



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:22 pm BST

PDB ID : 3JQE
Title : Crystal structure of pteridine reductase 1 (PTR1) from Trypanosoma brucei in ternary complex with cofactor (NADP+) and inhibitor 2-amino-6-(4-methoxyphenyl)-4-oxo-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidine-5-carbonitrile (DX8)
Authors : Tulloch, L.B.; Hunter, W.N.
Deposited on : 2009-09-06
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

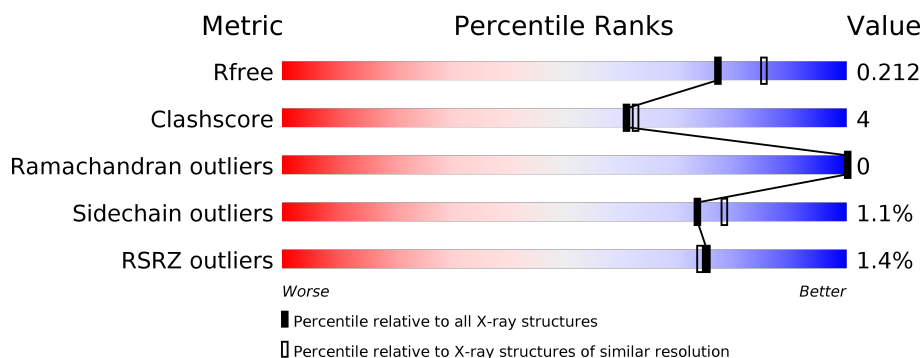
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	288	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 79%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 79% 7% 14% </div> </div>
1	B	288	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 79%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 79% 7% 14% </div> </div>
1	C	288	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 80%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 80% 6% 14% </div> </div>
1	D	288	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 78%, yellow 7%, orange 1%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 78% 7% 14% </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8639 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	7	0
			1878	1181	328	358	11			
1	B	248	Total	C	N	O	S	0	15	0
			1898	1198	330	359	11			
1	C	249	Total	C	N	O	S	0	9	0
			1868	1177	328	352	11			
1	D	249	Total	C	N	O	S	0	11	0
			1888	1189	329	359	11			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q581W1
A	-18	GLY	-	EXPRESSION TAG	UNP Q581W1
A	-17	SER	-	EXPRESSION TAG	UNP Q581W1
A	-16	SER	-	EXPRESSION TAG	UNP Q581W1
A	-15	HIS	-	EXPRESSION TAG	UNP Q581W1
A	-14	HIS	-	EXPRESSION TAG	UNP Q581W1
A	-13	HIS	-	EXPRESSION TAG	UNP Q581W1
A	-12	HIS	-	EXPRESSION TAG	UNP Q581W1
A	-11	HIS	-	EXPRESSION TAG	UNP Q581W1
A	-10	HIS	-	EXPRESSION TAG	UNP Q581W1
A	-9	SER	-	EXPRESSION TAG	UNP Q581W1
A	-8	SER	-	EXPRESSION TAG	UNP Q581W1
A	-7	GLY	-	EXPRESSION TAG	UNP Q581W1
A	-6	LEU	-	EXPRESSION TAG	UNP Q581W1
A	-5	VAL	-	EXPRESSION TAG	UNP Q581W1
A	-4	PRO	-	EXPRESSION TAG	UNP Q581W1
A	-3	ARG	-	EXPRESSION TAG	UNP Q581W1
A	-2	GLY	-	EXPRESSION TAG	UNP Q581W1
A	-1	SER	-	EXPRESSION TAG	UNP Q581W1
A	0	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-19	MET	-	EXPRESSION TAG	UNP Q581W1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	EXPRESSION TAG	UNP Q581W1
B	-17	SER	-	EXPRESSION TAG	UNP Q581W1
B	-16	SER	-	EXPRESSION TAG	UNP Q581W1
B	-15	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-14	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-13	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-12	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-11	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-10	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-9	SER	-	EXPRESSION TAG	UNP Q581W1
B	-8	SER	-	EXPRESSION TAG	UNP Q581W1
B	-7	GLY	-	EXPRESSION TAG	UNP Q581W1
B	-6	LEU	-	EXPRESSION TAG	UNP Q581W1
B	-5	VAL	-	EXPRESSION TAG	UNP Q581W1
B	-4	PRO	-	EXPRESSION TAG	UNP Q581W1
B	-3	ARG	-	EXPRESSION TAG	UNP Q581W1
B	-2	GLY	-	EXPRESSION TAG	UNP Q581W1
B	-1	SER	-	EXPRESSION TAG	UNP Q581W1
B	0	HIS	-	EXPRESSION TAG	UNP Q581W1
C	-19	MET	-	EXPRESSION TAG	UNP Q581W1
C	-18	GLY	-	EXPRESSION TAG	UNP Q581W1
C	-17	SER	-	EXPRESSION TAG	UNP Q581W1
C	-16	SER	-	EXPRESSION TAG	UNP Q581W1
C	-15	HIS	-	EXPRESSION TAG	UNP Q581W1
C	-14	HIS	-	EXPRESSION TAG	UNP Q581W1
C	-13	HIS	-	EXPRESSION TAG	UNP Q581W1
C	-12	HIS	-	EXPRESSION TAG	UNP Q581W1
C	-11	HIS	-	EXPRESSION TAG	UNP Q581W1
C	-10	HIS	-	EXPRESSION TAG	UNP Q581W1
C	-9	SER	-	EXPRESSION TAG	UNP Q581W1
C	-8	SER	-	EXPRESSION TAG	UNP Q581W1
C	-7	GLY	-	EXPRESSION TAG	UNP Q581W1
C	-6	LEU	-	EXPRESSION TAG	UNP Q581W1
C	-5	VAL	-	EXPRESSION TAG	UNP Q581W1
C	-4	PRO	-	EXPRESSION TAG	UNP Q581W1
C	-3	ARG	-	EXPRESSION TAG	UNP Q581W1
C	-2	GLY	-	EXPRESSION TAG	UNP Q581W1
C	-1	SER	-	EXPRESSION TAG	UNP Q581W1
C	0	HIS	-	EXPRESSION TAG	UNP Q581W1
D	-19	MET	-	EXPRESSION TAG	UNP Q581W1
D	-18	GLY	-	EXPRESSION TAG	UNP Q581W1
D	-17	SER	-	EXPRESSION TAG	UNP Q581W1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP Q581W1
D	-15	HIS	-	EXPRESSION TAG	UNP Q581W1
D	-14	HIS	-	EXPRESSION TAG	UNP Q581W1
D	-13	HIS	-	EXPRESSION TAG	UNP Q581W1
D	-12	HIS	-	EXPRESSION TAG	UNP Q581W1
D	-11	HIS	-	EXPRESSION TAG	UNP Q581W1
D	-10	HIS	-	EXPRESSION TAG	UNP Q581W1
D	-9	SER	-	EXPRESSION TAG	UNP Q581W1
D	-8	SER	-	EXPRESSION TAG	UNP Q581W1
D	-7	GLY	-	EXPRESSION TAG	UNP Q581W1
D	-6	LEU	-	EXPRESSION TAG	UNP Q581W1
D	-5	VAL	-	EXPRESSION TAG	UNP Q581W1
D	-4	PRO	-	EXPRESSION TAG	UNP Q581W1
D	-3	ARG	-	EXPRESSION TAG	UNP Q581W1
D	-2	GLY	-	EXPRESSION TAG	UNP Q581W1
D	-1	SER	-	EXPRESSION TAG	UNP Q581W1
D	0	HIS	-	EXPRESSION TAG	UNP Q581W1

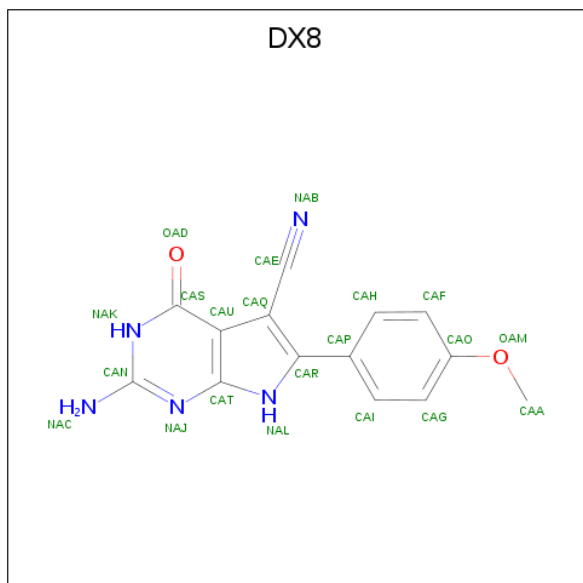
- # NAP
-
- The chemical structure of Naproxen (NAP) is shown, featuring a naphthalene ring system. The structure includes a carboxylic acid group (-COOH) at the 2-position, a chiral center at the 1-position, and a 6-methoxy group (-OCH₃). The stereochemistry is indicated by wedged and dashed bonds. The structure is labeled with various atoms and groups, including NH₂, COOH, OCH₃, and OCH₂.

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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-amino-6-(4-methoxyphenyl)-4-oxo-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidine-5-carbonitrile (three-letter code: DX8) (formula: C₁₄H₁₁N₅O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	14	5	2		
3	B	1	Total	C	N	O	0	0
			21	14	5	2		
3	C	1	Total	C	N	O	0	0
			21	14	5	2		
3	D	1	Total	C	N	O	0	0
			21	14	5	2		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	205	Total	O	0	0
			205	205		
5	B	208	Total	O	0	0
			208	208		
5	C	220	Total	O	0	0
			220	220		
5	D	194	Total	O	0	0
			194	194		

PRO	ASN	CYS	THR	SER	S152	V164	C168	H179	V206	E217	K220	R221	R222	R223	K224	R229	R230	E231	Q250	Y251	L265	A268
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.58Å 89.42Å 82.37Å 90.00° 115.56° 90.00°	Depositor
Resolution (Å)	34.32 – 2.00 34.31 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.2 (34.32-2.00) 94.1 (34.31-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.79 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.152 , 0.213 0.157 , 0.212	Depositor DCC
R_{free} test set	3179 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	1.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8639	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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 44.71 % 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 1.4671e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, DX8, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.58	0/1920	0.61	0/2604
1	B	0.60	0/1955	0.62	0/2652
1	C	0.59	0/1904	0.62	0/2582
1	D	0.57	0/1933	0.62	0/2621
All	All	0.59	0/7712	0.62	0/10459

There are no bond length outliers.

There are no bond angle outliers.

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	1878	0	1906	20	0
1	B	1898	0	1948	17	0
1	C	1868	0	1906	13	0
1	D	1888	0	1925	20	0
2	A	48	0	25	0	0
2	B	48	0	25	1	0
2	C	48	0	25	0	0
2	D	48	0	25	0	0
3	A	21	0	11	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	21	0	11	2	0
3	C	21	0	11	5	0
3	D	21	0	11	4	0
4	A	4	0	3	0	0
5	A	205	0	0	0	0
5	B	208	0	0	6	0
5	C	220	0	0	3	0
5	D	194	0	0	8	0
All	All	8639	0	7832	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 4.

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:B:168:CYS:SG	3:B:270:DX8:HAAB	2.19	0.81
1:C:168:CYS:SG	3:C:270:DX8:HAAB	2.20	0.81
1:C:75:GLU:OE1	5:C:484:HOH:O	2.00	0.79
3:D:270:DX8:CAE	3:D:270:DX8:HAH	2.12	0.79
1:A:168:CYS:SG	3:A:270:DX8:HAAB	2.24	0.78
1:D:222:ARG:HD3	1:D:231:GLU:OE2	1.85	0.75
3:C:270:DX8:HAG	5:C:427:HOH:O	1.85	0.74
1:D:168:CYS:SG	3:D:270:DX8:HAAB	2.27	0.74
1:C:75:GLU:HG2	5:C:364:HOH:O	1.92	0.68
1:A:247:GLY:HA2	1:A:250[B]:GLN:HG3	1.75	0.67
1:A:194:PRO:HG3	5:B:450:HOH:O	1.96	0.66
1:D:47:GLU:OE2	5:D:309:HOH:O	2.15	0.64
1:B:153:ASN:N	5:B:362:HOH:O	2.32	0.63
1:A:22:LYS:HG2	1:A:242:ILE:HG13	1.81	0.62
1:A:250[A]:GLN:HG2	5:B:271:HOH:O	1.98	0.62
1:D:217:GLU:HG3	5:D:299:HOH:O	2.01	0.61
3:A:270:DX8:HAH	3:A:270:DX8:CAE	2.31	0.61
1:B:164:VAL:HG22	1:B:179:HIS:CD2	2.36	0.60
3:C:270:DX8:HAH	3:C:270:DX8:CAE	2.32	0.60
1:A:161:ASP:HB3	1:A:164:VAL:HG13	1.85	0.59
1:C:9:THR:HA	1:C:33:HIS:HB3	1.87	0.56
1:A:9:THR:HA	1:A:33:HIS:HB3	1.86	0.56
1:D:9:THR:HA	1:D:33:HIS:HB3	1.88	0.55
1:A:250[A]:GLN:CD	1:B:236:GLN:HE21	2.09	0.55
1:B:223:ARG:HA	1:B:229:ARG:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:THR:HA	1:B:33:HIS:HB3	1.89	0.54
1:D:140:GLN:HG2	5:D:441:HOH:O	2.06	0.54
3:D:270:DX8:HAH	3:D:270:DX8:NAB	2.24	0.53
3:B:270:DX8:CAE	3:B:270:DX8:HAH	2.39	0.52
1:D:53:SER:CB	5:D:355:HOH:O	2.57	0.52
1:B:62:ASP:OD1	1:B:64[B]:THR:HG23	2.10	0.52
1:D:229:ARG:NH2	5:D:357:HOH:O	2.42	0.52
1:A:233:SER:H	1:A:236:GLN:HE21	1.57	0.52
1:C:232:ALA:HB2	1:D:251:TYR:CE2	2.45	0.52
1:D:132:PHE:CZ	1:D:136:MET:CE	2.94	0.51
1:D:250:GLN:HG3	5:D:443:HOH:O	2.12	0.50
1:A:103:VAL:HG21	1:C:195:TYR:OH	2.13	0.49
3:D:270:DX8:CAE	3:D:270:DX8:CAH	2.82	0.48
1:D:164:VAL:HG22	1:D:179:HIS:CD2	2.48	0.48
1:D:53:SER:HB2	5:D:355:HOH:O	2.13	0.47
3:C:270:DX8:CAH	3:C:270:DX8:CAE	2.92	0.47
1:B:64[B]:THR:CG2	1:B:122:GLU:HG2	2.45	0.47
1:A:193:ALA:N	1:A:194:PRO:CD	2.77	0.47
1:A:95:SER:CB	3:A:270:DX8:HNAC	2.28	0.46
1:B:229:ARG:NH1	5:B:450:HOH:O	2.48	0.46
1:D:220:LYS:O	1:D:224[A]:LYS:HG3	2.16	0.46
1:D:65:ASN:HA	1:D:69:LEU:HD22	1.97	0.46
1:A:67[A]:ASN:HA	1:C:117:GLU:HG3	1.98	0.46
1:C:232:ALA:HB2	1:D:251:TYR:CD2	2.52	0.45
1:B:160:CYS:HB3	5:B:383:HOH:O	2.16	0.45
1:A:254:GLY:HA3	1:B:265:LEU:HD11	1.99	0.45
1:C:210:PRO:HD3	3:C:270:DX8:NAB	2.32	0.45
1:A:65:ASN:HA	1:A:69:LEU:HD22	1.99	0.45
1:A:95:SER:HB3	3:A:270:DX8:NAC	2.32	0.44
1:C:138:PHE:O	1:C:142:GLN:HG2	2.17	0.44
1:D:132:PHE:CZ	1:D:136:MET:HE1	2.53	0.43
1:B:223:ARG:NH1	5:B:335:HOH:O	2.50	0.43
1:A:251:TYR:CE2	1:B:232:ALA:HB2	2.54	0.43
1:A:233:SER:H	1:A:236:GLN:NE2	2.17	0.43
1:A:232:ALA:HB2	1:B:251:TYR:CE2	2.54	0.42
1:B:247:GLY:HA2	1:B:250:GLN:HG3	2.02	0.42
3:A:270:DX8:CAE	3:A:270:DX8:CAH	2.95	0.41
1:C:254:GLY:HA3	1:D:265:LEU:HD11	2.02	0.41
1:B:64[B]:THR:HG22	1:B:122:GLU:HG2	2.03	0.41
1:B:35:HIS:HB2	2:B:269:NAP:C2A	2.51	0.41
1:C:65:ASN:HA	1:C:69:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:SER:HB3	3:A:270:DX8:HNAC	1.86	0.41
1:D:9:THR:O	1:D:93:ASN:HB3	2.21	0.41
1:C:22:LYS:HG2	1:C:242:ILE:HG13	2.03	0.40
1:D:220:LYS:HE3	5:D:346:HOH:O	2.20	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	247/288 (86%)	238 (96%)	9 (4%)	0	100	100
1	B	252/288 (88%)	245 (97%)	7 (3%)	0	100	100
1	C	246/288 (85%)	238 (97%)	8 (3%)	0	100	100
1	D	250/288 (87%)	242 (97%)	8 (3%)	0	100	100
All	All	995/1152 (86%)	963 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/231 (87%)	202 (100%)	0	100	100
1	B	207/231 (90%)	205 (99%)	2 (1%)	76	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	200/231 (87%)	197 (98%)	3 (2%)	65	69
1	D	204/231 (88%)	200 (98%)	4 (2%)	55	58
All	All	813/924 (88%)	804 (99%)	9 (1%)	73	78

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

Mol	Chain	Res	Type
1	B	229	ARG
1	B	230	ARG
1	C	164	VAL
1	C	216	GLU
1	C	250	GLN
1	D	47	GLU
1	D	53	SER
1	D	206	VAL
1	D	229	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	54	ASN
1	A	236	GLN
1	B	179	HIS
1	B	236	GLN
1	D	67[A]	ASN
1	D	166	GLN
1	D	179	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	DX8	D	270	-	22,23,23	2.27	3 (13%)	22,33,33	2.76	7 (31%)
3	DX8	B	270	-	22,23,23	2.17	3 (13%)	22,33,33	2.93	7 (31%)
4	ACT	A	271	-	1,3,3	1.15	0	0,3,3	0.00	-
3	DX8	C	270	-	22,23,23	2.12	3 (13%)	22,33,33	2.86	7 (31%)
3	DX8	A	270	-	22,23,23	2.11	3 (13%)	22,33,33	2.93	5 (22%)
2	NAP	B	269	-	45,52,52	1.67	4 (8%)	56,80,80	1.44	5 (8%)
2	NAP	A	269	-	45,52,52	1.78	4 (8%)	56,80,80	1.22	4 (7%)
2	NAP	D	269	-	45,52,52	1.58	4 (8%)	56,80,80	1.32	4 (7%)
2	NAP	C	269	-	45,52,52	1.52	4 (8%)	56,80,80	1.45	4 (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
2	NAP	A	269	-	-	0/31/67/67	0/5/5/5
3	DX8	B	270	-	-	4/6/8/8	0/3/3/3
3	DX8	C	270	-	-	2/6/8/8	0/3/3/3
3	DX8	A	270	-	-	4/6/8/8	0/3/3/3
2	NAP	B	269	-	-	1/31/67/67	0/5/5/5
3	DX8	D	270	-	-	4/6/8/8	0/3/3/3
2	NAP	D	269	-	-	0/31/67/67	0/5/5/5
2	NAP	C	269	-	-	0/31/67/67	0/5/5/5

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	269	NAP	O7N-C7N	8.84	1.41	1.24
2	B	269	NAP	O7N-C7N	8.31	1.40	1.24
3	D	270	DX8	CAP-CAR	-7.99	1.40	1.49
2	D	269	NAP	O7N-C7N	7.72	1.38	1.24
3	B	270	DX8	CAP-CAR	-7.72	1.40	1.49
3	A	270	DX8	CAP-CAR	-7.64	1.40	1.49
3	C	270	DX8	CAP-CAR	-7.59	1.40	1.49
2	C	269	NAP	O7N-C7N	7.25	1.38	1.24
3	D	270	DX8	CAS-NAK	4.89	1.41	1.33
3	B	270	DX8	CAS-NAK	4.49	1.40	1.33
2	B	269	NAP	C2A-N3A	4.38	1.39	1.32
3	C	270	DX8	CAS-NAK	4.36	1.40	1.33
2	A	269	NAP	C2A-N3A	4.28	1.39	1.32
3	A	270	DX8	CAS-NAK	4.06	1.40	1.33
2	D	269	NAP	C2A-N3A	3.96	1.38	1.32
2	C	269	NAP	C2A-N3A	3.81	1.38	1.32
3	D	270	DX8	CAN-NAK	3.79	1.42	1.35
2	A	269	NAP	C2N-N1N	3.57	1.39	1.35
3	C	270	DX8	CAN-NAK	3.42	1.41	1.35
3	B	270	DX8	CAN-NAK	3.21	1.41	1.35
3	A	270	DX8	CAN-NAK	3.04	1.40	1.35
2	D	269	NAP	C2A-N1A	2.94	1.39	1.33
2	B	269	NAP	C2A-N1A	2.82	1.39	1.33
2	A	269	NAP	C2A-N1A	2.68	1.38	1.33
2	C	269	NAP	C2A-N1A	2.63	1.38	1.33
2	C	269	NAP	C2N-N1N	2.25	1.37	1.35
2	B	269	NAP	C2N-N1N	2.20	1.37	1.35
2	D	269	NAP	O4B-C4B	-2.06	1.40	1.45

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	270	DX8	CAS-CAU-CAT	8.04	119.55	115.01
3	B	270	DX8	CAS-CAU-CAT	7.81	119.42	115.01
3	C	270	DX8	CAS-CAU-CAT	7.55	119.27	115.01
3	B	270	DX8	CAU-CAS-NAK	-7.19	117.71	124.09
3	D	270	DX8	CAS-CAU-CAT	6.81	118.85	115.01
3	D	270	DX8	CAU-CAS-NAK	-6.62	118.22	124.09
3	A	270	DX8	CAU-CAS-NAK	-6.45	118.36	124.09
3	C	270	DX8	CAU-CAS-NAK	-6.39	118.41	124.09
2	C	269	NAP	N3A-C2A-N1A	-5.96	119.37	128.68
2	D	269	NAP	N3A-C2A-N1A	-5.61	119.92	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	269	NAP	N3A-C2A-N1A	-5.57	119.97	128.68
3	C	270	DX8	NAJ-CAN-NAK	-5.53	119.84	127.22
3	A	270	DX8	CAN-NAJ-CAT	5.37	121.50	115.36
3	D	270	DX8	NAJ-CAN-NAK	-5.31	120.14	127.22
2	C	269	NAP	C3N-C7N-N7N	5.31	124.12	117.75
3	A	270	DX8	NAJ-CAN-NAK	-5.26	120.20	127.22
3	D	270	DX8	CAN-NAJ-CAT	5.21	121.30	115.36
3	C	270	DX8	CAN-NAJ-CAT	5.19	121.29	115.36
2	B	269	NAP	N3A-C2A-N1A	-5.07	120.75	128.68
3	B	270	DX8	CAN-NAJ-CAT	4.93	120.98	115.36
3	B	270	DX8	NAJ-CAN-NAK	-4.87	120.73	127.22
2	B	269	NAP	O7N-C7N-C3N	-4.83	113.85	119.63
2	B	269	NAP	C3N-C7N-N7N	4.69	123.38	117.75
2	C	269	NAP	O7N-C7N-C3N	-3.72	115.18	119.63
2	D	269	NAP	C3N-C7N-N7N	3.48	121.92	117.75
2	D	269	NAP	O7N-C7N-C3N	-3.29	115.69	119.63
2	A	269	NAP	C1B-N9A-C4A	-2.85	121.63	126.64
3	C	270	DX8	CAS-NAK-CAN	2.64	120.12	115.93
3	B	270	DX8	CAS-NAK-CAN	2.59	120.05	115.93
3	A	270	DX8	CAS-NAK-CAN	2.56	119.99	115.93
2	C	269	NAP	C1B-N9A-C4A	-2.54	122.17	126.64
3	D	270	DX8	CAS-NAK-CAN	2.49	119.89	115.93
3	B	270	DX8	CAI-CAP-CAR	-2.37	116.85	120.61
3	B	270	DX8	CAH-CAP-CAR	2.33	124.30	120.61
2	A	269	NAP	C3N-C7N-N7N	2.21	120.40	117.75
2	D	269	NAP	C1B-N9A-C4A	-2.20	122.77	126.64
3	C	270	DX8	NAC-CAN-NAJ	2.17	121.33	117.79
3	D	270	DX8	CAR-CAQ-CAE	-2.14	124.25	127.33
2	B	269	NAP	O3D-C3D-C4D	-2.13	104.89	111.05
2	B	269	NAP	C1B-N9A-C4A	-2.09	122.97	126.64
2	A	269	NAP	C4A-C5A-N7A	-2.07	107.24	109.40
3	D	270	DX8	NAC-CAN-NAK	2.06	120.45	117.25
3	C	270	DX8	CAI-CAP-CAR	-2.02	117.41	120.61

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	270	DX8	CAH-CAP-CAR-CAQ
3	B	270	DX8	CAH-CAP-CAR-CAQ
3	B	270	DX8	CAG-CAO-OAM-CAA
3	B	270	DX8	CAF-CAO-OAM-CAA

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Mol	Chain	Res	Type	Atoms
3	D	270	DX8	CAG-CAO-OAM-CAA
3	D	270	DX8	CAF-CAO-OAM-CAA
3	D	270	DX8	CAI-CAP-CAR-CAQ
3	A	270	DX8	CAG-CAO-OAM-CAA
3	A	270	DX8	CAF-CAO-OAM-CAA
3	A	270	DX8	CAH-CAP-CAR-CAQ
3	B	270	DX8	CAI-CAP-CAR-CAQ
3	A	270	DX8	CAI-CAP-CAR-CAQ
3	C	270	DX8	CAG-CAO-OAM-CAA
2	B	269	NAP	C5B-O5B-PA-O1A
3	C	270	DX8	CAH-CAP-CAR-CAQ

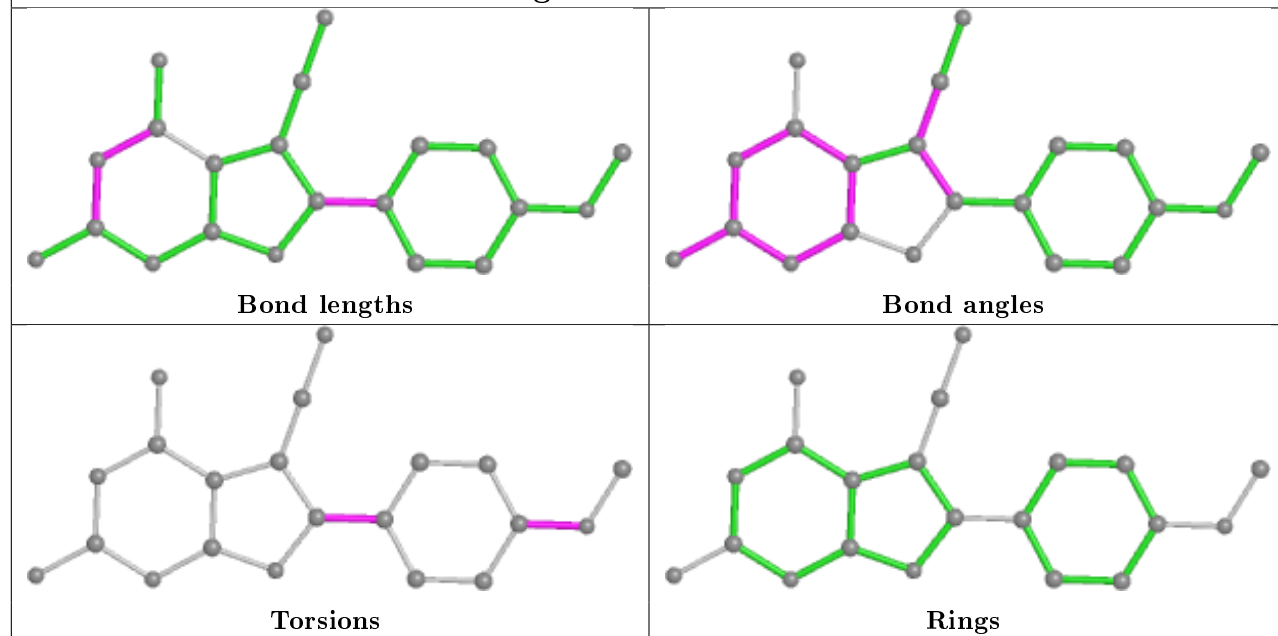
There are no ring outliers.

5 monomers are involved in 18 short contacts:

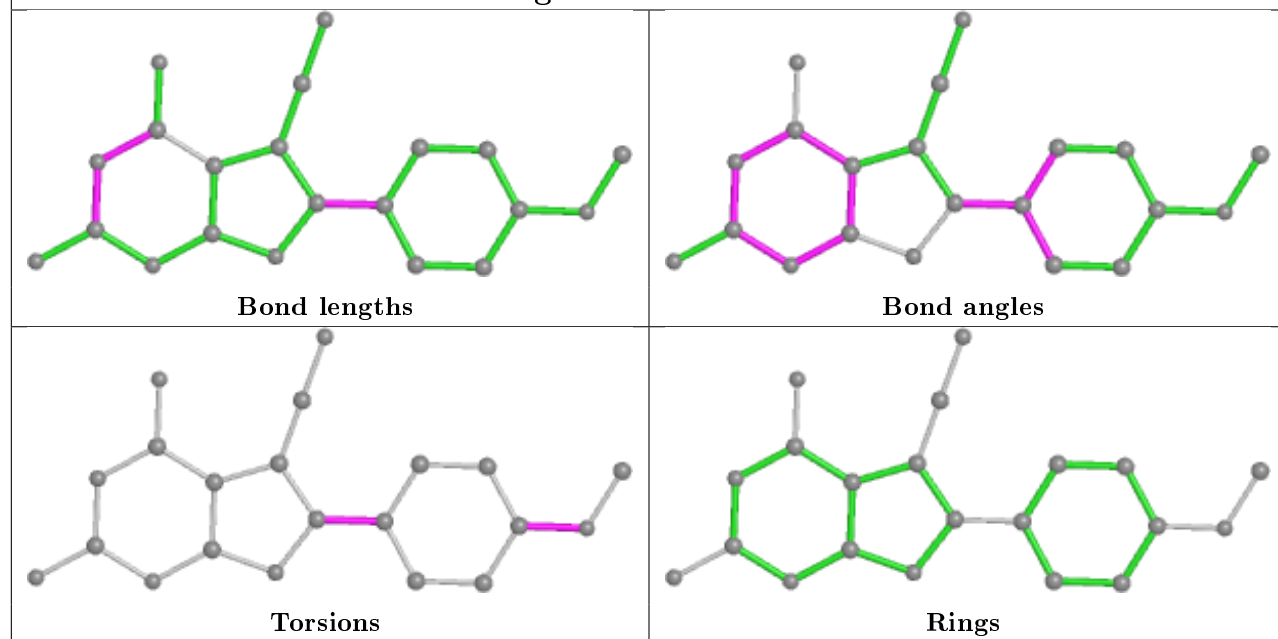
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	270	DX8	4	0
3	B	270	DX8	2	0
3	C	270	DX8	5	0
3	A	270	DX8	6	0
2	B	269	NAP	1	0

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.

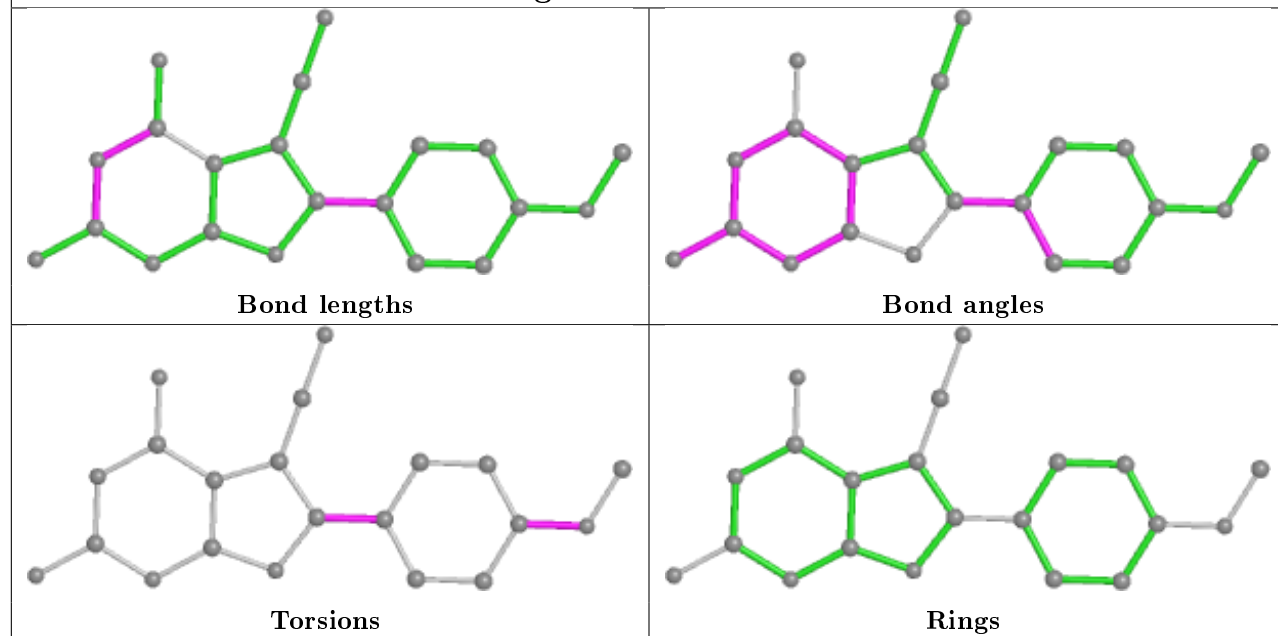
Ligand DX8 D 270



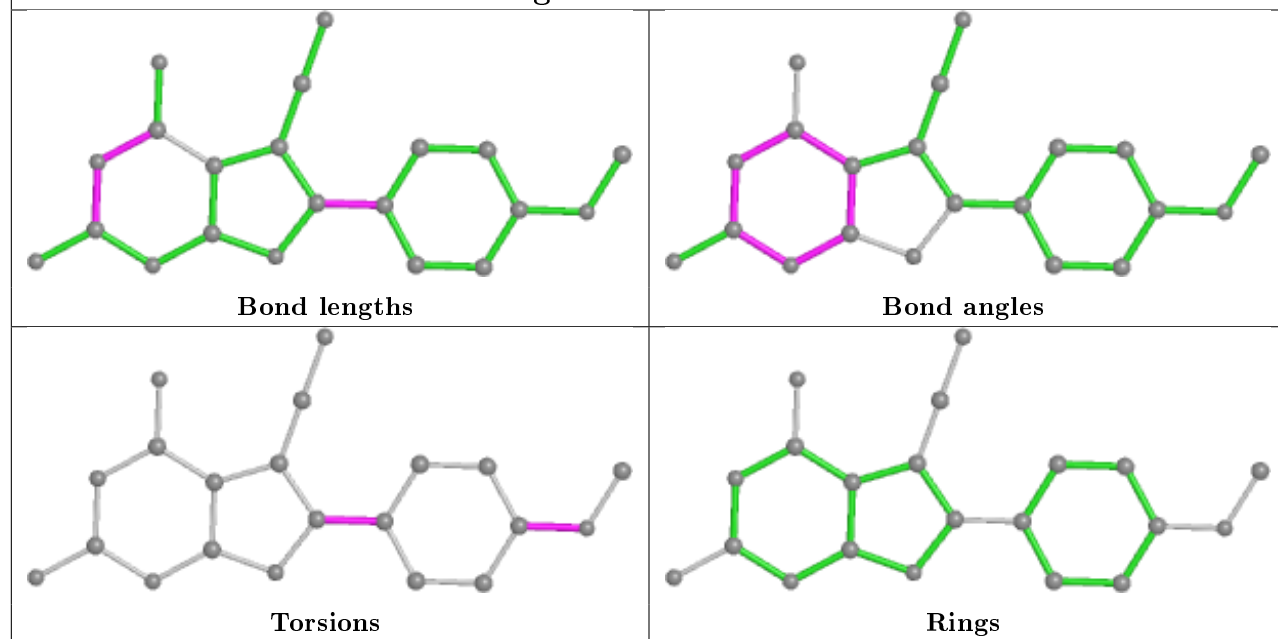
Ligand DX8 B 270

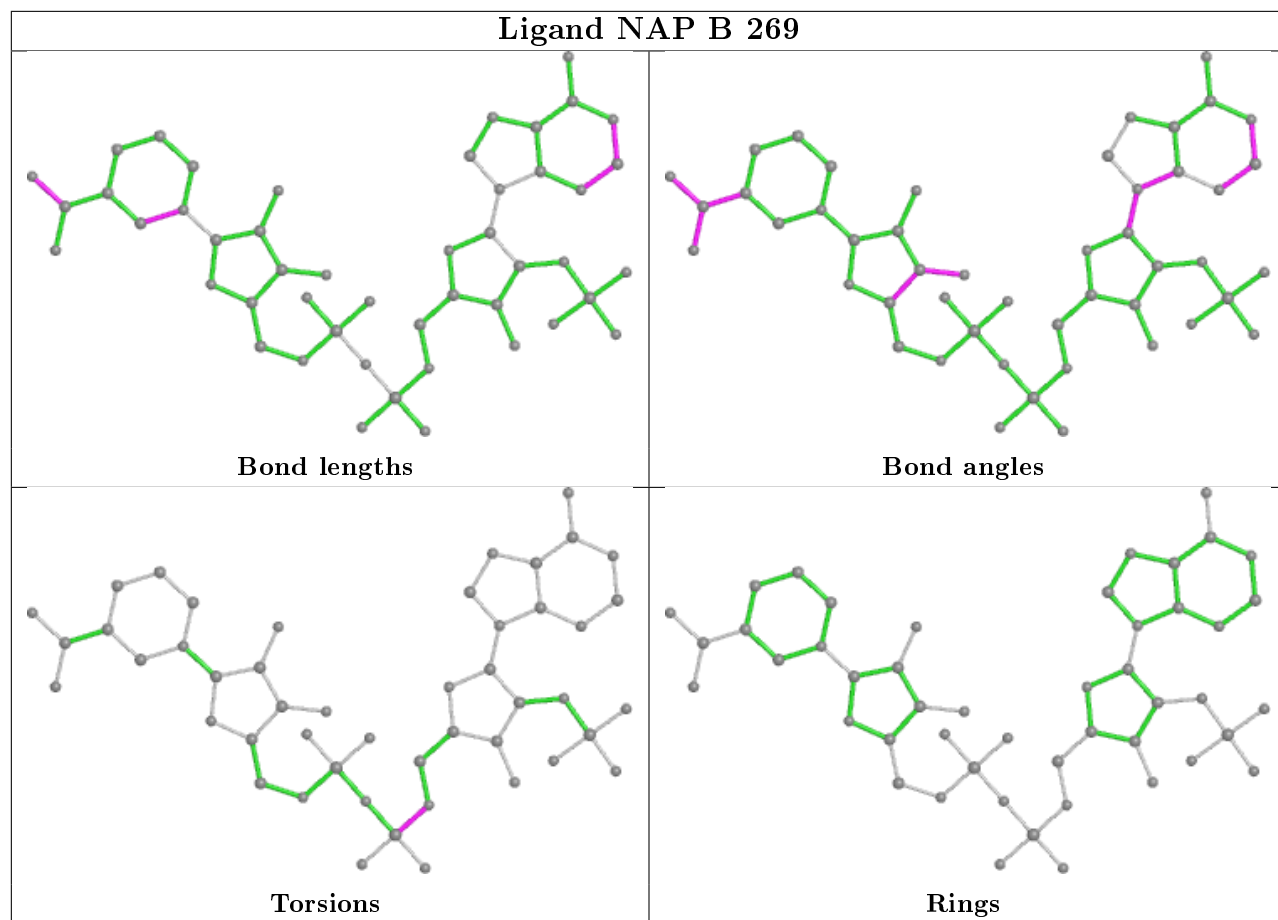


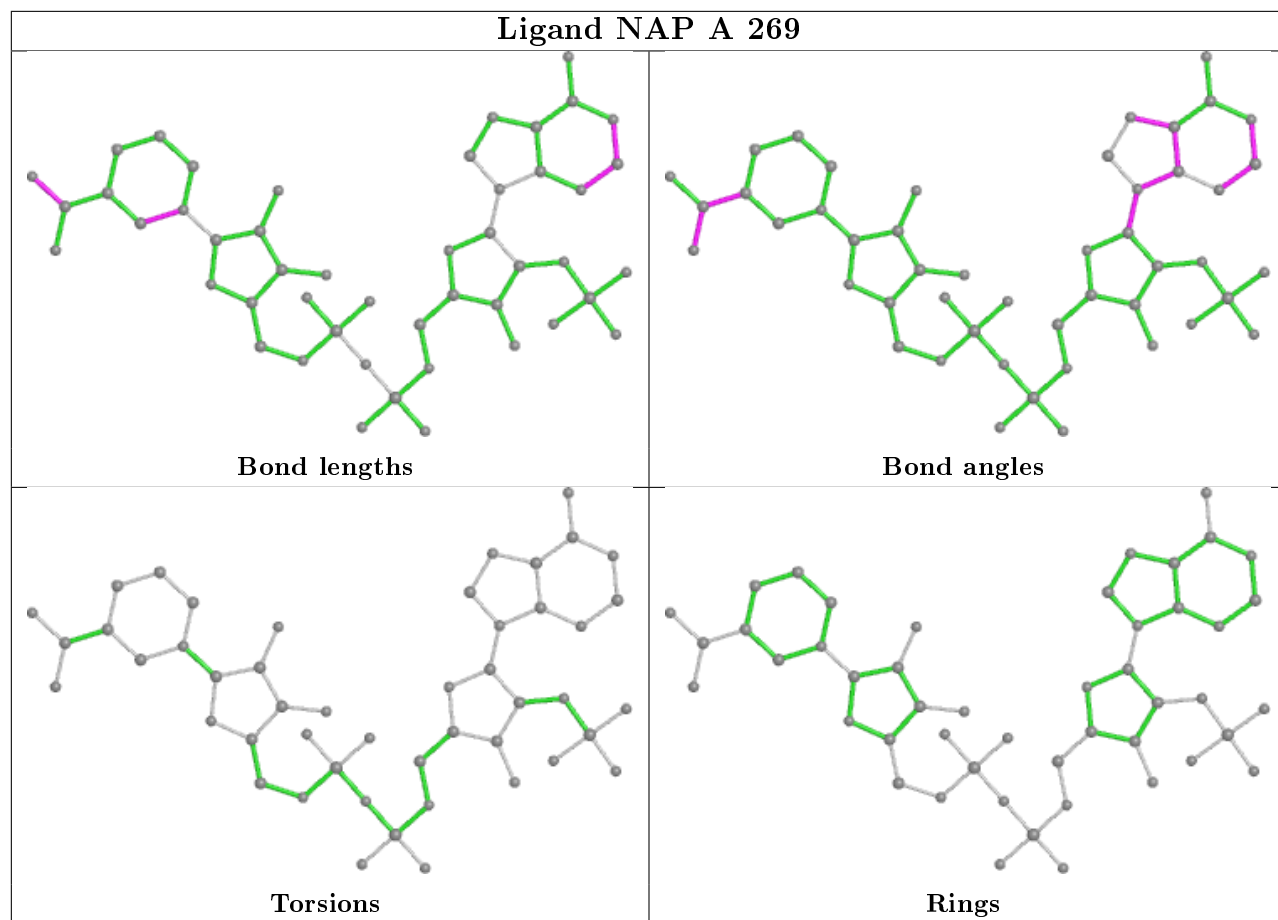
Ligand DX8 C 270

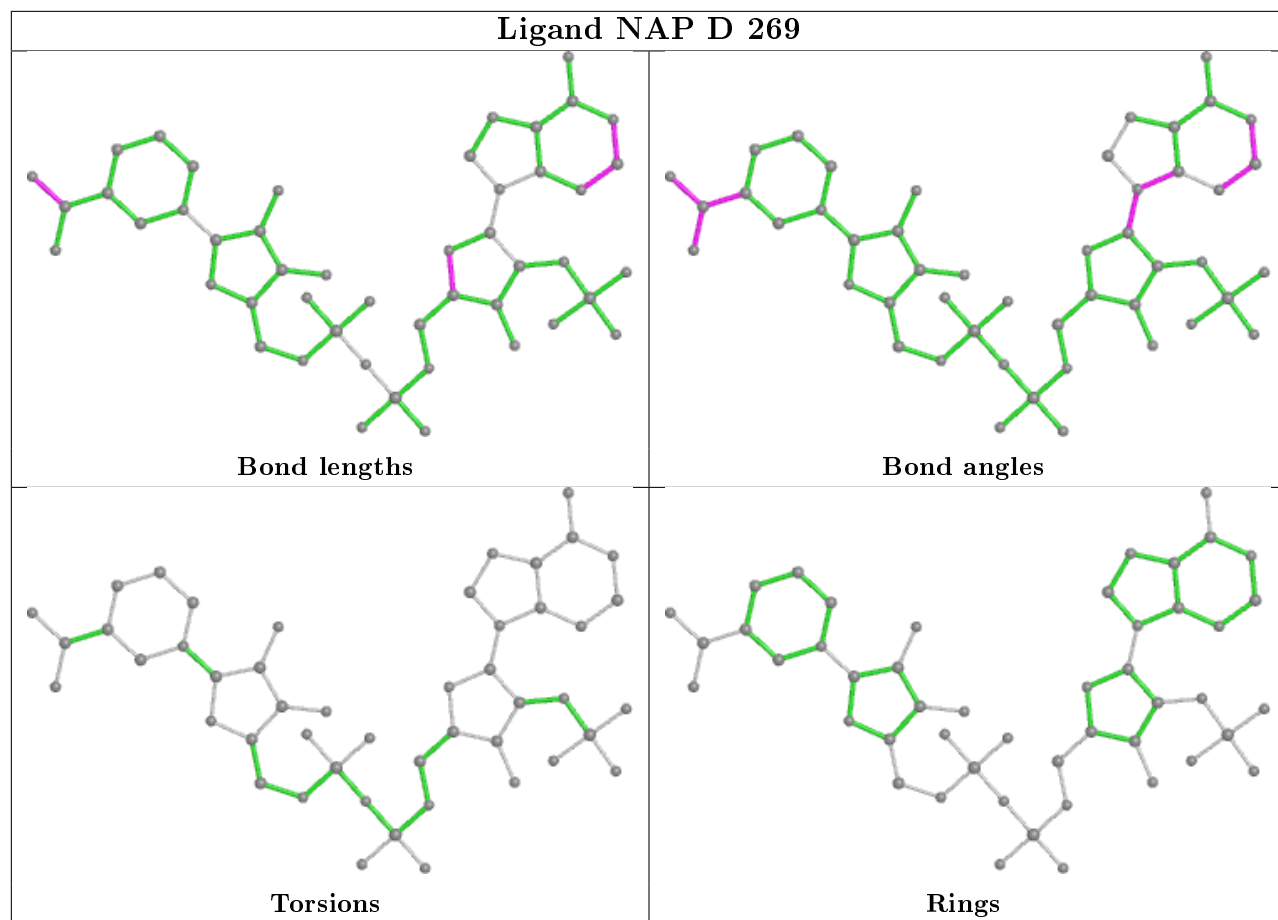


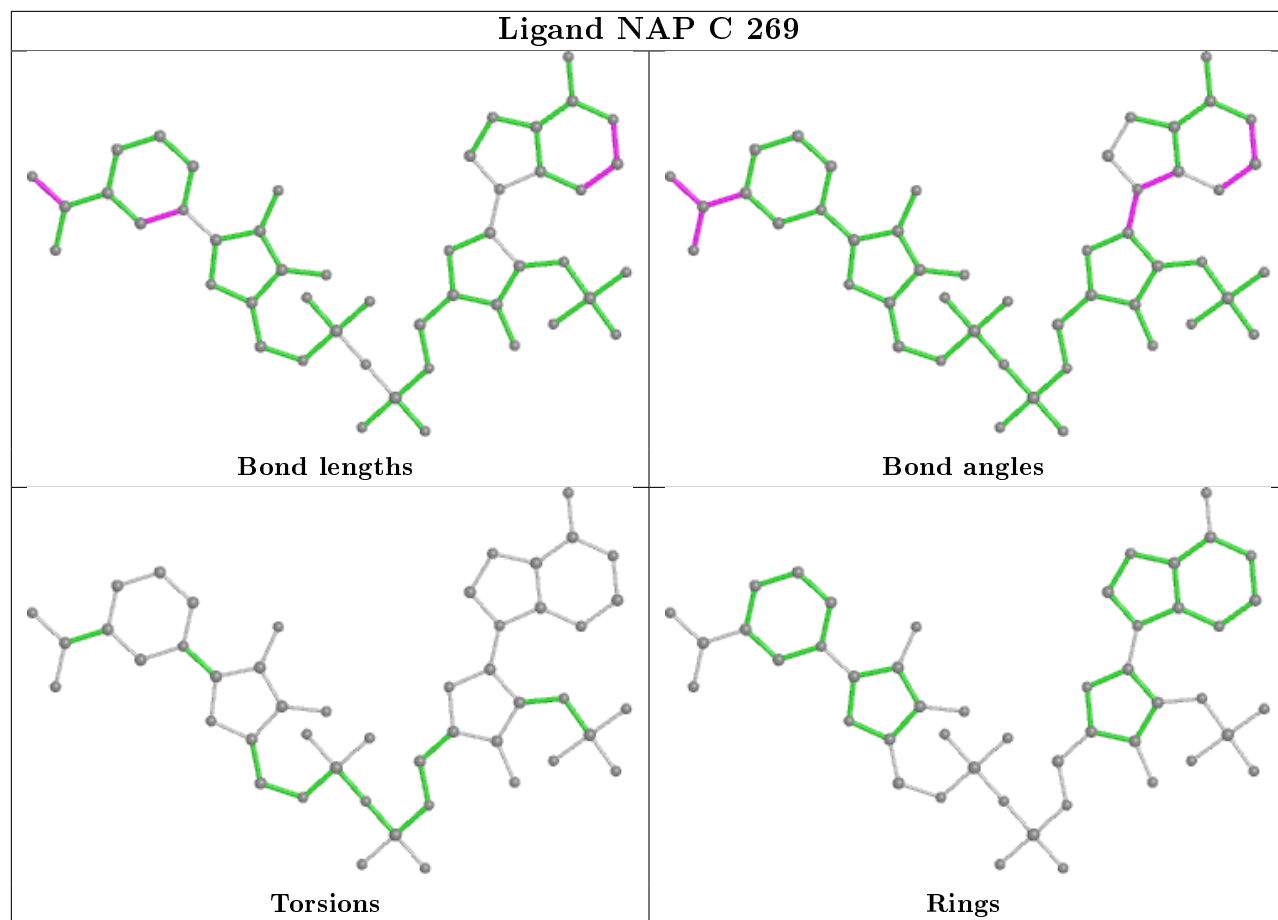
Ligand DX8 A 270











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	249/288 (86%)	-0.23	2 (0%) 86 85	9, 15, 22, 34	3 (1%)
1	B	248/288 (86%)	-0.32	4 (1%) 72 70	9, 14, 24, 35	0
1	C	249/288 (86%)	-0.17	7 (2%) 53 51	8, 14, 25, 48	1 (0%)
1	D	249/288 (86%)	-0.21	1 (0%) 92 92	9, 14, 24, 37	1 (0%)
All	All	995/1152 (86%)	-0.23	14 (1%) 75 74	8, 14, 24, 48	5 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	113	GLY	5.8
1	B	212	ALA	4.8
1	C	212	ALA	4.4
1	C	216	GLU	4.1
1	B	113	GLY	3.7
1	B	211	VAL	3.6
1	C	195	TYR	3.2
1	A	113	GLY	2.5
1	D	2	GLU	2.4
1	C	2	GLU	2.4
1	C	143	LYS	2.3
1	A	50	LYS	2.1
1	C	217[A]	GLU	2.0
1	B	2[A]	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

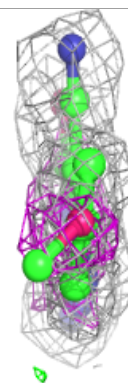
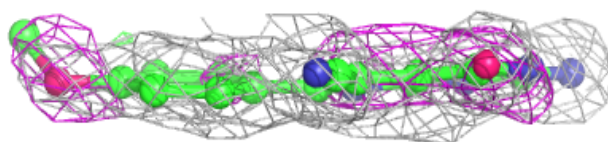
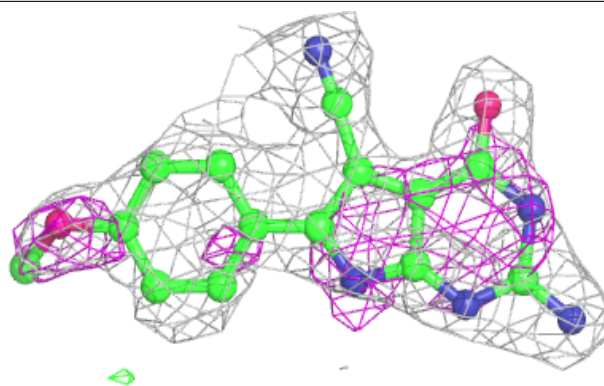
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	DX8	D	270	21/21	0.84	0.29	24,29,33,36	0
3	DX8	C	270	21/21	0.87	0.29	21,29,40,41	0
3	DX8	B	270	21/21	0.89	0.21	17,25,33,35	0
3	DX8	A	270	21/21	0.89	0.26	22,27,34,36	0
2	NAP	A	269	48/48	0.97	0.07	11,14,18,19	0
2	NAP	C	269	48/48	0.97	0.08	10,14,21,22	0
4	ACT	A	271	4/4	0.98	0.11	16,16,17,18	0
2	NAP	D	269	48/48	0.98	0.07	8,14,19,21	0
2	NAP	B	269	48/48	0.98	0.06	10,15,20,21	0

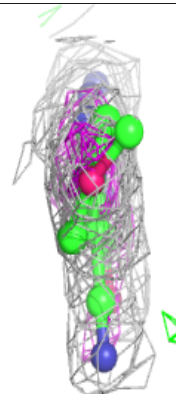
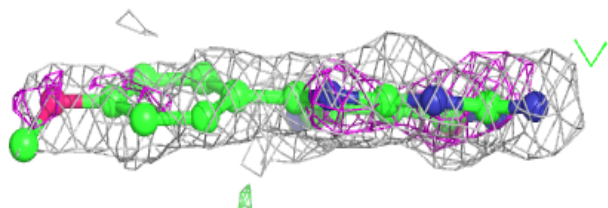
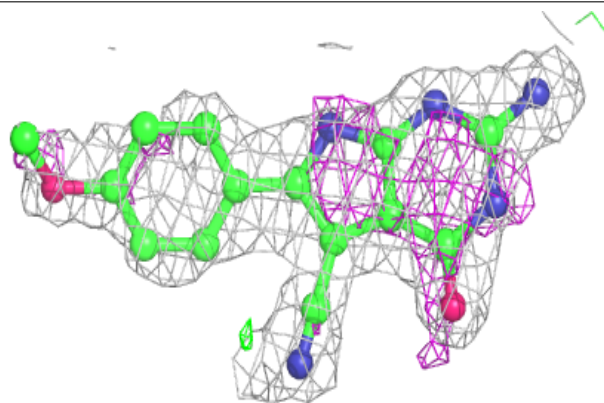
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DX8 D 270:

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

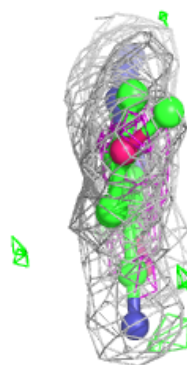
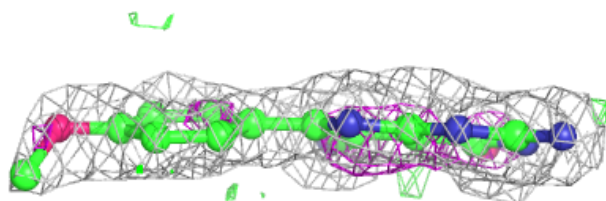
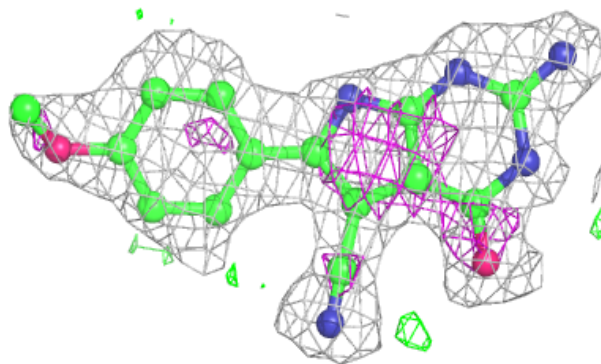
**Electron density around DX8 C 270:**

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

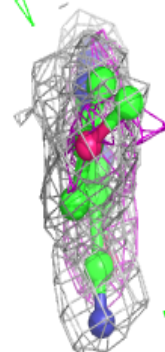
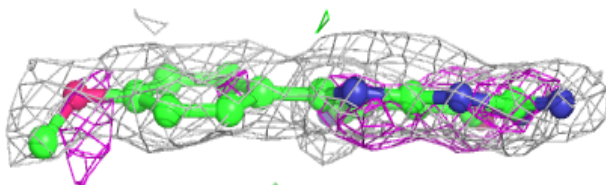
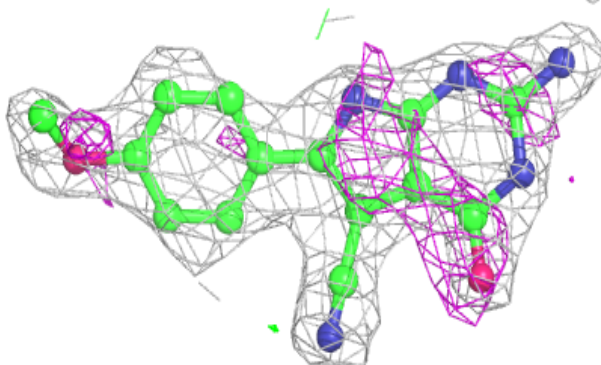


Electron density around DX8 B 270:

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

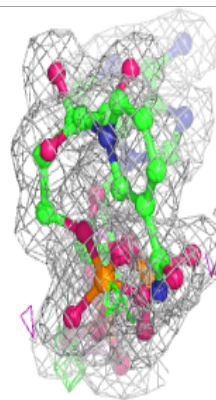
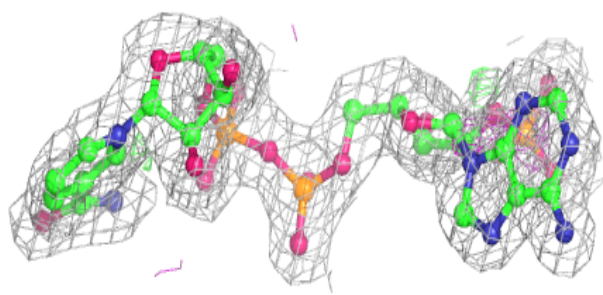
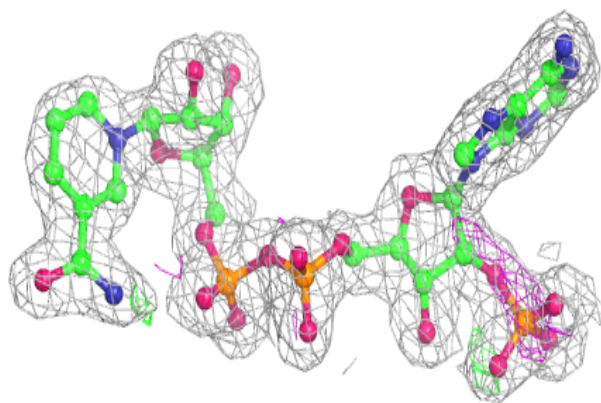
**Electron density around DX8 A 270:**

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

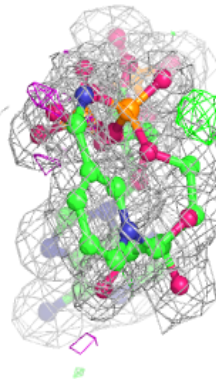
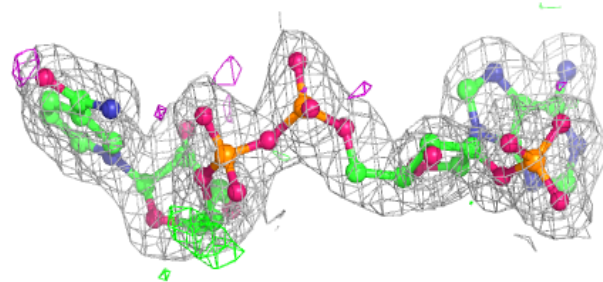
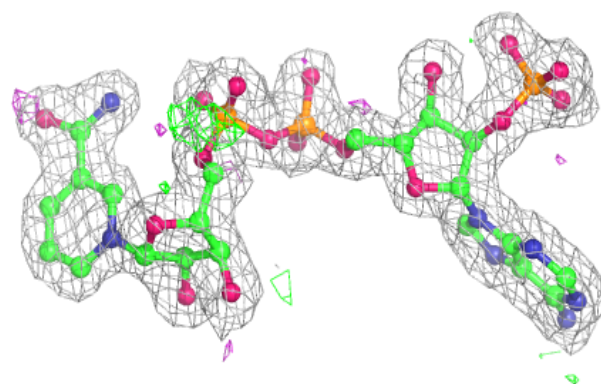


Electron density around NAP A 269:

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

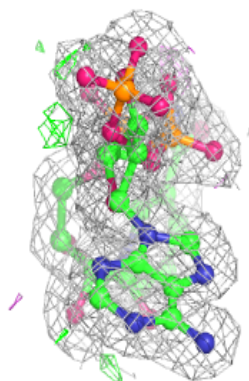
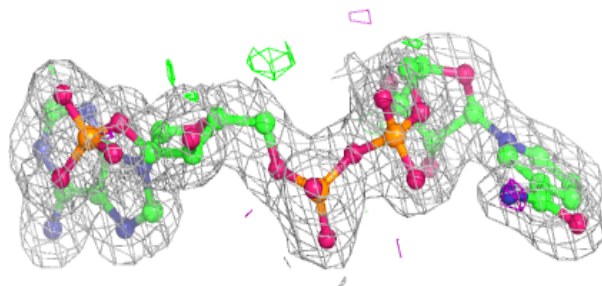
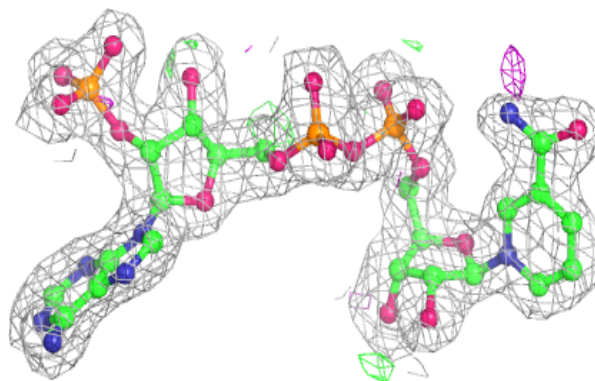
**Electron density around NAP C 269:**

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

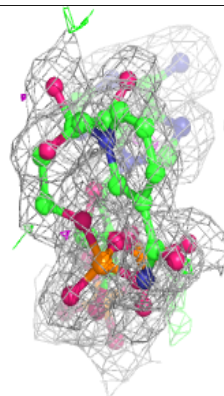
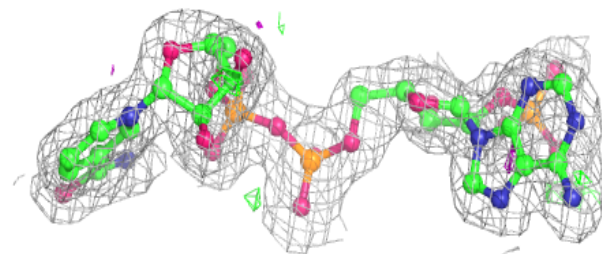
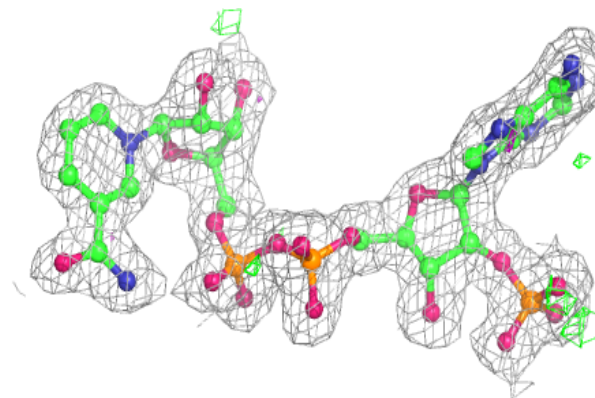


Electron density around NAP D 269:

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

**Electron density around NAP B 269:**

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



6.5 Other polymers

There are no such residues in this entry.