



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2025 – 03:02 PM EST

PDB ID : 9OHT / pdb\_00009oht  
Title : CD1c presenting GD3 ganglioside  
Authors : Cao, T.P.; Rossjohn, J.; Shahine, A.  
Deposited on : 2025-05-05  
Resolution : 2.98 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](mailto: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>.

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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 : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.47

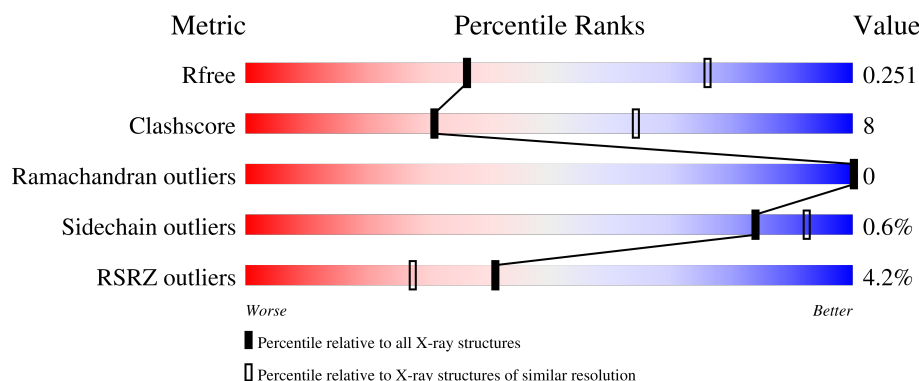
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.98 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))
$R_{free}$	164625	3360 (3.00-2.96)
Clashscore	180529	3751 (3.00-2.96)
Ramachandran outliers	177936	3628 (3.00-2.96)
Sidechain outliers	177891	3631 (3.00-2.96)
RSRZ outliers	164620	3372 (3.00-2.96)

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  $\geq 3$ , 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	281	
2	B	101	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MLA	A	304	-	X	-	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3145 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 T-cell surface glycoprotein CD1c/T-cell surface glycoprotein CD1b chimeric protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2196	1406	378	403	9			

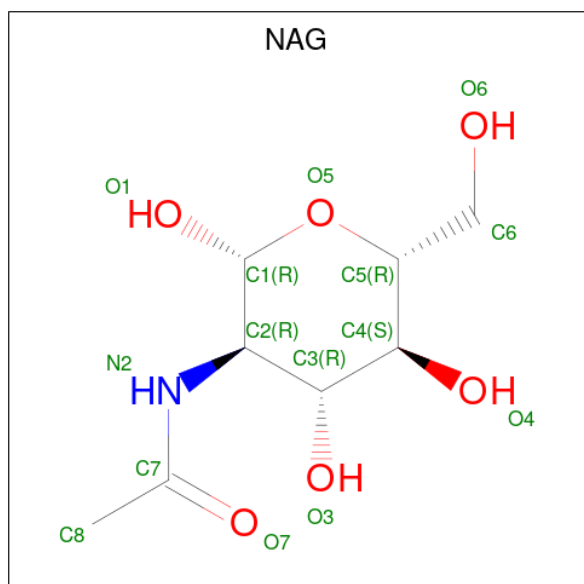
- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			782	500	136	144	2			

There is a discrepancy between the modelled and reference sequences:

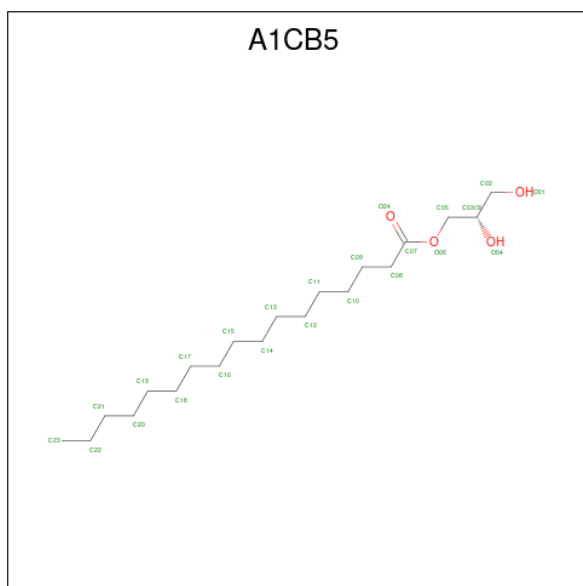
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ALA	-	expression tag	UNP P61769

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



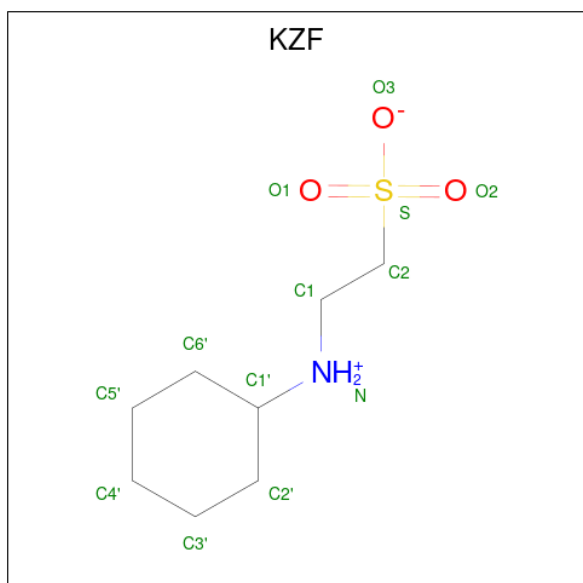
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is (2S)-2,3-dihydroxypropyl heptadecanoate (CCD ID: A1CB5) (formula:  $C_{20}H_{40}O_4$ ).



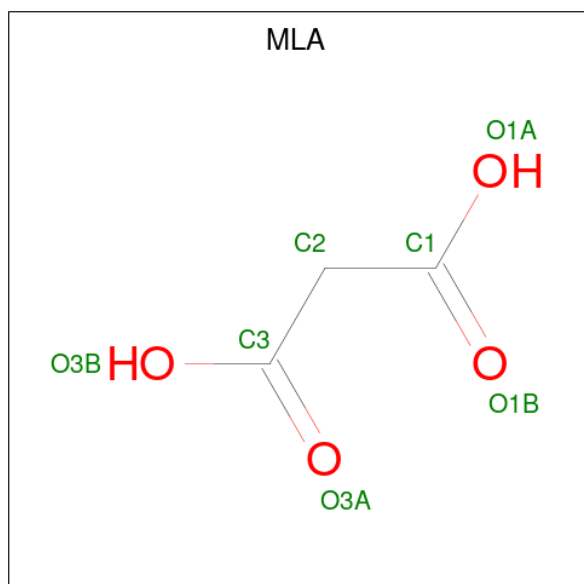
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			24	20	4		

- Molecule 5 is 2-(cyclohexylazanumyl)ethanesulfonate (CCD ID: KZF) (formula:  $C_8H_{17}NO_3S$ ).



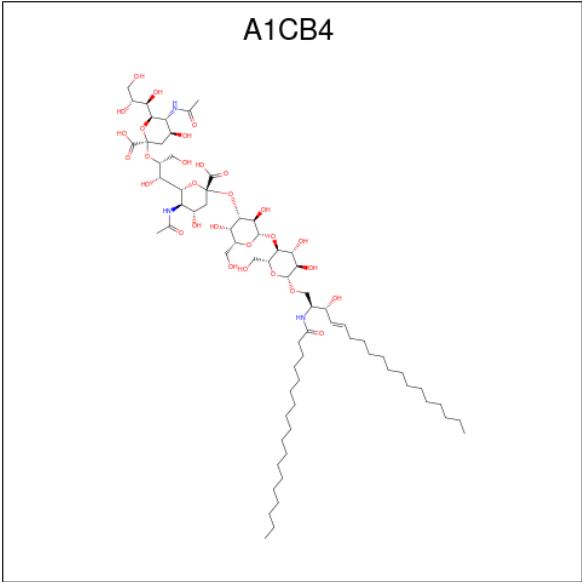
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 6 is MALONIC ACID (CCD ID: MLA) (formula:  $C_3H_4O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	3	4		
6	A	1	Total	C	O	0	0
			7	3	4		

- Molecule 7 is (2S,3R,4E)-3-hydroxy-2-octadecanamido-octadec-4-en-1-yl 5-acetamido-3,5-dideoxy-D-glycero- $\alpha$ -D-galacto-non-2-ulopyranonosyl-(2->8)-5-acetamido-3,5-dideoxy-D-glycero- $\alpha$ -D-galacto-non-2-ulopyranonosyl-(2->3)-beta-D-galactopyranosyl-(1->4)-beta-D-glucopyranoside (CCD ID: A1CB4) (formula:  $C_{70}H_{125}N_3O_{29}$ ) (labeled as "Ligand of Interest" by depositor).

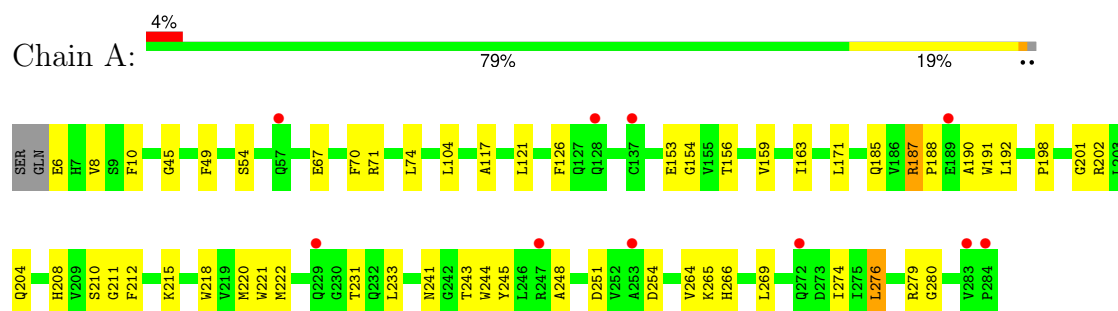


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	102	70	3	29	0	0

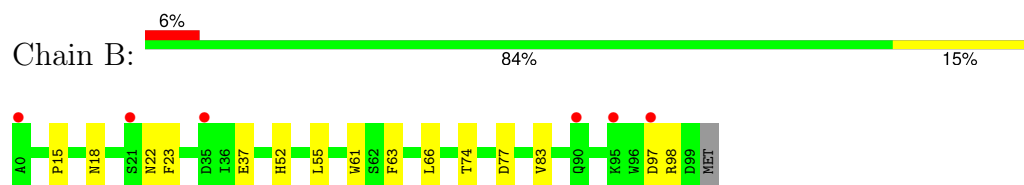
### 3 Residue-property plots [i](#)

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: T-cell surface glycoprotein CD1c/T-cell surface glycoprotein CD1b chimeric protein



- Molecule 2: Beta-2-microglobulin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.50Å 89.50Å 158.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.64 – 2.98 43.64 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.64-2.98) 99.8 (43.64-2.98)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 2.95Å)	Xtriage
Refinement program	PHENIX (1.21rc1_5107: ???)	Depositor
R, $R_{free}$	0.224 , 0.251 0.220 , 0.251	Depositor DCC
$R_{free}$ test set	793 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.8	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 67.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3145	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: KZF, MLA, NAG, A1CB4, A1CB5

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	0.50	0/2263	0.69	0/3080
2	B	0.55	0/805	0.70	0/1101
All	All	0.51	0/3068	0.69	0/4181

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	ARG	Sidechain

### 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	2196	0	2070	41	0
2	B	782	0	712	9	0
3	A	14	0	13	0	0
4	A	24	0	0	0	0
5	A	13	0	0	0	0
6	A	14	0	4	1	0
7	A	102	0	0	0	0
All	All	3145	0	2799	48	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 8.

All (48) 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:198:PRO:HG3	1:A:251:ASP:HB2	1.53	0.87
2:B:74:THR:HB	2:B:77:ASP:OD1	1.83	0.78
1:A:198:PRO:HG2	1:A:202:ARG:HB3	1.70	0.73
1:A:188:PRO:HB3	1:A:212:PHE:HB3	1.72	0.71
1:A:192:LEU:HD13	1:A:276:LEU:HD23	1.72	0.71
1:A:191:TRP:CD2	2:B:15:PRO:HG3	2.27	0.70
1:A:202:ARG:NH1	1:A:251:ASP:OD1	2.30	0.65
1:A:218:TRP:CE3	1:A:265:LYS:HG3	2.37	0.59
1:A:126:PHE:HE1	1:A:156:THR:HG23	1.70	0.57
1:A:153:GLU:OE2	1:A:153:GLU:HA	2.10	0.52
1:A:279:ARG:HG3	1:A:280:GLY:N	2.25	0.52
1:A:45:GLY:O	1:A:71:ARG:HD3	2.10	0.51
1:A:117:ALA:HB2	2:B:61:TRP:CE2	2.46	0.50
1:A:153:GLU:OE2	1:A:156:THR:HB	2.12	0.50
2:B:18:ASN:OD1	2:B:74:THR:HA	2.12	0.49
1:A:49:PHE:HB3	1:A:54:SER:HB2	1.93	0.49
1:A:201:GLY:O	1:A:254:ASP:HB2	2.13	0.49
1:A:190:ALA:HA	1:A:208:HIS:O	2.13	0.49
1:A:210:SER:HB2	1:A:245:TYR:HD1	1.78	0.48
1:A:241:ASN:ND2	6:A:305:MLA:O1B	2.35	0.48
1:A:218:TRP:CH2	1:A:220:MET:HB2	2.49	0.48
1:A:8:VAL:HG13	1:A:171:LEU:HD21	1.96	0.47
1:A:10:PHE:HB2	1:A:171:LEU:HD13	1.94	0.47
1:A:218:TRP:HE3	1:A:265:LYS:HG3	1.80	0.47
1:A:211:GLY:HA2	1:A:243:THR:HB	1.96	0.47
1:A:221:TRP:C	1:A:222:MET:HG2	2.41	0.46
2:B:22:ASN:OD1	2:B:23:PHE:N	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLN:HE21	1:A:185:GLN:HB3	1.56	0.45
1:A:233:LEU:HD23	1:A:248:ALA:HB2	1.99	0.44
1:A:198:PRO:HD3	1:A:204:GLN:HB2	2.00	0.44
1:A:67:GLU:O	1:A:71:ARG:HG3	2.19	0.43
2:B:55:LEU:HD11	2:B:63:PHE:HB3	2.00	0.43
1:A:104:LEU:HD12	1:A:104:LEU:HA	1.81	0.43
1:A:6:GLU:N	1:A:6:GLU:OE1	2.52	0.43
1:A:215:LYS:HD2	1:A:244:TRP:CZ2	2.55	0.42
1:A:153:GLU:CD	1:A:154:GLY:H	2.27	0.42
1:A:159:VAL:O	1:A:163:ILE:HG12	2.20	0.41
1:A:264:VAL:HB	1:A:274:ILE:HB	2.01	0.41
2:B:52:HIS:HA	2:B:66:LEU:O	2.21	0.41
1:A:70:PHE:O	1:A:74:LEU:HG	2.20	0.41
1:A:198:PRO:HG3	1:A:251:ASP:CB	2.39	0.41
1:A:215:LYS:HD2	1:A:244:TRP:CE2	2.55	0.41
1:A:187:ARG:HG2	1:A:269:LEU:HD23	2.02	0.41
1:A:126:PHE:CE1	1:A:156:THR:HG23	2.54	0.41
1:A:266:HIS:HB3	1:A:269:LEU:HG	2.02	0.41
2:B:37:GLU:O	2:B:83:VAL:HA	2.21	0.41
1:A:121:LEU:HA	1:A:121:LEU:HD23	1.87	0.40
2:B:97:ASP:OD1	2:B:98:ARG:N	2.55	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	277/281 (99%)	265 (96%)	12 (4%)	0	100	100
2	B	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
All	All	375/382 (98%)	359 (96%)	16 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	233/240 (97%)	231 (99%)	2 (1%)	75	88
2	B	81/94 (86%)	81 (100%)	0	100	100
All	All	314/334 (94%)	312 (99%)	2 (1%)	84	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	THR
1	A	276	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	25	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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	MLA	A	304	-	6,6,6	1.92	3 (50%)	7,7,7	1.16	1 (14%)
6	MLA	A	305	-	6,6,6	1.86	2 (33%)	7,7,7	1.67	2 (28%)
5	KZF	A	303	-	13,13,13	1.85	3 (23%)	16,17,17	2.41	4 (25%)
7	A1CB4	A	306	-	102,105,105	2.12	25 (24%)	130,141,141	1.54	17 (13%)
3	NAG	A	301	1	14,14,15	0.77	0	17,19,21	1.93	5 (29%)
4	A1CB5	A	302	-	23,23,23	1.00	1 (4%)	24,24,24	0.91	1 (4%)

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
6	MLA	A	304	-	-	3/4/4/4	-
6	MLA	A	305	-	-	2/4/4/4	-
5	KZF	A	303	-	-	1/7/15/15	0/1/1/1
7	A1CB4	A	306	-	-	52/101/179/179	0/4/4/4
3	NAG	A	301	1	-	2/6/23/26	0/1/1/1
4	A1CB5	A	302	-	-	10/23/23/23	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	306	A1CB4	C45-C46	-7.12	1.46	1.53
7	A	306	A1CB4	C56-C57	-6.91	1.47	1.53
7	A	306	A1CB4	C18-N20	6.13	1.47	1.34
5	A	303	KZF	C2-S	5.23	1.84	1.77
7	A	306	A1CB4	C67-N66	4.17	1.47	1.34
7	A	306	A1CB4	C49-C47	4.15	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	306	A1CB4	O48-C43	4.15	1.47	1.42
7	A	306	A1CB4	C76-N75	4.13	1.47	1.34
7	A	306	A1CB4	O29-C24	3.89	1.51	1.41
7	A	306	A1CB4	C49-C50	3.88	1.60	1.52
7	A	306	A1CB4	C86-C87	3.83	1.56	1.50
7	A	306	A1CB4	O42-C35	3.77	1.47	1.42
4	A	302	A1CB5	O06-C07	3.70	1.44	1.33
7	A	306	A1CB4	C60-C58	3.67	1.57	1.52
7	A	306	A1CB4	C44-C45	-3.61	1.47	1.53
7	A	306	A1CB4	O59-C54	3.46	1.46	1.42
7	A	306	A1CB4	C22-C21	3.23	1.57	1.51
7	A	306	A1CB4	O48-C47	3.23	1.48	1.44
7	A	306	A1CB4	C55-C56	-3.12	1.48	1.53
6	A	305	MLA	C2-C1	2.84	1.55	1.51
7	A	306	A1CB4	O59-C58	2.77	1.48	1.44
7	A	306	A1CB4	O23-C24	2.75	1.44	1.40
6	A	304	MLA	C2-C1	2.74	1.55	1.51
5	A	303	KZF	O1-S	2.36	1.51	1.45
5	A	303	KZF	O2-S	2.34	1.51	1.45
6	A	304	MLA	O3A-C3	2.28	1.29	1.22
7	A	306	A1CB4	C78-C76	2.27	1.55	1.50
7	A	306	A1CB4	O19-C18	-2.25	1.18	1.23
7	A	306	A1CB4	C69-C67	2.19	1.55	1.50
7	A	306	A1CB4	O32-C27	2.18	1.49	1.43
6	A	305	MLA	C2-C3	2.17	1.54	1.51
7	A	306	A1CB4	C26-C25	-2.14	1.46	1.52
6	A	304	MLA	C2-C3	2.04	1.54	1.51
7	A	306	A1CB4	O38-C33	2.03	1.47	1.41

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	306	A1CB4	O48-C47-C46	9.52	118.56	109.84
5	A	303	KZF	O2-S-C2	5.66	115.28	106.73
5	A	303	KZF	O2-S-O1	-5.42	96.20	113.82
7	A	306	A1CB4	O59-C58-C60	4.76	114.08	106.65
3	A	301	NAG	C1-O5-C5	4.66	118.43	112.19
7	A	306	A1CB4	C10-C09-C08	4.14	135.27	114.37
5	A	303	KZF	O1-S-C2	3.83	112.52	106.73
7	A	306	A1CB4	C58-C57-N66	-3.73	104.95	110.91
7	A	306	A1CB4	O59-C58-C57	3.11	112.69	109.84
3	A	301	NAG	C4-C3-C2	-3.06	106.53	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	306	A1CB4	C21-N20-C18	-3.03	118.36	123.40
4	A	302	A1CB5	O06-C07-C08	3.02	121.05	111.83
3	A	301	NAG	C1-C2-N2	3.01	115.18	110.43
7	A	306	A1CB4	C86-C87-C88	-2.91	118.65	124.69
7	A	306	A1CB4	C54-C55-C56	2.86	116.52	110.73
7	A	306	A1CB4	C25-C26-C27	2.74	115.91	109.68
7	A	306	A1CB4	C55-C56-C57	2.73	113.94	109.72
7	A	306	A1CB4	C54-O59-C58	-2.59	108.27	114.36
3	A	301	NAG	O4-C4-C5	2.56	115.63	109.32
7	A	306	A1CB4	C78-C76-N75	2.53	120.32	116.12
7	A	306	A1CB4	C33-O32-C27	-2.52	112.01	117.98
7	A	306	A1CB4	O29-C28-C27	2.48	114.85	109.72
7	A	306	A1CB4	C33-O38-C37	-2.46	108.91	113.72
3	A	301	NAG	O5-C1-C2	-2.46	107.48	111.29
5	A	303	KZF	C1-N-C1'	-2.32	109.72	114.18
6	A	305	MLA	O3B-C3-C2	2.12	121.08	114.51
6	A	305	MLA	C3-C2-C1	2.07	120.26	112.95
7	A	306	A1CB4	C17-C18-N20	2.06	119.50	115.86
6	A	304	MLA	O1A-C1-C2	2.04	120.83	114.51
7	A	306	A1CB4	O19-C18-N20	-2.01	119.55	122.95

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	306	A1CB4	C22-C21-C86-C87
7	A	306	A1CB4	C22-C21-C86-OA2
7	A	306	A1CB4	N20-C21-C86-OA2
7	A	306	A1CB4	C44-C43-O42-C35
7	A	306	A1CB4	O48-C43-O42-C35
7	A	306	A1CB4	C46-C47-C49-C50
7	A	306	A1CB4	C46-C47-C49-O74
7	A	306	A1CB4	O48-C47-C49-O74
7	A	306	A1CB4	C47-C49-C50-O53
7	A	306	A1CB4	O74-C49-C50-O53
7	A	306	A1CB4	O53-C54-C71-O73
7	A	306	A1CB4	C55-C54-O53-C50
7	A	306	A1CB4	O59-C54-O53-C50
7	A	306	A1CB4	C15-C16-C17-C18
7	A	306	A1CB4	O29-C28-C30-O31
7	A	306	A1CB4	C14-C15-C16-C17
4	A	302	A1CB5	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
7	A	306	A1CB4	C94-C95-C96-C97
7	A	306	A1CB4	O38-C37-C39-O40
7	A	306	A1CB4	C92-C93-C94-C95
7	A	306	A1CB4	C96-C97-C98-C99
7	A	306	A1CB4	C36-C37-C39-O40
7	A	306	A1CB4	C90-C91-C92-C93
7	A	306	A1CB4	C08-C09-C10-C11
7	A	306	A1CB4	C03-C04-C05-C06
3	A	301	NAG	C8-C7-N2-C2
3	A	301	NAG	O7-C7-N2-C2
7	A	306	A1CB4	C78-C76-N75-C46
7	A	306	A1CB4	O77-C76-N75-C46
7	A	306	A1CB4	O65-C60-C61-C62
7	A	306	A1CB4	C58-C60-C61-C62
7	A	306	A1CB4	C10-C11-C12-C13
7	A	306	A1CB4	C25-C24-O23-C22
7	A	306	A1CB4	C27-C28-C30-O31
7	A	306	A1CB4	O29-C24-O23-C22
7	A	306	A1CB4	C98-C99-CA0-CA1
4	A	302	A1CB5	C14-C15-C16-C17
4	A	302	A1CB5	C15-C16-C17-C18
7	A	306	A1CB4	C09-C10-C11-C12
7	A	306	A1CB4	C58-C60-C61-O64
7	A	306	A1CB4	C01-C02-C03-C04
7	A	306	A1CB4	C13-C14-C15-C16
7	A	306	A1CB4	C04-C05-C06-C07
4	A	302	A1CB5	C13-C14-C15-C16
4	A	302	A1CB5	C16-C17-C18-C19
7	A	306	A1CB4	C89-C90-C91-C92
4	A	302	A1CB5	C09-C10-C11-C12
4	A	302	A1CB5	C07-C08-C09-C10
4	A	302	A1CB5	C18-C19-C20-C21
7	A	306	A1CB4	C11-C12-C13-C14
7	A	306	A1CB4	O65-C60-C61-O64
4	A	302	A1CB5	C12-C13-C14-C15
6	A	305	MLA	O1A-C1-C2-C3
7	A	306	A1CB4	O64-C61-C62-O63
7	A	306	A1CB4	N20-C21-C86-C87
4	A	302	A1CB5	C10-C11-C12-C13
7	A	306	A1CB4	C02-C03-C04-C05
6	A	305	MLA	O1B-C1-C2-C3
7	A	306	A1CB4	C87-C88-C89-C90

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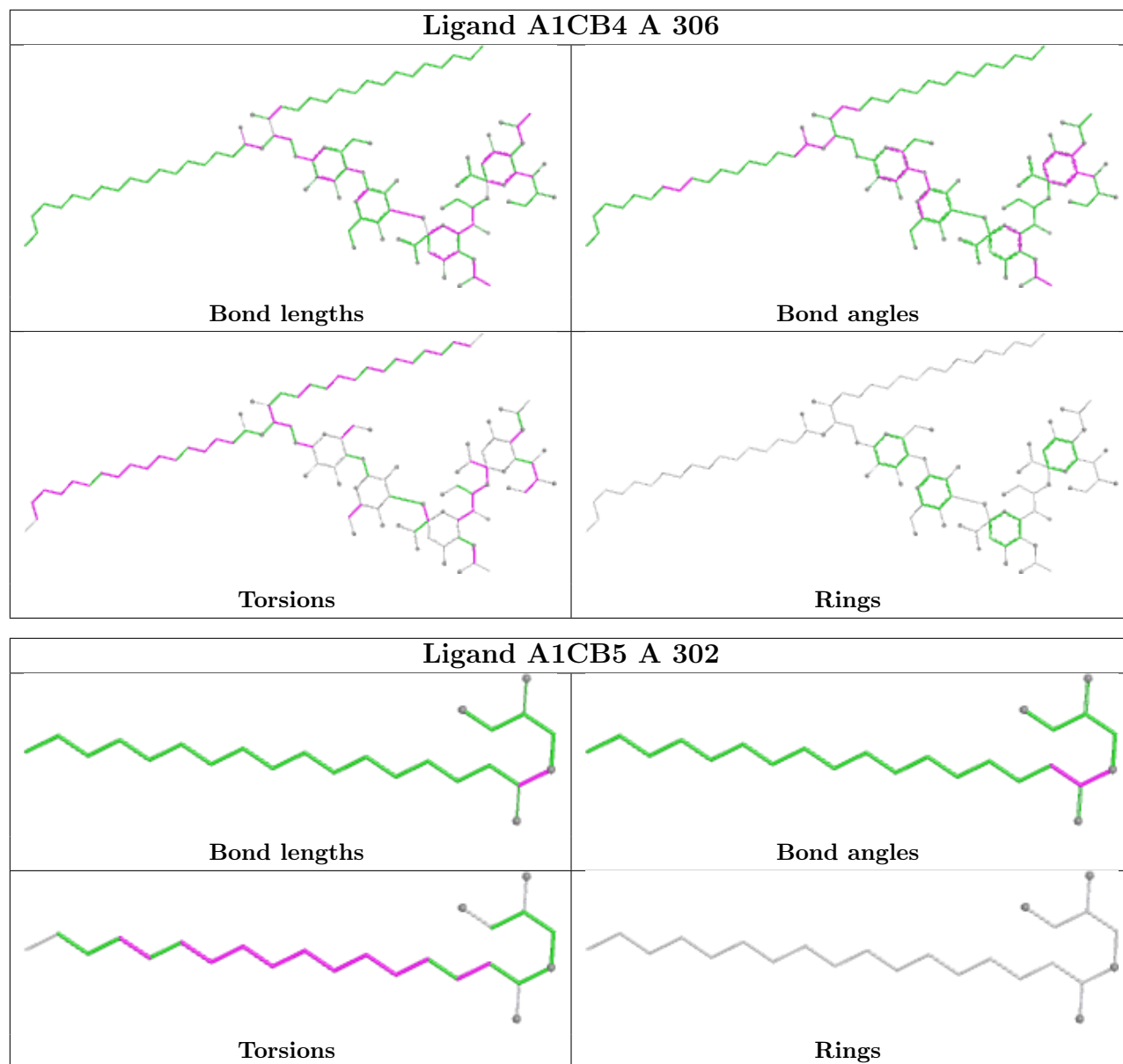
Mol	Chain	Res	Type	Atoms
7	A	306	A1CB4	N20-C21-C22-O23
7	A	306	A1CB4	O48-C47-C49-C50
6	A	304	MLA	C1-C2-C3-O3A
6	A	304	MLA	C1-C2-C3-O3B
5	A	303	KZF	C2-C1-N-C1'
7	A	306	A1CB4	C07-C08-C09-C10
7	A	306	A1CB4	C60-C61-C62-O63
7	A	306	A1CB4	C49-C50-O53-C54
6	A	304	MLA	O1A-C1-C2-C3
7	A	306	A1CB4	C56-C57-N66-C67
7	A	306	A1CB4	C05-C06-C07-C08

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	305	MLA	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 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 [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	279/281 (99%)	0.31	10 (3%) 46 31	43, 86, 121, 137	0
2	B	100/101 (99%)	0.50	6 (6%) 29 18	52, 70, 103, 108	0
All	All	379/382 (99%)	0.36	16 (4%) 41 27	43, 82, 118, 137	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	ARG	4.0
1	A	253	ALA	3.8
1	A	284	PRO	3.2
1	A	57	GLN	3.1
1	A	189	GLU	3.1
1	A	229	GLN	2.7
2	B	95	LYS	2.7
2	B	0	ALA	2.6
1	A	283	VAL	2.6
2	B	90	GLN	2.5
1	A	128	GLN	2.5
2	B	21	SER	2.4
2	B	35	ASP	2.4
2	B	97	ASP	2.4
1	A	137	CYS	2.4
1	A	272	GLN	2.1

### 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](#)

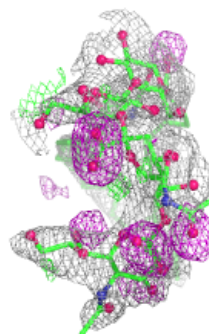
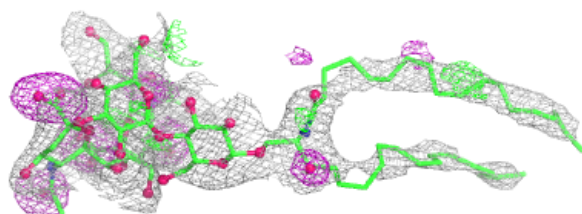
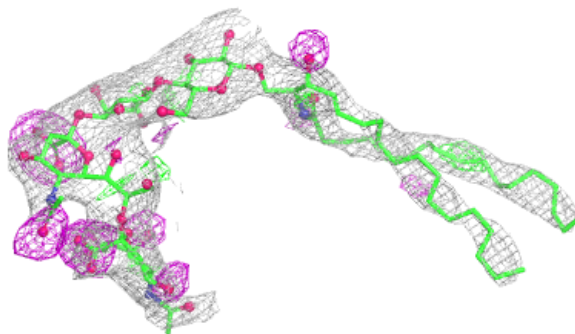
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	301	14/15	0.65	0.14	94,100,106,108	0
6	MLA	A	304	7/7	0.84	0.18	81,84,85,85	0
6	MLA	A	305	7/7	0.89	0.15	91,95,108,109	0
7	A1CB4	A	306	102/102	0.89	0.18	68,108,130,134	0
4	A1CB5	A	302	24/24	0.91	0.22	78,88,95,97	0
5	KZF	A	303	13/13	0.93	0.19	51,62,81,86	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.

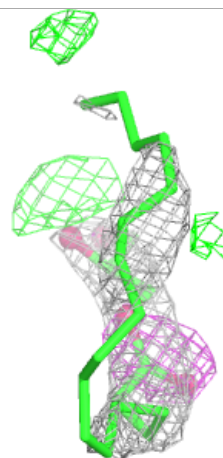
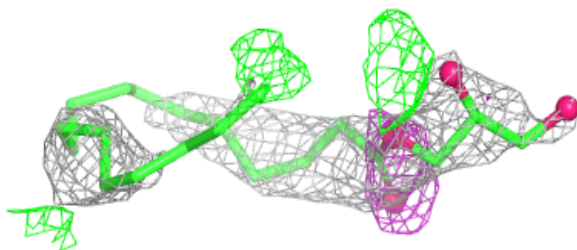
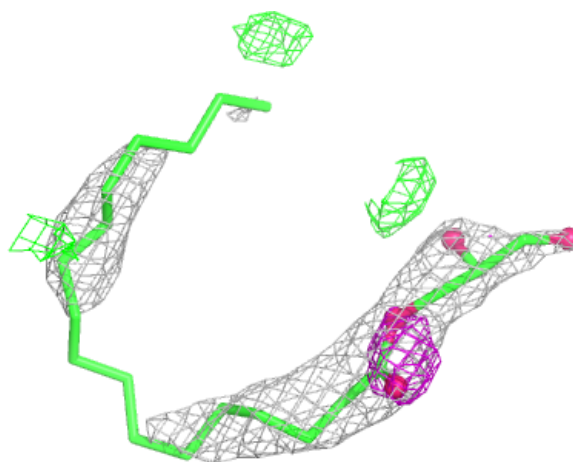
**Electron density around A1CB4 A 306:**

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



**Electron density around A1CB5 A 302:**

$2mF_o-DF_c$  (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.