



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 07:45 PM BST

PDB ID : 4CM8
Title : Crystal structure of pteridine reductase 1 (PTR1) from Trypanosoma brucei in ternary complex with cofactor and inhibitor
Authors : Barrack, K.L.; Hunter, W.N.
Deposited on : 2014-01-15
Resolution : 1.90 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 : 2.13.1
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) : 2.13.1

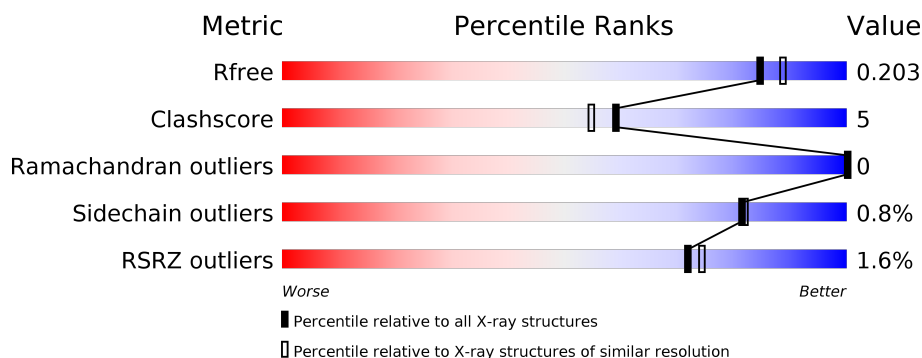
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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>2%</div> <div>80% 7% 13%</div> </div>
1	C	288	<div> <div>2%</div> <div>78% 8% 14%</div> </div>
1	D	288	<div> <div>2%</div> <div>78% 8% 13%</div> </div>
2	B	288	<div> <div>2%</div> <div>82% 5% 13%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	IZ9	C	1270	-	-	X	-
4	IZ9	D	1270	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8958 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	250	Total	C	N	O	S	0	5	0
			1888	1189	331	357	11			
1	C	249	Total	C	N	O	S	0	7	0
			1898	1192	335	360	11			
1	D	250	Total	C	N	O	S	0	9	0
			1926	1211	338	365	12			

There are 60 discrepancies between the modelled and reference sequences:

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

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

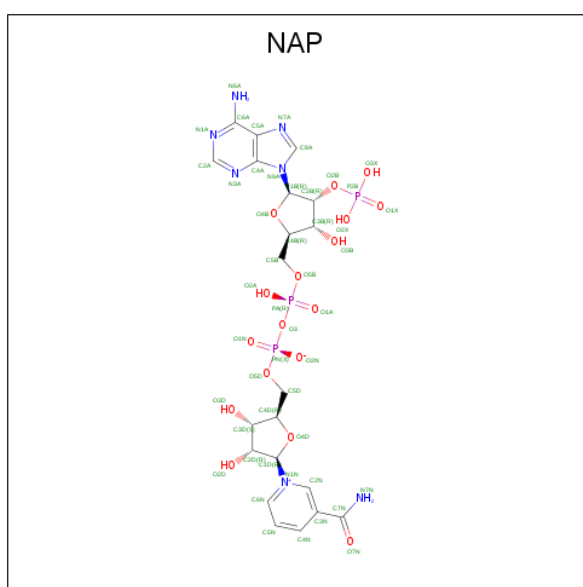
- Molecule 2 is a protein called PTERIDINE REDUCTASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	251	Total	C	N	O	S	0	3	0
			1889	1184	333	361	11			

There are 20 discrepancies between the modelled and reference sequences:

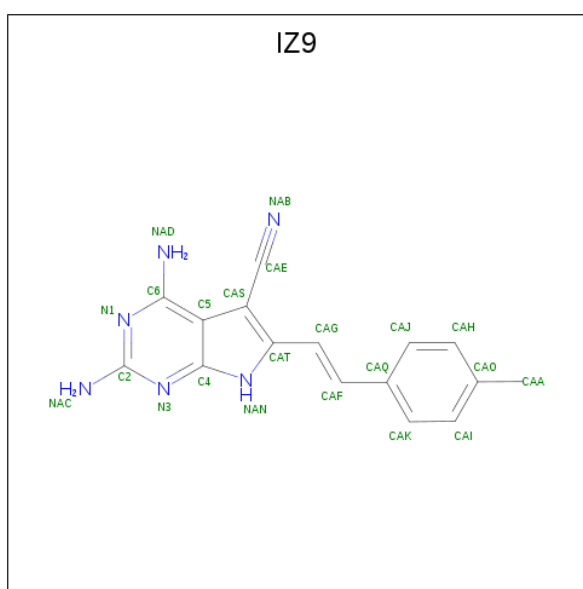
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP O76290
B	-18	GLY	-	expression tag	UNP O76290
B	-17	SER	-	expression tag	UNP O76290
B	-16	SER	-	expression tag	UNP O76290
B	-15	HIS	-	expression tag	UNP O76290
B	-14	HIS	-	expression tag	UNP O76290
B	-13	HIS	-	expression tag	UNP O76290
B	-12	HIS	-	expression tag	UNP O76290
B	-11	HIS	-	expression tag	UNP O76290
B	-10	HIS	-	expression tag	UNP O76290
B	-9	SER	-	expression tag	UNP O76290
B	-8	SER	-	expression tag	UNP O76290
B	-7	GLY	-	expression tag	UNP O76290
B	-6	LEU	-	expression tag	UNP O76290
B	-5	VAL	-	expression tag	UNP O76290
B	-4	PRO	-	expression tag	UNP O76290
B	-3	ARG	-	expression tag	UNP O76290
B	-2	GLY	-	expression tag	UNP O76290
B	-1	SER	-	expression tag	UNP O76290
B	0	HIS	-	expression tag	UNP O76290

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

- Molecule 4 is (E)-2,4-diamino-6-(4-methylstyryl)-7H-pyrrolo[2,3-d]pyrimidine-5-carbonitrile (three-letter code: IZ9) (formula: C₁₆H₁₄N₆).



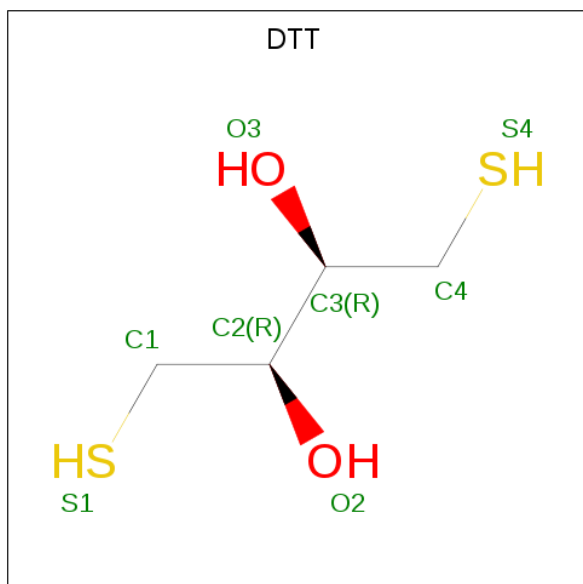
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			22	16	6		
4	B	1	Total	C	N	0	0
			22	16	6		
4	C	1	Total	C	N	0	0
			22	16	6		
4	D	1	Total	C	N	0	0
			22	16	6		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 6 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



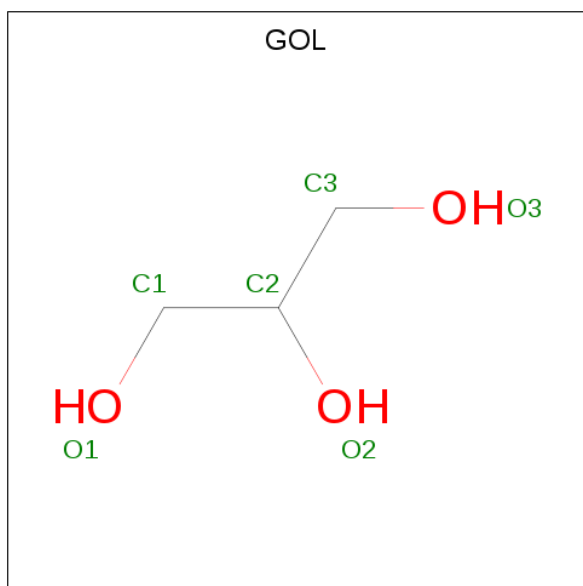
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	S	0
			8	4	2	2	

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



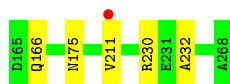
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	303	Total	O	0	0
			303	303		
8	B	290	Total	O	0	0
			290	290		
8	C	242	Total	O	0	0
			242	242		
8	D	206	Total	O	0	0
			206	206		

- Molecule 1: PTERIDINE REDUCTASE 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.60 Å 90.00 Å 82.60 Å 90.00° 115.57° 90.00°	Depositor
Resolution (Å)	15.50 – 1.90 15.43 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.0 (15.50-1.90) 92.2 (15.43-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 1.90 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.141 , 0.192 0.156 , 0.203	Depositor DCC
R_{free} test set	3576 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	12.3	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8958	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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 26.86 % 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 2.4410e-03. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAP, CSX, ACT, IZ9, DTT

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	0.71	0/1919	0.82	4/2603 (0.2%)
1	C	0.72	0/1931	0.79	3/2616 (0.1%)
1	D	0.71	0/1960	0.81	2/2658 (0.1%)
2	B	0.74	0/1919	0.80	0/2603
All	All	0.72	0/7729	0.80	9/10480 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	141	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	82	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	D	222	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	239	ASP	CB-CG-OD1	5.65	123.39	118.30
1	C	141	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	141	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	209	LEU	CA-CB-CG	-5.30	103.11	115.30
1	D	141	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	82	ARG	NE-CZ-NH1	5.26	122.93	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1888	0	1924	15	0
1	C	1898	0	1931	20	0
1	D	1926	0	1961	29	0
2	B	1889	0	1905	13	0
3	A	48	0	25	0	0
3	B	48	0	25	1	0
3	C	48	0	25	0	0
3	D	48	0	25	1	0
4	A	22	0	14	1	0
4	B	22	0	14	0	0
4	C	22	0	14	8	0
4	D	22	0	14	7	0
5	A	4	0	3	0	0
5	C	4	0	3	0	0
6	A	8	0	10	0	0
6	B	8	0	10	1	0
7	C	6	0	8	1	0
7	D	6	0	8	1	0
8	A	303	0	0	7	0
8	B	290	0	0	11	0
8	C	242	0	0	3	0
8	D	206	0	0	7	0
All	All	8958	0	7919	74	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 (74) 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:217:GLU:HG2	8:C:2194:HOH:O	1.52	1.09
2:B:117[B]:GLU:OE1	8:B:2174:HOH:O	1.86	0.94
2:B:211:VAL:O	8:B:2233:HOH:O	1.90	0.89
6:B:1271:DTT:S4	8:B:2290:HOH:O	2.42	0.77
1:D:175[A]:ASN:HB2	8:D:2159:HOH:O	1.84	0.75
1:D:164[B]:VAL:HG22	1:D:179:HIS:CD2	2.22	0.73
8:A:2214:HOH:O	1:C:175[A]:ASN:ND2	2.06	0.71
1:D:168:CSX:HG	4:D:1270:IZ9:CAH	2.04	0.71
1:D:175[B]:ASN:OD1	8:D:2150:HOH:O	2.11	0.68
1:C:168:CSX:HG	4:C:1270:IZ9:CAI	2.09	0.66
2:B:175[A]:ASN:HB2	8:B:2215:HOH:O	1.96	0.66
1:A:168:CSX:HG	4:A:1270:IZ9:CAI	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:GLU:OE1	8:B:2142:HOH:O	2.15	0.64
1:D:62:ASP:OD1	1:D:64[B]:THR:HG23	1.99	0.61
1:C:168:CSX:HG	4:C:1270:IZ9:CAK	2.13	0.61
1:D:168:CSX:HG	4:D:1270:IZ9:CAJ	2.13	0.60
2:B:104:GLN:HG2	1:D:140:GLN:HE22	1.66	0.59
8:B:2168:HOH:O	1:D:140:GLN:NE2	2.27	0.58
1:D:113:GLY:N	8:D:2122:HOH:O	2.36	0.57
8:B:2217:HOH:O	1:D:175[A]:ASN:ND2	2.13	0.57
1:D:210:PRO:HD3	4:D:1270:IZ9:NAB	2.19	0.56
1:C:168:CSX:SG	4:C:1270:IZ9:CAI	2.94	0.56
1:C:75:GLU:OE1	8:C:2117:HOH:O	2.18	0.56
1:D:164[B]:VAL:HG22	1:D:179:HIS:NE2	2.22	0.55
1:A:175[A]:ASN:HB2	8:A:2212:HOH:O	2.06	0.55
1:A:212:ALA:HB3	8:A:2129:HOH:O	2.07	0.53
1:A:175[B]:ASN:HB2	8:A:2212:HOH:O	2.09	0.53
1:A:46:ASP:O	1:A:50:LYS:HD3	2.08	0.53
1:A:65:ASN:HA	1:A:69:LEU:HD22	1.91	0.52
7:C:1272:GOL:H11	8:C:2242:HOH:O	2.09	0.52
1:D:168:CSX:SG	4:D:1270:IZ9:CAH	2.97	0.52
1:D:9:THR:HA	1:D:33:HIS:HB3	1.91	0.52
1:C:138:PHE:O	1:C:142[B]:GLN:HG2	2.10	0.51
1:D:46:ASP:CB	8:D:2059:HOH:O	2.60	0.50
1:A:22:LYS:HG2	1:A:242:ILE:HG12	1.94	0.49
1:A:46:ASP:O	1:A:50:LYS:CD	2.62	0.48
1:A:251:TYR:CE2	2:B:232:ALA:HB2	2.48	0.48
1:A:50:LYS:HD2	1:A:50:LYS:N	2.28	0.48
1:A:220:LYS:HD2	8:A:2247:HOH:O	2.14	0.48
2:B:102:LEU:O	1:D:136[B]:MET:HG3	2.14	0.48
1:D:161:ASP:HB3	1:D:164[A]:VAL:HG13	1.96	0.48
1:C:9:THR:HA	1:C:33:HIS:HB3	1.96	0.47
1:A:175[A]:ASN:ND2	8:A:2196:HOH:O	2.20	0.47
2:B:104:GLN:HG2	1:D:140:GLN:NE2	2.30	0.47
1:C:236:GLN:HE21	1:D:250[B]:GLN:CG	2.28	0.47
1:A:267:HIS:CD2	4:D:1270:IZ9:HAA3	2.50	0.47
1:D:46:ASP:HB3	8:D:2059:HOH:O	2.15	0.46
1:C:65:ASN:HA	1:C:69:LEU:HD22	1.99	0.45
1:A:9:THR:HA	1:A:33:HIS:HB3	1.98	0.45
1:C:163:MET:CE	4:C:1270:IZ9:HAA3	2.47	0.45
8:B:2217:HOH:O	1:D:175[B]:ASN:ND2	2.50	0.44
1:D:9:THR:O	1:D:93:ASN:HB3	2.17	0.44
2:B:230:ARG:HD2	8:B:2268:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175[B]:ASN:HB2	8:B:2215:HOH:O	2.18	0.44
1:D:65:ASN:HA	1:D:69:LEU:HD22	1.98	0.44
1:C:46:ASP:O	1:C:50:LYS:HG3	2.17	0.44
1:C:95:SER:CB	4:C:1270:IZ9:HAC2	2.31	0.43
1:D:213:MET:CE	7:D:1271:GOL:H11	2.49	0.43
1:C:221:TRP:HH2	4:C:1270:IZ9:HAA2	1.84	0.43
1:C:221:TRP:CH2	4:C:1270:IZ9:HAA2	2.55	0.42
1:A:17:ARG:HG3	1:A:44:LEU:HD22	2.01	0.41
3:D:1269:NAP:O2A	4:D:1270:IZ9:N1	2.53	0.41
2:B:15:ILE:HB	3:B:1269:NAP:H51N	2.01	0.41
1:C:193:ALA:N	1:C:194:PRO:CD	2.83	0.41
1:C:236:GLN:HE21	1:D:250[B]:GLN:CD	2.23	0.41
8:A:2214:HOH:O	1:C:175[B]:ASN:ND2	2.53	0.41
2:B:98:TYR:HB2	2:B:99:PRO:HD2	2.03	0.41
1:C:210:PRO:HD3	4:C:1270:IZ9:NAB	2.36	0.41
2:B:160:CYS:HB3	8:B:2192:HOH:O	2.20	0.41
1:C:33:HIS:HA	1:C:59:CYS:O	2.21	0.40
1:D:175[B]:ASN:HB2	8:D:2159:HOH:O	2.20	0.40
1:D:64[B]:THR:HG22	1:D:122:GLU:HG2	2.03	0.40
1:D:95:SER:CB	4:D:1270:IZ9:HAC2	2.35	0.40
1:D:220:LYS:CE	8:D:2176:HOH:O	2.69	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	248/288 (86%)	240 (97%)	8 (3%)	0	100	100
1	C	248/288 (86%)	240 (97%)	8 (3%)	0	100	100
1	D	253/288 (88%)	245 (97%)	8 (3%)	0	100	100
2	B	248/288 (86%)	242 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	997/1152 (86%)	967 (97%)	30 (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	202/230 (88%)	201 (100%)	1 (0%)	88	89
1	C	204/230 (89%)	203 (100%)	1 (0%)	88	89
1	D	207/230 (90%)	205 (99%)	2 (1%)	76	76
2	B	202/231 (87%)	200 (99%)	2 (1%)	76	76
All	All	815/921 (88%)	809 (99%)	6 (1%)	81	84

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
2	B	164	VAL
2	B	166	GLN
1	C	216	GLU
1	D	141	ARG
1	D	151	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	140	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

3 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	A	168	1	3,6,7	0.30	0	1,6,8	4.09	1 (100%)
1	CSX	D	168	1	3,6,7	0.62	0	1,6,8	2.69	1 (100%)
1	CSX	C	168	1	3,6,7	0.29	0	1,6,8	4.06	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	A	168	1	-	0/1/5/7	-
1	CSX	D	168	1	-	0/1/5/7	-
1	CSX	C	168	1	-	0/1/5/7	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	CSX	CA-CB-SG	-4.09	104.42	113.36
1	C	168	CSX	CA-CB-SG	-4.06	104.48	113.36
1	D	168	CSX	CA-CB-SG	-2.69	107.49	113.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	168	CSX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	168	CSX	3	0
1	C	168	CSX	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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$
7	GOL	C	1272	-	5,5,5	0.39	0	5,5,5	0.49	0
5	ACT	C	1271	-	1,3,3	3.27	1 (100%)	0,3,3	0.00	-
5	ACT	A	1271	-	1,3,3	1.83	0	0,3,3	0.00	-
7	GOL	D	1271	-	5,5,5	0.26	0	5,5,5	0.58	0
6	DTT	B	1271	-	7,7,7	0.52	0	4,8,8	0.68	0
4	IZ9	C	1270	-	23,24,24	1.55	5 (21%)	24,34,34	2.01	7 (29%)
3	NAP	B	1269	-	45,52,52	0.92	2 (4%)	56,80,80	1.38	6 (10%)
3	NAP	C	1269	-	45,52,52	0.80	1 (2%)	56,80,80	1.28	7 (12%)
6	DTT	A	1272	-	7,7,7	0.46	0	4,8,8	1.73	1 (25%)
4	IZ9	D	1270	-	23,24,24	1.51	4 (17%)	24,34,34	2.27	6 (25%)
3	NAP	A	1269	-	45,52,52	1.04	3 (6%)	56,80,80	1.23	7 (12%)
4	IZ9	B	1270	-	23,24,24	1.64	5 (21%)	24,34,34	1.59	5 (20%)
4	IZ9	A	1270	-	23,24,24	1.53	5 (21%)	24,34,34	2.23	7 (29%)
3	NAP	D	1269	-	45,52,52	0.88	2 (4%)	56,80,80	1.42	6 (10%)

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	NAP	B	1269	-	-	0/31/67/67	0/5/5/5
7	GOL	D	1271	-	-	2/4/4/4	-
6	DTT	B	1271	-	-	4/8/8/8	-
7	GOL	C	1272	-	-	0/4/4/4	-
4	IZ9	C	1270	-	-	0/3/7/7	0/3/3/3
3	NAP	C	1269	-	-	0/31/67/67	0/5/5/5
6	DTT	A	1272	-	-	4/8/8/8	-
4	IZ9	D	1270	-	-	0/3/7/7	0/3/3/3
3	NAP	A	1269	-	-	0/31/67/67	0/5/5/5
4	IZ9	B	1270	-	-	3/3/7/7	0/3/3/3
4	IZ9	A	1270	-	-	1/3/7/7	0/3/3/3
3	NAP	D	1269	-	-	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)
4	B	1270	IZ9	CAS-CAE	5.24	1.50	1.44
4	C	1270	IZ9	CAS-CAE	4.51	1.49	1.44
4	A	1270	IZ9	CAS-CAE	4.45	1.49	1.44
4	D	1270	IZ9	CAS-CAE	4.35	1.49	1.44
3	A	1269	NAP	P2B-O2B	3.51	1.65	1.59
5	C	1271	ACT	CH3-C	3.27	1.52	1.48
3	B	1269	NAP	O4D-C1D	3.26	1.45	1.41
4	C	1270	IZ9	C2-NAC	3.14	1.40	1.33
4	A	1270	IZ9	CAS-C5	-2.99	1.38	1.42
4	B	1270	IZ9	C6-NAD	2.91	1.44	1.34
4	D	1270	IZ9	C6-NAD	2.71	1.43	1.34
4	A	1270	IZ9	CAS-CAT	-2.70	1.37	1.41
4	B	1270	IZ9	C2-NAC	2.66	1.39	1.33
4	B	1270	IZ9	CAS-C5	-2.65	1.38	1.42
3	A	1269	NAP	C5A-C4A	2.63	1.47	1.40
4	D	1270	IZ9	CAS-CAT	-2.59	1.37	1.41
3	C	1269	NAP	C5A-C4A	2.59	1.47	1.40
3	D	1269	NAP	O4D-C1D	2.50	1.44	1.41
4	A	1270	IZ9	C2-NAC	2.47	1.38	1.33
3	D	1269	NAP	P2B-O2B	2.39	1.63	1.59
4	C	1270	IZ9	C6-NAD	2.39	1.42	1.34
4	A	1270	IZ9	C6-NAD	2.39	1.42	1.34
3	B	1269	NAP	C5A-C4A	2.25	1.46	1.40
4	D	1270	IZ9	CAS-C5	-2.24	1.39	1.42
3	A	1269	NAP	C2A-N3A	2.20	1.35	1.32
4	B	1270	IZ9	C2-N1	2.14	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1270	IZ9	CAS-C5	-2.05	1.39	1.42
4	C	1270	IZ9	CAT-CAG	2.04	1.49	1.46

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1270	IZ9	CAT-CAG-CAF	-6.63	115.92	123.97
4	D	1270	IZ9	CAT-CAG-CAF	-6.18	116.47	123.97
4	C	1270	IZ9	CAT-CAG-CAF	-5.06	117.82	123.97
3	D	1269	NAP	C3N-C7N-N7N	5.04	123.80	117.75
4	C	1270	IZ9	N3-C2-N1	-4.82	120.80	127.22
3	C	1269	NAP	N3A-C2A-N1A	-4.57	121.54	128.68
4	A	1270	IZ9	N3-C2-N1	-4.55	121.16	127.22
3	B	1269	NAP	C3N-C7N-N7N	4.40	123.03	117.75
4	D	1270	IZ9	N3-C2-N1	-4.36	121.40	127.22
4	D	1270	IZ9	C2-N3-C4	4.28	120.25	115.36
3	B	1269	NAP	N3A-C2A-N1A	-3.89	122.60	128.68
4	D	1270	IZ9	CAT-CAS-CAE	-3.63	122.12	127.33
4	B	1270	IZ9	CAT-CAG-CAF	-3.56	119.64	123.97
4	B	1270	IZ9	N3-C2-N1	-3.45	122.61	127.22
3	D	1269	NAP	O7N-C7N-C3N	-3.45	115.51	119.63
3	A	1269	NAP	N3A-C2A-N1A	-3.41	123.34	128.68
3	D	1269	NAP	C4A-C5A-N7A	-3.26	106.00	109.40
3	D	1269	NAP	N3A-C2A-N1A	-3.21	123.66	128.68
3	A	1269	NAP	O2N-PN-O1N	3.09	127.49	112.24
3	B	1269	NAP	C2A-N1A-C6A	3.08	124.02	118.75
4	C	1270	IZ9	CAT-CAS-CAE	-2.93	123.12	127.33
4	A	1270	IZ9	CAK-CAQ-CAJ	2.83	121.83	117.64
4	C	1270	IZ9	C2-N3-C4	2.82	118.58	115.36
3	C	1269	NAP	C2A-N1A-C6A	2.78	123.50	118.75
4	A	1270	IZ9	C2-N3-C4	2.75	118.50	115.36
3	B	1269	NAP	O3B-C3B-C2B	2.72	118.90	111.17
3	D	1269	NAP	C1B-N9A-C4A	-2.70	121.90	126.64
6	A	1272	DTT	C3-C4-S4	-2.66	106.75	114.47
4	A	1270	IZ9	CAT-CAS-CAE	-2.61	123.58	127.33
3	A	1269	NAP	C4A-C5A-N7A	-2.58	106.71	109.40
3	A	1269	NAP	C1B-N9A-C4A	-2.50	122.24	126.64
4	C	1270	IZ9	NAC-C2-N3	2.48	121.84	117.79
3	C	1269	NAP	C1B-N9A-C4A	-2.43	122.37	126.64
3	C	1269	NAP	O2N-PN-O1N	2.43	124.23	112.24
4	D	1270	IZ9	CAK-CAI-CAO	-2.39	118.18	121.38
4	D	1270	IZ9	CAK-CAQ-CAJ	2.37	121.15	117.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1270	IZ9	CAK-CAQ-CAJ	2.30	121.05	117.64
3	C	1269	NAP	N6A-C6A-N1A	2.23	123.20	118.57
4	C	1270	IZ9	CAK-CAQ-CAJ	2.22	120.92	117.64
3	C	1269	NAP	O2A-PA-O1A	2.21	123.15	112.24
4	B	1270	IZ9	C2-N3-C4	2.20	117.87	115.36
4	B	1270	IZ9	CAT-CAS-C5	-2.18	105.50	108.25
3	A	1269	NAP	C2A-N1A-C6A	2.16	122.44	118.75
3	B	1269	NAP	O7N-C7N-N7N	-2.12	119.56	122.58
4	C	1270	IZ9	CAJ-CAH-CAO	-2.11	118.55	121.38
3	D	1269	NAP	O3B-C3B-C2B	2.10	117.14	111.17
3	A	1269	NAP	PN-O3-PA	-2.07	125.72	132.83
4	A	1270	IZ9	CAK-CAI-CAO	-2.04	118.65	121.38
3	B	1269	NAP	C1B-N9A-C4A	-2.03	123.07	126.64
3	A	1269	NAP	C3D-C2D-C1D	2.02	104.02	100.98
4	A	1270	IZ9	CAQ-CAF-CAG	-2.01	117.93	125.87
3	C	1269	NAP	O2D-C2D-C1D	2.01	118.29	110.85

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1271	DTT	C1-C2-C3-O3
6	B	1271	DTT	C1-C2-C3-C4
6	B	1271	DTT	O2-C2-C3-O3
6	B	1271	DTT	O2-C2-C3-C4
6	A	1272	DTT	O2-C2-C3-C4
7	D	1271	GOL	O1-C1-C2-C3
7	D	1271	GOL	O1-C1-C2-O2
4	B	1270	IZ9	CAQ-CAF-CAG-CAT
6	A	1272	DTT	O3-C3-C4-S4
6	A	1272	DTT	C1-C2-C3-O3
4	B	1270	IZ9	CAG-CAF-CAQ-CAK
4	B	1270	IZ9	CAG-CAF-CAQ-CAJ
6	A	1272	DTT	O2-C2-C3-O3
4	A	1270	IZ9	CAQ-CAF-CAG-CAT

There are no ring outliers.

8 monomers are involved in 20 short contacts:

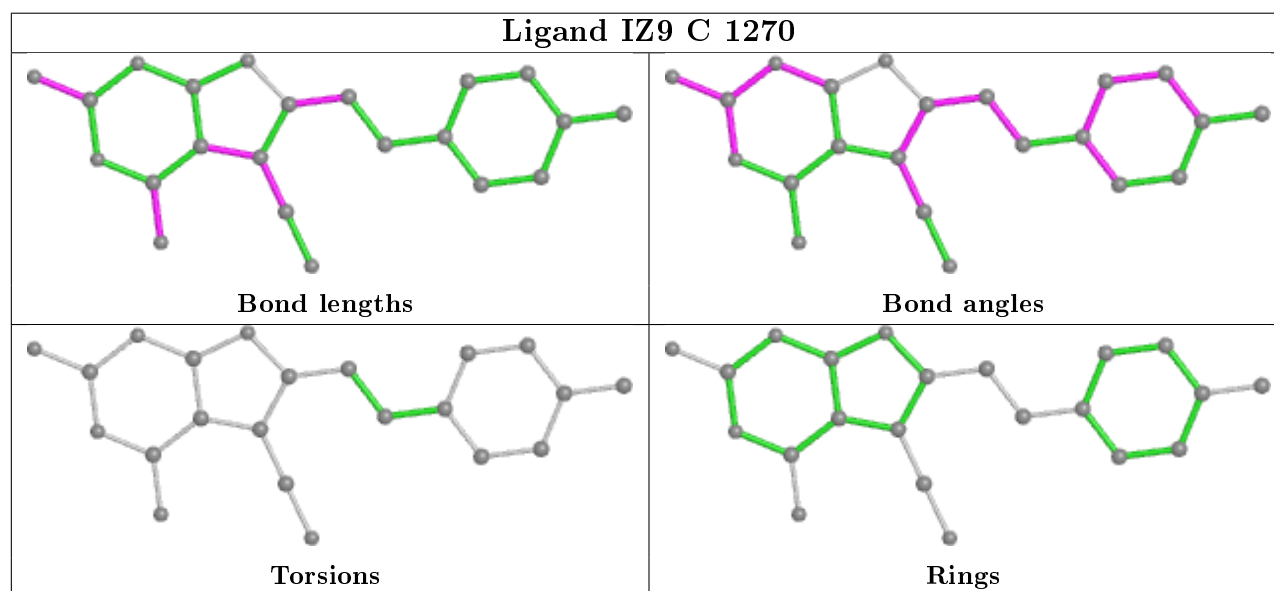
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1272	GOL	1	0

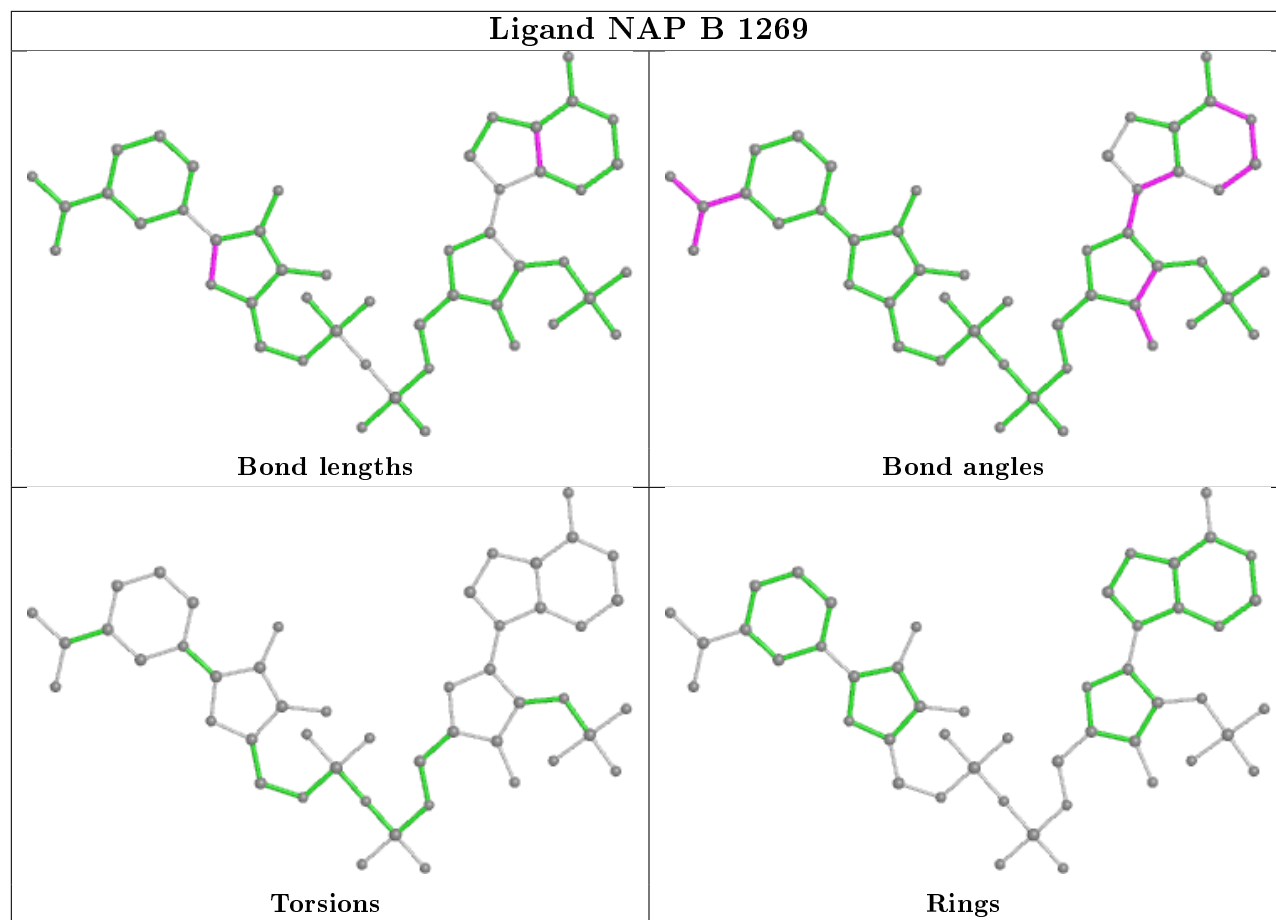
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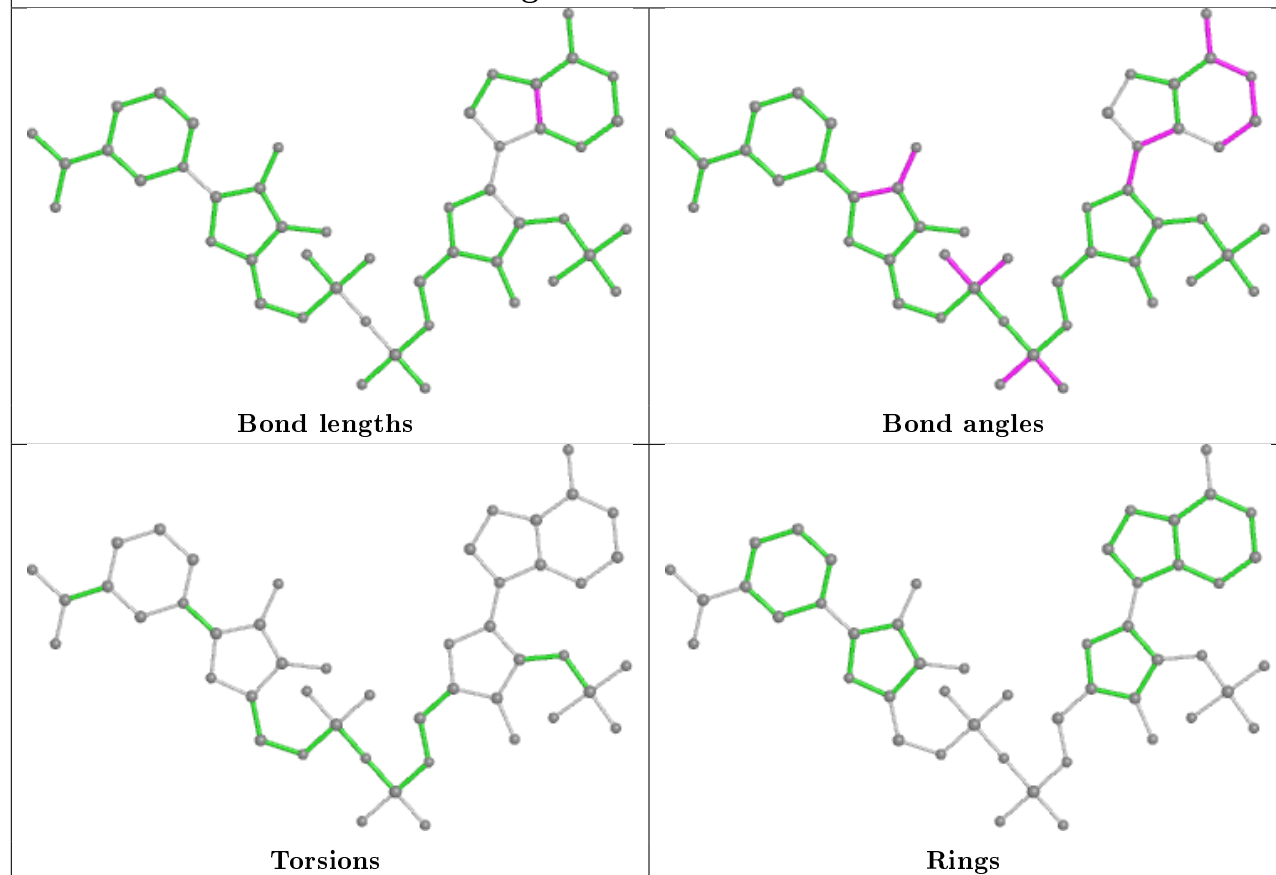
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1271	GOL	1	0
6	B	1271	DTT	1	0
4	C	1270	IZ9	8	0
3	B	1269	NAP	1	0
4	D	1270	IZ9	7	0
4	A	1270	IZ9	1	0
3	D	1269	NAP	1	0

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.

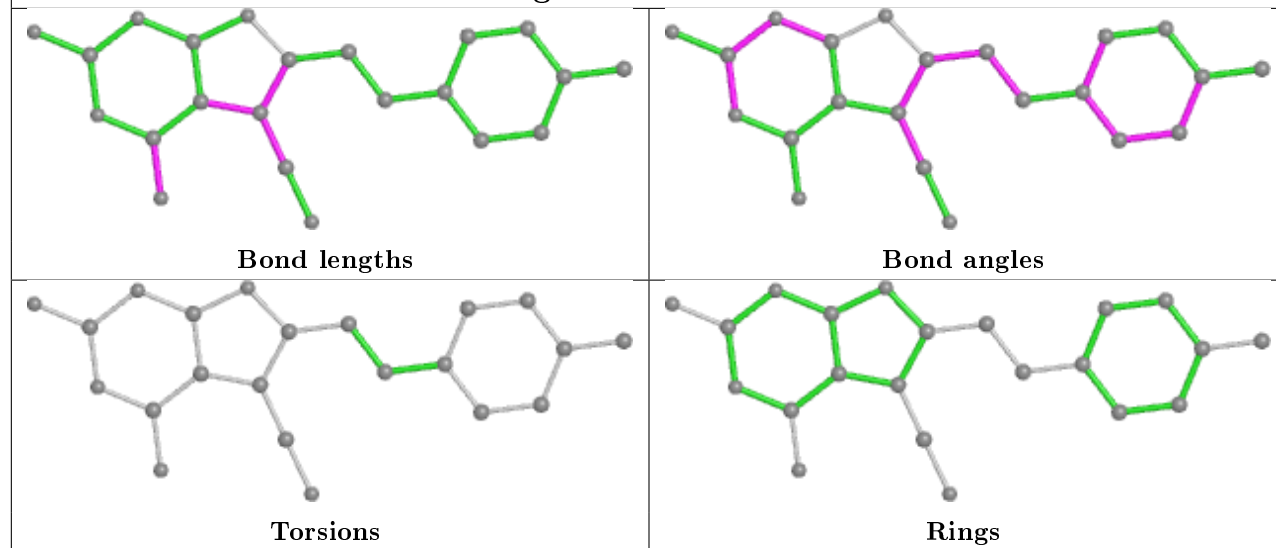




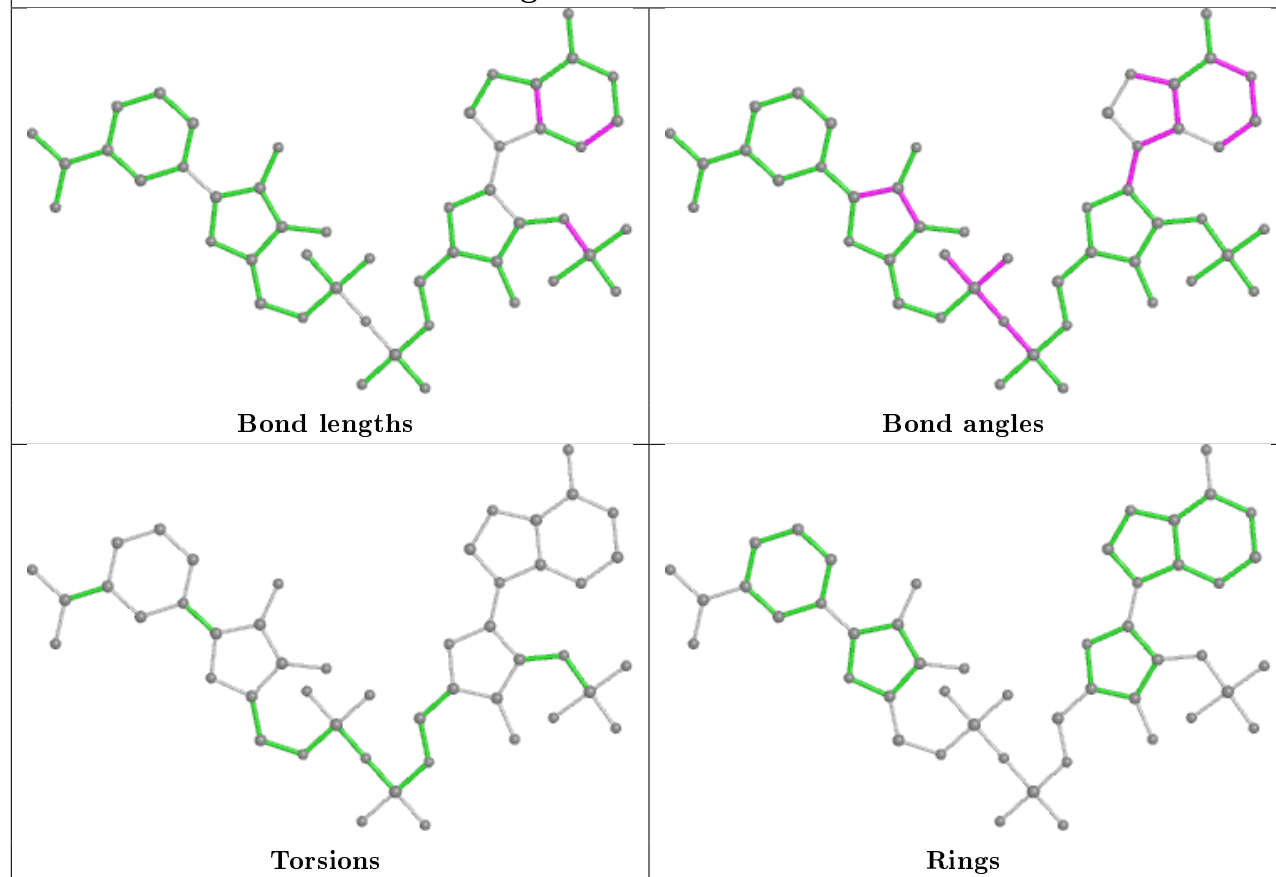
Ligand NAP C 1269



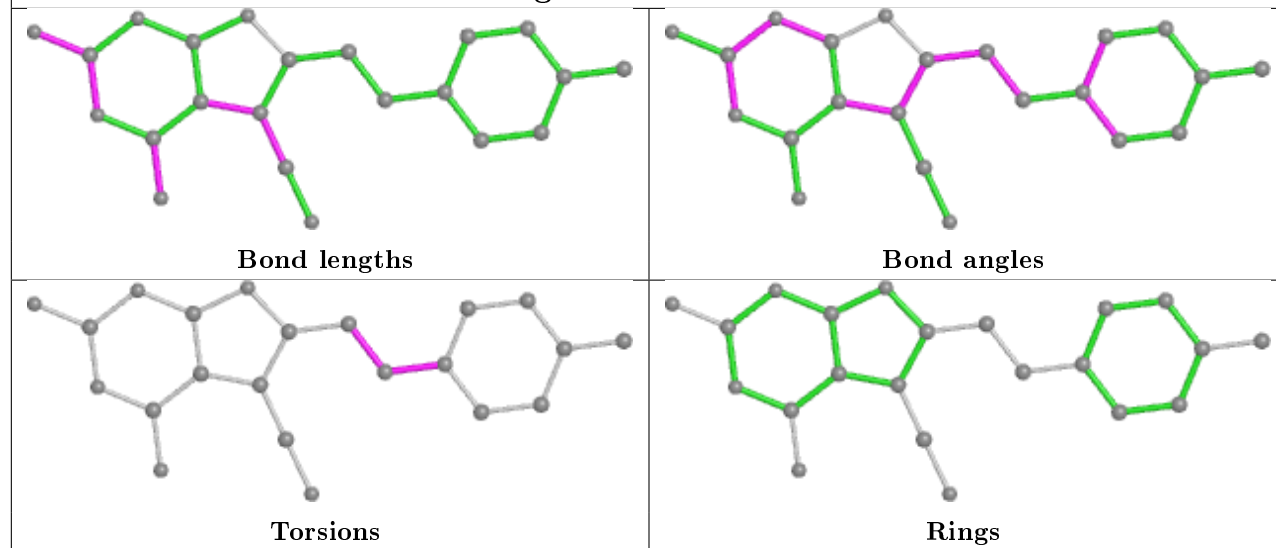
Ligand IZ9 D 1270

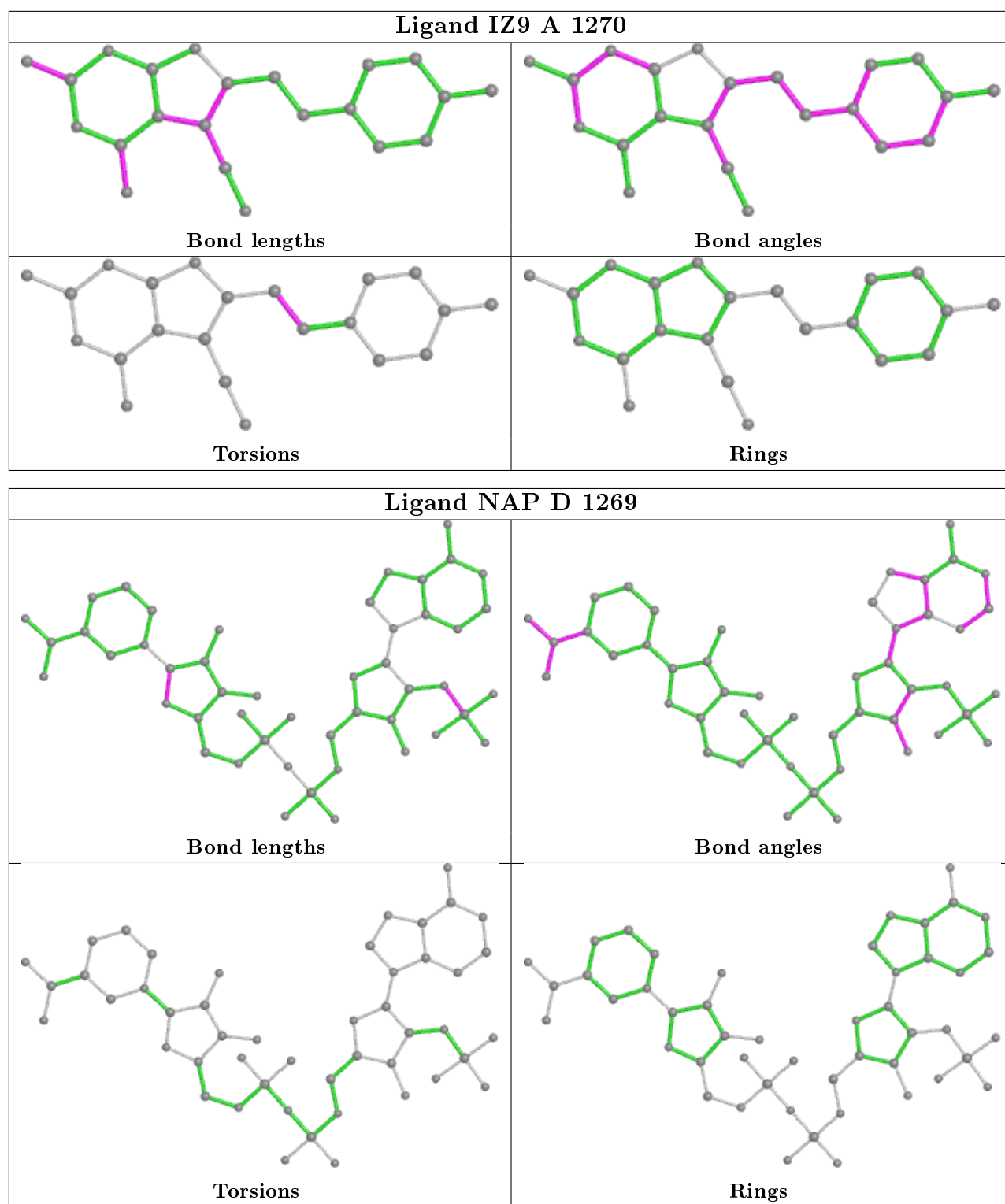


Ligand NAP A 1269



Ligand IZ9 B 1270





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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	249/288 (86%)	-0.52	2 (0%) 86 87	6, 12, 26, 44	0
1	C	248/288 (86%)	-0.50	4 (1%) 72 74	6, 12, 30, 52	0
1	D	249/288 (86%)	-0.47	5 (2%) 65 68	6, 12, 30, 50	0
2	B	251/288 (87%)	-0.57	5 (1%) 65 68	6, 11, 26, 58	0
All	All	997/1152 (86%)	-0.51	16 (1%) 72 74	6, 12, 28, 58	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	151	SER	4.9
2	B	151	SER	4.0
2	B	113	GLY	3.9
1	A	113	GLY	3.5
1	D	212	ALA	3.2
1	C	104	GLN	3.2
1	D	2	GLU	3.1
1	A	104	GLN	3.1
1	C	212	ALA	2.7
1	D	113	GLY	2.7
2	B	104	GLN	2.6
1	C	2	GLU	2.6
1	D	211	VAL	2.4
2	B	211	VAL	2.3
2	B	152	SER	2.3
1	C	211	VAL	2.2

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	0.09	13,16,37,38	0
1	CSX	D	168	7/8	0.94	0.09	14,17,31,37	0
1	CSX	C	168	7/8	0.96	0.09	12,14,29,35	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

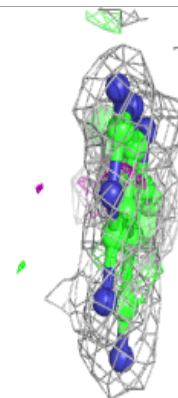
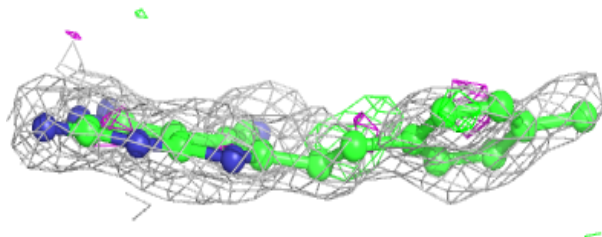
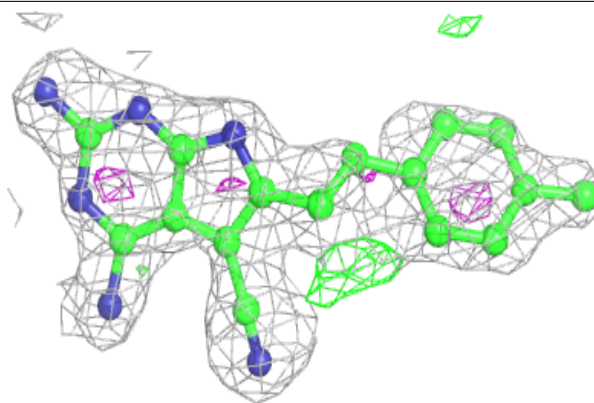
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	DTT	B	1271	8/8	0.66	0.29	60,69,73,77	0
6	DTT	A	1272	8/8	0.72	0.25	58,63,67,67	0
7	GOL	C	1272	6/6	0.82	0.19	51,54,56,57	0
4	IZ9	D	1270	22/22	0.86	0.19	23,28,39,40	0
7	GOL	D	1271	6/6	0.88	0.16	50,51,53,56	0
4	IZ9	C	1270	22/22	0.89	0.16	18,26,41,43	0
4	IZ9	A	1270	22/22	0.91	0.12	15,21,32,34	0
5	ACT	C	1271	4/4	0.92	0.11	21,25,25,25	0
4	IZ9	B	1270	22/22	0.94	0.11	13,20,32,34	0
5	ACT	A	1271	4/4	0.97	0.09	12,13,14,14	0
3	NAP	B	1269	48/48	0.98	0.06	6,9,10,11	0
3	NAP	A	1269	48/48	0.98	0.05	6,9,11,11	0
3	NAP	C	1269	48/48	0.99	0.05	7,10,12,12	0
3	NAP	D	1269	48/48	0.99	0.05	8,10,13,13	0

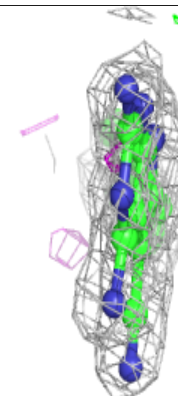
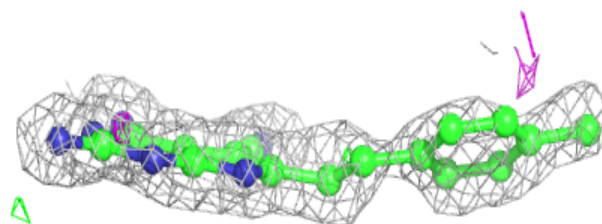
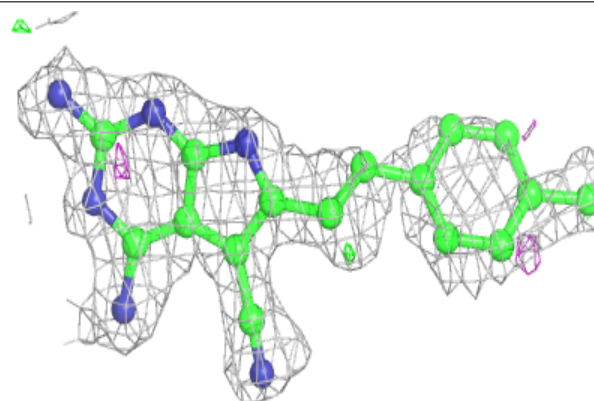
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around IZ9 D 1270:

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

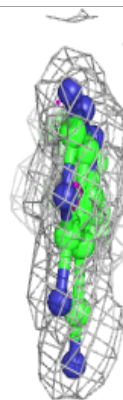
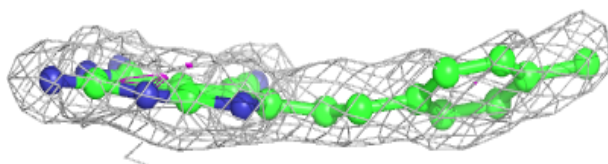
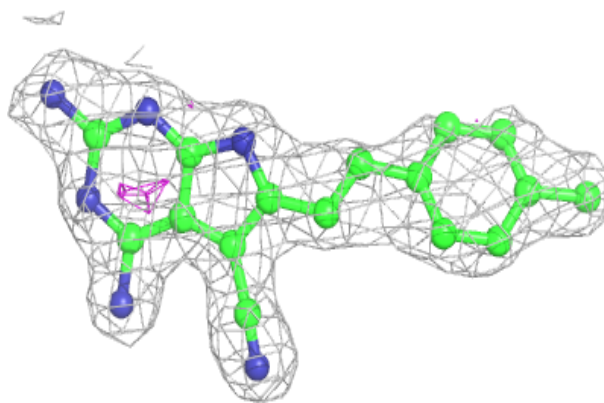
**Electron density around IZ9 C 1270:**

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

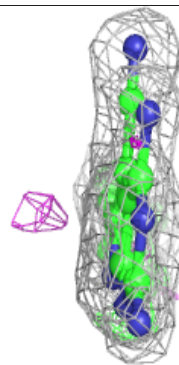
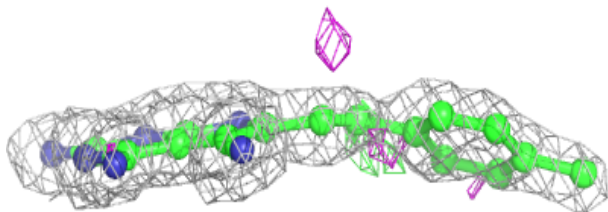
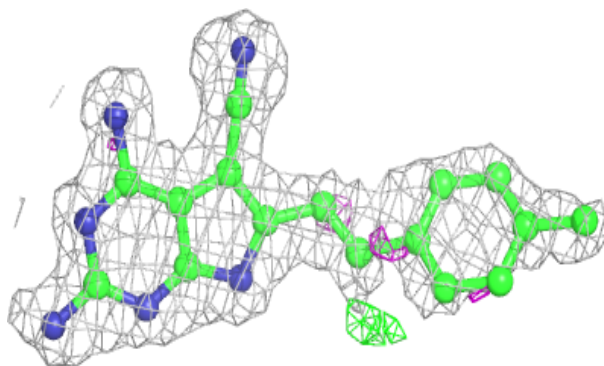


Electron density around IZ9 A 1270:

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

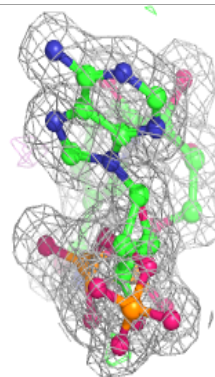
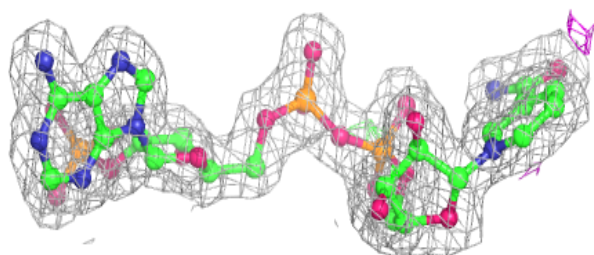
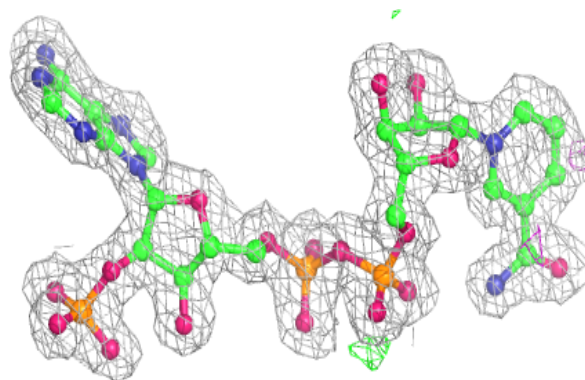
**Electron density around IZ9 B 1270:**

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

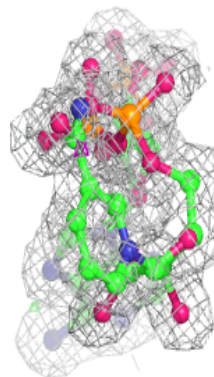
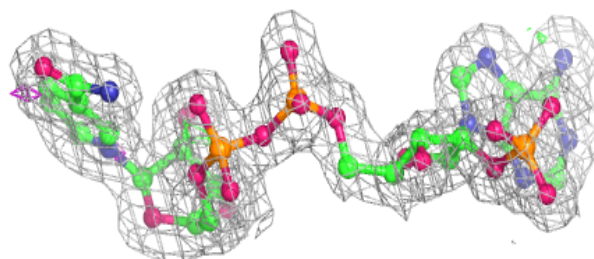
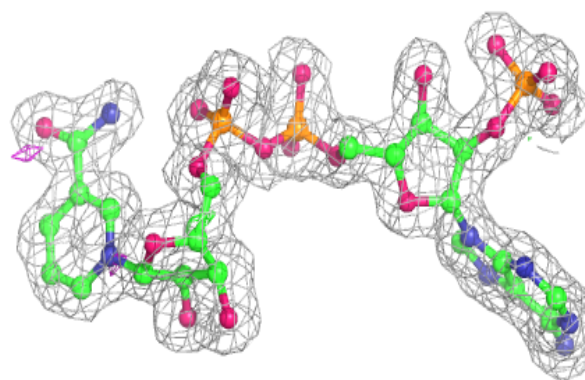


Electron density around NAP B 1269:

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

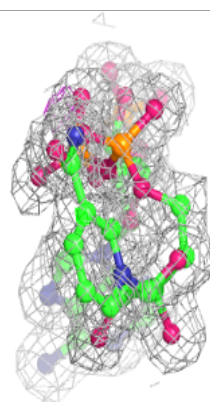
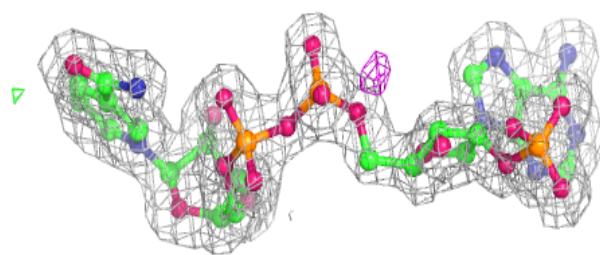
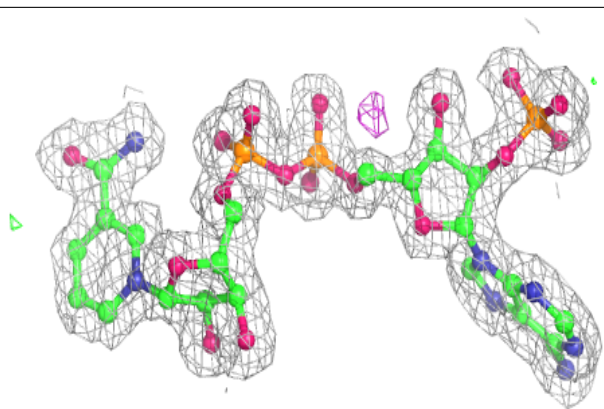
**Electron density around NAP A 1269:**

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

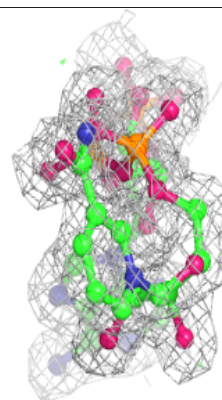
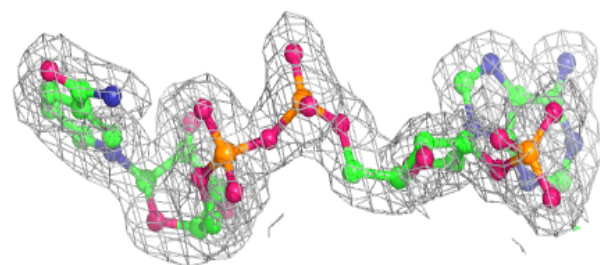
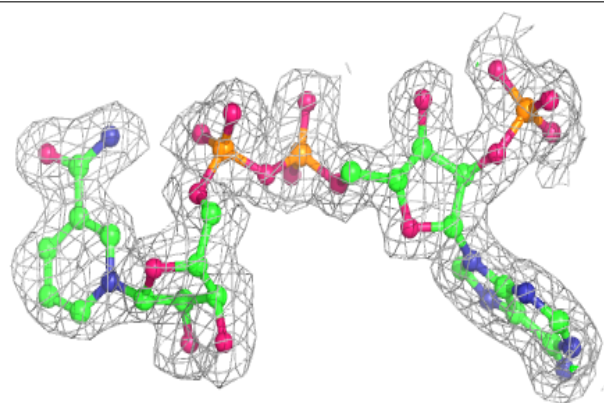


Electron density around NAP C 1269:

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

**Electron density around NAP D 1269:**

$2mF_o-DF_c$ (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.