



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:03 PM UTC

PDB ID : 9HUP / pdb_00009hup
Title : Trypanosoma brucei PTR1 (TbPTR1) in complex with inhibitor F194
Authors : Landi, G.; Pozzi, C.; Mangani, S.
Deposited on : 2024-12-23
Resolution : 1.76 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

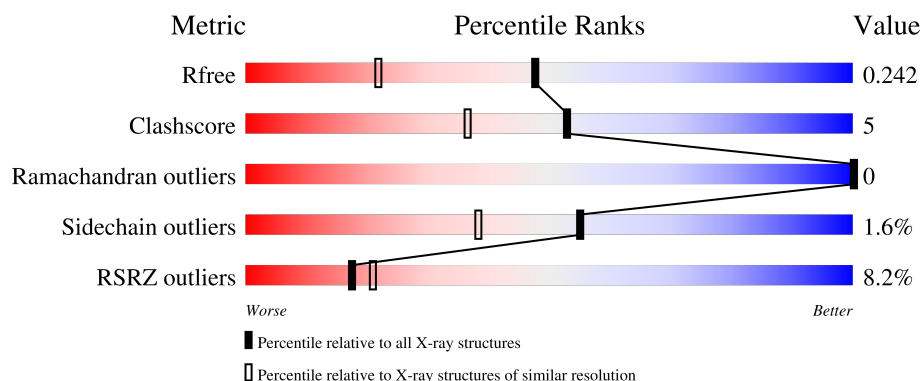
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	 3% 76% 10% 13%
1	B	289	 4% 75% 10% 14%
1	C	289	 18% 70% 13% 15%
1	D	289	 3% 80% 6% 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8163 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
			1867	1172	328	356	11			
1	B	248	Total	C	N	O	S	0	5	0
			1856	1169	319	357	11			
1	C	245	Total	C	N	O	S	0	3	0
			1784	1128	306	339	11			
1	D	250	Total	C	N	O	S	0	4	0
			1855	1169	324	351	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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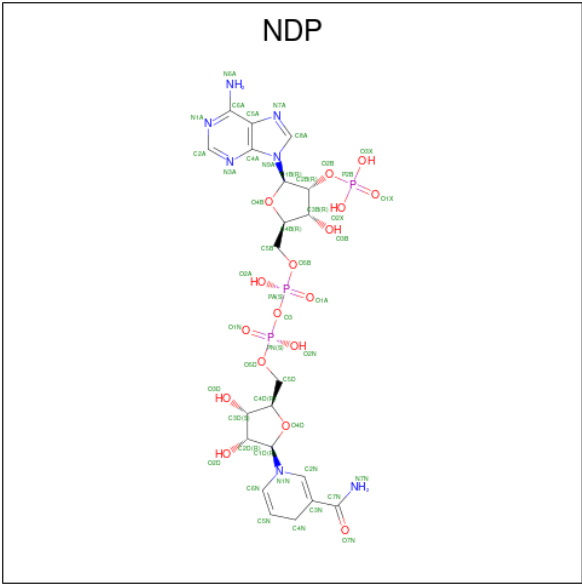
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	initiating methionine	UNP O76290
B	-19	GLY	-	expression tag	UNP O76290
B	-18	SER	-	expression tag	UNP O76290
B	-17	SER	-	expression tag	UNP O76290
B	-16	HIS	-	expression tag	UNP O76290
B	-15	HIS	-	expression tag	UNP O76290
B	-14	HIS	-	expression 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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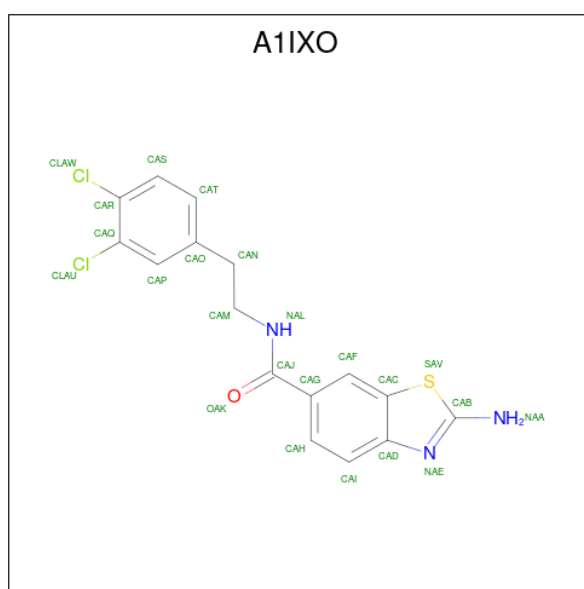
Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	initiating methionine	UNP O76290
D	-19	GLY	-	expression tag	UNP O76290
D	-18	SER	-	expression tag	UNP O76290
D	-17	SER	-	expression tag	UNP O76290
D	-16	HIS	-	expression tag	UNP O76290
D	-15	HIS	-	expression tag	UNP O76290
D	-14	HIS	-	expression 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: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



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-(3,4-dichlorophenyl)ethyl]-1,3-benzothiazole-6-carboxamide (CCD ID: A1IXO) (formula: C₁₆H₁₃Cl₂N₃OS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			23	16	2	3	1	1		
3	B	1	Total	C	Cl	N	O	S	0	0
			23	16	2	3	1	1		
3	D	1	Total	C	N	O	S		0	0
			15	10	3	1	1			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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		

- Molecule 5 is water.

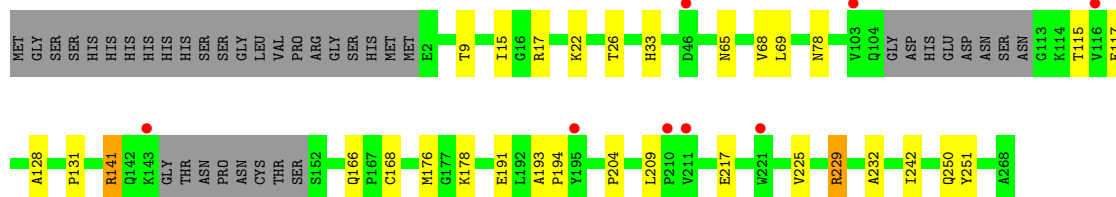
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	154	Total	O	0	1
			154	154		
5	B	158	Total	O	0	0
			158	158		
5	C	103	Total	O	0	0
			103	103		
5	D	125	Total	O	0	1
			125	125		

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.

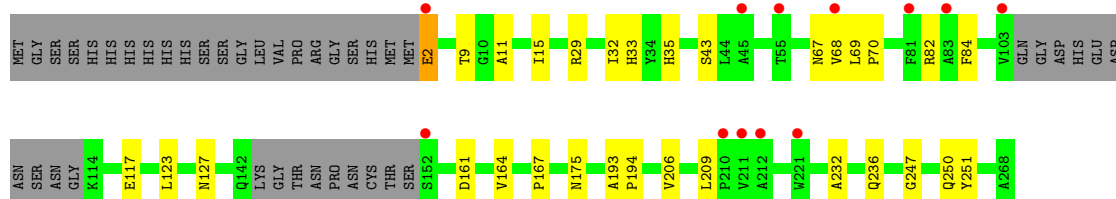
• Molecule 1: Pteridine reductase

Chain A: 



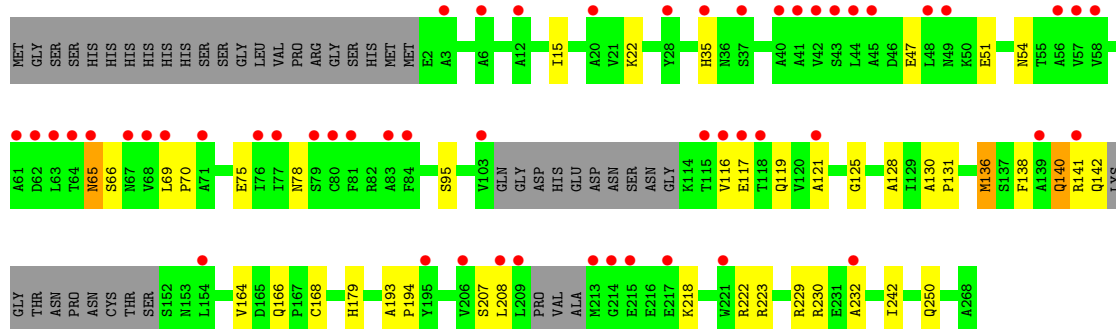
• Molecule 1: Pteridine reductase

Chain B: 



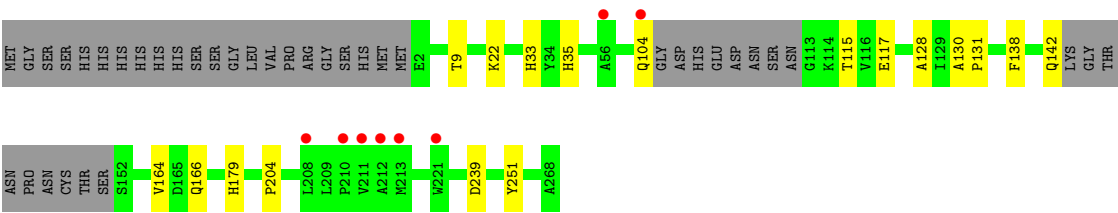
• Molecule 1: Pteridine reductase

Chain C: 



• Molecule 1: Pteridine reductase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.33Å 90.50Å 83.10Å 90.00° 115.43° 90.00°	Depositor
Resolution (Å)	66.17 – 1.76 66.17 – 1.76	Depositor EDS
% Data completeness (in resolution range)	98.7 (66.17-1.76) 98.7 (66.17-1.76)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.194 , 0.239 0.197 , 0.242	Depositor DCC
R_{free} test set	4991 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8163	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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 37.44 % 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 4.2887e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, NDP, CSX, A1IXO

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	0/1895	1.03	2/2572 (0.1%)
1	B	0.63	0/1887	1.02	0/2561
1	C	0.64	0/1810	1.13	2/2461 (0.1%)
1	D	0.59	0/1886	1.05	0/2561
All	All	0.62	0/7478	1.06	4/10155 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	75	GLU	CB-CG-CD	5.92	122.67	112.60
1	C	65	ASN	CA-CB-CG	5.77	118.37	112.60
1	A	204	PRO	CB-CA-C	-5.72	103.46	110.95
1	A	229	ARG	CB-CA-C	-5.51	104.07	111.89

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	1867	0	1869	19	0
1	B	1856	0	1850	20	0
1	C	1784	0	1748	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1855	0	1860	12	0
2	A	48	0	26	1	0
2	B	48	0	26	3	0
2	C	48	0	26	4	0
2	D	48	0	26	2	0
3	A	23	0	0	0	0
3	B	23	0	0	1	0
3	D	15	0	0	0	0
4	A	8	0	12	1	0
5	A	154	0	0	1	0
5	B	158	0	0	2	0
5	C	103	0	0	3	0
5	D	125	0	0	1	0
All	All	8163	0	7443	76	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 (76) 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:66:SER:HB3	5:C:427:HOH:O	1.37	1.21
1:D:22:LYS:HE3	1:D:239:ASP:OD1	1.81	0.79
1:C:164:VAL:HG22	1:C:179:HIS:CD2	2.18	0.78
1:A:78:ASN:OD1	1:A:141:ARG:NH1	2.21	0.74
1:B:2[A]:GLU:HA	1:B:2[A]:GLU:OE1	1.87	0.73
1:A:22:LYS:HG2	1:A:242:ILE:HG13	1.71	0.73
1:C:232:ALA:HB2	1:D:251:TYR:CE2	2.25	0.72
1:A:250:GLN:HG2	5:B:448:HOH:O	1.90	0.71
2:B:301:NDP:H41N	3:B:302:A1IXO:CAH	2.22	0.69
1:C:78:ASN:OD1	1:C:141:ARG:NH1	2.26	0.69
1:C:95:SER:HB3	2:C:301:NDP:H3D	1.77	0.67
1:A:17:ARG:HD3	4:A:303:EDO:H11	1.78	0.66
1:C:223:ARG:O	1:C:229:ARG:NH1	2.27	0.64
1:D:164:VAL:HG22	1:D:179:HIS:CD2	2.32	0.64
1:B:2[A]:GLU:OE1	1:B:2[A]:GLU:CA	2.47	0.62
1:B:67[A]:ASN:OD1	1:B:68:VAL:HG13	2.01	0.61
1:C:121:ALA:O	1:C:125:GLY:HA3	2.01	0.59
1:A:65:ASN:HA	1:A:69:LEU:HD22	1.86	0.56
1:C:138:PHE:O	1:C:142:GLN:HG2	2.04	0.56
1:B:167:PRO:HB3	1:B:175[B]:ASN:ND2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ASN:HB3	1:C:121:ALA:HA	1.89	0.54
1:C:69:LEU:HB3	1:C:70:PRO:HD3	1.90	0.54
1:D:9:THR:HA	1:D:33:HIS:HB3	1.89	0.54
1:B:161:ASP:HB3	1:B:164:VAL:HG13	1.90	0.52
1:C:164:VAL:HG22	1:C:179:HIS:NE2	2.24	0.52
1:A:250:GLN:CD	1:B:236:GLN:HE21	2.18	0.52
1:A:128:ALA:C	1:A:131:PRO:HD2	2.34	0.52
1:C:207:SER:O	1:C:208:LEU:C	2.53	0.52
1:A:251:TYR:CE2	1:B:232:ALA:HB2	2.45	0.51
1:C:232:ALA:HB2	1:D:251:TYR:CD2	2.46	0.50
1:C:35:HIS:HB2	2:C:301:NDP:C2A	2.42	0.50
1:A:9:THR:HA	1:A:33:HIS:HB3	1.93	0.50
1:C:230:ARG:HD2	5:C:414:HOH:O	2.12	0.49
1:D:138:PHE:O	1:D:142:GLN:HG2	2.13	0.49
1:D:104:GLN:HA	5:D:417:HOH:O	2.12	0.48
1:C:15:ILE:HB	2:C:301:NDP:H51N	1.93	0.48
1:C:22:LYS:HG2	1:C:242:ILE:HG13	1.96	0.48
1:C:54:ASN:HA	5:C:480:HOH:O	2.14	0.48
1:A:193:ALA:N	1:A:194:PRO:CD	2.76	0.48
1:D:204:PRO:HB2	2:D:301:NDP:H42N	1.96	0.48
1:D:130:ALA:HB3	1:D:131:PRO:HD3	1.97	0.47
1:A:115:THR:HB	1:A:117:GLU:OE1	2.14	0.47
1:B:69:LEU:N	1:B:70:PRO:CD	2.77	0.47
1:B:206:VAL:CG2	1:B:209:LEU:HD21	2.45	0.47
1:C:130:ALA:HB3	1:C:131:PRO:HD3	1.96	0.47
1:D:128:ALA:C	1:D:131:PRO:HD2	2.40	0.47
1:C:47:GLU:O	1:C:51[B]:GLU:HG2	2.15	0.46
1:B:15:ILE:HB	2:B:301:NDP:H51N	1.97	0.46
1:C:218:LYS:O	1:C:222:ARG:HG3	2.16	0.46
1:C:193:ALA:N	1:C:194:PRO:CD	2.78	0.46
1:C:116[A]:VAL:HG13	1:C:117:GLU:HG2	1.98	0.46
1:B:193:ALA:N	1:B:194:PRO:CD	2.80	0.45
1:A:178:LYS:NZ	5:A:409:HOH:O	2.49	0.45
1:B:123:LEU:O	1:B:127:ASN:HB2	2.15	0.45
1:D:115:THR:HB	1:D:117:GLU:OE2	2.16	0.45
1:B:247:GLY:O	1:B:250:GLN:HG3	2.17	0.44
1:C:128:ALA:C	1:C:131:PRO:HD2	2.43	0.44
1:D:35:HIS:HB2	2:D:301:NDP:C2A	2.48	0.44
1:C:65:ASN:HB2	1:C:125:GLY:HA3	2.00	0.43
1:A:232:ALA:HB2	1:B:251:TYR:CE2	2.53	0.43
1:B:9:THR:HA	1:B:33:HIS:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:VAL:O	1:A:229:ARG:HD3	2.19	0.42
1:A:15:ILE:HB	2:A:301:NDP:H51N	2.01	0.42
1:B:11:ALA:HB3	1:B:32:ILE:HG23	2.01	0.42
1:C:95:SER:CB	2:C:301:NDP:H3D	2.47	0.42
1:B:117:GLU:H	1:B:117:GLU:CD	2.28	0.42
1:C:136:MET:O	1:C:140:GLN:HB2	2.19	0.41
1:B:82:ARG:NE	5:B:411:HOH:O	2.53	0.41
1:B:29:ARG:HD2	1:B:84:PHE:CD1	2.55	0.41
1:C:69:LEU:N	1:C:70:PRO:CD	2.83	0.41
1:A:26:THR:HG22	1:A:26:THR:O	2.20	0.41
1:A:191:GLU:O	1:A:194:PRO:HD2	2.21	0.41
1:B:35:HIS:HB3	2:B:301:NDP:O3X	2.21	0.40
1:A:193:ALA:HB3	1:A:194:PRO:HD3	2.03	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	247/289 (86%)	237 (96%)	10 (4%)	0	100	100
1	B	245/289 (85%)	234 (96%)	11 (4%)	0	100	100
1	C	239/289 (83%)	230 (96%)	9 (4%)	0	100	100
1	D	247/289 (86%)	236 (96%)	11 (4%)	0	100	100
All	All	978/1156 (85%)	937 (96%)	41 (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	195/231 (84%)	190 (97%)	5 (3%)	40	20
1	B	193/231 (84%)	190 (98%)	3 (2%)	55	38
1	C	178/231 (77%)	174 (98%)	4 (2%)	45	26
1	D	192/231 (83%)	191 (100%)	1 (0%)	81	75
All	All	758/924 (82%)	745 (98%)	13 (2%)	55	36

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	VAL
1	A	141	ARG
1	A	166	GLN
1	A	209	LEU
1	A	217	GLU
1	B	2[A]	GLU
1	B	2[B]	GLU
1	B	43	SER
1	C	136	MET
1	C	140	GLN
1	C	166	GLN
1	C	250	GLN
1	D	166	GLN

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	65	ASN
1	A	92	ASN
1	A	127	ASN
1	A	140	GLN
1	A	250	GLN

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Mol	Chain	Res	Type
1	B	92	ASN
1	B	119	GLN
1	B	140	GLN
1	B	236	GLN
1	C	35	HIS
1	C	54	ASN
1	C	92	ASN
1	C	250	GLN
1	D	67	ASN
1	D	92	ASN
1	D	186	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	B	168	1	3,6,7	0.68	0	1,6,8	1.46	0
1	CSX	D	168	1	3,6,7	0.64	0	1,6,8	1.56	0
1	CSX	C	168	1	3,6,7	0.83	0	1,6,8	2.60	1 (100%)
1	CSX	A	168	1	3,6,7	0.67	0	1,6,8	2.86	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	B	168	1	-	0/2/5/7	-
1	CSX	D	168	1	-	0/2/5/7	-
1	CSX	C	168	1	-	0/2/5/7	-
1	CSX	A	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($^{\circ}$)	Ideal($^{\circ}$)
1	A	168	CSX	CA-CB-SG	-2.86	106.45	113.17
1	C	168	CSX	CA-CB-SG	-2.60	107.06	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](#)

9 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	A1IXO	B	302	-	25,25,25	3.46	8 (32%)	35,35,35	3.26	5 (14%)
2	NDP	A	301	-	51,52,52	0.71	1 (1%)	71,80,80	0.91	4 (5%)
2	NDP	D	301	-	51,52,52	0.72	1 (1%)	71,80,80	0.84	2 (2%)
2	NDP	C	301	-	51,52,52	0.54	0	71,80,80	0.70	1 (1%)
3	A1IXO	D	302	-	16,16,25	4.60	7 (43%)	22,22,35	4.40	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	303	-	3,3,3	0.26	0	2,2,2	1.26	0
4	EDO	A	304	-	3,3,3	0.19	0	2,2,2	0.36	0
3	A1IXO	A	302	-	25,25,25	3.60	8 (32%)	35,35,35	3.56	5 (14%)
2	NDP	B	301	-	51,52,52	0.86	2 (3%)	71,80,80	0.88	2 (2%)

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	A1IXO	B	302	-	-	3/10/10/10	0/3/3/3
2	NDP	A	301	-	-	1/34/77/77	0/5/5/5
2	NDP	D	301	-	-	2/34/77/77	0/5/5/5
2	NDP	C	301	-	-	5/34/77/77	0/5/5/5
3	A1IXO	D	302	-	-	0/7/7/10	0/2/2/3
4	EDO	A	303	-	-	1/1/1/1	-
4	EDO	A	304	-	-	0/1/1/1	-
3	A1IXO	A	302	-	-	3/10/10/10	0/3/3/3
2	NDP	B	301	-	-	1/34/77/77	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	A1IXO	CAB-SAV	-15.45	1.58	1.76
3	A	302	A1IXO	CAB-SAV	-13.96	1.60	1.76
3	B	302	A1IXO	CAB-SAV	-13.49	1.61	1.76
3	A	302	A1IXO	CAG-CAJ	-5.14	1.38	1.50
3	A	302	A1IXO	CAC-SAV	-5.03	1.64	1.74
3	B	302	A1IXO	CAG-CAJ	-4.96	1.39	1.50
3	D	302	A1IXO	CAG-CAJ	-4.88	1.39	1.50
3	D	302	A1IXO	CAC-SAV	-4.38	1.65	1.74
3	D	302	A1IXO	CAI-CAD	-4.37	1.33	1.40
3	B	302	A1IXO	CAN-CAO	-4.36	1.39	1.51
3	A	302	A1IXO	CAI-CAD	-4.35	1.33	1.40
3	B	302	A1IXO	CAC-SAV	-4.32	1.65	1.74
3	A	302	A1IXO	CAN-CAO	-4.28	1.39	1.51
3	B	302	A1IXO	CAI-CAD	-4.28	1.33	1.40
3	A	302	A1IXO	CAF-CAC	-3.86	1.33	1.39
3	B	302	A1IXO	CAF-CAC	-3.71	1.33	1.39
3	D	302	A1IXO	CAD-CAC	-3.68	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	A1IXO	CAD-CAC	-3.57	1.34	1.40
3	D	302	A1IXO	CAF-CAC	-3.51	1.33	1.39
3	B	302	A1IXO	CAD-CAC	-3.38	1.35	1.40
2	D	301	NDP	P2B-O2B	3.35	1.65	1.59
2	B	301	NDP	PA-O3	3.32	1.63	1.59
2	B	301	NDP	P2B-O2B	3.00	1.64	1.59
2	A	301	NDP	P2B-O2B	2.95	1.64	1.59
3	A	302	A1IXO	CAD-NAE	-2.76	1.34	1.39
3	B	302	A1IXO	CAD-NAE	-2.57	1.34	1.39
3	D	302	A1IXO	CAD-NAE	-2.57	1.34	1.39

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	A1IXO	CAC-SAV-CAB	15.33	96.14	88.89
3	A	302	A1IXO	CAC-SAV-CAB	14.89	95.93	88.89
3	B	302	A1IXO	CAC-SAV-CAB	13.64	95.34	88.89
3	A	302	A1IXO	SAV-CAB-NAE	-10.66	109.11	115.72
3	D	302	A1IXO	SAV-CAB-NAE	-10.17	109.41	115.72
3	B	302	A1IXO	SAV-CAB-NAE	-9.70	109.70	115.72
3	A	302	A1IXO	CAD-NAE-CAB	6.20	114.25	110.57
3	D	302	A1IXO	CAD-NAE-CAB	6.10	114.19	110.57
3	A	302	A1IXO	SAV-CAB-NAA	5.80	126.43	120.13
3	B	302	A1IXO	CAD-NAE-CAB	5.79	114.00	110.57
3	B	302	A1IXO	SAV-CAB-NAA	5.29	125.88	120.13
3	D	302	A1IXO	SAV-CAB-NAA	5.12	125.69	120.13
2	C	301	NDP	P2B-O2B-C2B	-3.87	113.10	123.43
3	A	302	A1IXO	CAI-CAH-CAG	-3.07	117.52	120.80
3	B	302	A1IXO	CAI-CAH-CAG	-2.95	117.65	120.80
3	D	302	A1IXO	CAI-CAH-CAG	-2.93	117.67	120.80
2	D	301	NDP	O4B-C1B-N9A	2.83	113.53	108.09
2	A	301	NDP	O2B-P2B-O1X	-2.67	99.80	109.33
2	A	301	NDP	O4B-C1B-N9A	2.42	112.74	108.09
3	D	302	A1IXO	CAF-CAC-SAV	2.16	131.45	126.07
2	A	301	NDP	C4B-O4B-C1B	-2.10	104.84	109.47
2	A	301	NDP	O2N-PN-O1N	2.08	122.13	112.44
2	B	301	NDP	O4B-C1B-N9A	2.06	112.04	108.09
2	B	301	NDP	C3N-C7N-N7N	2.00	121.23	117.67
2	D	301	NDP	O2N-PN-O1N	2.00	121.76	112.44

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	NDP	C5B-O5B-PA-O1A
2	C	301	NDP	C5B-O5B-PA-O3
2	C	301	NDP	O4D-C1D-N1N-C6N
3	A	302	A1IXO	NAL-CAM-CAN-CAO
2	B	301	NDP	O4D-C1D-N1N-C6N
4	A	303	EDO	O1-C1-C2-O2
3	A	302	A1IXO	CAM-CAN-CAO-CAP
2	A	301	NDP	O4D-C1D-N1N-C6N
3	A	302	A1IXO	CAM-CAN-CAO-CAT
3	B	302	A1IXO	CAM-CAN-CAO-CAP
3	B	302	A1IXO	CAM-CAN-CAO-CAT
2	D	301	NDP	O4D-C1D-N1N-C6N
3	B	302	A1IXO	CAN-CAM-NAL-CAJ
2	C	301	NDP	C5B-O5B-PA-O2A
2	C	301	NDP	C2B-O2B-P2B-O3X
2	D	301	NDP	C2N-C3N-C7N-N7N

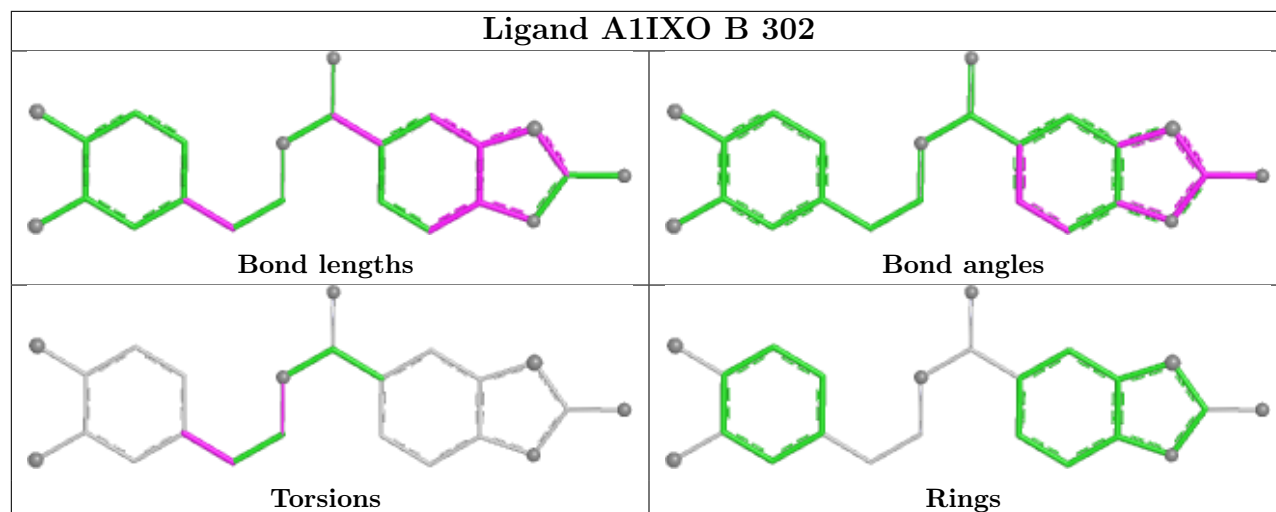
There are no ring outliers.

6 monomers are involved in 11 short contacts:

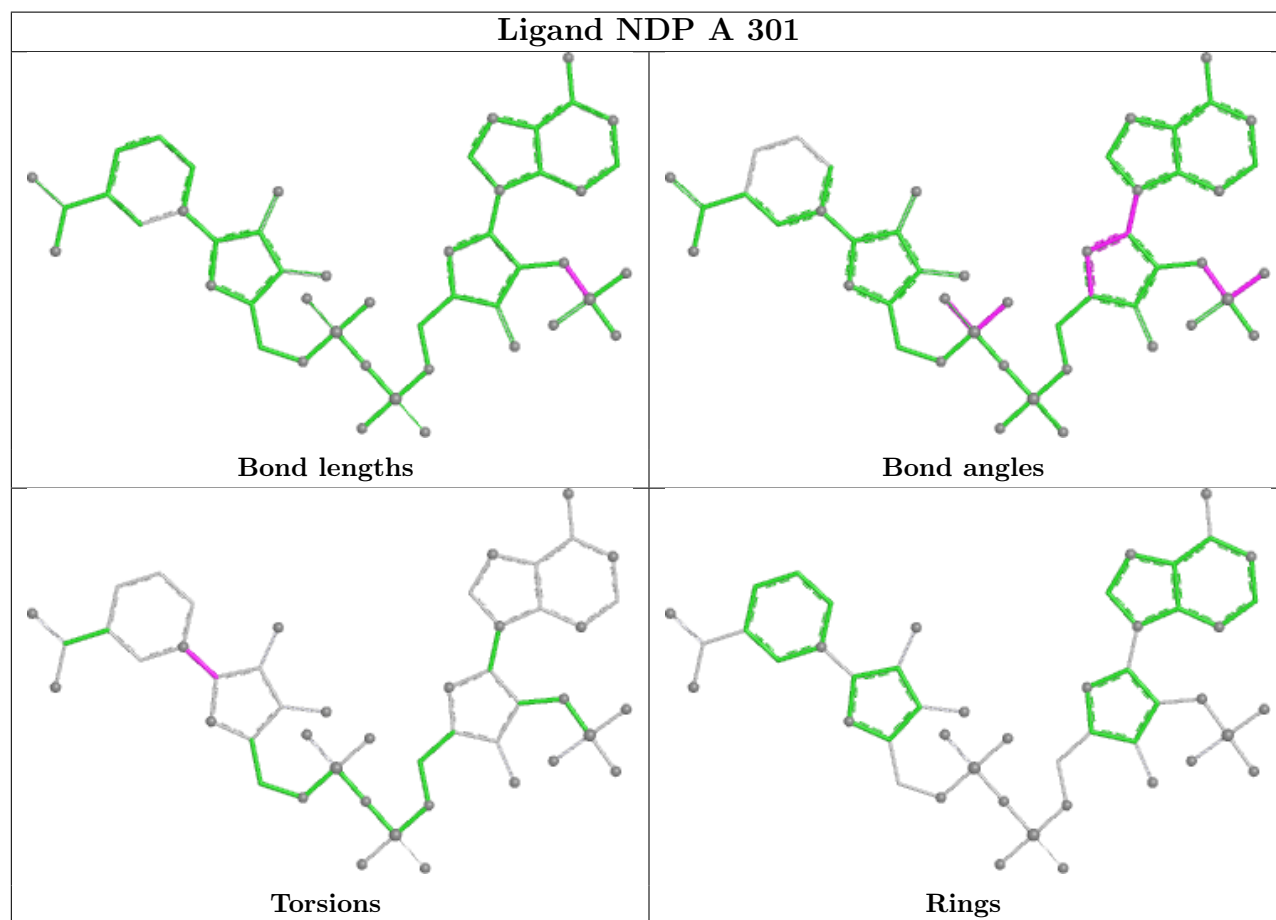
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	A1IXO	1	0
2	A	301	NDP	1	0
2	D	301	NDP	2	0
2	C	301	NDP	4	0
4	A	303	EDO	1	0
2	B	301	NDP	3	0

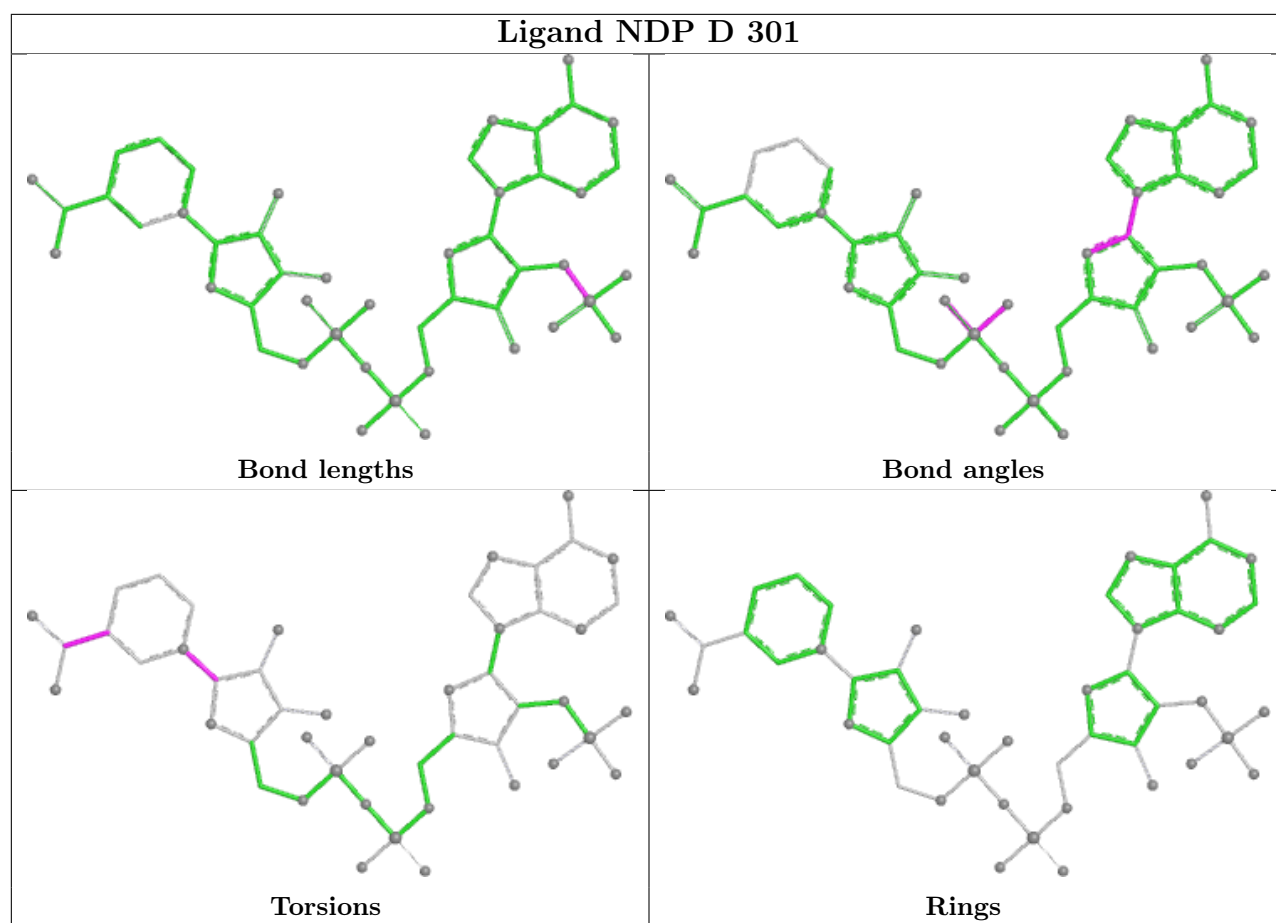
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

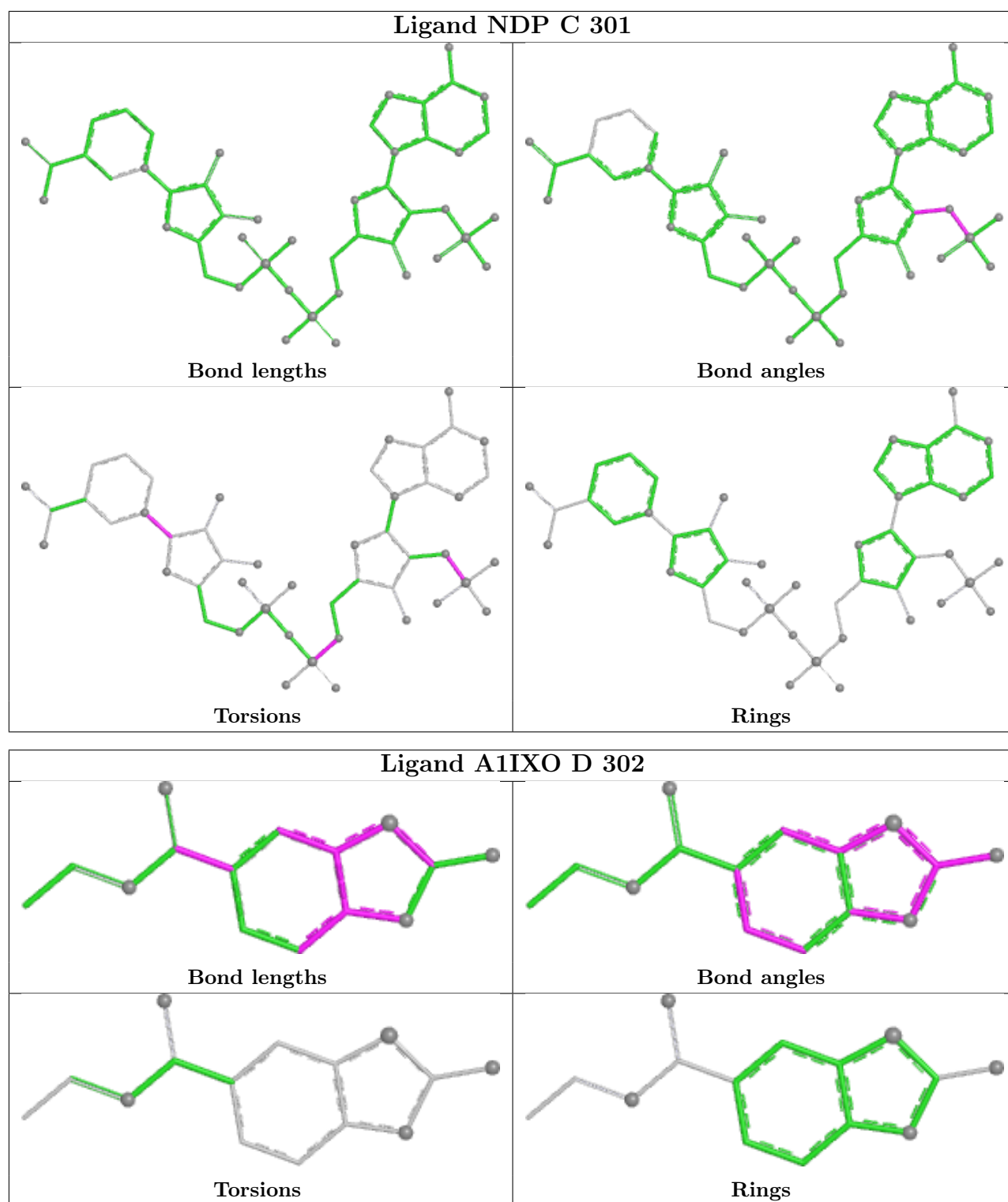
Ligand A1IXO B 302

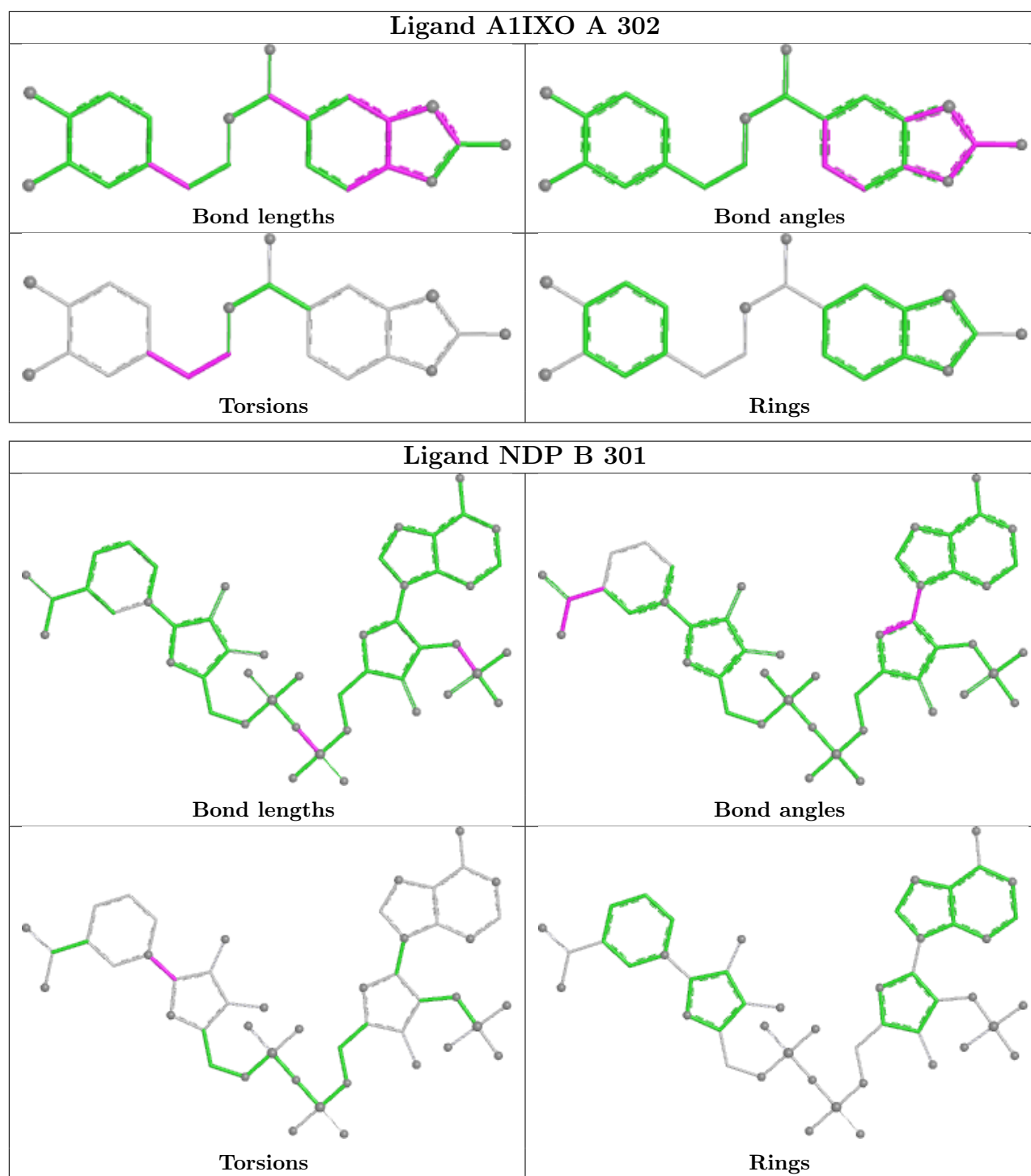


Ligand NDP A 301









5.7 Other polymers [i](#)

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

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	250/289 (86%)	0.26	8 (3%) 50 57	13, 28, 49, 73	14 (5%)
1	B	247/289 (85%)	0.28	12 (4%) 35 40	12, 27, 43, 60	15 (6%)
1	C	244/289 (84%)	1.16	53 (21%) 2 2	16, 34, 53, 74	25 (10%)
1	D	249/289 (86%)	0.44	8 (3%) 50 57	12, 30, 53, 81	17 (6%)
All	All	990/1156 (85%)	0.53	81 (8%) 17 21	12, 30, 49, 81	71 (7%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	209	LEU	5.3
1	C	214	GLY	4.4
1	C	208	LEU	4.2
1	C	37	SER	4.1
1	C	116[A]	VAL	4.1
1	C	64	THR	4.1
1	C	213	MET	3.9
1	C	232	ALA	3.7
1	C	206	VAL	3.4
1	B	211	VAL	3.3
1	C	118	THR	3.1
1	A	211	VAL	3.1
1	C	83	ALA	3.1
1	C	84	PHE	3.1
1	B	210	PRO	3.0
1	A	195	TYR	3.0
1	D	210	PRO	3.0
1	D	211	VAL	3.0
1	C	44	LEU	3.0
1	C	63	LEU	3.0
1	C	67	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	2[A]	GLU	2.8
1	C	42	VAL	2.8
1	C	195	TYR	2.8
1	C	6	ALA	2.8
1	B	212	ALA	2.7
1	C	45	ALA	2.7
1	A	143	LYS	2.7
1	C	221	TRP	2.7
1	B	55	THR	2.7
1	C	57	VAL	2.7
1	C	68	VAL	2.7
1	C	65	ASN	2.7
1	C	62	ASP	2.7
1	D	104	GLN	2.6
1	C	217	GLU	2.6
1	C	71	ALA	2.6
1	C	48	LEU	2.5
1	B	152	SER	2.5
1	C	35	HIS	2.5
1	D	212	ALA	2.4
1	C	77	ILE	2.4
1	D	208	LEU	2.4
1	C	81	PHE	2.4
1	B	103	VAL	2.4
1	C	141	ARG	2.4
1	B	45	ALA	2.4
1	B	83	ALA	2.4
1	D	56	ALA	2.4
1	C	117	GLU	2.3
1	C	20	ALA	2.3
1	C	40	ALA	2.3
1	C	76	ILE	2.3
1	D	221	TRP	2.3
1	C	3	ALA	2.3
1	C	12	ALA	2.3
1	B	221	TRP	2.2
1	C	115	THR	2.2
1	C	69	LEU	2.2
1	C	154	LEU	2.2
1	A	210	PRO	2.2
1	B	68	VAL	2.2
1	C	43	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	41	ALA	2.2
1	C	56	ALA	2.2
1	D	213	MET	2.2
1	A	221	TRP	2.2
1	C	58	VAL	2.1
1	C	215	GLU	2.1
1	C	121	ALA	2.1
1	C	103	VAL	2.1
1	C	79	SER	2.1
1	C	61	ALA	2.1
1	A	116	VAL	2.1
1	B	81	PHE	2.1
1	C	139	ALA	2.0
1	A	103	VAL	2.0
1	C	80	CYS	2.0
1	C	49	ASN	2.0
1	C	28	TYR	2.0
1	A	46	ASP	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	0.94	0.08	26,29,48,51	0
1	CSX	C	168	7/8	0.94	0.08	29,32,46,52	0
1	CSX	B	168	7/8	0.96	0.06	26,27,42,48	0
1	CSX	D	168	7/8	0.96	0.07	28,29,49,51	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

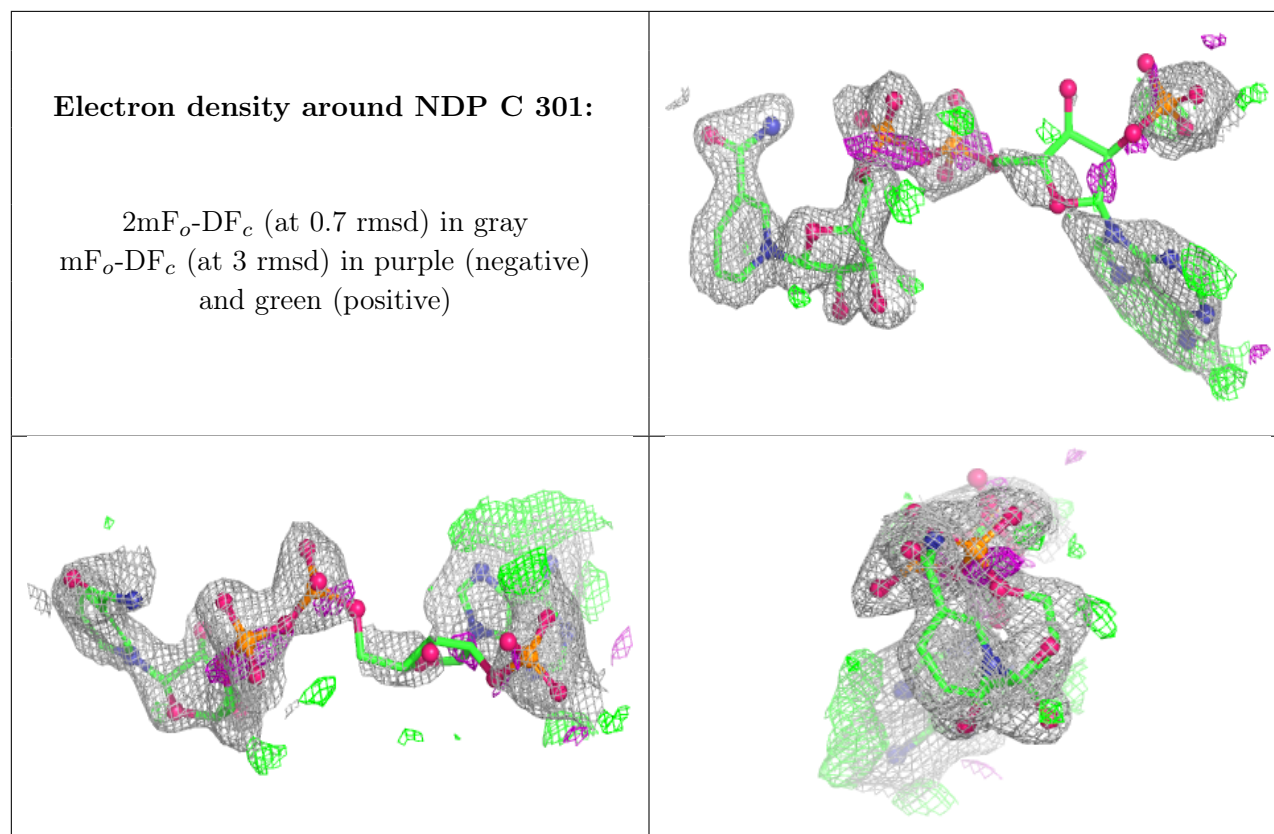
6.4 Ligands [i](#)

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.

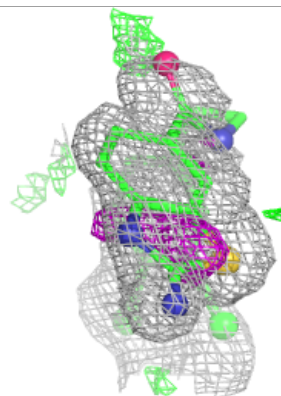
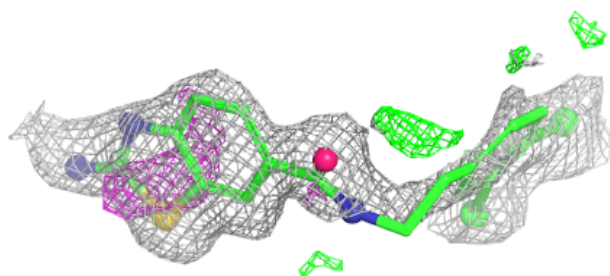
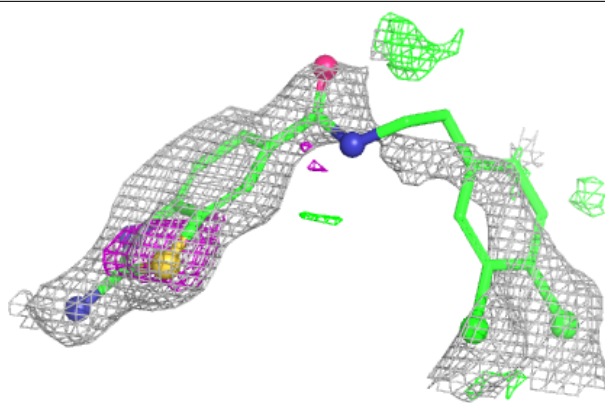
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NDP	C	301	48/48	0.74	0.17	33,44,56,57	48
3	A1IXO	A	302	23/23	0.74	0.24	43,61,67,70	10
3	A1IXO	B	302	23/23	0.75	0.27	44,65,75,76	23
3	A1IXO	D	302	15/23	0.75	0.19	45,46,51,52	15
4	EDO	A	304	4/4	0.84	0.14	47,52,57,57	0
4	EDO	A	303	4/4	0.88	0.14	32,38,45,49	0
2	NDP	B	301	48/48	0.92	0.09	23,30,38,40	48
2	NDP	D	301	48/48	0.93	0.09	25,34,40,50	0
2	NDP	A	301	48/48	0.94	0.08	24,30,35,39	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.

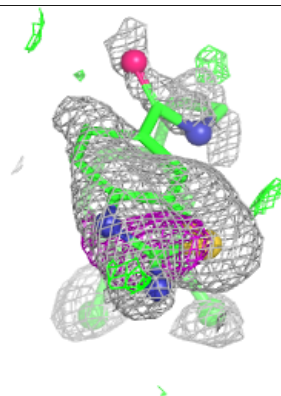
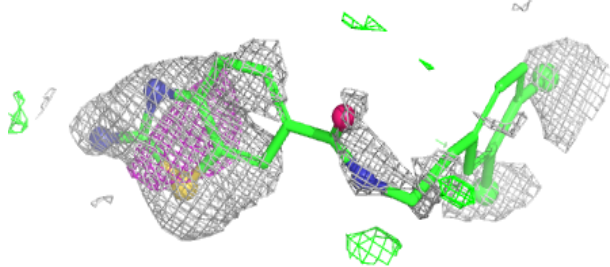
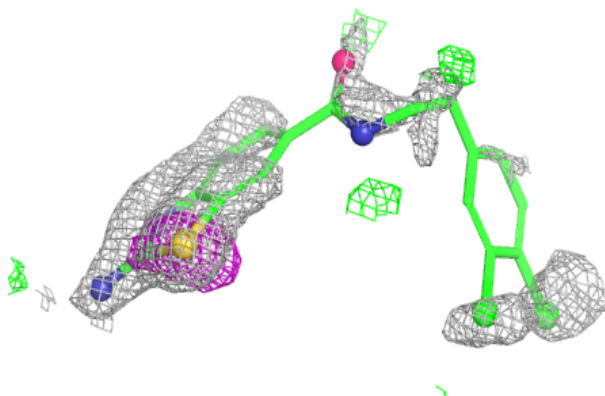


Electron density around A1IXO A 302:

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

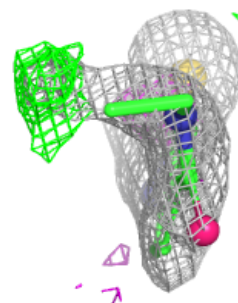
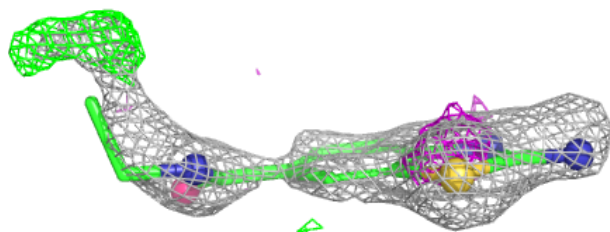
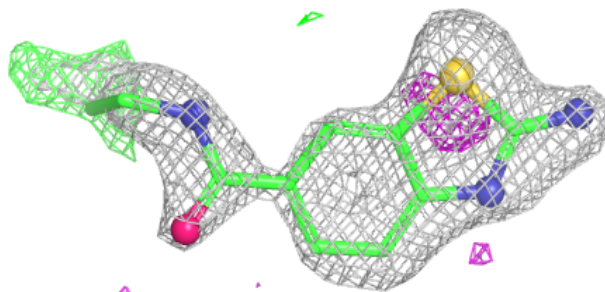
**Electron density around A1IXO B 302:**

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

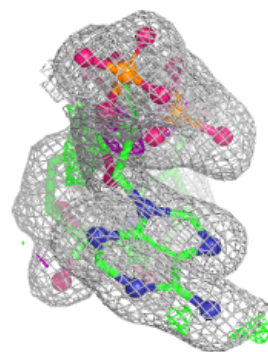
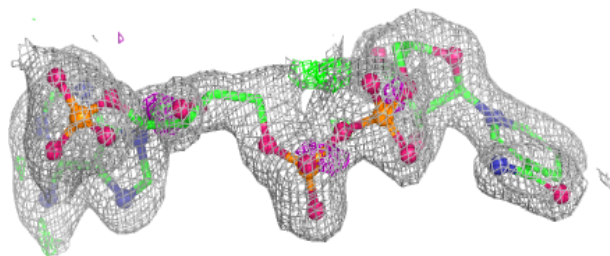
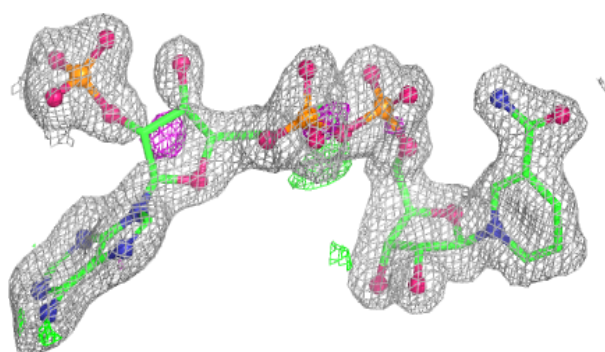


Electron density around A1IXO D 302:

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

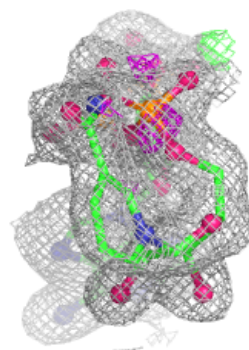
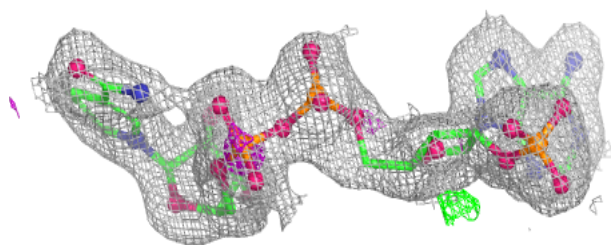
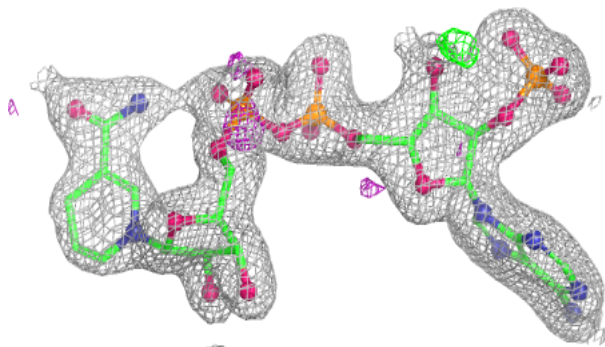
**Electron density around NDP B 301:**

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

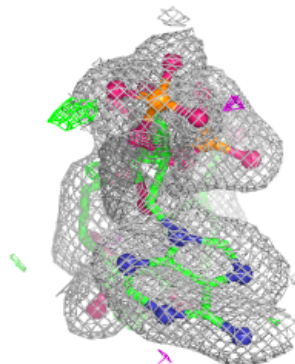
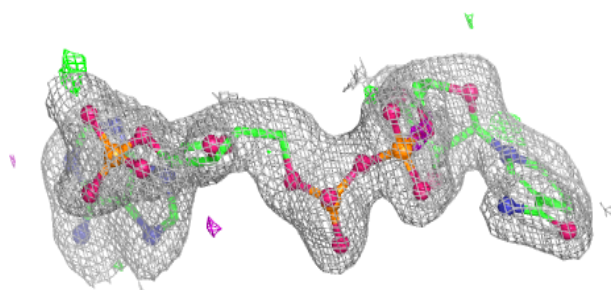
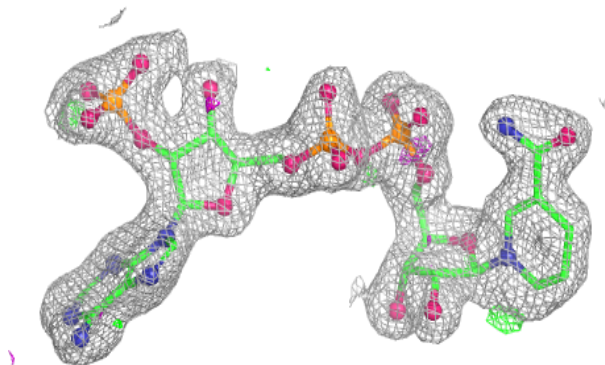


Electron density around NDP D 301:

$2mF_o-DF_c$ (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.