



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:54 AM UTC

PDB ID : 8F7U / pdb_00008f7u
Title : Macrocyclic Plasmin Inhibitor
Authors : Guojie, W.
Deposited on : 2022-11-20
Resolution : 1.47 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

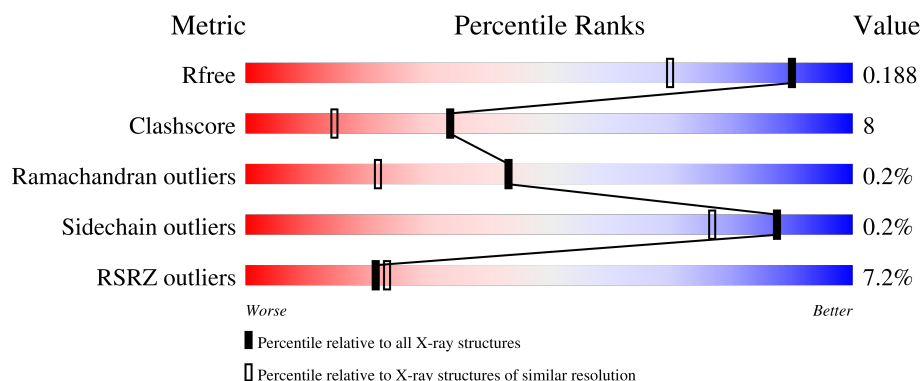
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.47 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	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

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	250	8% 85% 10% 5%
1	B	250	6% 86% 12% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4463 atoms, of which 96 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.

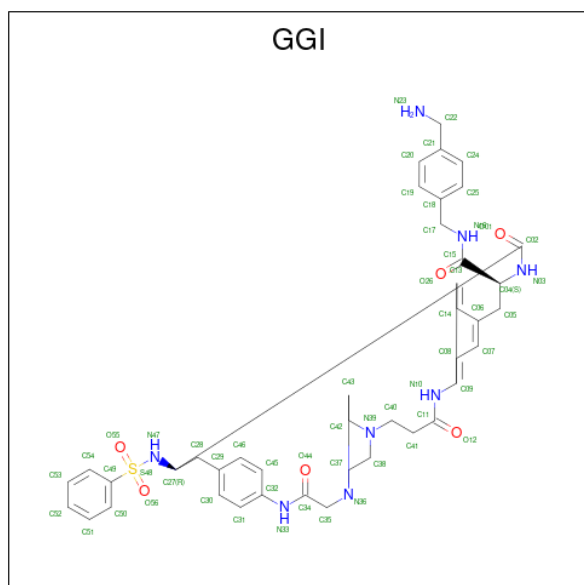
- Molecule 1 is a protein called Activation peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	2	1
			1824	1158	321	330	15			
1	B	250	Total	C	N	O	S	0	3	0
			1927	1226	338	347	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	741	ALA	SER	engineered mutation	UNP P00747
B	741	ALA	SER	engineered mutation	UNP P00747

- Molecule 2 is (5S,8R,18S,21R)-N-{{[4-(aminomethyl)phenyl]methyl}-21-[(benzenesulfonyl)amino]-3,11,20-trioxo-2,5,8,12,19-pentaazatetracyclo[21.2.2.2.2 5,8 .2 13,16]hentriaconta-1(25),13,15,23,26,28-hexaene-18-carboxamide (CCD ID: GGI) (formula: C₄₁H₄₈N₈O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 104	C 41	H 48	N 8	O 6	S 1	0	0
2	B	1	Total 104	C 41	H 48	N 8	O 6	S 1	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O S	0	0
			5 4 1			
3	A	1	Total	O S	0	0
			5 4 1			
3	B	1	Total	O S	0	0
			5 4 1			
3	B	1	Total	O S	0	0
			5 4 1			
3	B	1	Total	O S	0	0
			5 4 1			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

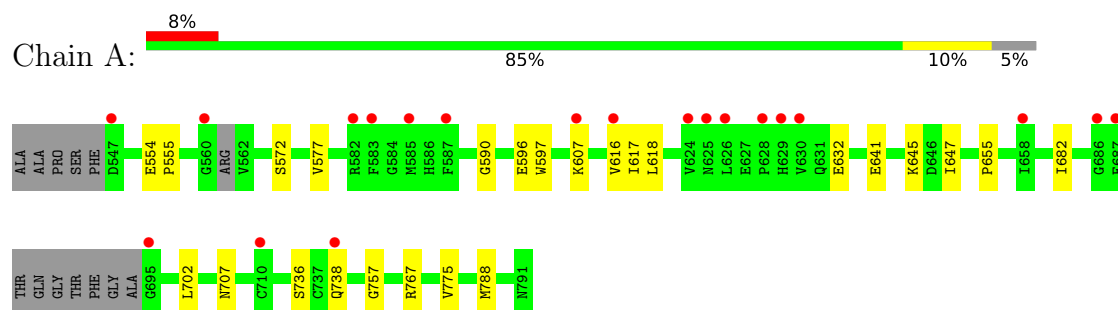
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	197	Total	O	0	0
			197	197		
5	B	268	Total	O	0	3
			271	271		

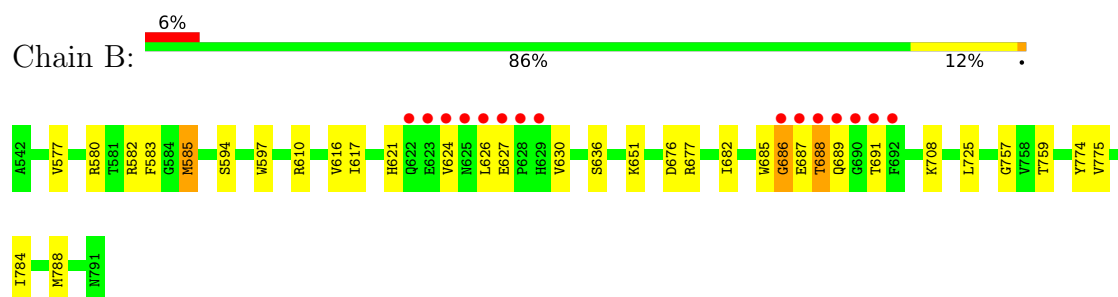
3 Residue-property plots [i](#)

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: Activation peptide



• Molecule 1: Activation peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.71Å 50.30Å 92.46Å 90.00° 93.11° 90.00°	Depositor
Resolution (Å)	48.64 – 1.47 48.64 – 1.47	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.64-1.47) 100.0 (48.64-1.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.82 (at 1.47Å)	Xtriage
Refinement program	PHENIX 1.19.2-4258	Depositor
R, R_{free}	0.173 , 0.189 0.172 , 0.188	Depositor DCC
R_{free} test set	3818 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4463	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% 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: GGI, GOL, SO4

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	0.69	5/1872 (0.3%)	0.78	0/2543
1	B	0.81	5/1983 (0.3%)	0.84	9/2693 (0.3%)
All	All	0.76	10/3855 (0.3%)	0.81	9/5236 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	688	THR	C-N	-22.46	0.95	1.34
1	B	585[A]	MET	C-O	8.45	1.34	1.24
1	B	585[B]	MET	C-O	8.45	1.34	1.24
1	A	645[A]	LYS	CA-C	8.26	1.63	1.52
1	A	645[B]	LYS	CA-C	8.26	1.63	1.52
1	A	707	ASN	C-N	-7.95	1.23	1.34
1	A	645[A]	LYS	C-O	7.28	1.33	1.23
1	A	645[B]	LYS	C-O	7.28	1.33	1.23
1	B	585[A]	MET	CA-C	5.87	1.60	1.52
1	B	585[B]	MET	CA-C	5.87	1.60	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	621	HIS	N-CA-C	-6.53	104.36	112.72
1	B	585[A]	MET	N-CA-C	6.46	119.14	109.25
1	B	585[B]	MET	N-CA-C	6.46	119.14	109.25
1	B	585[A]	MET	CA-C-O	6.41	127.92	120.49
1	B	585[B]	MET	CA-C-O	6.41	127.92	120.49
1	B	688	THR	O-C-N	-5.88	115.17	122.82
1	B	636[A]	SER	CA-C-O	5.44	125.56	119.41
1	B	636[B]	SER	CA-C-O	5.44	125.56	119.41
1	B	687	GLU	O-C-N	5.00	128.66	123.06

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	1824	0	1805	24	0
1	B	1927	0	1905	36	0
2	A	56	48	0	0	0
2	B	56	48	0	0	0
3	A	10	0	0	0	0
3	B	20	0	0	0	0
4	B	6	0	8	0	0
5	A	197	0	0	0	0
5	B	271	0	0	5	0
All	All	4367	96	3718	59	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 8.

All (59) 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:585[B]:MET:CE	1:B:689:GLN:HG3	1.91	1.01
1:A:577:VAL:HG12	1:A:618:LEU:HD22	1.42	0.98
1:B:577:VAL:HG13	1:B:616:VAL:HG13	1.47	0.96
1:B:585[B]:MET:HE1	1:B:689:GLN:HG3	1.54	0.88
1:B:597:TRP:CD1	1:B:788[B]:MET:HE3	2.15	0.82
1:B:585[B]:MET:HE1	1:B:689:GLN:CG	2.09	0.81
1:B:691:THR:HG22	5:B:1069:HOH:O	1.81	0.81
1:A:597:TRP:CD1	1:A:788[B]:MET:HE3	2.15	0.80
1:B:688:THR:HG21	5:B:1052[B]:HOH:O	1.80	0.80
1:A:577:VAL:CG1	1:A:618:LEU:HD22	2.12	0.78
1:A:617:ILE:CD1	1:A:632:GLU:HG2	2.15	0.76
1:B:577:VAL:CG1	1:B:616:VAL:HG13	2.20	0.71
1:B:688:THR:HG23	1:B:688:THR:O	1.91	0.70
1:A:682:ILE:HD12	1:A:736:SER:HB3	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:VAL:O	1:B:626:LEU:HD22	2.00	0.62
1:A:616:VAL:HG12	1:A:618:LEU:CD2	2.31	0.61
1:A:577:VAL:HG22	1:A:590:GLY:C	2.28	0.59
1:A:616:VAL:HG12	1:A:618:LEU:HD21	1.86	0.57
1:A:617:ILE:HD13	1:A:632:GLU:HG2	1.87	0.56
1:B:617:ILE:HG23	1:B:630:VAL:CG1	2.37	0.55
1:A:616:VAL:CG1	1:A:618:LEU:HD21	2.40	0.51
1:A:617:ILE:C	1:A:618:LEU:HD23	2.35	0.51
1:A:577:VAL:CG1	1:A:618:LEU:CD2	2.88	0.50
1:B:685:TRP:O	1:B:686:GLY:O	2.28	0.50
1:B:617:ILE:HG23	1:B:630:VAL:HG11	1.92	0.50
1:A:577:VAL:HG12	1:A:618:LEU:CD2	2.30	0.49
1:B:688:THR:O	1:B:688:THR:CG2	2.60	0.49
1:B:583:PHE:CZ	1:B:585[A]:MET:HE2	2.46	0.49
1:B:627:GLU:HB2	1:B:630:VAL:HG23	1.95	0.48
1:B:585[B]:MET:HE3	1:B:688:THR:O	2.13	0.48
1:A:617:ILE:HD12	1:A:632:GLU:HG2	1.93	0.47
1:B:580:ARG:HH12	1:B:626:LEU:HD11	1.78	0.47
1:A:767:ARG:HH22	1:B:582:ARG:HD3	1.79	0.47
1:B:624:VAL:O	1:B:626:LEU:CD2	2.61	0.47
1:B:594:SER:OG	1:B:788[B]:MET:HE3	2.14	0.47
1:B:626:LEU:HD22	1:B:626:LEU:N	2.30	0.46
1:B:725:LEU:C	1:B:725:LEU:HD12	2.40	0.46
1:B:594:SER:HB3	1:B:788[B]:MET:HE1	1.97	0.46
1:B:610:ARG:NH1	5:B:903:HOH:O	2.37	0.45
1:A:757:GLY:HA2	1:A:775:VAL:O	2.16	0.45
1:B:597:TRP:HD1	1:B:788[B]:MET:HE3	1.73	0.45
1:B:651:LYS:NZ	5:B:901:HOH:O	2.29	0.45
1:B:580:ARG:NH1	1:B:626:LEU:HD11	2.32	0.45
1:B:784:ILE:HG22	1:B:788[A]:MET:HE2	1.99	0.45
1:A:555:PRO:HA	1:A:572:SER:HB2	1.99	0.44
1:B:594:SER:OG	1:B:788[B]:MET:CE	2.66	0.44
1:A:616:VAL:HG12	1:A:618:LEU:HD23	1.99	0.43
1:B:682:ILE:C	1:B:682:ILE:HD12	2.43	0.43
1:B:594:SER:CB	1:B:788[B]:MET:HE1	2.49	0.43
1:B:708:LYS:HD2	5:B:923:HOH:O	2.18	0.43
1:A:607:LYS:HB2	1:A:607:LYS:HZ3	1.84	0.43
1:A:596:GLU:CG	1:A:655:PRO:HG3	2.49	0.42
1:A:682:ILE:HD13	1:A:702:LEU:CD1	2.49	0.42
1:A:641:GLU:HB2	1:A:647:ILE:HG23	2.01	0.42
1:B:757:GLY:HA2	1:B:775:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:676:ASP:C	1:B:677:ARG:HG2	2.45	0.42
1:A:555:PRO:CA	1:A:572:SER:HB2	2.50	0.41
1:A:738:GLN:HE21	1:A:738:GLN:HB3	1.66	0.41
1:B:759:THR:HA	1:B:774:TYR:CD2	2.56	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	233/250 (93%)	225 (97%)	8 (3%)	0	100	100
1	B	249/250 (100%)	237 (95%)	11 (4%)	1 (0%)	30	11
All	All	482/500 (96%)	462 (96%)	19 (4%)	1 (0%)	43	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	686	GLY

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	201/209 (96%)	200 (100%)	1 (0%)	81	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	211/209 (101%)	211 (100%)	0	100	100
All	All	412/418 (99%)	411 (100%)	1 (0%)	87	77

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	554	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	569	HIS
1	A	729	HIS
1	A	738	GLN
1	A	769	ASN
1	B	622	GLN
1	B	689	GLN
1	B	769	ASN

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](#)

9 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
3	SO4	B	803	-	4,4,4	0.39	0	6,6,6	0.10	0
3	SO4	B	804	-	4,4,4	0.40	0	6,6,6	0.13	0
3	SO4	B	806	-	4,4,4	0.35	0	6,6,6	0.08	0
4	GOL	B	805	-	5,5,5	0.88	0	5,5,5	1.06	1 (20%)
3	SO4	B	802	-	4,4,4	0.36	0	6,6,6	0.07	0
2	GGI	B	801	-	61,61,61	2.84	19 (31%)	84,84,84	1.80	19 (22%)
3	SO4	A	802	-	4,4,4	0.37	0	6,6,6	0.07	0
3	SO4	A	803	-	4,4,4	0.39	0	6,6,6	0.24	0
2	GGI	A	801	-	61,61,61	2.63	17 (27%)	84,84,84	1.56	18 (21%)

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	GGI	A	801	-	-	10/55/65/65	0/5/6/6
2	GGI	B	801	-	-	9/55/65/65	0/5/6/6
4	GOL	B	805	-	-	0/4/4/4	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	GGI	C40-N39	-9.12	1.26	1.47
2	A	801	GGI	C40-N39	-8.80	1.27	1.47
2	B	801	GGI	S48-N47	7.22	1.73	1.61
2	B	801	GGI	C35-N36	-6.49	1.33	1.47
2	B	801	GGI	C02-N03	6.33	1.47	1.34
2	B	801	GGI	C15-N16	6.13	1.48	1.33
2	B	801	GGI	C11-N10	6.13	1.48	1.35
2	A	801	GGI	C35-N36	-5.96	1.34	1.47
2	A	801	GGI	C15-N16	5.94	1.47	1.33
2	A	801	GGI	S48-N47	5.84	1.71	1.61
2	A	801	GGI	C02-N03	5.84	1.46	1.34
2	A	801	GGI	C11-N10	5.76	1.48	1.35
2	B	801	GGI	C34-N33	5.26	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	GGI	C49-S48	5.03	1.84	1.76
2	A	801	GGI	O56-S48	4.94	1.49	1.43
2	B	801	GGI	C43-N36	-4.22	1.35	1.46
2	A	801	GGI	C34-N33	4.04	1.44	1.35
2	A	801	GGI	C43-N36	-3.53	1.37	1.46
2	B	801	GGI	O44-C34	-3.49	1.16	1.23
2	A	801	GGI	C37-N36	-3.49	1.37	1.46
2	B	801	GGI	C37-N36	-3.43	1.37	1.46
2	B	801	GGI	O56-S48	3.32	1.47	1.43
2	B	801	GGI	C42-N39	-3.27	1.38	1.46
2	A	801	GGI	C42-N39	-3.03	1.38	1.46
2	A	801	GGI	C49-S48	2.99	1.81	1.76
2	B	801	GGI	C41-C11	2.93	1.57	1.51
2	A	801	GGI	C41-C11	2.90	1.57	1.51
2	B	801	GGI	O55-S48	2.85	1.46	1.43
2	A	801	GGI	O44-C34	-2.80	1.17	1.23
2	A	801	GGI	C35-C34	2.75	1.57	1.52
2	B	801	GGI	C05-C06	2.72	1.57	1.51
2	A	801	GGI	C28-C29	2.66	1.57	1.51
2	B	801	GGI	C28-C29	2.56	1.57	1.51
2	B	801	GGI	C35-C34	2.37	1.56	1.52
2	A	801	GGI	C05-C06	2.33	1.56	1.51
2	B	801	GGI	C19-C18	2.03	1.42	1.38

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	GGI	O56-S48-O55	-8.84	108.78	119.52
2	A	801	GGI	O56-S48-O55	-5.86	112.41	119.52
2	B	801	GGI	C18-C17-N16	-4.86	102.84	113.07
2	A	801	GGI	C18-C17-N16	-4.63	103.31	113.07
2	B	801	GGI	C35-N36-C37	3.46	116.53	111.14
2	B	801	GGI	C40-N39-C38	3.10	119.49	111.24
2	A	801	GGI	C40-N39-C38	3.00	119.24	111.24
2	B	801	GGI	C49-S48-N47	3.00	111.90	107.79
2	A	801	GGI	O44-C34-C35	2.98	126.22	121.02
2	A	801	GGI	O56-S48-C49	2.83	111.55	107.98
2	B	801	GGI	C06-C05-C04	-2.80	105.91	113.36
2	B	801	GGI	C46-C29-C30	2.78	122.37	118.23
2	A	801	GGI	C45-C32-C31	2.77	122.72	119.04
2	A	801	GGI	C02-C27-N47	-2.74	104.17	111.28
2	A	801	GGI	C15-C04-N03	-2.67	103.89	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	GGI	C46-C45-C32	-2.63	117.28	120.30
2	B	801	GGI	C15-C04-N03	-2.61	104.04	111.11
2	A	801	GGI	C31-C32-N33	-2.60	111.69	120.41
2	B	801	GGI	O55-S48-C49	2.57	111.22	107.98
2	B	801	GGI	C34-C35-N36	-2.56	107.46	113.41
2	B	801	GGI	C02-C27-N47	-2.53	104.72	111.28
2	A	801	GGI	C49-S48-N47	2.49	111.20	107.79
2	A	801	GGI	C46-C29-C30	2.43	121.85	118.23
2	B	801	GGI	C45-C46-C29	-2.42	117.81	121.00
2	B	801	GGI	O26-C15-C04	2.42	125.55	120.48
2	A	801	GGI	C31-C30-C29	-2.38	117.87	121.00
2	B	801	GGI	C45-C32-N33	-2.38	112.43	120.41
2	B	801	GGI	C43-N36-C37	2.25	113.69	108.84
2	A	801	GGI	C35-N36-C37	2.24	114.63	111.14
2	A	801	GGI	C06-C05-C04	-2.20	107.50	113.36
2	B	801	GGI	C30-C31-C32	-2.15	117.83	120.30
2	A	801	GGI	C42-C43-N36	2.15	114.98	110.65
2	B	801	GGI	O26-C15-N16	-2.08	118.57	122.98
2	B	801	GGI	C45-C32-C31	2.07	121.79	119.04
2	B	801	GGI	C28-C27-N47	2.07	113.15	110.64
2	A	801	GGI	C27-N47-S48	-2.07	116.76	121.30
4	B	805	GOL	C3-C2-C1	-2.05	104.28	111.80
2	A	801	GGI	C35-C34-N33	-2.02	110.48	114.23

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	GGI	N03-C02-C27-N47
2	B	801	GGI	N03-C02-C27-N47
2	A	801	GGI	C41-C40-N39-C38
2	B	801	GGI	C41-C40-N39-C38
2	A	801	GGI	C41-C40-N39-C42
2	B	801	GGI	C41-C40-N39-C42
2	A	801	GGI	C54-C49-S48-O55
2	B	801	GGI	O01-C02-C27-C28
2	A	801	GGI	C50-C49-S48-O55
2	B	801	GGI	N03-C02-C27-C28
2	A	801	GGI	C54-C49-S48-N47
2	A	801	GGI	O01-C02-C27-C28
2	A	801	GGI	C50-C49-S48-N47
2	A	801	GGI	N03-C02-C27-C28

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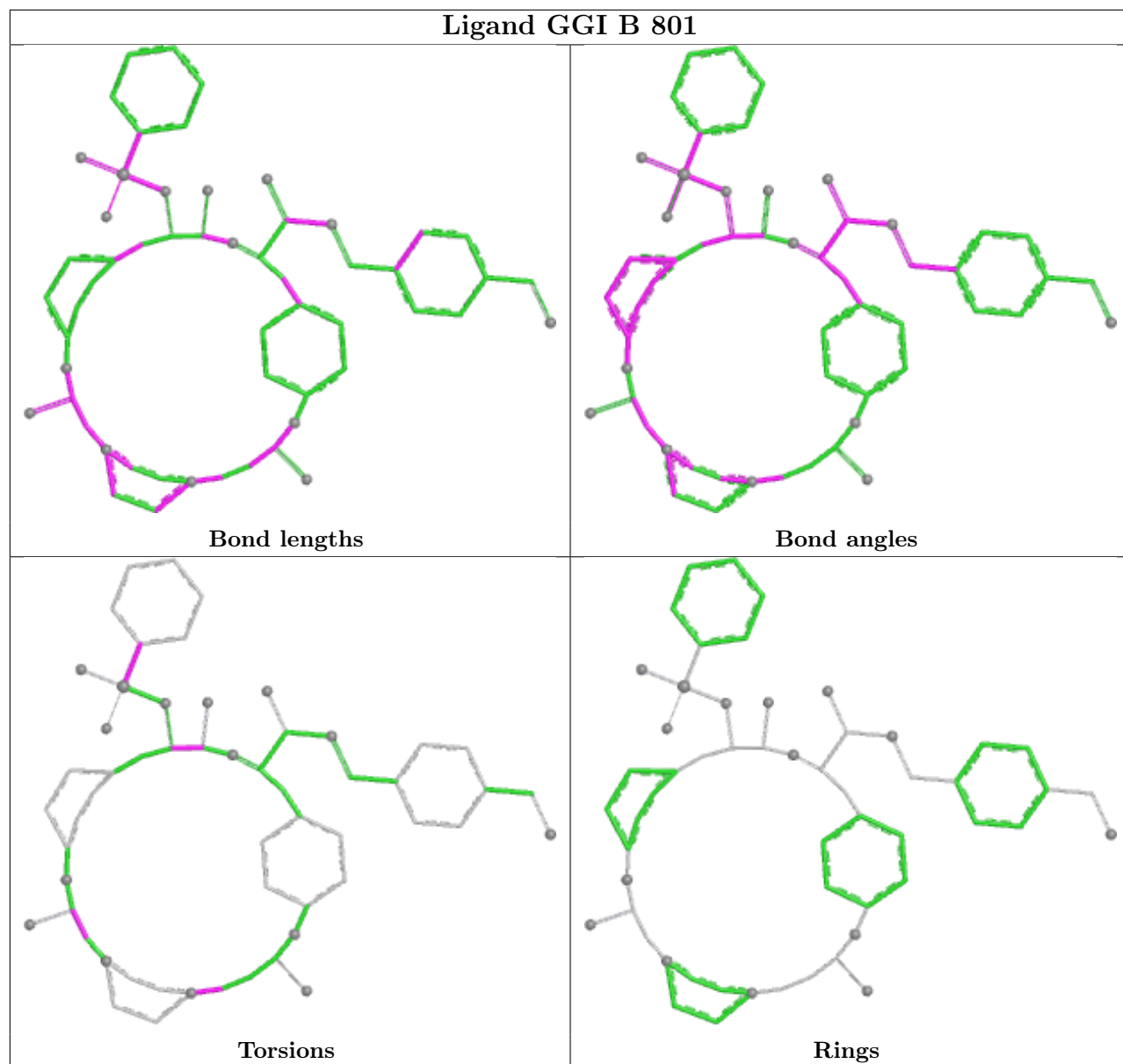
Mol	Chain	Res	Type	Atoms
2	A	801	GGI	O01-C02-C27-N47
2	B	801	GGI	O01-C02-C27-N47
2	B	801	GGI	C54-C49-S48-O56
2	B	801	GGI	C50-C49-S48-O56
2	B	801	GGI	O44-C34-C35-N36

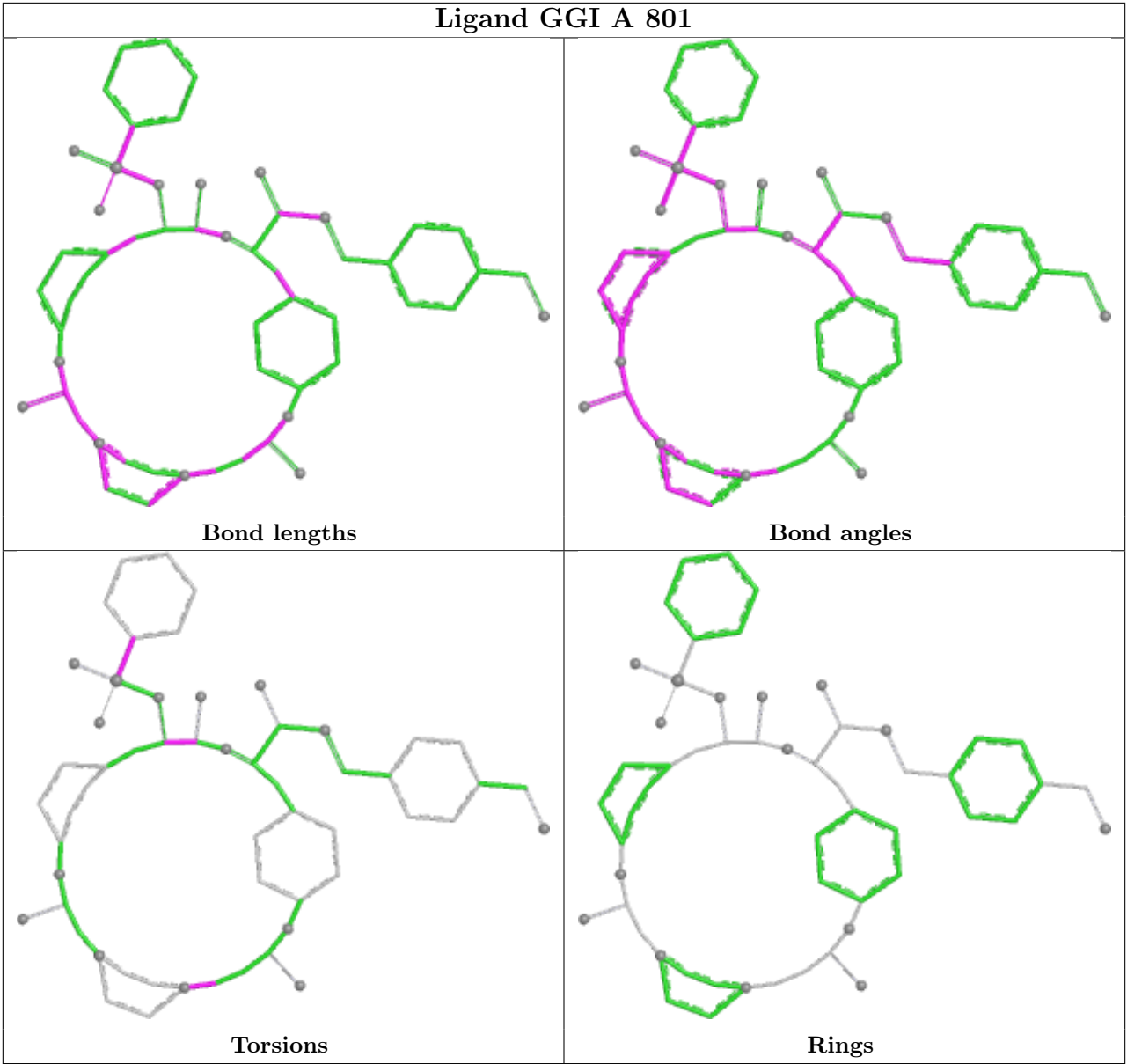
There are no ring outliers.

No monomer is involved in short contacts.

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 GGI B 801





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	561:ARG	C	562:VAL	N	19.36
1	B	688:THR	C	689:GLN	N	0.95

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	237/250 (94%)	0.52	20 (8%)	17 18	11, 22, 45, 61	2 (0%)
1	B	250/250 (100%)	0.13	15 (6%)	27 30	9, 15, 39, 66	3 (1%)
All	All	487/500 (97%)	0.32	35 (7%)	21 23	9, 17, 44, 66	5 (1%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	624	VAL	5.4
1	A	583	PHE	5.2
1	B	626	LEU	4.8
1	B	688	THR	4.6
1	B	629	HIS	4.3
1	B	625	ASN	4.3
1	A	560	GLY	4.2
1	A	686	GLY	4.2
1	B	691	THR	4.2
1	B	628	PRO	3.9
1	A	629	HIS	3.4
1	A	624	VAL	3.3
1	B	692	PHE	3.2
1	A	628	PRO	3.1
1	A	626	LEU	3.0
1	A	582	ARG	2.8
1	B	686	GLY	2.8
1	B	627	GLU	2.7
1	B	689	GLN	2.7
1	A	687	GLU	2.6
1	A	625	ASN	2.6
1	A	658	ILE	2.5
1	B	623	GLU	2.5
1	B	622	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	687	GLU	2.5
1	A	547	ASP	2.5
1	B	690	GLY	2.3
1	A	616	VAL	2.3
1	A	695	GLY	2.3
1	A	710	CYS	2.2
1	A	607	LYS	2.2
1	A	630	VAL	2.2
1	A	585	MET	2.1
1	A	587	PHE	2.0
1	A	738	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 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.

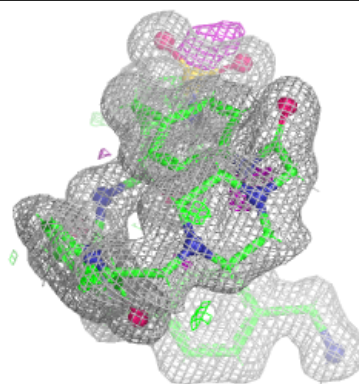
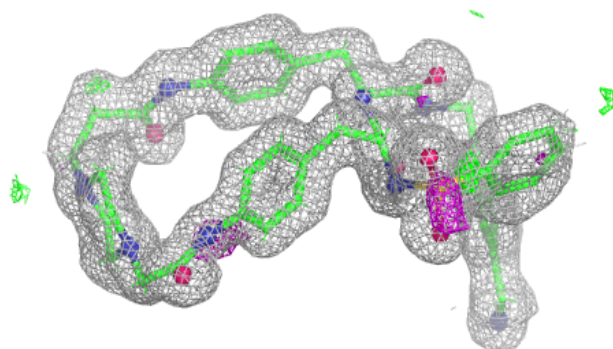
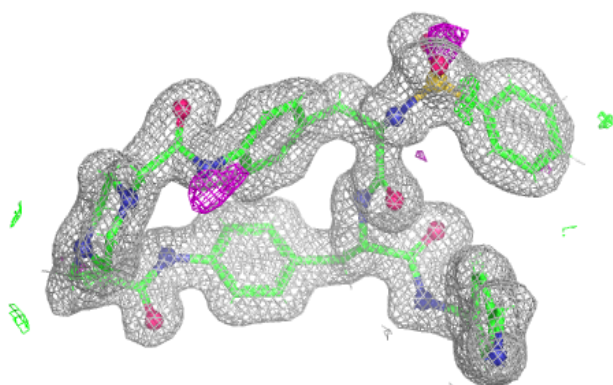
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	802	5/5	0.82	0.11	46,47,54,58	0
3	SO4	B	803	5/5	0.86	0.11	30,41,45,46	0
3	SO4	B	806	5/5	0.88	0.12	30,32,35,36	0
4	GOL	B	805	6/6	0.88	0.12	22,27,35,35	0
3	SO4	A	803	5/5	0.90	0.10	38,38,46,47	0
3	SO4	B	804	5/5	0.92	0.09	31,31,35,37	0
2	GGI	B	801	56/56	0.95	0.08	13,20,31,45	0
3	SO4	B	802	5/5	0.95	0.09	26,27,35,37	0
2	GGI	A	801	56/56	0.96	0.06	11,17,22,28	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.

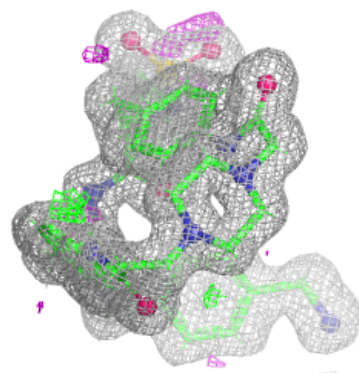
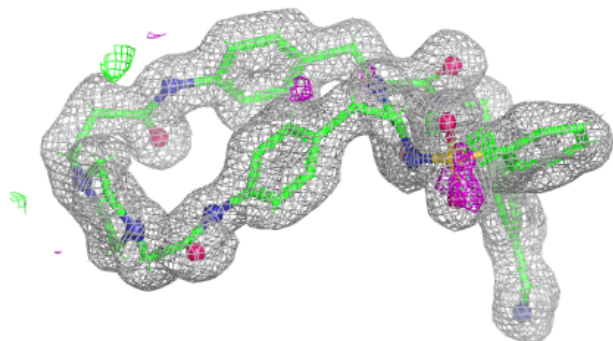
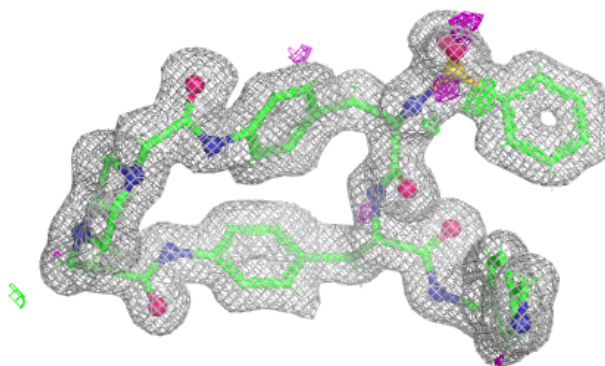
Electron density around GGI B 801:

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



Electron density around GGI A 801:

$2mF_o-DF_c$ (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.