



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 02:50 pm BST

PDB ID : 4CME
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 : 1.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

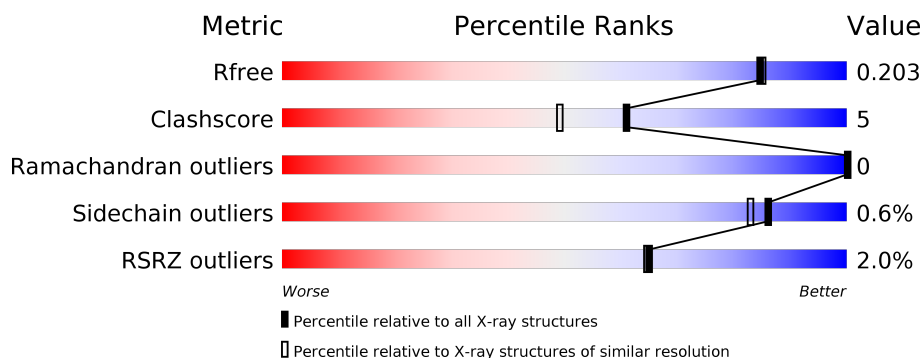
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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

Mol	Chain	Length	Quality of chain
1	A	288	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 9%, green 80%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 77% 9% 14% </div> </div>
1	B	288	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 7%, green 80%, grey 11%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 80% 7% 14% </div> </div>
2	C	288	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 9%, green 77%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 3% 77% 9% 13% </div> </div>
2	D	288	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 7%, green 80%, grey 11%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 80% 7% 14% </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8590 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	4	0
			1879	1180	329	358	12			
1	B	249	Total	C	N	O	S	0	11	0
			1931	1215	337	366	13			

There are 40 discrepancies between the modelled and reference sequences:

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

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

- Molecule 2 is a protein called PTERIDINE REDUCTASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	250	Total	C	N	O	S	0	2	0
			1877	1177	330	358	12			
2	D	249	Total	C	N	O	S	0	3	0
			1877	1177	330	358	12			

There are 40 discrepancies between the modelled and reference sequences:

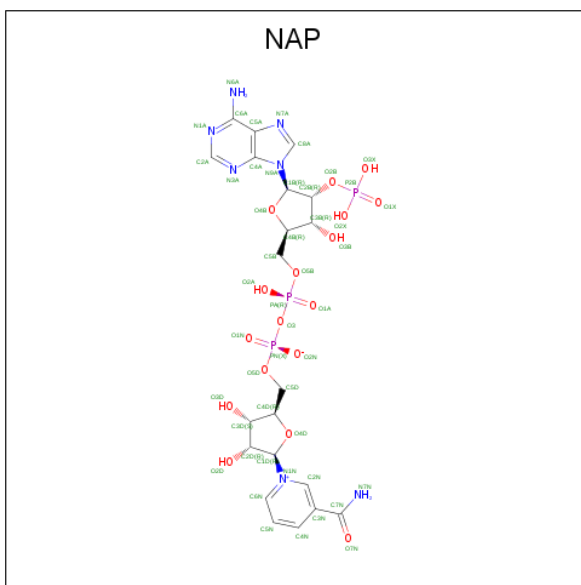
Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	expression tag	UNP O76290
C	-18	GLY	-	expression tag	UNP O76290
C	-17	SER	-	expression tag	UNP O76290
C	-16	SER	-	expression tag	UNP O76290
C	-15	HIS	-	expression tag	UNP O76290
C	-14	HIS	-	expression tag	UNP O76290
C	-13	HIS	-	expression tag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

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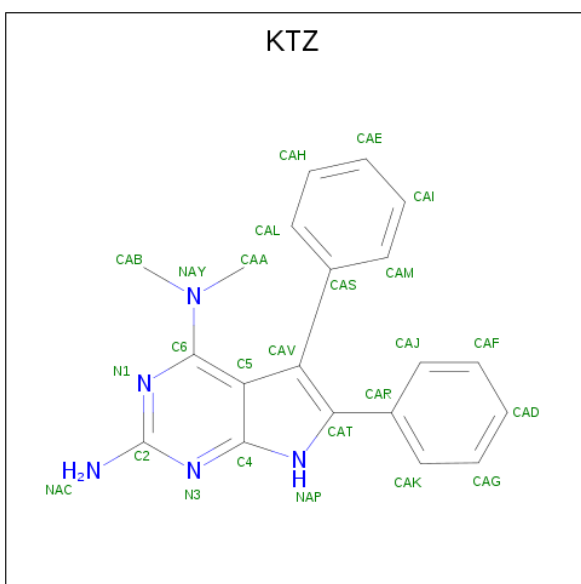
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP O76290
C	-3	ARG	-	expression tag	UNP O76290
C	-2	GLY	-	expression tag	UNP O76290
C	-1	SER	-	expression tag	UNP O76290
C	0	HIS	-	expression tag	UNP O76290
D	-19	MET	-	expression tag	UNP O76290
D	-18	GLY	-	expression tag	UNP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

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



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

- Molecule 4 is N4,N4-dimethyl-5,6-diphenyl-7H-pyrrolo[2,3-d]pyrimidine-2,4-diamine (three-letter code: KTZ) (formula: C₂₀H₁₉N₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			25	20	5		
4	B	1	Total	C	N	0	0
			25	20	5		
4	C	1	Total	C	N	0	0
			25	20	5		
4	D	1	Total	C	N	0	0
			25	20	5		

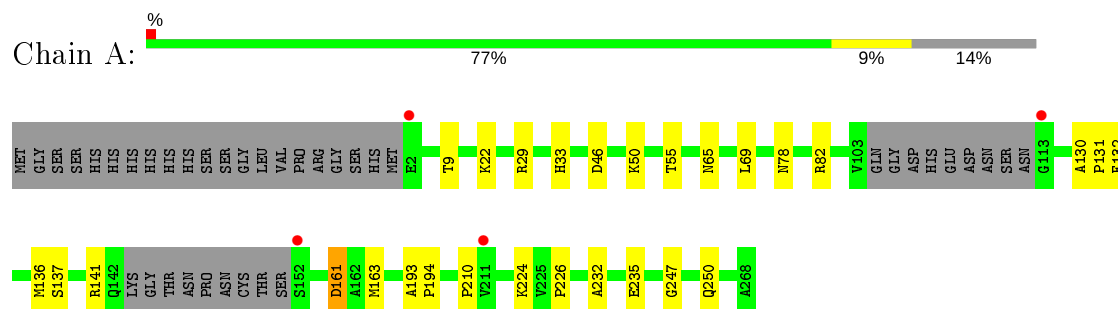
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	209	Total	O	0	0
			209	209		
5	B	190	Total	O	0	0
			190	190		
5	C	163	Total	O	0	0
			163	163		
5	D	172	Total	O	0	0
			172	172		

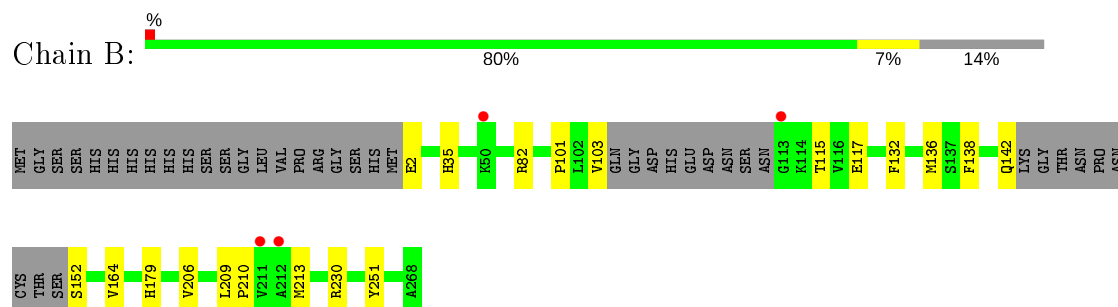
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

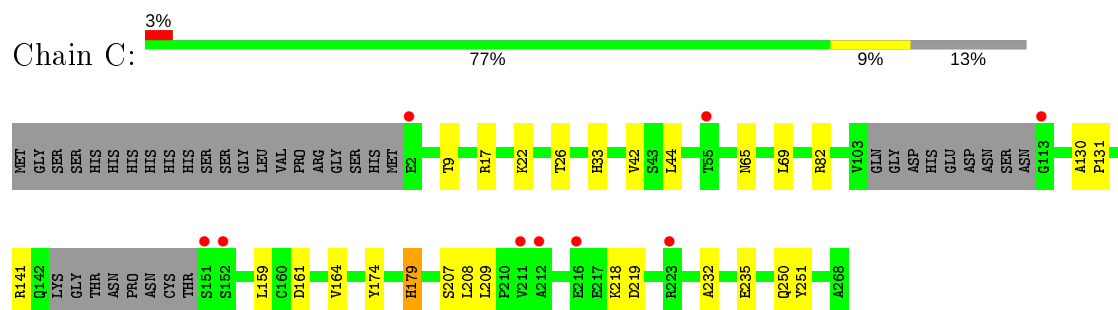
• Molecule 1: PTERIDINE REDUCTASE 1



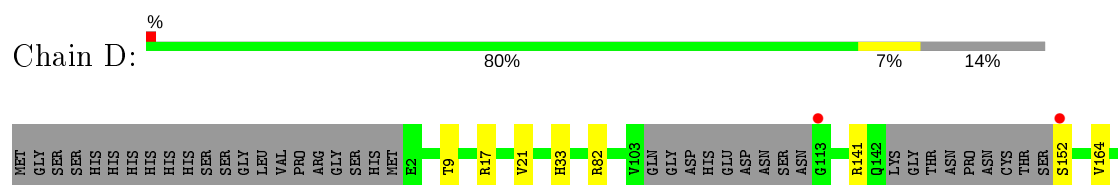
• Molecule 1: PTERIDINE REDUCTASE 1



• Molecule 2: PTERIDINE REDUCTASE 1



• Molecule 2: PTERIDINE REDUCTASE 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.05Å 88.42Å 84.22Å 90.00° 115.68° 90.00°	Depositor
Resolution (Å)	44.21 – 1.85 44.21 – 1.85	Depositor EDS
% Data completeness (in resolution range)	91.6 (44.21-1.85) 91.6 (44.21-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.150 , 0.194 0.163 , 0.203	Depositor DCC
R_{free} test set	3846 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	14.2	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8590	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.02% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.69	0/1912	0.79	2/2593 (0.1%)
1	B	0.69	0/1962	0.83	2/2663 (0.1%)
2	C	0.69	0/1896	0.83	4/2570 (0.2%)
2	D	0.69	0/1896	0.80	2/2570 (0.1%)
All	All	0.69	0/7666	0.81	10/10396 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	159	LEU	CA-CB-CG	-8.39	96.00	115.30
1	B	82	ARG	NE-CZ-NH1	7.71	124.16	120.30
2	D	82	ARG	NE-CZ-NH1	6.96	123.78	120.30
2	D	82	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	B	230	ARG	NE-CZ-NH1	5.74	123.17	120.30
2	C	159	LEU	CB-CG-CD2	5.39	120.16	111.00
1	A	161[A]	ASP	CB-CA-C	-5.19	100.02	110.40
1	A	161[B]	ASP	CB-CA-C	-5.19	100.02	110.40
2	C	219	ASP	CB-CG-OD1	5.16	122.94	118.30
2	C	82	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1879	0	1899	20	0
1	B	1931	0	1957	17	0
2	C	1877	0	1893	16	0
2	D	1877	0	1892	15	0
3	A	48	0	25	0	0
3	B	48	0	25	2	0
3	C	48	0	25	0	0
3	D	48	0	25	0	0
4	A	25	0	19	3	0
4	B	25	0	19	4	0
4	C	25	0	19	5	0
4	D	25	0	19	3	0
5	A	209	0	0	1	0
5	B	190	0	0	2	0
5	C	163	0	0	2	1
5	D	172	0	0	2	1
All	All	8590	0	7817	71	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 5.

All (71) 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:C:1270:KTZ:CAM	4:C:1270:KTZ:HAA2	2.11	0.81
4:D:1270:KTZ:HAB2	4:D:1270:KTZ:CAM	2.13	0.78
4:A:1270:KTZ:CAM	4:A:1270:KTZ:HAB2	2.22	0.70
1:B:209[B]:LEU:HB3	1:B:213[B]:MET:SD	2.34	0.68
2:C:209:LEU:HD23	4:C:1270:KTZ:HAI	1.75	0.68
1:B:210[B]:PRO:HD2	1:B:213[B]:MET:SD	2.36	0.65
4:D:1270:KTZ:CAS	4:D:1270:KTZ:HAB2	2.26	0.65
1:B:138:PHE:O	1:B:142:GLN:HG2	1.99	0.62
2:D:217:GLU:HA	2:D:220:LYS:HD3	1.85	0.59
2:D:141:ARG:HG2	5:D:2109:HOH:O	2.04	0.57
4:B:1270:KTZ:CAS	4:B:1270:KTZ:HAA2	2.36	0.56
1:B:152:SER:O	5:B:2120:HOH:O	2.18	0.56
2:C:164:VAL:HG22	2:C:179:HIS:CD2	2.40	0.55
4:C:1270:KTZ:HAA2	4:C:1270:KTZ:CAS	2.37	0.54
1:B:210[B]:PRO:O	1:B:213[B]:MET:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1270:KTZ:CAS	4:A:1270:KTZ:HAB2	2.37	0.54
1:B:164:VAL:HG22	1:B:179:HIS:CD2	2.44	0.52
2:D:209:LEU:HD23	4:D:1270:KTZ:HAI	1.91	0.52
1:B:209[B]:LEU:HD23	4:B:1270:KTZ:HAI	1.91	0.52
1:B:115:THR:HB	1:B:117:GLU:OE1	2.10	0.51
4:B:1270:KTZ:CAM	4:B:1270:KTZ:HAA2	2.40	0.51
1:B:132:PHE:CZ	1:B:136:MET:CE	2.93	0.51
1:A:22:LYS:HE3	1:A:235:GLU:HG3	1.91	0.51
1:A:232:ALA:HB2	1:B:251:TYR:CE2	2.47	0.50
1:A:210:PRO:HG3	4:A:1270:KTZ:HAB1	1.92	0.50
1:A:9:THR:HA	1:A:33:HIS:HB3	1.94	0.50
1:A:78:ASN:OD1	1:A:141:ARG:NH1	2.45	0.49
1:A:22:LYS:CE	1:A:235:GLU:HG3	2.43	0.49
2:D:208:LEU:HD22	2:D:234:ALA:HB2	1.94	0.49
2:C:65:ASN:HA	2:C:69:LEU:HD22	1.95	0.49
1:A:247:GLY:O	1:A:250:GLN:HG2	2.13	0.48
1:A:163[B]:MET:HE1	2:D:267:HIS:HB2	1.94	0.48
1:A:132:PHE:CZ	1:A:136:MET:CE	2.96	0.47
1:A:130:ALA:HB3	1:A:131:PRO:HD3	1.95	0.47
2:C:251:TYR:CE2	2:D:232:ALA:HB2	2.50	0.47
2:C:9:THR:HA	2:C:33:HIS:HB3	1.96	0.47
2:C:17:ARG:CZ	2:C:44:LEU:HD13	2.44	0.47
2:D:223:ARG:NH2	5:D:2144:HOH:O	2.47	0.47
2:C:141:ARG:HD3	5:C:2100:HOH:O	2.15	0.46
2:C:42:VAL:HG23	5:C:2036:HOH:O	2.15	0.46
1:A:161[B]:ASP:OD1	5:A:2127:HOH:O	2.20	0.46
2:C:232:ALA:HB2	2:D:251:TYR:CE2	2.50	0.46
2:D:207:SER:O	2:D:208:LEU:C	2.52	0.46
1:A:163[B]:MET:CE	2:D:267:HIS:HB2	2.45	0.46
1:A:65:ASN:HA	1:A:69:LEU:HD22	1.97	0.45
4:C:1270:KTZ:HAJ	4:C:1270:KTZ:CAS	2.45	0.45
2:C:130:ALA:HB3	2:C:131:PRO:HD3	1.98	0.45
3:B:1269:NAP:C7N	4:B:1270:KTZ:HAM	2.47	0.45
2:D:164:VAL:HG22	2:D:179:HIS:CD2	2.52	0.45
1:A:232:ALA:HB2	1:B:251:TYR:CD2	2.52	0.45
1:A:224:LYS:O	1:A:226:PRO:HD3	2.17	0.44
2:D:9:THR:HA	2:D:33:HIS:HB3	1.99	0.44
1:A:132:PHE:CZ	1:A:136:MET:HE1	2.53	0.44
1:A:193:ALA:N	1:A:194:PRO:CD	2.79	0.44
1:A:46:ASP:O	1:A:50:LYS:HG2	2.17	0.43
1:B:206[B]:VAL:HG13	1:B:206[B]:VAL:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:VAL:HG21	2:D:195:TYR:OH	2.18	0.43
1:A:137:SER:O	1:A:141:ARG:HG2	2.19	0.43
2:C:22:LYS:HE2	2:C:235:GLU:HG3	2.00	0.43
1:B:132:PHE:CE2	1:B:136:MET:CE	3.02	0.43
1:B:2:GLU:HG3	5:B:2001:HOH:O	2.19	0.42
2:C:161[A]:ASP:OD1	2:C:174:TYR:OH	2.38	0.42
1:B:35:HIS:HB2	3:B:1269:NAP:C2A	2.50	0.41
2:D:17:ARG:O	2:D:21:VAL:HG23	2.20	0.41
2:C:26:THR:HG22	2:C:26:THR:O	2.21	0.41
2:C:251:TYR:CD2	2:D:232:ALA:HB2	2.56	0.41
2:C:207:SER:O	2:C:208:LEU:C	2.60	0.41
1:B:206[B]:VAL:CG2	1:B:209[B]:LEU:HD21	2.51	0.40
2:C:209:LEU:HD13	2:C:218:LYS:HG2	2.02	0.40
4:C:1270:KTZ:CAA	4:C:1270:KTZ:CAS	3.00	0.40
1:A:29:ARG:HG2	1:A:55:THR:HG22	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)
5:C:2011:HOH:O	5:D:2138:HOH:O[2_656]	2.03	0.17

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	247/288 (86%)	237 (96%)	10 (4%)	0	100	100
1	B	254/288 (88%)	246 (97%)	8 (3%)	0	100	100
2	C	245/288 (85%)	237 (97%)	8 (3%)	0	100	100
2	D	245/288 (85%)	237 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	991/1152 (86%)	957 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	201/231 (87%)	200 (100%)	1 (0%)	88	86
1	B	207/231 (90%)	206 (100%)	1 (0%)	88	86
2	C	199/230 (86%)	197 (99%)	2 (1%)	76	69
2	D	199/230 (86%)	198 (100%)	1 (0%)	88	86
All	All	806/922 (87%)	801 (99%)	5 (1%)	86	83

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	B	101	PRO
2	C	179	HIS
2	C	250	GLN
2	D	152	SER

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

Mol	Chain	Res	Type
1	A	179	HIS
1	B	65	ASN
1	B	166	GLN
1	B	179	HIS
2	C	140	GLN
2	C	179	HIS
2	D	179	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CSX	D	168	2	3,6,7	0.80	0	1,6,8	0.18	0
2	CSX	C	168	2	3,6,7	0.94	0	1,6,8	1.59	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	D	168	2	-	0/1/5/7	-
2	CSX	C	168	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 ⓘ

There are no carbohydrates 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
4	KTZ	A	1270	-	26,28,28	1.35	4 (15%)	29,40,40	2.23	11 (37%)
4	KTZ	D	1270	-	26,28,28	1.52	5 (19%)	29,40,40	2.50	10 (34%)
4	KTZ	B	1270	-	26,28,28	1.30	4 (15%)	29,40,40	2.28	11 (37%)
3	NAP	B	1269	-	45,52,52	1.00	1 (2%)	56,80,80	1.18	5 (8%)
3	NAP	D	1269	-	45,52,52	1.13	4 (8%)	56,80,80	1.27	6 (10%)
3	NAP	A	1269	-	45,52,52	0.95	1 (2%)	56,80,80	1.27	6 (10%)
3	NAP	C	1269	-	45,52,52	0.95	2 (4%)	56,80,80	1.27	7 (12%)
4	KTZ	C	1270	-	26,28,28	1.28	3 (11%)	29,40,40	2.12	9 (31%)

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	KTZ	A	1270	-	-	2/12/12/12	0/4/4/4
4	KTZ	D	1270	-	-	1/12/12/12	0/4/4/4
4	KTZ	B	1270	-	-	6/12/12/12	0/4/4/4
3	NAP	B	1269	-	-	1/31/67/67	0/5/5/5
3	NAP	D	1269	-	-	1/31/67/67	0/5/5/5
3	NAP	A	1269	-	-	1/31/67/67	0/5/5/5
3	NAP	C	1269	-	-	0/31/67/67	0/5/5/5
4	KTZ	C	1270	-	-	4/12/12/12	0/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1270	KTZ	CAV-CAS	4.32	1.55	1.49
3	D	1269	NAP	P2B-O2B	3.82	1.66	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1269	NAP	P2B-O2B	3.71	1.66	1.59
4	A	1270	KTZ	C2-NAC	3.56	1.41	1.33
4	C	1270	KTZ	C2-NAC	3.56	1.41	1.33
4	B	1270	KTZ	C6-N1	3.11	1.36	1.32
3	C	1269	NAP	P2B-O2B	3.09	1.65	1.59
4	C	1270	KTZ	CAV-CAS	2.82	1.53	1.49
4	C	1270	KTZ	C6-N1	2.82	1.36	1.32
4	B	1270	KTZ	CAV-CAS	2.74	1.53	1.49
4	D	1270	KTZ	C2-NAC	2.69	1.39	1.33
4	A	1270	KTZ	CAV-CAS	2.66	1.53	1.49
3	C	1269	NAP	C2A-N3A	2.66	1.36	1.32
3	A	1269	NAP	P2B-O2B	2.65	1.64	1.59
4	B	1270	KTZ	C2-N1	2.60	1.40	1.35
4	B	1270	KTZ	C2-NAC	2.58	1.39	1.33
4	D	1270	KTZ	C2-N1	2.52	1.39	1.35
4	D	1270	KTZ	CAR-CAT	2.48	1.51	1.49
3	D	1269	NAP	C2A-N3A	2.39	1.35	1.32
4	D	1270	KTZ	C6-N1	2.34	1.35	1.32
4	A	1270	KTZ	C6-N1	2.27	1.35	1.32
4	A	1270	KTZ	CAV-C5	2.18	1.46	1.42
3	D	1269	NAP	P2B-O3X	-2.08	1.46	1.54
3	D	1269	NAP	C7N-N7N	2.03	1.36	1.33

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1270	KTZ	N3-C2-N1	-6.27	118.86	127.22
4	C	1270	KTZ	N3-C2-N1	-6.21	118.94	127.22
4	A	1270	KTZ	N3-C2-N1	-5.45	119.95	127.22
4	B	1270	KTZ	C5-C6-N1	-5.22	118.61	124.05
4	D	1270	KTZ	C2-N3-C4	5.11	121.19	115.36
4	B	1270	KTZ	N3-C2-N1	-4.97	120.60	127.22
4	D	1270	KTZ	CAJ-CAR-CAT	4.81	128.22	120.61
4	B	1270	KTZ	CAV-C5-C4	-4.80	103.71	107.54
4	D	1270	KTZ	CAK-CAR-CAT	-4.37	113.67	120.61
4	C	1270	KTZ	C5-C6-N1	-4.36	119.51	124.05
4	D	1270	KTZ	CAV-C5-C4	-4.19	104.20	107.54
3	A	1269	NAP	N3A-C2A-N1A	-4.14	122.20	128.68
3	C	1269	NAP	O7N-C7N-C3N	-3.85	115.02	119.63
4	D	1270	KTZ	C5-C6-N1	-3.75	120.14	124.05
4	A	1270	KTZ	C2-N3-C4	3.73	119.62	115.36
4	A	1270	KTZ	C5-C6-N1	-3.69	120.21	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1269	NAP	N3A-C2A-N1A	-3.68	122.92	128.68
3	A	1269	NAP	C3N-C7N-N7N	3.62	122.10	117.75
4	D	1270	KTZ	CAS-CAV-CAT	-3.51	119.92	126.88
3	C	1269	NAP	N3A-C2A-N1A	-3.51	123.19	128.68
4	C	1270	KTZ	C2-N1-C6	3.48	123.55	113.91
4	A	1270	KTZ	CAV-C5-C4	-3.47	104.77	107.54
4	A	1270	KTZ	CAK-CAR-CAT	-3.43	115.18	120.61
4	A	1270	KTZ	N1-C6-NAY	-3.39	110.32	115.67
4	A	1270	KTZ	CAJ-CAR-CAT	3.38	125.96	120.61
4	B	1270	KTZ	C2-N3-C4	3.24	119.06	115.36
3	D	1269	NAP	O7N-C7N-C3N	-3.21	115.79	119.63
3	D	1269	NAP	C3N-C7N-N7N	3.19	121.58	117.75
3	B	1269	NAP	N3A-C2A-N1A	-3.18	123.70	128.68
3	B	1269	NAP	C4A-C5A-N7A	-3.15	106.11	109.40
3	A	1269	NAP	C1B-N9A-C4A	-3.12	121.15	126.64
4	C	1270	KTZ	CAS-CAV-CAT	-3.12	120.69	126.88
4	C	1270	KTZ	CAV-C5-C4	-3.12	105.05	107.54
4	A	1270	KTZ	CAS-CAV-CAT	-3.09	120.75	126.88
3	D	1269	NAP	C1B-N9A-C4A	-3.08	121.23	126.64
4	B	1270	KTZ	CAK-CAR-CAT	-3.08	115.73	120.61
3	C	1269	NAP	C3N-C7N-N7N	2.97	121.31	117.75
4	B	1270	KTZ	NAC-C2-N1	2.95	121.85	117.25
4	C	1270	KTZ	C2-N3-C4	2.91	118.69	115.36
3	C	1269	NAP	C1B-N9A-C4A	-2.88	121.59	126.64
3	A	1269	NAP	O7N-C7N-C3N	-2.84	116.23	119.63
4	B	1270	KTZ	CAS-CAV-CAT	-2.84	121.24	126.88
4	B	1270	KTZ	CAJ-CAR-CAT	2.75	124.96	120.61
4	B	1270	KTZ	C2-N1-C6	2.69	121.38	113.91
4	C	1270	KTZ	NAC-C2-N3	2.67	122.15	117.79
4	A	1270	KTZ	C2-N1-C6	2.66	121.29	113.91
3	C	1269	NAP	PN-O3-PA	-2.66	123.70	132.83
3	C	1269	NAP	O4D-C1D-C2D	-2.65	103.06	106.93
4	C	1270	KTZ	CAK-CAR-CAT	-2.65	116.41	120.61
3	B	1269	NAP	C5A-C6A-N6A	2.63	124.35	120.35
4	D	1270	KTZ	C2-N1-C6	2.55	120.99	113.91
4	B	1270	KTZ	CAM-CAS-CAV	-2.53	116.93	120.77
3	D	1269	NAP	N6A-C6A-N1A	2.51	123.78	118.57
3	B	1269	NAP	C2A-N1A-C6A	2.45	122.95	118.75
3	A	1269	NAP	O2A-PA-O1A	2.26	123.41	112.24
4	B	1270	KTZ	CAL-CAS-CAV	2.24	124.16	120.77
4	A	1270	KTZ	CAM-CAS-CAV	-2.23	117.38	120.77
3	B	1269	NAP	O4B-C4B-C3B	-2.23	100.70	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1270	KTZ	N1-C6-NAY	-2.21	112.20	115.67
4	C	1270	KTZ	CAJ-CAR-CAT	2.18	124.07	120.61
3	D	1269	NAP	C5A-C6A-N6A	-2.08	117.19	120.35
4	A	1270	KTZ	CAL-CAS-CAV	2.07	123.91	120.77
4	D	1270	KTZ	NAC-C2-N1	2.03	120.41	117.25
3	C	1269	NAP	O2N-PN-O1N	2.02	122.23	112.24
3	A	1269	NAP	C2A-N1A-C6A	2.01	122.18	118.75

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1270	KTZ	C5-C6-NAY-CAB
4	B	1270	KTZ	CAL-CAS-CAV-C5
4	B	1270	KTZ	CAM-CAS-CAV-C5
4	B	1270	KTZ	C5-C6-NAY-CAA
4	C	1270	KTZ	CAL-CAS-CAV-C5
4	C	1270	KTZ	CAM-CAS-CAV-C5
4	A	1270	KTZ	C5-C6-NAY-CAB
4	C	1270	KTZ	C5-C6-NAY-CAA
3	D	1269	NAP	C3B-C2B-O2B-P2B
4	B	1270	KTZ	CAM-CAS-CAV-CAT
4	A	1270	KTZ	C5-C6-NAY-CAA
4	C	1270	KTZ	C5-C6-NAY-CAB
4	B	1270	KTZ	CAL-CAS-CAV-CAT
3	B	1269	NAP	C3B-C2B-O2B-P2B
3	A	1269	NAP	C3B-C2B-O2B-P2B
4	B	1270	KTZ	C5-C6-NAY-CAB

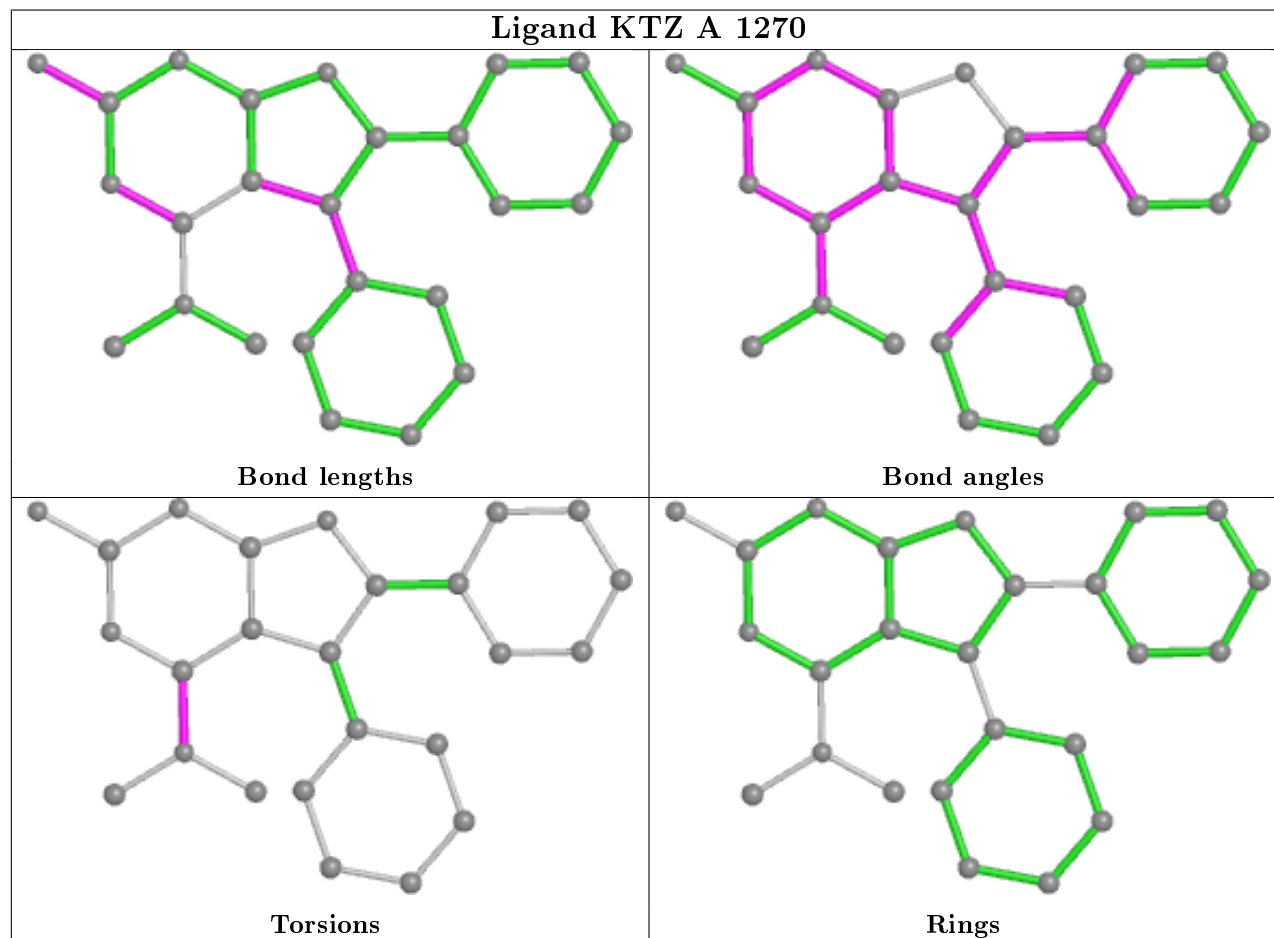
There are no ring outliers.

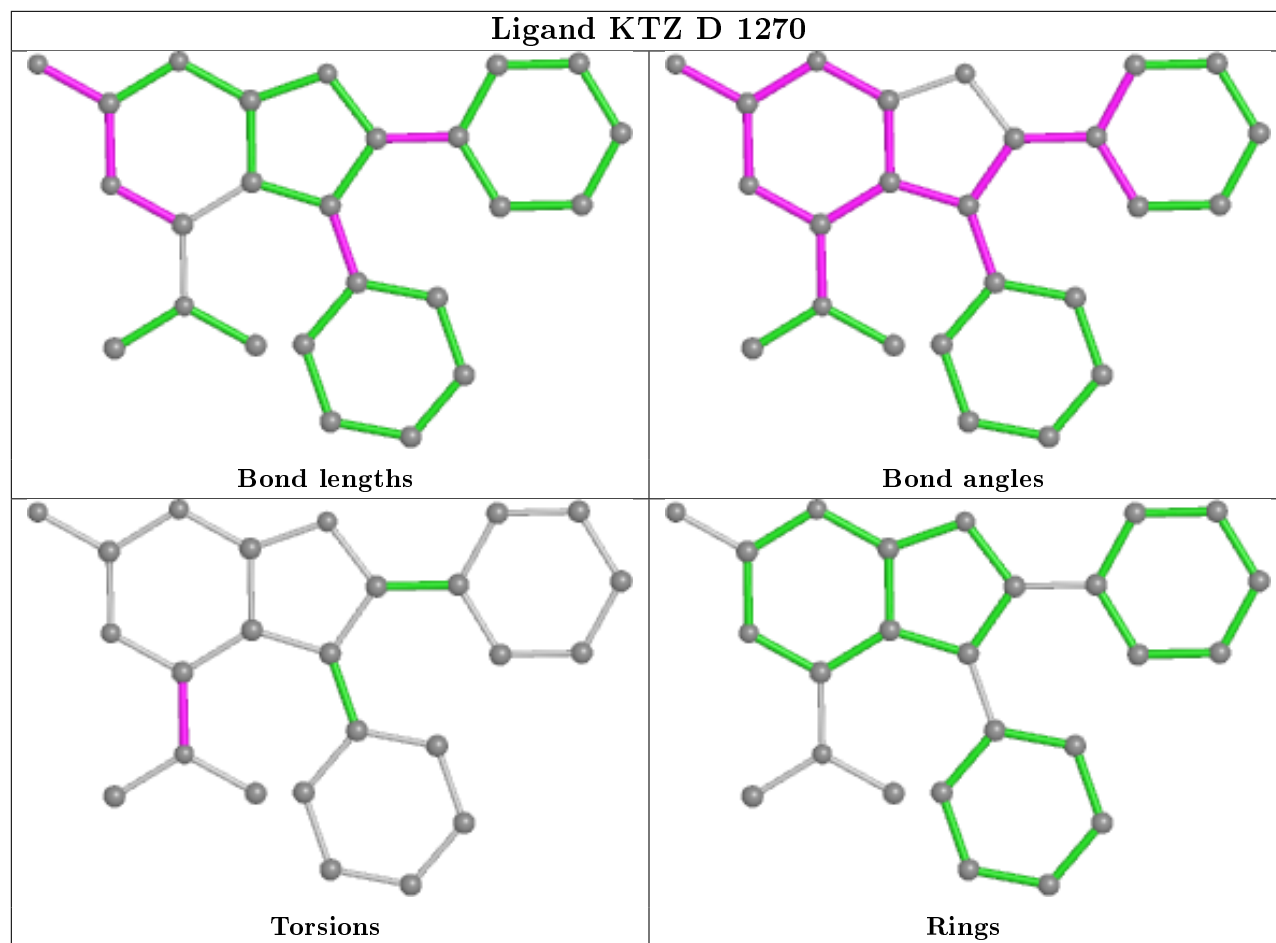
5 monomers are involved in 16 short contacts:

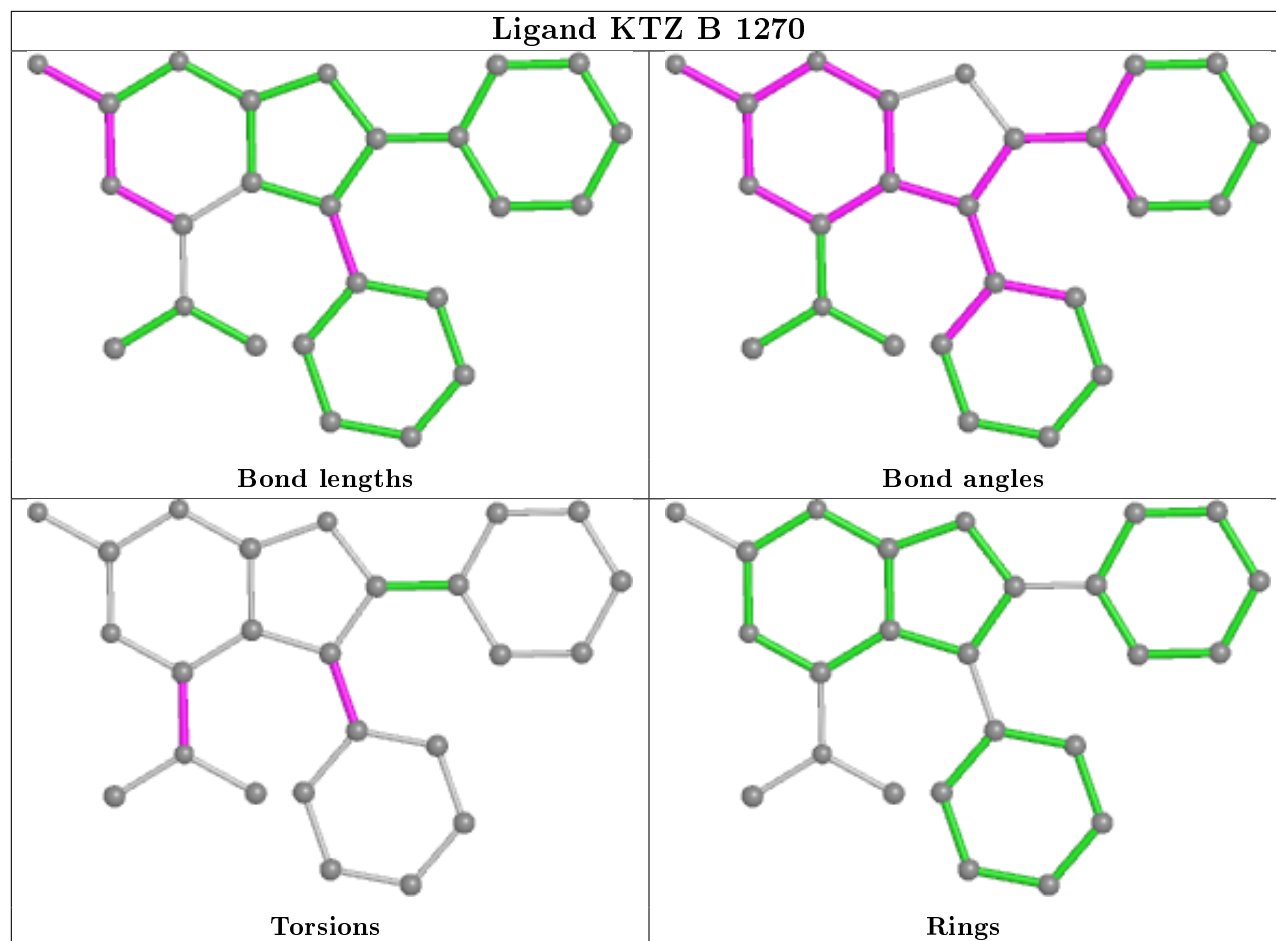
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1270	KTZ	3	0
4	D	1270	KTZ	3	0
4	B	1270	KTZ	4	0
3	B	1269	NAP	2	0
4	C	1270	KTZ	5	0

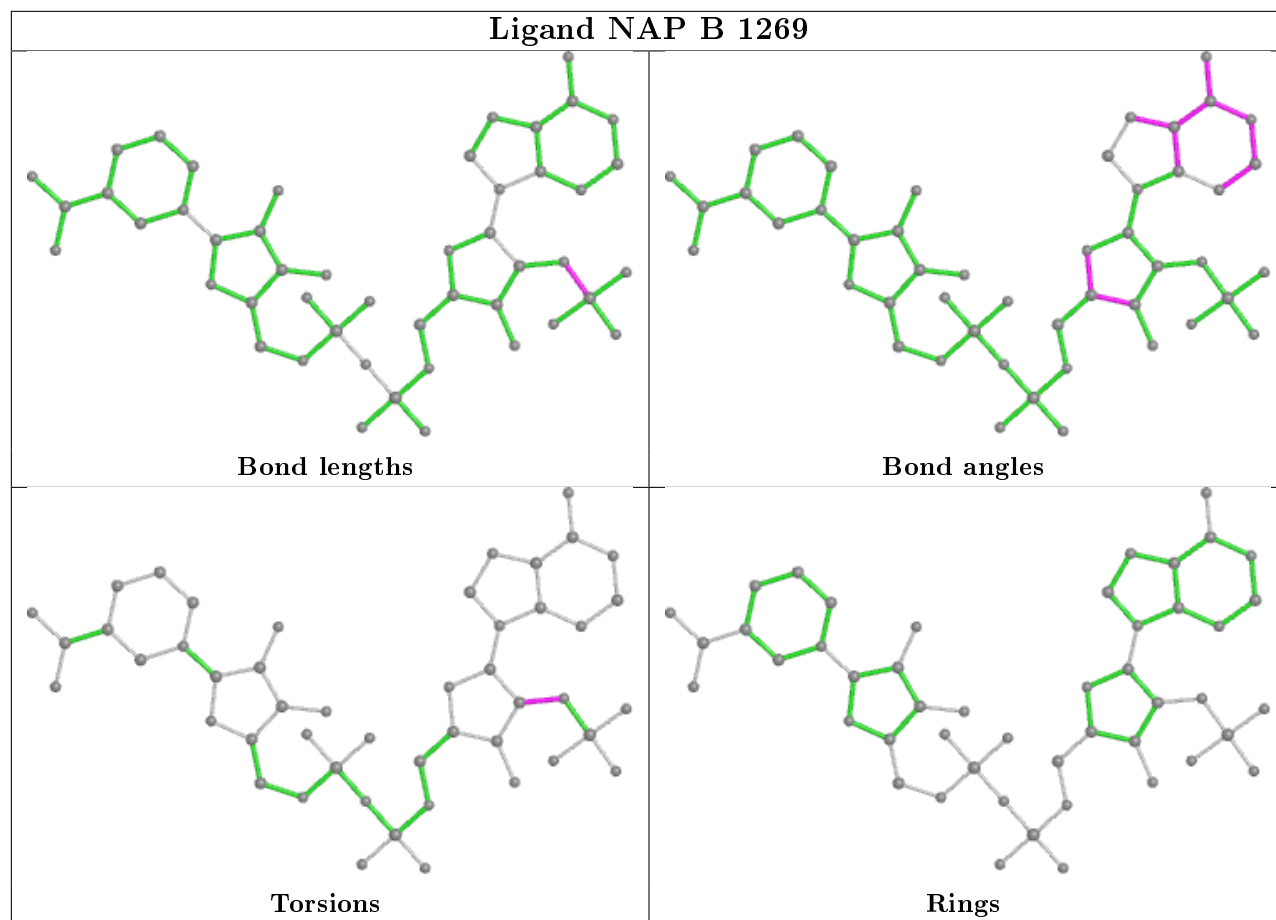
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

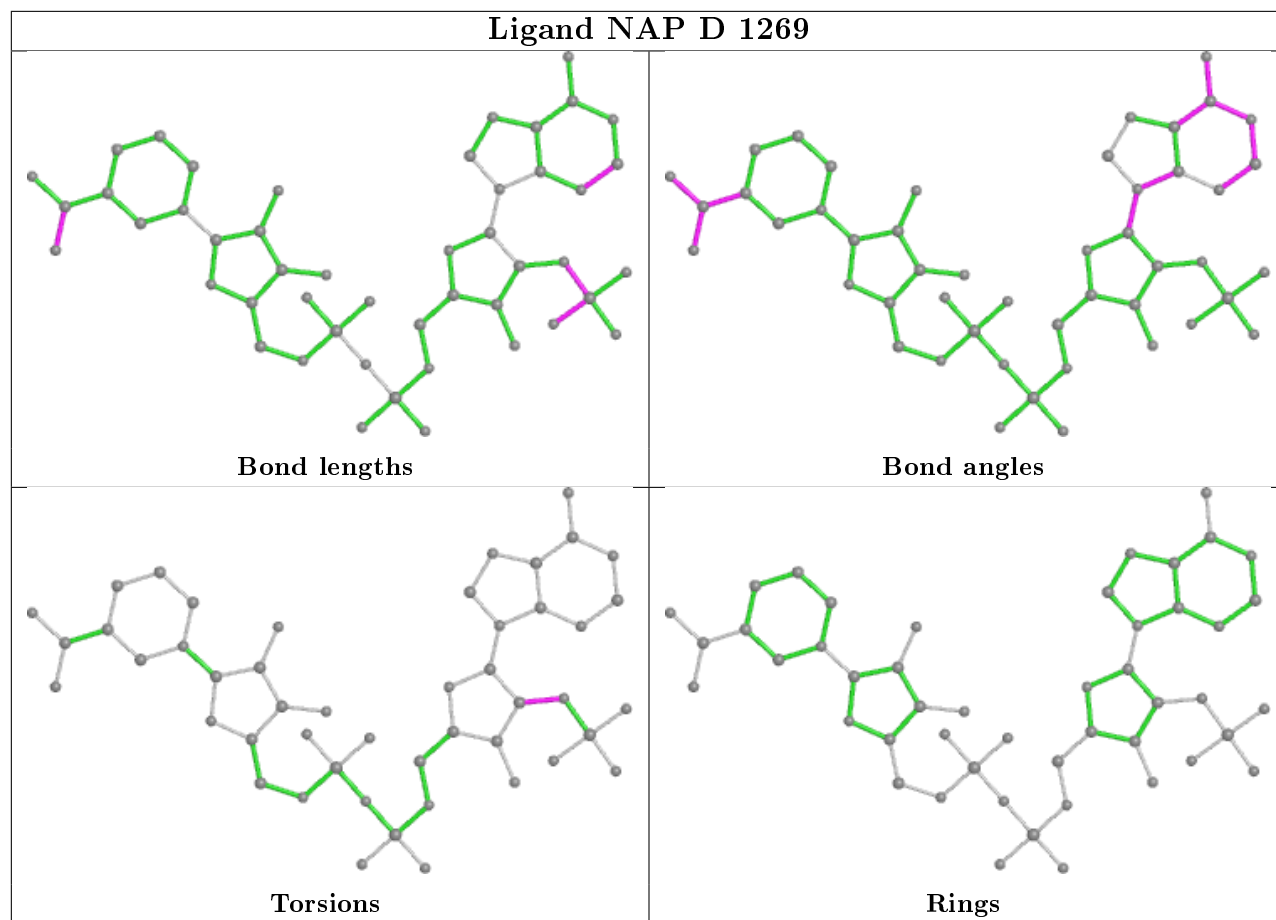
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

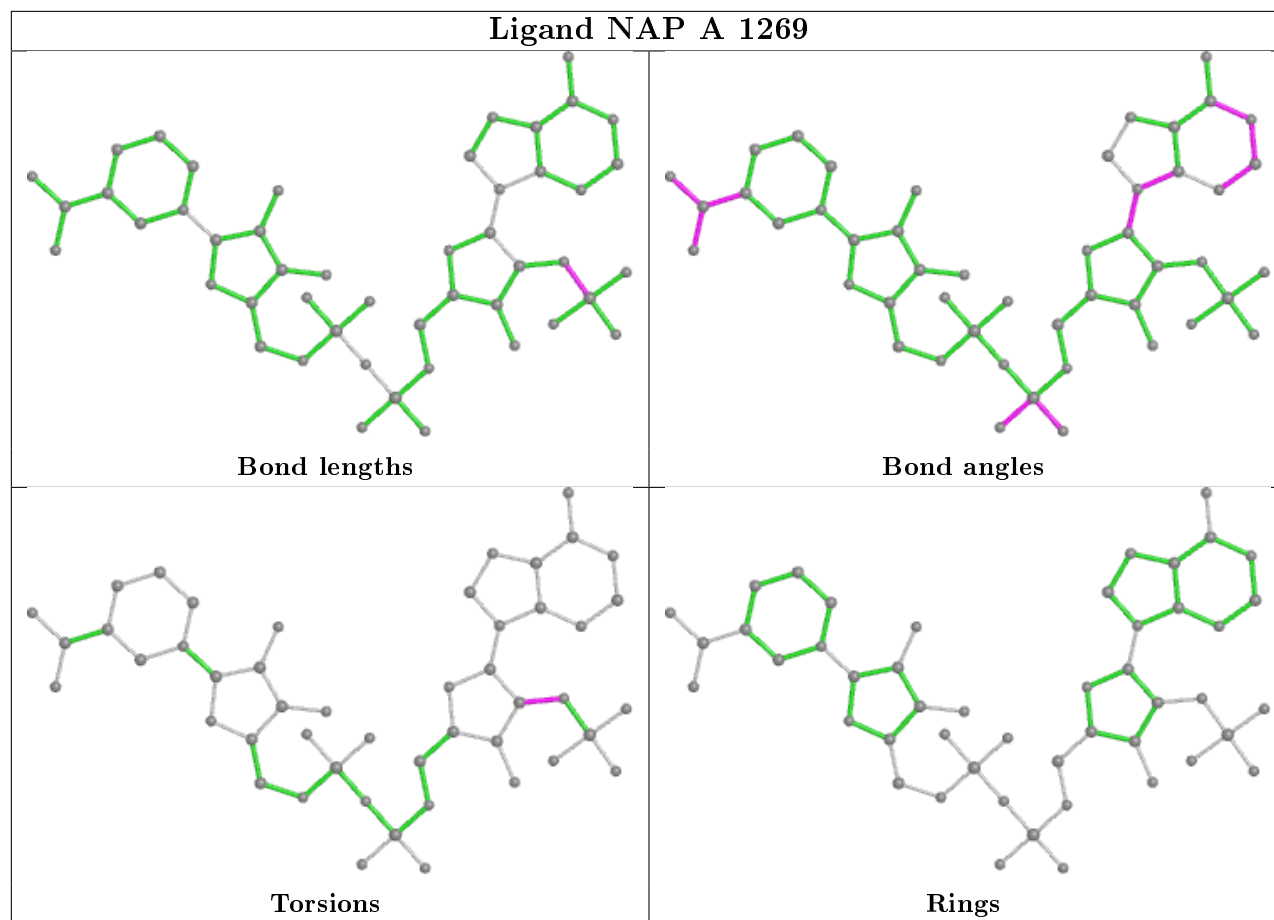


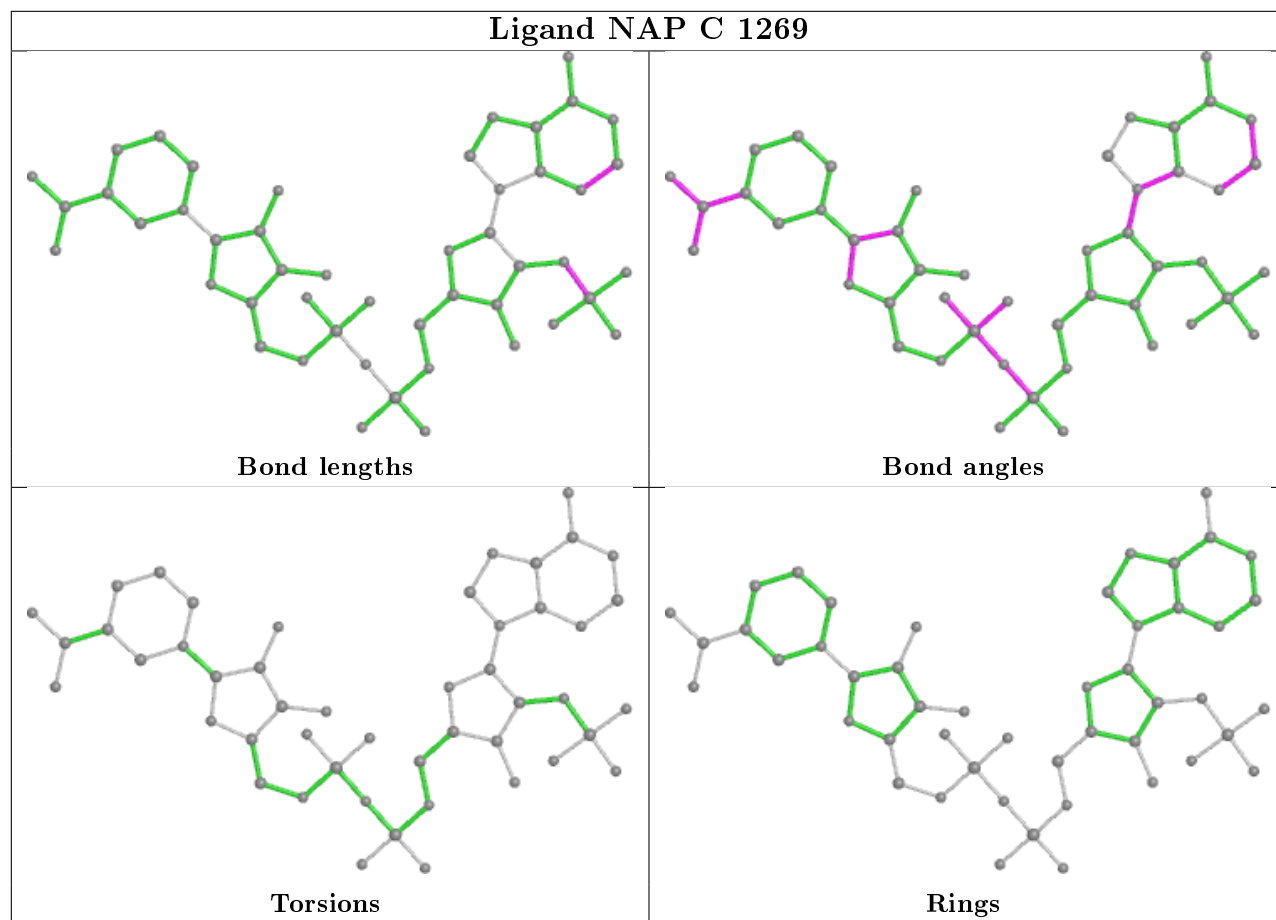


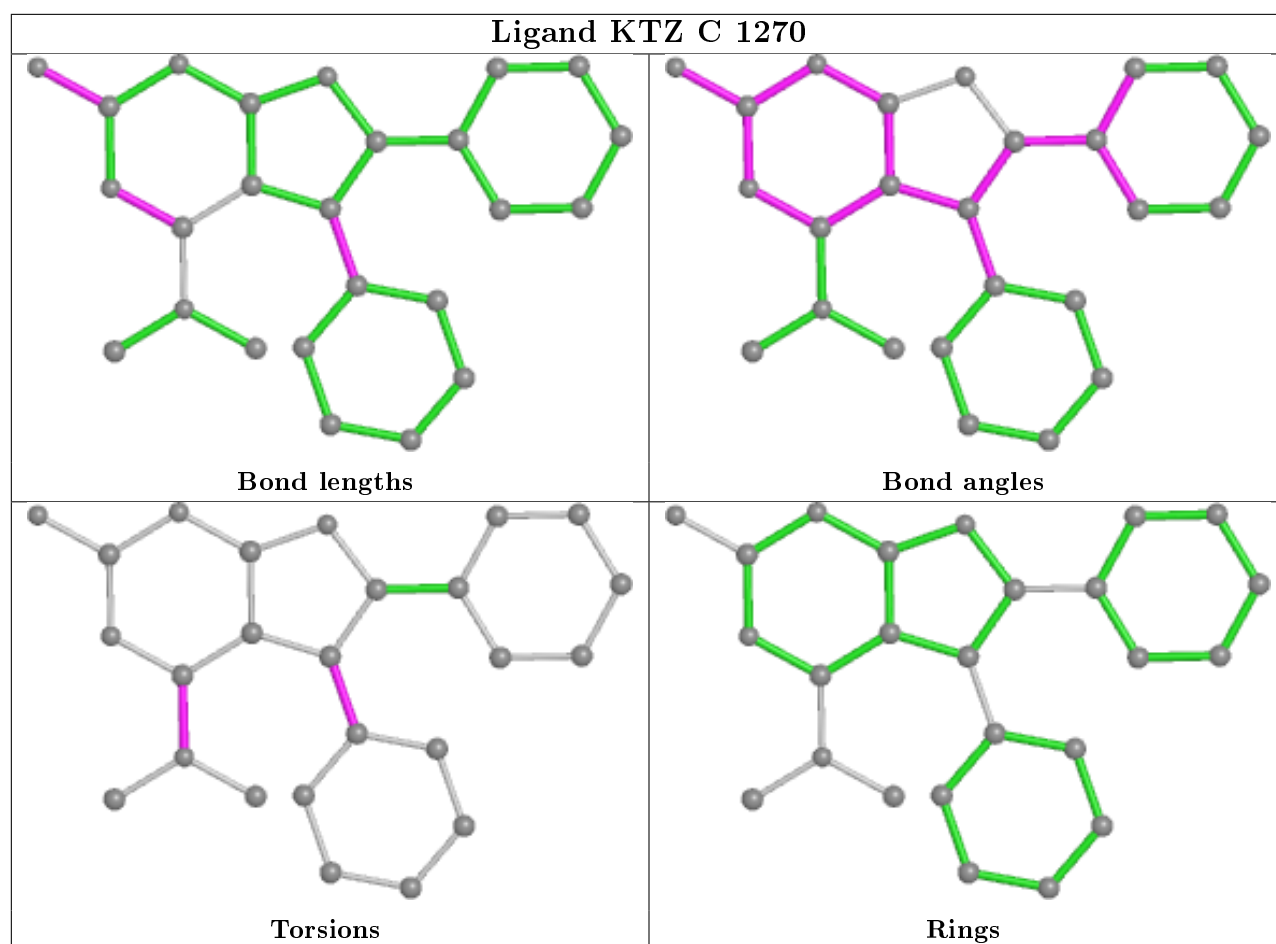












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	249/288 (86%)	-0.37	4 (1%) 72 72	6, 12, 29, 50	0
1	B	249/288 (86%)	-0.29	4 (1%) 72 72	7, 12, 29, 47	0
2	C	249/288 (86%)	-0.17	9 (3%) 42 40	7, 15, 36, 52	0
2	D	248/288 (86%)	-0.31	3 (1%) 79 79	7, 15, 31, 46	0
All	All	995/1152 (86%)	-0.29	20 (2%) 65 64	6, 14, 31, 52	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	113	GLY	4.2
2	D	113	GLY	4.1
2	C	151	SER	3.9
1	B	113	GLY	3.3
1	B	211[A]	VAL	3.3
1	B	212[A]	ALA	3.2
1	A	152	SER	3.2
2	C	113	GLY	3.1
2	C	212	ALA	2.9
2	D	152	SER	2.8
2	C	211	VAL	2.8
1	A	211	VAL	2.7
2	C	2	GLU	2.7
2	D	211	VAL	2.6
2	C	216	GLU	2.4
2	C	152	SER	2.4
1	B	50	LYS	2.3
1	A	2	GLU	2.3
2	C	223	ARG	2.1
2	C	55	THR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CSX	C	168	7/8	0.94	0.11	14,18,30,34	0
2	CSX	D	168	7/8	0.95	0.09	16,19,34,35	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

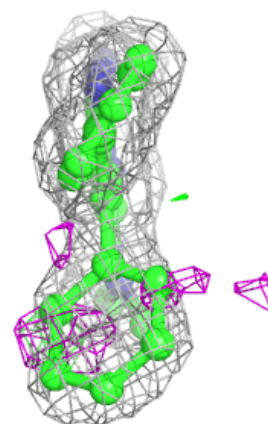
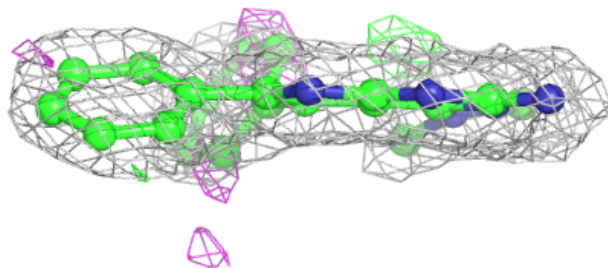
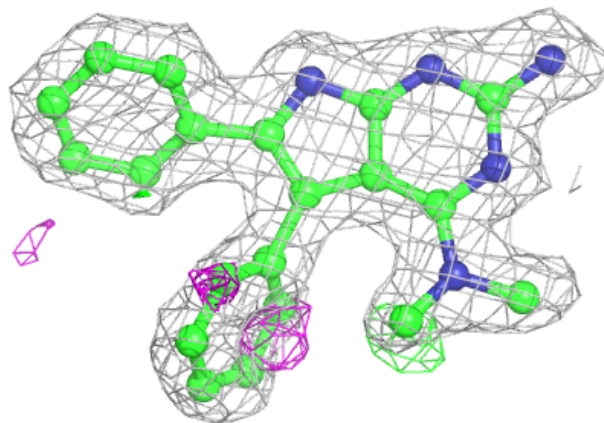
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	KTZ	D	1270	25/25	0.94	0.11	11,15,21,21	0
4	KTZ	C	1270	25/25	0.94	0.11	12,18,25,26	0
4	KTZ	B	1270	25/25	0.95	0.09	10,15,20,22	0
4	KTZ	A	1270	25/25	0.96	0.09	9,12,15,16	0
3	NAP	A	1269	48/48	0.98	0.06	7,10,11,12	0
3	NAP	C	1269	48/48	0.98	0.07	9,11,14,17	0
3	NAP	D	1269	48/48	0.98	0.07	9,11,13,13	0
3	NAP	B	1269	48/48	0.99	0.06	8,10,13,17	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.

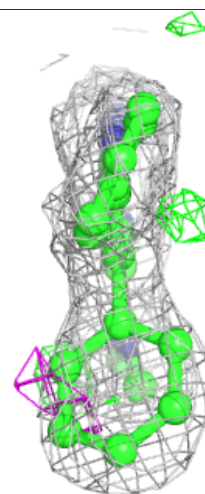
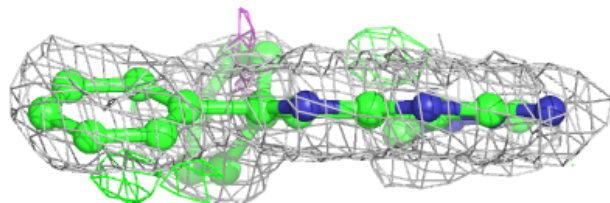
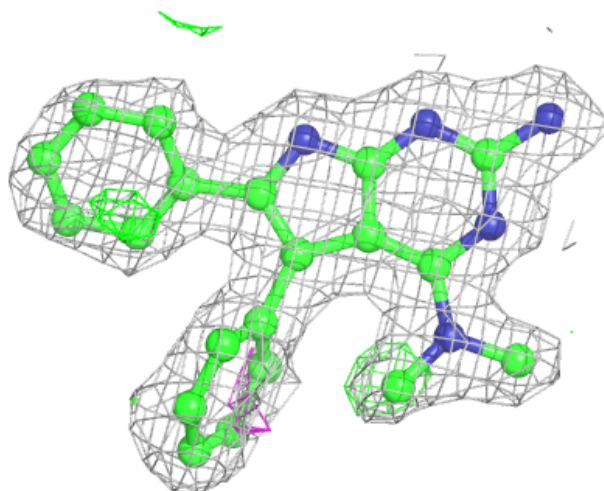
Electron density around KTZ D 1270:

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



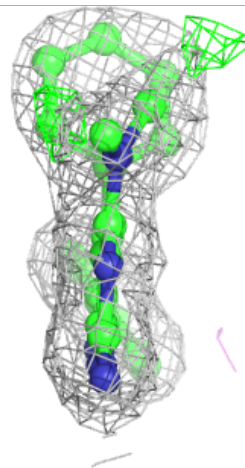
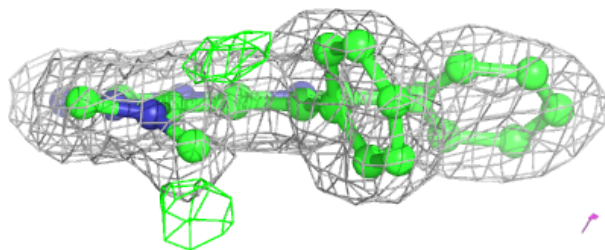
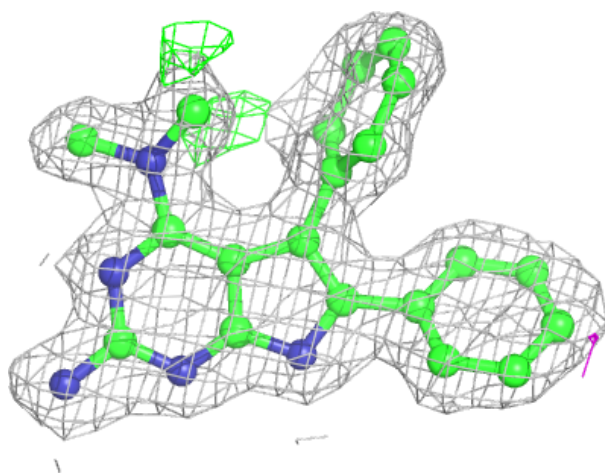
Electron density around KTZ C 1270:

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



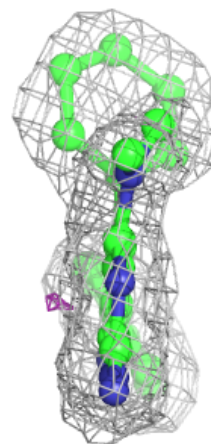
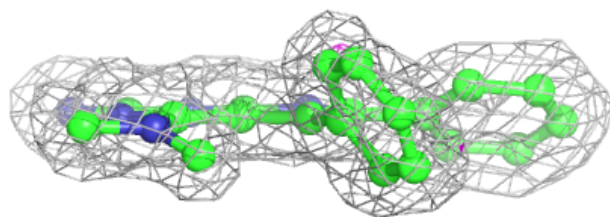
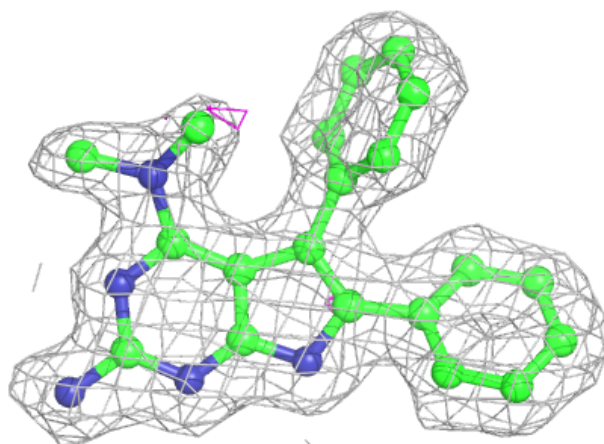
Electron density around KTZ B 1270:

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



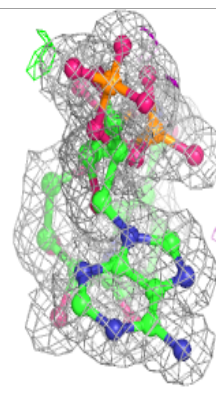
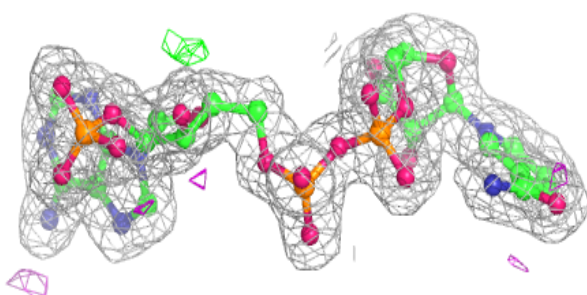
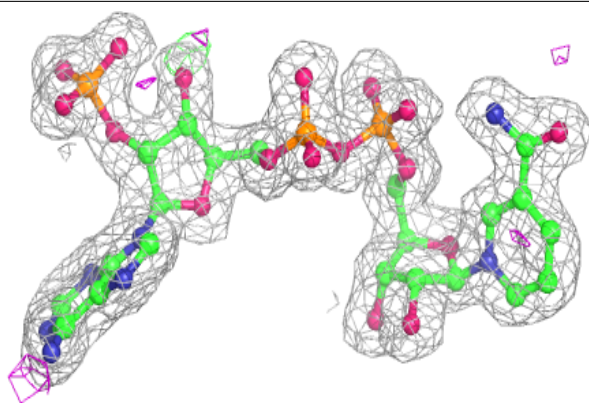
Electron density around KTZ A 1270:

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

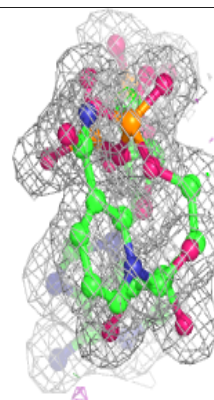
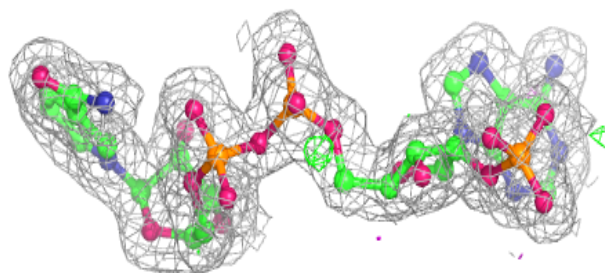
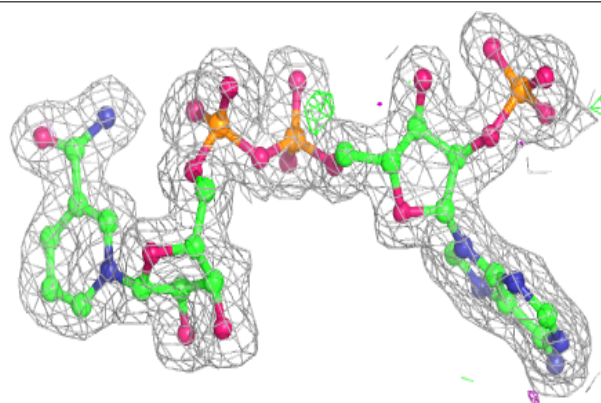


Electron density around NAP A 1269:

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

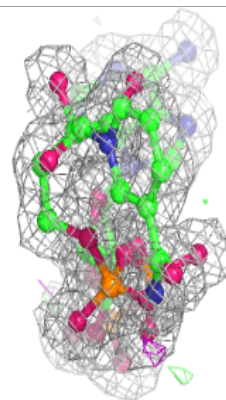
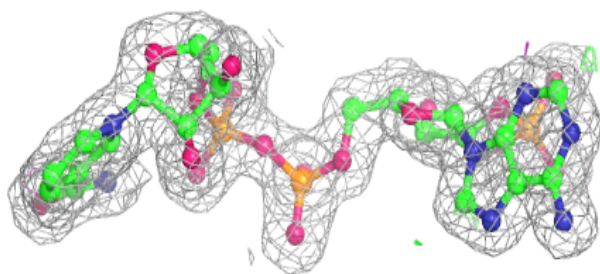
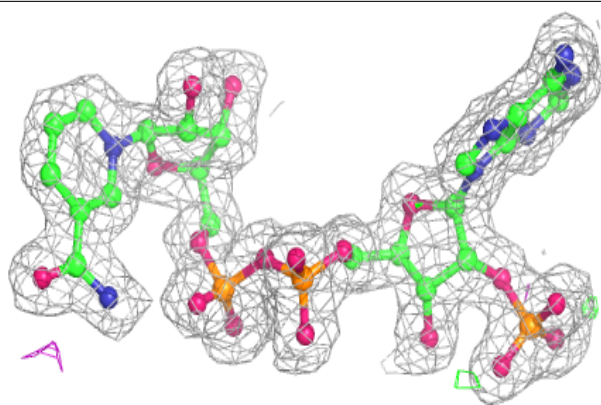
**Electron density around NAP C 1269:**

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

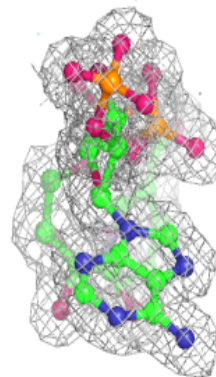
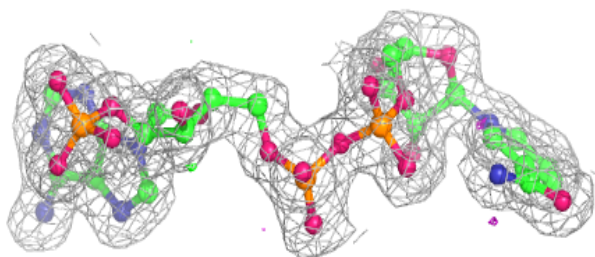
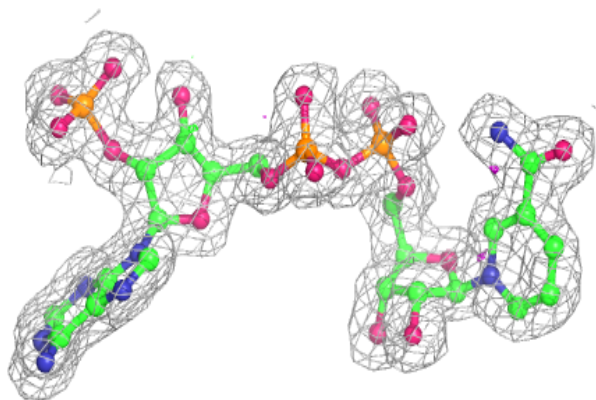


Electron density around NAP D 1269:

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

**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.