



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2021 – 12:18 PM EST

PDB ID : 7KU9
Title : The internal aldimine form of the wild-type Salmonella typhimurium Tryptophan Synthase with sodium ion at the metal coordination site, two molecules of F6F inhibitor at the enzyme alpha-site and another F6F molecule at the enzyme beta-site at 1.40 Angstrom resolution
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Deposited on : 2020-11-24
Resolution : 1.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

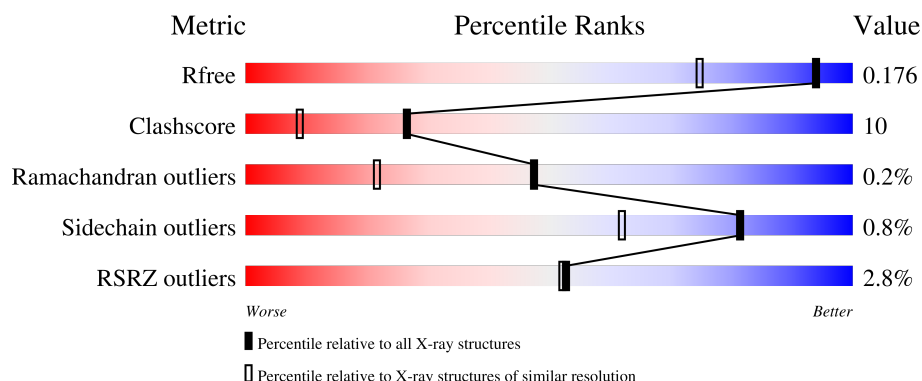
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	268	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>• •</div> </div> </div>
2	B	397	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>•</div> </div> </div>

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
3	F6F	A	309	-	-	X	-
4	DMS	A	302	-	-	X	-
4	DMS	B	1001	-	-	X	-
4	DMS	B	1022	-	-	X	-
5	EDO	B	1027	-	-	X	-
8	PEG	B	1015	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 6279 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.

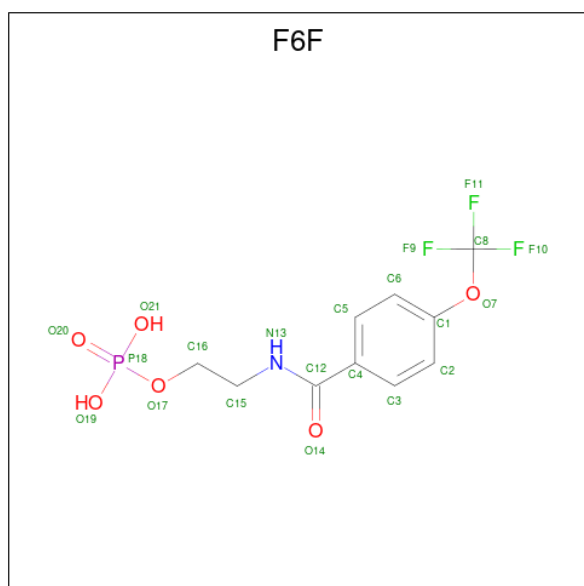
- Molecule 1 is a protein called Tryptophan synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	9	0
			2020	1282	347	383	8			

- Molecule 2 is a protein called Tryptophan synthase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	394	Total	C	N	O	S	0	17	0
			3128	1959	550	599	20			

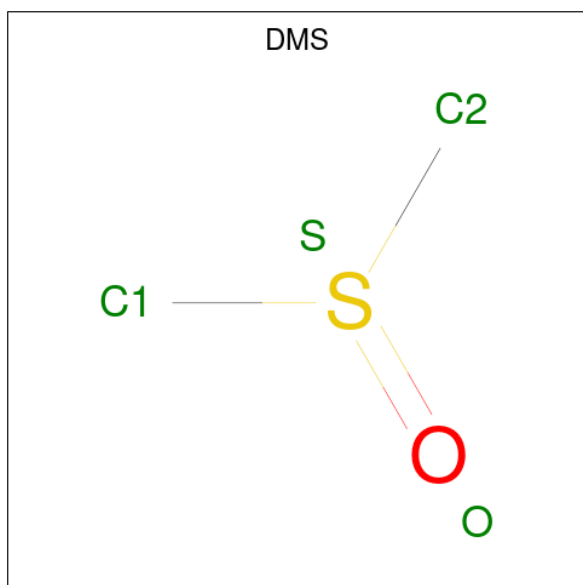
- Molecule 3 is 2-{[4-(TRIFLUOROMETHOXY)BENZOYL]AMINO}ETHYL DIHYDROGEN PHOSPHATE (three-letter code: F6F) (formula: C₁₀H₁₁F₃NO₆P) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	P	0	0
			21	10	3	1	6	1		
3	B	1	Total	C	F	N	O	P	0	0
			21	10	3	1	6	1		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).

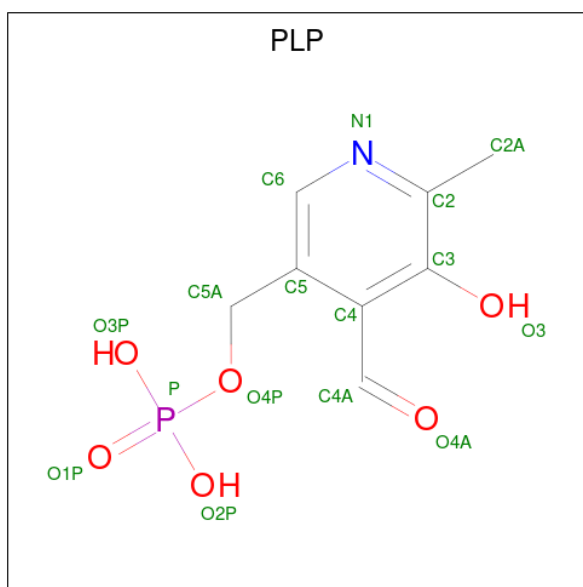


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0
6	B	2	Total Cl 2 2	0	0

- Molecule 7 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P) (labeled as "Ligand of Interest" by depositor).



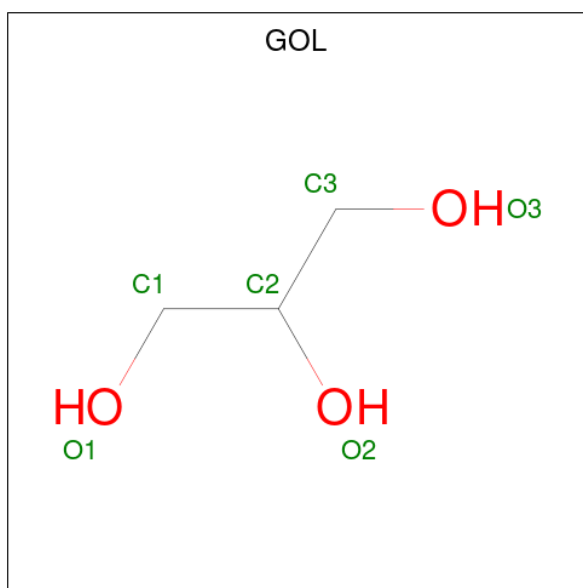
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			7	4	3		
8	B	1	Total	C	O	0	0
			7	4	3		
8	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Na	0	0
			1	1		

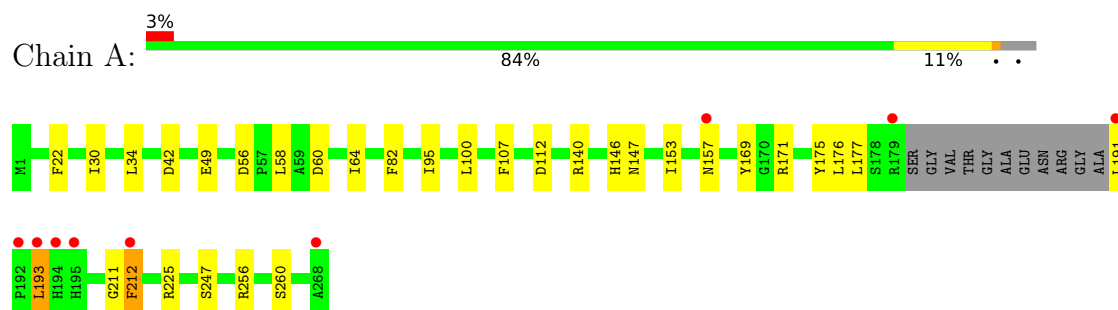
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	366	Total	O	0	3
			369	369		
11	B	518	Total	O	0	5
			523	523		

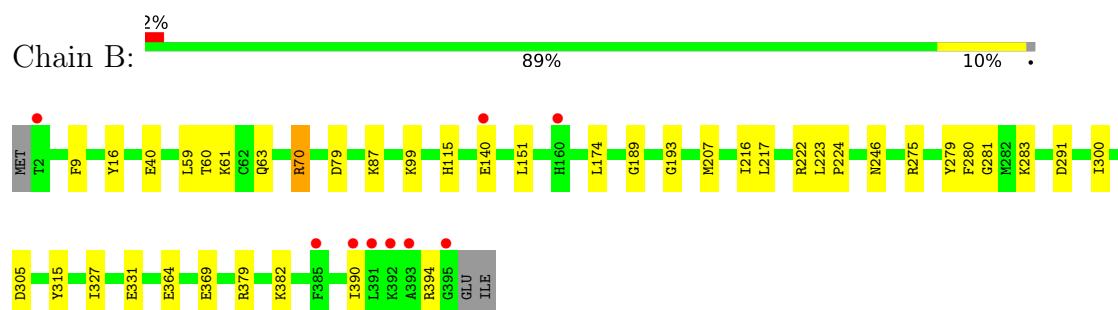
3 Residue-property plots

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: Tryptophan synthase alpha chain



• Molecule 2: Tryptophan synthase beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.26Å 58.90Å 67.23Å 90.00° 94.82° 90.00°	Depositor
Resolution (Å)	36.79 – 1.40 36.77 – 1.40	Depositor EDS
% Data completeness (in resolution range)	97.0 (36.79-1.40) 97.0 (36.77-1.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.136 , 0.177 0.135 , 0.176	Depositor DCC
R_{free} test set	6868 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	9.5	Xtriage
Anisotropy	1.549	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	6279	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PEG, F6F, GOL, DMS, EDO, PLP, 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	0.37	1/2059 (0.0%)	0.65	0/2795
2	B	0.42	0/3186	0.74	3/4298 (0.1%)
All	All	0.40	1/5245 (0.0%)	0.70	3/7093 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	LEU	C-N	-5.44	1.21	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	70[A]	ARG	CG-CD-NE	-6.14	98.90	111.80
2	B	70[B]	ARG	CG-CD-NE	-6.14	98.90	111.80
2	B	275	ARG	NE-CZ-NH2	-5.21	117.69	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2020	0	2014	37	0
2	B	3128	0	3082	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	42	0	18	7	0
3	B	21	0	9	0	0
4	A	20	0	30	10	0
4	B	76	0	114	25	0
5	A	12	0	18	9	0
5	B	16	0	24	8	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
7	B	15	0	6	1	0
8	B	21	0	30	7	0
9	B	12	0	16	4	0
10	B	1	0	0	0	0
11	A	369	0	0	14	0
11	B	523	0	0	24	0
All	All	6279	0	5361	111	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 10.

All (111) 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)
2:B:70[B]:ARG:HD3	2:B:369[B]:GLU:OE1	1.39	1.21
2:B:283:LYS:NZ	4:B:1001:DMS:C2	2.10	1.14
4:B:1022:DMS:H13	11:B:1237:HOH:O	1.47	1.11
2:B:283:LYS:HZ3	4:B:1001:DMS:C2	1.72	1.01
2:B:283:LYS:NZ	4:B:1001:DMS:H22	1.79	0.95
2:B:9:PHE:CZ	9:B:1029:GOL:H32	2.07	0.90
9:B:1029:GOL:H12	11:B:1485:HOH:O	1.70	0.89
2:B:283:LYS:HZ3	4:B:1001:DMS:H23	1.37	0.88
2:B:223:LEU:HD23	11:B:1397:HOH:O	1.75	0.86
5:B:1026:EDO:H22	11:B:1330:HOH:O	1.76	0.85
2:B:283:LYS:HZ1	4:B:1001:DMS:C2	1.80	0.83
2:B:222[B]:ARG:NH2	11:B:1101:HOH:O	2.13	0.81
1:A:260[B]:SER:OG	5:A:310:EDO:H11	1.82	0.80
2:B:283:LYS:NZ	4:B:1001:DMS:S	2.55	0.78
4:B:1022:DMS:H11	11:B:1504:HOH:O	1.84	0.77
1:A:157:ASN:CG	11:A:404:HOH:O	2.25	0.76
1:A:42[B]:ASP:OD2	11:A:401:HOH:O	2.06	0.74
5:A:308:EDO:H11	11:A:612:HOH:O	1.87	0.74
1:A:56:ASP:HB3	2:B:279:TYR:OH	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64[A]:ILE:HD12	3:A:309:F6F:P18	2.30	0.72
1:A:157:ASN:ND2	11:A:404:HOH:O	2.23	0.71
1:A:247:SER:OG	11:A:402:HOH:O	2.10	0.68
2:B:283:LYS:CE	4:B:1001:DMS:H22	2.25	0.67
2:B:217[A]:LEU:HG	11:B:1397:HOH:O	1.95	0.66
4:B:1011:DMS:C1	11:B:1349:HOH:O	2.43	0.66
2:B:9:PHE:CE2	9:B:1029:GOL:H32	2.31	0.65
4:A:307:DMS:C1	11:A:489:HOH:O	2.46	0.64
1:A:100[A]:LEU:HD13	1:A:100[A]:LEU:C	2.18	0.64
1:A:153:ILE:HG23	1:A:177:LEU:HG	1.79	0.64
2:B:99:LYS:NZ	11:B:1105:HOH:O	2.30	0.63
2:B:40[B]:GLU:CD	11:B:1111:HOH:O	2.37	0.63
1:A:147:ASN:HA	4:A:302:DMS:H21	1.80	0.63
1:A:225:ARG:HD3	5:A:308:EDO:O2	2.00	0.62
2:B:61[B]:LYS:H	8:B:1015:PEG:C1	2.14	0.61
1:A:176:LEU:HD21	1:A:193:LEU:HD12	1.82	0.61
1:A:34:LEU:HD11	4:A:306:DMS:C1	2.31	0.60
5:B:1030:EDO:H22	11:B:1120:HOH:O	2.01	0.60
4:A:307:DMS:H11	11:A:489:HOH:O	2.02	0.60
2:B:364:GLU:HA	9:B:1028:GOL:H2	1.85	0.59
2:B:291:ASP:HB3	5:B:1027:EDO:H22	1.84	0.58
2:B:63[A]:GLN:NE2	11:B:1113:HOH:O	2.37	0.58
2:B:70[B]:ARG:HH21	2:B:369[B]:GLU:CD	2.06	0.58
4:B:1011:DMS:H12	11:B:1349:HOH:O	2.02	0.58
2:B:61[A]:LYS:H	8:B:1015:PEG:C1	2.17	0.56
1:A:107:PHE:CE1	4:B:1001:DMS:C2	2.89	0.56
1:A:211:GLY:O	1:A:212:PHE:HB2	2.06	0.56
4:A:302:DMS:H23	11:A:448:HOH:O	2.04	0.56
2:B:216[A]:ILE:HG23	11:B:1397:HOH:O	2.05	0.56
4:A:302:DMS:H21	11:A:461:HOH:O	2.07	0.55
2:B:151:LEU:HA	5:B:1025:EDO:H12	1.88	0.54
1:A:147:ASN:HA	4:A:302:DMS:C2	2.38	0.54
2:B:291:ASP:HB3	5:B:1027:EDO:C2	2.38	0.54
5:A:303:EDO:H21	11:A:526:HOH:O	2.08	0.53
1:A:212:PHE:CZ	3:A:309:F6F:H161	2.43	0.53
1:A:260[B]:SER:OG	5:A:310:EDO:C1	2.56	0.53
1:A:140:ARG:HD3	1:A:169:TYR:HB3	1.91	0.53
1:A:107:PHE:HE1	4:B:1001:DMS:C2	2.22	0.53
4:B:1005:DMS:H12	11:B:1502:HOH:O	2.10	0.51
4:B:1011:DMS:H13	11:B:1349:HOH:O	2.06	0.51
2:B:59:LEU:O	8:B:1015:PEG:H12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64[A]:ILE:HD12	3:A:309:F6F:O19	2.12	0.50
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.46	0.50
1:A:82:PHE:CD1	5:A:303:EDO:H11	2.47	0.50
1:A:256:ARG:NH2	5:A:310:EDO:O2	2.45	0.49
1:A:95:ILE:HB	4:A:307:DMS:H12	1.95	0.49
5:A:303:EDO:C2	11:A:526:HOH:O	2.60	0.49
2:B:61[A]:LYS:HB2	8:B:1015:PEG:H11	1.95	0.49
1:A:30:ILE:CG2	4:A:306:DMS:H12	2.43	0.49
2:B:300:ILE:HD11	2:B:390:ILE:CD1	2.43	0.48
2:B:283:LYS:HE2	4:B:1001:DMS:H22	1.93	0.48
5:A:308:EDO:H22	11:A:612:HOH:O	2.13	0.48
2:B:60:THR:HA	8:B:1015:PEG:H12	1.94	0.48
1:A:22:PHE:HA	1:A:49:GLU:O	2.13	0.48
4:B:1001:DMS:H13	11:B:1600:HOH:O	2.13	0.47
2:B:283:LYS:NZ	4:B:1001:DMS:H23	2.03	0.47
1:A:64[A]:ILE:HD12	3:A:309:F6F:O20	2.14	0.47
2:B:193:GLY:HA2	2:B:280:PHE:O	2.14	0.46
2:B:216[B]:ILE:HG22	2:B:222[B]:ARG:O	2.15	0.46
1:A:112:ASP:OD1	1:A:146:HIS:HE1	1.97	0.46
4:B:1022:DMS:C1	11:B:1237:HOH:O	2.24	0.46
4:B:1022:DMS:C1	11:B:1504:HOH:O	2.54	0.46
2:B:382:LYS:HD2	4:B:1017:DMS:O	2.17	0.45
1:A:60:ASP:OD1	3:A:309:F6F:O20	2.35	0.45
2:B:291:ASP:CA	5:B:1027:EDO:H22	2.47	0.44
1:A:56:ASP:HB3	2:B:279:TYR:CZ	2.52	0.44
3:A:301:F6F:O20	3:A:309:F6F:O19	2.35	0.44
2:B:216[A]:ILE:CG2	11:B:1397:HOH:O	2.64	0.44
4:B:1005:DMS:C1	11:B:1502:HOH:O	2.63	0.44
2:B:216[A]:ILE:HG21	2:B:224:PRO:HD3	2.01	0.43
1:A:58:LEU:HD11	2:B:174:LEU:HB2	1.99	0.43
1:A:107:PHE:CE1	4:B:1001:DMS:H22	2.54	0.43
2:B:300:ILE:HD11	2:B:390:ILE:HD13	2.01	0.43
2:B:305[B]:ASP:OD1	2:B:305[B]:ASP:C	2.57	0.43
2:B:79:ASP:HB2	2:B:379:ARG:HB3	2.01	0.43
1:A:212:PHE:CE1	3:A:309:F6F:H161	2.54	0.43
1:A:191:LEU:N	11:A:414:HOH:O	2.51	0.42
4:A:302:DMS:C2	11:A:448:HOH:O	2.64	0.42
2:B:61[B]:LYS:HB2	8:B:1015:PEG:H11	2.01	0.42
2:B:291:ASP:HA	5:B:1027:EDO:H22	2.01	0.42
2:B:87:LYS:NZ	7:B:1002:PLP:O3	2.47	0.42
1:A:153:ILE:CG2	1:A:177:LEU:HG	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:LYS:HZ3	4:B:1001:DMS:H22	1.53	0.42
2:B:16:TYR:O	2:B:281:GLY:HA2	2.20	0.41
1:A:100[A]:LEU:C	1:A:100[A]:LEU:CD1	2.88	0.41
2:B:61[B]:LYS:NZ	11:B:1110:HOH:O	2.34	0.41
4:B:1018:DMS:C1	11:B:1540:HOH:O	2.68	0.41
2:B:315:TYR:CE2	5:B:1030:EDO:H21	2.56	0.41
2:B:246:ASN:CB	8:B:1013:PEG:H22	2.51	0.41
1:A:153:ILE:HD13	1:A:175:TYR:CG	2.57	0.40
2:B:63[B]:GLN:HG2	11:B:1119:HOH:O	2.21	0.40
2:B:327:ILE:HG23	2:B:331:GLU:HB2	2.02	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	263/268 (98%)	261 (99%)	1 (0%)	1 (0%)	34	12
2	B	409/397 (103%)	401 (98%)	8 (2%)	0	100	100
All	All	672/665 (101%)	662 (98%)	9 (1%)	1 (0%)	47	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	PHE

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	212/208 (102%)	211 (100%)	1 (0%)	88	74
2	B	325/311 (104%)	322 (99%)	3 (1%)	78	58
All	All	537/519 (104%)	533 (99%)	4 (1%)	81	66

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	ARG
2	B	140	GLU
2	B	207	MET
2	B	394	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	HIS

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 44 ligands modelled in this entry, 4 are monoatomic - leaving 40 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	DMS	B	1004	-	3,3,3	0.25	0	3,3,3	0.18	0
4	DMS	B	1007	-	3,3,3	0.48	0	3,3,3	0.10	0
4	DMS	B	1016	-	3,3,3	0.22	0	3,3,3	0.19	0
4	DMS	B	1017	-	3,3,3	0.24	0	3,3,3	0.24	0
4	DMS	B	1008	-	3,3,3	0.25	0	3,3,3	0.05	0
8	PEG	B	1023	-	6,6,6	0.14	0	5,5,5	0.10	0
4	DMS	B	1009	-	3,3,3	0.32	0	3,3,3	0.11	0
4	DMS	B	1011	-	3,3,3	0.23	0	3,3,3	0.06	0
4	DMS	B	1005	-	3,3,3	0.27	0	3,3,3	0.34	0
4	DMS	A	306	-	3,3,3	0.28	0	3,3,3	0.15	0
5	EDO	A	310	-	3,3,3	0.04	0	2,2,2	0.29	0
5	EDO	B	1026	-	3,3,3	0.18	0	2,2,2	0.20	0
4	DMS	B	1019	-	3,3,3	0.22	0	3,3,3	0.12	0
4	DMS	B	1020	-	3,3,3	0.24	0	3,3,3	0.09	0
5	EDO	A	303	-	3,3,3	0.09	0	2,2,2	0.51	0
4	DMS	B	1022	-	3,3,3	0.56	0	3,3,3	0.38	0
4	DMS	B	1024	-	3,3,3	0.31	0	3,3,3	0.26	0
8	PEG	B	1013	-	6,6,6	0.36	0	5,5,5	0.29	0
4	DMS	A	307	-	3,3,3	0.25	0	3,3,3	0.25	0
8	PEG	B	1015	-	6,6,6	0.57	0	5,5,5	0.45	0
4	DMS	B	1014	-	3,3,3	0.16	0	3,3,3	0.07	0
5	EDO	B	1030	-	3,3,3	0.17	0	2,2,2	0.32	0
9	GOL	B	1028	-	5,5,5	0.14	0	5,5,5	0.55	0
5	EDO	B	1025	-	3,3,3	0.07	0	2,2,2	0.10	0
4	DMS	B	1001	-	3,3,3	0.21	0	3,3,3	0.36	0
7	PLP	B	1002	2	15,15,16	0.87	1 (6%)	20,22,23	1.37	2 (10%)
4	DMS	B	1021	-	3,3,3	0.18	0	3,3,3	0.30	0
3	F6F	A	301	-	21,21,21	0.49	0	29,30,30	0.36	0
5	EDO	B	1027	-	3,3,3	0.10	0	2,2,2	0.34	0
5	EDO	A	308	-	3,3,3	0.10	0	2,2,2	0.29	0
4	DMS	B	1010	-	3,3,3	0.22	0	3,3,3	0.14	0
3	F6F	B	1003	-	21,21,21	0.44	0	29,30,30	0.55	0
4	DMS	A	302	-	3,3,3	0.43	0	3,3,3	0.19	0
4	DMS	B	1006	-	3,3,3	0.24	0	3,3,3	0.09	0
4	DMS	B	1018	-	3,3,3	0.49	0	3,3,3	0.15	0
4	DMS	A	304	-	3,3,3	0.32	0	3,3,3	0.34	0
4	DMS	A	305	-	3,3,3	0.24	0	3,3,3	0.24	0
3	F6F	A	309	-	21,21,21	0.35	0	29,30,30	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GOL	B	1029	-	5,5,5	0.25	0	5,5,5	0.54	0
4	DMS	B	1012	-	3,3,3	0.18	0	3,3,3	0.15	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
5	EDO	B	1025	-	-	1/1/1/1	-
3	F6F	B	1003	-	-	2/17/17/17	0/1/1/1
9	GOL	B	1028	-	-	2/4/4/4	-
5	EDO	B	1026	-	-	0/1/1/1	-
8	PEG	B	1023	-	-	1/4/4/4	-
5	EDO	A	303	-	-	0/1/1/1	-
3	F6F	A	309	-	-	9/17/17/17	0/1/1/1
7	PLP	B	1002	2	-	0/6/6/8	0/1/1/1
8	PEG	B	1013	-	-	1/4/4/4	-
9	GOL	B	1029	-	-	4/4/4/4	-
8	PEG	B	1015	-	-	2/4/4/4	-
3	F6F	A	301	-	-	4/17/17/17	0/1/1/1
5	EDO	B	1027	-	-	1/1/1/1	-
5	EDO	A	308	-	-	1/1/1/1	-
5	EDO	B	1030	-	-	0/1/1/1	-
5	EDO	A	310	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1002	PLP	C4A-C4	-2.15	1.47	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1002	PLP	O4P-C5A-C5	3.45	115.92	109.35
7	B	1002	PLP	C4A-C4-C5	3.27	124.31	120.94

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	1029	GOL	O1-C1-C2-C3
9	B	1029	GOL	O1-C1-C2-O2
8	B	1013	PEG	O1-C1-C2-O2
9	B	1029	GOL	C1-C2-C3-O3
9	B	1029	GOL	O2-C2-C3-O3
8	B	1015	PEG	O2-C3-C4-O4
3	A	309	F6F	C4-C12-N13-C15
5	B	1025	EDO	O1-C1-C2-O2
3	A	309	F6F	O14-C12-C4-C3
3	A	309	F6F	O14-C12-C4-C5
5	A	308	EDO	O1-C1-C2-O2
5	A	310	EDO	O1-C1-C2-O2
8	B	1015	PEG	C1-C2-O2-C3
3	A	309	F6F	O14-C12-N13-C15
3	A	301	F6F	C16-O17-P18-O20
5	B	1027	EDO	O1-C1-C2-O2
3	B	1003	F6F	C2-C1-O7-C8
3	B	1003	F6F	C6-C1-O7-C8
9	B	1028	GOL	O1-C1-C2-O2
3	A	309	F6F	N13-C12-C4-C3
3	A	309	F6F	N13-C12-C4-C5
3	A	301	F6F	C6-C1-O7-C8
3	A	301	F6F	C2-C1-O7-C8
8	B	1023	PEG	C4-C3-O2-C2
3	A	309	F6F	C2-C1-O7-C8
3	A	309	F6F	C6-C1-O7-C8
9	B	1028	GOL	O1-C1-C2-C3
3	A	301	F6F	C15-C16-O17-P18
3	A	309	F6F	C15-C16-O17-P18

There are no ring outliers.

23 monomers are involved in 71 short contacts:

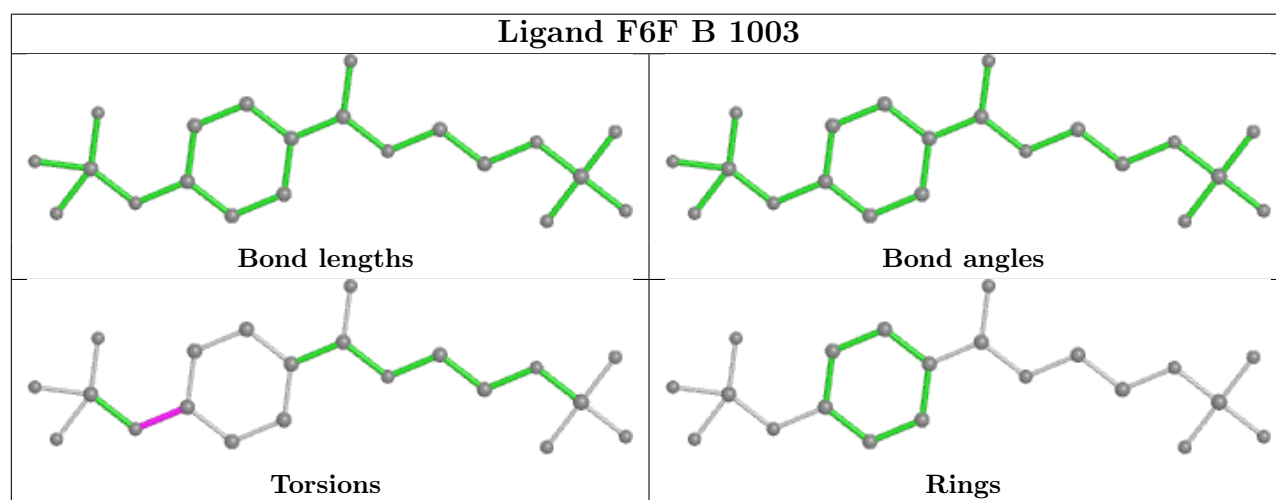
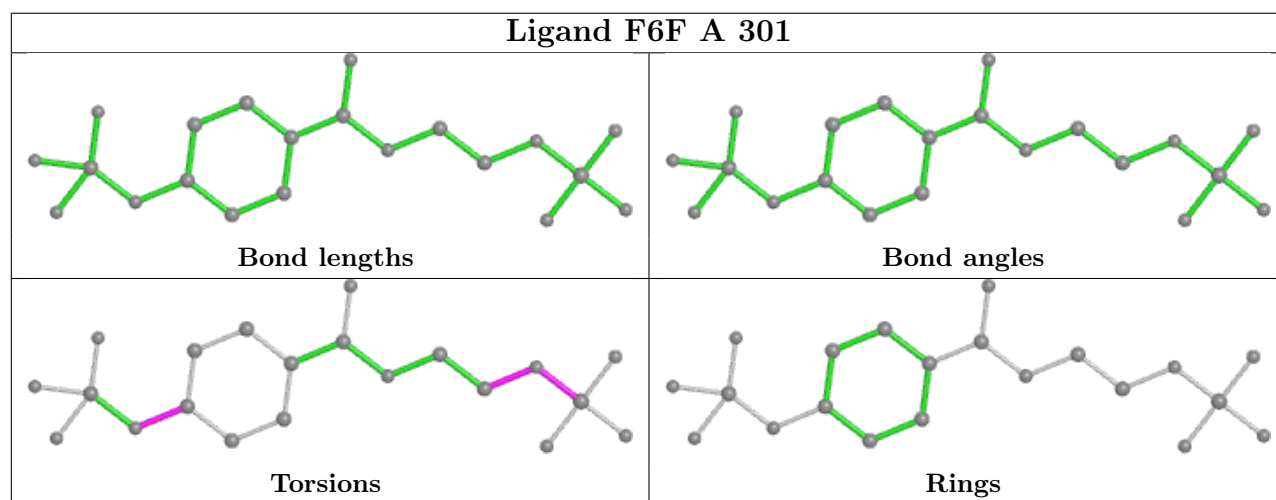
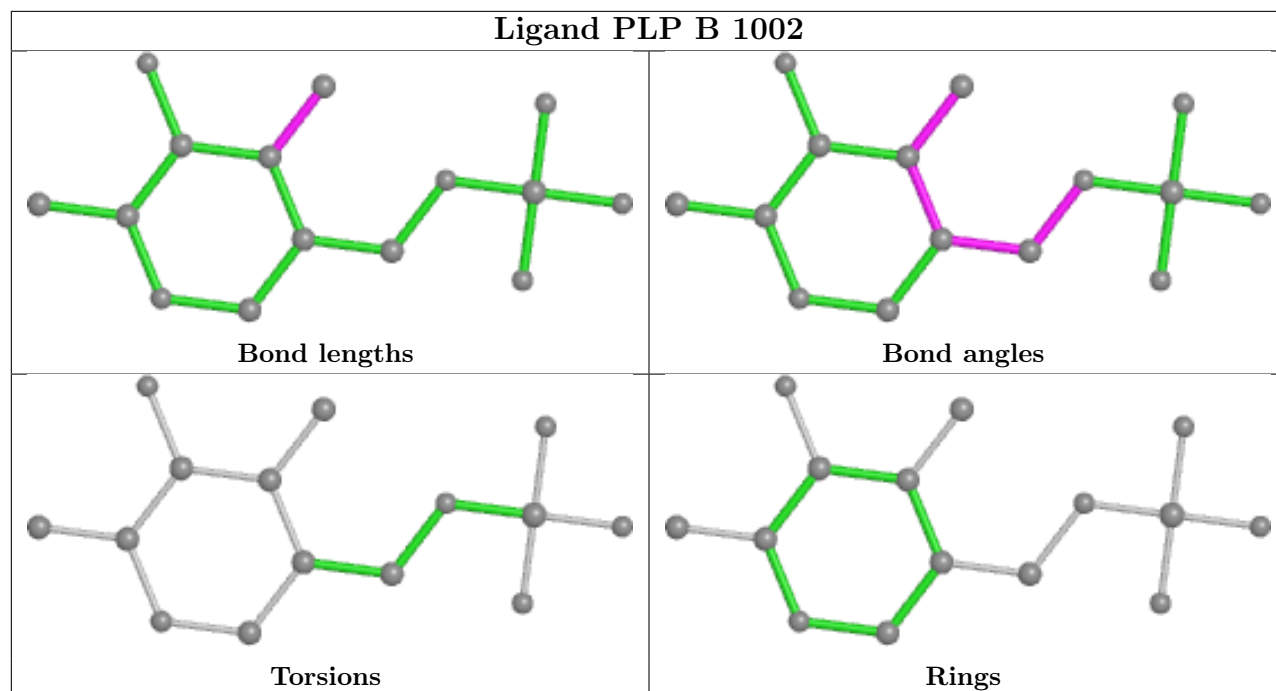
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1017	DMS	1	0
4	B	1011	DMS	3	0
4	B	1005	DMS	2	0
4	A	306	DMS	2	0
5	A	310	EDO	3	0
5	B	1026	EDO	1	0
5	A	303	EDO	3	0
4	B	1022	DMS	4	0
8	B	1013	PEG	1	0

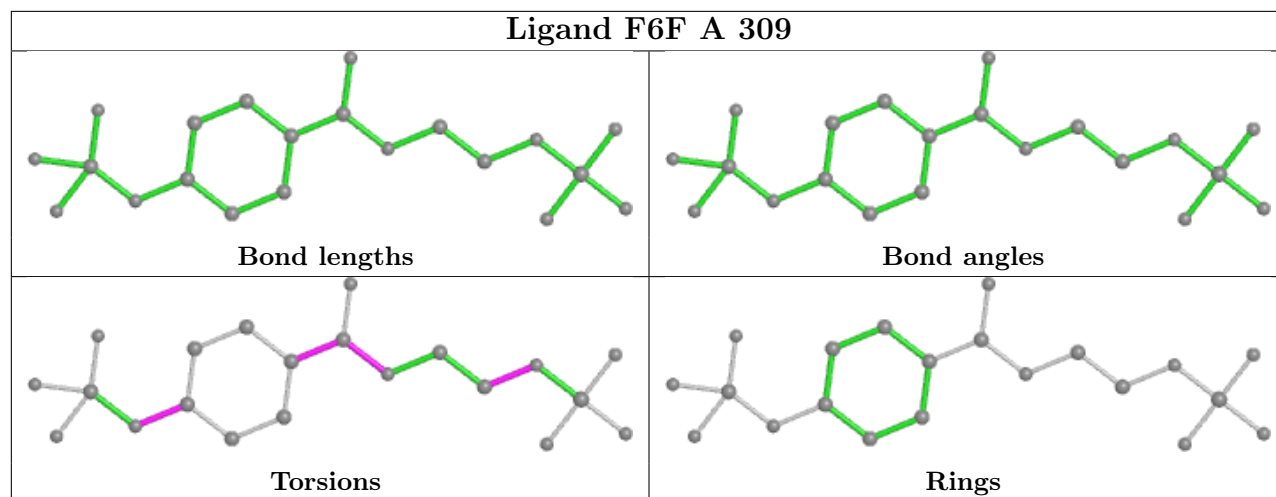
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	307	DMS	3	0
8	B	1015	PEG	6	0
5	B	1030	EDO	2	0
9	B	1028	GOL	1	0
5	B	1025	EDO	1	0
4	B	1001	DMS	14	0
7	B	1002	PLP	1	0
3	A	301	F6F	1	0
5	B	1027	EDO	4	0
5	A	308	EDO	3	0
4	A	302	DMS	5	0
4	B	1018	DMS	1	0
3	A	309	F6F	7	0
9	B	1029	GOL	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	257/268 (95%)	-0.20	9 (3%)	44 43	10, 16, 33, 60	0
2	B	394/397 (99%)	-0.08	9 (2%)	60 60	9, 12, 33, 56	0
All	All	651/665 (97%)	-0.13	18 (2%)	53 52	9, 14, 33, 60	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	LEU	7.7
1	A	193	LEU	5.9
2	B	391	LEU	4.6
2	B	395	GLY	4.5
1	A	194	HIS	4.4
1	A	212	PHE	4.2
2	B	393	ALA	3.8
1	A	268	ALA	3.3
2	B	390	ILE	3.2
2	B	392	LYS	3.1
1	A	179	ARG	3.0
1	A	192	PRO	3.0
2	B	385	PHE	2.9
2	B	160	HIS	2.4
2	B	140	GLU	2.2
1	A	157	ASN	2.2
2	B	2	THR	2.1
1	A	195	HIS	2.1

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, 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(\AA^2)	Q<0.9
5	EDO	B	1030	4/4	0.70	0.22	21,24,29,36	0
8	PEG	B	1013	7/7	0.77	0.25	32,41,49,53	0
4	DMS	B	1007	4/4	0.81	0.26	31,41,41,48	0
4	DMS	B	1014	4/4	0.82	0.22	30,108,118,125	0
9	GOL	B	1029	6/6	0.83	0.22	23,27,28,31	0
8	PEG	B	1023	7/7	0.84	0.26	39,47,51,52	0
5	EDO	A	310	4/4	0.84	0.25	35,43,45,50	0
4	DMS	A	304	4/4	0.86	0.15	26,28,38,47	0
5	EDO	B	1025	4/4	0.86	0.19	42,42,44,47	0
4	DMS	B	1006	4/4	0.86	0.24	27,48,53,63	0
4	DMS	B	1009	4/4	0.87	0.21	32,40,41,44	0
4	DMS	B	1008	4/4	0.87	0.22	52,57,60,64	0
9	GOL	B	1028	6/6	0.89	0.18	29,33,34,39	0
4	DMS	B	1016	4/4	0.89	0.26	47,51,61,66	0
6	CL	B	1032	1/1	0.90	0.04	68,68,68,68	0
6	CL	B	1033	1/1	0.90	0.22	75,75,75,75	0
5	EDO	B	1026	4/4	0.90	0.12	23,28,33,40	0
8	PEG	B	1015	7/7	0.91	0.18	23,29,32,48	0
4	DMS	B	1001	4/4	0.91	0.29	38,39,44,47	0
5	EDO	A	303	4/4	0.91	0.12	22,25,31,32	0
3	F6F	A	309	21/21	0.91	0.17	26,40,47,55	21
4	DMS	B	1010	4/4	0.92	0.21	59,72,74,74	0
4	DMS	A	307	4/4	0.92	0.21	20,27,32,36	0
4	DMS	B	1005	4/4	0.92	0.13	30,32,32,39	0
4	DMS	B	1018	4/4	0.92	0.12	36,43,47,48	0
4	DMS	B	1019	4/4	0.92	0.23	32,44,47,51	0
4	DMS	B	1021	4/4	0.92	0.25	37,41,53,57	0
4	DMS	B	1020	4/4	0.93	0.20	34,36,40,47	0
4	DMS	A	305	4/4	0.93	0.14	33,39,40,47	0
4	DMS	B	1011	4/4	0.93	0.28	52,53,55,57	0
5	EDO	B	1027	4/4	0.93	0.26	44,47,47,55	0
6	CL	A	311	1/1	0.94	0.03	66,66,66,66	0

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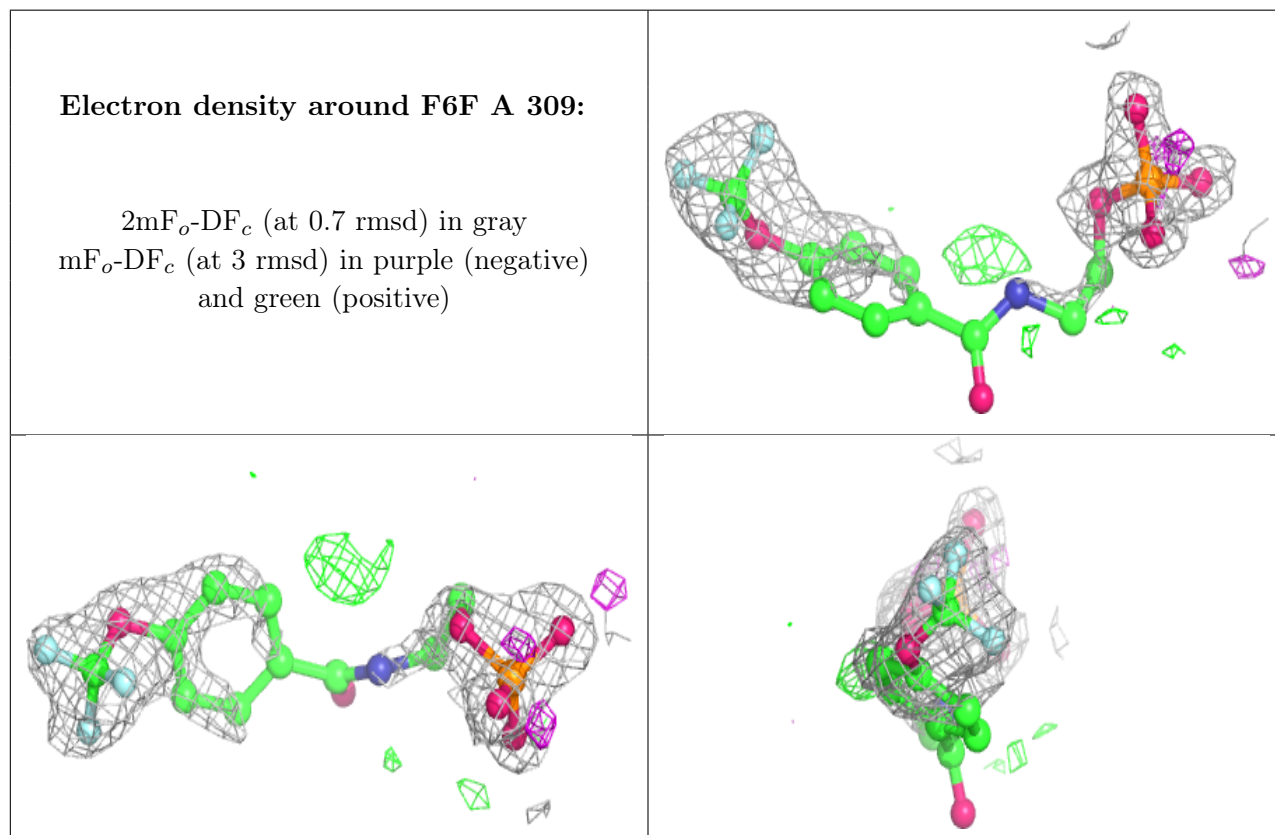
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	A	308	4/4	0.94	0.18	34,35,35,48	0
4	DMS	B	1024	4/4	0.94	0.22	41,43,44,48	0
3	F6F	B	1003	21/21	0.94	0.10	22,24,27,27	0
4	DMS	A	306	4/4	0.95	0.26	43,43,50,52	0
4	DMS	B	1012	4/4	0.95	0.17	63,66,66,72	0
3	F6F	A	301	21/21	0.95	0.09	18,21,26,31	0
4	DMS	A	302	4/4	0.95	0.11	20,24,24,30	0
4	DMS	B	1017	4/4	0.96	0.19	29,32,33,37	0
4	DMS	B	1004	4/4	0.97	0.19	37,46,46,52	0
7	PLP	B	1002	15/16	0.99	0.12	10,11,13,14	0
4	DMS	B	1022	4/4	0.99	0.17	14,20,24,27	0
10	NA	B	1031	1/1	1.00	0.11	15,15,15,15	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.

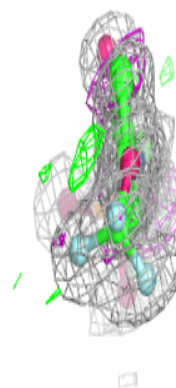
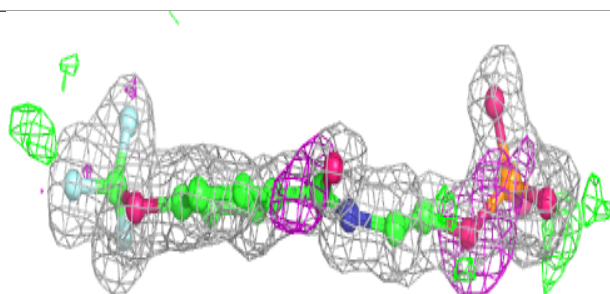
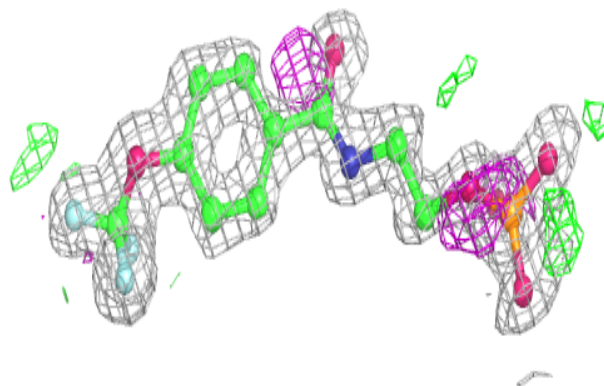
Electron density around F6F A 309:

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

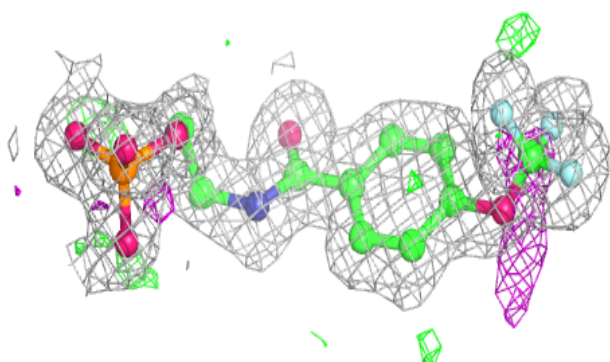
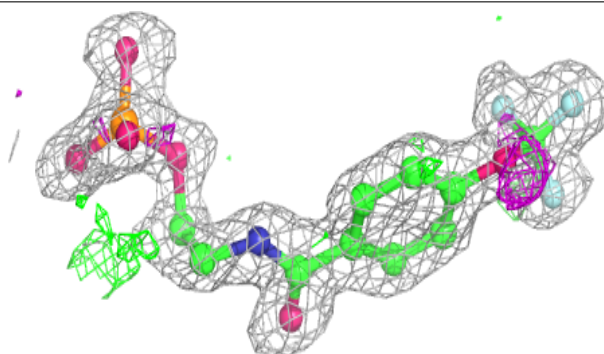


Electron density around F6F B 1003:

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

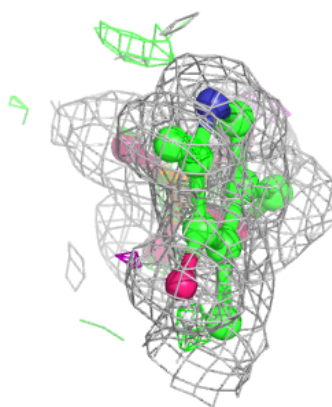
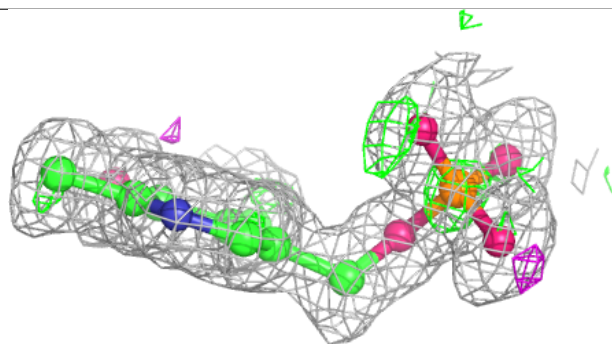
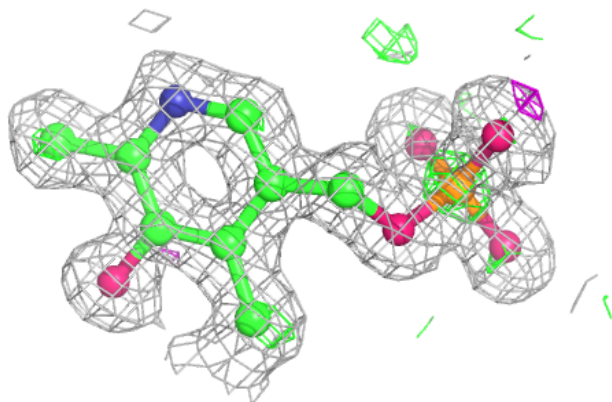
**Electron density around F6F A 301:**

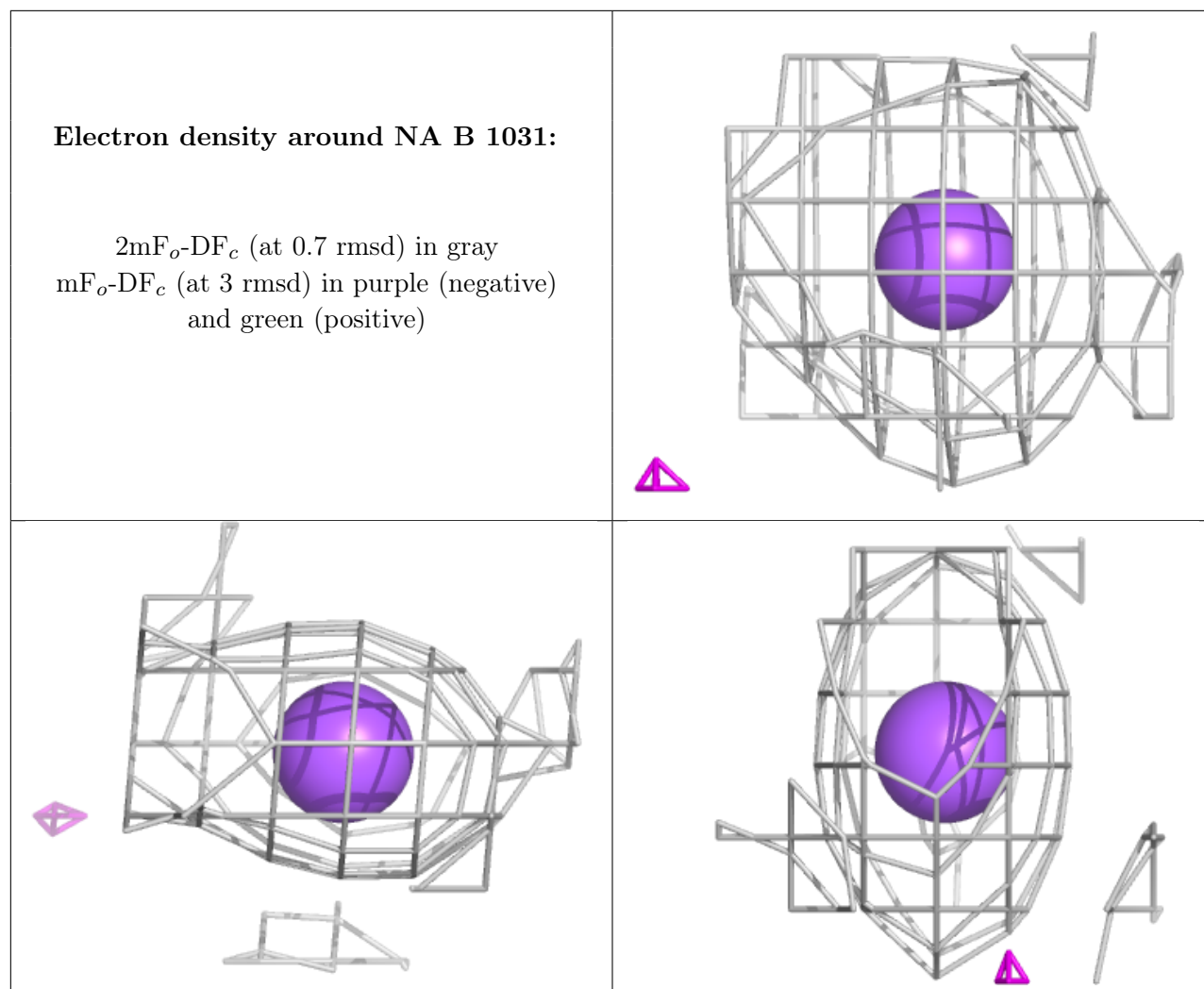
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PLP B 1002:

$2mF_o-DF_c$ (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.