



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2024 – 02:56 AM EDT

PDB ID : 4CLO
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 : 1.88 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

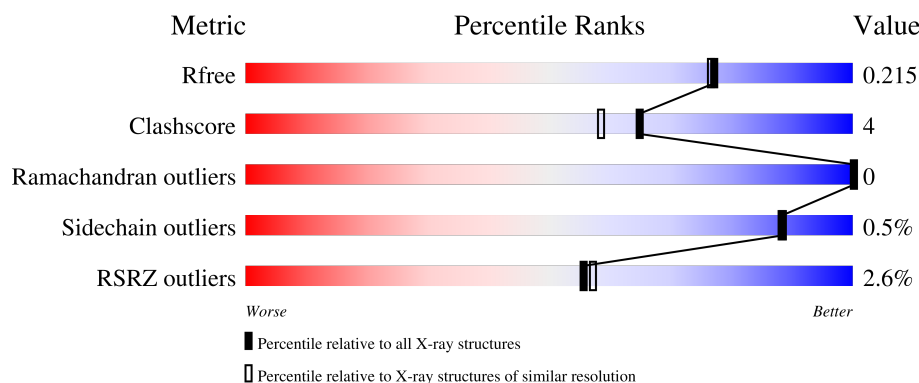
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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

Mol	Chain	Length	Quality of chain
1	A	288	
1	D	288	
2	B	288	
2	C	288	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	D	1271	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8632 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	251	Total	C	N	O	S	0	3	0
			1884	1183	331	359	11			
1	D	249	Total	C	N	O	S	0	8	0
			1890	1193	329	357	11			

There are 40 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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	252	Total	C	N	O	S	0	4	0
			1895	1189	331	364	11			
2	C	251	Total	C	N	O	S	0	5	0
			1894	1192	333	358	11			

There are 40 discrepancies between the modelled and reference sequences:

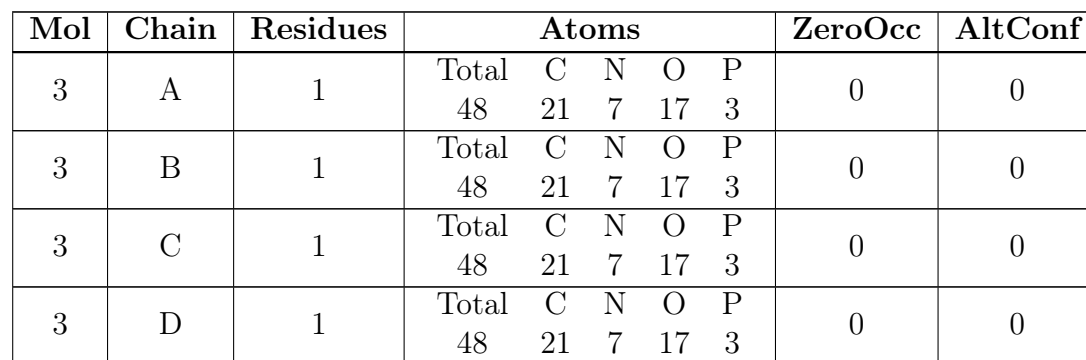
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP O76290
B	-18	GLY	-	expression tag	UNP O76290
B	-17	SER	-	expression tag	UNP O76290
B	-16	SER	-	expression tag	UNP O76290
B	-15	HIS	-	expression tag	UNP O76290
B	-14	HIS	-	expression tag	UNP O76290
B	-13	HIS	-	expression tag	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
C	-19	MET	-	expression tag	UNP O76290
C	-18	GLY	-	expression tag	UNP O76290
C	-17	SER	-	expression tag	UNP O76290
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

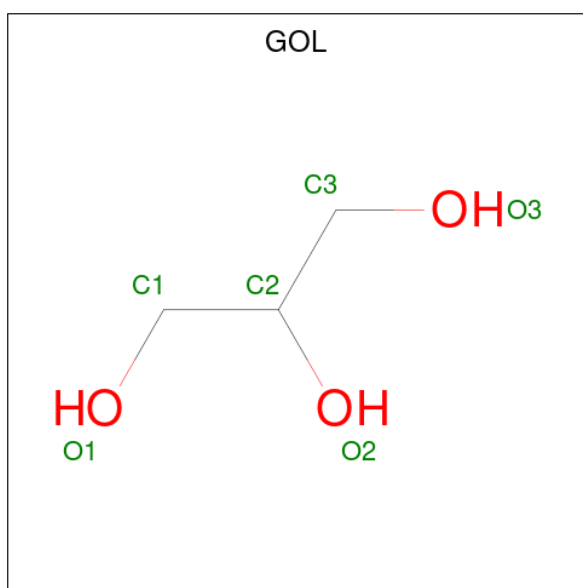
- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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- XP0
- The chemical structure of XP0 is a complex molecule featuring a purine-like core. The core consists of a fused bicyclic system with nitrogen atoms at positions N1, N3, and N9. Substituents are labeled with three-letter codes: NAA (amino group at C2), NAW (methyl group at N9), CAM (methyl group at N9), CAK (methyl group at N9), CAJ (methyl group at N9), CAL (methyl group at N9), CAG (methyl group at N9), CAE (methyl group at N9), CAF (methyl group at N9), CAH (methyl group at N9), CAD (methyl group at N9), CAB (methyl group at N9), CAC (methyl group at N9), CAS (methyl group at N9), CAI (methyl group at N9), C6 (methyl group at N9), C5 (methyl group at N9), C4 (methyl group at N9), C2 (methyl group at N9), and C1 (methyl group at N9).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			23	18	5		
4	B	1	Total	C	N	0	0
			23	18	5		
4	C	1	Total	C	N	0	0
			23	18	5		
4	D	1	Total	C	N	0	0
			23	18	5		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

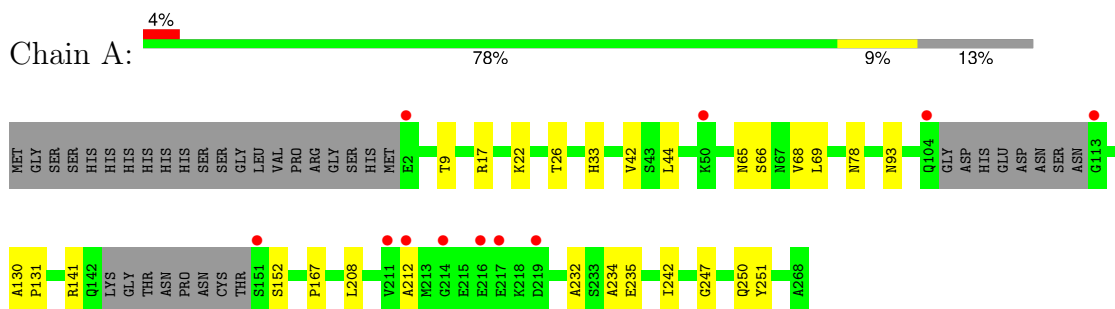
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	215	Total	O	0	0
			215	215		
6	B	196	Total	O	0	0
			196	196		
6	C	185	Total	O	0	0
			185	185		
6	D	183	Total	O	0	0
			183	183		

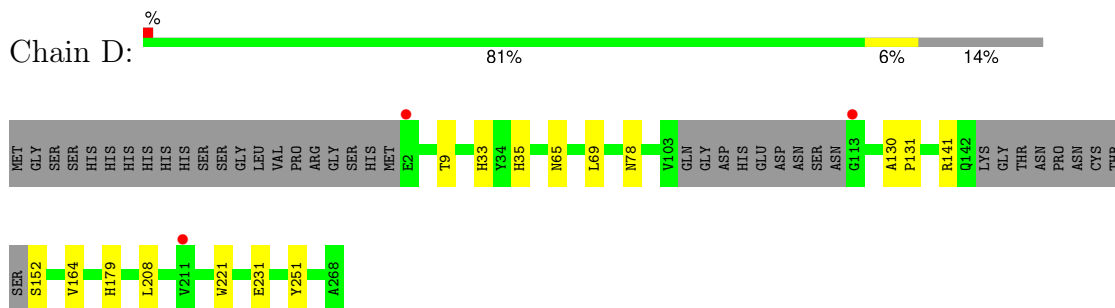
3 Residue-property plots [i](#)

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.

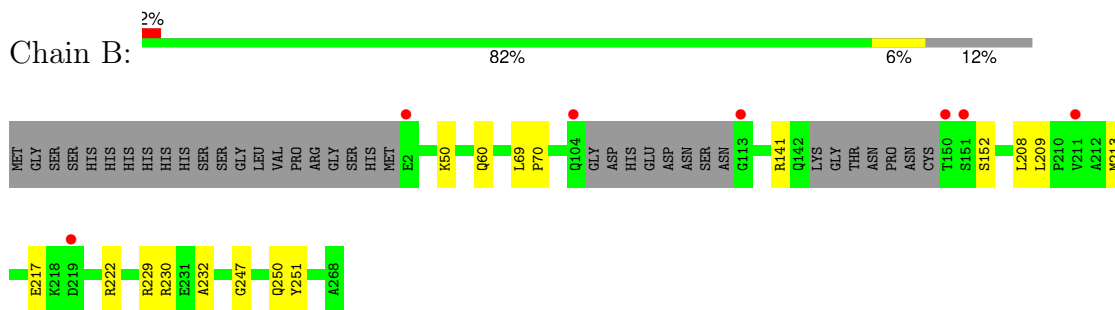
• Molecule 1: PTERIDINE REDUCTASE 1



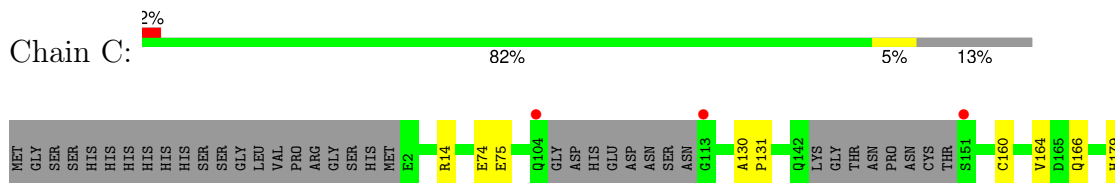
• Molecule 1: PTERIDINE REDUCTASE 1

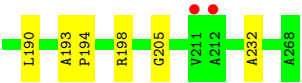


• Molecule 2: PTERIDINE REDUCTASE 1



• Molecule 2: 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	74.12Å 89.24Å 84.38Å 90.00° 115.27° 90.00°	Depositor
Resolution (Å)	19.73 – 1.88 19.73 – 1.88	Depositor EDS
% Data completeness (in resolution range)	93.4 (19.73-1.88) 93.6 (19.73-1.88)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.13 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.157 , 0.204 0.172 , 0.215	Depositor DCC
R_{free} test set	3772 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	16.1	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8632	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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 27.04 % 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 2.3603e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CSX, XP0, GOL, NAP

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	0.64	0/1920	0.76	0/2604
1	D	0.68	0/1938	0.77	0/2631
2	B	0.68	0/1926	0.78	1/2611 (0.0%)
2	C	0.70	0/1928	0.78	1/2613 (0.0%)
All	All	0.67	0/7712	0.77	2/10459 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	141	ARG	NE-CZ-NH2	-5.44	117.58	120.30
2	C	198	ARG	NE-CZ-NH1	5.22	122.91	120.30

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	1884	0	1909	21	0
1	D	1890	0	1934	13	0
2	B	1895	0	1919	13	0
2	C	1894	0	1935	10	0
3	A	48	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	25	0	0
3	C	48	0	25	1	0
3	D	48	0	25	1	0
4	A	23	0	17	1	0
4	B	23	0	17	7	0
4	C	23	0	17	1	0
4	D	23	0	17	4	0
5	D	6	0	8	4	0
6	A	215	0	0	6	2
6	B	196	0	0	3	2
6	C	185	0	0	4	1
6	D	183	0	0	1	1
All	All	8632	0	7873	64	3

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 (64) 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)
4:B:1270:XP0:CAC	4:B:1270:XP0:CAQ	2.35	1.03
4:B:1270:XP0:CAB	4:B:1270:XP0:CAS	2.39	0.98
2:B:50:LYS:NZ	6:B:2053:HOH:O	2.01	0.93
4:B:1270:XP0:CAC	4:B:1270:XP0:CAB	0.94	0.89
1:A:22:LYS:HG2	1:A:242:ILE:HG13	1.59	0.83
1:D:78:ASN:OD1	1:D:141:ARG:NH1	2.12	0.82
4:D:1270:XP0:HAM1	4:D:1270:XP0:CAC	2.23	0.69
1:A:22:LYS:NZ	1:A:235:GLU:HG3	2.14	0.63
2:B:60:GLN:OE1	6:B:2065:HOH:O	2.16	0.61
1:A:212:ALA:HB3	6:A:2099:HOH:O	2.03	0.59
1:D:231:GLU:OE2	5:D:1271:GOL:H31	2.04	0.58
2:B:213:MET:HE2	2:B:217[B]:GLU:HB3	1.85	0.57
1:A:247:GLY:O	1:A:250[A]:GLN:HG2	2.07	0.55
1:A:42:VAL:HG23	6:A:2044:HOH:O	2.05	0.55
1:D:164:VAL:HG22	1:D:179:HIS:CD2	2.42	0.54
1:A:250[B]:GLN:HG2	6:A:2195:HOH:O	2.07	0.54
1:A:42:VAL:CG2	6:A:2044:HOH:O	2.56	0.54
2:C:74:GLU:OE1	6:C:2076:HOH:O	2.19	0.53
4:D:1270:XP0:HAM1	4:D:1270:XP0:CAB	2.40	0.52
1:A:17:ARG:CZ	1:A:44:LEU:HD13	2.40	0.51
2:C:160:CYS:HB3	6:C:2112:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:GLU:CD	5:D:1271:GOL:H31	2.31	0.51
2:C:164:VAL:HG22	2:C:179:HIS:CD2	2.45	0.51
1:A:9:THR:HA	1:A:33:HIS:HB3	1.93	0.50
4:B:1270:XP0:CAC	4:B:1270:XP0:CAM	2.91	0.49
2:C:130:ALA:HB3	2:C:131:PRO:HD3	1.93	0.49
2:B:247:GLY:O	2:B:250:GLN:HG2	2.12	0.48
1:D:141:ARG:HG2	6:D:2128:HOH:O	2.12	0.48
2:C:205:GLY:O	3:C:1269:NAP:H4N	2.14	0.48
2:C:14:ARG:HD3	6:C:2185:HOH:O	2.13	0.48
4:D:1270:XP0:CAC	4:D:1270:XP0:CAM	2.92	0.48
1:D:65:ASN:HA	1:D:69:LEU:HD22	1.96	0.47
1:D:9:THR:HA	1:D:33:HIS:HB3	1.97	0.47
2:C:193:ALA:N	2:C:194:PRO:CD	2.77	0.47
4:B:1270:XP0:CAC	4:B:1270:XP0:HAM1	2.45	0.47
1:D:35:HIS:HB2	3:D:1269:NAP:C2A	2.45	0.46
1:A:251:TYR:CE2	2:B:232:ALA:HB2	2.51	0.46
1:D:208:LEU:HA	5:D:1271:GOL:H32	1.98	0.46
1:A:167:PRO:HG2	2:C:190[B]:LEU:HD12	1.98	0.45
2:B:213:MET:CE	2:B:217[B]:GLU:OE1	2.65	0.45
1:A:232:ALA:HB2	2:B:251:TYR:CE2	2.51	0.45
2:B:222:ARG:HB3	2:B:229:ARG:O	2.16	0.45
1:D:130:ALA:HB3	1:D:131:PRO:HD3	1.98	0.45
2:B:213:MET:HE2	2:B:217[B]:GLU:CB	2.47	0.44
2:C:232:ALA:HB2	1:D:251:TYR:CE2	2.51	0.44
2:B:209:LEU:CD2	4:B:1270:XP0:CAE	2.96	0.44
4:B:1270:XP0:CAB	4:B:1270:XP0:HAM1	2.48	0.44
1:A:9:THR:O	1:A:93:ASN:HB3	2.17	0.43
2:C:75:GLU:HB2	6:C:2074:HOH:O	2.19	0.43
4:A:1270:XP0:CAM	4:A:1270:XP0:CAC	2.97	0.43
1:D:221:TRP:CD2	4:D:1270:XP0:HAF	2.53	0.42
1:A:208:LEU:HD22	1:A:234:ALA:HB2	2.00	0.42
1:A:65:ASN:HA	1:A:69:LEU:HD22	2.01	0.42
1:A:250[A]:GLN:OE1	1:A:250[A]:GLN:HA	2.20	0.42
2:B:208:LEU:HA	6:B:2154:HOH:O	2.20	0.42
1:A:26:THR:HG22	1:A:26:THR:O	2.20	0.41
1:A:66:SER:OG	1:A:68:VAL:HG22	2.21	0.41
2:B:222:ARG:HG2	2:B:230:ARG:HA	2.02	0.41
2:B:69:LEU:N	2:B:70:PRO:CD	2.84	0.41
1:A:130:ALA:HB3	1:A:131:PRO:HD3	2.03	0.41
4:C:1270:XP0:CAM	4:C:1270:XP0:CAC	3.00	0.40
1:D:231:GLU:OE2	5:D:1271:GOL:C3	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ASN:ND2	6:A:2096:HOH:O	2.43	0.40
1:A:141:ARG:CD	6:A:2092:HOH:O	2.68	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2009:HOH:O	6:B:2158:HOH:O[2_555]	2.13	0.07
6:A:2020:HOH:O	6:D:2024:HOH:O[1_455]	2.18	0.02
6:B:2047:HOH:O	6:C:2054:HOH:O[1_554]	2.18	0.02

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	D	251/288 (87%)	244 (97%)	7 (3%)	0	100	100
2	B	249/288 (86%)	239 (96%)	10 (4%)	0	100	100
2	C	249/288 (86%)	239 (96%)	10 (4%)	0	100	100
All	All	997/1152 (86%)	962 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/231 (87%)	201 (100%)	1 (0%)	88	88
1	D	205/231 (89%)	204 (100%)	1 (0%)	88	88
2	B	203/230 (88%)	202 (100%)	1 (0%)	88	88
2	C	203/230 (88%)	202 (100%)	1 (0%)	88	88
All	All	813/922 (88%)	809 (100%)	4 (0%)	88	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	SER
2	B	152	SER
2	C	166	GLN
1	D	152	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	175	ASN
2	B	236	GLN
1	D	25	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z > 2$
2	CSX	B	168	2	3,6,7	0.82	0	1,6,8	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CSX	C	168	2	3,6,7	0.30	0	1,6,8	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSX	B	168	2	-	0/2/5/7	-
2	CSX	C	168	2	-	0/2/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	NAP	D	1269	-	46,52,52	1.03	3 (6%)	61,80,80	1.46	9 (14%)
3	NAP	C	1269	-	46,52,52	1.05	2 (4%)	61,80,80	1.52	9 (14%)
4	XP0	D	1270	-	25,26,26	1.93	5 (20%)	28,36,36	2.77	8 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	XP0	B	1270	-	25,26,26	2.82	5 (20%)	28,36,36	2.85	10 (35%)
3	NAP	B	1269	-	46,52,52	1.05	2 (4%)	61,80,80	1.48	9 (14%)
5	GOL	D	1271	-	5,5,5	0.44	0	5,5,5	0.83	0
4	XP0	C	1270	-	25,26,26	2.21	9 (36%)	28,36,36	3.03	11 (39%)
3	NAP	A	1269	-	46,52,52	1.26	3 (6%)	61,80,80	1.45	11 (18%)
4	XP0	A	1270	-	25,26,26	1.93	5 (20%)	28,36,36	2.77	8 (28%)

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	D	1269	-	-	2/31/67/67	0/5/5/5
3	NAP	C	1269	-	-	0/31/67/67	0/5/5/5
4	XP0	D	1270	-	-	0/7/16/16	0/4/4/4
4	XP0	B	1270	-	-	0/7/16/16	0/4/4/4
3	NAP	B	1269	-	-	2/31/67/67	0/5/5/5
5	GOL	D	1271	-	-	0/4/4/4	-
4	XP0	C	1270	-	-	0/7/16/16	0/4/4/4
3	NAP	A	1269	-	-	1/31/67/67	0/5/5/5
4	XP0	A	1270	-	-	0/7/16/16	0/4/4/4

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1270	XP0	CAB-CAC	-10.38	0.94	1.19
4	C	1270	XP0	CAL-NAW	5.19	1.55	1.46
3	A	1269	NAP	PN-O3	4.86	1.64	1.59
4	B	1270	XP0	CAL-NAW	4.74	1.54	1.46
4	D	1270	XP0	C6-N1	4.74	1.37	1.32
4	B	1270	XP0	C6-N1	4.35	1.37	1.32
4	A	1270	XP0	C6-C5	-4.33	1.37	1.43
4	B	1270	XP0	C6-C5	-4.27	1.37	1.43
4	A	1270	XP0	CAL-NAW	4.20	1.53	1.46
4	D	1270	XP0	CAL-NAW	4.12	1.53	1.46
4	B	1270	XP0	CAS-C5	-4.11	1.36	1.42
4	A	1270	XP0	CAB-CAC	-4.01	1.09	1.19
4	A	1270	XP0	C6-N1	3.98	1.36	1.32
4	C	1270	XP0	CAS-C5	-3.95	1.37	1.42
4	C	1270	XP0	CAB-CAC	-3.73	1.10	1.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1270	XP0	CAS-C5	-3.72	1.37	1.42
4	D	1270	XP0	CAB-CAC	-3.64	1.10	1.19
4	C	1270	XP0	C6-C5	-3.59	1.38	1.43
4	A	1270	XP0	CAS-C5	-3.54	1.37	1.42
3	C	1269	NAP	PA-O3	3.40	1.63	1.59
4	C	1270	XP0	CAS-CAC	-3.40	1.37	1.44
4	D	1270	XP0	C6-C5	-3.28	1.38	1.43
3	A	1269	NAP	P2B-O2B	3.21	1.65	1.59
3	B	1269	NAP	P2B-O2B	3.17	1.65	1.59
4	C	1270	XP0	CAQ-CAB	-3.15	1.36	1.44
3	B	1269	NAP	PA-O3	3.07	1.62	1.59
3	C	1269	NAP	P2B-O2B	3.03	1.64	1.59
4	C	1270	XP0	CAM-NAW	2.96	1.51	1.46
4	C	1270	XP0	C6-N1	2.62	1.35	1.32
3	D	1269	NAP	P2B-O2B	2.35	1.63	1.59
4	C	1270	XP0	CAI-NAP	-2.25	1.32	1.36
3	A	1269	NAP	O4D-C1D	2.15	1.43	1.40
3	D	1269	NAP	C2N-N1N	2.09	1.37	1.35
3	D	1269	NAP	O7N-C7N	-2.03	1.20	1.24

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1270	XP0	CAI-CAS-CAC	-9.42	114.51	126.64
4	C	1270	XP0	CAI-CAS-CAC	-9.25	114.72	126.64
4	D	1270	XP0	CAI-CAS-CAC	-9.21	114.77	126.64
4	B	1270	XP0	CAI-CAS-CAC	-7.40	117.11	126.64
4	B	1270	XP0	N3-C2-N1	-6.89	118.45	127.21
4	D	1270	XP0	N3-C2-N1	-6.29	119.21	127.21
4	A	1270	XP0	N3-C2-N1	-5.64	120.04	127.21
4	C	1270	XP0	N3-C2-N1	-5.61	120.08	127.21
4	B	1270	XP0	N1-C6-NAW	-5.34	113.35	117.17
4	C	1270	XP0	N1-C6-NAW	-5.27	113.40	117.17
3	B	1269	NAP	C4B-O4B-C1B	-5.17	105.19	109.92
4	D	1270	XP0	C2-N3-C4	4.99	120.86	115.48
3	D	1269	NAP	O4B-C1B-N9A	4.84	115.16	108.75
4	B	1270	XP0	C2-N3-C4	4.79	120.65	115.48
3	C	1269	NAP	N3A-C2A-N1A	-4.66	122.35	128.67
4	C	1270	XP0	C5-C6-NAW	4.65	127.88	120.14
3	C	1269	NAP	O4B-C1B-N9A	4.62	114.88	108.75
4	A	1270	XP0	C5-C6-N1	-4.37	117.38	123.30
3	D	1269	NAP	C4B-O4B-C1B	-4.33	105.96	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1270	XP0	C5-C6-NAW	4.26	127.24	120.14
3	C	1269	NAP	C4B-O4B-C1B	-4.08	106.19	109.92
3	D	1269	NAP	C2B-C1B-N9A	-4.08	103.51	112.56
3	A	1269	NAP	C2B-C1B-N9A	-4.04	103.59	112.56
4	A	1270	XP0	C5-C6-NAW	3.87	126.58	120.14
4	C	1270	XP0	CAH-CAQ-CAB	-3.84	113.98	120.78
3	A	1269	NAP	C1B-N9A-C4A	-3.83	119.90	126.64
4	C	1270	XP0	C2-N3-C4	3.80	119.58	115.48
3	B	1269	NAP	C2B-C1B-N9A	-3.72	104.30	112.56
4	D	1270	XP0	C5-C6-NAW	3.64	126.19	120.14
4	A	1270	XP0	C2-N1-C6	3.63	123.27	113.52
3	C	1269	NAP	C2B-C1B-N9A	-3.61	104.55	112.56
4	A	1270	XP0	CAK-CAM-NAW	3.58	108.27	103.47
3	B	1269	NAP	N3A-C2A-N1A	-3.57	123.83	128.67
4	D	1270	XP0	N1-C6-NAW	-3.54	114.64	117.17
4	C	1270	XP0	C5-C6-N1	-3.40	118.70	123.30
3	A	1269	NAP	N3A-C2A-N1A	-3.29	124.21	128.67
4	C	1270	XP0	C2-N1-C6	3.29	122.36	113.52
3	B	1269	NAP	O7N-C7N-C3N	-3.25	115.63	119.60
3	A	1269	NAP	O4B-C1B-N9A	3.21	113.00	108.75
4	B	1270	XP0	C2-N1-C6	3.18	122.06	113.52
3	B	1269	NAP	C3N-C7N-N7N	3.09	121.54	117.74
4	D	1270	XP0	C5-C6-N1	-3.08	119.13	123.30
4	D	1270	XP0	C2-N1-C6	3.00	121.58	113.52
3	A	1269	NAP	C4B-O4B-C1B	-2.94	107.24	109.92
4	B	1270	XP0	C5-C6-N1	-2.88	119.40	123.30
4	B	1270	XP0	NAA-C2-N1	2.85	121.50	117.22
4	C	1270	XP0	CAG-CAQ-CAB	2.83	125.78	120.78
3	C	1269	NAP	C1B-N9A-C4A	-2.81	121.70	126.64
4	B	1270	XP0	CAK-CAM-NAW	2.75	107.16	103.47
4	A	1270	XP0	CAM-NAW-CAL	-2.74	106.29	111.50
3	A	1269	NAP	C3N-C7N-N7N	2.68	121.04	117.74
3	D	1269	NAP	C1B-N9A-C4A	-2.67	121.96	126.64
3	D	1269	NAP	O2N-PN-O1N	2.64	124.74	112.44
3	C	1269	NAP	O2A-PA-O1A	2.64	124.73	112.44
3	A	1269	NAP	O3X-P2B-O2X	2.64	117.69	107.80
3	B	1269	NAP	O4B-C1B-N9A	2.50	112.06	108.75
4	C	1270	XP0	NAA-C2-N1	2.46	120.91	117.22
3	A	1269	NAP	O2X-P2B-O2B	-2.42	96.42	105.85
3	D	1269	NAP	O3-PN-O1N	-2.41	103.47	110.70
3	D	1269	NAP	C4A-C5A-N7A	-2.39	106.81	109.34
3	B	1269	NAP	C5N-C4N-C3N	-2.36	118.04	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1269	NAP	O2N-PN-O1N	2.36	123.41	112.44
4	C	1270	XP0	CAS-C5-C4	-2.32	102.47	106.55
3	D	1269	NAP	O2A-PA-O1A	2.30	123.16	112.44
3	A	1269	NAP	O3-PN-O1N	-2.30	103.78	110.70
4	D	1270	XP0	NAA-C2-N1	2.26	120.61	117.22
3	B	1269	NAP	C6N-N1N-C2N	-2.24	119.97	121.88
3	B	1269	NAP	O2N-PN-O1N	2.24	122.86	112.44
3	A	1269	NAP	O2N-PN-O3	2.24	113.32	107.27
3	C	1269	NAP	C4A-C5A-N7A	-2.22	106.99	109.34
4	A	1270	XP0	CAM-NAW-C6	2.19	130.38	123.31
3	C	1269	NAP	O2B-P2B-O1X	-2.18	101.56	109.33
4	B	1270	XP0	CAH-CAQ-CAB	-2.15	116.98	120.78
3	A	1269	NAP	C4D-O4D-C1D	2.07	111.83	109.92
3	D	1269	NAP	O2B-C2B-C3B	2.00	118.86	111.68

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1269	NAP	C5B-O5B-PA-O1A
3	B	1269	NAP	C5B-O5B-PA-O1A
3	B	1269	NAP	C5B-O5B-PA-O3
3	D	1269	NAP	C5B-O5B-PA-O1A
3	D	1269	NAP	C3B-C2B-O2B-P2B

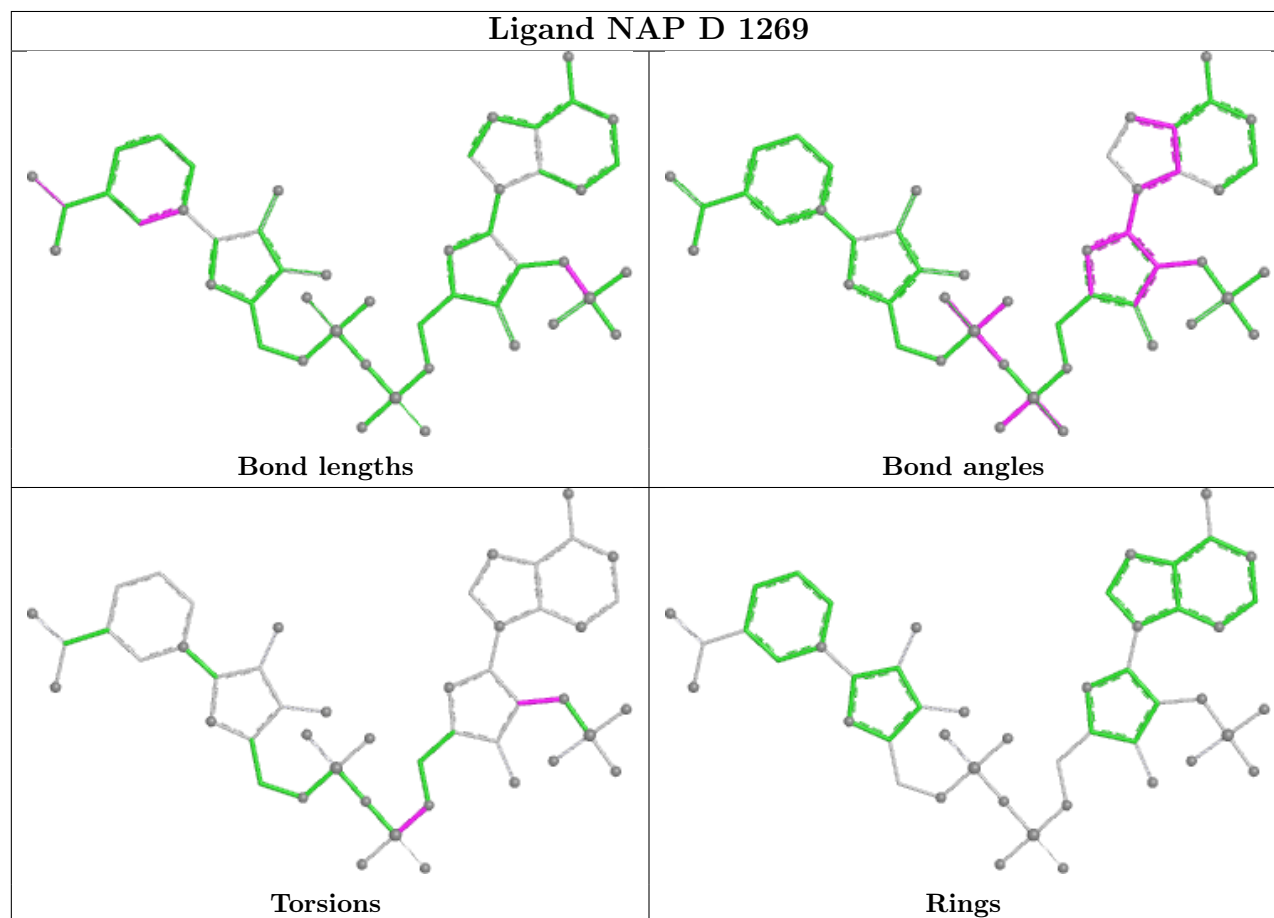
There are no ring outliers.

7 monomers are involved in 19 short contacts:

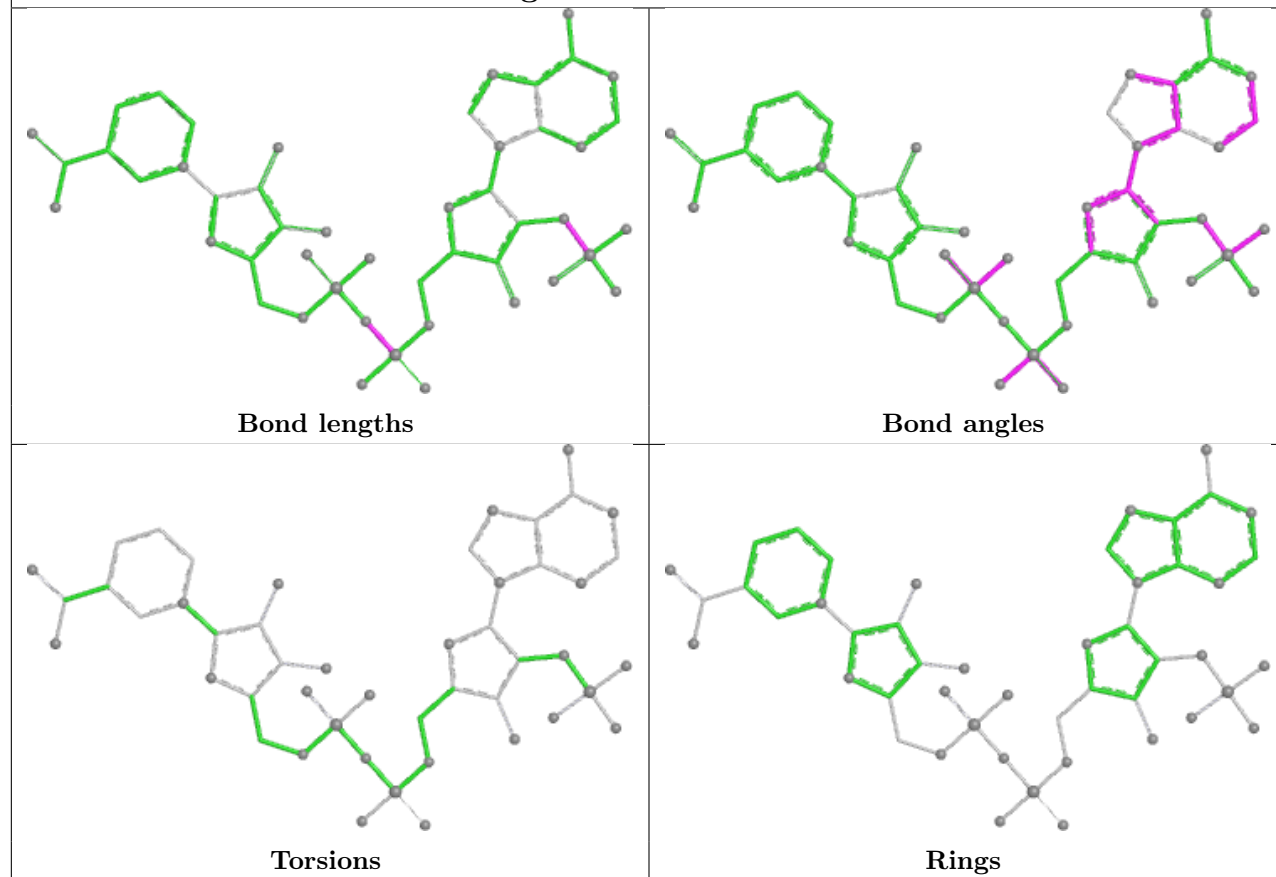
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1269	NAP	1	0
3	C	1269	NAP	1	0
4	D	1270	XP0	4	0
4	B	1270	XP0	7	0
5	D	1271	GOL	4	0
4	C	1270	XP0	1	0
4	A	1270	XP0	1	0

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.

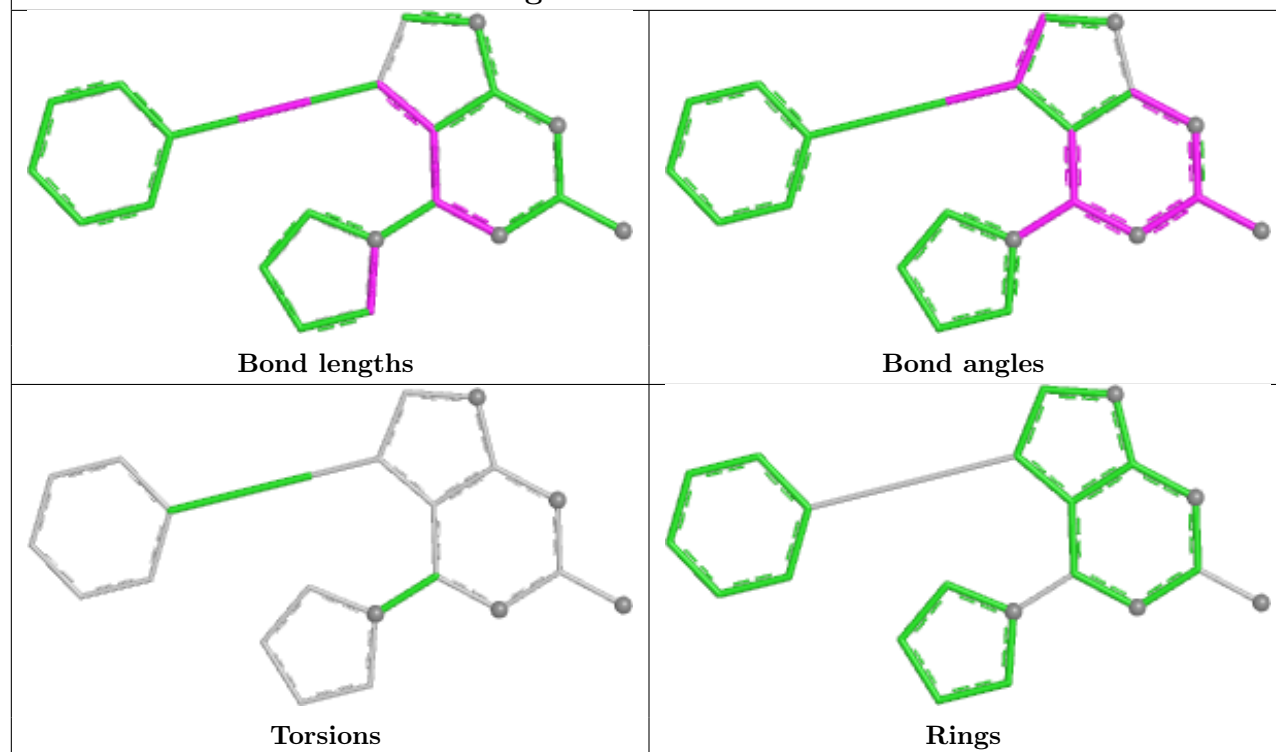
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

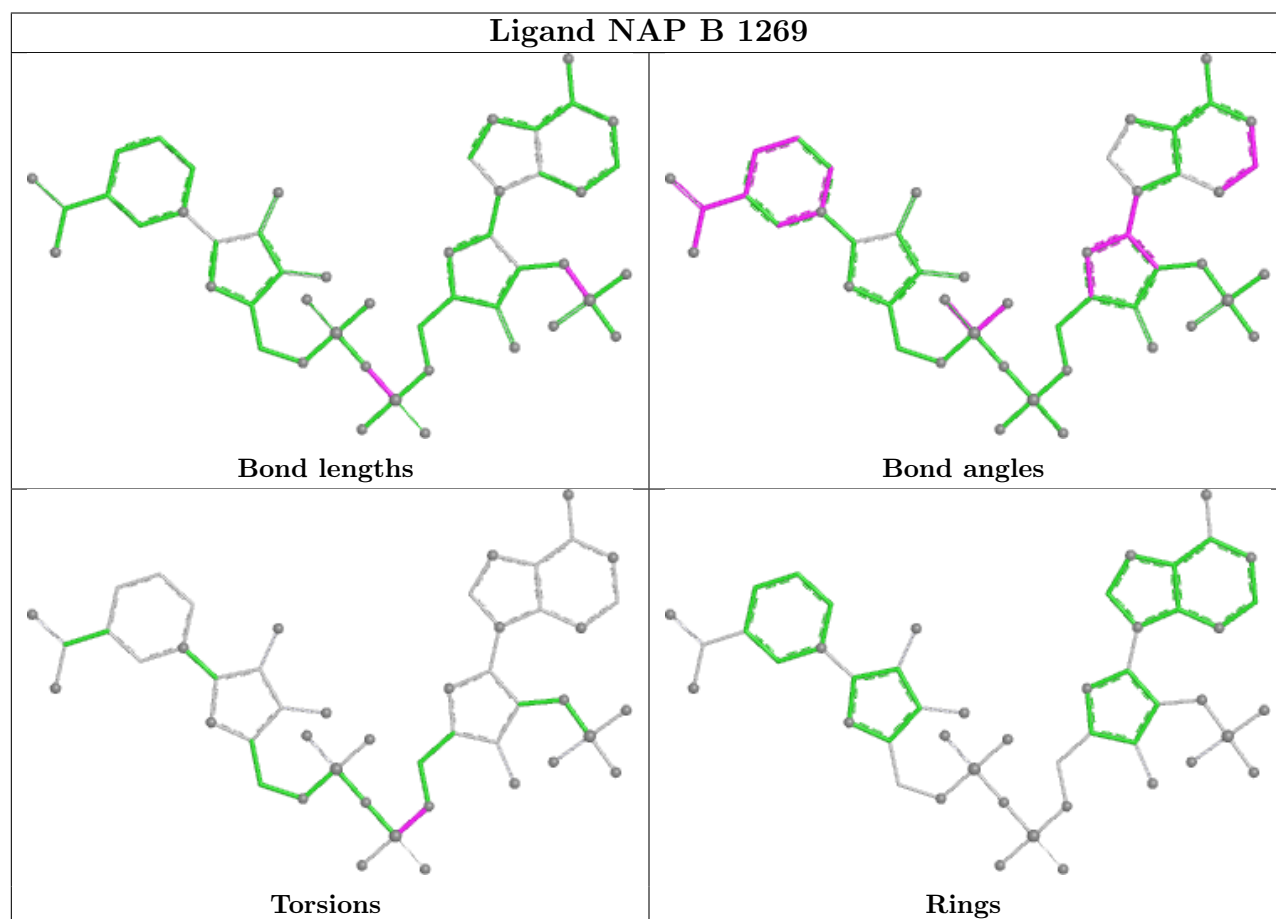
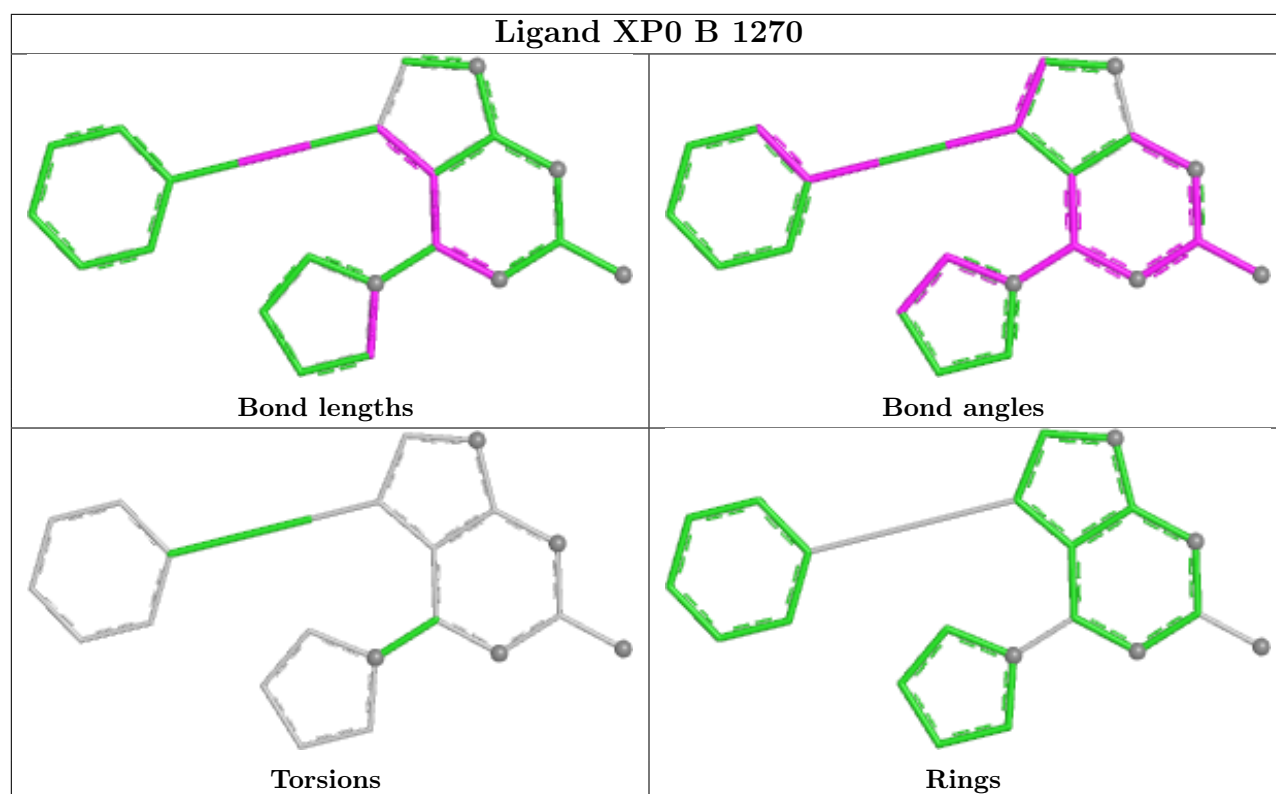


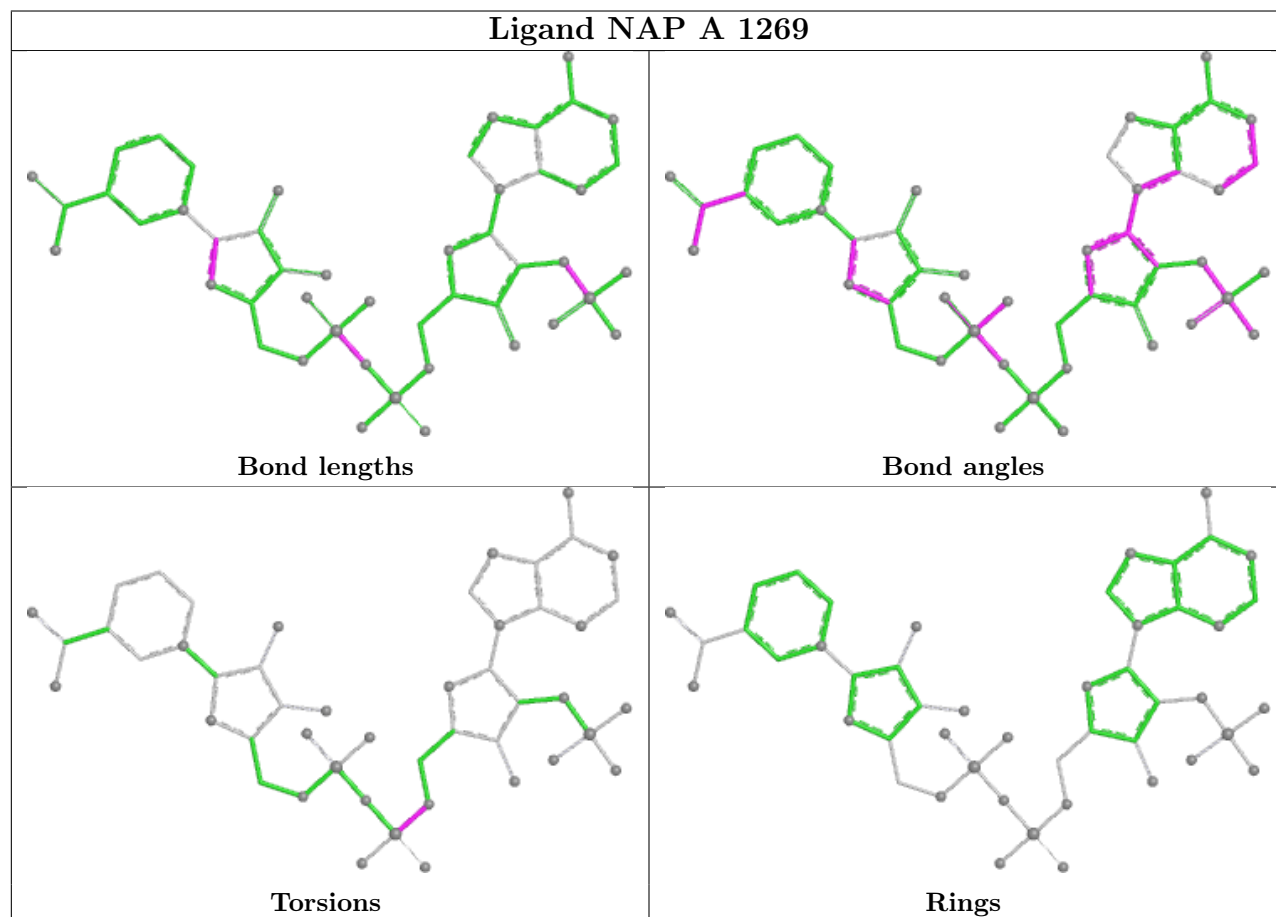
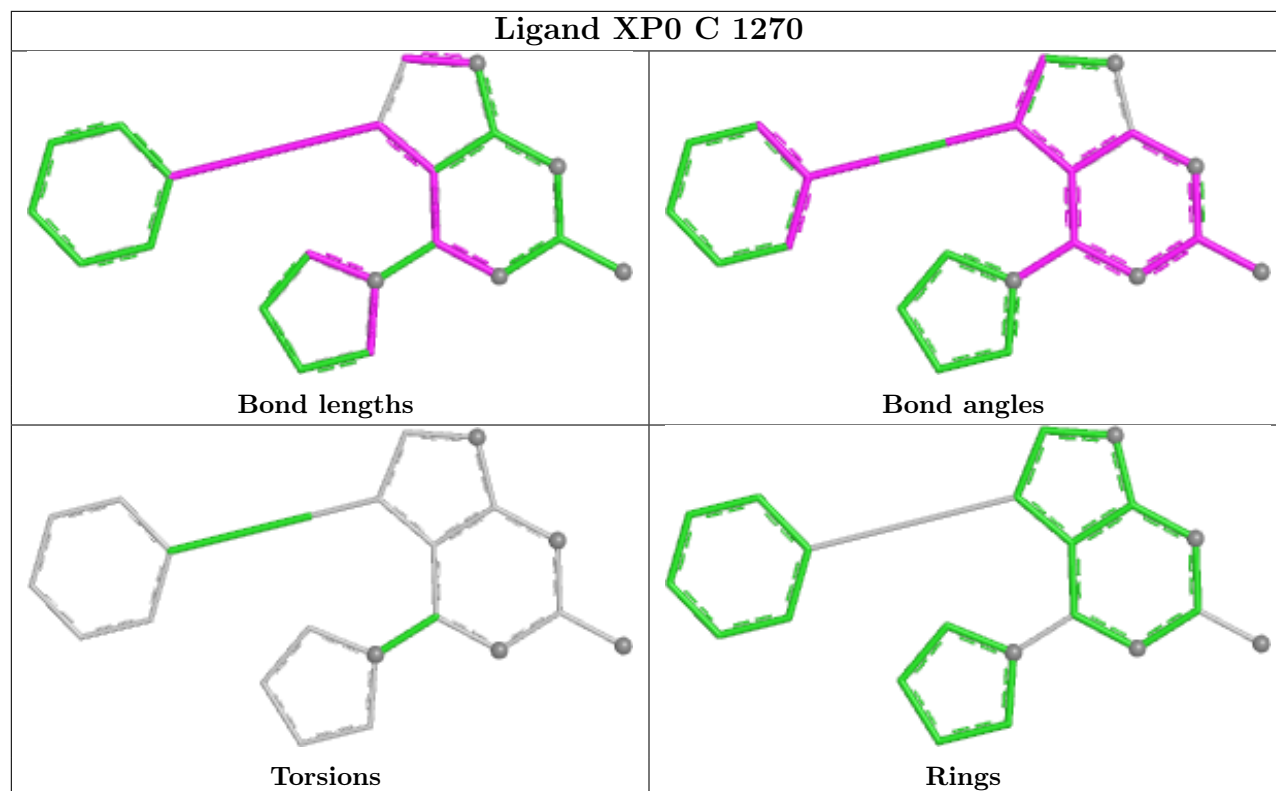
Ligand NAP C 1269

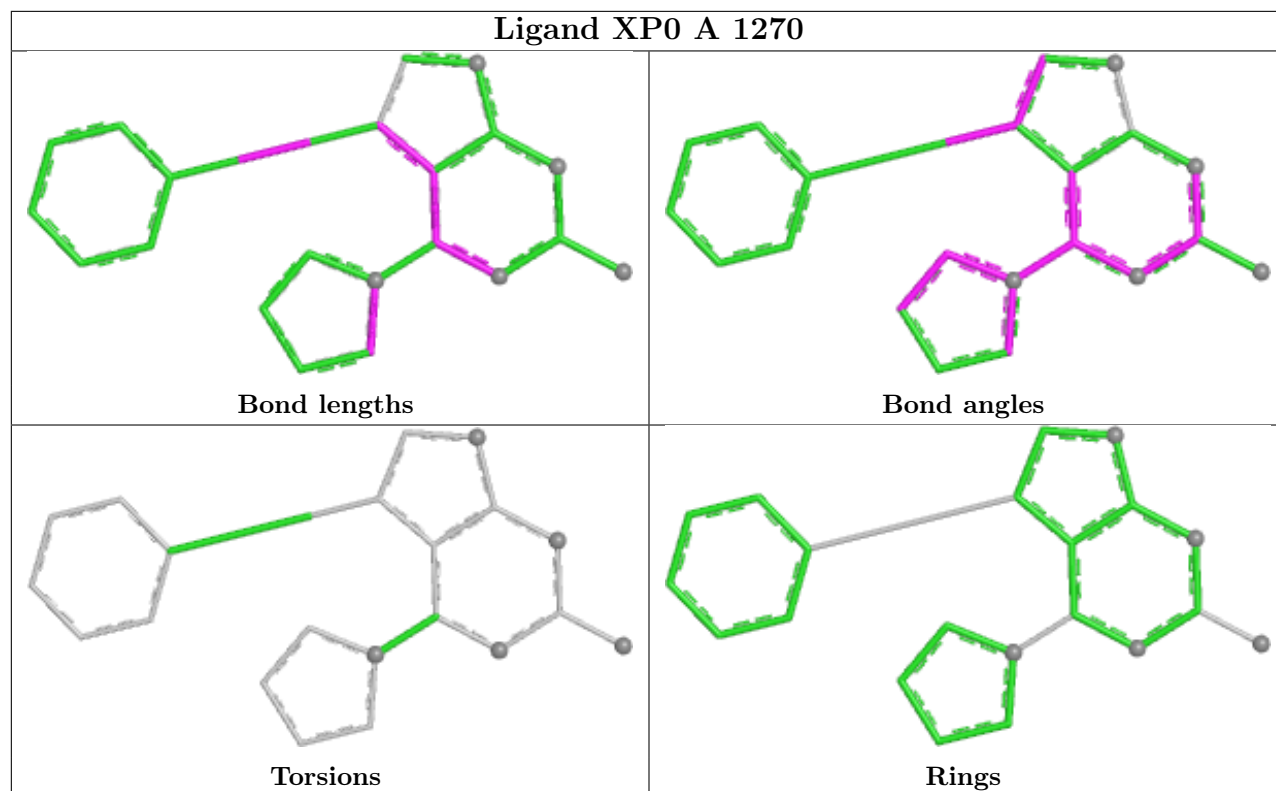


Ligand XP0 D 1270









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	251/288 (87%)	-0.05	11 (4%) 34 35	9, 19, 44, 63	0
1	D	249/288 (86%)	-0.39	3 (1%) 79 80	8, 15, 32, 47	0
2	B	251/288 (87%)	-0.30	7 (2%) 53 54	9, 17, 36, 60	0
2	C	250/288 (86%)	-0.31	5 (2%) 65 67	8, 15, 35, 57	0
All	All	1001/1152 (86%)	-0.26	26 (2%) 56 57	8, 16, 37, 63	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	113	GLY	8.0
1	A	212	ALA	6.5
2	B	113	GLY	5.6
2	C	151	SER	5.5
1	A	211	VAL	5.1
2	B	150	THR	5.1
1	A	113	GLY	4.4
2	B	104	GLN	4.2
2	B	151	SER	4.2
1	A	216	GLU	4.2
2	C	212	ALA	4.1
1	D	113	GLY	3.9
1	A	151	SER	3.8
2	C	104	GLN	3.7
1	A	214	GLY	3.6
1	A	50	LYS	3.4
1	A	104	GLN	3.3
1	A	2	GLU	3.2
2	C	211	VAL	3.1
2	B	211	VAL	2.9
1	D	2	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	2	GLU	2.3
1	A	217	GLU	2.3
1	A	219	ASP	2.3
2	B	219	ASP	2.3
1	D	211	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	CSX	C	168	7/8	0.91	0.10	17,20,40,42	0
2	CSX	B	168	7/8	0.94	0.08	18,20,39,42	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

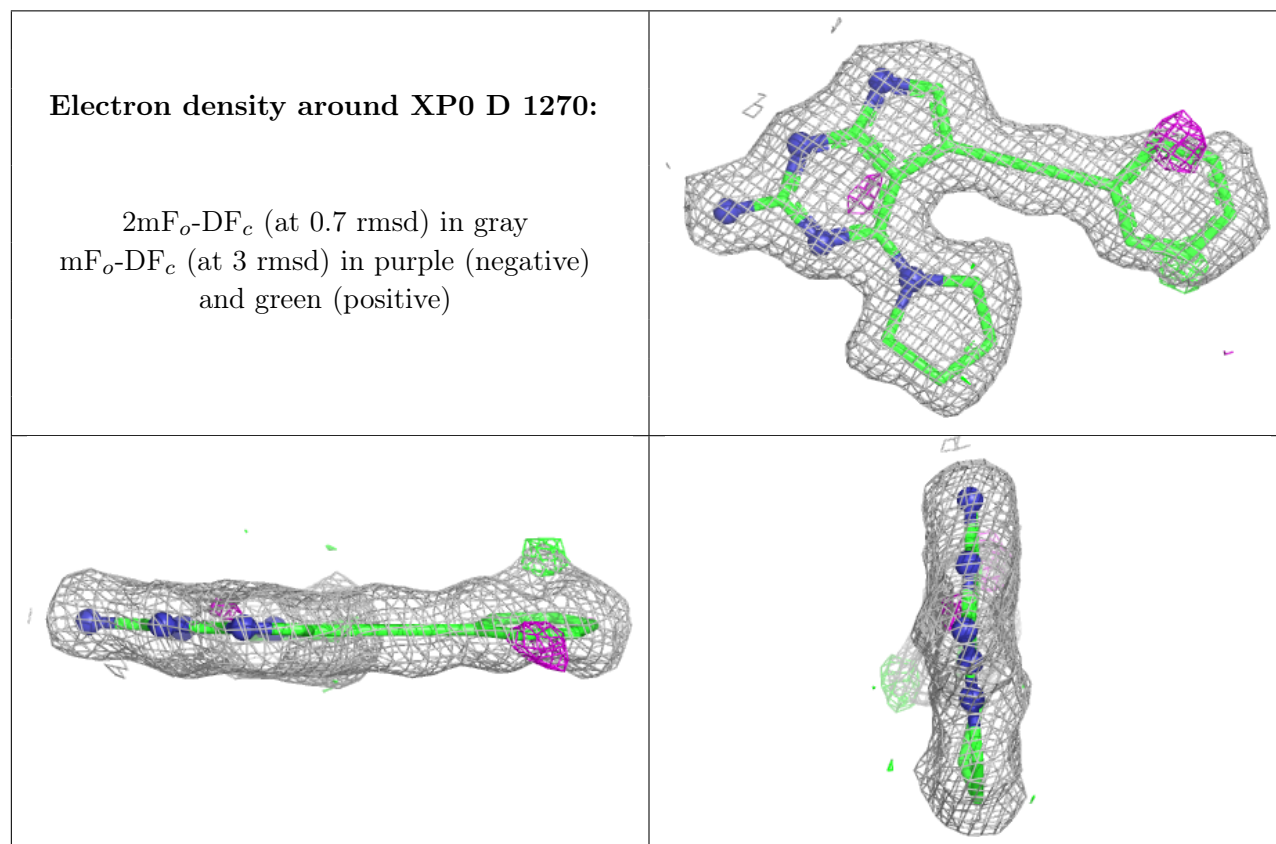
6.4 Ligands [i](#)

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
5	GOL	D	1271	6/6	0.78	0.25	35,39,40,44	0
4	XP0	D	1270	23/23	0.91	0.10	12,17,27,28	0
4	XP0	C	1270	23/23	0.92	0.10	15,23,40,42	0
4	XP0	B	1270	23/23	0.93	0.10	13,18,42,44	0
4	XP0	A	1270	23/23	0.93	0.10	16,23,36,37	0
3	NAP	A	1269	48/48	0.97	0.07	12,15,21,22	0
3	NAP	D	1269	48/48	0.98	0.06	10,13,17,21	0
3	NAP	B	1269	48/48	0.98	0.06	10,14,17,20	0
3	NAP	C	1269	48/48	0.98	0.06	9,12,16,16	0

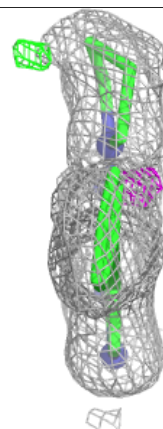
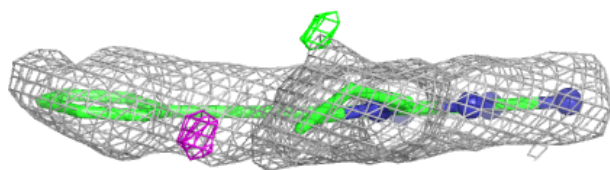
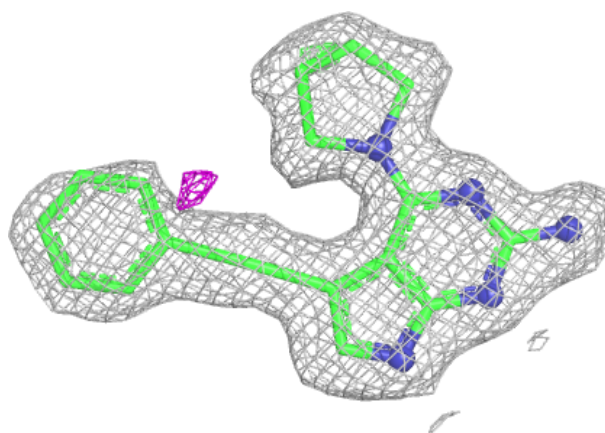
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

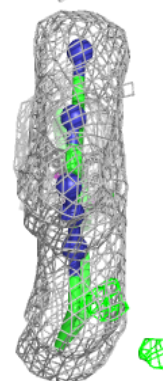
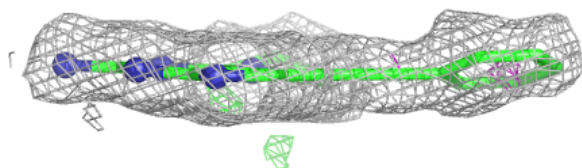
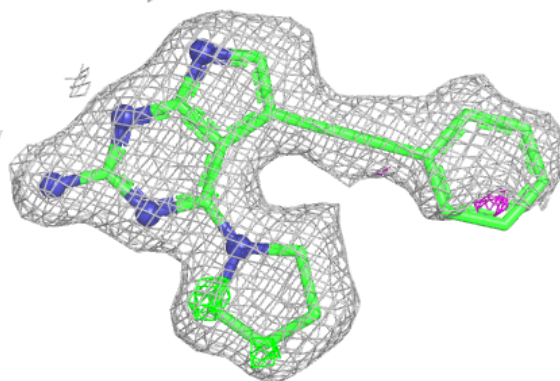


Electron density around XP0 C 1270:

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

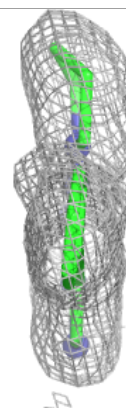
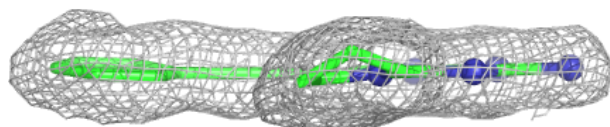
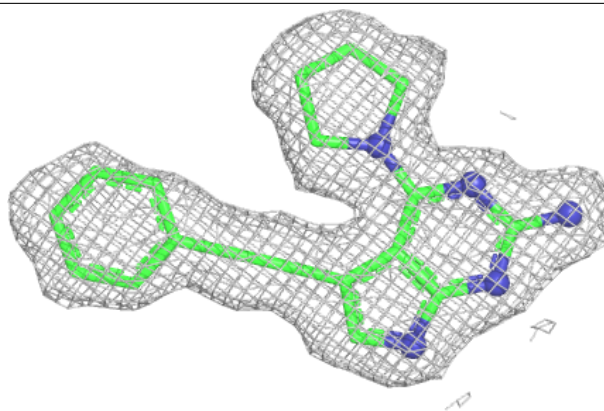
**Electron density around XP0 B 1270:**

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

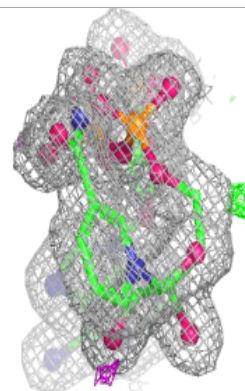
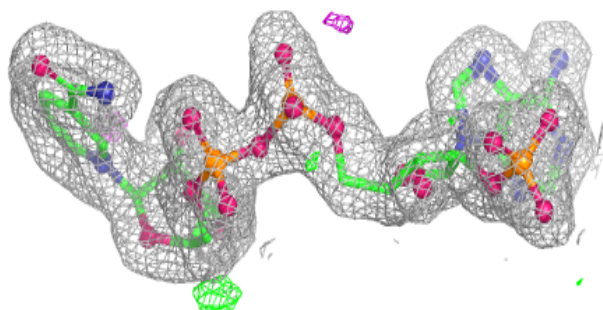
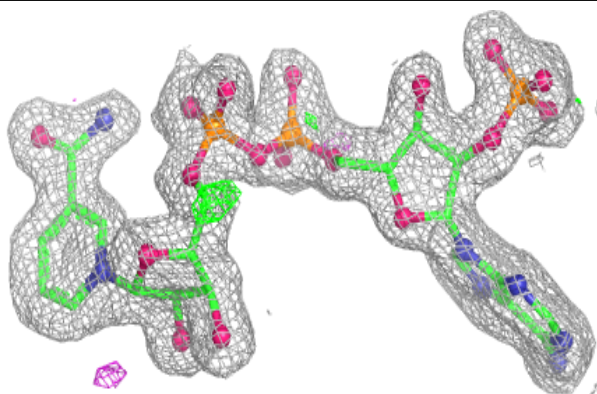


Electron density around XP0 A 1270:

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

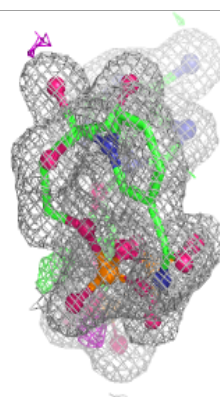
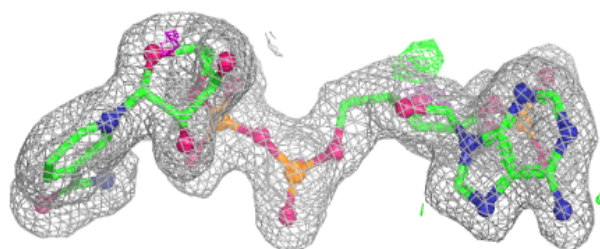
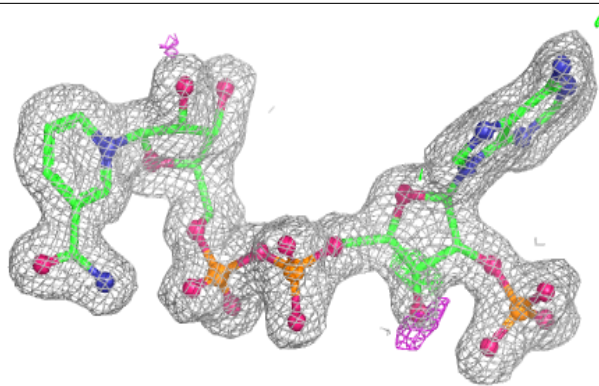
**Electron density around NAP A 1269:**

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

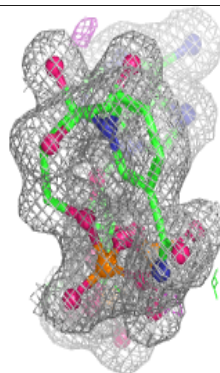
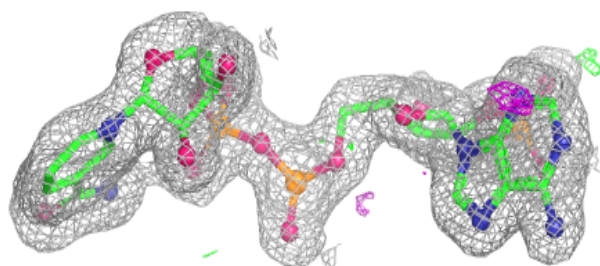
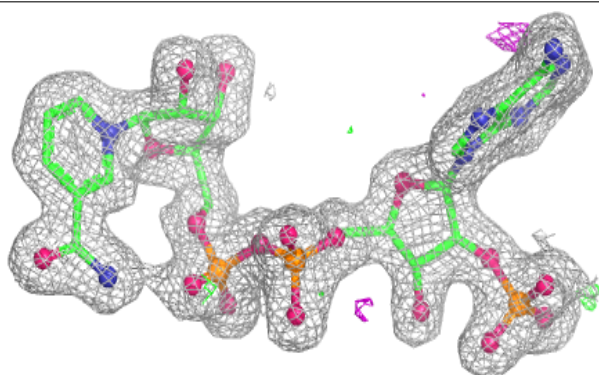


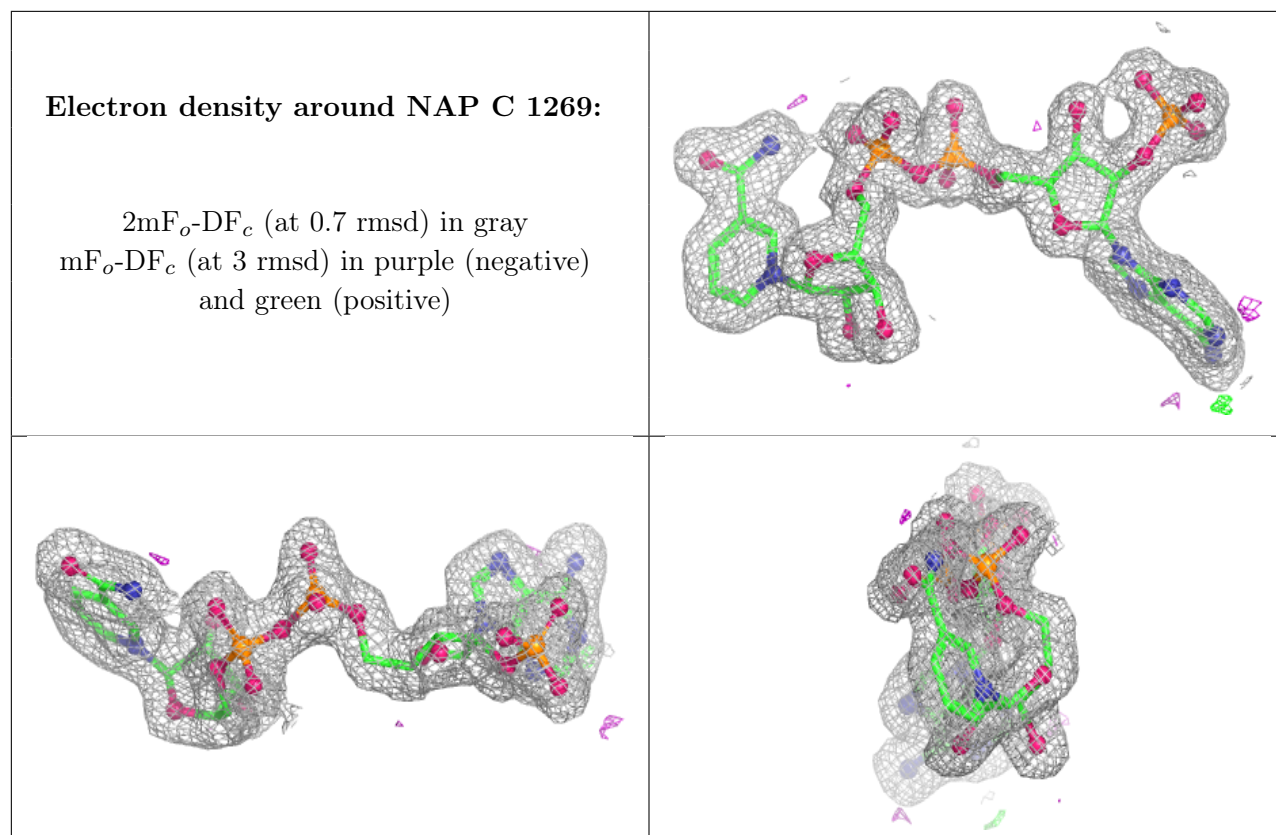
Electron density around NAP D 1269:

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

**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)





6.5 Other polymers [i](#)

There are no such residues in this entry.