Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 08:13 AM EDT

PDB ID	:	3JQF
Title	:	Crystal structure of pteridine reductase 1 (PTR1) from Trypanosoma brucei in ternary complex with cofactor (NADP+) and inhibitor 1,3,5-triazine-2,4,6-triamine (AX2)
Authors	:	Tulloch, L.B.; Hunter, W.N.
Deposited on	:	2009-09-06
Resolution	:	1.60 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:

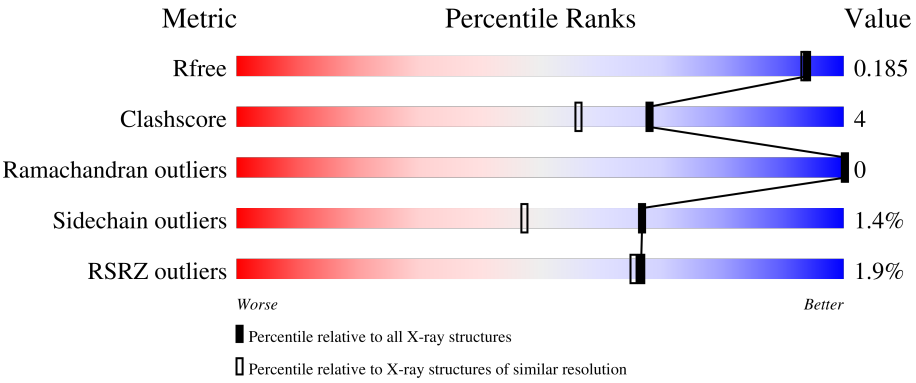
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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% 6% 14%
1	B	288	78% 8% 14%
1	D	288	79% 6% 14%
2	C	288	80% 6% 14%

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
4	AX2	A	270	-	X	-	-
4	AX2	B	270	-	X	-	-
4	AX2	C	272	-	X	-	-
4	AX2	D	270	-	X	-	-
5	DTT	A	271	X	-	-	-
5	DTT	A	276[B]	X	-	-	-
5	DTT	B	271	X	-	-	-
5	DTT	C	273	X	-	-	-
5	DTT	D	271	X	-	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 9055 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pteridine reductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	12	0
			1901	1207	330	353	11			
1	B	248	Total	C	N	O	S	0	21	0
			1937	1229	335	361	12			
1	D	249	Total	C	N	O	S	0	16	0
			1908	1207	331	358	12			

There are 60 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

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

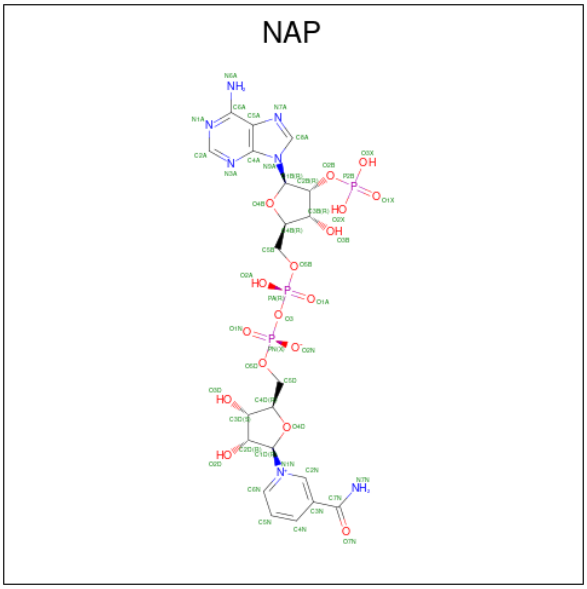
- Molecule 2 is a protein called Pteridine reductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	248	Total	C	N	O	S	0	17	0
			1906	1206	330	358	12			

There are 20 discrepancies between the modelled and reference sequences:

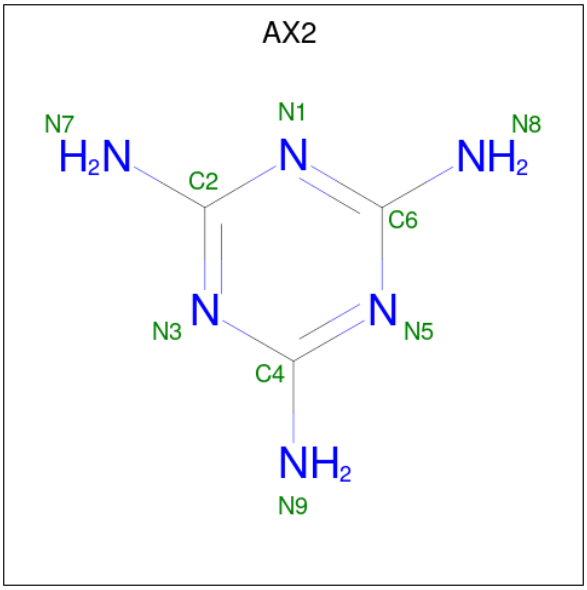
Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	expression tag	UNP Q581W1
C	-18	GLY	-	expression tag	UNP Q581W1
C	-17	SER	-	expression tag	UNP Q581W1
C	-16	SER	-	expression tag	UNP Q581W1
C	-15	HIS	-	expression tag	UNP Q581W1
C	-14	HIS	-	expression tag	UNP Q581W1
C	-13	HIS	-	expression tag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

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



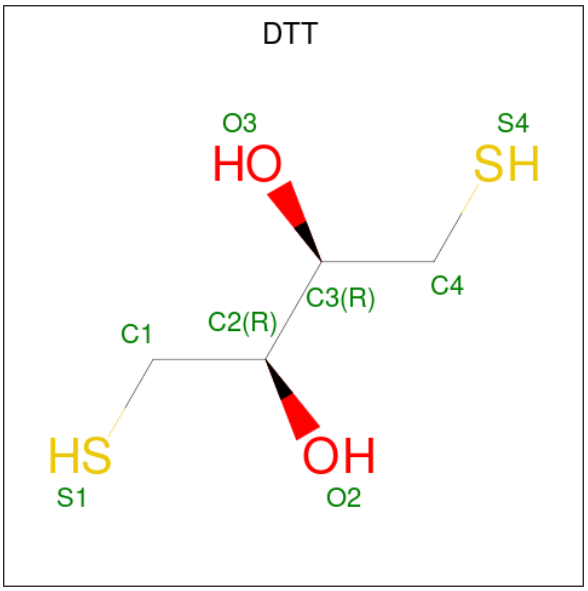
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is 1,3,5-triazine-2,4,6-triamine (three-letter code: AX2) (formula: $C_3H_6N_6$).



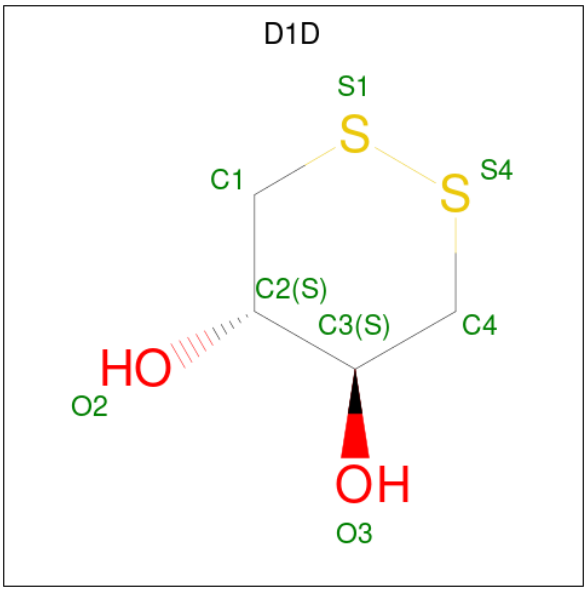
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N		0	0
			9	3	6			
4	B	1	Total	C	N		0	0
			9	3	6			
4	C	1	Total	C	N		0	0
			9	3	6			
4	D	1	Total	C	N		0	0
			9	3	6			

- Molecule 5 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



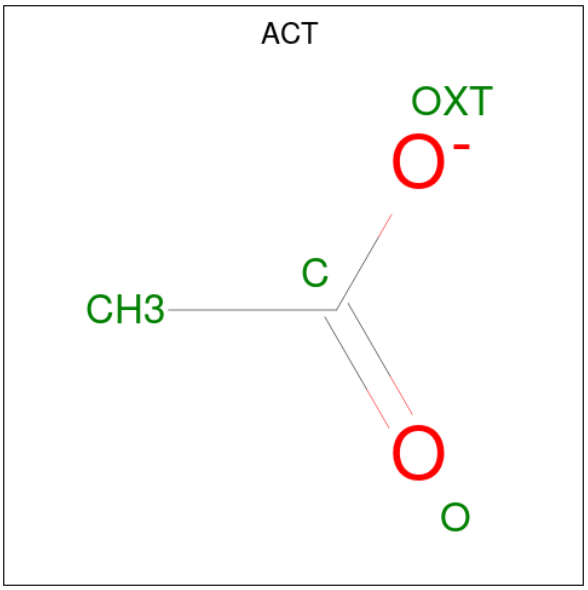
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O S 8 4 2 2	0	0
5	A	1	Total C O S 8 4 2 2	0	1
5	B	1	Total C O S 8 4 2 2	0	0
5	C	1	Total C O S 8 4 2 2	0	0
5	D	1	Total C O S 8 4 2 2	0	0

- Molecule 6 is (4S,5S)-1,2-DITHIANE-4,5-DIOL (three-letter code: D1D) (formula: $C_4H_8O_2S_2$).



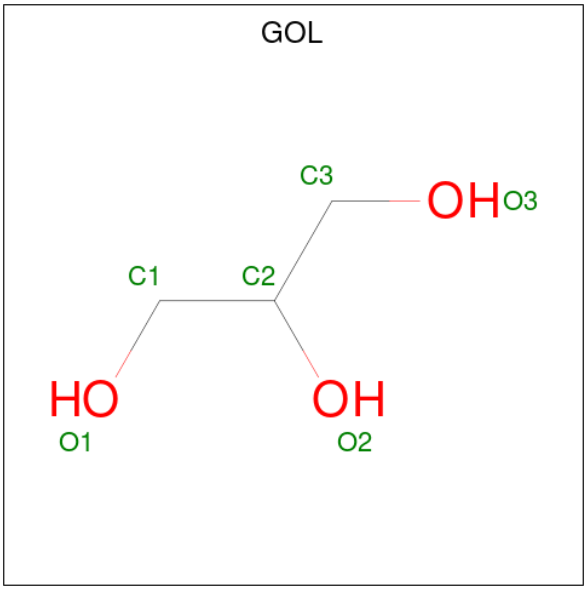
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O S 8 4 2 2	0	0
6	B	1	Total C O S 8 4 2 2	0	0
6	C	1	Total C O S 8 4 2 2	0	0
6	D	1	Total C O S 8 4 2 2	0	0

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	316	Total O 319 319	0	3
9	B	261	Total O 262 262	0	1

Continued on next page...

Continued from previous page...

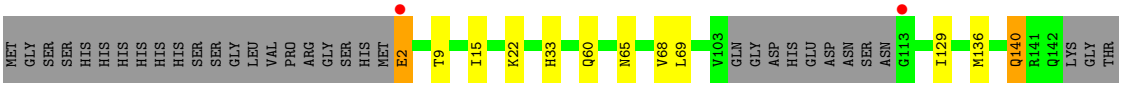
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	245	Total O 247 247	0	2
9	D	237	Total O 239 239	0	2

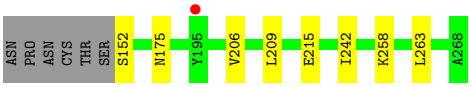
3 Residue-property plots (i)

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

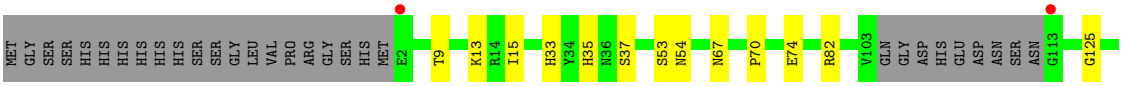
Chain A:





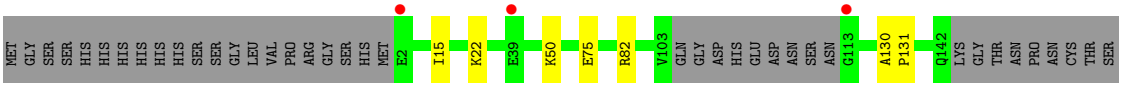
• Molecule 1: Pteridine reductase 1

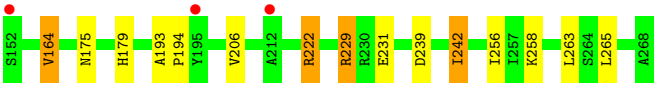
Chain B:



• Molecule 1: Pteridine reductase 1

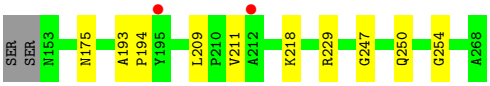
Chain D:





• Molecule 2: Pteridine reductase 1

Chain C:


SER
SER
N153
N175
A193
P194
Y195
L209
P210
V211
A212
K218
R229
G247
Q250
G254
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	74.55Å 90.24Å 82.41Å 90.00° 115.57° 90.00°	Depositor
Resolution (Å)	23.38 – 1.60 22.93 – 1.60	Depositor EDS
% Data completeness (in resolution range)	92.2 (23.38-1.60) 92.2 (22.93-1.60)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.03	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 1.60Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.145 , 0.186 0.143 , 0.185	Depositor DCC
R_{free} test set	5999 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	18.1	Xtriage
Anisotropy	0.635	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 61.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	9055	wwPDB-VP
Average B, all atoms (Å^2)	21.0	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 30.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2842e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSX, DTT, NAP, D1D, GOL, AX2, 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	0.79	0/1958	0.70	0/2655
1	B	0.81	0/2012	0.75	1/2726 (0.0%)
1	D	0.78	0/1965	0.75	2/2665 (0.1%)
2	C	0.78	0/1958	0.70	0/2653
All	All	0.79	0/7893	0.73	3/10699 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	222	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	D	82	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	B	198	ARG	NE-CZ-NH1	5.66	123.13	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1901	0	1976	17	0
1	B	1937	0	2015	15	0
1	D	1908	0	1965	15	0
2	C	1906	0	1964	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	48	0	25	1	0
3	B	48	0	25	2	0
3	C	48	0	25	2	0
3	D	48	0	25	1	0
4	A	9	0	6	0	0
4	B	9	0	6	0	0
4	C	9	0	6	0	0
4	D	9	0	6	0	0
5	A	16	0	12	2	0
5	B	8	0	9	1	0
5	C	8	0	9	1	0
5	D	8	0	9	0	0
6	A	8	0	8	1	0
6	B	8	0	8	2	0
6	C	8	0	8	0	0
6	D	8	0	8	0	0
7	A	12	0	9	1	0
7	C	8	0	6	1	0
7	D	4	0	3	0	0
8	A	6	0	8	0	0
8	C	6	0	8	0	0
9	A	319	0	0	4	0
9	B	262	0	0	7	0
9	C	247	0	0	3	0
9	D	239	0	0	5	0
All	All	9055	0	8149	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)
1:A:175:ASN:HB2	9:A:542:HOH:O	1.47	1.13
1:B:175:ASN:HB2	9:B:648:HOH:O	1.69	0.91
1:B:54[B]:ASN:ND2	9:B:604:HOH:O	1.92	0.91
2:C:175:ASN:HB2	9:C:630:HOH:O	1.70	0.89
6:B:272:D1D:S4	9:B:633:HOH:O	2.38	0.81
1:D:175[B]:ASN:OD1	9:D:586:HOH:O	1.99	0.79
1:D:164[A]:VAL:HG22	1:D:179:HIS:CD2	2.20	0.77
2:C:39:GLU:HB2	9:C:629:HOH:O	1.86	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206[A]:VAL:HG23	1:D:263:LEU:HD22	1.71	0.72
1:D:222:ARG:HD3	1:D:231:GLU:OE2	1.94	0.67
1:D:50:LYS:HG3	9:D:628:HOH:O	1.96	0.66
1:B:70:PRO:O	1:B:74[B]:GLU:HG3	1.97	0.63
1:D:75:GLU:OE2	9:D:606:HOH:O	2.16	0.63
1:A:136:MET:O	1:A:140:GLN:HG3	1.99	0.62
5:A:271:DTT:H12	6:A:272:D1D:H1C1	1.84	0.59
1:A:206[B]:VAL:HG23	1:A:263:LEU:HD22	1.85	0.57
1:A:136:MET:O	1:A:140:GLN:CG	2.54	0.56
1:B:13[A]:LYS:HE2	1:B:37:SER:OG	2.05	0.55
1:D:229:ARG:NH2	9:D:544:HOH:O	2.40	0.54
1:A:22:LYS:HG2	1:A:242:ILE:HG13	1.91	0.53
1:B:153:ASN:HA	9:B:611:HOH:O	2.09	0.52
5:B:271:DTT:H12	6:B:272:D1D:H1C1	1.91	0.51
1:A:206[B]:VAL:CG1	1:A:209[B]:LEU:HD11	2.41	0.51
1:B:82:ARG:NH1	9:B:564:HOH:O	2.44	0.50
1:A:175:ASN:ND2	9:A:442:HOH:O	2.46	0.49
2:C:65:ASN:HA	2:C:69:LEU:HD22	1.94	0.49
2:C:247:GLY:HA2	2:C:250:GLN:HG3	1.95	0.48
1:D:258[A]:LYS:HD3	9:D:542[A]:HOH:O	2.13	0.48
1:D:22:LYS:HE3	1:D:239:ASP:OD1	2.13	0.48
1:A:258[B]:LYS:HE2	7:A:275:ACT:O	2.14	0.47
1:B:9:THR:HA	1:B:33:HIS:HB3	1.97	0.47
1:A:206[B]:VAL:HG23	1:A:263:LEU:CD2	2.45	0.47
1:B:160:CYS:HB3	9:B:514:HOH:O	2.14	0.46
2:C:211:VAL:HG22	9:C:436:HOH:O	2.16	0.45
2:C:9:THR:HA	2:C:33:HIS:HB3	1.99	0.45
1:B:35:HIS:HB2	3:B:269:NAP:C2A	2.47	0.45
2:C:254:GLY:HA3	1:D:265:LEU:HD11	1.99	0.44
1:A:2:GLU:HA	9:A:588:HOH:O	2.18	0.44
1:A:65:ASN:HA	1:A:69:LEU:HD22	2.00	0.44
5:A:271:DTT:H42	5:A:271:DTT:H11	1.76	0.44
2:C:209[B]:LEU:HG	2:C:218:LYS:HG2	2.00	0.43
1:A:129[A]:ILE:HD12	9:A:477:HOH:O	2.18	0.43
1:B:229:ARG:NE	9:B:629:HOH:O	2.34	0.43
1:A:9:THR:HA	1:A:33:HIS:HB3	2.01	0.43
1:B:15:ILE:HB	3:B:269:NAP:H51N	2.00	0.43
5:C:273:DTT:H41	5:C:273:DTT:H11	1.85	0.43
1:A:206[B]:VAL:HG13	1:A:209[B]:LEU:HD11	2.01	0.42
1:B:206[A]:VAL:HG12	1:B:231:GLU:HB2	2.01	0.42
1:A:15:ILE:HB	3:A:269:NAP:H51N	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:274:ACT:H3	1:D:256:ILE:HD12	2.01	0.42
2:C:35:HIS:HB2	3:C:269:NAP:C2A	2.50	0.41
1:B:206[A]:VAL:HG12	1:B:231:GLU:CB	2.50	0.41
1:D:193:ALA:N	1:D:194:PRO:HD2	2.36	0.41
1:B:125:GLY:HA2	1:B:129[B]:ILE:HB	2.03	0.41
1:D:130:ALA:HB3	1:D:131:PRO:HD3	2.02	0.41
2:C:15:ILE:HB	3:C:269:NAP:H51N	2.03	0.40
1:D:15:ILE:HB	3:D:269:NAP:H51N	2.03	0.40
1:D:242:ILE:HD12	1:D:242:ILE:C	2.41	0.40
1:B:206[B]:VAL:CG2	1:B:209[B]:LEU:HD11	2.52	0.40
2:C:193:ALA:HB3	2:C:194:PRO:HD3	2.03	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	253/288 (88%)	245 (97%)	8 (3%)	0	100	100
1	B	258/288 (90%)	249 (96%)	9 (4%)	0	100	100
1	D	254/288 (88%)	246 (97%)	8 (3%)	0	100	100
2	C	252/288 (88%)	242 (96%)	10 (4%)	0	100	100
All	All	1017/1152 (88%)	982 (97%)	35 (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	207/231 (90%)	203 (98%)	4 (2%)	57	34
1	B	213/231 (92%)	210 (99%)	3 (1%)	67	47
1	D	208/231 (90%)	204 (98%)	4 (2%)	57	34
2	C	206/230 (90%)	204 (99%)	2 (1%)	76	61
All	All	834/923 (90%)	821 (98%)	13 (2%)	67	41

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	60	GLN
1	A	140	GLN
1	A	152	SER
1	B	53	SER
1	B	67[A]	ASN
1	B	67[B]	ASN
2	C	141	ARG
2	C	229	ARG
1	D	164[A]	VAL
1	D	164[B]	VAL
1	D	229	ARG
1	D	242	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	60	GLN
1	A	140	GLN
1	A	166	GLN
1	A	175	ASN
1	A	186	GLN
1	B	65	ASN
1	B	166	GLN
1	B	175	ASN
1	B	186	GLN
2	C	175	ASN
2	C	186	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	67[A]	ASN
1	D	140	GLN
1	D	166	GLN
1	D	186	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	C	59	2	3,6,7	0.86	0	1,6,8	1.60	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	C	59	2	-	0/1/5/7	-

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)

25 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	$\#\|Z\| > 2$
4	AX2	A	270	-	9,9,9	1.46	1 (11%)	12,12,12	2.61	8 (66%)
6	D1D	D	272	-	6,8,8	0.81	0	6,10,10	0.78	0
7	ACT	A	275	-	3,3,3	0.66	0	3,3,3	1.47	0
4	AX2	D	270	-	9,9,9	0.95	0	12,12,12	2.55	9 (75%)
3	NAP	C	269	-	45,52,52	1.57	6 (13%)	56,80,80	1.36	8 (14%)
7	ACT	D	273	-	3,3,3	0.76	0	3,3,3	1.59	1 (33%)
5	DTT	B	271	-	7,7,7	0.40	0	4,8,8	1.07	0
7	ACT	A	273	-	3,3,3	0.67	0	3,3,3	1.17	0
4	AX2	C	272	-	9,9,9	0.90	0	12,12,12	2.68	9 (75%)
6	D1D	C	270	-	6,8,8	0.74	0	6,10,10	1.22	0
4	AX2	B	270	-	9,9,9	1.19	0	12,12,12	2.81	9 (75%)
3	NAP	A	269	-	45,52,52	1.54	5 (11%)	56,80,80	1.32	6 (10%)
6	D1D	A	272	-	6,8,8	0.81	0	6,10,10	1.12	0
7	ACT	A	274	-	3,3,3	0.82	0	3,3,3	1.00	0
6	D1D	B	272	-	6,8,8	0.77	0	6,10,10	0.96	0
5	DTT	A	271	-	7,7,7	0.34	0	4,8,8	0.98	0
8	GOL	C	275	-	5,5,5	0.62	0	5,5,5	0.75	0
3	NAP	B	269	-	45,52,52	1.60	6 (13%)	56,80,80	1.40	5 (8%)
7	ACT	C	271	-	3,3,3	0.88	0	3,3,3	1.17	0
7	ACT	C	274	-	3,3,3	0.65	0	3,3,3	1.68	2 (66%)
5	DTT	D	271	-	7,7,7	0.63	0	4,8,8	0.81	0
8	GOL	A	277	-	5,5,5	0.27	0	5,5,5	0.73	0
5	DTT	C	273	-	7,7,7	0.60	0	4,8,8	0.68	0
3	NAP	D	269	-	45,52,52	1.71	4 (8%)	56,80,80	1.60	5 (8%)

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
4	AX2	A	270	-	-	-	0/1/1/1
6	D1D	D	272	-	-	-	0/0/1/1
4	AX2	D	270	-	-	-	0/1/1/1
3	NAP	C	269	-	-	0/31/67/67	0/5/5/5
5	DTT	B	271	-	1/1/2/2	1/8/8/8	-
4	AX2	C	272	-	-	-	0/1/1/1
6	D1D	C	270	-	-	-	0/0/1/1
5	DTT	A	276[B]	-	1/1/2/2	-	-
4	AX2	B	270	-	-	-	0/1/1/1
3	NAP	A	269	-	-	0/31/67/67	0/5/5/5
6	D1D	A	272	-	-	-	0/0/1/1
6	D1D	B	272	-	-	-	0/0/1/1
5	DTT	A	271	-	1/1/2/2	2/8/8/8	-
8	GOL	C	275	-	-	2/4/4/4	-
3	NAP	B	269	-	-	0/31/67/67	0/5/5/5
5	DTT	D	271	-	1/1/2/2	5/8/8/8	-
8	GOL	A	277	-	-	0/4/4/4	-
5	DTT	C	273	-	1/1/2/2	5/8/8/8	-
3	NAP	D	269	-	-	0/31/67/67	0/5/5/5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	269	NAP	O7N-C7N	7.55	1.38	1.24
3	C	269	NAP	O7N-C7N	7.41	1.38	1.24
3	B	269	NAP	O7N-C7N	6.88	1.37	1.24
3	A	269	NAP	O7N-C7N	6.33	1.36	1.24
3	D	269	NAP	C2A-N3A	5.22	1.40	1.32
3	B	269	NAP	C2A-N3A	4.32	1.39	1.32
3	A	269	NAP	C2A-N3A	4.27	1.39	1.32
3	C	269	NAP	C2A-N3A	3.88	1.38	1.32
4	A	270	AX2	C6-N1	3.05	1.40	1.35
3	A	269	NAP	C2A-N1A	2.84	1.39	1.33
3	B	269	NAP	P2B-O2B	2.79	1.64	1.59
3	B	269	NAP	C2A-N1A	2.67	1.38	1.33
3	D	269	NAP	C2A-N1A	2.54	1.38	1.33
3	B	269	NAP	C4N-C3N	2.53	1.43	1.39
3	A	269	NAP	C4N-C3N	2.53	1.43	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	269	NAP	P2B-O2B	2.31	1.63	1.59
3	B	269	NAP	O4B-C4B	-2.28	1.39	1.45
3	C	269	NAP	C2N-N1N	2.24	1.37	1.35
3	D	269	NAP	C4N-C3N	2.21	1.43	1.39
3	C	269	NAP	C2A-N1A	2.09	1.37	1.33
3	C	269	NAP	O4B-C4B	-2.06	1.40	1.45
3	C	269	NAP	C4N-C3N	2.01	1.42	1.39

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	269	NAP	N3A-C2A-N1A	-6.09	119.16	128.68
3	B	269	NAP	N3A-C2A-N1A	-6.06	119.21	128.68
3	C	269	NAP	N3A-C2A-N1A	-5.56	119.99	128.68
3	D	269	NAP	C3N-C7N-N7N	5.44	124.28	117.75
3	A	269	NAP	N3A-C2A-N1A	-5.41	120.23	128.68
3	D	269	NAP	O7N-C7N-C3N	-4.51	114.23	119.63
4	C	272	AX2	N1-C6-N5	-3.94	119.24	125.42
4	B	270	AX2	N1-C2-N3	-3.76	119.53	125.42
4	A	270	AX2	N1-C6-N5	-3.74	119.56	125.42
3	B	269	NAP	C1B-N9A-C4A	-3.73	120.09	126.64
3	A	269	NAP	O7N-C7N-C3N	-3.72	115.18	119.63
4	B	270	AX2	N3-C4-N5	-3.70	119.61	125.42
4	D	270	AX2	N3-C4-N5	-3.65	119.70	125.42
3	D	269	NAP	C1B-N9A-C4A	-3.60	120.32	126.64
4	B	270	AX2	C6-N5-C4	3.57	120.87	114.83
4	A	270	AX2	N1-C2-N3	-3.56	119.84	125.42
4	B	270	AX2	N1-C6-N5	-3.54	119.87	125.42
4	C	272	AX2	N3-C4-N5	-3.33	120.19	125.42
3	A	269	NAP	C3N-C7N-N7N	3.33	121.75	117.75
3	C	269	NAP	C1B-N9A-C4A	-3.26	120.91	126.64
4	C	272	AX2	C6-N5-C4	3.24	120.30	114.83
4	D	270	AX2	C4-N3-C2	3.21	120.25	114.83
4	D	270	AX2	N1-C6-N5	-3.21	120.39	125.42
4	B	270	AX2	C6-N1-C2	3.18	120.20	114.83
4	C	272	AX2	N8-C6-N5	3.08	122.04	117.25
4	A	270	AX2	C6-N5-C4	3.04	119.96	114.83
4	C	272	AX2	N1-C2-N3	-3.01	120.70	125.42
4	C	272	AX2	C6-N1-C2	3.01	119.91	114.83
4	D	270	AX2	N1-C2-N3	-3.00	120.71	125.42
4	A	270	AX2	C4-N3-C2	2.95	119.82	114.83
4	B	270	AX2	C4-N3-C2	2.95	119.81	114.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	270	AX2	N7-C2-N1	2.94	121.82	117.25
3	B	269	NAP	O4D-C4D-C3D	2.88	110.81	105.11
4	A	270	AX2	C6-N1-C2	2.87	119.68	114.83
4	C	272	AX2	C4-N3-C2	2.84	119.63	114.83
4	D	270	AX2	C6-N5-C4	2.83	119.61	114.83
4	A	270	AX2	N3-C4-N5	-2.82	120.99	125.42
3	C	269	NAP	C5A-C6A-N6A	2.77	124.57	120.35
3	C	269	NAP	C3N-C7N-N7N	2.68	120.96	117.75
4	D	270	AX2	C6-N1-C2	2.66	119.33	114.83
4	D	270	AX2	N8-C6-N1	2.65	121.38	117.25
3	B	269	NAP	C4A-C5A-N7A	-2.64	106.65	109.40
4	B	270	AX2	N7-C2-N1	2.59	121.28	117.25
4	C	272	AX2	N9-C4-N5	2.58	121.26	117.25
3	C	269	NAP	O7N-C7N-C3N	-2.48	116.66	119.63
4	B	270	AX2	N9-C4-N3	2.42	121.02	117.25
3	D	269	NAP	O3B-C3B-C2B	2.37	117.90	111.17
3	A	269	NAP	C2A-N1A-C6A	2.34	122.77	118.75
3	C	269	NAP	C2A-N1A-C6A	2.32	122.72	118.75
4	A	270	AX2	N8-C6-N1	2.31	120.84	117.25
4	B	270	AX2	N8-C6-N1	2.28	120.80	117.25
3	C	269	NAP	C4A-C5A-N7A	-2.26	107.04	109.40
4	D	270	AX2	N7-C2-N3	2.23	120.72	117.25
3	A	269	NAP	C6N-N1N-C2N	2.22	124.00	121.97
3	C	269	NAP	O2N-PN-O1N	2.18	123.04	112.24
3	B	269	NAP	C3N-C7N-N7N	2.15	120.33	117.75
7	D	273	ACT	OXT-C-O	-2.09	114.35	122.05
3	A	269	NAP	C1B-N9A-C4A	-2.09	122.98	126.64
7	C	274	ACT	OXT-C-CH3	2.07	123.72	115.18
7	C	274	ACT	OXT-C-O	-2.05	114.49	122.05
4	D	270	AX2	N9-C4-N5	2.04	120.43	117.25
4	C	272	AX2	N7-C2-N1	2.03	120.41	117.25

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	271	DTT	C3
5	A	276[B]	DTT	C3
5	B	271	DTT	C3
5	C	273	DTT	C3
5	D	271	DTT	C3

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	271	DTT	S1-C1-C2-O2
5	A	271	DTT	C1-C2-C3-C4
5	B	271	DTT	C1-C2-C3-C4
5	C	273	DTT	S1-C1-C2-O2
5	C	273	DTT	C1-C2-C3-O3
5	C	273	DTT	C1-C2-C3-C4
5	C	273	DTT	O2-C2-C3-O3
5	C	273	DTT	O2-C2-C3-C4
5	D	271	DTT	S1-C1-C2-O2
5	D	271	DTT	C1-C2-C3-O3
5	D	271	DTT	C1-C2-C3-C4
5	D	271	DTT	O2-C2-C3-O3
5	D	271	DTT	O2-C2-C3-C4
8	C	275	GOL	O1-C1-C2-O2
8	C	275	GOL	O1-C1-C2-C3

There are no ring outliers.

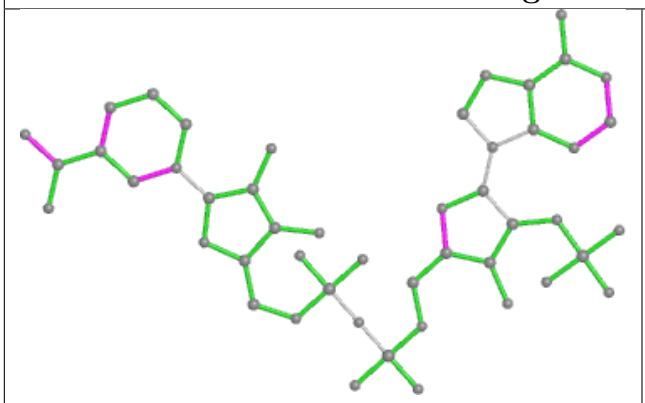
11 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	275	ACT	1	0
3	C	269	NAP	2	0
5	B	271	DTT	1	0
3	A	269	NAP	1	0
6	A	272	D1D	1	0
6	B	272	D1D	2	0
5	A	271	DTT	2	0
3	B	269	NAP	2	0
7	C	274	ACT	1	0
5	C	273	DTT	1	0
3	D	269	NAP	1	0

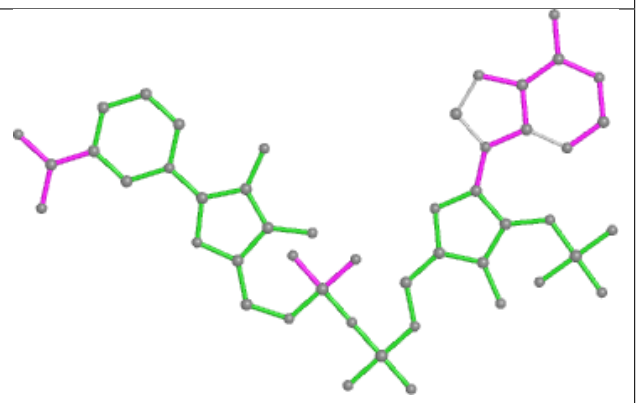
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

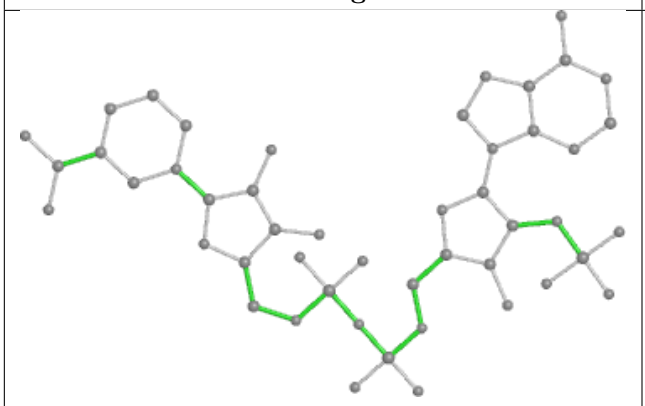
Ligand NAP C 269



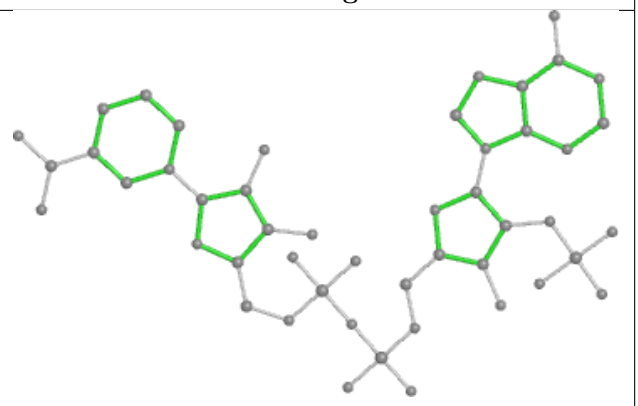
Bond lengths



Bond angles

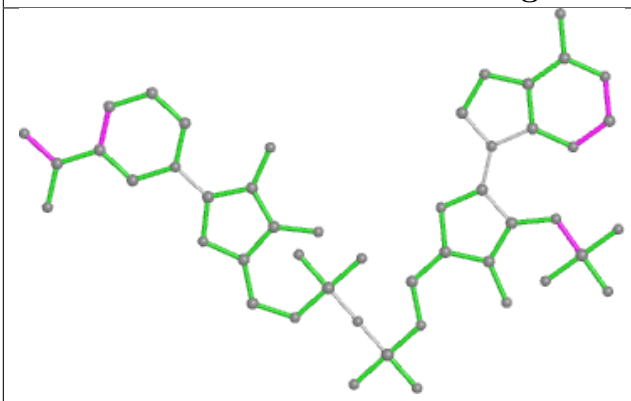


Torsions

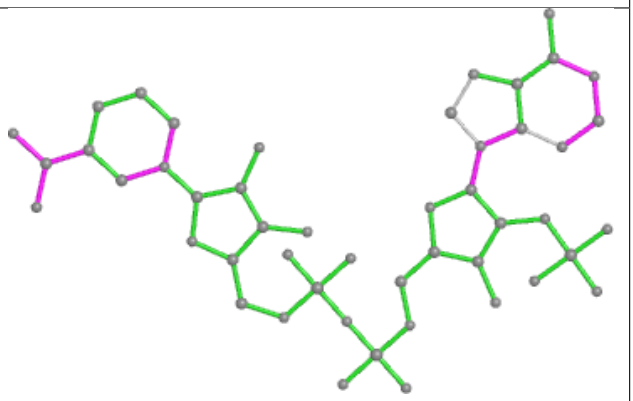


Rings

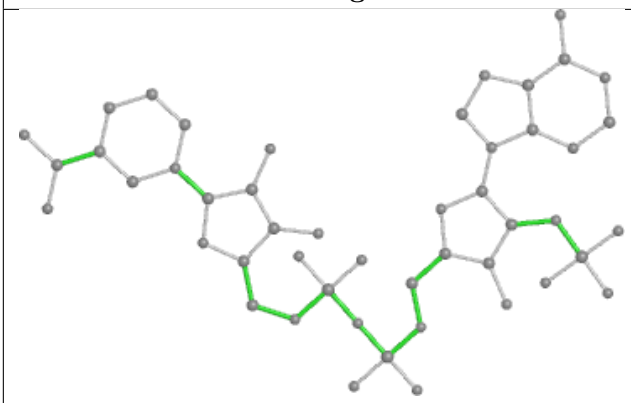
Ligand NAP A 269



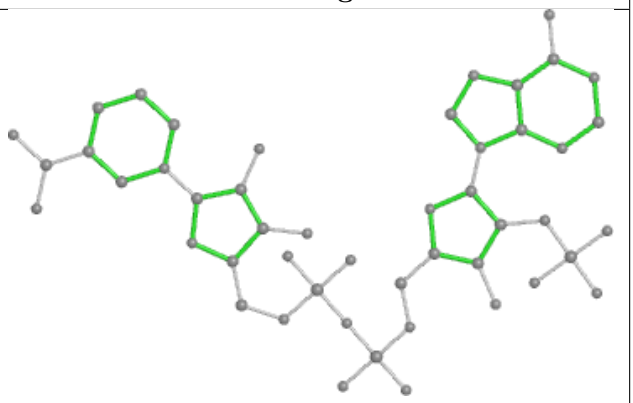
Bond lengths



Bond angles

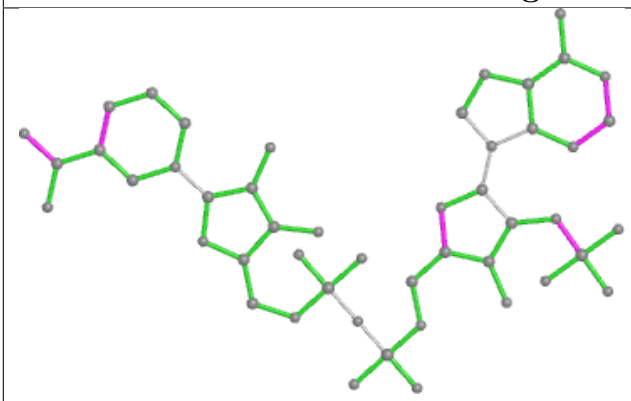


Torsions

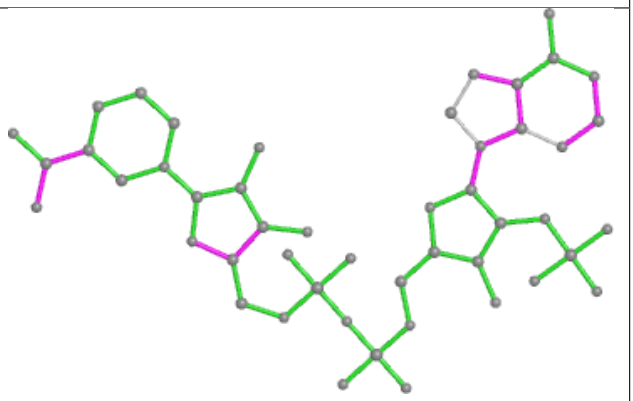


Rings

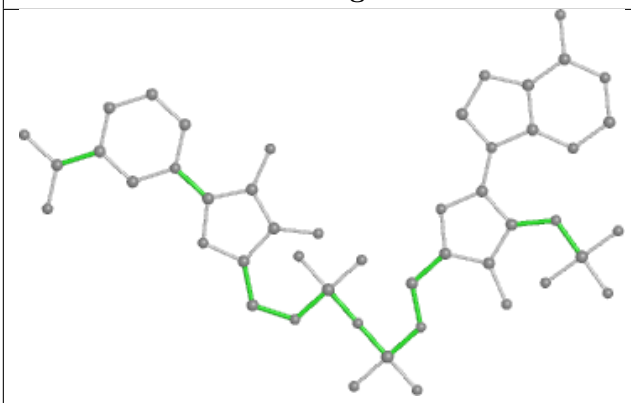
Ligand NAP B 269



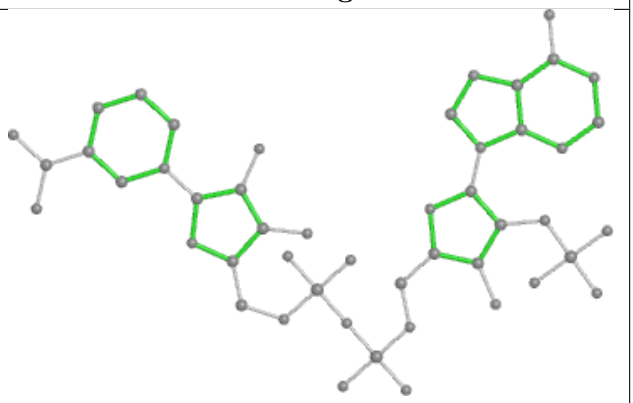
Bond lengths



Bond angles

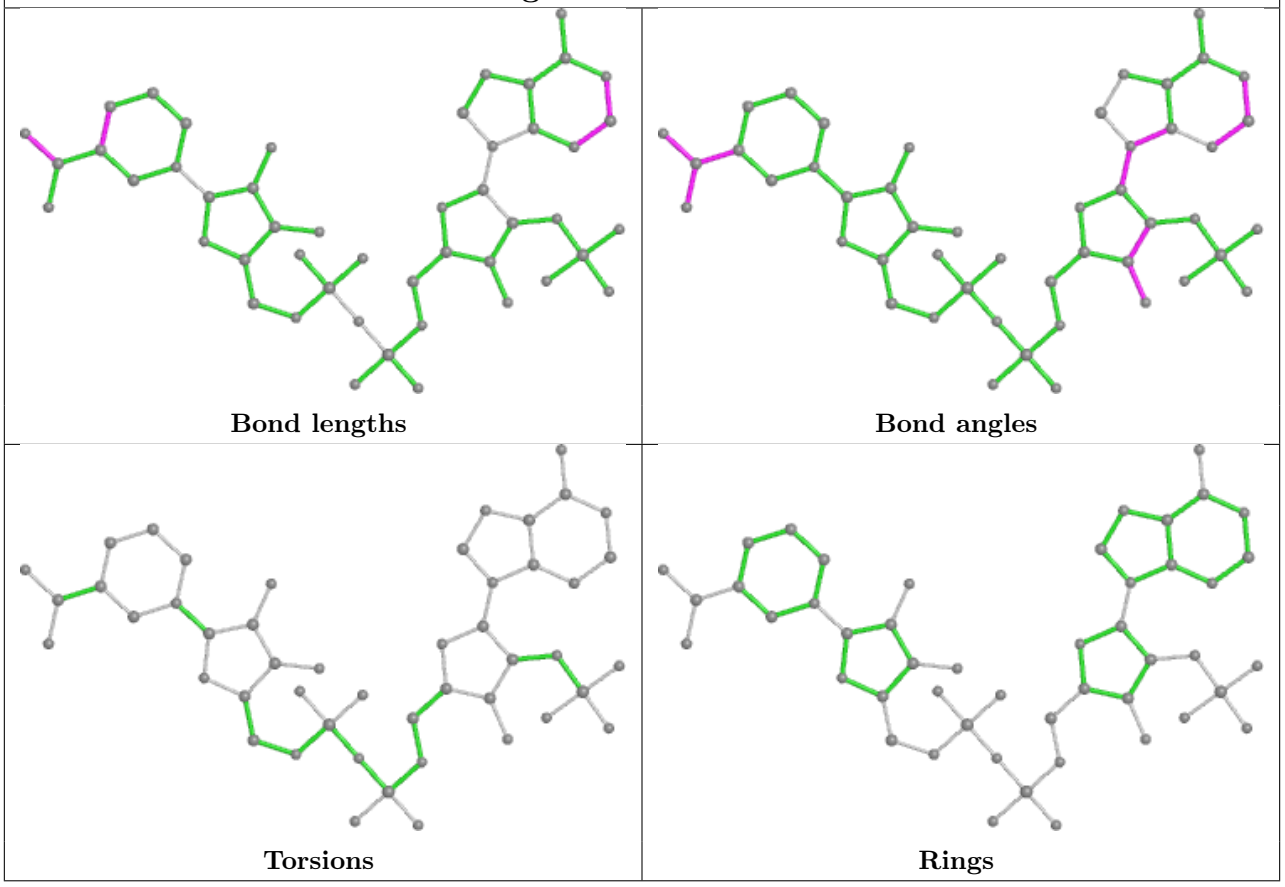


Torsions



Rings

Ligand NAP D 269



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	249/288 (86%)	-0.24	3 (1%)	79	78	14, 17, 28, 49	7 (2%)
1	B	248/288 (86%)	-0.27	4 (1%)	72	71	13, 16, 29, 45	2 (0%)
1	D	249/288 (86%)	-0.18	6 (2%)	59	56	14, 18, 30, 43	6 (2%)
2	C	247/288 (85%)	-0.16	6 (2%)	59	56	14, 17, 31, 44	5 (2%)
All	All	993/1152 (86%)	-0.21	19 (1%)	66	65	13, 17, 30, 49	20 (2%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	113	GLY	7.8
2	C	113	GLY	7.0
1	D	113	GLY	6.2
1	B	212	ALA	5.2
1	A	113	GLY	3.7
2	C	212	ALA	3.7
1	D	152	SER	3.3
1	D	2	GLU	3.3
1	B	2[A]	GLU	3.0
1	B	211	VAL	3.0
1	A	2	GLU	2.8
2	C	195	TYR	2.8
2	C	2	GLU	2.7
1	D	212	ALA	2.5
1	A	195	TYR	2.3
1	D	195	TYR	2.2
2	C	3	ALA	2.2
2	C	103	VAL	2.1
1	D	39	GLU	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, 95^{th} 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	59	7/8	0.98	0.10	15,17,24,35	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	DTT	A	276[B]	8/8	0.84	0.15	25,37,52,56	1
8	GOL	C	275	6/6	0.90	0.12	24,33,41,44	0
8	GOL	A	277	6/6	0.92	0.12	23,34,35,40	0
7	ACT	D	273	4/4	0.92	0.16	23,26,27,28	0
7	ACT	A	275	4/4	0.94	0.20	24,27,29,29	0
5	DTT	B	271	8/8	0.94	0.15	23,47,60,61	8
6	D1D	A	272	8/8	0.94	0.09	24,33,42,44	1
6	D1D	D	272	8/8	0.94	0.11	25,35,42,44	0
5	DTT	C	273	8/8	0.95	0.11	27,45,51,61	8
6	D1D	B	272	8/8	0.95	0.14	20,31,38,46	0
5	DTT	D	271	8/8	0.95	0.13	28,48,51,63	8
7	ACT	A	274	4/4	0.95	0.14	23,24,27,28	0
6	D1D	C	270	8/8	0.96	0.08	22,30,37,38	0
5	DTT	A	271	8/8	0.96	0.12	28,45,51,53	8
7	ACT	C	274	4/4	0.96	0.12	25,26,28,30	0
3	NAP	A	269	48/48	0.97	0.06	10,15,18,18	0
3	NAP	D	269	48/48	0.97	0.08	11,17,20,21	0
4	AX2	D	270	9/9	0.97	0.07	15,17,18,19	0
7	ACT	C	271	4/4	0.98	0.08	15,17,17,18	0
3	NAP	C	269	48/48	0.98	0.07	14,16,19,21	0
4	AX2	A	270	9/9	0.98	0.05	14,15,19,19	0

Continued on next page...

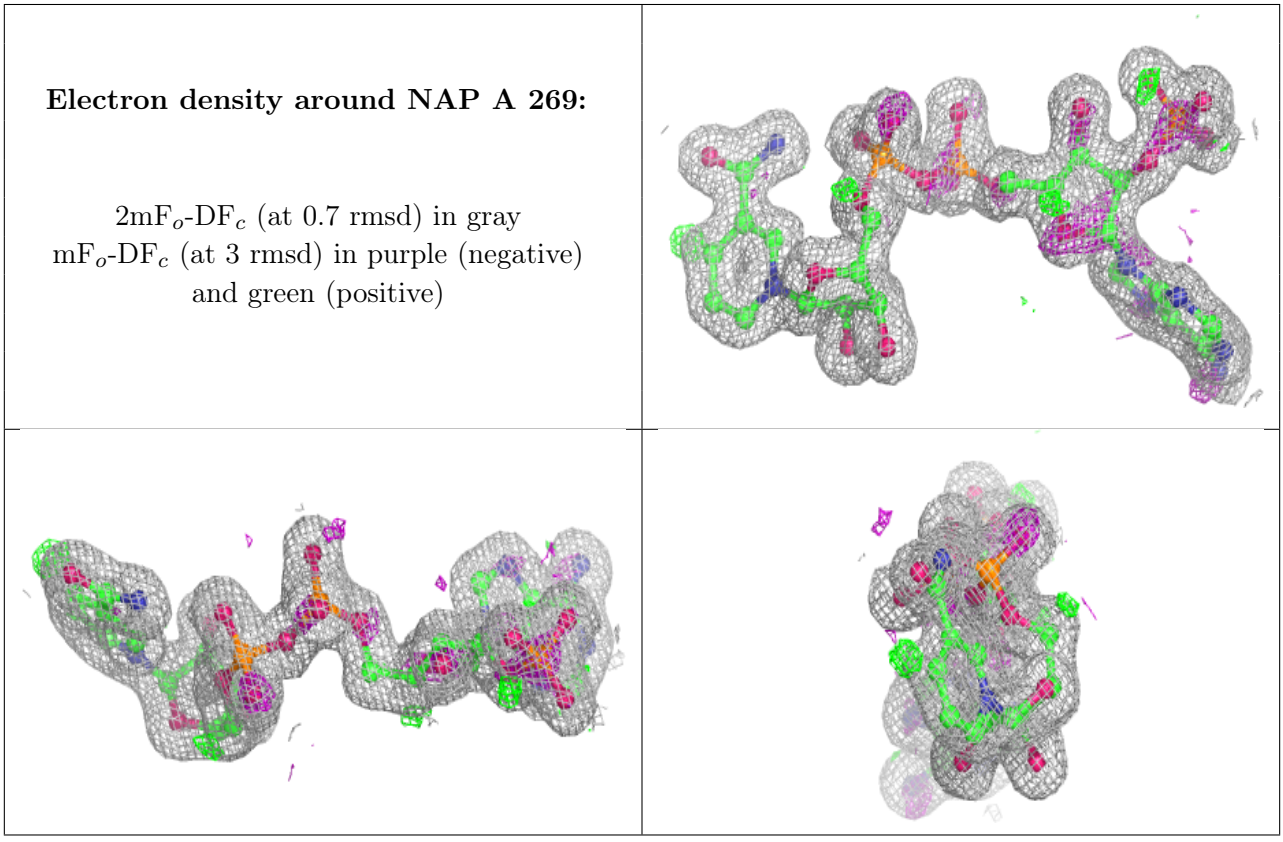
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	AX2	B	270	9/9	0.98	0.04	12,14,16,17	0
4	AX2	C	272	9/9	0.98	0.05	14,16,19,20	0
7	ACT	A	273	4/4	0.99	0.10	21,21,24,26	0
3	NAP	B	269	48/48	0.99	0.05	11,15,17,18	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.

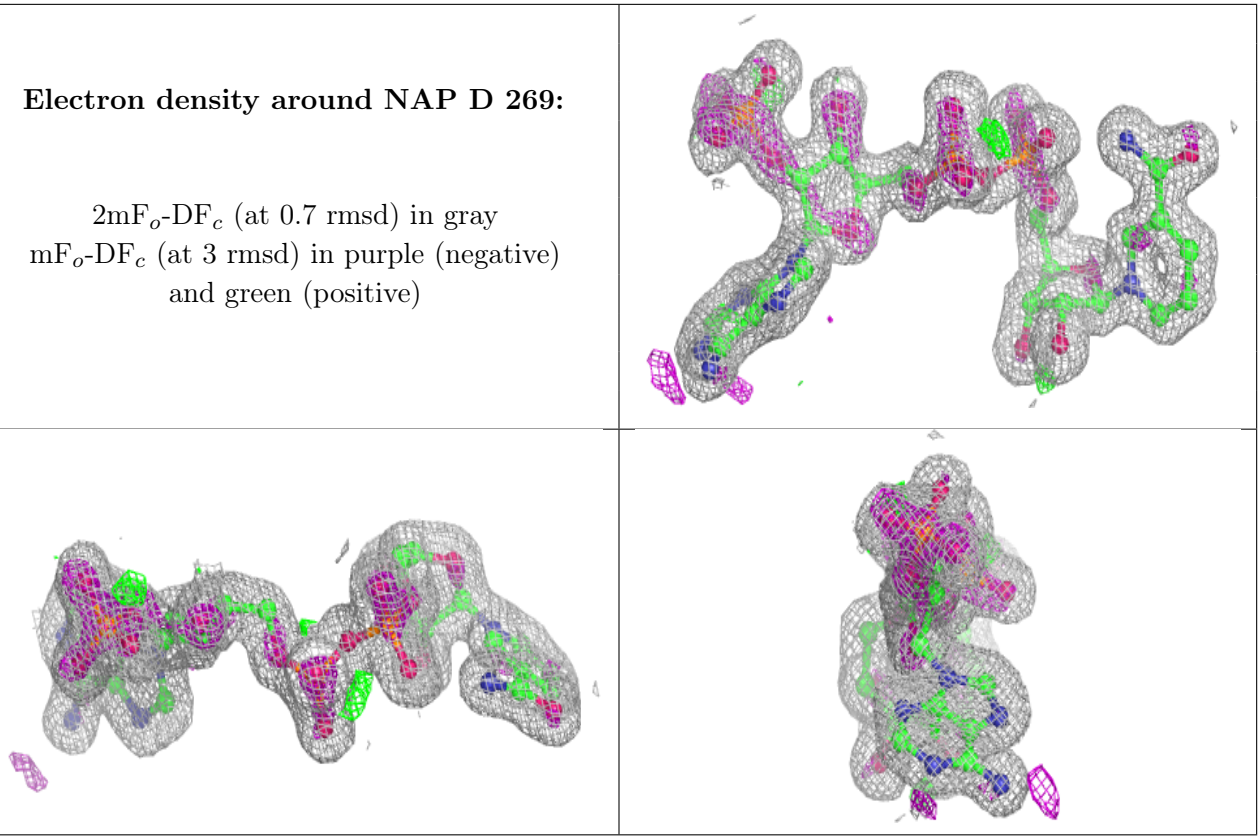
Electron density around NAP A 269:

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



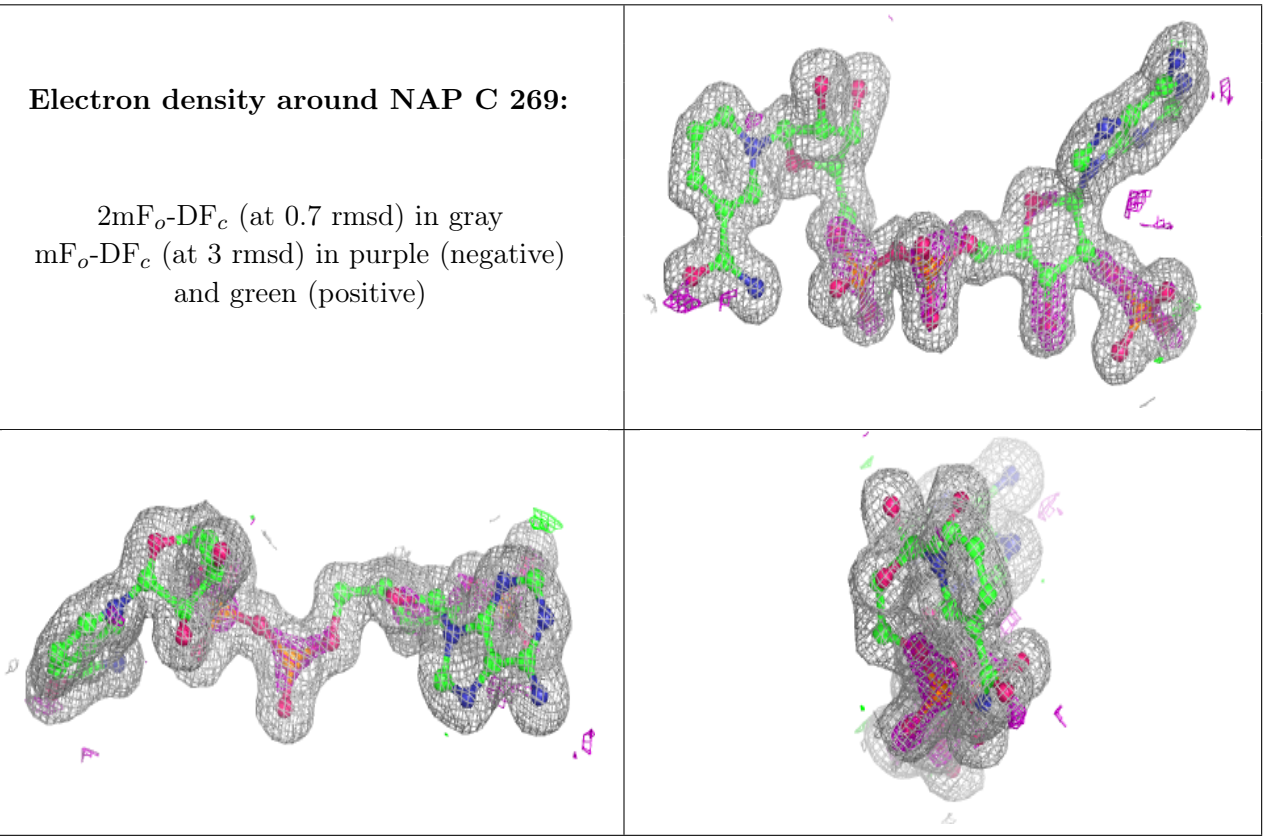
Electron density around NAP D 269:

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



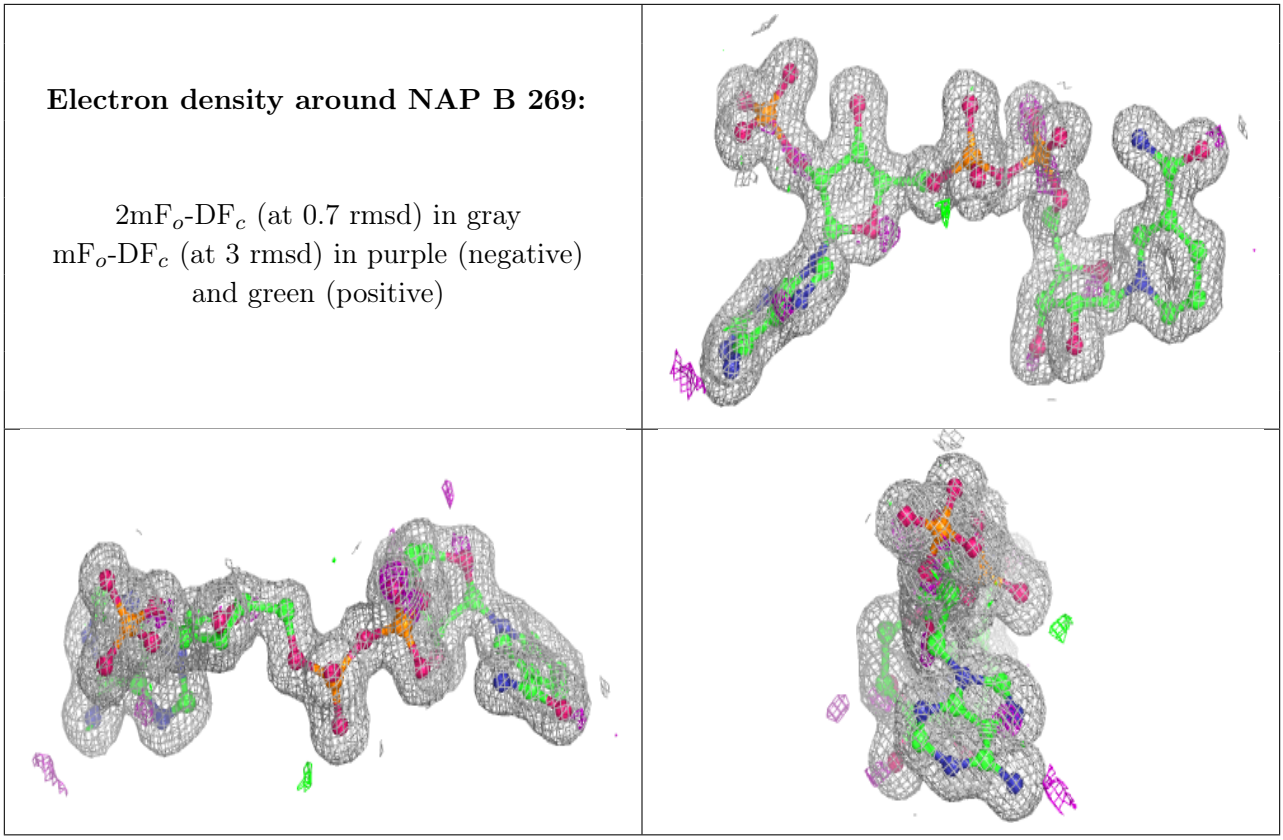
Electron density around NAP C 269:

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



Electron density around NAP B 269:

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



6.5 Other polymers (i)

There are no such residues in this entry.