



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:35 PM UTC

PDB ID : 8SWE / pdb_00008swe
Title : FGFR2 Kinase Domain Bound to Reversible Inhibitor Cmpd 3
Authors : Valverde, R.; Foster, L.
Deposited on : 2023-05-18
Resolution : 2.24 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

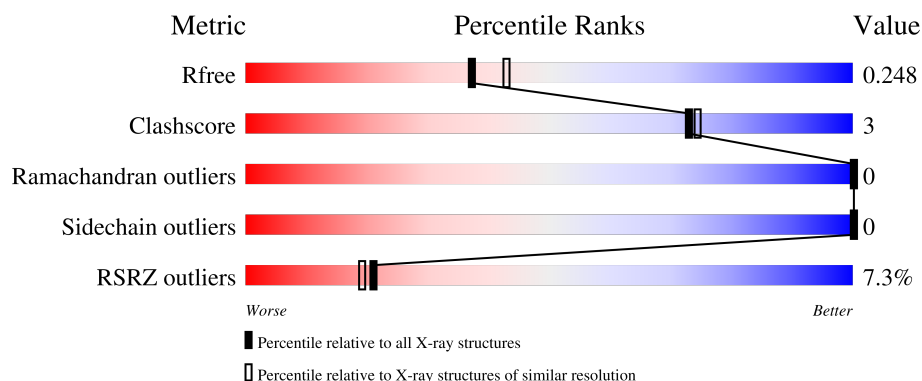
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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}	180053	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	316	6% 83% 7% 10%
1	B	316	8% 85% 5% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9535 atoms, of which 4691 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.

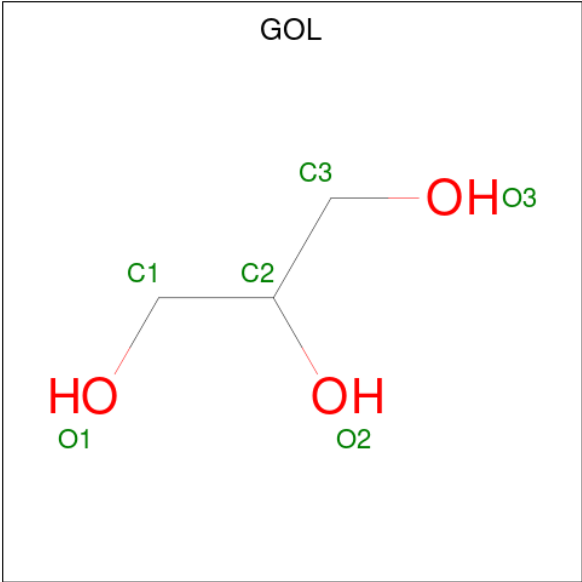
- Molecule 1 is a protein called Fibroblast growth factor receptor 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	284	Total	C	H	N	O	S	0	2	0
			4578	1454	2296	388	418	22			
1	B	288	Total	C	H	N	O	S	0	0	0
			4619	1466	2314	391	427	21			

There are 10 discrepancies between the modelled and reference sequences:

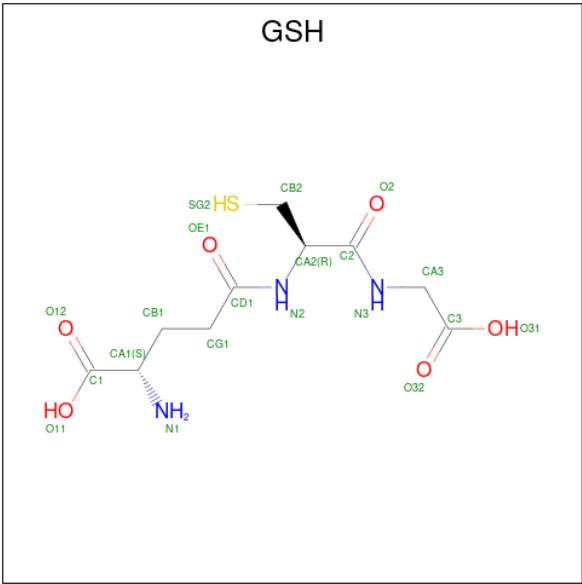
Chain	Residue	Modelled	Actual	Comment	Reference
A	453	SER	-	expression tag	UNP P21802
A	454	HIS	-	expression tag	UNP P21802
A	455	MET	-	expression tag	UNP P21802
A	456	GLY	-	expression tag	UNP P21802
A	457	SER	-	expression tag	UNP P21802
B	453	SER	-	expression tag	UNP P21802
B	454	HIS	-	expression tag	UNP P21802
B	455	MET	-	expression tag	UNP P21802
B	456	GLY	-	expression tag	UNP P21802
B	457	SER	-	expression tag	UNP P21802

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



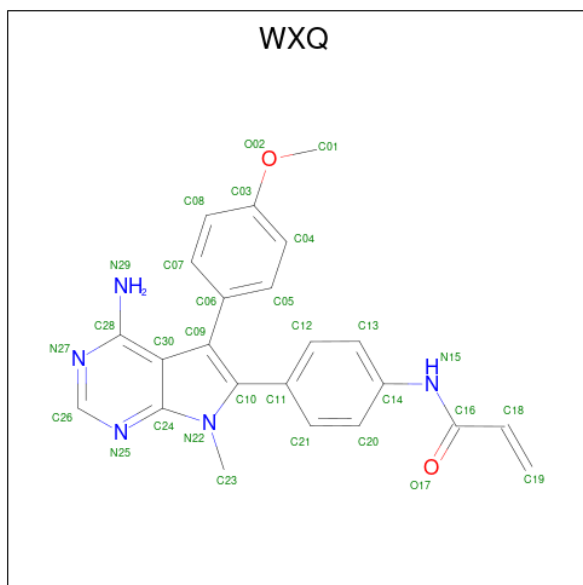
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O		0	0
			6	3	3			
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is GLUTATHIONE (CCD ID: GSH) (formula: C₁₀H₁₇N₃O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	
			35	10	15	3	6	1	
								0	0

- Molecule 4 is N-{4-[4-amino-5-(4-methoxyphenyl)-7-methyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl]phenyl}prop-2-enamide (CCD ID: WXQ) (formula: C₂₃H₂₁N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O		
			51	23	21	5	2		
4	B	1	Total	C	H	N	O		
			51	23	21	5	2		
								0	0

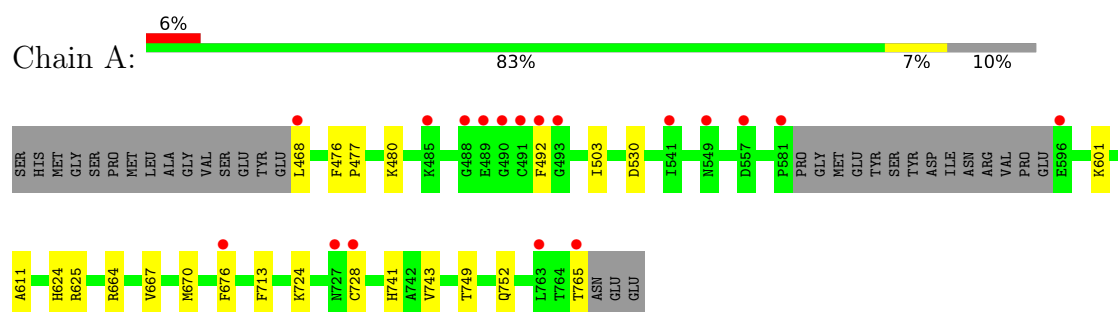
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	81	Total	O		
			81	81		
					0	0
5	B	72	Total	O		
			72	72		
					0	0

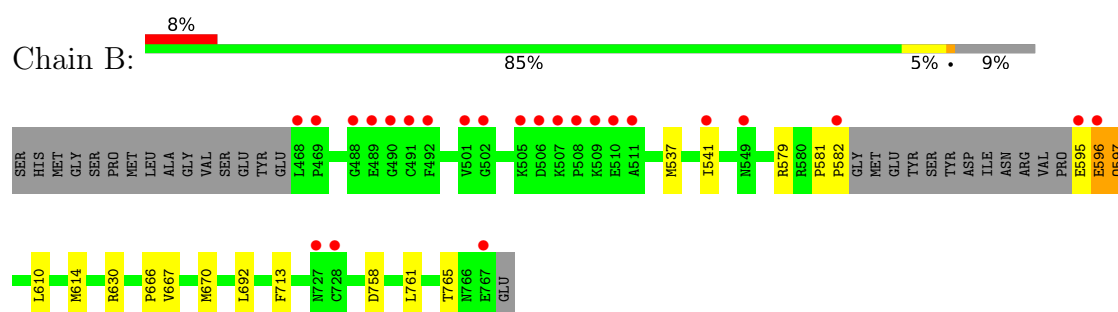
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Fibroblast growth factor receptor 2



- Molecule 1: Fibroblast growth factor receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.46Å 117.13Å 64.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.37 – 2.24 78.37 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.0 (78.37-2.24) 98.9 (78.37-2.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.66 (at 2.25Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.211 , 0.250 0.212 , 0.248	Depositor DCC
R_{free} test set	2000 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9535	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, GSH, WXQ

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	0.32	1/2336 (0.0%)	0.43	1/3154 (0.0%)
1	B	0.23	0/2353	0.39	3/3178 (0.1%)
All	All	0.28	1/4689 (0.0%)	0.41	4/6332 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	611	ALA	C-N	-8.45	1.22	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	596	GLU	N-CA-C	-7.42	98.91	109.96
1	B	596	GLU	CB-CA-C	6.87	120.05	110.16
1	A	492	PHE	N-CA-C	-5.71	105.43	112.90
1	B	597	GLN	N-CA-C	-5.41	102.47	110.48

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2282	2296	2300	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2305	2314	2313	16	0
2	A	6	0	8	1	0
2	B	18	24	24	2	0
3	A	20	15	15	0	0
4	A	30	21	0	0	0
4	B	30	21	0	0	0
5	A	81	0	0	2	0
5	B	72	0	0	0	0
All	All	4844	4691	4660	30	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 3.

All (30) 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:579:ARG:HG2	1:B:596:GLU:O	1.85	0.77
1:B:630:ARG:NH2	1:B:666:PRO:HG2	2.07	0.70
1:B:758:ASP:OD1	2:B:802:GOL:H32	1.95	0.67
1:A:724:LYS:NZ	1:A:728:CYS:O	2.29	0.66
1:B:582:PRO:HD3	1:B:597:GLN:NE2	2.16	0.60
1:B:761:LEU:HD23	2:B:802:GOL:H12	1.84	0.59
1:B:630:ARG:HH22	1:B:666:PRO:HG2	1.68	0.59
1:B:595:GLU:HG2	1:B:595:GLU:O	2.03	0.58
1:A:667:VAL:HG13	1:A:713:PHE:CE1	2.39	0.58
1:B:582:PRO:HD3	1:B:597:GLN:HE21	1.69	0.57
1:A:667:VAL:HG13	1:A:713:PHE:HE1	1.70	0.55
1:A:667:VAL:HA	1:A:670:MET:HE2	1.88	0.55
1:A:530:ASP:OD2	1:A:664:ARG:NH2	2.42	0.52
1:A:468:LEU:N	5:A:904:HOH:O	2.42	0.51
1:B:761:LEU:O	1:B:765:THR:HG22	2.12	0.49
1:A:601:LYS:NZ	1:A:765:THR:OG1	2.45	0.49
1:A:749:THR:OG1	1:A:752:GLN:HG3	2.14	0.48
1:B:667:VAL:HG13	1:B:713:PHE:CE2	2.48	0.48
2:A:801:GOL:O1	5:A:901:HOH:O	2.20	0.46
1:B:581:PRO:HA	1:B:597:GLN:NE2	2.30	0.46
1:B:610:LEU:HD13	1:B:692:LEU:HD21	1.98	0.45
1:A:477:PRO:HG2	1:A:480:LYS:HE3	2.00	0.44
1:B:537:MET:O	1:B:541:ILE:HG12	2.20	0.41
1:A:676:PHE:CZ	1:A:713:PHE:HD2	2.38	0.41
1:B:582:PRO:CD	1:B:597:GLN:NE2	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:667:VAL:HA	1:B:670:MET:HE2	2.03	0.41
1:A:476:PHE:CD1	1:A:503:ILE:HD12	2.56	0.41
1:A:741[A]:HIS:HD2	1:A:743:VAL:H	1.68	0.41
1:B:614:MET:HE3	1:B:614:MET:HA	2.03	0.40
1:A:624:HIS:O	1:A:625:ARG:HB2	2.21	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	282/316 (89%)	278 (99%)	4 (1%)	0	100	100
1	B	284/316 (90%)	277 (98%)	7 (2%)	0	100	100
All	All	566/632 (90%)	555 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	251/277 (91%)	251 (100%)	0	100	100
1	B	253/277 (91%)	253 (100%)	0	100	100
All	All	504/554 (91%)	504 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	494	GLN
1	A	546	ASN
1	B	549	ASN
1	B	556	GLN
1	B	597	GLN
1	B	620	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
4	WXQ	B	804	-	33,33,33	2.83	16 (48%)	43,47,47	3.52	17 (39%)
2	GOL	B	802	-	5,5,5	0.08	0	5,5,5	0.22	0
4	WXQ	A	803	-	33,33,33	2.83	15 (45%)	43,47,47	3.27	17 (39%)
2	GOL	A	801	-	5,5,5	0.91	0	5,5,5	1.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	803	-	5,5,5	0.08	0	5,5,5	0.24	0
3	GSH	A	802	-	18,19,19	2.15	4 (22%)	21,24,24	1.49	4 (19%)
2	GOL	B	801	-	5,5,5	0.59	0	5,5,5	1.02	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	WXQ	B	804	-	-	2/16/16/16	0/4/4/4
2	GOL	B	802	-	-	2/4/4/4	-
4	WXQ	A	803	-	-	4/16/16/16	0/4/4/4
2	GOL	A	801	-	-	2/4/4/4	-
2	GOL	B	803	-	-	2/4/4/4	-
3	GSH	A	802	-	-	7/24/24/24	-
2	GOL	B	801	-	-	2/4/4/4	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	804	WXQ	C16-N15	6.07	1.46	1.35
4	A	803	WXQ	C16-N15	5.85	1.46	1.35
3	A	802	GSH	C2-N3	5.55	1.46	1.33
3	A	802	GSH	CD1-N2	5.49	1.45	1.34
4	A	803	WXQ	C30-C24	5.48	1.48	1.40
4	B	804	WXQ	C30-C24	5.39	1.47	1.40
4	B	804	WXQ	C30-C28	-5.35	1.36	1.42
4	A	803	WXQ	C10-N22	-5.24	1.29	1.38
4	B	804	WXQ	C10-N22	-5.23	1.29	1.38
4	A	803	WXQ	C30-C28	-5.07	1.36	1.42
4	B	804	WXQ	C19-C18	4.96	1.54	1.30
4	A	803	WXQ	C19-C18	4.86	1.53	1.30
4	A	803	WXQ	C11-C10	4.81	1.55	1.48
4	B	804	WXQ	C11-C10	4.64	1.55	1.48
4	A	803	WXQ	C28-N29	4.61	1.46	1.34
4	B	804	WXQ	C28-N29	4.58	1.45	1.34
4	A	803	WXQ	C18-C16	3.45	1.53	1.48
4	B	804	WXQ	C18-C16	3.41	1.53	1.48
4	A	803	WXQ	C14-N15	2.88	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	804	WXQ	O17-C16	-2.87	1.18	1.24
4	B	804	WXQ	C14-N15	2.79	1.47	1.41
4	B	804	WXQ	C06-C09	2.76	1.54	1.49
4	A	803	WXQ	O17-C16	-2.76	1.19	1.24
4	A	803	WXQ	C06-C09	2.71	1.54	1.49
4	A	803	WXQ	C30-C09	2.61	1.53	1.46
4	A	803	WXQ	C21-C11	-2.58	1.35	1.39
4	A	803	WXQ	C13-C14	2.42	1.43	1.39
4	B	804	WXQ	C13-C14	2.32	1.43	1.39
4	B	804	WXQ	C30-C09	2.32	1.52	1.46
4	B	804	WXQ	O02-C03	2.28	1.42	1.37
4	B	804	WXQ	C21-C11	-2.25	1.36	1.39
3	A	802	GSH	O2-C2	-2.21	1.19	1.23
3	A	802	GSH	OE1-CD1	-2.14	1.19	1.23
4	A	803	WXQ	O02-C03	2.13	1.41	1.37
4	B	804	WXQ	C26-N27	2.06	1.37	1.33

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	804	WXQ	C18-C16-N15	9.79	120.49	113.84
4	B	804	WXQ	C19-C18-C16	-8.88	112.46	122.22
4	A	803	WXQ	C19-C18-C16	-8.66	112.71	122.22
4	B	804	WXQ	C23-N22-C24	-7.51	114.62	124.69
4	A	803	WXQ	C18-C16-N15	7.22	118.74	113.84
4	A	803	WXQ	C23-N22-C24	-7.14	115.12	124.69
4	B	804	WXQ	N25-C24-N22	6.88	139.28	124.88
4	A	803	WXQ	N25-C24-N22	6.79	139.10	124.88
4	B	804	WXQ	C24-C30-C09	-6.74	101.51	107.32
4	A	803	WXQ	C24-C30-C09	-6.73	101.52	107.32
4	B	804	WXQ	C09-C10-N22	-6.10	98.20	108.32
4	A	803	WXQ	C09-C10-N22	-6.01	98.35	108.32
4	B	804	WXQ	C11-C10-N22	5.48	131.29	121.91
4	B	804	WXQ	C30-C24-N25	-5.23	121.42	126.97
4	A	803	WXQ	C30-C24-N25	-5.12	121.54	126.97
4	A	803	WXQ	C11-C10-N22	5.06	130.58	121.91
4	B	804	WXQ	N27-C26-N25	-4.67	121.52	128.58
4	A	803	WXQ	C23-N22-C10	-4.55	117.69	126.69
4	B	804	WXQ	C14-N15-C16	-4.32	119.95	128.07
4	B	804	WXQ	C23-N22-C10	-4.30	118.18	126.69
4	A	803	WXQ	N27-C26-N25	-4.25	122.15	128.58
3	A	802	GSH	CA2-CB2-SG2	-3.73	109.96	114.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	WXQ	C14-N15-C16	-3.24	121.97	128.07
4	B	804	WXQ	C26-N25-C24	2.92	118.97	111.83
3	A	802	GSH	CB1-CG1-CD1	-2.82	106.78	113.06
4	A	803	WXQ	C26-N25-C24	2.79	118.66	111.83
4	A	803	WXQ	C30-C09-C06	-2.41	121.52	127.01
4	B	804	WXQ	C30-C28-N29	-2.35	120.30	123.40
4	B	804	WXQ	O17-C16-C18	-2.33	119.21	122.70
4	B	804	WXQ	C30-C09-C06	-2.31	121.76	127.01
4	A	803	WXQ	C20-C21-C11	2.20	123.15	120.80
3	A	802	GSH	C2-CA2-N2	-2.15	105.29	111.11
4	B	804	WXQ	O17-C16-N15	-2.14	120.30	123.11
4	B	804	WXQ	C20-C14-C13	-2.08	116.28	119.04
4	A	803	WXQ	C20-C14-C13	-2.07	116.30	119.04
4	A	803	WXQ	C21-C11-C10	-2.06	117.46	120.56
4	A	803	WXQ	C30-C28-N29	-2.01	120.75	123.40
3	A	802	GSH	O31-C3-CA3	2.01	120.44	112.81

There are no chirality outliers.

All (21) torsion outliers are listed below:

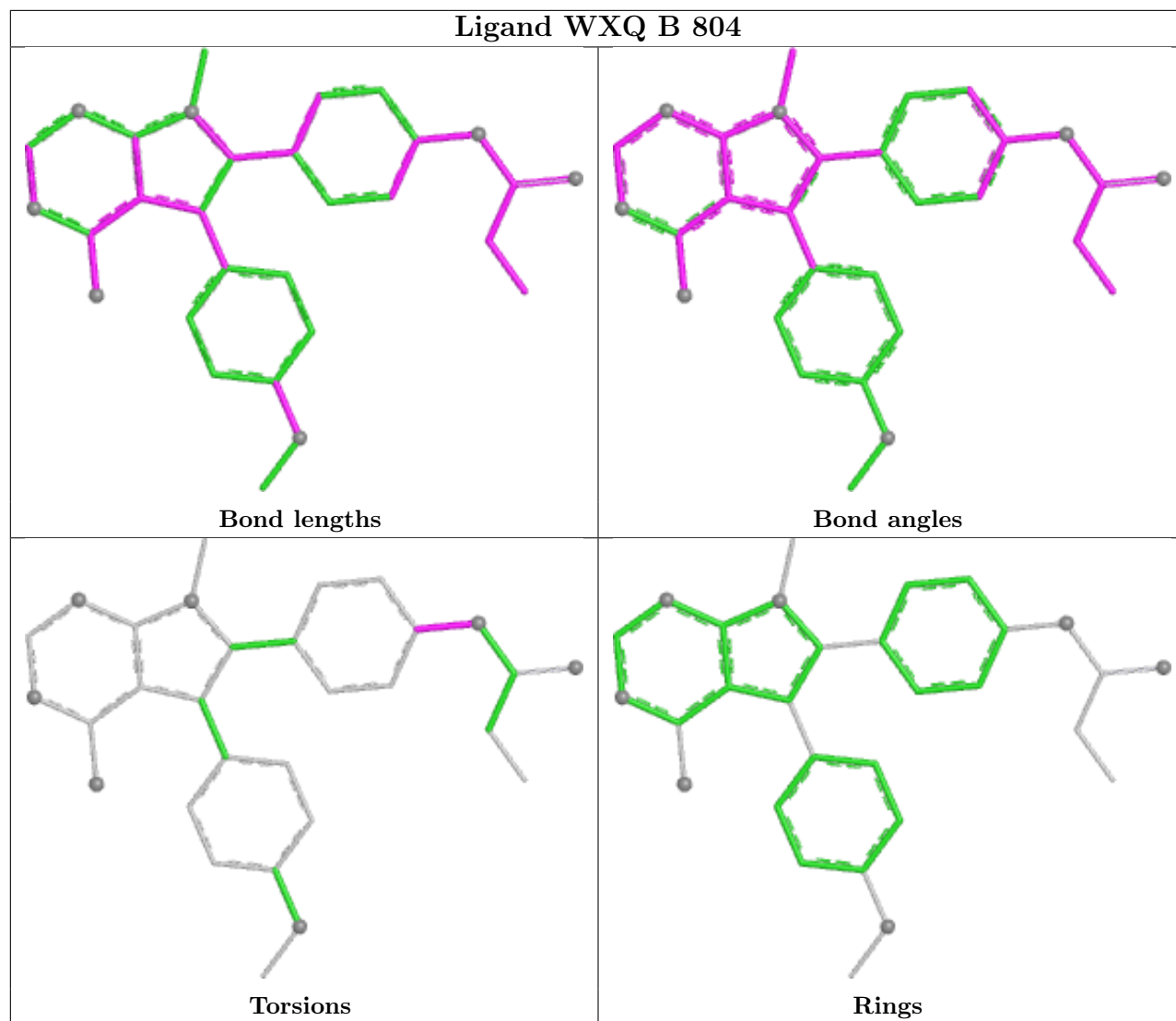
Mol	Chain	Res	Type	Atoms
2	A	801	GOL	C1-C2-C3-O3
2	B	802	GOL	C1-C2-C3-O3
2	B	803	GOL	C1-C2-C3-O3
3	A	802	GSH	N2-CA2-CB2-SG2
3	A	802	GSH	C2-CA2-CB2-SG2
4	A	803	WXQ	N15-C16-C18-C19
4	A	803	WXQ	O17-C16-C18-C19
4	A	803	WXQ	C13-C14-N15-C16
4	A	803	WXQ	C20-C14-N15-C16
3	A	802	GSH	O31-C3-CA3-N3
2	B	801	GOL	O1-C1-C2-C3
3	A	802	GSH	CA1-CB1-CG1-CD1
2	A	801	GOL	O2-C2-C3-O3
2	B	801	GOL	O1-C1-C2-O2
2	B	802	GOL	O2-C2-C3-O3
3	A	802	GSH	O32-C3-CA3-N3
2	B	803	GOL	O2-C2-C3-O3
4	B	804	WXQ	C13-C14-N15-C16
4	B	804	WXQ	C20-C14-N15-C16
3	A	802	GSH	OE1-CD1-CG1-CB1
3	A	802	GSH	N2-CD1-CG1-CB1

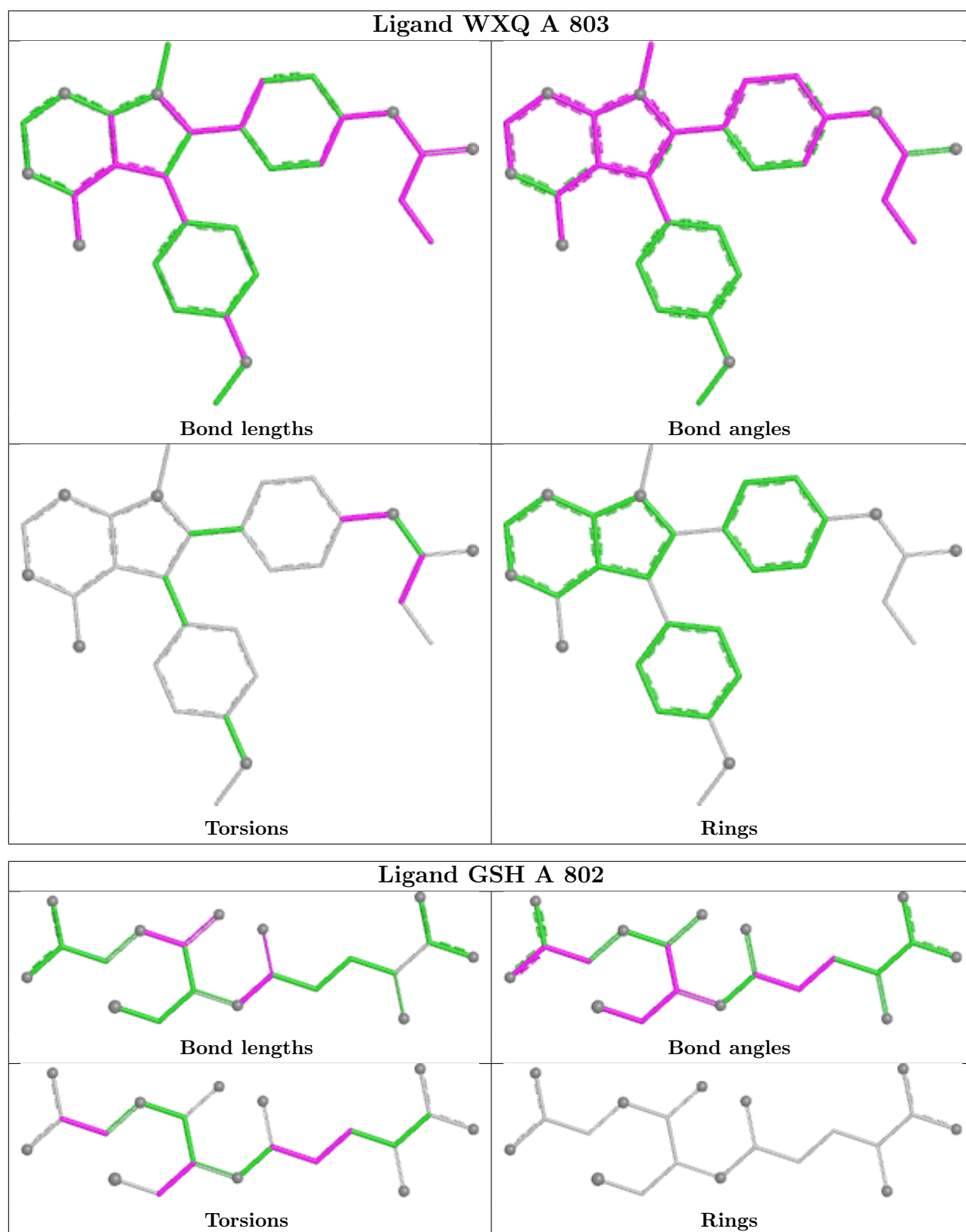
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	802	GOL	2	0
2	A	801	GOL	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 ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	284/316 (89%)	0.55	18 (6%) 26 24	23, 48, 74, 116	2 (0%)
1	B	288/316 (91%)	0.51	24 (8%) 17 15	33, 47, 85, 121	0
All	All	572/632 (90%)	0.53	42 (7%) 21 19	23, 47, 81, 121	2 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	492	PHE	7.7
1	A	491	CYS	5.5
1	A	581	PRO	5.4
1	B	490	GLY	5.3
1	B	492	PHE	5.2
1	A	490	GLY	4.9
1	B	491	CYS	4.5
1	B	595	GLU	4.2
1	A	765	THR	4.2
1	B	508	PRO	4.1
1	B	596	GLU	3.8
1	B	489	GLU	3.6
1	A	728	CYS	3.6
1	B	541	ILE	3.4
1	B	510	GLU	3.2
1	B	505	LYS	3.2
1	A	596	GLU	3.1
1	B	582	PRO	3.1
1	B	468	LEU	3.0
1	A	763	LEU	2.9
1	B	501	VAL	2.9
1	B	727	ASN	2.8
1	A	485	LYS	2.7
1	A	489	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	767	GLU	2.6
1	B	469	PRO	2.6
1	B	509	LYS	2.6
1	A	676	PHE	2.5
1	A	557	ASP	2.5
1	A	488	GLY	2.5
1	A	493	GLY	2.5
1	A	468	LEU	2.5
1	B	728	CYS	2.4
1	A	541	ILE	2.4
1	B	507	LYS	2.4
1	A	549	ASN	2.3
1	B	506	ASP	2.3
1	B	511	ALA	2.2
1	B	488	GLY	2.1
1	B	549	ASN	2.1
1	B	502	GLY	2.1
1	A	727	ASN	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

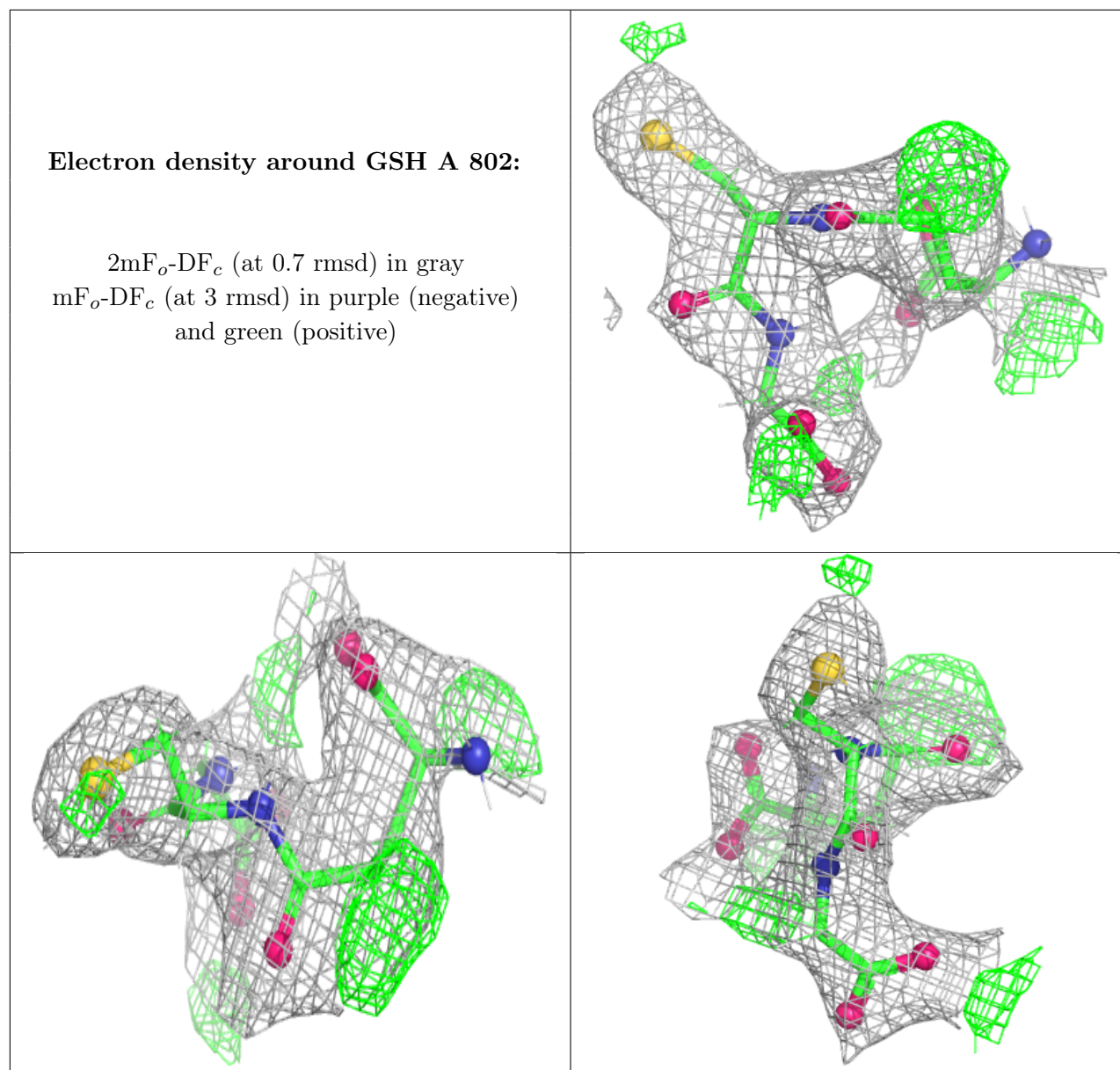
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	B	803	6/6	0.50	0.24	33,40,73,78	0
3	GSH	A	802	20/20	0.77	0.18	62,79,109,113	0
2	GOL	B	801	6/6	0.78	0.16	46,56,67,67	0
2	GOL	A	801	6/6	0.81	0.23	38,48,63,78	0
2	GOL	B	802	6/6	0.81	0.20	52,68,78,93	0

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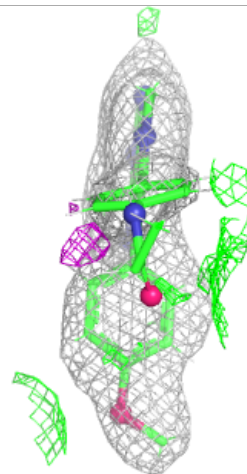
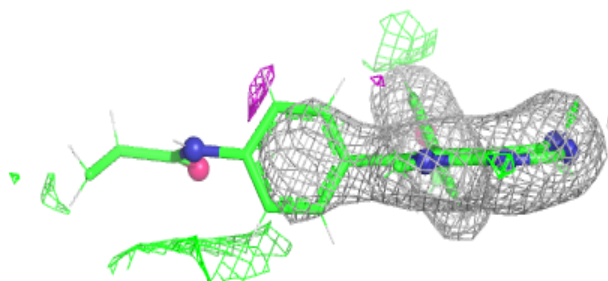
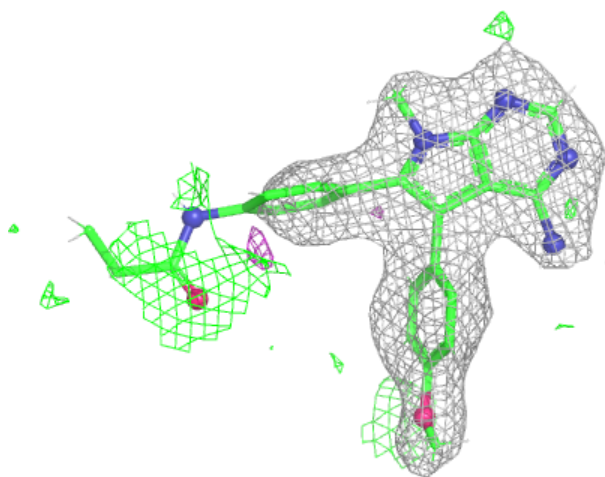
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	WXQ	A	803	30/30	0.88	0.20	41,58,117,130	0
4	WXQ	B	804	30/30	0.89	0.17	34,52,95,113	0

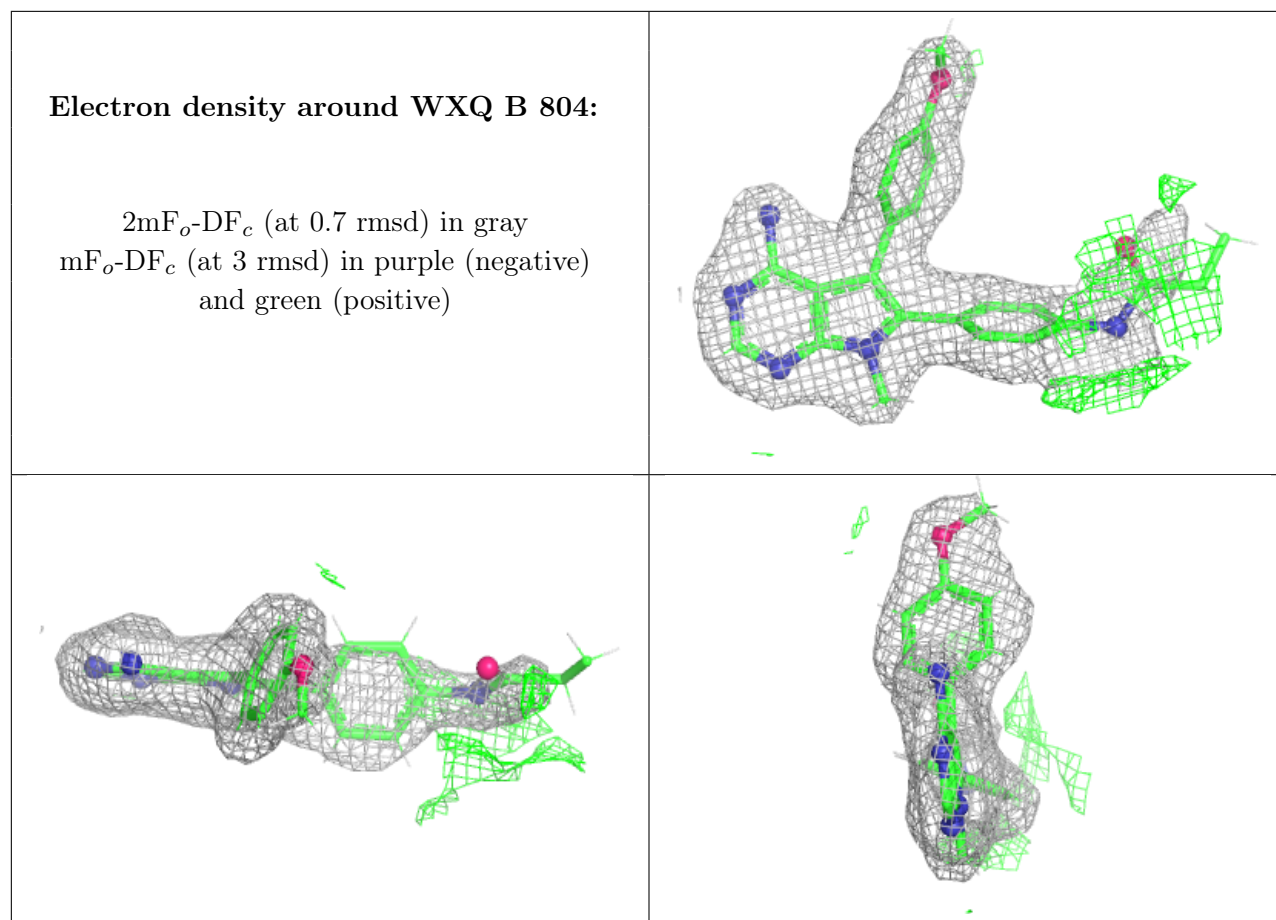
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around WXQ A 803:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.