Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 03:35 AM EDT

PDB ID	:	4CM1
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 (i) 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 (i)) were used in the production of this report:

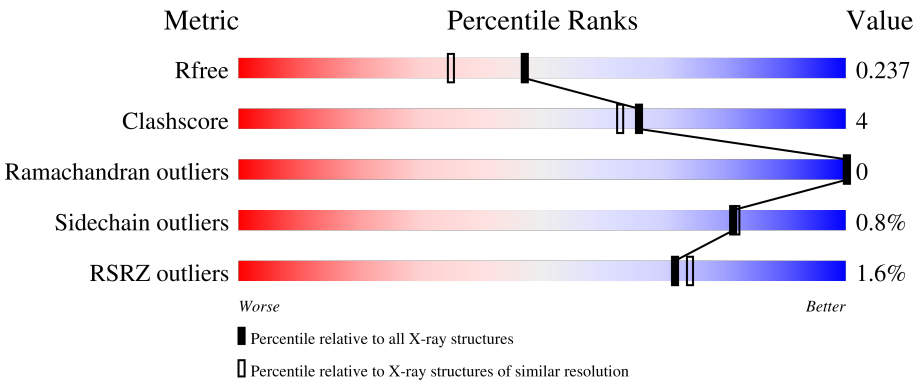
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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 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 <=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	80% 7% 13%
1	B	288	% 82% 5% 14%
1	C	288	2% 80% 6% • 13%
1	D	288	2% 78% 8% 13%

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
2	DTT	B	1168	-	X	-	-
4	IQW	C	1270[B]	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8691 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
			Total	C	N	O	S			
1	A	251	1877	1181	331	354	11	0	1	0
1	B	249	1862	1170	329	352	11	0	1	0
1	C	250	1863	1170	329	353	11	0	0	0
1	D	250	1863	1170	329	353	11	0	0	0

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

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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

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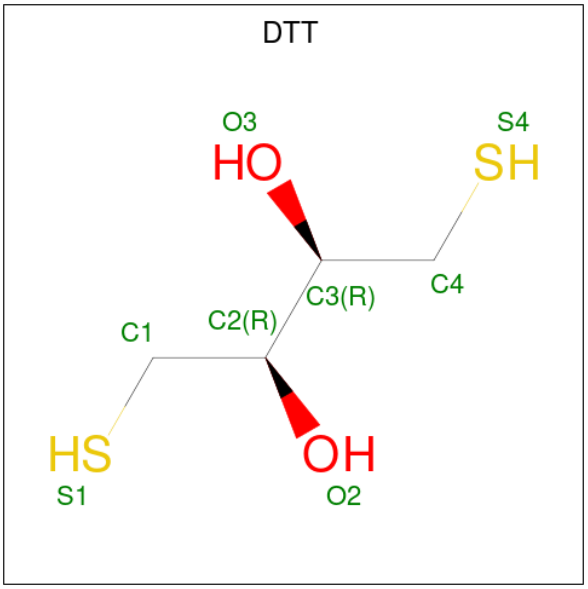
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP O76290
D	-15	HIS	-	expression tag	UNP O76290
D	-14	HIS	-	expression tag	UNP O76290
D	-13	HIS	-	expression tag	UNP O76290
D	-12	HIS	-	expression tag	UNP O76290
D	-11	HIS	-	expression tag	UNP O76290
D	-10	HIS	-	expression tag	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

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



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

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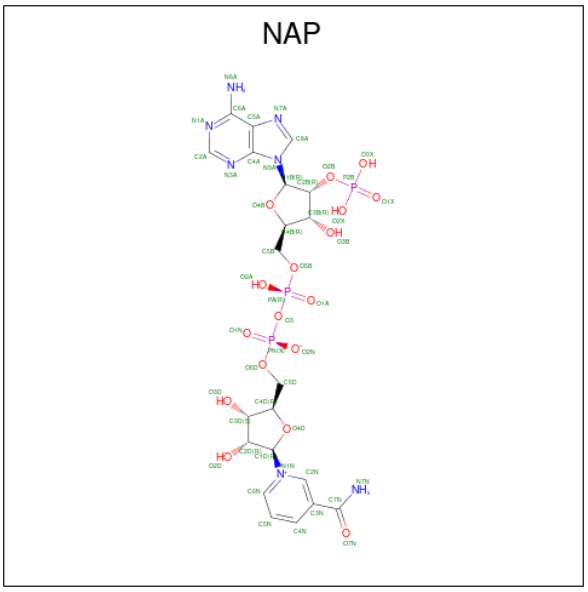
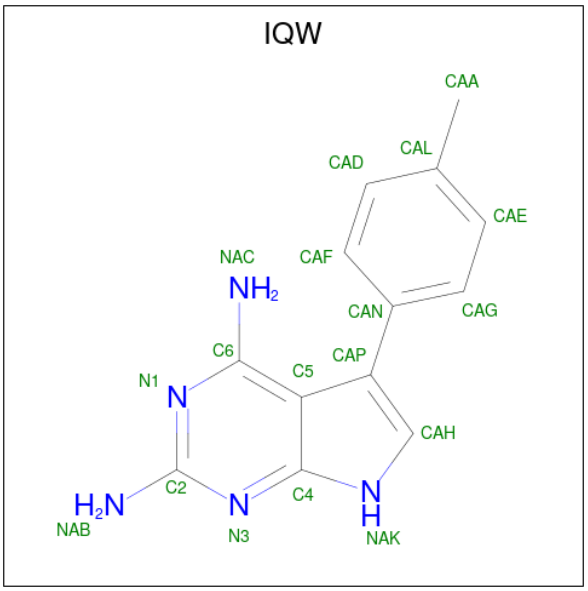
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
2	C	1	8	4	2	2	0	0
			Total	C	O	S		
2	D	1	8	4	2	2	0	0

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



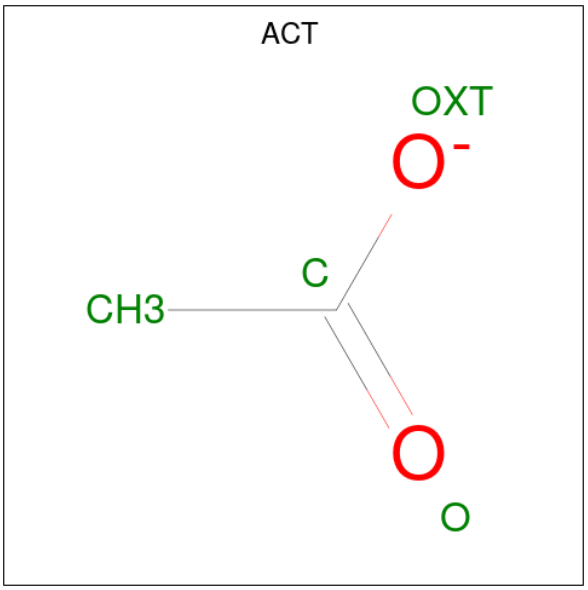
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
3	B	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
3	C	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
3	D	1	48	21	7	17	3	0	0

- Molecule 4 is 5-(p-tolyl)-7H-pyrrolo[2,3-d]pyrimidine-2,4-diamine (three-letter code: IQW) (formula: $C_{13}H_{13}N_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
4	A	1	36	26	10	0	1
			Total	C	N		
4	B	1	18	13	5	0	0
			Total	C	N		
4	C	1	36	26	10	0	1
			Total	C	N		
4	D	1	18	13	5	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is water.

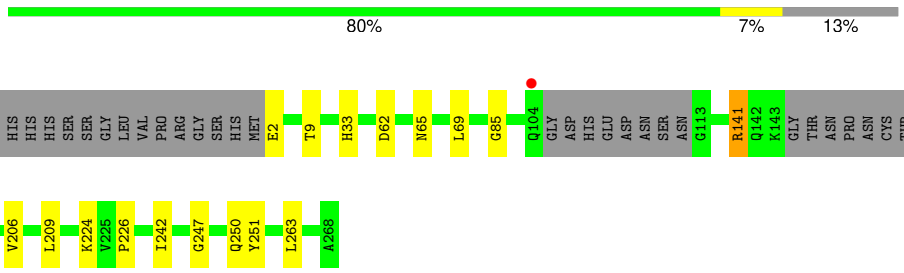
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	250	250	250	0	0
			Total	O		
6	B	259	259	259	0	0
			Total	O		
6	C	206	206	206	0	0
			Total	O		
6	D	171	171	171	0	0

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.

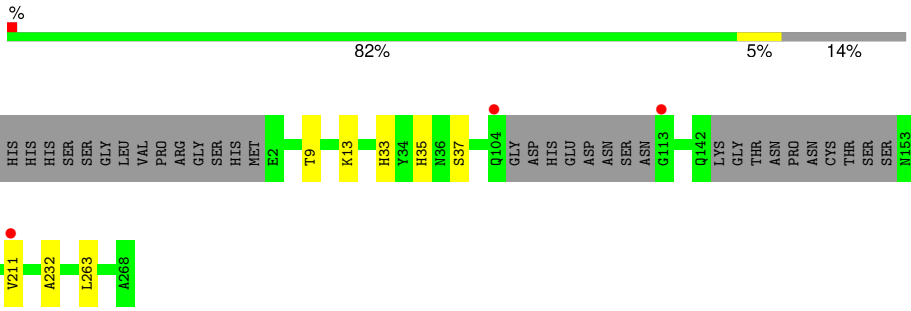
• Molecule 1: PTERIDINE REDUCTASE 1

Chain A:



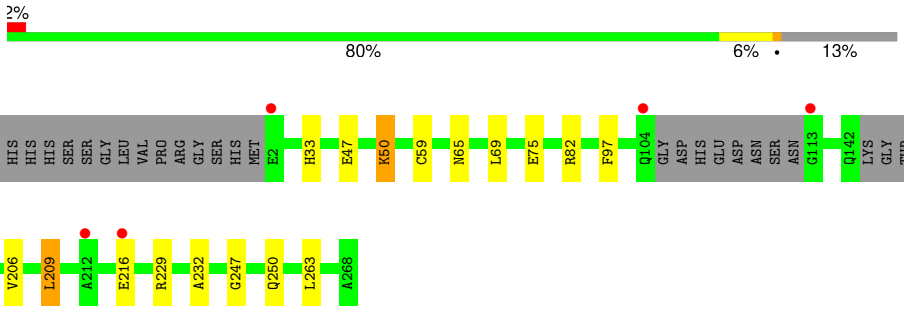
• Molecule 1: PTERIDINE REDUCTASE 1

Chain B:



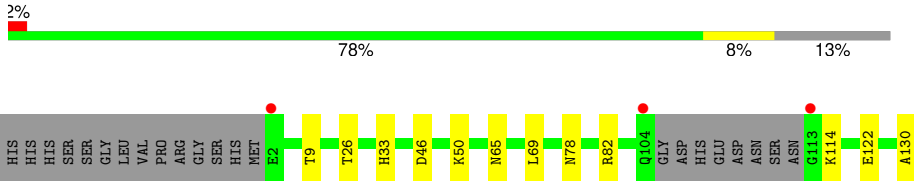
• Molecule 1: PTERIDINE REDUCTASE 1

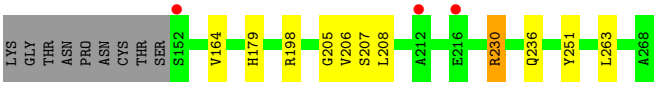
Chain C:



• Molecule 1: PTERIDINE REDUCTASE 1

Chain D:




LYS
GLY
THR
ASN
PRO
ASN
CYS
THR
SER
S152
V164
H179
R198
G205
V206
S207
L208
A212
E216
R230
Q236
Y251
L263
A268

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.70Å 90.87Å 82.67Å 90.00° 115.74° 90.00°	Depositor
Resolution (Å)	45.44 – 1.90 45.44 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (45.44-1.90) 97.9 (45.44-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.184 , 0.233 0.195 , 0.237	Depositor DCC
R_{free} test set	3868 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	10.1	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8691	wwPDB-VP
Average B, all atoms (Å^2)	13.0	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 23.36 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7346e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: DTT, NAP, IQW, ACT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.64	0/1907	0.78	3/2586 (0.1%)
1	B	0.68	0/1892	0.78	0/2567
1	C	0.66	0/1890	0.81	4/2564 (0.2%)
1	D	0.69	0/1890	0.80	5/2564 (0.2%)
All	All	0.67	0/7579	0.79	12/10281 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	230	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	D	82	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	D	230	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	C	229	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	C	209	LEU	CA-CB-CG	-6.15	101.15	115.30
1	A	141	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	C	165	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	A	62	ASP	CB-CG-OD1	5.67	123.41	118.30
1	C	82	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	D	198	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	D	82	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	A	209	LEU	CA-CB-CG	-5.29	103.13	115.30

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	1877	0	1908	13	0
1	B	1862	0	1885	11	0
1	C	1863	0	1884	13	0
1	D	1863	0	1884	17	0
2	A	8	0	9	1	0
2	B	8	0	9	0	0
2	C	8	0	9	0	0
2	D	8	0	9	0	0
3	A	48	0	25	1	0
3	B	48	0	25	1	0
3	C	48	0	25	1	0
3	D	48	0	25	1	0
4	A	36	0	26	6	0
4	B	18	0	13	0	0
4	C	36	0	26	8	0
4	D	18	0	13	0	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	250	0	0	9	0
6	B	259	0	0	3	0
6	C	206	0	0	5	0
6	D	171	0	0	1	0
All	All	8691	0	7781	62	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (62) 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:A:1270[B]:IQW:HAG	6:A:2190:HOH:O	1.15	1.26
4:C:1270[B]:IQW:HAF	6:C:2164:HOH:O	1.03	1.19
4:A:1270[B]:IQW:CAG	6:A:2190:HOH:O	1.69	1.12
4:C:1270[B]:IQW:HAH	6:C:2164:HOH:O	1.51	1.10
4:C:1270[B]:IQW:CAH	6:C:2164:HOH:O	2.01	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1270[B]:IQW:HAH	6:A:2190:HOH:O	1.65	0.94
4:A:1270[B]:IQW:CAH	6:A:2190:HOH:O	2.16	0.92
1:C:47:GLU:O	1:C:50:LYS:HG3	1.79	0.83
4:C:1270[B]:IQW:CAF	6:C:2164:HOH:O	1.80	0.78
1:B:175:ASN:HB2	6:B:2191:HOH:O	1.91	0.70
1:B:211:VAL:O	6:B:2207:HOH:O	2.12	0.67
1:A:164:VAL:HG22	1:A:179:HIS:CD2	2.31	0.65
1:D:164:VAL:HG22	1:D:179:HIS:CD2	2.31	0.65
1:D:206:VAL:HG23	1:D:263:LEU:HD22	1.80	0.64
1:C:247:GLY:O	1:C:250:GLN:HG3	1.98	0.62
1:C:75:GLU:OE1	6:C:2105:HOH:O	2.16	0.61
1:C:206:VAL:HG23	1:C:263:LEU:HD22	1.84	0.59
1:A:85:GLY:O	6:A:2112:HOH:O	2.16	0.57
1:D:78:ASN:OD1	1:D:141:ARG:NH1	2.35	0.57
1:A:194:PRO:HG3	6:A:2187:HOH:O	2.04	0.57
1:B:206:VAL:HG23	1:B:263:LEU:HD22	1.87	0.56
1:A:206:VAL:HG22	4:A:1270[B]:IQW:HAA	1.87	0.56
1:C:47:GLU:O	1:C:50:LYS:CG	2.53	0.55
1:D:130:ALA:HB3	1:D:131:PRO:HD3	1.87	0.55
1:A:247:GLY:O	1:A:250:GLN:HG2	2.07	0.54
1:B:164:VAL:HG22	1:B:179:HIS:CD2	2.43	0.53
1:C:206:VAL:HG22	4:C:1270[B]:IQW:HAAB	1.90	0.53
1:D:46:ASP:O	1:D:50:LYS:HG3	2.08	0.53
1:D:65:ASN:HA	1:D:69:LEU:HD22	1.91	0.51
1:D:9:THR:HA	1:D:33:HIS:HB3	1.93	0.50
1:A:65:ASN:HA	1:A:69:LEU:HD22	1.95	0.49
1:B:9:THR:HA	1:B:33:HIS:HB3	1.94	0.49
1:D:230:ARG:HH22	1:D:236:GLN:HE22	1.60	0.48
1:A:164:VAL:HG22	1:A:179:HIS:NE2	2.29	0.47
1:C:247:GLY:O	1:C:250:GLN:CG	2.63	0.47
3:A:1269:NAP:O2A	4:A:1270[B]:IQW:N3	2.48	0.46
1:A:141:ARG:HG2	6:A:2146:HOH:O	2.16	0.46
1:D:78:ASN:HB3	6:D:2090:HOH:O	2.15	0.46
3:C:1269:NAP:O2A	4:C:1270[B]:IQW:N3	2.49	0.46
1:D:26:THR:O	1:D:26:THR:HG22	2.15	0.46
1:D:164:VAL:HG22	1:D:179:HIS:NE2	2.32	0.45
1:D:205:GLY:O	3:D:1269:NAP:H4N	2.16	0.45
1:B:13:LYS:HE2	1:B:37:SER:OG	2.16	0.45
1:B:164:VAL:HG22	1:B:179:HIS:NE2	2.32	0.44
1:C:97:PHE:CZ	4:C:1270[B]:IQW:HAG	2.52	0.44
1:C:209:LEU:CD2	4:C:1270[A]:IQW:HAAA	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:ALA:HB2	1:D:251:TYR:CD2	2.53	0.44
1:A:224:LYS:O	1:A:226:PRO:HD3	2.18	0.44
1:B:160:CYS:HB3	6:B:2172:HOH:O	2.16	0.44
1:B:206:VAL:HG23	1:B:263:LEU:CD2	2.49	0.43
1:A:251:TYR:CE2	1:B:232:ALA:HB2	2.54	0.42
1:D:114:LYS:NZ	1:D:122:GLU:OE1	2.42	0.42
1:C:65:ASN:HA	1:C:69:LEU:HD22	2.01	0.42
1:B:35:HIS:HB2	3:B:1269:NAP:C2A	2.49	0.42
1:A:2:GLU:N	6:A:2001:HOH:O	2.52	0.42
1:A:9:THR:HA	1:A:33:HIS:HB3	2.01	0.42
1:A:206:VAL:HG23	1:A:263:LEU:HD22	2.03	0.41
2:A:1168:DTT:S4	6:A:2170:HOH:O	2.62	0.41
1:D:207:SER:O	1:D:208:LEU:C	2.59	0.41
1:C:33:HIS:HA	1:C:59:CYS:O	2.20	0.41
1:C:232:ALA:HB2	1:D:251:TYR:CE2	2.56	0.40
1:D:206:VAL:HG23	1:D:263:LEU:CD2	2.51	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	246/288 (85%)	239 (97%)	7 (3%)	0	100	100
1	B	244/288 (85%)	238 (98%)	6 (2%)	0	100	100
1	C	244/288 (85%)	235 (96%)	9 (4%)	0	100	100
1	D	244/288 (85%)	236 (97%)	8 (3%)	0	100	100
All	All	978/1152 (85%)	948 (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	200/231 (87%)	197 (98%)	3 (2%)	65	62
1	B	198/231 (86%)	198 (100%)	0	100	100
1	C	198/231 (86%)	195 (98%)	3 (2%)	65	62
1	D	198/231 (86%)	198 (100%)	0	100	100
All	All	794/924 (86%)	788 (99%)	6 (1%)	81	82

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

Mol	Chain	Res	Type
1	A	152	SER
1	A	172	SER
1	A	242	ILE
1	C	50	LYS
1	C	166	GLN
1	C	216	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	166	GLN
1	A	175	ASN
1	B	166	GLN
1	D	166	GLN
1	D	175	ASN
1	D	250	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

16 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	C	1269	-	46,52,52	0.96	2 (4%)	61,80,80	1.48	9 (14%)
2	DTT	C	1168	1	7,7,7	0.41	0	4,8,8	3.16	2 (50%)
4	IQW	A	1270[B]	-	19,20,20	1.29	2 (10%)	20,29,29	2.29	5 (25%)
4	IQW	D	1270	-	19,20,20	1.13	2 (10%)	20,29,29	2.34	6 (30%)
4	IQW	C	1270[B]	-	19,20,20	1.23	2 (10%)	20,29,29	2.14	3 (15%)
3	NAP	B	1269	-	46,52,52	1.04	3 (6%)	61,80,80	1.79	8 (13%)
5	ACT	B	1271	-	3,3,3	0.80	0	3,3,3	0.84	0
3	NAP	D	1269	-	46,52,52	1.13	4 (8%)	61,80,80	1.79	10 (16%)
2	DTT	D	1168	1	7,7,7	1.23	1 (14%)	4,8,8	1.99	2 (50%)
2	DTT	B	1168	1	7,7,7	1.46	1 (14%)	4,8,8	1.66	1 (25%)
4	IQW	A	1270[A]	-	19,20,20	1.30	2 (10%)	20,29,29	2.52	4 (20%)
4	IQW	C	1270[A]	-	19,20,20	1.39	2 (10%)	20,29,29	2.41	4 (20%)
3	NAP	A	1269	-	46,52,52	0.89	1 (2%)	61,80,80	1.44	7 (11%)
4	IQW	B	1270	-	19,20,20	1.22	2 (10%)	20,29,29	2.24	6 (30%)
5	ACT	A	1271	-	3,3,3	0.79	0	3,3,3	1.10	0
2	DTT	A	1168	1	7,7,7	1.34	1 (14%)	4,8,8	2.16	2 (50%)

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	C	1269	-	-	0/31/67/67	0/5/5/5
2	DTT	C	1168	1	-	2/8/8/8	-
4	IQW	A	1270[B]	-	-	0/4/4/4	0/3/3/3
4	IQW	D	1270	-	-	1/4/4/4	0/3/3/3
4	IQW	C	1270[B]	-	-	0/4/4/4	0/3/3/3
3	NAP	B	1269	-	-	0/31/67/67	0/5/5/5
3	NAP	D	1269	-	-	0/31/67/67	0/5/5/5
2	DTT	D	1168	1	-	3/8/8/8	-
2	DTT	B	1168	1	-	8/8/8/8	-
4	IQW	A	1270[A]	-	-	1/4/4/4	0/3/3/3
4	IQW	C	1270[A]	-	-	1/4/4/4	0/3/3/3
3	NAP	A	1269	-	-	1/31/67/67	0/5/5/5
4	IQW	B	1270	-	-	1/4/4/4	0/3/3/3
2	DTT	A	1168	1	-	2/8/8/8	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1270[A]	IQW	C2-NAB	4.19	1.42	1.33
4	A	1270[A]	IQW	C2-NAB	4.15	1.42	1.33
4	A	1270[B]	IQW	C2-NAB	3.75	1.41	1.33
3	D	1269	NAP	PA-O3	3.74	1.63	1.59
4	C	1270[B]	IQW	C2-NAB	3.54	1.41	1.33
4	B	1270	IQW	C2-NAB	3.36	1.40	1.33
3	A	1269	NAP	P2B-O2B	3.25	1.65	1.59
3	B	1269	NAP	O4D-C1D	3.00	1.44	1.40
3	B	1269	NAP	PN-O3	2.99	1.62	1.59
3	C	1269	NAP	C2A-N3A	2.96	1.36	1.32
2	A	1168	DTT	C4-S4	2.71	1.87	1.81
4	A	1270[B]	IQW	C6-NAC	2.65	1.43	1.34
3	D	1269	NAP	P2B-O2B	2.59	1.64	1.59
4	D	1270	IQW	C6-NAC	2.55	1.43	1.34
4	D	1270	IQW	C2-NAB	2.42	1.38	1.33
2	D	1168	DTT	C4-S4	2.29	1.86	1.81
4	C	1270[A]	IQW	C6-NAC	2.25	1.42	1.34
4	C	1270[B]	IQW	C6-NAC	2.25	1.42	1.34
3	D	1269	NAP	O4D-C1D	2.23	1.43	1.40
3	B	1269	NAP	PA-O3	2.22	1.61	1.59
4	A	1270[A]	IQW	C6-NAC	2.14	1.41	1.34
4	B	1270	IQW	C6-NAC	2.10	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1269	NAP	PN-O3	2.09	1.61	1.59
2	B	1168	DTT	C1-C2	2.06	1.57	1.51
3	D	1269	NAP	C1B-N9A	-2.00	1.45	1.49

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1269	NAP	O4B-C1B-N9A	8.12	119.51	108.75
4	C	1270[A]	IQW	N3-C2-N1	-6.94	118.39	127.21
4	A	1270[A]	IQW	N3-C2-N1	-6.93	118.40	127.21
4	A	1270[B]	IQW	N3-C2-N1	-6.54	118.89	127.21
3	D	1269	NAP	C4B-O4B-C1B	-6.10	104.34	109.92
4	D	1270	IQW	N3-C2-N1	-6.05	119.52	127.21
4	C	1270[B]	IQW	N3-C2-N1	-5.99	119.59	127.21
3	A	1269	NAP	C4B-O4B-C1B	-5.95	104.48	109.92
3	D	1269	NAP	O4B-C1B-N9A	5.70	116.30	108.75
3	B	1269	NAP	C4B-O4B-C1B	-5.42	104.96	109.92
4	B	1270	IQW	N3-C2-N1	-5.15	120.67	127.21
4	A	1270[A]	IQW	C2-N3-C4	5.07	120.95	115.48
2	C	1168	DTT	C2-C1-S1	-4.89	100.76	114.43
4	C	1270[A]	IQW	C2-N3-C4	4.88	120.74	115.48
3	C	1269	NAP	C4B-O4B-C1B	-4.61	105.70	109.92
3	B	1269	NAP	N3A-C2A-N1A	-4.60	122.43	128.67
3	C	1269	NAP	O4B-C1B-N9A	4.56	114.79	108.75
3	D	1269	NAP	C1B-N9A-C4A	-4.47	118.79	126.64
4	A	1270[B]	IQW	C2-N3-C4	4.42	120.25	115.48
4	C	1270[B]	IQW	CAP-C5-C4	-4.36	104.06	107.54
4	D	1270	IQW	CAP-C5-C4	-4.27	104.13	107.54
4	B	1270	IQW	CAP-C5-C4	-4.25	104.14	107.54
4	A	1270[A]	IQW	NAB-C2-N1	4.18	123.49	117.22
2	C	1168	DTT	C3-C4-S4	-3.98	103.31	114.43
3	B	1269	NAP	C3N-C7N-N7N	3.95	122.60	117.74
4	B	1270	IQW	NAB-C2-N1	3.95	123.14	117.22
4	C	1270[A]	IQW	NAB-C2-N1	3.88	123.04	117.22
3	C	1269	NAP	N3A-C2A-N1A	-3.82	123.49	128.67
4	A	1270[A]	IQW	CAP-C5-C4	-3.78	104.52	107.54
4	C	1270[B]	IQW	C2-N3-C4	3.73	119.51	115.48
3	D	1269	NAP	C3N-C7N-N7N	3.69	122.28	117.74
3	C	1269	NAP	C2B-C1B-N9A	-3.62	104.51	112.56
4	C	1270[A]	IQW	CAP-C5-C4	-3.62	104.65	107.54
4	D	1270	IQW	C2-N3-C4	3.56	119.33	115.48
3	D	1269	NAP	C2B-C1B-N9A	-3.56	104.65	112.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1270	IQW	NAB-C2-N1	3.45	122.39	117.22
4	A	1270[B]	IQW	CAP-C5-C4	-3.33	104.88	107.54
4	B	1270	IQW	C2-N3-C4	3.31	119.05	115.48
3	A	1269	NAP	N3A-C2A-N1A	-3.28	124.22	128.67
3	D	1269	NAP	C6N-N1N-C2N	-3.25	119.11	121.88
3	A	1269	NAP	O4B-C1B-N9A	3.22	113.02	108.75
4	D	1270	IQW	CAF-CAN-CAP	-3.18	115.59	120.87
2	A	1168	DTT	C2-C1-S1	-3.10	105.78	114.43
3	D	1269	NAP	O2N-PN-O3	3.03	115.45	107.27
3	B	1269	NAP	C2B-C1B-N9A	-2.93	106.04	112.56
3	B	1269	NAP	C1B-N9A-C4A	-2.92	121.52	126.64
3	D	1269	NAP	C4A-C5A-N7A	-2.85	106.33	109.34
3	C	1269	NAP	C1B-N9A-C4A	-2.81	121.70	126.64
2	B	1168	DTT	C3-C4-S4	-2.77	106.68	114.43
3	B	1269	NAP	O7N-C7N-C3N	-2.72	116.27	119.60
4	B	1270	IQW	CAF-CAN-CAP	-2.69	116.41	120.87
3	D	1269	NAP	C4D-O4D-C1D	2.67	112.37	109.92
3	D	1269	NAP	N3A-C2A-N1A	-2.65	125.07	128.67
3	C	1269	NAP	O7N-C7N-C3N	-2.63	116.39	119.60
3	A	1269	NAP	C1B-N9A-C4A	-2.57	122.12	126.64
4	D	1270	IQW	CAG-CAE-CAL	-2.57	118.41	121.37
2	D	1168	DTT	C2-C1-S1	-2.50	107.44	114.43
3	A	1269	NAP	O3X-P2B-O2X	2.48	117.11	107.80
4	B	1270	IQW	CAG-CAE-CAL	-2.48	118.51	121.37
3	C	1269	NAP	O2N-PN-O1N	2.48	123.97	112.44
2	A	1168	DTT	O3-C3-C2	-2.41	104.52	109.57
3	A	1269	NAP	C2B-C1B-N9A	-2.39	107.24	112.56
4	A	1270[B]	IQW	CAF-CAN-CAP	-2.31	117.04	120.87
4	A	1270[B]	IQW	NAB-C2-N1	2.23	120.56	117.22
3	C	1269	NAP	N6A-C6A-N1A	2.22	123.09	118.33
3	A	1269	NAP	C4A-C5A-N7A	-2.13	107.08	109.34
3	B	1269	NAP	C4A-C5A-N7A	-2.13	107.09	109.34
2	D	1168	DTT	O3-C3-C2	-2.06	105.24	109.57
3	C	1269	NAP	C2N-C3N-C4N	2.01	120.59	118.26

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1168	DTT	S1-C1-C2-O2
2	A	1168	DTT	S1-C1-C2-C3
2	B	1168	DTT	S1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	B	1168	DTT	S1-C1-C2-C3
2	B	1168	DTT	C1-C2-C3-O3
2	B	1168	DTT	C1-C2-C3-C4
2	B	1168	DTT	O2-C2-C3-O3
2	B	1168	DTT	O2-C2-C3-C4
2	B	1168	DTT	C2-C3-C4-S4
2	B	1168	DTT	O3-C3-C4-S4
2	C	1168	DTT	C2-C3-C4-S4
2	C	1168	DTT	O3-C3-C4-S4
2	D	1168	DTT	S1-C1-C2-O2
2	D	1168	DTT	C1-C2-C3-C4
4	B	1270	IQW	CAG-CAN-CAP-C5
4	C	1270[A]	IQW	CAF-CAN-CAP-C5
4	A	1270[A]	IQW	CAF-CAN-CAP-C5
4	D	1270	IQW	CAG-CAN-CAP-C5
3	A	1269	NAP	C5B-O5B-PA-O1A
2	D	1168	DTT	S1-C1-C2-C3

There are no ring outliers.

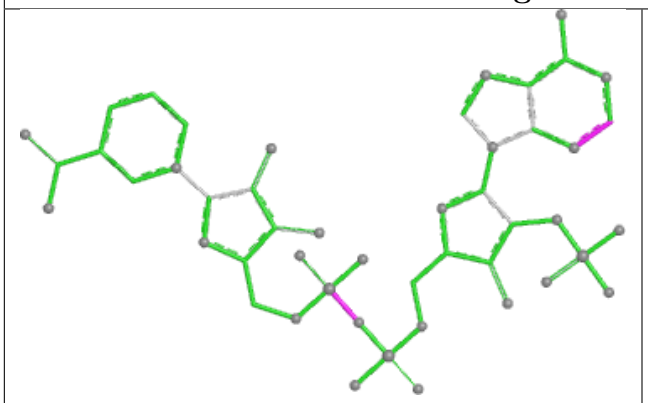
8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1269	NAP	1	0
4	A	1270[B]	IQW	6	0
4	C	1270[B]	IQW	7	0
3	B	1269	NAP	1	0
3	D	1269	NAP	1	0
4	C	1270[A]	IQW	1	0
3	A	1269	NAP	1	0
2	A	1168	DTT	1	0

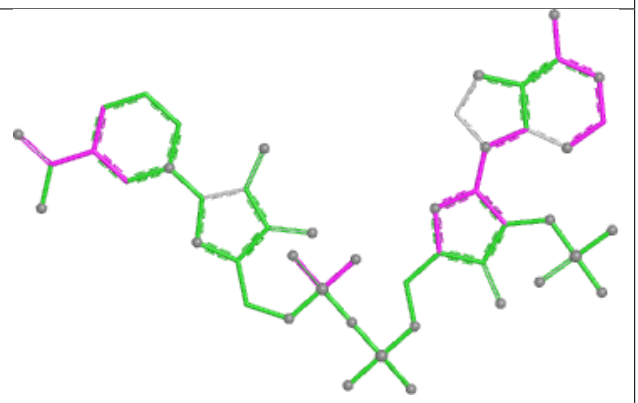
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

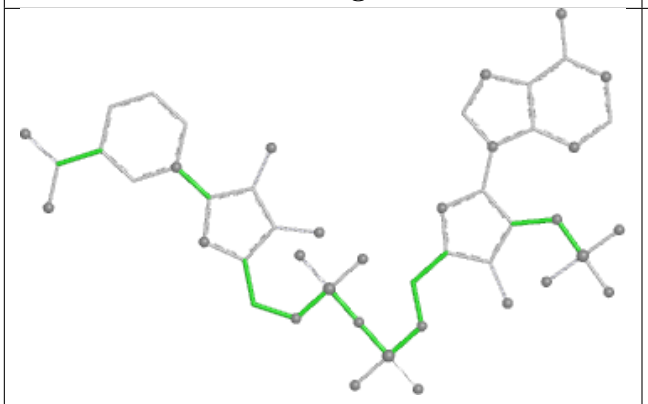
Ligand NAP C 1269



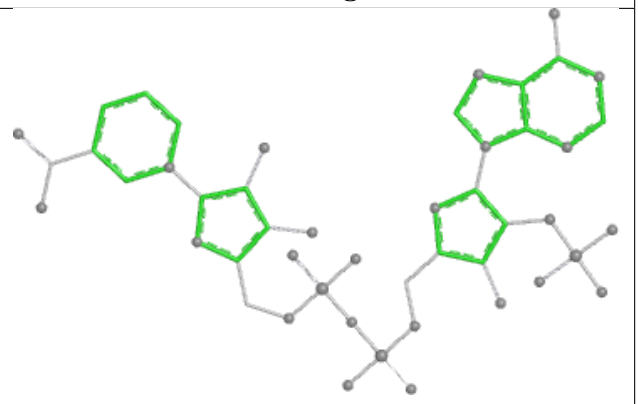
Bond lengths



Bond angles

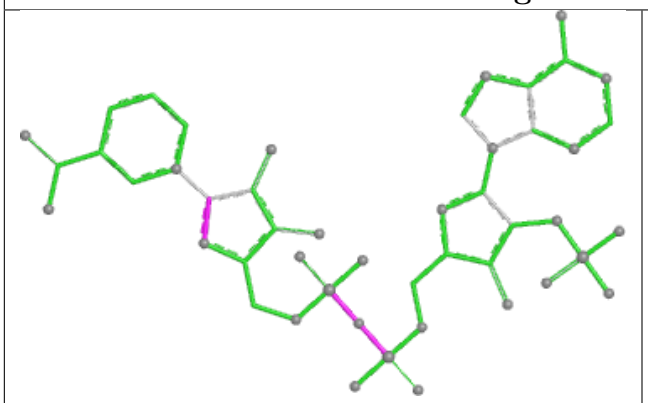


Torsions

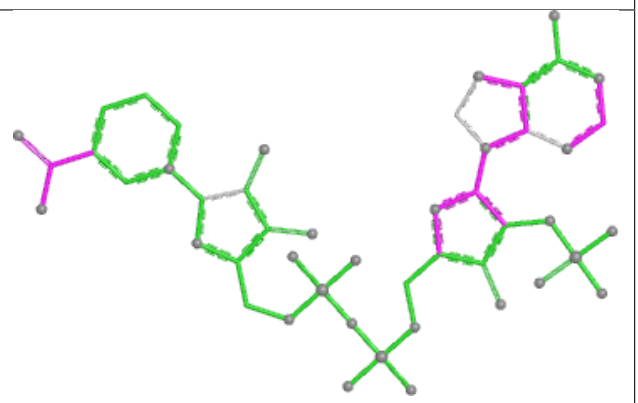


Rings

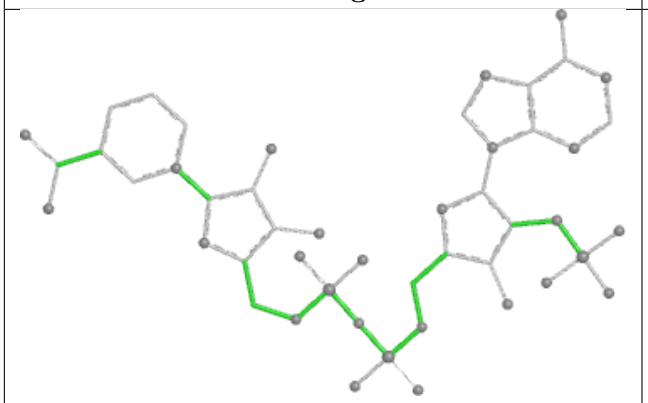
Ligand NAP B 1269



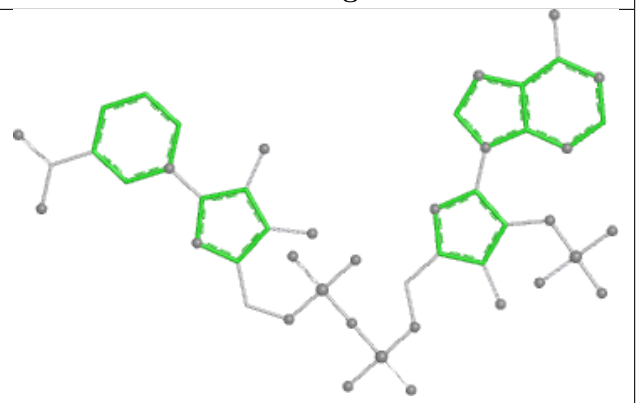
Bond lengths



Bond angles

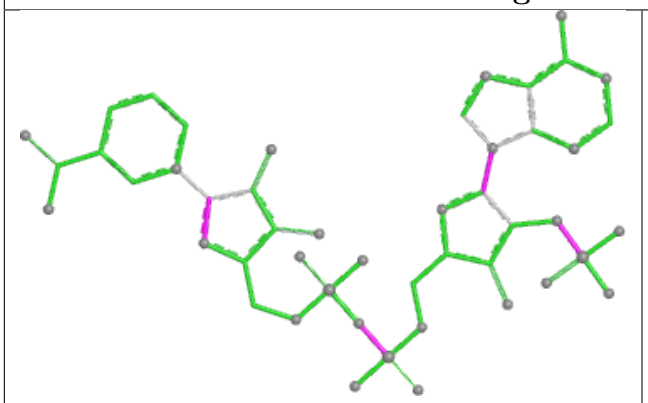


Torsions

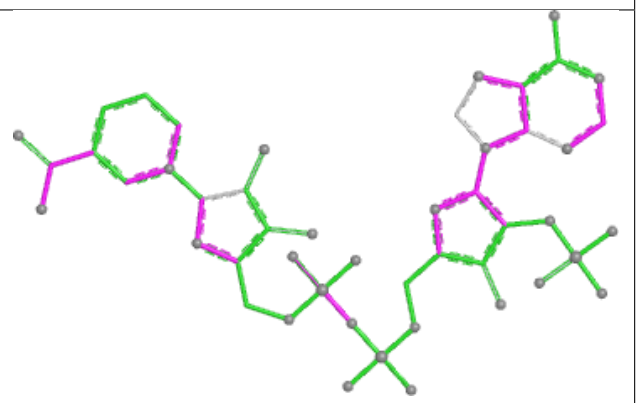


Rings

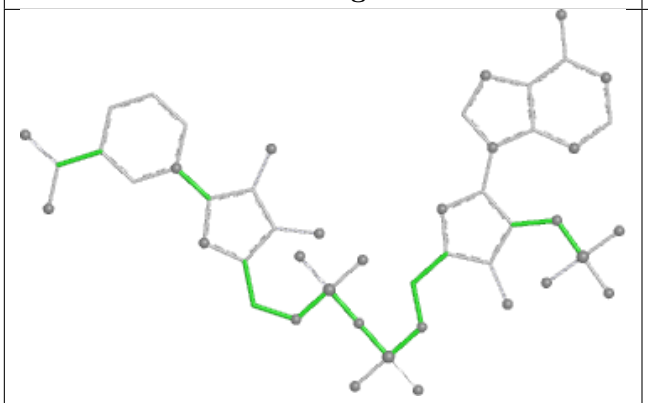
Ligand NAP D 1269



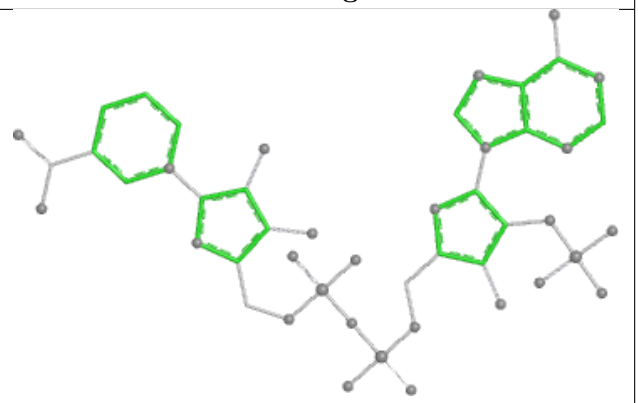
Bond lengths



Bond angles

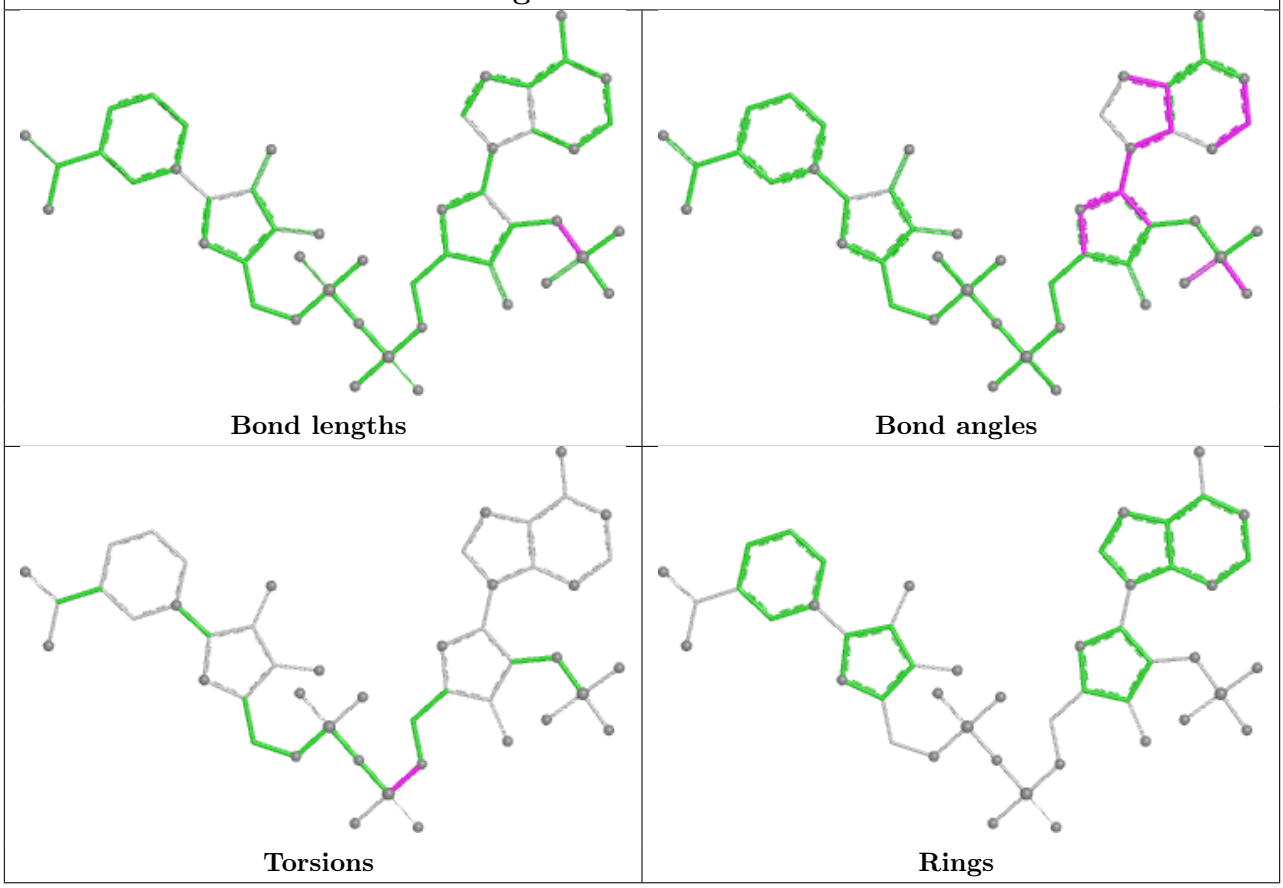


Torsions



Rings

Ligand NAP A 1269



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%)	-0.33	1 (0%)	92	93	4, 10, 24, 49	0
1	B	249/288 (86%)	-0.38	3 (1%)	79	81	5, 9, 22, 47	0
1	C	250/288 (86%)	-0.33	6 (2%)	59	62	5, 10, 28, 51	0
1	D	250/288 (86%)	-0.28	6 (2%)	59	62	5, 11, 28, 49	0
All	All	1000/1152 (86%)	-0.33	16 (1%)	72	74	4, 10, 27, 51	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	104	GLN	5.1
1	A	104	GLN	3.9
1	C	113	GLY	3.3
1	D	2	GLU	3.2
1	D	113	GLY	3.1
1	B	211	VAL	3.1
1	C	212	ALA	3.0
1	B	113	GLY	2.9
1	C	104	GLN	2.7
1	C	2	GLU	2.5
1	C	152	SER	2.4
1	B	104	GLN	2.3
1	D	152	SER	2.3
1	D	216	GLU	2.3
1	C	216	GLU	2.1
1	D	212	ALA	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

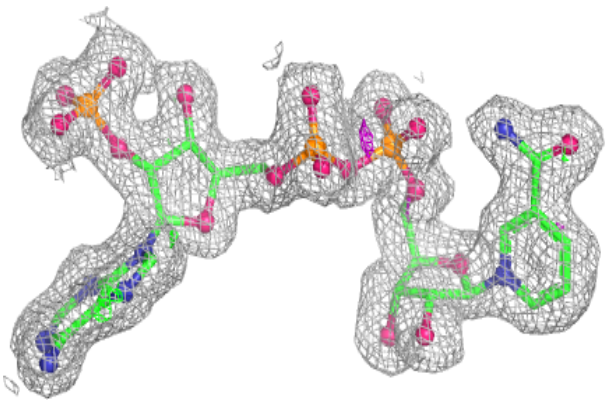
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

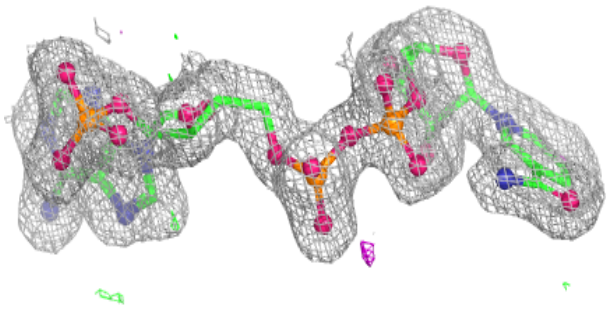
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DTT	D	1168	8/8	0.86	0.14	31,39,48,50	0
4	IQW	D	1270	18/18	0.86	0.15	12,15,24,24	0
5	ACT	B	1271	4/4	0.87	0.13	16,19,19,19	0
2	DTT	B	1168	8/8	0.89	0.17	28,43,49,54	0
2	DTT	C	1168	8/8	0.91	0.17	29,41,48,57	0
2	DTT	A	1168	8/8	0.91	0.12	31,35,42,52	0
4	IQW	B	1270	18/18	0.92	0.12	9,11,19,20	0
4	IQW	A	1270[B]	18/18	0.95	0.13	7,8,9,9	18
4	IQW	A	1270[A]	18/18	0.95	0.13	7,8,9,9	18
4	IQW	C	1270[A]	18/18	0.96	0.14	9,10,12,13	18
4	IQW	C	1270[B]	18/18	0.96	0.14	8,8,10,10	18
3	NAP	D	1269	48/48	0.98	0.07	7,8,10,10	0
3	NAP	A	1269	48/48	0.98	0.06	6,8,9,9	0
3	NAP	B	1269	48/48	0.98	0.07	5,7,10,10	0
5	ACT	A	1271	4/4	0.98	0.06	13,13,13,14	0
3	NAP	C	1269	48/48	0.98	0.06	5,7,8,8	0

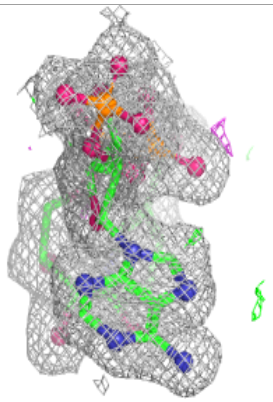
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

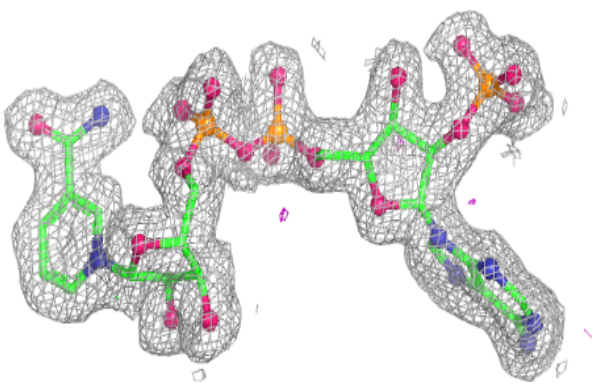


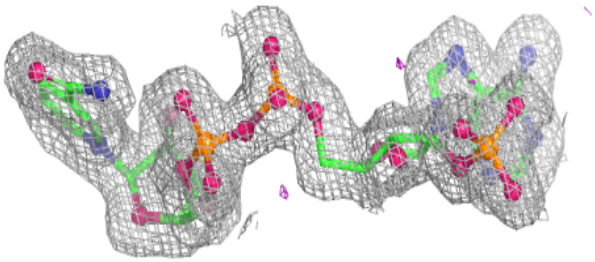


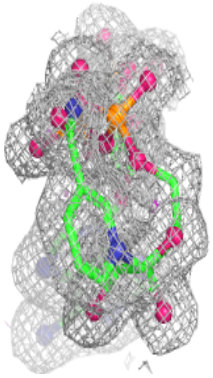


Electron density around NAP A 1269:

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

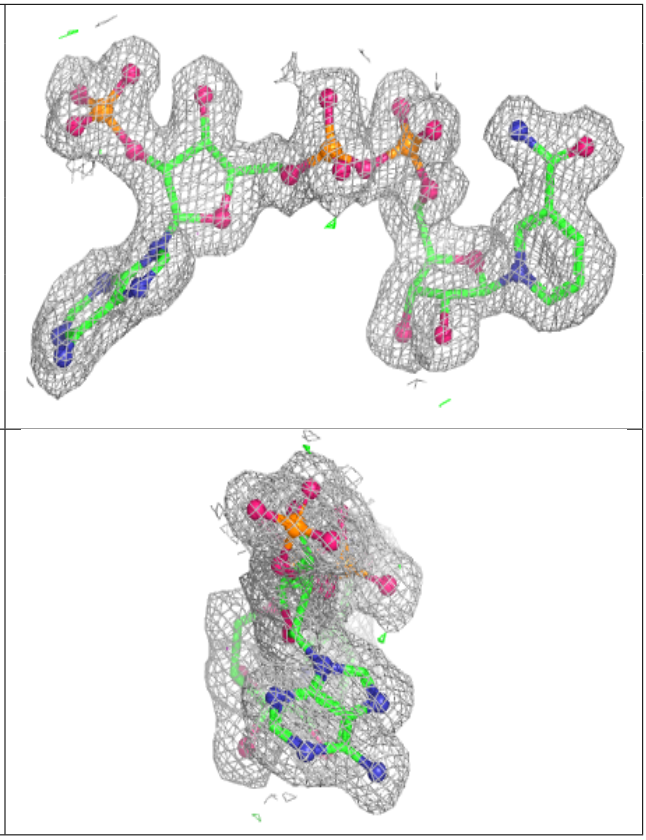






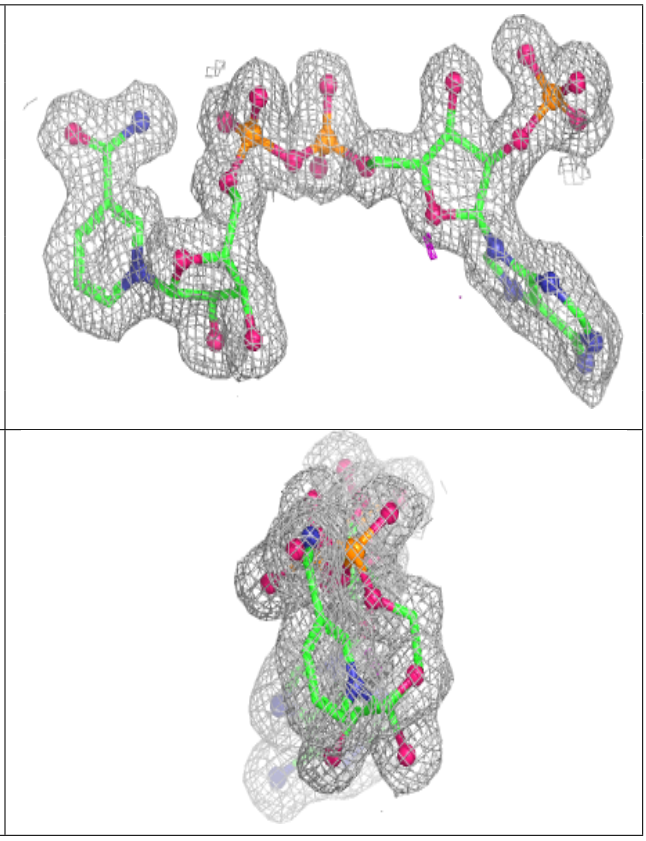
Electron density around NAP B 1269:

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



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)



6.5 Other polymers (i)

There are no such residues in this entry.