



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:01 AM UTC

PDB ID : 4CMJ / pdb_00004cmj
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 : 2014-01-16
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

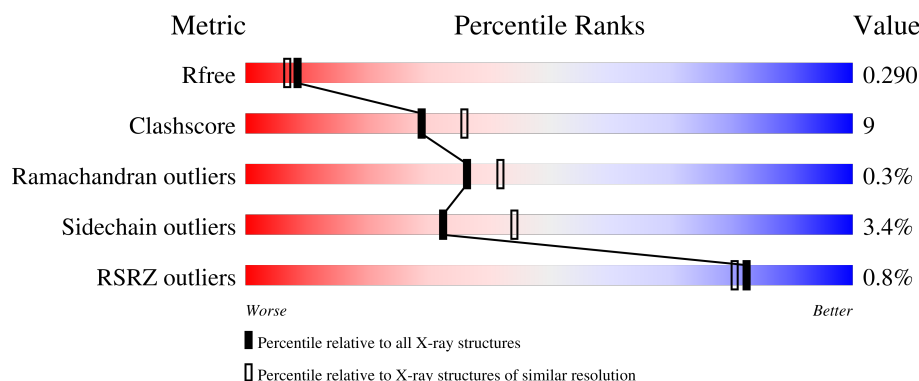
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	B	288	
1	C	288	
1	D	288	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8112 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	0	0
			1869	1173	330	355	11			
1	B	251	Total	C	N	O	S	0	1	0
			1877	1179	332	355	11			
1	C	251	Total	C	N	O	S	0	0	0
			1869	1173	330	355	11			
1	D	249	Total	C	N	O	S	0	0	0
			1854	1165	327	351	11			

There are 80 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
B	-19	MET	-	expression tag	UNP O76290

Continued on next page...

Continued from previous page...

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

Continued on next page...

Chain	Residue	Modelled	Actual	Comment	Reference
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

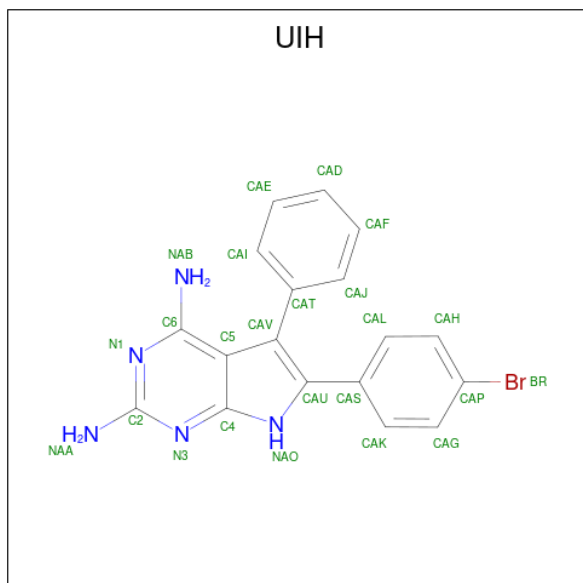
- # NAP
-
- The chemical structure of Naproxen (NAP) is shown, featuring a 2-naphthol core with a 6-methoxy group and a 1-(4-chlorophenyl)propyl side chain. The stereochemistry is indicated with wedges and dashes at the chiral centers. The numbering of atoms is provided for each part of the molecule.

Continued on next page...

Continued from previous page...

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 6-(4-bromophenyl)-5-phenyl-7H-pyrrolo[2,3-d]pyrimidine-2,4-diamine (CCD ID: UIH) (formula: C₁₈H₁₄BrN₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	Br	C	N	0	0
			24	1	18	5		
3	B	1	Total	Br	C	N	0	0
			24	1	18	5		
3	C	1	Total	Br	C	N	0	0
			24	1	18	5		
3	D	1	Total	Br	C	N	0	0
			24	1	18	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total	O	0	0
			108	108		
4	B	104	Total	O	0	0
			104	104		
4	C	84	Total	O	0	0
			84	84		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	59	Total	O	0	0
			59	59		

• Molecule 1: PTERIDINE REDUCTASE 1

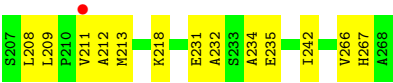
[illegible]

● Molecule 1: PTERIDINE REDUCTASE 1

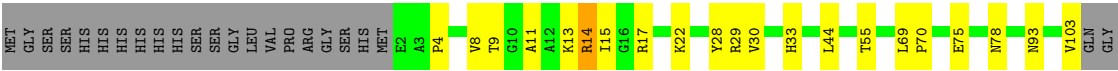
[illegible]

● Molecule 1: PTERIDINE REDUCTASE 1

[illegible]



● 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	74.30Å 90.20Å 82.19Å 90.00° 115.65° 90.00°	Depositor
Resolution (Å)	13.94 – 2.20 13.94 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.8 (13.94-2.20) 93.9 (13.94-2.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.205 , 0.285 0.212 , 0.290	Depositor DCC
R_{free} test set	2348 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8112	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

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

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	0.97	1/1896 (0.1%)	1.07	2/2572 (0.1%)
1	B	1.00	1/1907 (0.1%)	1.12	4/2586 (0.2%)
1	C	0.94	1/1896 (0.1%)	1.10	5/2572 (0.2%)
1	D	0.97	1/1881 (0.1%)	1.11	2/2552 (0.1%)
All	All	0.97	4/7580 (0.1%)	1.10	13/10282 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	ARG	CA-C	6.33	1.59	1.53
1	C	157	VAL	C-O	-5.92	1.18	1.24
1	D	200	ASN	C-O	-5.36	1.17	1.23
1	B	97	PHE	N-CA	-5.05	1.40	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	182	VAL	N-CA-C	-6.92	103.56	110.62
1	C	76	ILE	N-CA-C	-6.86	103.79	110.72
1	B	225	VAL	N-CA-C	6.55	113.52	107.56
1	B	209	LEU	CA-C-N	-6.31	113.47	119.90
1	B	209	LEU	C-N-CA	-6.31	113.47	119.90
1	C	130	ALA	CA-C-N	-6.26	112.39	119.28
1	C	130	ALA	C-N-CA	-6.26	112.39	119.28
1	C	23	LEU	N-CA-C	-6.18	104.62	111.36
1	C	211	VAL	N-CA-C	5.67	116.41	110.62
1	D	181	LEU	N-CA-C	5.54	117.75	111.11
1	A	26	THR	N-CA-C	-5.26	106.82	113.18
1	D	30	VAL	N-CA-C	5.26	116.23	108.45
1	A	13	LYS	N-CA-C	5.16	115.85	108.74

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	1869	0	1890	33	0
1	B	1877	0	1904	31	0
1	C	1869	0	1890	36	0
1	D	1854	0	1877	32	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0
2	C	48	0	25	1	0
2	D	48	0	25	1	0
3	A	24	0	14	5	0
3	B	24	0	14	3	0
3	C	24	0	14	6	0
3	D	24	0	14	4	0
4	A	108	0	0	10	0
4	B	104	0	0	8	1
4	C	84	0	0	5	1
4	D	59	0	0	3	0
All	All	8112	0	7717	134	1

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 9.

All (134) 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:A:197:ILE:HG23	4:A:2052:HOH:O	1.62	1.00
1:A:155:SER:HA	4:A:2052:HOH:O	1.69	0.93
3:D:1270:UIH:CAI	3:D:1270:UIH:HAL	2.01	0.90
1:B:217:GLU:HB2	4:B:2084:HOH:O	1.79	0.83
1:C:198:ARG:HD3	4:C:2044:HOH:O	1.84	0.78
1:B:66:SER:HA	4:B:2035:HOH:O	1.84	0.78
3:C:1270:UIH:CAT	3:C:1270:UIH:HAL	2.16	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:VAL:HG22	1:A:179:HIS:CD2	2.28	0.68
3:A:1270:UIH:HAK	3:A:1270:UIH:CAT	2.26	0.65
1:A:78:ASN:OD1	1:A:141:ARG:NH1	2.31	0.64
1:D:160:CYS:HB3	4:D:2040:HOH:O	1.98	0.63
1:A:93:ASN:OD1	1:A:159:LEU:HD13	2.01	0.61
1:B:198:ARG:HD3	4:B:2057:HOH:O	1.99	0.61
1:B:206:VAL:HG22	3:B:1270:UIH:HAF	1.83	0.61
1:A:140:GLN:HE22	1:C:104:GLN:H	1.48	0.60
1:A:251:TYR:CE2	1:B:232:ALA:HB2	2.37	0.59
1:A:163:MET:HG2	4:A:2056:HOH:O	2.03	0.58
1:C:232:ALA:HB2	1:D:251:TYR:CD2	2.38	0.58
1:A:172:SER:O	1:A:176:MET:HG3	2.02	0.58
1:D:29:ARG:HG2	1:D:55:THR:HG22	1.86	0.58
1:D:169:MET:O	1:D:170:ALA:HB3	2.04	0.58
3:D:1270:UIH:HAL	3:D:1270:UIH:CAT	2.33	0.57
1:D:213:MET:HB3	1:D:218:LYS:HG3	1.86	0.57
1:C:208:LEU:O	4:C:2059:HOH:O	2.18	0.56
1:C:164:VAL:HG22	1:C:179:HIS:CD2	2.40	0.55
1:A:68:VAL:HG22	4:A:2026:HOH:O	2.06	0.55
1:D:205:GLY:O	2:D:1269:NAP:H4N	2.07	0.55
1:C:97:PHE:CE2	3:C:1270:UIH:HAJ	2.42	0.55
1:D:130:ALA:HB3	1:D:131:PRO:HD3	1.88	0.54
3:D:1270:UIH:CAI	3:D:1270:UIH:CAL	2.82	0.54
1:B:164:VAL:HG22	1:B:179:HIS:CD2	2.42	0.54
1:D:153:ASN:ND2	1:D:245:VAL:O	2.40	0.54
1:C:232:ALA:HB2	1:D:251:TYR:CE2	2.42	0.54
1:A:250:GLN:HE21	1:A:250:GLN:HA	1.73	0.53
3:A:1270:UIH:CAK	3:A:1270:UIH:CAJ	2.87	0.53
1:B:24:HIS:O	1:B:52:ARG:NH2	2.42	0.53
1:B:140:GLN:HE22	1:B:143:LYS:HE2	1.74	0.53
1:D:8:VAL:CG1	1:D:11:ALA:HB2	2.40	0.52
1:A:168:CYS:SG	3:A:1270:UIH:CAG	2.97	0.52
1:C:61:ALA:HB3	1:C:76:ILE:HD11	1.91	0.52
1:C:117:GLU:HB2	4:C:2038:HOH:O	2.10	0.52
1:A:9:THR:HA	1:A:33:HIS:HB3	1.91	0.52
3:C:1270:UIH:HAL	3:C:1270:UIH:CAI	2.39	0.52
1:B:38:ALA:O	1:B:42:VAL:HG22	2.10	0.52
1:B:31:VAL:HG21	1:B:80:CYS:HB2	1.93	0.51
1:C:97:PHE:CZ	3:C:1270:UIH:HAJ	2.46	0.51
1:D:4:PRO:HB2	1:D:28:TYR:CD2	2.45	0.50
1:C:42:VAL:CG2	4:C:2016:HOH:O	2.60	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ASN:HA	1:A:69:LEU:HD22	1.94	0.49
1:D:223:ARG:O	1:D:229:ARG:NH1	2.42	0.49
1:A:268:ALA:OXT	1:D:224:LYS:HE3	2.12	0.49
1:A:124:ILE:HG22	1:A:129:ILE:CD1	2.42	0.49
1:A:197:ILE:CG2	4:A:2052:HOH:O	2.39	0.49
3:A:1270:UIH:HAK	3:A:1270:UIH:CAJ	2.43	0.49
1:A:232:ALA:HB2	1:B:251:TYR:CE2	2.48	0.49
4:A:2066:HOH:O	1:C:191:GLU:HB2	2.13	0.48
1:C:158:ASN:HB3	1:C:181:LEU:HD11	1.96	0.48
1:C:175:ASN:ND2	4:C:2048:HOH:O	2.46	0.48
1:D:4:PRO:HB2	1:D:28:TYR:CE2	2.49	0.48
3:C:1270:UIH:CAT	3:C:1270:UIH:CAL	2.88	0.48
1:B:209:LEU:O	1:B:210:PRO:C	2.54	0.48
1:A:155:SER:CA	4:A:2052:HOH:O	2.40	0.47
1:D:9:THR:HA	1:D:33:HIS:HB3	1.96	0.47
1:C:69:LEU:N	1:C:70:PRO:CD	2.77	0.47
1:B:33:HIS:CG	1:B:34:TYR:N	2.82	0.47
1:C:159:LEU:HD22	2:C:1269:NAP:H4D	1.96	0.47
1:A:9:THR:O	1:A:93:ASN:HB3	2.15	0.47
1:A:250:GLN:HA	1:A:250:GLN:NE2	2.29	0.47
2:B:1269:NAP:O1A	3:B:1270:UIH:N1	2.48	0.47
1:C:15:ILE:HA	1:C:234:ALA:HB1	1.96	0.47
1:C:49:ASN:HA	1:C:52:ARG:O	2.14	0.47
1:A:161:ASP:OD1	1:A:161:ASP:C	2.57	0.47
3:C:1270:UIH:HAL	3:C:1270:UIH:CAJ	2.44	0.47
1:B:193:ALA:N	1:B:194:PRO:CD	2.78	0.46
1:A:88:ASP:O	1:A:154:LEU:HA	2.16	0.46
1:C:172:SER:O	1:C:176:MET:HG3	2.14	0.46
1:D:224:LYS:O	1:D:226:PRO:HD3	2.15	0.46
1:B:66:SER:HB3	4:B:2038:HOH:O	2.15	0.46
1:C:38:ALA:O	1:C:42:VAL:HG13	2.16	0.46
1:A:160:CYS:O	2:A:1269:NAP:H6N	2.16	0.46
3:B:1270:UIH:CAT	3:B:1270:UIH:HAK	2.46	0.45
1:C:17:ARG:NH1	1:C:44:LEU:HD13	2.31	0.45
1:D:15:ILE:HG13	4:D:2008:HOH:O	2.14	0.45
1:A:179:HIS:ND1	4:A:2067:HOH:O	2.04	0.45
1:C:86:ARG:HD3	1:C:88:ASP:OD2	2.16	0.45
1:D:200:ASN:HB3	1:D:255:SER:O	2.16	0.45
1:A:232:ALA:HB2	1:B:251:TYR:CD2	2.51	0.45
3:A:1270:UIH:CAT	3:A:1270:UIH:CAK	2.90	0.45
1:C:88:ASP:O	1:C:154:LEU:HA	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:PRO:O	1:D:218:LYS:HD3	2.16	0.45
1:D:242:ILE:HA	1:D:245:VAL:HG22	1.98	0.45
1:B:6:ALA:HB2	1:B:89:VAL:HB	1.99	0.45
1:C:9:THR:O	1:C:93:ASN:HB3	2.17	0.45
1:D:69:LEU:HB3	1:D:70:PRO:HD3	1.98	0.45
1:D:163:MET:HG3	3:D:1270:UIH:BR	2.72	0.45
1:B:26:THR:HG22	1:B:26:THR:O	2.17	0.44
1:C:266:VAL:HG12	1:C:267:HIS:O	2.17	0.44
1:A:117:GLU:HG2	1:C:67:ASN:HA	1.98	0.44
1:D:93:ASN:OD1	1:D:159:LEU:HD13	2.18	0.44
1:C:33:HIS:CG	1:C:34:TYR:N	2.86	0.44
1:C:130:ALA:HB3	1:C:131:PRO:HD3	1.99	0.44
1:B:10:GLY:HA2	4:B:2005:HOH:O	2.17	0.44
1:A:4:PRO:HB2	1:A:28:TYR:CE2	2.52	0.43
1:B:128:ALA:O	1:D:176:MET:HE1	2.18	0.43
1:B:140:GLN:NE2	1:B:143:LYS:HE2	2.32	0.43
1:C:212:ALA:O	1:C:213:MET:C	2.62	0.43
1:A:130:ALA:HB3	1:A:131:PRO:HD3	1.99	0.43
1:B:207:SER:O	1:B:208:LEU:C	2.60	0.43
1:B:11:ALA:HB3	1:B:32:ILE:HG23	2.00	0.43
1:D:75:GLU:HA	1:D:78:ASN:HB2	2.01	0.43
1:B:117:GLU:HG3	1:D:70:PRO:HG2	2.01	0.43
1:C:151:SER:O	1:C:151:SER:OG	2.30	0.42
1:B:227:LEU:HD12	1:B:227:LEU:HA	1.91	0.42
1:A:229:ARG:NH1	4:A:2084:HOH:O	2.52	0.42
1:B:157:VAL:HG11	1:B:241:VAL:HG13	2.02	0.42
1:C:52:ARG:HD2	1:C:55:THR:HG21	2.01	0.42
4:A:2067:HOH:O	1:C:179:HIS:ND1	2.21	0.42
1:D:103:VAL:O	1:D:103:VAL:HG12	2.18	0.42
1:B:155:SER:HA	1:B:198:ARG:O	2.20	0.42
1:B:66:SER:CB	4:B:2038:HOH:O	2.68	0.42
1:D:164:VAL:HG22	1:D:179:HIS:CD2	2.54	0.42
1:D:192:LEU:HB3	1:D:197:ILE:HB	2.02	0.42
1:B:35:HIS:CD2	1:B:62:ASP:HA	2.55	0.41
1:A:120:VAL:HG11	1:C:129:ILE:HD13	2.02	0.41
1:C:209:LEU:HD22	1:C:218:LYS:HA	2.00	0.41
1:A:207:SER:O	1:A:208:LEU:C	2.63	0.41
4:B:2063:HOH:O	1:D:186:GLN:NE2	2.26	0.41
1:A:19:ILE:CD1	1:A:159:LEU:HD11	2.51	0.41
1:D:14:ARG:HB3	4:D:2008:HOH:O	2.21	0.40
1:C:231:GLU:OE1	1:C:231:GLU:N	2.41	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:LEU:O	4:B:2009:HOH:O	2.22	0.40
1:C:65:ASN:HA	1:C:69:LEU:HD22	2.03	0.40
1:B:9:THR:O	1:B:10:GLY:C	2.64	0.40
1:D:13:LYS:HA	1:D:17:ARG:HD2	2.04	0.40

All (1) 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)
4:B:2019:HOH:O	4:C:2020:HOH:O[1_454]	1.97	0.23

5.3 Torsion angles

5.3.1 Protein backbone

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	245/288 (85%)	230 (94%)	14 (6%)	1 (0%)	30	34
1	B	246/288 (85%)	230 (94%)	16 (6%)	0	100	100
1	C	245/288 (85%)	230 (94%)	15 (6%)	0	100	100
1	D	243/288 (84%)	230 (95%)	11 (4%)	2 (1%)	16	16
All	All	979/1152 (85%)	920 (94%)	56 (6%)	3 (0%)	36	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	208	LEU
1	A	223	ARG
1	D	14	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/231 (86%)	192 (96%)	7 (4%)	32	43
1	B	200/231 (87%)	192 (96%)	8 (4%)	28	38
1	C	199/231 (86%)	193 (97%)	6 (3%)	36	49
1	D	197/231 (85%)	191 (97%)	6 (3%)	36	49
All	All	795/924 (86%)	768 (97%)	27 (3%)	32	44

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	44	LEU
1	A	151	SER
1	A	166	GLN
1	A	242	ILE
1	A	245	VAL
1	A	250	GLN
1	B	79	SER
1	B	95	SER
1	B	104	GLN
1	B	152	SER
1	B	159	LEU
1	B	179	HIS
1	B	206	VAL
1	B	250	GLN
1	C	42	VAL
1	C	140	GLN
1	C	166	GLN
1	C	206	VAL
1	C	235	GLU
1	C	242	ILE
1	D	22	LYS
1	D	44	LEU
1	D	117	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	159	LEU
1	D	208	LEU
1	D	213	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	140	GLN
1	A	175	ASN
1	A	250	GLN
1	A	267	HIS
1	B	92	ASN
1	B	140	GLN
1	B	158	ASN
1	B	179	HIS
1	B	250	GLN
1	C	25	GLN
1	C	65	ASN
1	C	175	ASN
1	D	35	HIS
1	D	119	GLN
1	D	142	GLN
1	D	175	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

8 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$
2	NAP	B	1269	-	50,52,52	1.43	7 (14%)	71,80,80	2.03	17 (23%)
3	UIH	B	1270	-	27,27,27	1.72	6 (22%)	37,39,39	1.78	9 (24%)
2	NAP	A	1269	-	50,52,52	1.31	6 (12%)	71,80,80	1.90	17 (23%)
3	UIH	C	1270	-	27,27,27	1.58	5 (18%)	37,39,39	1.86	11 (29%)
2	NAP	C	1269	-	50,52,52	1.34	6 (12%)	71,80,80	1.89	21 (29%)
3	UIH	A	1270	-	27,27,27	1.73	6 (22%)	37,39,39	1.94	9 (24%)
2	NAP	D	1269	-	50,52,52	1.35	10 (20%)	71,80,80	2.05	18 (25%)
3	UIH	D	1270	-	27,27,27	1.80	5 (18%)	37,39,39	1.52	6 (16%)

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	B	1269	-	-	0/35/67/67	0/5/5/5
3	UIH	B	1270	-	-	0/8/8/8	0/4/4/4
2	NAP	A	1269	-	-	0/35/67/67	0/5/5/5
3	UIH	C	1270	-	-	1/8/8/8	0/4/4/4
2	NAP	C	1269	-	-	3/35/67/67	0/5/5/5
3	UIH	A	1270	-	-	0/8/8/8	0/4/4/4
2	NAP	D	1269	-	-	0/35/67/67	0/5/5/5
3	UIH	D	1270	-	-	2/8/8/8	0/4/4/4

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1269	NAP	C5A-C4A	4.83	1.47	1.39
2	A	1269	NAP	C5A-C4A	4.75	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1269	NAP	C5A-C4A	4.52	1.47	1.39
3	A	1270	UIH	C2-NAA	4.52	1.42	1.33
3	D	1270	UIH	C2-NAA	4.41	1.42	1.33
3	D	1270	UIH	C5-CAV	-4.21	1.35	1.46
3	D	1270	UIH	C6-NAB	4.21	1.45	1.34
2	B	1269	NAP	PN-O3	4.15	1.64	1.59
3	B	1270	UIH	C2-NAA	4.02	1.41	1.33
2	C	1269	NAP	PN-O3	3.93	1.63	1.59
3	A	1270	UIH	C5-CAV	-3.84	1.36	1.46
3	B	1270	UIH	C6-NAB	3.71	1.43	1.34
2	D	1269	NAP	C5A-C4A	3.65	1.45	1.39
3	C	1270	UIH	C5-CAV	-3.58	1.36	1.46
3	A	1270	UIH	C5-C6	-3.50	1.38	1.42
3	D	1270	UIH	C5-C6	-3.39	1.38	1.42
3	B	1270	UIH	BR-CAP	3.38	1.97	1.90
3	C	1270	UIH	C2-NAA	3.36	1.40	1.33
2	B	1269	NAP	PA-O3	3.35	1.63	1.59
3	A	1270	UIH	C6-NAB	3.34	1.42	1.34
3	B	1270	UIH	C5-CAV	-3.27	1.37	1.46
3	C	1270	UIH	C5-C6	-3.10	1.38	1.42
2	B	1269	NAP	O7N-C7N	-3.08	1.18	1.24
2	A	1269	NAP	C5A-N7A	-3.01	1.33	1.39
2	A	1269	NAP	C4A-N9A	-2.93	1.31	1.37
2	D	1269	NAP	P2B-O2B	2.92	1.64	1.59
2	A	1269	NAP	C5A-C6A	2.84	1.48	1.41
2	D	1269	NAP	C3N-C7N	-2.77	1.46	1.50
3	B	1270	UIH	C5-C6	-2.76	1.39	1.42
3	D	1270	UIH	BR-CAP	2.72	1.95	1.90
3	C	1270	UIH	C6-NAB	2.71	1.41	1.34
2	B	1269	NAP	C8A-N7A	2.71	1.36	1.31
3	C	1270	UIH	CAS-CAU	2.67	1.51	1.47
2	D	1269	NAP	C5A-C6A	2.66	1.48	1.41
2	C	1269	NAP	C5A-C6A	2.66	1.48	1.41
2	D	1269	NAP	C8A-N7A	2.64	1.36	1.31
2	D	1269	NAP	PA-O3	2.63	1.62	1.59
2	A	1269	NAP	P2B-O2B	2.62	1.64	1.59
2	A	1269	NAP	C8A-N7A	2.52	1.36	1.31
3	A	1270	UIH	C5-C4	-2.42	1.37	1.41
2	D	1269	NAP	O7N-C7N	-2.34	1.19	1.24
2	C	1269	NAP	PA-O3	2.28	1.62	1.59
2	B	1269	NAP	C5A-C6A	2.22	1.47	1.41
3	A	1270	UIH	BR-CAP	2.22	1.94	1.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1269	NAP	O4B-C1B	2.21	1.47	1.42
2	B	1269	NAP	C5A-N7A	-2.18	1.35	1.39
2	C	1269	NAP	C8A-N7A	2.15	1.35	1.31
3	B	1270	UIH	C5-C4	-2.11	1.38	1.41
2	D	1269	NAP	C5A-N7A	-2.11	1.35	1.39
2	D	1269	NAP	PN-O3	2.08	1.61	1.59
2	C	1269	NAP	C4A-N9A	-2.06	1.33	1.37

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1269	NAP	C2B-C1B-N9A	-7.24	101.84	113.75
2	B	1269	NAP	C3N-C7N-N7N	6.13	125.29	117.74
2	D	1269	NAP	C5A-C4A-N3A	-6.07	118.36	126.72
2	A	1269	NAP	O4B-C1B-N9A	5.65	118.95	108.09
2	B	1269	NAP	N3A-C2A-N1A	-5.27	120.61	128.58
2	D	1269	NAP	C4A-C5A-N7A	-5.22	104.61	110.58
2	C	1269	NAP	C2B-C1B-N9A	-4.94	105.62	113.75
2	D	1269	NAP	O4B-C1B-N9A	4.82	117.35	108.09
2	A	1269	NAP	C5A-C4A-N3A	-4.72	120.22	126.72
3	A	1270	UIH	N3-C2-N1	-4.70	118.27	125.48
2	C	1269	NAP	C4A-N9A-C8A	4.61	110.58	105.74
2	B	1269	NAP	C5A-C4A-N3A	-4.60	120.38	126.72
2	D	1269	NAP	O2A-PA-O3	4.43	119.26	107.27
3	B	1270	UIH	NAA-C2-N1	4.41	123.84	117.22
2	D	1269	NAP	C2A-N3A-C4A	4.41	122.59	111.83
2	B	1269	NAP	O7N-C7N-C3N	-4.39	114.23	119.60
2	A	1269	NAP	C4A-C5A-N7A	-4.36	105.60	110.58
3	B	1270	UIH	N3-C2-N1	-4.24	118.98	125.48
2	B	1269	NAP	C4D-O4D-C1D	-4.22	106.06	109.92
2	C	1269	NAP	C5A-C4A-N3A	-4.09	121.09	126.72
3	A	1270	UIH	C2-N1-C6	4.05	122.14	117.28
2	D	1269	NAP	C5A-N7A-C8A	4.02	109.77	103.45
2	D	1269	NAP	N3A-C2A-N1A	-3.95	122.60	128.58
3	C	1270	UIH	CAT-CAV-CAU	-3.94	119.28	126.60
2	B	1269	NAP	O4B-C1B-N9A	3.92	115.62	108.09
2	B	1269	NAP	C2A-N3A-C4A	3.89	121.34	111.83
2	C	1269	NAP	C4A-C5A-N7A	-3.84	106.20	110.58
3	A	1270	UIH	C5-CAV-CAU	3.82	108.34	106.54
3	C	1270	UIH	N3-C2-N1	-3.80	119.66	125.48
3	D	1270	UIH	N3-C2-N1	-3.77	119.70	125.48
2	C	1269	NAP	N3A-C4A-N9A	3.75	133.54	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1269	NAP	N3A-C4A-N9A	3.71	133.48	127.17
3	C	1270	UIH	C2-N1-C6	3.66	121.67	117.28
2	B	1269	NAP	C4A-C5A-N7A	-3.64	106.42	110.58
2	D	1269	NAP	C2B-C1B-N9A	-3.62	107.79	113.75
2	C	1269	NAP	O7N-C7N-N7N	-3.54	117.50	122.62
2	B	1269	NAP	N3A-C4A-N9A	3.48	133.09	127.17
3	C	1270	UIH	CAS-CAU-CAV	-3.46	128.05	131.65
3	A	1270	UIH	CAT-CAV-CAU	-3.46	120.18	126.60
2	C	1269	NAP	N3A-C2A-N1A	-3.46	123.35	128.58
2	B	1269	NAP	C2A-N1A-C6A	3.44	124.39	118.73
3	D	1270	UIH	C2-N1-C6	3.44	121.40	117.28
2	D	1269	NAP	C6A-C5A-N7A	3.42	138.69	132.09
3	A	1270	UIH	NAA-C2-N1	3.40	122.33	117.22
3	B	1270	UIH	C2-N1-C6	3.40	121.37	117.28
3	D	1270	UIH	CAK-CAS-CAU	-3.38	116.74	120.76
2	B	1269	NAP	C5A-N7A-C8A	3.32	108.67	103.45
3	D	1270	UIH	C5-CAV-CAU	3.29	108.09	106.54
3	A	1270	UIH	CAS-CAU-CAV	-3.20	128.32	131.65
2	D	1269	NAP	N9A-C8A-N7A	-3.17	109.44	113.94
2	C	1269	NAP	O3X-P2B-O2X	3.16	119.64	107.80
2	A	1269	NAP	C3N-C7N-N7N	3.15	121.62	117.74
2	B	1269	NAP	N9A-C8A-N7A	-3.15	109.47	113.94
2	D	1269	NAP	C3N-C7N-N7N	3.12	121.59	117.74
2	B	1269	NAP	O2B-P2B-O1X	-3.10	98.28	109.33
2	C	1269	NAP	N9A-C8A-N7A	-3.08	109.57	113.94
2	C	1269	NAP	C5A-N7A-C8A	3.07	108.28	103.45
2	B	1269	NAP	C6A-C5A-N7A	3.06	137.99	132.09
3	A	1270	UIH	C5-C4-NAO	3.03	111.84	109.24
2	B	1269	NAP	C2B-C1B-N9A	-3.03	108.77	113.75
2	B	1269	NAP	C4A-N9A-C8A	3.02	108.91	105.74
2	D	1269	NAP	C4B-O4B-C1B	-3.02	102.81	109.47
2	D	1269	NAP	O3-PN-O1N	-2.95	101.82	110.70
3	C	1270	UIH	C5-CAV-CAU	2.92	107.92	106.54
2	C	1269	NAP	C6A-C5A-N7A	2.92	137.71	132.09
2	C	1269	NAP	C2A-N3A-C4A	2.91	118.95	111.83
3	C	1270	UIH	NAA-C2-N3	2.91	121.58	117.22
3	B	1270	UIH	CAS-CAU-CAV	-2.90	128.63	131.65
3	D	1270	UIH	CAS-CAU-CAV	-2.83	128.70	131.65
2	A	1269	NAP	C2A-N3A-C4A	2.82	118.72	111.83
3	B	1270	UIH	CAI-CAT-CAV	-2.81	116.06	120.91
2	C	1269	NAP	O2N-PN-O1N	2.72	125.10	112.44
3	D	1270	UIH	NAA-C2-N1	2.66	121.22	117.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1269	NAP	C2A-N1A-C6A	2.66	123.10	118.73
2	A	1269	NAP	C5A-N7A-C8A	2.63	107.59	103.45
2	A	1269	NAP	N3A-C4A-N9A	2.61	131.60	127.17
3	C	1270	UIH	NAB-C6-N1	-2.57	113.56	117.03
3	C	1270	UIH	C5-CAV-CAT	2.55	132.80	127.01
2	A	1269	NAP	N3A-C2A-N1A	-2.53	124.75	128.58
3	B	1270	UIH	CAT-CAV-CAU	-2.53	121.90	126.60
2	C	1269	NAP	C2A-N1A-C6A	2.48	122.81	118.73
2	C	1269	NAP	C4D-O4D-C1D	-2.47	107.67	109.92
2	C	1269	NAP	O4B-C1B-N9A	2.45	112.80	108.09
2	A	1269	NAP	C4B-O4B-C1B	-2.45	104.05	109.47
2	D	1269	NAP	O2B-P2B-O1X	-2.42	100.70	109.33
3	B	1270	UIH	CAJ-CAT-CAV	2.42	125.08	120.91
3	B	1270	UIH	CAK-CAS-CAU	-2.39	117.92	120.76
3	C	1270	UIH	C6-C5-C4	-2.32	113.98	115.71
2	C	1269	NAP	C3N-C7N-N7N	2.28	120.55	117.74
2	A	1269	NAP	C6A-C5A-N7A	2.24	136.42	132.09
2	A	1269	NAP	O3X-P2B-O2X	2.23	116.15	107.80
2	C	1269	NAP	C5N-C6N-N1N	-2.22	117.35	120.38
2	B	1269	NAP	O4D-C4D-C3D	2.22	109.56	105.15
2	D	1269	NAP	C4A-N9A-C8A	2.22	108.06	105.74
3	A	1270	UIH	C2-N3-C4	2.21	119.85	114.59
2	C	1269	NAP	P2B-O2B-C2B	2.20	129.31	123.43
2	A	1269	NAP	O2A-PA-O3	2.18	113.18	107.27
3	A	1270	UIH	C6-C5-C4	-2.16	114.10	115.71
2	C	1269	NAP	C4A-N9A-C1B	-2.13	121.64	126.63
2	A	1269	NAP	O2B-P2B-O1X	-2.11	101.82	109.33
2	D	1269	NAP	C5A-C4A-N9A	2.09	108.09	105.81
3	C	1270	UIH	C5-C4-NAO	2.09	111.04	109.24
3	B	1270	UIH	C5-CAV-CAU	2.08	107.52	106.54
2	C	1269	NAP	O5B-PA-O1A	-2.08	100.70	108.94
2	D	1269	NAP	C2N-C3N-C4N	2.08	120.67	118.26
2	A	1269	NAP	C4D-O4D-C1D	-2.06	108.04	109.92
2	A	1269	NAP	C5A-C4A-N9A	2.06	108.05	105.81
3	C	1270	UIH	CAL-CAS-CAU	2.04	123.19	120.76

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1269	NAP	C5B-O5B-PA-O2A
2	C	1269	NAP	C5B-O5B-PA-O1A

Continued on next page...

Continued from previous page...

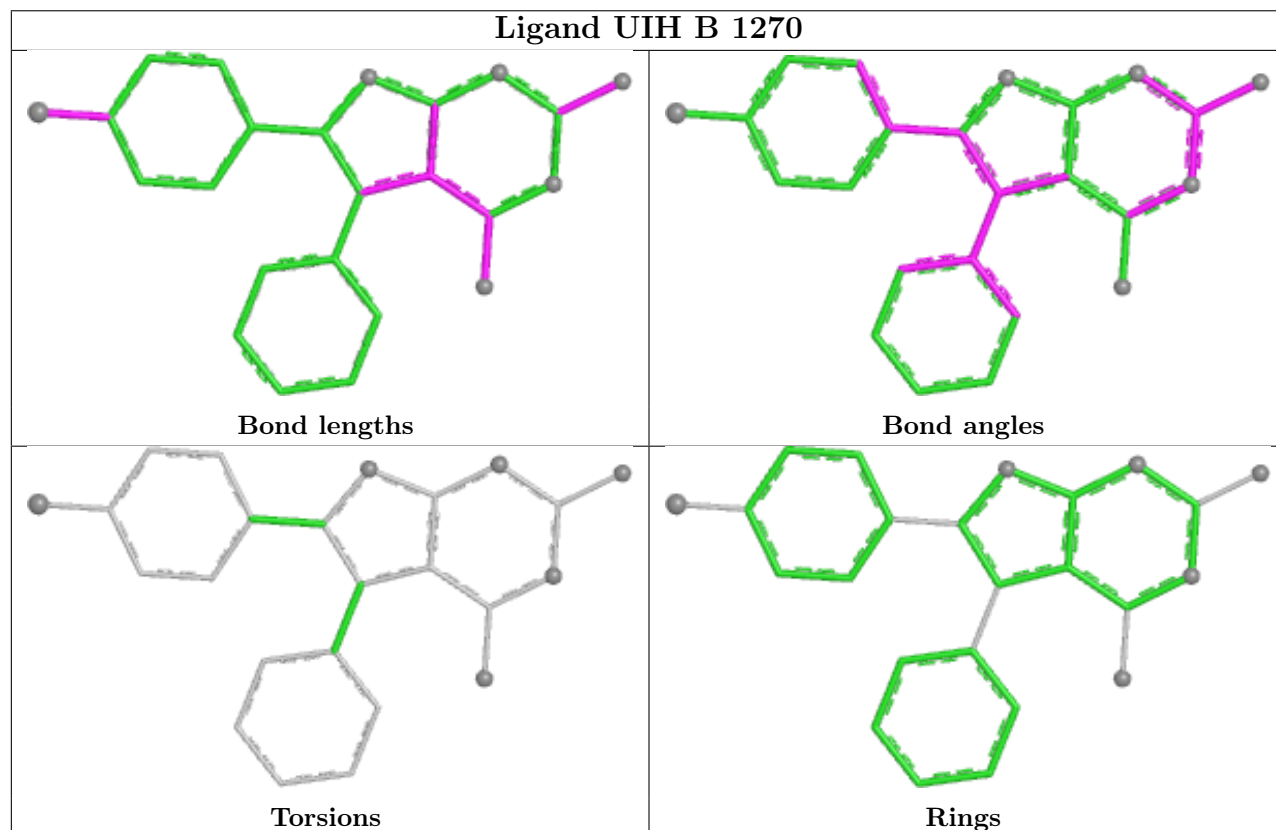
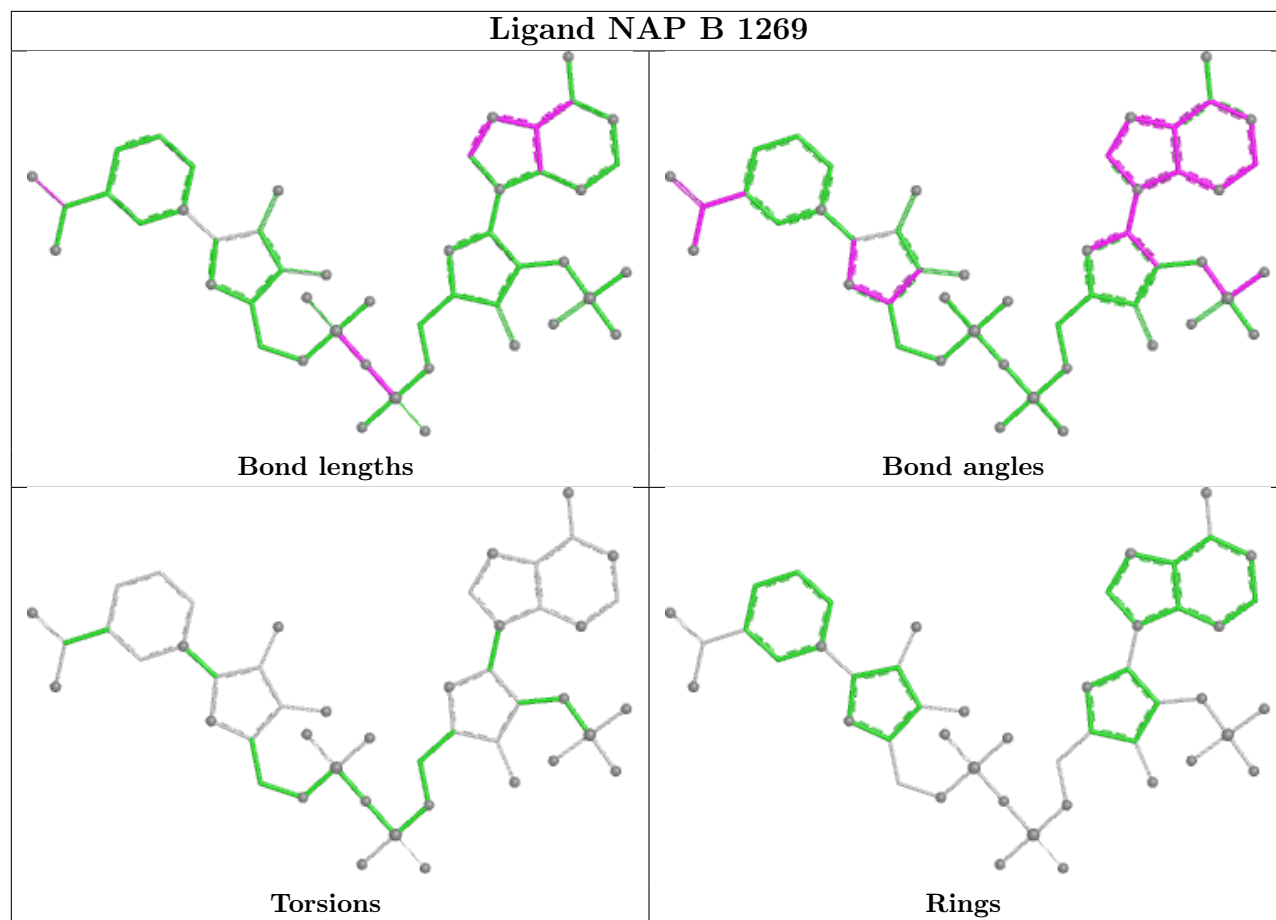
Mol	Chain	Res	Type	Atoms
2	C	1269	NAP	C5B-O5B-PA-O3
3	D	1270	UIH	CAK-CAS-CAU-NAO
3	C	1270	UIH	CAK-CAS-CAU-NAO
3	D	1270	UIH	CAL-CAS-CAU-CAV

There are no ring outliers.

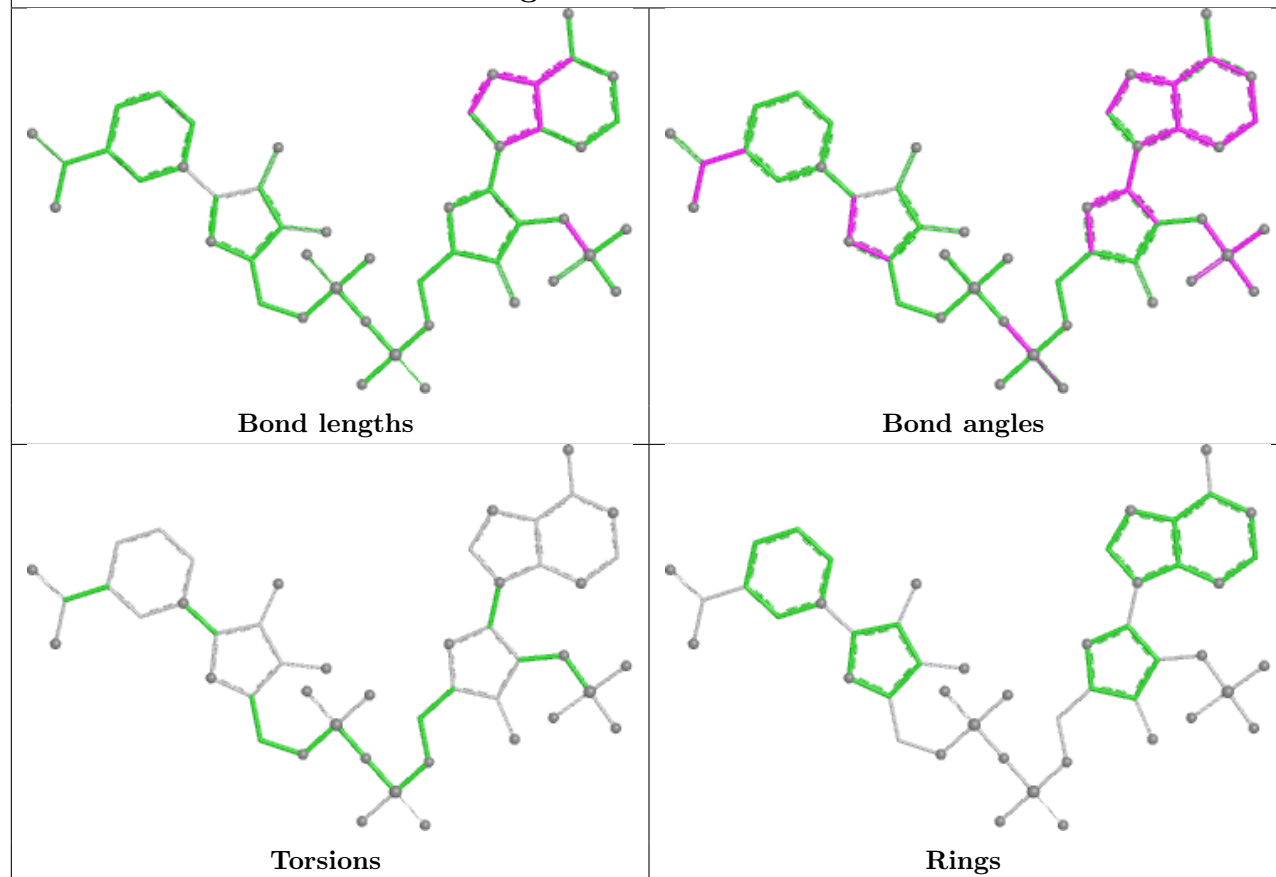
8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1269	NAP	1	0
3	B	1270	UIH	3	0
2	A	1269	NAP	1	0
3	C	1270	UIH	6	0
2	C	1269	NAP	1	0
3	A	1270	UIH	5	0
2	D	1269	NAP	1	0
3	D	1270	UIH	4	0

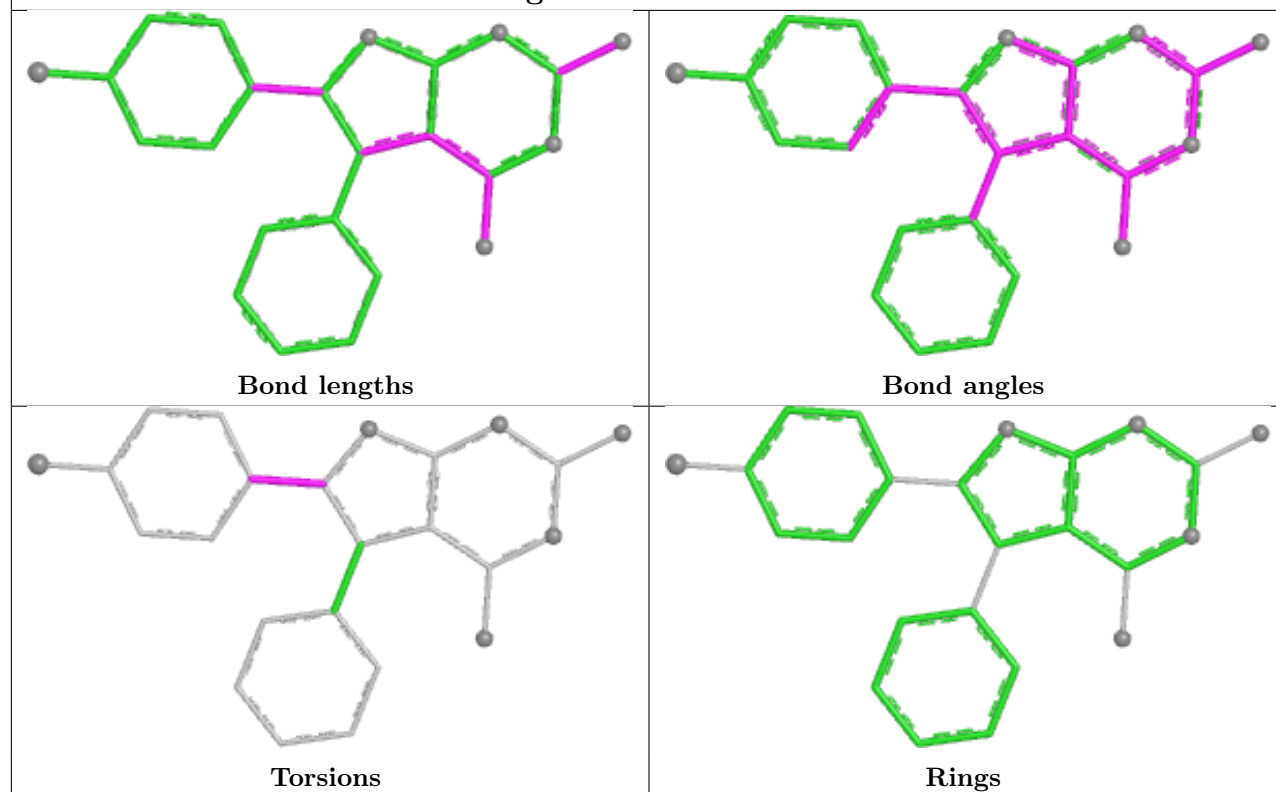
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



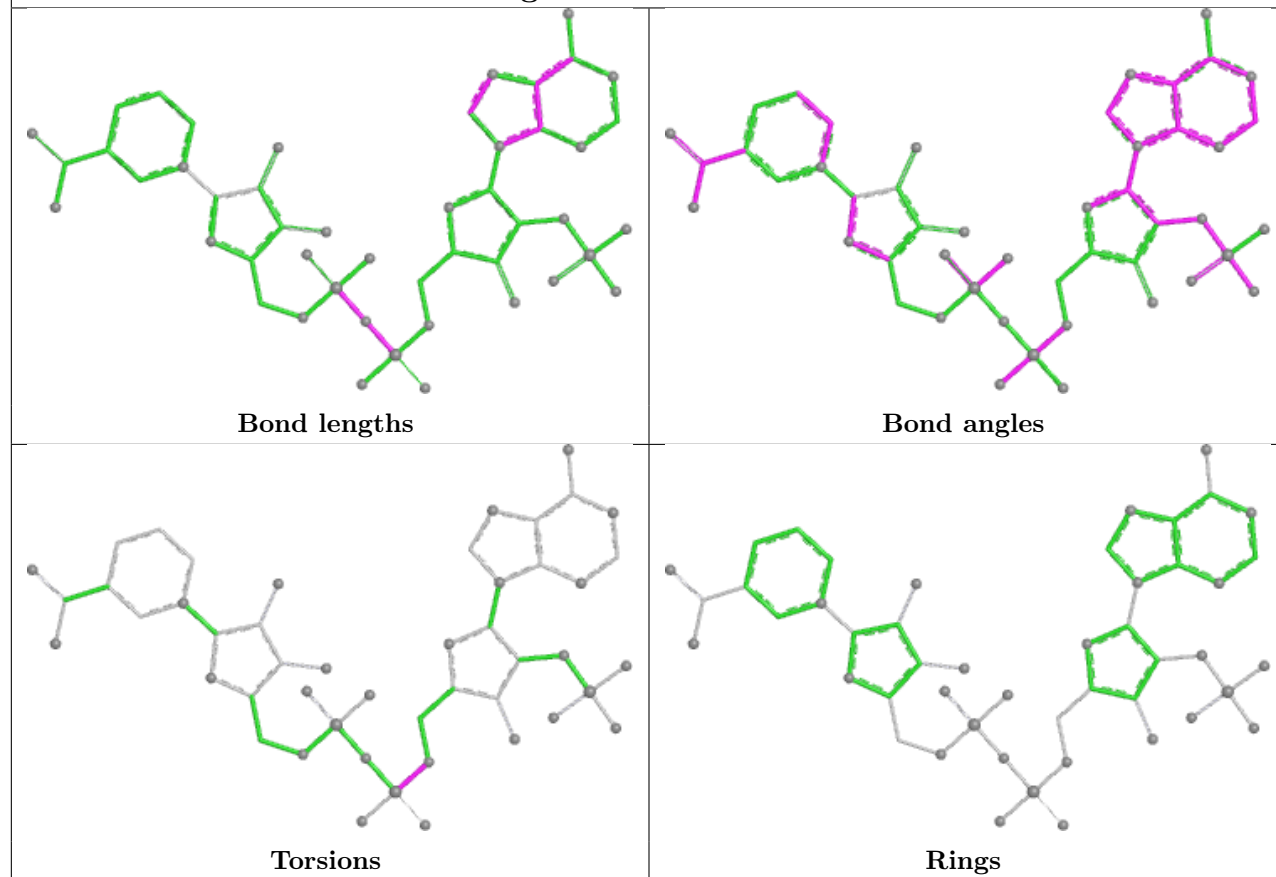
Ligand NAP A 1269



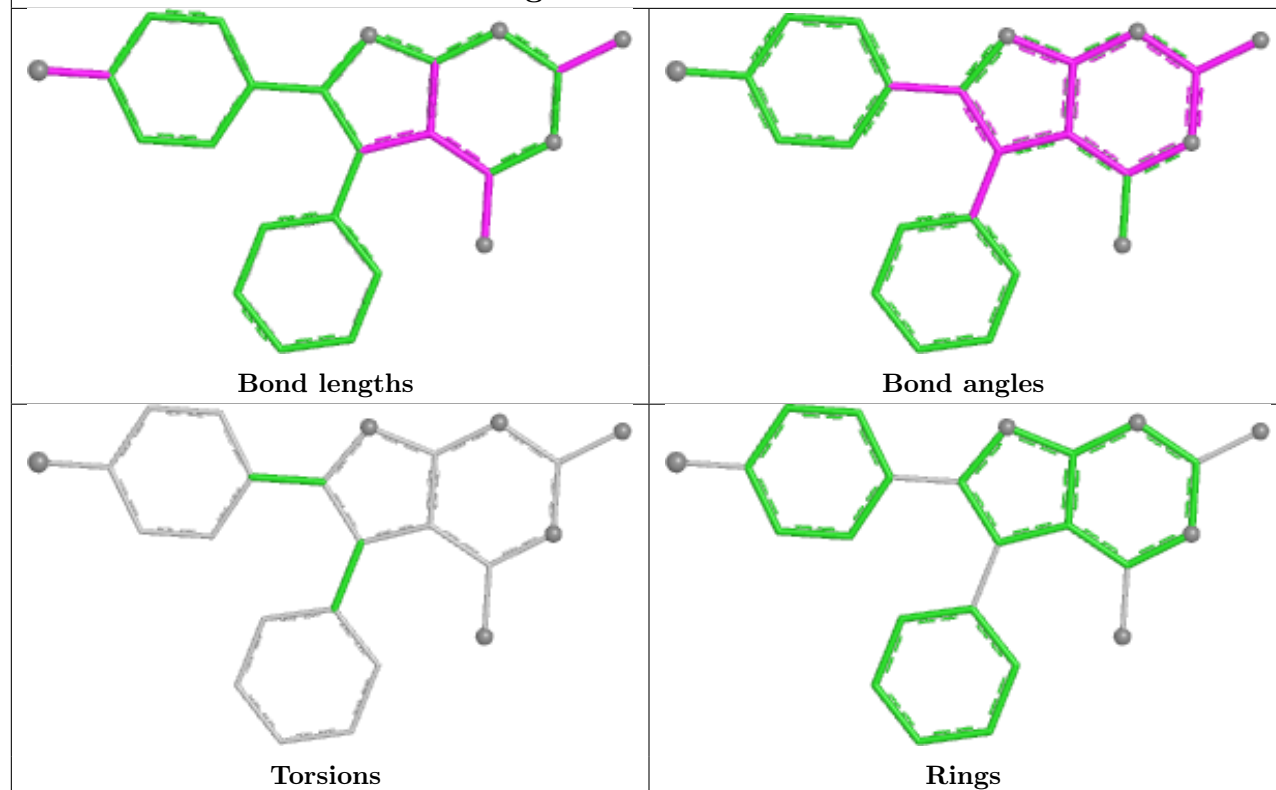
Ligand UIH C 1270



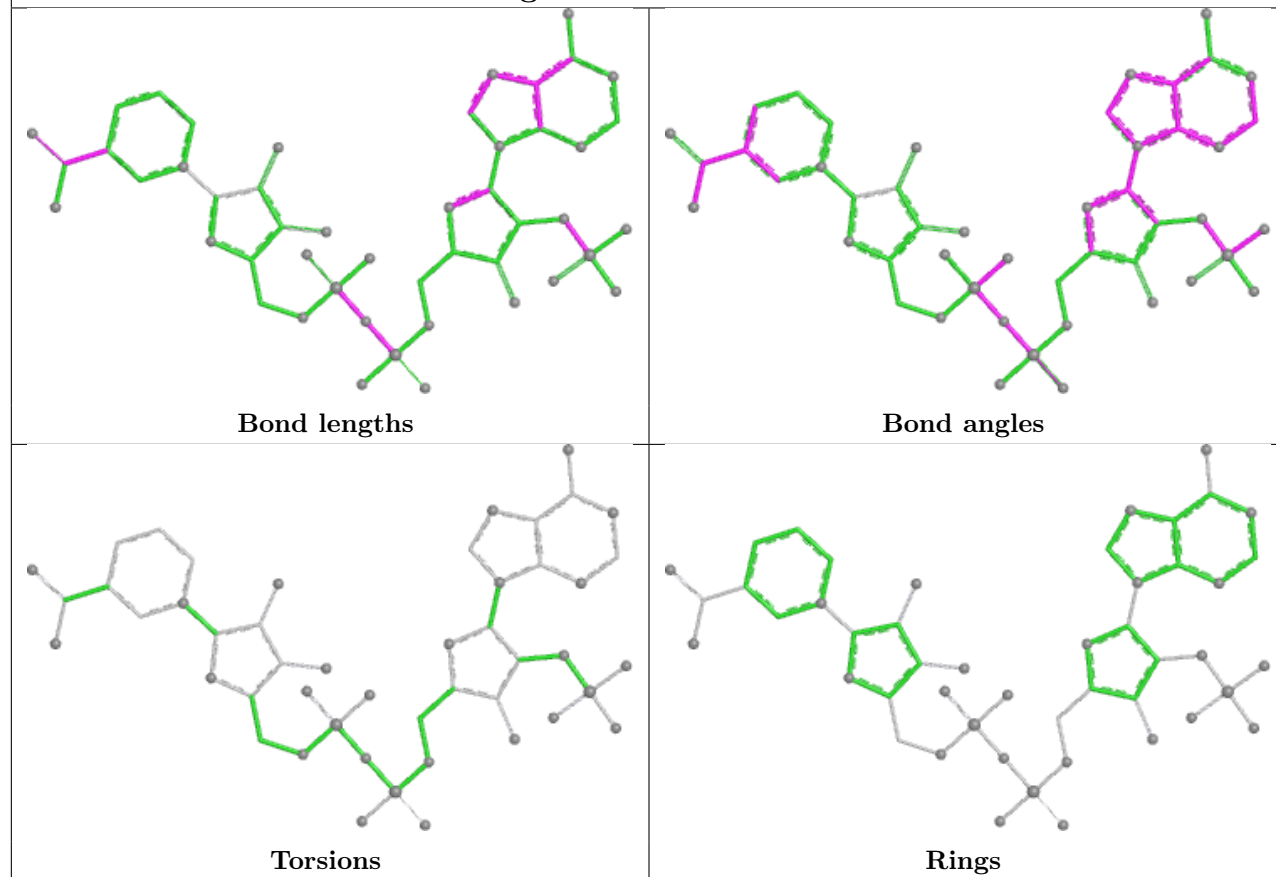
Ligand NAP C 1269



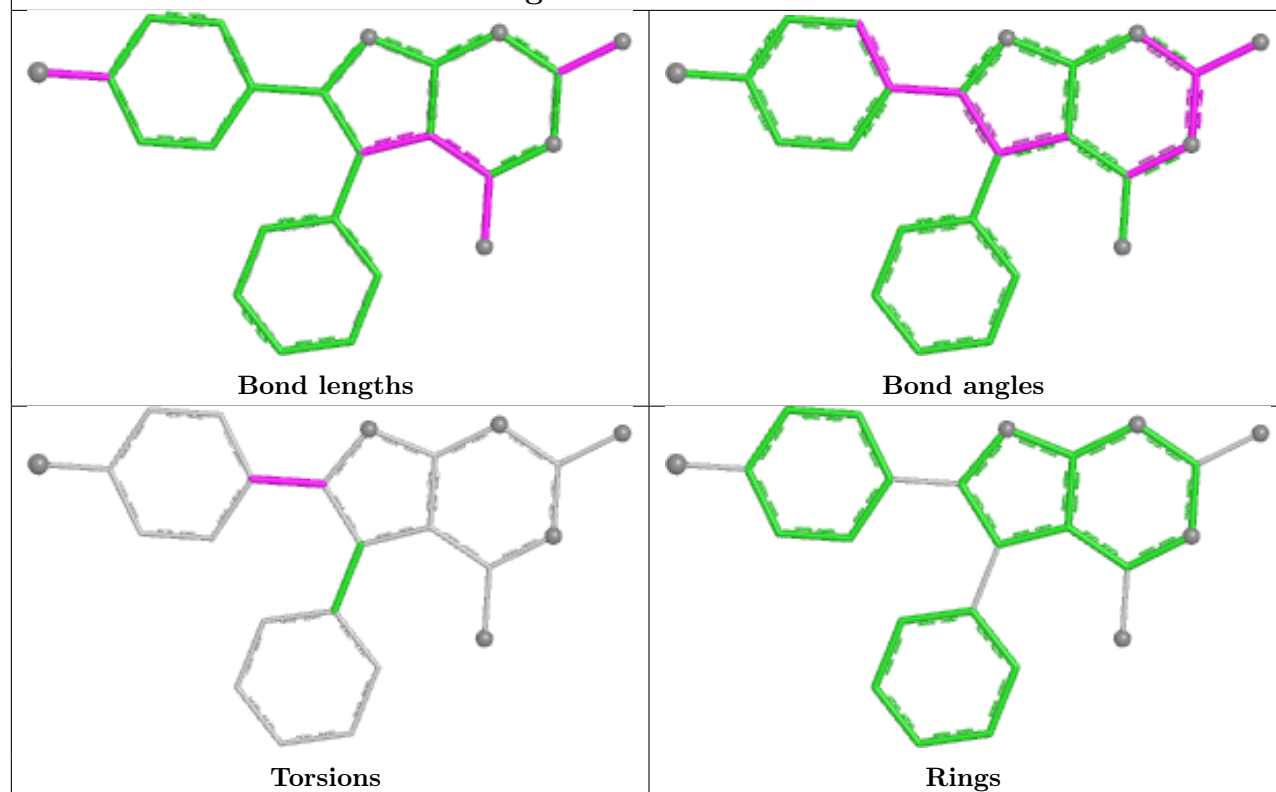
Ligand UIH A 1270



Ligand NAP D 1269



Ligand UIH 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 [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	251/288 (87%)	-0.22	1 (0%) 88 87	6, 14, 30, 54	0
1	B	251/288 (87%)	-0.17	1 (0%) 88 87	6, 14, 29, 48	1 (0%)
1	C	251/288 (87%)	-0.09	1 (0%) 88 87	8, 15, 38, 54	0
1	D	249/288 (86%)	-0.08	5 (2%) 65 62	7, 15, 38, 73	0
All	All	1002/1152 (86%)	-0.14	8 (0%) 82 80	6, 15, 34, 73	1 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	212	ALA	6.1
1	D	211	VAL	4.1
1	D	210	PRO	3.0
1	C	211	VAL	3.0
1	D	218	LYS	3.0
1	B	211	VAL	2.5
1	A	104	GLN	2.1
1	D	213	MET	2.0

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

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

6.3 Carbohydrates [i](#)

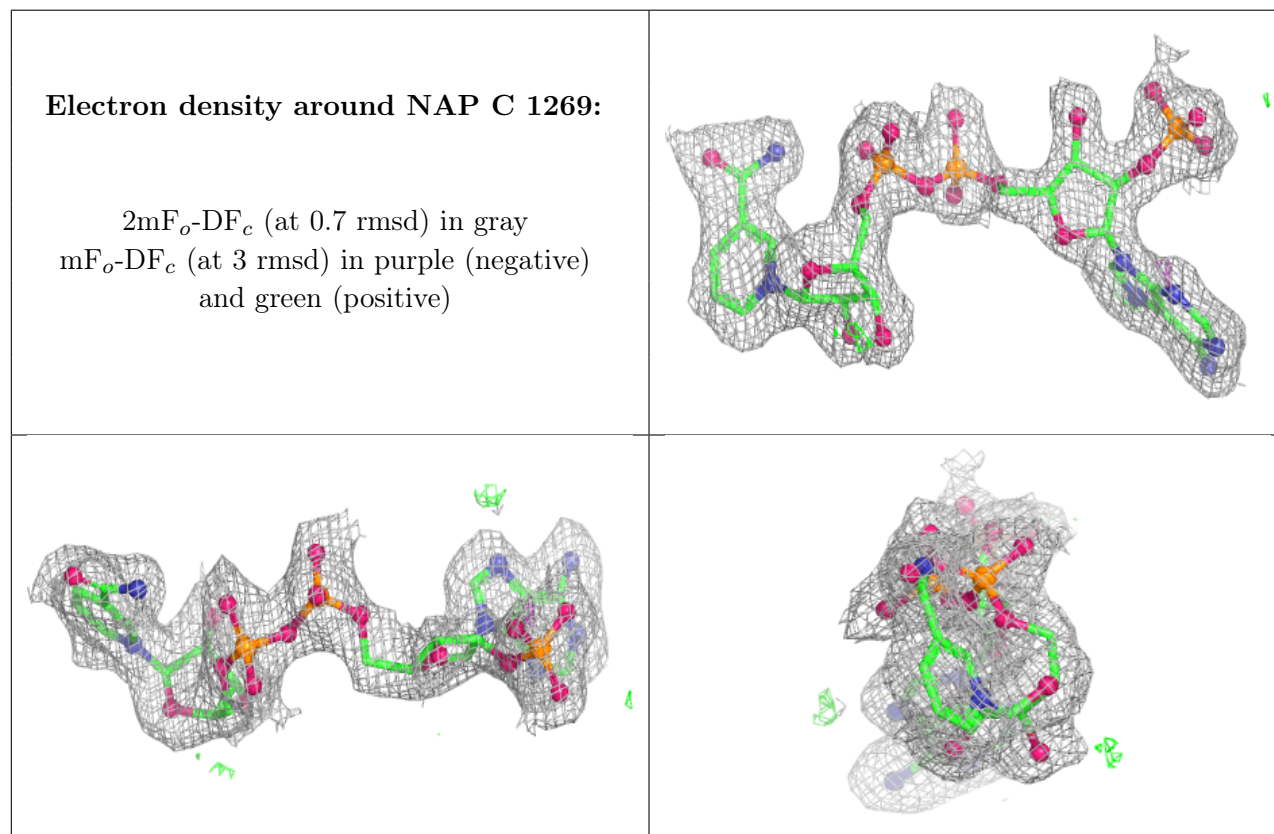
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

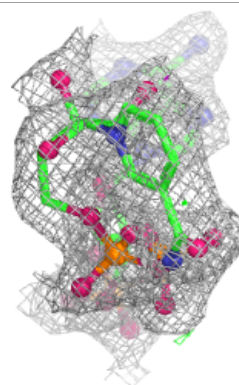
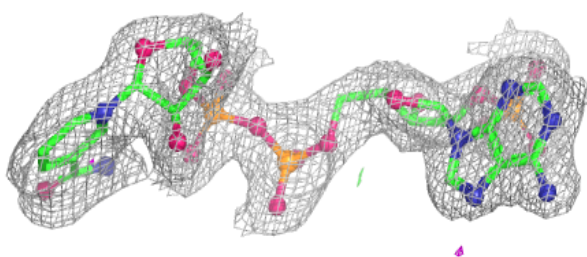
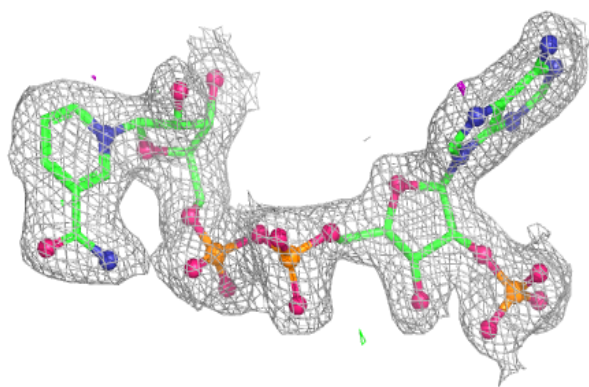
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAP	C	1269	48/48	0.96	0.06	9,12,14,15	0
2	NAP	D	1269	48/48	0.96	0.06	10,13,17,18	0
3	UIH	C	1270	24/24	0.96	0.09	18,26,31,33	0
3	UIH	D	1270	24/24	0.96	0.08	16,21,24,27	0
3	UIH	B	1270	24/24	0.97	0.08	14,17,20,23	0
2	NAP	A	1269	48/48	0.97	0.06	7,9,13,13	0
2	NAP	B	1269	48/48	0.97	0.06	5,9,11,12	0
3	UIH	A	1270	24/24	0.98	0.07	15,20,22,25	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.

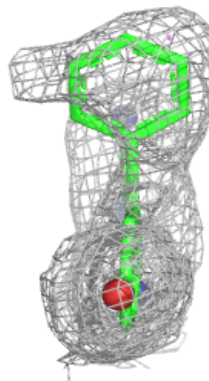
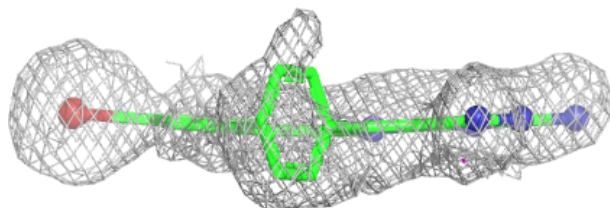
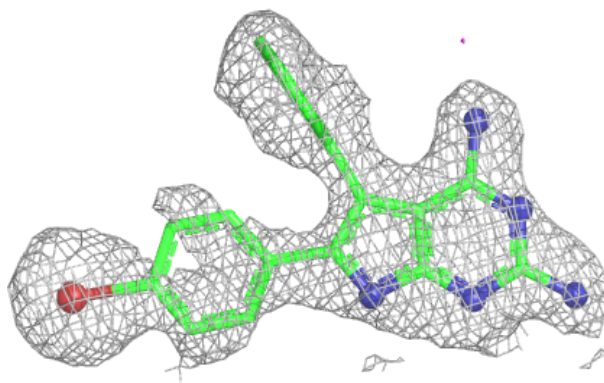


Electron density around NAP D 1269:

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

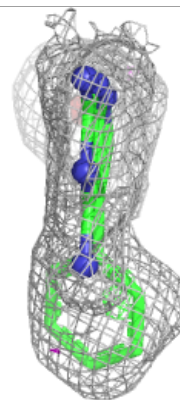
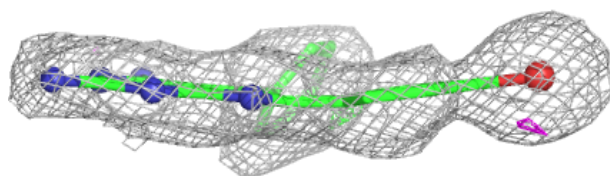
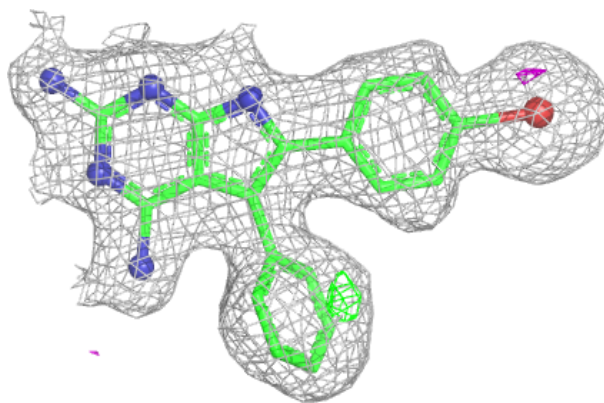
**Electron density around UIH C 1270:**

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

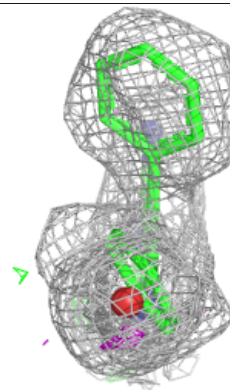
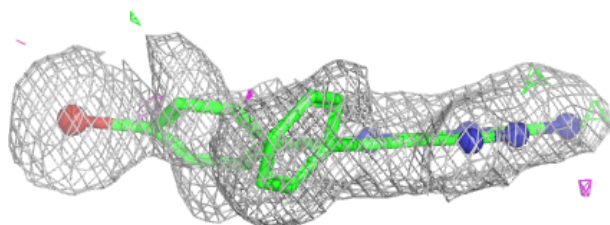
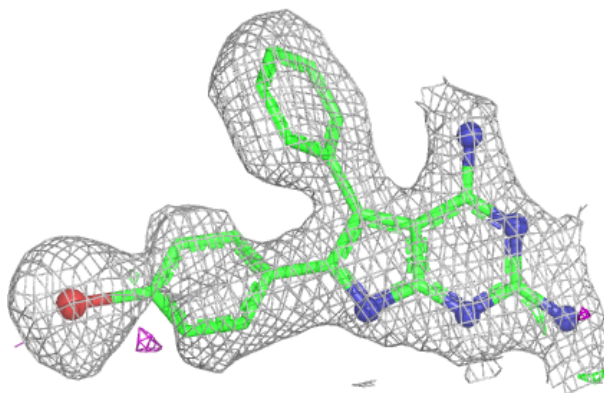


Electron density around UIH D 1270:

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

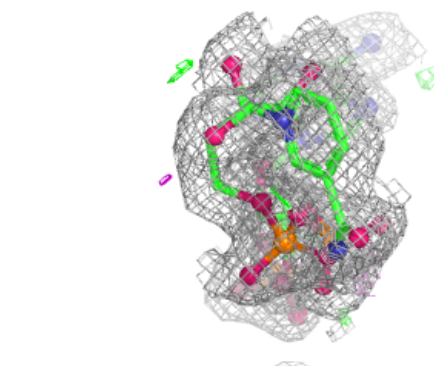
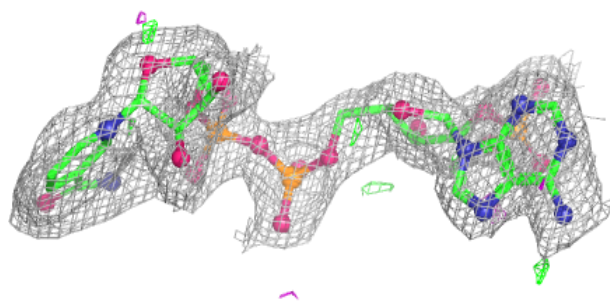
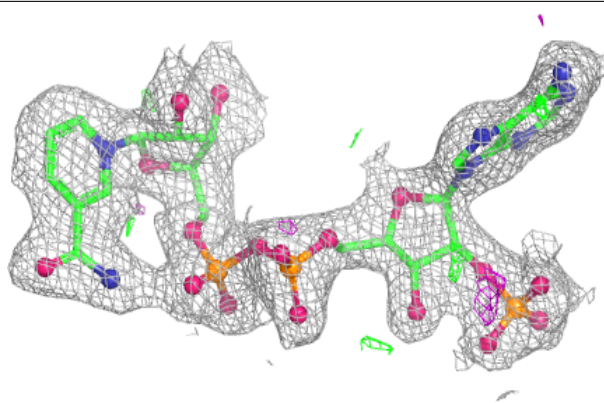
**Electron density around UIH B 1270:**

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

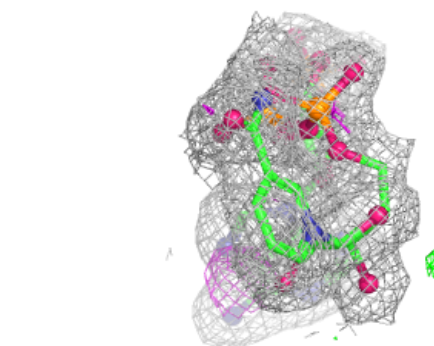
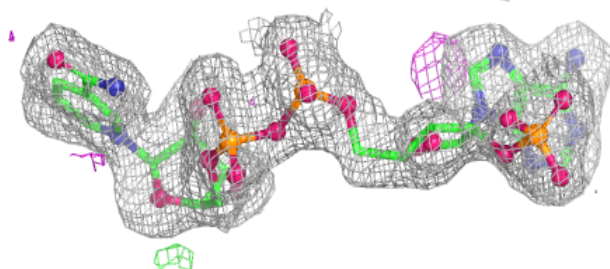
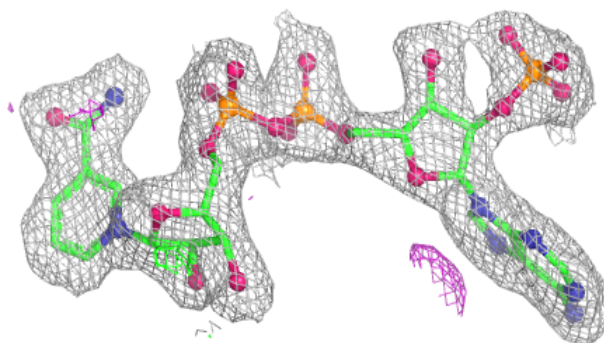


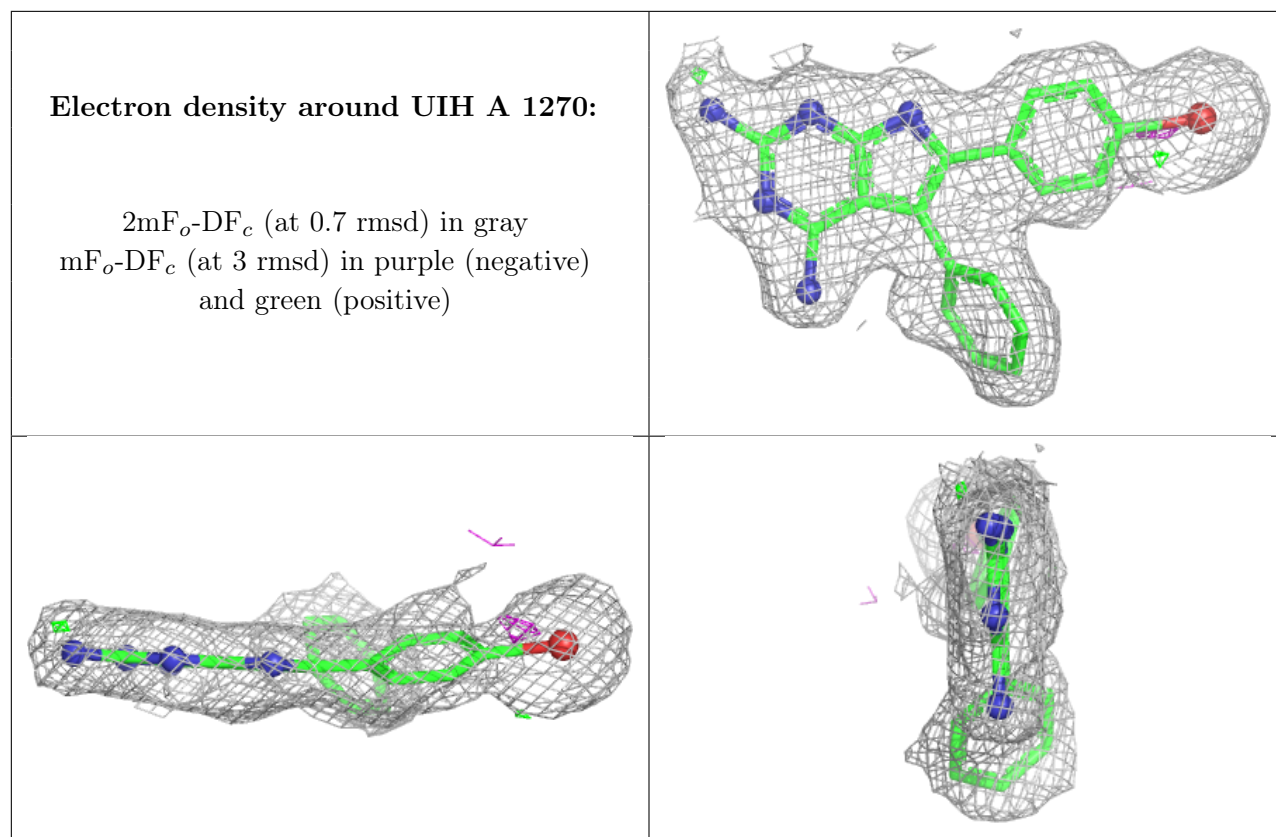
Electron density around NAP A 1269:

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

**Electron density around NAP 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.