



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 26, 2020 – 04:12 PM EST

PDB ID : 7KHS  
Title : OgOGA IN COMPLEX WITH LIGAND 55  
Authors : Shaffer, P.L.  
Deposited on : 2020-10-21  
Resolution : 1.78 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 : 2.14.6  
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) : 2.14.6

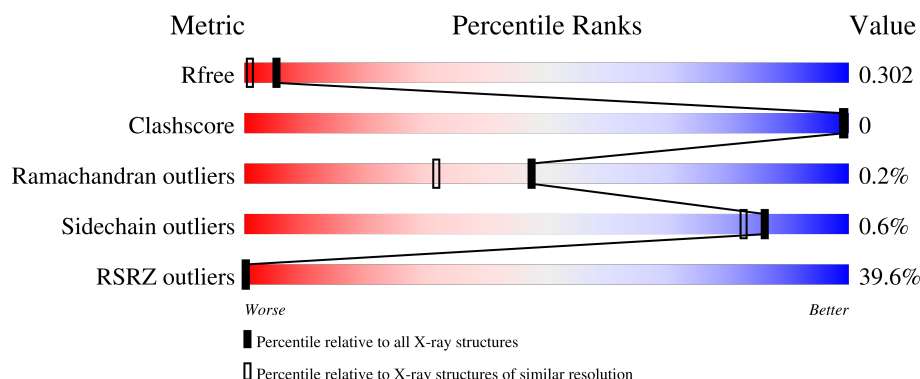
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	449	<div> <div>19%</div> <div>95%</div> <div>5%</div> </div>
1	B	449	<div> <div>51%</div> <div>91%</div> <div>• •</div> </div>
1	C	449	<div> <div>63%</div> <div>92%</div> <div>• 5%</div> </div>
1	D	449	<div> <div>21%</div> <div>96%</div> <div>•</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28033 atoms, of which 13715 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.

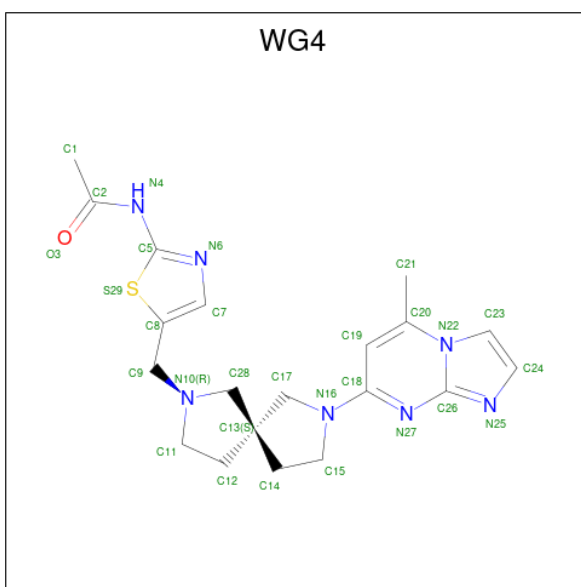
- Molecule 1 is a protein called Protein O-GlcNAcase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	449	Total	C	H	N	O	S	198	2	0
			7042	2263	3474	652	641	12			
1	B	430	Total	C	H	N	O	S	218	0	0
			6715	2159	3317	619	608	12			
1	C	427	Total	C	H	N	O	S	386	2	0
			6710	2156	3316	622	604	12			
1	D	448	Total	C	H	N	O	S	133	4	0
			7059	2268	3484	653	642	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q2CEE3
A	0	SER	-	expression tag	UNP Q2CEE3
B	-1	GLY	-	expression tag	UNP Q2CEE3
B	0	SER	-	expression tag	UNP Q2CEE3
C	-1	GLY	-	expression tag	UNP Q2CEE3
C	0	SER	-	expression tag	UNP Q2CEE3
D	-1	GLY	-	expression tag	UNP Q2CEE3
D	0	SER	-	expression tag	UNP Q2CEE3

- Molecule 2 is N-(5-([(5S)-7-(5-methylimidazo[1,2-a]pyrimidin-7-yl)-2,7-diazaspiro[4.4]nonan-2-yl)methyl]-1,3-thiazol-2-yl)acetamide (three-letter code: WG4) (formula: C<sub>20</sub>H<sub>25</sub>N<sub>7</sub>OS) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			54	20	25	7	1	1		
2	B	1	Total	C	H	N	O	S	0	0
			54	20	25	7	1	1		
2	C	1	Total	C	H	N	O	S	0	0
			54	20	25	7	1	1		
2	D	1	Total	C	H	N	O	S	0	0
			54	20	25	7	1	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 5 is water.

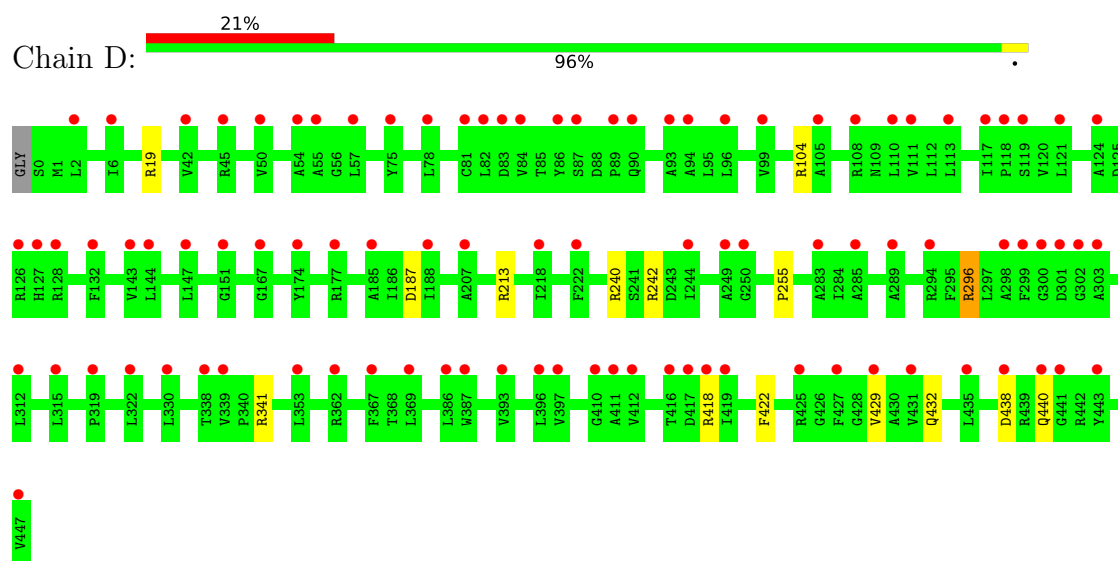
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	116	Total	H	O	0	0
			118	2	116		
5	B	38	Total	H	O	0	0
			46	8	38		
5	C	18	Total	O		0	0
			18	18			
5	D	89	Total	H	O	0	0
			97	8	89		



● Molecule 1: Protein O-GlcNAcase



● Molecule 1: Protein O-GlcNAcase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.23Å 83.08Å 122.96Å 90.00° 90.25° 90.00°	Depositor
Resolution (Å)	44.79 – 1.78 44.67 – 1.79	Depositor EDS
% Data completeness (in resolution range)	87.4 (44.79-1.78) 87.4 (44.67-1.79)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.273 , 0.296 0.277 , 0.302	Depositor DCC
$R_{free}$ test set	2508 reflections (1.42%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.9	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 17.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.399 for h,-k,-l	Xtriage
Reported twinning fraction	0.625 for H, K, L 0.375 for -h,-k,l	Depositor
Outliers	0 of 176418 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	28033	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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: WG4, CA, EDO

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	0.84	0/3666	0.99	20/4999 (0.4%)
1	B	0.76	0/3488	0.95	17/4754 (0.4%)
1	C	0.74	1/3484 (0.0%)	0.93	11/4747 (0.2%)
1	D	0.80	0/3673	0.97	11/5009 (0.2%)
All	All	0.79	1/14311 (0.0%)	0.96	59/19509 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	350	ARG	CD-NE	10.34	1.64	1.46

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	A	240	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	D	213	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	C	296	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	B	296	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	D	187	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	A	296	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	A	57	LEU	CB-CG-CD1	6.47	122.00	111.00
1	B	47	ARG	CD-NE-CZ	6.44	132.62	123.60
1	D	240	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	A	418	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	B	19	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	A	59	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	D	187	ASP	CB-CG-OD1	6.17	123.86	118.30
1	C	240	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	C	19	ARG	NE-CZ-NH1	6.14	123.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	GLN	CA-CB-CG	6.09	126.80	113.40
1	B	425	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	B	418	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	D	242	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	C	418	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	D	19	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	70	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	D	341	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	328	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	B	242	ARG	CD-NE-CZ	5.73	131.62	123.60
1	C	215	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	C	350	ARG	CD-NE-CZ	5.62	131.47	123.60
1	B	15	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	282	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	341	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	350	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	D	104	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	19	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	377	ASP	CB-CG-OD1	5.38	123.14	118.30
1	D	418	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	C	282	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	B	70	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	213	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	213	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	B	361	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	D	418	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	282	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	D	296	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	C	1	MET	CG-SD-CE	5.27	108.62	100.20
1	A	418	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	362	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	242	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	215	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	B	104	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	B	240	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	C	59	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	341	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	145	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	41	ASP	CB-CG-OD1	5.10	122.89	118.30
1	C	350	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	12	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	377	ASP	CB-CG-OD2	-5.06	113.74	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	ASP	CB-CG-OD2	5.06	122.86	118.30

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	3568	3474	3459	2	0
1	B	3398	3317	3305	2	0
1	C	3394	3316	3302	3	0
1	D	3575	3484	3469	2	0
2	A	29	25	0	0	0
2	B	29	25	0	1	0
2	C	29	25	0	0	0
2	D	29	25	0	1	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	C	4	6	6	0	0
5	A	116	2	0	0	0
5	B	38	8	0	0	0
5	C	18	0	0	0	0
5	D	89	8	0	0	0
All	All	14318	13715	13541	9	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 0.

All (9) 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:294[B]:ARG:HB2	1:C:294[B]:ARG:HH11	1.31	0.91
1:C:294[B]:ARG:NH1	1:C:294[B]:ARG:HB2	2.09	0.65
1:D:429:VAL:HA	1:D:432:GLN:HG2	1.80	0.64
1:A:227:TYR:CE1	1:B:422:PHE:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ARG:HD2	1:B:272:TYR:O	2.17	0.45
1:A:99:VAL:HG21	1:A:143:VAL:HG13	2.02	0.41
2:B:501:WG4:S29	2:B:501:WG4:O3	2.79	0.41
1:C:227:TYR:CE1	1:D:422:PHE:HB2	2.56	0.41
2:D:501:WG4:S29	2:D:501:WG4:O3	2.78	0.41

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	449/449 (100%)	435 (97%)	13 (3%)	1 (0%)	47	32
1	B	424/449 (94%)	411 (97%)	12 (3%)	1 (0%)	47	32
1	C	423/449 (94%)	409 (97%)	13 (3%)	1 (0%)	47	32
1	D	450/449 (100%)	436 (97%)	13 (3%)	1 (0%)	47	32
All	All	1746/1796 (97%)	1691 (97%)	51 (3%)	4 (0%)	47	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	255	PRO
1	A	255	PRO
1	C	255	PRO
1	D	255	PRO

### 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	358/356 (101%)	355 (99%)	3 (1%)	81	76
1	B	339/356 (95%)	338 (100%)	1 (0%)	92	90
1	C	338/356 (95%)	336 (99%)	2 (1%)	86	82
1	D	360/356 (101%)	357 (99%)	3 (1%)	81	76
All	All	1395/1424 (98%)	1386 (99%)	9 (1%)	86	82

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	347	PRO
1	A	350	ARG
1	A	438	ASP
1	B	438	ASP
1	C	218	ILE
1	C	438	ASP
1	D	296	ARG
1	D	438	ASP
1	D	440	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	390	GLN
1	B	390	GLN
1	C	390	GLN
1	D	109	ASN
1	D	390	GLN

### 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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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
2	WG4	C	501	-	27,33,33	1.79	5 (18%)	24,49,49	2.59	12 (50%)
2	WG4	A	501	-	27,33,33	1.60	4 (14%)	24,49,49	2.92	10 (41%)
2	WG4	D	501	-	27,33,33	1.53	7 (25%)	24,49,49	2.84	11 (45%)
4	EDO	C	502	-	3,3,3	0.47	0	2,2,2	0.52	0
2	WG4	B	501	-	27,33,33	1.55	6 (22%)	24,49,49	2.38	7 (29%)

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	WG4	C	501	-	-	2/9/34/34	0/5/5/5
2	WG4	A	501	-	-	4/9/34/34	0/5/5/5
2	WG4	D	501	-	-	2/9/34/34	0/5/5/5
4	EDO	C	502	-	-	1/1/1/1	-
2	WG4	B	501	-	-	2/9/34/34	0/5/5/5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	WG4	C28-N10	6.45	1.52	1.46
2	A	501	WG4	C28-N10	5.25	1.51	1.46
2	D	501	WG4	C28-N10	4.09	1.50	1.46
2	B	501	WG4	C7-N6	-3.47	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	WG4	C9-C8	-3.38	1.47	1.51
2	D	501	WG4	C7-N6	-3.06	1.31	1.36
2	B	501	WG4	C28-N10	3.01	1.49	1.46
2	C	501	WG4	C7-N6	-2.93	1.31	1.36
2	B	501	WG4	C9-C8	-2.56	1.48	1.51
2	A	501	WG4	C7-N6	-2.50	1.32	1.36
2	B	501	WG4	C19-C18	2.49	1.43	1.39
2	C	501	WG4	C19-C18	2.45	1.43	1.39
2	C	501	WG4	C9-C8	-2.45	1.49	1.51
2	D	501	WG4	C26-N25	-2.34	1.32	1.35
2	B	501	WG4	C26-N25	-2.28	1.32	1.35
2	D	501	WG4	C17-N16	2.24	1.50	1.46
2	A	501	WG4	C19-C18	2.18	1.42	1.39
2	D	501	WG4	C7-C8	-2.17	1.32	1.37
2	B	501	WG4	C7-C8	-2.15	1.32	1.37
2	C	501	WG4	C26-N25	-2.10	1.32	1.35
2	D	501	WG4	C19-C18	2.08	1.42	1.39
2	D	501	WG4	C14-C15	2.01	1.56	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	WG4	C9-N10-C28	7.49	122.44	112.93
2	D	501	WG4	C18-N27-C26	7.01	122.92	117.65
2	C	501	WG4	C9-N10-C28	6.52	121.21	112.93
2	B	501	WG4	C9-N10-C28	5.61	120.06	112.93
2	D	501	WG4	C9-N10-C28	5.47	119.87	112.93
2	B	501	WG4	C15-N16-C17	-5.32	104.75	112.36
2	A	501	WG4	C18-N27-C26	4.83	121.28	117.65
2	C	501	WG4	C18-N27-C26	4.82	121.27	117.65
2	D	501	WG4	C15-N16-C17	-4.80	105.49	112.36
2	A	501	WG4	C15-N16-C18	4.68	129.33	123.60
2	C	501	WG4	C15-N16-C17	-4.66	105.69	112.36
2	A	501	WG4	C15-N16-C17	-4.49	105.93	112.36
2	A	501	WG4	C14-C15-N16	4.37	107.36	103.61
2	B	501	WG4	C18-N27-C26	4.19	120.80	117.65
2	A	501	WG4	C24-C23-N22	4.02	110.13	106.83
2	D	501	WG4	C15-N16-C18	3.90	128.37	123.60
2	A	501	WG4	C11-N10-C28	-3.89	100.21	104.02
2	B	501	WG4	C17-N16-C18	3.74	128.18	123.60
2	B	501	WG4	C14-C15-N16	3.73	106.81	103.61
2	D	501	WG4	O3-C2-C1	-3.67	115.25	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	WG4	C17-N16-C18	3.24	127.57	123.60
2	D	501	WG4	C24-C23-N22	3.12	109.39	106.83
2	C	501	WG4	C24-C23-N22	3.11	109.38	106.83
2	D	501	WG4	C7-C8-S29	-3.00	109.02	112.00
2	D	501	WG4	O3-C2-N4	2.94	126.91	123.04
2	B	501	WG4	C15-N16-C18	2.84	127.07	123.60
2	D	501	WG4	C12-C13-C17	2.83	119.17	113.42
2	C	501	WG4	O3-C2-C1	-2.68	117.07	122.06
2	C	501	WG4	C15-N16-C18	2.55	126.72	123.60
2	D	501	WG4	C9-N10-C11	2.54	116.88	113.18
2	C	501	WG4	C11-C12-C13	2.53	108.14	104.25
2	C	501	WG4	N27-C18-N16	-2.51	115.21	117.43
2	C	501	WG4	C7-C8-S29	-2.45	109.57	112.00
2	B	501	WG4	C7-C8-S29	-2.44	109.58	112.00
2	C	501	WG4	C1-C2-N4	2.41	118.52	114.98
2	A	501	WG4	O3-C2-C1	-2.34	117.72	122.06
2	C	501	WG4	C14-C13-C12	2.29	114.37	110.49
2	A	501	WG4	O3-C2-N4	2.08	125.77	123.04
2	A	501	WG4	C12-C11-N10	2.07	109.08	104.02
2	D	501	WG4	C17-N16-C18	2.03	126.08	123.60

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	WG4	C8-C9-N10-C11
2	C	501	WG4	C8-C9-N10-C28
2	A	501	WG4	C8-C9-N10-C11
2	A	501	WG4	C8-C9-N10-C28
2	D	501	WG4	C8-C9-N10-C28
2	B	501	WG4	C8-C9-N10-C11
2	B	501	WG4	C8-C9-N10-C28
2	D	501	WG4	C8-C9-N10-C11
4	C	502	EDO	O1-C1-C2-O2
2	A	501	WG4	N27-C18-N16-C15
2	A	501	WG4	C19-C18-N16-C15

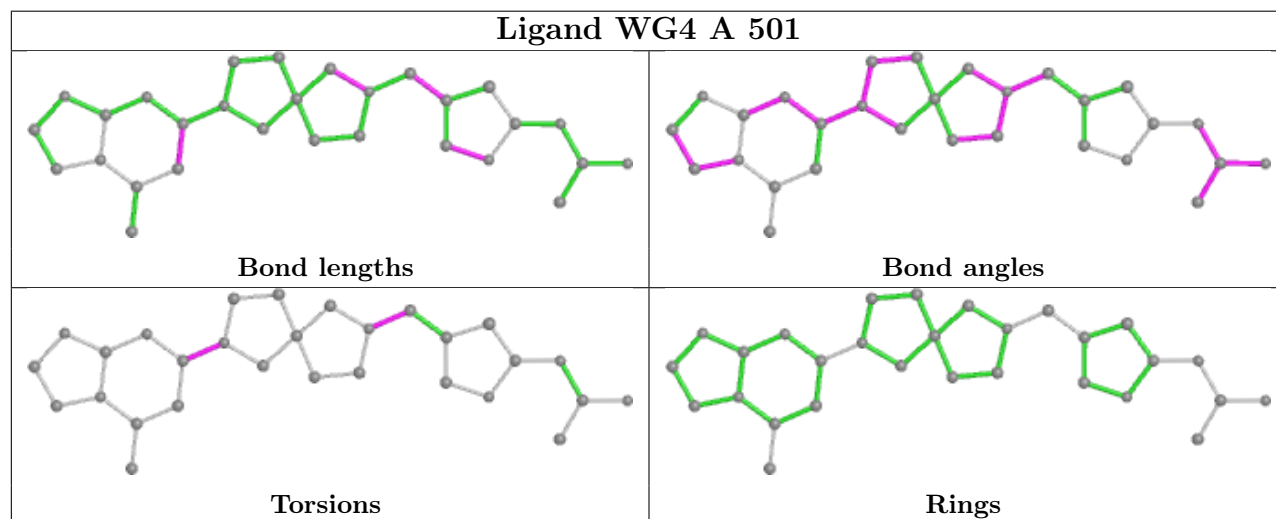
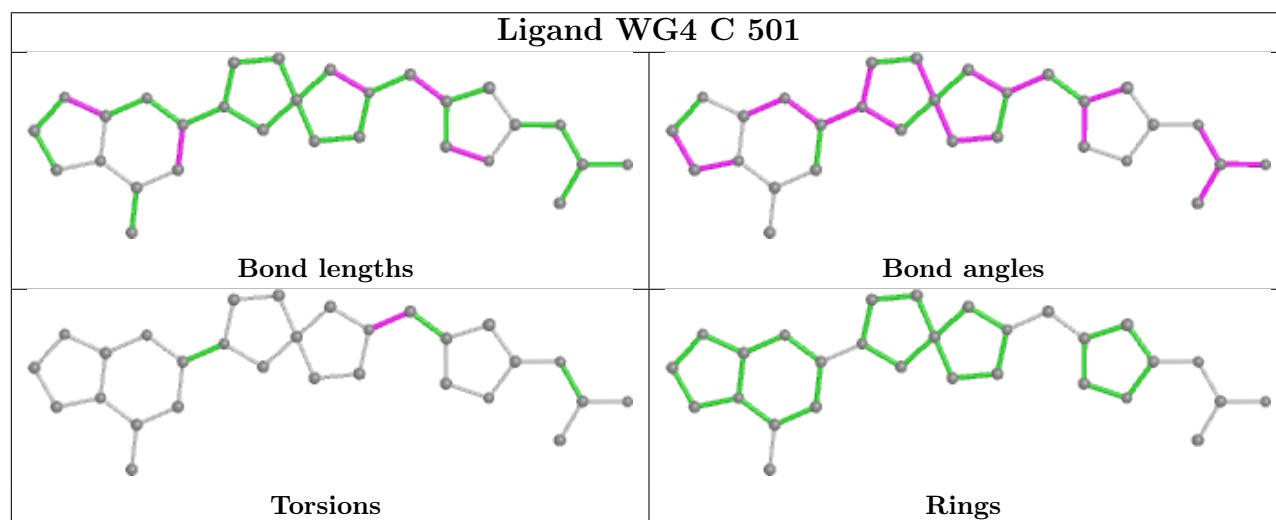
There are no ring outliers.

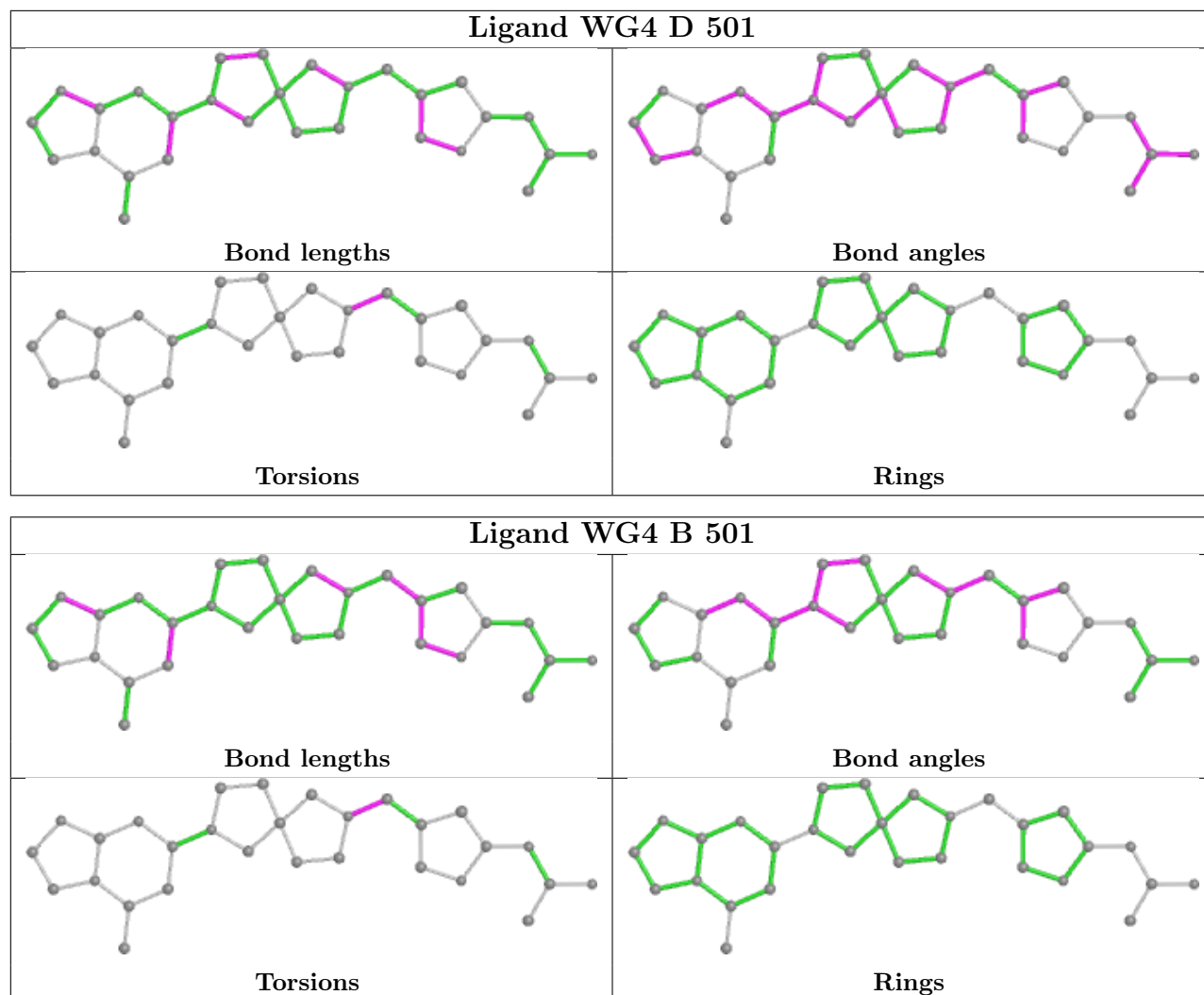
2 monomers are involved in 2 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	WG4	1	0
2	B	501	WG4	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 [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	449/449 (100%)	1.39	86 (19%) <b>1</b> <b>1</b>	20, 29, 52, 73	18 (4%)
1	B	430/449 (95%)	2.56	231 (53%) <b>0</b> <b>0</b>	23, 39, 65, 94	20 (4%)
1	C	427/449 (95%)	3.09	284 (66%) <b>0</b> <b>0</b>	25, 49, 72, 89	39 (9%)
1	D	448/449 (99%)	1.52	94 (20%) <b>1</b> <b>0</b>	20, 30, 48, 65	10 (2%)
All	All	1754/1796 (97%)	2.13	695 (39%) <b>0</b> <b>0</b>	20, 35, 65, 94	87 (4%)

All (695) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	LEU	16.6
1	B	86	TYR	12.5
1	B	112	LEU	12.2
1	D	299	PHE	12.2
1	C	132	PHE	11.5
1	C	274	ALA	11.5
1	C	137	ALA	11.3
1	B	175	LEU	11.1
1	C	406	ALA	11.0
1	C	96	LEU	10.9
1	B	299	PHE	10.9
1	C	84	VAL	10.9
1	D	118	PRO	10.7
1	C	299	PHE	10.6
1	B	117	ILE	10.1
1	B	87	SER	9.9
1	C	85	THR	9.8
1	C	337	LEU	9.8
1	B	81	CYS	8.9
1	B	182	LEU	8.6
1	C	151	GLY	8.3

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Mol	Chain	Res	Type	RSRZ
1	C	339	VAL	8.2
1	C	333	LEU	8.2
1	D	82	LEU	8.2
1	C	245	LEU	8.1
1	B	178	LEU	8.0
1	C	139	LEU	8.0
1	C	332	ALA	7.9
1	B	343	ASP	7.6
1	C	303	ALA	7.4
1	B	151	GLY	7.4
1	B	44	VAL	7.4
1	B	84	VAL	7.3
1	C	134	GLU	7.3
1	C	93	ALA	7.2
1	C	278	TYR	7.1
1	B	408	PRO	7.1
1	C	102	LEU	7.0
1	C	200	ILE	7.0
1	B	208	VAL	7.0
1	C	153	VAL	7.0
1	C	189	PHE	7.0
1	B	406	ALA	6.9
1	C	133	ALA	6.9
1	C	410	GLY	6.8
1	C	165	ALA	6.8
1	C	247	LEU	6.7
1	D	124	ALA	6.7
1	B	251	TRP	6.6
1	B	48	TRP	6.6
1	C	336	ALA	6.5
1	B	82	LEU	6.5
1	B	348	ALA	6.5
1	C	1	MET	6.4
1	C	244	ILE	6.4
1	B	147	LEU	6.3
1	C	349	TRP	6.3
1	B	409	PRO	6.2
1	B	347	PRO	6.2
1	C	2	LEU	6.2
1	D	410	GLY	6.2
1	C	330	LEU	6.2
1	C	251	TRP	6.2

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Mol	Chain	Res	Type	RSRZ
1	C	335	ALA	6.2
1	C	212	LEU	6.1
1	B	349	TRP	6.0
1	C	54	ALA	6.0
1	D	447	VAL	6.0
1	C	193	PRO	5.9
1	B	42	VAL	5.9
1	C	345	SER	5.8
1	C	207	ALA	5.8
1	C	447	VAL	5.8
1	B	217	VAL	5.8
1	C	48	TRP	5.8
1	A	447	VAL	5.8
1	C	186	ILE	5.8
1	B	342	PRO	5.8
1	B	188	ILE	5.7
1	C	211	VAL	5.7
1	B	83	ASP	5.7
1	B	133	ALA	5.7
1	C	53	ASP	5.7
1	A	299	PHE	5.6
1	C	205	LEU	5.6
1	C	316	PHE	5.6
1	C	343	ASP	5.6
1	C	97	ALA	5.6
1	A	132	PHE	5.6
1	C	114	PHE	5.6
1	C	202	ALA	5.6
1	C	78	LEU	5.5
1	B	80	PRO	5.5
1	C	248	VAL	5.5
1	C	271	ALA	5.4
1	C	80	PRO	5.4
1	A	96	LEU	5.4
1	B	92	ARG	5.4
1	C	182	LEU	5.3
1	C	46	ALA	5.3
1	A	127	HIS	5.3
1	B	155	PHE	5.3
1	A	118	PRO	5.2
1	B	152	HIS	5.2
1	B	114	PHE	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	415	ALA	5.2
1	C	249	ALA	5.1
1	D	429	VAL	5.1
1	B	300	GLY	5.1
1	B	185	ALA	5.1
1	C	50	VAL	5.1
1	B	165	ALA	5.1
1	C	413	PHE	5.0
1	C	252	ILE	5.0
1	C	273	LEU	5.0
1	D	119	SER	5.0
1	C	188	ILE	4.9
1	B	339	VAL	4.9
1	A	119	SER	4.9
1	B	134	GLU	4.8
1	D	117	ILE	4.8
1	B	153	VAL	4.8
1	B	412	VAL	4.8
1	D	151	GLY	4.8
1	C	272	TYR	4.7
1	C	417	ASP	4.7
1	B	184	PRO	4.7
1	B	209	GLY	4.7
1	B	298	ALA	4.7
1	B	216	PRO	4.7
1	C	107	LEU	4.6
1	D	2	LEU	4.6
1	C	71	GLY	4.6
1	C	58	ALA	4.6
1	B	78	LEU	4.6
1	C	63	LEU	4.6
1	C	216	PRO	4.6
1	C	164	MET	4.6
1	C	176	GLN	4.6
1	B	95	LEU	4.5
1	C	217	VAL	4.5
1	C	174	TYR	4.5
1	B	404	ASP	4.5
1	B	169	PRO	4.5
1	C	92	ARG	4.5
1	D	418	ARG	4.5
1	B	137	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	115	ASP	4.5
1	B	30	GLY	4.5
1	B	351	ALA	4.5
1	C	143	VAL	4.4
1	C	409	PRO	4.4
1	B	113	LEU	4.4
1	C	315	LEU	4.4
1	C	393	VAL	4.4
1	C	412	VAL	4.4
1	C	218	ILE	4.4
1	D	127	HIS	4.4
1	B	399	TYR	4.4
1	B	250	GLY	4.4
1	C	403	LEU	4.4
1	B	411	ALA	4.4
1	B	101	GLN	4.3
1	C	246	PRO	4.3
1	B	50	VAL	4.3
1	B	405	GLU	4.3
1	B	141	ASN	4.3
1	C	35	ILE	4.3
1	C	27	ALA	4.3
1	C	155	PHE	4.3
1	B	202	ALA	4.3
1	C	297	LEU	4.3
1	A	446	GLY	4.2
1	B	249	ALA	4.2
1	D	81	CYS	4.2
1	B	150	ALA	4.2
1	C	411	ALA	4.2
1	C	25	TRP	4.2
1	C	192	GLY	4.2
1	C	312	LEU	4.2
1	B	28	ALA	4.2
1	C	263	PHE	4.2
1	A	126	ARG	4.2
1	C	326	THR	4.2
1	B	108	ARG	4.2
1	C	203	ALA	4.2
1	C	95	LEU	4.2
1	C	208	VAL	4.2
1	C	288	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	345	SER	4.2
1	B	245	LEU	4.1
1	C	52	TYR	4.1
1	C	60	LEU	4.1
1	C	342	PRO	4.1
1	C	145	ARG	4.1
1	C	44	VAL	4.1
1	C	302	GLY	4.1
1	D	302	GLY	4.1
1	A	46	ALA	4.1
1	B	189	PHE	4.1
1	B	74	PHE	4.0
1	D	55	ALA	4.0
1	B	393	VAL	4.0
1	B	190	TRP	4.0
1	B	156	CYS	4.0
1	C	301	ASP	4.0
1	C	286	ALA	3.9
1	C	347	PRO	3.9
1	C	279	ALA	3.9
1	B	55	ALA	3.8
1	B	99	VAL	3.8
1	B	447	VAL	3.8
1	B	213	ARG	3.8
1	D	443	TYR	3.8
1	B	140	SER	3.8
1	C	31	MET	3.8
1	C	329	ILE	3.8
1	C	111	VAL	3.8
1	C	317	TRP	3.8
1	D	303	ALA	3.8
1	B	36	TYR	3.8
1	D	427	PHE	3.8
1	B	403	LEU	3.8
1	C	353	LEU	3.8
1	C	171	GLY	3.8
1	C	239	GLY	3.8
1	B	79	ALA	3.8
1	B	427	PHE	3.7
1	B	54	ALA	3.7
1	B	96	LEU	3.7
1	B	304	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	431	VAL	3.7
1	C	39	LYS	3.7
1	B	143	VAL	3.7
1	C	419	ILE	3.7
1	C	160	TYR	3.6
1	A	81	CYS	3.6
1	C	47	ARG	3.6
1	C	57	LEU	3.6
1	C	180	SER	3.6
1	A	412	VAL	3.6
1	C	209	GLY	3.6
1	B	135	ALA	3.6
1	A	117	ILE	3.6
1	C	306	SER	3.6
1	C	29	ALA	3.6
1	A	410	GLY	3.6
1	B	14	TRP	3.6
1	B	205	LEU	3.6
1	C	356	LEU	3.6
1	C	103	ALA	3.5
1	C	135	ALA	3.5
1	C	402	TRP	3.5
1	A	175	LEU	3.5
1	B	322	LEU	3.5
1	B	344	PRO	3.5
1	C	82	LEU	3.5
1	A	2	LEU	3.5
1	C	190	TRP	3.5
1	B	111	VAL	3.5
1	C	400	CYS	3.5
1	B	285	ALA	3.5
1	C	20	ALA	3.5
1	C	98	ARG	3.5
1	B	102	LEU	3.5
1	C	322	LEU	3.5
1	D	113	LEU	3.5
1	B	402	TRP	3.5
1	C	195	ILE	3.5
1	B	37	GLY	3.5
1	C	169	PRO	3.5
1	A	393	VAL	3.4
1	B	167	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	144	LEU	3.4
1	C	51	PRO	3.4
1	C	181	THR	3.4
1	B	58	ALA	3.4
1	C	234	ALA	3.4
1	C	167	GLY	3.4
1	C	323	GLY	3.4
1	C	34	TYR	3.4
1	B	2	LEU	3.4
1	C	237	LEU	3.4
1	C	284	ILE	3.4
1	B	336	ALA	3.4
1	C	45	ARG	3.4
1	C	69	ALA	3.4
1	C	415	ALA	3.4
1	C	3	THR	3.4
1	B	363	ILE	3.4
1	B	98	ARG	3.4
1	C	61	THR	3.4
1	C	351	ALA	3.4
1	C	404	ASP	3.4
1	C	407	PRO	3.4
1	D	90	GLN	3.4
1	A	48	TRP	3.4
1	B	301	ASP	3.3
1	B	334	ARG	3.3
1	C	108	ARG	3.3
1	B	353	LEU	3.3
1	D	417	ASP	3.3
1	B	367	PHE	3.3
1	C	185	ALA	3.3
1	C	295	PHE	3.3
1	C	397	VAL	3.3
1	C	250	GLY	3.3
1	D	300	GLY	3.3
1	B	51	PRO	3.3
1	C	201	VAL	3.3
1	B	85	THR	3.3
1	D	132	PHE	3.3
1	B	154	VAL	3.3
1	B	145	ARG	3.2
1	B	324	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	212	LEU	3.2
1	C	298	ALA	3.2
1	B	387	TRP	3.2
1	C	91	ASP	3.2
1	C	243	ASP	3.2
1	C	283	ALA	3.2
1	C	359	LEU	3.2
1	C	75	TYR	3.2
1	C	399	TYR	3.2
1	B	38	PRO	3.2
1	B	11	GLY	3.2
1	C	159	GLU	3.2
1	C	196	VAL	3.2
1	D	99	VAL	3.2
1	A	89	PRO	3.2
1	B	148	ARG	3.2
1	B	218	ILE	3.2
1	B	136	GLN	3.2
1	B	357	ARG	3.2
1	A	115	ASP	3.2
1	C	141	ASN	3.2
1	C	110	LEU	3.2
1	C	147	LEU	3.2
1	B	201	VAL	3.1
1	B	46	ALA	3.1
1	B	191	THR	3.1
1	A	121	LEU	3.1
1	B	161	CYS	3.1
1	C	281	GLU	3.1
1	A	86	TYR	3.1
1	A	417	ASP	3.1
1	C	113	LEU	3.1
1	C	291	TRP	3.1
1	D	315	LEU	3.1
1	C	369	LEU	3.1
1	C	378	LEU	3.1
1	D	285	ALA	3.1
1	D	298	ALA	3.1
1	D	387	TRP	3.1
1	B	164	MET	3.0
1	B	416	THR	3.0
1	A	155	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	363	ILE	3.0
1	D	440	GLN	3.0
1	C	83	ASP	3.0
1	C	431	VAL	3.0
1	A	387	TRP	3.0
1	C	191	THR	3.0
1	B	356	LEU	3.0
1	A	123	GLU	3.0
1	C	340	PRO	3.0
1	A	129	PHE	3.0
1	B	244	ILE	3.0
1	B	277	ASP	3.0
1	C	307	ASP	3.0
1	C	311	LEU	3.0
1	D	143	VAL	3.0
1	C	156	CYS	3.0
1	D	393	VAL	3.0
1	C	282	ARG	2.9
1	B	34	TYR	2.9
1	B	75	TYR	2.9
1	C	367	PHE	2.9
1	B	431	VAL	2.9
1	C	37	GLY	2.9
1	C	184	PRO	2.9
1	C	314	ASP	2.9
1	C	386	LEU	2.9
1	D	338	THR	2.9
1	C	267	HIS	2.9
1	D	425	ARG	2.9
1	C	280	PRO	2.9
1	C	414	PRO	2.9
1	B	352	ALA	2.9
1	C	81	CYS	2.9
1	B	25	TRP	2.9
1	B	107	LEU	2.9
1	B	276	PRO	2.9
1	B	419	ILE	2.9
1	C	79	ALA	2.9
1	C	253	THR	2.9
1	B	247	LEU	2.8
1	B	315	LEU	2.8
1	C	175	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	277	ASP	2.8
1	A	442	ARG	2.8
1	C	12	ARG	2.8
1	B	29	ALA	2.8
1	A	114	PHE	2.8
1	A	367	PHE	2.8
1	B	308	LEU	2.8
1	C	346	ASP	2.8
1	B	239	GLY	2.8
1	B	252	ILE	2.8
1	C	179	GLY	2.8
1	B	49	ARG	2.8
1	C	215	ARG	2.8
1	A	212	LEU	2.8
1	B	57	LEU	2.8
1	B	359	LEU	2.8
1	C	112	LEU	2.8
1	B	210	GLU	2.8
1	C	275	ASP	2.8
1	D	244	ILE	2.8
1	C	142	MET	2.8
1	C	154	VAL	2.8
1	A	441	GLY	2.8
1	C	372	GLU	2.8
1	C	43	HIS	2.8
1	C	321	ALA	2.8
1	A	122	PRO	2.8
1	B	181	THR	2.7
1	C	178	LEU	2.7
1	C	320	PHE	2.7
1	C	384[A]	ASN	2.7
1	B	47	ARG	2.7
1	B	43	HIS	2.7
1	B	171	GLY	2.7
1	D	174	TYR	2.7
1	C	240	ARG	2.7
1	D	42	VAL	2.7
1	C	74	PHE	2.7
1	C	405	GLU	2.7
1	D	167	GLY	2.7
1	C	177	ARG	2.7
1	D	128	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	290	ALA	2.7
1	A	190	TRP	2.7
1	B	110	LEU	2.7
1	B	144	LEU	2.7
1	D	353	LEU	2.7
1	B	166	GLY	2.7
1	B	242	ARG	2.7
1	D	177	ARG	2.7
1	B	271	ALA	2.7
1	A	204	HIS	2.7
1	D	6	ILE	2.7
1	A	120	VAL	2.7
1	A	271	ALA	2.6
1	B	146	HIS	2.6
1	C	289	ALA	2.6
1	C	232	VAL	2.6
1	C	423	TYR	2.6
1	C	172	SER	2.6
1	B	364	ASN	2.6
1	C	287	ALA	2.6
1	B	397	VAL	2.6
1	B	407	PRO	2.6
1	C	146	HIS	2.6
1	B	174	TYR	2.6
1	A	398	ALA	2.6
1	A	427	PHE	2.6
1	C	379	PHE	2.6
1	A	444	HIS	2.6
1	A	130	ASP	2.6
1	B	6	ILE	2.6
1	A	339	VAL	2.6
1	B	94	ALA	2.6
1	B	335	ALA	2.6
1	B	433	ASP	2.6
1	D	83	ASP	2.6
1	D	94	ALA	2.6
1	A	222	PHE	2.5
1	C	105	ALA	2.5
1	A	440	GLN	2.5
1	B	200	ILE	2.5
1	D	218	ILE	2.5
1	A	273	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	330	LEU	2.5
1	C	227	TYR	2.5
1	A	158	THR	2.5
1	B	172	SER	2.5
1	C	219	TRP	2.5
1	C	344	PRO	2.5
1	D	301	ASP	2.5
1	B	269	THR	2.5
1	B	327	THR	2.5
1	C	327	THR	2.5
1	D	435	LEU	2.5
1	B	52	TYR	2.5
1	C	210	GLU	2.5
1	C	325	GLU	2.5
1	D	126	ARG	2.5
1	D	294[A]	ARG	2.5
1	A	103	ALA	2.5
1	C	162	GLY	2.5
1	D	289	ALA	2.5
1	A	90	GLN	2.5
1	C	387	TRP	2.5
1	A	429	VAL	2.5
1	C	99	VAL	2.5
1	A	333	LEU	2.5
1	D	144	LEU	2.5
1	C	241	SER	2.5
1	D	87	SER	2.5
1	C	394	GLY	2.5
1	A	298	ALA	2.5
1	B	69	ALA	2.5
1	C	214	ARG	2.5
1	C	168	ASP	2.5
1	D	438	ASP	2.5
1	C	422	PHE	2.5
1	D	222	PHE	2.5
1	A	245	LEU	2.5
1	B	177	ARG	2.4
1	B	255	PRO	2.4
1	B	341	ARG	2.4
1	D	93	ALA	2.4
1	D	105	ALA	2.4
1	C	49	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	84	VAL	2.4
1	A	1	MET	2.4
1	C	26	ILE	2.4
1	C	304	VAL	2.4
1	D	188	ILE	2.4
1	A	60	LEU	2.4
1	D	57	LEU	2.4
1	D	312	LEU	2.4
1	B	438	ASP	2.4
1	D	185	ALA	2.4
1	B	338	THR	2.4
1	B	282	ARG	2.4
1	D	250	GLY	2.4
1	A	154	VAL	2.4
1	C	429	VAL	2.4
1	C	350	ARG	2.4
1	B	253	THR	2.4
1	C	416	THR	2.4
1	B	8	GLY	2.4
1	B	278	TYR	2.4
1	A	88	ASP	2.4
1	A	20	ALA	2.4
1	B	203	ALA	2.4
1	D	283	ALA	2.4
1	B	365	LYS	2.4
1	C	22	VAL	2.4
1	D	78	LEU	2.4
1	D	96	LEU	2.4
1	D	322	LEU	2.4
1	D	419	ILE	2.4
1	D	89	PRO	2.4
1	D	75	TYR	2.4
1	B	446	GLY	2.4
1	C	9	PHE	2.3
1	A	162	GLY	2.3
1	C	94	ALA	2.3
1	C	398	ALA	2.3
1	B	417	ASP	2.3
1	D	339	VAL	2.3
1	B	297	LEU	2.3
1	B	142	MET	2.3
1	A	411	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	86	TYR	2.3
1	B	418	ARG	2.3
1	A	78	LEU	2.3
1	B	311	LEU	2.3
1	D	147	LEU	2.3
1	A	146	HIS	2.3
1	B	199	GLU	2.3
1	C	161	CYS	2.3
1	B	160	TYR	2.3
1	C	140	SER	2.3
1	B	67	ALA	2.3
1	C	224	ALA	2.3
1	A	413	PHE	2.3
1	B	9	PHE	2.3
1	A	153	VAL	2.2
1	A	102	LEU	2.2
1	B	103	ALA	2.2
1	D	441	GLY	2.2
1	B	64	ARG	2.2
1	C	23	MET	2.2
1	C	242	ARG	2.2
1	B	187	ASP	2.2
1	A	133	ALA	2.2
1	C	285	ALA	2.2
1	A	50	VAL	2.2
1	D	396	LEU	2.2
1	B	384	ASN	2.2
1	B	346	ASP	2.2
1	B	379	PHE	2.2
1	B	422	PHE	2.2
1	C	313	CYS	2.2
1	A	128	ARG	2.2
1	A	97	ALA	2.2
1	B	97	ALA	2.2
1	C	446	GLY	2.2
1	D	249	ALA	2.2
1	B	5	VAL	2.2
1	D	84	VAL	2.2
1	D	397	VAL	2.2
1	B	273	LEU	2.2
1	C	401	ASP	2.2
1	C	38	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	47	ARG	2.2
1	C	170	ARG	2.2
1	C	318	GLN	2.2
1	A	-1	GLY	2.2
1	B	10	TYR	2.2
1	B	274	ALA	2.2
1	B	279	ALA	2.2
1	C	66	ALA	2.2
1	C	430	ALA	2.2
1	D	50	VAL	2.2
1	D	386	LEU	2.2
1	C	32	ASN	2.2
1	C	149	GLY	2.2
1	B	168	ASP	2.2
1	C	138	ASP	2.2
1	B	180	SER	2.1
1	B	227	TYR	2.1
1	B	423	TYR	2.1
1	C	328	ARG	2.1
1	D	108	ARG	2.1
1	A	44	VAL	2.1
1	A	431	VAL	2.1
1	B	73	VAL	2.1
1	D	111	VAL	2.1
1	A	378	LEU	2.1
1	D	121	LEU	2.1
1	A	373	ILE	2.1
1	D	45	ARG	2.1
1	A	0	SER	2.1
1	C	354	GLU	2.1
1	D	54	ALA	2.1
1	C	257	ASN	2.1
1	B	4	GLY	2.1
1	B	215	ARG	2.1
1	B	292	GLN	2.1
1	C	59	ARG	2.1
1	B	312	LEU	2.1
1	C	158	THR	2.1
1	A	306	SER	2.1
1	C	197	SER	2.1
1	B	173	ALA	2.1
1	D	411	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	319	PRO	2.1
1	B	170	ARG	2.1
1	B	214	ARG	2.1
1	B	302	GLY	2.1
1	C	418	ARG	2.1
1	B	248	VAL	2.1
1	A	247	LEU	2.1
1	B	27	ALA	2.1
1	B	237	LEU	2.1
1	C	434	ILE	2.1
1	C	360	LYS	2.1
1	C	358	ASP	2.1
1	A	85	THR	2.1
1	C	33	THR	2.1
1	B	104	ARG	2.1
1	C	222	PHE	2.1
1	B	68	ALA	2.1
1	B	219	TRP	2.1
1	B	317	TRP	2.1
1	C	348	ALA	2.1
1	A	106	GLY	2.1
1	D	110	LEU	2.1
1	B	355	ASP	2.1
1	C	364	ASN	2.1
1	A	131	SER	2.1
1	D	362	ARG	2.0
1	B	368	THR	2.0
1	B	149	GLY	2.0
1	B	88	ASP	2.0
1	C	116	ASP	2.0
1	D	412	VAL	2.0
1	A	334	ARG	2.0
1	C	296	ARG	2.0
1	D	369	LEU	2.0
1	C	21	THR	2.0
1	B	115	ASP	2.0
1	C	72	MET	2.0
1	A	430	ALA	2.0
1	D	207	ALA	2.0
1	A	422	PHE	2.0
1	B	139	LEU	2.0
1	D	367	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	416	THR	2.0
1	A	349	TRP	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

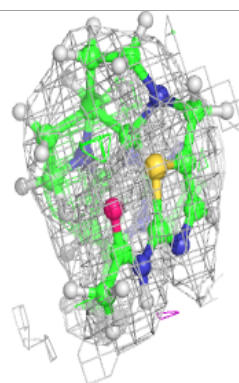
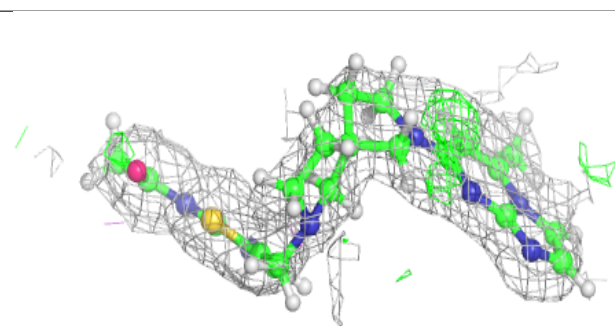
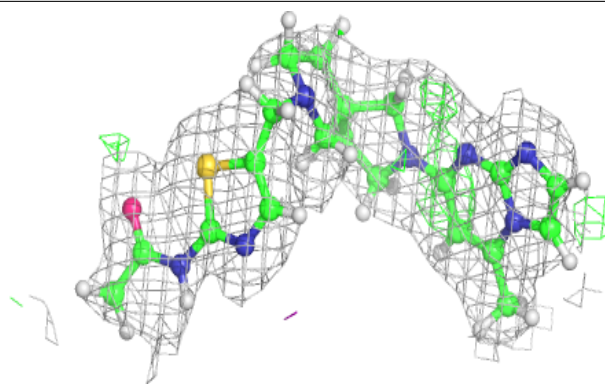
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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	CA	B	502	1/1	0.80	0.07	37,37,37,37	0
2	WG4	C	501	29/29	0.81	0.17	25,31,40,44	0
2	WG4	B	501	29/29	0.83	0.18	20,30,43,50	0
2	WG4	A	501	29/29	0.84	0.15	24,31,38,41	0
2	WG4	D	501	29/29	0.91	0.13	19,25,40,44	0
4	EDO	C	502	4/4	0.92	0.17	18,19,25,26	1
3	CA	D	502	1/1	0.98	0.07	29,29,29,29	0

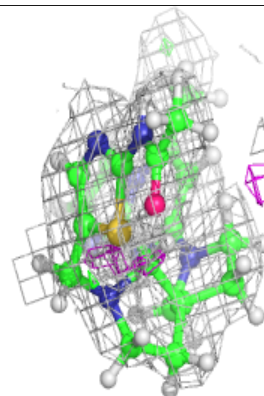
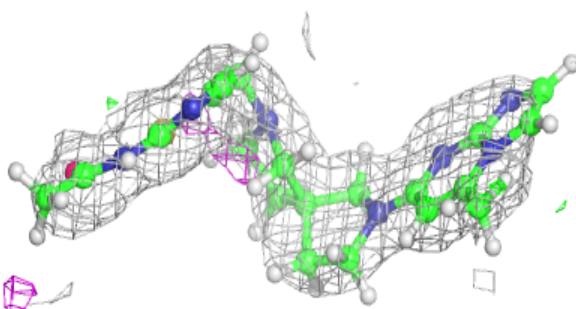
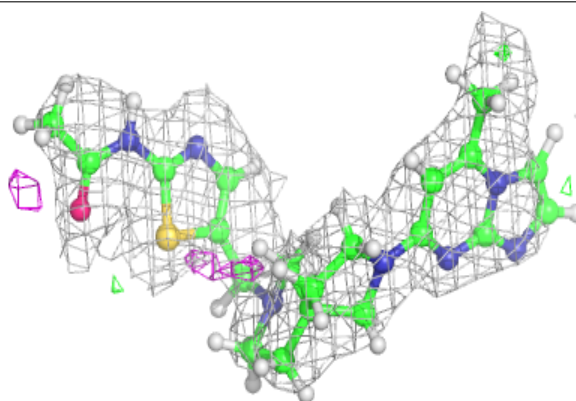
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around WG4 C 501:**

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

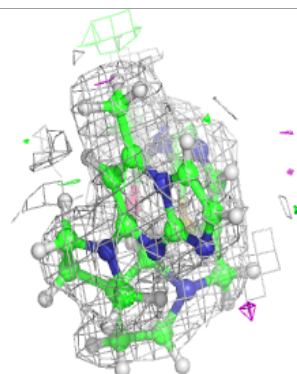
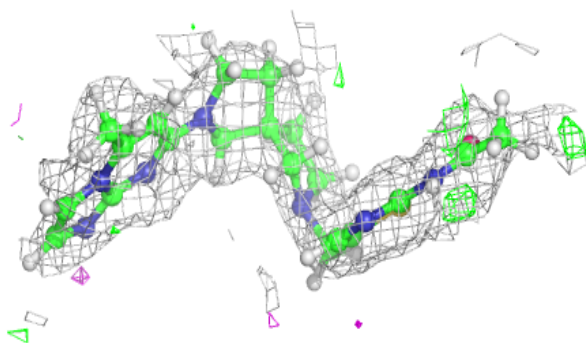
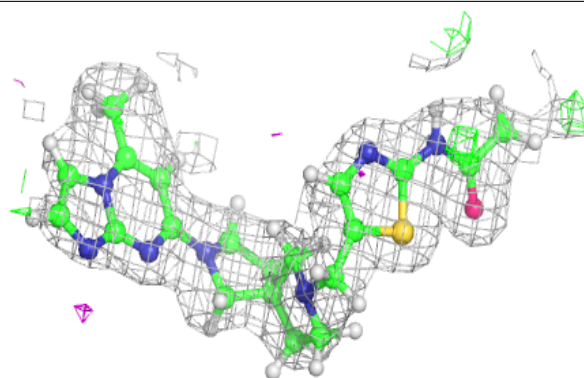
**Electron density around WG4 B 501:**

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

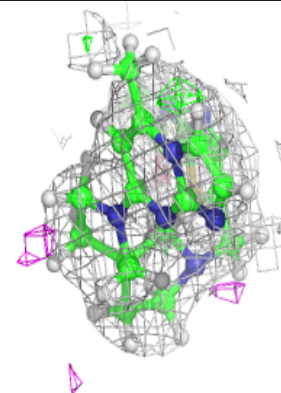
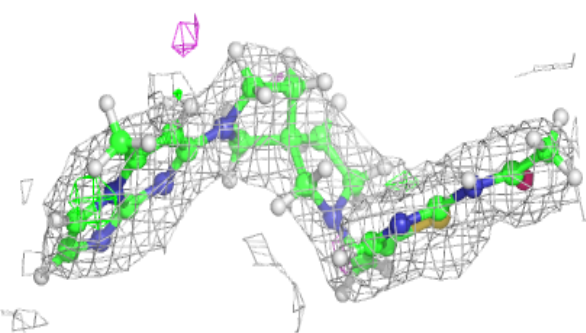
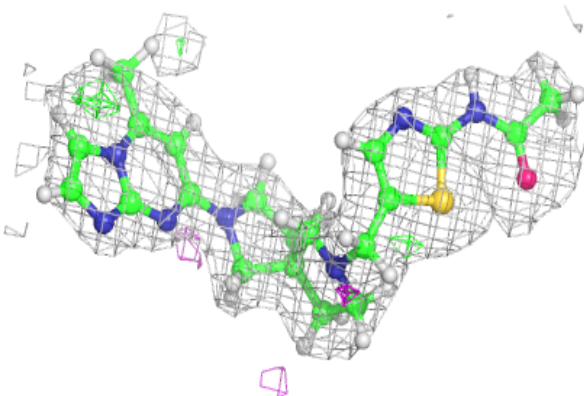


**Electron density around WG4 A 501:**

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

**Electron density around WG4 D 501:**

$2mF_o-DF_c$  (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.