

Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 08:23 PM EDT

PDB ID	:	6CX5
Title	:	Structure of alpha-GSA[8,8P] bound by CD1d and in complex with the
		Va14Vb8.2 TCR
Authors	:	Wang, J.; Zajonc, D.
Deposited on	:	2018-04-02
Resolution	:	2.40 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:

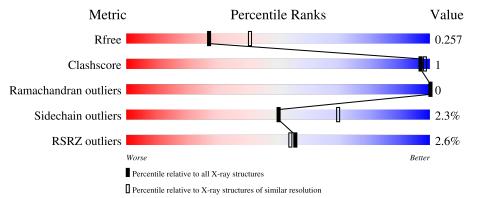
MolProbity	:	4.02b-467 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)		
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.40 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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		
			3%		
1	А	285	87%	6%	7%
			5%		
2	В	99	95%		••
			%		
3	С	209	95%		·
			<u>2%</u>		
4	D	241	94%		5%•
5	Ε	2	50% 50%		

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Mol	Chain	Length	Quality of chain
6	F	3	100%



2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 6623 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 Antigen-presenting glycoprotein CD1d1.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
1	А	264	Total 2130	C 1361	N 363	O 393	S 13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	280	HIS	-	expression tag	UNP A0A0R4J090
А	281	HIS	-	expression tag	UNP A0A0R4J090
А	282	HIS	-	expression tag	UNP A0A0R4J090
А	283	HIS	-	expression tag	UNP A0A0R4J090
А	284	HIS	-	expression tag	UNP A0A0R4J090
А	285	HIS	-	expression tag	UNP A0A0R4J090

• Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	98	Total 810	C 517	N 137	0 149	S 7	0	0	0

• Molecule 3 is a protein called Chimeric T cell antigen receptor alpha chain Va14, Va24, Ja18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	С	200	Total 1529	C 947	N 261	0 313	S 8	0	0	0

• Molecule 4 is a protein called Chimeric T cell antigen receptor beta chain Vb8.2, vb11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	239	Total 1869	C 1174	N 333	O 356	S 6	0	0	0

• Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a



cetamido-2-deoxy-beta-D-glucopyranose.

$$\beta$$
 4 β

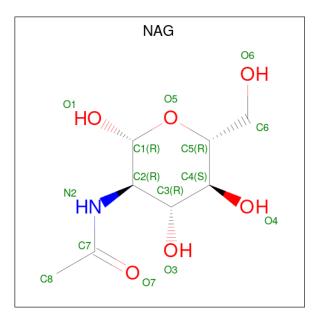
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Е	2	Total 28	C 16	N 2	O 10	0	0	0

• Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[al pha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf	Trace
6	F	3	Total 38	C 22	N 2	0 14	0	0	0

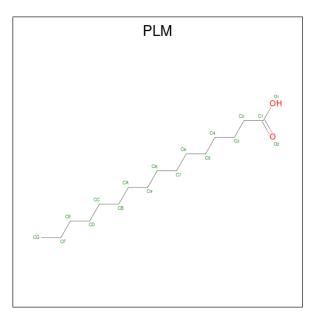
• Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	А	1	Total 14	C 8	N 1	O 5	0	0

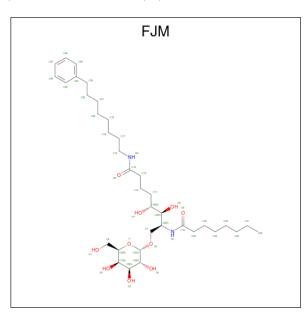


• Molecule 8 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	А	1	Total C 18 16	0 2	0	0

• Molecule 9 is (5R,6S,7S)-5,6-dihydroxy-7-(octanoylamino)-N-(8-phenyloctyl)-8-{[(2S,3R, 4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl]oxy}octanamide (non-preferred name) (three-letter code: FJM) (formula: $C_{36}H_{62}N_2O_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	А	1	Total 48	C 36	N 2	0 10	0	0



• Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	А	1	Total Na 1 1	0	0

• Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	А	44	Total O 44 44	0	0
11	В	8	Total O 8 8	0	0
11	С	34	Total O 34 34	0	0
11	D	52	$\begin{array}{cc} \text{Total} & \text{O} \\ 52 & 52 \end{array}$	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.

- Chain A: 87% 7% 6% SER ALA HIS GLY HIS SER SIH SIH SIH • Molecule 2: Beta-2-microglobulin Chain B: 95% • Molecule 3: Chimeric T cell antigen receptor alpha chain Va14,Va24,Ja18 Chain C: 95% • Molecule 4: Chimeric T cell antigen receptor beta chain Vb8.2, vb11 Chain D: 94% 5%•
- Molecule 1: Antigen-presenting glycoprotein CD1d1

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:	50%	50%



NAG1 NAG2

 • Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)] 2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

100%

NAG1 NAG2 FUC3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	78.77Å 190.79Å 150.88Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 - 2.40	Depositor
Resolution (A)	35.39 - 2.40	EDS
% Data completeness	99.8 (40.00-2.40)	Depositor
(in resolution range)	99.8 (35.39-2.40)	EDS
R _{merge}	0.11	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.36 (at 2.39 Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
D D.	0.214 , 0.258	Depositor
R, R_{free}	0.216 , 0.257	DCC
R_{free} test set	2265 reflections $(5.04%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	39.7	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32, 28.6	EDS
L-test for twinning ²	$ \langle L \rangle = 0.49, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6623	wwPDB-VP
Average B, all atoms $(Å^2)$	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.

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.



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: NAG, FJM, NA, FUC, PLM

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.48	0/2189	0.66	2/2970~(0.1%)	
2	В	0.43	0/836	0.61	0/1133	
3	С	0.55	0/1555	0.69	0/2114	
4	D	0.47	0/1920	0.65	0/2618	
All	All	0.49	0/6500	0.66	2/8835~(0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	А	79	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	А	79	ARG	NE-CZ-NH2	-5.95	117.32	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	А	2130	0	2040	8	0
2	В	810	0	783	1	0
3	С	1529	0	1443	2	0
4	D	1869	0	1772	2	0
5	Е	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	38	0	34	0	0
7	А	14	0	13	0	0
8	А	18	0	31	0	0
9	А	48	0	0	0	0
10	А	1	0	0	0	0
11	А	44	0	0	0	0
11	В	8	0	0	0	0
11	С	34	0	0	0	0
11	D	52	0	0	0	0
All	All	6623	0	6141	11	0

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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 1.

All (11) 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:152:ALA:C	1:A:153:ASP:CA	2.48	0.81
1:A:83:GLU:HG3	4:D:50:TYR:OH	2.03	0.57
3:C:184:ASP:N	3:C:184:ASP:OD1	2.38	0.55
1:A:35:LEU:HD12	1:A:183:LEU:HD23	1.94	0.50
1:A:87:MET:HE3	1:A:145:LEU:HG	1.98	0.45
4:D:176:GLU:OE2	4:D:186:SER:OG	2.32	0.45
1:A:267:HIS:HD2	1:A:269:SER:OG	2.00	0.45
1:A:219:TRP:CZ2	1:A:221:MET:HG3	2.53	0.43
3:C:2:THR:O	3:C:2:THR:HG23	2.19	0.43
1:A:209:HIS:CE1	2:B:99:MET:HA	2.55	0.41
1:A:219:TRP:HB3	1:A:266:LYS:HB2	2.02	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	Percer	ntiles
1	А	256/285~(90%)	250~(98%)	6(2%)	0	100	100
2	В	96/99~(97%)	92~(96%)	4 (4%)	0	100	100
3	С	194/209~(93%)	181 (93%)	13 (7%)	0	100	100
4	D	$237/241 \ (98\%)$	234~(99%)	3(1%)	0	100	100
All	All	783/834~(94%)	757~(97%)	26 (3%)	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 side chain 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	А	231/249~(93%)	228~(99%)	3~(1%)	69 84
2	В	92/93~(99%)	89~(97%)	3~(3%)	38 57
3	С	174/188~(93%)	173~(99%)	1 (1%)	86 94
4	D	201/208~(97%)	192~(96%)	9~(4%)	27 44
All	All	698/738~(95%)	682~(98%)	16 (2%)	50 70

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	91	LYS
1	А	180	LYS
1	А	196	VAL
2	В	44	LYS
2	В	48	LYS
2	В	70	PHE
3	С	184	ASP
4	D	25	GLN
4	D	54	SER
4	D	79	GLU
4	D	115	ARG
4	D	168	CYS
4	D	172	GLN

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Mol	Chain	Res	Type
4	D	190	ARG
4	D	215	SER
4	D	235	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	267	HIS
4	D	24	ASN
4	D	230	GLN

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)

5 monosaccharides 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	Chain	Res	Link	Bond lengths				Bond angles		
NIOI		nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2		
5	NAG	Е	1	5,1	14,14,15	0.59	0	$17,\!19,\!21$	0.94	2 (11%)	
5	NAG	Е	2	5	14,14,15	0.37	0	17,19,21	0.90	0	
6	NAG	F	1	1,6	14,14,15	0.39	0	$17,\!19,\!21$	1.08	1 (5%)	
6	NAG	F	2	6	14,14,15	0.45	0	17,19,21	1.55	1 (5%)	
6	FUC	F	3	6	10,10,11	0.74	0	14,14,16	0.83	1 (7%)	



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
5	NAG	Е	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	Е	2	5	-	0/6/23/26	0/1/1/1
6	NAG	F	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
6	FUC	F	3	6	-	-	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
6	F	2	NAG	C1-O5-C5	5.53	119.69	112.19
6	F	1	NAG	O5-C5-C6	2.96	111.85	107.20
5	Е	1	NAG	C1-O5-C5	2.25	115.23	112.19
5	Е	1	NAG	O5-C1-C2	-2.06	108.04	111.29
6	F	3	FUC	C1-C2-C3	2.01	112.14	109.67

There are no chirality outliers.

All (3) torsion outliers are listed below:

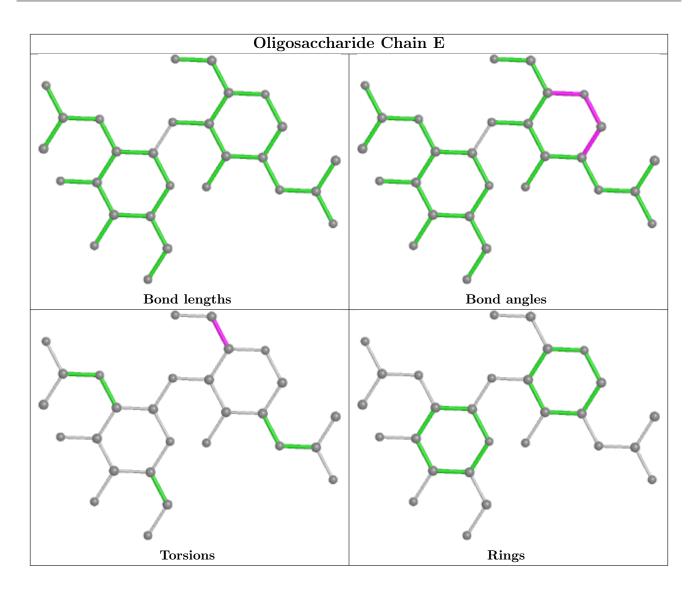
Mol	Chain	Res	Type	Atoms
6	F	1	NAG	O5-C5-C6-O6
5	Ε	1	NAG	C4-C5-C6-O6
5	Ε	1	NAG	O5-C5-C6-O6

There are no ring outliers.

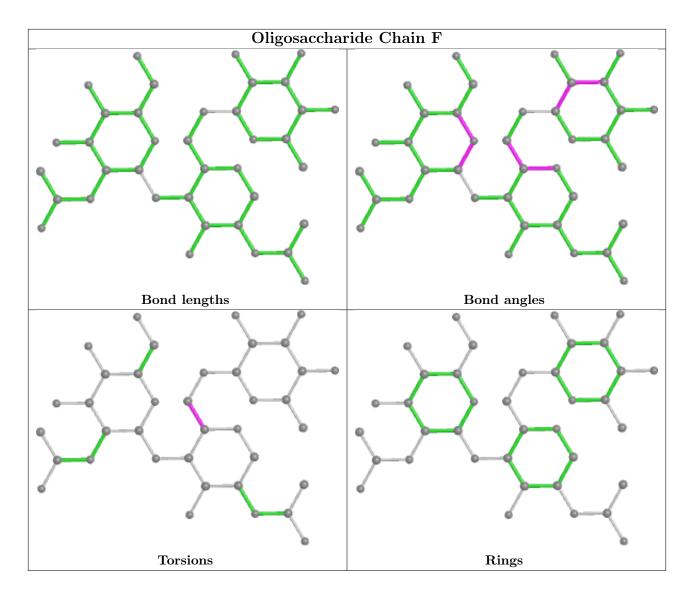
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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 C	Chain	Res	Link	Bo	Bond lengths			Bond angles		
	Type	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	А	301	1	$14,\!14,\!15$	0.56	0	17,19,21	1.45	<mark>3 (17%)</mark>
8	PLM	А	307	-	17,17,17	0.59	0	17,17,17	1.62	4 (23%)
9	FJM	А	308	-	49,49,49	0.92	4 (8%)	57,61,61	1.13	3 (5%)



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	NAG	А	301	1	-	2/6/23/26	0/1/1/1
8	PLM	А	307	-	-	7/15/15/15	-
9	FJM	А	308	-	-	8/44/64/64	0/2/2/2

Chain \mathbf{Z} Mol Res Type Atoms Observed(Å) Ideal(Å) 9 308 FJM C36-C15 3.051.571.51А 9 308 FJM 1.50А C8-N1 2.651.469 А 308 FJM C23-C24-2.541.441.519 FJM C13-C14 А 308 2.311.551.51

All (4) bond length outliers are listed below:

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
8	А	307	PLM	C4-C3-C2	-3.36	101.12	113.19
7	А	301	NAG	C1-O5-C5	2.96	116.20	112.19
7	А	301	NAG	C8-C7-N2	2.92	121.05	116.10
9	А	308	FJM	C4-O-C5	2.72	119.03	113.69
8	А	307	PLM	C6-C5-C4	-2.48	101.81	114.42
7	А	301	NAG	C2-N2-C7	2.44	126.38	122.90
9	А	308	FJM	O1-C6-C5	-2.23	103.63	111.29
9	А	308	FJM	C20-C19-C18	-2.17	103.43	114.42
8	А	307	PLM	CA-C9-C8	-2.05	104.00	114.42
8	А	307	PLM	O1-C1-O2	2.05	128.40	123.30

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	А	308	FJM	N2-C16-C17-C18
7	А	301	NAG	C8-C7-N2-C2
7	А	301	NAG	O7-C7-N2-C2
8	А	307	PLM	C1-C2-C3-C4
8	А	307	PLM	C3-C4-C5-C6
8	А	307	PLM	C5-C6-C7-C8
9	А	308	FJM	C20-C21-C22-C23

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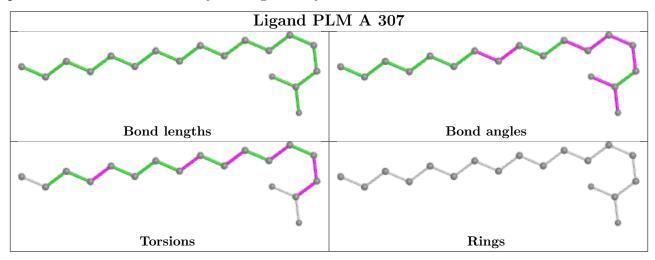
Mol	Chain	Res	Type	Atoms
8	А	307	PLM	С7-С8-С9-СА
9	А	308	FJM	C19-C20-C21-C22
8	А	307	PLM	O1-C1-C2-C3
9	А	308	FJM	C22-C23-C24-C25
9	А	308	FJM	C22-C23-C24-C29
8	А	307	PLM	O2-C1-C2-C3
9	А	308	FJM	C1-C5-C6-O1
9	А	308	FJM	O9-C15-C36-C35
9	А	308	FJM	C18-C19-C20-C21
8	А	307	PLM	CB-CC-CD-CE

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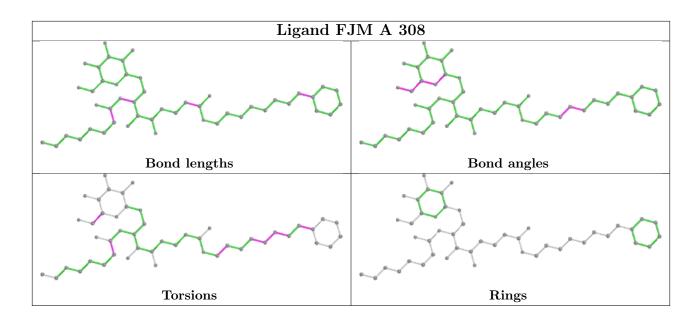
There are no ring outliers.

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)

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 $>$	#RSRZ>2		$OWAB(Å^2)$	Q<0.9	
1	А	264/285~(92%)	-0.05	9~(3%)	45	44	24, 38, 86, 111	0
2	В	98/99~(98%)	0.09	5(5%)	28	26	31, 54, 87, 118	0
3	С	200/209~(95%)	-0.21	3(1%)	73	72	24, 41, 78, 93	0
4	D	239/241~(99%)	-0.37	4 (1%)	70	68	25, 37, 58, 81	0
All	All	801/834~(96%)	-0.17	21 (2%)	56	54	24, 40, 80, 118	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	99	MET	6.7
1	А	256	GLY	6.1
2	В	3	LYS	4.5
2	В	97	ARG	4.3
1	А	204	ARG	4.1
1	А	255	ALA	3.8
4	D	179	ALA	3.7
3	С	184	ASP	3.4
1	А	254	GLU	3.3
1	А	253	VAL	3.0
3	С	154	SER	2.9
2	В	2	GLN	2.8
4	D	180	LEU	2.8
1	А	257	GLU	2.6
1	А	259	ALA	2.5
1	А	230	GLN	2.4
4	D	3	ALA	2.4
3	С	181	ASN	2.2
1	А	206	LEU	2.1
2	В	31	HIS	2.0
4	D	217	ASN	2.0



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

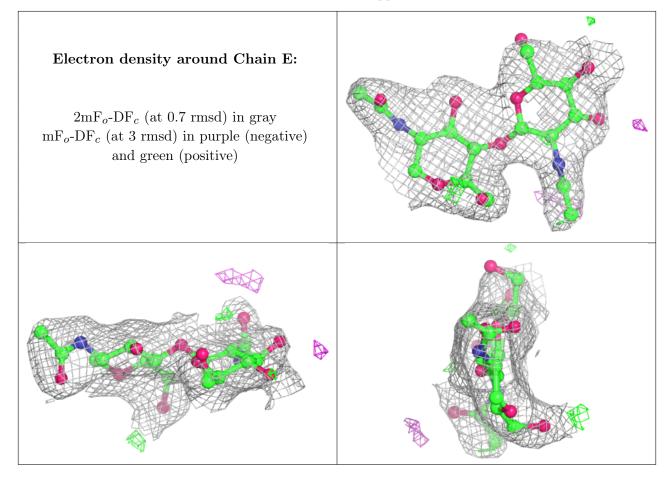
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

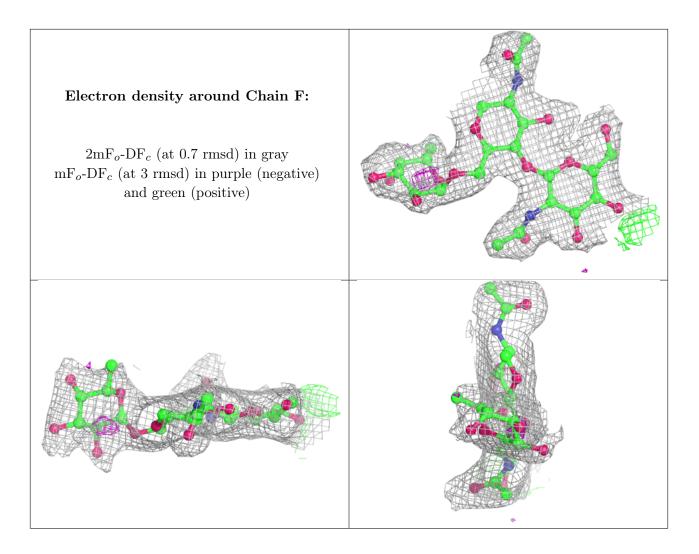
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	FUC	F	3	10/11	0.82	0.28	$65,\!67,\!68,\!68$	0
5	NAG	Е	2	14/15	0.83	0.27	68,72,83,86	0
6	NAG	F	2	14/15	0.91	0.21	51,55,60,60	0
6	NAG	F	1	14/15	0.95	0.14	35,38,49,58	0
5	NAG	Е	1	14/15	0.96	0.14	38,41,46,56	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.







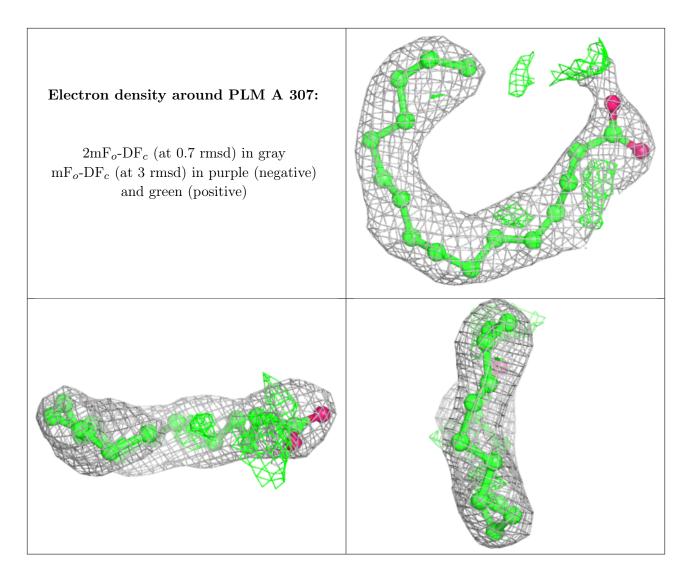
6.4 Ligands (i)

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.

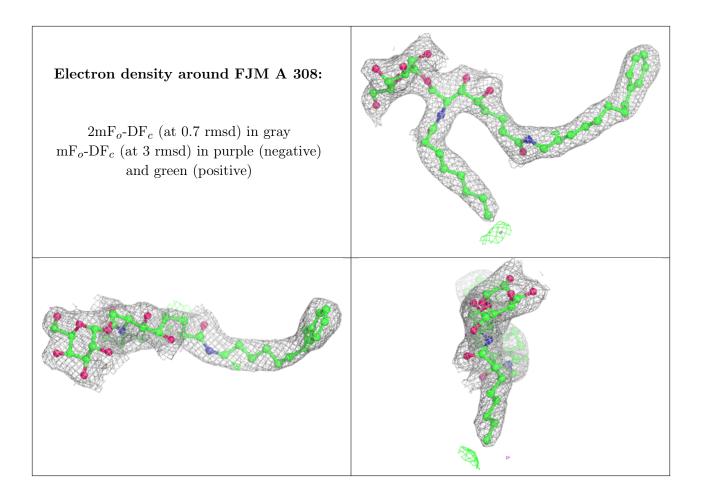
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q < 0.9
7	NAG	А	301	14/15	0.87	0.17	59,67,71,72	0
8	PLM	А	307	18/18	0.87	0.25	$48,\!51,\!69,\!72$	0
9	FJM	А	308	48/48	0.95	0.20	24,30,50,52	0
10	NA	А	309	1/1	0.96	0.19	34,34,34,34	0

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.

