



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:45 AM UTC

PDB ID : 3ZEP / pdb_00003zep
Title : Crystal Structure of JAK3 Kinase Domain in Complex with a Pyrrolopyrazin
e-2-phenyl Ether Inhibitor
Authors : Kuglstatter, A.; Jestel, A.; Nagel, S.; Boettcher, J.; Blaesse, M.
Deposited on : 2012-12-06
Resolution : 2.35 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

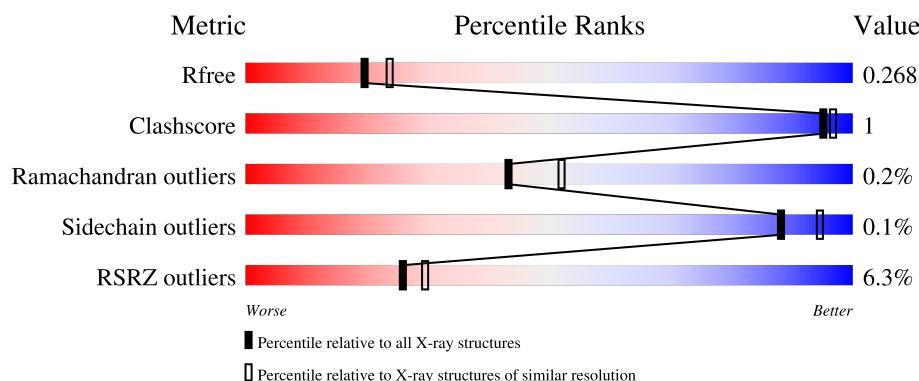
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	 4% 91% 5% •
1	B	288	 8% 91% • 6%
1	C	288	 6% 94% • •
1	D	288	 6% 93% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9259 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.

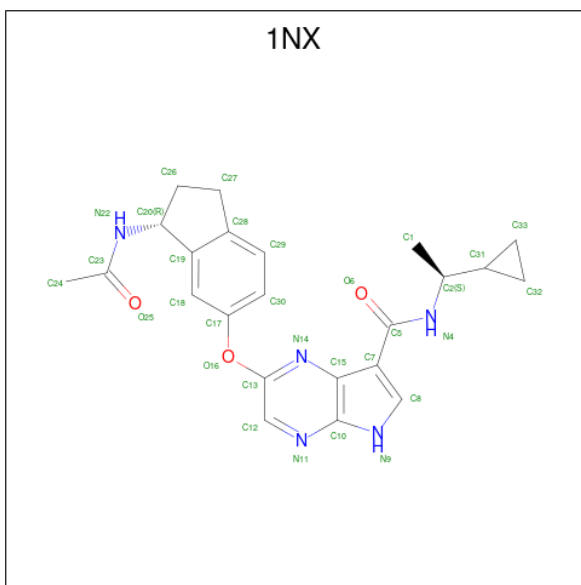
- Molecule 1 is a protein called TYROSINE-PROTEIN KINASE JAK3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	P	S	41	0	0
			2215	1407	385	407	2	14			
1	B	270	Total	C	N	O	P	S	54	1	0
			2188	1392	382	398	2	14			
1	C	278	Total	C	N	O	P	S	57	0	0
			2240	1421	390	413	2	14			
1	D	274	Total	C	N	O	P	S	41	0	0
			2207	1405	383	403	2	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1040	SER	CYS	engineered mutation	UNP P52333
A	1048	SER	CYS	engineered mutation	UNP P52333
B	1040	SER	CYS	engineered mutation	UNP P52333
B	1048	SER	CYS	engineered mutation	UNP P52333
C	1040	SER	CYS	engineered mutation	UNP P52333
C	1048	SER	CYS	engineered mutation	UNP P52333
D	1040	SER	CYS	engineered mutation	UNP P52333
D	1048	SER	CYS	engineered mutation	UNP P52333

- Molecule 2 is 2-[[[(3R)-3-acetamido-2,3-dihydro-1H-inden-5-yl]oxy]-N-[(1S)-1-cyclopropylethyl]-5H-pyrrolo[2,3-b]pyrazine-7-carboxamide (CCD ID: 1NX) (formula: C₂₃H₂₅N₅O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	23	5	3		
2	B	1	Total	C	N	O	0	0
			31	23	5	3		
2	C	1	Total	C	N	O	0	0
			31	23	5	3		
2	D	1	Total	C	N	O	0	0
			31	23	5	3		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

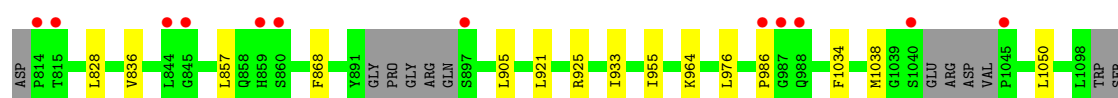
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	74	Total	O	0	0
			74	74		
4	B	69	Total	O	0	0
			69	69		
4	C	71	Total	O	0	0
			71	71		
4	D	65	Total	O	0	0
			65	65		

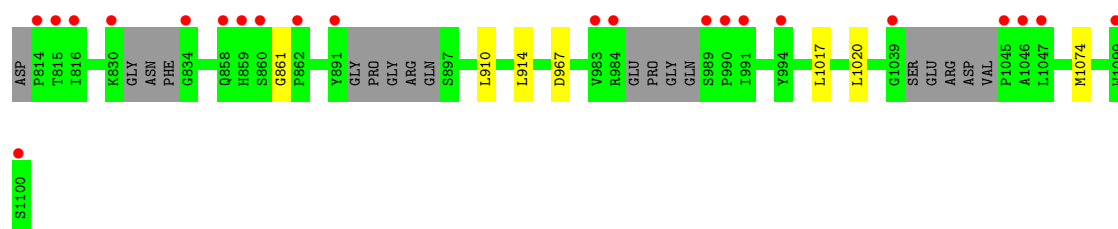
3 Residue-property plots

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.

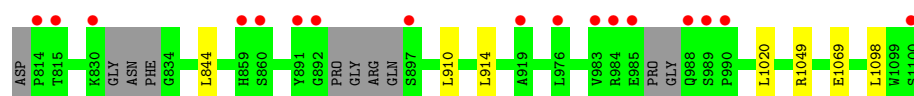
• Molecule 1: TYROSINE-PROTEIN KINASE JAK3



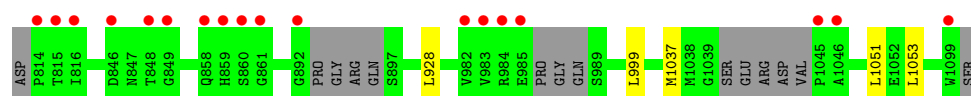
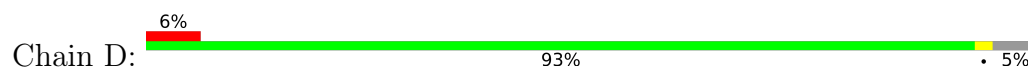
• Molecule 1: TYROSINE-PROTEIN KINASE JAK3



• Molecule 1: TYROSINE-PROTEIN KINASE JAK3



• Molecule 1: TYROSINE-PROTEIN KINASE JAK3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.55Å 114.08Å 104.20Å 90.00° 96.82° 90.00°	Depositor
Resolution (Å)	103.70 – 2.35 103.46 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.8 (103.70-2.35) 96.9 (103.46-2.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.226 , 0.265 0.227 , 0.268	Depositor DCC
R_{free} test set	924 reflections (1.66%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9259	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: GOL, 1NX, PTR

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	0/2232	0.80	0/3012
1	B	0.69	0/2203	0.80	0/2970
1	C	0.71	1/2256 (0.0%)	0.79	0/3044
1	D	0.70	0/2224	0.81	0/3000
All	All	0.70	1/8915 (0.0%)	0.80	0/12026

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1049	ARG	NE-CZ	5.45	1.39	1.33

There are no bond angle outliers.

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	2215	0	2192	11	0
1	B	2188	0	2171	4	0
1	C	2240	0	2212	3	0
1	D	2207	0	2181	4	0
2	A	31	0	25	0	0
2	B	31	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	31	0	25	0	0
2	D	31	0	25	0	0
3	C	6	0	8	0	0
4	A	74	0	0	0	0
4	B	69	0	0	0	0
4	C	71	0	0	0	0
4	D	65	0	0	0	0
All	All	9259	0	8864	21	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 1.

All (21) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1038:MET:HE2	1:A:1050:LEU:HB2	1.81	0.62
1:B:910:LEU:HD21	1:B:1020:LEU:HD21	1.82	0.61
1:C:910:LEU:HD21	1:C:1020:LEU:HD21	1.86	0.56
1:A:1038:MET:CE	1:A:1050:LEU:HD13	2.36	0.55
1:B:1017:LEU:HB3	1:B:1074:MET:HE2	1.87	0.54
1:C:914:LEU:HD11	1:C:1020:LEU:HD23	1.89	0.54
1:B:914:LEU:HD11	1:B:1020:LEU:HD23	1.92	0.51
1:A:1034:PHE:HB3	1:A:1038:MET:HE3	1.93	0.50
1:D:999:LEU:HB3	1:D:1051:LEU:HD11	1.95	0.47
1:A:905:LEU:HD11	1:A:964:LYS:HD2	1.97	0.47
1:D:1037:MET:CB	1:D:1053:LEU:HD11	2.45	0.46
1:A:933:ILE:CD1	1:A:955:ILE:HD13	2.47	0.45
1:D:1037:MET:HB3	1:D:1053:LEU:HD11	1.99	0.45
1:A:1038:MET:HE3	1:A:1050:LEU:HD13	2.00	0.44
1:A:828:LEU:HD12	1:A:836:VAL:HG12	1.98	0.44
1:A:857:LEU:HD11	1:A:868:PHE:HB2	1.99	0.43
1:B:967:ASP:HB2	2:B:2101:1NX:H331	2.00	0.43
1:A:921:LEU:HD22	1:A:925:ARG:HG2	1.99	0.43
1:A:976:LEU:HD12	1:D:928:LEU:HA	2.01	0.42
1:C:1069:GLU:HB3	1:C:1098:LEU:HD21	2.01	0.42
1:A:1038:MET:HE2	1:A:1050:LEU:CB	2.48	0.41

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	268/288 (93%)	259 (97%)	8 (3%)	1 (0%)	30	34
1	B	259/288 (90%)	250 (96%)	8 (3%)	1 (0%)	30	34
1	C	268/288 (93%)	261 (97%)	7 (3%)	0	100	100
1	D	264/288 (92%)	258 (98%)	6 (2%)	0	100	100
All	All	1059/1152 (92%)	1028 (97%)	29 (3%)	2 (0%)	43	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	986	PRO
1	B	861	GLY

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	240/250 (96%)	240 (100%)	0	100	100
1	B	237/250 (95%)	237 (100%)	0	100	100
1	C	243/250 (97%)	242 (100%)	1 (0%)	84	91
1	D	238/250 (95%)	238 (100%)	0	100	100
All	All	958/1000 (96%)	957 (100%)	1 (0%)	88	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	844	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	847	ASN
1	A	856	GLN
1	A	873	GLN
1	B	847	ASN
1	B	856	GLN
1	C	827	GLN
1	D	832	ASN
1	D	856	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	$\# Z > 2$
1	PTR	B	980	1	15,16,17	0.79	0	17,22,24	0.81	0
1	PTR	B	981	1	15,16,17	0.78	0	17,22,24	0.86	0
1	PTR	A	981	1	15,16,17	0.83	0	17,22,24	0.73	0
1	PTR	C	980	1	15,16,17	0.81	0	17,22,24	0.81	0
1	PTR	C	981	1	15,16,17	0.80	0	17,22,24	0.77	0
1	PTR	A	980	1	15,16,17	0.77	0	17,22,24	0.77	0
1	PTR	D	981	1	15,16,17	0.81	0	17,22,24	0.72	0
1	PTR	D	980	1	15,16,17	0.77	0	17,22,24	0.77	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
1	PTR	B	980	1	-	0/10/11/13	0/1/1/1
1	PTR	B	981	1	-	0/10/11/13	0/1/1/1
1	PTR	A	981	1	-	0/10/11/13	0/1/1/1
1	PTR	C	980	1	-	0/10/11/13	0/1/1/1
1	PTR	C	981	1	-	0/10/11/13	0/1/1/1
1	PTR	A	980	1	-	1/10/11/13	0/1/1/1
1	PTR	D	981	1	-	0/10/11/13	0/1/1/1
1	PTR	D	980	1	-	0/10/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	980	PTR	CZ-OH-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	GOL	C	2102	-	5,5,5	0.30	0	5,5,5	0.24	0
2	1NX	C	2101	-	34,35,35	0.68	0	44,51,51	1.95	10 (22%)
2	1NX	A	2099	-	34,35,35	0.66	0	44,51,51	2.03	11 (25%)
2	1NX	D	2100	-	34,35,35	0.67	0	44,51,51	2.01	10 (22%)
2	1NX	B	2101	-	34,35,35	0.70	0	44,51,51	2.09	11 (25%)

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	GOL	C	2102	-	-	1/4/4/4	-
2	1NX	C	2101	-	-	3/20/31/31	0/5/5/5
2	1NX	A	2099	-	-	5/20/31/31	0/5/5/5
2	1NX	D	2100	-	-	4/20/31/31	0/5/5/5
2	1NX	B	2101	-	-	1/20/31/31	0/5/5/5

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2101	1NX	C12-C13-N14	-7.14	118.02	122.99
2	A	2099	1NX	C12-C13-N14	-7.09	118.05	122.99
2	D	2100	1NX	C12-C13-N14	-6.99	118.12	122.99
2	C	2101	1NX	C12-C13-N14	-6.70	118.33	122.99
2	D	2100	1NX	N9-C10-N11	4.97	134.74	126.69
2	B	2101	1NX	N9-C10-N11	4.94	134.70	126.69
2	C	2101	1NX	N9-C10-N11	4.91	134.65	126.69
2	A	2099	1NX	N9-C10-N11	4.76	134.40	126.69
2	B	2101	1NX	C10-N9-C8	4.63	110.66	108.48
2	C	2101	1NX	C10-N9-C8	4.25	110.49	108.48
2	D	2100	1NX	C10-N9-C8	4.23	110.47	108.48
2	A	2099	1NX	C10-N9-C8	4.07	110.40	108.48
2	B	2101	1NX	C26-C20-C19	4.07	106.20	103.17
2	A	2099	1NX	C17-O16-C13	3.36	128.04	119.06
2	D	2100	1NX	C15-N14-C13	3.32	121.09	116.55
2	B	2101	1NX	C15-N14-C13	3.26	121.01	116.55
2	D	2100	1NX	C17-O16-C13	3.21	127.65	119.06
2	A	2099	1NX	C15-N14-C13	3.13	120.83	116.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2101	1NX	C15-N14-C13	2.97	120.61	116.55
2	B	2101	1NX	C1-C2-C31	-2.78	108.14	114.11
2	C	2101	1NX	C17-O16-C13	2.61	126.03	119.06
2	D	2100	1NX	C27-C26-C20	-2.59	101.57	105.59
2	B	2101	1NX	C17-O16-C13	2.53	125.81	119.06
2	B	2101	1NX	C7-C5-N4	2.47	119.54	116.24
2	A	2099	1NX	O16-C13-N14	2.34	123.86	118.89
2	D	2100	1NX	C31-C2-N4	-2.34	105.60	110.07
2	C	2101	1NX	C1-C2-C31	-2.33	109.10	114.11
2	D	2100	1NX	C1-C2-C31	-2.27	109.24	114.11
2	A	2099	1NX	C27-C26-C20	-2.25	102.09	105.59
2	B	2101	1NX	C26-C27-C28	2.20	105.43	103.27
2	A	2099	1NX	C26-C20-C19	2.19	104.81	103.17
2	A	2099	1NX	C26-C20-N22	-2.16	109.99	114.49
2	A	2099	1NX	C32-C31-C2	-2.15	117.14	120.28
2	A	2099	1NX	C12-N11-C10	2.12	120.34	116.19
2	D	2100	1NX	C32-C31-C2	-2.07	117.26	120.28
2	C	2101	1NX	C27-C26-C20	-2.06	102.39	105.59
2	D	2100	1NX	C12-N11-C10	2.05	120.21	116.19
2	C	2101	1NX	C18-C19-C28	-2.05	119.59	121.21
2	C	2101	1NX	C33-C31-C2	-2.04	117.29	120.28
2	B	2101	1NX	C26-C20-N22	-2.03	110.26	114.49
2	B	2101	1NX	C12-N11-C10	2.03	120.16	116.19
2	C	2101	1NX	C26-C20-N22	-2.03	110.27	114.49

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2099	1NX	C1-C2-C31-C32
2	A	2099	1NX	C1-C2-C31-C33
2	C	2101	1NX	C1-C2-C31-C33
2	C	2101	1NX	C1-C2-C31-C32
2	D	2100	1NX	C1-C2-C31-C32
2	D	2100	1NX	C1-C2-C31-C33
2	D	2100	1NX	C30-C17-O16-C13
2	A	2099	1NX	C30-C17-O16-C13
2	D	2100	1NX	C18-C17-O16-C13
3	C	2102	GOL	O2-C2-C3-O3
2	A	2099	1NX	C18-C17-O16-C13
2	A	2099	1NX	N4-C5-C7-C15
2	B	2101	1NX	N4-C5-C7-C15

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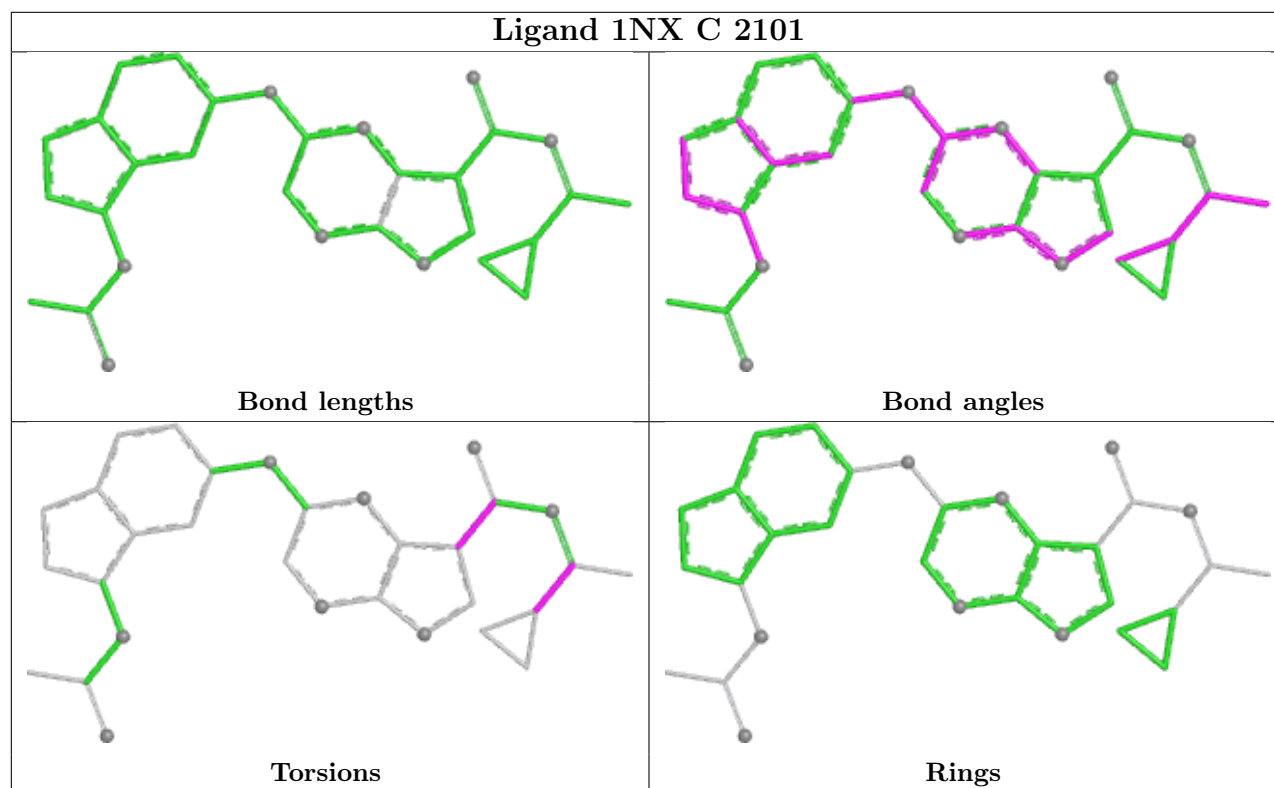
Mol	Chain	Res	Type	Atoms
2	C	2101	1NX	N4-C5-C7-C15

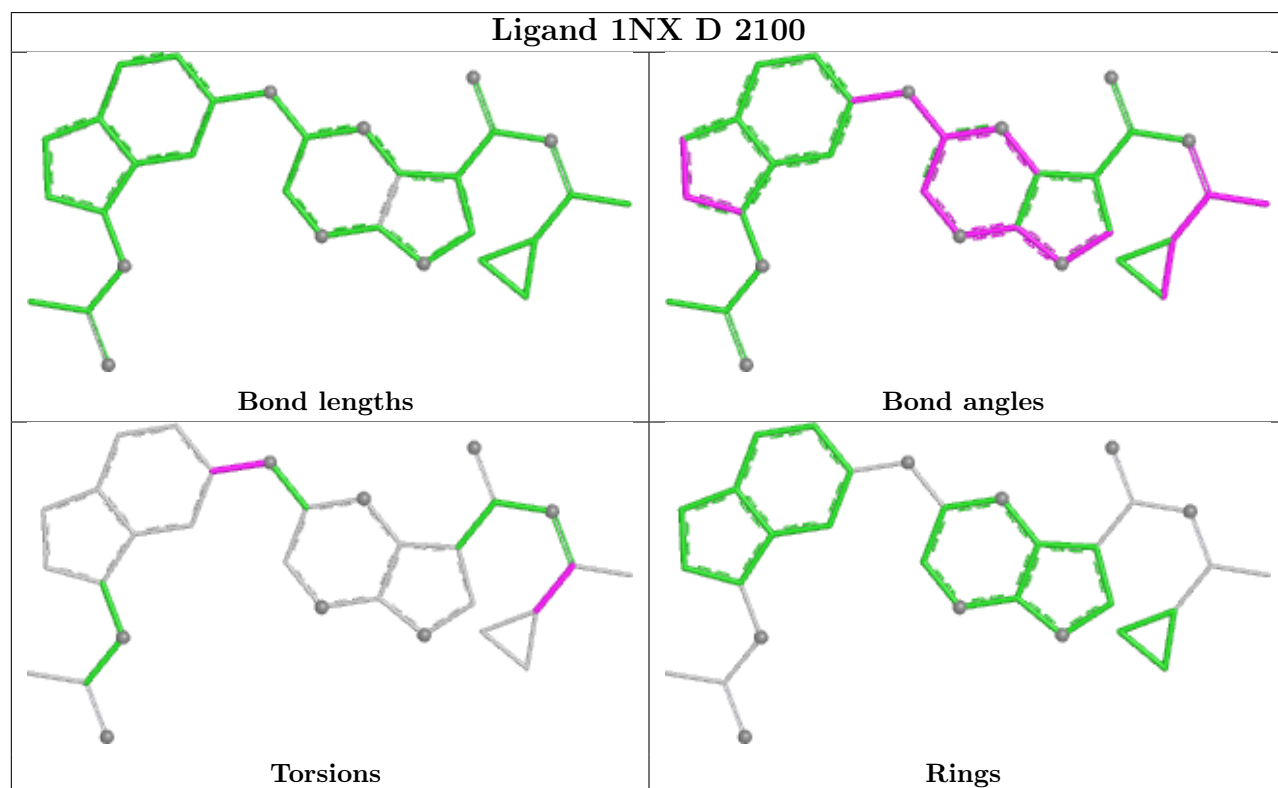
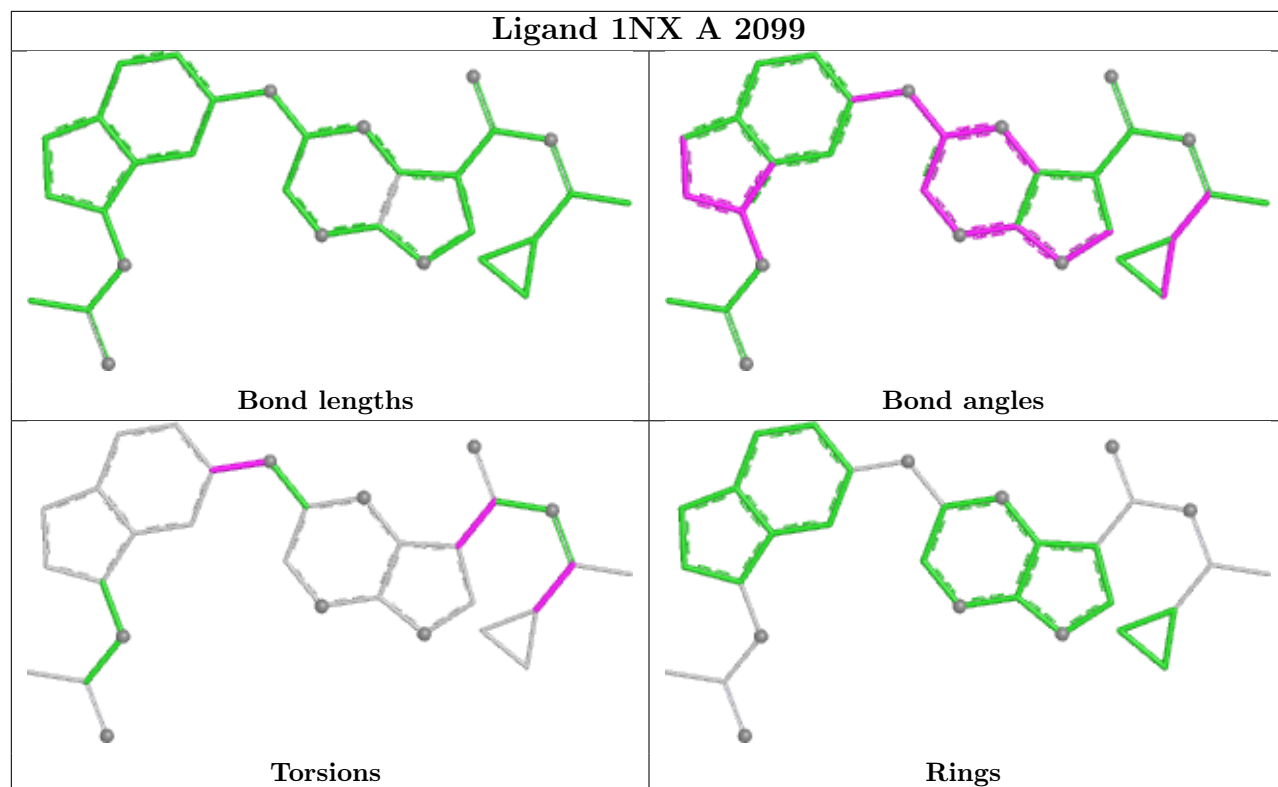
There are no ring outliers.

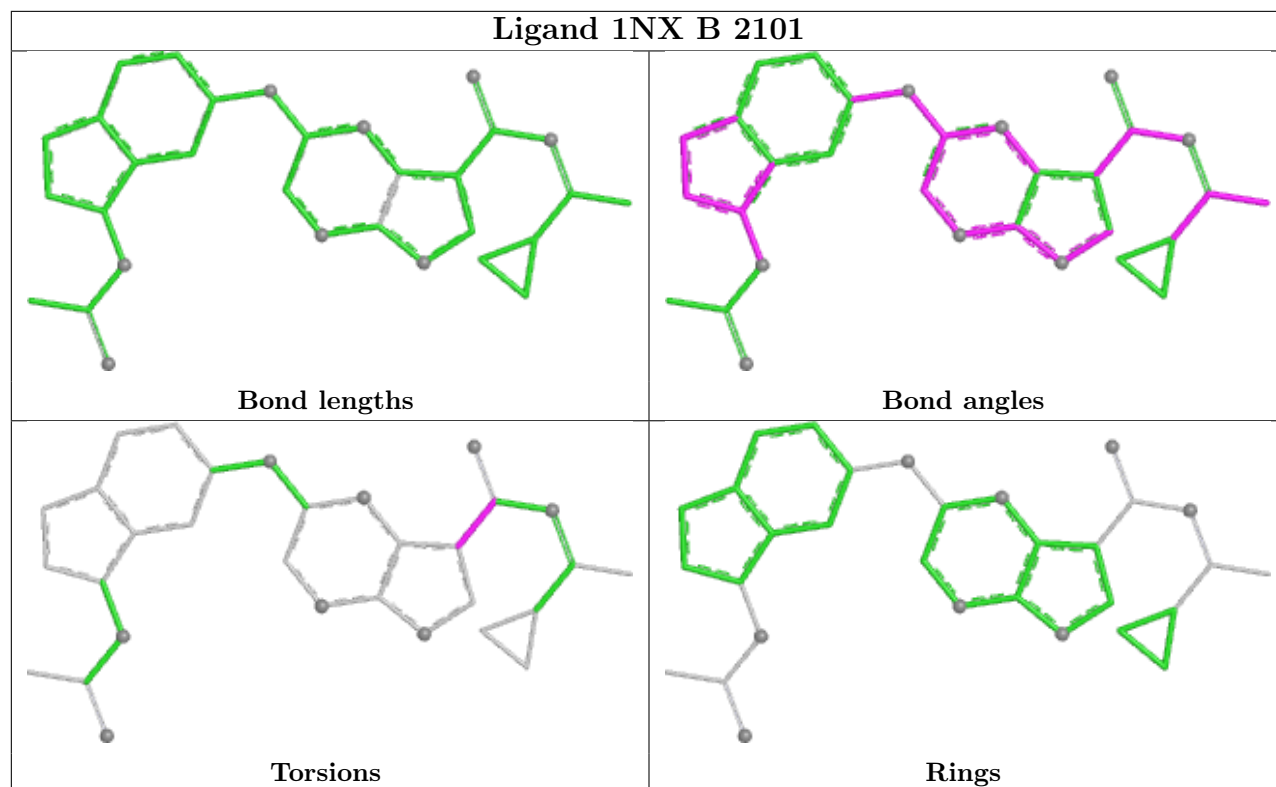
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2101	1NX	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	274/288 (95%)	0.32	12 (4%)	39 45	18, 35, 61, 89	11 (4%)
1	B	268/288 (93%)	0.48	22 (8%)	17 20	20, 37, 69, 96	13 (4%)
1	C	276/288 (95%)	0.51	17 (6%)	26 30	19, 37, 63, 88	15 (5%)
1	D	272/288 (94%)	0.37	18 (6%)	24 27	15, 35, 68, 88	10 (3%)
All	All	1090/1152 (94%)	0.42	69 (6%)	26 29	15, 36, 66, 96	49 (4%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	814	PRO	4.6
1	B	1100	SER	4.5
1	D	1045	PRO	4.1
1	A	986	PRO	4.0
1	B	1099	TRP	4.0
1	D	892	GLY	4.0
1	B	989	SER	4.0
1	C	892	GLY	3.8
1	B	860	SER	3.7
1	D	1099	TRP	3.6
1	B	814	PRO	3.6
1	D	814	PRO	3.4
1	B	983	VAL	3.4
1	C	815	THR	3.3
1	B	859	HIS	3.2
1	B	984	ARG	3.2
1	D	984	ARG	3.1
1	C	989	SER	3.0
1	A	987	GLY	3.0
1	C	1100	SER	3.0
1	B	830	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	845	GLY	2.9
1	B	1045	PRO	2.9
1	A	844	LEU	2.9
1	D	816	ILE	2.9
1	C	990	PRO	2.9
1	A	1040	SER	2.9
1	D	859	HIS	2.8
1	A	815	THR	2.7
1	A	859	HIS	2.7
1	B	1046	ALA	2.7
1	B	858	GLN	2.7
1	C	984	ARG	2.7
1	C	859	HIS	2.6
1	B	815	THR	2.6
1	B	990	PRO	2.6
1	A	860	SER	2.6
1	A	897	SER	2.5
1	D	982	VAL	2.5
1	D	861	GLY	2.5
1	D	858	GLN	2.5
1	B	994	TYR	2.5
1	D	860	SER	2.4
1	C	891	TYR	2.4
1	C	988	GLN	2.4
1	C	919	ALA	2.3
1	D	848	THR	2.3
1	C	985	GLU	2.3
1	D	983	VAL	2.3
1	C	976	LEU	2.3
1	B	891	TYR	2.3
1	C	897	SER	2.2
1	B	816	ILE	2.2
1	B	834	GLY	2.2
1	A	814	PRO	2.2
1	D	985	GLU	2.2
1	D	815	THR	2.2
1	C	983	VAL	2.1
1	D	849	GLY	2.1
1	B	1047	LEU	2.1
1	A	988	GLN	2.1
1	C	860	SER	2.1
1	B	1039	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	991	ILE	2.0
1	A	1045	PRO	2.0
1	D	1046	ALA	2.0
1	D	846	ASP	2.0
1	B	862	PRO	2.0
1	C	830	LYS	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(Å ²)	Q<0.9
1	PTR	B	981	16/17	0.83	0.17	53,83,92,96	0
1	PTR	C	981	16/17	0.83	0.17	56,82,97,99	0
1	PTR	A	981	16/17	0.87	0.13	45,54,76,83	0
1	PTR	D	981	16/17	0.87	0.15	50,66,81,85	0
1	PTR	C	980	16/17	0.88	0.14	51,67,90,94	0
1	PTR	D	980	16/17	0.89	0.11	46,49,69,69	0
1	PTR	B	980	16/17	0.90	0.12	47,55,80,87	0
1	PTR	A	980	16/17	0.92	0.11	40,52,65,67	0

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
3	GOL	C	2102	6/6	0.83	0.17	61,64,70,70	0
2	1NX	D	2100	31/31	0.90	0.16	46,54,58,59	0
2	1NX	C	2101	31/31	0.93	0.18	41,49,54,56	0
2	1NX	B	2101	31/31	0.94	0.16	46,52,59,64	0

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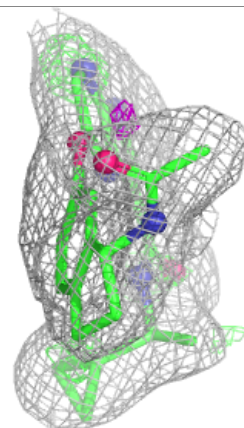
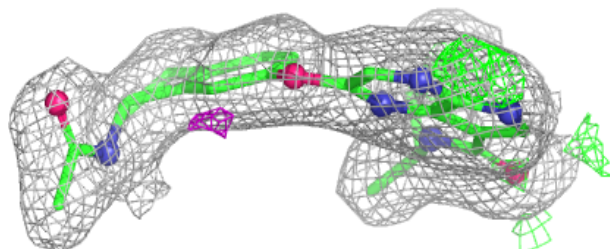
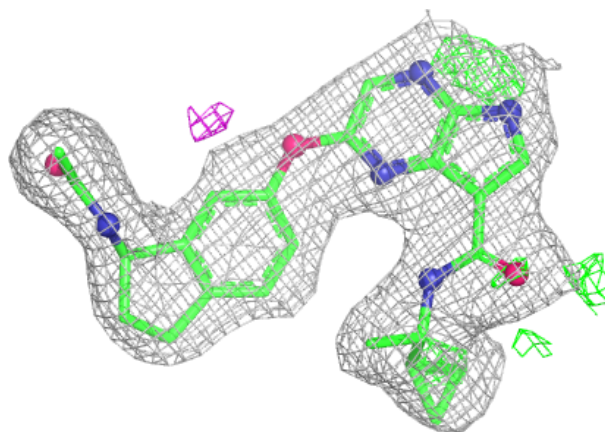
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	1NX	A	2099	31/31	0.95	0.15	40,48,59,64	0

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.

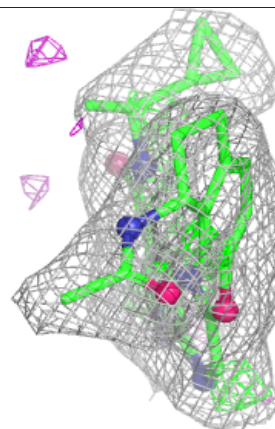
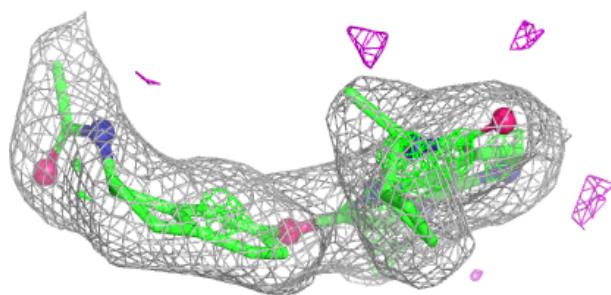
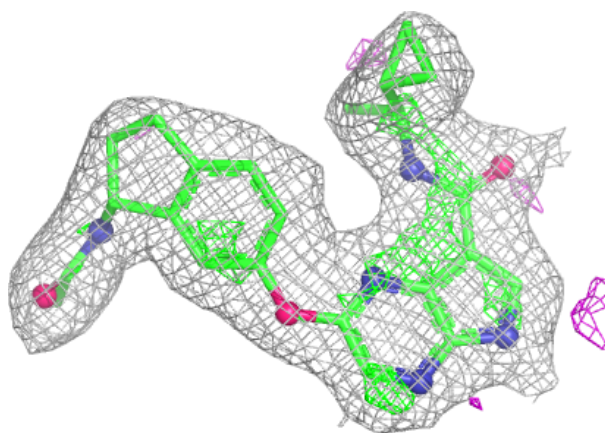
Electron density around 1NX D 2100:

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



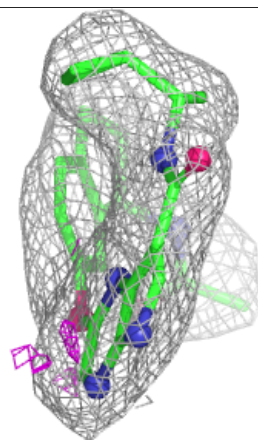
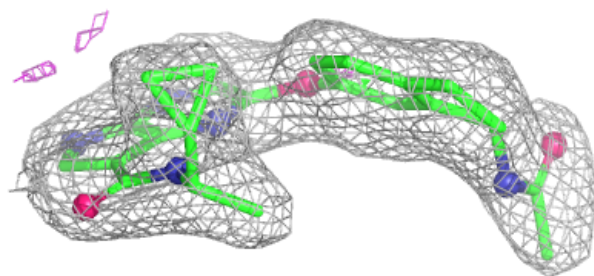
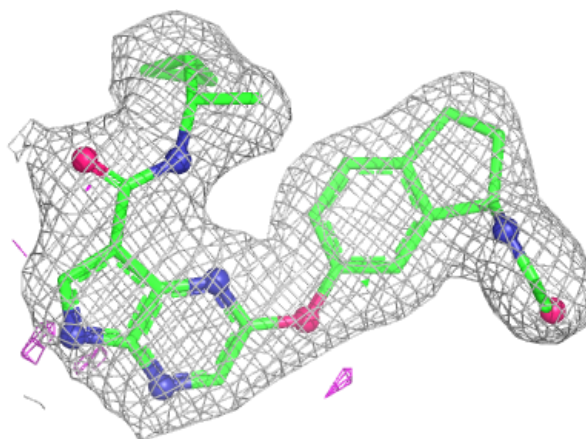
Electron density around 1NX C 2101:

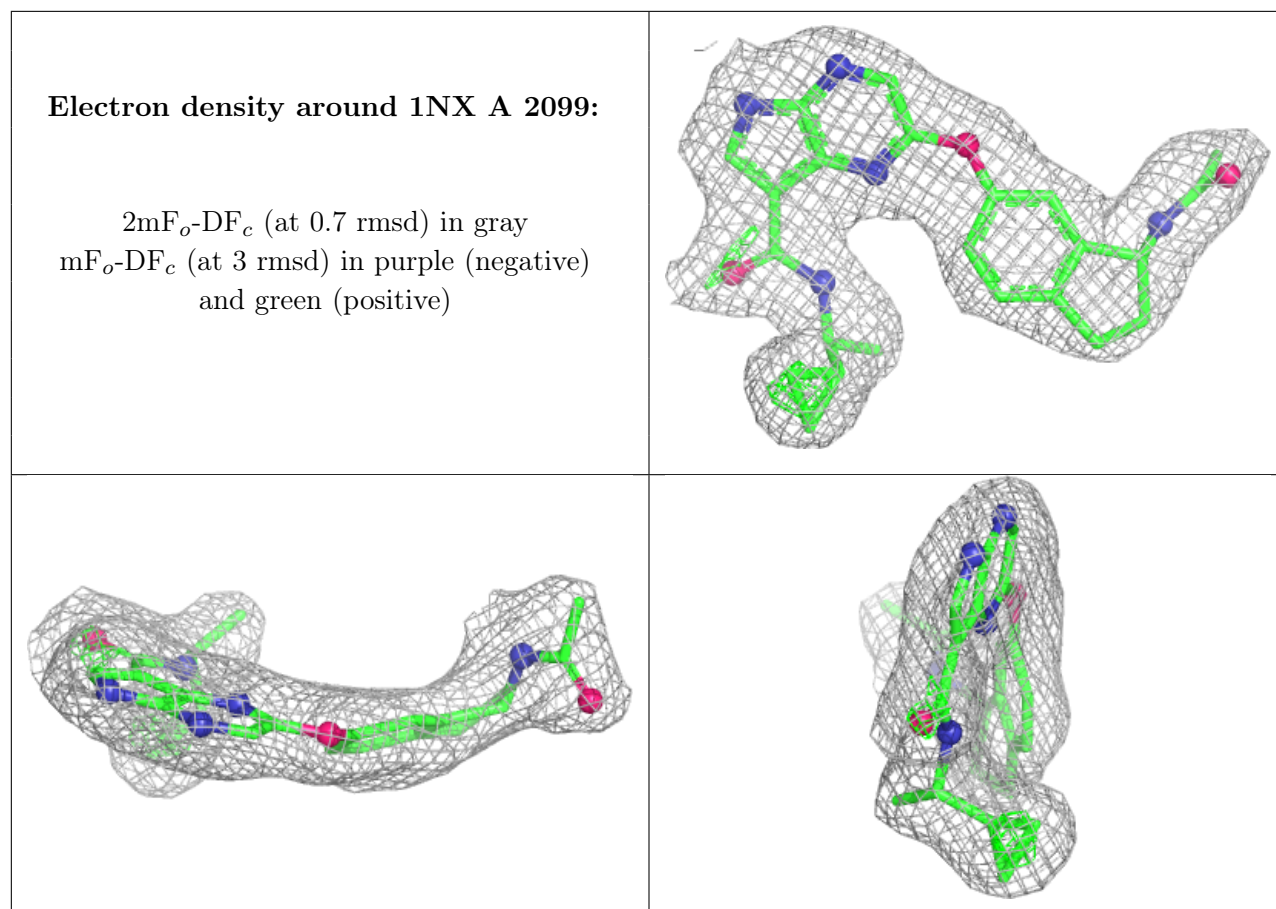
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 1NX B 2101:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.