



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2025 – 04:24 am BST

PDB ID : 9HUU / pdb\_00009huu  
Title : Trypanosoma brucei PTR1 (TbPTR1) in complex with inhibitor F223  
Authors : Landi, G.; Pozzi, C.; Mangani, S.  
Deposited on : 2024-12-23  
Resolution : 1.85 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](mailto: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>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

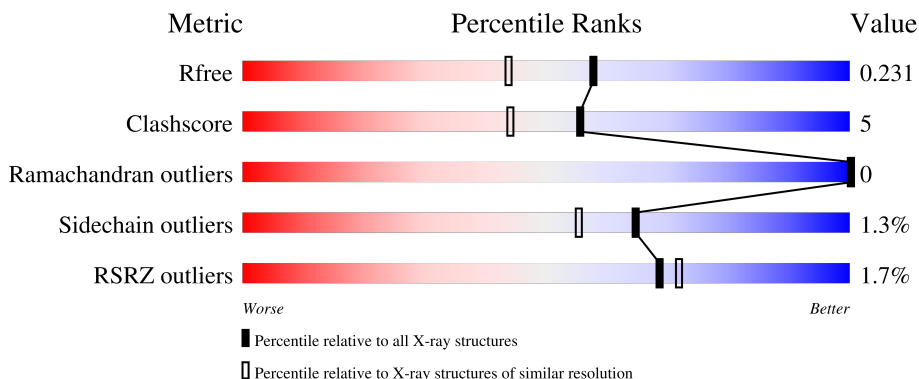
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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))
$R_{free}$	164625	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (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  $\geq 3$ , 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 7 unique types of molecules in this entry. The entry contains 8266 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	2	0
			1865	1170	329	355	11			
1	B	249	Total	C	N	O	S	0	8	0
			1888	1186	328	363	11			
1	C	250	Total	C	N	O	S	0	3	0
			1835	1157	321	346	11			
1	D	250	Total	C	N	O	S	0	5	0
			1864	1174	325	354	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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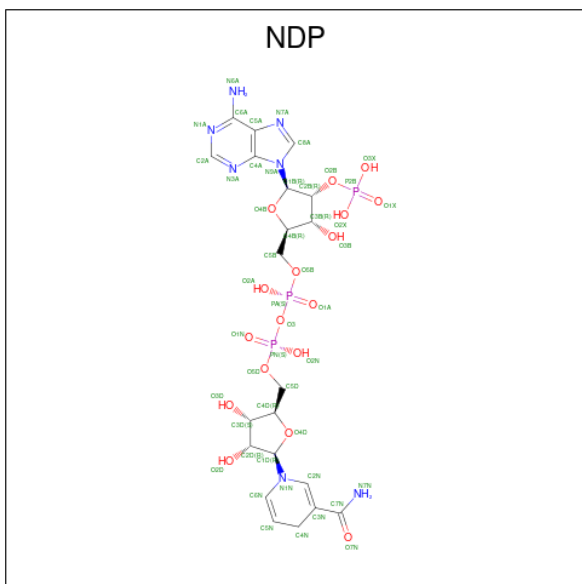
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	initiating methionine	UNP O76290
B	-19	GLY	-	expression tag	UNP O76290
B	-18	SER	-	expression tag	UNP O76290
B	-17	SER	-	expression tag	UNP O76290
B	-16	HIS	-	expression tag	UNP O76290
B	-15	HIS	-	expression tag	UNP O76290
B	-14	HIS	-	expression 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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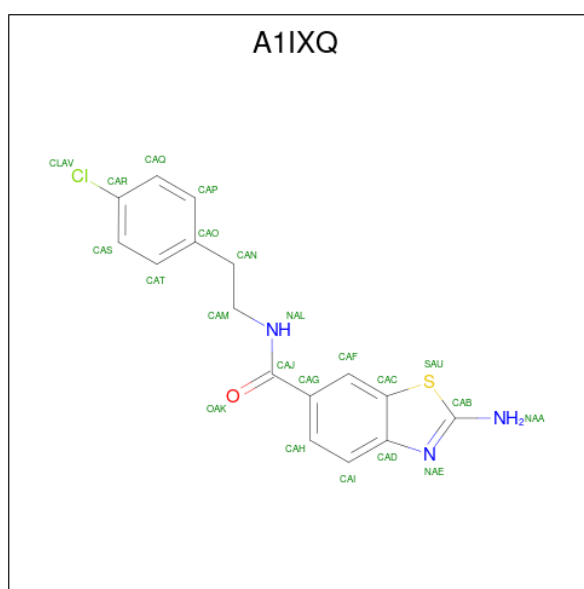
Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	initiating methionine	UNP O76290
D	-19	GLY	-	expression tag	UNP O76290
D	-18	SER	-	expression tag	UNP O76290
D	-17	SER	-	expression tag	UNP O76290
D	-16	HIS	-	expression tag	UNP O76290
D	-15	HIS	-	expression tag	UNP O76290
D	-14	HIS	-	expression 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 2-azanyl- {N}-[2-(4-chlorophenyl)ethyl]-1,3-benzothiazole-6-carboxamide (CCD ID: A1IXQ) (formula: C<sub>16</sub>H<sub>14</sub>ClN<sub>3</sub>OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			22	16	1	3	1	1		
3	B	1	Total	C	Cl	N	O	S	0	0
			22	16	1	3	1	1		
3	D	1	Total	C	Cl	N	O	S	0	0
			22	16	1	3	1	1		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total 1	Cl 1	0	0

- Molecule 7 is water.

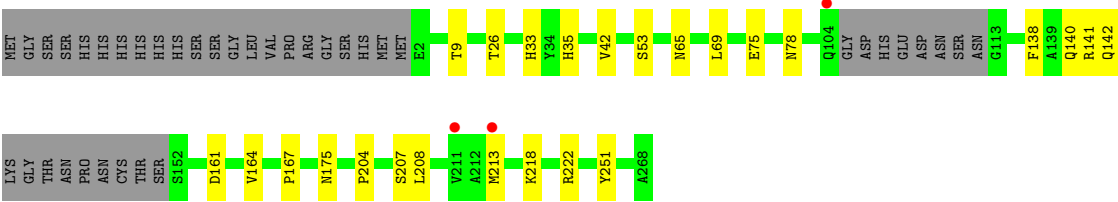
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	142	Total 142	O 142	0	2
7	B	162	Total 162	O 162	0	1
7	C	107	Total 107	O 107	0	1
7	D	128	Total 128	O 128	0	1





- Molecule 1: Pteridine reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.55Å 90.58Å 83.14Å 90.00° 115.62° 90.00°	Depositor
Resolution (Å)	54.04 – 1.85 54.04 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.2 (54.04-1.85) 99.2 (54.04-1.85)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.180 , 0.231 0.181 , 0.231	Depositor DCC
$R_{free}$ test set	4190 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8266	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	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 35.90 % 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 5.4315e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NDP, CSX, ACT, A1IXQ, EDO, CL

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	0.60	0/1887	1.02	1/2562 (0.0%)
1	B	0.63	0/1928	1.01	0/2615
1	C	0.61	0/1860	1.04	1/2529 (0.0%)
1	D	0.60	0/1898	1.03	1/2576 (0.0%)
All	All	0.61	0/7573	1.03	3/10282 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	75	GLU	CB-CG-CD	6.91	124.35	112.60
1	D	75	GLU	CB-CG-CD	5.62	122.16	112.60
1	A	117	GLU	CB-CA-C	-5.57	101.22	110.68

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	1865	0	1867	18	0
1	B	1888	0	1902	19	0
1	C	1835	0	1816	26	0
1	D	1864	0	1875	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	48	0	26	0	0
2	B	48	0	26	2	0
2	C	48	0	26	3	0
2	D	48	0	26	2	0
3	A	22	0	0	1	0
3	B	22	0	0	1	0
3	D	22	0	0	0	0
4	A	4	0	3	0	0
5	A	8	0	12	3	0
5	D	4	0	6	0	0
6	C	1	0	0	1	0
7	A	142	0	0	3	0
7	B	162	0	0	1	0
7	C	107	0	0	0	0
7	D	128	0	0	0	0
All	All	8266	0	7585	70	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 (70) 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:78:ASN:OD1	1:C:141:ARG:NH1	2.22	0.71
1:D:167:PRO:HB3	1:D:175[B]:ASN:ND2	2.07	0.70
1:C:167:PRO:HB3	1:C:175[B]:ASN:ND2	2.07	0.69
1:C:65:ASN:HA	1:C:69:LEU:HD12	1.75	0.68
1:C:164:VAL:HG22	1:C:179:HIS:CD2	2.29	0.66
1:C:223:ARG:O	1:C:229:ARG:NH1	2.24	0.65
1:C:232:ALA:HB2	1:D:251:TYR:CE2	2.34	0.62
1:B:2[A]:GLU:HA	1:B:2[A]:GLU:OE1	2.00	0.61
5:A:304:EDO:H11	1:B:258:LYS:HE2	1.81	0.61
2:B:301:NDP:H41N	3:B:302:A1IXQ:CAH	2.31	0.60
1:C:95:SER:HB3	2:C:301:NDP:H3D	1.82	0.60
1:A:161:ASP:HB3	1:A:164:VAL:HG13	1.83	0.60
1:A:65:ASN:HA	1:A:69:LEU:HD22	1.84	0.59
1:C:123:LEU:O	1:C:127:ASN:HB2	2.03	0.58
7:A:485:HOH:O	1:C:169:MET:HE1	2.04	0.57
1:A:22:LYS:HG2	1:A:242:ILE:HG13	1.86	0.57
1:D:65:ASN:HA	1:D:69:LEU:HD22	1.89	0.54
1:D:161:ASP:HB3	1:D:164:VAL:HG13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:ALA:O	1:C:125:GLY:HA3	2.08	0.54
1:D:78:ASN:OD1	1:D:141:ARG:NH1	2.43	0.52
1:A:9:THR:HA	1:A:33:HIS:HB3	1.92	0.51
1:B:2[A]:GLU:OE1	1:B:2[A]:GLU:CA	2.58	0.51
1:A:251:TYR:CE2	1:B:232:ALA:HB2	2.47	0.50
1:C:193:ALA:N	1:C:194:PRO:CD	2.74	0.50
1:C:64:THR:O	1:C:69:LEU:HG	2.13	0.49
1:A:2:GLU:HA	7:A:478:HOH:O	2.12	0.48
1:A:232:ALA:HB2	1:B:251:TYR:CE2	2.48	0.48
1:B:218:LYS:O	1:B:222:ARG:HG3	2.13	0.48
1:B:69:LEU:HB3	1:B:70:PRO:HD3	1.96	0.48
1:C:205:GLY:O	2:C:301:NDP:H42N	2.14	0.47
1:C:9:THR:HA	1:C:33:HIS:HB3	1.96	0.47
1:B:138:PHE:O	1:B:142:GLN:HG2	2.15	0.47
1:C:218:LYS:O	1:C:222:ARG:HG3	2.15	0.47
1:D:218:LYS:O	1:D:222:ARG:HG3	2.15	0.46
1:A:136:MET:HG2	1:C:102:LEU:HD23	1.97	0.46
1:C:38:ALA:O	1:C:42:VAL:HG23	2.15	0.46
1:B:193:ALA:N	1:B:194:PRO:CD	2.79	0.46
1:C:69:LEU:N	1:C:70:PRO:CD	2.79	0.45
1:D:204:PRO:HB2	2:D:301:NDP:H42N	1.97	0.45
1:C:117:GLU:HB2	6:C:302:CL:CL	2.53	0.45
1:D:26:THR:O	1:D:26:THR:HG22	2.16	0.45
1:B:117:GLU:H	1:B:117:GLU:CD	2.24	0.44
1:D:9:THR:HA	1:D:33:HIS:HB3	1.99	0.44
1:B:115:THR:HB	1:B:117:GLU:OE2	2.17	0.44
1:B:69:LEU:N	1:B:70:PRO:CD	2.80	0.44
1:A:72:SER:HA	5:A:305:EDO:H22	2.00	0.44
1:B:65:ASN:HA	1:B:69:LEU:HD22	2.00	0.44
1:A:250:GLN:HG3	1:B:236:GLN:HE21	1.82	0.44
1:C:138:PHE:O	1:C:142:GLN:HG2	2.18	0.43
1:C:116[B]:VAL:O	1:C:119:GLN:HB2	2.18	0.43
1:D:138:PHE:O	1:D:142:GLN:HG2	2.19	0.43
1:C:126:THR:HG21	2:C:301:NDP:N6A	2.33	0.43
1:B:35:HIS:HB2	2:B:301:NDP:C2A	2.49	0.43
1:C:230:ARG:HH12	1:C:236:GLN:HE22	1.67	0.43
1:D:207:SER:O	1:D:208:LEU:C	2.62	0.42
1:A:250:GLN:HG3	1:B:236:GLN:NE2	2.34	0.42
1:C:232:ALA:HB2	1:D:251:TYR:CD2	2.53	0.42
1:A:152:SER:N	7:A:412:HOH:O	2.52	0.41
1:C:75:GLU:O	1:C:78:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:HIS:HB2	2:D:301:NDP:C2A	2.50	0.41
1:A:69:LEU:N	1:A:70:PRO:CD	2.82	0.41
1:A:210:PRO:HG2	3:A:302:A1IXQ:CAS	2.50	0.41
1:A:61:ALA:HB2	5:A:305:EDO:H21	2.03	0.41
1:A:128:ALA:C	1:A:131:PRO:HD2	2.45	0.41
1:A:250:GLN:HG2	7:B:428:HOH:O	2.19	0.41
1:B:9:THR:HA	1:B:33:HIS:HB3	2.03	0.40
1:B:130:ALA:HB3	1:B:131:PRO:HD3	2.03	0.40
1:C:98:TYR:HB2	1:C:99:PRO:HD2	2.02	0.40
1:A:225:VAL:O	1:A:229:ARG:HD3	2.22	0.40
1:B:136:MET:HE2	1:B:136:MET:HB3	1.89	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/289 (85%)	237 (96%)	9 (4%)	0	100	100
1	B	249/289 (86%)	240 (96%)	9 (4%)	0	100	100
1	C	246/289 (85%)	236 (96%)	10 (4%)	0	100	100
1	D	247/289 (86%)	240 (97%)	7 (3%)	0	100	100
All	All	988/1156 (86%)	953 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	195/231 (84%)	193 (99%)	2 (1%)	73	67
1	B	201/231 (87%)	200 (100%)	1 (0%)	86	84
1	C	185/231 (80%)	182 (98%)	3 (2%)	58	46
1	D	195/231 (84%)	191 (98%)	4 (2%)	48	34
All	All	776/924 (84%)	766 (99%)	10 (1%)	65	55

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	209	LEU
1	A	217	GLU
1	B	117	GLU
1	C	69	LEU
1	C	95	SER
1	C	140	GLN
1	D	42	VAL
1	D	53	SER
1	D	140	GLN
1	D	213	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	36	ASN
1	A	65	ASN
1	A	92	ASN
1	A	127	ASN
1	A	140	GLN
1	A	250	GLN
1	B	65	ASN
1	B	92	ASN
1	B	186	GLN
1	B	236	GLN
1	C	65	ASN
1	C	92	ASN
1	C	127	ASN
1	D	65	ASN

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Mol	Chain	Res	Type
1	D	92	ASN
1	D	127	ASN
1	D	186	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	B	168	1	3,6,7	0.56	0	1,6,8	0.96	0
1	CSX	D	168	1	3,6,7	0.66	0	1,6,8	0.69	0
1	CSX	A	168	1	3,6,7	0.69	0	1,6,8	0.83	0
1	CSX	C	168	1	3,6,7	0.72	0	1,6,8	1.39	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	1	-	0/1/5/7	-
1	CSX	D	168	1	-	0/1/5/7	-
1	CSX	A	168	1	-	0/1/5/7	-
1	CSX	C	168	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

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](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	ACT	A	303	-	3,3,3	1.25	0	3,3,3	0.90	0
5	EDO	D	303	-	3,3,3	0.15	0	2,2,2	0.12	0
3	A1IXQ	A	302	-	21,24,24	2.06	4 (19%)	28,33,33	1.33	4 (14%)
5	EDO	A	305	-	3,3,3	0.31	0	2,2,2	1.12	0
2	NDP	B	301	-	45,52,52	0.85	1 (2%)	53,80,80	0.87	1 (1%)
2	NDP	A	301	-	45,52,52	0.73	1 (2%)	53,80,80	0.84	1 (1%)
3	A1IXQ	B	302	-	21,24,24	2.00	5 (23%)	28,33,33	1.24	4 (14%)
2	NDP	D	301	-	45,52,52	0.81	1 (2%)	53,80,80	0.99	2 (3%)
5	EDO	A	304	-	3,3,3	0.23	0	2,2,2	0.65	0
2	NDP	C	301	-	45,52,52	0.71	1 (2%)	53,80,80	0.85	1 (1%)
3	A1IXQ	D	302	-	21,24,24	2.07	4 (19%)	28,33,33	1.34	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	D	303	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1IXQ	A	302	-	-	3/10/10/10	0/3/3/3
5	EDO	A	305	-	-	1/1/1/1	-
2	NDP	B	301	-	-	1/30/77/77	0/5/5/5
2	NDP	A	301	-	-	1/30/77/77	0/5/5/5
3	A1IXQ	B	302	-	-	3/10/10/10	0/3/3/3
2	NDP	D	301	-	-	3/30/77/77	0/5/5/5
5	EDO	A	304	-	-	0/1/1/1	-
2	NDP	C	301	-	-	2/30/77/77	0/5/5/5
3	A1IXQ	D	302	-	-	0/10/10/10	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	A1IXQ	CAG-CAJ	-5.44	1.38	1.50
3	A	302	A1IXQ	CAI-CAD	-5.29	1.32	1.41
3	D	302	A1IXQ	CAG-CAJ	-5.16	1.39	1.50
3	D	302	A1IXQ	CAI-CAD	-5.06	1.33	1.41
3	B	302	A1IXQ	CAG-CAJ	-5.01	1.39	1.50
3	B	302	A1IXQ	CAI-CAD	-4.96	1.33	1.41
3	D	302	A1IXQ	CAN-CAO	-4.57	1.38	1.51
3	B	302	A1IXQ	CAN-CAO	-4.34	1.39	1.51
3	A	302	A1IXQ	CAN-CAO	-3.95	1.40	1.51
2	B	301	NDP	P2B-O2B	3.29	1.65	1.59
2	D	301	NDP	P2B-O2B	3.21	1.65	1.59
2	A	301	NDP	P2B-O2B	2.76	1.64	1.59
3	A	302	A1IXQ	CAD-CAC	-2.28	1.34	1.42
2	C	301	NDP	P2B-O2B	2.27	1.63	1.59
3	B	302	A1IXQ	CAD-CAC	-2.23	1.35	1.42
3	D	302	A1IXQ	CAD-CAC	-2.21	1.35	1.42
3	B	302	A1IXQ	CAF-CAC	-2.00	1.33	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	A1IXQ	CAD-CAC-SAU	-3.48	107.24	111.85
3	D	302	A1IXQ	CAF-CAC-SAU	3.19	131.48	125.10
3	A	302	A1IXQ	CAF-CAC-SAU	3.18	131.47	125.10
3	A	302	A1IXQ	CAI-CAH-CAG	-3.12	117.26	120.79
3	A	302	A1IXQ	CAD-CAC-SAU	-3.11	107.73	111.85
3	B	302	A1IXQ	CAD-CAC-SAU	-2.99	107.89	111.85
3	B	302	A1IXQ	CAF-CAC-SAU	2.89	130.87	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NDP	C5A-C6A-N6A	2.69	124.44	120.35
2	B	301	NDP	C5A-C6A-N6A	2.66	124.39	120.35
3	D	302	A1IXQ	CAI-CAH-CAG	-2.51	117.95	120.79
3	A	302	A1IXQ	CAC-CAD-NAE	2.51	113.88	108.04
2	C	301	NDP	C5A-C6A-N6A	2.42	124.04	120.35
3	B	302	A1IXQ	CAI-CAH-CAG	-2.36	118.12	120.79
2	D	301	NDP	C1B-N9A-C4A	-2.28	122.63	126.64
3	D	302	A1IXQ	CAC-CAD-NAE	2.25	113.29	108.04
3	B	302	A1IXQ	CAC-CAD-NAE	2.05	112.82	108.04
2	A	301	NDP	O2D-C2D-C3D	2.03	118.38	111.82
3	D	302	A1IXQ	CAM-CAN-CAO	-2.02	108.18	112.87

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	NDP	O4D-C1D-N1N-C6N
2	C	301	NDP	C2N-C3N-C7N-N7N
2	B	301	NDP	O4D-C1D-N1N-C6N
3	B	302	A1IXQ	CAN-CAM-NAL-CAJ
2	A	301	NDP	O4D-C1D-N1N-C6N
5	D	303	EDO	O1-C1-C2-O2
3	A	302	A1IXQ	CAM-CAN-CAO-CAT
3	A	302	A1IXQ	CAM-CAN-CAO-CAP
2	D	301	NDP	O4D-C1D-N1N-C6N
3	B	302	A1IXQ	CAM-CAN-CAO-CAP
3	B	302	A1IXQ	CAM-CAN-CAO-CAT
5	A	305	EDO	O1-C1-C2-O2
3	A	302	A1IXQ	CAN-CAM-NAL-CAJ
2	D	301	NDP	C5B-O5B-PA-O1A
2	D	301	NDP	C2N-C3N-C7N-N7N

There are no ring outliers.

7 monomers are involved in 11 short contacts:

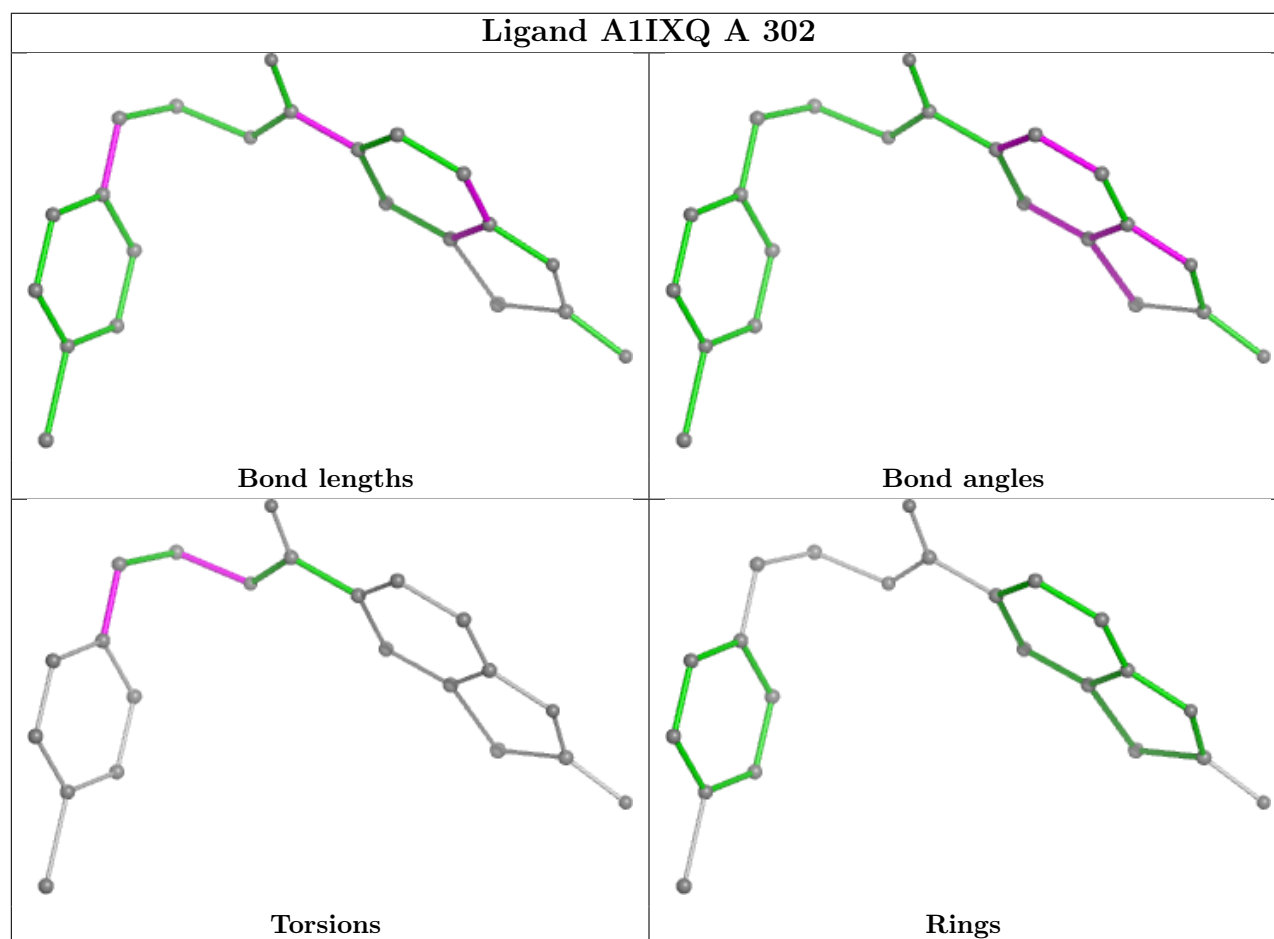
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	A1IXQ	1	0
5	A	305	EDO	2	0
2	B	301	NDP	2	0
3	B	302	A1IXQ	1	0
2	D	301	NDP	2	0

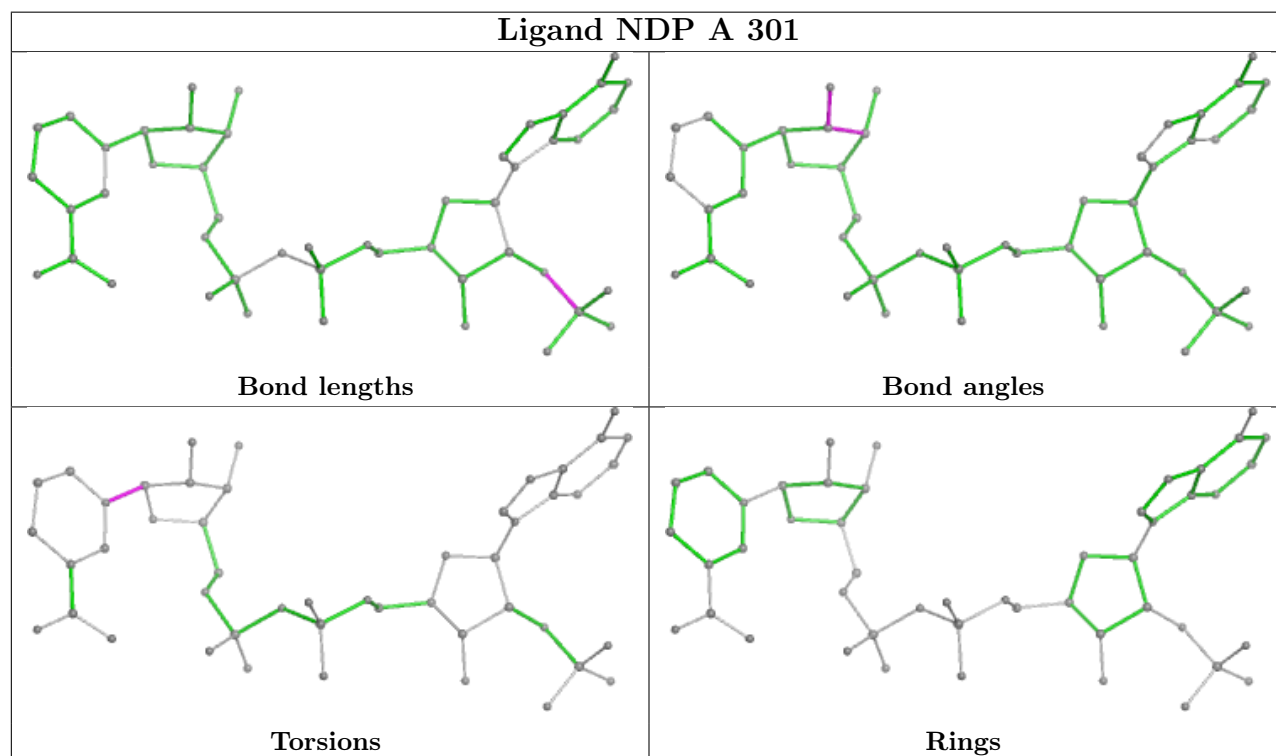
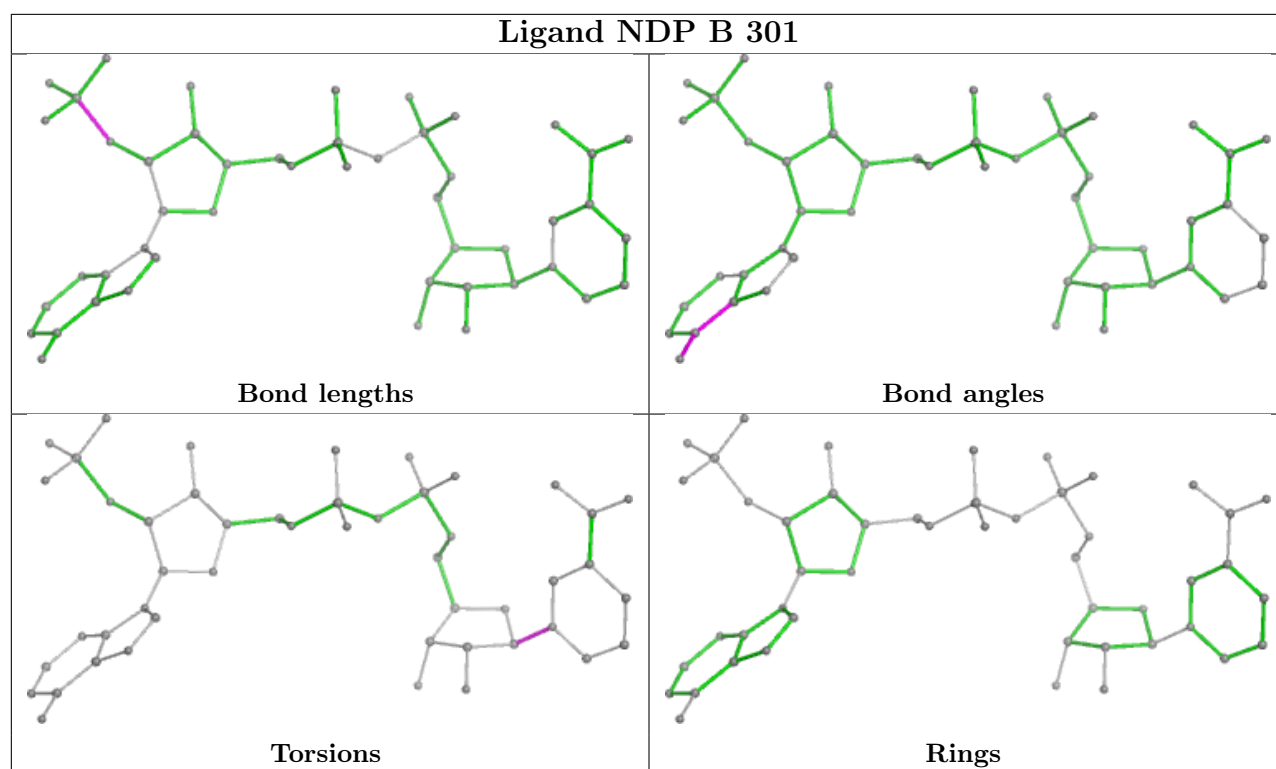
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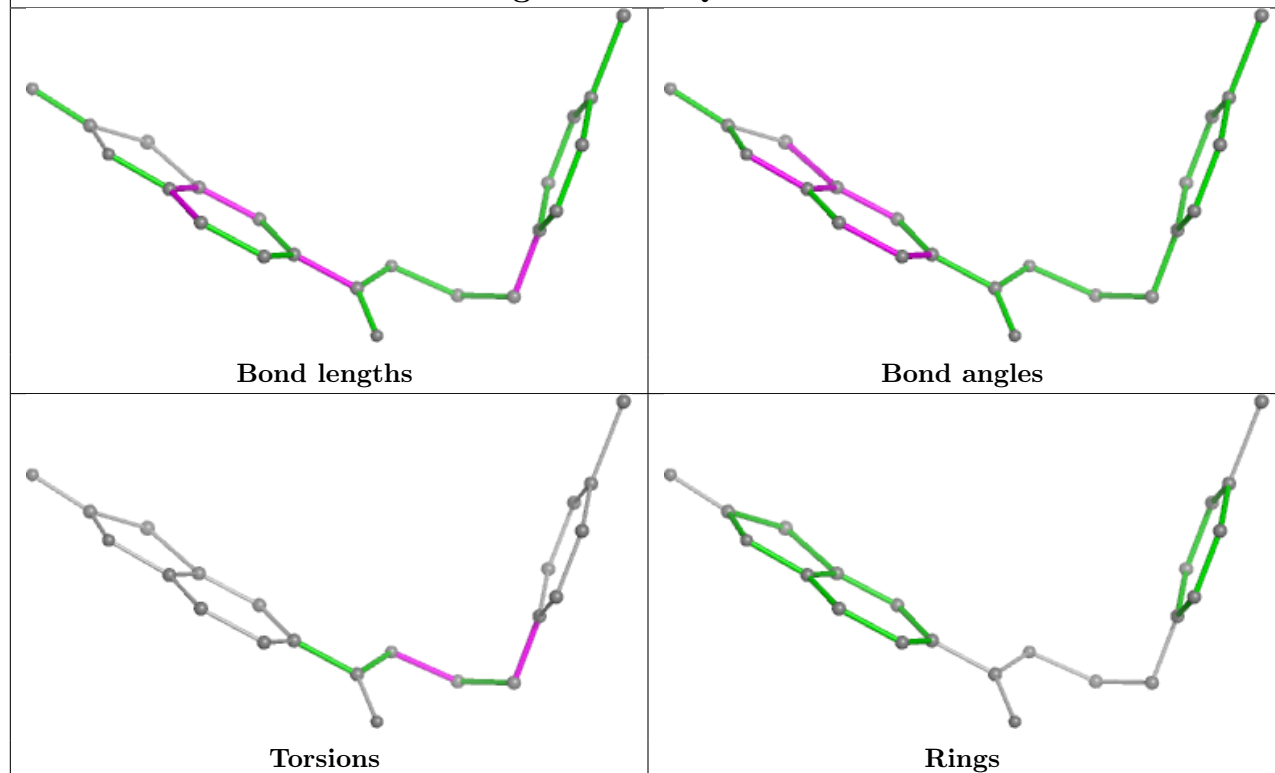
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	304	EDO	1	0
2	C	301	NDP	3	0

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.

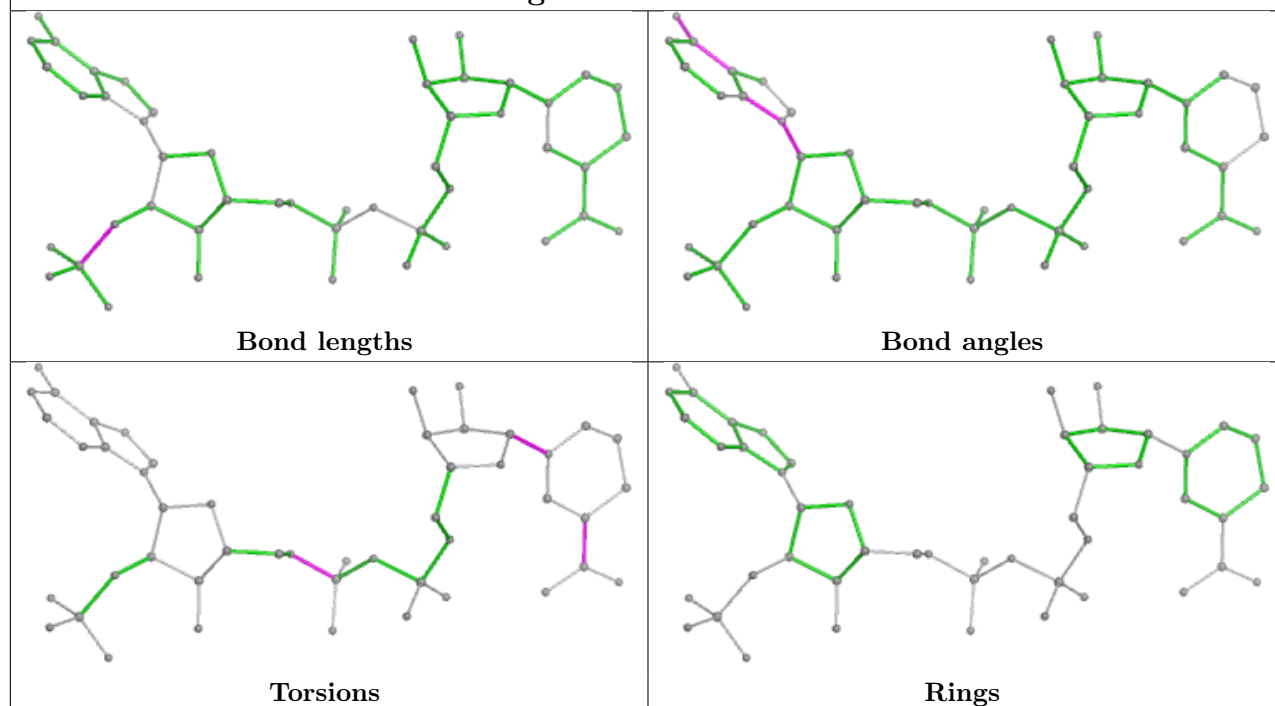


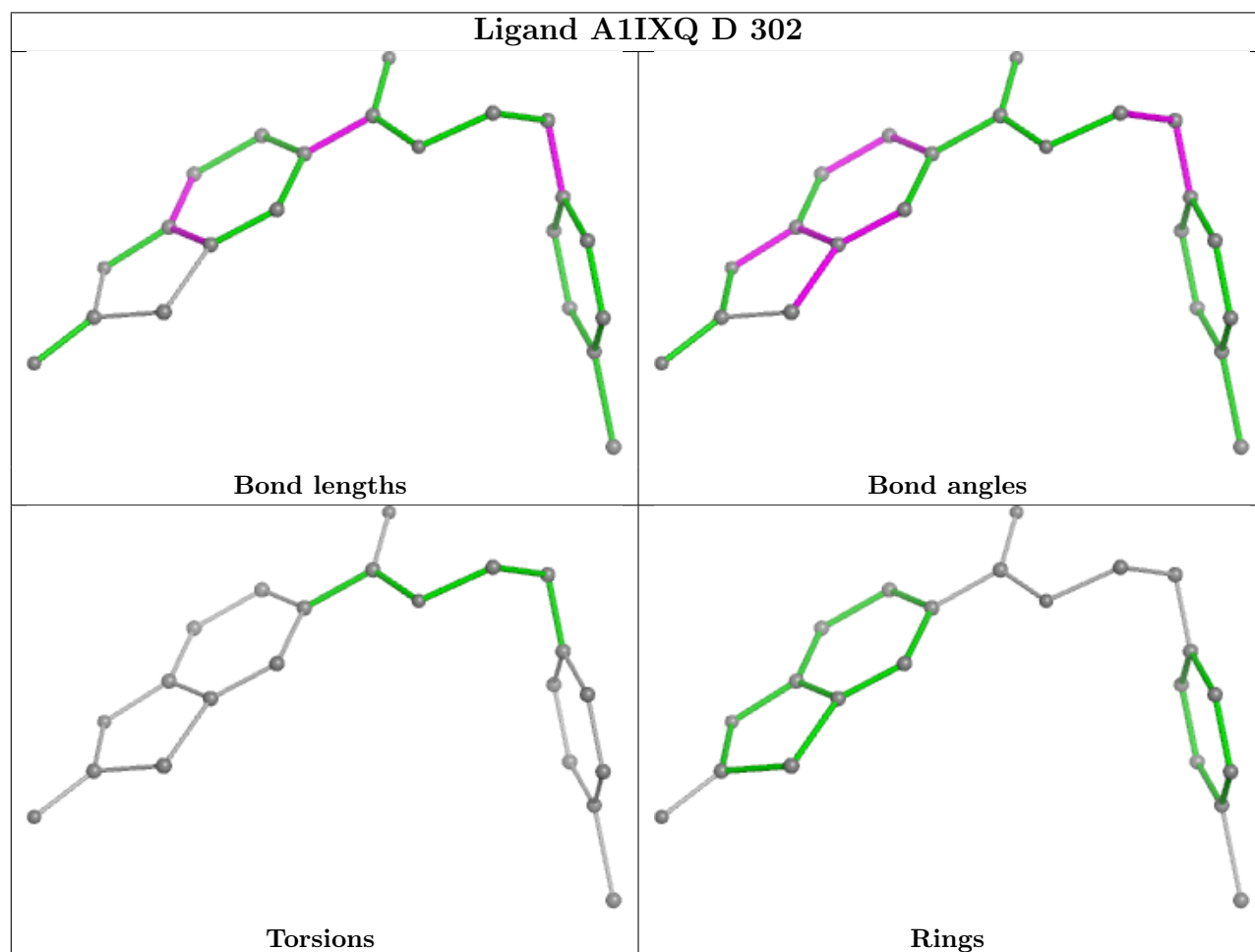
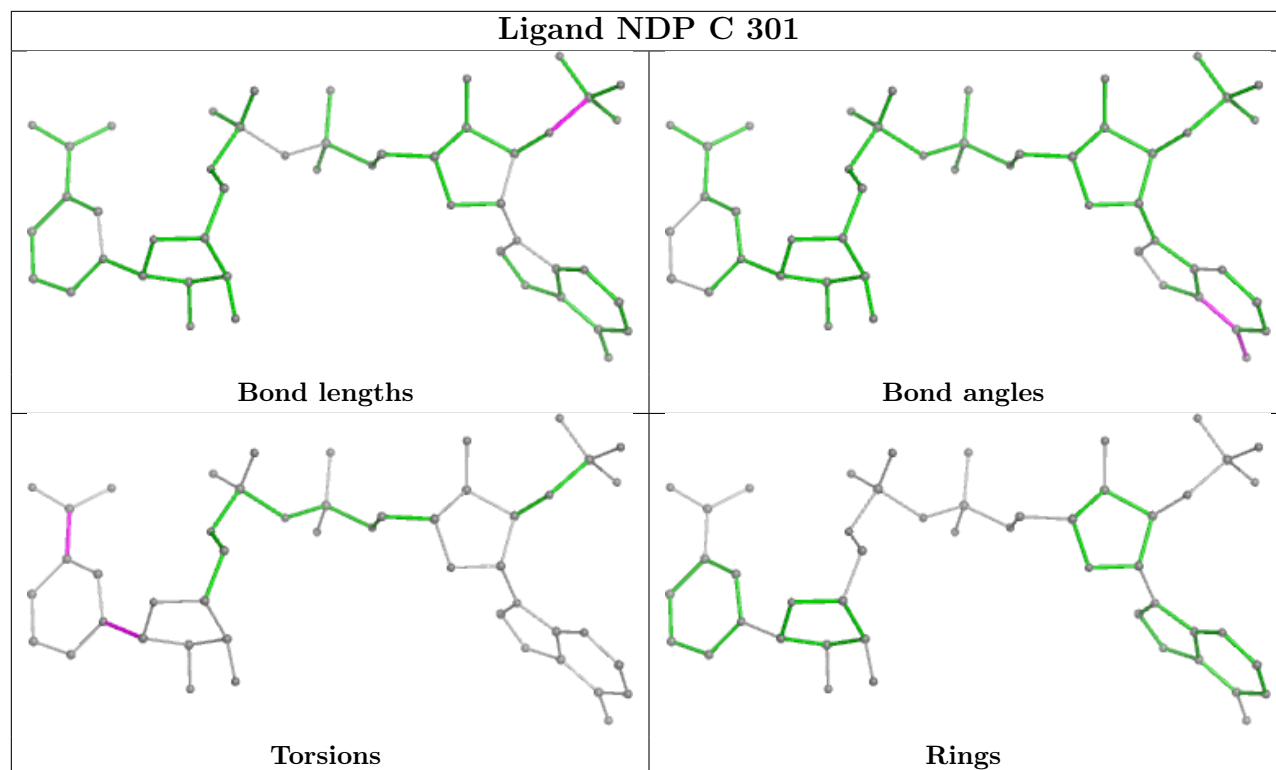


## Ligand A1IXQ B 302



## Ligand NDP D 301







## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	250/289 (86%)	-0.29	1 (0%) 89 91	11, 27, 49, 72	8 (3%)
1	B	248/289 (85%)	-0.32	1 (0%) 89 91	11, 25, 40, 67	18 (7%)
1	C	249/289 (86%)	0.31	12 (4%) 36 39	12, 31, 59, 93	18 (7%)
1	D	249/289 (86%)	-0.13	3 (1%) 76 79	11, 28, 51, 78	10 (4%)
All	All	996/1156 (86%)	-0.11	17 (1%) 69 72	11, 28, 50, 93	54 (5%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	209	LEU	3.4
1	C	213	MET	3.2
1	C	116[A]	VAL	2.9
1	C	208	LEU	2.8
1	C	2	GLU	2.4
1	D	211	VAL	2.4
1	D	213	MET	2.4
1	D	104	GLN	2.3
1	C	113	GLY	2.2
1	C	64	THR	2.1
1	B	211	VAL	2.1
1	C	103	VAL	2.1
1	C	151	SER	2.1
1	A	104	GLN	2.1
1	C	212	ALA	2.1
1	C	37	SER	2.0
1	C	42	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	CSX	A	168	7/8	0.93	0.08	26,28,52,53	0
1	CSX	C	168	7/8	0.94	0.07	24,28,49,52	0
1	CSX	B	168	7/8	0.95	0.07	24,26,41,42	0
1	CSX	D	168	7/8	0.97	0.06	25,28,47,47	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

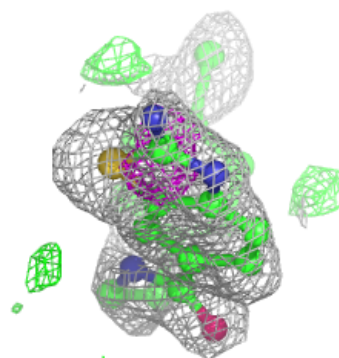
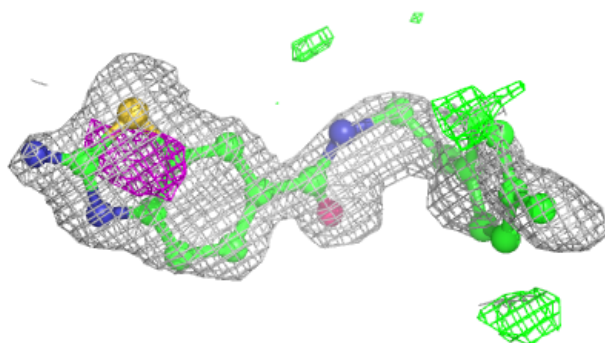
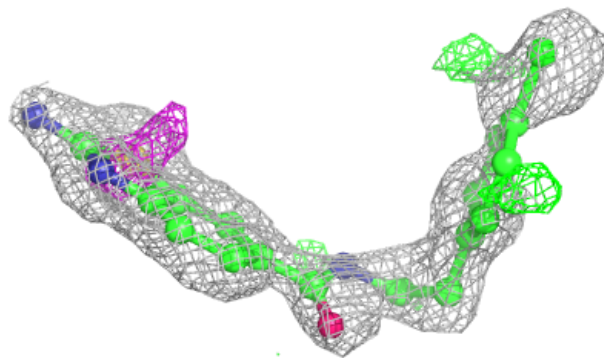
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	EDO	D	303	4/4	0.82	0.16	39,45,45,47	0
3	A1IXQ	B	302	22/22	0.84	0.19	33,45,68,69	22
3	A1IXQ	D	302	22/22	0.84	0.18	41,51,71,79	8
3	A1IXQ	A	302	22/22	0.84	0.17	34,49,64,66	9
5	EDO	A	305	4/4	0.85	0.14	37,45,49,52	0
2	NDP	C	301	48/48	0.85	0.15	28,35,43,48	48
5	EDO	A	304	4/4	0.88	0.15	30,39,41,45	0
6	CL	C	302	1/1	0.88	0.19	60,60,60,60	1
4	ACT	A	303	4/4	0.92	0.10	30,32,32,32	0
2	NDP	B	301	48/48	0.94	0.09	20,29,33,35	48
2	NDP	D	301	48/48	0.94	0.07	25,33,40,46	0
2	NDP	A	301	48/48	0.96	0.07	24,31,35,39	0

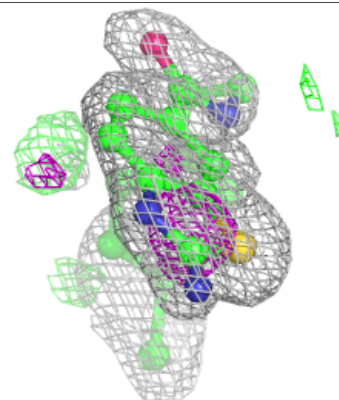
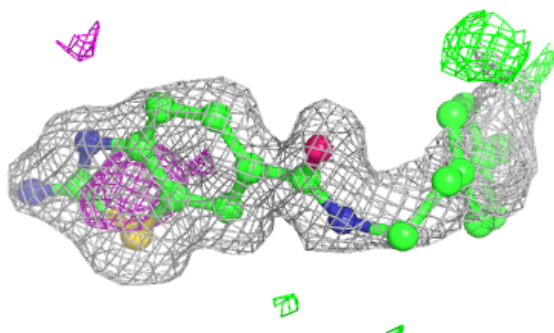
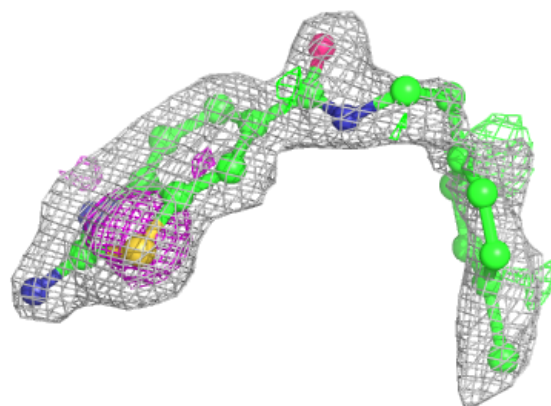
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A1IXQ 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)

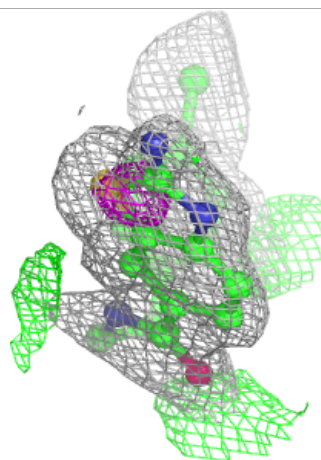
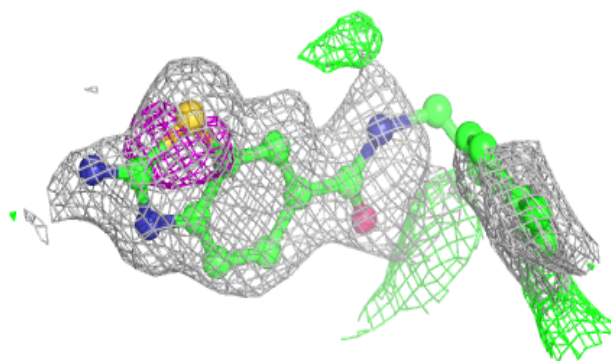
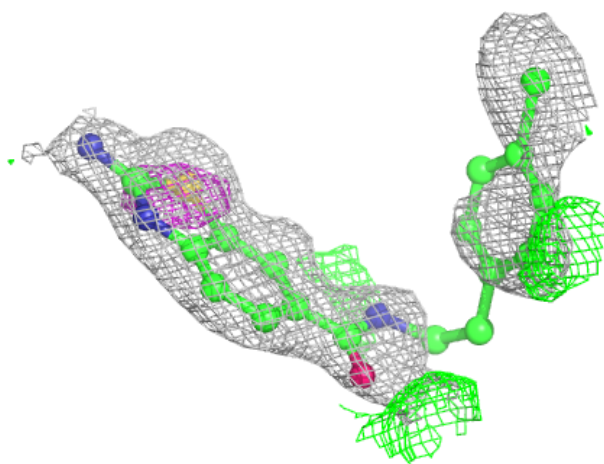
**Electron density around A1IXQ D 302:**

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



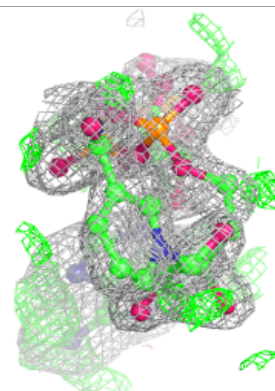
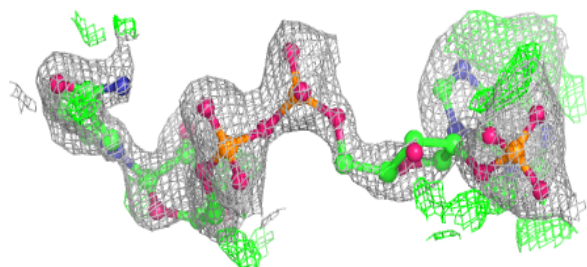
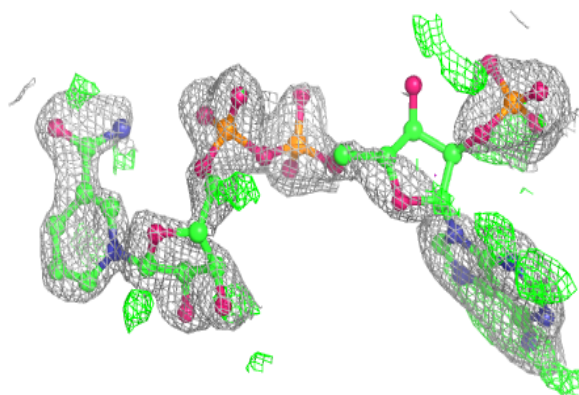
**Electron density around A1IXQ A 302:**

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

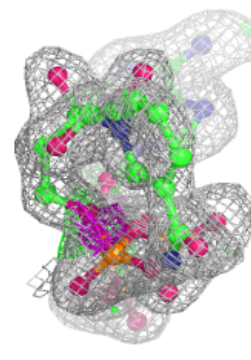
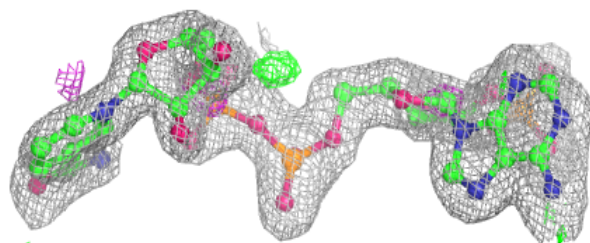
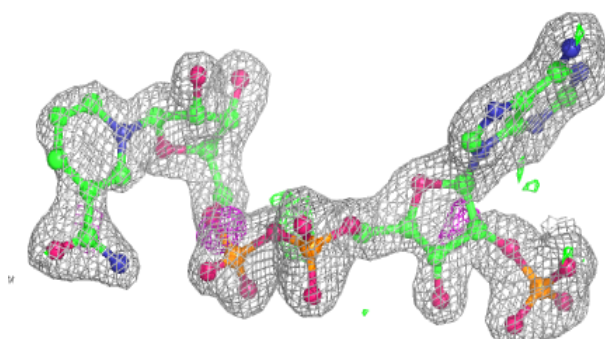


**Electron density around NDP C 301:**

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

**Electron density around NDP B 301:**

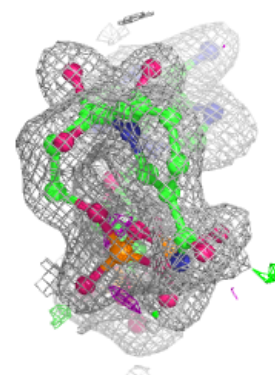
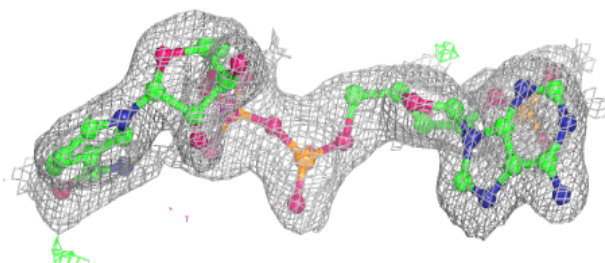
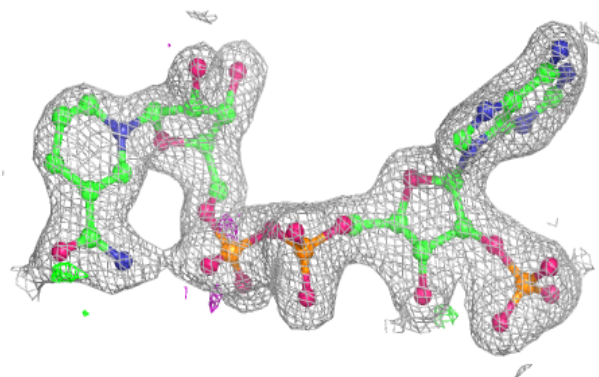
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



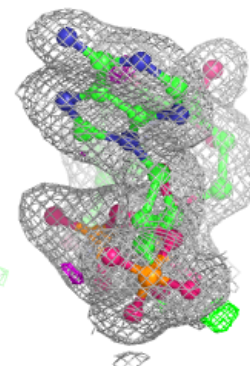
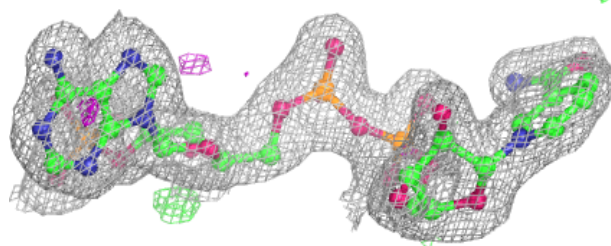
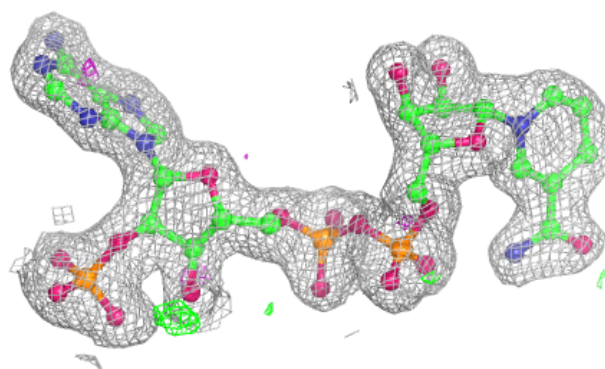


**Electron density around NDP D 301:**

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

**Electron density around 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.