Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2022 – 01:44 pm BST

PDB ID	:	7A2A
Title	:	Crystal Structure of EGFR-T790M/V948R in Complex with Spebrutinib and EAI001
Authors	:	Niggenaber, J.; Mueller, M.P.; Rauh, D.
Deposited on	:	2020-08-17
Resolution	:	1.90 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 (i) 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 (i)) were used in the production of this report:

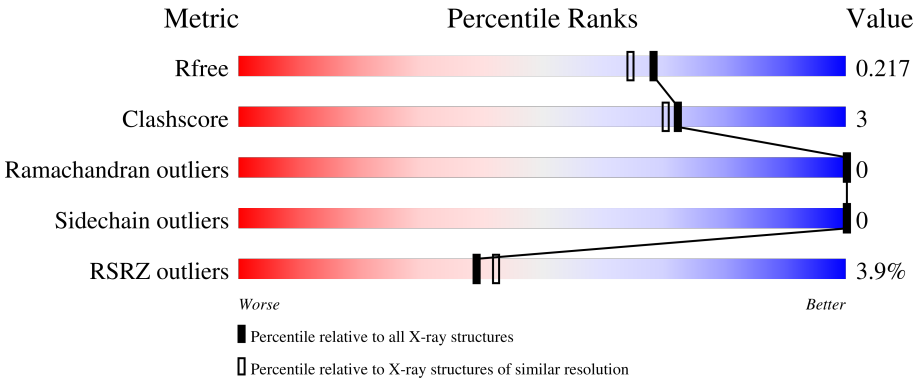
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	333	2% 75% 5% 20%
1	B	333	5% 74% 7% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	B	1104	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4385 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.

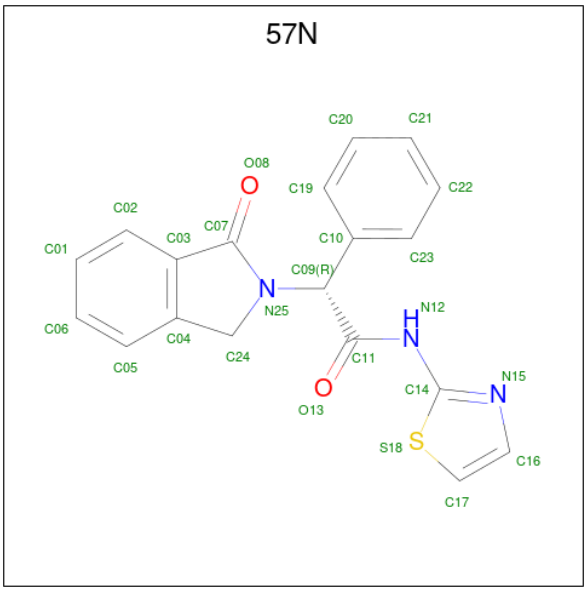
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	1	0
			2055	1330	345	364	16			
1	B	268	Total	C	N	O	S	0	3	0
			2081	1339	354	373	15			

There are 14 discrepancies between the modelled and reference sequences:

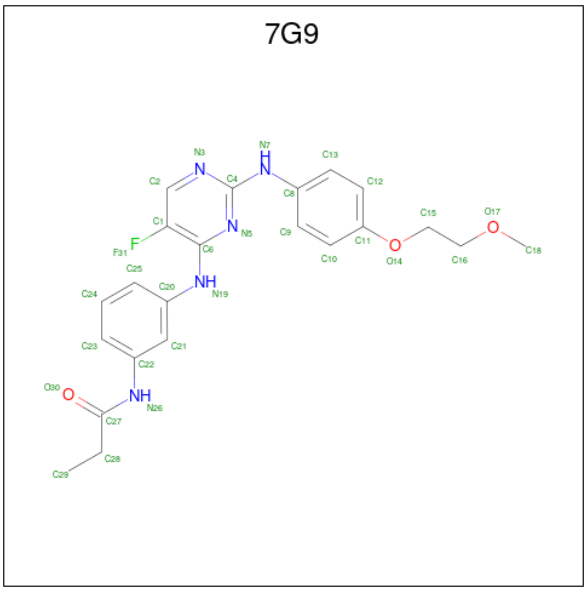
Chain	Residue	Modelled	Actual	Comment	Reference
A	690	GLY	-	expression tag	UNP P00533
A	691	SER	-	expression tag	UNP P00533
A	692	HIS	-	expression tag	UNP P00533
A	693	MET	-	expression tag	UNP P00533
A	694	ALA	-	expression tag	UNP P00533
A	790	MET	THR	engineered mutation	UNP P00533
A	948	ARG	VAL	engineered mutation	UNP P00533
B	690	GLY	-	expression tag	UNP P00533
B	691	SER	-	expression tag	UNP P00533
B	692	HIS	-	expression tag	UNP P00533
B	693	MET	-	expression tag	UNP P00533
B	694	ALA	-	expression tag	UNP P00533
B	790	MET	THR	engineered mutation	UNP P00533
B	948	ARG	VAL	engineered mutation	UNP P00533

- Molecule 2 is (2R)-2-(1-oxo-1,3-dihydro-2H-isoindol-2-yl)-2-phenyl-N-(1,3-thiazol-2-yl)acetamide (three-letter code: 57N) (formula: $C_{19}H_{15}N_3O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			25	19	3	2	1		
2	B	1	Total	C	N	O	S	0	0
			25	19	3	2	1		

- Molecule 3 is {N}-[3-[[5-fluoranyl-2-[[4-(2-methoxyethoxy)phenyl]amino]pyrimidin-4-yl]amino]phenyl]propanamide (three-letter code: 7G9) (formula: $C_{22}H_{24}FN_5O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			31	22	1	5	3		

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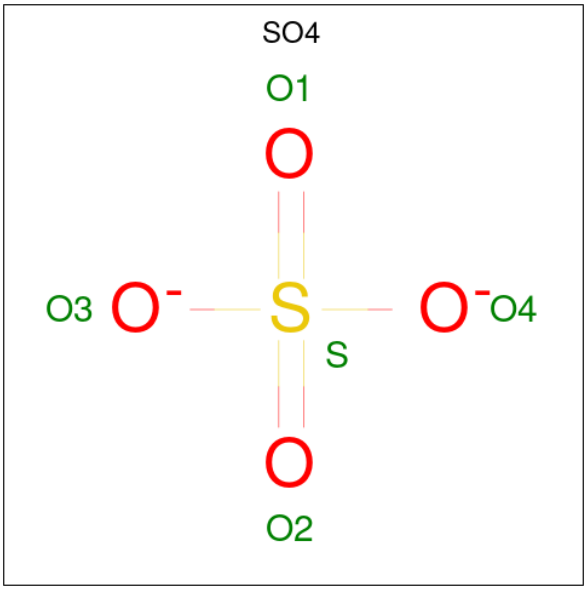
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C F N O 31 22 1 5 3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	64	Total O 64 64	0	0

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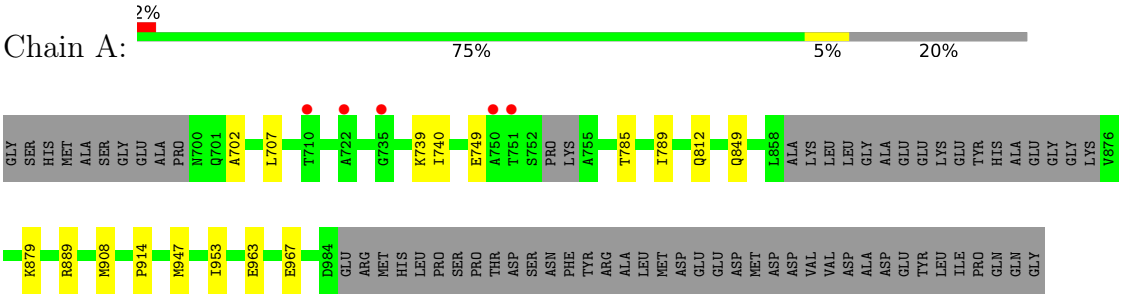
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	52	Total O 52 52	0	0

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.

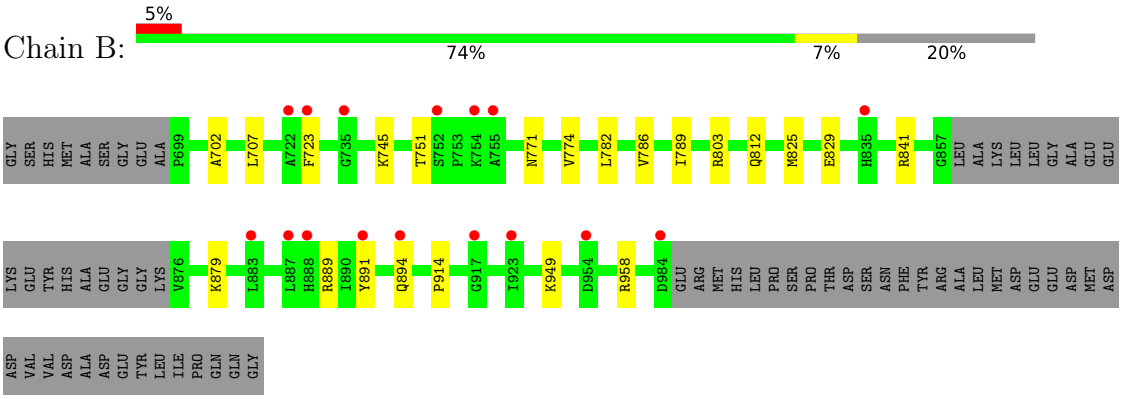
• Molecule 1: Epidermal growth factor receptor

Chain A:



• Molecule 1: Epidermal growth factor receptor

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.18Å 83.73Å 92.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.84 – 1.90 47.84 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.84-1.90) 100.0 (47.84-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.194 , 0.217 0.194 , 0.217	Depositor DCC
R_{free} test set	2331 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	44.6	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4385	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, 57N, 7G9, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.33	0/2103	0.51	0/2860
1	B	0.34	0/2138	0.52	0/2910
All	All	0.34	0/4241	0.51	0/5770

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	2055	0	2027	13	0
1	B	2081	0	2031	19	0
2	A	25	0	0	0	0
2	B	25	0	0	0	0
3	A	31	0	0	0	0
3	B	31	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	2	0
5	A	1	0	0	0	0
6	A	64	0	0	0	0
6	B	52	0	0	0	0
All	All	4385	0	4058	28	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 (28) 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:841[B]:ARG:NH2	4:B:1104:SO4:O3	2.20	0.74
1:B:803:ARG:NH2	4:B:1104:SO4:O4	2.24	0.65
1:A:749[A]:GLU:HG2	1:A:785:THR:HG22	1.80	0.62
1:B:723:PHE:CD1	1:B:745:LYS:HE3	2.38	0.59
1:A:702:ALA:HB3	1:B:812:GLN:HG2	1.85	0.58
1:B:825:MET:O	1:B:829:GLU:HG2	2.04	0.57
1:A:908:MET:HG3	1:A:947:MET:HE1	1.87	0.56
1:B:889:ARG:O	1:B:889:ARG:NH1	2.34	0.54
1:B:751:THR:HG22	1:B:786:VAL:HG23	1.89	0.53
1:B:707:LEU:HD12	1:B:789:ILE:HD13	1.89	0.53
1:B:723:PHE:HD1	1:B:745:LYS:HE3	1.75	0.52
1:B:894:GLN:NE2	1:B:958:ARG:HB2	2.27	0.48
1:A:707:LEU:HD12	1:A:789:ILE:HD13	1.95	0.47
1:A:739:LYS:C	1:A:740:ILE:HD13	2.36	0.46
1:A:702:ALA:CB	1:B:812:GLN:HG2	2.45	0.46
1:A:879:LYS:HD3	1:A:914:PRO:O	2.17	0.45
1:A:953:ILE:HD13	1:A:953:ILE:HA	1.86	0.44
1:B:879:LYS:HD3	1:B:914:PRO:O	2.19	0.43
1:A:740:ILE:HD13	1:A:740:ILE:N	2.34	0.42
1:A:963:GLU:O	1:A:967:GLU:HG3	2.20	0.42
1:B:751:THR:HG22	1:B:786:VAL:CG2	2.50	0.42
1:B:771:ASN:HB3	1:B:774[B]:VAL:HG22	2.00	0.41
1:B:782:LEU:HD23	1:B:782:LEU:HA	1.94	0.41
1:A:812:GLN:HG2	1:B:702:ALA:CB	2.50	0.41
1:A:889:ARG:HD3	1:A:889:ARG:HA	1.79	0.40
1:B:889:ARG:NH1	1:B:891:TYR:HD2	2.19	0.40
1:B:949:LYS:O	1:B:958:ARG:HG2	2.21	0.40
1:A:849:GLN:HG3	1:B:702:ALA:O	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	261/333 (78%)	257 (98%)	4 (2%)	0	100	100
1	B	267/333 (80%)	263 (98%)	4 (2%)	0	100	100
All	All	528/666 (79%)	520 (98%)	8 (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	215/291 (74%)	215 (100%)	0	100	100
1	B	217/291 (75%)	217 (100%)	0	100	100
All	All	432/582 (74%)	432 (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. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	B	1104	-	4,4,4	0.17	0	6,6,6	0.11	0
2	57N	B	1101	-	26,28,28	2.54	11 (42%)	30,39,39	3.61	9 (30%)
4	SO4	A	1103	-	4,4,4	0.19	0	6,6,6	0.18	0
4	SO4	A	1104	-	4,4,4	0.15	0	6,6,6	0.15	0
4	SO4	B	1103	-	4,4,4	0.15	0	6,6,6	0.19	0
3	7G9	A	1102	1	33,33,33	1.61	7 (21%)	43,43,43	1.82	5 (11%)
2	57N	A	1101	-	26,28,28	2.52	10 (38%)	30,39,39	3.94	7 (23%)
3	7G9	B	1102	1	33,33,33	1.60	5 (15%)	43,43,43	1.66	4 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	7G9	B	1102	1	-	3/19/19/19	0/3/3/3
2	57N	A	1101	-	-	0/14/28/28	0/4/4/4
3	7G9	A	1102	1	-	5/19/19/19	0/3/3/3
2	57N	B	1101	-	-	1/14/28/28	0/4/4/4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	57N	C07-N25	8.41	1.44	1.36
2	A	1101	57N	C07-N25	8.33	1.44	1.36
3	B	1102	7G9	C6-N19	4.56	1.44	1.36
3	A	1102	7G9	C4-N7	4.42	1.45	1.36
3	B	1102	7G9	C4-N7	4.37	1.45	1.36
2	B	1101	57N	C11-N12	4.30	1.45	1.35
2	A	1101	57N	C14-N12	4.25	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1102	7G9	C27-N26	4.12	1.44	1.35
3	A	1102	7G9	C27-N26	4.06	1.44	1.35
3	A	1102	7G9	C6-N19	4.00	1.43	1.36
2	A	1101	57N	C11-N12	3.97	1.44	1.35
2	B	1101	57N	C24-C04	3.73	1.55	1.50
2	A	1101	57N	C03-C07	3.72	1.54	1.48
2	B	1101	57N	C14-N12	3.62	1.43	1.36
2	B	1101	57N	C03-C07	3.36	1.54	1.48
2	A	1101	57N	C24-C04	3.29	1.54	1.50
2	A	1101	57N	C09-C11	-2.65	1.51	1.54
2	B	1101	57N	C09-C11	-2.52	1.51	1.54
2	B	1101	57N	C09-N25	-2.51	1.44	1.46
3	A	1102	7G9	C8-N7	2.49	1.46	1.40
2	A	1101	57N	O13-C11	-2.45	1.18	1.23
2	B	1101	57N	C24-N25	-2.45	1.45	1.46
3	B	1102	7G9	C20-N19	2.43	1.46	1.40
2	A	1101	57N	C24-N25	-2.34	1.45	1.46
2	B	1101	57N	C17-S18	-2.34	1.59	1.71
3	B	1102	7G9	C8-N7	2.24	1.45	1.40
3	A	1102	7G9	O30-C27	-2.19	1.18	1.23
2	A	1101	57N	C17-S18	-2.14	1.60	1.71
2	A	1101	57N	C16-N15	2.13	1.47	1.37
2	B	1101	57N	O08-C07	-2.05	1.18	1.22
3	A	1102	7G9	C20-N19	2.04	1.45	1.40
2	B	1101	57N	O13-C11	-2.04	1.19	1.23
3	A	1102	7G9	C6-C1	-2.03	1.37	1.40

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1101	57N	C04-C24-N25	16.34	107.62	102.18
2	B	1101	57N	C04-C24-N25	14.34	106.96	102.18
2	A	1101	57N	C24-N25-C07	-11.10	108.55	113.12
2	B	1101	57N	C24-N25-C07	-10.06	108.98	113.12
3	A	1102	7G9	N3-C4-N5	-6.65	120.25	126.55
3	B	1102	7G9	C1-C2-N3	-5.88	117.59	122.77
3	A	1102	7G9	C1-C2-N3	-5.87	117.60	122.77
3	B	1102	7G9	N3-C4-N5	-5.26	121.56	126.55
3	A	1102	7G9	C20-N19-C6	-4.69	117.61	129.39
3	B	1102	7G9	C20-N19-C6	-4.63	117.75	129.39
2	B	1101	57N	C24-N25-C09	4.41	127.98	123.86
2	A	1101	57N	C24-N25-C09	4.32	127.90	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1102	7G9	C2-N3-C4	4.28	122.34	115.88
2	B	1101	57N	C11-C09-N25	-3.76	104.78	110.16
3	B	1102	7G9	C2-N3-C4	3.72	121.50	115.88
2	A	1101	57N	C11-C09-N25	-3.52	105.12	110.16
2	A	1101	57N	C14-N12-C11	-3.49	121.25	129.02
2	B	1101	57N	C14-N12-C11	-3.42	121.41	129.02
2	A	1101	57N	C24-C04-C03	-2.76	108.03	109.75
2	B	1101	57N	C03-C07-N25	2.51	107.93	106.44
2	B	1101	57N	C10-C09-C11	-2.38	107.39	112.06
2	B	1101	57N	C24-C04-C03	-2.25	108.34	109.75
2	A	1101	57N	C03-C07-N25	2.25	107.77	106.44
2	B	1101	57N	C04-C03-C07	-2.15	107.79	108.94
3	A	1102	7G9	C4-N5-C6	2.07	121.12	116.39

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102	7G9	C12-C11-O14-C15
3	A	1102	7G9	C10-C11-O14-C15
3	A	1102	7G9	C21-C20-N19-C6
3	A	1102	7G9	C25-C20-N19-C6
3	B	1102	7G9	C25-C20-N19-C6
3	B	1102	7G9	C15-C16-O17-C18
3	B	1102	7G9	C21-C20-N19-C6
3	A	1102	7G9	C15-C16-O17-C18
2	B	1101	57N	C10-C09-N25-C24

There are no ring outliers.

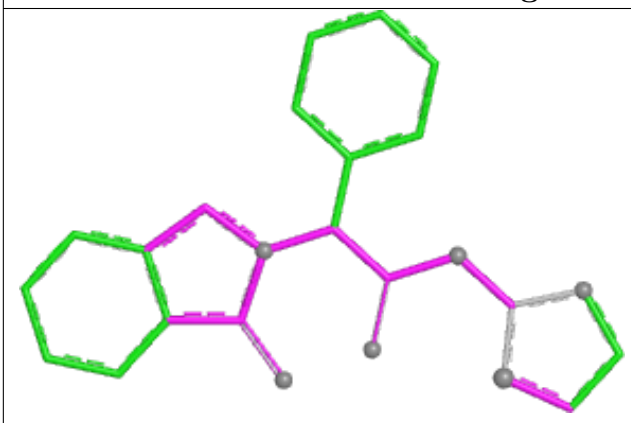
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1104	SO4	2	0

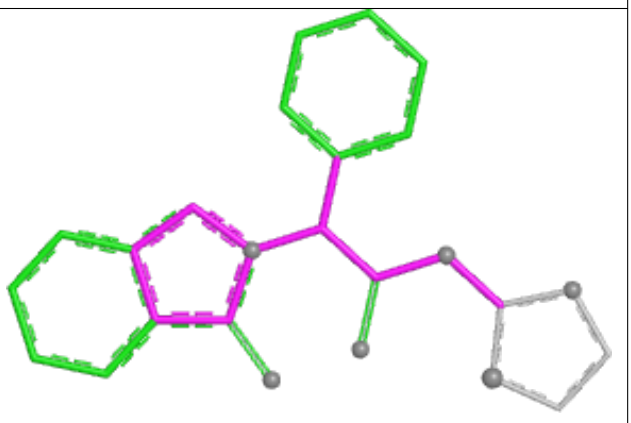
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

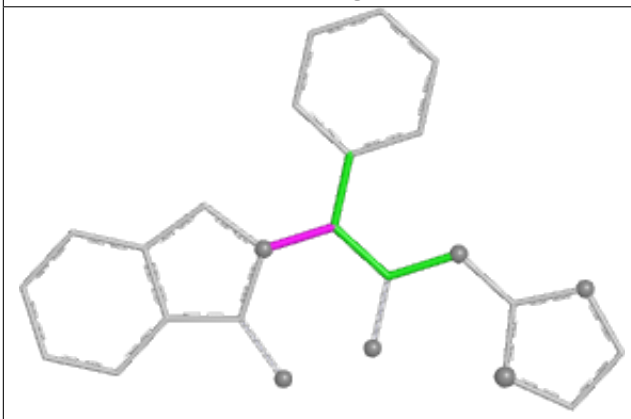
Ligand 57N B 1101



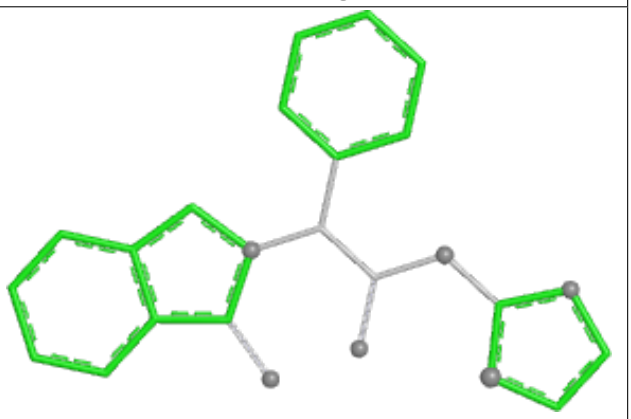
Bond lengths



Bond angles

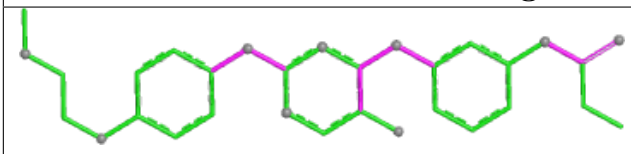


Torsions

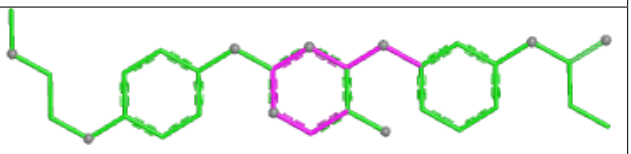


Rings

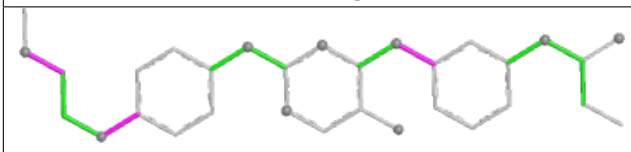
Ligand 7G9 A 1102



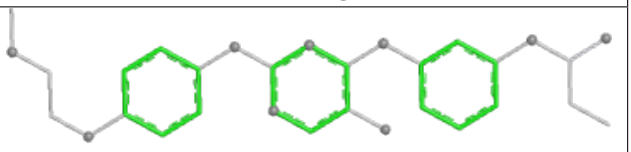
Bond lengths



Bond angles

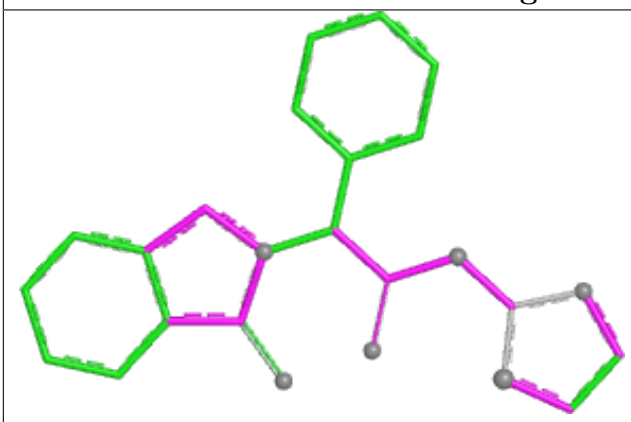


Torsions

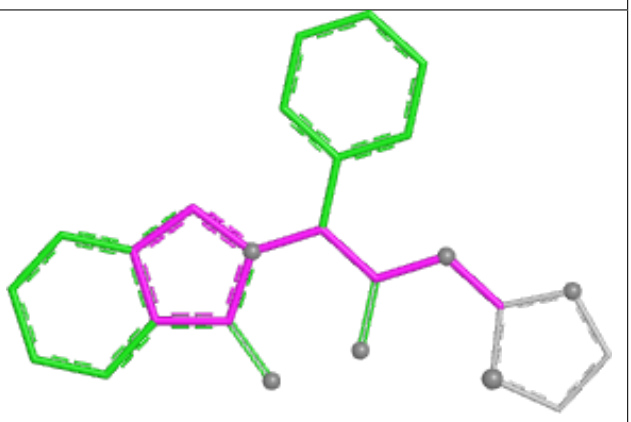


Rings

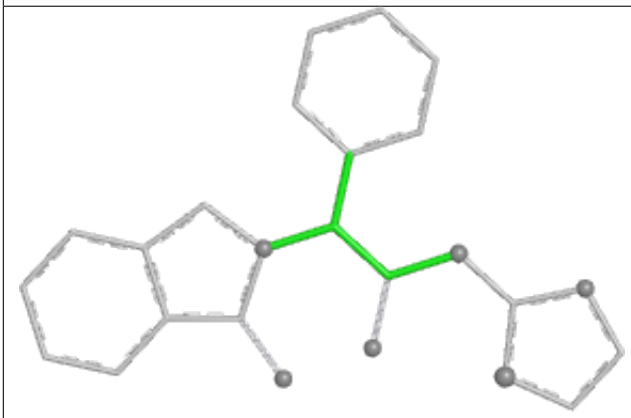
Ligand 57N A 1101



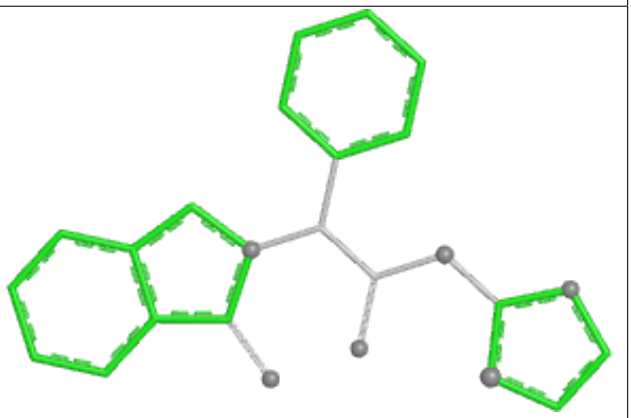
Bond lengths



Bond angles

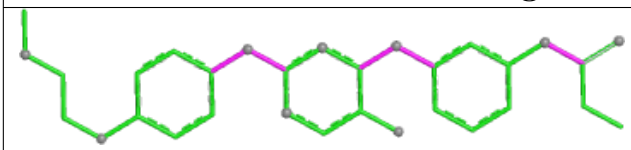


Torsions

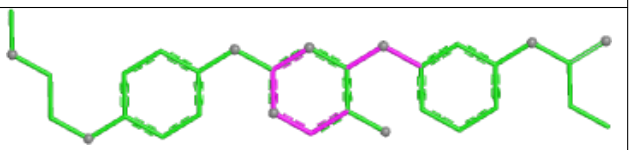


Rings

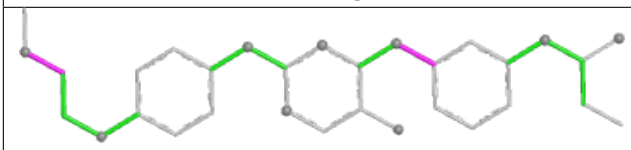
Ligand 7G9 B 1102



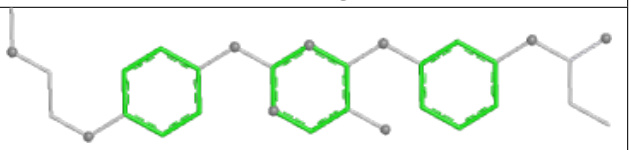
Bond lengths



Bond angles



Torsions



Rings

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^{th} 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	266/333 (79%)	0.26	5 (1%)	66	69	33, 51, 81, 104	0
1	B	268/333 (80%)	0.50	16 (5%)	21	24	34, 62, 98, 120	0
All	All	534/666 (80%)	0.38	21 (3%)	39	42	33, 55, 93, 120	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	755	ALA	6.0
1	A	735	GLY	4.6
1	A	751	THR	4.1
1	B	735	GLY	3.9
1	B	752	SER	3.9
1	A	710	THR	3.7
1	A	722	ALA	3.1
1	B	835	HIS	3.0
1	B	984	ASP	2.9
1	B	723	PHE	2.7
1	B	754	LYS	2.6
1	B	917	GLY	2.6
1	A	750	ALA	2.5
1	B	894	GLN	2.4
1	B	923	ILE	2.2
1	B	883	LEU	2.2
1	B	891	TYR	2.1
1	B	888	HIS	2.1
1	B	954	ASP	2.1
1	B	722	ALA	2.0
1	B	887	LEU	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)

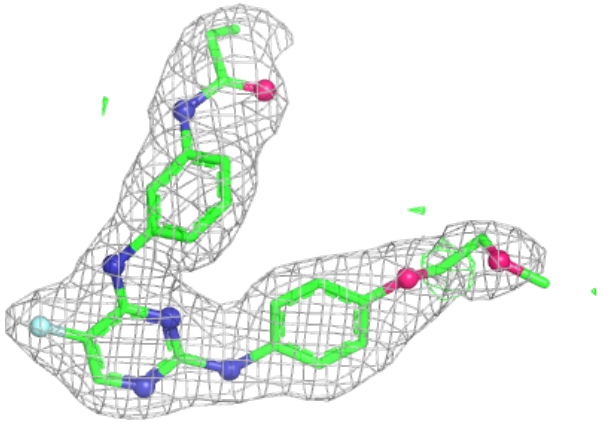
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

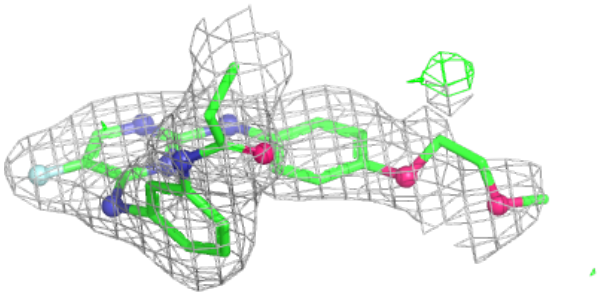
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	A	1105	1/1	0.75	0.18	85,85,85,85	0
4	SO4	B	1104	5/5	0.90	0.26	100,103,104,105	0
3	7G9	A	1102	31/31	0.94	0.12	37,50,89,93	0
2	57N	B	1101	25/25	0.95	0.14	36,42,52,54	0
2	57N	A	1101	25/25	0.95	0.14	41,44,60,61	0
3	7G9	B	1102	31/31	0.96	0.12	36,49,77,83	0
4	SO4	A	1103	5/5	0.98	0.11	47,49,52,56	0
4	SO4	B	1103	5/5	0.98	0.14	54,58,60,67	0
4	SO4	A	1104	5/5	0.99	0.14	49,50,53,57	0

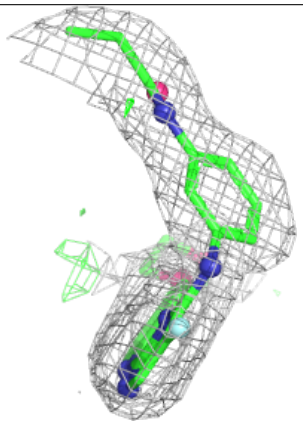
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7G9 A 1102:

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

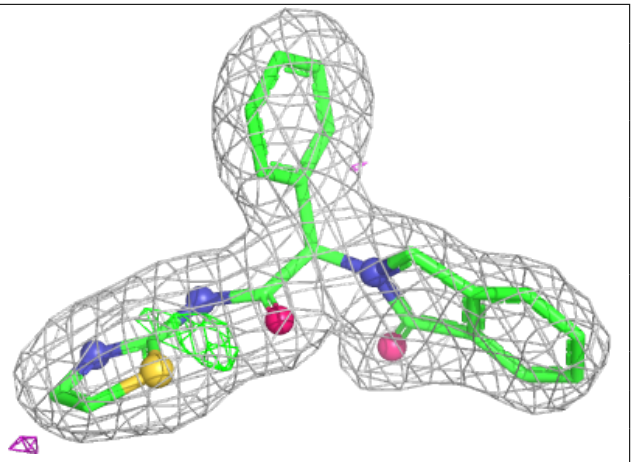


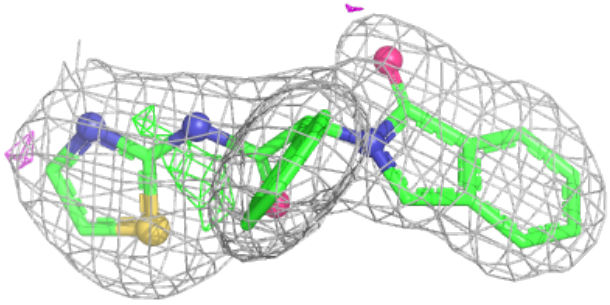


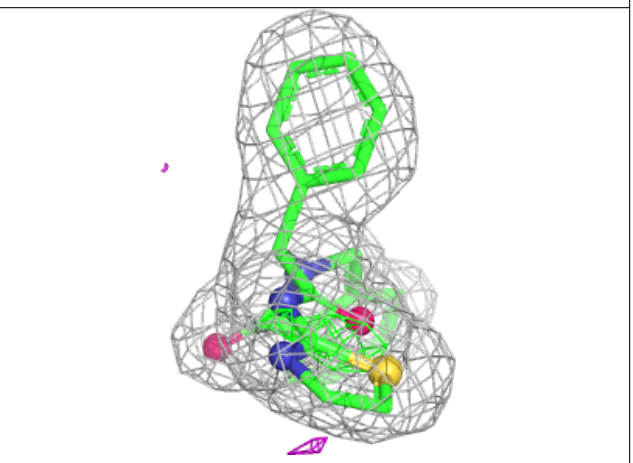


Electron density around 57N B 1101:

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

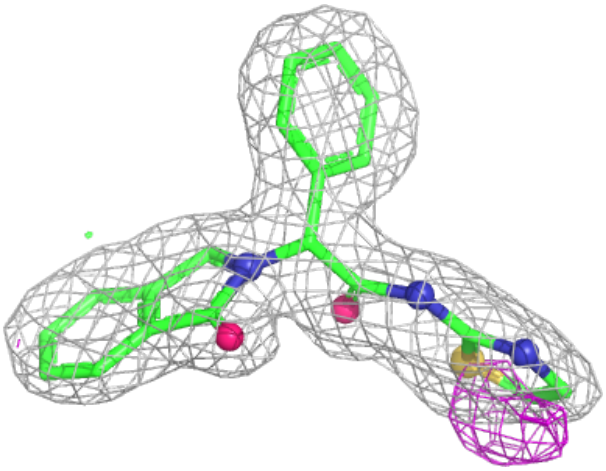


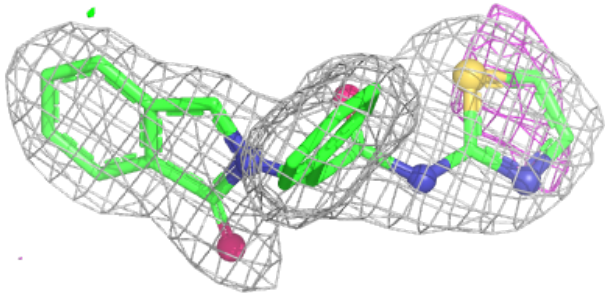


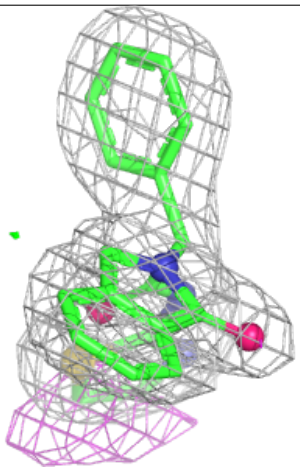


Electron density around 57N A 1101:

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

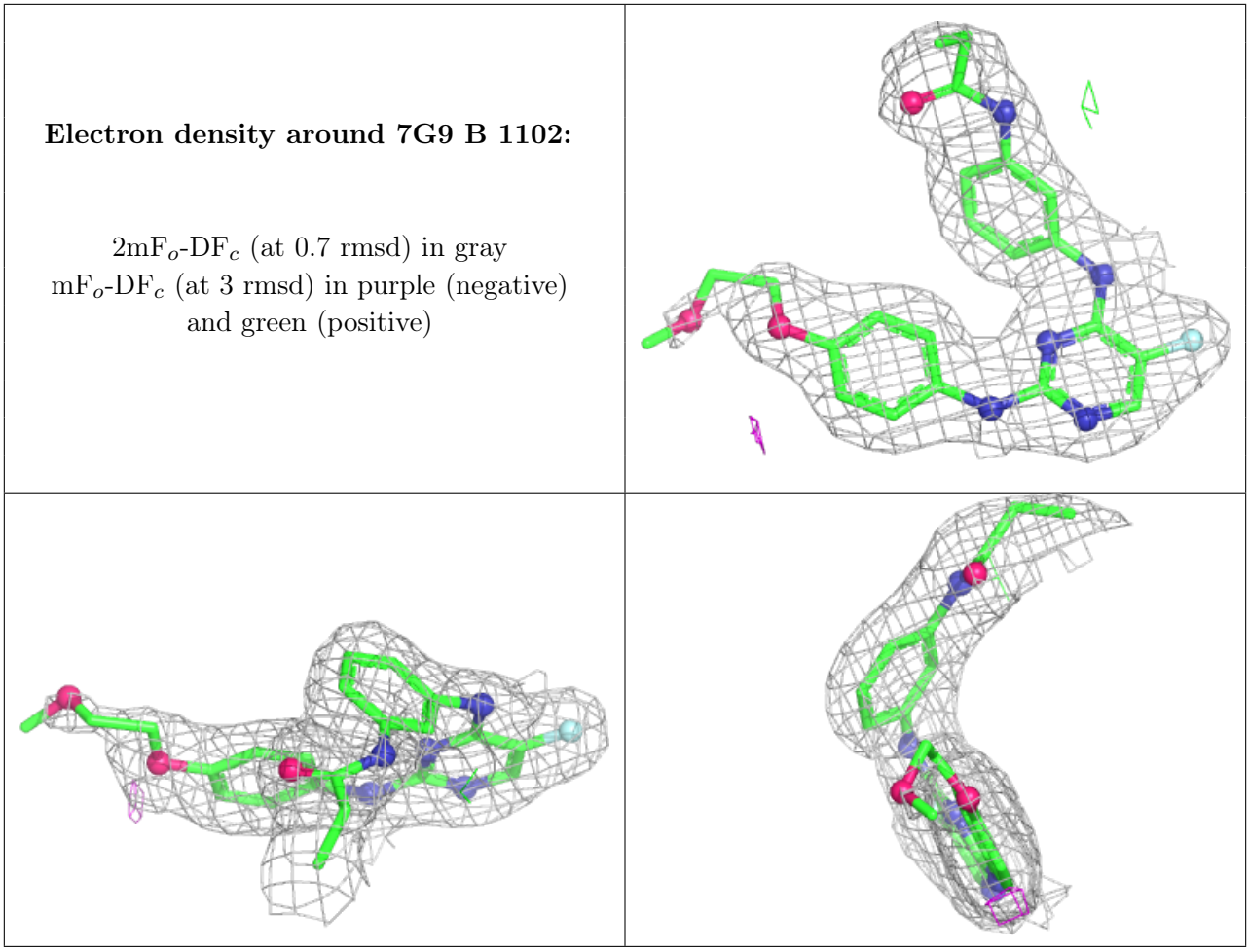






Electron density around 7G9 B 1102:

$2mF_o$-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.