



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:31 AM UTC

PDB ID : 6CWB / pdb_00006cwb
Title : Structure of alpha-GSA[8,4P] bound by CD1d and in complex with the Va14Vb8.2 TCR
Authors : Wang, J.; Zajonc, D.
Deposited on : 2018-03-30
Resolution : 2.85 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

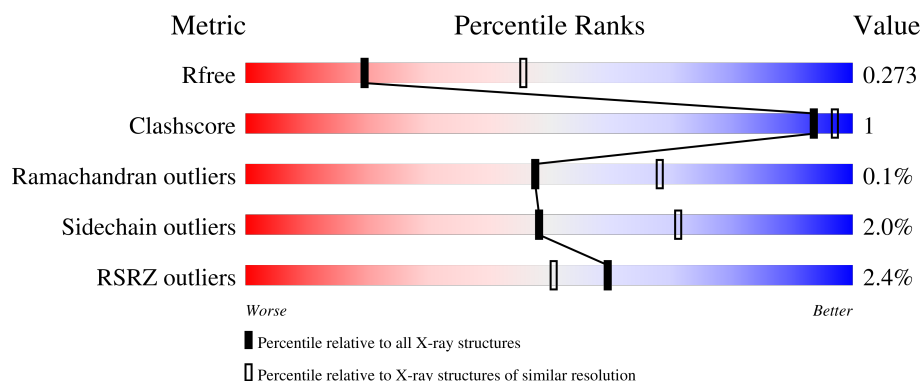
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	A	285	2% 86% 7% 7%
2	B	99	4% 95% ..
3	C	209	2% 90% 5% .
4	D	241	% 95% ..
5	E	3	33% 67%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6441 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	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	2	0
			2125	1361	358	393	13			

There are 6 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			790	504	130	149	7			

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

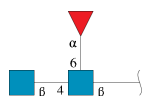
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	201	Total	C	N	O	S	0	0	0
			1521	943	260	310	8			

- 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	C	N	O	S	0	0	0
			1876	1178	334	358	6			

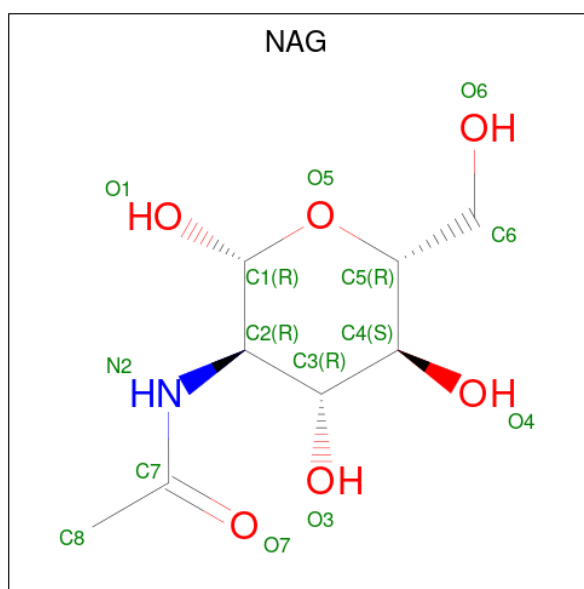
- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[al

pha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



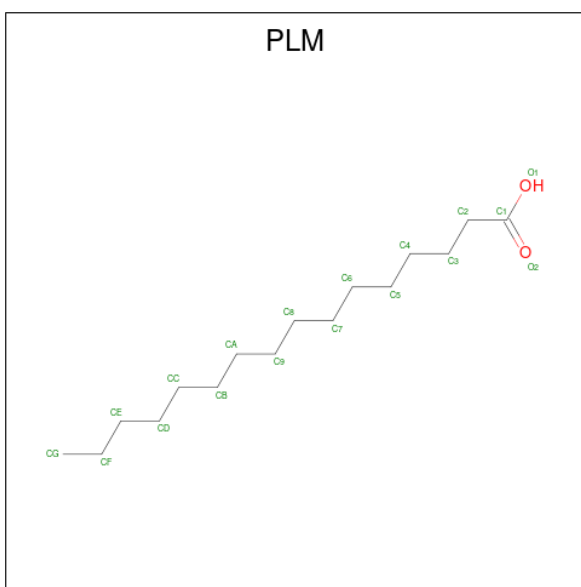
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



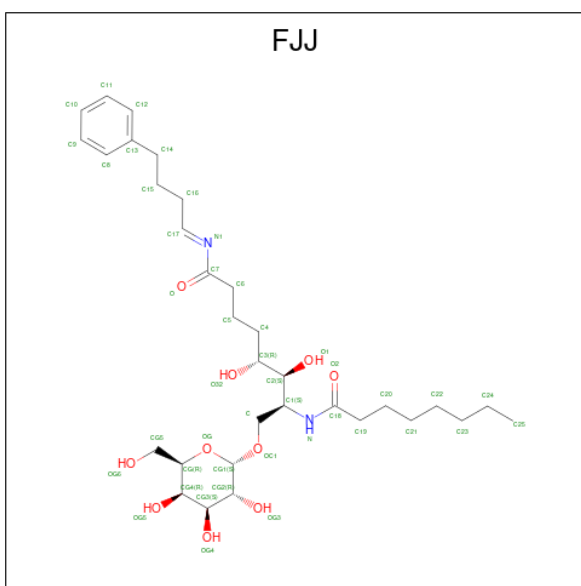
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			18	16	2		

- Molecule 8 is (5R,6S,7S)-5,6-dihydroxy-7-(octanoylamino)-N-[(1E)-4-phenylbutylidene]-8-[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl]oxy}octanamide (non-preferred name) (CCD ID: FJJ) (formula: C₃₂H₅₂N₂O₁₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			44	32	2	10		

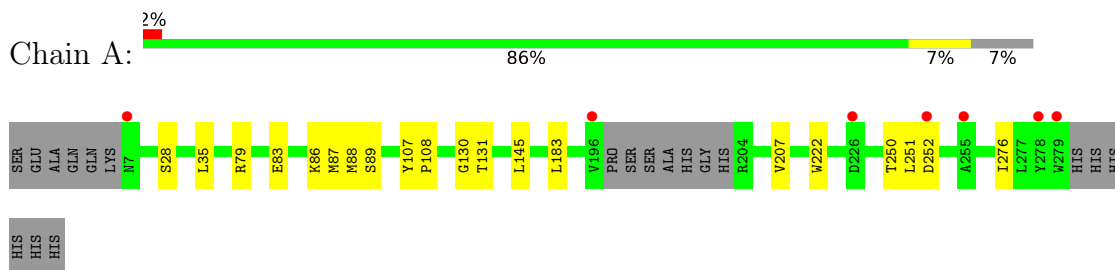
- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total	Na	0	0
			1	1		

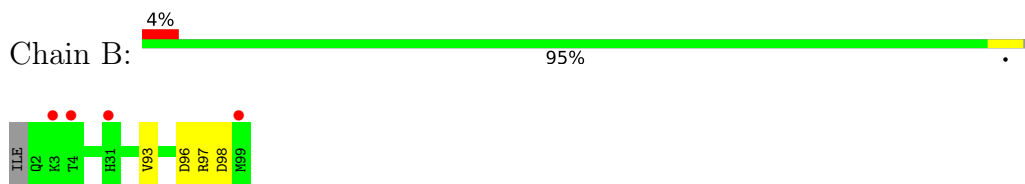
3 Residue-property plots

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.

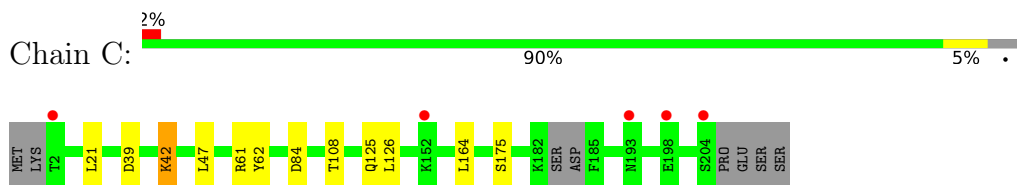
- Molecule 1: Antigen-presenting glycoprotein CD1d1



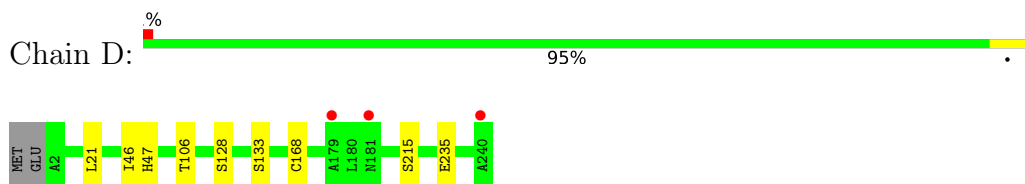
- Molecule 2: Beta-2-microglobulin



- Molecule 3: Chimeric T cell antigen receptor alpha chain Va14,Va24,Ja18



- Molecule 4: Chimeric T cell antigen receptor beta chain Vb8.2, vb11



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	78.31Å 190.27Å 151.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.22 – 2.85 35.22 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (35.22-2.85) 99.6 (35.22-2.85)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.215 , 0.275 0.218 , 0.273	Depositor DCC
R_{free} test set	1380 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 11.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6441	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: FUC, PLM, NA, FJJ, NAG

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	A	0.59	0/2192	0.79	0/2982
2	B	0.60	0/816	0.74	0/1112
3	C	0.61	0/1548	0.78	0/2108
4	D	0.57	0/1927	0.74	0/2626
All	All	0.59	0/6483	0.77	0/8828

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	A	2125	0	2020	9	0
2	B	790	0	732	1	0
3	C	1521	0	1428	6	0
4	D	1876	0	1785	2	0
5	E	38	0	34	0	0
6	A	28	0	26	0	0
7	A	18	0	31	0	0
8	A	44	0	0	0	0
9	D	1	0	0	0	0
All	All	6441	0	6056	18	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 1.

All (18) 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:88:MET:HE1	1:A:145:LEU:HD23	1.66	0.76
3:C:61:ARG:NH2	3:C:84:ASP:OD2	2.21	0.73
1:A:35:LEU:HD12	1:A:183:LEU:HD23	1.71	0.72
4:D:21:LEU:HD22	4:D:106:THR:HG21	1.91	0.52
3:C:21:LEU:HG	3:C:108:THR:HG21	1.93	0.50
1:A:83:GLU:HA	1:A:86:LYS:HD2	1.93	0.50
3:C:125:GLN:C	3:C:126:LEU:HD12	2.41	0.47
3:C:47:LEU:HD22	3:C:62:TYR:CE2	2.51	0.46
3:C:164:LEU:C	3:C:164:LEU:HD12	2.42	0.45
1:A:87:MET:C	1:A:88:MET:HE2	2.43	0.44
3:C:39:ASP:HB2	3:C:42:LYS:HG3	1.99	0.44
4:D:46:ILE:HG22	4:D:47:HIS:CD2	2.53	0.43
1:A:107:TYR:HB3	1:A:108:PRO:HD2	2.00	0.43
1:A:207:VAL:HG22	1:A:250:THR:HG22	2.02	0.42
1:A:35:LEU:CD1	1:A:183:LEU:HD23	2.46	0.41
1:A:131:THR:O	1:A:131:THR:HG22	2.21	0.41
2:B:96:ASP:O	2:B:98:ASP:N	2.53	0.40
1:A:222:TRP:CD1	1:A:251:LEU:HB2	2.56	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	A	264/285 (93%)	256 (97%)	7 (3%)	1 (0%)	30	48
2	B	96/99 (97%)	90 (94%)	6 (6%)	0	100	100
3	C	197/209 (94%)	186 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	237/241 (98%)	233 (98%)	4 (2%)	0	100	100
All	All	794/834 (95%)	765 (96%)	28 (4%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	GLY

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	A	228/249 (92%)	223 (98%)	5 (2%)	45	69
2	B	87/93 (94%)	85 (98%)	2 (2%)	44	68
3	C	171/188 (91%)	169 (99%)	2 (1%)	63	80
4	D	203/208 (98%)	198 (98%)	5 (2%)	42	66
All	All	689/738 (93%)	675 (98%)	14 (2%)	48	71

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	79	ARG
1	A	89	SER
1	A	252	ASP
1	A	276	ILE
2	B	93	VAL
2	B	97	ARG
3	C	42	LYS
3	C	175	SER
4	D	128	SER
4	D	133	SER
4	D	168	CYS
4	D	215	SER

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Mol	Chain	Res	Type
4	D	235	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	117	HIS
1	A	134	GLN
1	A	229	GLN
1	A	267	HIS
2	B	8	GLN
3	C	76	HIS
4	D	24	ASN

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 ⓘ

3 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	E	1	5,1	14,14,15	0.51	0	17,19,21	1.13	1 (5%)
5	NAG	E	2	5	14,14,15	0.36	0	17,19,21	1.49	1 (5%)
5	FUC	E	3	5	10,10,11	0.66	0	14,14,16	0.77	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
5	NAG	E	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	FUC	E	3	5	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	2	NAG	C1-O5-C5	4.95	118.81	112.19
5	E	1	NAG	C1-C2-N2	2.68	114.66	110.43

There are no chirality outliers.

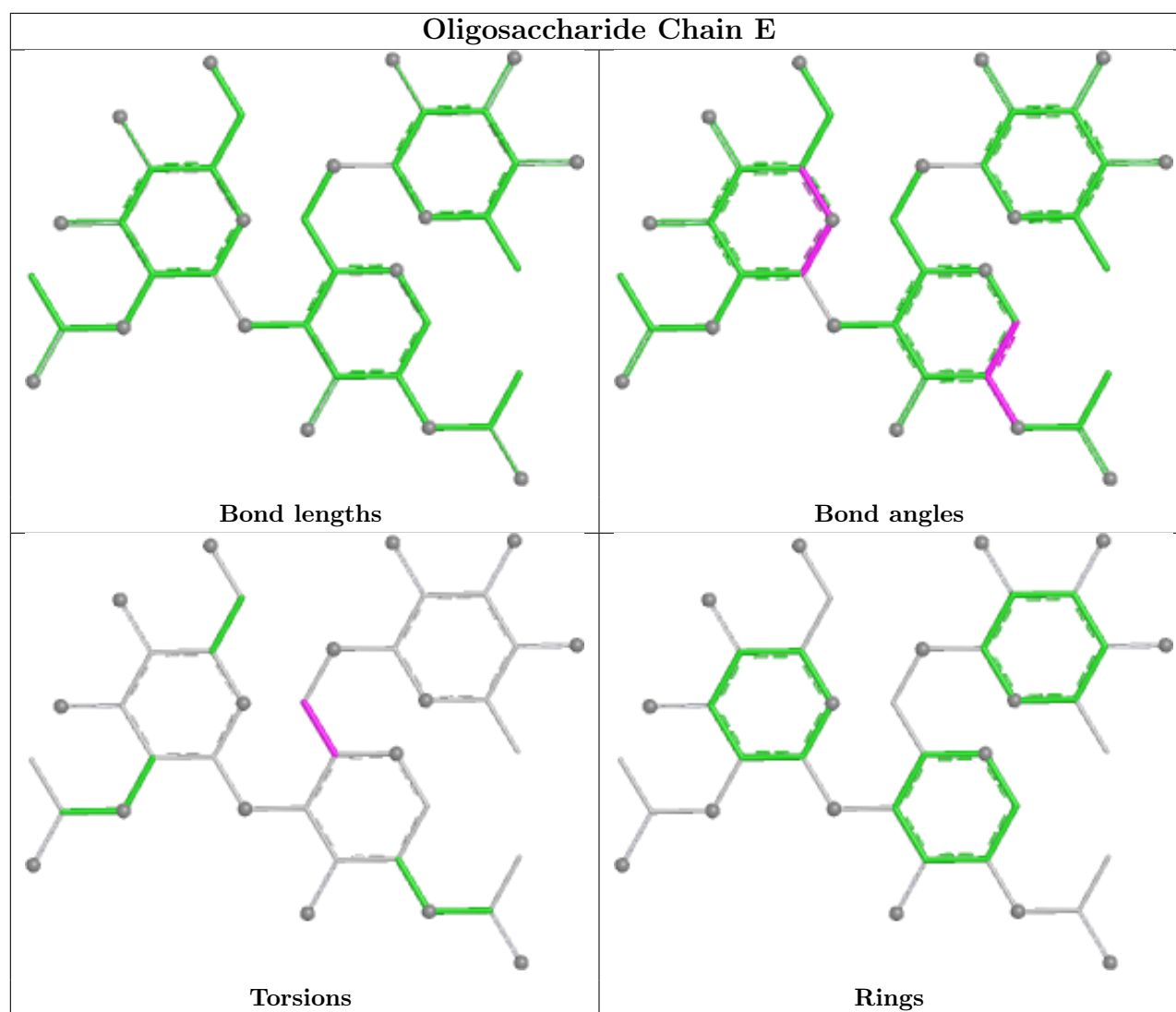
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
7	PLM	A	306	-	17,17,17	0.64	0	17,17,17	1.49	3 (17%)
8	FJJ	A	307	-	44,45,45	1.77	7 (15%)	49,57,57	1.65	9 (18%)
6	NAG	A	301	1	14,14,15	0.42	0	17,19,21	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	302	1	14,14,15	0.59	0	17,19,21	1.55	1 (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	PLM	A	306	-	-	10/15/15/15	-
8	FJJ	A	307	-	-	6/37/60/60	0/2/2/2
6	NAG	A	301	1	-	2/6/23/26	0/1/1/1
6	NAG	A	302	1	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	307	FJJ	C16-C17	7.48	1.56	1.49
8	A	307	FJJ	C17-N1	5.77	1.47	1.26
8	A	307	FJJ	OC1-CG1	3.27	1.45	1.40
8	A	307	FJJ	C19-C18	2.70	1.56	1.51
8	A	307	FJJ	C14-C13	-2.20	1.45	1.51
8	A	307	FJJ	C11-C12	2.10	1.42	1.38
8	A	307	FJJ	C9-C8	2.03	1.42	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	307	FJJ	C5-C4-C3	-6.87	102.86	114.11
6	A	302	NAG	C1-O5-C5	5.35	119.36	112.19
7	A	306	PLM	C4-C3-C2	-3.00	102.12	113.13
8	A	307	FJJ	C9-C10-C11	-2.69	116.18	119.87
7	A	306	PLM	CC-CB-CA	-2.67	100.86	114.37
8	A	307	FJJ	OG6-CG5-CG	-2.63	102.39	111.33
7	A	306	PLM	C6-C5-C4	-2.44	102.03	114.37
8	A	307	FJJ	C-C1-N	-2.41	106.22	109.66
8	A	307	FJJ	C4-C3-C2	2.34	117.68	113.97
8	A	307	FJJ	C12-C13-C8	-2.27	114.86	118.23
8	A	307	FJJ	C10-C11-C12	2.10	122.84	120.24
8	A	307	FJJ	C9-C8-C13	2.10	123.57	120.61
8	A	307	FJJ	C15-C16-C17	2.06	120.58	114.31

There are no chirality outliers.

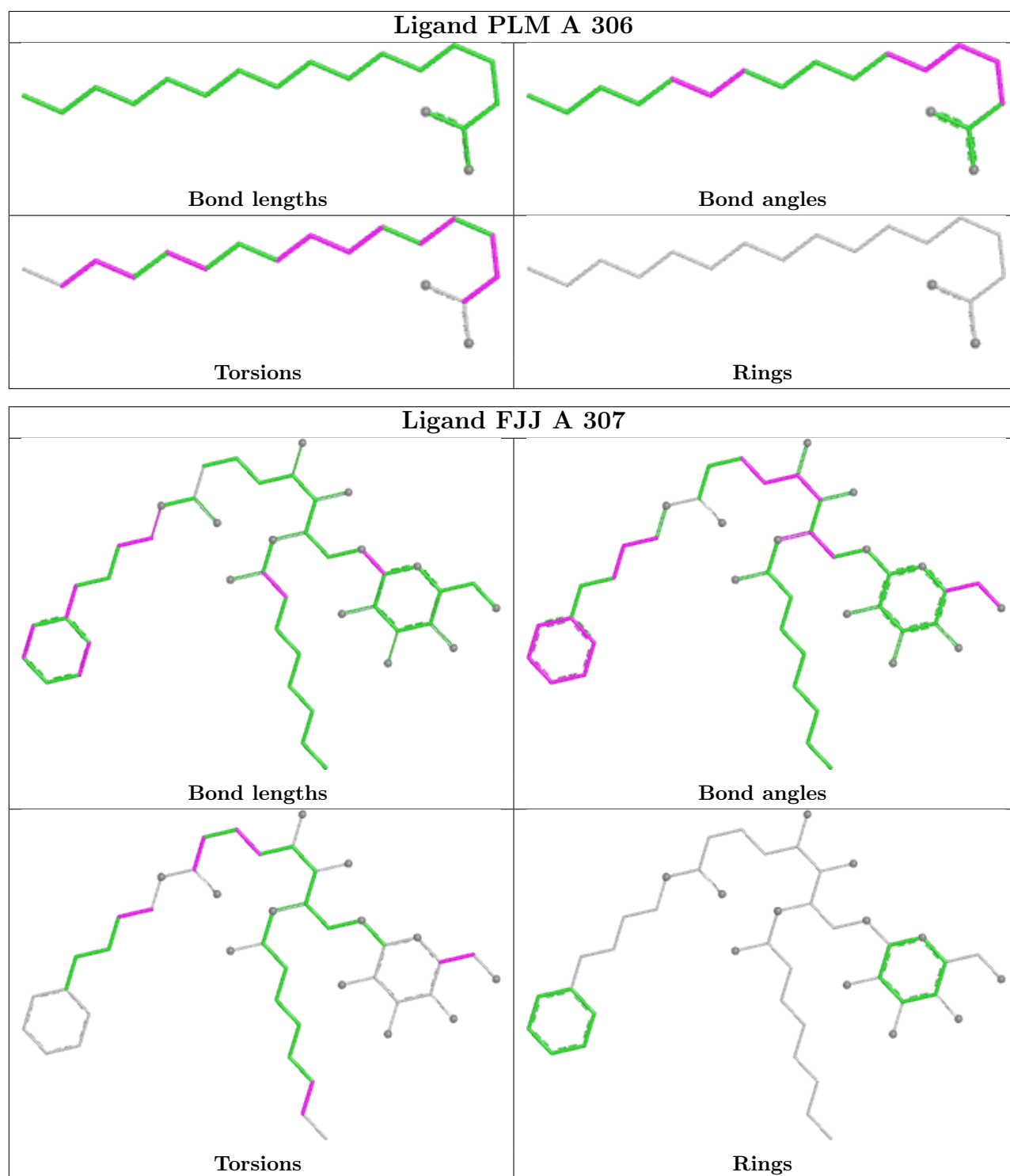
All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	307	FJJ	C15-C16-C17-N1
6	A	302	NAG	O5-C5-C6-O6
6	A	302	NAG	C4-C5-C6-O6
7	A	306	PLM	C7-C8-C9-CA
7	A	306	PLM	C1-C2-C3-C4
7	A	306	PLM	C3-C4-C5-C6
6	A	301	NAG	O5-C5-C6-O6
7	A	306	PLM	C6-C7-C8-C9
7	A	306	PLM	CD-CE-CF-CG
8	A	307	FJJ	C22-C23-C24-C25
7	A	306	PLM	CC-CD-CE-CF
7	A	306	PLM	C5-C6-C7-C8
8	A	307	FJJ	CG4-CG-CG5-OG6
7	A	306	PLM	O2-C1-C2-C3
7	A	306	PLM	CA-CB-CC-CD
7	A	306	PLM	O1-C1-C2-C3
8	A	307	FJJ	OG-CG-CG5-OG6
6	A	301	NAG	C1-C2-N2-C7
8	A	307	FJJ	C3-C4-C5-C6
8	A	307	FJJ	C5-C6-C7-N1

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 ⓘ

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	A	266/285 (93%)	0.04	7 (2%) 57 48	21, 45, 89, 106	2 (0%)
2	B	98/99 (98%)	0.21	4 (4%) 41 32	40, 58, 82, 109	0
3	C	201/209 (96%)	0.04	5 (2%) 58 49	29, 48, 84, 113	0
4	D	239/241 (99%)	-0.23	3 (1%) 75 68	30, 44, 65, 85	0
All	All	804/834 (96%)	-0.02	19 (2%) 59 51	21, 47, 83, 113	2 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	152	LYS	4.3
1	A	226	ASP	3.7
1	A	196	VAL	2.7
4	D	179	ALA	2.7
4	D	240	ALA	2.7
2	B	3	LYS	2.5
3	C	193	ASN	2.5
3	C	204	SER	2.5
1	A	7	ASN	2.5
2	B	99	MET	2.4
3	C	198	GLU	2.3
2	B	4	THR	2.3
1	A	255	ALA	2.2
4	D	181	ASN	2.2
3	C	2	THR	2.2
2	B	31	HIS	2.1
1	A	278	TYR	2.1
1	A	279	TRP	2.0
1	A	252	ASP	2.0

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

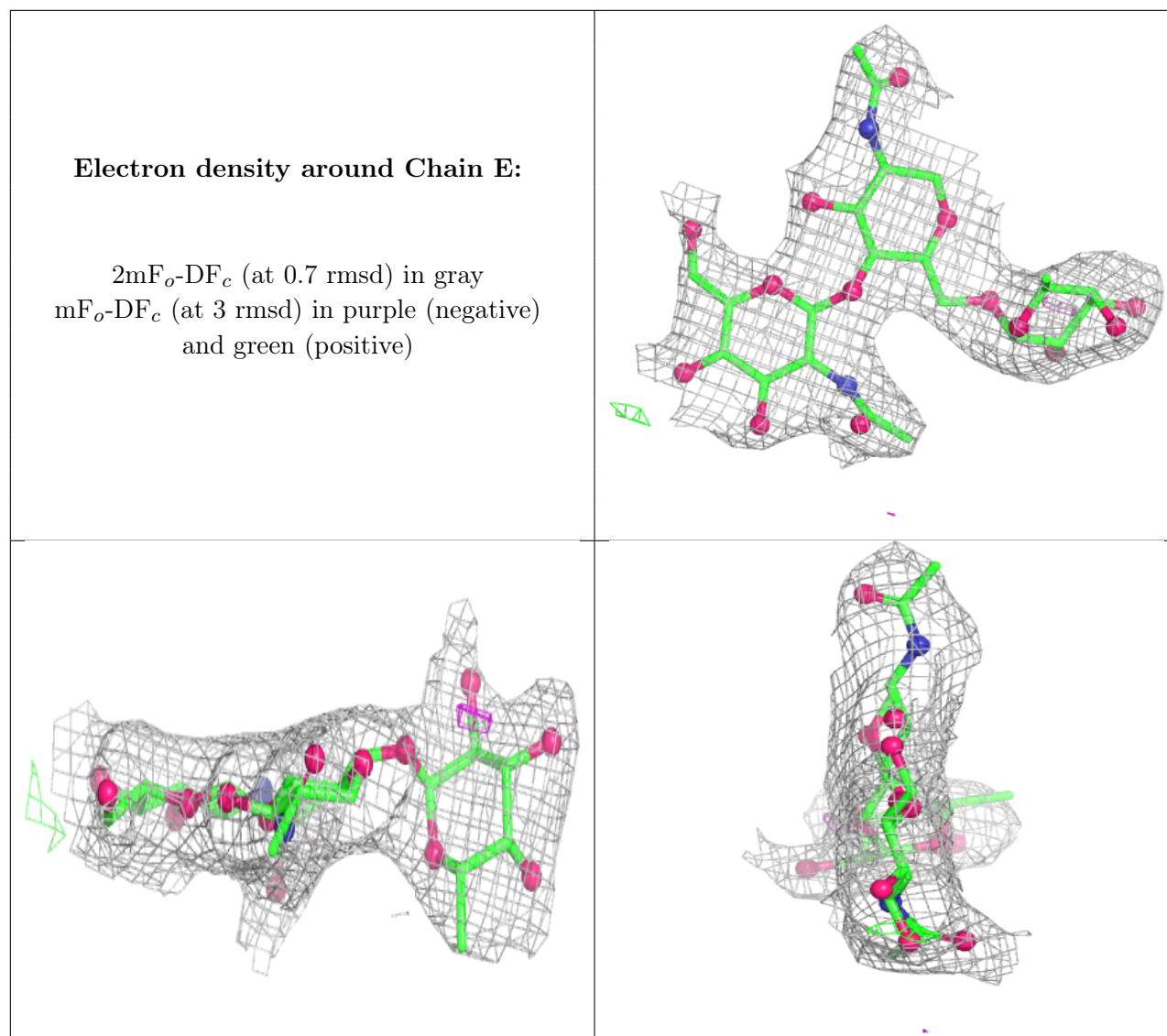
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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($\text{\AA}^2$)	Q<0.9
5	NAG	E	2	14/15	0.79	0.12	62,65,68,68	0
5	FUC	E	3	10/11	0.88	0.13	66,72,77,78	0
5	NAG	E	1	14/15	0.94	0.08	51,53,60,66	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.



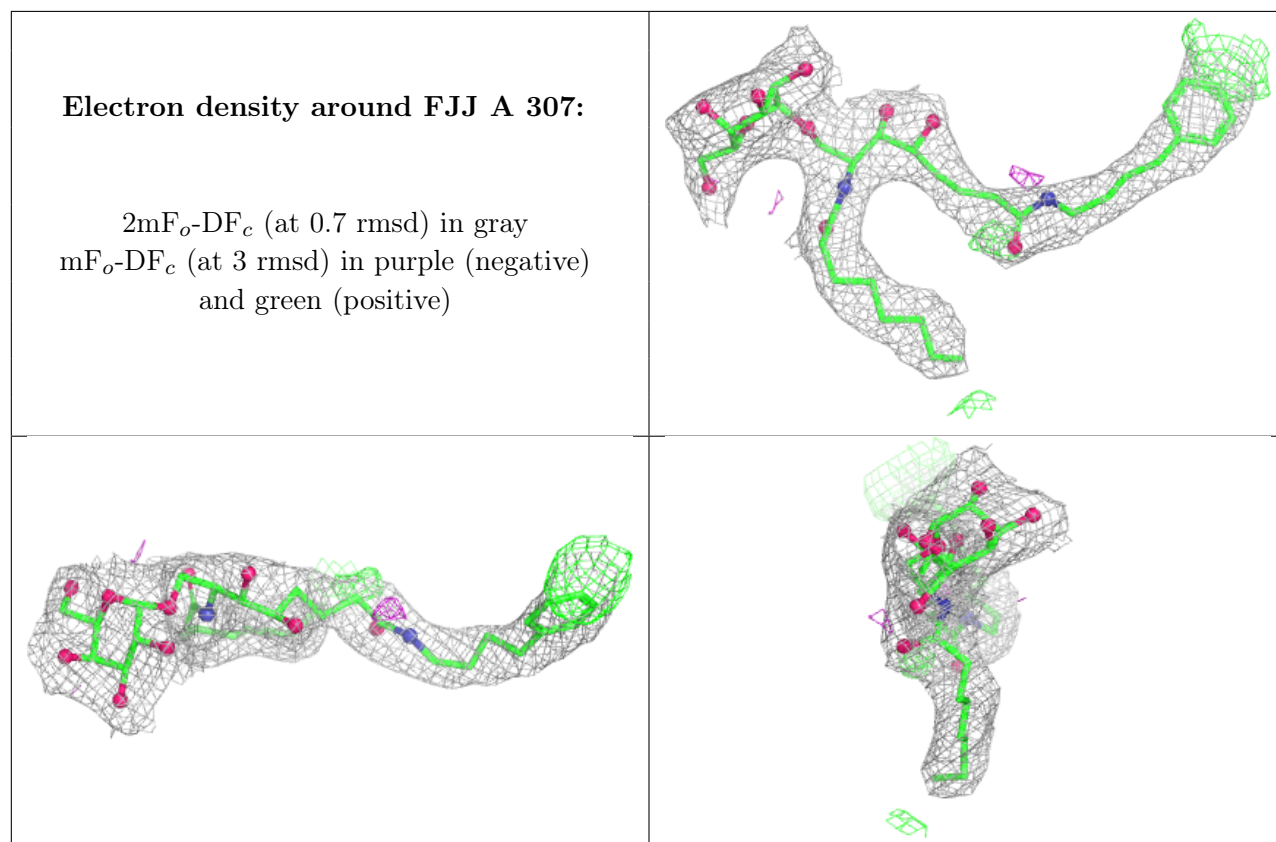
6.4 Ligands ⓘ

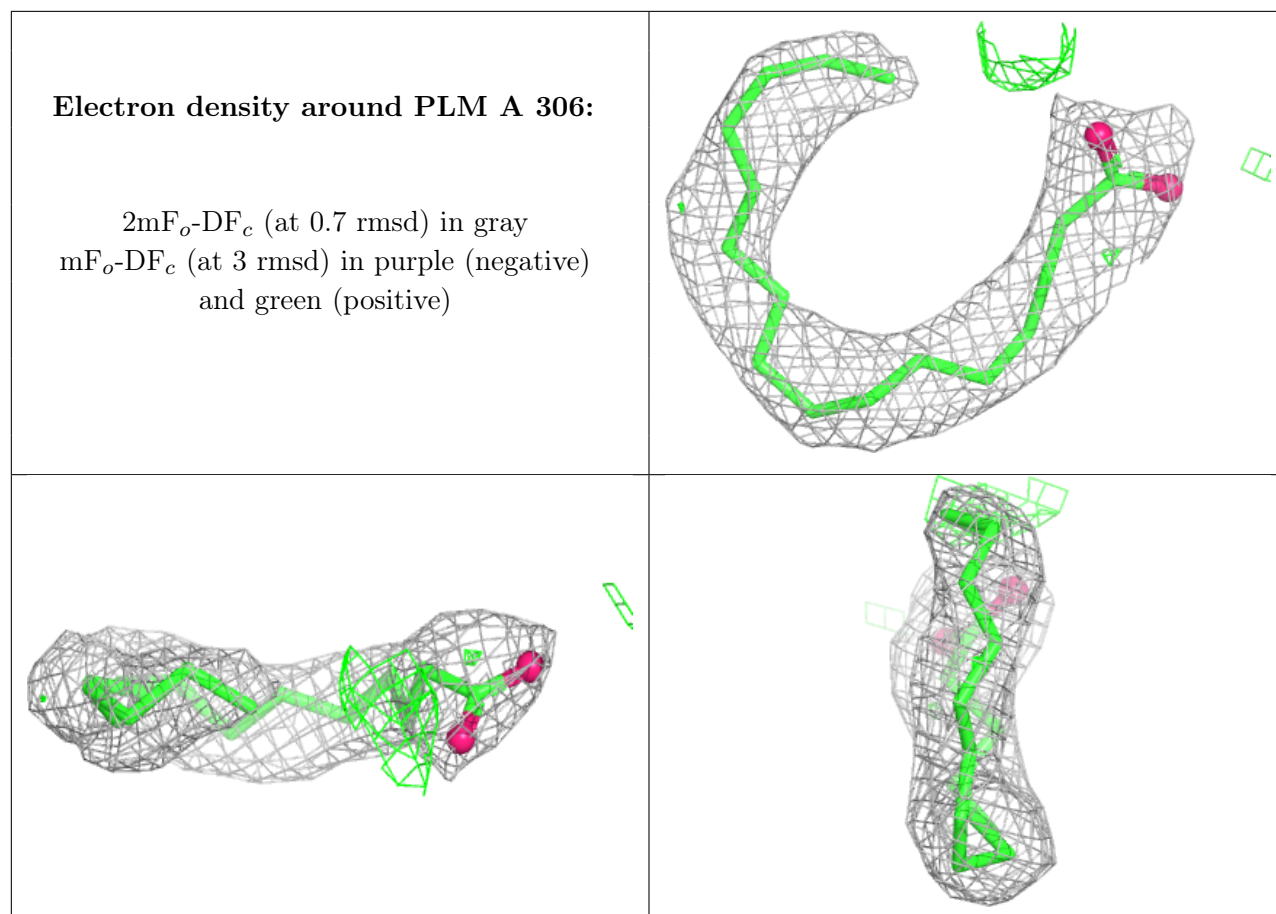
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	A	301	14/15	0.77	0.13	69,73,74,79	0
6	NAG	A	302	14/15	0.89	0.10	39,40,46,46	0
8	FJJ	A	307	44/44	0.90	0.12	31,39,58,59	0
7	PLM	A	306	18/18	0.92	0.19	60,65,72,74	0
9	NA	D	301	1/1	0.93	0.07	42,42,42,42	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.