



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:33 pm BST

PDB ID : 3G2Q  
Title : Crystal Structure of the Glycopeptide N-methyltransferase MtfA complexed with sinefungin  
Authors : Shi, R.; Matte, A.; Cygler, M.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)  
Deposited on : 2009-01-31  
Resolution : 2.18 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

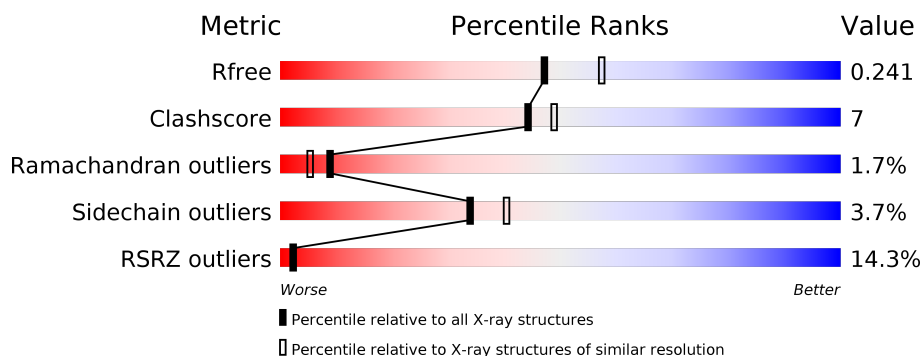
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.18 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	299	
1	B	299	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3812 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 PCZA361.24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	1	0
			1873	1173	334	358	8			
1	B	230	Total	C	N	O	S	0	1	0
			1761	1102	320	331	8			

There are 38 discrepancies between the modelled and reference sequences:

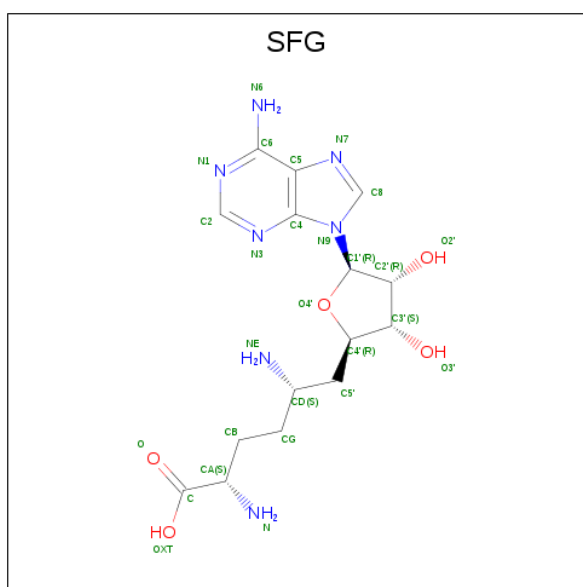
Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	EXPRESSION TAG	UNP O52805
A	-17	GLY	-	EXPRESSION TAG	UNP O52805
A	-16	SER	-	EXPRESSION TAG	UNP O52805
A	-15	SER	-	EXPRESSION TAG	UNP O52805
A	-14	HIS	-	EXPRESSION TAG	UNP O52805
A	-13	HIS	-	EXPRESSION TAG	UNP O52805
A	-12	HIS	-	EXPRESSION TAG	UNP O52805
A	-11	HIS	-	EXPRESSION TAG	UNP O52805
A	-10	HIS	-	EXPRESSION TAG	UNP O52805
A	-9	HIS	-	EXPRESSION TAG	UNP O52805
A	-8	SER	-	EXPRESSION TAG	UNP O52805
A	-7	GLY	-	EXPRESSION TAG	UNP O52805
A	-6	GLY	-	EXPRESSION TAG	UNP O52805
A	-5	LEU	-	EXPRESSION TAG	UNP O52805
A	-4	VAL	-	EXPRESSION TAG	UNP O52805
A	-3	PRO	-	EXPRESSION TAG	UNP O52805
A	-2	ARG	-	EXPRESSION TAG	UNP O52805
A	-1	GLY	-	EXPRESSION TAG	UNP O52805
A	0	SER	-	EXPRESSION TAG	UNP O52805
B	-18	MET	-	EXPRESSION TAG	UNP O52805
B	-17	GLY	-	EXPRESSION TAG	UNP O52805
B	-16	SER	-	EXPRESSION TAG	UNP O52805
B	-15	SER	-	EXPRESSION TAG	UNP O52805
B	-14	HIS	-	EXPRESSION TAG	UNP O52805
B	-13	HIS	-	EXPRESSION TAG	UNP O52805

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	EXPRESSION TAG	UNP O52805
B	-11	HIS	-	EXPRESSION TAG	UNP O52805
B	-10	HIS	-	EXPRESSION TAG	UNP O52805
B	-9	HIS	-	EXPRESSION TAG	UNP O52805
B	-8	SER	-	EXPRESSION TAG	UNP O52805
B	-7	GLY	-	EXPRESSION TAG	UNP O52805
B	-6	GLY	-	EXPRESSION TAG	UNP O52805
B	-5	LEU	-	EXPRESSION TAG	UNP O52805
B	-4	VAL	-	EXPRESSION TAG	UNP O52805
B	-3	PRO	-	EXPRESSION TAG	UNP O52805
B	-2	ARG	-	EXPRESSION TAG	UNP O52805
B	-1	GLY	-	EXPRESSION TAG	UNP O52805
B	0	SER	-	EXPRESSION TAG	UNP O52805

- Molecule 2 is SINEFUNGIN (three-letter code: SFG) (formula:  $C_{15}H_{23}N_7O_5$ ).



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	69	Total	O	0	0
			69	69		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.61Å 71.92Å 75.06Å 90.00° 103.82° 90.00°	Depositor
Resolution (Å)	50.00 – 2.18 44.68 – 2.18	Depositor EDS
% Data completeness (in resolution range)	92.0 (50.00-2.18) 92.0 (44.68-2.18)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 2.18Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.226 , 0.253 0.220 , 0.241	Depositor DCC
$R_{free}$ test set	1589 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.6	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 54.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3812	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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: SFG

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	0.53	0/1906	0.66	0/2580
1	B	0.59	0/1794	0.69	0/2424
All	All	0.56	0/3700	0.67	0/5004

There are no bond length outliers.

There are no bond angle outliers.

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	1873	0	1863	22	0
1	B	1761	0	1746	29	0
2	A	27	0	22	0	0
2	B	27	0	22	1	0
3	A	55	0	0	3	0
3	B	69	0	0	2	0
All	All	3812	0	3653	48	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 7.

All (48) 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:B:63:VAL:HG22	1:B:63:VAL:O	1.54	1.07
1:A:95:THR:HG22	1:A:120:GLN:HE22	1.30	0.93
1:A:95:THR:CG2	1:A:120:GLN:HE22	1.83	0.91
1:B:128:LEU:H	1:B:160:HIS:HE1	1.19	0.91
1:A:95:THR:HG22	1:A:120:GLN:NE2	2.00	0.75
1:B:63:VAL:CG2	1:B:63:VAL:O	2.30	0.74
1:B:63:VAL:O	1:B:64:SER:C	2.30	0.70
1:B:14:HIS:CE1	1:B:214:HIS:CE1	2.80	0.69
1:A:175:GLU:HG3	3:A:369:HOH:O	1.93	0.67
1:B:214:HIS:HD2	3:B:378:HOH:O	1.78	0.66
1:B:156:SER:O	1:B:160:HIS:HD2	1.79	0.66
1:B:14:HIS:HE1	1:B:214:HIS:CE1	2.14	0.65
1:B:62:PRO:O	1:B:62:PRO:CD	2.46	0.63
1:B:12:THR:HB	1:B:13:PRO:HD2	1.81	0.63
1:A:203:LEU:HD11	1:B:229[A]:ARG:NH1	2.15	0.61
1:B:214:HIS:CD2	3:B:378:HOH:O	2.50	0.61
1:B:210:GLU:OE2	1:B:229[A]:ARG:NH1	2.35	0.59
1:A:98:LEU:HD22	1:A:118[B]:LEU:HG	1.87	0.56
1:B:59:ARG:HG3	1:B:267:LEU:HD22	1.88	0.56
1:B:62:PRO:CG	1:B:62:PRO:O	2.54	0.55
1:A:254:PRO:HB2	1:A:263:LYS:HD3	1.88	0.55
1:A:95:THR:HG23	1:A:120:GLN:HE22	1.72	0.54
1:A:258:GLY:O	1:A:260:ALA:N	2.41	0.54
1:B:14:HIS:O	1:B:14:HIS:CG	2.63	0.51
1:B:62:PRO:HD2	1:B:62:PRO:O	2.10	0.51
1:B:123:MET:HG2	2:B:500:SFG:N1	2.25	0.51
1:B:63:VAL:O	1:B:64:SER:O	2.30	0.50
1:A:60:THR:HG22	1:A:168:LEU:HD21	1.93	0.50
1:B:128:LEU:H	1:B:160:HIS:CE1	2.12	0.50
1:A:138:SER:CB	3:A:375:HOH:O	2.61	0.49
1:A:197:VAL:O	1:B:214:HIS:CB	2.60	0.49
1:B:126:PHE:CE2	1:B:156:SER:HB3	2.48	0.48
1:B:10:VAL:O	1:B:227:THR:HG21	2.13	0.48
1:A:141:SER:O	1:A:144:GLU:HB2	2.14	0.47
1:A:55:GLU:HG3	1:A:255:PHE:CD1	2.51	0.45
1:A:254:PRO:HA	1:A:265:MET:O	2.17	0.45
1:A:11:ARG:HD3	1:A:16:ASP:OD1	2.18	0.44
1:B:128:LEU:C	1:B:130:LYS:H	2.20	0.44
1:A:90:ALA:HB3	1:A:118[A]:LEU:HD23	1.99	0.44
1:B:61:GLY:HA3	1:B:62:PRO:HD3	1.87	0.44
1:A:216:ALA:HA	1:B:197:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:THR:OG1	1:A:61:GLY:N	2.51	0.43
1:B:166:LYS:HD3	1:B:168:LEU:HD21	2.00	0.43
1:A:146:ASP:O	1:A:150:ARG:HG3	2.20	0.41
1:B:254:PRO:HA	1:B:265:MET:O	2.21	0.41
1:A:184:ARG:O	1:A:184:ARG:HG3	2.20	0.41
1:B:188:LEU:HA	1:B:189:PRO:HD3	1.90	0.41
1:A:138:SER:HB3	3:A:375:HOH:O	2.20	0.40

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	240/299 (80%)	222 (92%)	12 (5%)	6 (2%)	5	2
1	B	221/299 (74%)	215 (97%)	4 (2%)	2 (1%)	17	15
All	All	461/598 (77%)	437 (95%)	16 (4%)	8 (2%)	9	5

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	GLU
1	A	259	GLY
1	B	64	SER
1	B	189	PRO
1	A	219	THR
1	A	220	THR
1	A	221	ASP
1	A	217	ASP

### 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	197/240 (82%)	190 (96%)	7 (4%)	35	42
1	B	184/240 (77%)	177 (96%)	7 (4%)	33	39
All	All	381/480 (79%)	367 (96%)	14 (4%)	34	40

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	59	ARG
1	A	101	PHE
1	A	166	LYS
1	A	168	LEU
1	A	224	VAL
1	A	267	LEU
1	B	64	SER
1	B	74	MET
1	B	101	PHE
1	B	195	ARG
1	B	211	ILE
1	B	227	THR
1	B	267	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	B	14	HIS
1	B	160	HIS
1	B	199	HIS
1	B	214	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SFG	B	500	-	22,29,29	1.23	3 (13%)	18,42,42	1.85	5 (27%)
2	SFG	A	400	-	22,29,29	1.21	3 (13%)	18,42,42	1.89	5 (27%)

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	SFG	B	500	-	-	0/9/33/33	0/3/3/3
2	SFG	A	400	-	-	1/9/33/33	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	SFG	C5-C4	2.93	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	SFG	O4'-C1'	2.84	1.45	1.41
2	A	400	SFG	C2-N3	2.37	1.35	1.32
2	B	500	SFG	C5-C4	2.32	1.47	1.40
2	B	500	SFG	C2-N3	2.15	1.35	1.32
2	A	400	SFG	O4'-C1'	2.09	1.44	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	SFG	N3-C2-N1	-4.12	122.25	128.68
2	B	500	SFG	N3-C2-N1	-4.11	122.25	128.68
2	A	400	SFG	C2-N1-C6	3.22	124.26	118.75
2	B	500	SFG	C2-N1-C6	3.02	123.92	118.75
2	B	500	SFG	N6-C6-N1	2.83	124.46	118.57
2	A	400	SFG	N6-C6-N1	2.67	124.12	118.57
2	B	500	SFG	C1'-N9-C4	-2.55	122.15	126.64
2	A	400	SFG	O3'-C3'-C4'	-2.54	103.70	111.05
2	B	500	SFG	O3'-C3'-C4'	-2.27	104.50	111.05
2	A	400	SFG	C1'-N9-C4	-2.08	122.99	126.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	SFG	C4'-C5'-CD-CG

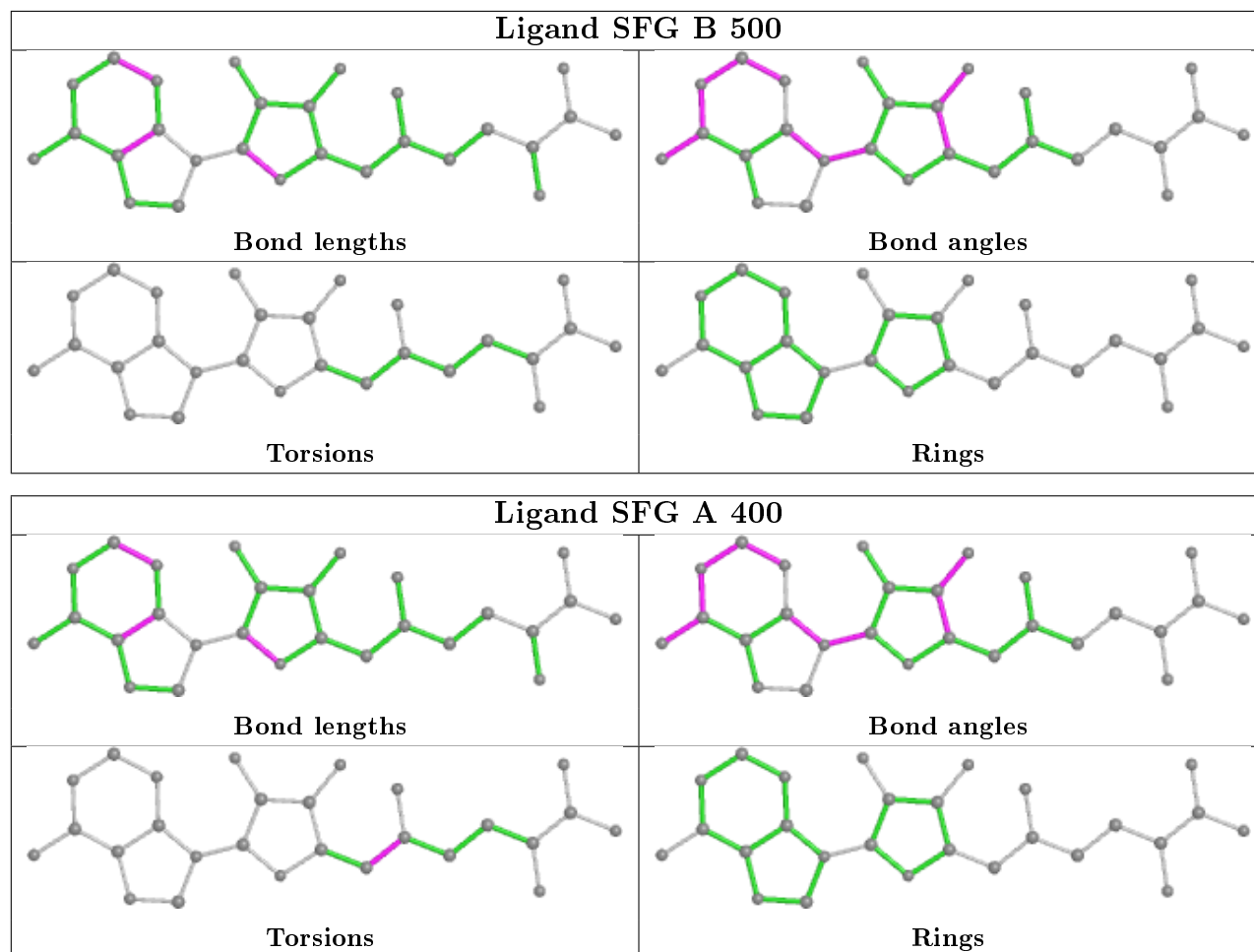
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	SFG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	247/299 (82%)	1.11	36 (14%) 2 2	29, 48, 73, 80	3 (1%)
1	B	230/299 (76%)	1.06	32 (13%) 2 2	30, 45, 77, 116	4 (1%)
All	All	477/598 (79%)	1.09	68 (14%) 2 2	29, 47, 74, 116	7 (1%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	216	ALA	9.3
1	A	197	VAL	8.5
1	B	225	VAL	7.1
1	A	199	HIS	6.3
1	A	47	ALA	6.2
1	A	225	VAL	6.0
1	B	215	PRO	5.7
1	B	14	HIS	5.6
1	A	185	LYS	5.3
1	A	198	LEU	5.2
1	B	190	GLY	4.9
1	A	22	VAL	4.4
1	B	129	ASP	4.4
1	A	25	ARG	4.4
1	A	220	THR	4.4
1	B	62	PRO	4.4
1	A	186	GLN	4.2
1	B	213	ILE	4.2
1	B	193	GLY	4.1
1	A	222	PRO	4.0
1	B	47	ALA	3.9
1	A	182	LEU	3.9
1	A	223	PHE	3.9
1	B	196	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	217	ASP	3.8
1	B	214	HIS	3.6
1	A	111	ASP	3.5
1	B	63	VAL	3.5
1	A	33	ASP	3.4
1	B	31	PHE	3.3
1	A	221	ASP	3.3
1	B	212	THR	3.2
1	B	29	CYS	3.2
1	B	195	ARG	3.1
1	A	219	THR	3.1
1	A	183	GLU	3.1
1	A	79	PHE	3.1
1	A	224	VAL	3.0
1	A	26	GLY	2.9
1	B	15	ALA	2.9
1	B	188	LEU	2.9
1	B	61	GLY	2.8
1	A	24	GLU	2.8
1	B	226	CYS	2.8
1	B	9	PRO	2.7
1	A	48	ASP	2.7
1	A	20	ALA	2.6
1	A	113	ARG	2.6
1	A	184	ARG	2.6
1	B	234	ALA	2.6
1	B	194	ARG	2.5
1	A	37	ALA	2.5
1	B	189	PRO	2.4
1	B	205	ALA	2.4
1	B	272	MET	2.4
1	A	23	GLY	2.4
1	A	215	PRO	2.3
1	B	233	LEU	2.3
1	A	142	ILE	2.3
1	A	34	GLU	2.3
1	B	30	ASP	2.3
1	A	8	GLY	2.2
1	A	274	GLY	2.2
1	B	32	TYR	2.2
1	A	112	VAL	2.2
1	A	21	SER	2.0

*Continued on next page...*



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Mol	Chain	Res	Type	RSRZ
1	B	184	ARG	2.0
1	A	64	SER	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](#)

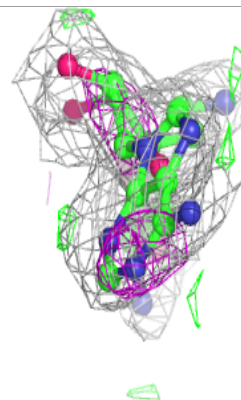
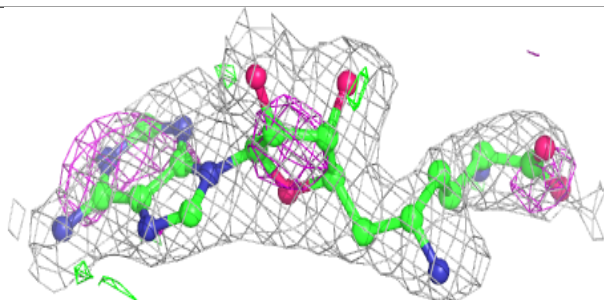
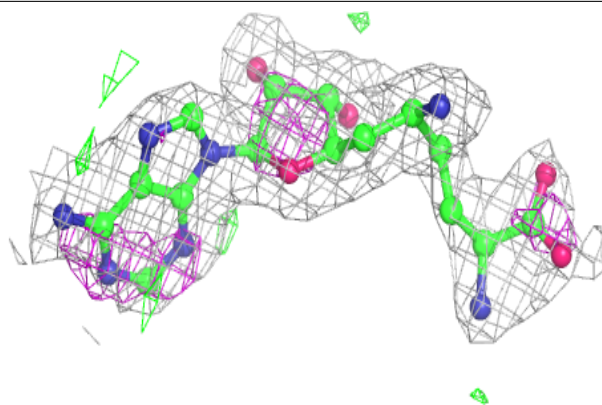
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	SFG	B	500	27/27	0.87	0.17	42,46,65,65	0
2	SFG	A	400	27/27	0.95	0.11	35,41,59,59	0

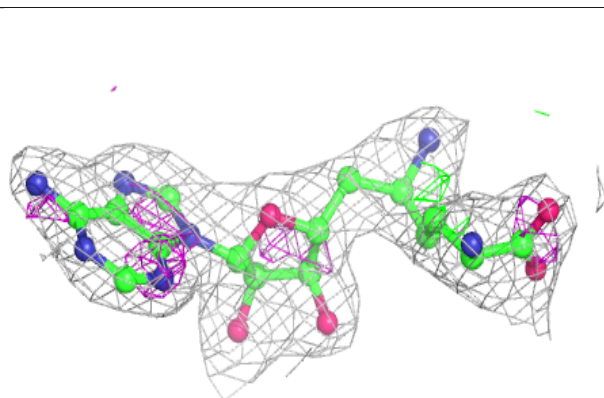
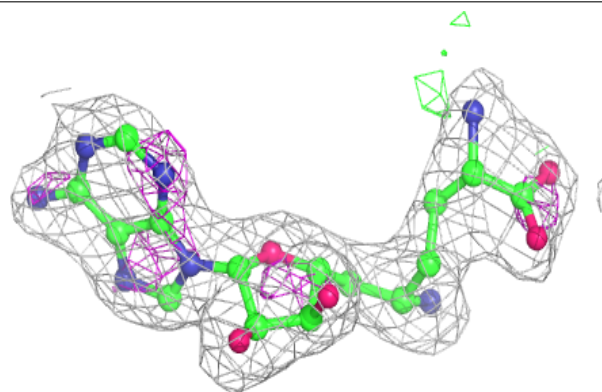
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around SFG 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 SFG A 400:**

$2mF_o-DF_c$  (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.