



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 01:58 am BST

PDB ID : 3JQC
Title : Crystal structure of pteridine reductase 1 (PTR1) from Trypanosoma brucei in ternary complex with cofactor (NADP+) and inhibitor 2-amino-6-bromo-4-oxo-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidine-5-carbonitrile (JU2)
Authors : Tulloch, L.B.; Hunter, W.N.
Deposited on : 2009-09-06
Resolution : 1.80 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

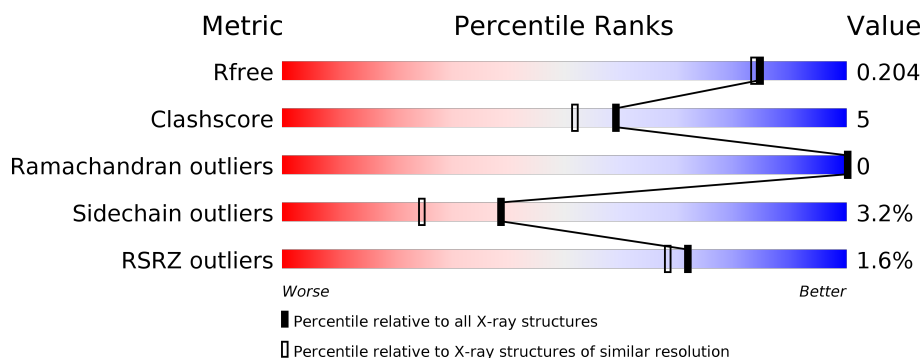
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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>%</div> <div> <div></div> <div>79%</div> <div>7%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	288	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>11%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	288	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>10%</div> <div>•</div> <div>13%</div> </div> </div>
1	D	288	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>10%</div> <div>•</div> <div>14%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8546 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	6	0
			1871	1179	328	353	11			
1	B	250	Total	C	N	O	S	0	12	0
			1901	1196	334	360	11			
1	C	250	Total	C	N	O	S	0	14	0
			1907	1199	334	362	12			
1	D	249	Total	C	N	O	S	0	11	0
			1888	1188	333	356	11			

There are 80 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

Continued on next page...

Continued from previous page...

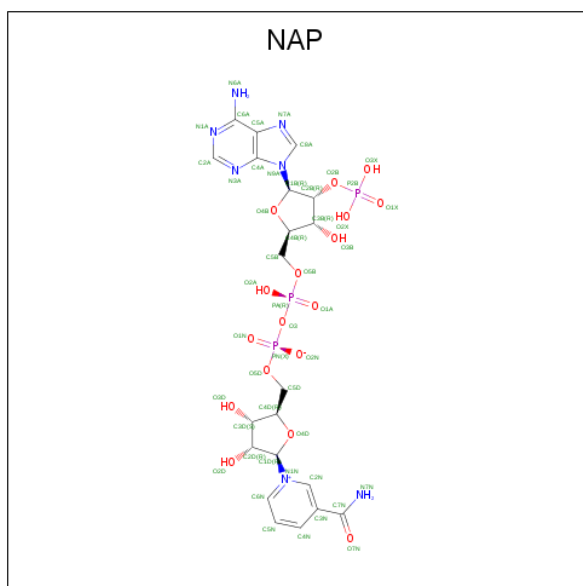
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	EXPRESSION TAG	UNP Q581W1
B	-17	SER	-	EXPRESSION TAG	UNP Q581W1
B	-16	SER	-	EXPRESSION TAG	UNP Q581W1
B	-15	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-14	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-13	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-12	HIS	-	EXPRESSION TAG	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
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
D	-19	MET	-	EXPRESSION TAG	UNP Q581W1
D	-18	GLY	-	EXPRESSION TAG	UNP Q581W1
D	-17	SER	-	EXPRESSION TAG	UNP Q581W1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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 NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $\text{C}_{21}\text{H}_{28}\text{N}_7\text{O}_{17}\text{P}_3$).



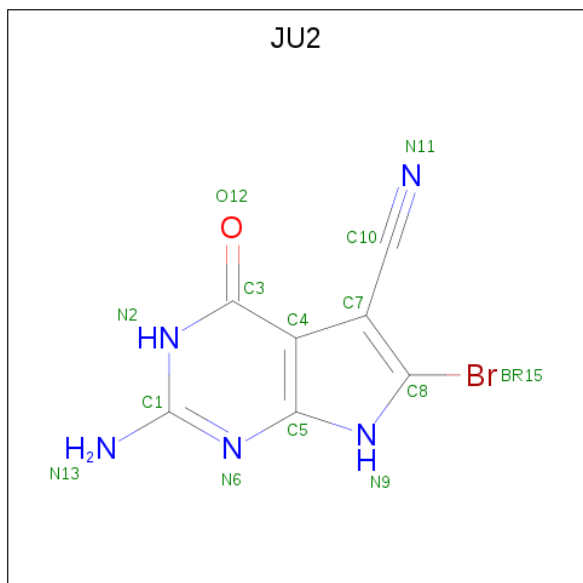
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 3 is 2-amino-6-bromo-4-oxo-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidine-5-carbonitrile (three-letter code: JU2) (formula: C₇H₄BrN₅O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	0	0
			14	1	7	5	1		
3	B	1	Total	Br	C	N	O	0	0
			14	1	7	5	1		
3	C	1	Total	Br	C	N	O	0	0
			14	1	7	5	1		
3	D	1	Total	Br	C	N	O	0	0
			14	1	7	5	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	190	Total	O	0	0
			190	190		
4	B	183	Total	O	0	0
			183	183		
4	C	187	Total	O	0	0
			187	187		

Continued on next page...

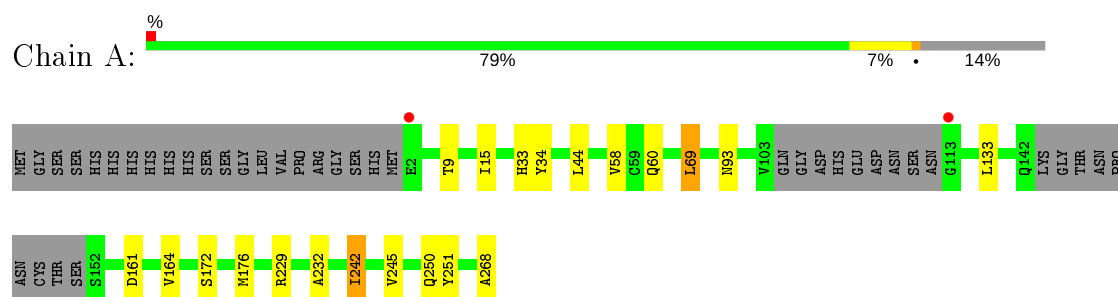
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	171	Total	O	0	0
			171	171		

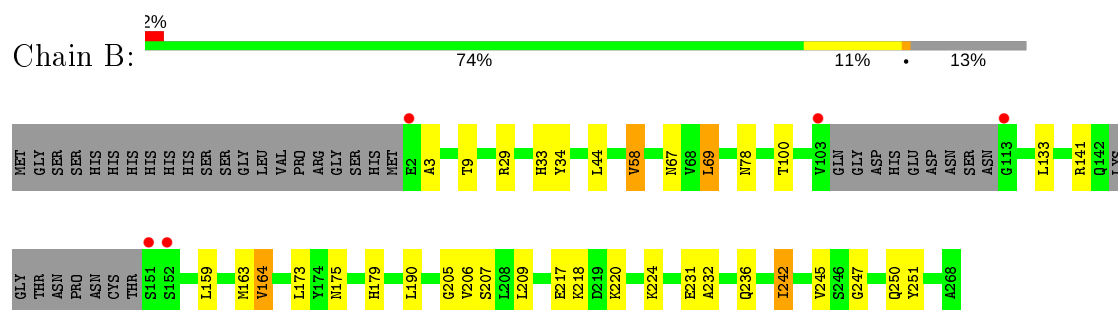
3 Residue-property plots

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.

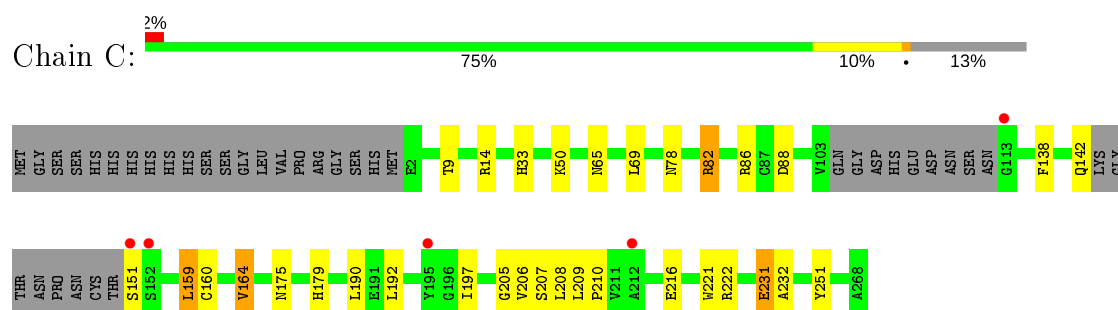
• Molecule 1: Pteridine reductase 1



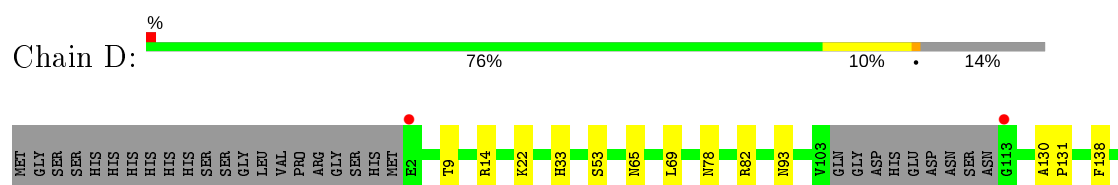
• Molecule 1: Pteridine reductase 1

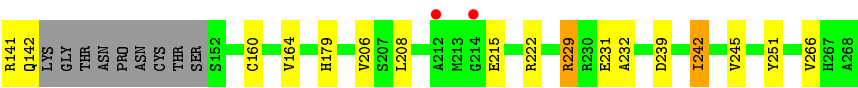


• Molecule 1: Pteridine reductase 1



• Molecule 1: Pteridine reductase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.86 Å 89.11 Å 84.25 Å 90.00° 116.08° 90.00°	Depositor
Resolution (Å)	27.65 – 1.80 27.65 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.8 (27.65-1.80) 92.8 (27.65-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.80 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.168 , 0.204 0.169 , 0.204	Depositor DCC
R_{free} test set	4262 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.849	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8546	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.14% 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: JU2, NAP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/1910	0.54	0/2590
1	B	0.41	0/1943	0.57	0/2635
1	C	0.43	0/1943	0.57	1/2637 (0.0%)
1	D	0.41	0/1927	0.52	0/2614
All	All	0.42	0/7723	0.55	1/10476 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	159	LEU	CA-CB-CG	-5.16	103.44	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	1871	0	1911	13	0
1	B	1901	0	1937	21	0
1	C	1907	0	1938	25	0
1	D	1888	0	1924	21	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	48	0	25	1	0
2	D	48	0	25	0	0
3	A	14	0	4	0	0
3	B	14	0	4	0	0
3	C	14	0	4	1	0
3	D	14	0	4	0	0
4	A	190	0	0	0	1
4	B	183	0	0	1	0
4	C	187	0	0	4	0
4	D	171	0	0	6	1
All	All	8546	0	7826	73	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 (73) 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:D:231:GLU:HB2	4:D:711:HOH:O	1.26	1.30
1:C:82:ARG:HG2	1:C:82:ARG:HH21	1.32	0.94
1:D:206:VAL:HG12	4:D:711:HOH:O	1.68	0.92
1:B:207:SER:O	1:B:231[A]:GLU:HB2	1.79	0.83
1:A:34:TYR:HE2	1:A:58:VAL:HG13	1.49	0.76
1:B:34[A]:TYR:HE2	1:B:58:VAL:HG13	1.52	0.74
1:C:207[A]:SER:O	1:C:231:GLU:HB3	1.89	0.72
1:D:164:VAL:HG22	1:D:179:HIS:CD2	2.27	0.69
1:D:231:GLU:CB	4:D:711:HOH:O	2.04	0.67
1:C:82:ARG:CG	1:C:82:ARG:HH21	2.07	0.66
1:B:205:GLY:O	2:B:269:NAP:H4N	1.96	0.65
1:C:222:ARG:HE	1:C:231:GLU:CD	2.01	0.64
1:C:151:SER:N	4:C:598:HOH:O	2.32	0.63
1:C:205[A]:GLY:O	2:C:269:NAP:H4N	1.99	0.62
1:B:164:VAL:HG22	1:B:179:HIS:CD2	2.35	0.62
1:C:206[A]:VAL:HG22	4:C:372:HOH:O	2.00	0.61
1:B:207:SER:O	1:B:231[B]:GLU:HB3	2.02	0.59
1:D:206:VAL:C	4:D:711:HOH:O	2.39	0.59
1:D:222:ARG:HD3	1:D:231:GLU:OE2	2.04	0.57
1:B:247:GLY:O	1:B:250:GLN:HG2	2.07	0.55
1:B:9:THR:HA	1:B:33:HIS:HB3	1.89	0.55
1:C:9:THR:HA	1:C:33:HIS:HB3	1.89	0.55
1:A:9:THR:HA	1:A:33:HIS:HB3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:VAL:HG22	1:C:179:HIS:CD2	2.42	0.55
1:D:22:LYS:HE2	1:D:239:ASP:OD1	2.06	0.55
1:A:69:LEU:HD13	1:A:133:LEU:HD12	1.89	0.54
1:D:9:THR:HA	1:D:33:HIS:HB3	1.90	0.53
1:B:209:LEU:HD13	1:B:218:LYS:HA	1.90	0.52
1:C:78[B]:ASN:HD21	1:C:82:ARG:CZ	2.24	0.51
1:D:229:ARG:NH2	4:D:513:HOH:O	2.45	0.50
1:A:250:GLN:HG3	1:B:236:GLN:HE21	1.78	0.49
1:A:9:THR:O	1:A:93:ASN:HB3	2.11	0.49
1:C:210:PRO:HD3	3:C:270:JU2:N11	2.28	0.48
1:C:65:ASN:HA	1:C:69:LEU:HD22	1.94	0.48
1:A:34:TYR:CE2	1:A:58:VAL:HG13	2.39	0.48
1:B:67:ASN:HB2	4:B:360:HOH:O	2.13	0.48
1:B:242[A]:ILE:HA	1:B:245:VAL:HG22	1.97	0.47
1:C:86:ARG:HD3	1:C:88:ASP:OD1	2.14	0.47
1:C:82:ARG:NH2	1:C:82:ARG:CG	2.72	0.47
1:A:251:TYR:CE2	1:B:232:ALA:HB2	2.50	0.47
1:A:232:ALA:HB2	1:B:251:TYR:CE2	2.50	0.47
1:C:232:ALA:HB2	1:D:251:TYR:CE2	2.50	0.46
1:A:172:SER:O	1:A:176:MET:HG3	2.15	0.46
1:B:163:MET:HG3	1:B:206:VAL:HG23	1.98	0.45
1:C:231:GLU:HG2	4:C:373:HOH:O	2.16	0.45
1:D:78:ASN:OD1	1:D:141:ARG:NH1	2.49	0.45
1:D:242:ILE:HA	1:D:245:VAL:HG22	1.98	0.45
1:D:65:ASN:HA	1:D:69:LEU:HD22	1.97	0.45
1:B:69:LEU:HD13	1:B:133:LEU:HD12	1.99	0.45
1:B:220:LYS:O	1:B:224:LYS:HE2	2.17	0.44
1:D:130:ALA:HB3	1:D:131:PRO:HD3	1.99	0.44
1:C:232:ALA:HB2	1:D:251:TYR:CD2	2.53	0.44
1:A:242:ILE:HA	1:A:245:VAL:HG22	1.99	0.44
1:C:209[A]:LEU:HA	1:C:210:PRO:HD3	1.81	0.44
1:C:251:TYR:CE2	1:D:232:ALA:HB2	2.53	0.44
1:D:14:ARG:NH2	1:D:208:LEU:O	2.51	0.43
1:C:160:CYS:HB3	4:C:347:HOH:O	2.19	0.43
1:A:268:ALA:HB2	1:D:266:VAL:HB	1.99	0.43
1:A:15:ILE:HB	2:A:269:NAP:H51N	2.00	0.43
1:B:220:LYS:O	1:B:224:LYS:HG3	2.20	0.42
1:B:164:VAL:HA	1:B:175:ASN:HD21	1.84	0.42
1:C:164:VAL:HA	1:C:175:ASN:HD21	1.83	0.42
1:D:9:THR:O	1:D:93:ASN:HB3	2.19	0.42
1:A:161:ASP:HB3	1:A:164:VAL:HG13	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ALA:O	1:B:29:ARG:NH2	2.52	0.42
1:C:138:PHE:O	1:C:142:GLN:HG2	2.20	0.42
1:B:78[A]:ASN:OD1	1:B:141:ARG:NH2	2.53	0.41
1:D:160:CYS:HB3	4:D:302:HOH:O	2.20	0.41
1:B:100:THR:HG21	1:B:173:LEU:HD12	2.03	0.41
1:D:138:PHE:O	1:D:142:GLN:HG2	2.21	0.40
1:C:206[A]:VAL:HG21	1:C:221:TRP:CZ3	2.56	0.40
1:C:192:LEU:HB3	1:C:197:ILE:HB	2.04	0.40
1:C:14:ARG:NH2	1:C:208[B]:LEU:O	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:336:HOH:O	4:D:337:HOH:O[1_655]	2.19	0.01

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	251/288 (87%)	245 (98%)	6 (2%)	0	100	100
1	C	252/288 (88%)	241 (96%)	11 (4%)	0	100	100
1	D	249/288 (86%)	240 (96%)	9 (4%)	0	100	100
All	All	999/1152 (87%)	963 (96%)	36 (4%)	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%)	196 (98%)	5 (2%)	47	34
1	B	205/231 (89%)	195 (95%)	10 (5%)	25	11
1	C	205/231 (89%)	198 (97%)	7 (3%)	37	22
1	D	203/231 (88%)	198 (98%)	5 (2%)	47	34
All	All	814/924 (88%)	787 (97%)	27 (3%)	39	23

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

Mol	Chain	Res	Type
1	A	44	LEU
1	A	60	GLN
1	A	69	LEU
1	A	229	ARG
1	A	242	ILE
1	B	44	LEU
1	B	58	VAL
1	B	69	LEU
1	B	159[A]	LEU
1	B	159[B]	LEU
1	B	164	VAL
1	B	190	LEU
1	B	217	GLU
1	B	242[A]	ILE
1	B	242[B]	ILE
1	C	50	LYS
1	C	82	ARG
1	C	159	LEU
1	C	164	VAL
1	C	190	LEU
1	C	216	GLU
1	C	231	GLU
1	D	53	SER
1	D	82	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	215	GLU
1	D	229	ARG
1	D	242	ILE

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

Mol	Chain	Res	Type
1	A	60	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
1	C	35	HIS
1	C	175	ASN
1	C	186	GLN
1	D	67[A]	ASN
1	D	166	GLN
1	D	175	ASN
1	D	179	HIS
1	D	186	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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
3	JU2	A	270	-	12,15,15	2.97	4 (33%)	9,22,22	4.56	5 (55%)
3	JU2	B	270	-	12,15,15	2.97	4 (33%)	9,22,22	4.66	5 (55%)
3	JU2	D	270	-	12,15,15	2.99	4 (33%)	9,22,22	4.57	5 (55%)
2	NAP	C	269	-	45,52,52	1.66	3 (6%)	56,80,80	1.23	3 (5%)
2	NAP	A	269	-	45,52,52	1.64	4 (8%)	56,80,80	1.18	3 (5%)
2	NAP	D	269	-	45,52,52	1.67	4 (8%)	56,80,80	1.07	2 (3%)
2	NAP	B	269	-	45,52,52	1.68	3 (6%)	56,80,80	1.16	4 (7%)
3	JU2	C	270	-	12,15,15	3.08	4 (33%)	9,22,22	4.39	5 (55%)

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	JU2	A	270	-	-	0/0/2/2	0/2/2/2
3	JU2	B	270	-	-	0/0/2/2	0/2/2/2
3	JU2	D	270	-	-	0/0/2/2	0/2/2/2
2	NAP	C	269	-	-	1/31/67/67	0/5/5/5
2	NAP	A	269	-	-	0/31/67/67	0/5/5/5
2	NAP	D	269	-	-	0/31/67/67	0/5/5/5
2	NAP	B	269	-	-	1/31/67/67	0/5/5/5
3	JU2	C	270	-	-	0/0/2/2	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	269	NAP	O7N-C7N	8.68	1.40	1.24
2	D	269	NAP	O7N-C7N	8.55	1.40	1.24
2	C	269	NAP	O7N-C7N	8.49	1.40	1.24
2	A	269	NAP	O7N-C7N	8.36	1.40	1.24
3	A	270	JU2	C7-C10	-8.27	1.34	1.44
3	D	270	JU2	C7-C10	-8.20	1.34	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	270	JU2	C7-C10	-8.12	1.34	1.44
3	B	270	JU2	C7-C10	-7.94	1.34	1.44
3	C	270	JU2	BR15-C8	4.70	1.97	1.90
3	D	270	JU2	BR15-C8	4.40	1.96	1.90
2	B	269	NAP	C2A-N3A	4.22	1.38	1.32
3	B	270	JU2	BR15-C8	4.21	1.96	1.90
3	A	270	JU2	BR15-C8	4.09	1.96	1.90
2	C	269	NAP	C2A-N3A	4.07	1.38	1.32
2	D	269	NAP	C2A-N3A	4.02	1.38	1.32
2	A	269	NAP	C2A-N3A	3.87	1.38	1.32
3	C	270	JU2	C7-C4	3.76	1.46	1.42
3	B	270	JU2	C7-C4	3.51	1.46	1.42
3	D	270	JU2	C7-C4	3.06	1.46	1.42
3	A	270	JU2	C7-C4	3.01	1.45	1.42
3	B	270	JU2	C4-C5	2.94	1.50	1.43
2	D	269	NAP	C2N-N1N	2.84	1.38	1.35
3	D	270	JU2	C4-C5	2.83	1.50	1.43
3	A	270	JU2	C4-C5	2.76	1.50	1.43
3	C	270	JU2	C4-C5	2.74	1.50	1.43
2	D	269	NAP	C2A-N1A	2.55	1.38	1.33
2	C	269	NAP	C2A-N1A	2.51	1.38	1.33
2	A	269	NAP	C2A-N1A	2.44	1.38	1.33
2	B	269	NAP	C2A-N1A	2.43	1.38	1.33
2	A	269	NAP	C2N-N1N	2.36	1.37	1.35

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	270	JU2	C4-C3-N2	-8.98	116.12	124.09
3	A	270	JU2	C4-C3-N2	-8.86	116.23	124.09
3	D	270	JU2	C4-C3-N2	-8.79	116.29	124.09
3	C	270	JU2	C4-C3-N2	-8.45	116.59	124.09
3	D	270	JU2	C3-C4-C5	7.82	119.43	115.01
3	B	270	JU2	C3-C4-C5	7.75	119.39	115.01
3	A	270	JU2	C3-C4-C5	7.50	119.25	115.01
3	C	270	JU2	C3-C4-C5	6.92	118.92	115.01
2	C	269	NAP	N3A-C2A-N1A	-6.08	119.17	128.68
2	A	269	NAP	N3A-C2A-N1A	-6.07	119.20	128.68
2	D	269	NAP	N3A-C2A-N1A	-5.49	120.10	128.68
2	B	269	NAP	N3A-C2A-N1A	-5.34	120.33	128.68
3	B	270	JU2	C1-N6-C5	4.81	120.85	115.36
3	C	270	JU2	C1-N6-C5	4.80	120.84	115.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	270	JU2	C1-N6-C5	4.51	120.51	115.36
3	D	270	JU2	C1-N6-C5	4.49	120.48	115.36
3	D	270	JU2	C3-N2-C1	4.34	122.83	115.93
3	B	270	JU2	C3-N2-C1	4.29	122.74	115.93
3	A	270	JU2	C3-N2-C1	4.28	122.72	115.93
3	C	270	JU2	C3-N2-C1	4.12	122.47	115.93
2	B	269	NAP	O7N-C7N-C3N	-3.04	115.99	119.63
2	A	269	NAP	C3N-C7N-N7N	2.87	121.20	117.75
2	A	269	NAP	C1B-N9A-C4A	-2.82	121.69	126.64
3	C	270	JU2	N6-C1-N2	-2.72	123.60	127.22
3	A	270	JU2	N6-C1-N2	-2.67	123.66	127.22
3	D	270	JU2	N6-C1-N2	-2.64	123.70	127.22
2	B	269	NAP	C3N-C7N-N7N	2.64	120.91	117.75
3	B	270	JU2	N6-C1-N2	-2.60	123.75	127.22
2	C	269	NAP	O7N-C7N-C3N	-2.51	116.62	119.63
2	B	269	NAP	C1B-N9A-C4A	-2.40	122.42	126.64
2	C	269	NAP	C3N-C7N-N7N	2.22	120.41	117.75
2	D	269	NAP	C1B-N9A-C4A	-2.14	122.89	126.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	269	NAP	C5B-O5B-PA-O1A
2	B	269	NAP	C5B-O5B-PA-O1A

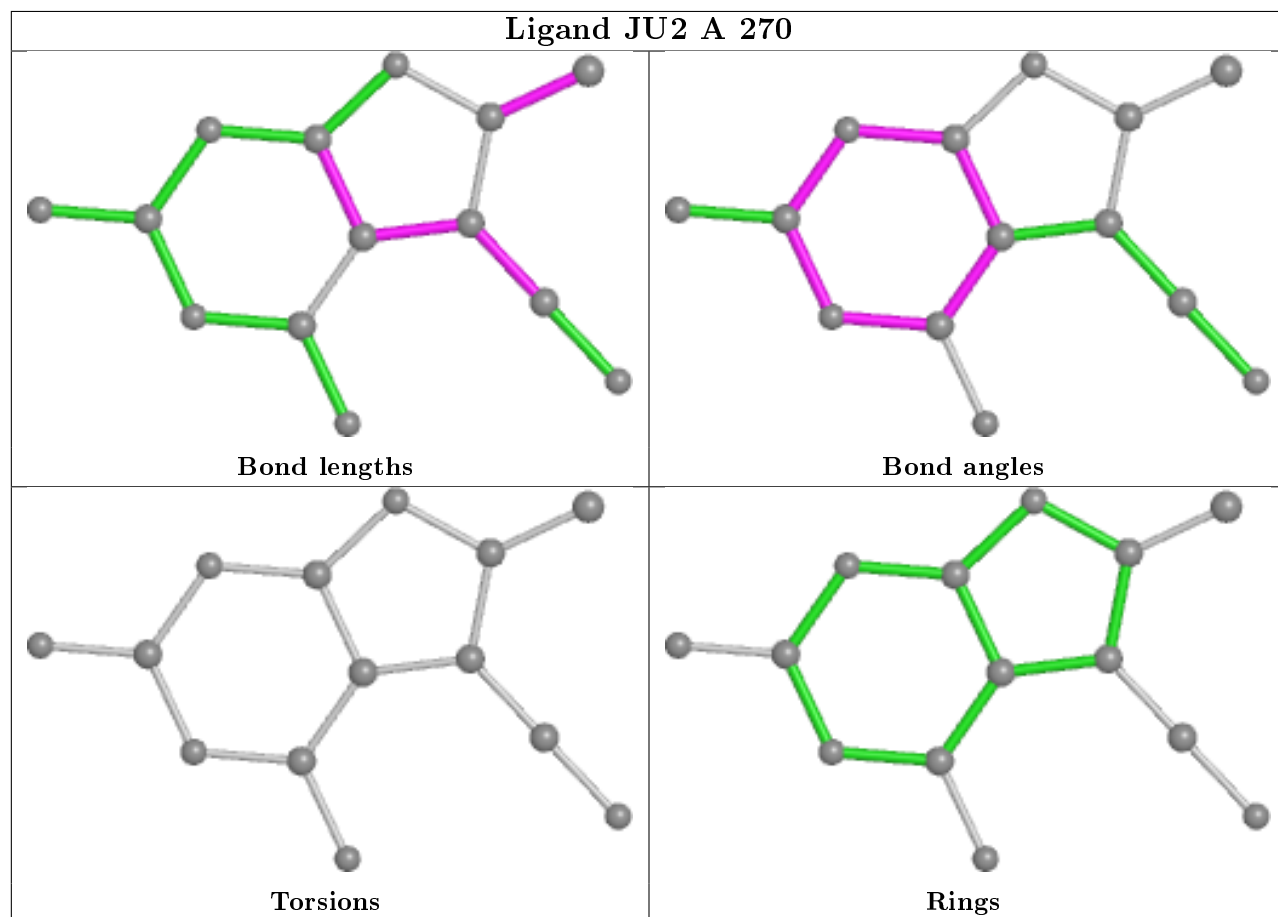
There are no ring outliers.

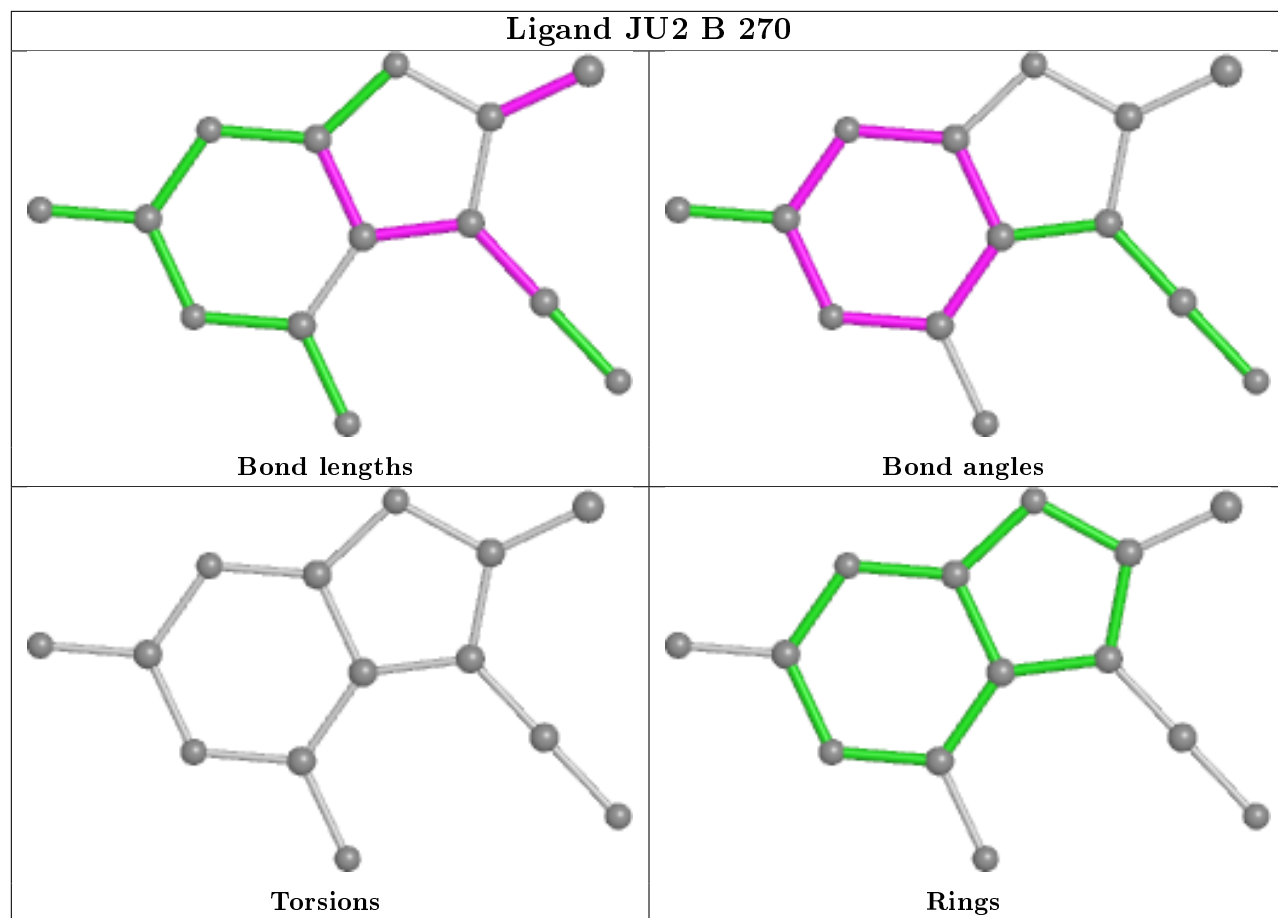
4 monomers are involved in 4 short contacts:

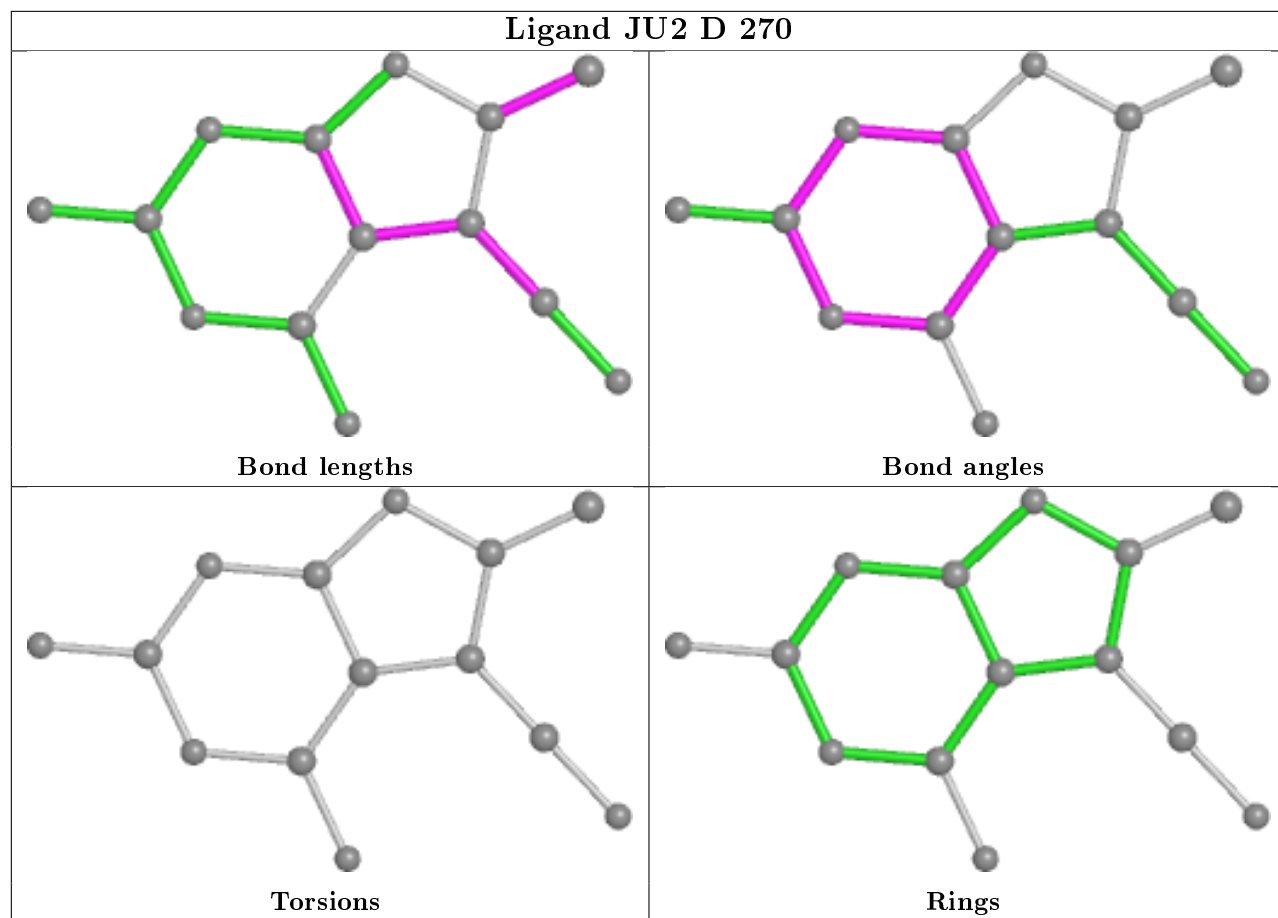
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	269	NAP	1	0
2	A	269	NAP	1	0
2	B	269	NAP	1	0
3	C	270	JU2	1	0

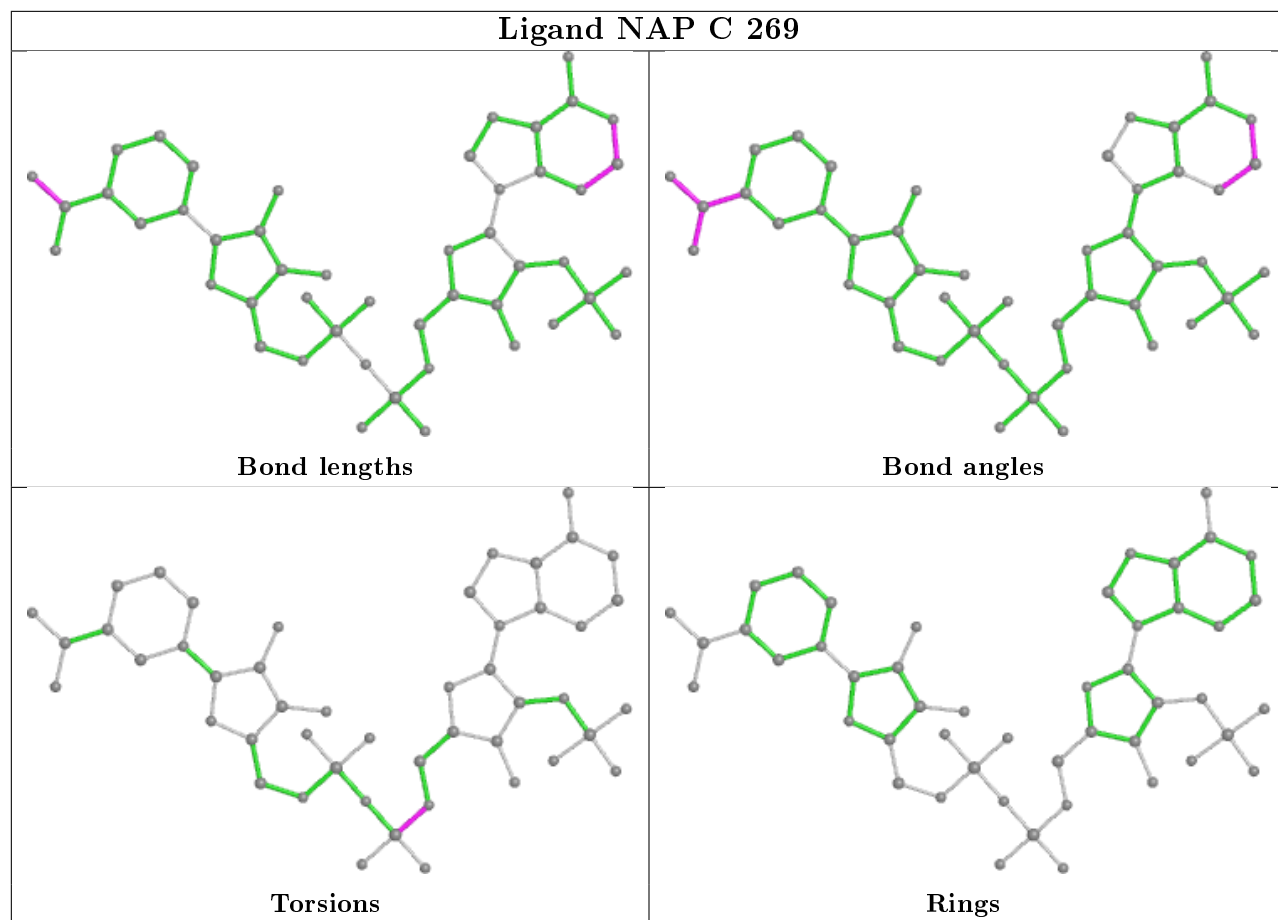
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

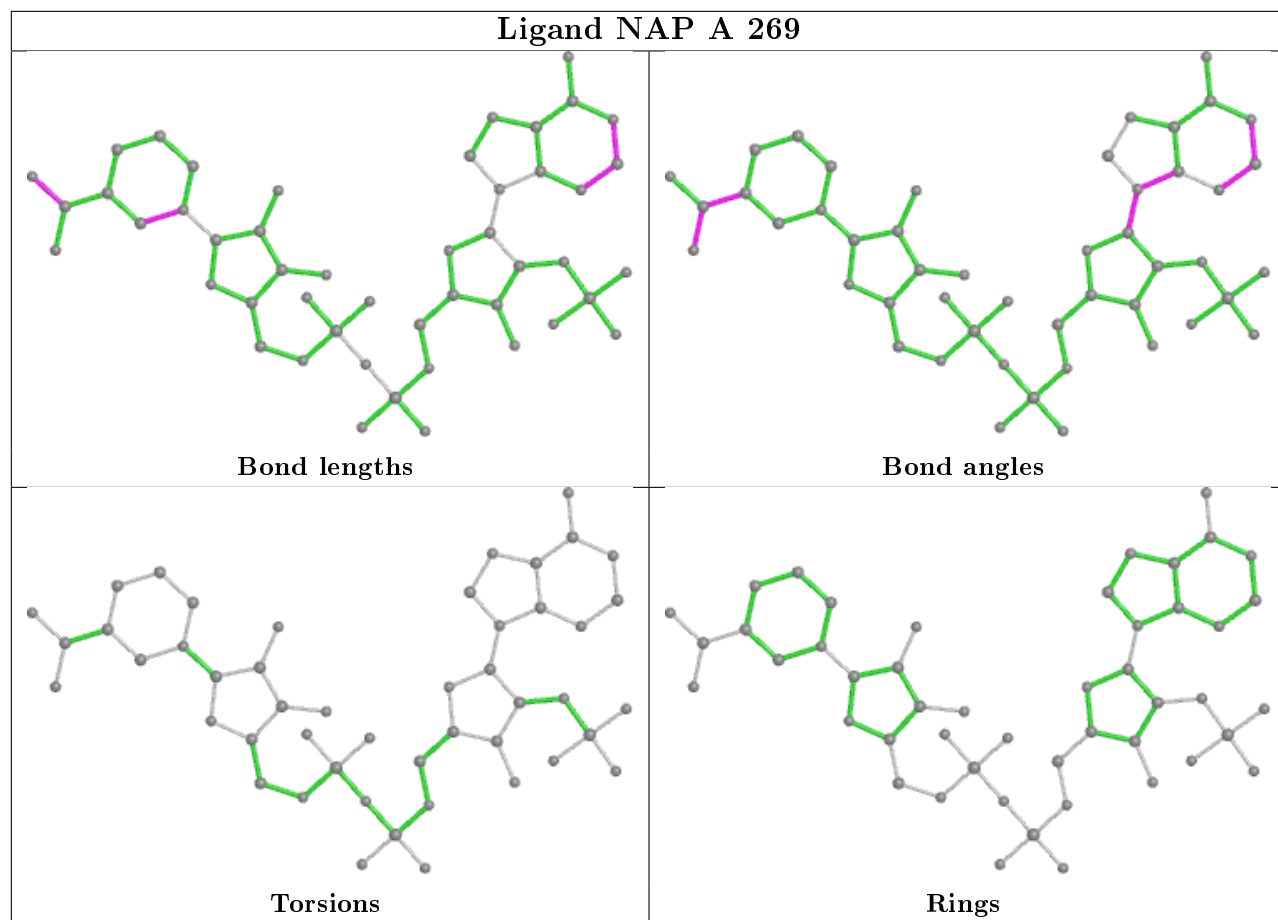
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

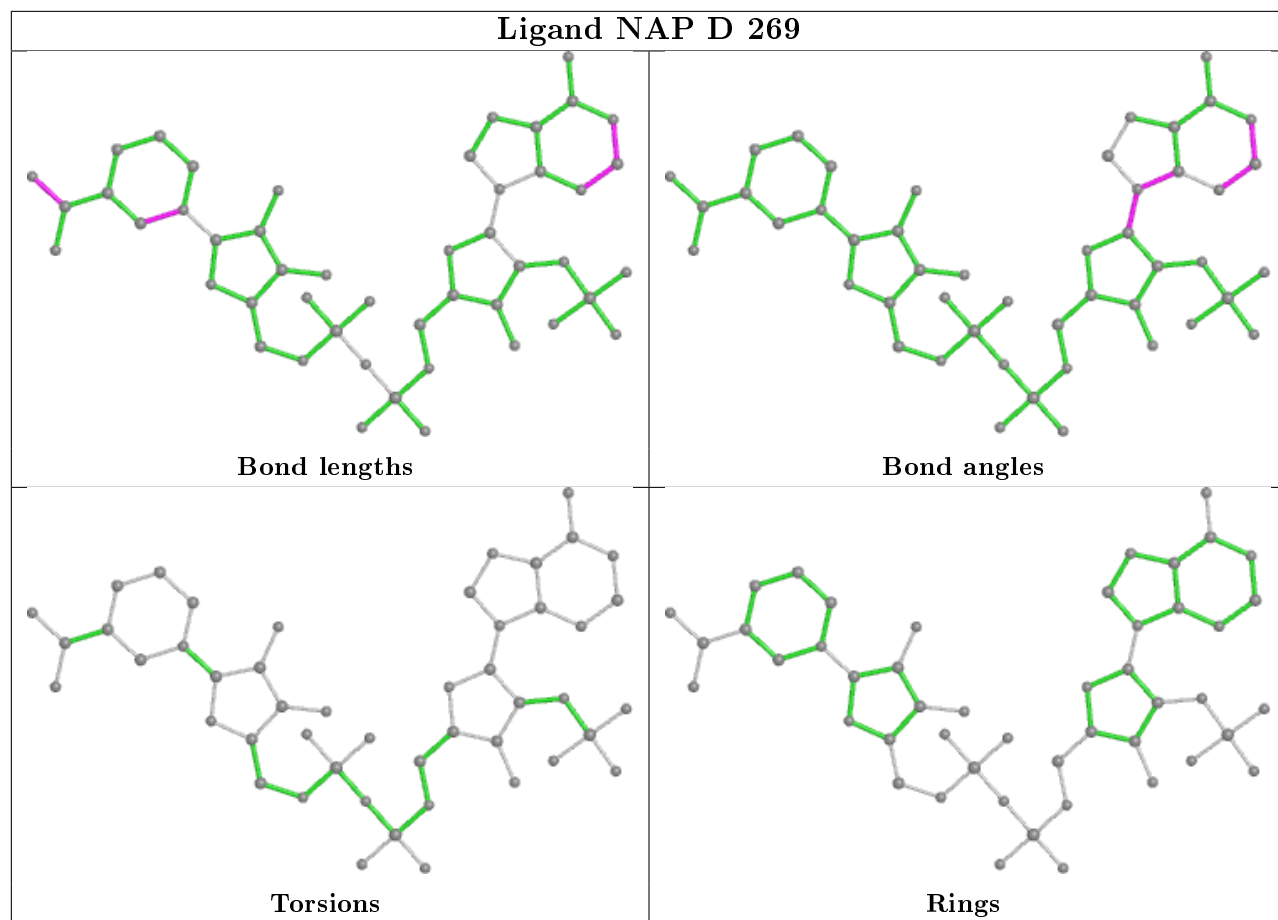


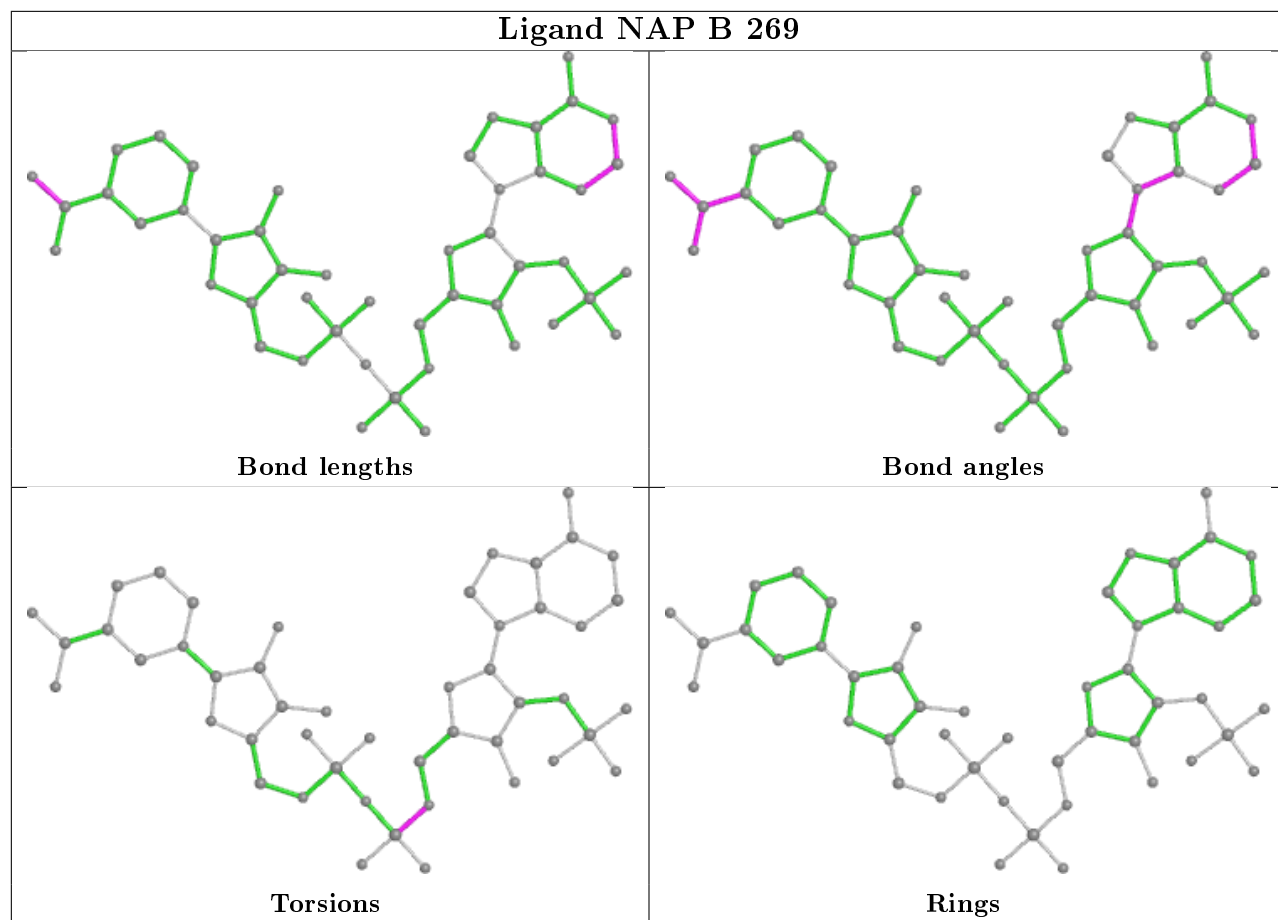


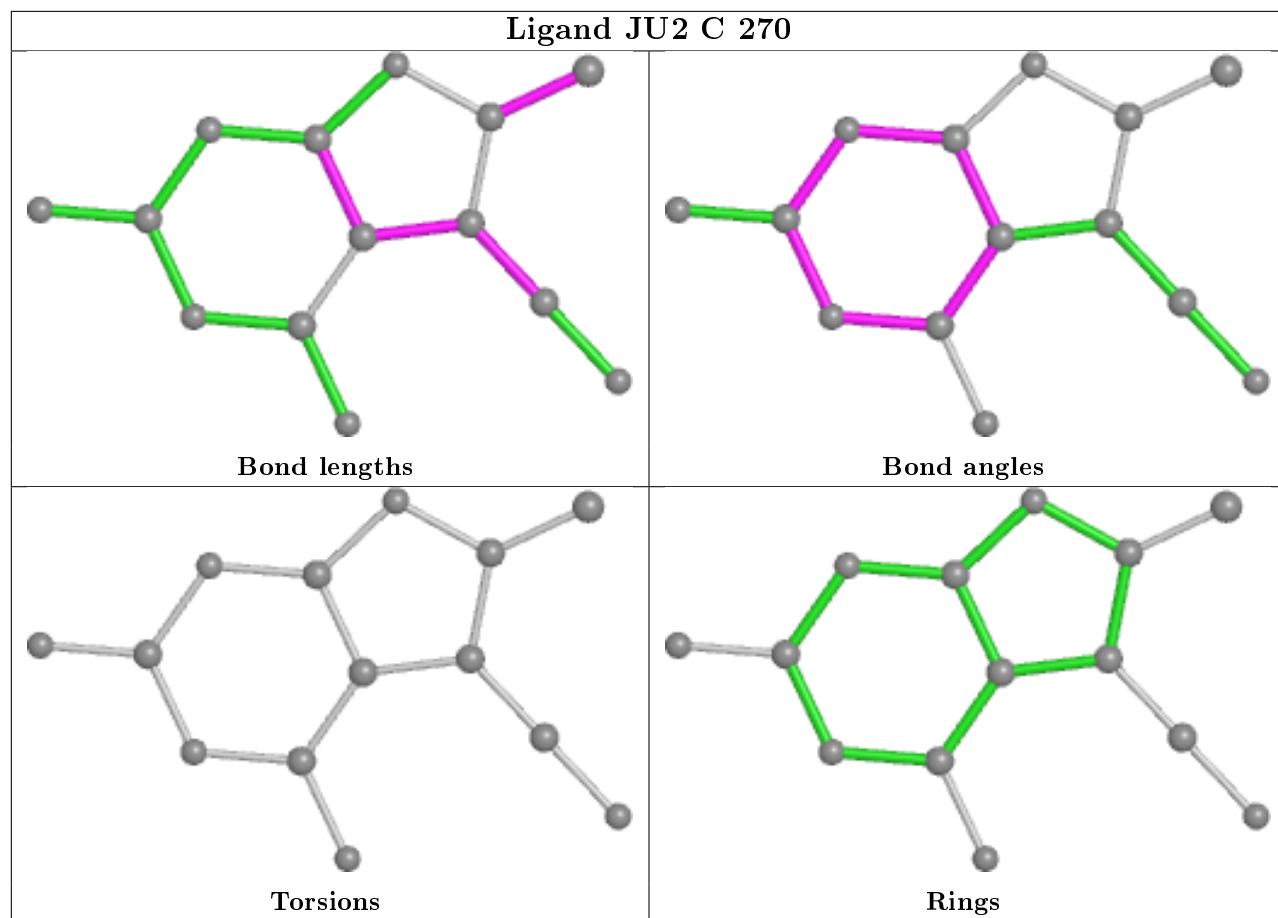












5.7 Other polymers [i](#)

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%)	-0.35	2 (0%) 86 84	11, 15, 28, 39	3 (1%)
1	B	250/288 (86%)	-0.35	5 (2%) 65 61	10, 15, 29, 47	0
1	C	250/288 (86%)	-0.25	5 (2%) 65 61	11, 15, 30, 46	2 (0%)
1	D	249/288 (86%)	-0.26	4 (1%) 72 68	10, 15, 28, 36	6 (2%)
All	All	998/1152 (86%)	-0.30	16 (1%) 72 68	10, 15, 29, 47	11 (1%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	113	GLY	5.8
1	C	151	SER	5.0
1	A	113	GLY	4.5
1	C	113	GLY	4.2
1	D	113	GLY	4.1
1	A	2	GLU	3.1
1	B	151	SER	3.0
1	C	152	SER	3.0
1	B	2	GLU	2.9
1	D	2	GLU	2.7
1	C	195	TYR	2.4
1	D	212	ALA	2.3
1	B	103	VAL	2.2
1	B	152	SER	2.2
1	D	214	GLY	2.1
1	C	212	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

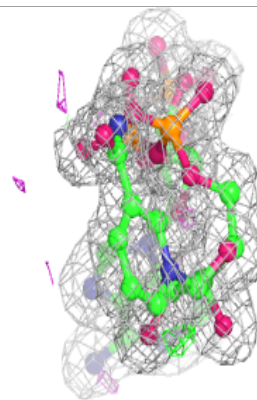
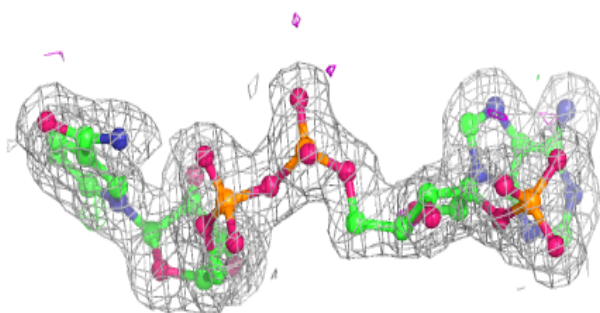
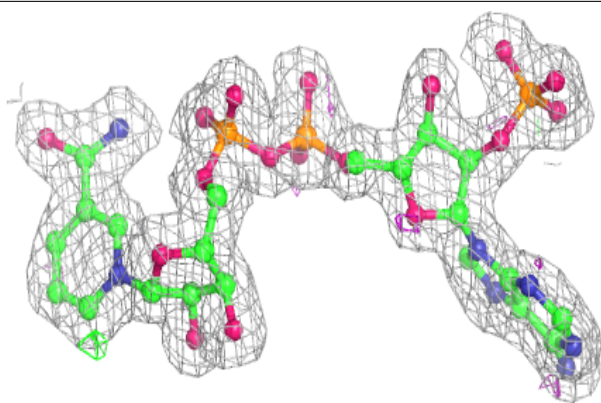
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAP	C	269	48/48	0.97	0.06	8,15,20,21	0
2	NAP	A	269	48/48	0.98	0.06	11,15,19,20	0
2	NAP	D	269	48/48	0.98	0.06	9,15,20,21	0
2	NAP	B	269	48/48	0.98	0.06	9,14,19,20	0
3	JU2	B	270	14/14	0.99	0.06	12,16,20,21	0
3	JU2	D	270	14/14	0.99	0.07	14,20,23,23	0
3	JU2	A	270	14/14	0.99	0.07	12,16,20,20	0
3	JU2	C	270	14/14	0.99	0.07	13,16,19,22	0

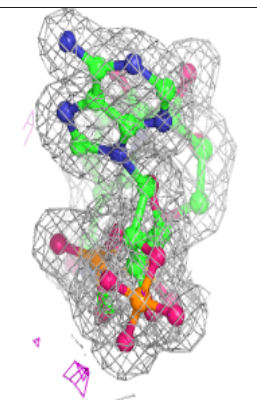
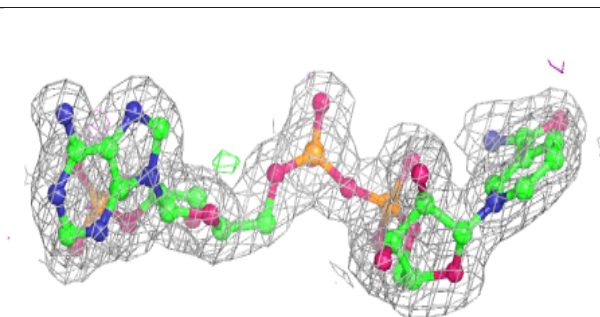
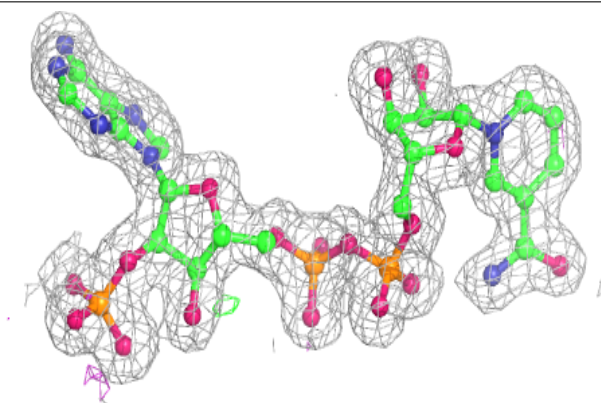
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP 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)

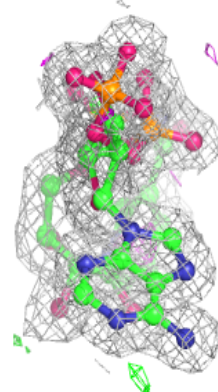
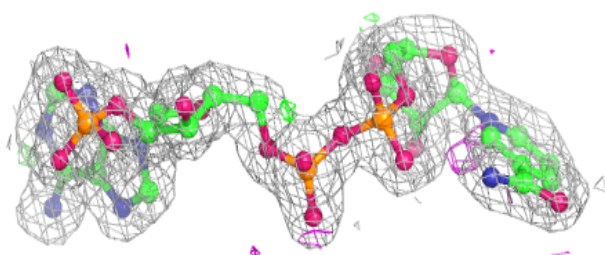
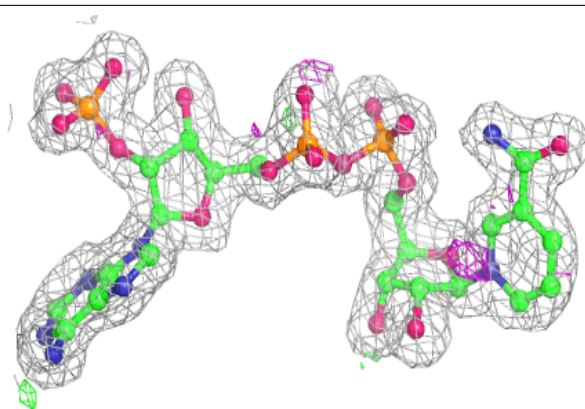
**Electron density around NAP A 269:**

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

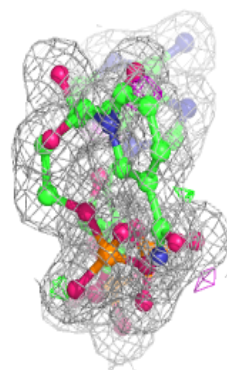
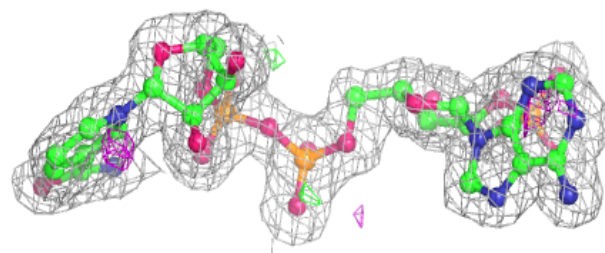
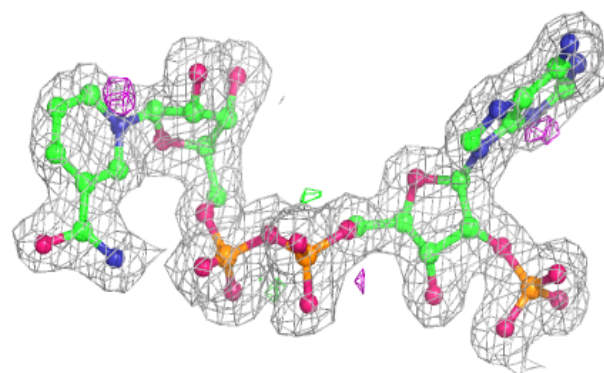


Electron density around NAP D 269:

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

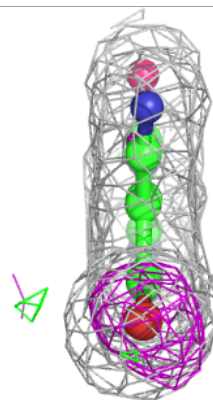
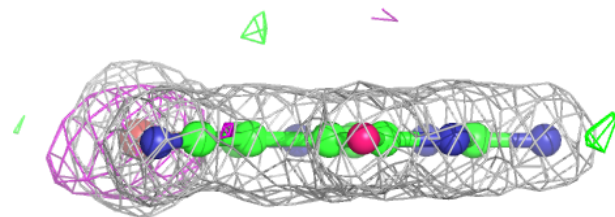
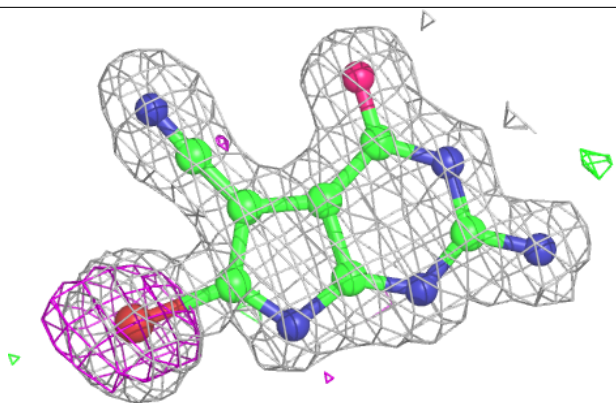
**Electron density around NAP B 269:**

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

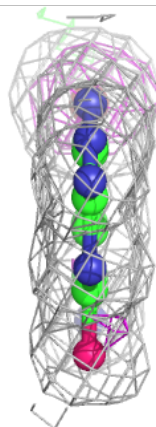
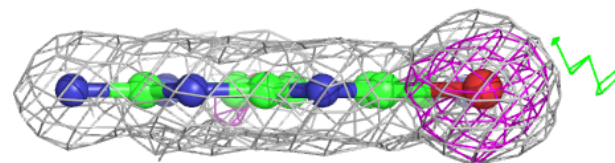
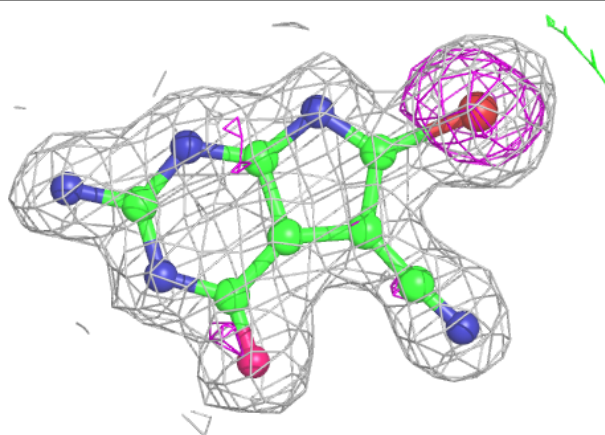


Electron density around JU2 B 270:

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

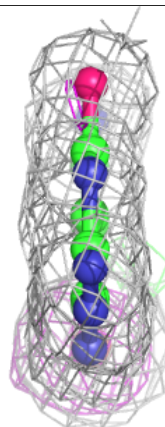
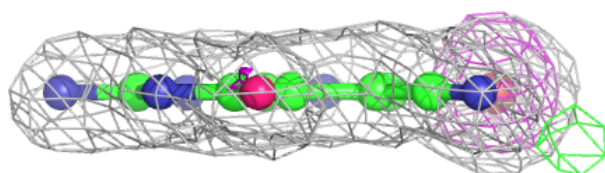
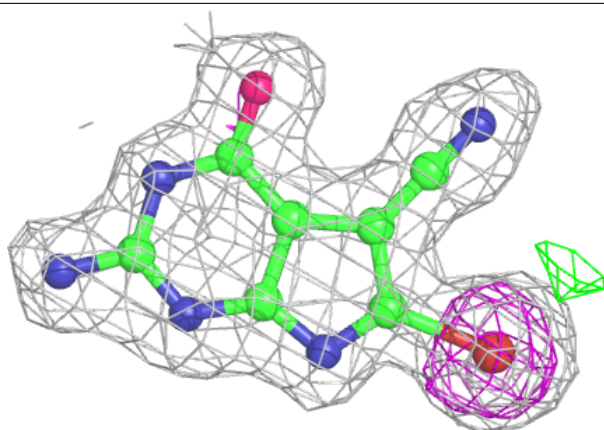
**Electron density around JU2 D 270:**

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

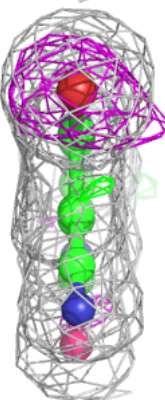
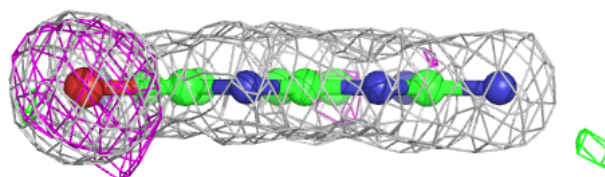
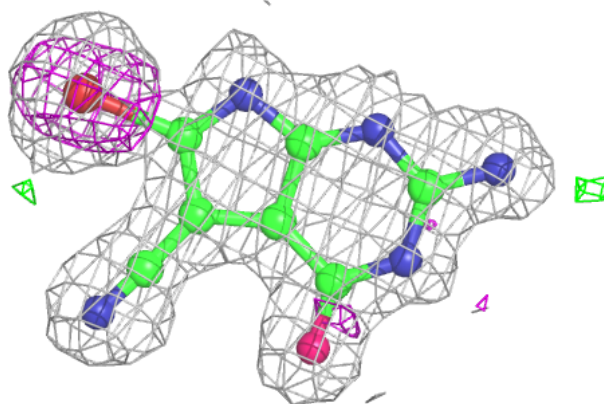


Electron density around JU2 A 270:

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

**Electron density around JU2 C 270:**

$2mF_o-DF_c$ (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.