



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:53 pm BST

PDB ID : 5FU8  
Title : Pseudomonas aeruginosa RmlA in complex with allosteric inhibitor  
Authors : Alphey, M.S.; Tran, F.; Westwood, N.J.; Naismith, J.H.  
Deposited on : 2016-01-21  
Resolution : 2.20 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](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.

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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 : 2.11  
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) : 2.11

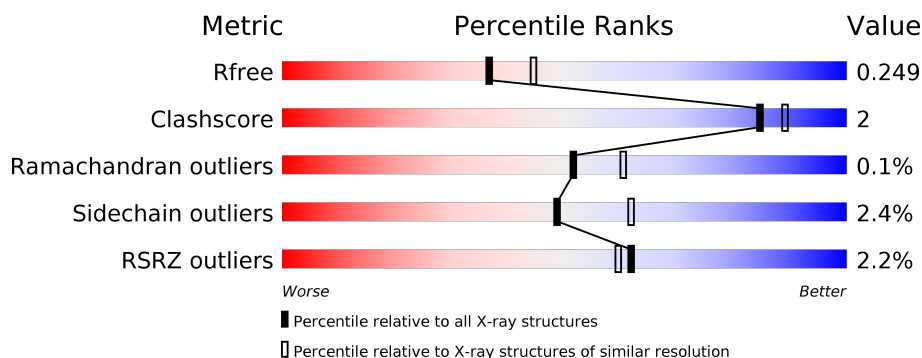
# 1 Overall quality at a glance

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 on 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	303	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div>•</div> </div> </div>
1	B	303	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>•</div> </div> </div>
1	C	303	<div> <div>4%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>•</div> </div> </div>
1	D	303	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>•</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10061 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 GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	1	0
			2339	1495	399	440	5			
1	B	293	Total	C	N	O	S	0	1	0
			2299	1471	387	436	5			
1	C	295	Total	C	N	O	S	0	1	0
			2321	1484	395	438	4			
1	D	292	Total	C	N	O	S	0	1	0
			2291	1466	386	435	4			

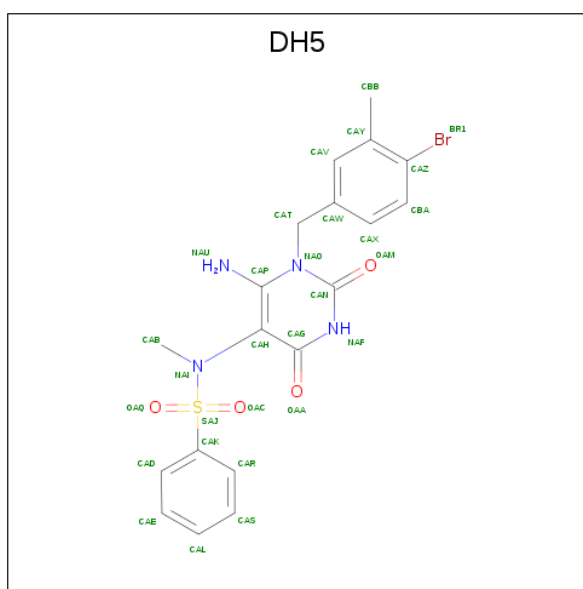
There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	HIS	-	expression tag	UNP Q9HU22
A	-8	HIS	-	expression tag	UNP Q9HU22
A	-7	HIS	-	expression tag	UNP Q9HU22
A	-6	HIS	-	expression tag	UNP Q9HU22
A	-5	HIS	-	expression tag	UNP Q9HU22
A	-4	HIS	-	expression tag	UNP Q9HU22
A	-3	GLY	-	expression tag	UNP Q9HU22
A	-2	SER	-	expression tag	UNP Q9HU22
A	-1	MET	-	expression tag	UNP Q9HU22
A	0	ALA	-	expression tag	UNP Q9HU22
B	-9	HIS	-	expression tag	UNP Q9HU22
B	-8	HIS	-	expression tag	UNP Q9HU22
B	-7	HIS	-	expression tag	UNP Q9HU22
B	-6	HIS	-	expression tag	UNP Q9HU22
B	-5	HIS	-	expression tag	UNP Q9HU22
B	-4	HIS	-	expression tag	UNP Q9HU22
B	-3	GLY	-	expression tag	UNP Q9HU22
B	-2	SER	-	expression tag	UNP Q9HU22
B	-1	MET	-	expression tag	UNP Q9HU22
B	0	ALA	-	expression tag	UNP Q9HU22

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	HIS	-	expression tag	UNP Q9HU22
C	-8	HIS	-	expression tag	UNP Q9HU22
C	-7	HIS	-	expression tag	UNP Q9HU22
C	-6	HIS	-	expression tag	UNP Q9HU22
C	-5	HIS	-	expression tag	UNP Q9HU22
C	-4	HIS	-	expression tag	UNP Q9HU22
C	-3	GLY	-	expression tag	UNP Q9HU22
C	-2	SER	-	expression tag	UNP Q9HU22
C	-1	MET	-	expression tag	UNP Q9HU22
C	0	ALA	-	expression tag	UNP Q9HU22
D	-9	HIS	-	expression tag	UNP Q9HU22
D	-8	HIS	-	expression tag	UNP Q9HU22
D	-7	HIS	-	expression tag	UNP Q9HU22
D	-6	HIS	-	expression tag	UNP Q9HU22
D	-5	HIS	-	expression tag	UNP Q9HU22
D	-4	HIS	-	expression tag	UNP Q9HU22
D	-3	GLY	-	expression tag	UNP Q9HU22
D	-2	SER	-	expression tag	UNP Q9HU22
D	-1	MET	-	expression tag	UNP Q9HU22
D	0	ALA	-	expression tag	UNP Q9HU22

- Molecule 2 is N-(6-amino-1-(4-bromo-3-methylbenzyl)-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-5-yl)-N-methylbenzenesulfonamide (three-letter code: DH5) (formula:  $C_{19}H_{19}BrN_4O_4S$ ).



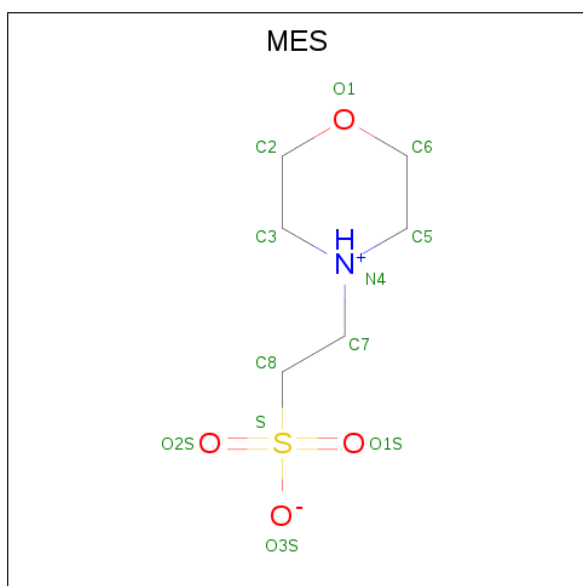
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	S	0	0
			29	1	19	4	4	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	Br	C	N	O	S	0	0
			29	1	19	4	4	1		
2	C	1	Total	Br	C	N	O	S	0	0
			29	1	19	4	4	1		
2	D	1	Total	Br	C	N	O	S	0	0
			29	1	19	4	4	1		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	182	Total	O	0	0
			182	182		
5	B	153	Total	O	0	0
			153	153		
5	C	158	Total	O	0	0
			158	158		
5	D	150	Total	O	0	0
			150	150		

**i**

● Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.18 Å   154.48 Å   134.75 Å 90.00°   92.34°   90.00°	Depositor
Resolution (Å)	134.64 – 2.20 25.88 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (134.64-2.20) 96.2 (25.88-2.20)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.200   ,   0.249 0.207   ,   0.249	Depositor DCC
$R_{free}$ test set	3158 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34   ,   40.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.095 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10061	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DH5, MES, CL

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	0.57	0/2395	0.75	2/3247 (0.1%)
1	B	0.57	0/2352	0.78	1/3190 (0.0%)
1	C	0.59	0/2376	0.79	4/3222 (0.1%)
1	D	0.54	0/2344	0.73	0/3180
All	All	0.57	0/9467	0.76	7/12839 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	B	128	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	A	62	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	245	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	3	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	C	69	ASP	CB-CG-OD1	5.08	122.87	118.30
1	C	286	ARG	NE-CZ-NH1	5.07	122.84	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	2339	0	2322	12	0
1	B	2299	0	2292	8	0
1	C	2321	0	2303	15	0
1	D	2291	0	2280	16	0
2	A	29	0	0	0	0
2	B	29	0	0	0	0
2	C	29	0	0	0	0
2	D	29	0	0	3	0
3	A	12	0	13	2	0
3	B	12	0	13	0	0
3	C	12	0	13	0	0
3	D	12	0	13	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	182	0	0	0	0
5	B	153	0	0	2	0
5	C	158	0	0	0	0
5	D	150	0	0	0	0
All	All	10061	0	9249	43	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 2.

All (43) 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:C:237[A]:GLN:OE1	1:D:237[A]:GLN:OE1	1.71	1.07
1:D:119:HIS:CD2	2:D:500:DH5:BR1	2.96	0.73
1:C:23:ILE:HD11	1:C:28:LEU:HD23	1.76	0.68
1:C:237[A]:GLN:OE1	1:D:237[A]:GLN:HG2	1.98	0.64
1:C:237[A]:GLN:OE1	1:D:237[A]:GLN:CD	2.37	0.64
1:C:237[A]:GLN:CD	1:D:237[A]:GLN:OE1	2.36	0.61
1:A:226:THR:O	1:A:226:THR:HG22	2.03	0.58
1:B:12:SER:O	1:B:15:ARG:HG2	2.04	0.57
1:C:237[A]:GLN:OE1	1:D:237[A]:GLN:CG	2.53	0.57
1:C:237[A]:GLN:CG	1:D:237[A]:GLN:OE1	2.53	0.56
1:C:237[A]:GLN:HG2	1:D:237[A]:GLN:OE1	2.07	0.55
1:A:214:VAL:O	3:A:550:MES:H82	2.07	0.54
1:D:119:HIS:NE2	2:D:500:DH5:BR1	2.97	0.53
1:C:35:MET:CE	1:C:226:THR:HG21	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:GLU:HA	1:B:237[A]:GLN:HE21	1.74	0.52
1:D:226:THR:HG22	1:D:226:THR:O	2.11	0.50
1:A:142:PRO:HG2	1:A:166:PRO:HG2	1.94	0.49
1:B:122:LEU:CD2	1:B:175:LEU:HD21	2.43	0.49
1:A:234:GLU:HA	1:A:237[A]:GLN:HE21	1.77	0.49
1:C:30:VAL:HG11	1:C:112:LEU:HD21	1.95	0.48
1:A:62:ARG:NH1	1:B:62:ARG:HD2	2.28	0.48
1:C:128:ARG:NH1	1:C:133:SER:OG	2.46	0.48
1:A:30:VAL:HG11	1:A:112:LEU:HD21	1.95	0.48
1:A:154:GLY:O	3:A:550:MES:C7	2.62	0.47
1:C:226:THR:HG22	1:C:226:THR:O	2.15	0.47
1:D:64:GLN:HG2	1:D:79:TYR:CD1	2.50	0.47
1:B:32:ASP:HB2	5:B:2018:HOH:O	2.16	0.44
1:A:35:MET:CE	1:A:226:THR:HG21	2.47	0.44
1:C:189:LEU:HD11	1:C:202:VAL:HG23	1.98	0.44
1:D:234:GLU:HA	1:D:237[A]:GLN:HE21	1.82	0.44
1:A:224:LEU:HD11	1:A:238:PHE:CD2	2.54	0.43
1:B:189:LEU:HD11	1:B:202:VAL:HG23	2.00	0.43
1:C:24:SER:HB2	1:C:59:ASP:OD2	2.18	0.43
1:A:35:MET:O	1:A:39:PRO:HD2	2.18	0.42
1:D:35:MET:CE	1:D:226:THR:HG21	2.49	0.42
1:B:141:ASP:OD2	1:B:144:ARG:HD3	2.20	0.42
1:D:45:LEU:HD22	2:D:500:DH5:CAR	2.49	0.42
1:D:90:GLN:HG2	1:D:197:LEU:HD12	2.01	0.42
1:B:194:ARG:HD3	5:B:2107:HOH:O	2.19	0.42
1:D:141:ASP:OD2	1:D:144:ARG:HD3	2.20	0.41
1:C:60:THR:HB	1:C:61:PRO:HD3	2.03	0.41
1:A:35:MET:HE1	1:A:226:THR:HG21	2.04	0.40
1:A:1:MET:HB3	1:A:129:GLN:OE1	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	294/303 (97%)	290 (99%)	4 (1%)	0	100	100
1	B	292/303 (96%)	284 (97%)	8 (3%)	0	100	100
1	C	292/303 (96%)	287 (98%)	4 (1%)	1 (0%)	41	46
1	D	291/303 (96%)	286 (98%)	5 (2%)	0	100	100
All	All	1169/1212 (96%)	1147 (98%)	21 (2%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	31	TYR

### 5.3.2 Protein sidechains ⓘ

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	245/248 (99%)	240 (98%)	5 (2%)	55	69
1	B	241/248 (97%)	233 (97%)	8 (3%)	38	49
1	C	243/248 (98%)	240 (99%)	3 (1%)	71	83
1	D	240/248 (97%)	233 (97%)	7 (3%)	42	54
All	All	969/992 (98%)	946 (98%)	23 (2%)	49	62

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	190	LYS
1	A	194	ARG
1	A	232	LEU
1	A	277	LYS
1	B	2	LYS
1	B	17	HIS
1	B	58	GLN
1	B	111	ASN
1	B	190	LYS

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Mol	Chain	Res	Type
1	B	194	ARG
1	B	275	LEU
1	B	285	LYS
1	C	2	LYS
1	C	190	LYS
1	C	194	ARG
1	D	2	LYS
1	D	17	HIS
1	D	24	SER
1	D	84	SER
1	D	111	ASN
1	D	124	SER
1	D	155	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MES	A	550	-	12,12,12	2.16	1 (8%)	14,16,16	1.64	3 (21%)
2	DH5	D	500	-	29,31,31	3.19	7 (24%)	34,46,46	2.49	8 (23%)
3	MES	C	550	-	12,12,12	2.04	1 (8%)	14,16,16	2.19	6 (42%)
2	DH5	A	500	-	29,31,31	2.92	7 (24%)	34,46,46	2.18	6 (17%)
3	MES	B	550	-	12,12,12	2.14	1 (8%)	14,16,16	1.38	2 (14%)
2	DH5	C	500	-	29,31,31	3.41	8 (27%)	34,46,46	2.39	7 (20%)
3	MES	D	550	-	12,12,12	2.12	1 (8%)	14,16,16	1.79	2 (14%)
2	DH5	B	500	-	29,31,31	2.97	7 (24%)	34,46,46	2.06	7 (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
3	MES	A	550	-	-	2/6/14/14	0/1/1/1
2	DH5	D	500	-	-	2/20/20/20	0/3/3/3
3	MES	C	550	-	-	3/6/14/14	0/1/1/1
2	DH5	A	500	-	-	4/20/20/20	0/3/3/3
3	MES	B	550	-	-	1/6/14/14	0/1/1/1
2	DH5	C	500	-	-	3/20/20/20	0/3/3/3
3	MES	D	550	-	-	3/6/14/14	0/1/1/1
2	DH5	B	500	-	-	2/20/20/20	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	DH5	OAQ-SAJ	9.93	1.54	1.43
2	B	500	DH5	OAC-SAJ	9.34	1.53	1.43
2	C	500	DH5	OAC-SAJ	9.27	1.53	1.43
2	D	500	DH5	OAC-SAJ	8.20	1.52	1.43
2	A	500	DH5	OAC-SAJ	8.14	1.52	1.43
2	D	500	DH5	CAH-NAI	-8.02	1.35	1.45
2	B	500	DH5	OAQ-SAJ	7.72	1.52	1.43
2	C	500	DH5	CAH-NAI	-7.42	1.35	1.45
2	D	500	DH5	OAQ-SAJ	7.40	1.51	1.43
2	A	500	DH5	OAQ-SAJ	7.34	1.51	1.43
3	B	550	MES	C8-S	-6.97	1.67	1.77
3	D	550	MES	C8-S	-6.90	1.67	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	550	MES	C8-S	-6.89	1.67	1.77
3	C	550	MES	C8-S	-6.56	1.68	1.77
2	A	500	DH5	CAH-NAI	-6.12	1.37	1.45
2	B	500	DH5	CAH-NAI	-6.11	1.37	1.45
2	C	500	DH5	CBB-CAY	-5.54	1.39	1.51
2	A	500	DH5	SAJ-NAI	5.50	1.72	1.64
2	A	500	DH5	CBB-CAY	-5.39	1.40	1.51
2	D	500	DH5	SAJ-NAI	5.06	1.71	1.64
2	D	500	DH5	CBB-CAY	-5.03	1.40	1.51
2	D	500	DH5	CAG-NAF	4.89	1.41	1.33
2	B	500	DH5	CBB-CAY	-4.78	1.41	1.51
2	B	500	DH5	CAT-CAW	-4.46	1.40	1.51
2	C	500	DH5	CAT-CAW	-4.43	1.40	1.51
2	D	500	DH5	CAT-CAW	-3.95	1.41	1.51
2	C	500	DH5	CAK-SAJ	-3.90	1.71	1.76
2	C	500	DH5	SAJ-NAI	3.56	1.69	1.64
2	A	500	DH5	CAT-CAW	-3.41	1.43	1.51
2	B	500	DH5	CAG-NAF	3.30	1.38	1.33
2	B	500	DH5	SAJ-NAI	3.01	1.68	1.64
2	A	500	DH5	CAG-NAF	2.82	1.37	1.33
2	C	500	DH5	CAG-NAF	2.68	1.37	1.33

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	DH5	OAC-SAJ-OAQ	-6.92	108.31	119.52
2	D	500	DH5	OAC-SAJ-OAQ	-6.41	109.14	119.52
2	A	500	DH5	CAG-NAF-CAN	6.35	120.51	115.14
2	C	500	DH5	OAC-SAJ-NAI	6.35	113.20	106.77
2	D	500	DH5	OAC-SAJ-NAI	6.18	113.04	106.77
2	D	500	DH5	CAG-CAH-CAP	6.17	120.38	114.57
2	C	500	DH5	CAG-NAF-CAN	6.03	120.23	115.14
2	D	500	DH5	CAG-NAF-CAN	6.02	120.23	115.14
2	B	500	DH5	OAC-SAJ-NAI	5.93	112.78	106.77
2	A	500	DH5	OAC-SAJ-OAQ	-5.74	110.22	119.52
2	A	500	DH5	OAC-SAJ-NAI	5.73	112.58	106.77
3	D	550	MES	O3S-S-C8	5.31	114.36	105.77
2	B	500	DH5	CAG-NAF-CAN	5.27	119.59	115.14
2	C	500	DH5	CAG-CAH-CAP	5.04	119.32	114.57
2	B	500	DH5	OAC-SAJ-OAQ	-5.00	111.43	119.52
3	C	550	MES	C2-C3-N4	4.76	117.32	110.10
2	B	500	DH5	CAG-CAH-CAP	4.40	118.71	114.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	DH5	CAG-CAH-CAP	4.09	118.42	114.57
3	C	550	MES	O3S-S-C8	3.67	111.71	105.77
3	A	550	MES	C6-O1-C2	3.56	121.78	109.89
2	D	500	DH5	CAB-NAI-SAJ	3.50	122.75	116.83
2	D	500	DH5	OAQ-SAJ-NAI	3.18	110.00	106.77
2	A	500	DH5	OAQ-SAJ-NAI	2.81	109.62	106.77
3	C	550	MES	O1S-S-C8	2.77	110.26	106.92
3	B	550	MES	O1S-S-C8	2.76	110.24	106.92
3	B	550	MES	O3S-S-C8	2.66	110.07	105.77
2	D	500	DH5	CAH-CAG-NAF	-2.56	117.87	123.14
3	D	550	MES	C2-C3-N4	2.53	113.94	110.10
2	C	500	DH5	CAV-CAY-CAZ	2.49	120.65	116.87
2	B	500	DH5	OAQ-SAJ-NAI	2.40	109.20	106.77
3	A	550	MES	O1S-S-C8	2.37	109.77	106.92
3	C	550	MES	O2S-S-C8	-2.35	104.08	106.92
2	B	500	DH5	NAU-CAP-NAO	2.30	123.23	120.12
3	A	550	MES	O2S-S-C8	2.24	109.61	106.92
2	C	500	DH5	CAB-NAI-SAJ	2.23	120.60	116.83
2	D	500	DH5	CAV-CAY-CAZ	2.23	120.25	116.87
2	A	500	DH5	OAQ-SAJ-CAK	2.07	110.67	108.05
2	C	500	DH5	CAH-CAG-NAF	-2.04	118.94	123.14
2	B	500	DH5	CAB-NAI-SAJ	2.03	120.27	116.83
3	C	550	MES	C7-N4-C3	2.01	116.39	111.23
3	C	550	MES	C6-O1-C2	2.01	116.60	109.89

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	550	MES	C8-C7-N4-C3
2	D	500	DH5	CAB-NAI-SAJ-OAQ
2	D	500	DH5	CAB-NAI-SAJ-OAC
3	C	550	MES	C8-C7-N4-C3
2	A	500	DH5	CAB-NAI-SAJ-OAQ
2	A	500	DH5	CAB-NAI-SAJ-OAC
3	B	550	MES	N4-C7-C8-S
2	C	500	DH5	CAB-NAI-SAJ-OAQ
2	C	500	DH5	CAB-NAI-SAJ-OAC
3	D	550	MES	C7-C8-S-O1S
3	D	550	MES	C7-C8-S-O3S
2	B	500	DH5	CAB-NAI-SAJ-OAQ
3	C	550	MES	C7-C8-S-O3S

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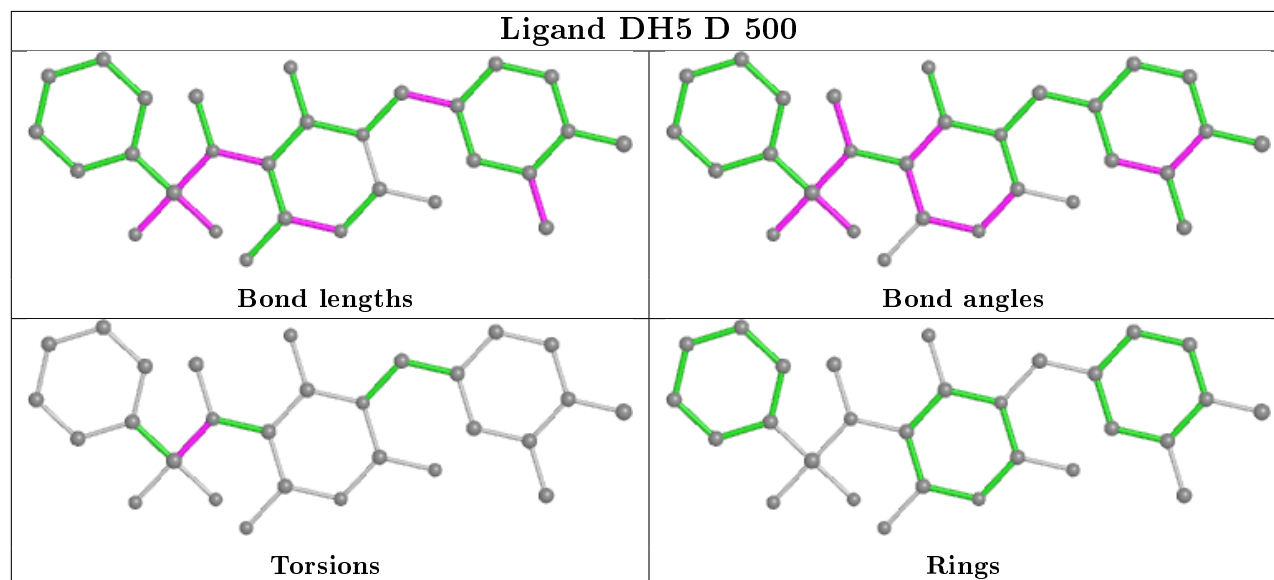
Mol	Chain	Res	Type	Atoms
2	B	500	DH5	CAB-NAI-SAJ-OAC
3	D	550	MES	C7-C8-S-O2S
3	A	550	MES	C8-C7-N4-C5
2	A	500	DH5	NAO-CAT-CAW-CAV
3	C	550	MES	C7-C8-S-O1S
2	C	500	DH5	NAO-CAT-CAW-CAV
2	A	500	DH5	NAO-CAT-CAW-CAX

There are no ring outliers.

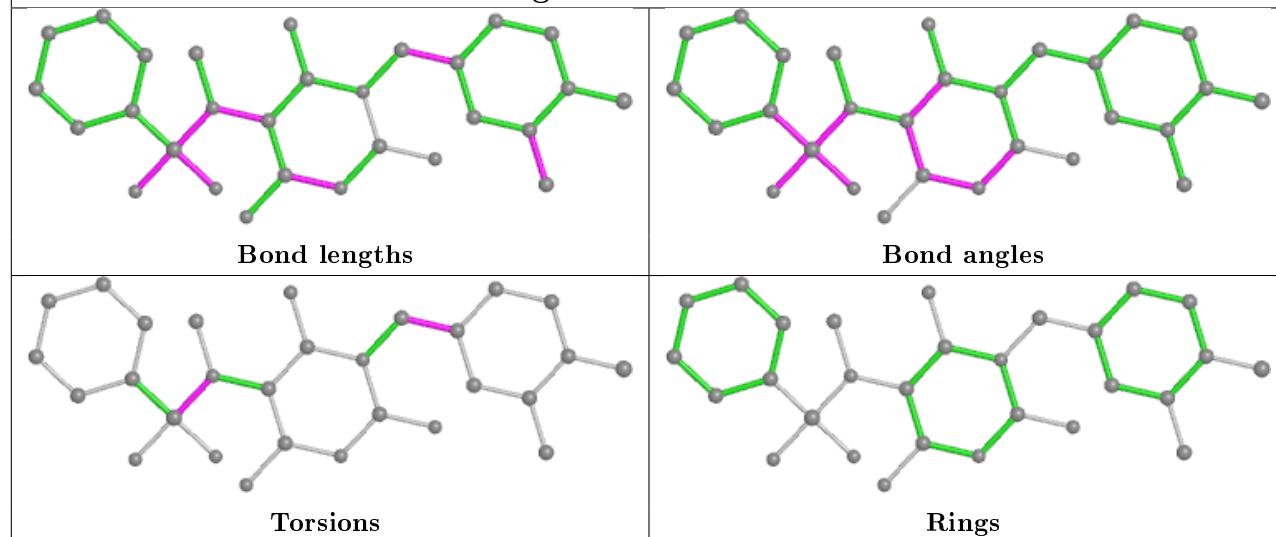
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	550	MES	2	0
2	D	500	DH5	3	0

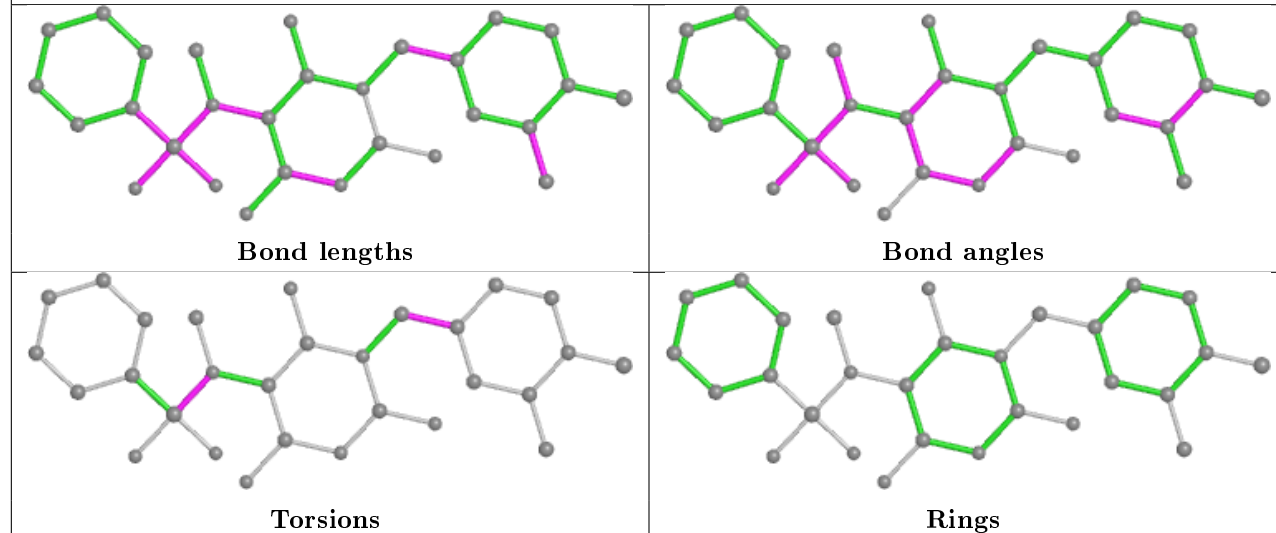
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.



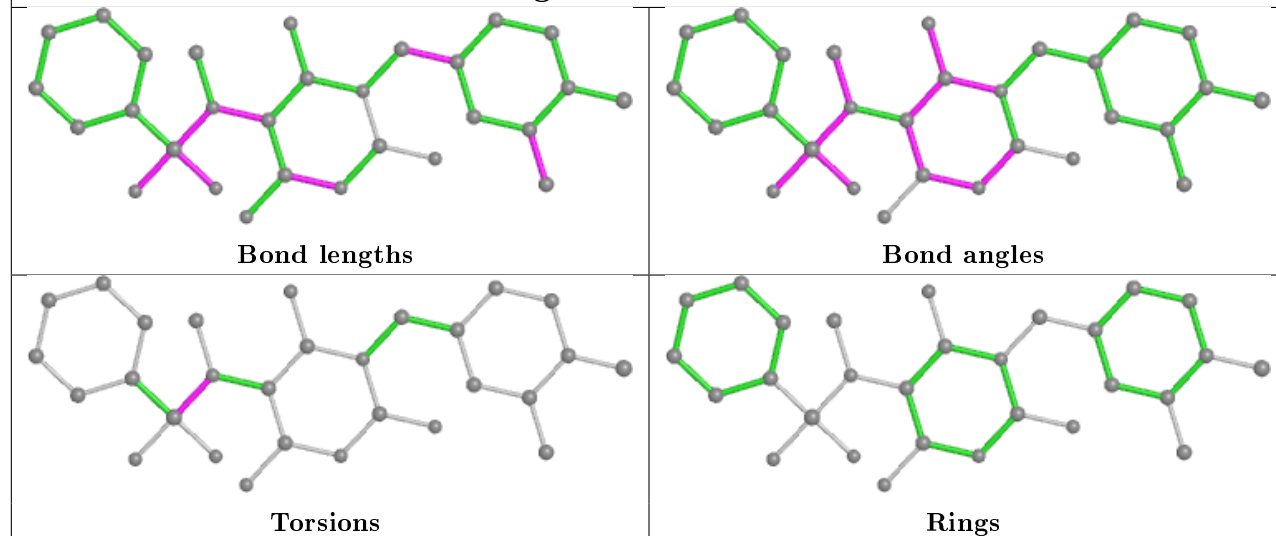
## Ligand DH5 A 500



## Ligand DH5 C 500



## Ligand DH5 B 500



## 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<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	297/303 (98%)	-0.38	3 (1%) 82 81	12, 21, 43, 82	0
1	B	293/303 (96%)	-0.27	4 (1%) 75 73	15, 25, 43, 69	0
1	C	295/303 (97%)	-0.26	12 (4%) 37 35	10, 22, 52, 93	0
1	D	292/303 (96%)	-0.19	7 (2%) 59 56	13, 27, 47, 86	0
All	All	1177/1212 (97%)	-0.28	26 (2%) 62 59	10, 24, 47, 93	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	194	ARG	4.8
1	C	189	LEU	4.0
1	A	194	ARG	3.7
1	D	194	ARG	3.7
1	C	193	PRO	3.3
1	C	190	LYS	3.3
1	D	22	ALA	3.3
1	C	195	GLY	3.2
1	C	-5	HIS	3.2
1	B	194	ARG	3.0
1	D	193	PRO	2.9
1	D	190	LYS	2.9
1	A	11	GLY	2.7
1	C	11	GLY	2.6
1	D	127	GLN	2.4
1	C	23	ILE	2.4
1	C	127	GLN	2.4
1	D	195	GLY	2.4
1	D	13	GLY	2.3
1	B	195	GLY	2.2
1	B	13	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	-4	HIS	2.1
1	A	190	LYS	2.1
1	C	277	LYS	2.1
1	B	1	MET	2.0
1	C	152	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

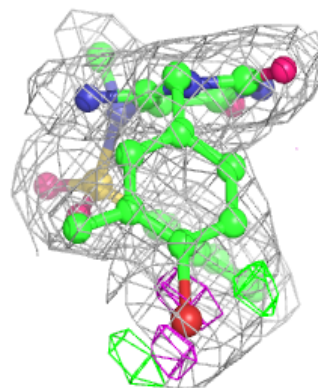
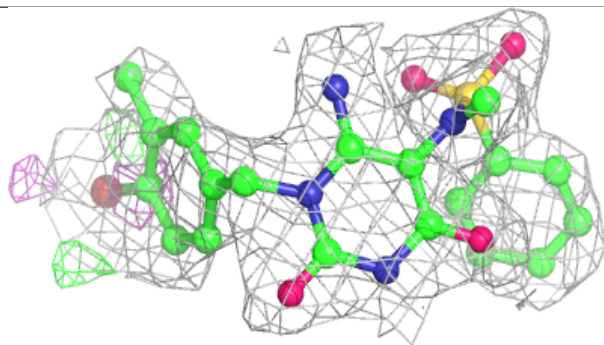
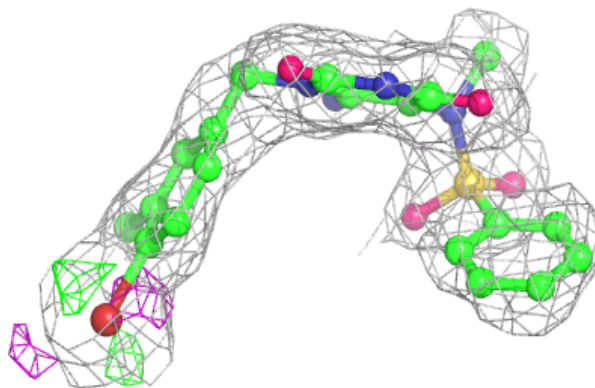
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MES	B	550	12/12	0.61	0.35	80,88,91,97	0
3	MES	D	550	12/12	0.86	0.18	64,66,70,74	0
3	MES	A	550	12/12	0.88	0.25	46,51,54,59	0
3	MES	C	550	12/12	0.91	0.18	39,44,47,48	0
2	DH5	D	500	29/29	0.95	0.12	22,28,44,59	0
2	DH5	B	500	29/29	0.95	0.11	20,24,47,53	0
2	DH5	C	500	29/29	0.96	0.12	17,19,31,38	0
4	CL	D	3001	1/1	0.96	0.06	41,41,41,41	0
2	DH5	A	500	29/29	0.97	0.10	16,19,27,35	0
4	CL	C	3001	1/1	0.98	0.05	37,37,37,37	0
4	CL	A	3001	1/1	0.99	0.04	30,30,30,30	0
4	CL	B	3001	1/1	0.99	0.05	32,32,32,32	0

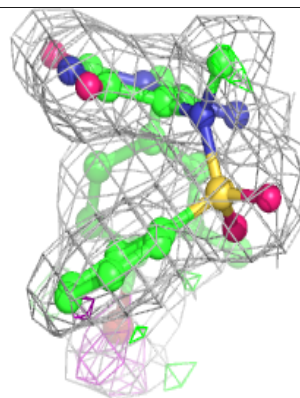
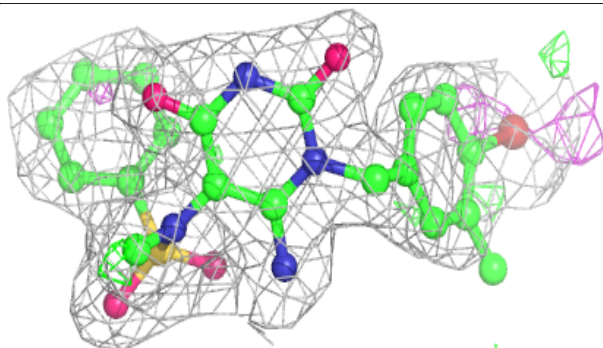
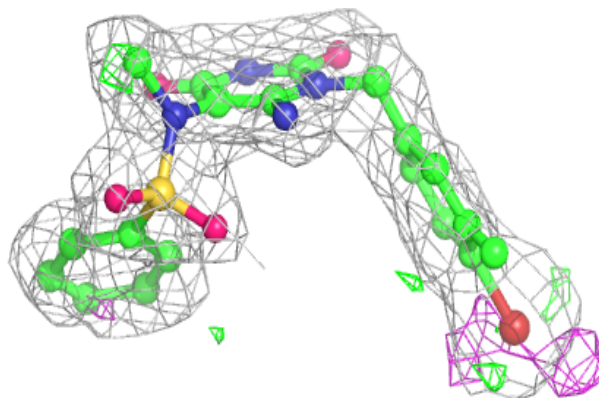
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around DH5 D 500:**

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

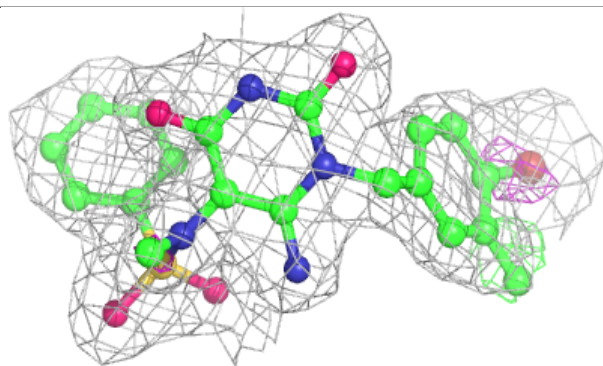
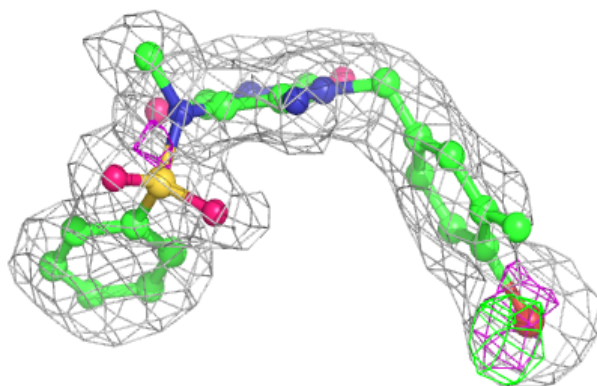
**Electron density around DH5 B 500:**

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

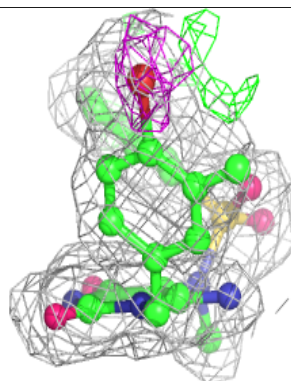
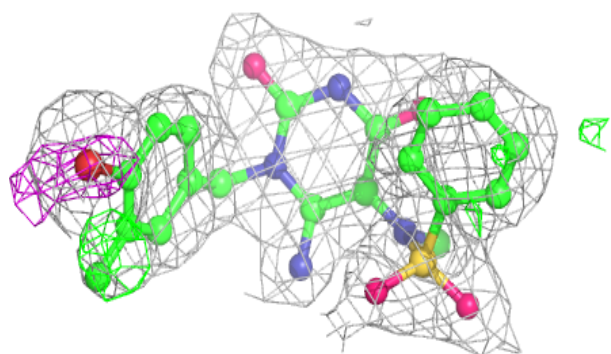
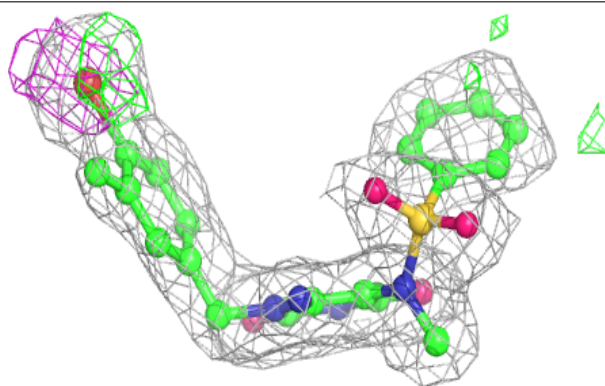


**Electron density around DH5 C 500:**

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

**Electron density around DH5 A 500:**

$2mF_o-DF_c$  (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.