wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2022 – 12:07 PM EDT

PDB ID	:	5SGI
Title	:	Crystal Structure of human phosphodiesterase 10 in complex with 6-(3-methylphenoxy)-2-(4-pyridin-2-ylpiperazin-1-yl)-9H-purine
Authors	:	Joseph, C.; Benz, J.; Flohr, A.; Brunner, M.; Rudolph, M.G.
Deposited on	:	2022-02-01
Resolution	:	1.97 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:

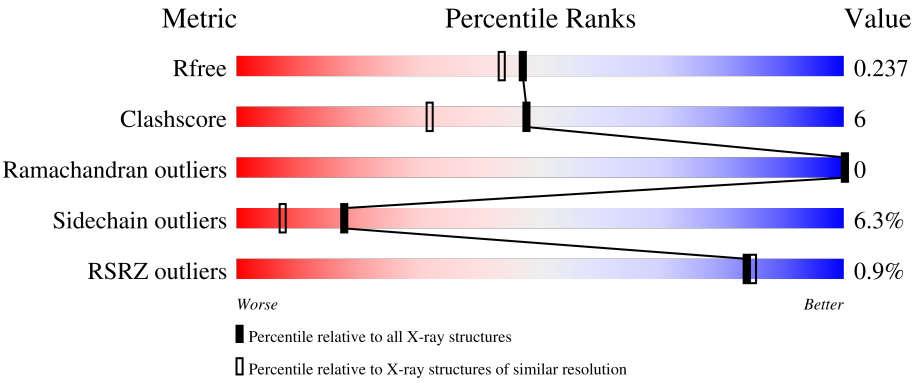
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 1.97 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	80% 10% • 8%
1	B	343	75% 14% • 8%
1	C	343	78% 12% • 9%
1	D	343	76% 14% • 9%

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	GOL	A	803	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11121 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	314	Total	C	N	O	S	0	6	0
			2578	1648	436	468	26			
1	B	315	Total	C	N	O	S	0	5	0
			2579	1648	437	469	25			
1	C	313	Total	C	N	O	S	0	7	0
			2576	1648	437	466	25			
1	D	313	Total	C	N	O	S	0	5	0
			2566	1641	437	463	25			

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

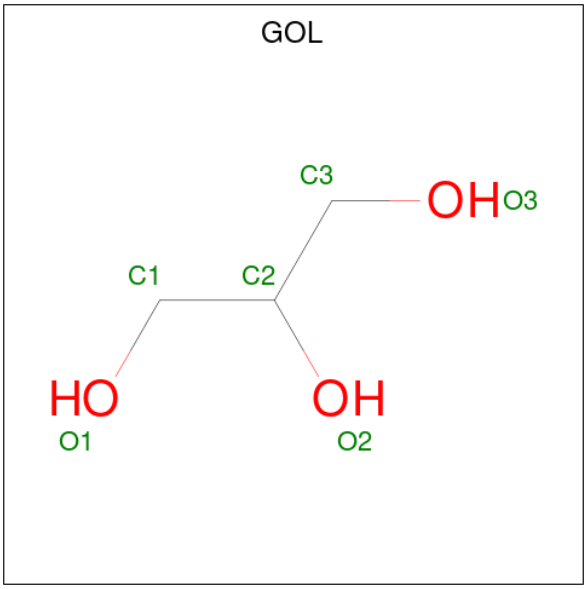
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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).

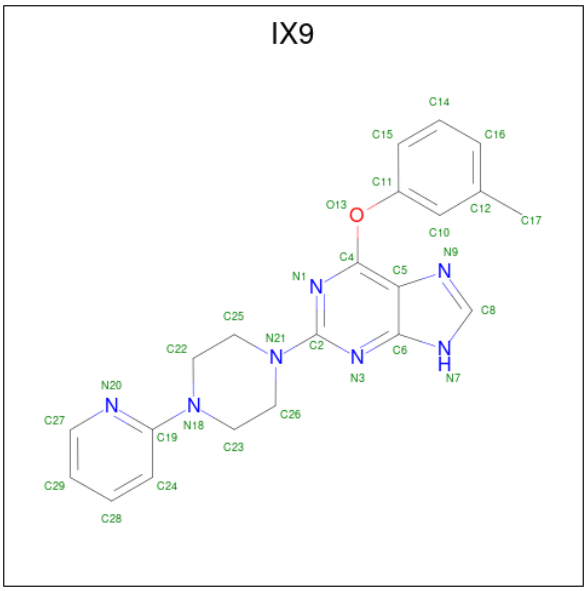
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is 6-(3-methylphenoxy)-2-[4-(pyridin-2-yl)piperazin-1-yl]-9H-purine (three-letter code: IX9) (formula: $C_{21}H_{21}N_7O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 29 21 7 1	0	0
5	B	1	Total C N O 29 21 7 1	0	0
5	C	1	Total C N O 29 21 7 1	0	0
5	D	1	Total C N O 29 21 7 1	0	0

- Molecule 6 is water.

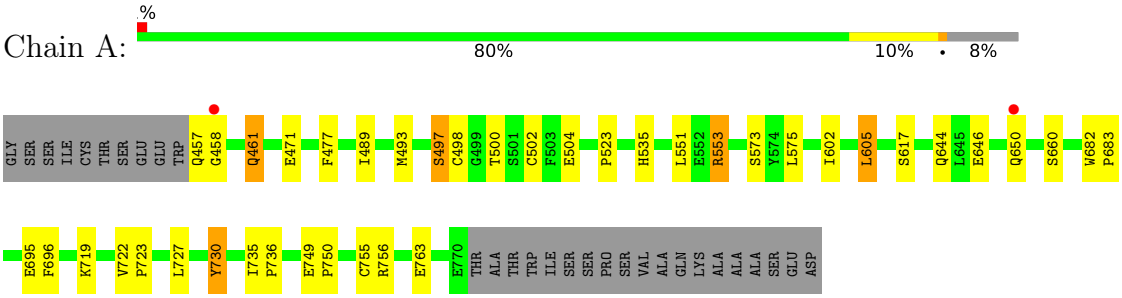
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	167	Total O 167 167	0	0
6	B	190	Total O 190 190	0	0
6	C	187	Total O 187 187	0	0
6	D	142	Total O 142 142	0	0

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.

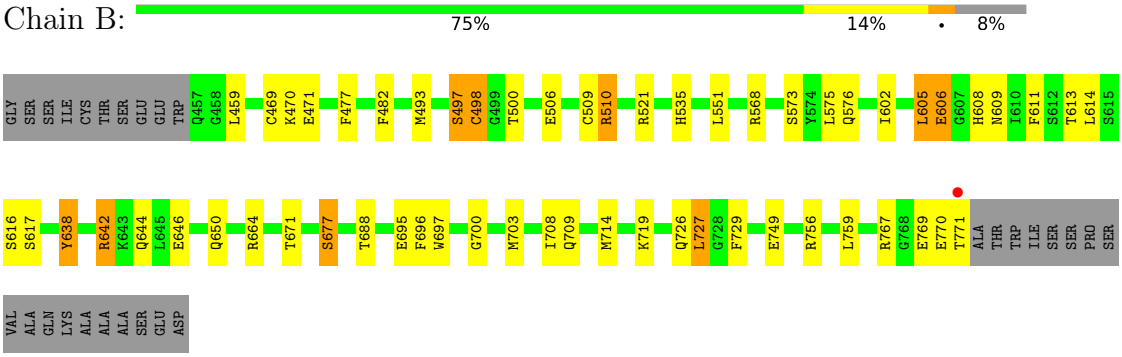
• Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

Chain A:



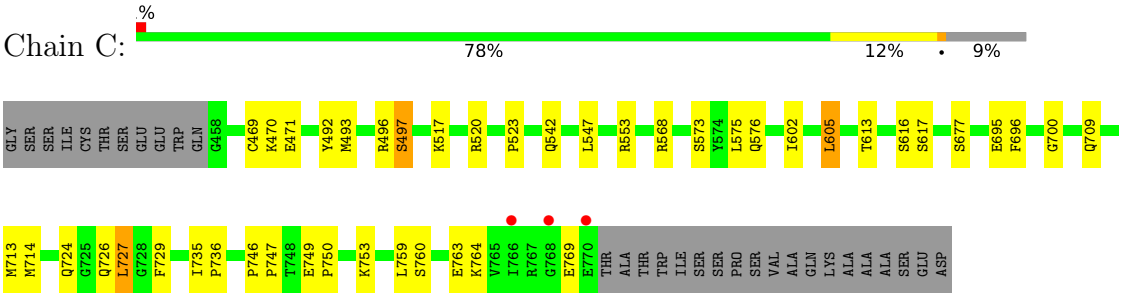
• Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

Chain B:



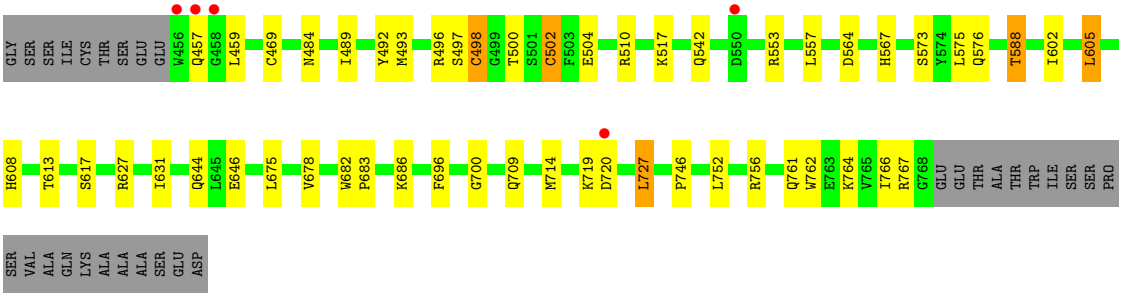
• Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

Chain C:



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

Chain D:


GLY SER SER ILE CYS THR SER GLU GLU W456 Q457 G458 L459 C469 N484 I489 Y492 M493 R496 S497 C498 G499 T500 S501 C502 F503 E504 R510 K517 Q542 D550 R553 L557 D564 H567 S573 Y574 L575 Q576 T588 I602 L605
H608 T613 S617 R627 I631 Q644 L645 E646 L675 V678 W682 P683 K686 F696 G700 Q709 M714 K719 D720 L727 P746 L752 R756 Q761 W762 E763 K764 V765 I766 R767 G768 GLU GLU THR ALA THR TRP ILE SER SER PRO
SER VAL ALA GLN LYS ALA ALA ALA SER GLU ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	135.86Å 135.86Å 235.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.63 – 1.97 41.60 – 1.97	Depositor EDS
% Data completeness (in resolution range)	85.5 (41.63-1.97) 85.6 (41.60-1.97)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.64 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.182 , 0.235 0.189 , 0.237	Depositor DCC
R_{free} test set	5440 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	26.9	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.031 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11121	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: MG, CME, GOL, ZN, IX9

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	0.83	1/2647 (0.0%)	0.92	0/3580
1	B	0.83	1/2645 (0.0%)	0.95	5/3578 (0.1%)
1	C	0.82	0/2648	0.91	1/3581 (0.0%)
1	D	0.81	0/2632	0.91	0/3560
All	All	0.82	2/10572 (0.0%)	0.93	6/14299 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	695	GLU	CD-OE2	-5.79	1.19	1.25
1	A	730	TYR	C-O	5.19	1.33	1.23

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	642	ARG	NE-CZ-NH1	-7.78	116.41	120.30
1	B	510	ARG	NE-CZ-NH2	6.01	123.30	120.30
1	B	498	CYS	CB-CA-C	5.46	121.32	110.40
1	C	470	LYS	N-CA-CB	-5.32	101.02	110.60
1	B	664	ARG	NE-CZ-NH1	5.09	122.85	120.30

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	2578	0	2554	31	0
1	B	2579	0	2549	35	0
1	C	2576	0	2566	26	0
1	D	2566	0	2547	34	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	6	0	8	4	0
4	B	6	0	8	3	0
5	A	29	0	0	1	0
5	B	29	0	0	4	0
5	C	29	0	0	4	0
5	D	29	0	0	2	0
6	A	167	0	0	3	0
6	B	190	0	0	5	0
6	C	187	0	0	5	0
6	D	142	0	0	4	0
All	All	11121	0	10232	125	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.

The worst 5 of 125 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:457:GLN:CB	1:A:458:GLY:HA2	1.93	0.99
1:D:469:CYS:SG	6:D:1028:HOH:O	2.27	0.92
1:A:461:GLN:NE2	1:A:461:GLN:HA	1.92	0.84
1:D:493:MET:O	1:D:497:SER:HB2	1.79	0.83
1:B:606:GLU:HG2	6:B:1067:HOH:O	1.82	0.78

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	317/343 (92%)	308 (97%)	9 (3%)	0	100	100
1	B	317/343 (92%)	308 (97%)	9 (3%)	0	100	100
1	C	317/343 (92%)	311 (98%)	6 (2%)	0	100	100
1	D	315/343 (92%)	304 (96%)	11 (4%)	0	100	100
All	All	1266/1372 (92%)	1231 (97%)	35 (3%)	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	287/305 (94%)	276 (96%)	11 (4%)	33	21
1	B	286/305 (94%)	263 (92%)	23 (8%)	12	3
1	C	288/305 (94%)	268 (93%)	20 (7%)	15	6
1	D	285/305 (93%)	262 (92%)	23 (8%)	11	3
All	All	1146/1220 (94%)	1069 (93%)	77 (7%)	18	6

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	500	THR
1	D	646	GLU
1	D	502[B]	CYS

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Mol	Chain	Res	Type
1	D	576	GLN
1	D	727	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	542	GLN
1	C	743	GLN
1	D	731	ASN
1	C	709	GLN
1	D	484	ASN

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	B	509	1	8,9,10	0.58	0	5,9,11	1.03	0
1	CME	A	509	1	8,9,10	0.44	0	5,9,11	0.52	0
1	CME	D	509	1	8,9,10	0.31	0	5,9,11	0.61	0
1	CME	C	509	1	8,9,10	0.68	0	5,9,11	1.05	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	CME	B	509	1	-	1/5/8/10	-
1	CME	A	509	1	-	1/5/8/10	-
1	CME	D	509	1	-	2/5/8/10	-
1	CME	C	509	1	-	1/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	509	CME	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	$\#\|Z\|>2$
5	IX9	B	804	-	30,33,33	1.38	6 (20%)	35,46,46	2.92	21 (60%)
5	IX9	A	804	-	30,33,33	1.32	2 (6%)	35,46,46	3.39	17 (48%)
4	GOL	A	803	-	5,5,5	0.19	0	5,5,5	0.89	0
4	GOL	B	803	-	5,5,5	0.30	0	5,5,5	0.65	0
5	IX9	D	803	-	30,33,33	1.24	4 (13%)	35,46,46	2.38	13 (37%)
5	IX9	C	803	-	30,33,33	1.40	7 (23%)	35,46,46	2.49	15 (42%)

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
5	IX9	B	804	-	-	3/12/22/22	0/5/5/5
5	IX9	A	804	-	-	2/12/22/22	0/5/5/5
4	GOL	A	803	-	-	4/4/4/4	-
4	GOL	B	803	-	-	2/4/4/4	-
5	IX9	D	803	-	-	3/12/22/22	0/5/5/5
5	IX9	C	803	-	-	3/12/22/22	0/5/5/5

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	804	IX9	C6-N3	-3.15	1.30	1.36
5	C	803	IX9	C2-N21	2.93	1.41	1.35
5	D	803	IX9	O13-C11	-2.89	1.33	1.39
5	C	803	IX9	C15-C11	2.68	1.44	1.38
5	B	804	IX9	O13-C11	-2.68	1.33	1.39

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	804	IX9	C26-N21-C2	-11.45	102.72	121.69
5	B	804	IX9	C26-N21-C2	-8.05	108.34	121.69
5	A	804	IX9	C25-N21-C2	-8.01	108.40	121.69
5	D	803	IX9	C26-N21-C2	-7.38	109.46	121.69
5	C	803	IX9	C26-N21-C2	-6.75	110.50	121.69

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	GOL	O1-C1-C2-O2
4	A	803	GOL	O1-C1-C2-C3
4	B	803	GOL	C1-C2-C3-O3
4	B	803	GOL	O2-C2-C3-O3
5	A	804	IX9	N1-C2-N21-C25

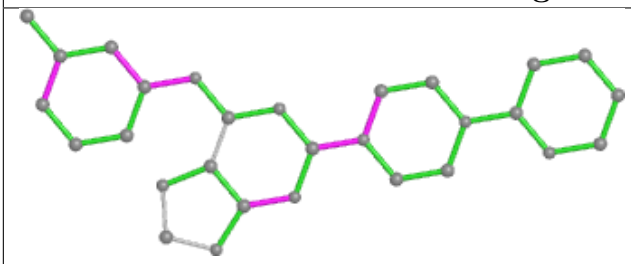
There are no ring outliers.

6 monomers are involved in 18 short contacts:

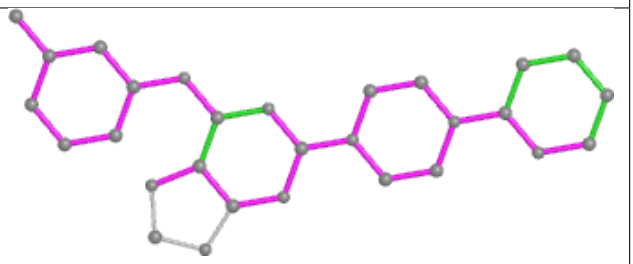
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	804	IX9	4	0
5	A	804	IX9	1	0
4	A	803	GOL	4	0
4	B	803	GOL	3	0
5	D	803	IX9	2	0
5	C	803	IX9	4	0

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.

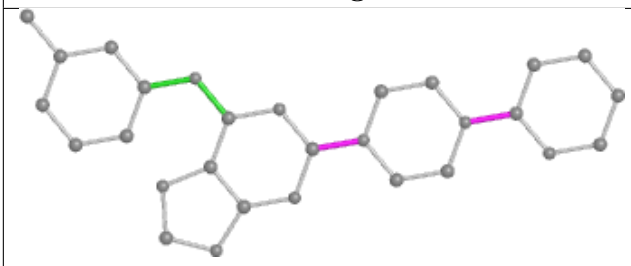
Ligand IX9 B 804



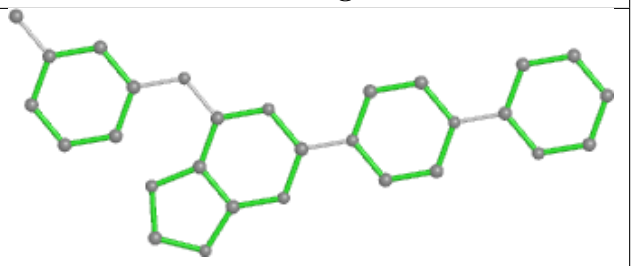
Bond lengths



Bond angles

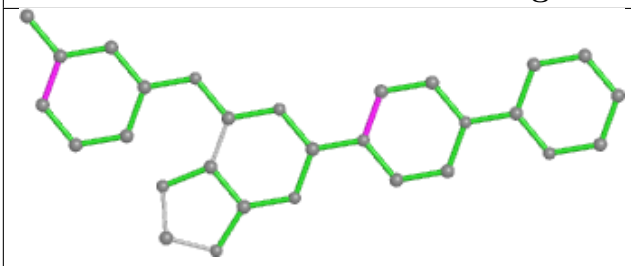


Torsions

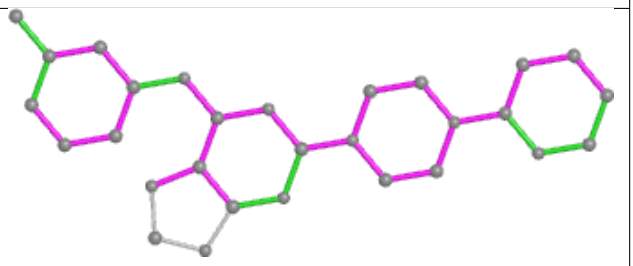


Rings

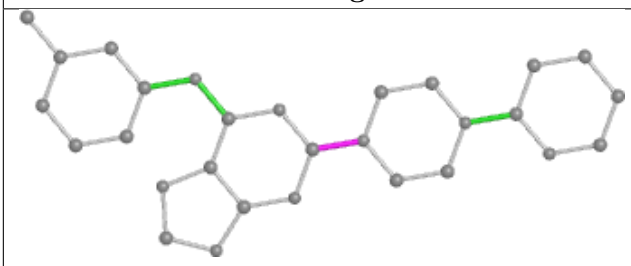
Ligand IX9 A 804



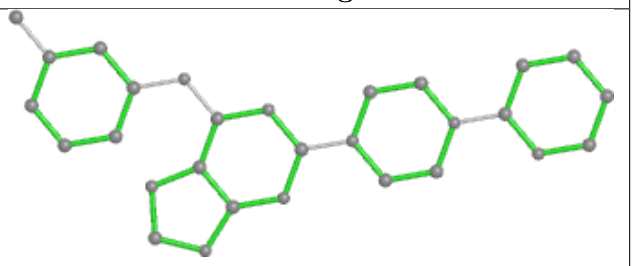
Bond lengths



Bond angles

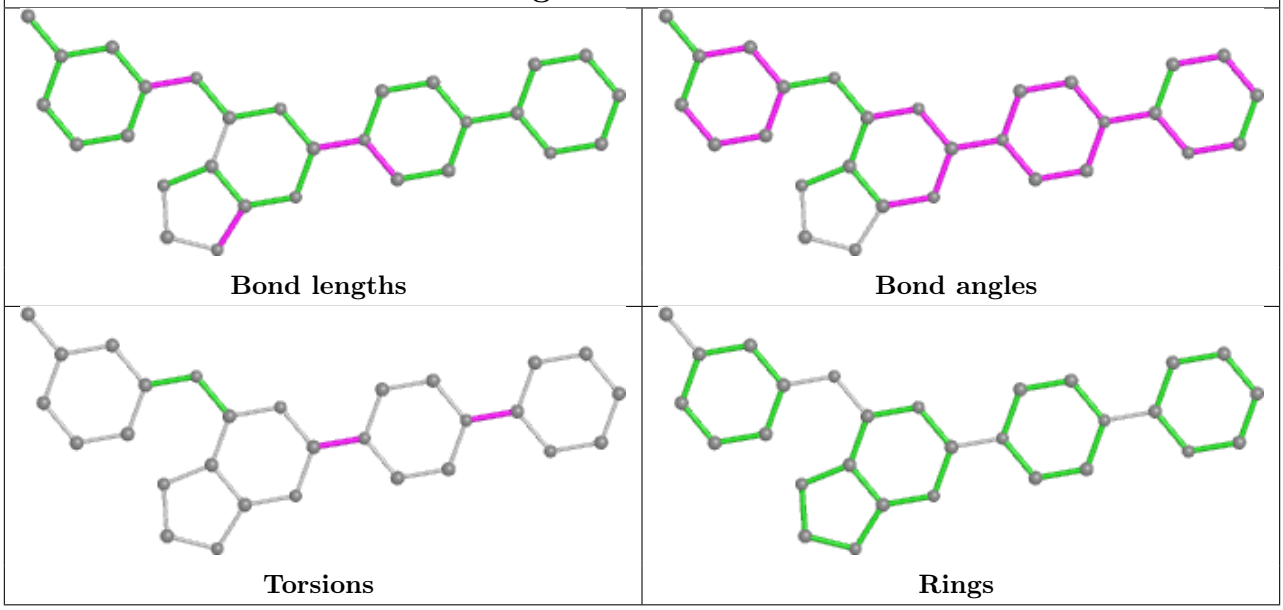


Torsions

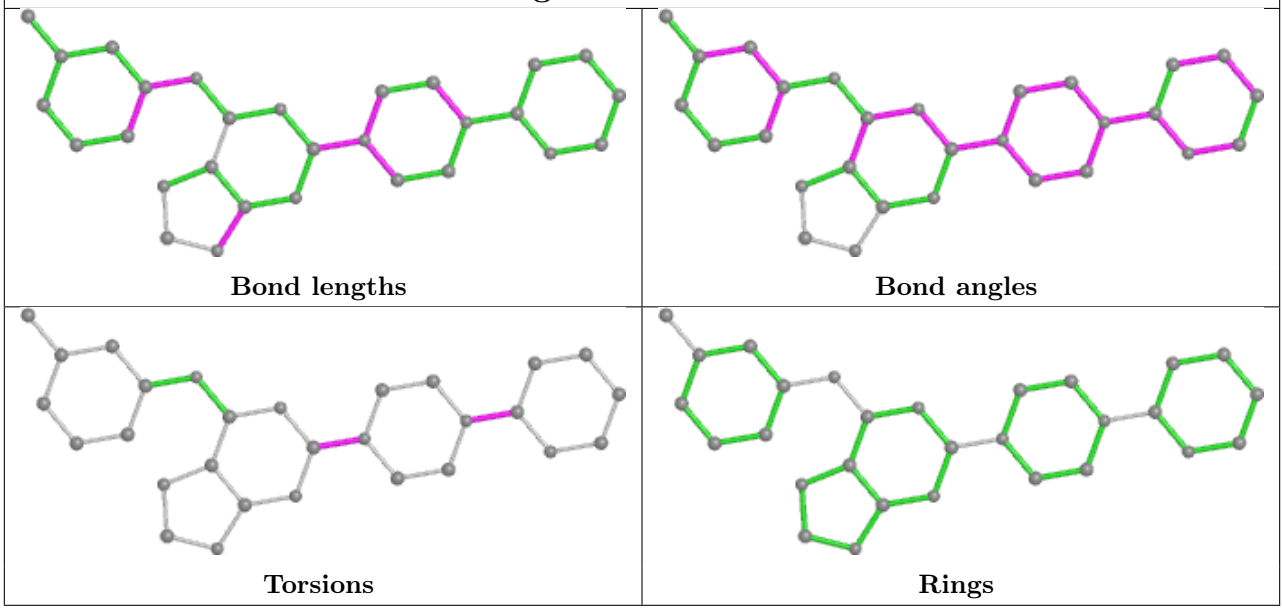


Rings

Ligand IX9 D 803



Ligand IX9 C 803



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, 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	313/343 (91%)	-0.24	2 (0%)	89	90	21, 31, 57, 92	0
1	B	314/343 (91%)	-0.28	1 (0%)	94	94	19, 30, 53, 89	0
1	C	312/343 (90%)	-0.38	3 (0%)	82	83	20, 31, 53, 93	0
1	D	312/343 (90%)	-0.24	5 (1%)	72	73	25, 38, 63, 104	0
All	All	1251/1372 (91%)	-0.28	11 (0%)	84	85	19, 33, 58, 104	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	771	THR	4.9
1	D	457	GLN	3.7
1	D	720	ASP	2.9
1	C	770	GLU	2.9
1	D	456	TRP	2.5

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	B	509	10/11	0.93	0.12	33,41,71,72	0
1	CME	A	509	10/11	0.94	0.10	34,42,77,82	0
1	CME	C	509	10/11	0.95	0.09	33,36,80,87	0
1	CME	D	509	10/11	0.95	0.10	37,48,89,99	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

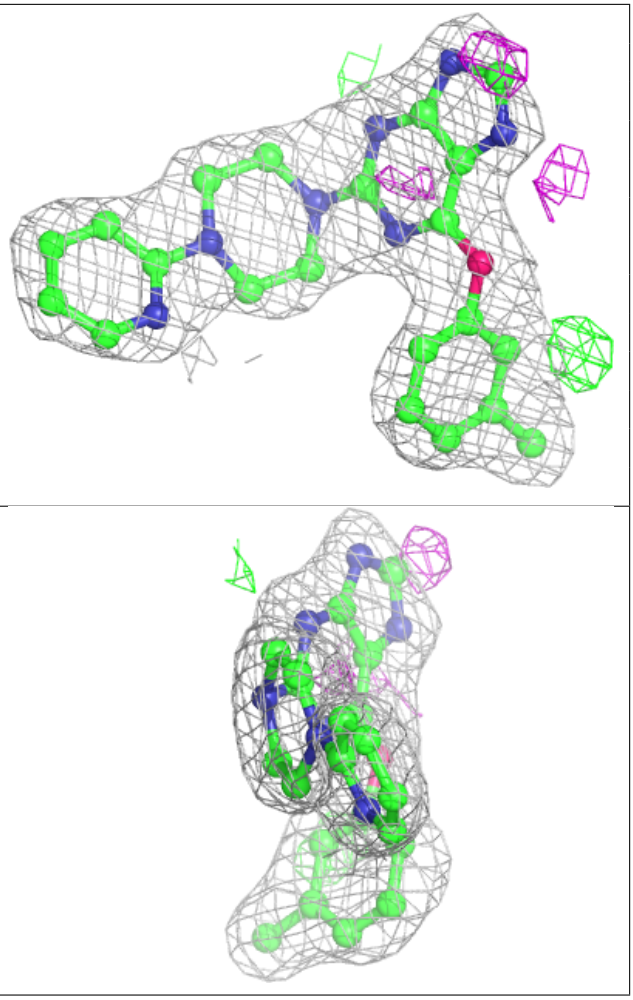
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	MG	D	802	1/1	0.87	0.29	46,46,46,46	0
4	GOL	A	803	6/6	0.88	0.19	47,53,61,61	0
4	GOL	B	803	6/6	0.88	0.17	43,49,51,53	0
3	MG	A	802	1/1	0.91	0.25	32,32,32,32	0
5	IX9	A	804	29/29	0.92	0.12	27,37,40,47	0
5	IX9	D	803	29/29	0.93	0.13	41,46,51,58	0
5	IX9	B	804	29/29	0.94	0.15	28,33,38,39	0
5	IX9	C	803	29/29	0.94	0.15	31,40,49,50	0
3	MG	B	802	1/1	0.94	0.26	26,26,26,26	0
3	MG	C	802	1/1	0.95	0.35	34,34,34,34	0
2	ZN	C	801	1/1	0.99	0.11	29,29,29,29	0
2	ZN	D	801	1/1	0.99	0.10	33,33,33,33	0
2	ZN	A	801	1/1	0.99	0.10	27,27,27,27	0
2	ZN	B	801	1/1	0.99	0.10	26,26,26,26	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.

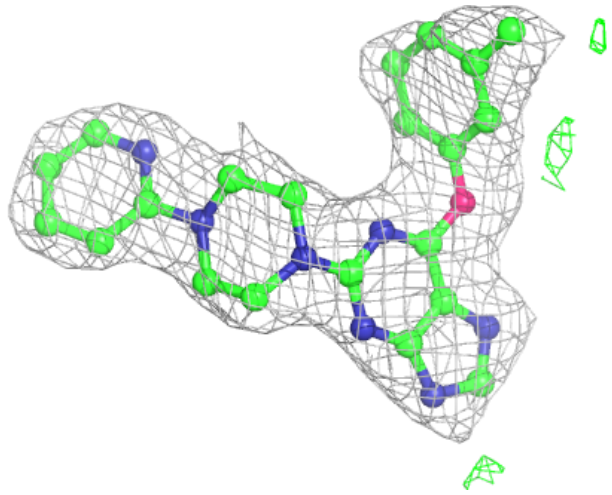
Electron density around IX9 A 804:

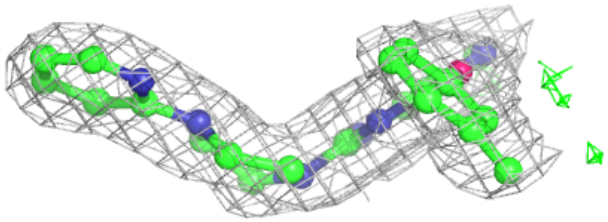
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

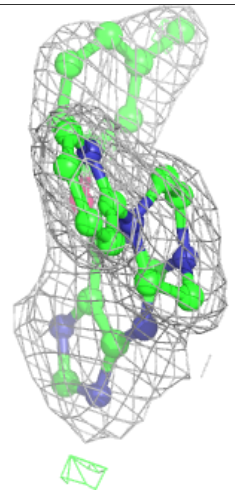


Electron density around IX9 D 803:

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

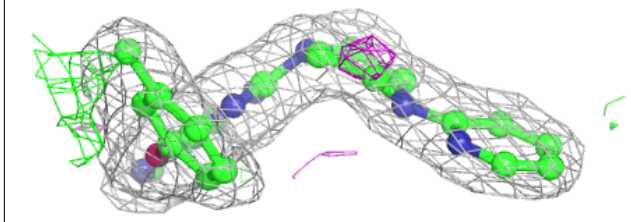


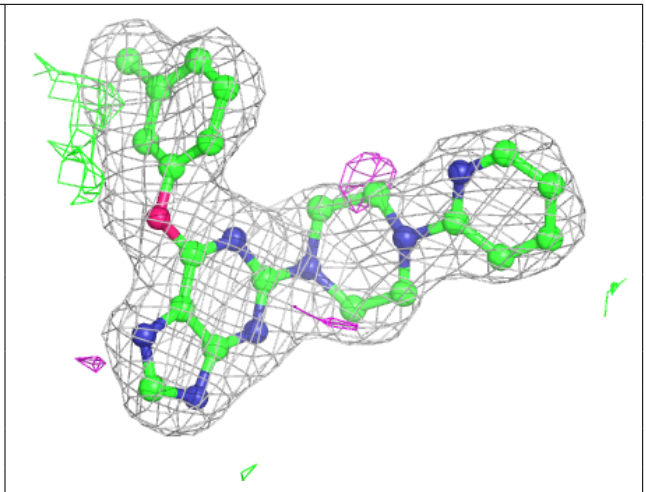


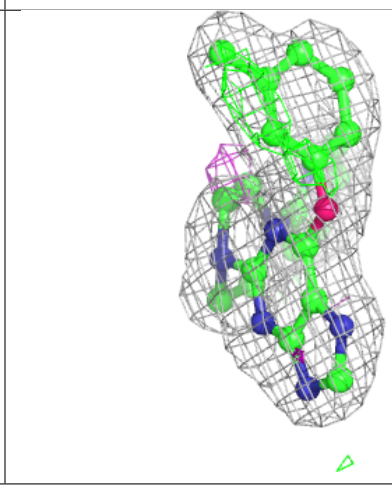


Electron density around IX9 B 804:

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

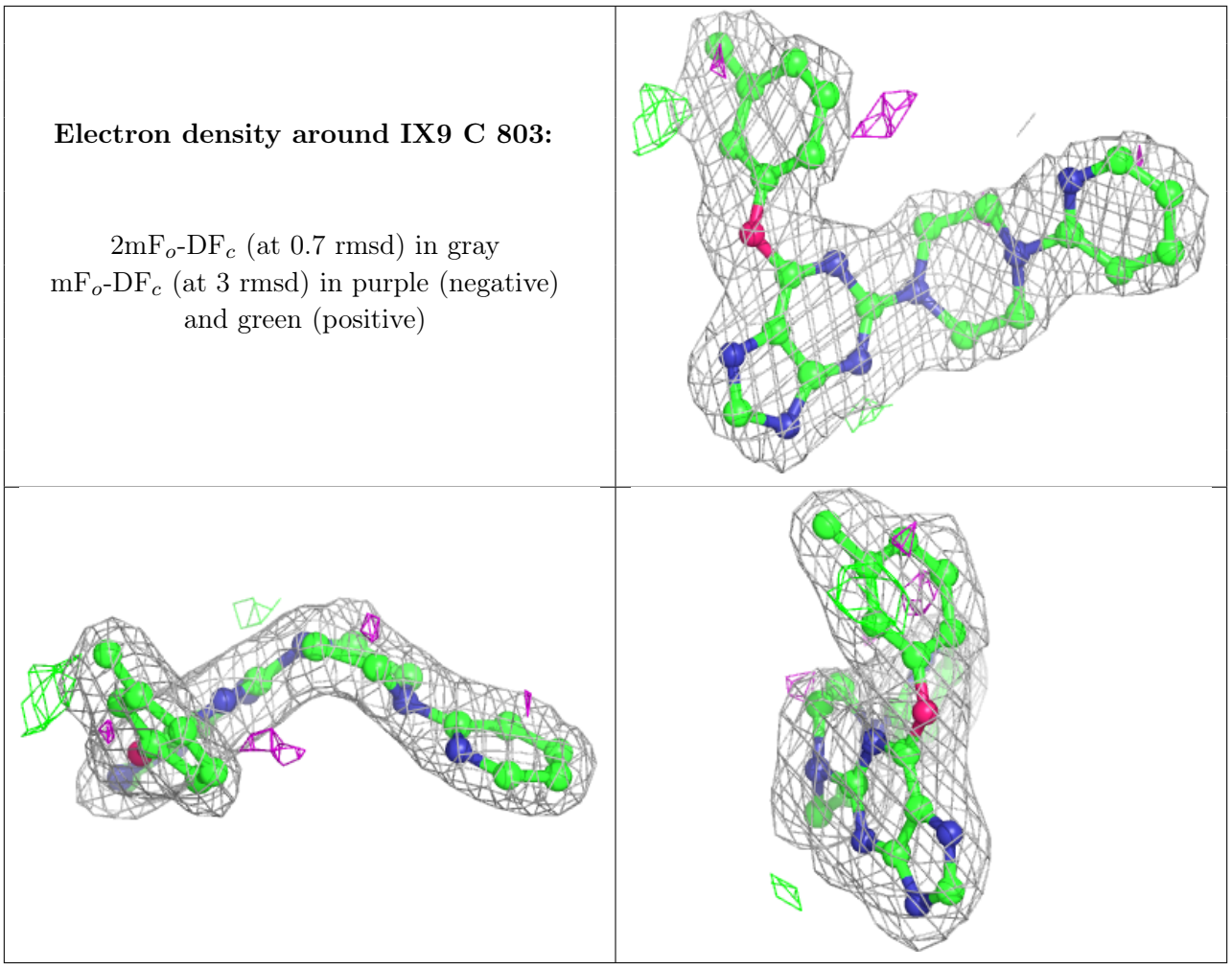






Electron density around IX9 C 803:

$2mF_o$-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.