



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 02:53 PM UTC

PDB ID : 8BP2 / pdb_00008bp2
Title : 2.8A STRUCTURE OF ZOLIFLODACIN WITH S.AUREUS DNA GYRASE
AND DNA
Authors : Bax, B.D.; Morgan, H.; Warren, A.J.
Deposited on : 2022-11-15
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

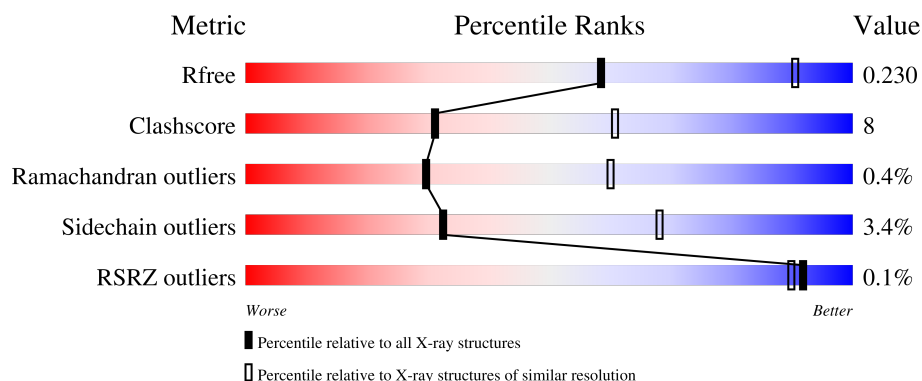
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	BBB	189	76% 23% .
1	DDD	189	73% 25% ..
2	AAA	490	82% 16% ..
2	CCC	490	81% 17% ..
3	EEE	20	30% 10% 60%

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Mol	Chain	Length	Quality of chain
3	EbE	20	30%25%5%40%
3	FFF	20	5%20%20%60%
3	FbF	20	15%20%25%40%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11777 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 DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BBB	189	Total	C	N	O	S	0	0	0
			1470	922	256	283	9			
1	DDD	189	Total	C	N	O	S	0	0	0
			1468	925	255	279	9			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	?	-	LEU	deletion	UNP P66937
BBB	?	-	TYR	deletion	UNP P66937
BBB	?	-	LYS	deletion	UNP P66937
BBB	?	-	LEU	deletion	UNP P66937
BBB	?	-	THR	deletion	UNP P66937
BBB	?	-	GLN	deletion	UNP P66937
BBB	?	-	GLY	deletion	UNP P66937
BBB	?	-	LYS	deletion	UNP P66937
BBB	?	-	GLN	deletion	UNP P66937
BBB	?	-	LYS	deletion	UNP P66937
BBB	?	-	TYR	deletion	UNP P66937
BBB	?	-	TYR	deletion	UNP P66937
BBB	?	-	VAL	deletion	UNP P66937
BBB	?	-	TYR	deletion	UNP P66937
BBB	?	-	ASN	deletion	UNP P66937
BBB	?	-	ASP	deletion	UNP P66937
BBB	?	-	ARG	deletion	UNP P66937
BBB	?	-	GLU	deletion	UNP P66937
BBB	?	-	LEU	deletion	UNP P66937
BBB	?	-	ASP	deletion	UNP P66937
BBB	?	-	LYS	deletion	UNP P66937
BBB	?	-	LEU	deletion	UNP P66937
BBB	?	-	LYS	deletion	UNP P66937
BBB	?	-	SER	deletion	UNP P66937
BBB	?	-	GLU	deletion	UNP P66937

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	?	-	LEU	deletion	UNP P66937
BBB	?	-	ASN	deletion	UNP P66937
BBB	?	-	PRO	deletion	UNP P66937
BBB	?	-	THR	deletion	UNP P66937
BBB	?	-	PRO	deletion	UNP P66937
BBB	?	-	LYS	deletion	UNP P66937
BBB	?	-	TRP	deletion	UNP P66937
BBB	?	-	SER	deletion	UNP P66937
BBB	?	-	ILE	deletion	UNP P66937
BBB	?	-	ALA	deletion	UNP P66937
BBB	?	-	ARG	deletion	UNP P66937
BBB	544	THR	-	linker	UNP P66937
BBB	545	GLY	-	linker	UNP P66937
DDD	?	-	LEU	deletion	UNP P66937
DDD	?	-	TYR	deletion	UNP P66937
DDD	?	-	LYS	deletion	UNP P66937
DDD	?	-	LEU	deletion	UNP P66937
DDD	?	-	THR	deletion	UNP P66937
DDD	?	-	GLN	deletion	UNP P66937
DDD	?	-	GLY	deletion	UNP P66937
DDD	?	-	LYS	deletion	UNP P66937
DDD	?	-	GLN	deletion	UNP P66937
DDD	?	-	LYS	deletion	UNP P66937
DDD	?	-	TYR	deletion	UNP P66937
DDD	?	-	TYR	deletion	UNP P66937
DDD	?	-	VAL	deletion	UNP P66937
DDD	?	-	TYR	deletion	UNP P66937
DDD	?	-	ASN	deletion	UNP P66937
DDD	?	-	ASP	deletion	UNP P66937
DDD	?	-	ARG	deletion	UNP P66937
DDD	?	-	GLU	deletion	UNP P66937
DDD	?	-	LEU	deletion	UNP P66937
DDD	?	-	ASP	deletion	UNP P66937
DDD	?	-	LYS	deletion	UNP P66937
DDD	?	-	LEU	deletion	UNP P66937
DDD	?	-	LYS	deletion	UNP P66937
DDD	?	-	SER	deletion	UNP P66937
DDD	?	-	GLU	deletion	UNP P66937
DDD	?	-	LEU	deletion	UNP P66937
DDD	?	-	ASN	deletion	UNP P66937
DDD	?	-	PRO	deletion	UNP P66937
DDD	?	-	THR	deletion	UNP P66937

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	?	-	PRO	deletion	UNP P66937
DDD	?	-	LYS	deletion	UNP P66937
DDD	?	-	TRP	deletion	UNP P66937
DDD	?	-	SER	deletion	UNP P66937
DDD	?	-	ILE	deletion	UNP P66937
DDD	?	-	ALA	deletion	UNP P66937
DDD	?	-	ARG	deletion	UNP P66937
DDD	544	THR	-	linker	UNP P66937
DDD	545	GLY	-	linker	UNP P66937

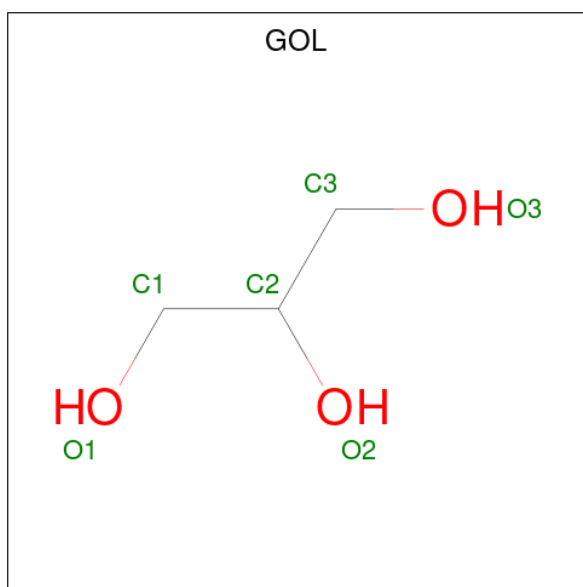
- Molecule 2 is a protein called DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AAA	482	Total	C	N	O	S	0	0	0
			3805	2367	693	729	16			
2	CCC	481	Total	C	N	O	S	0	3	0
			3831	2382	698	735	16			

- Molecule 3 is a DNA chain called DNA (20-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	EEE	8	Total	C	N	O	P	0	0	0
			163	78	33	45	7			
3	EbE	12	Total	C	N	O	P	0	1	0
			265	126	45	81	13			
3	FFF	8	Total	C	N	O	P	0	0	0
			163	78	33	45	7			
3	FbF	12	Total	C	N	O	P	0	2	0
			255	116	43	82	14			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	BBB	1	Total	C	O	0	0
			6	3	3		
4	AAA	1	Total	C	O	0	0
			6	3	3		
4	AAA	1	Total	C	O	0	0
			6	3	3		
4	AAA	1	Total	C	O	0	0
			6	3	3		
4	AAA	1	Total	C	O	0	0
			6	3	3		
4	CCC	1	Total	C	O	0	0
			6	3	3		
4	FbF	1	Total	C	O	0	0
			6	3	3		

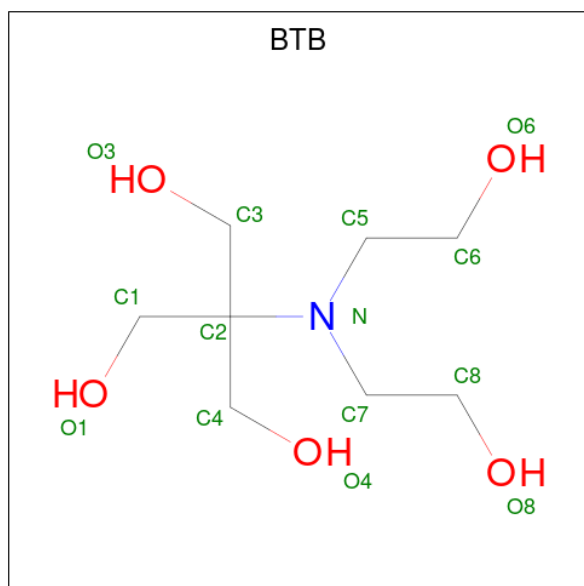
- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	BBB	1	Total	Mn	0	0
			1	1		
5	DDD	1	Total	Mn	0	0
			1	1		
5	CCC	1	Total	Mn	0	0
			1	1		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

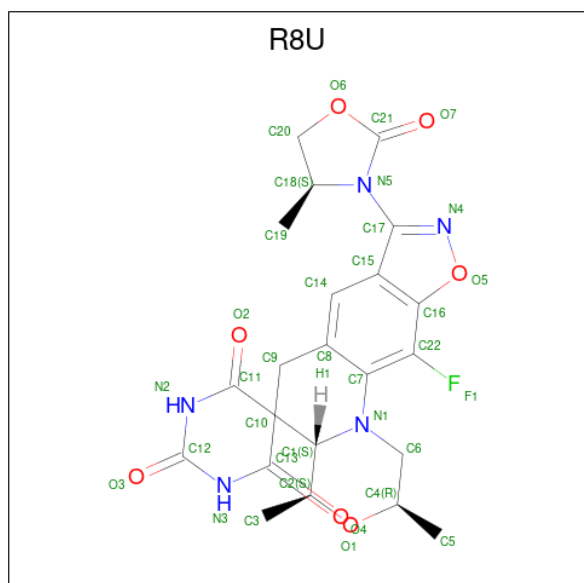
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	AAA	1	Total	Na		0	0
			1	1			

- Molecule 7 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	CCC	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is Zoliflodacin (CCD ID: R8U) (formula: $C_{22}H_{22}FN_5O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	EbE	1	Total	C	F	N	O	0	0
			35	22	1	5	7		
8	FbF	1	Total	C	F	N	O	0	0
			35	22	1	5	7		

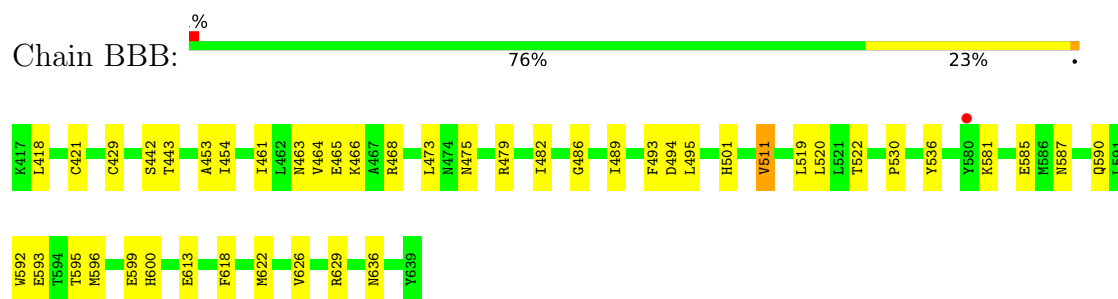
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	BBB	22	Total	O	0	0
			22	22		
9	AAA	76	Total	O	0	0
			76	76		
9	DDD	15	Total	O	0	0
			15	15		
9	CCC	66	Total	O	0	0
			66	66		
9	EEE	11	Total	O	0	0
			11	11		
9	EbE	8	Total	O	0	0
			8	8		
9	FFF	11	Total	O	0	0
			11	11		
9	FbF	18	Total	O	0	0
			18	18		

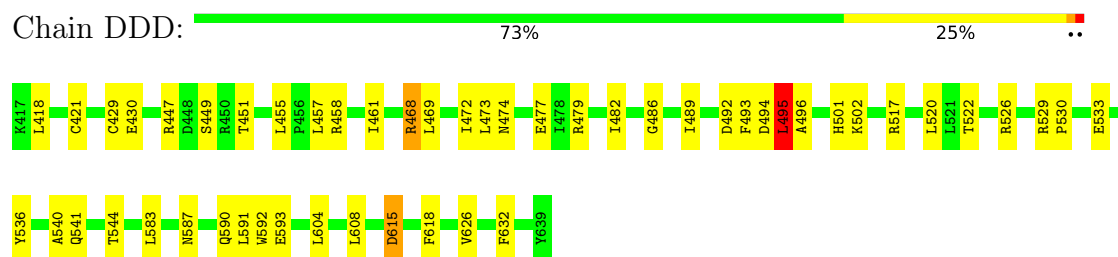
3 Residue-property plots

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.

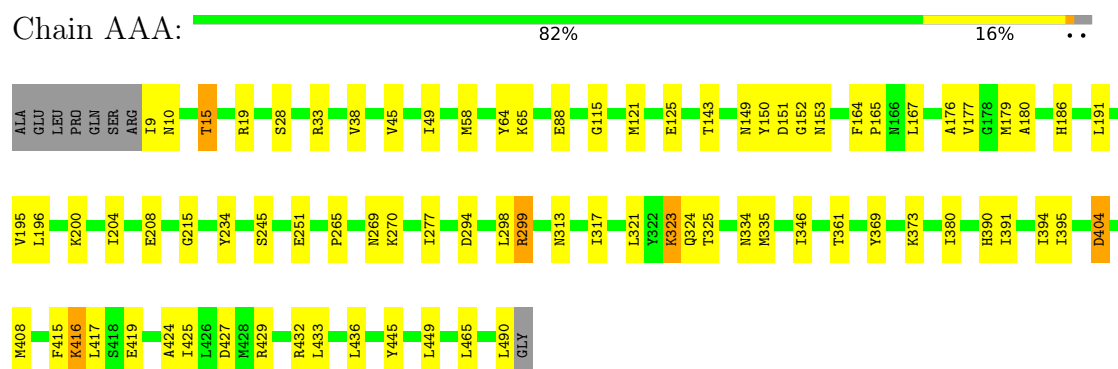
• Molecule 1: DNA gyrase subunit B



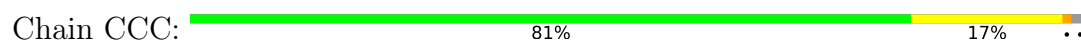
• Molecule 1: DNA gyrase subunit B



• Molecule 2: DNA gyrase subunit A

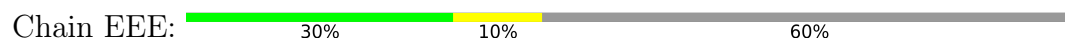


• Molecule 2: DNA gyrase subunit A

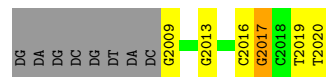
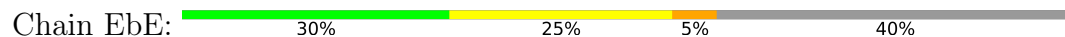




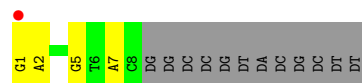
- Molecule 3: DNA (20-MER)



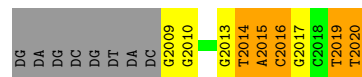
- Molecule 3: DNA (20-MER)



- Molecule 3: DNA (20-MER)



- Molecule 3: DNA (20-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	94.54Å 94.54Å 417.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.85 – 2.80 24.85 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (24.85-2.80) 99.4 (24.85-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.191 , 0.231 0.189 , 0.230	Depositor DCC
R_{free} test set	2538 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	76.5	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.127 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11777	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: NA, R8U, GOL, MN, BTB

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	BBB	0.56	0/1493	1.09	2/2016 (0.1%)
1	DDD	0.55	0/1492	1.07	1/2015 (0.0%)
2	AAA	0.61	0/3853	1.10	4/5196 (0.1%)
2	CCC	0.59	0/3879	1.14	2/5228 (0.0%)
3	EEE	0.60	0/183	1.34	2/281 (0.7%)
3	EbE	0.61	0/294	1.18	2/449 (0.4%)
3	FFF	0.57	0/183	1.20	2/281 (0.7%)
3	FbF	1.27	6/280 (2.1%)	1.59	9/429 (2.1%)
All	All	0.61	6/11657 (0.1%)	1.13	24/15895 (0.2%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	FbF	2019[A]	DT	O3'-P	7.59	1.72	1.61
3	FbF	2019[B]	DT	O3'-P	7.59	1.72	1.61
3	FbF	2020[A]	DT	P-OP2	7.01	1.62	1.48
3	FbF	2020[B]	DT	P-OP2	7.01	1.62	1.48
3	FbF	2020[A]	DT	P-OP1	6.01	1.60	1.48

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	FbF	2019[A]	DT	P-O3'-C3'	-10.74	104.09	120.20
3	FbF	2019[B]	DT	P-O3'-C3'	-10.74	104.09	120.20
3	FFF	5	DG	O3'-P-O5'	-8.14	91.79	104.00
2	AAA	361	THR	CA-CB-OG1	-6.85	99.33	109.60
3	FbF	2014	DT	P-O3'-C3'	-6.49	110.46	120.20

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	BBB	1470	0	1439	32	0
1	DDD	1468	0	1439	37	0
2	AAA	3805	0	3832	57	0
2	CCC	3831	0	3866	56	0
3	EEE	163	0	91	0	0
3	EbE	265	0	149	14	0
3	FFF	163	0	91	2	0
3	FbF	255	0	134	14	0
4	AAA	24	0	32	1	0
4	BBB	6	0	8	1	0
4	CCC	6	0	8	0	0
4	FbF	6	0	8	0	0
5	BBB	1	0	0	0	0
5	CCC	1	0	0	0	0
5	DDD	1	0	0	0	0
6	AAA	1	0	0	0	0
7	CCC	14	0	15	0	0
8	EbE	35	0	0	1	0
8	FbF	35	0	0	1	0
9	AAA	76	0	0	3	0
9	BBB	22	0	0	1	0
9	CCC	66	0	0	2	0
9	DDD	15	0	0	0	0
9	EEE	11	0	0	0	0
9	EbE	8	0	0	2	0
9	FFF	11	0	0	0	0
9	FbF	18	0	0	4	0
All	All	11777	0	11112	183	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.

The worst 5 of 183 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)
3:FbF:2019[A]:DT:H4'	3:FbF:2020[A]:DT:OP1	1.33	1.16
3:FbF:2019[A]:DT:H2''	3:FbF:2020[A]:DT:O5'	1.48	1.13
2:CCC:183:ILE:HG12	2:CCC:335:MET:HG2	1.63	0.80
1:DDD:495:LEU:H	1:DDD:495:LEU:HD12	1.47	0.80
1:DDD:632:PHE:HE1	2:CCC:19:ARG:HH11	1.33	0.76

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	BBB	187/189 (99%)	174 (93%)	11 (6%)	2 (1%)	11	36
1	DDD	187/189 (99%)	174 (93%)	12 (6%)	1 (0%)	24	55
2	AAA	480/490 (98%)	459 (96%)	20 (4%)	1 (0%)	43	72
2	CCC	482/490 (98%)	462 (96%)	19 (4%)	1 (0%)	43	72
All	All	1336/1358 (98%)	1269 (95%)	62 (5%)	5 (0%)	30	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AAA	33	ARG
2	CCC	33	ARG
1	BBB	599	GLU
1	DDD	495	LEU
1	BBB	486	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	BBB	153/158 (97%)	146 (95%)	7 (5%)	24	58
1	DDD	151/158 (96%)	144 (95%)	7 (5%)	24	58
2	AAA	408/423 (96%)	398 (98%)	10 (2%)	42	76
2	CCC	413/423 (98%)	398 (96%)	15 (4%)	31	66
All	All	1125/1162 (97%)	1086 (96%)	39 (4%)	32	67

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	CCC	147	ILE
2	CCC	423	GLN
2	CCC	279	GLU
2	CCC	357	GLU
2	CCC	431[B]	ARG

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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
8	R8U	EbE	2101	-	36,40,40	0.75	1 (2%)	45,64,64	1.17	6 (13%)
4	GOL	FbF	2101	-	5,5,5	0.13	0	5,5,5	0.40	0
4	GOL	BBB	701	-	5,5,5	0.10	0	5,5,5	0.38	0
8	R8U	FbF	2102	-	36,40,40	0.69	1 (2%)	45,64,64	0.98	3 (6%)
4	GOL	AAA	501	-	5,5,5	0.11	0	5,5,5	0.39	0
7	BTB	CCC	902	5	13,13,13	1.45	3 (23%)	7,16,16	0.83	0
4	GOL	AAA	503	-	5,5,5	0.10	0	5,5,5	0.30	0
4	GOL	CCC	903	-	5,5,5	0.11	0	5,5,5	0.44	0
4	GOL	AAA	505	-	5,5,5	0.13	0	5,5,5	0.38	0
4	GOL	AAA	504	-	5,5,5	0.13	0	5,5,5	0.38	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
8	R8U	EbE	2101	-	-	0/0/68/68	0/6/6/6
4	GOL	FbF	2101	-	-	0/4/4/4	-
4	GOL	BBB	701	-	-	0/4/4/4	-
8	R8U	FbF	2102	-	-	0/0/68/68	0/6/6/6
4	GOL	AAA	501	-	-	2/4/4/4	-
7	BTB	CCC	902	5	-	2/21/21/21	-
4	GOL	AAA	503	-	-	0/4/4/4	-
4	GOL	CCC	903	-	-	2/4/4/4	-
4	GOL	AAA	505	-	-	3/4/4/4	-
4	GOL	AAA	504	-	-	4/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	CCC	902	BTB	C2-N	3.71	1.55	1.48
8	EbE	2101	R8U	C15-C17	-3.08	1.40	1.47
8	FbF	2102	R8U	C15-C17	-2.66	1.41	1.47
7	CCC	902	BTB	C5-N	2.49	1.51	1.48
7	CCC	902	BTB	C7-N	2.00	1.50	1.48

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	EbE	2101	R8U	C19-C18-C20	-3.39	111.00	113.79
8	EbE	2101	R8U	C9-C10-C13	-3.00	101.97	108.36
8	FbF	2102	R8U	C9-C10-C13	-2.81	102.37	108.36
8	FbF	2102	R8U	C15-C17-N5	2.53	132.78	126.40
8	EbE	2101	R8U	C18-N5-C17	2.48	125.71	121.34

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	505	GOL	O1-C1-C2-O2
4	AAA	505	GOL	O1-C1-C2-C3
4	CCC	903	GOL	O2-C2-C3-O3
4	AAA	501	GOL	C1-C2-C3-O3
4	AAA	504	GOL	O1-C1-C2-C3

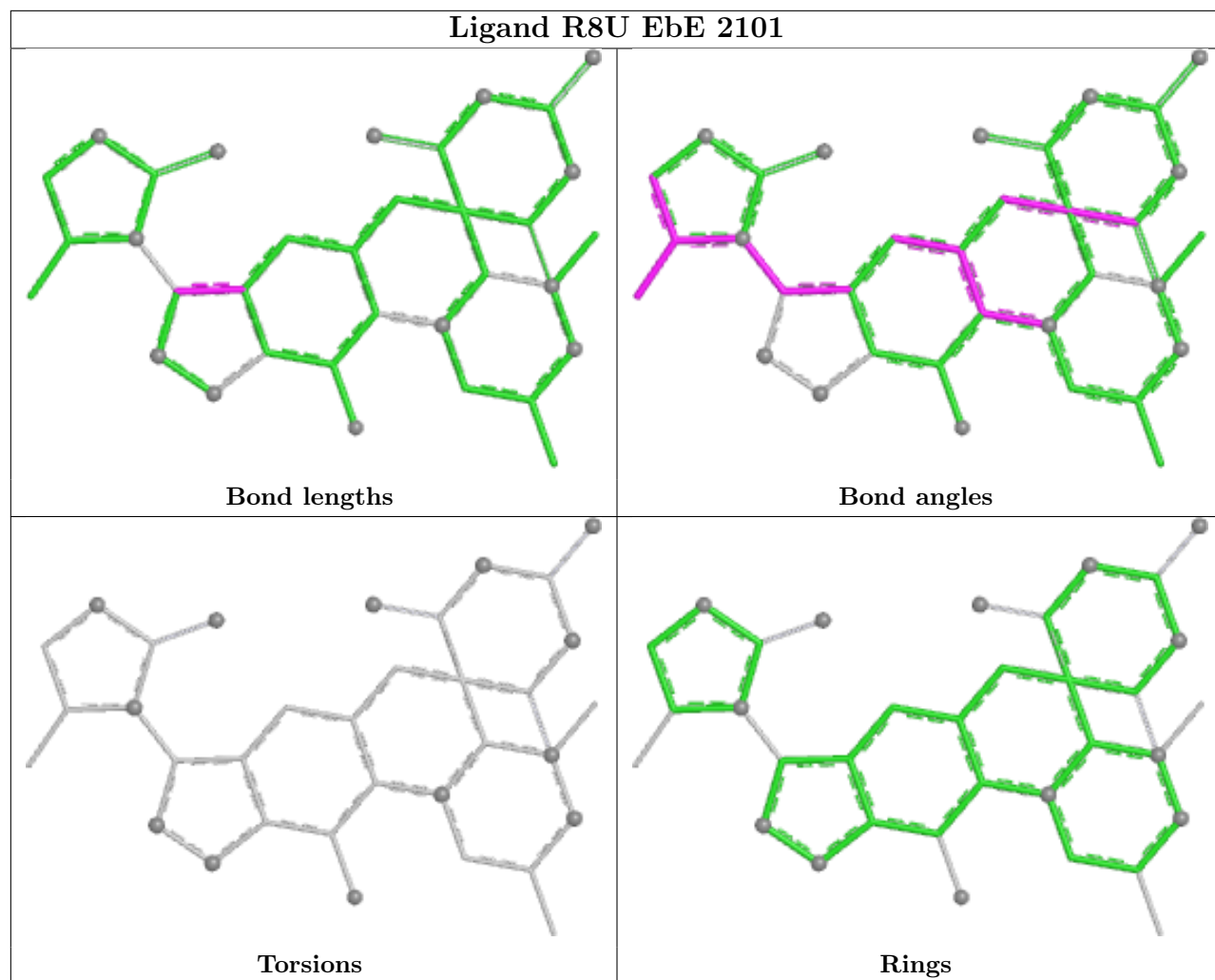
There are no ring outliers.

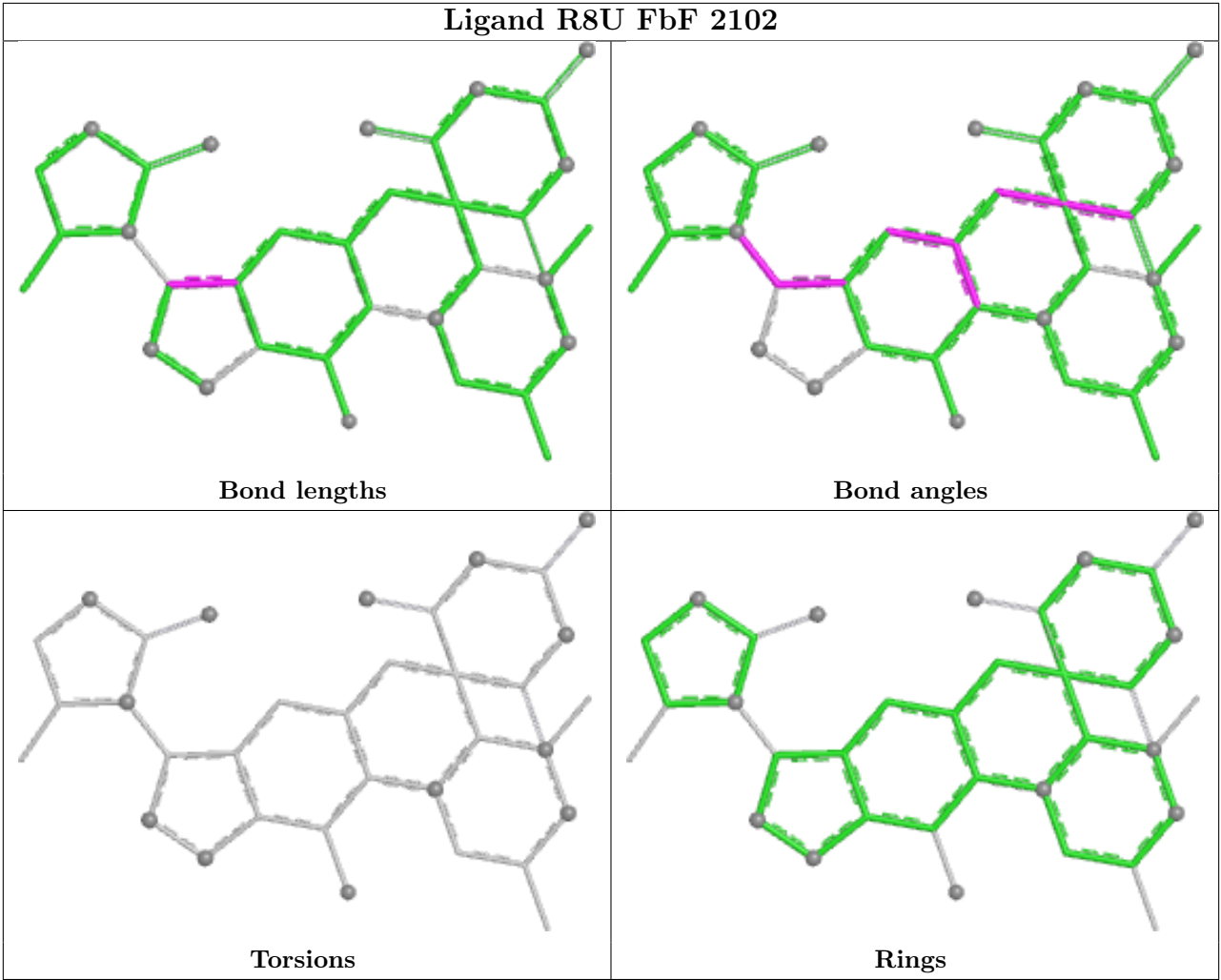
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	EbE	2101	R8U	1	0
4	BBB	701	GOL	1	0
8	FbF	2102	R8U	1	0
4	AAA	504	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.

Ligand R8U EbE 2101





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
3	FbF	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	FbF	2019[A]:DT	O3'	2020[A]:DT	P	1.86

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, 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	BBB	189/189 (100%)	-0.41	1 (0%) 87 82	87, 117, 160, 190	0
1	DDD	189/189 (100%)	-0.54	0 100 100	89, 113, 147, 160	0
2	AAA	482/490 (98%)	-0.96	0 100 100	56, 84, 112, 163	0
2	CCC	481/490 (98%)	-0.94	0 100 100	41, 81, 112, 141	3 (0%)
3	EEE	8/20 (40%)	-0.78	0 100 100	72, 77, 83, 89	0
3	EbE	12/20 (60%)	-0.88	0 100 100	45, 79, 110, 151	1 (8%)
3	FFF	8/20 (40%)	-0.51	1 (12%) 8 6	54, 70, 96, 121	1 (12%)
3	FbF	12/20 (60%)	-0.33	0 100 100	43, 79, 115, 116	2 (16%)
All	All	1381/1438 (96%)	-0.81	2 (0%) 92 90	41, 90, 136, 190	7 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	FFF	1	DG	4.9
1	BBB	580	TYR	2.4

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

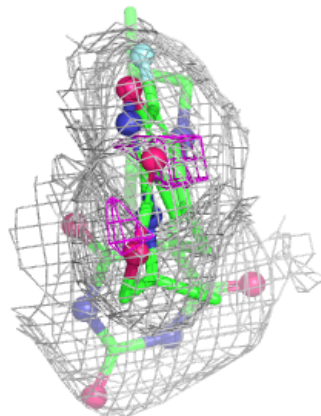
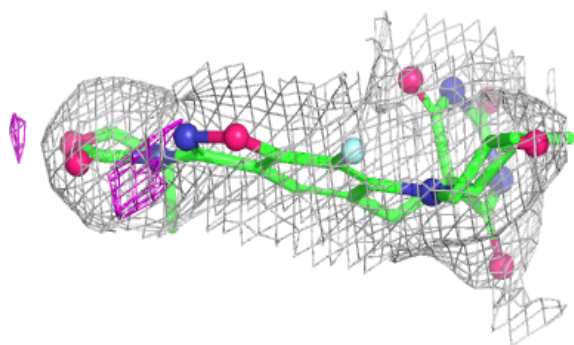
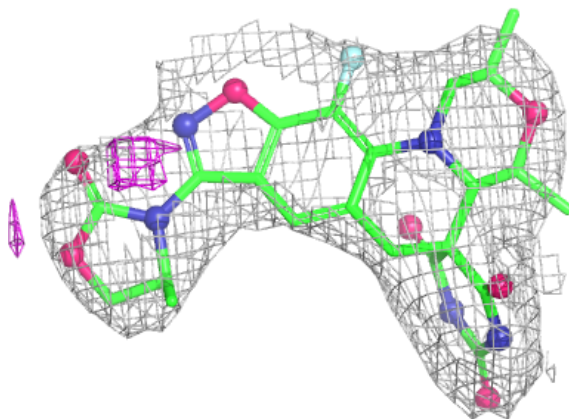
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	FbF	2101	6/6	0.83	0.16	87,90,90,90	0
4	GOL	AAA	503	6/6	0.87	0.12	89,90,90,90	0
4	GOL	AAA	505	6/6	0.92	0.09	90,90,90,90	0
4	GOL	AAA	501	6/6	0.92	0.09	90,90,90,90	0
4	GOL	CCC	903	6/6	0.93	0.10	90,90,90,90	0
4	GOL	AAA	504	6/6	0.93	0.13	82,90,90,90	0
7	BTB	CCC	902	14/14	0.93	0.19	77,88,90,90	14
4	GOL	BBB	701	6/6	0.95	0.06	81,85,87,90	0
6	NA	AAA	502	1/1	0.96	0.10	68,68,68,68	0
8	R8U	EbE	2101	35/35	0.96	0.06	71,84,90,90	0
8	R8U	FbF	2102	35/35	0.96	0.06	64,82,90,90	0
5	MN	BBB	702	1/1	0.99	0.04	87,87,87,87	0
5	MN	CCC	901	1/1	0.99	0.08	90,90,90,90	0
5	MN	DDD	701	1/1	1.00	0.02	84,84,84,84	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.

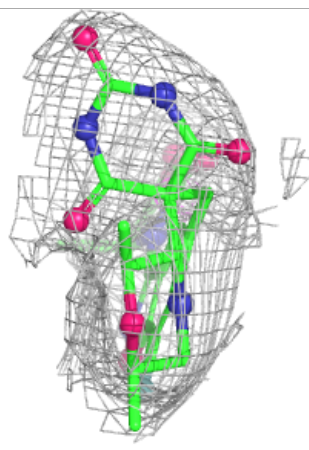
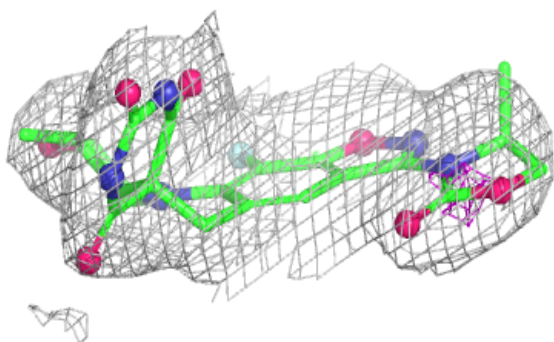
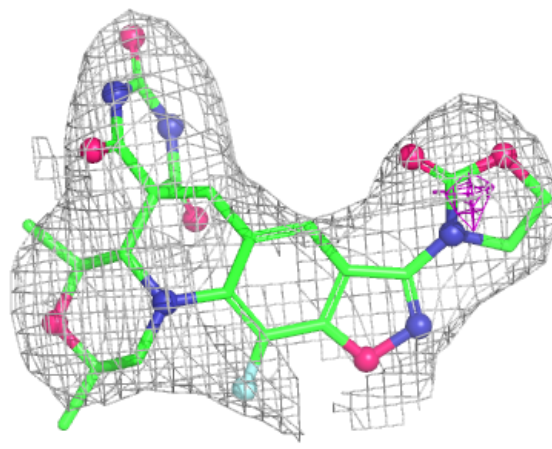
Electron density around R8U EbE 2101:

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



Electron density around R8U FbF 2102:

$2mF_o-DF_c$ (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.