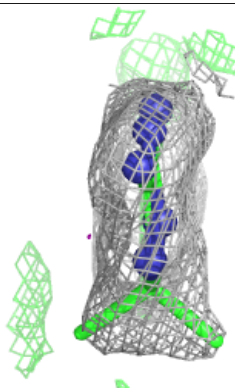
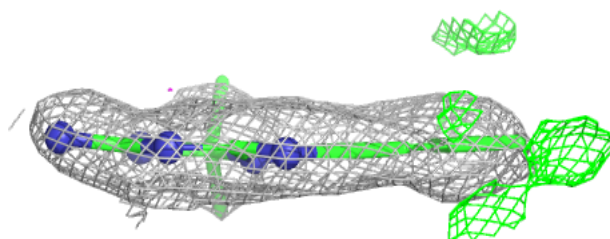
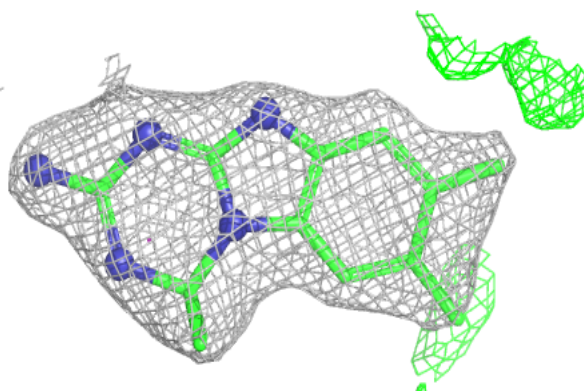
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1H0S 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)

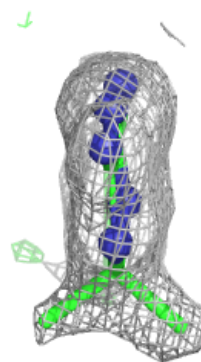
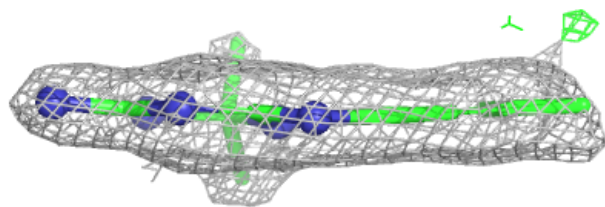
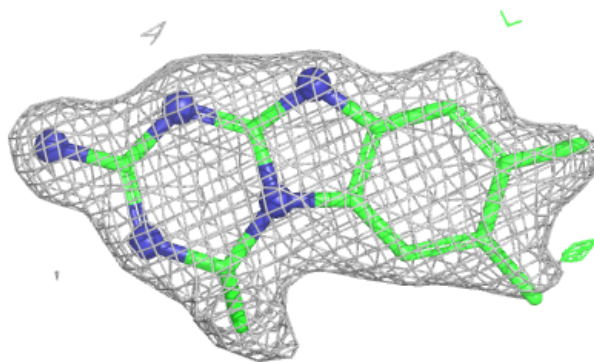
**Electron density around A1H0S D 302:**

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

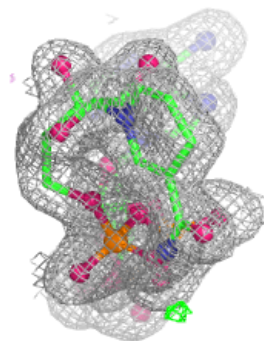
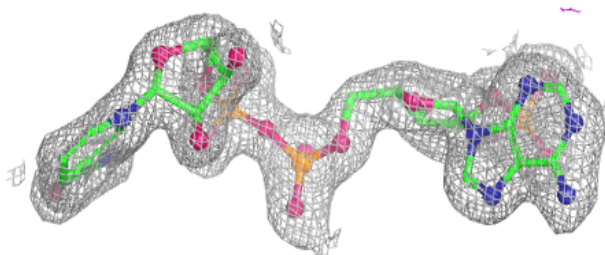
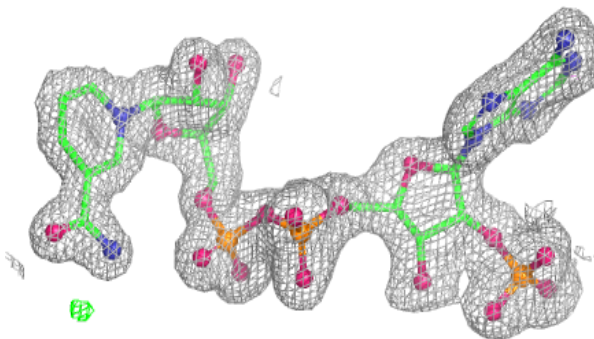


Electron density around A1H0S A 302:

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

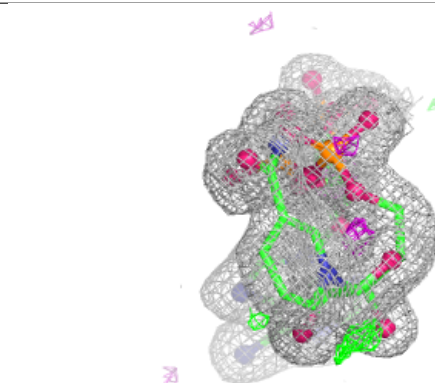
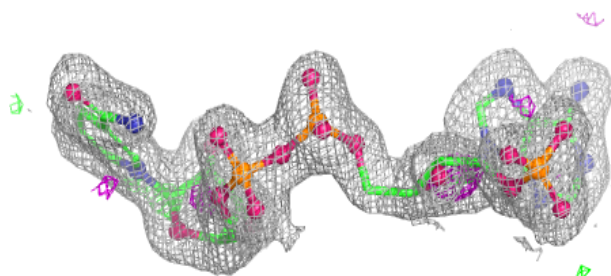
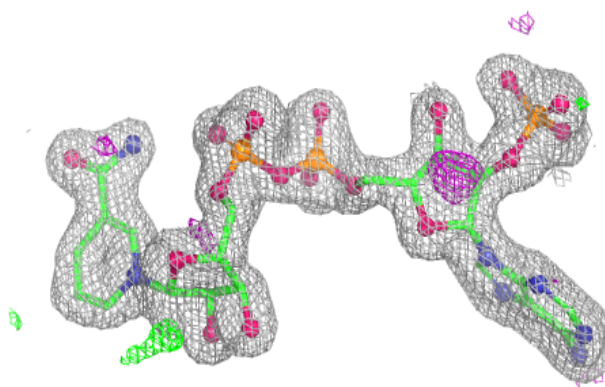
**Electron density around NDP B 301:**

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

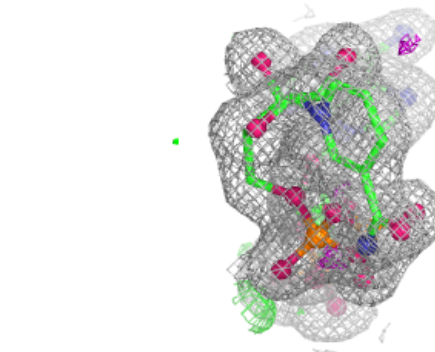
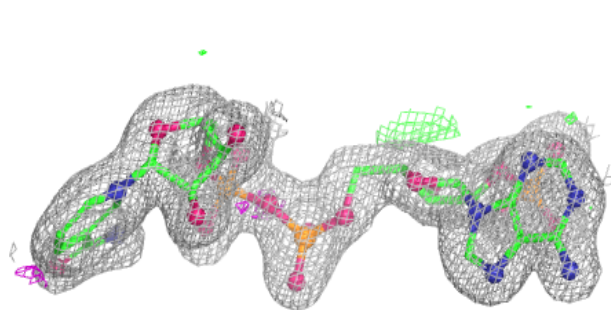
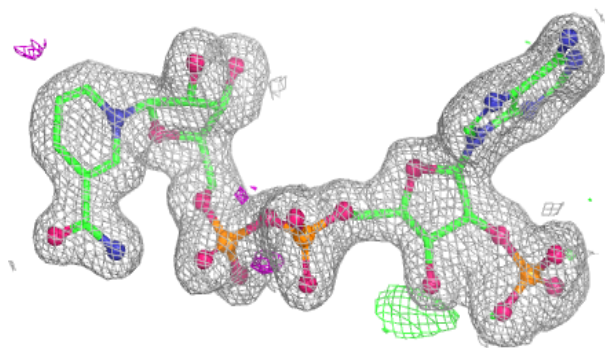


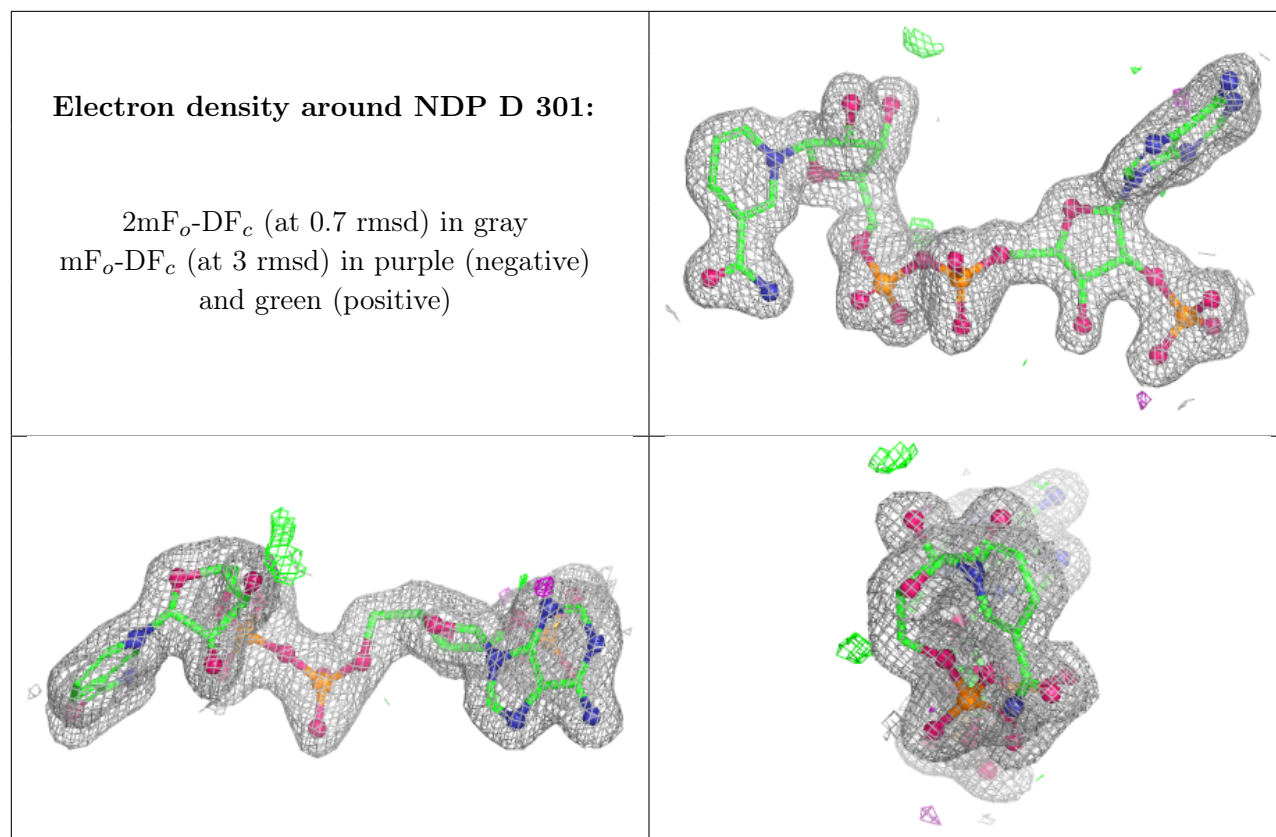
Electron density around NDP C 301:

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

**Electron density around NDP 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.