



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:23 AM UTC

PDB ID : 7QXE / pdb_00007qxe
Title : Recognition of Staphylococcus aureus wall teichoic acid analogue TB87 (compound 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

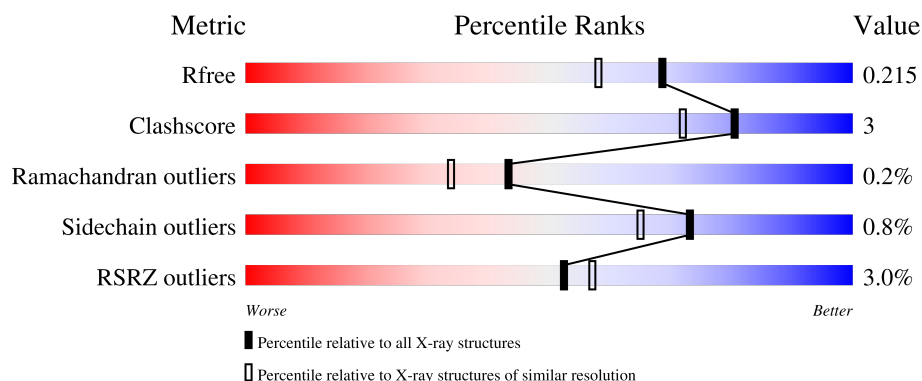
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	HHH	236	4% 83% 8% 9%
1	KKK	236	3% 84% 7% 9%
2	LLL	220	3% 92% 8%
2	MMM	220	2% 95% .

2 Entry composition

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.

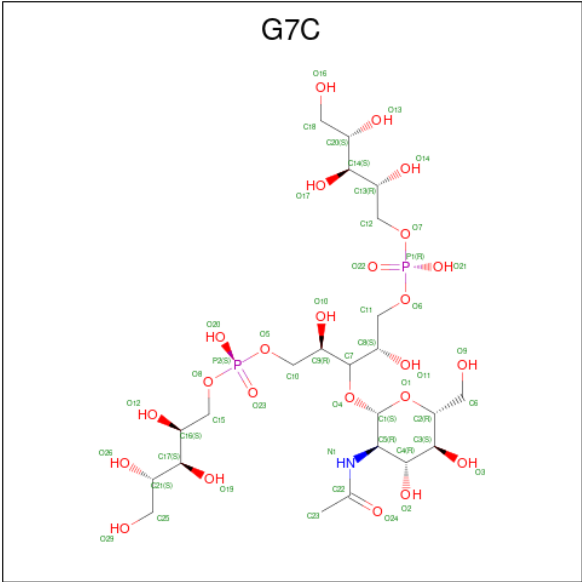
- Molecule 1 is a protein called Antibody Fab 4497 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	HHH	215	Total	C	N	O	S	0	1	0
			1608	1012	274	316	6			
1	KKK	215	Total	C	N	O	S	0	2	0
			1608	1012	274	316	6			

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

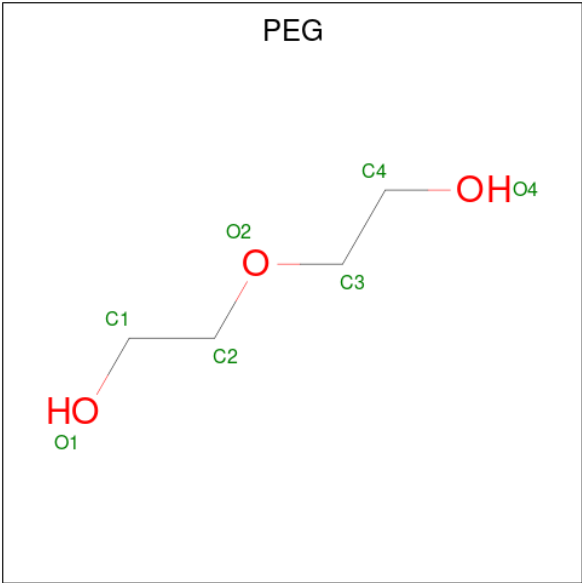
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	LLL	219	Total	C	N	O	S	0	0	0
			1718	1078	296	340	4			
2	MMM	219	Total	C	N	O	S	0	0	0
			1718	1078	296	340	4			

- Molecule 3 is [(2 {S},4 {R})-3-[(2 {S},3 {R},4 {R},5 {S},6 {R})-3-acetamido-6-(hydroxy methyl)-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 (CCD ID: G7C) (formula: C₂₃H₄₇NO₂₄P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	HHH	1	Total	C	N	O	P	0
			42	20	1	19	2	
3	KKK	1	Total	C	N	O	P	0
			49	23	1	23	2	

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).

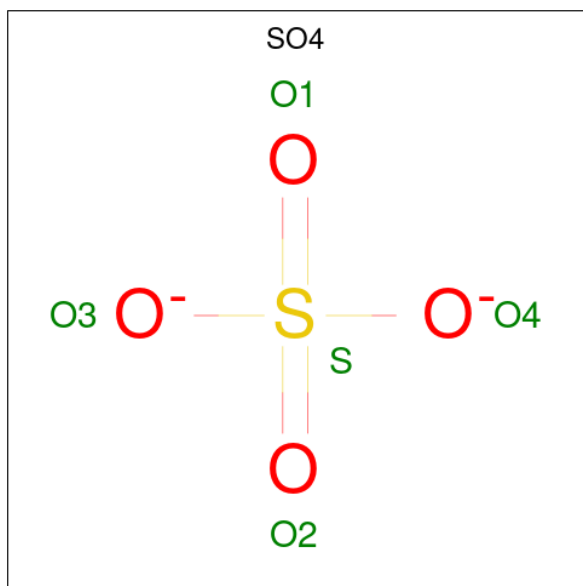


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	HHH	1	Total	C	O	0	0
			7	4	3		
4	LLL	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

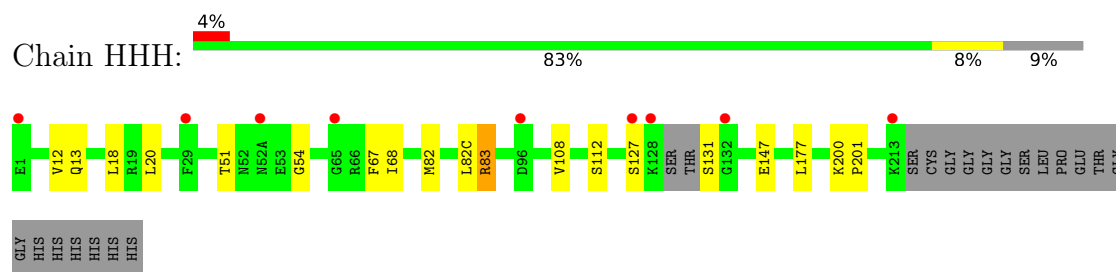
- Molecule 8 is water.

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

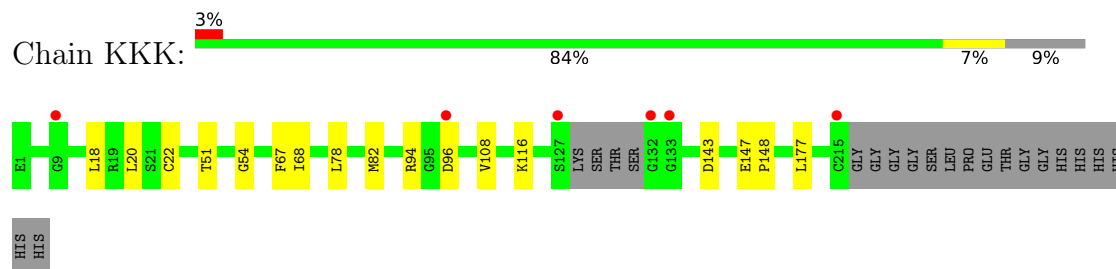
3 Residue-property plots [i](#)

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 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.

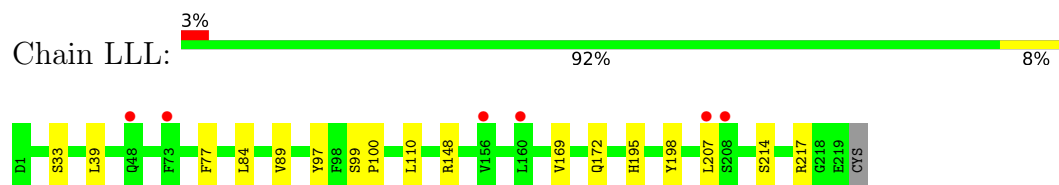
- Molecule 1: Antibody Fab 4497 heavy chain



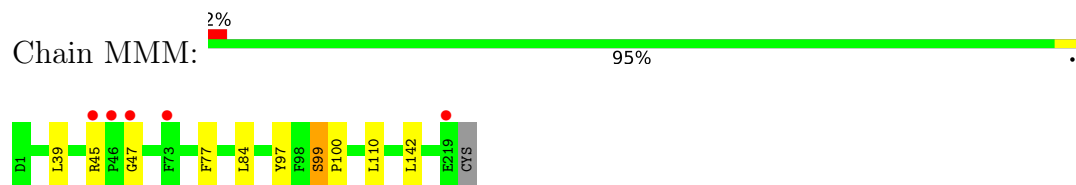
- Molecule 1: Antibody Fab 4497 heavy chain



- Molecule 2: Antibody 4497 light chain



- Molecule 2: Antibody 4497 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.03Å 112.92Å 154.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.00 – 1.84 46.00 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.00-1.84) 99.8 (46.00-1.84)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.188 , 0.218 (Not available) , 0.215	Depositor DCC
R_{free} test set	4991 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
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.*

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: CL, SO4, G7C, GOL, PEG

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	0.98	0/1648	1.21	2/2243 (0.1%)
1	KKK	0.96	0/1651	1.19	0/2248
2	LLL	0.99	1/1757 (0.1%)	1.21	0/2385
2	MMM	0.95	0/1757	1.21	0/2385
All	All	0.97	1/6813 (0.0%)	1.21	2/9261 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	LLL	33	SER	C-N	13.47	1.53	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	HHH	83	ARG	CA-C-N	5.26	125.92	120.03
1	HHH	83	ARG	C-N-CA	5.26	125.92	120.03

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	1570	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	KKK	1608	0	1566	10	0
2	LLL	1718	0	1675	8	0
2	MMM	1718	0	1675	7	0
3	HHH	42	0	0	0	0
3	KKK	49	0	0	0	0
4	HHH	7	0	10	0	0
4	LLL	7	0	10	0	0
5	HHH	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	HHH	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	35	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 3.

All (35) 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
1:KKK:20:LEU:HG	1:KKK:82:MET:HE2	1.81	0.62
2:MMM:47:GLY:C	8:MMM:428:HOH:O	2.44	0.59
1:HHH:20:LEU:HG	1:HHH:82:MET:HE2	1.84	0.59
1:HHH:177:LEU:C	1:HHH:177:LEU:HD12	2.29	0.57
1:KKK:177:LEU:C	1:KKK:177:LEU:HD12	2.30	0.56
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
2:LLL:89:VAL:HG21	2:LLL:172:GLN:HB3	1.90	0.52
2:LLL:84:LEU:HD11	2:LLL:110:LEU:HD21	1.91	0.51
1:HHH:82:MET:HE1	1:HHH:108:VAL:HG21	1.93	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:KKK:82:MET:HE1	1:KKK:108:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:KKK:18:LEU:HB2	1:KKK:82:MET:HE3	2.03	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	Interatomic distance (Å)	Clash overlap (Å)
8:HHH:416:HOH:O	8:KKK:513:HOH:O[2_554]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	212/236 (90%)	207 (98%)	4 (2%)	1 (0%)	24	12
1	KKK	213/236 (90%)	208 (98%)	4 (2%)	1 (0%)	24	12
2	LLL	217/220 (99%)	213 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	MMM	217/220 (99%)	213 (98%)	4 (2%)	0	100	100
All	All	859/912 (94%)	841 (98%)	16 (2%)	2 (0%)	43	34

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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	180/194 (93%)	178 (99%)	2 (1%)	65	54
1	KKK	180/194 (93%)	179 (99%)	1 (1%)	78	72
2	LLL	195/196 (100%)	194 (100%)	1 (0%)	81	75
2	MMM	195/196 (100%)	193 (99%)	2 (1%)	68	58
All	All	750/780 (96%)	744 (99%)	6 (1%)	73	65

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

Mol	Chain	Res	Type
1	HHH	83	ARG
1	HHH	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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PEG	LLL	301	-	6,6,6	0.27	0	5,5,5	0.20	0
4	PEG	HHH	302	-	6,6,6	0.21	0	5,5,5	0.16	0
6	SO4	LLL	303	-	4,4,4	0.32	0	6,6,6	0.06	0
6	SO4	LLL	302	-	4,4,4	0.20	0	6,6,6	0.15	0
3	G7C	HHH	301	-	42,42,50	0.53	0	58,60,71	1.34	8 (13%)
6	SO4	MMM	301	-	4,4,4	0.27	0	6,6,6	0.25	0
6	SO4	MMM	302	-	4,4,4	0.32	0	6,6,6	0.13	0
3	G7C	KKK	301	-	49,49,50	0.42	0	68,70,71	1.05	5 (7%)
7	GOL	KKK	302	-	5,5,5	0.12	0	5,5,5	0.29	0
6	SO4	MMM	303	-	4,4,4	0.28	0	6,6,6	0.16	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	PEG	LLL	301	-	-	2/4/4/4	-
4	PEG	HHH	302	-	-	2/4/4/4	-
3	G7C	HHH	301	-	-	26/46/66/82	0/1/1/1
3	G7C	KKK	301	-	-	24/60/80/82	0/1/1/1
7	GOL	KKK	302	-	-	0/4/4/4	-

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	HHH	301	G7C	O4-C7-C9	5.67	115.79	107.98
3	KKK	301	G7C	O4-C7-C8	3.31	112.54	107.98
3	HHH	301	G7C	C1-O4-C7	3.07	125.26	117.98
3	HHH	301	G7C	O10-C9-C10	-2.93	103.53	109.99
3	HHH	301	G7C	O11-C8-C7	-2.82	102.43	109.18
3	KKK	301	G7C	C8-C7-C9	-2.78	107.70	113.59
3	KKK	301	G7C	C13-C14-C20	2.75	118.15	113.57
3	HHH	301	G7C	O10-C9-C7	2.71	115.65	109.18
3	HHH	301	G7C	C11-C8-C7	2.48	116.40	111.62
3	HHH	301	G7C	O4-C1-C5	-2.17	104.55	108.07
3	HHH	301	G7C	O21-P1-O22	2.11	122.27	112.44
3	KKK	301	G7C	O21-P1-O22	2.07	122.06	112.44
3	KKK	301	G7C	O4-C1-O1	-2.06	105.28	110.69

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	HHH	301	G7C	O4-C7-C8-O11
3	HHH	301	G7C	C8-C7-C9-C10
3	HHH	301	G7C	C8-C7-C9-O10
3	HHH	301	G7C	O4-C7-C9-C10
3	HHH	301	G7C	O4-C7-C9-O10
3	HHH	301	G7C	C8-C7-O4-C1
3	HHH	301	G7C	C9-C7-O4-C1
3	HHH	301	G7C	O7-C12-C13-O14
3	HHH	301	G7C	O7-C12-C13-C14
3	HHH	301	G7C	O8-C15-C16-O12
3	HHH	301	G7C	C11-O6-P1-O22
3	HHH	301	G7C	C12-O7-P1-O22
3	HHH	301	G7C	C12-C13-C14-C20

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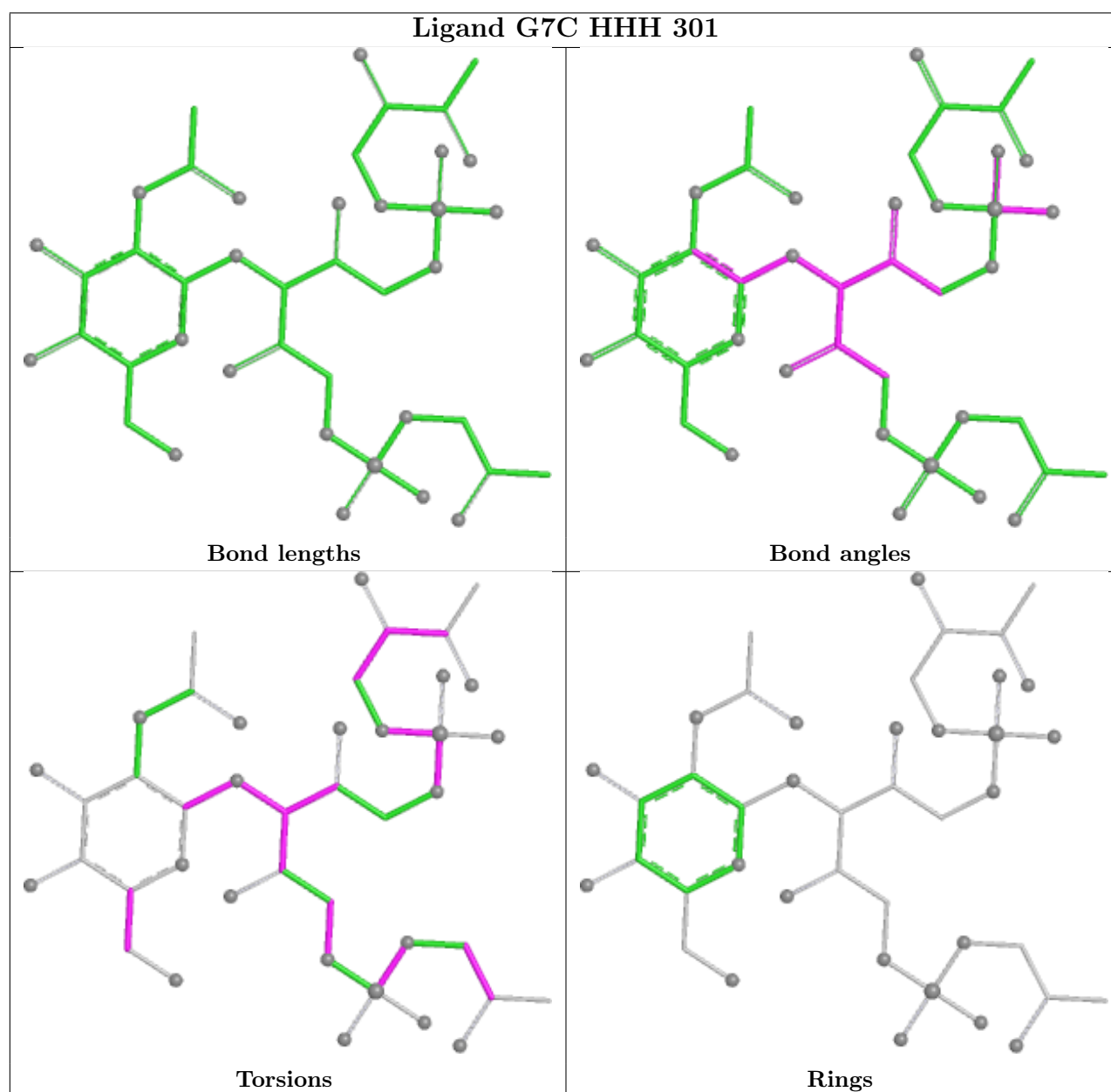
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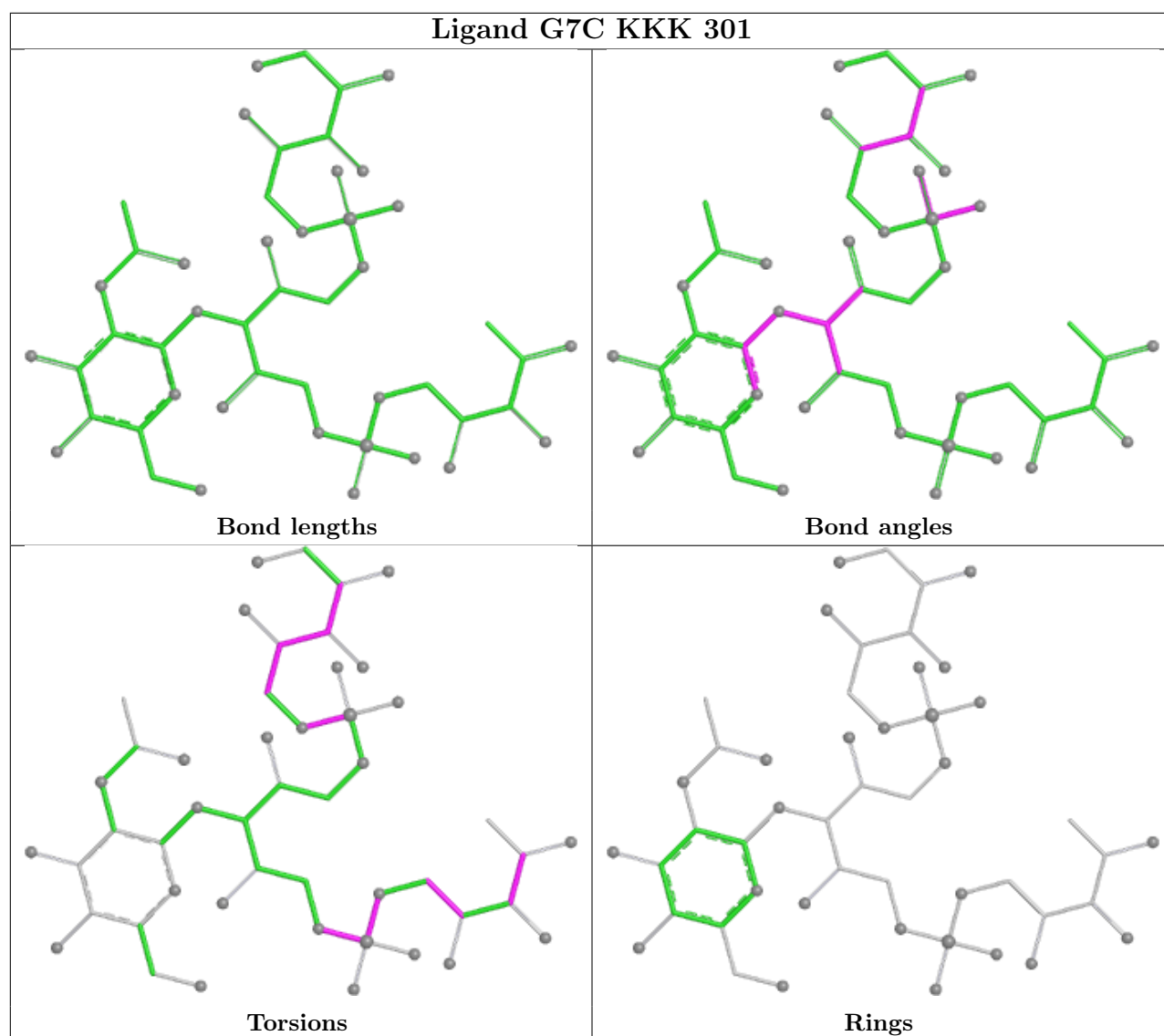
Mol	Chain	Res	Type	Atoms
3	HHH	301	G7C	C15-O8-P2-O5
3	HHH	301	G7C	C15-O8-P2-O20
3	HHH	301	G7C	C15-O8-P2-O23
3	KKK	301	G7C	O7-C12-C13-O14
3	KKK	301	G7C	O7-C12-C13-C14
3	KKK	301	G7C	O8-C15-C16-C17
3	KKK	301	G7C	C16-C17-C21-C25
3	KKK	301	G7C	C16-C17-C21-O26
3	KKK	301	G7C	O19-C17-C21-O26
3	KKK	301	G7C	C10-O5-P2-O8
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
3	KKK	301	G7C	C15-O8-P2-O5
3	KKK	301	G7C	C15-O8-P2-O20
3	KKK	301	G7C	C15-O8-P2-O23
3	KKK	301	G7C	O19-C17-C21-C25
3	KKK	301	G7C	C12-C13-C14-O17
3	KKK	301	G7C	C13-C14-C20-C18
3	KKK	301	G7C	C12-C13-C14-C20
4	LLL	301	PEG	O1-C1-C2-O2
3	HHH	301	G7C	O1-C1-O4-C7
3	KKK	301	G7C	C13-C14-C20-O13
3	KKK	301	G7C	O17-C14-C20-C18
3	KKK	301	G7C	O17-C14-C20-O13
4	HHH	302	PEG	O1-C1-C2-O2
4	LLL	301	PEG	O2-C3-C4-O4
3	HHH	301	G7C	O8-C15-C16-C17
3	HHH	301	G7C	O14-C13-C14-C20
3	HHH	301	G7C	C12-C13-C14-O17
3	KKK	301	G7C	O8-C15-C16-O12
3	HHH	301	G7C	C11-O6-P1-O7
3	HHH	301	G7C	C12-O7-P1-O21
3	HHH	301	G7C	C12-O7-P1-O6
3	KKK	301	G7C	C10-O5-P2-O23
4	HHH	302	PEG	O2-C3-C4-O4
3	HHH	301	G7C	O14-C13-C14-O17
3	HHH	301	G7C	C9-C10-O5-P2
3	HHH	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 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	HHH	215/236 (91%)	0.39	9 (4%) 40 43	21, 39, 59, 94	1 (0%)
1	KKK	215/236 (91%)	0.13	6 (2%) 55 60	19, 36, 59, 84	2 (0%)
2	LLL	219/220 (99%)	0.35	6 (2%) 56 61	29, 41, 63, 89	0
2	MMM	219/220 (99%)	0.00	5 (2%) 61 67	26, 33, 55, 76	0
All	All	868/912 (95%)	0.22	26 (2%) 52 57	19, 37, 60, 94	3 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	KKK	215	CYS	5.0
1	KKK	132	GLY	4.8
1	HHH	128	LYS	4.0
2	LLL	73	PHE	3.3
2	MMM	46	PRO	3.2
1	KKK	96	ASP	3.0
1	KKK	127	SER	2.9
1	KKK	133	GLY	2.9
2	MMM	73	PHE	2.7
2	MMM	45	ARG	2.6
2	MMM	47	GLY	2.6
1	HHH	1	GLU	2.5
1	HHH	127	SER	2.5
2	LLL	160	LEU	2.3
1	HHH	29	PHE	2.3
2	LLL	207	LEU	2.3
2	LLL	208	SER	2.2
2	MMM	219	GLU	2.2
1	HHH	96	ASP	2.2
1	HHH	132	GLY	2.1
2	LLL	156	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	HHH	52(A)	ASN	2.1
1	KKK	9	GLY	2.1
1	HHH	213	LYS	2.0
1	HHH	65	GLY	2.0
2	LLL	48	GLN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

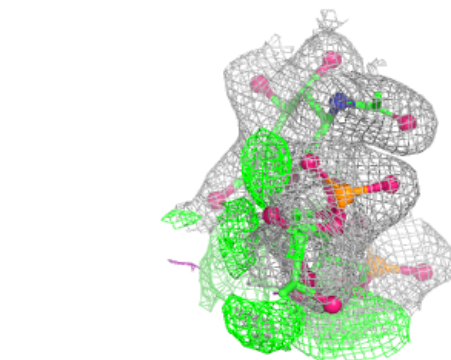
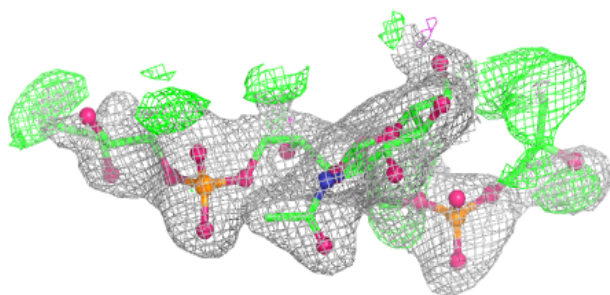
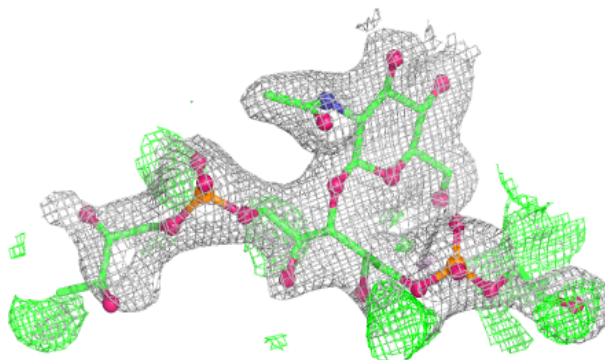
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PEG	HHH	302	7/7	0.66	0.26	74,84,86,88	0
6	SO4	MMM	303	5/5	0.69	0.13	85,99,102,103	0
4	PEG	LLL	301	7/7	0.74	0.21	73,75,82,83	0
7	GOL	KKK	302	6/6	0.74	0.17	64,71,76,85	0
6	SO4	MMM	302	5/5	0.75	0.11	90,92,103,111	0
6	SO4	MMM	301	5/5	0.76	0.14	60,74,84,91	0
6	SO4	LLL	302	5/5	0.79	0.12	67,68,73,75	0
3	G7C	HHH	301	42/50	0.81	0.17	39,68,104,106	0
6	SO4	LLL	303	5/5	0.85	0.09	95,97,98,99	0
3	G7C	KKK	301	49/50	0.91	0.11	33,54,90,106	0
5	CL	HHH	303	1/1	0.99	0.05	36,36,36,36	0

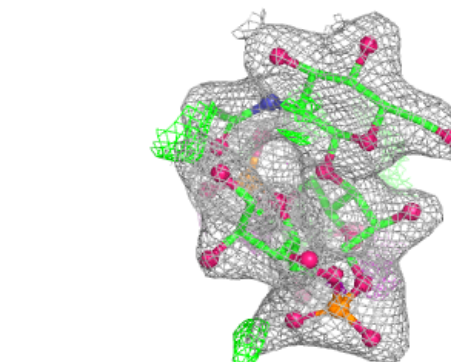
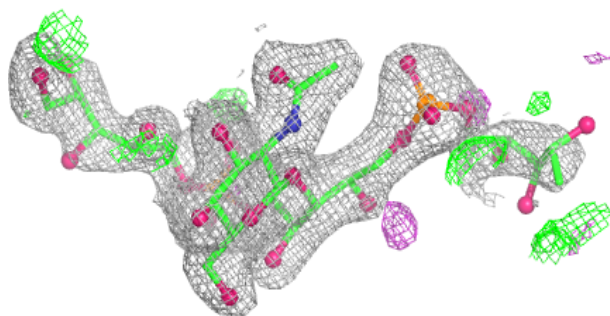
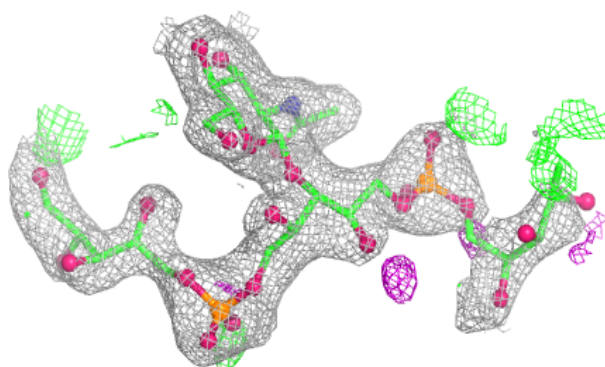
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around G7C HHH 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 G7C KKK 301:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.