

Full wwPDB X-ray Structure Validation Report (i)

Aug 25, 2022 – 04:43 pm BST

PDB ID : 7QXC

Title: Recognition of Staphylococcus aureus wall teichoic acid analogue SA533 (com-

pound 1) by Fab4461

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

Deposited on : 2022-01-26

Resolution : 1.45 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 : 2.30

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0267$

CCP4 : 7.1.010 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

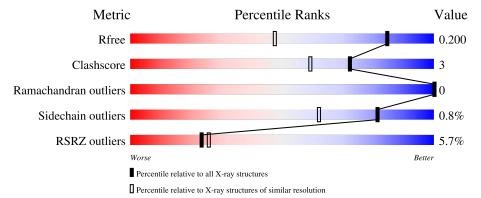
Validation Pipeline (wwPDB-VP) : 2.30

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 1.45 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	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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% 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	ННН	239	8% 85% 5%	• 10%			
2	LLL	220	93%	6%			



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3835 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.

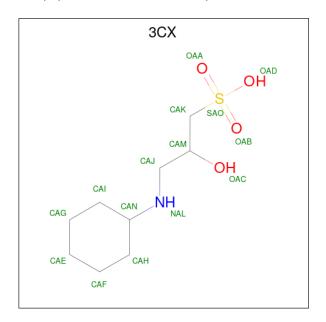
• Molecule 1 is a protein called Fab 4461 heavy chain.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	иии	216	Total	С	N	О	S	0	1	0
1	111111	210	1609	1013	270	317	9		1	

• Molecule 2 is a protein called Fab 4461 light chain.

Mol C	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	LLL	219	Total	C 1072	N 293	O 344	S	0	0	0

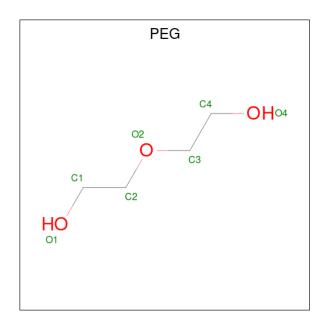
• Molecule 3 is (2S)-3-(cyclohexylamino)-2-hydroxypropane-1-sulfonic acid (three-letter code: 3CX) (formula: C₉H₁₉NO₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
3	иии	1	Total	С	N	О	S	0	0
9	111111	1	15	9	1	4	1		0

• Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).

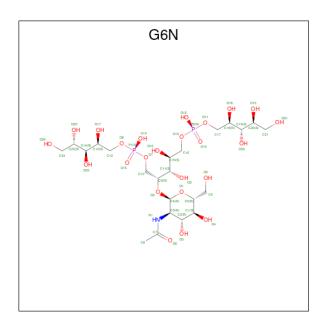




Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	ННН	1	Total C O 7 4 3	0	0
4	LLL	1	Total C O 7 4 3	0	0
4	LLL	1	Total C O 7 4 3	0	0
4	LLL	1	Total C O 7 4 3	0	0

• Molecule 5 is [(2 {S},3 {S},4 {R})-4-[(2 {R},3 {R},4 {R},5 {S},6 {R})-3-acetamido-6-(hydroxymethyl)-4,5-bis(oxidanyl)oxan-2-yl]oxy-2,3-bis(oxidanyl)-5-[oxidanyl-[(2 {R})-2-oxidanyl-propoxy]phosphoryl]oxy-pentyl] [(2 {R},3 {S},4 {S})-2,3,4,5-tetrakis(oxidanyl)pentyl] hydrogen phosphate (three-letter code: G6N) (formula: $C_{23}H_{47}NO_{24}P_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
E	ттт	1	Total	С	N	О	Р	0	0
) 3	יויויד	1	45	21	1	21	2	U	0

• Molecule 6 is water.

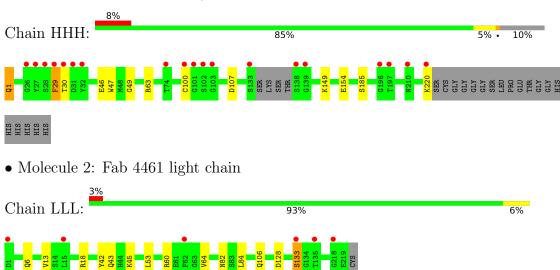
\mathbf{Mol}	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
6	ННН	188	Total O 188 188	0	0
6	LLL	236	Total O 236 236	0	0



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 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: Fab 4461 heavy chain





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	58.19Å 65.45Å 74.34Å	Depositor
a, b, c, α , β , γ	90.00° 112.90° 90.00°	Depositor
Resolution (Å)	53.51 - 1.45	Depositor
Resolution (A)	53.51 - 1.45	EDS
% Data completeness	96.5 (53.51-1.45)	Depositor
(in resolution range)	96.5 (53.51 - 1.45)	EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.52 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D.	0.174 , 0.200	Depositor
R, R_{free}	0.174 , 0.200	DCC
R_{free} test set	4371 reflections $(4.99%)$	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3835	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.43% 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: G6N, 3CX, 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		
Moi Chain		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	ННН	0.65	0/1651	0.77	0/2249	
2	LLL	0.67	0/1752	0.76	0/2379	
All	All	0.66	0/3403	0.77	0/4628	

There are no bond length outliers.

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	1609	0	1562	13	0
2	LLL	1714	0	1654	10	0
3	ННН	15	0	18	0	0
4	ННН	7	0	10	0	0
4	LLL	21	0	30	1	0
5	LLL	45	0	0	0	0
6	ННН	188	0	0	4	0
6	LLL	236	0	0	6	0
All	All	3835	0	3274	23	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 3.



All (23) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}(\mathring{\rm A})$	overlap (Å)
2:LLL:106:GLN:OE1	6:LLL:401:HOH:O	1.55	1.21
1:HHH:154[B]:GLU:OE1	6:HHH:401:HOH:O	1.62	1.15
1:HHH:185:SER:OG	6:HHH:402:HOH:O	1.89	0.84
1:HHH:100:CYS:SG	6:HHH:572:HOH:O	2.33	0.84
2:LLL:18:ARG:NH1	2:LLL:82:ASN:OD1	2.12	0.82
2:LLL:42:TYR:OH	6:LLL:402:HOH:O	1.97	0.80
1:HHH:1:GLN:N	1:HHH:1:GLN:OE1	2.15	0.79
1:HHH:1:GLN:NE2	6:HHH:403:HOH:O	1.96	0.75
2:LLL:133:SER:HB2	6:LLL:581:HOH:O	1.93	0.68
2:LLL:45:LYS:HE3	6:LLL:505:HOH:O	1.95	0.66
1:HHH:107:ASP:OD2	6:LLL:402:HOH:O	2.14	0.65
1:HHH:46:GLU:OE2	1:HHH:63:ARG:HD3	2.00	0.62
1:HHH:29:PHE:CE1	1:HHH:30:THR:HG23	2.38	0.59
2:LLL:43:GLN:HB2	2:LLL:53:LEU:HD11	1.88	0.55
2:LLL:6:GLN:O	2:LLL:106:GLN:NE2	2.38	0.54
1:HHH:149:LYS:HE2	6:LLL:431:HOH:O	2.07	0.53
1:HHH:220:LYS:NZ	2:LLL:128:ASP:OD2	2.41	0.52
4:LLL:303:PEG:O4	4:LLL:304:PEG:O4	2.15	0.45
1:HHH:47:TRP:CH2	1:HHH:49:GLY:HA2	2.54	0.43
2:LLL:13:VAL:HB	2:LLL:84:LEU:HD22	2.02	0.41
2:LLL:60:ARG:HG2	2:LLL:64:VAL:HB	2.02	0.41
1:HHH:29:PHE:CD1	1:HHH:30:THR:HG23	2.55	0.40
1:HHH:1:GLN:H3	1:HHH:1:GLN:CD	2.23	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	ННН	213/239 (89%)	206 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
2	LLL	217/220 (99%)	215 (99%)	2 (1%)	0	100	100
All	All	430/459 (94%)	421 (98%)	9 (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	ННН	178/195 (91%)	176 (99%)	2 (1%)	73 48		
2	LLL	193/194 (100%)	192 (100%)	1 (0%)	88 75		
All	All	371/389 (95%)	368 (99%)	3 (1%)	81 62		

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	ННН	1	GLN
1	ННН	29	PHE
2	LLL	133	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)

6 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	Mol Type Chain Res 1		Link	Вс	ond leng	ths	Bond angles			
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PEG	LLL	302	-	6,6,6	0.12	0	5,5,5	0.06	0
4	PEG	ННН	302	-	6,6,6	0.14	0	5,5,5	0.09	0
4	PEG	LLL	304	-	6,6,6	0.18	0	5,5,5	0.10	0
3	3CX	ННН	301	-	15,15,15	0.86	1 (6%)	16,20,20	2.31	2 (12%)
5	G6N	LLL	301	-	44,45,50	0.34	0	59,64,71	0.86	2 (3%)
4	PEG	LLL	303	-	6,6,6	0.17	0	5,5,5	0.10	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	302	-	-	2/4/4/4	-
4	PEG	ННН	302	-	-	3/4/4/4	-
4	PEG	LLL	304	-	-	3/4/4/4	-
3	3CX	ННН	301	-	-	1/10/18/18	0/1/1/1
5	G6N	LLL	301	-	-	7/52/72/82	0/1/1/1
4	PEG	LLL	303	-	-	3/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$Ideal(\AA)$
3	ННН	301	3CX	OAB-SAO	2.97	1.53	1.45



All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	ННН	301	3CX	OAB-SAO-CAK	-8.71	96.59	106.94
5	LLL	301	G6N	O19-C20-C19	2.10	114.20	109.10
3	ННН	301	3CX	OAD-SAO-OAA	2.04	116.27	111.27
5	LLL	301	G6N	C2-C3-N1	2.04	114.47	110.62

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	ННН	301	3CX	SAO-CAK-CAM-OAC
5	LLL	301	G6N	C8-C7-N1-C3
5	LLL	301	G6N	O8-C12-C13-C14
5	LLL	301	G6N	O8-C12-C13-O17
5	LLL	301	G6N	O6-C7-N1-C3
4	ННН	302	PEG	O2-C3-C4-O4
4	ННН	302	PEG	O1-C1-C2-O2
4	LLL	304	PEG	O2-C3-C4-O4
4	LLL	303	PEG	O2-C3-C4-O4
4	ННН	302	PEG	C1-C2-O2-C3
4	LLL	302	PEG	C1-C2-O2-C3
4	LLL	302	PEG	O2-C3-C4-O4
4	LLL	303	PEG	C1-C2-O2-C3
4	LLL	304	PEG	O1-C1-C2-O2
4	LLL	304	PEG	C1-C2-O2-C3
4	LLL	303	PEG	O1-C1-C2-O2
5	LLL	301	G6N	C10-C9-O2-C4
5	LLL	301	G6N	C11-C9-O2-C4
5	LLL	301	G6N	C2-C3-N1-C7

There are no ring outliers.

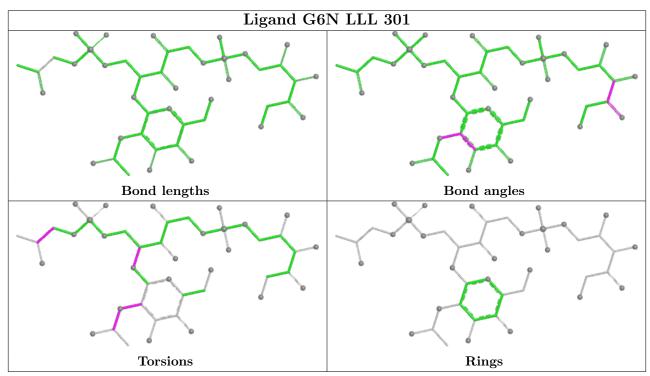
2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	LLL	304	PEG	1	0
4	LLL	303	PEG	1	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 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)

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, 95^{th} 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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	ННН	216/239 (90%)	0.46	19 (8%) 10 11	14, 20, 54, 102	0
2	LLL	$219/220 \ (99\%)$	0.09	6 (2%) 54 56	14, 20, 33, 54	0
All	All	435/459 (94%)	0.28	25 (5%) 23 26	14, 20, 44, 102	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	ННН	29	PHE	11.7
1	ННН	30	THR	10.7
1	ННН	27	TYR	10.4
1	ННН	28	SER	8.1
1	ННН	139	GLY	7.3
1	ННН	102	SER	6.3
1	ННН	103	GLY	6.1
1	ННН	138	SER	4.3
1	ННН	197	THR	4.2
1	ННН	101	GLY	4.1
1	ННН	100	CYS	3.9
1	ННН	196	GLY	3.7
1	ННН	26	GLY	3.1
2	LLL	133	SER	2.8
1	ННН	31	ASP	2.6
2	LLL	135	THR	2.6
2	LLL	15	LEU	2.6
2	LLL	218	GLY	2.6
1	ННН	220	LYS	2.6
1	ННН	133	SER	2.6
1	ННН	32	TYR	2.5
2	LLL	62	PHE	2.5
1	ННН	210	ASN	2.4
2	LLL	1	ASP	2.4

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		-		
Mol	Chain	Res	Type	RSRZ
1	ННН	74	THR	2.4

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.

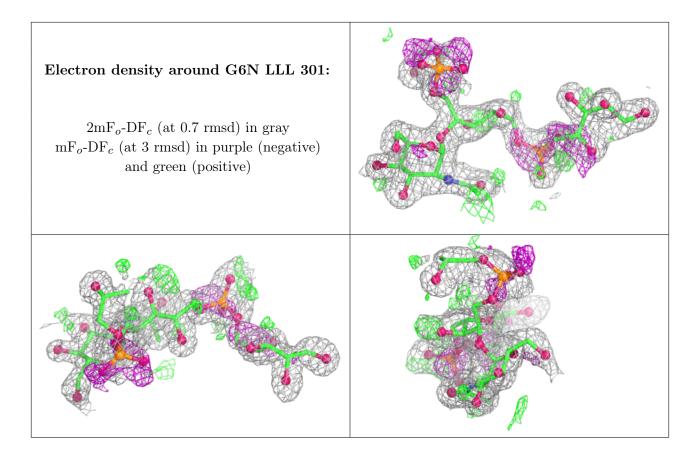
6.4 Ligands (i)

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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	PEG	LLL	304	7/7	0.71	0.17	41,42,43,45	0
4	PEG	ННН	302	7/7	0.78	0.23	61,62,64,64	0
4	PEG	LLL	303	7/7	0.82	0.16	34,43,46,47	0
4	PEG	LLL	302	7/7	0.84	0.13	43,45,48,51	0
5	G6N	LLL	301	45/50	0.87	0.16	25,33,49,58	0
3	3CX	ННН	301	15/15	0.93	0.10	23,25,38,38	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.





6.5 Other polymers (i)

There are no such residues in this entry.

