



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 22, 2024 – 01:50 PM EDT

PDB ID : 5EDE  
Title : human PDE10A in complex with 1-(4-Chloro-phenyl)-3-methyl-1H-thieno[2,3-c]pyrazole-5-carboxylic acid (tetrahydro-furan-2-ylmethyl)-amide at 2.2Å  
Authors : Joseph, C.; Rudolph, M.G.  
Deposited on : 2015-10-21  
Resolution : 2.20 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
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) : 2.37.1

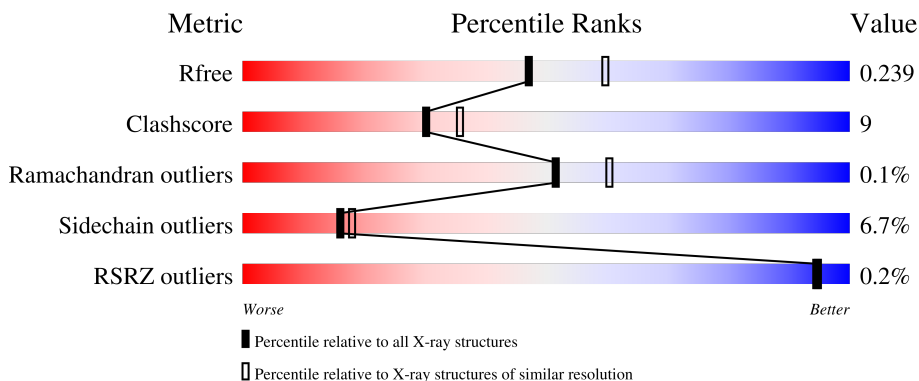
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	316	<div> <div style="width: 76%;"></div> <div style="width: 21%;"></div> <div style="width: 3%;"></div> </div> <div>76% 21% ..</div>
1	C	316	<div> <div style="width: 77%;"></div> <div style="width: 20%;"></div> <div style="width: 3%;"></div> </div> <div>77% 20% ..</div>
1	D	316	<div> <div style="width: 76%;"></div> <div style="width: 22%;"></div> <div style="width: 2%;"></div> </div> <div>76% 22% ..</div>
2	B	315	<div> <div style="width: 78%;"></div> <div style="width: 17%;"></div> <div style="width: 5%;"></div> </div> <div>78% 17% .</div>

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
5	GOL	A	803	-	X	-	-
5	GOL	B	803	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11207 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
			2580	1648	438	468	26			
1	C	313	Total	C	N	O	S	0	7	0
			2578	1648	439	466	25			
1	D	313	Total	C	N	O	S	0	5	0
			2568	1641	439	463	25			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	ALA	-	expression tag	UNP Q9Y233
A	470	ARG	LYS	conflict	UNP Q9Y233
A	771	ALA	-	expression tag	UNP Q9Y233
C	456	ALA	-	expression tag	UNP Q9Y233
C	470	ARG	LYS	conflict	UNP Q9Y233
C	771	ALA	-	expression tag	UNP Q9Y233
D	456	ALA	-	expression tag	UNP Q9Y233
D	470	ARG	LYS	conflict	UNP Q9Y233
D	771	ALA	-	expression tag	UNP Q9Y233

- Molecule 2 is a protein called cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	315	Total	C	N	O	S	0	5	0
			2581	1648	439	469	25			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	457	ALA	-	expression tag	UNP Q9Y233

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Chain	Residue	Modelled	Actual	Comment	Reference
B	470	ARG	LYS	conflict	UNP Q9Y233
B	771	ALA	-	expression tag	UNP Q9Y233

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

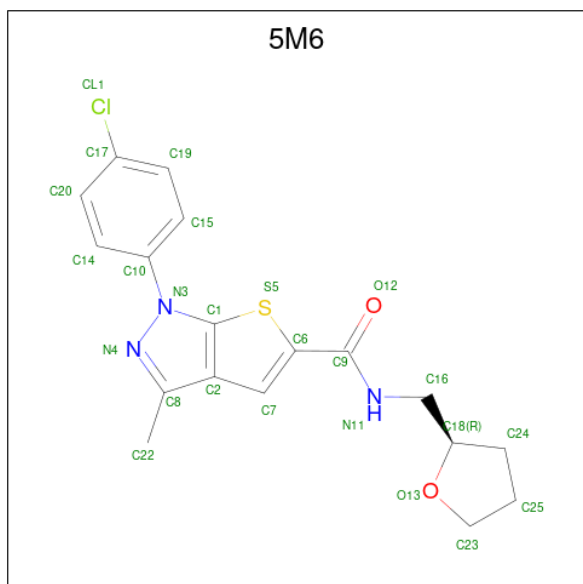
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 6 is 1-(4-chlorophenyl)-3-methyl- {N}-[[2 {R}]-oxolan-2-yl]methyl]thieno[2,3-c]pyrazole-5-carboxamide (three-letter code: 5M6) (formula: C<sub>18</sub>H<sub>18</sub>ClN<sub>3</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	Cl	N	O	S	0	0
			25	18	1	3	2	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total 25	C 18	Cl 1	N 3	O 2	S 1	0	0
6	C	1	Total 25	C 18	Cl 1	N 3	O 2	S 1	0	0
6	D	1	Total 25	C 18	Cl 1	N 3	O 2	S 1	0	0

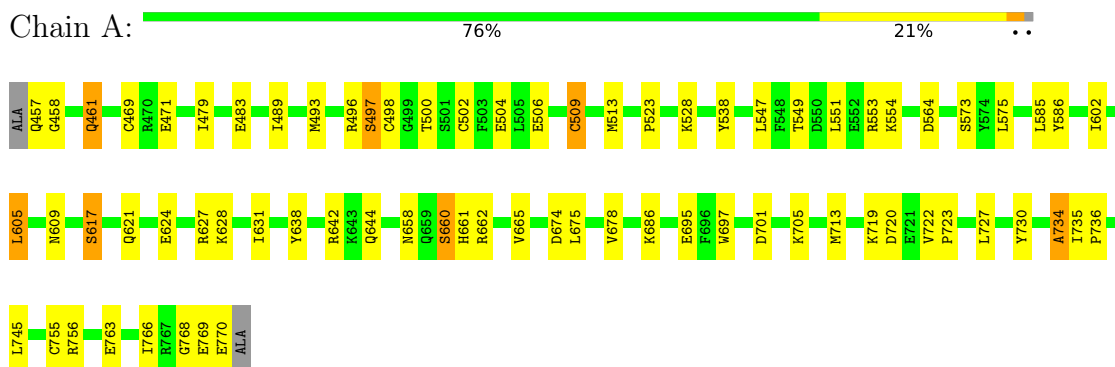
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	191	Total 191	O 191	0	0
7	B	219	Total 219	O 219	0	0
7	C	215	Total 215	O 215	0	0
7	D	155	Total 155	O 155	0	0

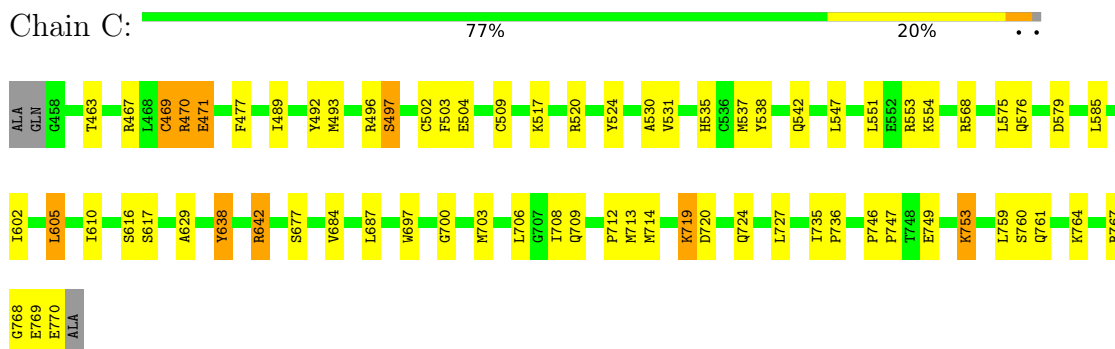
### 3 Residue-property plots

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.

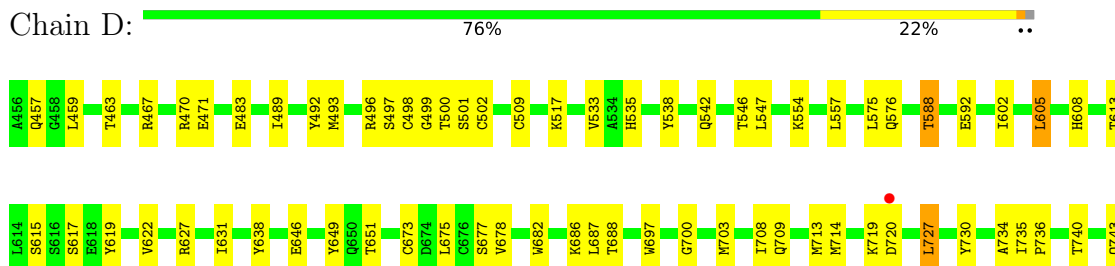
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



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



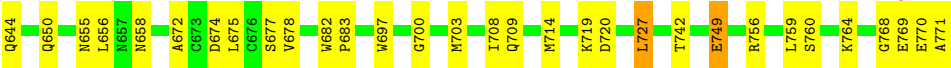
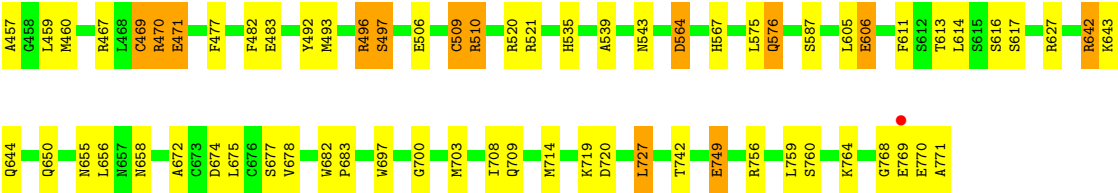
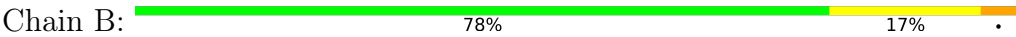
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A







- Molecule 2: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.61Å 135.61Å 235.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.73 – 2.20 43.74 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.0 (43.73-2.20) 96.0 (43.74-2.20)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.183 , 0.242 0.186 , 0.239	Depositor DCC
$R_{free}$ test set	4074 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 58.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11207	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CME, ZN, MG, 5M6, GOL

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	1.18	4/2649 (0.2%)	1.12	5/3583 (0.1%)
1	C	1.18	4/2650 (0.2%)	1.12	5/3584 (0.1%)
1	D	1.08	1/2634 (0.0%)	1.10	0/3563
2	B	1.22	5/2647 (0.2%)	1.14	5/3581 (0.1%)
All	All	1.17	14/10580 (0.1%)	1.12	15/14311 (0.1%)

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	606	GLU	CG-CD	10.19	1.67	1.51
1	C	524	TYR	CE2-CZ	-6.69	1.29	1.38
1	C	530	ALA	CA-CB	6.63	1.66	1.52
2	B	606	GLU	CB-CG	6.58	1.64	1.52
1	C	531	VAL	CB-CG2	5.88	1.65	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	642	ARG	NE-CZ-NH1	-9.61	115.49	120.30
1	A	674	ASP	CB-CG-OD2	-8.65	110.52	118.30
1	C	642	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	C	537	MET	CG-SD-CE	6.08	109.93	100.20
1	C	585	LEU	CB-CG-CD2	-6.08	100.67	111.00

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	2580	0	2554	54	0
1	C	2578	0	2566	52	0
1	D	2568	0	2550	45	0
2	B	2581	0	2555	41	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	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	6	0	8	3	0
5	B	6	0	8	4	0
6	A	25	0	0	1	0
6	B	25	0	0	1	0
6	C	25	0	0	1	0
6	D	25	0	0	2	0
7	A	191	0	0	8	0
7	B	219	0	0	5	0
7	C	215	0	0	9	0
7	D	155	0	0	4	0
All	All	11207	0	10241	191	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 9.

The worst 5 of 191 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	1.67	1.22
2:B:770:GLU:HG3	2:B:771:ALA:H	1.10	1.08
1:A:457:GLN:CB	1:A:458:GLY:CA	2.29	1.07
2:B:770:GLU:HG3	2:B:771:ALA:N	1.59	1.05
1:D:727:LEU:CD1	1:D:766:ILE:HD12	1.88	1.03

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	317/316 (100%)	306 (96%)	11 (4%)	0	100	100
1	C	317/316 (100%)	310 (98%)	7 (2%)	0	100	100
1	D	315/316 (100%)	308 (98%)	6 (2%)	1 (0%)	41	46
2	B	317/315 (101%)	310 (98%)	7 (2%)	0	100	100
All	All	1266/1263 (100%)	1234 (98%)	31 (2%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	615	SER

### 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	287/282 (102%)	274 (96%)	13 (4%)	27	34
1	C	288/282 (102%)	265 (92%)	23 (8%)	12	12
1	D	285/282 (101%)	265 (93%)	20 (7%)	15	16
2	B	286/281 (102%)	263 (92%)	23 (8%)	12	12
All	All	1146/1127 (102%)	1067 (93%)	79 (7%)	16	16

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	753	LYS
1	D	613	THR
1	D	457	GLN
1	D	517	LYS
1	D	709	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	644	GLN
1	D	761	GLN
1	C	604	GLN
1	D	621	GLN
1	C	542	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\# Z  > 2$
2	CME	B	509	2	8,9,10	0.67	0	5,9,11	3.39	2 (40%)
1	CME	C	509	1	8,9,10	0.76	0	5,9,11	2.78	1 (20%)
1	CME	D	509	1	8,9,10	0.71	0	5,9,11	3.07	1 (20%)
1	CME	A	509	1	8,9,10	0.72	0	5,9,11	3.06	1 (20%)

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	509	CME	CE-SD-SG	7.04	135.90	103.45
1	A	509	CME	CE-SD-SG	6.68	134.25	103.45
1	D	509	CME	CE-SD-SG	6.32	132.57	103.45
1	C	509	CME	CE-SD-SG	5.63	129.38	103.45
2	B	509	CME	CB-SG-SD	-2.63	97.01	103.82

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

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	GOL	B	803	-	5,5,5	0.91	0	5,5,5	1.18	1 (20%)
6	5M6	C	803	-	22,28,28	1.33	3 (13%)	25,40,40	1.61	5 (20%)
6	5M6	D	803	-	22,28,28	1.22	3 (13%)	25,40,40	2.16	6 (24%)
5	GOL	A	803	-	5,5,5	0.90	0	5,5,5	1.37	2 (40%)
6	5M6	A	804	-	22,28,28	1.70	3 (13%)	25,40,40	2.11	5 (20%)
6	5M6	B	804	-	22,28,28	1.83	4 (18%)	25,40,40	1.94	5 (20%)

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	GOL	B	803	-	-	2/4/4/4	-
6	5M6	C	803	-	-	2/11/20/20	0/4/4/4
6	5M6	D	803	-	-	5/11/20/20	0/4/4/4
5	GOL	A	803	-	-	4/4/4/4	-
6	5M6	A	804	-	-	3/11/20/20	0/4/4/4
6	5M6	B	804	-	-	3/11/20/20	0/4/4/4

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	804	5M6	C6-S5	5.48	1.79	1.72
6	A	804	5M6	C6-S5	4.67	1.78	1.72
6	A	804	5M6	C16-C18	3.18	1.55	1.51
6	B	804	5M6	C16-C18	3.08	1.55	1.51
6	D	803	5M6	C16-C18	2.48	1.54	1.51



The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	804	5M6	C10-N3-C1	-6.92	122.57	129.77
6	D	803	5M6	C10-N3-C1	-5.61	123.93	129.77
6	B	804	5M6	C6-C9-N11	5.53	123.32	115.59
6	C	803	5M6	C10-N3-C1	-4.59	124.99	129.77
6	D	803	5M6	C22-C8-N4	4.45	129.43	119.65

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	803	GOL	O1-C1-C2-C3
5	A	803	GOL	C1-C2-C3-O3
6	A	804	5M6	C15-C10-N3-C1
6	A	804	5M6	C14-C10-N3-C1
6	B	804	5M6	C15-C10-N3-C1

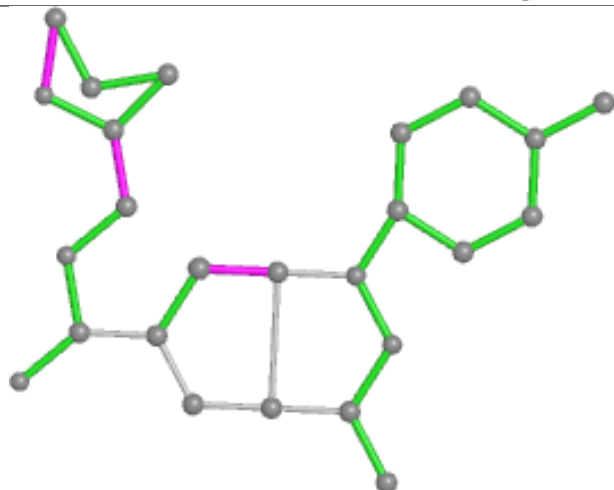
There are no ring outliers.

6 monomers are involved in 12 short contacts:

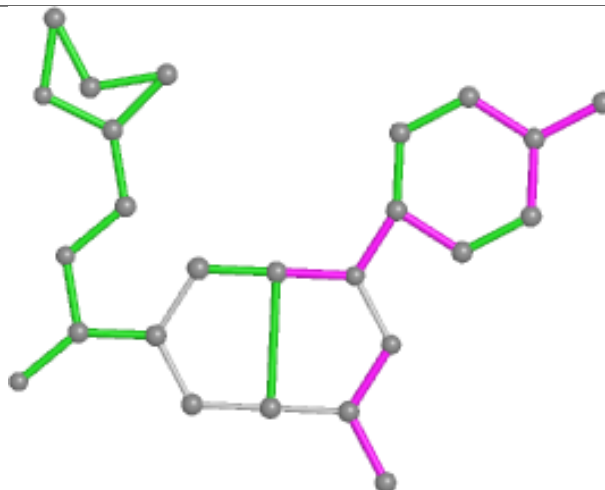
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	803	GOL	4	0
6	C	803	5M6	1	0
6	D	803	5M6	2	0
5	A	803	GOL	3	0
6	A	804	5M6	1	0
6	B	804	5M6	1	0

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.

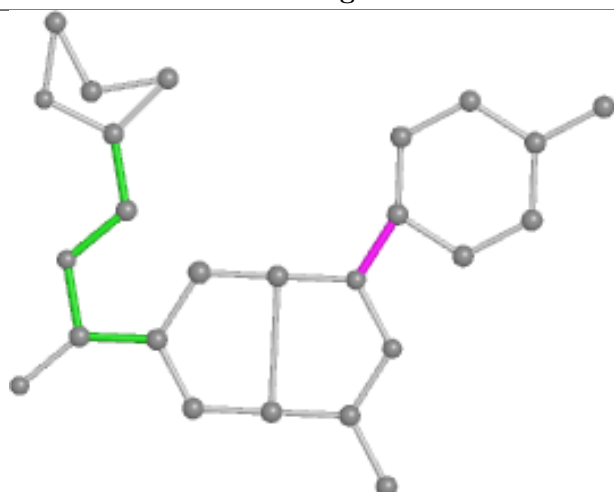
## Ligand 5M6 C 803



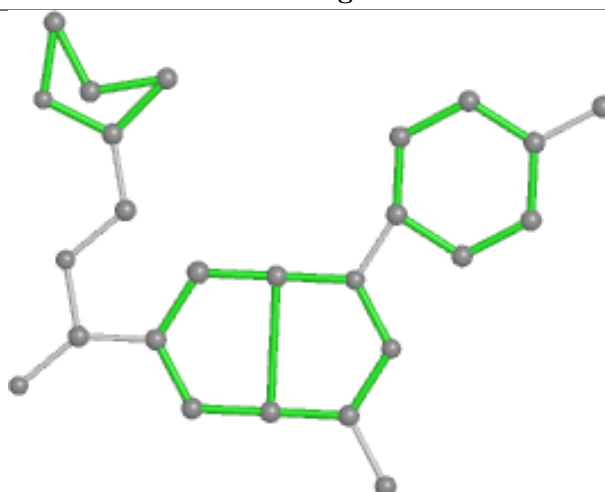
Bond lengths



Bond angles

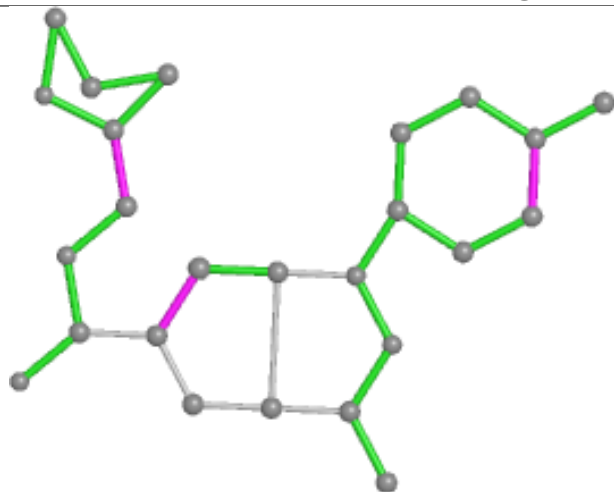


Torsions

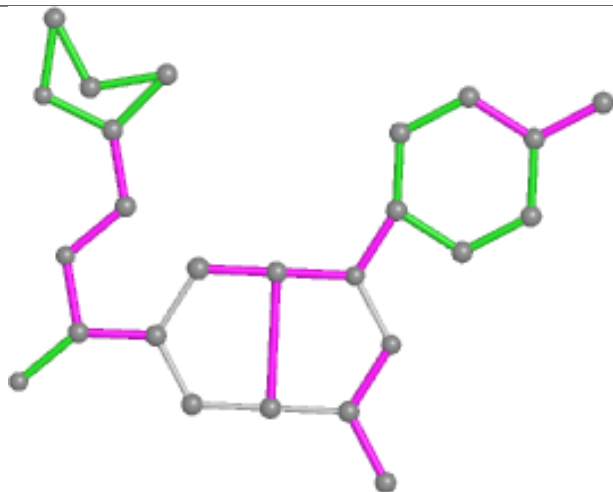


Rings

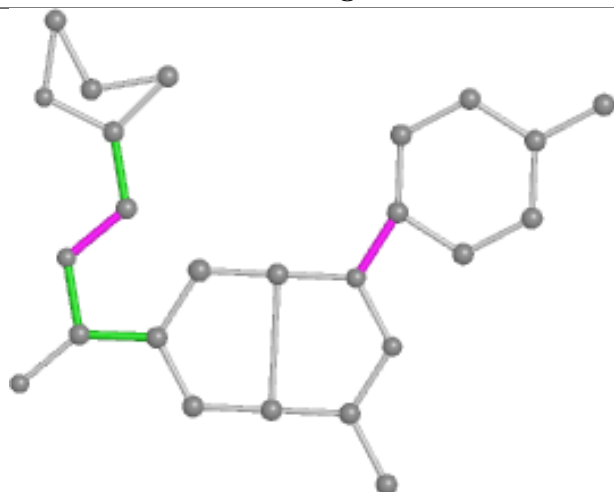
## Ligand 5M6 D 803



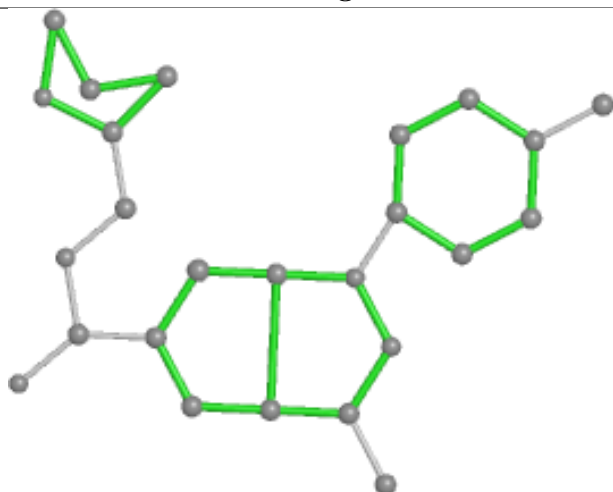
Bond lengths



Bond angles

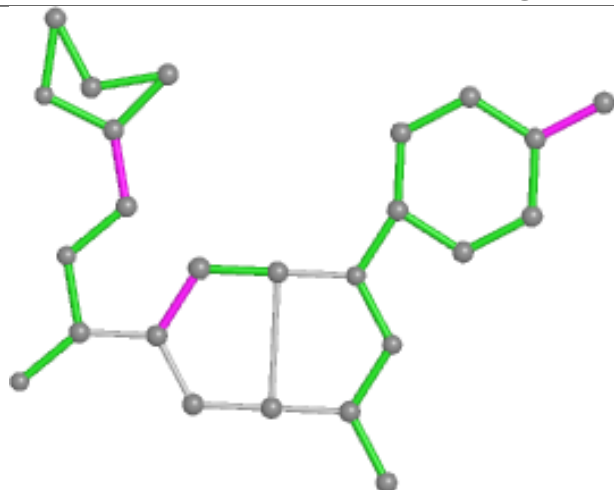


Torsions

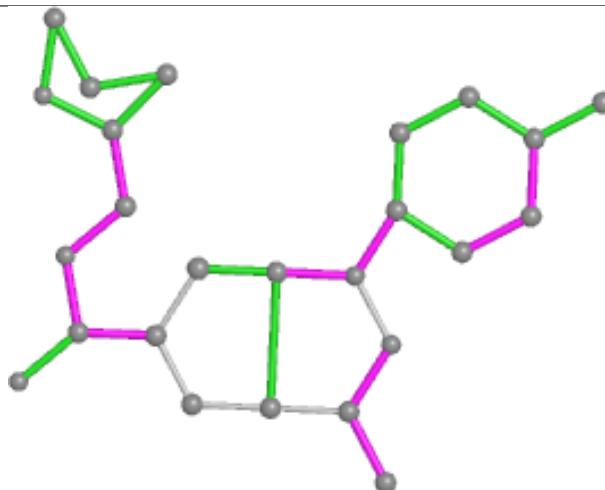


Rings

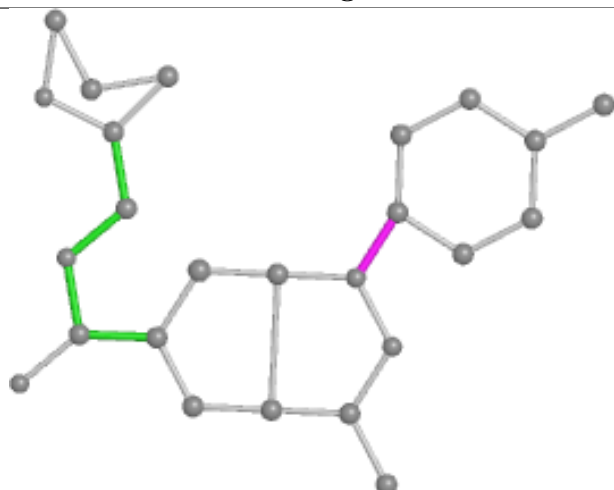
## Ligand 5M6 A 804



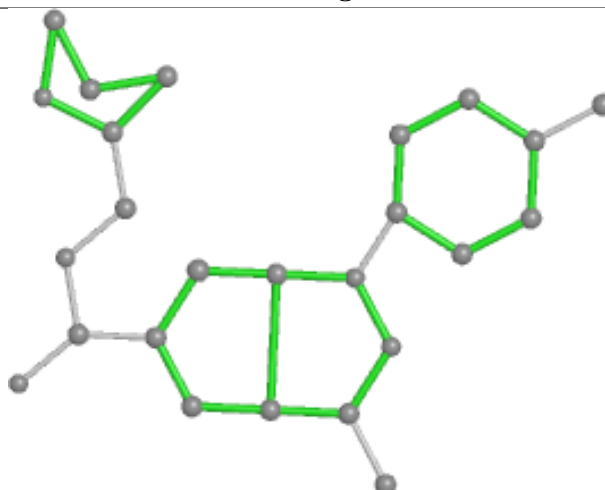
Bond lengths



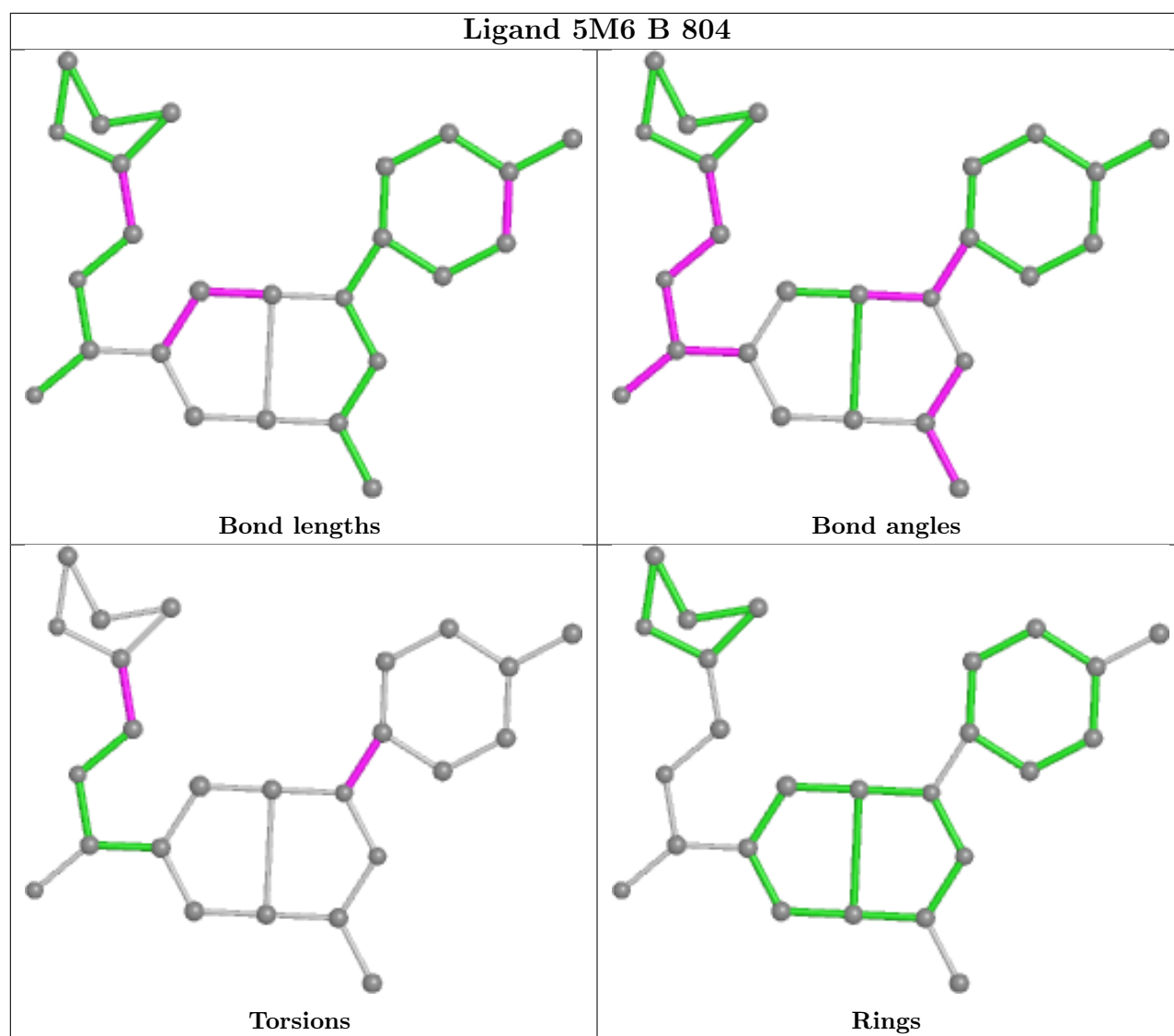
Bond angles



Torsions



Rings



## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	313/316 (99%)	-0.52	0	100 100	20, 32, 53, 80	0
1	C	312/316 (98%)	-0.68	0	100 100	19, 32, 52, 73	0
1	D	312/316 (98%)	-0.39	1 (0%)	94 93	25, 40, 60, 80	0
2	B	314/315 (99%)	-0.45	1 (0%)	94 93	18, 31, 53, 75	0
All	All	1251/1263 (99%)	-0.51	2 (0%)	95 94	18, 34, 56, 80	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	769	GLU	2.6
1	D	720	ASP	2.4

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	CME	A	509	10/11	0.87	0.16	38,43,65,66	0
2	CME	B	509	10/11	0.91	0.14	32,40,68,69	0
1	CME	C	509	10/11	0.91	0.13	35,38,64,67	0
1	CME	D	509	10/11	0.92	0.13	40,43,69,71	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

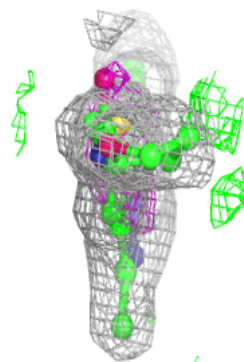
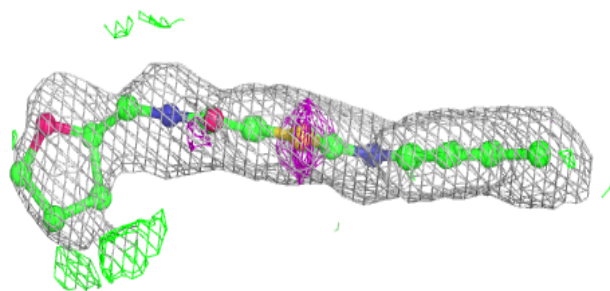
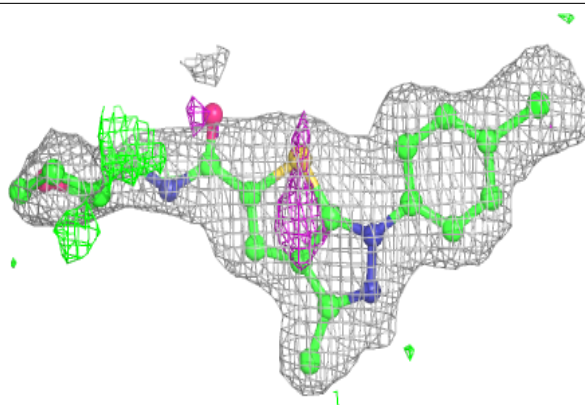
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	B	803	6/6	0.86	0.14	37,42,43,44	0
5	GOL	A	803	6/6	0.91	0.15	43,46,49,49	0
6	5M6	D	803	25/25	0.92	0.15	36,43,69,71	0
6	5M6	B	804	25/25	0.93	0.12	29,38,58,62	0
6	5M6	A	804	25/25	0.93	0.14	32,36,58,61	0
6	5M6	C	803	25/25	0.94	0.16	32,36,58,63	0
4	MG	D	802	1/1	0.97	0.05	31,31,31,31	0
4	MG	B	802	1/1	0.99	0.11	12,12,12,12	0
4	MG	C	802	1/1	0.99	0.06	22,22,22,22	0
4	MG	A	802	1/1	0.99	0.08	25,25,25,25	0
3	ZN	C	801	1/1	1.00	0.09	26,26,26,26	0
3	ZN	D	801	1/1	1.00	0.08	33,33,33,33	0
3	ZN	A	801	1/1	1.00	0.11	28,28,28,28	0
3	ZN	B	801	1/1	1.00	0.10	24,24,24,24	0

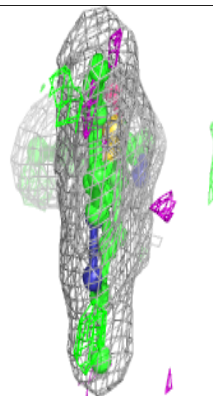
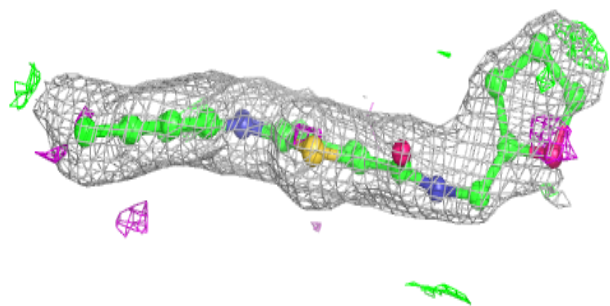
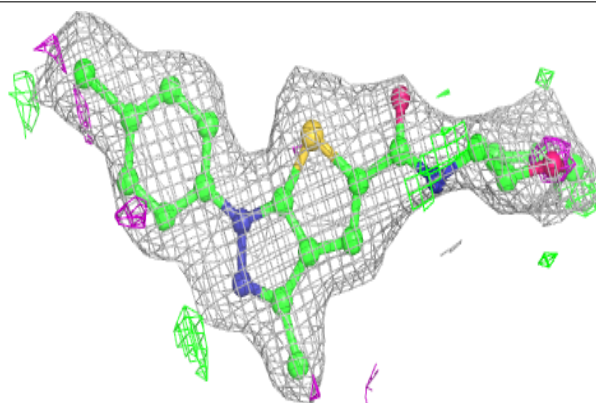
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 5M6 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 5M6 B 804:**

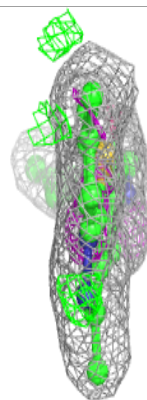
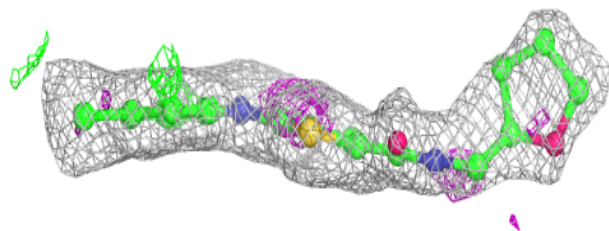
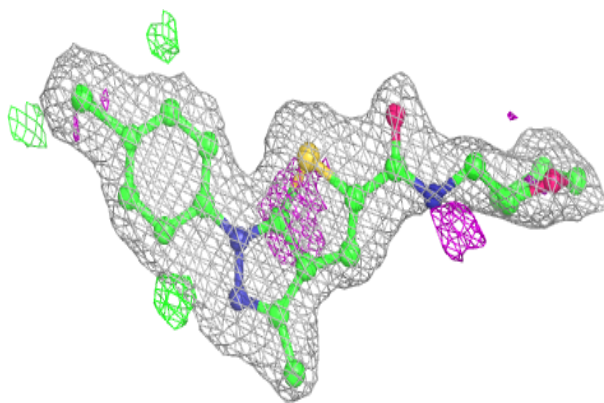
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



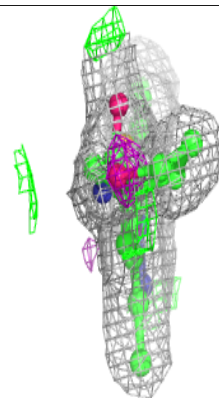
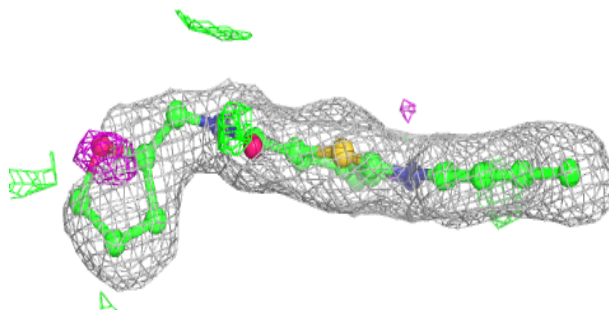
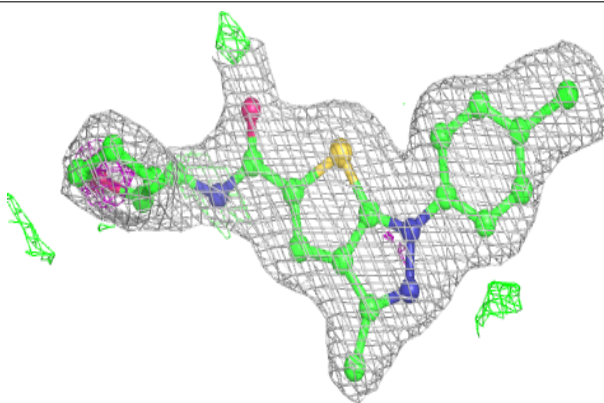


**Electron density around 5M6 A 804:**

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

**Electron density around 5M6 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.