



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:38 PM UTC

PDB ID : 8RHY / pdb_00008rhy
Title : Crystal Structure of Trypanosoma brucei PTR1 in complex with the cofactor and inhibitor P34
Authors : Pozzi, C.; Mangani, S.; Landi, G.
Deposited on : 2023-12-17
Resolution : 1.86 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

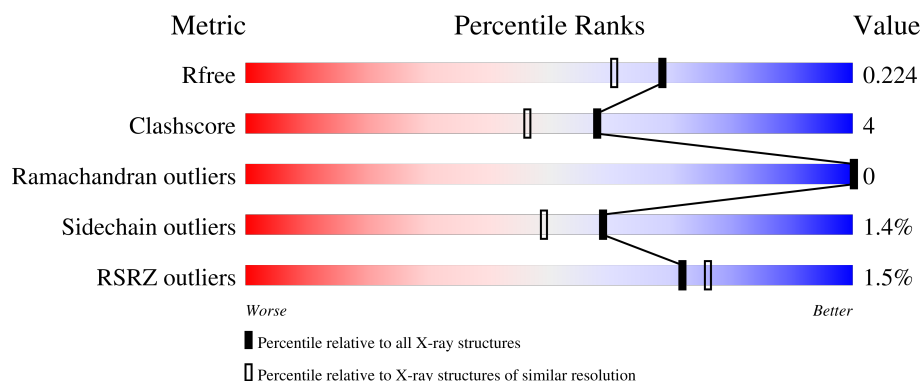
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

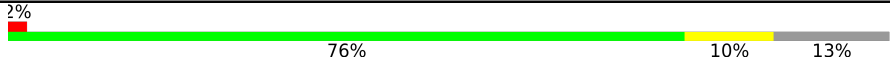
The reported resolution of this entry is 1.86 Å.

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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	
1	B	289	
1	C	289	
1	D	289	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8397 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	251	Total	C	N	O	S	0	3	0
			1858	1168	324	355	11			
1	B	249	Total	C	N	O	S	0	3	0
			1834	1158	325	340	11			
1	C	251	Total	C	N	O	S	0	5	0
			1860	1172	324	353	11			
1	D	250	Total	C	N	O	S	0	8	0
			1895	1191	334	359	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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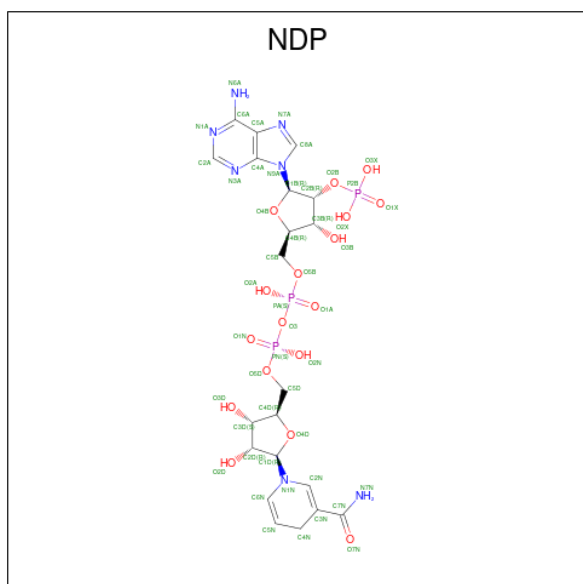
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	initiating methionine	UNP O76290
B	-19	GLY	-	expression tag	UNP O76290
B	-18	SER	-	expression tag	UNP O76290
B	-17	SER	-	expression tag	UNP O76290
B	-16	HIS	-	expression tag	UNP O76290
B	-15	HIS	-	expression tag	UNP O76290
B	-14	HIS	-	expression 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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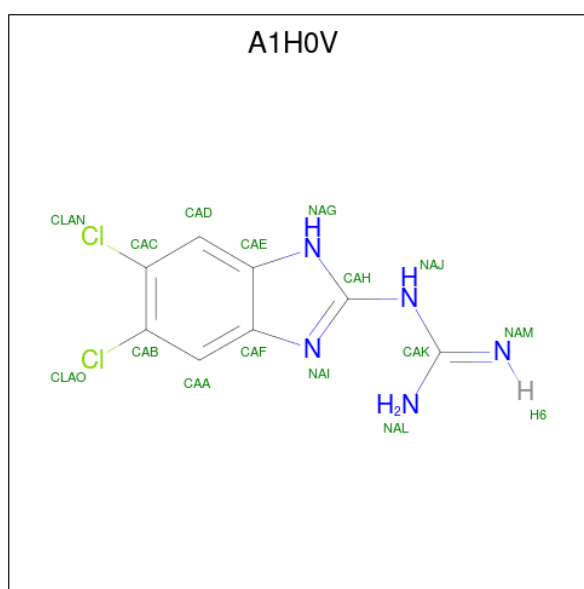
Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	initiating methionine	UNP O76290
D	-19	GLY	-	expression tag	UNP O76290
D	-18	SER	-	expression tag	UNP O76290
D	-17	SER	-	expression tag	UNP O76290
D	-16	HIS	-	expression tag	UNP O76290
D	-15	HIS	-	expression tag	UNP O76290
D	-14	HIS	-	expression 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: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).



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 1-[5,6-bis(chloranyl)-1 {H}-benzimidazol-2-yl]guanidine (CCD ID: A1H0V) (formula: C₈H₇Cl₂N₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	0	0
			15	8	2	5		
3	B	1	Total	C	Cl	N	0	0
			15	8	2	5		
3	C	1	Total	C	Cl	N	0	0
			15	8	2	5		
3	D	1	Total	C	Cl	N	0	0
			15	8	2	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	165	Total	O	0	0
			165	165		

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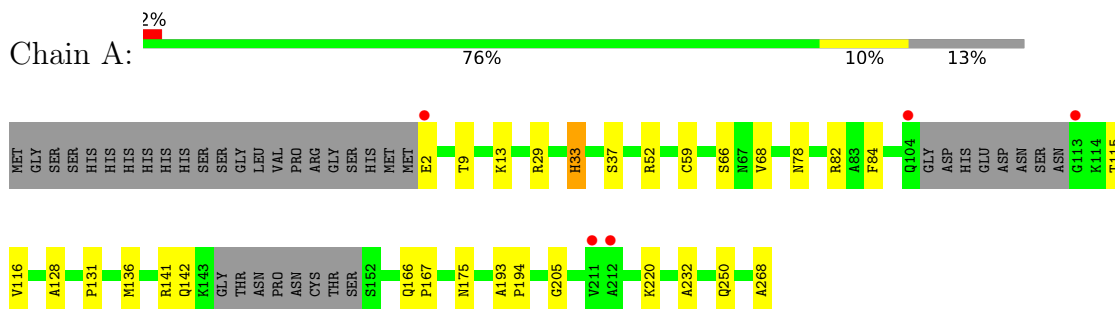
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	167	Total 167	O 167	0	3
4	C	189	Total 189	O 189	0	2
4	D	177	Total 177	O 177	0	3

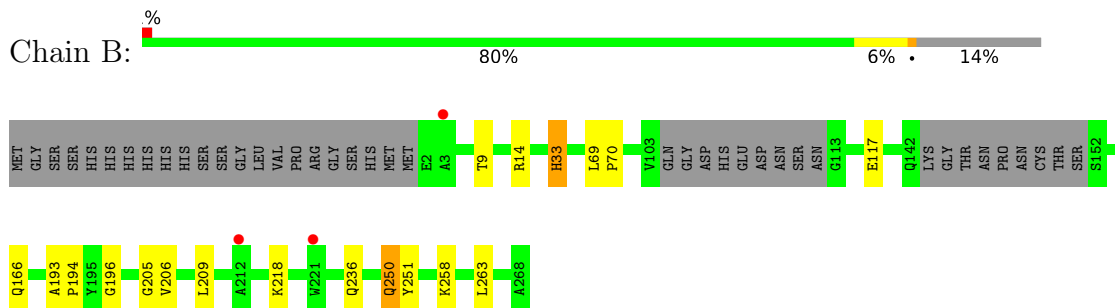
3 Residue-property plots [i](#)

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

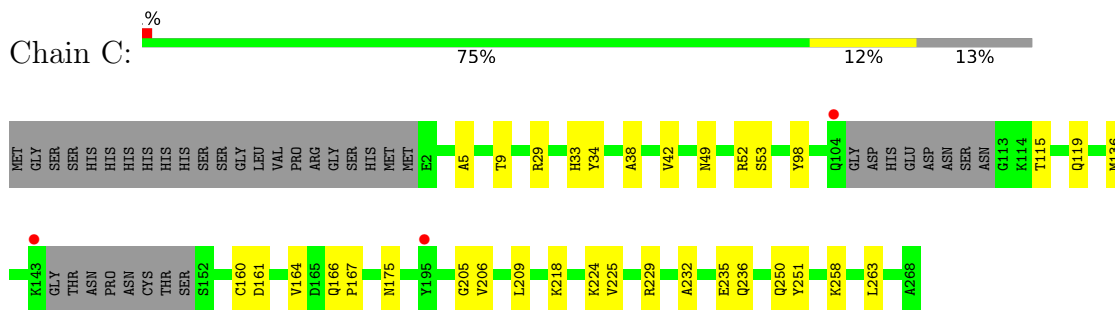
- Molecule 1: Pteridine reductase



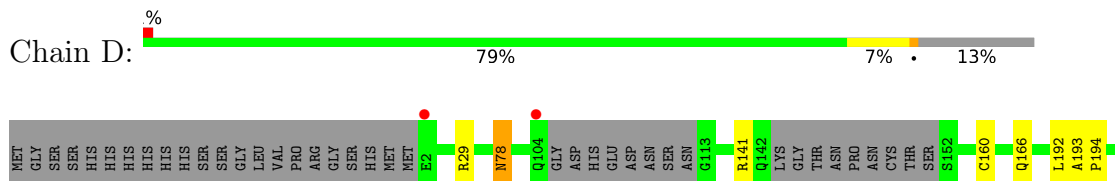
- Molecule 1: Pteridine reductase

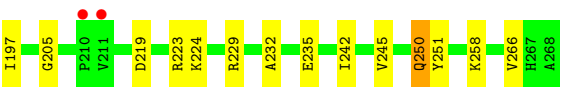


- Molecule 1: Pteridine reductase



- Molecule 1: Pteridine reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.36Å 99.09Å 84.45Å 90.00° 115.86° 90.00°	Depositor
Resolution (Å)	75.84 – 1.86 75.84 – 1.86	Depositor EDS
% Data completeness (in resolution range)	94.7 (75.84-1.86) 94.7 (75.84-1.86)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.183 , 0.223 0.183 , 0.224	Depositor DCC
R_{free} test set	4713 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	9.4	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8397	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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 22.94 % 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 5.1476e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1H0V, NDP

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	0.65	0/1894	1.20	7/2574 (0.3%)
1	B	0.66	0/1870	1.22	4/2542 (0.2%)
1	C	0.68	0/1899	1.16	4/2582 (0.2%)
1	D	0.69	2/1946 (0.1%)	1.22	5/2641 (0.2%)
All	All	0.67	2/7609 (0.0%)	1.20	20/10339 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	78[A]	ASN	C-O	5.46	1.30	1.24
1	D	78[B]	ASN	C-O	5.46	1.30	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	78[A]	ASN	CA-C-O	7.41	128.64	120.63
1	D	78[B]	ASN	CA-C-O	7.41	128.64	120.63
1	D	235	GLU	CB-CG-CD	7.19	124.82	112.60
1	A	115	THR	CA-CB-OG1	-6.64	99.64	109.60
1	C	136	MET	CB-CA-C	-6.31	100.97	110.88
1	C	115	THR	CA-CB-OG1	-6.07	100.50	109.60
1	C	258	LYS	CB-CA-C	-5.74	100.70	109.89
1	D	258	LYS	CB-CA-C	-5.72	100.74	109.89
1	A	116	VAL	N-CA-CB	5.57	118.11	110.54
1	A	82	ARG	CA-CB-CG	-5.55	102.99	114.10
1	B	196	GLY	CA-C-N	-5.53	115.96	122.93
1	B	196	GLY	C-N-CA	-5.53	115.96	122.93
1	A	220	LYS	CB-CA-C	5.52	119.95	110.79
1	D	224	LYS	CG-CD-CE	5.47	123.88	111.30
1	A	33	HIS	CA-CB-CG	-5.35	108.45	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	224	LYS	CG-CD-CE	5.27	123.41	111.30
1	A	136	MET	CB-CA-C	-5.15	102.57	110.81
1	B	33	HIS	CA-CB-CG	-5.12	108.68	113.80
1	B	258	LYS	N-CA-CB	5.05	117.78	109.95
1	A	52	ARG	CA-CB-CG	5.03	124.17	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1858	0	1849	19	0
1	B	1834	0	1844	15	0
1	C	1860	0	1861	22	0
1	D	1895	0	1920	16	0
2	A	48	0	26	3	0
2	B	48	0	26	3	0
2	C	48	0	26	2	0
2	D	48	0	26	3	0
3	A	15	0	0	3	0
3	B	15	0	0	1	0
3	C	15	0	0	1	0
3	D	15	0	0	3	0
4	A	165	0	0	3	0
4	B	167	0	0	0	0
4	C	189	0	0	2	0
4	D	177	0	0	2	0
All	All	8397	0	7578	68	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 (68) 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)
2:D:301:NDP:H41N	3:D:302:A1H0V:CAE	2.18	0.73
1:C:225:VAL:O	1:C:229:ARG:HD3	1.94	0.67
1:A:250:GLN:HG2	4:A:495:HOH:O	1.96	0.65
2:A:301:NDP:H41N	3:A:302:A1H0V:CAE	2.27	0.65
1:C:232:ALA:HB2	1:D:251:TYR:CE2	2.34	0.63
1:B:9:THR:HA	1:B:33:HIS:HB3	1.81	0.62
1:D:250[B]:GLN:HG2	4:D:470:HOH:O	1.99	0.62
1:A:250:GLN:HG3	1:B:236:GLN:HE21	1.63	0.61
1:D:78[B]:ASN:OD1	1:D:141:ARG:NH1	2.36	0.59
1:D:223[A]:ARG:NH2	1:D:229:ARG:O	2.37	0.57
1:A:205:GLY:O	2:A:301:NDP:H42N	2.05	0.57
1:C:160:CYS:HB3	4:C:509:HOH:O	2.05	0.57
1:A:167:PRO:HB3	1:A:175[A]:ASN:OD1	2.05	0.56
1:D:205:GLY:O	2:D:301:NDP:H42N	2.06	0.55
1:A:250:GLN:CD	1:B:236:GLN:HE21	2.15	0.55
1:A:142:GLN:HB3	4:A:402:HOH:O	2.06	0.54
1:B:205:GLY:O	2:B:301:NDP:H42N	2.07	0.54
1:D:160:CYS:HB3	4:D:493:HOH:O	2.06	0.54
1:A:250:GLN:HG3	1:B:236:GLN:NE2	2.23	0.54
1:B:69:LEU:N	1:B:70:PRO:CD	2.73	0.52
1:C:167:PRO:HB3	1:C:175[B]:ASN:OD1	2.09	0.52
1:A:250:GLN:CG	1:B:236:GLN:HE21	2.23	0.51
1:C:206[B]:VAL:HG21	1:C:209:LEU:HD21	1.92	0.50
1:C:232:ALA:HB2	1:D:251:TYR:CD2	2.46	0.50
1:C:236:GLN:HE21	1:D:250[B]:GLN:HG3	1.77	0.50
2:C:301:NDP:H41N	3:C:302:A1H0V:CAF	2.41	0.50
1:A:29:ARG:HD2	1:A:84:PHE:CD1	2.47	0.50
1:A:128:ALA:C	1:A:131:PRO:HD2	2.38	0.49
1:B:250:GLN:HE21	1:B:250:GLN:HA	1.78	0.49
1:C:251:TYR:CE2	1:D:232:ALA:HB2	2.48	0.49
1:C:206[B]:VAL:CG2	1:C:209:LEU:HD21	2.42	0.48
1:A:232:ALA:HB2	1:B:251:TYR:CE2	2.49	0.47
1:C:9:THR:HA	1:C:33:HIS:HB3	1.95	0.47
1:C:38:ALA:O	1:C:42:VAL:HG23	2.15	0.47
1:A:78[B]:ASN:OD1	1:A:141:ARG:NH2	2.48	0.47
1:B:206:VAL:HG23	1:B:263:LEU:CD2	2.45	0.46
1:A:2:GLU:N	4:A:410:HOH:O	2.48	0.46
1:C:49:ASN:HA	1:C:52:ARG:O	2.16	0.46
1:B:209:LEU:HD13	1:B:218:LYS:CB	2.46	0.45
1:B:193:ALA:N	1:B:194:PRO:CD	2.80	0.45
1:C:161:ASP:HB3	1:C:164:VAL:HG13	1.99	0.45
1:D:242:ILE:HD13	1:D:242:ILE:HA	1.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:GLN:NE2	1:D:250[B]:GLN:HG3	2.33	0.44
1:A:193:ALA:N	1:A:194:PRO:CD	2.81	0.44
1:C:251:TYR:CD2	1:D:232:ALA:HB2	2.53	0.44
1:C:206[A]:VAL:HG23	1:C:263:LEU:CD2	2.48	0.43
1:D:192:LEU:HB3	1:D:197:ILE:HB	2.01	0.43
1:A:33:HIS:HA	1:A:59:CYS:O	2.18	0.43
1:A:13:LYS:HE2	1:A:37:SER:OG	2.19	0.43
2:A:301:NDP:H41N	3:A:302:A1H0V:CAD	2.48	0.43
1:C:205:GLY:O	2:C:301:NDP:H42N	2.18	0.43
1:C:5:ALA:HA	1:C:29:ARG:O	2.19	0.42
1:C:98:TYR:HE1	1:C:119:GLN:HG2	1.84	0.42
1:C:235:GLU:HG3	4:C:494:HOH:O	2.19	0.42
3:D:302:A1H0V:NAI	3:D:302:A1H0V:NAL	2.67	0.42
1:C:209:LEU:HD13	1:C:218:LYS:HA	2.02	0.42
1:B:209:LEU:HD13	1:B:218:LYS:HB3	2.01	0.42
1:C:34:TYR:CE2	1:C:38:ALA:HA	2.55	0.42
2:D:301:NDP:H41N	3:D:302:A1H0V:CAD	2.49	0.41
1:A:9:THR:HA	1:A:33:HIS:HB3	2.02	0.41
3:A:302:A1H0V:NAL	3:A:302:A1H0V:NAI	2.66	0.41
1:A:66:SER:OG	1:A:68:VAL:HG22	2.19	0.41
2:B:301:NDP:H41N	3:B:302:A1H0V:CAF	2.51	0.41
1:A:268:ALA:HB2	1:D:266:VAL:HB	2.03	0.41
1:B:14:ARG:HD3	2:B:301:NDP:O1A	2.21	0.41
1:D:193:ALA:N	1:D:194:PRO:CD	2.84	0.40
1:D:219:ASP:O	1:D:223[B]:ARG:HG2	2.22	0.40
1:B:206:VAL:HG23	1:B:263:LEU:HD22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/289 (86%)	239 (96%)	9 (4%)	0	100	100
1	B	246/289 (85%)	237 (96%)	9 (4%)	0	100	100
1	C	249/289 (86%)	240 (96%)	9 (4%)	0	100	100
1	D	252/289 (87%)	242 (96%)	10 (4%)	0	100	100
All	All	995/1156 (86%)	958 (96%)	37 (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	193/232 (83%)	192 (100%)	1 (0%)	81	77
1	B	189/232 (82%)	186 (98%)	3 (2%)	55	44
1	C	195/232 (84%)	192 (98%)	3 (2%)	57	47
1	D	203/232 (88%)	198 (98%)	5 (2%)	42	27
All	All	780/928 (84%)	768 (98%)	12 (2%)	59	47

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	B	117	GLU
1	B	166	GLN
1	B	250	GLN
1	C	53	SER
1	C	166	GLN
1	C	250	GLN
1	D	29	ARG
1	D	166	GLN
1	D	245	VAL
1	D	250[A]	GLN
1	D	250[B]	GLN

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	25	GLN
1	A	65	ASN
1	A	92	ASN
1	A	127	ASN
1	A	250	GLN
1	B	92	ASN
1	B	236	GLN
1	B	250	GLN
1	C	54	ASN
1	C	92	ASN
1	C	236	GLN
1	D	92	ASN
1	D	119	GLN
1	D	140	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	A1H0V	C	302	-	16,16,16	1.81	6 (37%)	21,23,23	1.57	5 (23%)
2	NDP	B	301	-	51,52,52	0.82	2 (3%)	71,80,80	0.99	4 (5%)
2	NDP	C	301	-	51,52,52	0.72	1 (1%)	71,80,80	0.94	3 (4%)
3	A1H0V	A	302	-	16,16,16	2.80	6 (37%)	21,23,23	1.44	4 (19%)
2	NDP	A	301	-	51,52,52	0.79	2 (3%)	71,80,80	0.91	3 (4%)
3	A1H0V	D	302	-	16,16,16	2.04	6 (37%)	21,23,23	1.01	2 (9%)
3	A1H0V	B	302	-	16,16,16	2.77	7 (43%)	21,23,23	1.37	2 (9%)
2	NDP	D	301	-	51,52,52	0.93	3 (5%)	71,80,80	1.02	5 (7%)

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	A1H0V	C	302	-	-	0/4/4/4	0/2/2/2
2	NDP	B	301	-	-	1/34/77/77	0/5/5/5
2	NDP	C	301	-	-	1/34/77/77	0/5/5/5
3	A1H0V	A	302	-	-	0/4/4/4	0/2/2/2
2	NDP	A	301	-	-	2/34/77/77	0/5/5/5
3	A1H0V	D	302	-	-	0/4/4/4	0/2/2/2
3	A1H0V	B	302	-	-	0/4/4/4	0/2/2/2
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	A1H0V	CAC-CLAN	8.17	1.92	1.73
3	B	302	A1H0V	CAB-CLAO	7.37	1.91	1.73
3	A	302	A1H0V	CAB-CLAO	4.88	1.85	1.73
2	D	301	NDP	P2B-O2B	3.72	1.66	1.59
3	B	302	A1H0V	CAF-NAI	-3.65	1.32	1.39
3	B	302	A1H0V	CAH-NAJ	-3.60	1.30	1.37
3	D	302	A1H0V	CAH-NAJ	-3.29	1.30	1.37
3	C	302	A1H0V	CAD-CAE	-3.19	1.34	1.39
3	D	302	A1H0V	CAA-CAF	-3.13	1.35	1.40
3	B	302	A1H0V	CAE-NAG	-3.03	1.33	1.38
2	B	301	NDP	P2B-O2B	3.02	1.64	1.59
3	B	302	A1H0V	CAE-CAF	-2.98	1.35	1.40
3	D	302	A1H0V	CAE-NAG	-2.92	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NDP	P2B-O2B	2.78	1.64	1.59
3	C	302	A1H0V	CAE-CAF	-2.75	1.36	1.40
3	C	302	A1H0V	CAA-CAF	-2.73	1.35	1.40
3	D	302	A1H0V	CAB-CLAO	2.72	1.80	1.73
3	B	302	A1H0V	CAD-CAE	-2.57	1.35	1.39
3	A	302	A1H0V	CAH-NAI	2.57	1.36	1.32
3	D	302	A1H0V	CAC-CLAN	2.57	1.79	1.73
3	C	302	A1H0V	CAF-NAI	-2.56	1.34	1.39
2	B	301	NDP	PN-O3	2.52	1.62	1.59
2	D	301	NDP	PA-O3	2.43	1.62	1.59
2	A	301	NDP	PA-O3	2.41	1.62	1.59
3	A	302	A1H0V	CAE-CAF	-2.36	1.36	1.40
2	C	301	NDP	C4N-C3N	-2.35	1.45	1.50
3	D	302	A1H0V	CAE-CAF	-2.32	1.36	1.40
2	D	301	NDP	PN-O3	2.24	1.61	1.59
3	A	302	A1H0V	CAA-CAF	-2.23	1.36	1.40
3	B	302	A1H0V	CAC-CLAN	2.21	1.78	1.73
3	C	302	A1H0V	CAB-CLAO	2.21	1.78	1.73
3	A	302	A1H0V	CAE-NAG	-2.17	1.34	1.38
3	C	302	A1H0V	CAC-CLAN	2.13	1.78	1.73

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	A1H0V	CAF-NAI-CAH	3.40	108.21	104.21
3	B	302	A1H0V	CAF-CAE-NAG	3.07	109.39	105.71
3	C	302	A1H0V	CAF-CAE-NAG	3.06	109.39	105.71
2	D	301	NDP	O4B-C1B-N9A	3.04	113.92	108.09
3	C	302	A1H0V	NAG-CAH-NAI	-2.98	109.40	113.73
3	A	302	A1H0V	CAF-CAE-NAG	2.92	109.22	105.71
2	C	301	NDP	O4B-C1B-N9A	2.84	113.54	108.09
2	B	301	NDP	O4B-C1B-N9A	2.80	113.46	108.09
3	B	302	A1H0V	CAA-CAB-CAC	-2.72	116.66	120.28
3	A	302	A1H0V	NAG-CAH-NAI	-2.68	109.83	113.73
2	C	301	NDP	C2B-C1B-N9A	-2.65	109.39	113.75
2	A	301	NDP	C3N-C7N-N7N	2.53	122.15	117.67
2	B	301	NDP	C3N-C7N-N7N	2.48	122.08	117.67
3	A	302	A1H0V	CAD-CAC-CAB	-2.42	117.06	120.28
2	A	301	NDP	O4B-C1B-N9A	2.37	112.64	108.09
2	B	301	NDP	C2B-C1B-N9A	-2.31	109.96	113.75
3	D	302	A1H0V	CAD-CAC-CLAN	2.28	122.19	118.45
2	D	301	NDP	O2D-C2D-C3D	2.27	119.10	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NDP	C4B-O4B-C1B	-2.23	104.55	109.47
2	A	301	NDP	O2B-P2B-O1X	-2.22	101.43	109.33
2	D	301	NDP	C3N-C7N-N7N	2.19	121.55	117.67
3	C	302	A1H0V	NAG-CAH-NAJ	2.09	128.01	123.05
3	C	302	A1H0V	CAA-CAF-CAE	2.08	123.41	120.50
2	D	301	NDP	O7N-C7N-C3N	-2.03	117.06	120.90
3	D	302	A1H0V	NAJ-CAH-NAI	2.03	126.73	122.77
2	D	301	NDP	P2B-O2B-C2B	-2.02	118.04	123.43
3	A	302	A1H0V	NAJ-CAH-NAI	2.02	126.70	122.77
2	C	301	NDP	O3B-C3B-C2B	2.00	116.79	111.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	A	301	NDP	O4D-C1D-N1N-C6N
2	A	301	NDP	C5B-O5B-PA-O1A

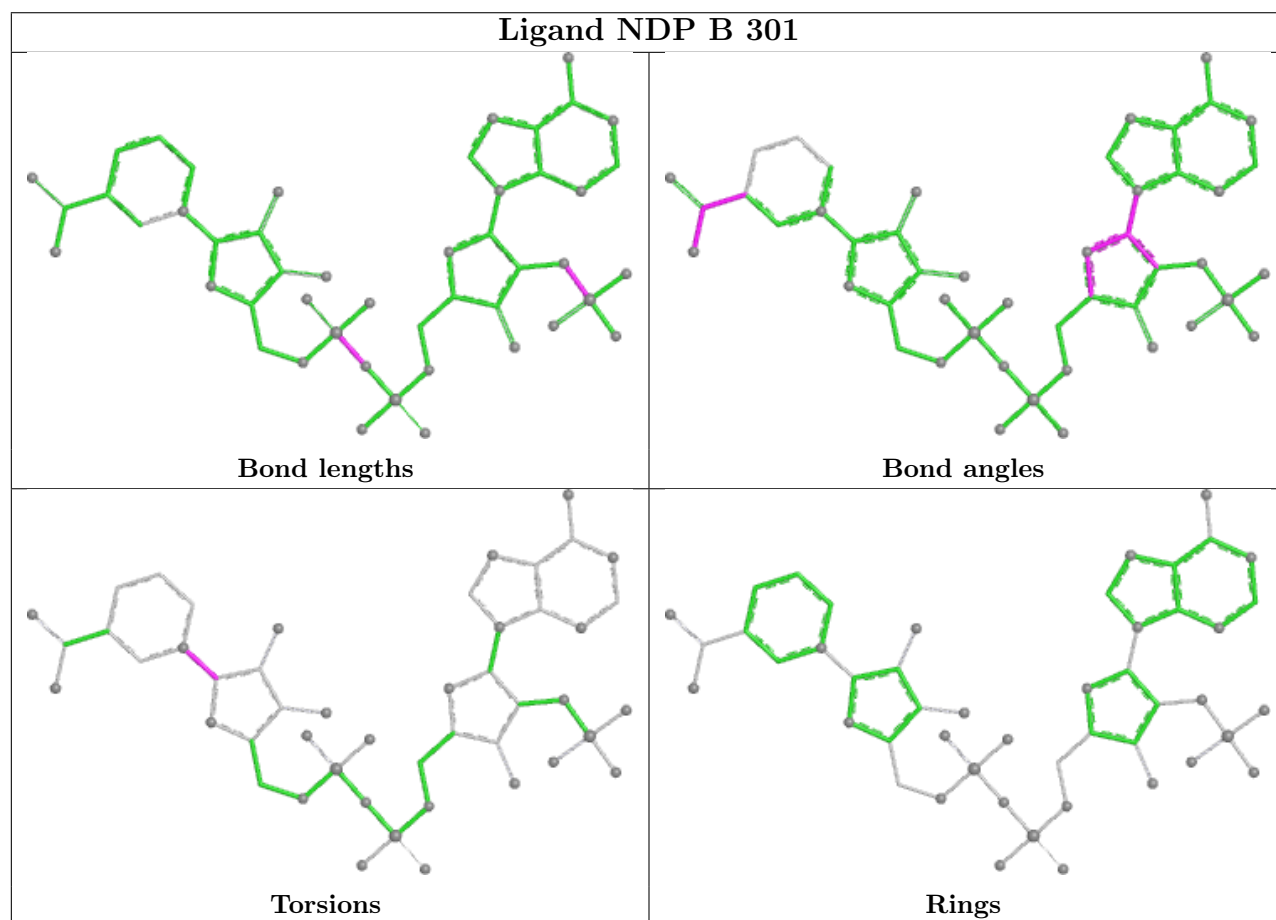
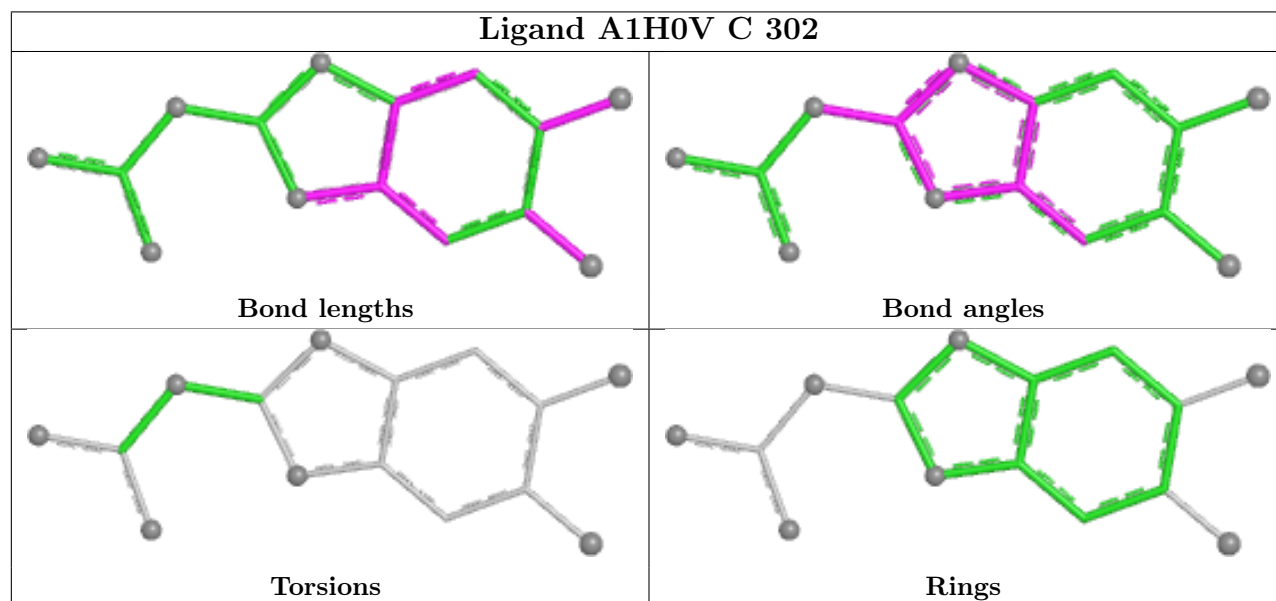
There are no ring outliers.

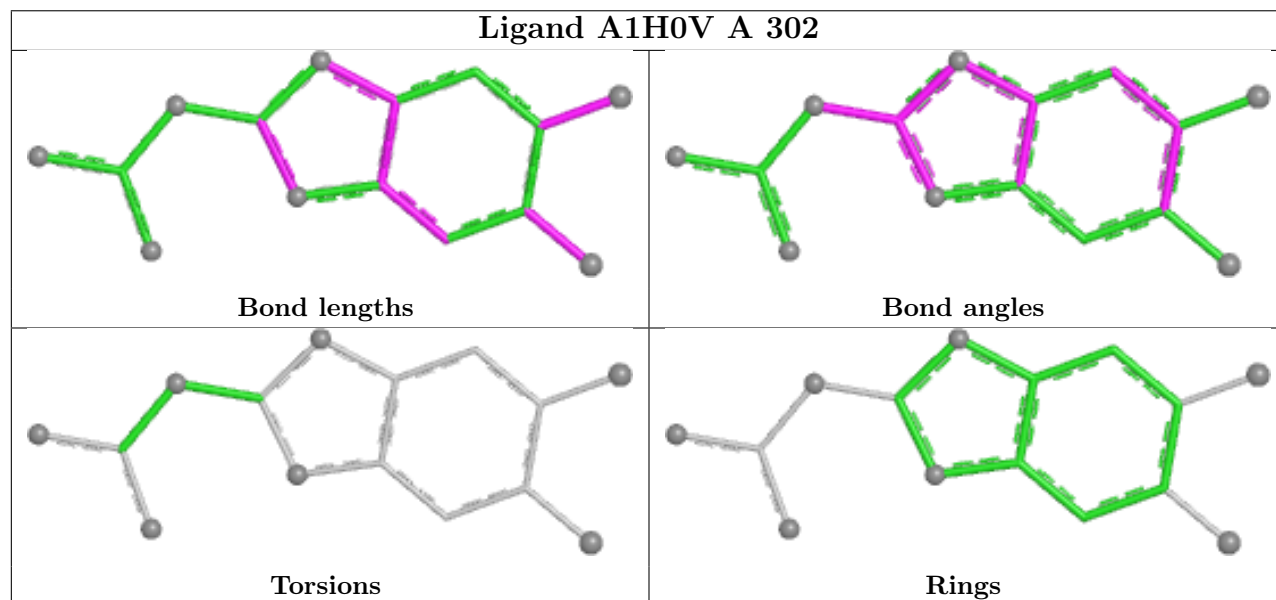
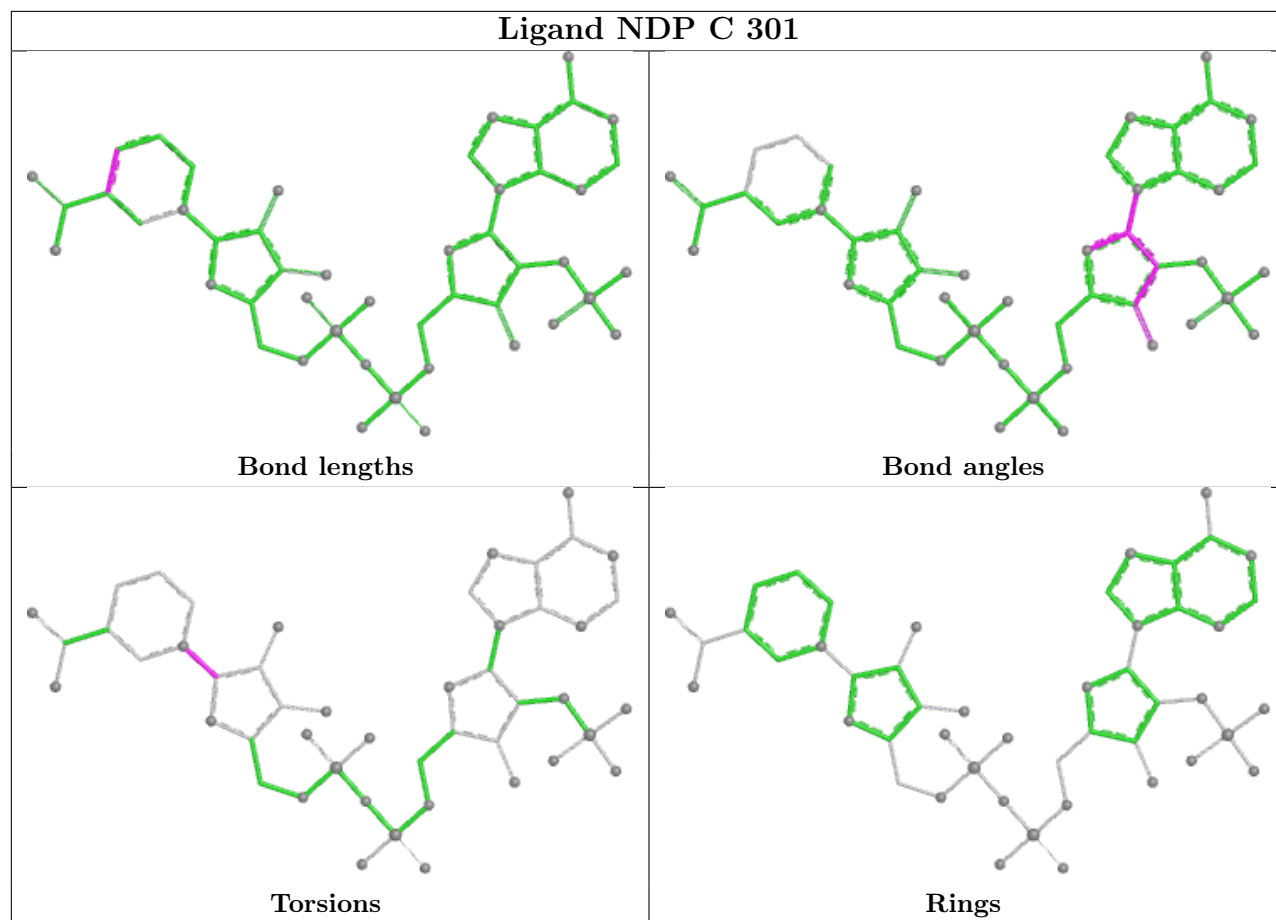
8 monomers are involved in 13 short contacts:

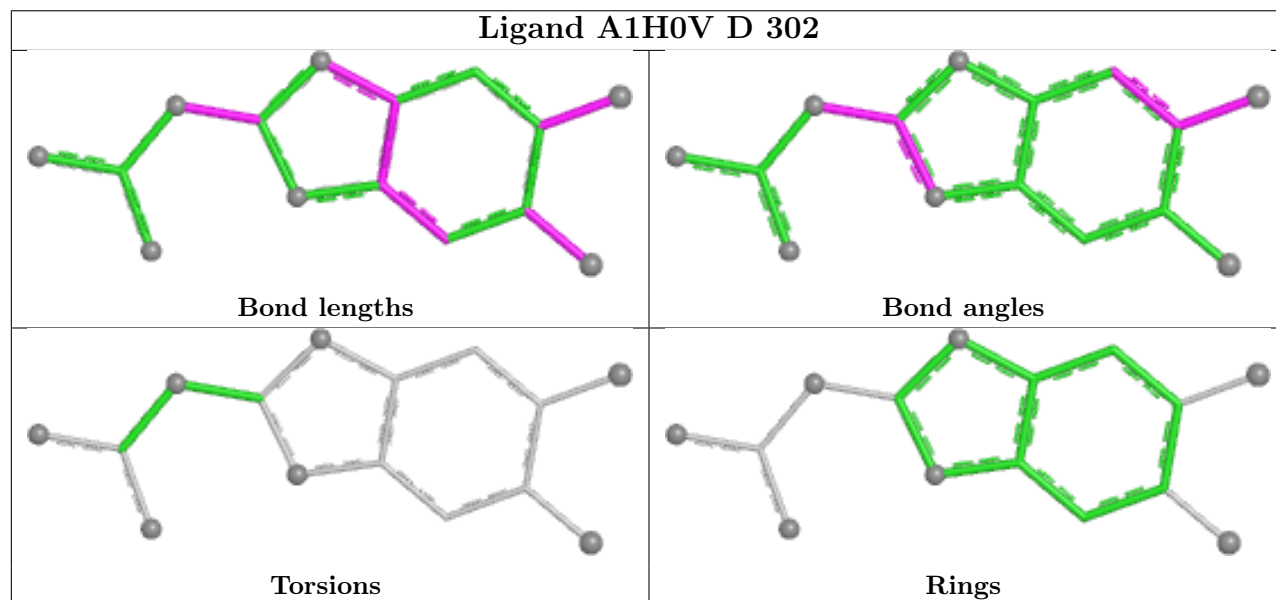
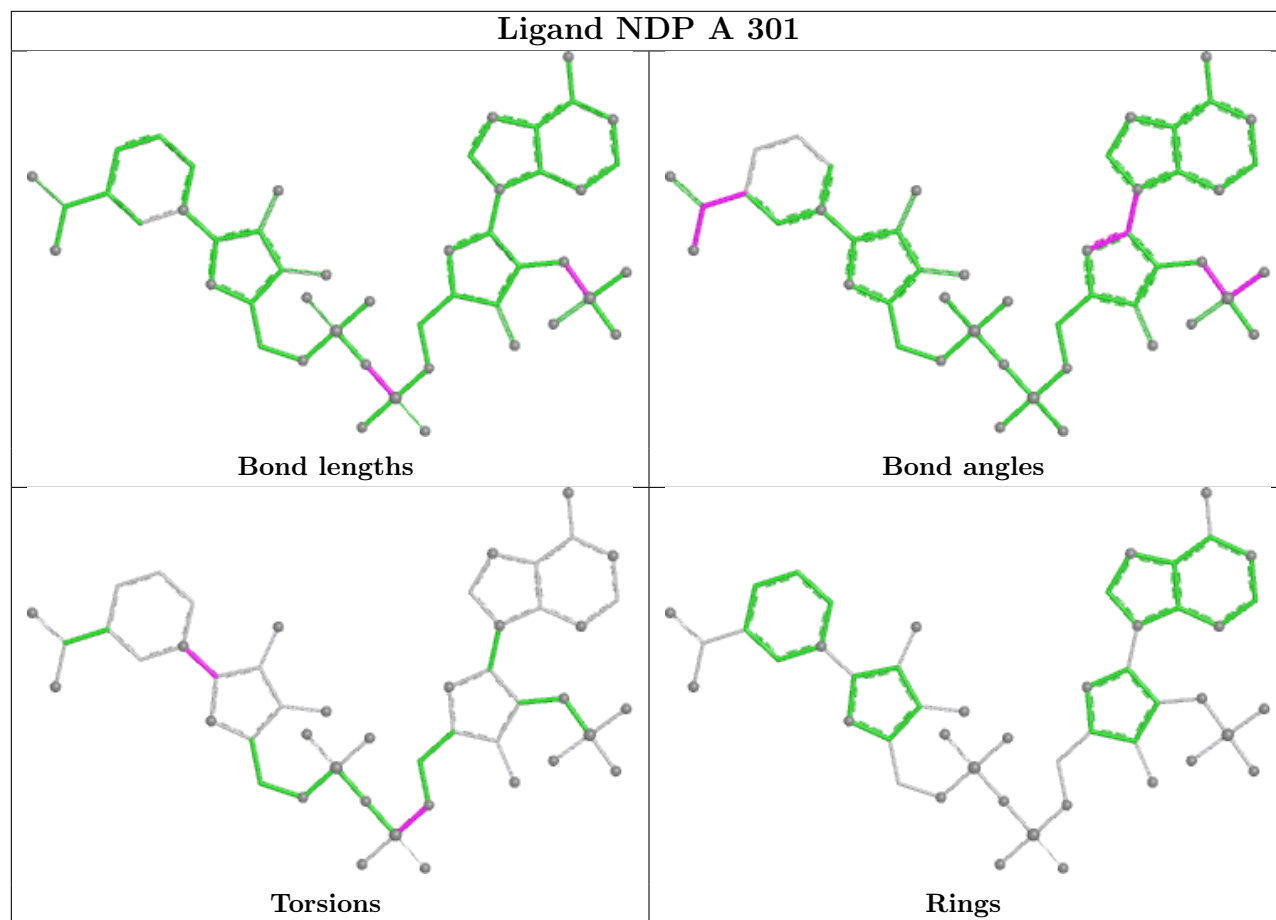
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	302	A1H0V	1	0
2	B	301	NDP	3	0
2	C	301	NDP	2	0
3	A	302	A1H0V	3	0
2	A	301	NDP	3	0
3	D	302	A1H0V	3	0
3	B	302	A1H0V	1	0
2	D	301	NDP	3	0

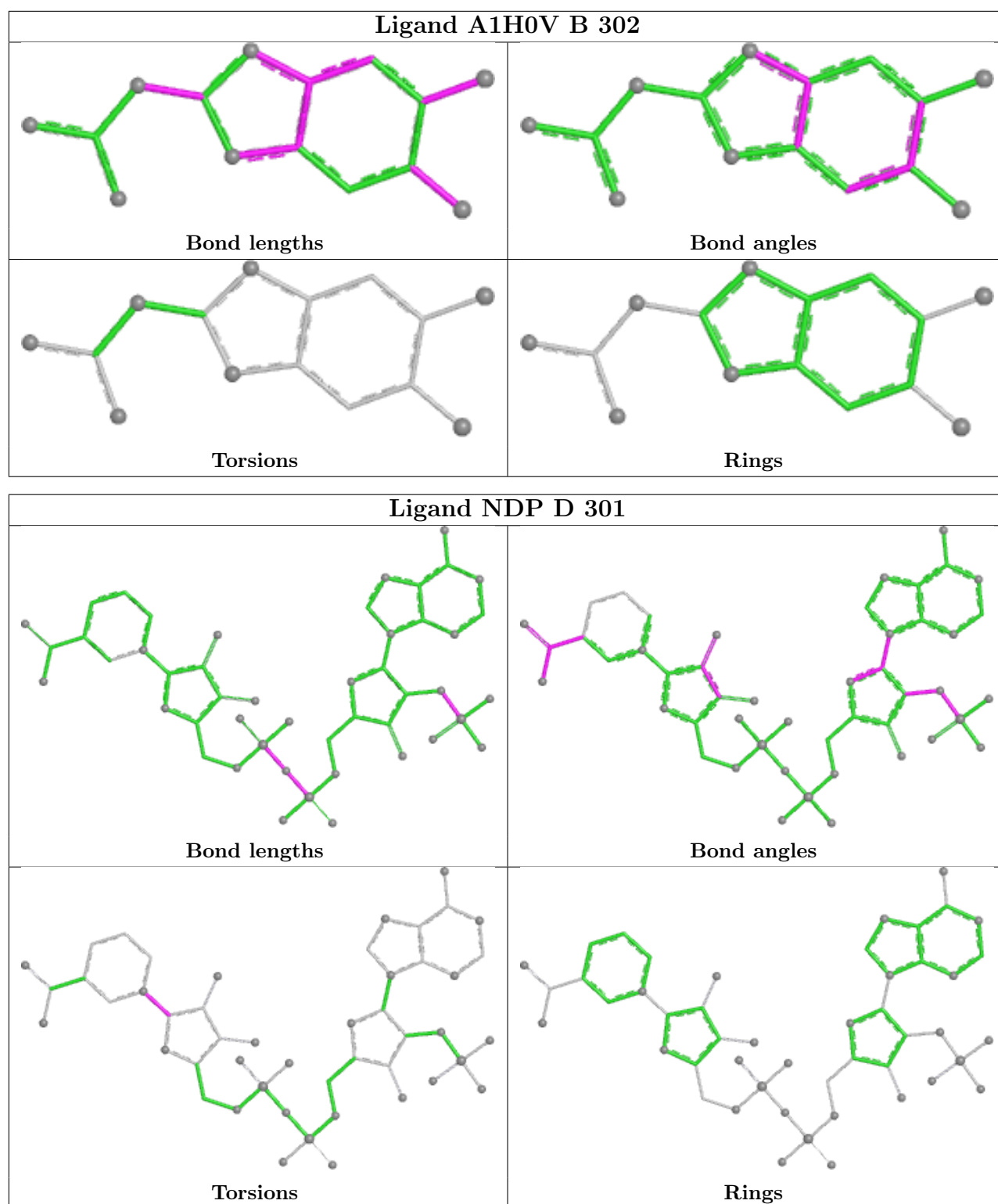
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	251/289 (86%)	-0.22	5 (1%) 65 68	2, 8, 25, 43	10 (3%)
1	B	249/289 (86%)	-0.03	3 (1%) 76 80	2, 10, 26, 45	8 (3%)
1	C	251/289 (86%)	-0.18	3 (1%) 76 80	2, 8, 22, 38	12 (4%)
1	D	250/289 (86%)	-0.22	4 (1%) 70 74	2, 8, 21, 40	15 (6%)
All	All	1001/1156 (86%)	-0.17	15 (1%) 72 76	2, 8, 24, 45	45 (4%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	104	GLN	3.2
1	A	104	GLN	2.8
1	B	212	ALA	2.8
1	D	2	GLU	2.5
1	A	2	GLU	2.4
1	C	195	TYR	2.3
1	C	104	GLN	2.3
1	D	211	VAL	2.3
1	D	210	PRO	2.2
1	C	143	LYS	2.2
1	A	113	GLY	2.1
1	A	212	ALA	2.1
1	B	3	ALA	2.1
1	B	221	TRP	2.0
1	A	211	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

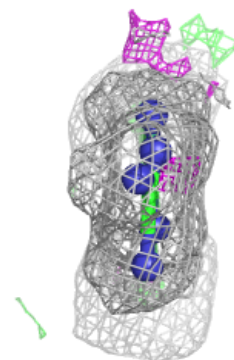
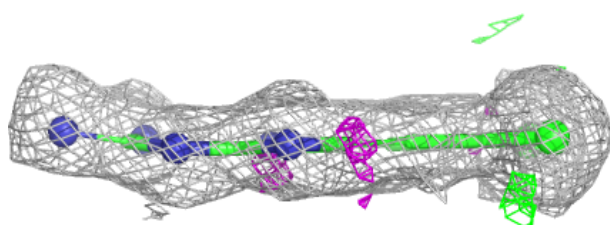
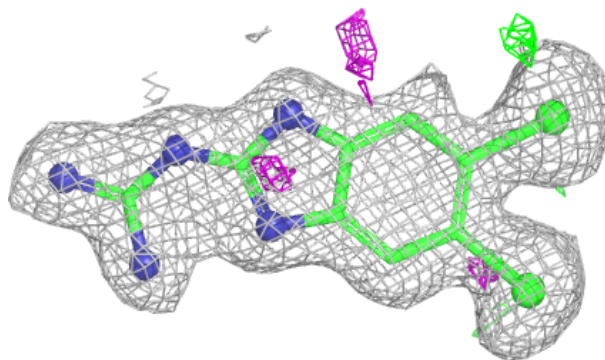
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	A1H0V	A	302	15/15	0.94	0.08	14,18,30,38	0
3	A1H0V	B	302	15/15	0.94	0.08	13,16,33,45	0
2	NDP	D	301	48/48	0.95	0.07	8,13,17,20	0
3	A1H0V	C	302	15/15	0.95	0.07	8,10,18,29	0
3	A1H0V	D	302	15/15	0.95	0.07	14,16,25,28	0
2	NDP	B	301	48/48	0.96	0.06	8,13,16,19	0
2	NDP	C	301	48/48	0.97	0.05	4,9,11,12	0
2	NDP	A	301	48/48	0.97	0.06	9,11,14,15	0

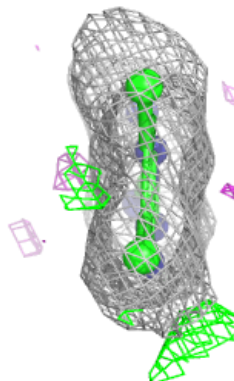
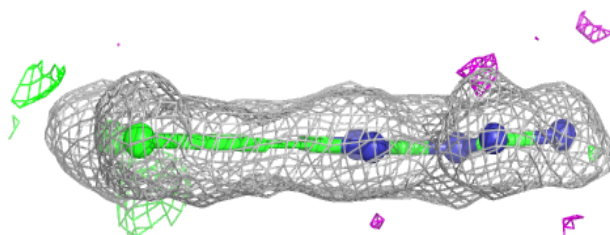
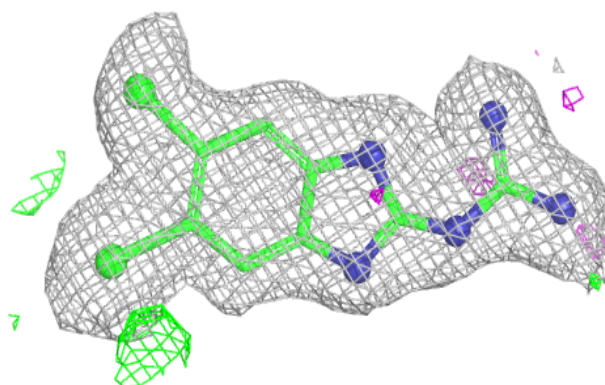
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1H0V 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)

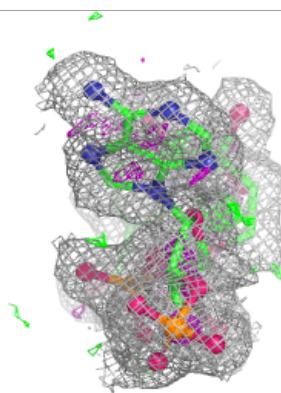
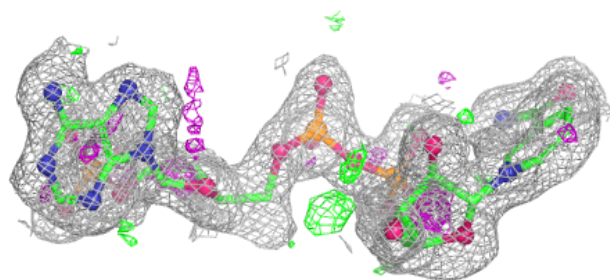
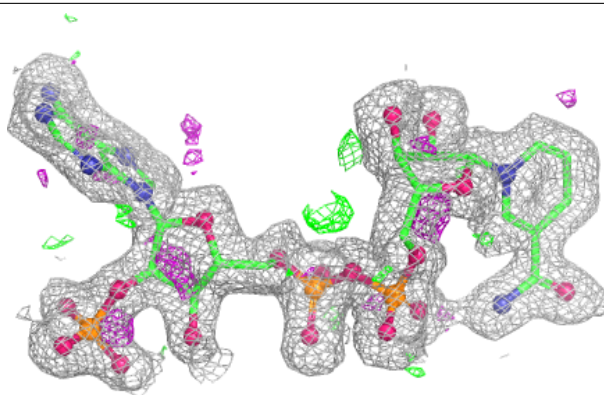
**Electron density around A1H0V B 302:**

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

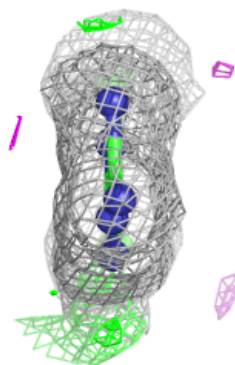
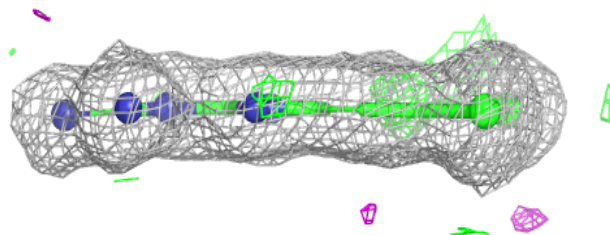
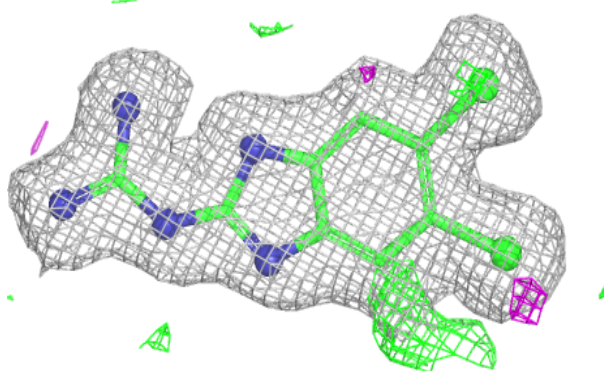


Electron density around NDP D 301:

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

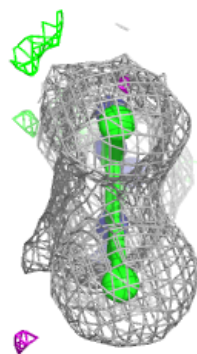
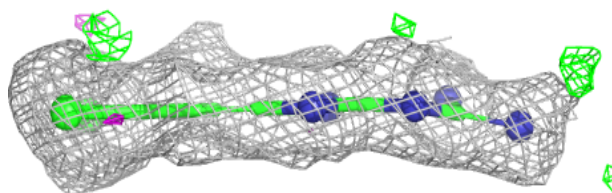
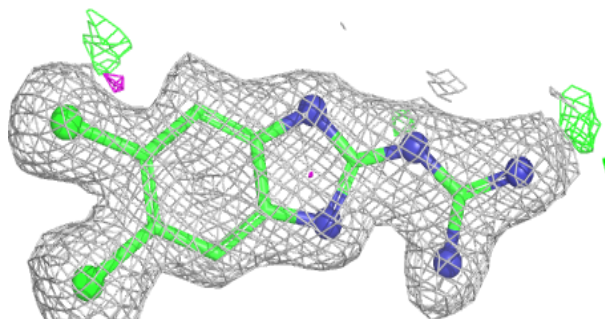
**Electron density around A1H0V C 302:**

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

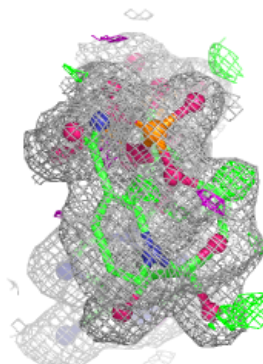
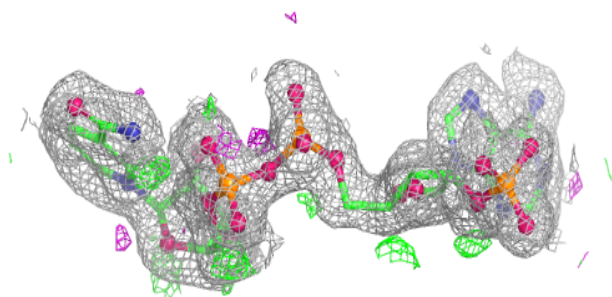
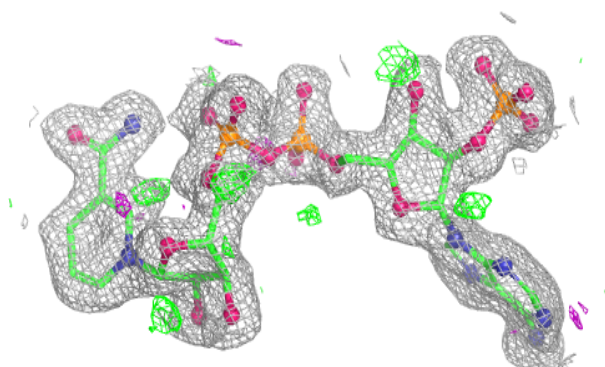


Electron density around A1H0V D 302:

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

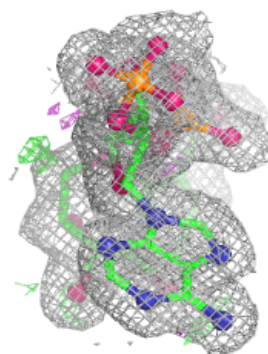
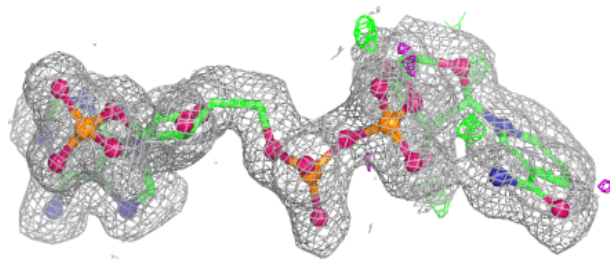
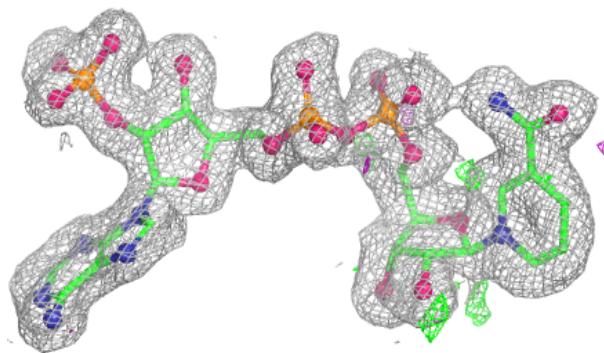
**Electron density around NDP B 301:**

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

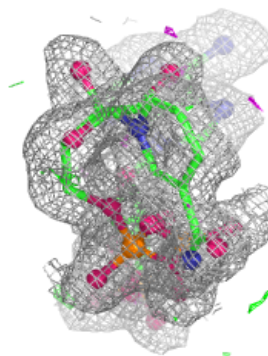
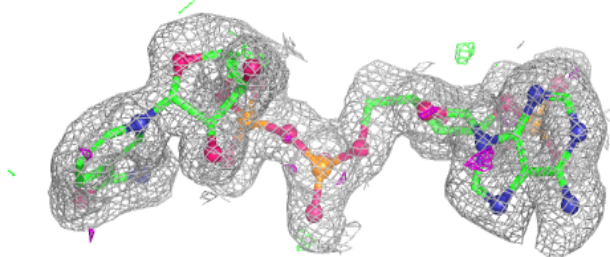
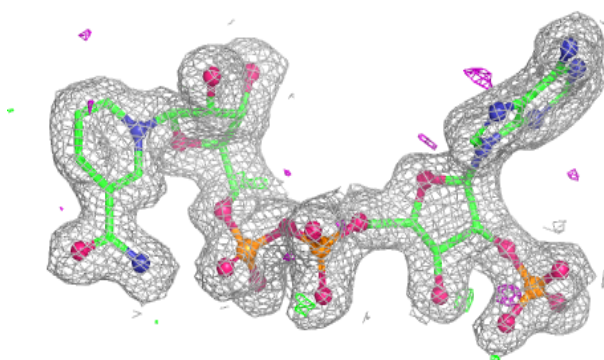


Electron density around NDP C 301:

$2mF_o-DF_c$ (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.