



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:39 AM UTC

PDB ID : 9OHW / pdb_00009ohw
Title : CD1c presenting GM1 ganglioside
Authors : Cao, T.P.; Rossjohn, J.; Shahine, A.
Deposited on : 2025-05-05
Resolution : 2.50 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

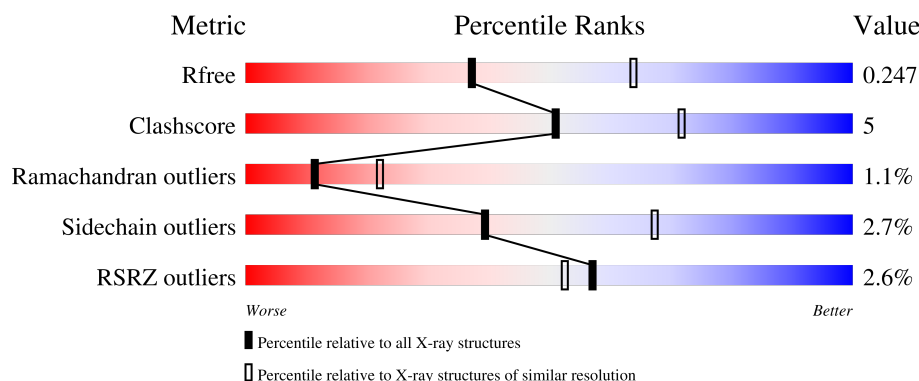
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	
2	B	99	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 3311 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.

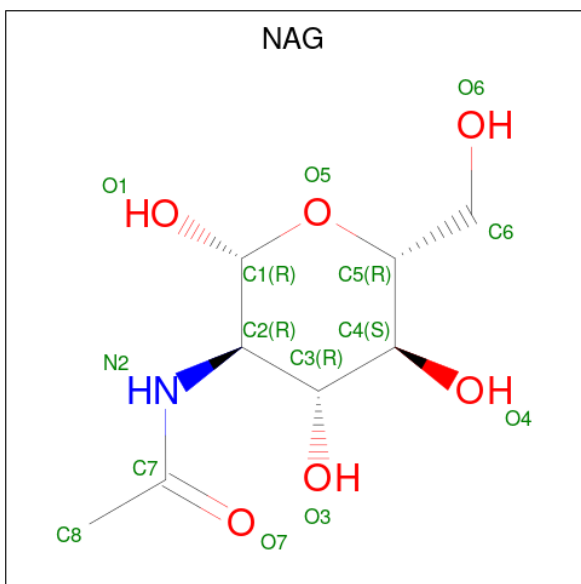
- Molecule 1 is a protein called T-cell surface glycoprotein CD1c/T-cell surface glycoprotein CD1b chimeric protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	1	0
			2227	1427	383	408	9			

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

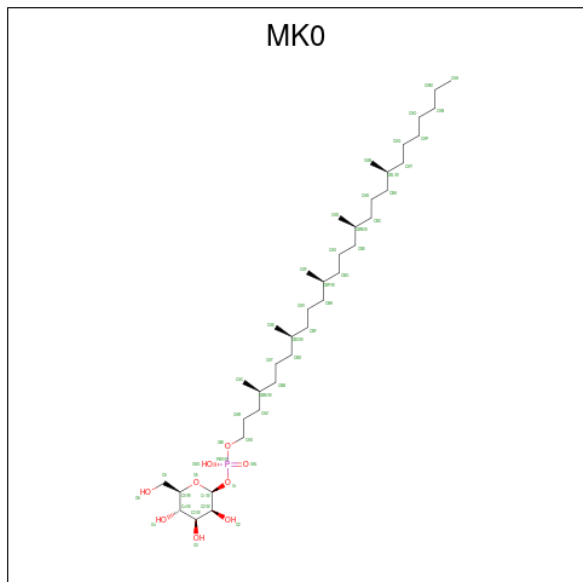
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			811	519	136	154	2			

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



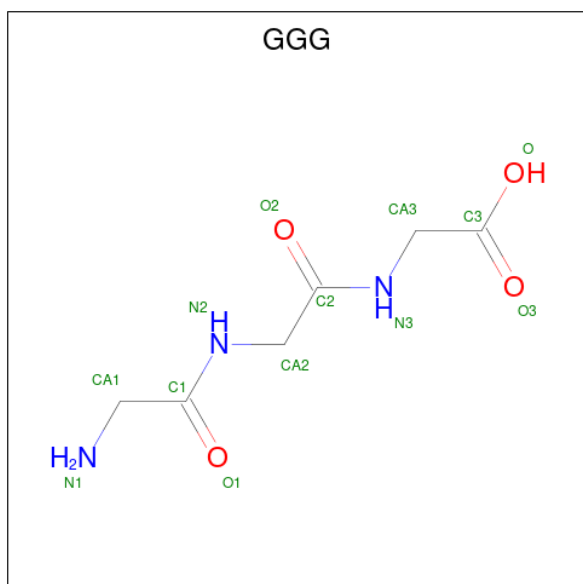
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is 1-O-[(S)-hydroxy{[(4S,8S,16S,20S)-4,8,12,16,20-pentamethylheptacosyl]oxy}phosphoryl]-beta-D-mannopyranose (CCD ID: MK0) (formula: $C_{38}H_{77}O_9P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			48	38	9	1		

- Molecule 5 is glycylglycylglycine (CCD ID: GGG) (formula: $C_6H_{11}N_3O_4$).



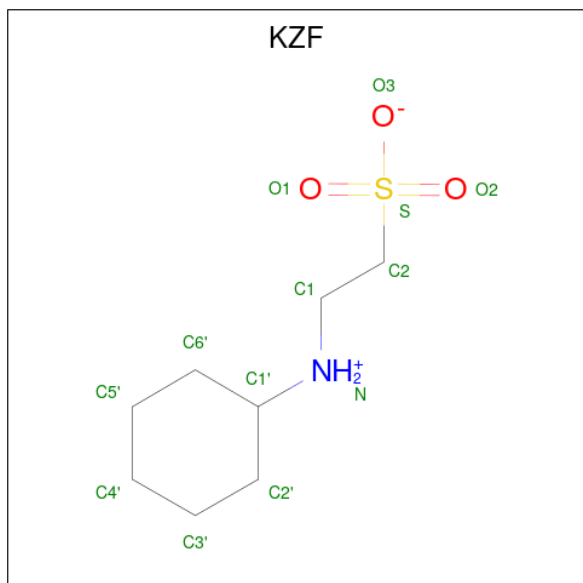
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			13	6	3	4		

Continued on next page...

Continued from previous page...

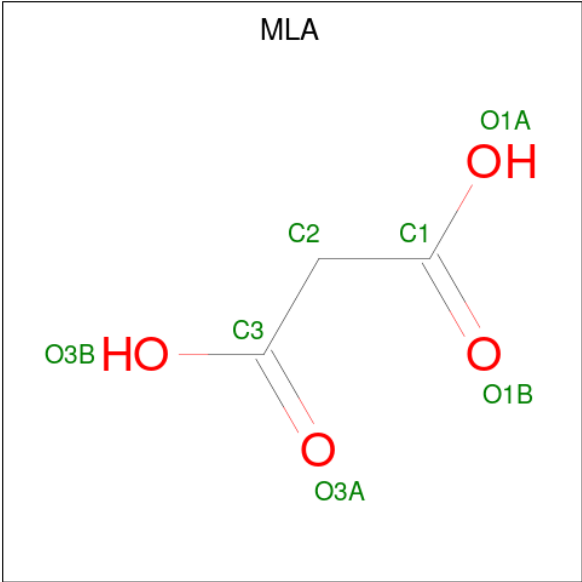
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			13	6	3	4		
5	B	1	Total	C	N	O	0	0
			13	6	3	4		

- Molecule 6 is 2-(cyclohexylazaniumyl)ethanesulfonate (CCD ID: KZF) (formula: $C_8H_{17}NO_3S$).



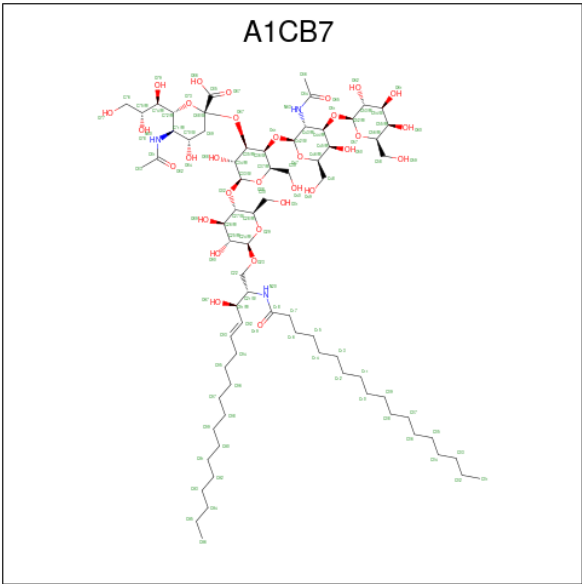
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
6	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
6	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 7 is MALONIC ACID (CCD ID: MLA) (formula: $C_3H_4O_4$).



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

- 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->3)-2-acetamido-2-deoxy- β -D-galactopyranosyl-(1->4)]- β -D-galactopyranosyl-(1->4)- β -D-glucopyranoside (CCD ID: A1CB7) (formula: $C_{73}H_{131}N_3O_{31}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			107	73	3	31		

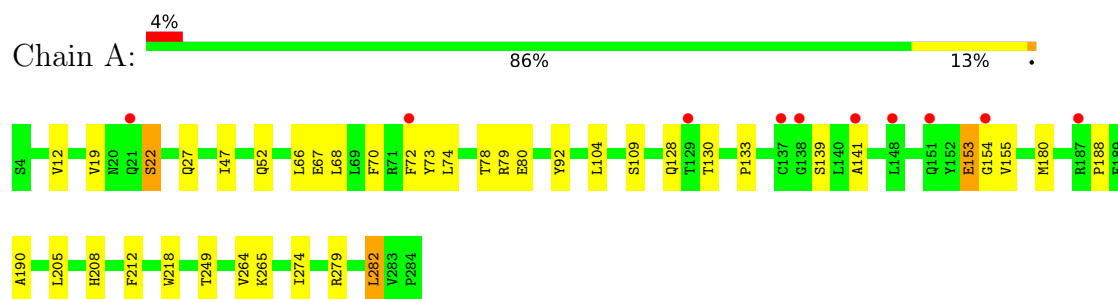
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	17	Total	O	0	0
			17	17		
9	B	2	Total	O	0	0
			2	2		

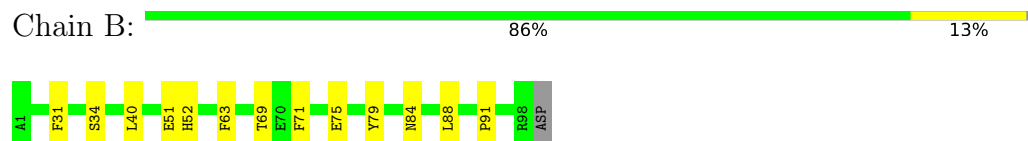
3 Residue-property plots [i](#)

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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.62Å 86.56Å 91.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.83 – 2.50 48.83 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.83-2.50) 99.1 (48.83-2.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.207 , 0.246 0.207 , 0.247	Depositor DCC
R_{free} test set	794 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3311	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% 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: NAG, A1CB7, MLA, KZF, MK0, GGG

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	0.39	0/2298	0.59	0/3125
2	B	0.34	0/834	0.53	0/1131
All	All	0.38	0/3132	0.57	0/4256

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	2227	0	2109	23	1
2	B	811	0	775	7	0
3	A	14	0	13	0	0
4	A	48	0	76	9	0
5	A	26	0	20	2	0
5	B	13	0	10	2	0
6	A	26	0	0	0	0
6	B	13	0	0	0	0
7	A	7	0	2	0	0
8	A	107	0	0	0	0
9	A	17	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	2	0	0	0	0
All	All	3311	0	3005	33	1

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 5.

All (33) 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:73:TYR:HB2	4:A:302:MK0:HBO	1.64	0.79
1:A:188:PRO:HB3	1:A:212:PHE:HB3	1.76	0.66
1:A:78:THR:HG22	5:A:306:GGG:HN1	1.59	0.66
2:B:84:ASN:ND2	2:B:91:PRO:HG3	2.16	0.59
1:A:70:PHE:HE1	4:A:302:MK0:HBGA	1.70	0.55
4:A:302:MK0:H1	4:A:302:MK0:HACB	1.88	0.55
1:A:66:LEU:HD13	4:A:302:MK0:HABB	1.90	0.53
1:A:74:LEU:O	1:A:78:THR:HG23	2.10	0.51
1:A:155:VAL:HG22	4:A:302:MK0:HBBA	1.95	0.49
1:A:218:TRP:HB3	1:A:265:LYS:HB2	1.95	0.48
1:A:133:PRO:HB3	1:A:141:ALA:HB1	1.96	0.48
2:B:40:LEU:HD13	2:B:69:THR:HG22	1.96	0.47
1:A:264:VAL:HB	1:A:274:ILE:HB	1.95	0.47
1:A:79:ARG:NH1	1:A:80:GLU:HG2	2.29	0.47
1:A:19:VAL:O	1:A:92:TYR:HB3	2.15	0.46
1:A:279:ARG:O	1:A:282:LEU:HB2	2.16	0.46
1:A:79:ARG:HH11	1:A:80:GLU:HG2	1.80	0.46
1:A:47:ILE:HG13	1:A:67:GLU:HG2	1.97	0.45
4:A:302:MK0:HABA	4:A:302:MK0:HAQ	1.77	0.45
1:A:78:THR:CG2	5:A:306:GGG:HN1	2.26	0.44
2:B:51:GLU:HA	5:B:101:GGG:HA3A	1.98	0.44
1:A:27:GLN:HE21	1:A:27:GLN:HB2	1.59	0.44
2:B:34:SER:HB3	2:B:63:PHE:CE2	2.53	0.43
1:A:153:GLU:C	1:A:155:VAL:H	2.26	0.43
2:B:52:HIS:H	5:B:101:GGG:HA3A	1.84	0.42
1:A:72[A]:PHE:CE2	4:A:302:MK0:HAC	2.54	0.42
1:A:180:MET:HE3	1:A:180:MET:HB3	1.84	0.42
1:A:205:LEU:O	1:A:249:THR:HA	2.20	0.42
1:A:72[A]:PHE:HE2	4:A:302:MK0:HAC	1.84	0.42
1:A:190:ALA:HA	1:A:208:HIS:O	2.20	0.41
2:B:31:PHE:CE2	2:B:63:PHE:HB2	2.56	0.41
4:A:302:MK0:HAFB	4:A:302:MK0:HAUA	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:PHE:HD2	2:B:79:TYR:CZ	2.39	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:SER:OG	1:A:52:GLN:OE1[3_545]	2.06	0.14

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	280/281 (100%)	268 (96%)	8 (3%)	4 (1%)	9	17
2	B	96/99 (97%)	90 (94%)	6 (6%)	0	100	100
All	All	376/380 (99%)	358 (95%)	14 (4%)	4 (1%)	11	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	GLU
1	A	139	SER
1	A	128	GLN
1	A	154	GLY

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	238/240 (99%)	231 (97%)	7 (3%)	37	65
2	B	91/93 (98%)	89 (98%)	2 (2%)	45	73
All	All	329/333 (99%)	320 (97%)	9 (3%)	39	67

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	22	SER
1	A	68	LEU
1	A	104	LEU
1	A	109	SER
1	A	130	THR
1	A	282	LEU
2	B	75	GLU
2	B	88	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	82	GLN
1	A	146	HIS
2	B	84	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

10 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$
3	NAG	A	301	1	14,14,15	0.94	0	17,19,21	1.45	3 (17%)
4	MK0	A	302	-	47,48,48	1.34	5 (10%)	60,61,61	1.12	4 (6%)
6	KZF	B	102	-	13,13,13	1.56	3 (23%)	16,17,17	2.45	6 (37%)
5	GGG	A	306	-	11,12,12	2.33	3 (27%)	11,14,14	1.40	1 (9%)
5	GGG	A	303	-	11,12,12	2.61	4 (36%)	11,14,14	1.25	1 (9%)
5	GGG	B	101	-	11,12,12	2.65	3 (27%)	11,14,14	1.97	2 (18%)
7	MLA	A	307	-	6,6,6	1.43	0	7,7,7	1.20	0
6	KZF	A	305	-	13,13,13	1.41	3 (23%)	16,17,17	1.97	6 (37%)
6	KZF	A	304	-	13,13,13	1.37	3 (23%)	16,17,17	1.88	2 (12%)
8	A1CB7	A	308	-	109,111,111	2.19	23 (21%)	141,149,149	1.43	23 (16%)

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	-	2/6/23/26	0/1/1/1
4	MK0	A	302	-	-	26/46/66/66	0/1/1/1
6	KZF	B	102	-	-	4/7/15/15	0/1/1/1
5	GGG	A	306	-	-	5/12/12/12	-
5	GGG	A	303	-	-	4/12/12/12	-
5	GGG	B	101	-	-	5/12/12/12	-
7	MLA	A	307	-	-	2/4/4/4	-
6	KZF	A	305	-	-	4/7/15/15	0/1/1/1
6	KZF	A	304	-	-	3/7/15/15	0/1/1/1
8	A1CB7	A	308	-	-	41/93/192/192	0/5/5/5

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	308	A1CB7	O67-C35	8.07	1.52	1.42
8	A	308	A1CB7	C18-N20	7.53	1.50	1.34
8	A	308	A1CB7	C70-C71	-6.07	1.47	1.53
5	B	101	GGG	C1-N2	5.69	1.46	1.33
5	B	101	GGG	C2-N3	5.56	1.46	1.33
8	A	308	A1CB7	C81-N80	5.55	1.52	1.34
5	A	303	GGG	C2-N3	5.51	1.46	1.33
8	A	308	A1CB7	C91-C92	5.43	1.58	1.50
5	A	303	GGG	C1-N2	5.39	1.46	1.33
8	A	308	A1CB7	C22-C21	5.12	1.61	1.51
5	A	306	GGG	C1-N2	4.92	1.45	1.33
5	A	306	GGG	C2-N3	4.83	1.44	1.33
8	A	308	A1CB7	O73-C72	4.78	1.51	1.44
8	A	308	A1CB7	C64-N63	4.35	1.48	1.34
8	A	308	A1CB7	O23-C24	4.32	1.47	1.40
4	A	302	MK0	PBV-O1	4.17	1.71	1.59
4	A	302	MK0	O5-C5	4.05	1.54	1.44
8	A	308	A1CB7	C75-C74	4.04	1.60	1.53
6	B	102	KZF	C2-S	3.82	1.82	1.77
6	A	305	KZF	C2-S	3.40	1.82	1.77
8	A	308	A1CB7	O41-C42	3.31	1.51	1.41
8	A	308	A1CB7	O73-C68	3.28	1.46	1.42
8	A	308	A1CB7	C17-C18	3.11	1.57	1.51
6	A	304	KZF	C2-S	2.89	1.81	1.77
8	A	308	A1CB7	O41-C36	-2.78	1.36	1.43
8	A	308	A1CB7	O38-C33	2.78	1.49	1.41
4	A	302	MK0	PBV-OBI	2.77	1.70	1.59
8	A	308	A1CB7	C44-C43	-2.73	1.48	1.53
8	A	308	A1CB7	O19-C18	-2.63	1.18	1.23
6	A	304	KZF	O1-S	2.61	1.52	1.45
6	B	102	KZF	O2-S	2.58	1.52	1.45
8	A	308	A1CB7	C74-C72	2.57	1.56	1.52
8	A	308	A1CB7	O65-C64	-2.50	1.17	1.23
4	A	302	MK0	O5-C1	2.47	1.48	1.41
8	A	308	A1CB7	O57-C52	2.41	1.48	1.41
6	A	305	KZF	O2-S	2.40	1.51	1.45
6	B	102	KZF	O1-S	2.40	1.51	1.45
8	A	308	A1CB7	C83-C81	2.38	1.55	1.50
4	A	302	MK0	CAR-CAZ	2.34	1.62	1.52
5	A	303	GGG	O1-C1	-2.32	1.18	1.23
6	A	304	KZF	O2-S	2.22	1.51	1.45
8	A	308	A1CB7	C34-C35	-2.12	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	308	A1CB7	C68-C85	-2.11	1.49	1.54
5	B	101	GGG	O1-C1	-2.10	1.19	1.23
5	A	303	GGG	O2-C2	-2.09	1.19	1.23
6	A	305	KZF	O1-S	2.08	1.51	1.45
5	A	306	GGG	O2-C2	-2.02	1.19	1.23

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	308	A1CB7	C66-C64-N63	5.05	124.49	116.12
6	A	304	KZF	O2-S-O1	-4.68	98.61	113.82
8	A	308	A1CB7	C17-C18-N20	4.66	124.07	115.86
5	B	101	GGG	C2-CA2-N2	4.56	126.32	113.04
6	B	102	KZF	C3'-C2'-C1'	4.51	119.17	111.09
6	A	305	KZF	O3-S-O1	-4.21	100.86	111.40
6	A	304	KZF	O1-S-C2	4.17	113.03	106.73
6	B	102	KZF	C6'-C1'-C2'	4.16	117.98	110.80
4	A	302	MK0	C3-C4-C5	3.98	117.45	110.23
6	B	102	KZF	O2-S-C2	3.93	112.66	106.73
6	B	102	KZF	O3-S-O1	-3.89	101.66	111.40
8	A	308	A1CB7	O73-C72-C71	3.80	113.33	109.84
5	A	306	GGG	C3-CA3-N3	-3.59	101.92	113.06
8	A	308	A1CB7	C33-O32-C27	-3.52	109.64	117.98
6	A	305	KZF	O2-S-C2	3.50	112.01	106.73
8	A	308	A1CB7	O19-C18-N20	-3.47	117.08	122.95
4	A	302	MK0	CAS-CBC-CBN	-3.34	104.87	115.97
8	A	308	A1CB7	C42-O41-C36	-3.28	110.20	117.98
3	A	301	NAG	O5-C1-C2	-3.07	106.54	111.29
8	A	308	A1CB7	C44-C43-N63	-3.02	106.09	110.91
8	A	308	A1CB7	C91-C92-C93	-2.99	118.50	124.69
8	A	308	A1CB7	C42-O47-C46	-2.98	107.90	113.72
8	A	308	A1CB7	O41-C42-C43	2.97	112.89	108.07
6	B	102	KZF	C1-N-C1'	-2.93	108.53	114.18
8	A	308	A1CB7	O73-C72-C74	2.91	111.19	106.65
6	A	305	KZF	O3-S-C2	2.79	111.47	106.00
3	A	301	NAG	C1-O5-C5	2.73	115.85	112.19
4	A	302	MK0	C4-C3-C2	2.68	115.54	110.83
6	B	102	KZF	O1-S-C2	2.67	110.77	106.73
6	A	305	KZF	C1-N-C1'	-2.67	109.05	114.18
8	A	308	A1CB7	O65-C64-N63	-2.61	117.38	121.98
8	A	308	A1CB7	C52-O51-C44	-2.56	111.90	117.98
8	A	308	A1CB7	C75-C74-C72	-2.53	108.30	113.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	308	A1CB7	C52-C53-C54	2.50	115.27	110.01
8	A	308	A1CB7	C91-C21-N20	2.44	113.80	109.66
6	A	305	KZF	O1-S-C2	2.42	110.39	106.73
8	A	308	A1CB7	C42-C43-N63	-2.41	106.88	110.92
4	A	302	MK0	O5-C5-C4	2.37	113.96	109.70
5	A	303	GGG	O1-C1-N2	-2.28	118.55	123.03
8	A	308	A1CB7	C55-C54-C53	2.23	114.75	110.83
8	A	308	A1CB7	O65-C64-C66	-2.20	118.13	122.05
8	A	308	A1CB7	O77-C76-C75	-2.19	106.56	111.16
5	B	101	GGG	O2-C2-N3	-2.18	118.74	123.03
3	A	301	NAG	C1-C2-N2	2.18	113.86	110.43
8	A	308	A1CB7	C72-C71-N80	-2.08	107.58	110.91
8	A	308	A1CB7	O57-C56-C58	2.03	111.47	106.44
6	A	305	KZF	C6'-C1'-C2'	2.03	114.31	110.80
8	A	308	A1CB7	C83-C81-N80	2.02	119.47	116.12

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	302	MK0	O5-C1-O1-PBV
5	A	306	GGG	O3-C3-CA3-N3
5	B	101	GGG	O1-C1-CA1-N1
5	B	101	GGG	N2-C1-CA1-N1
5	B	101	GGG	C2-CA2-N2-C1
5	B	101	GGG	O3-C3-CA3-N3
5	B	101	GGG	O-C3-CA3-N3
6	A	304	KZF	C2'-C1'-N-C1
6	A	304	KZF	C2-C1-N-C1'
6	A	305	KZF	C1-C2-S-O1
6	B	102	KZF	C2'-C1'-N-C1
6	B	102	KZF	N-C1-C2-S
8	A	308	A1CB7	N20-C21-C22-O23
8	A	308	A1CB7	C91-C21-N20-C18
8	A	308	A1CB7	O29-C24-O23-C22
8	A	308	A1CB7	O67-C68-C85-O86
8	A	308	A1CB7	O73-C68-C85-O86
8	A	308	A1CB7	C72-C74-C75-C76
8	A	308	A1CB7	O79-C74-C75-C76
8	A	308	A1CB7	O79-C74-C75-O78
8	A	308	A1CB7	C74-C75-C76-O77
8	A	308	A1CB7	O78-C75-C76-O77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	308	A1CB7	C17-C18-N20-C21
8	A	308	A1CB7	O57-C56-C58-O59
4	A	302	MK0	O5-C5-C6-O6
8	A	308	A1CB7	C72-C74-C75-O78
8	A	308	A1CB7	O19-C18-N20-C21
8	A	308	A1CB7	C55-C56-C58-O59
4	A	302	MK0	C4-C5-C6-O6
8	A	308	A1CB7	O29-C28-C30-O31
5	A	303	GGG	O1-C1-N2-CA2
5	A	303	GGG	O2-C2-N3-CA3
8	A	308	A1CB7	O38-C37-C39-O40
4	A	302	MK0	CAU-CBG-CBP-CAF
5	A	306	GGG	O-C3-CA3-N3
8	A	308	A1CB7	C45-C46-C48-O49
8	A	308	A1CB7	C95-C96-C97-C98
8	A	308	A1CB7	C27-C28-C30-O31
3	A	301	NAG	C8-C7-N2-C2
3	A	301	NAG	O7-C7-N2-C2
8	A	308	A1CB7	C66-C64-N63-C43
8	A	308	A1CB7	O65-C64-N63-C43
4	A	302	MK0	CAP-CAQ-CAY-CBL
4	A	302	MK0	CBG-CAU-CBE-CBN
8	A	308	A1CB7	C36-C37-C39-O40
4	A	302	MK0	CBB-CAT-CBD-CBO
8	A	308	A1CB7	O47-C46-C48-O49
5	A	303	GGG	CA1-C1-N2-CA2
5	A	303	GGG	CA2-C2-N3-CA3
5	A	306	GGG	O1-C1-CA1-N1
4	A	302	MK0	CBH-CAV-CBF-CBO
5	A	306	GGG	N2-C1-CA1-N1
8	A	308	A1CB7	C03-C04-C05-C06
8	A	308	A1CB7	C99-CA0-CA1-CA2
4	A	302	MK0	CAO-CAP-CAQ-CAY
8	A	308	A1CB7	C96-C97-C98-C99
4	A	302	MK0	CAN-CAO-CAP-CAQ
4	A	302	MK0	CBD-CAT-CBB-CBM
8	A	308	A1CB7	C12-C13-C14-C15
4	A	302	MK0	CAU-CBE-CBN-CBC
8	A	308	A1CB7	CA3-CA4-CA5-CA6
4	A	302	MK0	CAR-CAZ-CBM-CAC
4	A	302	MK0	CAU-CBE-CBN-CAD
4	A	302	MK0	CAV-CBF-CBO-CAE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	308	A1CB7	C08-C09-C10-C11
4	A	302	MK0	CAR-CAZ-CBM-CBB
4	A	302	MK0	CAV-CBF-CBO-CBD
4	A	302	MK0	CAU-CBG-CBP-CBH
8	A	308	A1CB7	C05-C06-C07-C08
8	A	308	A1CB7	C04-C05-C06-C07
8	A	308	A1CB7	C97-C98-C99-CA0
6	A	304	KZF	C6'-C1'-N-C1
8	A	308	A1CB7	CA2-CA3-CA4-CA5
4	A	302	MK0	CAX-OBI-PBV-O1
4	A	302	MK0	CAX-OBI-PBV-OAG
4	A	302	MK0	CAX-OBI-PBV-OAL
8	A	308	A1CB7	O38-C33-O32-C27
8	A	308	A1CB7	C94-C95-C96-C97
6	B	102	KZF	C2-C1-N-C1'
4	A	302	MK0	CBC-CAS-CBA-CBL
8	A	308	A1CB7	C22-C21-N20-C18
8	A	308	A1CB7	O67-C68-C85-O87
6	A	305	KZF	C2'-C1'-N-C1
6	A	305	KZF	C6'-C1'-N-C1
6	B	102	KZF	C6'-C1'-N-C1
6	A	305	KZF	C1-C2-S-O2
8	A	308	A1CB7	C92-C93-C94-C95
4	A	302	MK0	C1-O1-PBV-OAG
4	A	302	MK0	CAZ-CAR-CAX-OBI
8	A	308	A1CB7	C34-C33-O32-C27
4	A	302	MK0	CAA-CAM-CAN-CAO
4	A	302	MK0	CBE-CAU-CBG-CBP
7	A	307	MLA	C1-C2-C3-O3A
8	A	308	A1CB7	C10-C11-C12-C13
7	A	307	MLA	C1-C2-C3-O3B
5	A	306	GGG	C3-CA3-N3-C2

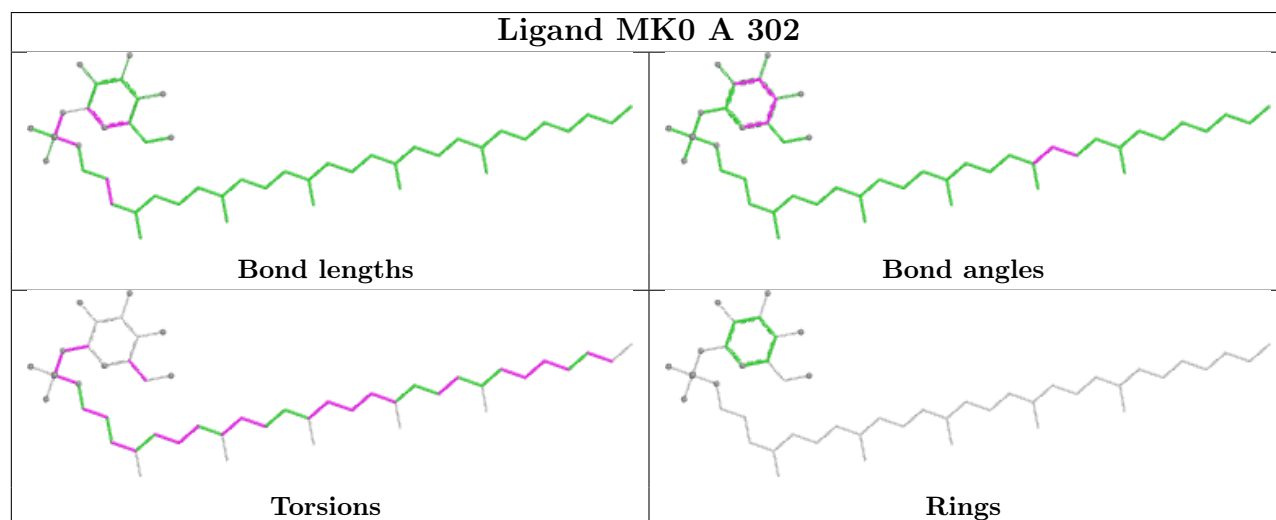
There are no ring outliers.

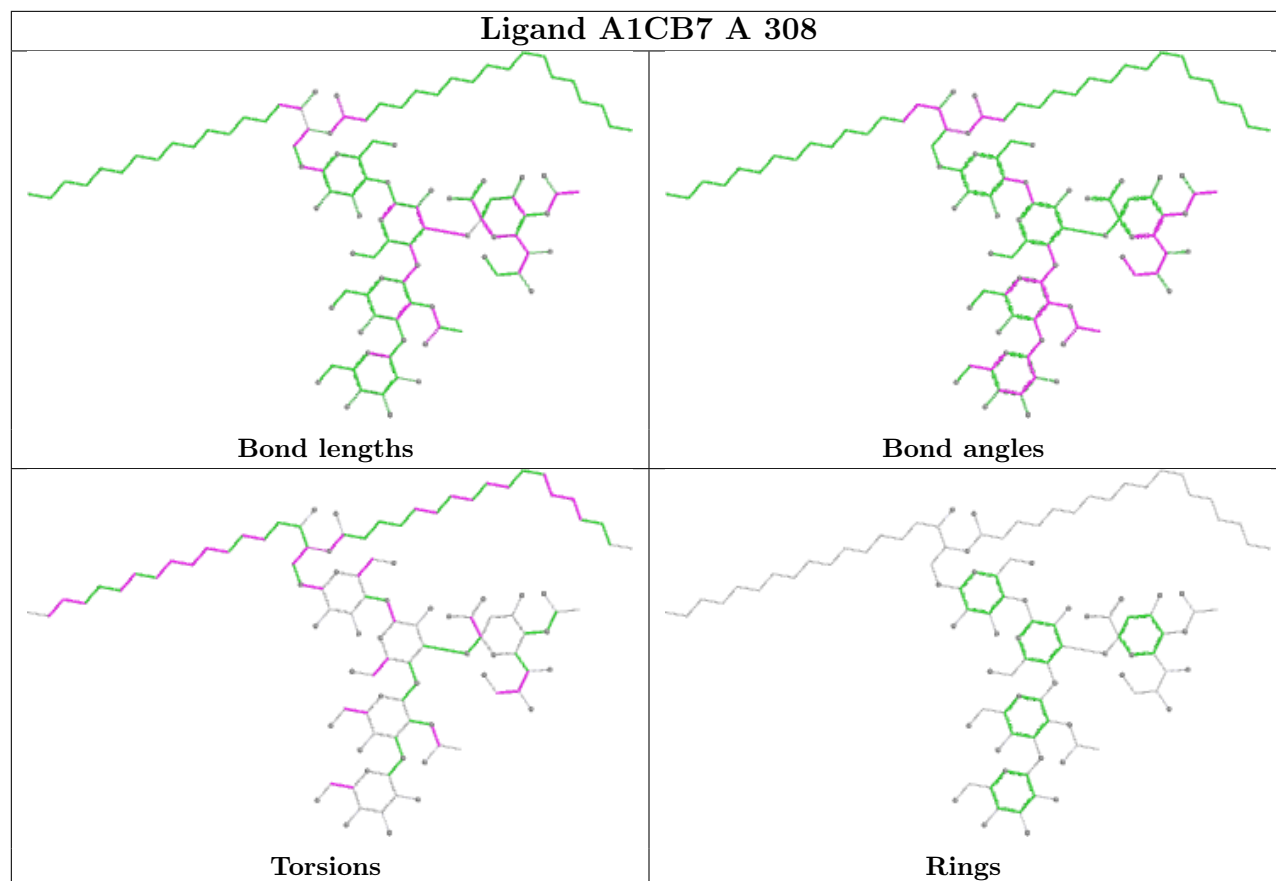
3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	302	MK0	9	0
5	A	306	GGG	2	0
5	B	101	GGG	2	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, 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	281/281 (100%)	0.15	10 (3%) 46 41	23, 40, 77, 97	1 (0%)
2	B	98/99 (98%)	0.34	0 100 100	28, 48, 76, 85	0
All	All	379/380 (99%)	0.20	10 (2%) 57 52	23, 43, 77, 97	1 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	GLN	2.9
1	A	141	ALA	2.8
1	A	137	CYS	2.8
1	A	154	GLY	2.3
1	A	129	THR	2.3
1	A	187	ARG	2.3
1	A	151	GLN	2.2
1	A	148	LEU	2.2
1	A	72[A]	PHE	2.1
1	A	138	GLY	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](#)

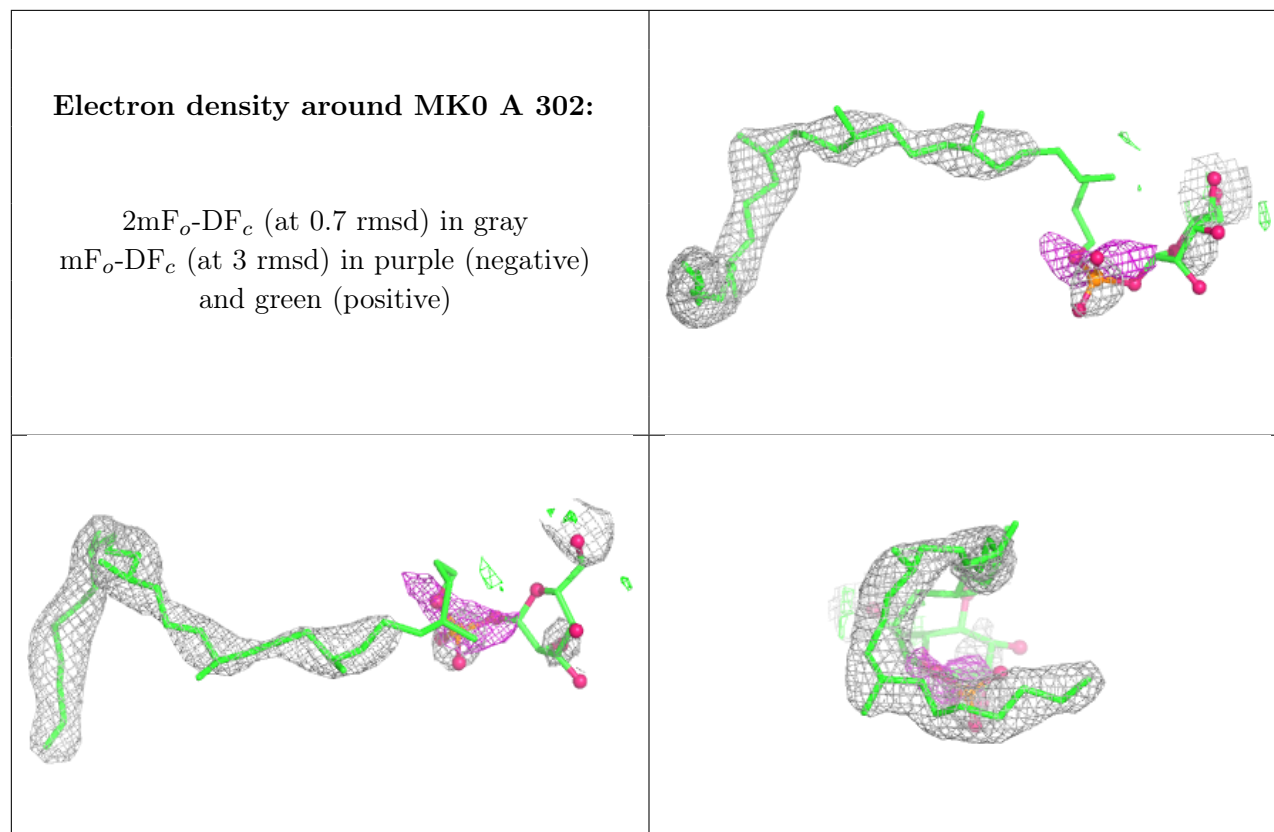
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

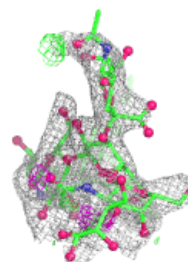
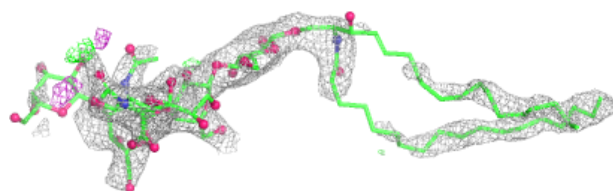
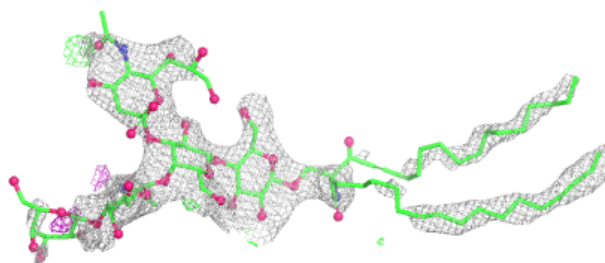
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MLA	A	307	7/7	0.63	0.15	68,80,99,102	0
5	GGG	A	303	13/13	0.69	0.16	63,76,80,81	0
5	GGG	B	101	13/13	0.73	0.15	38,51,64,70	0
4	MK0	A	302	48/48	0.80	0.18	21,62,107,115	2
6	KZF	B	102	13/13	0.80	0.14	50,64,90,93	0
5	GGG	A	306	13/13	0.80	0.17	62,66,83,87	0
8	A1CB7	A	308	107/107	0.83	0.15	44,84,108,115	0
6	KZF	A	305	13/13	0.91	0.12	46,55,72,74	0
3	NAG	A	301	14/15	0.92	0.08	39,44,51,51	0
6	KZF	A	304	13/13	0.97	0.07	34,39,47,50	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 A1CB7 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.