



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 07:53 PM UTC

PDB ID : 2X9N / pdb_00002x9n
Title : High resolution structure of TbPTR1 in complex with cyromazine
Authors : Dawson, A.; Tulloch, L.B.; Barrack, K.L.; Hunter, W.N.
Deposited on : 2010-03-23
Resolution : 1.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

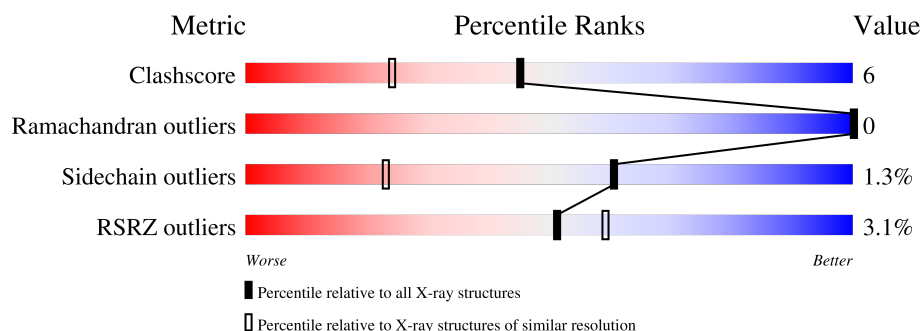
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.15 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))
Clashscore	190562	1393 (1.16-1.12)
Ramachandran outliers	187476	1369 (1.16-1.12)
Sidechain outliers	187428	1369 (1.16-1.12)
RSRZ outliers	180081	1379 (1.16-1.12)

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

Mol	Chain	Length	Quality of chain
1	A	288	2% 78% 7% 14%
1	B	288	3% 77% 8% 14%
1	C	288	2% 76% 9% 14%
1	D	288	4% 75% 10% 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
3	AX3	B	1270[B]	-	-	X	-
3	AX3	C	1270[B]	-	-	X	-
3	AX3	D	1270[B]	-	-	X	-
6	D1D	D	1271[B]	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9198 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	7	0
			1878	1184	329	353	12			
1	B	248	Total	C	N	O	S	0	9	0
			1890	1197	328	353	12			
1	C	249	Total	C	N	O	S	0	6	0
			1885	1190	329	355	11			
1	D	247	Total	C	N	O	S	0	10	0
			1869	1184	329	344	12			

There are 80 discrepancies between the modelled and reference sequences:

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

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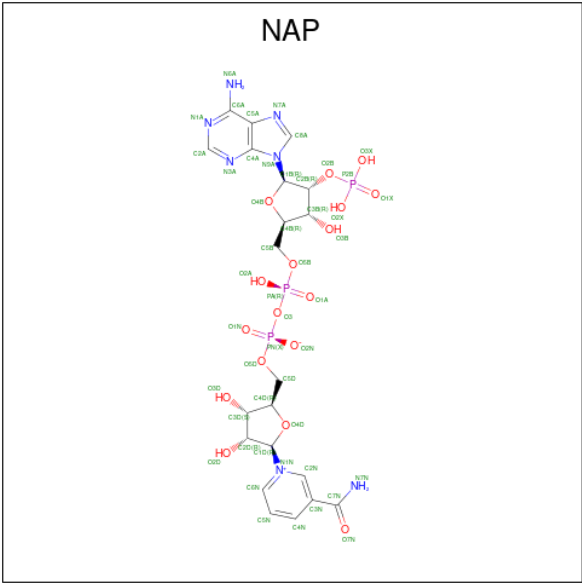
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP O76290
B	-17	SER	-	expression tag	UNP O76290
B	-16	SER	-	expression tag	UNP O76290
B	-15	HIS	-	expression tag	UNP O76290
B	-14	HIS	-	expression tag	UNP O76290
B	-13	HIS	-	expression tag	UNP O76290
B	-12	HIS	-	expression tag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

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

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



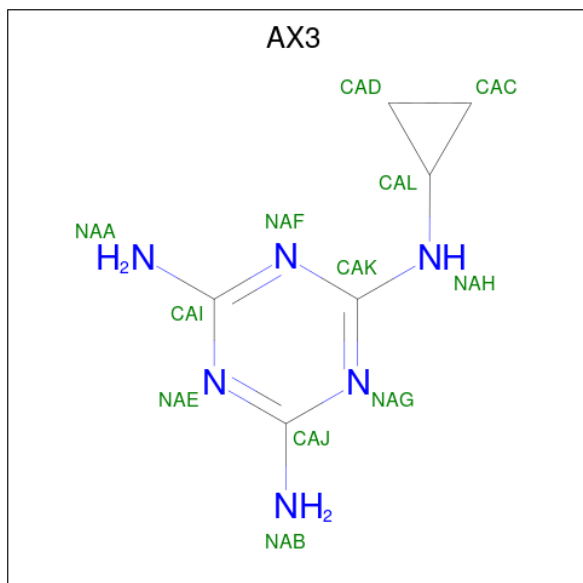
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

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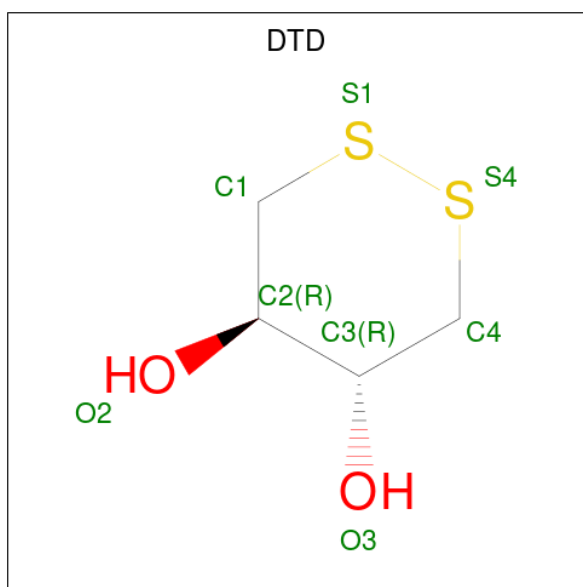
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is N²-cyclopropyl-1,3,5-triazine-2,4,6-triamine (CCD ID: AX3) (formula: C₆H₁₀N₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			12	6	6		
3	B	1	Total	C	N	0	1
			16	9	7		
3	C	1	Total	C	N	0	1
			16	9	7		
3	D	1	Total	C	N	0	1
			16	9	7		

- Molecule 4 is DITHIANE DIOL (CCD ID: DTD) (formula: C₄H₈O₂S₂).

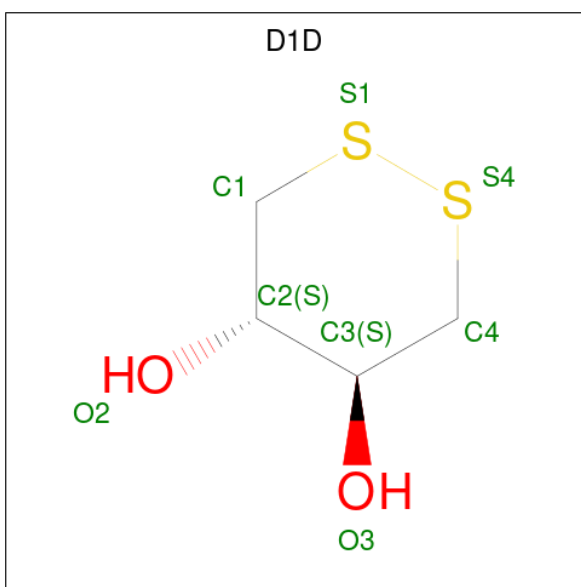


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	1
			9	4	2	3		
4	C	1	Total	C	O	S	0	1
			9	4	2	3		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

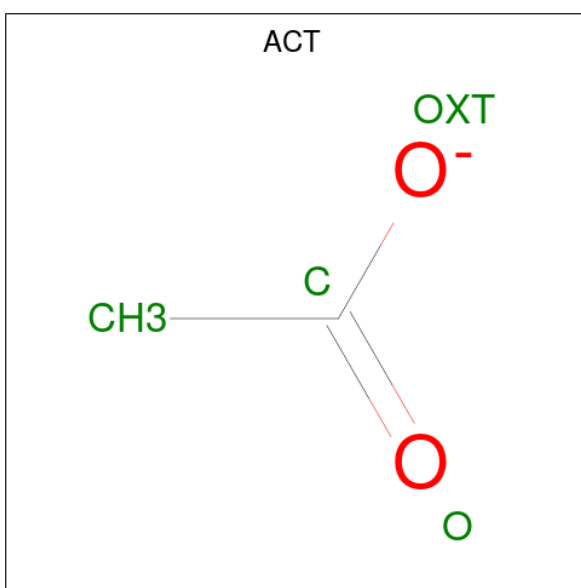
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		
5	D	1	Total	Na	0	0
			1	1		

- Molecule 6 is (4S,5S)-1,2-DITHIANE-4,5-DIOL (CCD ID: D1D) (formula: C₄H₈O₂S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	S	0	1
			9	4	2	3		
6	D	1	Total	C	O	S	0	1
			9	4	2	3		

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).



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

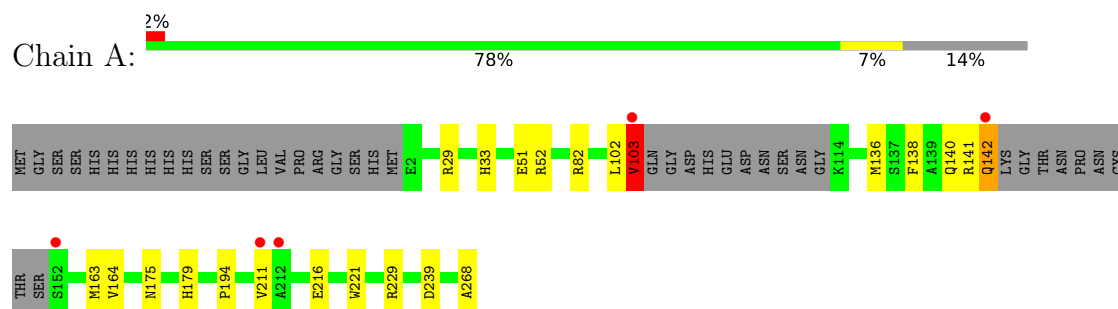
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	382	Total 382	O 382	0	0
8	B	321	Total 321	O 321	0	0
8	C	356	Total 356	O 356	0	0
8	D	323	Total 323	O 323	0	0

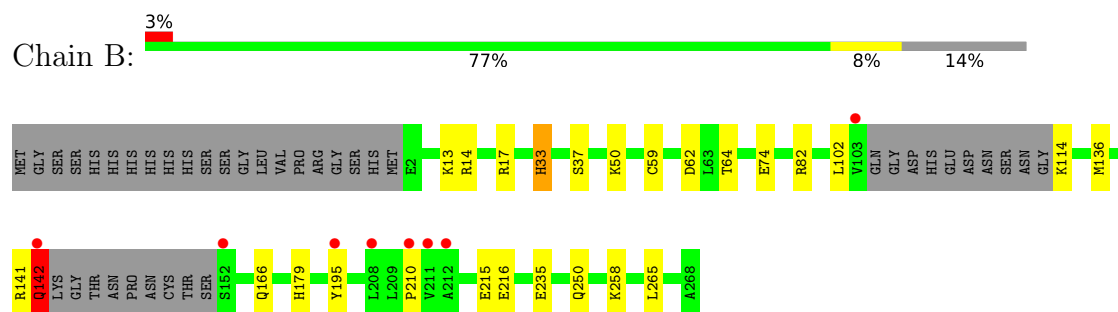
3 Residue-property plots

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.

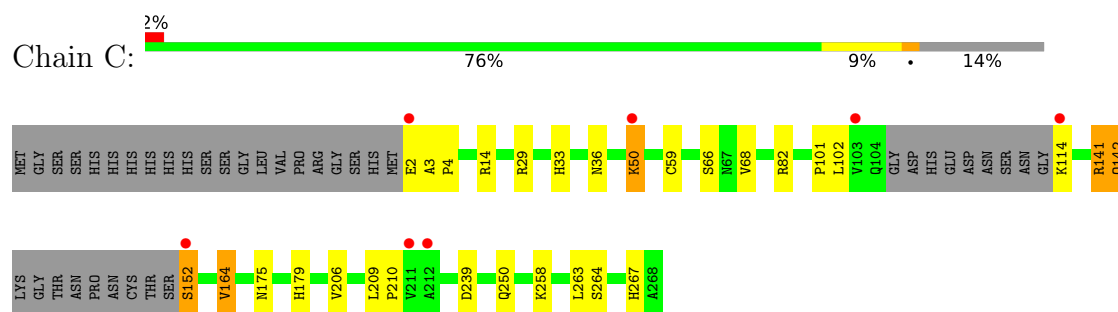
• Molecule 1: PTERIDINE REDUCTASE



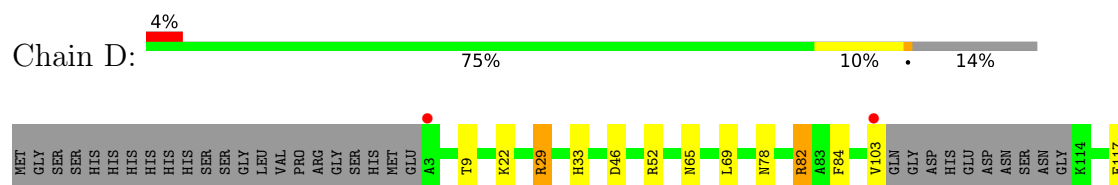
• Molecule 1: PTERIDINE REDUCTASE

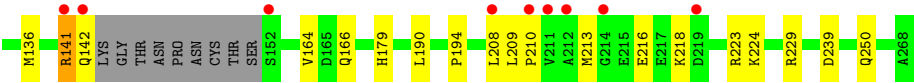


• Molecule 1: PTERIDINE REDUCTASE



• Molecule 1: PTERIDINE REDUCTASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.50Å 90.00Å 82.40Å 90.00° 115.50° 90.00°	Depositor
Resolution (Å)	20.00 – 1.15 20.00 – 1.15	Depositor EDS
% Data completeness (in resolution range)	93.2 (20.00-1.15) 96.0 (20.00-1.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 1.10Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.126 , 0.152 0.133 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	7.0	Xtriage
Anisotropy	0.838	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 72.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9198	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, NAP, AX3, NA, DTD, D1D

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	1.01	1/1943 (0.1%)	1.34	12/2637 (0.5%)
1	B	0.99	1/1967 (0.1%)	1.37	15/2669 (0.6%)
1	C	1.02	0/1946	1.39	12/2641 (0.5%)
1	D	0.99	0/1946	1.36	16/2641 (0.6%)
All	All	1.00	2/7802 (0.0%)	1.36	55/10588 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	179	HIS	CG-ND1	-5.85	1.31	1.38
1	A	179	HIS	CG-ND1	-5.47	1.32	1.38

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	GLN	CA-CB-CG	16.17	146.45	114.10
1	C	141	ARG	CD-NE-CZ	12.56	141.99	124.40
1	A	142	GLN	CB-CG-CD	12.44	133.75	112.60
1	A	82	ARG	CD-NE-CZ	9.79	138.11	124.40
1	A	141	ARG	CD-NE-CZ	9.23	137.32	124.40
1	C	114	LYS	CA-C-O	-8.83	105.79	120.80
1	C	250	GLN	CB-CG-CD	8.78	127.52	112.60
1	A	103	VAL	N-CA-CB	-8.70	96.71	111.50
1	D	29	ARG	CD-NE-CZ	-8.32	112.75	124.40
1	B	142	GLN	OE1-CD-NE2	8.18	130.78	122.60
1	C	29	ARG	NE-CZ-NH2	-8.08	111.93	119.20
1	A	216	GLU	CB-CG-CD	7.70	125.70	112.60
1	B	250	GLN	CB-CG-CD	7.59	125.50	112.60
1	B	82	ARG	CD-NE-CZ	7.57	135.00	124.40
1	D	52	ARG	CD-NE-CZ	7.22	134.51	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	VAL	O-C-N	7.11	129.05	121.87
1	D	82[A]	ARG	CD-NE-CZ	-6.86	114.80	124.40
1	D	82[B]	ARG	CD-NE-CZ	-6.86	114.80	124.40
1	B	142	GLN	CG-CD-NE2	-6.74	106.29	116.40
1	C	141	ARG	NE-CZ-NH2	6.73	125.26	119.20
1	A	102	LEU	CA-C-N	6.66	133.68	121.70
1	A	102	LEU	C-N-CA	6.66	133.68	121.70
1	D	82[A]	ARG	NE-CZ-NH2	-6.56	113.29	119.20
1	D	82[B]	ARG	NE-CZ-NH2	-6.56	113.29	119.20
1	B	142	GLN	CB-CG-CD	-6.51	101.54	112.60
1	D	46	ASP	CA-CB-CG	6.36	118.96	112.60
1	C	239	ASP	CA-CB-CG	6.33	118.93	112.60
1	C	114	LYS	N-CA-CB	6.08	120.84	110.50
1	D	239	ASP	CA-CB-CG	6.08	118.68	112.60
1	B	215	GLU	CB-CG-CD	6.02	122.83	112.60
1	B	258[A]	LYS	N-CA-CB	5.97	118.74	109.97
1	B	258[B]	LYS	N-CA-CB	5.97	118.74	109.97
1	B	17	ARG	NE-CZ-NH1	-5.95	115.55	121.50
1	C	142	GLN	CA-C-O	-5.81	110.92	120.80
1	B	141	ARG	CG-CD-NE	5.79	124.74	112.00
1	D	141	ARG	CB-CG-CD	5.72	124.46	111.30
1	D	229	ARG	NE-CZ-NH2	5.72	124.34	119.20
1	A	140	GLN	OE1-CD-NE2	-5.67	116.93	122.60
1	B	74	GLU	CB-CG-CD	-5.61	103.06	112.60
1	D	213	MET	CA-C-O	-5.53	114.96	121.16
1	D	194	PRO	CB-CA-C	-5.51	104.03	111.85
1	C	36	ASN	OD1-CG-ND2	5.43	128.03	122.60
1	D	216	GLU	O-C-N	5.40	128.31	122.15
1	C	82	ARG	NE-CZ-NH2	-5.39	114.35	119.20
1	D	103	VAL	CA-C-O	-5.37	111.67	120.80
1	A	29	ARG	NE-CZ-NH2	-5.34	114.39	119.20
1	B	142	GLN	N-CA-CB	5.29	119.49	110.50
1	A	33	HIS	ND1-CE1-NE2	5.21	113.61	108.40
1	C	250	GLN	N-CA-C	5.18	119.22	113.01
1	D	142	GLN	CB-CG-CD	-5.15	103.85	112.60
1	C	267	HIS	CA-CB-CG	5.14	118.94	113.80
1	B	33	HIS	CA-CB-CG	-5.13	108.67	113.80
1	A	239	ASP	CA-CB-CG	5.10	117.70	112.60
1	D	117	GLU	CB-CG-CD	5.09	121.25	112.60
1	B	141	ARG	CD-NE-CZ	5.04	131.45	124.40

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	1878	0	1908	14	0
1	B	1890	0	1938	19	0
1	C	1885	0	1919	28	0
1	D	1869	0	1914	23	0
2	A	48	0	25	0	0
2	B	48	0	25	2	0
2	C	48	0	25	1	0
2	D	48	0	25	2	0
3	A	12	0	10	1	0
3	B	16	0	9	11	0
3	C	16	0	12	10	0
3	D	16	0	11	12	0
4	A	9	0	4	1	0
4	C	9	0	4	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	B	9	0	4	1	0
6	D	9	0	4	4	0
7	C	4	0	3	0	0
8	A	382	0	0	6	0
8	B	321	0	0	8	0
8	C	356	0	0	13	0
8	D	323	0	0	8	0
All	All	9198	0	7840	93	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 6.

All (93) 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:208:LEU:O	3:D:1270[B]:AX3:HAD	1.70	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1270[B]:AX3:CAC	6:D:1271[B]:D1D:H4C2	2.10	0.81
1:C:152:SER:HB3	8:C:2196:HOH:O	1.83	0.79
1:C:210:PRO:HB3	3:C:1270[A]:AX3:HADA	1.63	0.79
1:A:175:ASN:HB2	8:A:2279:HOH:O	1.84	0.77
1:C:175:ASN:HB2	8:C:2267:HOH:O	1.85	0.75
1:C:14:ARG:NH2	3:C:1270[B]:AX3:HAC	2.02	0.74
1:A:194:PRO:HG3	8:C:2304:HOH:O	1.89	0.73
1:B:62:ASP:OD1	1:B:64[B]:THR:HG23	1.88	0.73
1:B:50:LYS:HG3	8:B:2084:HOH:O	1.88	0.71
1:B:210:PRO:CA	3:B:1270[B]:AX3:HADA	2.20	0.71
1:C:3:ALA:HA	8:C:2055:HOH:O	1.90	0.71
1:C:210:PRO:N	3:C:1270[B]:AX3:HACA	2.08	0.69
2:B:1269:NAP:N7N	3:B:1270[B]:AX3:HACA	2.07	0.69
1:D:210:PRO:HG3	3:D:1270[B]:AX3:HAC	1.74	0.68
1:A:51:GLU:OE1	1:A:52[B]:ARG:HG3	1.95	0.67
3:B:1270[A]:AX3:HAD	8:B:2249:HOH:O	1.96	0.66
3:B:1270[B]:AX3:HAL	6:B:1271[B]:D1D:H1C2	1.78	0.66
1:A:163:MET:HG3	8:A:2382:HOH:O	1.95	0.66
3:D:1270[B]:AX3:HACA	6:D:1271[B]:D1D:S4	2.36	0.65
1:D:164:VAL:HG22	1:D:179:HIS:CE1	2.32	0.65
1:C:210:PRO:CA	3:C:1270[B]:AX3:HACA	2.28	0.64
1:C:258[B]:LYS:HE2	1:C:264:SER:OG	1.97	0.64
3:D:1270[B]:AX3:HACA	6:D:1271[B]:D1D:H4C2	1.78	0.63
2:B:1269:NAP:C7N	3:B:1270[B]:AX3:HACA	2.29	0.62
3:C:1270[A]:AX3:HAD	8:C:2206:HOH:O	1.98	0.62
1:B:142:GLN:HG3	8:B:2173:HOH:O	2.02	0.60
1:B:210:PRO:N	3:B:1270[B]:AX3:HADA	2.17	0.59
1:B:210:PRO:HD3	3:B:1270[B]:AX3:HAC	1.84	0.59
1:D:179:HIS:HD2	8:D:2242:HOH:O	1.86	0.58
1:B:142:GLN:HB2	8:B:2213:HOH:O	2.02	0.58
1:A:52[B]:ARG:HD2	8:A:2125:HOH:O	2.04	0.57
1:A:164:VAL:HA	8:A:2281:HOH:O	2.04	0.57
3:D:1270[A]:AX3:HACA	8:D:2188:HOH:O	2.04	0.56
1:C:210:PRO:CB	3:C:1270[A]:AX3:HADA	2.34	0.56
1:C:102:LEU:O	1:D:136[A]:MET:HG3	2.05	0.56
3:A:1270:AX3:HACA	4:A:1271[B]:DTD:S1	2.47	0.54
1:C:210:PRO:HD3	3:C:1270[B]:AX3:HAD	1.89	0.54
1:D:164:VAL:HG22	1:D:179:HIS:ND1	2.21	0.54
1:B:210:PRO:HA	3:B:1270[B]:AX3:HADA	1.89	0.54
1:D:210:PRO:N	3:D:1270[B]:AX3:HADA	2.23	0.54
2:D:1269:NAP:PA	3:D:1270[A]:AX3:HADA	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:PRO:HG3	8:C:2210:HOH:O	2.08	0.53
1:C:14:ARG:HH22	3:C:1270[B]:AX3:HAC	1.73	0.53
1:B:210:PRO:HG3	3:B:1270[B]:AX3:CAL	2.40	0.51
1:B:13:LYS:HE2	1:B:37:SER:OG	2.10	0.51
1:C:179:HIS:HD2	8:D:2242:HOH:O	1.94	0.50
1:D:78:ASN:O	1:D:82[B]:ARG:HG2	2.13	0.49
1:C:4:PRO:HD2	8:C:2055:HOH:O	2.12	0.49
1:C:210:PRO:HG3	3:C:1270[B]:AX3:CAL	2.43	0.49
1:A:103:VAL:HG11	1:B:195:TYR:CE2	2.49	0.48
1:D:210:PRO:CA	3:D:1270[B]:AX3:HADA	2.44	0.48
1:C:66:SER:OG	1:C:68[C]:VAL:HG22	2.13	0.48
3:D:1270[B]:AX3:HAC	6:D:1271[B]:D1D:H4C1	1.95	0.48
1:C:258[B]:LYS:HD3	8:C:2340:HOH:O	2.13	0.47
1:D:210:PRO:HG3	3:D:1270[B]:AX3:CAC	2.41	0.47
8:A:2238:HOH:O	1:B:136[B]:MET:HE1	2.14	0.47
1:C:3:ALA:CB	8:C:2055:HOH:O	2.63	0.47
1:B:14:ARG:NH2	3:B:1270[B]:AX3:CAD	2.78	0.46
1:C:142:GLN:NE2	8:C:2241:HOH:O	2.48	0.46
1:B:114:LYS:N	8:B:2188:HOH:O	2.49	0.46
1:A:136[B]:MET:HE1	8:B:2185:HOH:O	2.15	0.46
1:C:206[A]:VAL:HG23	1:C:263:LEU:HD22	1.98	0.46
3:B:1270[A]:AX3:HACA	8:B:2180:HOH:O	2.15	0.45
1:B:33:HIS:HA	1:B:59:CYS:O	2.17	0.45
1:D:82[B]:ARG:NH2	8:D:2171:HOH:O	2.48	0.45
1:D:223:ARG:NH1	8:D:2267:HOH:O	2.49	0.45
1:D:250:GLN:NE2	8:D:2299:HOH:O	2.49	0.45
1:C:50:LYS:HZ3	1:C:50:LYS:HG3	1.63	0.44
1:D:29:ARG:HD2	1:D:84:PHE:CD1	2.53	0.44
1:C:152:SER:N	8:C:2246:HOH:O	2.49	0.44
1:D:209:LEU:HD13	1:D:218:LYS:HB3	1.99	0.44
1:C:3:ALA:CA	8:C:2055:HOH:O	2.59	0.44
1:A:268:ALA:OXT	1:D:224:LYS:HE2	2.18	0.43
1:A:136[B]:MET:HG3	1:B:102:LEU:O	2.18	0.43
1:D:82[A]:ARG:HH21	1:D:82[A]:ARG:HD3	1.09	0.42
1:D:22[A]:LYS:HG2	8:D:2054:HOH:O	2.19	0.42
1:A:103:VAL:HG11	1:B:195:TYR:CZ	2.54	0.42
1:B:265:LEU:HB2	1:D:190[B]:LEU:HD21	2.02	0.42
2:C:1269:NAP:C7N	3:C:1270[B]:AX3:HADA	2.50	0.42
1:D:136[A]:MET:HG2	8:D:2211:HOH:O	2.18	0.42
1:C:33:HIS:HA	1:C:59:CYS:O	2.20	0.42
1:C:206[C]:VAL:CG2	1:C:209:LEU:HD21	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ARG:NH2	8:A:2324:HOH:O	2.53	0.42
1:B:235:GLU:HG2	8:B:2012:HOH:O	2.20	0.41
1:C:164:VAL:O	1:C:179:HIS:HE1	2.04	0.41
1:D:65:ASN:HA	1:D:69:LEU:HD22	2.02	0.41
1:A:138:PHE:O	1:A:142:GLN:HG2	2.22	0.40
2:D:1269:NAP:O2A	3:D:1270[A]:AX3:HADA	2.21	0.40
1:C:141:ARG:HG2	8:C:2230:HOH:O	2.21	0.40
1:D:9:THR:HA	1:D:33:HIS:HB3	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	251/288 (87%)	242 (96%)	9 (4%)	0	100	100
1	B	254/288 (88%)	245 (96%)	9 (4%)	0	100	100
1	C	251/288 (87%)	242 (96%)	9 (4%)	0	100	100
1	D	253/288 (88%)	244 (96%)	9 (4%)	0	100	100
All	All	1009/1152 (88%)	973 (96%)	36 (4%)	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	205/231 (89%)	204 (100%)	1 (0%)	81	58
1	B	209/231 (90%)	206 (99%)	3 (1%)	59	21
1	C	206/231 (89%)	202 (98%)	4 (2%)	50	11
1	D	205/231 (89%)	203 (99%)	2 (1%)	68	34
All	All	825/924 (89%)	815 (99%)	10 (1%)	61	26

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	VAL
1	B	142	GLN
1	B	166	GLN
1	B	216	GLU
1	C	2	GLU
1	C	50	LYS
1	C	152	SER
1	C	164	VAL
1	D	141	ARG
1	D	166	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	186	GLN
1	B	92	ASN
1	B	175	ASN
1	C	54	ASN
1	C	92	ASN
1	C	175	ASN
1	C	179	HIS
1	C	250	GLN
1	D	54	ASN
1	D	92	ASN
1	D	175	ASN
1	D	179	HIS
1	D	250	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 for Mogul analysis.

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	AX3	C	1270[B]	-	13,13,13	2.25	4 (30%)	18,18,18	4.80	9 (50%)
2	NAP	A	1269	-	50,52,52	1.07	2 (4%)	71,80,80	1.24	7 (9%)
3	AX3	A	1270	-	13,13,13	1.27	1 (7%)	18,18,18	1.80	7 (38%)
4	DTD	C	1271[A]	-	8,8,8	1.93	3 (37%)	6,10,10	3.65	4 (66%)
2	NAP	D	1269	-	50,52,52	1.06	2 (4%)	71,80,80	1.28	7 (9%)
6	D1D	B	1271[A]	-	8,8,8	0.43	0	6,10,10	1.96	3 (50%)
3	AX3	B	1270[A]	-	13,13,13	1.47	1 (7%)	18,18,18	2.99	7 (38%)
3	AX3	D	1270[B]	-	13,13,13	1.45	2 (15%)	18,18,18	7.25	11 (61%)
3	AX3	C	1270[A]	-	13,13,13	1.45	2 (15%)	18,18,18	3.98	9 (50%)
2	NAP	C	1269	-	50,52,52	1.00	4 (8%)	71,80,80	0.97	3 (4%)
2	NAP	B	1269	-	50,52,52	1.17	4 (8%)	71,80,80	1.33	9 (12%)
6	D1D	D	1271[B]	-	8,8,8	1.68	1 (12%)	6,10,10	2.93	3 (50%)
3	AX3	D	1270[A]	-	13,13,13	1.33	1 (7%)	18,18,18	4.29	8 (44%)
4	DTD	A	1271[B]	-	8,8,8	1.96	1 (12%)	6,10,10	2.50	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	D1D	D	1271[A]	-	8,8,8	1.24	0	6,10,10	2.93	3 (50%)
4	DTD	C	1271[B]	-	8,8,8	1.41	2 (25%)	6,10,10	3.65	4 (66%)
4	DTD	A	1271[A]	-	8,8,8	0.95	0	6,10,10	2.50	2 (33%)
6	D1D	B	1271[B]	-	8,8,8	1.00	1 (12%)	6,10,10	1.96	3 (50%)
7	ACT	C	1272	-	3,3,3	1.04	0	3,3,3	0.94	0
3	AX3	B	1270[B]	-	13,13,13	3.12	4 (30%)	18,18,18	6.96	10 (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	AX3	C	1270[B]	-	-	0/4/6/6	0/2/2/2
2	NAP	A	1269	-	-	0/35/67/67	0/5/5/5
3	AX3	A	1270	-	-	0/4/6/6	0/2/2/2
4	DTD	C	1271[A]	-	-	-	0/1/1/1
2	NAP	D	1269	-	-	0/35/67/67	0/5/5/5
6	D1D	B	1271[A]	-	-	-	1/1/1/1
3	AX3	B	1270[A]	-	-	3/4/6/6	0/2/2/2
3	AX3	D	1270[B]	-	-	2/4/6/6	0/2/2/2
3	AX3	C	1270[A]	-	-	2/4/6/6	0/2/2/2
2	NAP	C	1269	-	-	0/35/67/67	0/5/5/5
2	NAP	B	1269	-	-	0/35/67/67	0/5/5/5
6	D1D	D	1271[B]	-	-	-	1/1/1/1
3	AX3	D	1270[A]	-	-	3/4/6/6	0/2/2/2
4	DTD	A	1271[B]	-	-	-	1/1/1/1
6	D1D	D	1271[A]	-	-	-	0/1/1/1
4	DTD	C	1271[B]	-	-	-	0/1/1/1
4	DTD	A	1271[A]	-	-	-	0/1/1/1
6	D1D	B	1271[B]	-	-	-	0/1/1/1
3	AX3	B	1270[B]	-	-	0/4/6/6	0/2/2/2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1270[B]	AX3	CAK-NAH	-9.58	1.23	1.34
3	C	1270[B]	AX3	CAK-NAH	-5.94	1.27	1.34
4	A	1271[B]	DTD	C1-S1	4.88	1.87	1.82
3	B	1270[A]	AX3	CAI-NAA	-4.29	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1270[B]	AX3	CAI-NAA	-4.29	1.25	1.33
6	D	1271[B]	D1D	C4-S4	3.77	1.86	1.82
4	C	1271[A]	DTD	C4-S4	3.75	1.86	1.82
3	C	1270[B]	AX3	CAL-NAH	2.73	1.52	1.46
2	C	1269	NAP	C2N-N1N	2.70	1.38	1.35
3	D	1270[A]	AX3	CAI-NAA	-2.64	1.28	1.33
3	D	1270[B]	AX3	CAI-NAA	-2.64	1.28	1.33
4	C	1271[A]	DTD	C3-C2	-2.64	1.47	1.52
4	C	1271[B]	DTD	C3-C2	-2.64	1.47	1.52
2	D	1269	NAP	PA-O3	2.63	1.62	1.59
2	B	1269	NAP	PN-O3	2.62	1.62	1.59
6	B	1271[B]	D1D	C1-S1	2.62	1.85	1.82
3	C	1270[B]	AX3	CAD-CAL	2.56	1.54	1.48
3	C	1270[A]	AX3	CAK-NAH	2.52	1.37	1.34
2	A	1269	NAP	PN-O3	2.50	1.62	1.59
2	D	1269	NAP	C8A-N9A	-2.45	1.33	1.37
4	C	1271[A]	DTD	C1-S1	-2.41	1.79	1.82
4	C	1271[B]	DTD	C1-S1	-2.41	1.79	1.82
3	A	1270	AX3	CAD-CAL	2.39	1.54	1.48
2	A	1269	NAP	C2N-N1N	2.39	1.37	1.35
3	B	1270[B]	AX3	CAL-NAH	2.32	1.51	1.46
2	C	1269	NAP	C4N-C3N	2.27	1.42	1.39
3	B	1270[B]	AX3	CAC-CAL	2.23	1.54	1.48
2	C	1269	NAP	PA-O3	-2.23	1.57	1.59
2	B	1269	NAP	C8A-N7A	2.22	1.35	1.31
2	B	1269	NAP	PA-O3	2.21	1.61	1.59
2	B	1269	NAP	C2A-N1A	-2.21	1.30	1.33
3	D	1270[B]	AX3	CAL-NAH	2.19	1.51	1.46
3	C	1270[A]	AX3	CAJ-NAB	-2.13	1.29	1.33
3	C	1270[B]	AX3	CAJ-NAB	-2.13	1.29	1.33
2	C	1269	NAP	C6N-N1N	2.03	1.40	1.35

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1270[B]	AX3	CAK-NAH-CAL	-24.63	86.03	124.32
3	B	1270[B]	AX3	CAD-CAL-NAH	-22.87	70.42	118.06
3	C	1270[B]	AX3	CAC-CAL-NAH	-17.20	82.25	118.06
3	B	1270[B]	AX3	CAK-NAH-CAL	-14.99	101.01	124.32
3	C	1270[A]	AX3	CAK-NAH-CAL	-14.15	102.33	124.32
3	D	1270[A]	AX3	NAA-CAI-NAE	11.30	134.16	117.22
3	D	1270[B]	AX3	NAA-CAI-NAE	11.30	134.16	117.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1270[A]	AX3	CAD-CAL-NAH	8.31	135.38	118.06
3	D	1270[B]	AX3	CAD-CAL-NAH	-8.08	101.24	118.06
3	C	1270[B]	AX3	CAK-NAH-CAL	-7.72	112.32	124.32
3	D	1270[A]	AX3	NAA-CAI-NAF	-7.25	106.35	117.22
3	D	1270[B]	AX3	NAA-CAI-NAF	-7.25	106.35	117.22
3	B	1270[A]	AX3	CAC-CAL-NAH	7.07	132.79	118.06
3	B	1270[A]	AX3	NAA-CAI-NAE	5.97	126.17	117.22
3	B	1270[B]	AX3	NAA-CAI-NAE	5.97	126.17	117.22
4	C	1271[A]	DTD	C4-C3-C2	5.94	124.18	112.45
4	C	1271[B]	DTD	C4-C3-C2	5.94	124.18	112.45
6	D	1271[A]	D1D	O3-C3-C4	-5.62	100.37	109.81
6	D	1271[B]	D1D	O3-C3-C4	-5.62	100.37	109.81
3	B	1270[A]	AX3	NAA-CAI-NAF	-5.51	108.96	117.22
3	B	1270[B]	AX3	NAA-CAI-NAF	-5.51	108.96	117.22
4	A	1271[A]	DTD	O3-C3-C4	-5.28	100.94	109.81
4	A	1271[B]	DTD	O3-C3-C4	-5.28	100.94	109.81
4	C	1271[A]	DTD	O3-C3-C2	5.20	121.61	110.20
4	C	1271[B]	DTD	O3-C3-C2	5.20	121.61	110.20
3	D	1270[A]	AX3	CAJ-NAE-CAI	4.34	121.81	114.76
3	D	1270[B]	AX3	CAJ-NAE-CAI	4.34	121.81	114.76
2	B	1269	NAP	C5N-C4N-C3N	-4.21	116.23	120.36
3	C	1270[A]	AX3	NAH-CAK-NAF	-4.03	110.76	117.09
3	D	1270[A]	AX3	NAE-CAI-NAF	-3.91	119.48	125.48
3	D	1270[B]	AX3	NAE-CAI-NAF	-3.91	119.48	125.48
3	C	1270[A]	AX3	CAC-CAL-NAH	3.81	126.00	118.06
3	D	1270[A]	AX3	NAE-CAJ-NAG	-3.73	119.77	125.48
3	D	1270[B]	AX3	NAE-CAJ-NAG	-3.73	119.77	125.48
3	D	1270[A]	AX3	NAB-CAJ-NAE	3.69	122.76	117.22
3	D	1270[B]	AX3	NAB-CAJ-NAE	3.69	122.76	117.22
3	A	1270	AX3	CAI-NAF-CAK	3.57	119.69	113.77
2	A	1269	NAP	C5N-C4N-C3N	-3.43	117.00	120.36
3	C	1270[A]	AX3	NAB-CAJ-NAE	3.42	122.35	117.22
3	C	1270[B]	AX3	NAB-CAJ-NAE	3.42	122.35	117.22
3	A	1270	AX3	NAE-CAI-NAF	-3.32	120.39	125.48
3	D	1270[B]	AX3	CAC-CAL-NAH	3.32	124.97	118.06
3	C	1270[A]	AX3	NAH-CAK-NAG	3.30	122.27	117.09
2	D	1269	NAP	C4A-C5A-N7A	-3.23	106.89	110.58
3	B	1270[A]	AX3	NAB-CAJ-NAE	3.16	121.97	117.22
3	B	1270[B]	AX3	NAB-CAJ-NAE	3.16	121.97	117.22
6	D	1271[A]	D1D	O2-C2-C1	-3.14	104.53	109.81
6	D	1271[B]	D1D	O2-C2-C1	-3.14	104.53	109.81
2	B	1269	NAP	N9A-C8A-N7A	-3.08	109.57	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1269	NAP	C6N-C5N-C4N	3.07	123.88	119.45
2	B	1269	NAP	C4A-N9A-C8A	3.06	108.95	105.74
3	B	1270[B]	AX3	CAC-CAD-CAL	2.99	62.40	59.80
4	C	1271[A]	DTD	C1-C2-C3	2.98	118.34	112.45
4	C	1271[B]	DTD	C1-C2-C3	2.98	118.34	112.45
3	B	1270[B]	AX3	NAH-CAK-NAF	-2.98	112.40	117.09
3	B	1270[A]	AX3	NAF-CAK-NAG	2.98	131.14	126.26
3	B	1270[B]	AX3	NAF-CAK-NAG	2.98	131.14	126.26
2	D	1269	NAP	N9A-C8A-N7A	-2.97	109.73	113.94
6	B	1271[A]	D1D	O2-C2-C1	-2.96	104.85	109.81
6	B	1271[B]	D1D	O2-C2-C1	-2.96	104.85	109.81
3	C	1270[A]	AX3	CAJ-NAE-CAI	2.92	119.52	114.76
3	C	1270[B]	AX3	CAJ-NAE-CAI	2.92	119.52	114.76
2	B	1269	NAP	O7N-C7N-C3N	-2.89	116.06	119.60
2	B	1269	NAP	C6N-N1N-C2N	-2.86	119.45	121.88
3	C	1270[A]	AX3	NAA-CAI-NAE	2.77	121.38	117.22
3	C	1270[B]	AX3	NAA-CAI-NAE	2.77	121.38	117.22
3	D	1270[A]	AX3	CAI-NAF-CAK	2.77	118.36	113.77
3	D	1270[B]	AX3	CAI-NAF-CAK	2.77	118.36	113.77
3	A	1270	AX3	CAD-CAL-NAH	-2.76	112.31	118.06
2	A	1269	NAP	C6N-C5N-C4N	2.76	123.43	119.45
6	B	1271[A]	D1D	C1-C2-C3	2.76	117.91	112.45
6	B	1271[B]	D1D	C1-C2-C3	2.76	117.91	112.45
3	B	1270[A]	AX3	NAH-CAK-NAG	-2.74	112.77	117.09
2	D	1269	NAP	C4A-N9A-C8A	2.72	108.59	105.74
3	C	1270[B]	AX3	CAD-CAC-CAL	2.68	62.13	59.80
2	C	1269	NAP	N9A-C8A-N7A	-2.66	110.16	113.94
3	C	1270[B]	AX3	CAD-CAL-CAC	-2.60	57.82	60.40
4	A	1271[A]	DTD	O3-C3-C2	-2.58	104.54	110.20
4	A	1271[B]	DTD	O3-C3-C2	-2.58	104.54	110.20
2	D	1269	NAP	C5A-N7A-C8A	2.54	107.45	103.45
6	D	1271[A]	D1D	C1-C2-C3	2.53	117.45	112.45
6	D	1271[B]	D1D	C1-C2-C3	2.53	117.45	112.45
2	A	1269	NAP	O3B-C3B-C2B	2.51	118.21	111.19
2	A	1269	NAP	C4B-O4B-C1B	-2.50	103.95	109.47
2	A	1269	NAP	C5A-C4A-N3A	-2.47	123.32	126.72
4	C	1271[A]	DTD	O2-C2-C3	2.44	115.56	110.20
4	C	1271[B]	DTD	O2-C2-C3	2.44	115.56	110.20
2	B	1269	NAP	C5A-C4A-N3A	-2.34	123.49	126.72
2	D	1269	NAP	C3N-C7N-N7N	2.33	120.60	117.74
3	B	1270[B]	AX3	CAD-CAC-CAL	-2.32	57.79	59.80
3	A	1270	AX3	NAA-CAI-NAE	2.31	120.68	117.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1269	NAP	C4A-C5A-N7A	-2.29	107.96	110.58
3	C	1270[A]	AX3	NAE-CAI-NAF	-2.26	122.02	125.48
3	C	1270[B]	AX3	NAE-CAI-NAF	-2.26	122.02	125.48
2	D	1269	NAP	O7N-C7N-C3N	-2.24	116.86	119.60
3	A	1270	AX3	NAF-CAK-NAG	-2.21	122.63	126.26
2	C	1269	NAP	C4B-O4B-C1B	-2.18	104.65	109.47
3	A	1270	AX3	NAH-CAK-NAG	2.15	120.46	117.09
3	C	1270[A]	AX3	NAE-CAJ-NAG	-2.13	122.21	125.48
3	C	1270[B]	AX3	NAE-CAJ-NAG	-2.13	122.21	125.48
2	B	1269	NAP	O3B-C3B-C2B	2.12	117.11	111.19
2	D	1269	NAP	C4B-O4B-C1B	-2.10	104.82	109.47
3	A	1270	AX3	CAK-NAH-CAL	-2.07	121.10	124.32
3	B	1270[A]	AX3	CAJ-NAE-CAI	2.07	118.12	114.76
3	B	1270[B]	AX3	CAJ-NAE-CAI	2.07	118.12	114.76
2	B	1269	NAP	C4A-N9A-C1B	-2.04	121.86	126.63
2	A	1269	NAP	C5N-C6N-N1N	-2.02	117.63	120.38
3	D	1270[B]	AX3	CAD-CAC-CAL	2.01	61.55	59.80
6	B	1271[A]	D1D	O2-C2-C3	-2.01	105.80	110.20
6	B	1271[B]	D1D	O2-C2-C3	-2.01	105.80	110.20
2	C	1269	NAP	C6N-N1N-C2N	-2.00	120.17	121.88

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1270[A]	AX3	CAC-CAL-NAH-CAK
3	B	1270[A]	AX3	NAG-CAK-NAH-CAL
3	B	1270[A]	AX3	NAF-CAK-NAH-CAL
3	C	1270[A]	AX3	NAG-CAK-NAH-CAL
3	D	1270[A]	AX3	CAC-CAL-NAH-CAK
3	D	1270[A]	AX3	NAG-CAK-NAH-CAL
3	D	1270[A]	AX3	NAF-CAK-NAH-CAL
3	D	1270[B]	AX3	NAG-CAK-NAH-CAL
3	D	1270[B]	AX3	NAF-CAK-NAH-CAL
3	C	1270[A]	AX3	NAF-CAK-NAH-CAL

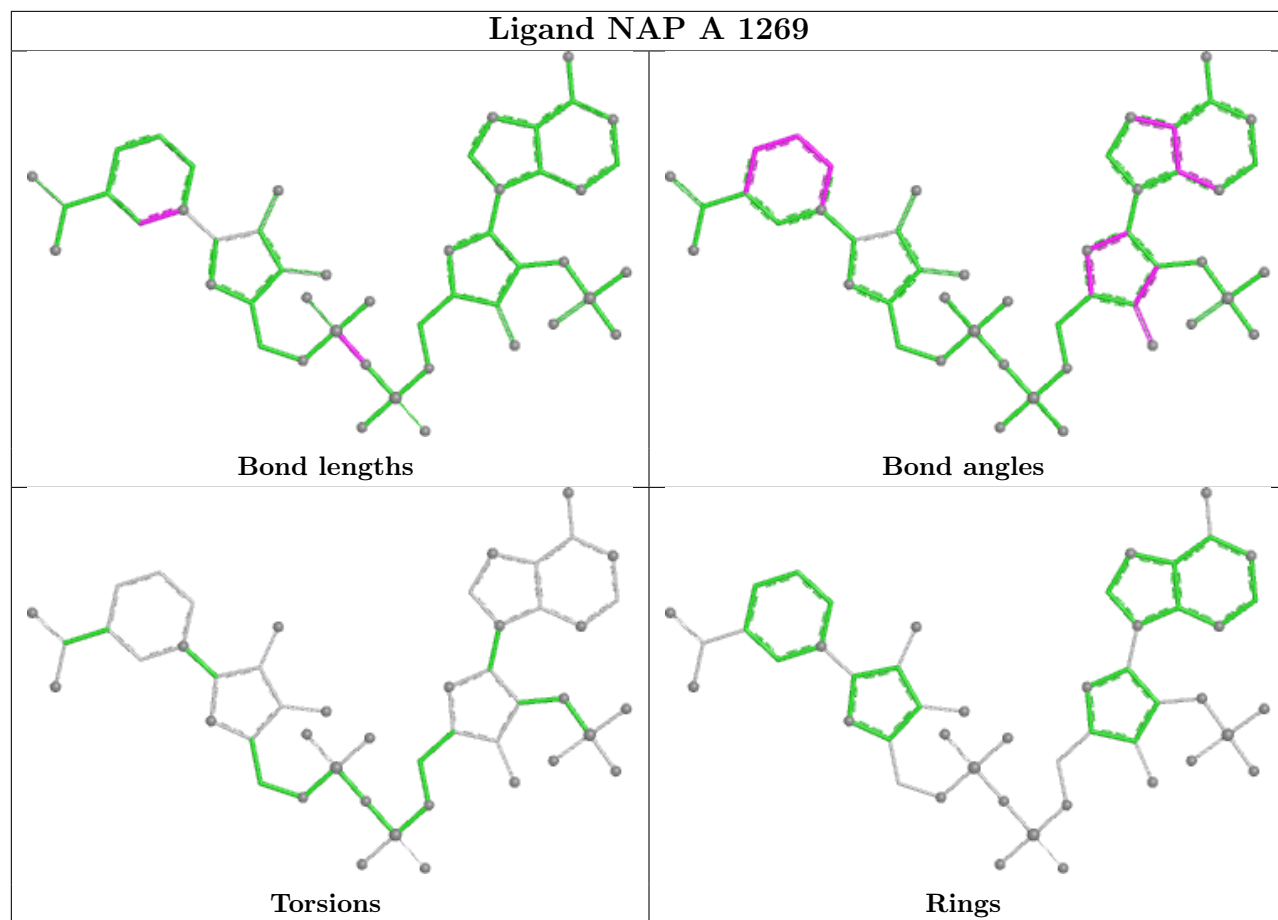
All (3) ring outliers are listed below:

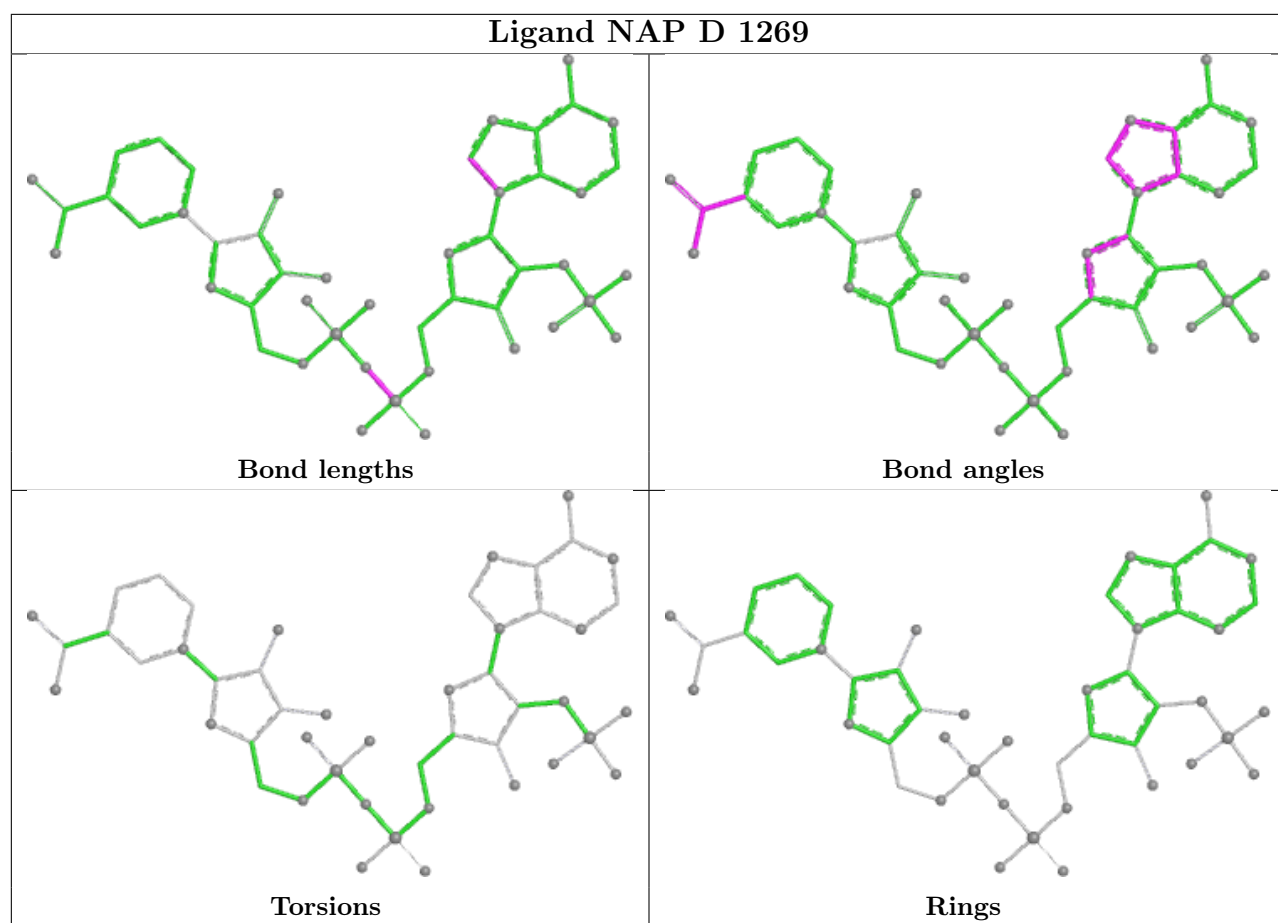
Mol	Chain	Res	Type	Atoms
6	D	1271[B]	D1D	C1-C2-C3-C4-S1-S4
6	B	1271[A]	D1D	C1-C2-C3-C4-S1-S4
4	A	1271[B]	DTD	C1-C2-C3-C4-S1-S4

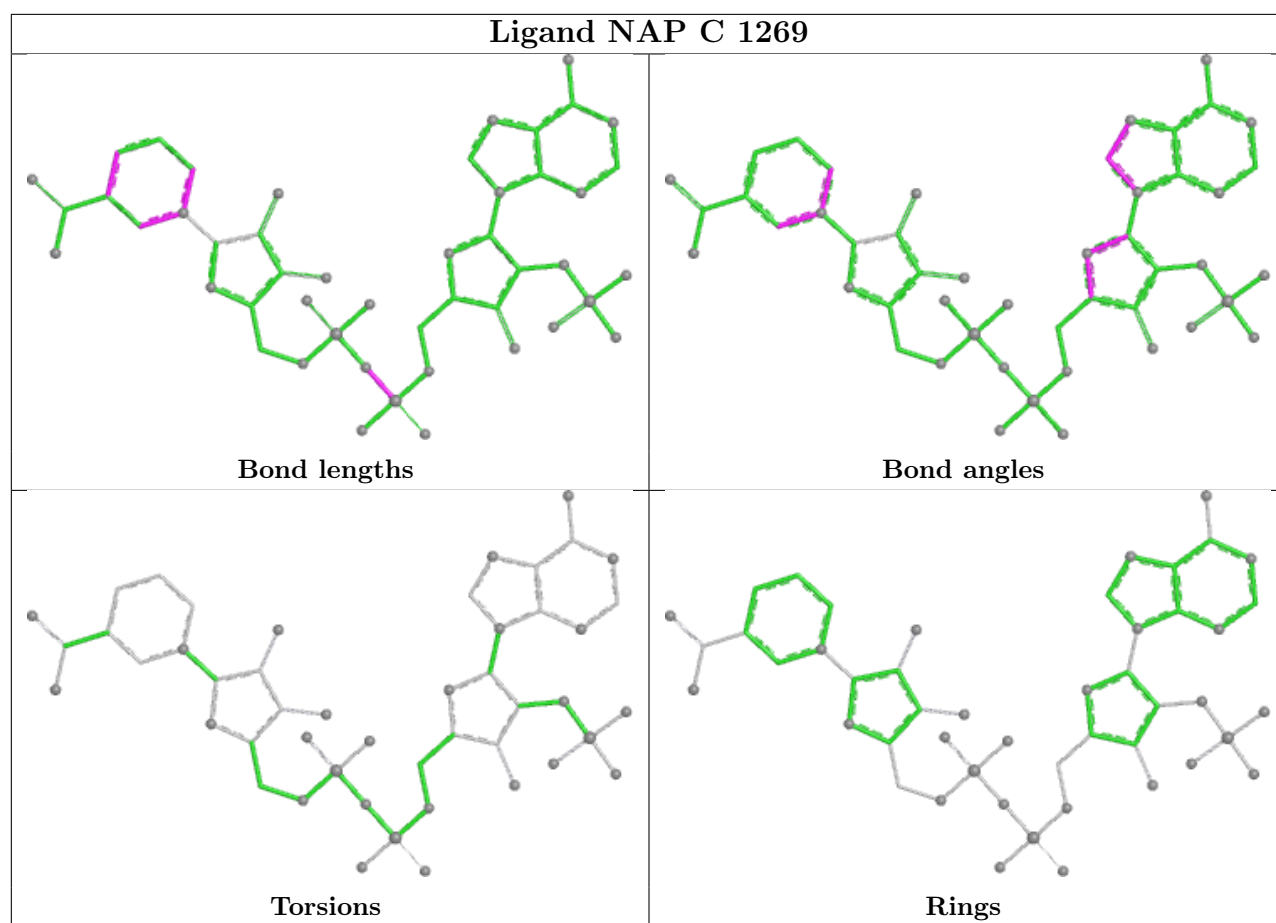
13 monomers are involved in 34 short contacts:

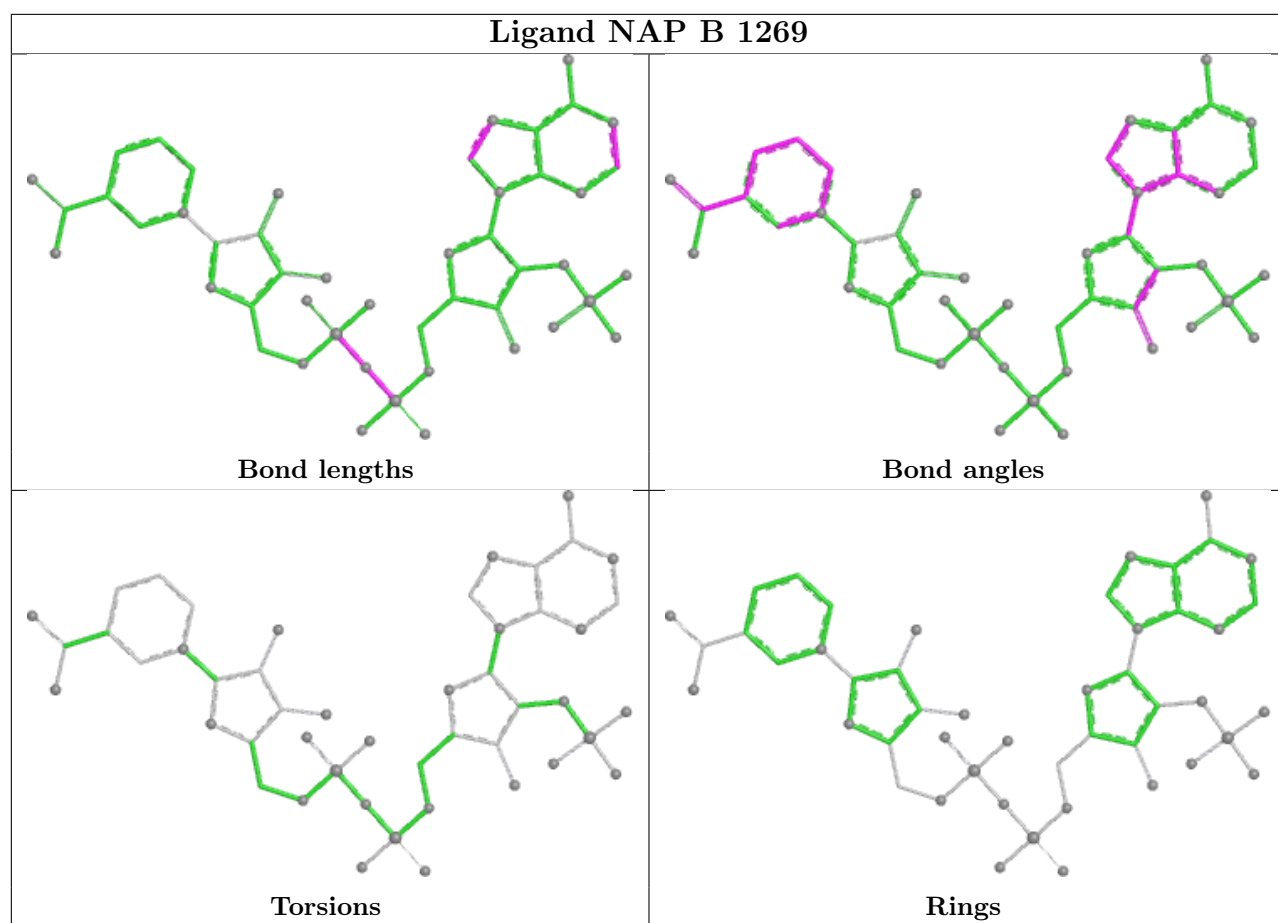
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1270[B]	AX3	7	0
3	A	1270	AX3	1	0
2	D	1269	NAP	2	0
3	B	1270[A]	AX3	2	0
3	D	1270[B]	AX3	9	0
3	C	1270[A]	AX3	3	0
2	C	1269	NAP	1	0
2	B	1269	NAP	2	0
6	D	1271[B]	D1D	4	0
3	D	1270[A]	AX3	3	0
4	A	1271[B]	DTD	1	0
6	B	1271[B]	D1D	1	0
3	B	1270[B]	AX3	9	0

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	248/288 (86%)	-0.11	5 (2%)	65	74	4, 9, 21, 40	7 (2%)
1	B	248/288 (86%)	0.05	8 (3%)	50	58	5, 10, 26, 40	11 (4%)
1	C	249/288 (86%)	0.03	7 (2%)	55	63	5, 10, 27, 41	6 (2%)
1	D	247/288 (85%)	0.06	11 (4%)	38	45	4, 10, 26, 39	10 (4%)
All	All	992/1152 (86%)	0.01	31 (3%)	51	59	4, 10, 26, 41	34 (3%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	211	VAL	4.9
1	C	211	VAL	4.1
1	D	103	VAL	3.7
1	A	103	VAL	3.6
1	D	211	VAL	3.5
1	B	142	GLN	3.5
1	D	142	GLN	3.5
1	B	212	ALA	3.3
1	C	152	SER	3.1
1	D	212	ALA	3.1
1	C	114	LYS	2.7
1	D	219	ASP	2.6
1	A	211	VAL	2.6
1	B	210	PRO	2.6
1	B	195	TYR	2.4
1	D	152	SER	2.4
1	C	50	LYS	2.4
1	A	212	ALA	2.3
1	B	152	SER	2.3
1	D	3	ALA	2.3
1	A	142	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	141	ARG	2.2
1	D	214	GLY	2.2
1	C	2	GLU	2.2
1	B	208	LEU	2.2
1	D	208	LEU	2.2
1	C	212	ALA	2.1
1	B	103	VAL	2.1
1	C	103	VAL	2.1
1	D	210	PRO	2.1
1	A	152	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

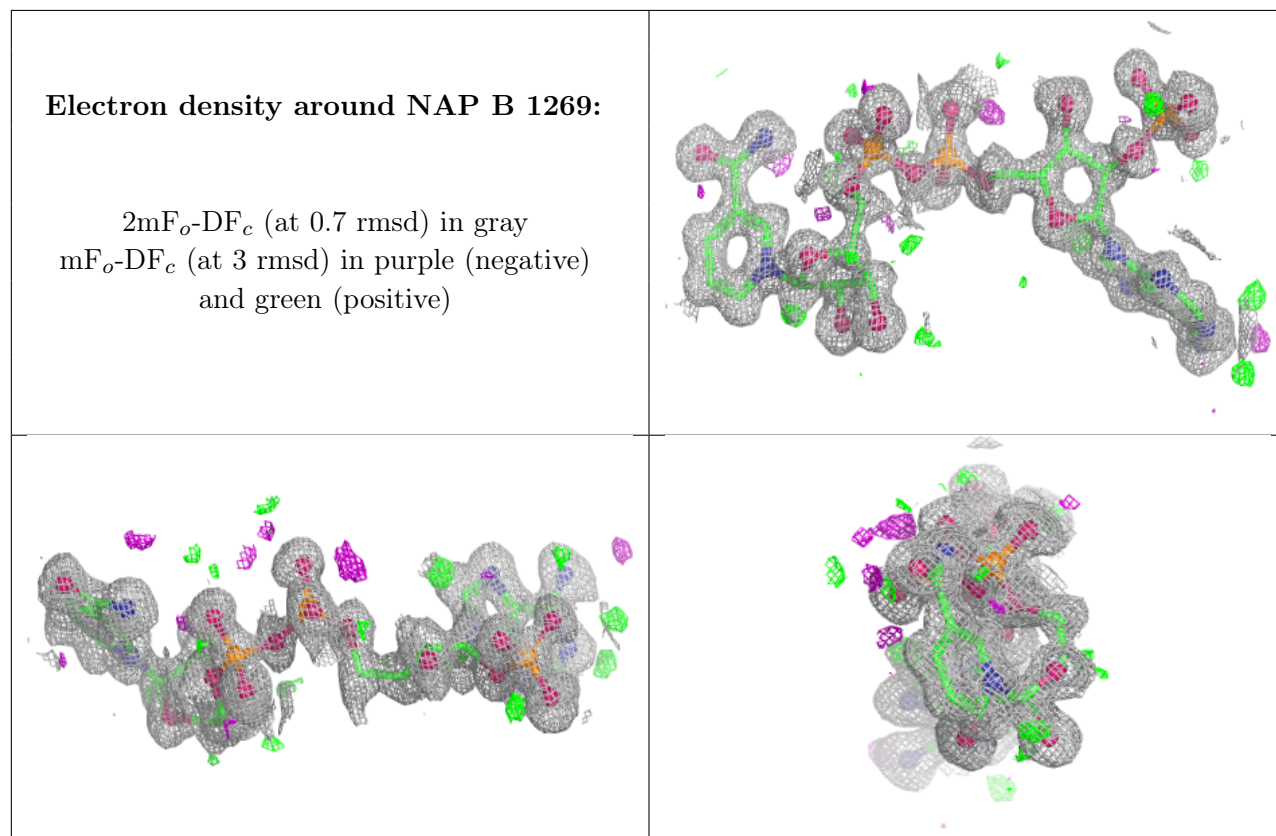
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	D1D	D	1271[A]	8/8	0.88	0.16	19,22,23,25	8
6	D1D	D	1271[B]	8/8	0.88	0.16	19,23,25,26	8
3	AX3	D	1270[A]	12/12	0.90	0.14	16,21,24,24	4
3	AX3	D	1270[B]	12/12	0.90	0.14	16,22,30,31	4
4	DTD	C	1271[A]	8/8	0.91	0.14	26,31,33,36	1
4	DTD	C	1271[B]	8/8	0.91	0.14	28,31,33,36	1
3	AX3	B	1270[A]	12/12	0.91	0.12	14,19,21,22	4
3	AX3	B	1270[B]	12/12	0.91	0.12	14,20,22,23	4
6	D1D	B	1271[A]	8/8	0.92	0.12	28,32,34,38	1
6	D1D	B	1271[B]	8/8	0.92	0.12	26,32,34,38	1
4	DTD	A	1271[A]	8/8	0.94	0.12	13,25,31,39	1
4	DTD	A	1271[B]	8/8	0.94	0.12	13,25,31,39	1
3	AX3	C	1270[A]	12/12	0.94	0.10	17,19,22,23	4

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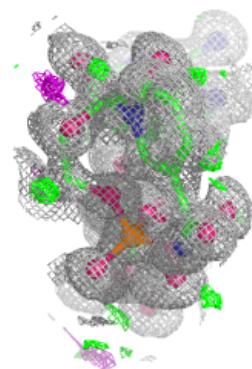
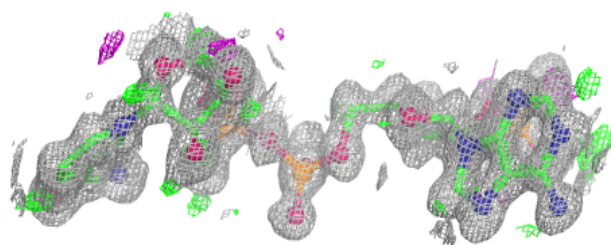
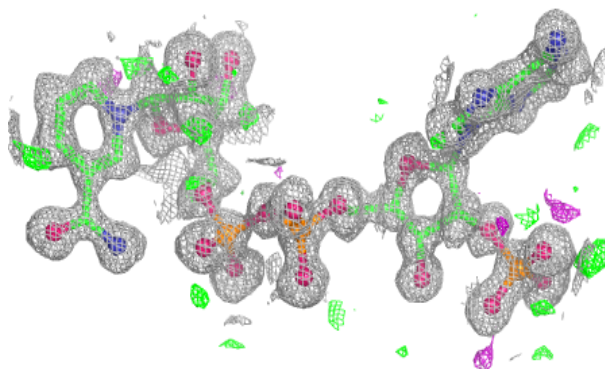
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	AX3	C	1270[B]	12/12	0.94	0.10	17,20,22,22	4
5	NA	A	1272	1/1	0.96	0.09	31,31,31,31	0
5	NA	D	1272	1/1	0.98	0.21	26,26,26,26	0
2	NAP	B	1269	48/48	0.99	0.03	6,8,11,15	0
2	NAP	C	1269	48/48	0.99	0.03	5,8,11,13	0
2	NAP	D	1269	48/48	0.99	0.04	7,8,11,12	0
3	AX3	A	1270	12/12	0.99	0.04	6,7,16,17	0
7	ACT	C	1272	4/4	0.99	0.05	11,11,12,14	0
2	NAP	A	1269	48/48	1.00	0.03	5,7,9,11	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.

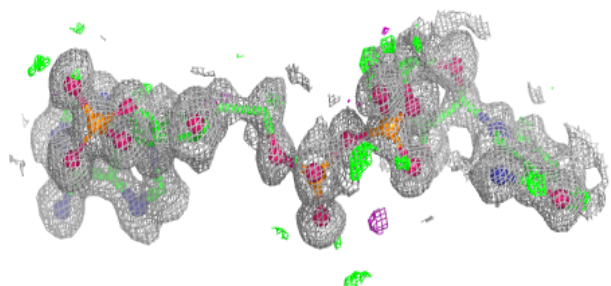
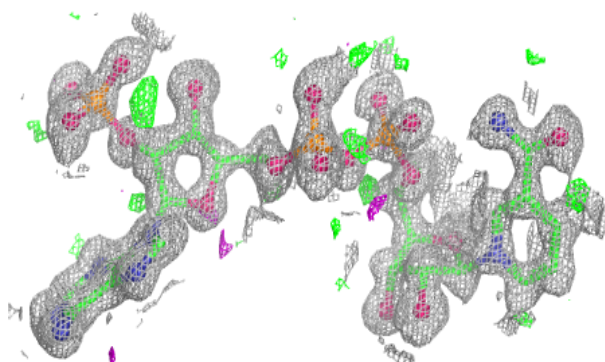


Electron density around NAP C 1269:

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

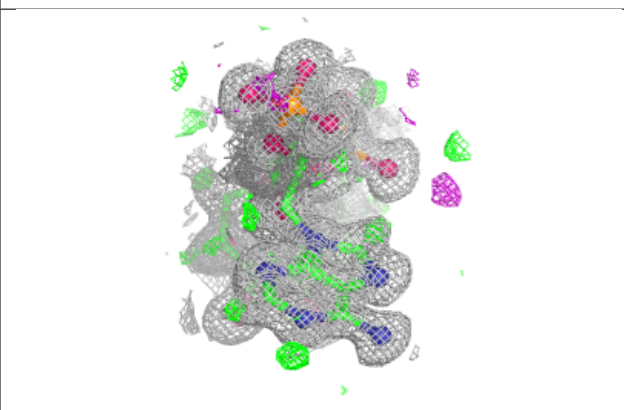
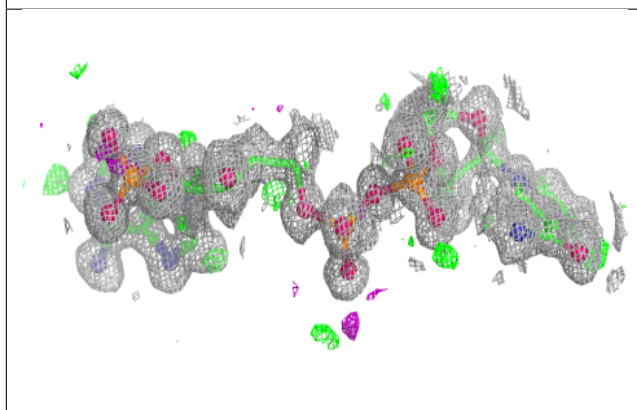
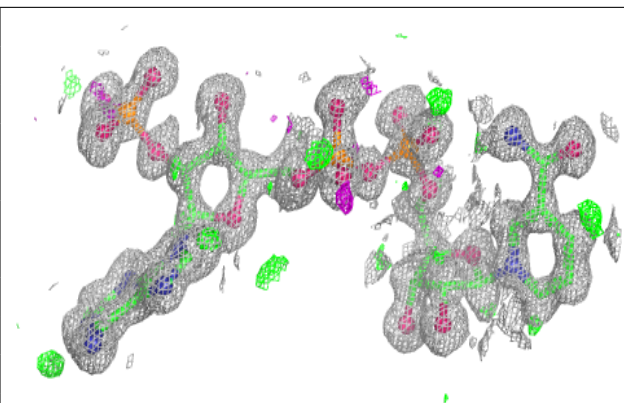
**Electron density around NAP D 1269:**

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



Electron density around NAP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.