



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:40 AM UTC

PDB ID : 9OHU / pdb_00009ohu
Title : CD1c presenting GM3 ganglioside
Authors : Cao, T.P.; Rossjohn, J.; Shahine, A.
Deposited on : 2025-05-05
Resolution : 2.90 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

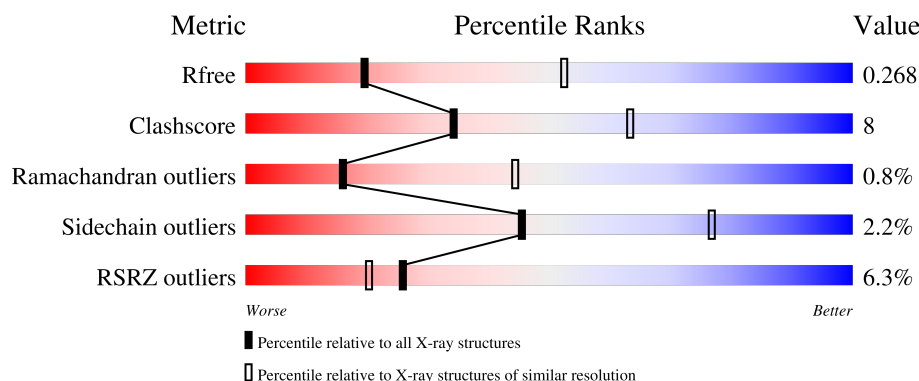
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	281	5% 77% 22% .
2	B	101	9% 87% 13%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 3130 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
			2187	1403	376	399	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	101	Total	C	N	O	S	0	0	0
			794	507	137	147	3			

There is a discrepancy between the modelled and reference sequences:

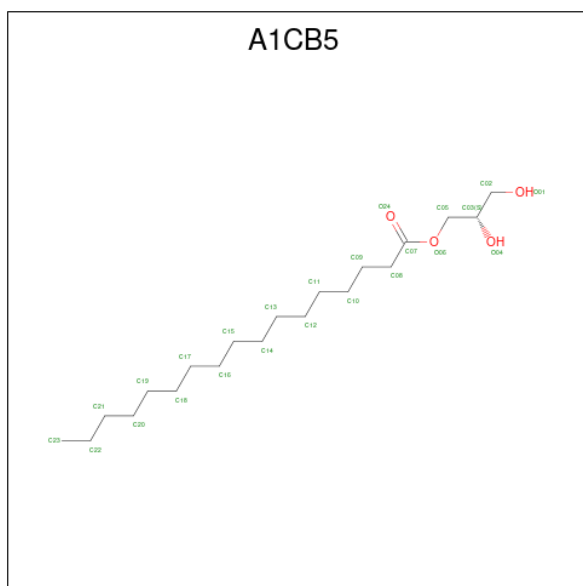
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ALA	-	expression tag	UNP P61769

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



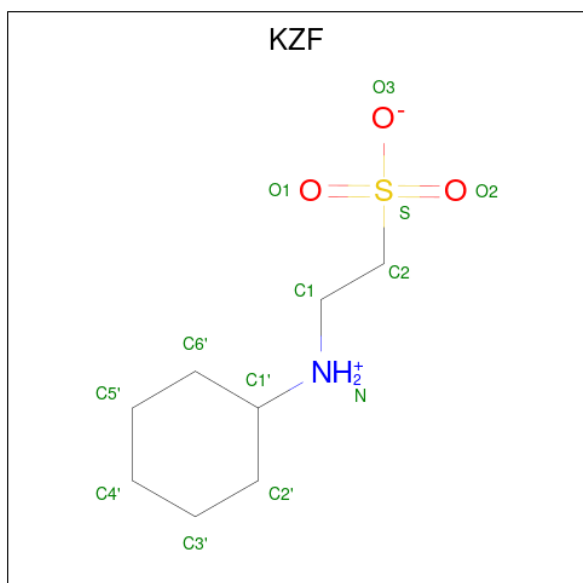
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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



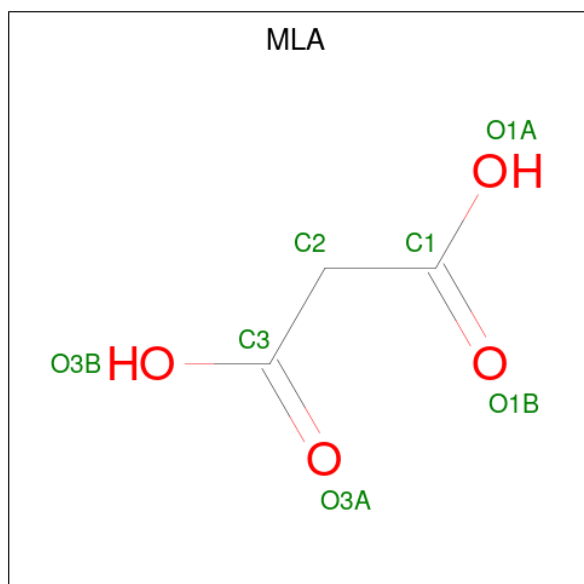
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			24	20	4		

- 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: $C_3H_4O_4$).

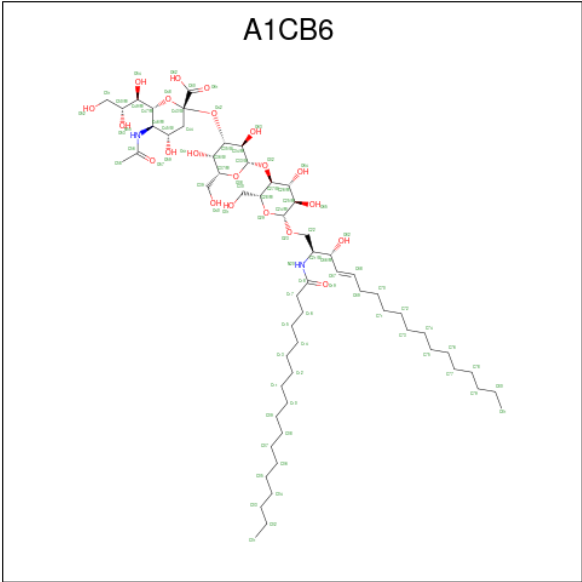


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	3	4		
6	A	1	Total	C	O	0	0
			7	3	4		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Cl	0	0
			2	2		

- Molecule 8 is (2S,3R,4E)-3-hydroxy-2-octadecanamido-octadec-4-en-1-yl 5-acetamido-3,5-dideoxy-D-glycero- α -D-galacto-non-2-ulopyranonosyl-(2->3)- β -D-galactopyranosyl-(1->4)- β -D-glucopyranoside (CCD ID: A1CB6) (formula: $C_{59}H_{108}N_2O_{21}$) (labeled as "Ligand of Interest" by depositor).

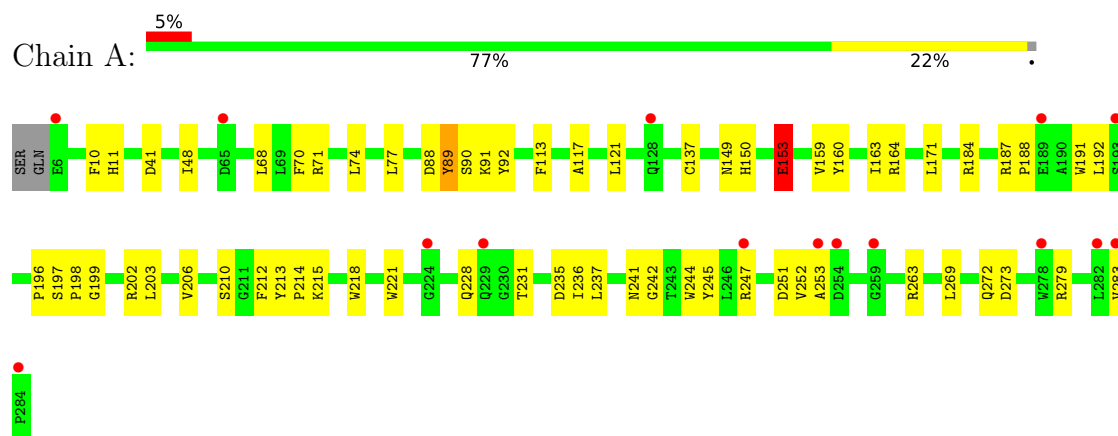


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			82	59	2	21		

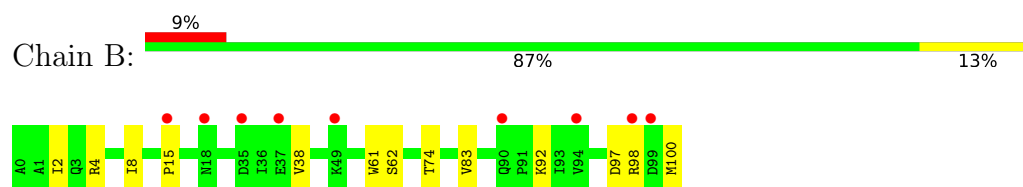
3 Residue-property plots

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: 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, α , β , γ	88.80Å 88.80Å 157.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.40 – 2.90 44.40 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.40-2.90) 100.0 (44.40-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.21rc1_5107: ???)	Depositor
R, R_{free}	0.234 , 0.272 0.226 , 0.268	Depositor DCC
R_{free} test set	844 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	84.3	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 80.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3130	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.11% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1CB6, A1CB5, KZF, MLA, CL, 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	0.19	0/2254	0.43	0/3068
2	B	0.17	0/817	0.40	0/1116
All	All	0.18	0/3071	0.42	0/4184

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

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	2187	0	2064	40	0
2	B	794	0	725	11	0
3	A	14	0	13	0	0
4	A	24	0	0	0	0
5	A	13	0	0	1	0
6	A	14	0	4	1	0
7	A	2	0	0	0	0
8	A	82	0	0	0	0
All	All	3130	0	2806	45	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 (45) 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:188:PRO:HB3	1:A:212:PHE:HB3	1.65	0.78
1:A:198:PRO:HG2	1:A:202:ARG:HB3	1.68	0.76
1:A:206:VAL:HG21	2:B:100:MET:HE3	1.69	0.72
1:A:218:TRP:HZ3	1:A:263:ARG:HG2	1.63	0.63
2:B:38:VAL:HG22	2:B:83:VAL:HG22	1.80	0.63
2:B:74:THR:O	2:B:98:ARG:NH2	2.31	0.63
1:A:221:TRP:HB2	1:A:231:THR:HG22	1.79	0.63
1:A:191:TRP:CD2	2:B:15:PRO:HG3	2.36	0.61
1:A:196:PRO:HD3	2:B:100:MET:HE1	1.82	0.60
1:A:153:GLU:N	1:A:153:GLU:OE1	2.38	0.56
1:A:88:ASP:O	1:A:90:SER:N	2.41	0.54
1:A:247:ARG:NH1	2:B:100:MET:HE2	2.23	0.54
1:A:269:LEU:HD23	1:A:273:ASP:HA	1.91	0.53
1:A:10:PHE:HB2	1:A:171:LEU:HD13	1.90	0.51
1:A:228:GLN:O	1:A:231:THR:HG23	2.11	0.51
1:A:198:PRO:HG3	1:A:251:ASP:HB2	1.93	0.50
1:A:121:LEU:HD21	2:B:2:ILE:HB	1.94	0.49
1:A:41:ASP:HB2	1:A:48:ILE:HD11	1.95	0.49
1:A:117:ALA:HB2	2:B:61:TRP:CE2	2.47	0.49
1:A:198:PRO:HG3	1:A:251:ASP:CB	2.43	0.48
1:A:213:TYR:CG	1:A:214:PRO:HA	2.47	0.48
2:B:8:ILE:HG12	2:B:83:VAL:HG21	1.95	0.48
1:A:149:ASN:O	1:A:150:HIS:ND1	2.47	0.48
1:A:210:SER:HB2	1:A:245:TYR:HD1	1.77	0.48
1:A:160:TYR:O	1:A:164:ARG:HB2	2.15	0.47
2:B:97:ASP:HB3	2:B:100:MET:HB2	1.97	0.47
1:A:70:PHE:O	1:A:74:LEU:HD23	2.15	0.46
1:A:215:LYS:HG3	1:A:236:ILE:HG21	1.97	0.46
1:A:203:LEU:O	1:A:251:ASP:HA	2.17	0.45
1:A:159:VAL:O	1:A:163:ILE:HG12	2.17	0.45
1:A:11:HIS:CD2	1:A:113:PHE:HE1	2.34	0.45
1:A:197:SER:C	1:A:199:GLY:H	2.25	0.44
1:A:68:LEU:HD22	1:A:71:ARG:HH12	1.83	0.43
1:A:235:ASP:HB2	1:A:237:LEU:HD21	2.00	0.43
2:B:4:ARG:HD2	2:B:62:SER:HB3	2.00	0.43
1:A:89:TYR:HA	1:A:92:TYR:CD2	2.54	0.42
1:A:221:TRP:H	1:A:231:THR:HG21	1.84	0.42
1:A:184:ARG:NH2	1:A:242:GLY:O	2.52	0.42
1:A:279:ARG:CZ	1:A:283:VAL:HG21	2.51	0.41
1:A:252:VAL:HG22	1:A:253:ALA:H	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:TYR:CD1	1:A:214:PRO:HA	2.55	0.41
1:A:11:HIS:HD2	1:A:113:PHE:HE1	1.68	0.41
1:A:244:TRP:NE1	5:A:303:KZF:O3	2.53	0.41
1:A:241:ASN:ND2	6:A:305:MLA:O1B	2.54	0.41
1:A:68:LEU:HD22	1:A:71:ARG:NH1	2.37	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%)	264 (95%)	10 (4%)	3 (1%)	11	36
2	B	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
All	All	376/382 (98%)	359 (96%)	14 (4%)	3 (1%)	16	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	TYR
1	A	153	GLU
1	A	272	GLN

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	A	231/240 (96%)	225 (97%)	6 (3%)	40	73
2	B	83/94 (88%)	82 (99%)	1 (1%)	63	86
All	All	314/334 (94%)	307 (98%)	7 (2%)	45	77

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU
1	A	91	LYS
1	A	137	CYS
1	A	153	GLU
1	A	187	ARG
1	A	192	LEU
2	B	92	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	87	GLN
1	A	226	GLN
1	A	228	GLN
2	B	25	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\# Z > 2$
3	NAG	A	301	1	14,14,15	0.67	0	17,19,21	1.41	3 (17%)
6	MLA	A	305	-	6,6,6	1.36	0	7,7,7	1.14	0
4	A1CB5	A	302	-	23,23,23	0.83	1 (4%)	24,24,24	0.79	1 (4%)
5	KZF	A	303	-	13,13,13	1.36	3 (23%)	16,17,17	2.00	7 (43%)
6	MLA	A	304	-	6,6,6	1.35	0	7,7,7	1.22	0
8	A1CB6	A	308	-	82,84,84	1.99	20 (24%)	103,109,109	1.33	9 (8%)

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
3	NAG	A	301	1	-	4/6/23/26	0/1/1/1
6	MLA	A	305	-	-	4/4/4/4	-
4	A1CB5	A	302	-	-	12/23/23/23	-
5	KZF	A	303	-	-	4/7/15/15	0/1/1/1
6	MLA	A	304	-	-	3/4/4/4	-
8	A1CB6	A	308	-	-	48/77/136/136	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	308	A1CB6	C18-N20	8.08	1.51	1.34
8	A	308	A1CB6	C45-C46	-7.39	1.46	1.53
8	A	308	A1CB6	C22-C21	5.84	1.62	1.51
8	A	308	A1CB6	C44-C45	-4.09	1.47	1.53
8	A	308	A1CB6	C56-N55	3.90	1.46	1.34
8	A	308	A1CB6	O42-C35	3.36	1.46	1.42
5	A	303	KZF	C2-S	3.14	1.82	1.77
8	A	308	A1CB6	C66-C67	3.05	1.55	1.50
8	A	308	A1CB6	O23-C22	2.95	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	308	A1CB6	O23-C24	2.93	1.45	1.40
8	A	308	A1CB6	O48-C43	2.72	1.45	1.42
4	A	302	A1CB5	O06-C07	2.67	1.41	1.33
8	A	308	A1CB6	C17-C18	2.57	1.56	1.51
8	A	308	A1CB6	C43-C60	-2.49	1.48	1.54
8	A	308	A1CB6	O82-C66	-2.43	1.39	1.43
5	A	303	KZF	O2-S	2.32	1.51	1.45
8	A	308	A1CB6	C21-N20	2.27	1.50	1.46
8	A	308	A1CB6	O19-C18	-2.24	1.18	1.23
8	A	308	A1CB6	O29-C24	2.23	1.47	1.41
8	A	308	A1CB6	O48-C47	2.20	1.47	1.44
8	A	308	A1CB6	O38-C33	2.11	1.47	1.41
5	A	303	KZF	O1-S	2.11	1.51	1.45
8	A	308	A1CB6	O57-C56	-2.04	1.18	1.23
8	A	308	A1CB6	O59-C45	-2.01	1.39	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	308	A1CB6	C66-C21-N20	-5.65	100.08	109.66
8	A	308	A1CB6	C21-N20-C18	4.22	130.44	123.40
8	A	308	A1CB6	C22-O23-C24	4.11	122.61	113.80
5	A	303	KZF	O3-S-O1	-4.02	101.35	111.40
8	A	308	A1CB6	O23-C24-C25	3.70	113.89	108.27
3	A	301	NAG	C1-O5-C5	3.57	116.98	112.19
8	A	308	A1CB6	C33-O32-C27	-3.23	110.31	117.98
5	A	303	KZF	O2-S-C2	3.01	111.27	106.73
5	A	303	KZF	O3-S-C2	2.97	111.81	106.00
4	A	302	A1CB5	O06-C07-C08	2.75	120.21	111.83
5	A	303	KZF	C1-N-C1'	-2.73	108.93	114.18
8	A	308	A1CB6	O19-C18-C17	-2.56	117.38	122.02
5	A	303	KZF	C5'-C6'-C1'	2.54	115.65	111.09
5	A	303	KZF	C6'-C1'-C2'	2.52	115.15	110.80
3	A	301	NAG	O5-C1-C2	-2.48	107.46	111.29
5	A	303	KZF	O1-S-C2	2.32	110.24	106.73
8	A	308	A1CB6	C58-C56-N55	2.30	119.94	116.12
3	A	301	NAG	C4-C3-C2	-2.20	107.79	111.02
8	A	308	A1CB6	C24-C25-C26	2.16	114.54	110.01
8	A	308	A1CB6	C44-C45-C46	2.01	112.83	109.72

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	302	A1CB5	O01-C02-C03-C05
5	A	303	KZF	C6'-C1'-N-C1
5	A	303	KZF	C1-C2-S-O1
8	A	308	A1CB6	C66-C21-C22-O23
8	A	308	A1CB6	N20-C21-C22-O23
8	A	308	A1CB6	C22-C21-C66-C67
8	A	308	A1CB6	C22-C21-C66-O82
8	A	308	A1CB6	N20-C21-C66-C67
8	A	308	A1CB6	N20-C21-C66-O82
8	A	308	A1CB6	C22-C21-N20-C18
8	A	308	A1CB6	C25-C24-O23-C22
8	A	308	A1CB6	C44-C43-O42-C35
8	A	308	A1CB6	O48-C43-O42-C35
8	A	308	A1CB6	C46-C47-C49-C50
8	A	308	A1CB6	C46-C47-C49-O54
8	A	308	A1CB6	O48-C47-C49-C50
8	A	308	A1CB6	O48-C47-C49-O54
8	A	308	A1CB6	C49-C50-C51-O52
8	A	308	A1CB6	O53-C50-C51-O52
8	A	308	A1CB6	O38-C37-C39-O40
8	A	308	A1CB6	C36-C37-C39-O40
8	A	308	A1CB6	C74-C75-C76-C77
8	A	308	A1CB6	C11-C12-C13-C14
8	A	308	A1CB6	C72-C73-C74-C75
8	A	308	A1CB6	C13-C14-C15-C16
3	A	301	NAG	C8-C7-N2-C2
3	A	301	NAG	O7-C7-N2-C2
8	A	308	A1CB6	C58-C56-N55-C46
8	A	308	A1CB6	O57-C56-N55-C46
8	A	308	A1CB6	C05-C06-C07-C08
4	A	302	A1CB5	C11-C12-C13-C14
3	A	301	NAG	O5-C5-C6-O6
8	A	308	A1CB6	C07-C08-C09-C10
3	A	301	NAG	C4-C5-C6-O6
8	A	308	A1CB6	C06-C07-C08-C09
8	A	308	A1CB6	C76-C77-C78-C79
4	A	302	A1CB5	O01-C02-C03-O04
4	A	302	A1CB5	C15-C16-C17-C18
4	A	302	A1CB5	C14-C15-C16-C17
8	A	308	A1CB6	C70-C71-C72-C73
8	A	308	A1CB6	C08-C09-C10-C11
8	A	308	A1CB6	C01-C02-C03-C04
8	A	308	A1CB6	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	308	A1CB6	C71-C72-C73-C74
8	A	308	A1CB6	C67-C68-C69-C70
8	A	308	A1CB6	C04-C05-C06-C07
4	A	302	A1CB5	C09-C10-C11-C12
4	A	302	A1CB5	C13-C14-C15-C16
6	A	304	MLA	O1A-C1-C2-C3
8	A	308	A1CB6	C16-C17-C18-O19
8	A	308	A1CB6	C75-C76-C77-C78
8	A	308	A1CB6	C78-C79-C80-C81
8	A	308	A1CB6	C47-C49-C50-C51
6	A	304	MLA	O1B-C1-C2-C3
8	A	308	A1CB6	C47-C49-C50-O53
8	A	308	A1CB6	C16-C17-C18-N20
8	A	308	A1CB6	C77-C78-C79-C80
8	A	308	A1CB6	C02-C03-C04-C05
8	A	308	A1CB6	O54-C49-C50-O53
6	A	305	MLA	O1A-C1-C2-C3
6	A	305	MLA	C1-C2-C3-O3A
4	A	302	A1CB5	C16-C17-C18-C19
4	A	302	A1CB5	C10-C11-C12-C13
8	A	308	A1CB6	C69-C70-C71-C72
6	A	305	MLA	O1B-C1-C2-C3
6	A	305	MLA	C1-C2-C3-O3B
8	A	308	A1CB6	C73-C74-C75-C76
5	A	303	KZF	C2'-C1'-N-C1
8	A	308	A1CB6	O42-C43-C60-O62
8	A	308	A1CB6	O48-C43-C60-O62
5	A	303	KZF	C1-C2-S-O2
4	A	302	A1CB5	O06-C07-C08-C09
4	A	302	A1CB5	C12-C13-C14-C15
6	A	304	MLA	C1-C2-C3-O3A
4	A	302	A1CB5	O24-C07-C08-C09

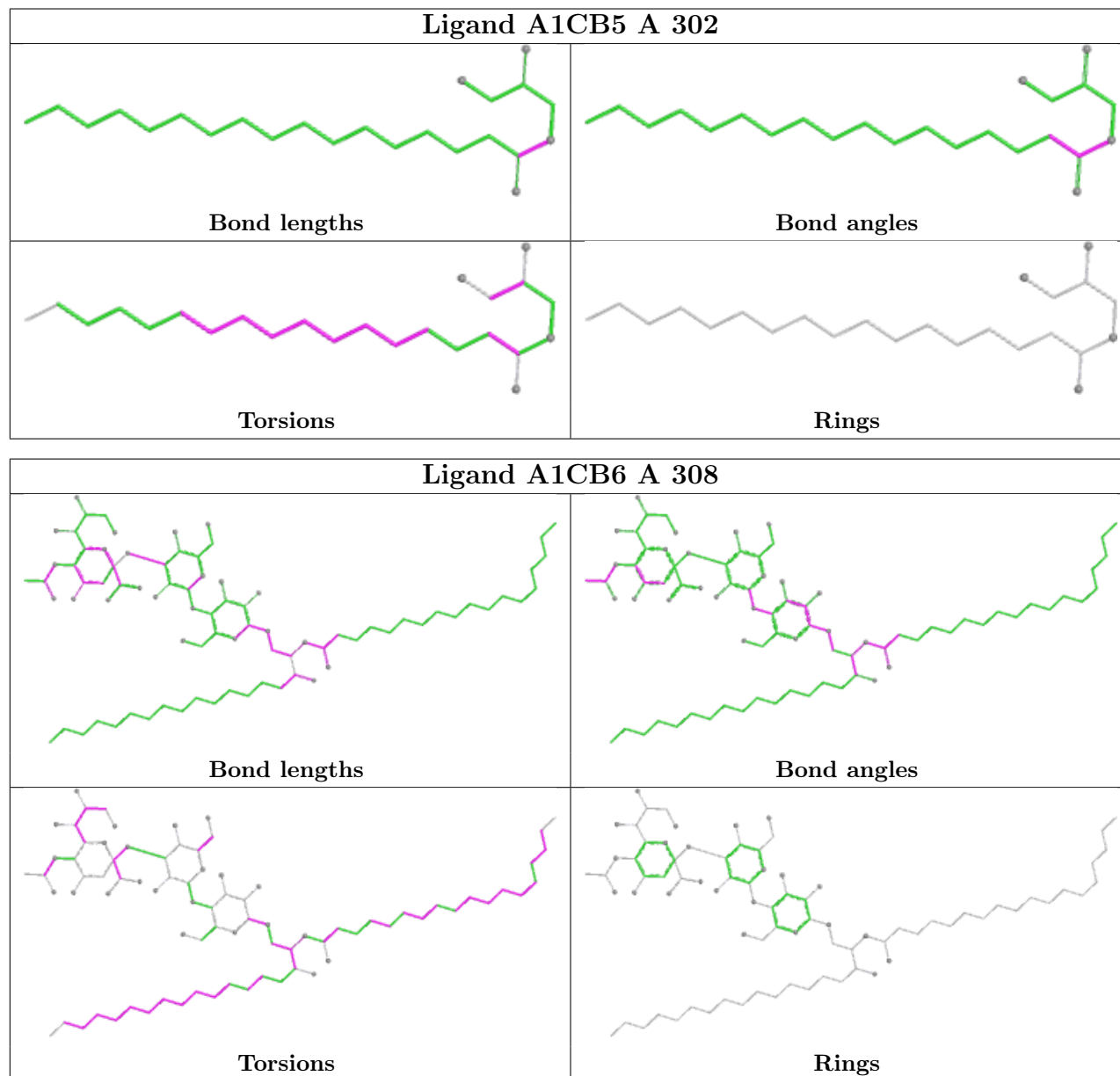
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	305	MLA	1	0
5	A	303	KZF	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 ⓘ

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	279/281 (99%)	0.44	15 (5%) 31 24	50, 93, 131, 151	0
2	B	101/101 (100%)	0.61	9 (8%) 15 13	52, 74, 111, 142	0
All	All	380/382 (99%)	0.48	24 (6%) 26 20	50, 88, 129, 151	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	284	PRO	4.7
1	A	247	ARG	3.9
1	A	254	ASP	3.5
1	A	259	GLY	3.3
1	A	253	ALA	3.1
2	B	99	ASP	2.9
2	B	35	ASP	2.8
1	A	229	GLN	2.8
1	A	189	GLU	2.8
1	A	6	GLU	2.7
2	B	37	GLU	2.7
1	A	278	TRP	2.6
1	A	282	LEU	2.6
2	B	15	PRO	2.3
2	B	18	ASN	2.3
1	A	65	ASP	2.2
1	A	193	SER	2.2
2	B	90	GLN	2.1
1	A	128	GLN	2.1
1	A	283	VAL	2.1
2	B	98	ARG	2.1
1	A	224	GLY	2.0
2	B	49	LYS	2.0
2	B	94	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

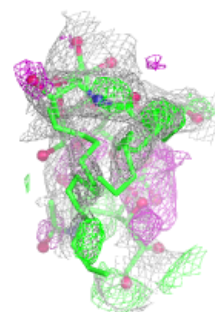
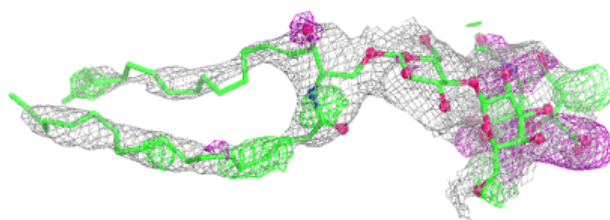
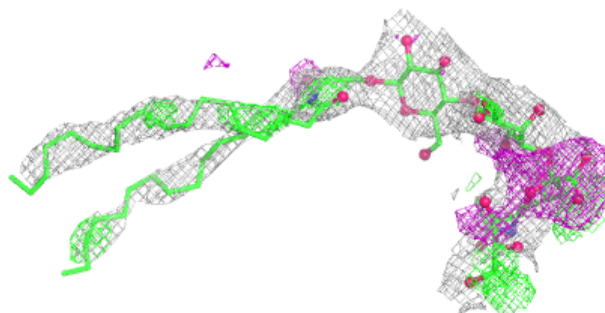
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MLA	A	305	7/7	0.65	0.14	102,112,137,138	0
7	CL	A	306	1/1	0.66	0.14	138,138,138,138	0
3	NAG	A	301	14/15	0.73	0.12	79,92,108,113	0
8	A1CB6	A	308	82/82	0.85	0.22	68,132,167,178	0
7	CL	A	307	1/1	0.87	0.20	108,108,108,108	0
6	MLA	A	304	7/7	0.89	0.17	79,96,104,110	0
5	KZF	A	303	13/13	0.91	0.22	56,72,89,98	1
4	A1CB5	A	302	24/24	0.92	0.24	76,90,99,112	0

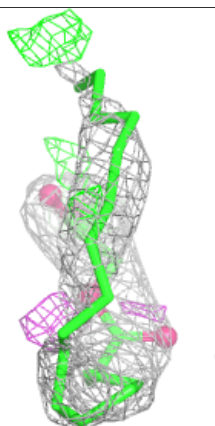
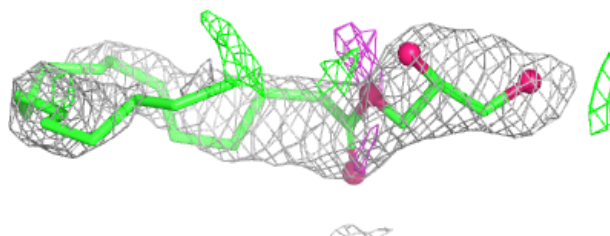
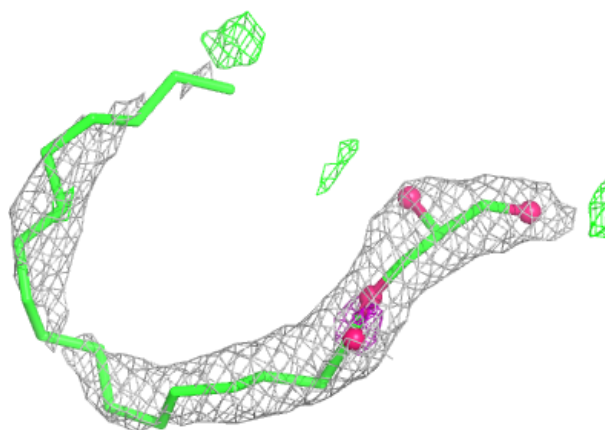
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1CB6 A 308:

$2mF_o-DF_c$ (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.