



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2021 – 04:18 PM EDT

PDB ID : 4HT3
Title : The crystal structure of Salmonella typhimurium Tryptophan Synthase at 1.30Å complexed with N-(4'-TRIFLUOROMETHOXYBENZENESULFONYL)-2-AMINO-1-ETHYLPHOSPHATE (F9) inhibitor in the alpha site, internal aldimine
Authors : Hilario, E.; Niks, D.; Dunn, M.F.; Mueller, L.J.; Fan, L.
Deposited on : 2012-10-31
Resolution : 1.30 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 : 2.23.1
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) : 2.23.1

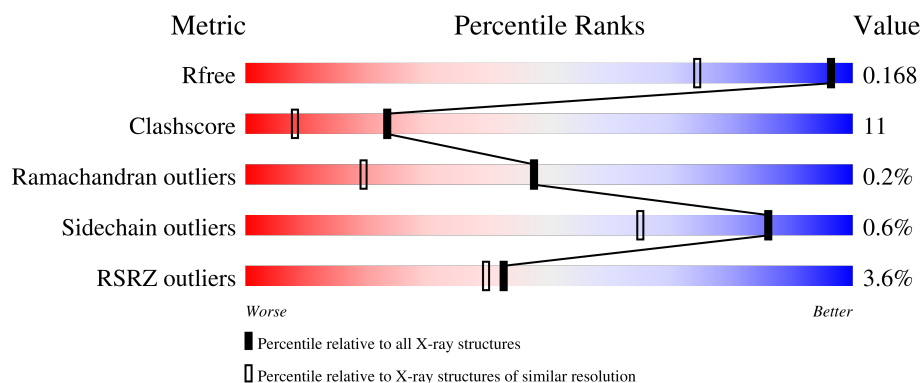
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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>5%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
2	B	397	<div> <div>3%</div> <div>87%</div> <div>12%</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
11	PEG	B	416	-	-	X	-
5	CL	B	423	-	-	X	-
7	PGE	A	305	-	-	X	-
7	PGE	B	403	-	-	X	-
8	PG5	A	306	-	-	X	-
9	EDO	B	402	-	-	X	-
9	EDO	B	409	-	-	X	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 6251 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.

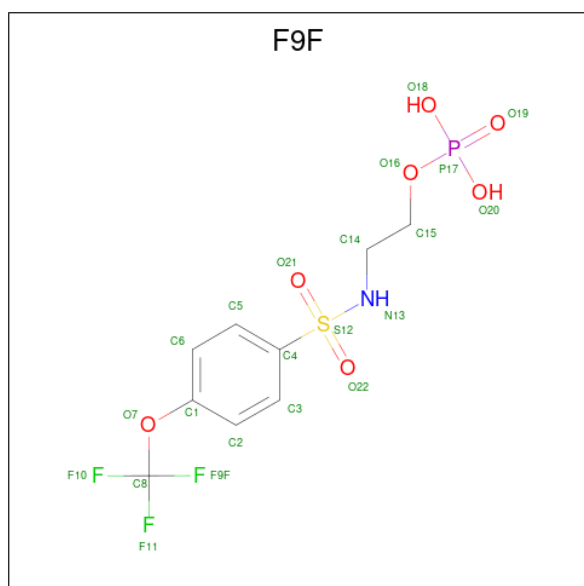
- Molecule 1 is a protein called Tryptophan synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	18	0
			2104	1340	363	392	9			

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

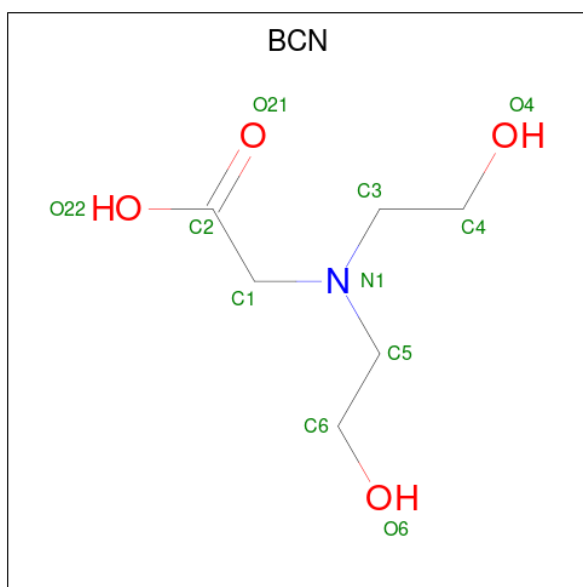
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	393	Total	C	N	O	S	0	35	0
			3190	2026	545	595	24			

- Molecule 3 is 2-([4-(TRIFLUOROMETHOXY)PHENYL]SULFONYL)AMINO)ETHYL DIHYDROGEN PHOSPHATE (three-letter code: F9F) (formula: C₉H₁₁F₃NO₇PS).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	P	S	0	0
			22	9	3	1	7	1	1		

- Molecule 4 is BICINE (three-letter code: BCN) (formula: C₆H₁₃NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			11	6	1	4		
4	B	1	Total	C	N	O	0	0
			11	6	1	4		
4	B	1	Total	C	N	O	0	0
			11	6	1	4		
4	B	1	Total	C	N	O	0	0
			11	6	1	4		

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

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

- Molecule 6 is CESIUM ION (three-letter code: CS) (formula: Cs).

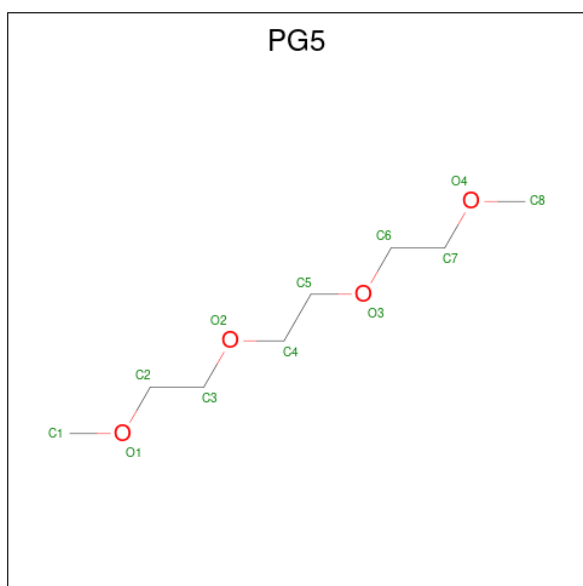
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cs	0	0
			1	1		
6	B	2	Total	Cs	0	1
			4	4		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



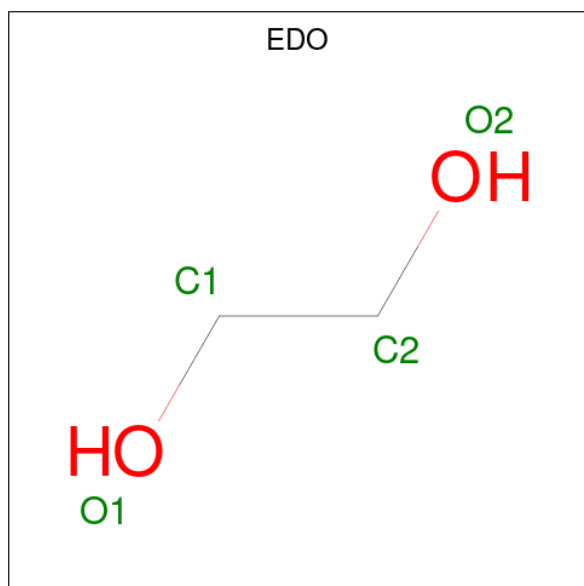
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	6	4		
7	B	1	Total	C	O	0	0
			10	6	4		
7	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is 1-METHOXY-2-[2-(2-METHOXY-ETHOXY)]-ETHANE (three-letter code: PG5) (formula: $C_8H_{18}O_4$).



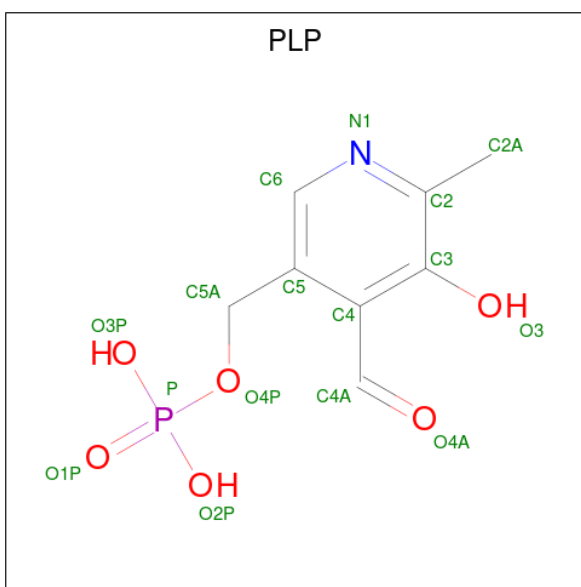
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			12	8	4		

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



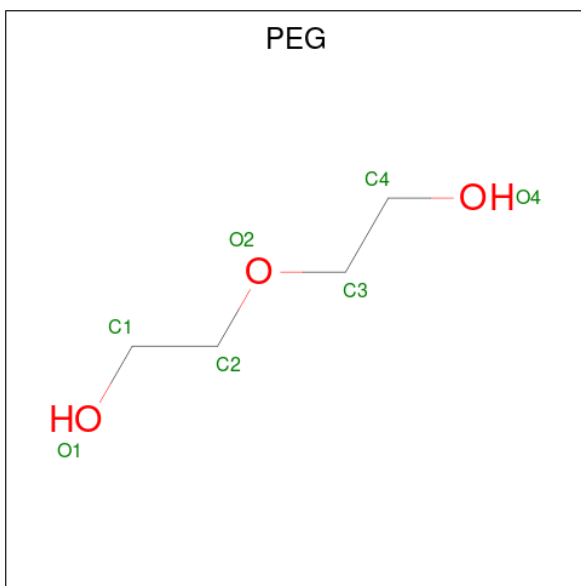
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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

- Molecule 11 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

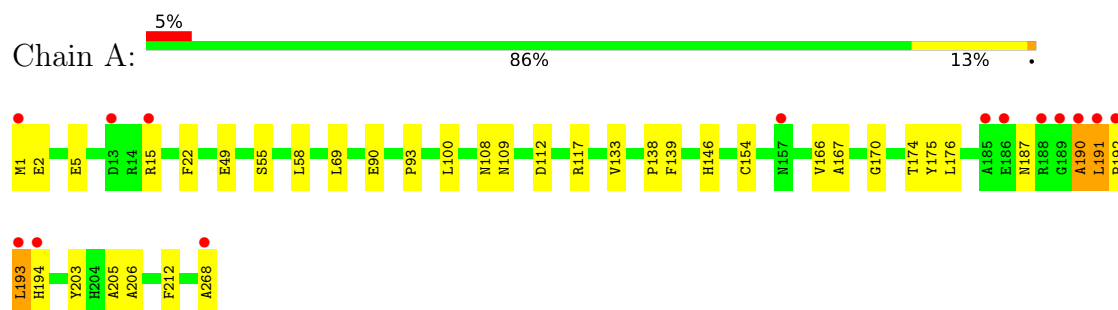
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	306	Total 306	O 306	0	0
12	B	459	Total 462	O 462	0	3

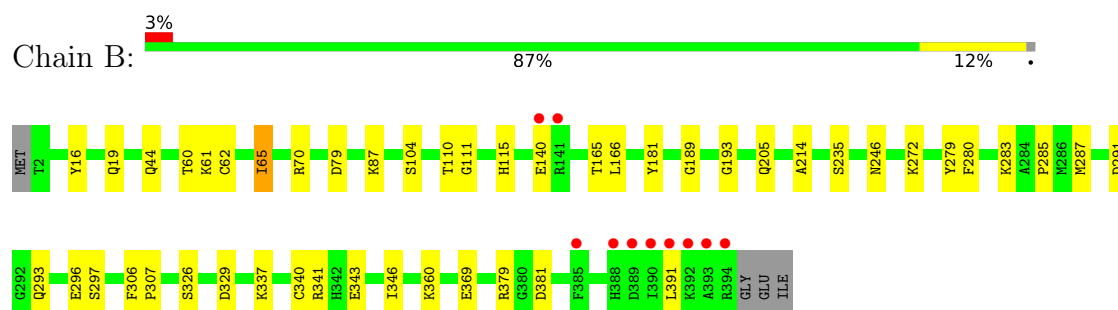
3 Residue-property plots

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	181.85Å 59.14Å 67.30Å 90.00° 94.74° 90.00°	Depositor
Resolution (Å)	18.36 – 1.30 18.36 – 1.30	Depositor EDS
% Data completeness (in resolution range)	95.1 (18.36-1.30) 95.2 (18.36-1.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.89 (at 1.30Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.131 , 0.169 0.129 , 0.168	Depositor DCC
R_{free} test set	8300 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	10.1	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 59.7	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	0.97	EDS
Total number of atoms	6251	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.14% 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: CS, F9F, PG5, PEG, PLP, EDO, BCN, PGE, 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	0.56	0/2198	0.73	0/2982
2	B	0.58	0/3341	0.75	2/4505 (0.0%)
All	All	0.57	0/5539	0.74	2/7487 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	291	ASP	CB-CG-OD2	-5.43	113.41	118.30
2	B	329	ASP	CB-CG-OD2	-5.03	113.77	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190	ALA	Peptide

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	2104	0	2159	51	0
2	B	3190	0	3260	58	0
3	A	22	0	9	1	0
4	A	11	0	12	0	0
4	B	33	0	36	1	0
5	A	1	0	0	0	0
5	B	6	0	0	4	0
6	A	1	0	0	0	0
6	B	4	0	0	0	0
7	A	10	0	14	13	0
7	B	20	0	28	12	0
8	A	12	0	18	12	0
9	A	12	0	18	5	0
9	B	28	0	42	15	0
10	B	15	0	6	0	0
11	B	14	0	20	7	0
12	A	306	0	0	4	0
12	B	462	0	0	19	0
All	All	6251	0	5622	125	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 11.

All (125) 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:A:90:GLU:OE2	9:A:309:EDO:H12	1.14	1.27
1:A:2:GLU:HB3	1:A:5:GLU:OE1	1.38	1.23
7:A:305:PGE:C3	2:B:283:LYS:HZ1	1.63	1.12
1:A:69:LEU:HD11	12:B:926:HOH:O	1.51	1.09
1:A:90:GLU:OE2	9:A:309:EDO:C1	2.01	1.08
1:A:190:ALA:HB1	1:A:191:LEU:CB	1.85	1.07
1:A:190:ALA:CB	1:A:191:LEU:HB3	1.87	1.04
1:A:170:GLY:O	8:A:306:PG5:H32	1.58	1.02
1:A:190:ALA:HB1	1:A:191:LEU:HB3	1.01	1.00
7:A:305:PGE:H3	2:B:283:LYS:HZ1	1.27	0.97
2:B:165[B]:THR:HG22	12:B:899:HOH:O	1.69	0.90
2:B:165[B]:THR:HG22	2:B:166:LEU:H	1.39	0.87
7:A:305:PGE:C3	2:B:283:LYS:NZ	2.38	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296[B]:GLU:HG3	12:B:950:HOH:O	1.75	0.86
1:A:58:LEU:HD21	12:B:955:HOH:O	1.75	0.85
1:A:139:PHE:HE2	7:A:305:PGE:H12	1.43	0.83
2:B:60:THR:CG2	11:B:416:PEG:H12	2.11	0.80
1:A:203:TYR:O	8:A:306:PG5:H72	1.81	0.80
7:A:305:PGE:H3	2:B:283:LYS:NZ	1.98	0.79
1:A:2:GLU:CB	1:A:5:GLU:OE1	2.29	0.77
2:B:165[B]:THR:CG2	12:B:899:HOH:O	2.29	0.77
7:B:403:PGE:H6	5:B:423:CL:CL	2.23	0.76
1:A:139:PHE:HE2	7:A:305:PGE:C1	1.99	0.75
7:B:403:PGE:O4	5:B:423:CL:CL	2.41	0.74
1:A:58:LEU:CD2	12:B:955:HOH:O	2.33	0.73
1:A:138:PRO:HG2	7:A:305:PGE:H1	1.71	0.72
2:B:61:LYS:O	11:B:416:PEG:H21	1.89	0.72
7:A:305:PGE:H32	2:B:283:LYS:NZ	2.05	0.71
1:A:206:ALA:H	8:A:306:PG5:C2	2.03	0.71
2:B:104:SER:OG	12:B:916:HOH:O	2.04	0.70
1:A:69:LEU:CD1	12:B:926:HOH:O	2.24	0.70
1:A:90:GLU:CD	9:A:309:EDO:H12	2.09	0.69
2:B:379[B]:ARG:NH1	12:B:912:HOH:O	2.25	0.69
2:B:272:LYS:HD2	7:B:403:PGE:H22	1.75	0.69
7:B:403:PGE:C6	5:B:423:CL:CL	2.77	0.69
2:B:62[B]:CYS:SG	2:B:65[B]:ILE:HD11	2.33	0.68
2:B:165[B]:THR:HG21	2:B:296[B]:GLU:OE2	1.95	0.67
2:B:111:GLY:N	9:B:402:EDO:O2	2.26	0.65
1:A:206:ALA:H	8:A:306:PG5:H22	1.59	0.65
1:A:93:PRO:CG	9:A:308:EDO:H22	2.27	0.65
1:A:167:ALA:O	8:A:306:PG5:H21	1.98	0.64
2:B:60:THR:HG21	11:B:416:PEG:H12	1.80	0.64
2:B:87:LYS:HE2	9:B:402:EDO:H12	1.79	0.63
1:A:1:MET:O	1:A:2:GLU:HG2	2.02	0.60
2:B:306[A]:PHE:CD1	2:B:307[A]:PRO:HD2	2.36	0.60
1:A:139:PHE:CE2	7:A:305:PGE:C1	2.83	0.60
7:A:305:PGE:H52	12:A:435:HOH:O	2.01	0.60
1:A:205:ALA:HA	8:A:306:PG5:H22	1.83	0.58
9:B:409:EDO:H12	11:B:416:PEG:O4	2.04	0.57
1:A:112:ASP:OD1	1:A:146:HIS:HE1	1.87	0.57
8:A:306:PG5:H11	12:A:663:HOH:O	2.03	0.57
2:B:140:GLU:HG3	12:B:832:HOH:O	2.05	0.56
2:B:111:GLY:H	9:B:402:EDO:C2	2.19	0.56
2:B:306[A]:PHE:CD1	2:B:307[A]:PRO:CD	2.90	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55[B]:SER:OG	2:B:293:GLN:HB3	2.07	0.54
2:B:62[B]:CYS:HB2	2:B:343:GLU:CD	2.27	0.54
1:A:192:PRO:N	1:A:193:LEU:HA	2.21	0.54
2:B:360[A]:LYS:HG3	12:B:547:HOH:O	2.06	0.54
2:B:341[A]:ARG:HD2	12:B:566:HOH:O	2.08	0.54
2:B:165[B]:THR:HG22	2:B:166:LEU:N	2.17	0.53
1:A:15:ARG:O	1:A:268:ALA:HB2	2.08	0.53
7:A:305:PGE:H2	2:B:16:TYR:OH	2.09	0.52
2:B:44[A]:GLN:HG3	12:B:682:HOH:O	2.08	0.52
1:A:117[B]:ARG:NH2	12:A:628:HOH:O	2.43	0.52
2:B:326:SER:OG	9:B:410:EDO:H12	2.10	0.52
1:A:187:ASN:ND2	12:A:672:HOH:O	2.43	0.52
2:B:87:LYS:HE2	9:B:402:EDO:C1	2.40	0.51
2:B:110:THR:HG1	9:B:402:EDO:C2	2.23	0.51
2:B:214:ALA:HB3	7:B:417:PGE:H62	1.92	0.51
1:A:139:PHE:CE2	7:A:305:PGE:H1	2.45	0.50
2:B:181[B]:TYR:CE1	12:B:525:HOH:O	2.63	0.50
1:A:166:VAL:O	8:A:306:PG5:H13	2.12	0.49
1:A:192:PRO:HB2	1:A:193:LEU:HA	1.93	0.49
1:A:93:PRO:HG2	9:A:308:EDO:H22	1.94	0.49
2:B:379[B]:ARG:HD2	2:B:381:ASP:OD2	2.13	0.48
1:A:192:PRO:CB	1:A:193:LEU:HA	2.42	0.48
9:B:409:EDO:H21	11:B:416:PEG:O4	2.13	0.48
1:A:175:TYR:CE2	3:A:301:F9F:H5	2.48	0.48
2:B:285:PRO:HG3	5:B:423:CL:CL	2.51	0.48
2:B:115:HIS:HB3	9:B:402:EDO:H22	1.95	0.47
2:B:272:LYS:CD	7:B:403:PGE:H22	2.43	0.47
1:A:154[B]:CYS:SG	1:A:166:VAL:HG11	2.54	0.47
1:A:133[B]:VAL:HG23	2:B:19:GLN:OE1	2.14	0.47
1:A:190:ALA:HB1	1:A:191:LEU:CA	2.41	0.47
7:B:403:PGE:H1	7:B:403:PGE:H3	1.32	0.46
2:B:296[B]:GLU:HG2	2:B:297[B]:SER:O	2.16	0.45
9:B:409:EDO:C1	11:B:416:PEG:O4	2.65	0.45
7:B:403:PGE:O4	7:B:403:PGE:O2	2.35	0.45
9:B:413:EDO:O2	9:B:414:EDO:H11	2.16	0.45
9:B:413:EDO:O2	9:B:414:EDO:C1	2.64	0.45
11:B:416:PEG:H21	11:B:416:PEG:H41	1.79	0.44
1:A:22:PHE:HA	1:A:49:GLU:O	2.17	0.44
2:B:306[A]:PHE:HA	2:B:307[A]:PRO:HD3	1.78	0.44
1:A:206:ALA:N	8:A:306:PG5:H22	2.30	0.44
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:305:PGE:C2	2:B:16:TYR:OH	2.65	0.43
2:B:70:ARG:CZ	2:B:369[B]:GLU:HG2	2.48	0.43
2:B:272:LYS:CE	7:B:403:PGE:H22	2.47	0.43
2:B:287[B]:MET:HA	2:B:287[B]:MET:CE	2.48	0.43
2:B:337:LYS:HD3	2:B:391:LEU:HD11	2.00	0.43
4:B:405:BCN:O6	9:B:414:EDO:H21	2.19	0.43
1:A:100:LEU:C	1:A:100:LEU:HD13	2.39	0.43
2:B:166:LEU:HD11	9:B:419:EDO:H21	2.01	0.42
1:A:193:LEU:HB2	1:A:194:HIS:H	1.71	0.42
2:B:205:GLN:HG3	2:B:235[B]:SER:OG	2.19	0.42
1:A:108[B]:ASN:HD22	1:A:108[B]:ASN:HA	1.47	0.42
1:A:192:PRO:HB2	1:A:193:LEU:CA	2.49	0.42
2:B:61:LYS:HE2	12:B:820:HOH:O	2.19	0.42
2:B:340[B]:CYS:SG	2:B:346:ILE:HG12	2.59	0.41
1:A:108[A]:ASN:ND2	1:A:109:ASN:OD1	2.53	0.41
1:A:174:THR:OG1	8:A:306:PG5:H12	2.21	0.41
2:B:44[B]:GLN:HG3	12:B:658:HOH:O	2.20	0.41
2:B:246:ASN:HB2	12:B:894:HOH:O	2.21	0.41
9:B:409:EDO:H22	12:B:553:HOH:O	2.19	0.41
2:B:62[B]:CYS:HB2	2:B:343:GLU:OE2	2.19	0.41
1:A:167:ALA:O	8:A:306:PG5:C2	2.68	0.41
2:B:193:GLY:HA2	2:B:280:PHE:O	2.21	0.41
2:B:279:TYR:CG	2:B:280:PHE:N	2.89	0.41
2:B:79:ASP:HB2	2:B:379[A]:ARG:HB3	2.03	0.40
7:B:417:PGE:H5	12:B:756[A]:HOH:O	2.22	0.40
1:A:170:GLY:HA3	8:A:306:PG5:H13	2.02	0.40
1:A:176:LEU:HD21	1:A:192:PRO:HB3	2.02	0.40
1:A:190:ALA:CA	1:A:191:LEU:HB3	2.49	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	284/268 (106%)	279 (98%)	4 (1%)	1 (0%)	34	10
2	B	428/397 (108%)	420 (98%)	8 (2%)	0	100	100
All	All	712/665 (107%)	699 (98%)	12 (2%)	1 (0%)	47	20

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	226/208 (109%)	224 (99%)	2 (1%)	78	53
2	B	345/311 (111%)	343 (99%)	2 (1%)	86	65
All	All	571/519 (110%)	567 (99%)	4 (1%)	86	61

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

Mol	Chain	Res	Type
1	A	191	LEU
1	A	193	LEU
2	B	65[A]	ILE
2	B	65[B]	ILE

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 34 ligands modelled in this entry, 12 are monoatomic - leaving 22 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	$\# Z > 2$
11	PEG	B	416	-	6,6,6	0.88	0	5,5,5	1.38	0
9	EDO	B	421	-	3,3,3	0.51	0	2,2,2	0.14	0
7	PGE	B	403	-	9,9,9	0.49	0	8,8,8	0.93	0
9	EDO	A	309	-	3,3,3	0.36	0	2,2,2	0.40	0
4	BCN	B	406	-	7,10,10	0.50	0	8,11,11	1.55	1 (12%)
8	PG5	A	306	-	11,11,11	0.91	0	10,10,10	1.19	2 (20%)
9	EDO	A	307	-	3,3,3	0.49	0	2,2,2	0.46	0
3	F9F	A	301	-	22,22,22	1.57	3 (13%)	32,33,33	1.44	6 (18%)
9	EDO	B	410	-	3,3,3	0.96	0	2,2,2	0.63	0
4	BCN	B	407	-	7,10,10	0.45	0	8,11,11	0.78	0
9	EDO	B	414	-	3,3,3	0.53	0	2,2,2	0.14	0
11	PEG	B	415	-	6,6,6	0.37	0	5,5,5	0.46	0
9	EDO	B	413	-	3,3,3	0.31	0	2,2,2	0.57	0
4	BCN	A	302	-	7,10,10	0.38	0	8,11,11	1.47	1 (12%)
9	EDO	B	419	-	3,3,3	0.68	0	2,2,2	0.19	0
9	EDO	A	308	-	3,3,3	0.38	0	2,2,2	0.69	0
4	BCN	B	405	-	7,10,10	0.42	0	8,11,11	1.33	1 (12%)
9	EDO	B	402	-	3,3,3	0.28	0	2,2,2	0.88	0
10	PLP	B	401	2	15,15,16	2.04	3 (20%)	20,22,23	1.72	5 (25%)
7	PGE	B	417	-	9,9,9	0.64	0	8,8,8	0.47	0
7	PGE	A	305	-	9,9,9	0.69	0	8,8,8	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	EDO	B	409	-	3,3,3	0.51	0	2,2,2	0.36	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
11	PEG	B	416	-	-	1/4/4/4	-
9	EDO	B	421	-	-	1/1/1/1	-
7	PGE	B	403	-	-	4/7/7/7	-
9	EDO	A	309	-	-	1/1/1/1	-
4	BCN	B	406	-	-	2/8/10/10	-
8	PG5	A	306	-	-	7/9/9/9	-
9	EDO	A	307	-	-	1/1/1/1	-
3	F9F	A	301	-	-	6/20/20/20	0/1/1/1
9	EDO	B	410	-	-	1/1/1/1	-
4	BCN	B	407	-	-	3/8/10/10	-
9	EDO	B	414	-	-	1/1/1/1	-
11	PEG	B	415	-	-	4/4/4/4	-
9	EDO	B	413	-	-	1/1/1/1	-
4	BCN	A	302	-	-	5/8/10/10	-
9	EDO	B	419	-	-	1/1/1/1	-
9	EDO	A	308	-	-	1/1/1/1	-
4	BCN	B	405	-	-	2/8/10/10	-
9	EDO	B	402	-	-	1/1/1/1	-
10	PLP	B	401	2	-	0/6/6/8	0/1/1/1
7	PGE	B	417	-	-	3/7/7/7	-
7	PGE	A	305	-	-	5/7/7/7	-
9	EDO	B	409	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	401	PLP	C5-C4	5.99	1.47	1.40
3	A	301	F9F	C4-S12	-5.89	1.67	1.76
10	B	401	PLP	C2-N1	-2.35	1.29	1.33
3	A	301	F9F	C5-C4	2.28	1.42	1.38
10	B	401	PLP	C3-C2	2.08	1.43	1.40
3	A	301	F9F	C3-C4	2.01	1.42	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	302	BCN	C2-C1-N1	-3.83	108.02	113.48
3	A	301	F9F	O22-S12-O21	-3.76	114.93	119.55
10	B	401	PLP	C6-N1-C2	3.75	126.11	119.17
4	B	406	BCN	C2-C1-N1	-3.38	108.66	113.48
4	B	405	BCN	C2-C1-N1	-3.34	108.73	113.48
10	B	401	PLP	O4P-C5A-C5	3.05	115.16	109.35
3	A	301	F9F	C5-C4-C3	-2.98	116.28	120.44
10	B	401	PLP	C3-C4-C5	-2.89	115.62	118.74
3	A	301	F9F	C5-C4-S12	2.70	122.70	119.77
3	A	301	F9F	C6-C5-C4	2.60	122.14	119.45
10	B	401	PLP	C2A-C2-N1	2.54	122.63	117.67
3	A	301	F9F	O21-S12-C4	2.51	111.06	107.97
10	B	401	PLP	C4A-C4-C5	2.47	123.48	120.94
8	A	306	PG5	C1-O1-C2	2.13	126.21	112.96
8	A	306	PG5	O2-C3-C2	2.10	119.85	110.39
3	A	301	F9F	C14-N13-S12	-2.09	113.65	120.41

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	403	PGE	C1-C2-O2-C3
11	B	415	PEG	O1-C1-C2-O2
11	B	416	PEG	C4-C3-O2-C2
7	A	305	PGE	C6-C5-O3-C4
7	B	417	PGE	O3-C5-C6-O4
7	A	305	PGE	O1-C1-C2-O2
4	A	302	BCN	C2-C1-N1-C3
7	A	305	PGE	O3-C5-C6-O4
9	A	308	EDO	O1-C1-C2-O2
9	A	309	EDO	O1-C1-C2-O2
9	B	413	EDO	O1-C1-C2-O2
7	B	403	PGE	O2-C3-C4-O3
8	A	306	PG5	O2-C4-C5-O3
3	A	301	F9F	C3-C4-S12-O21
7	B	417	PGE	O1-C1-C2-O2
11	B	415	PEG	O2-C3-C4-O4
9	B	414	EDO	O1-C1-C2-O2
4	A	302	BCN	C2-C1-N1-C5
4	B	407	BCN	N1-C3-C4-O4
3	A	301	F9F	C5-C4-S12-O21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	B	419	EDO	O1-C1-C2-O2
4	B	407	BCN	C2-C1-N1-C3
7	B	403	PGE	O3-C5-C6-O4
4	B	406	BCN	C2-C1-N1-C5
7	A	305	PGE	C4-C3-O2-C2
11	B	415	PEG	C4-C3-O2-C2
3	A	301	F9F	N13-C14-C15-O16
11	B	415	PEG	C1-C2-O2-C3
7	A	305	PGE	C1-C2-O2-C3
7	B	403	PGE	C4-C3-O2-C2
8	A	306	PG5	C7-C6-O3-C5
4	B	405	BCN	C2-C1-N1-C3
4	B	406	BCN	C2-C1-N1-C3
9	A	307	EDO	O1-C1-C2-O2
8	A	306	PG5	C6-C7-O4-C8
4	A	302	BCN	C4-C3-N1-C5
4	B	407	BCN	C2-C1-N1-C5
3	A	301	F9F	C3-C4-S12-N13
3	A	301	F9F	C6-C1-O7-C8
8	A	306	PG5	C4-C5-O3-C6
4	A	302	BCN	C6-C5-N1-C3
4	A	302	BCN	C6-C5-N1-C1
3	A	301	F9F	C2-C1-O7-C8
4	B	405	BCN	C2-C1-N1-C5
8	A	306	PG5	C2-C3-O2-C4
8	A	306	PG5	O1-C2-C3-O2
7	B	417	PGE	C6-C5-O3-C4
9	B	402	EDO	O1-C1-C2-O2
9	B	409	EDO	O1-C1-C2-O2
9	B	410	EDO	O1-C1-C2-O2
9	B	421	EDO	O1-C1-C2-O2
8	A	306	PG5	O3-C6-C7-O4

There are no ring outliers.

15 monomers are involved in 62 short contacts:

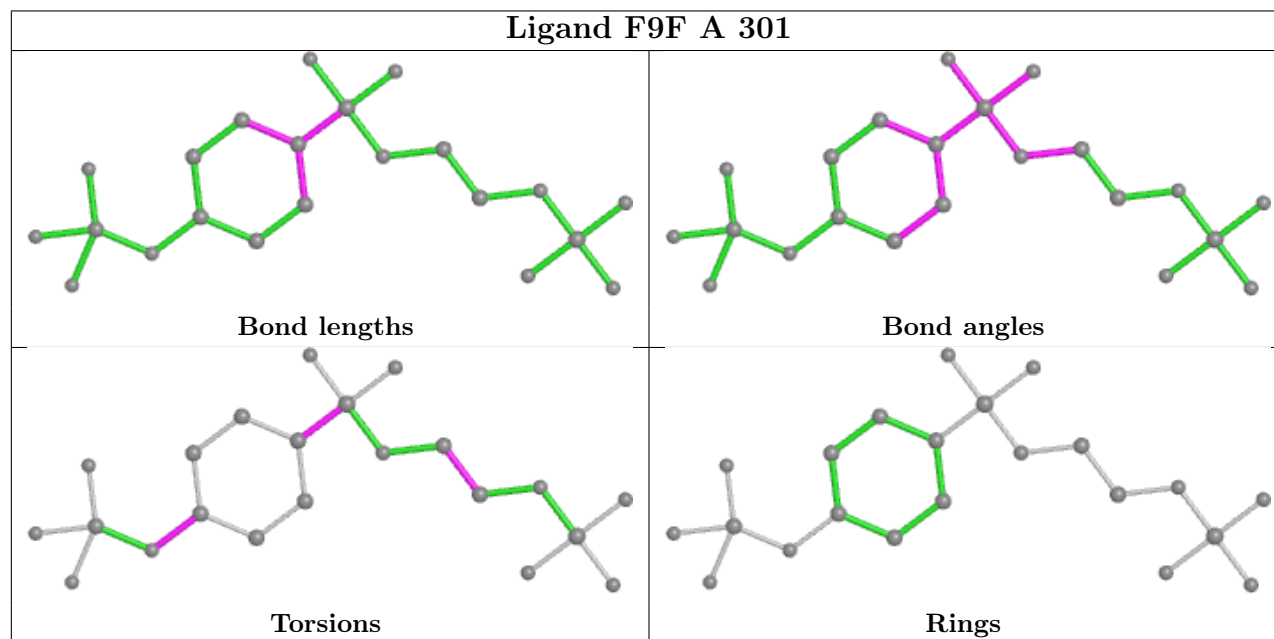
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	416	PEG	7	0
7	B	403	PGE	10	0
9	A	309	EDO	3	0
8	A	306	PG5	12	0
3	A	301	F9F	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	410	EDO	1	0
9	B	414	EDO	3	0
9	B	413	EDO	2	0
9	B	419	EDO	1	0
9	A	308	EDO	2	0
4	B	405	BCN	1	0
9	B	402	EDO	6	0
7	B	417	PGE	2	0
7	A	305	PGE	13	0
9	B	409	EDO	4	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

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	268/268 (100%)	-0.09	14 (5%) 27 24	7, 14, 32, 59	8 (2%)
2	B	393/397 (98%)	-0.25	10 (2%) 57 56	6, 11, 24, 75	5 (1%)
All	All	661/665 (99%)	-0.18	24 (3%) 42 39	6, 13, 30, 75	13 (1%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	LEU	14.4
1	A	193	LEU	6.3
2	B	393	ALA	6.1
2	B	392	LYS	5.7
1	A	192	PRO	5.5
2	B	391	LEU	5.4
1	A	1	MET	4.2
2	B	385	PHE	4.1
1	A	190	ALA	4.1
2	B	394	ARG	4.0
2	B	390	ILE	3.8
1	A	13	ASP	3.3
1	A	268	ALA	3.1
1	A	157[A]	ASN	3.1
1	A	189	GLY	2.9
2	B	141	ARG	2.8
1	A	194	HIS	2.6
1	A	186	GLU	2.5
2	B	140	GLU	2.4
1	A	15	ARG	2.4
2	B	388	HIS	2.3
1	A	185	ALA	2.3
2	B	389	ASP	2.1
1	A	188	ARG	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, 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.

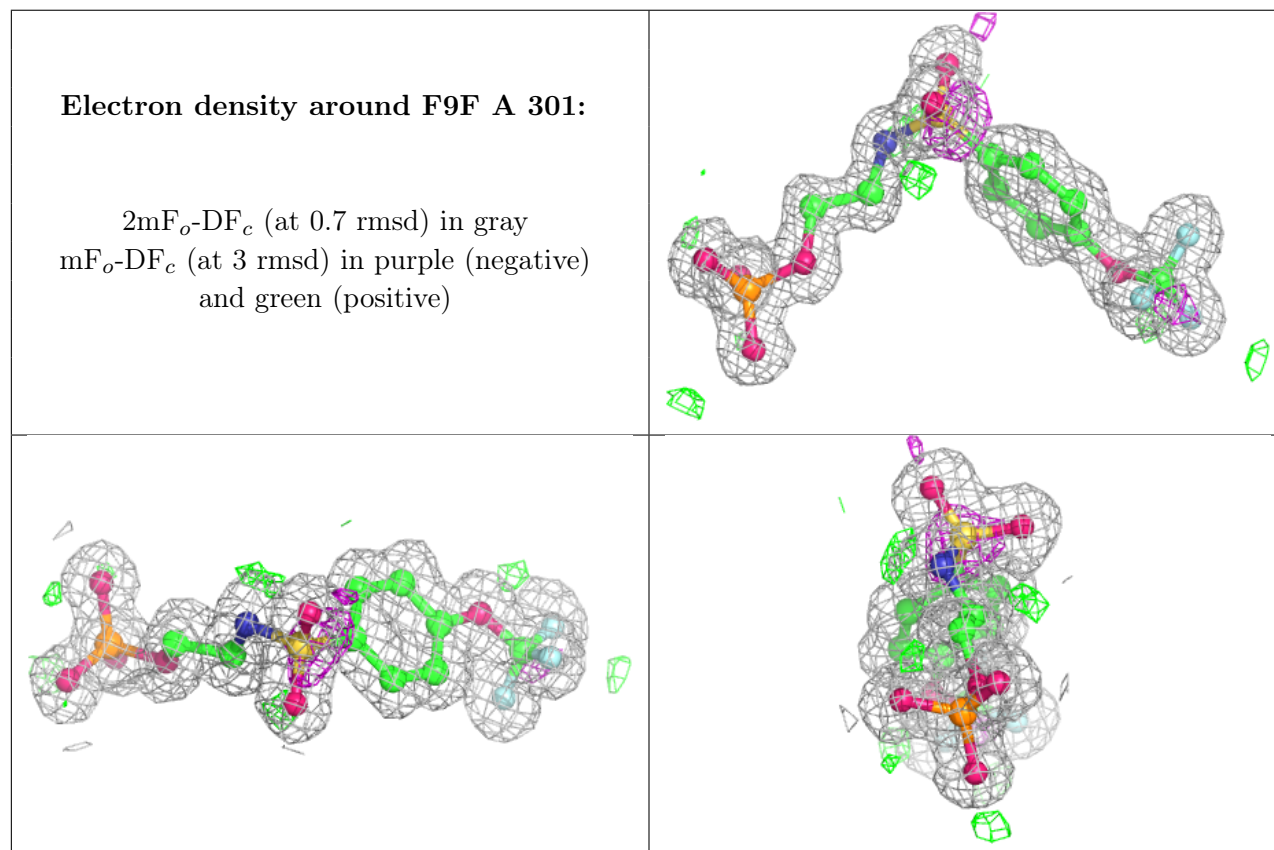
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	PEG	B	415	7/7	0.73	0.19	39,44,58,59	0
9	EDO	B	421	4/4	0.79	0.26	34,35,43,43	0
8	PG5	A	306	12/12	0.83	0.23	13,27,38,42	0
7	PGE	B	403	10/10	0.84	0.20	16,27,34,41	0
11	PEG	B	416	7/7	0.84	0.20	16,18,27,36	0
7	PGE	B	417	10/10	0.85	0.18	23,33,40,48	0
9	EDO	B	409	4/4	0.86	0.18	24,28,31,45	0
9	EDO	B	419	4/4	0.87	0.14	28,28,32,32	0
9	EDO	B	410	4/4	0.90	0.18	15,23,32,35	0
4	BCN	B	405	11/11	0.90	0.19	15,27,36,44	0
9	EDO	A	309	4/4	0.90	0.26	30,32,37,40	0
9	EDO	B	402	4/4	0.90	0.17	19,23,26,29	0
7	PGE	A	305	10/10	0.90	0.14	20,25,33,34	0
9	EDO	B	414	4/4	0.91	0.18	34,35,36,39	0
5	CL	B	418	1/1	0.92	0.12	65,65,65,65	0
4	BCN	B	407	11/11	0.92	0.22	19,29,40,40	0
9	EDO	B	413	4/4	0.93	0.24	25,29,30,42	0
4	BCN	A	302	11/11	0.93	0.28	27,40,56,62	0
9	EDO	A	308	4/4	0.93	0.25	30,32,35,37	0
4	BCN	B	406	11/11	0.94	0.10	11,19,22,22	0
9	EDO	A	307	4/4	0.95	0.20	25,26,36,50	0
5	CL	B	420	1/1	0.95	0.14	44,44,44,44	0
5	CL	B	404	1/1	0.96	0.22	58,58,58,58	0
5	CL	B	408	1/1	0.96	0.09	57,57,57,57	0
5	CL	A	303	1/1	0.98	0.08	41,41,41,41	0
5	CL	B	423	1/1	0.99	0.13	30,30,30,30	0
6	CS	B	412[A]	1/1	0.99	0.04	10,10,10,10	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	CS	B	412[B]	1/1	0.99	0.04	14,14,14,14	1
10	PLP	B	401	15/16	0.99	0.04	7,9,16,18	0
6	CS	B	412[C]	1/1	0.99	0.04	15,15,15,15	1
3	F9F	A	301	22/22	0.99	0.04	11,12,15,17	0
6	CS	B	411	1/1	1.00	0.04	12,12,12,12	1
5	CL	B	422	1/1	1.00	0.02	21,21,21,21	0
6	CS	A	304	1/1	1.00	0.04	12,12,12,12	1

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.



6.5 Other polymers ⓘ

There are no such residues in this entry.