wwPDB X-ray Structure Validation Summary Report (i)

Oct 8, 2024 – 10:11 AM EDT

PDB ID	:	5SJ4
Title	:	CRYSTAL STRUCTURE OF HUMAN PHOSPHODIESTERASE 10 IN COMPLEX WITH c1(ccccc1)c2cn(C)c(n2)CCC3=Nc4c(C(N3)=O)cnn4C, micromolar IC50=0.04979
Authors	:	Joseph, C.; Benz, J.; Flohr, A.; Groebke-Zbinden, K.; Rudolph, M.G.
Deposited on	:	2022-02-01
Resolution	:	2.77 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

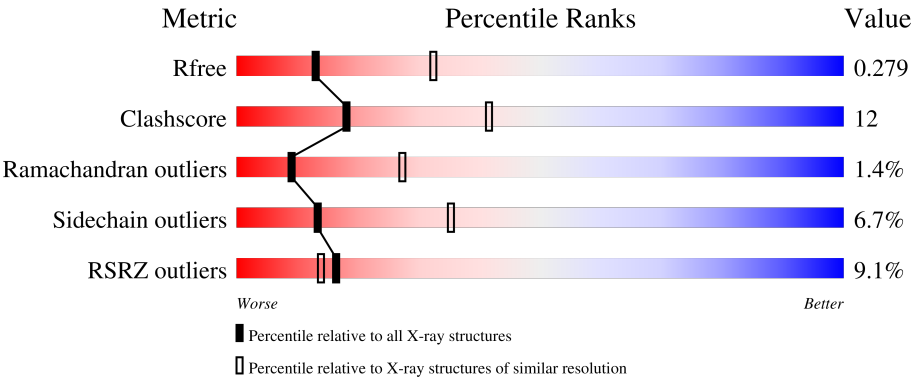
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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}	164625	4924 (2.80-2.76)
Clashscore	180529	5458 (2.80-2.76)
Ramachandran outliers	177936	5386 (2.80-2.76)
Sidechain outliers	177891	5388 (2.80-2.76)
RSRZ outliers	164620	4926 (2.80-2.76)

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

Mol	Chain	Length	Quality of chain
1	A	343	9% 63% 25% • 9%
1	B	343	8% 61% 28% • 8%
1	C	343	7% 62% 27% • 9%
1	D	343	10% 65% 24% • 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	JXI	A	803	X	-	-	-
4	JXI	B	803	X	-	-	-
4	JXI	C	803	X	-	-	-
4	JXI	D	803	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10464 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 cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	1	0
			2549	1629	435	461	24			
1	B	315	Total	C	N	O	S	0	1	0
			2559	1635	437	463	24			
1	C	313	Total	C	N	O	S	0	2	0
			2557	1634	438	461	24			
1	D	310	Total	C	N	O	S	0	0	0
			2519	1612	429	454	24			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	447	GLY	-	expression tag	UNP Q9Y233
A	448	SER	-	expression tag	UNP Q9Y233
B	447	GLY	-	expression tag	UNP Q9Y233
B	448	SER	-	expression tag	UNP Q9Y233
C	447	GLY	-	expression tag	UNP Q9Y233
C	448	SER	-	expression tag	UNP Q9Y233
D	447	GLY	-	expression tag	UNP Q9Y233
D	448	SER	-	expression tag	UNP Q9Y233

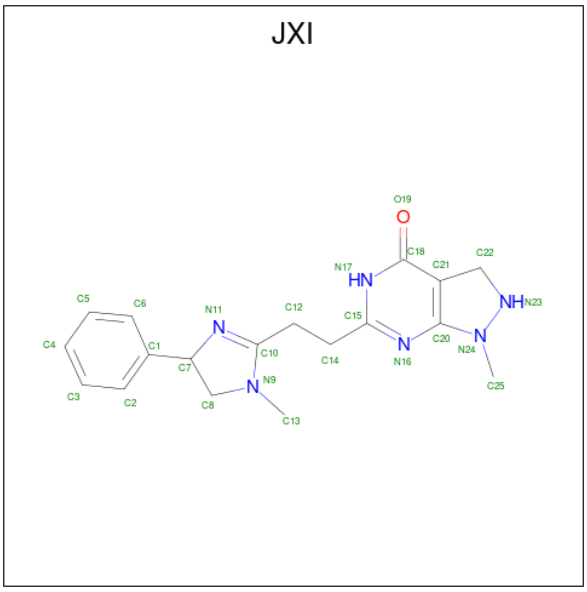
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is 1-methyl-6-{2-[(4R)-1-methyl-4-phenyl-4,5-dihydro-1H-imidazol-2-yl]ethyl }-1,2,3,5-tetrahydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (three-letter code: JXI) (formula: $C_{18}H_{22}N_6O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 25 18 6 1	0	0
4	B	1	Total C N O 25 18 6 1	0	0
4	C	1	Total C N O 25 18 6 1	0	0
4	D	1	Total C N O 25 18 6 1	0	0

- Molecule 5 is water.

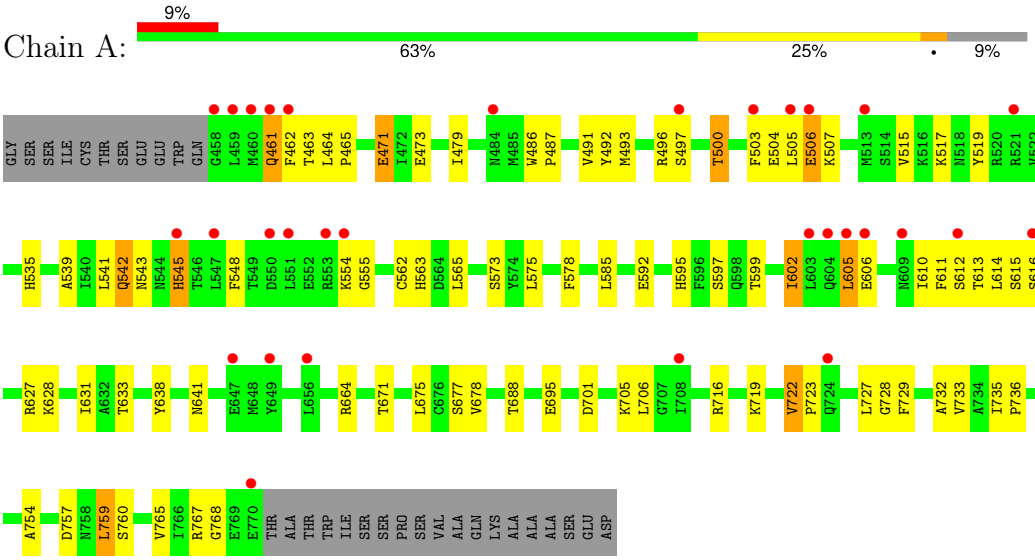
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	45	Total O 45 45	0	0
5	B	45	Total O 45 45	0	0
5	C	50	Total O 50 50	0	0
5	D	32	Total O 32 32	0	0

3 Residue-property plots (i)

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

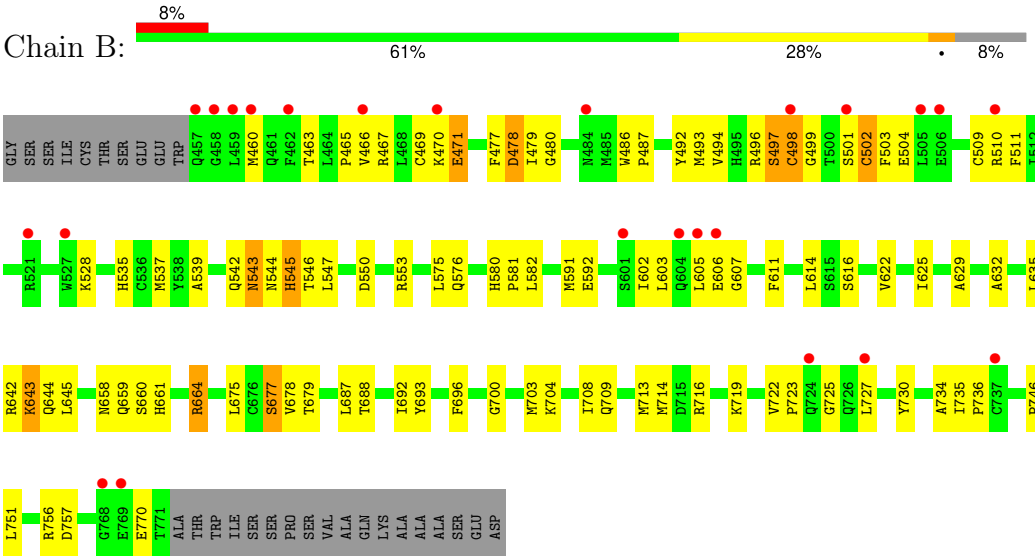
• Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

Chain A:



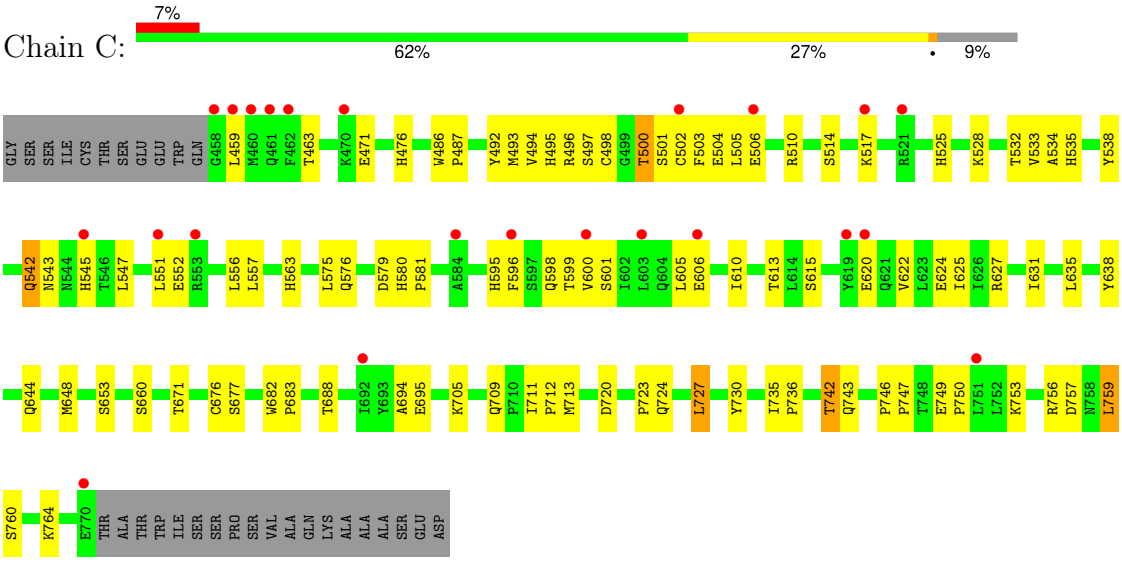
• Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

Chain B:



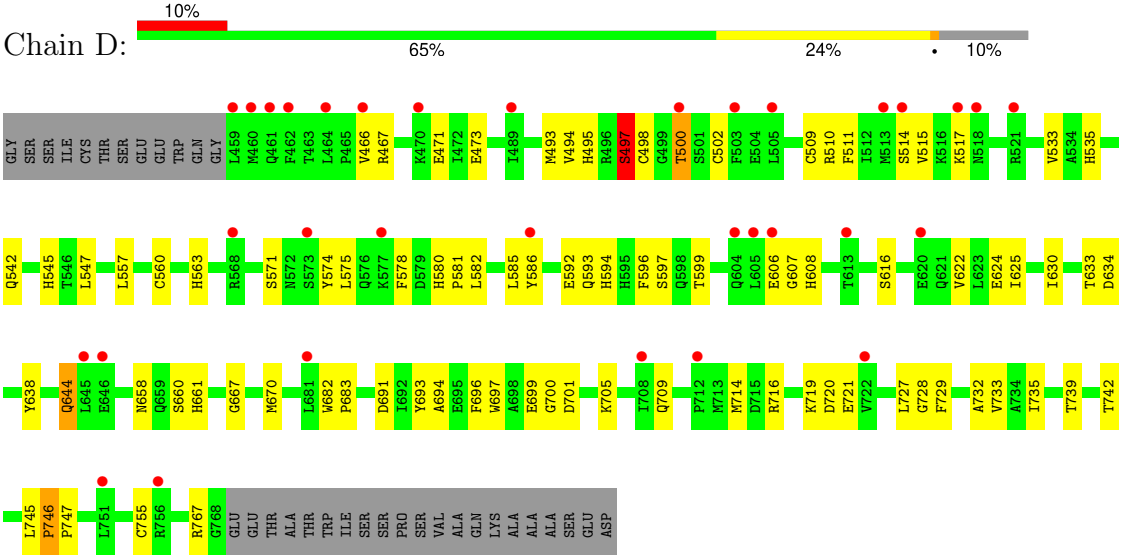
• Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

Chain C:



• Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	135.14Å 135.14Å 235.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.48 – 2.77 43.48 – 2.77	Depositor EDS
% Data completeness (in resolution range)	86.8 (43.48-2.77) 86.8 (43.48-2.77)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.92 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.195 , 0.278 0.202 , 0.279	Depositor DCC
R_{free} test set	1999 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	58.4	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.046 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	10464	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CME, MG, JXI

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	0.90	2/2603 (0.1%)	1.11	2/3521 (0.1%)
1	B	0.87	1/2613 (0.0%)	1.12	4/3535 (0.1%)
1	C	0.91	4/2614 (0.2%)	1.09	6/3535 (0.2%)
1	D	0.86	1/2570 (0.0%)	1.06	0/3478
All	All	0.89	8/10400 (0.1%)	1.10	12/14069 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	GLU	CD-OE2	7.32	1.33	1.25
1	C	620	GLU	CD-OE1	7.24	1.33	1.25
1	C	620	GLU	CG-CD	6.30	1.61	1.51
1	D	473	GLU	CD-OE1	5.63	1.31	1.25
1	C	606	GLU	CG-CD	5.63	1.60	1.51

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	664	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	C	620	GLU	OE1-CD-OE2	-6.64	115.33	123.30
1	C	606	GLU	OE1-CD-OE2	-5.83	116.31	123.30
1	C	620	GLU	CB-CG-CD	5.76	129.75	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	620	GLU	CG-CD-OE1	5.70	129.71	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	497	SER	Peptide

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	2549	0	2524	59	1
1	B	2559	0	2528	71	1
1	C	2557	0	2537	61	0
1	D	2519	0	2496	59	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	25	0	0	0	0
4	B	25	0	0	3	0
4	C	25	0	0	0	0
4	D	25	0	0	0	0
5	A	45	0	0	2	0
5	B	45	0	0	0	0
5	C	50	0	0	8	0
5	D	32	0	0	2	0
All	All	10464	0	10085	244	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 12.

The worst 5 of 244 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:644:GLN:HE21	1:D:644:GLN:HA	1.23	1.02
1:B:470:LYS:HD2	1:D:742:THR:HG22	1.44	1.00
1:A:542:GLN:HA	1:A:542:GLN:NE2	1.79	0.97
1:A:542:GLN:HA	1:A:542:GLN:HE21	1.31	0.95
1:B:543:ASN:N	1:B:543:ASN:HD22	1.63	0.92

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)
1:A:606:GLU:OE1	1:B:606:GLU:OE2[3_555]	2.01	0.19

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	311/343 (91%)	282 (91%)	23 (7%)	6 (2%)	6 20
1	B	313/343 (91%)	284 (91%)	25 (8%)	4 (1%)	10 29
1	C	312/343 (91%)	284 (91%)	26 (8%)	2 (1%)	22 48
1	D	307/343 (90%)	276 (90%)	26 (8%)	5 (2%)	8 24
All	All	1243/1372 (91%)	1126 (91%)	100 (8%)	17 (1%)	9 27

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	554	LYS
1	B	502	CYS
1	A	506	GLU
1	B	659	GLN
1	C	502	CYS

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	282/305 (92%)	263 (93%)	19 (7%)	13	35
1	B	282/305 (92%)	260 (92%)	22 (8%)	10	28
1	C	283/305 (93%)	261 (92%)	22 (8%)	10	28
1	D	279/305 (92%)	267 (96%)	12 (4%)	25	54
All	All	1126/1220 (92%)	1051 (93%)	75 (7%)	13	35

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	676	CYS
1	D	660	SER
1	C	711	ILE
1	D	517	LYS
1	B	497	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	461	GLN
1	D	658	ASN
1	D	495	HIS
1	D	593	GLN
1	D	761	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)

4 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	CME	C	509	1	8,9,10	0.49	0	6,9,11	0.78	0
1	CME	B	509	1	8,9,10	0.60	0	6,9,11	1.20	1 (16%)
1	CME	A	509	1	8,9,10	0.64	0	6,9,11	0.79	0
1	CME	D	509	1	8,9,10	0.55	0	6,9,11	1.03	1 (16%)

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	CME	C	509	1	-	1/5/8/10	-
1	CME	B	509	1	-	2/5/8/10	-
1	CME	A	509	1	-	1/5/8/10	-
1	CME	D	509	1	-	2/5/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	509	CME	CB-SG-SD	2.36	109.97	103.86
1	D	509	CME	CB-SG-SD	2.02	109.09	103.86

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	509	CME	SD-CE-CZ-OH
1	C	509	CME	SD-CE-CZ-OH
1	D	509	CME	N-CA-CB-SG
1	B	509	CME	SD-CE-CZ-OH
1	D	509	CME	SD-CE-CZ-OH

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)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	JXI	C	803	-	20,28,28	2.14	9 (45%)	20,40,40	3.68	9 (45%)
4	JXI	D	803	-	20,28,28	2.29	5 (25%)	20,40,40	4.12	9 (45%)
4	JXI	A	803	-	20,28,28	2.65	5 (25%)	20,40,40	4.01	11 (55%)
4	JXI	B	803	-	20,28,28	2.14	8 (40%)	20,40,40	4.04	9 (45%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	JXI	C	803	-	1/1/4/5	5/9/30/30	0/4/4/4
4	JXI	D	803	-	1/1/4/5	4/9/30/30	0/4/4/4
4	JXI	A	803	-	1/1/4/5	5/9/30/30	0/4/4/4
4	JXI	B	803	-	1/1/4/5	2/9/30/30	0/4/4/4

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	JXI	C7-N11	-6.82	1.38	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	803	JXI	C7-N11	-6.04	1.40	1.48
4	A	803	JXI	C1-C7	-5.74	1.43	1.51
4	C	803	JXI	C7-N11	-5.19	1.41	1.48
4	A	803	JXI	C10-N9	4.93	1.43	1.35

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	803	JXI	C21-C18-N17	-11.06	107.30	115.70
4	A	803	JXI	C12-C14-C15	10.59	123.48	112.55
4	D	803	JXI	C14-C12-C10	9.52	120.62	111.62
4	D	803	JXI	C12-C14-C15	9.43	122.28	112.55
4	C	803	JXI	C14-C12-C10	8.84	119.98	111.62

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	803	JXI	C7
4	B	803	JXI	C7
4	C	803	JXI	C7
4	D	803	JXI	C7

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	JXI	C2-C1-C7-C8
4	C	803	JXI	C2-C1-C7-C8
4	D	803	JXI	C2-C1-C7-C8
4	D	803	JXI	C6-C1-C7-C8
4	C	803	JXI	C6-C1-C7-C8

There are no ring outliers.

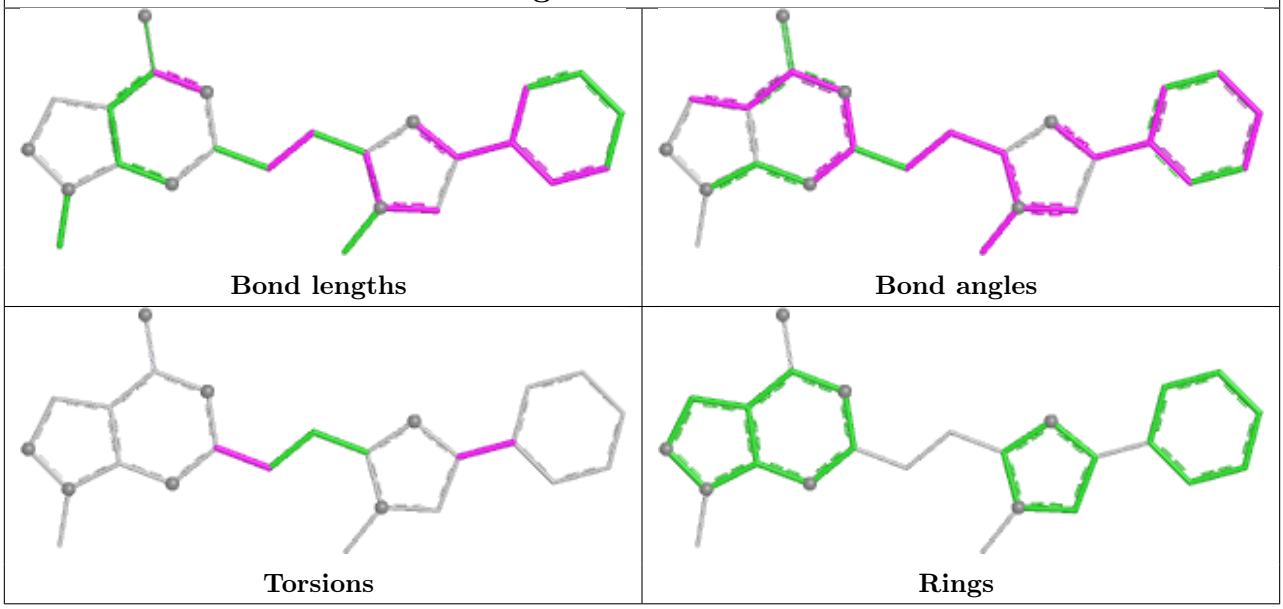
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	803	JXI	3	0

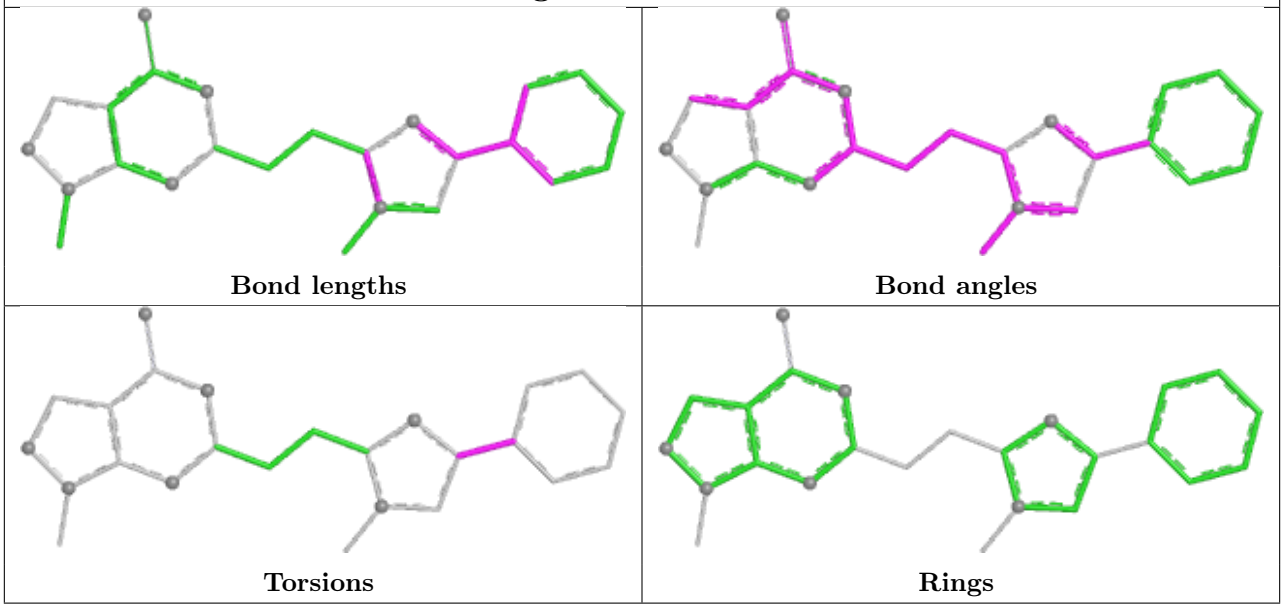
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

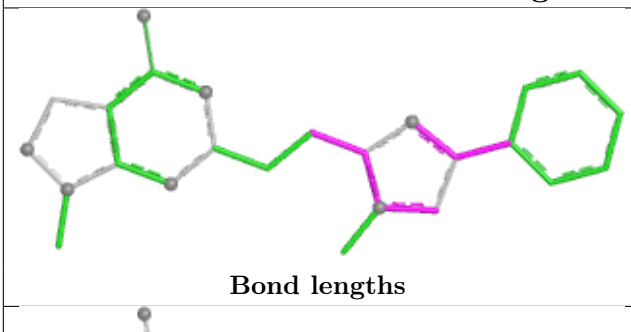
Ligand JXI C 803



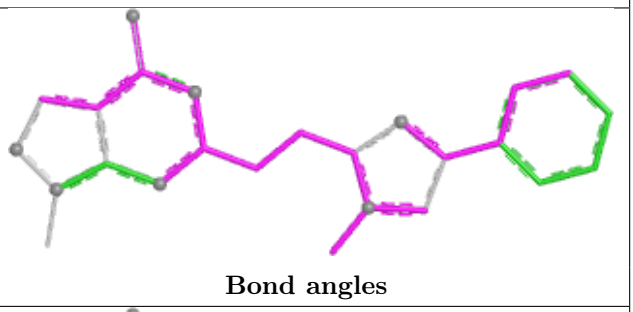
Ligand JXI D 803



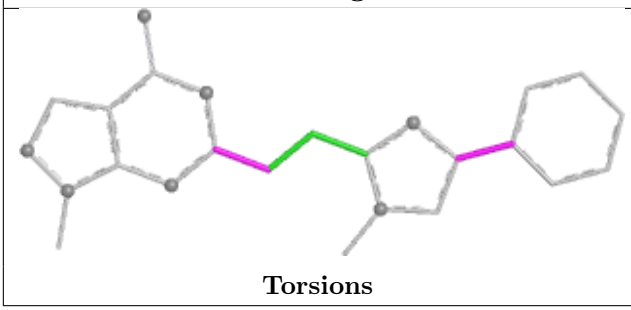
Ligand JXI A 803



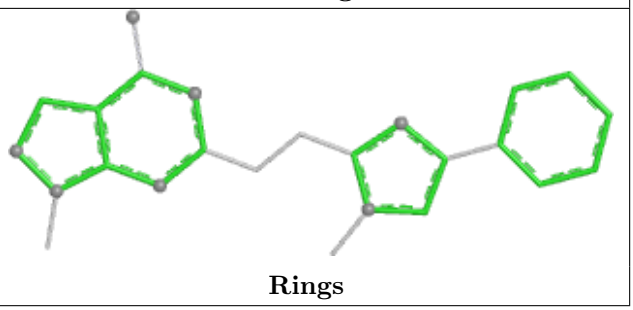
Bond lengths



Bond angles

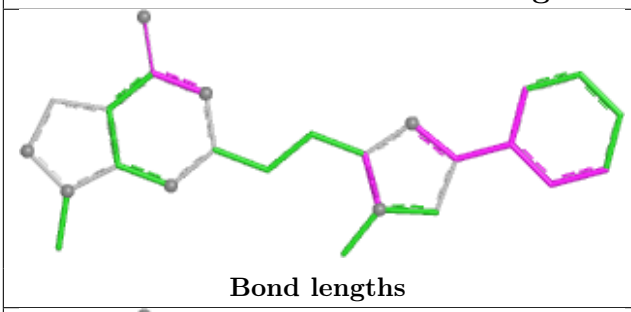


Torsions

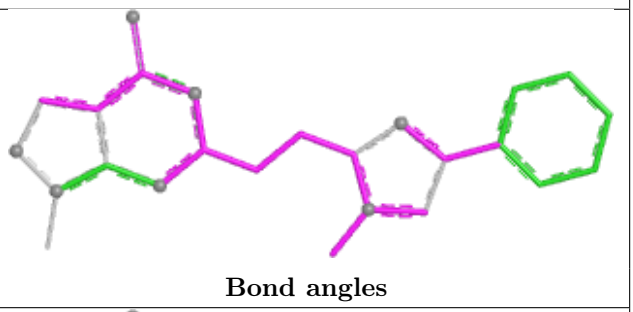


Rings

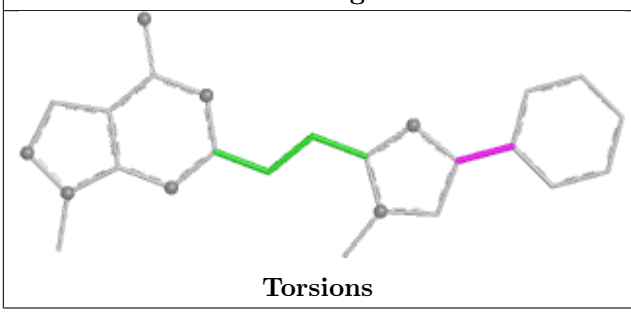
Ligand JXI B 803



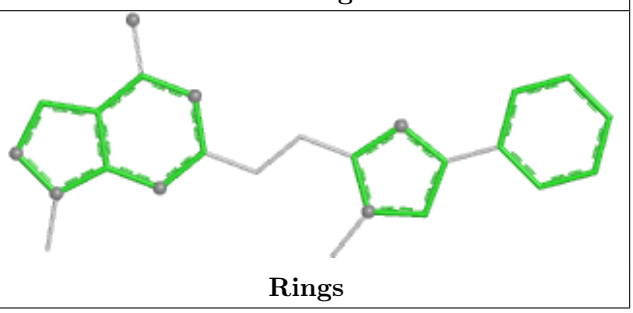
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	312/343 (90%)	0.86	31 (9%)	14	12	32, 62, 91, 112	1 (0%)
1	B	314/343 (91%)	0.86	27 (8%)	18	15	40, 62, 97, 118	1 (0%)
1	C	312/343 (90%)	0.81	23 (7%)	22	19	40, 64, 92, 121	2 (0%)
1	D	309/343 (90%)	1.11	33 (10%)	12	11	50, 73, 98, 111	0
All	All	1247/1372 (90%)	0.91	114 (9%)	16	14	32, 66, 97, 121	4 (0%)

The worst 5 of 114 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	458	GLY	4.5
1	D	459	LEU	4.3
1	A	459	LEU	4.1
1	B	460	MET	4.0
1	C	606	GLU	3.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CME	D	509	10/11	0.69	0.25	61,91,129,132	0
1	CME	C	509	10/11	0.75	0.19	64,78,126,127	0
1	CME	A	509	10/11	0.79	0.20	58,93,131,135	0
1	CME	B	509	10/11	0.80	0.32	66,94,102,109	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

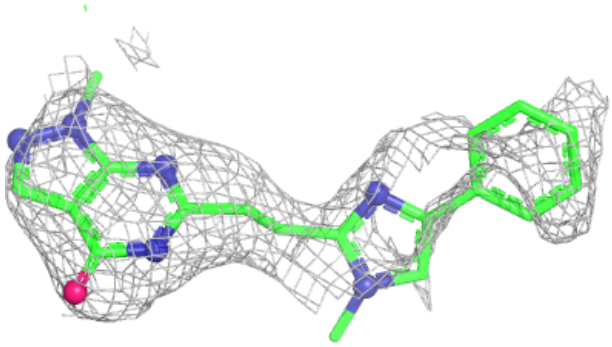
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

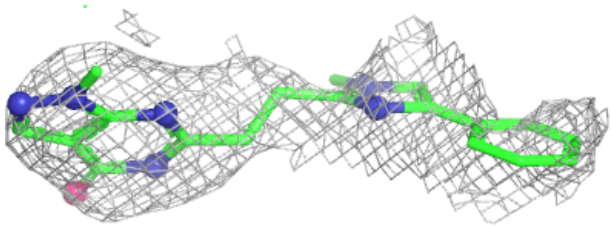
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	JXI	D	803	25/25	0.80	0.20	58,102,135,145	0
4	JXI	B	803	25/25	0.87	0.15	53,76,95,102	0
4	JXI	A	803	25/25	0.87	0.14	54,67,78,86	0
4	JXI	C	803	25/25	0.88	0.17	51,72,117,121	0
3	MG	B	802	1/1	0.93	0.07	58,58,58,58	0
3	MG	C	802	1/1	0.96	0.05	44,44,44,44	0
3	MG	D	802	1/1	0.96	0.07	54,54,54,54	0
2	ZN	D	801	1/1	0.97	0.04	60,60,60,60	0
2	ZN	A	801	1/1	0.99	0.03	51,51,51,51	0
3	MG	A	802	1/1	0.99	0.03	90,90,90,90	0
2	ZN	C	801	1/1	0.99	0.02	46,46,46,46	0
2	ZN	B	801	1/1	1.00	0.02	51,51,51,51	0

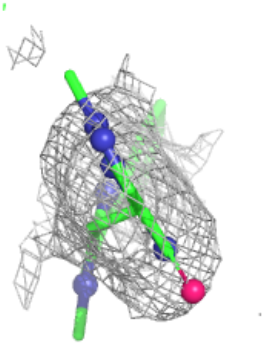
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JXI D 803:

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

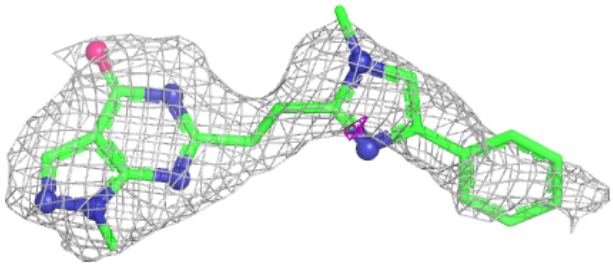


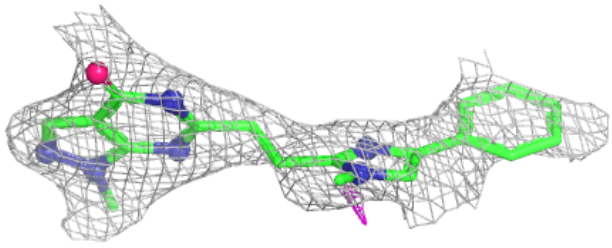


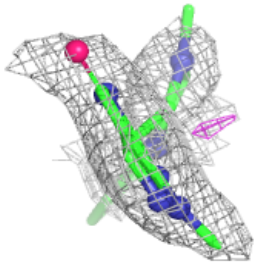


Electron density around JXI B 803:

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

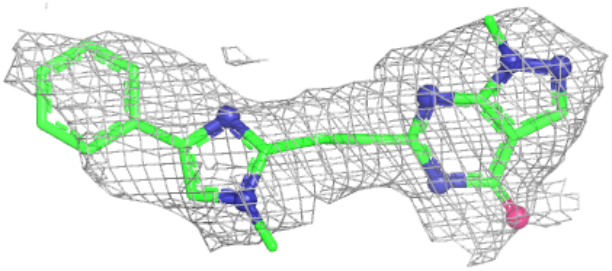


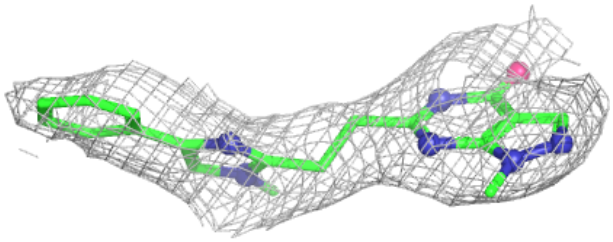


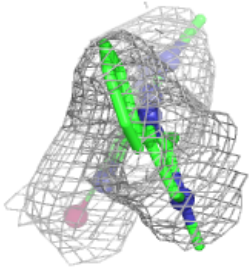


Electron density around JXI A 803:

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

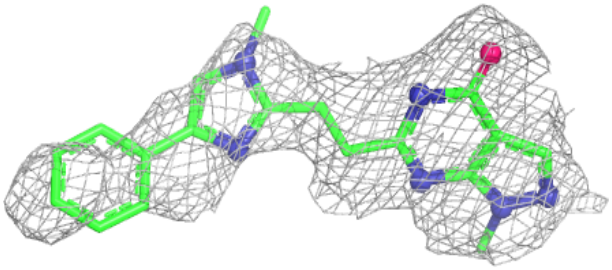


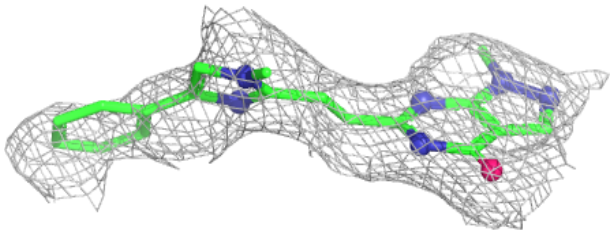


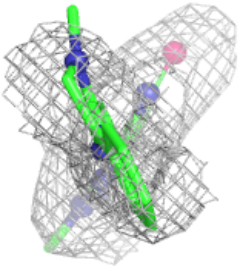


Electron density around JXI C 803:

$2mF_o$-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.