

Full wwPDB X-ray Structure Validation Report (i)

Aug 25, 2022 – 04:09 pm BST

PDB ID : 7QXE

Title: Recognition of Staphylococcus aureus wall teichoic acid analogue TB87 (com-

pound 3) by Fab4497

Authors: Soriano-Maldonado, P.; van Raaij, M.J.

Deposited on : 2022-01-26

Resolution : 1.84 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (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)

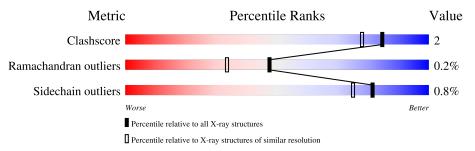
Validation Pipeline (wwPDB-VP) : 2.30

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 1.84 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain		
1	ННН	236	84%	7%	9%
1	KKK	236	86%	6%	9%
2	LLL	220	92%		8%
2	MMM	220	95%		•



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7296 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.

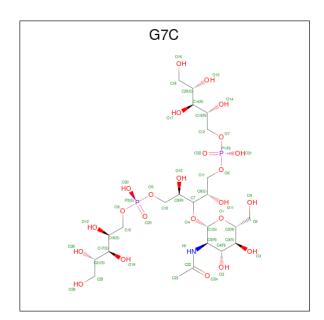
Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
1	ННН	215	Total 1608	C 1012	N 274	O 316	S 6	0	1	0
1	KKK	215	Total 1608	C 1012	N 274	O 316	S 6	0	2	0

• Molecule 2 is a protein called Antibody 4497 light chain.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	2 LLL	219	Total	С	N	О	S	0	0	0
		213	1718	1078	296	340	4			
9	ммм	219	Total	С	N	O	S	0	0	0
2	MMM	219	1718	1078	296	340	4		U	

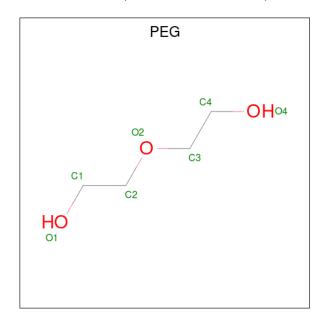
• Molecule 3 is [(2 {S},4 {R})-3-[(2 {S},3 {R},4 {R},5 {S},6 {R})-3-acetamido-6-(hydroxyme thyl)-4,5-bis(oxidanyl)oxan-2-yl]oxy-2,4-bis(oxidanyl)-5-[oxidanyl-[(2 {S})-2,3,4,5-tetrakis(oxidanyl)pentoxy]phosphoryl]oxy-pentyl] [(2 {R},3 {S})-2,3,4,5-tetrakis(oxidanyl)pentyl] hydrogen phosphate (three-letter code: G7C) (formula: C₂₃H₄₇NO₂₄P₂) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	ннн	1	Total	С	N	О	Р	0	0
3	111111		42	20	1	19	2	U	
9	KKK	1	Total	С	N	О	Р	0	0
3	3 KKK	1	49	23	1	23	2	U	0

 $\bullet \ \, \text{Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$)}. \\$



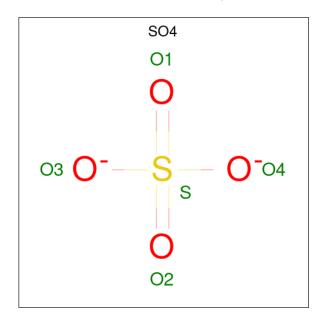
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	ННН	1	Total C O 7 4 3	0	0
4	LLL	1	Total C O 7 4 3	0	0



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

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

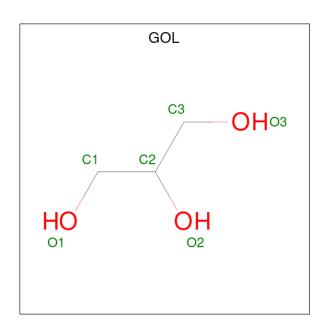
 \bullet Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: $\mathrm{O_4S}).$



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

 \bullet Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $\mathrm{C_3H_8O_3}).$





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

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	ННН	118	Total O 118 118	0	0
8	LLL	103	Total O 103 103	0	0
8	KKK	138	Total O 138 138	0	0
8	MMM	148	Total O 148 148	0	0

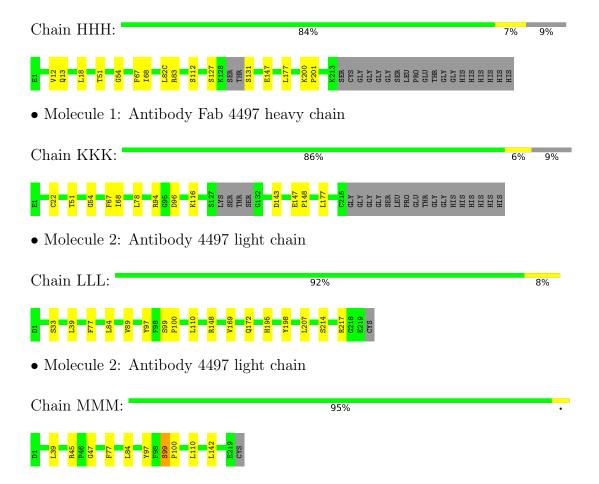


3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS failed to run properly.

• Molecule 1: Antibody Fab 4497 heavy chain





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	64.03Å 112.92Å 154.99Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.00 - 1.84	Depositor
% Data completeness	99.8 (46.00-1.84)	Depositor
(in resolution range)	33.0 (10.00 1.01)	_
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.52 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.188 , 0.218	Depositor
Wilson B-factor (\mathring{A}^2)	34.1	Xtriage
Anisotropy	0.358	Xtriage
L-test for twinning ²	$ < L > = 0.50, < L^2> = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7296	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: CL, GOL, PEG, SO4, G7C

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	Bo	nd lengths	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	ННН	0.67	0/1648	0.83	0/2243	
1	KKK	0.66	0/1651	0.83	0/2248	
2	LLL	0.66	1/1757 (0.1%)	0.83	0/2385	
2	MMM	0.66	0/1757	0.85	0/2385	
All	All	0.66	1/6813 (0.0%)	0.83	0/9261	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$Ideal(\AA)$
2	LLL	33	SER	C-N	8.47	1.53	1.34

There are no bond angle outliers.

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	ННН	1608	0	1570	8	0
1	KKK	1608	0	1566	7	0
2	LLL	1718	0	1675	8	0
2	MMM	1718	0	1675	7	0
3	ННН	42	0	0	0	0
3	KKK	49	0	0	0	0



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Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
4	ННН	7	0	10	0	0
4	LLL	7	0	10	0	0
5	ННН	1	0	0	0	0
6	LLL	10	0	0	0	0
6	MMM	15	0	0	0	0
7	KKK	6	0	8	0	0
8	ННН	118	0	0	1	1
8	KKK	138	0	0	2	1
8	LLL	103	0	0	1	0
8	MMM	148	0	0	1	0
All	All	7296	0	6514	30	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 (30) 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:LLL:207:LEU:O	8:LLL:401:HOH:O	2.01	0.77
1:HHH:147:GLU:OE2	8:HHH:401:HOH:O	2.15	0.64
2:MMM:47:GLY:C	8:MMM:428:HOH:O	2.44	0.55
1:KKK:116:LYS:HE3	8:KKK:444:HOH:O	2.07	0.55
2:LLL:195:HIS:O	2:LLL:217:ARG:NH1	2.39	0.55
1:KKK:67:PHE:O	1:KKK:68:ILE:HD13	2.07	0.55
1:HHH:67:PHE:O	1:HHH:68:ILE:HD13	2.07	0.55
1:HHH:177:LEU:C	1:HHH:177:LEU:HD12	2.29	0.52
2:LLL:89:VAL:HG21	2:LLL:172:GLN:HB3	1.90	0.52
1:KKK:177:LEU:C	1:KKK:177:LEU:HD12	2.30	0.52
2:LLL:84:LEU:HD11	2:LLL:110:LEU:HD21	1.91	0.51
1:KKK:51:THR:OG1	1:KKK:54:GLY:HA2	2.12	0.50
1:HHH:51:THR:OG1	1:HHH:54:GLY:HA2	2.14	0.48
1:KKK:147:GLU:OE2	8:KKK:401:HOH:O	2.20	0.48
1:HHH:200:LYS:N	1:HHH:201:PRO:CD	2.80	0.44
1:KKK:94:ARG:NH2	1:KKK:96:ASP:OD2	2.50	0.44
2:MMM:39:LEU:HD22	2:MMM:77:PHE:CG	2.52	0.44
2:MMM:45:ARG:HB3	2:MMM:45:ARG:CZ	2.48	0.44
2:LLL:39:LEU:HD22	2:LLL:77:PHE:CG	2.54	0.43
1:KKK:22:CYS:HB3	1:KKK:78:LEU:HB3	2.01	0.42
1:HHH:13:GLN:OE1	1:HHH:112:SER:HA	2.19	0.42
2:MMM:142:LEU:HD12	2:MMM:142:LEU:N	2.35	0.42
1:HHH:12:VAL:HG11	1:HHH:82(C):LEU:HD13	2.01	0.42



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Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	$\text{distance } (\text{\AA})$	overlap (Å)
2:MMM:84:LEU:HD11	2:MMM:110:LEU:HD21	2.01	0.42
2:LLL:99:SER:HA	2:LLL:100:PRO:HD3	1.96	0.42
1:HHH:18:LEU:HD12	1:HHH:18:LEU:HA	1.90	0.41
2:LLL:148:ARG:NH2	2:LLL:169:VAL:HG21	2.35	0.41
2:MMM:39:LEU:HD22	2:MMM:77:PHE:CB	2.50	0.40
2:LLL:198:TYR:O	2:LLL:214:SER:HA	2.21	0.40
2:MMM:99:SER:HA	2:MMM:100:PRO:HD3	1.98	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	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
8:HHH:416:HOH:O	8:KKK:513:HOH:O[2_554]	2.17	0.03

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	Perce	ntiles
1	ННН	212/236~(90%)	207 (98%)	4 (2%)	1 (0%)	29	15
1	KKK	213/236~(90%)	208 (98%)	4 (2%)	1 (0%)	29	15
2	LLL	217/220~(99%)	213 (98%)	4 (2%)	0	100	100
2	MMM	217/220~(99%)	213 (98%)	4 (2%)	0	100	100
All	All	859/912 (94%)	841 (98%)	16 (2%)	2 (0%)	47	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	ННН	127	SER
1	KKK	143	ASP



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	Perc		$_{ m ntiles}$
1	ННН	180/194~(93%)	178 (99%)	2 (1%)		73	64
1	KKK	180/194 (93%)	179 (99%)	1 (1%)		86	82
2	LLL	195/196 (100%)	194 (100%)	1 (0%)		88	85
2	MMM	195/196 (100%)	193 (99%)	2 (1%)		76	68
All	All	750/780 (96%)	744 (99%)	6 (1%)		81	75

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	ННН	83	ARG
1	ННН	131	SER
2	LLL	97	TYR
1	KKK	148	PRO
2	MMM	97	TYR
2	MMM	99	SER

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.



5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 1 is 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	Trmo	Chain	Res	Link	Во	ond leng	ths	В	ond ang	cles
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	LLL	302	-	4,4,4	0.23	0	6,6,6	0.17	0
6	SO4	MMM	301	-	4,4,4	0.29	0	6,6,6	0.25	0
7	GOL	KKK	302	-	5,5,5	0.11	0	5, 5, 5	0.29	0
3	G7C	ННН	301	-	41,42,50	0.52	0	56,60,71	1.35	8 (14%)
4	PEG	LLL	301	-	6,6,6	0.27	0	5,5,5	0.21	0
6	SO4	MMM	302	-	4,4,4	0.35	0	6,6,6	0.10	0
4	PEG	ННН	302	-	6,6,6	0.21	0	5,5,5	0.16	0
6	SO4	MMM	303	-	4,4,4	0.32	0	6,6,6	0.14	0
3	G7C	KKK	301	-	48,49,50	0.41	0	65,70,71	1.04	3 (4%)
6	SO4	LLL	303	-	4,4,4	0.35	0	6,6,6	0.06	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
7	GOL	KKK	302	_	-	1/4/4/4	-
3	G7C	ННН	301	-	-	28/46/66/82	0/1/1/1
4	PEG	LLL	301	-	-	2/4/4/4	-
4	PEG	ННН	302	-	-	2/4/4/4	_
3	G7C	KKK	301	-	-	24/60/80/82	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathbf{Ideal}(^{o})$
3	ННН	301	G7C	O4-C7-C9	5.67	115.79	107.98
3	KKK	301	G7C	O4-C7-C8	3.31	112.54	107.98



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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
3	ННН	301	G7C	C1-O4-C7	2.95	125.26	117.96
3	ННН	301	G7C	O10-C9-C10	-2.84	103.53	109.92
3	ННН	301	G7C	O11-C8-C7	-2.80	102.43	109.14
3	KKK	301	G7C	C8-C7-C9	-2.78	107.70	113.59
3	ННН	301	G7C	O10-C9-C7	2.71	115.65	109.14
3	ННН	301	G7C	C11-C8-C7	2.44	116.40	111.61
3	KKK	301	G7C	C13-C14-C20	2.30	118.15	113.36
3	ННН	301	G7C	O4-C1-C5	-2.14	104.55	108.24
3	ННН	301	G7C	O21-P1-O22	2.03	122.27	112.24

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	ННН	301	G7C	O4-C7-C8-O11
3	ННН	301	G7C	C8-C7-C9-C10
3	ННН	301	G7C	C8-C7-C9-O10
3	ННН	301	G7C	O4-C7-C9-C10
3	ННН	301	G7C	O4-C7-C9-O10
3	ННН	301	G7C	C8-C7-O4-C1
3	ННН	301	G7C	C9-C7-O4-C1
3	ННН	301	G7C	O7-C12-C13-O14
3	ННН	301	G7C	O7-C12-C13-C14
3	ННН	301	G7C	O8-C15-C16-O12
3	ННН	301	G7C	C11-O6-P1-O22
3	ННН	301	G7C	C12-O7-P1-O22
3	ННН	301	G7C	C12-C13-C14-C20
3	ННН	301	G7C	C12-C13-C14-O17
3	ННН	301	G7C	C15-O8-P2-O5
3	ННН	301	G7C	C15-O8-P2-O20
3	ННН	301	G7C	C15-O8-P2-O23
3	KKK	301	G7C	O7-C12-C13-O14
3	KKK	301	G7C	O7-C12-C13-C14
3	KKK	301	G7C	O8-C15-C16-C17
3	KKK	301	G7C	C16-C17-C21-C25
3	KKK	301	G7C	C16-C17-C21-O26
3	KKK	301	G7C	O19-C17-C21-O26
3	KKK	301	G7C	C12-O7-P1-O21
3	KKK	301	G7C	C12-O7-P1-O22
3	KKK	301	G7C	C12-O7-P1-O6
3	KKK	301	G7C	O14-C13-C14-C20
3	KKK	301	G7C	O14-C13-C14-O17



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Mol	Chain	Res	Type	Atoms
3	KKK	301	G7C	C15-O8-P2-O5
3	KKK	301	G7C	C15-O8-P2-O20
3	KKK	301	G7C	C15-O8-P2-O23
4	LLL	301	PEG	O1-C1-C2-O2
3	KKK	301	G7C	O19-C17-C21-C25
3	KKK	301	G7C	O17-C14-C20-C18
3	KKK	301	G7C	C12-C13-C14-O17
3	KKK	301	G7C	C13-C14-C20-C18
3	KKK	301	G7C	C12-C13-C14-C20
3	ННН	301	G7C	O1-C1-O4-C7
3	KKK	301	G7C	C13-C14-C20-O13
3	KKK	301	G7C	C10-O5-P2-O8
4	ННН	302	PEG	O1-C1-C2-O2
3	KKK	301	G7C	O17-C14-C20-O13
4	LLL	301	PEG	O2-C3-C4-O4
3	ННН	301	G7C	O14-C13-C14-C20
3	ННН	301	G7C	C12-O7-P1-O6
3	ННН	301	G7C	O8-C15-C16-C17
3	ННН	301	G7C	C10-O5-P2-O8
3	ННН	301	G7C	C12-O7-P1-O21
3	KKK	301	G7C	C10-O5-P2-O23
3	KKK	301	G7C	O8-C15-C16-O12
4	ННН	302	PEG	O2-C3-C4-O4
3	ННН	301	G7C	C11-O6-P1-O7
3	ННН	301	G7C	C9-C10-O5-P2
7	KKK	302	GOL	C1-C2-C3-O3
3	ННН	301	G7C	O14-C13-C14-O17
3	ННН	301	G7C	C11-O6-P1-O21
3	ННН	301	G7C	C3-C2-C6-O9

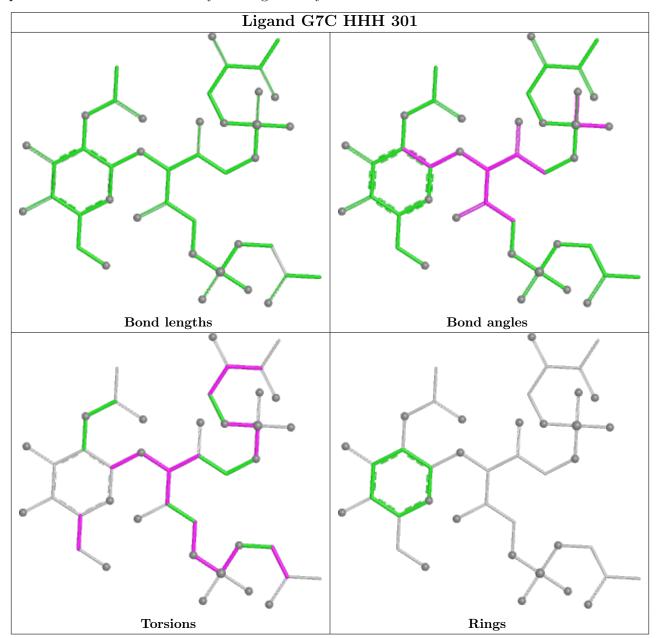
There are no ring outliers.

No monomer is involved in short contacts.

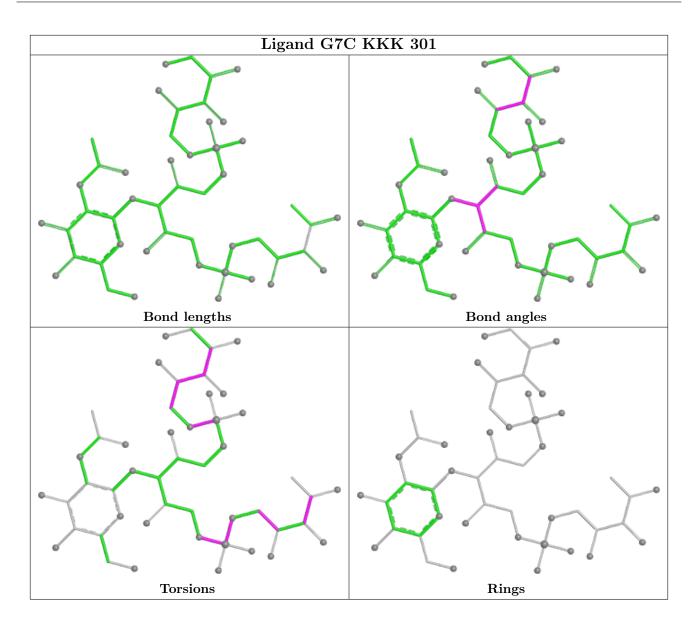
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.



The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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.

