



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2022 – 04:49 pm BST

PDB ID : 7QXD
Title : Recognition of Staphylococcus aureus wall teichoic acid analogue SA475 (compound 2) by Fab4497
Authors : Soriano-Maldonado, P.; van Raaij, M.J.
Deposited on : 2022-01-26
Resolution : 1.65 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.30

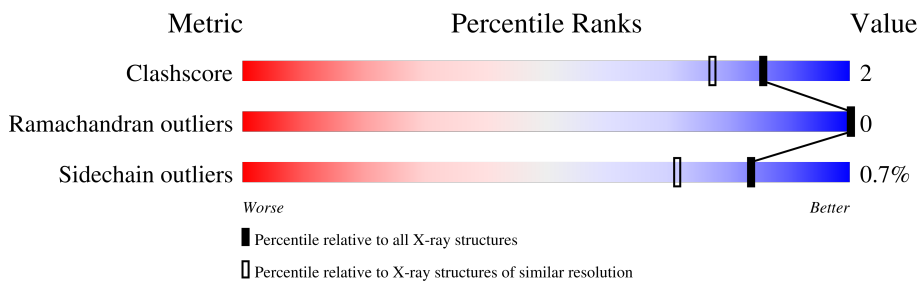
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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))
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)

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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	HHH	236	
1	KKK	236	
2	LLL	220	
2	MMM	220	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7623 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.

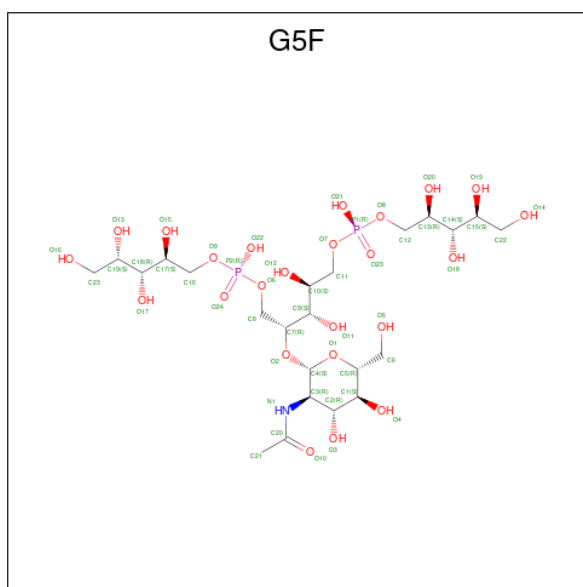
- Molecule 1 is a protein called Antibody Fab 4497 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	HHH	214	Total 1608	C 1014	N 272	O 316	S 6	0	3	0
1	KKK	215	Total 1614	C 1017	N 274	O 317	S 6	0	2	0

- Molecule 2 is a protein called Antibody Fab 4497 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	LLL	219	Total 1721	C 1080	N 296	O 341	S 4	0	1	0
2	MMM	219	Total 1726	C 1083	N 299	O 340	S 4	0	1	0

- Molecule 3 is [(2 {S},3 {S},4 {R})-4-[(2 {S},3 {R},4 {R},5 {S},6 {R})-3-acetamido-6-(hydroxymethyl)-4,5-bis(oxidanyl)oxan-2-yl]oxy-5-[[2 {S},3 {R})-2,3-bis(oxidanyl)butoxy]-oxidanyl-phosphoryl]oxy-2,3-bis(oxidanyl)pentyl] [(2 {R},3 {S},4 {S})-2,3,4,5-tetrakis(oxidanyl)pentyl] hydrogen phosphate (three-letter code: G5F) (formula: C₂₃H₄₇NO₂₄P₂) (labeled as "Ligand of Interest" by depositor).



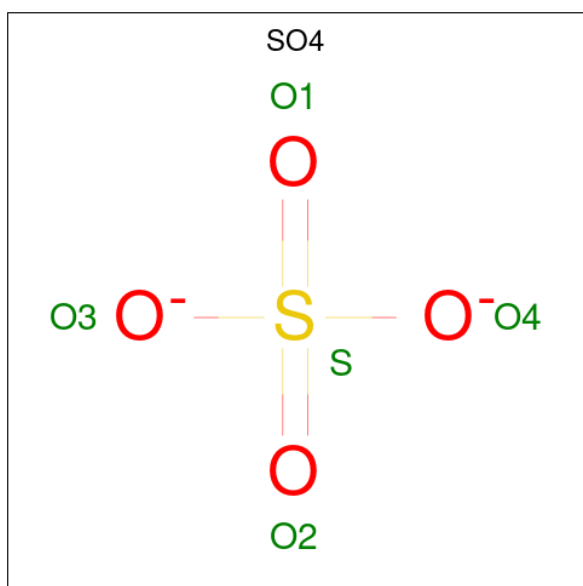
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
3	HHH	1	47	22	1	22	2	0	0
3	MMM	1	49	23	1	23	2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



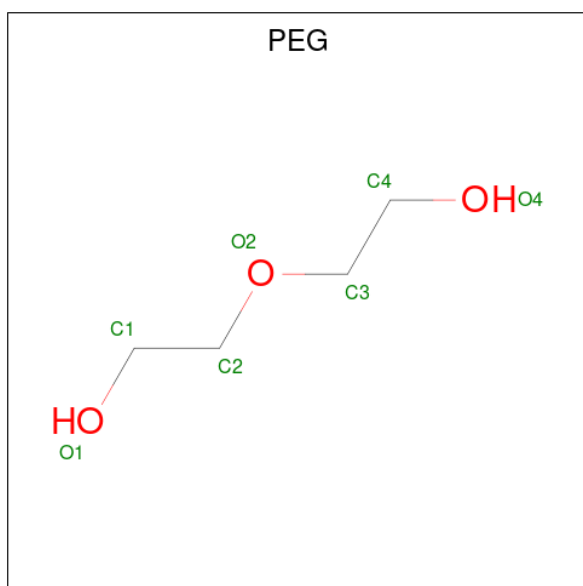
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C O		
4	LLL	1	6	3 3	0	0
4	KKK	1	6	3 3	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	LLL	1	Total	O	S	0	0
			5	4	1		
5	MMM	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	KKK	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	HHH	195	Total O 197 197	0	2
7	LLL	176	Total O 178 178	0	2
7	KKK	188	Total O 192 192	0	4
7	MMM	259	Total O 262 262	0	3

4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.39Å 113.37Å 154.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.02 – 1.65	Depositor
% Data completeness (in resolution range)	93.0 (90.02-1.65)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 1.65Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.175 , 0.202	Depositor
Wilson B-factor (Å ²)	23.3	Xtrriage
Anisotropy	0.230	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7623	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: PEG, GOL, G5F, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	HHH	0.70	1/1654 (0.1%)	0.83	0/2251
1	KKK	0.70	0/1657	0.82	0/2256
2	LLL	0.67	0/1763	0.83	1/2393 (0.0%)
2	MMM	0.71	0/1768	0.88	1/2399 (0.0%)
All	All	0.69	1/6842 (0.0%)	0.84	2/9299 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	HHH	151	GLU	CD-OE2	5.79	1.32	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	LLL	31	ARG	NE-CZ-NH2	-6.40	117.10	120.30
2	MMM	148	ARG	NE-CZ-NH1	6.09	123.35	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	HHH	1608	0	1567	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	KKK	1614	0	1578	8	1
2	LLL	1721	0	1680	7	1
2	MMM	1726	0	1688	7	0
3	HHH	47	0	0	0	0
3	MMM	49	0	0	0	0
4	KKK	6	0	8	2	0
4	LLL	6	0	8	0	0
5	LLL	5	0	0	0	0
5	MMM	5	0	0	0	0
6	KKK	7	0	10	0	0
7	HHH	197	0	0	0	0
7	KKK	192	0	0	2	0
7	LLL	178	0	0	0	0
7	MMM	262	0	0	1	0
All	All	7623	0	6539	29	1

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 2.

All (29) 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:KKK:104:ASP:OD1	2:MMM:51[A]:ARG:NH2	2.08	0.84
2:LLL:155:LYS:NZ	2:LLL:201:GLU:OE1	2.24	0.67
4:KKK:302:GOL:H11	7:KKK:441:HOH:O	1.96	0.66
2:MMM:51[A]:ARG:HG3	7:MMM:519:HOH:O	1.99	0.60
4:KKK:302:GOL:C1	7:KKK:441:HOH:O	2.51	0.58
1:KKK:68:PHE:O	1:KKK:69:ILE:HD13	2.09	0.52
2:MMM:51[A]:ARG:HH11	2:MMM:52:LEU:H	1.55	0.52
2:MMM:51[A]:ARG:NH1	2:MMM:52:LEU:H	2.07	0.52
1:HHH:181:LEU:C	1:HHH:181:LEU:HD12	2.34	0.48
1:HHH:202:ASN:ND2	1:HHH:209:LYS:HE2	2.29	0.48
2:LLL:39:LEU:HD22	2:LLL:77:PHE:CG	2.48	0.48
2:MMM:39:LEU:HD22	2:MMM:77:PHE:CG	2.49	0.47
2:MMM:39:LEU:HD22	2:MMM:77:PHE:CB	2.44	0.47
2:LLL:100:PRO:HA	2:LLL:101:PRO:C	2.35	0.46
1:KKK:22:CYS:HB3	1:KKK:79:LEU:HB3	1.97	0.46
1:HHH:22:CYS:HB3	1:HHH:79:LEU:HB3	1.99	0.45
1:KKK:181:LEU:C	1:KKK:181:LEU:HD12	2.37	0.45
2:LLL:205:GLN:O	1:KKK:1:GLU:HB2	2.16	0.45
1:HHH:51:THR:OG1	1:HHH:55:GLY:HA2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LLL:84:LEU:HD11	2:LLL:110:LEU:HD21	1.99	0.44
1:HHH:98:ARG:CZ	1:HHH:100[A]:ASP:OD1	2.65	0.44
1:HHH:83:MET:HB3	1:HHH:86:LEU:HD21	1.99	0.43
2:MMM:100:PRO:HA	2:MMM:101:PRO:C	2.38	0.43
2:LLL:89:VAL:HG21	2:LLL:172:GLN:HB3	2.01	0.42
1:KKK:48:ILE:HD13	1:KKK:48:ILE:HA	1.86	0.42
2:LLL:39:LEU:HD22	2:LLL:77:PHE:CB	2.51	0.41
1:HHH:204:LYS:N	1:HHH:205:PRO:CD	2.84	0.41
1:KKK:83:MET:HE2	1:KKK:86:LEU:HD21	2.03	0.40
1:KKK:204:LYS:N	1:KKK:205:PRO:CD	2.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LLL:33:SER:O	1:KKK:31:SER:OG[3_544]	2.10	0.10

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	HHH	213/236 (90%)	207 (97%)	6 (3%)	0	100	100
1	KKK	213/236 (90%)	207 (97%)	6 (3%)	0	100	100
2	LLL	218/220 (99%)	215 (99%)	3 (1%)	0	100	100
2	MMM	218/220 (99%)	215 (99%)	3 (1%)	0	100	100
All	All	862/912 (94%)	844 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	HHH	179/194 (92%)	177 (99%)	2 (1%)	73	55
1	KKK	181/194 (93%)	180 (99%)	1 (1%)	86	75
2	LLL	196/196 (100%)	195 (100%)	1 (0%)	88	80
2	MMM	196/196 (100%)	195 (100%)	1 (0%)	88	80
All	All	752/780 (96%)	747 (99%)	5 (1%)	84	71

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	HHH	50	PHE
1	HHH	132	LYS
2	LLL	97	TYR
1	KKK	50	PHE
2	MMM	97	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	LLL	301	-	5,5,5	0.21	0	5,5,5	0.65	0
4	GOL	KKK	302	-	5,5,5	0.06	0	5,5,5	0.29	0
5	SO4	LLL	302	-	4,4,4	0.15	0	6,6,6	0.12	0
3	G5F	HHH	301	-	47,47,50	0.43	0	64,67,71	0.78	4 (6%)
3	G5F	MMM	301	-	48,49,50	0.48	0	64,70,71	0.78	2 (3%)
6	PEG	KKK	301	-	6,6,6	0.35	0	5,5,5	0.31	0
5	SO4	MMM	302	-	4,4,4	0.25	0	6,6,6	0.26	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
4	GOL	LLL	301	-	-	4/4/4/4	-
4	GOL	KKK	302	-	-	2/4/4/4	-
3	G5F	HHH	301	-	-	6/56/76/82	0/1/1/1
3	G5F	MMM	301	-	-	7/60/80/82	0/1/1/1
6	PEG	KKK	301	-	-	1/4/4/4	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	MMM	301	G5F	O17-C18-C17	2.91	115.85	108.81
3	HHH	301	G5F	C4-C3-N1	-2.46	106.77	111.00
3	HHH	301	G5F	O21-P1-O23	2.18	123.01	112.24
3	HHH	301	G5F	O9-C16-C17	2.05	114.83	109.36
3	HHH	301	G5F	O9-P2-O24	-2.01	101.23	109.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	MMM	301	G5F	O22-P2-O24	2.00	122.14	112.24

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	HHH	301	G5F	O19-C15-C22-O14
3	MMM	301	G5F	C16-C17-C18-O17
3	MMM	301	G5F	O15-C17-C18-C19
3	MMM	301	G5F	O15-C17-C18-O17
3	MMM	301	G5F	C17-C18-C19-O13
4	LLL	301	GOL	O1-C1-C2-C3
4	LLL	301	GOL	C1-C2-C3-O3
4	KKK	302	GOL	C1-C2-C3-O3
3	HHH	301	G5F	C14-C15-C22-O14
3	MMM	301	G5F	C16-C17-C18-C19
3	MMM	301	G5F	C17-C18-C19-C23
3	MMM	301	G5F	O17-C18-C19-O13
4	LLL	301	GOL	O2-C2-C3-O3
6	KKK	301	PEG	C1-C2-O2-C3
3	HHH	301	G5F	C16-O9-P2-O22
3	HHH	301	G5F	C13-C14-C15-O19
4	KKK	302	GOL	O2-C2-C3-O3
3	HHH	301	G5F	C16-O9-P2-O6
4	LLL	301	GOL	O1-C1-C2-O2
3	HHH	301	G5F	C16-O9-P2-O24

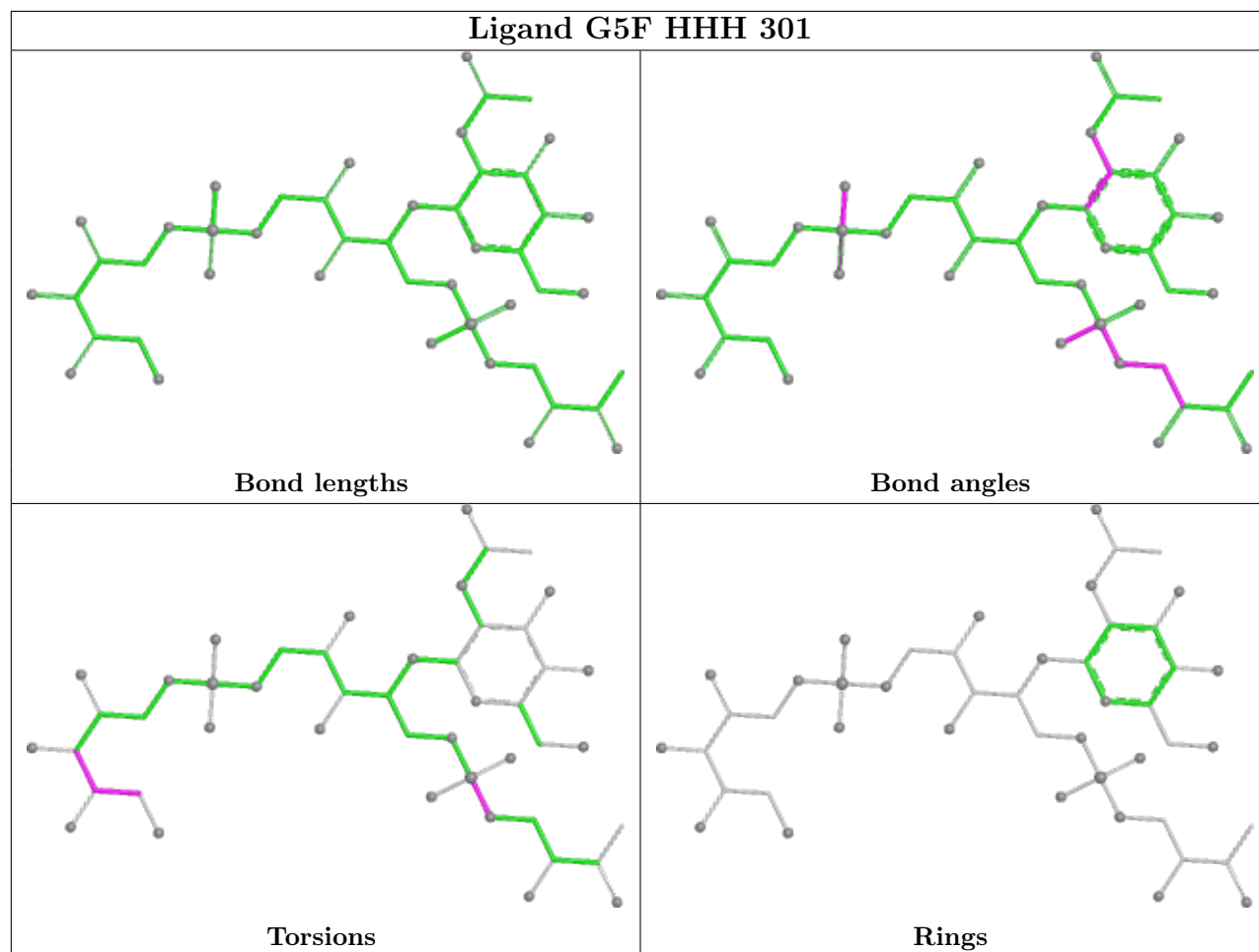
There are no ring outliers.

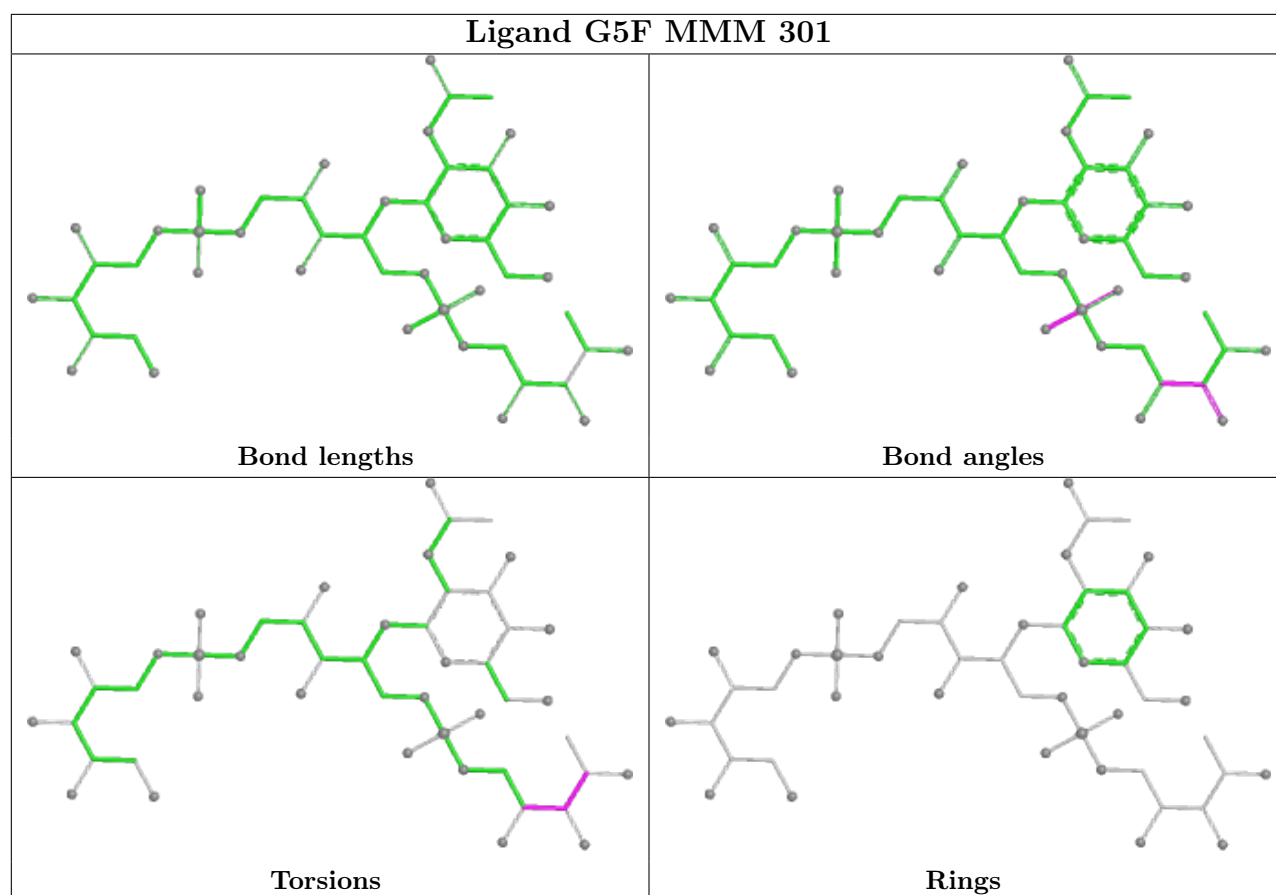
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	KKK	302	GOL	2	0

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

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.