



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2025 – 10:12 AM EST

PDB ID : 9OHV / pdb_00009ohv
Title : CD1c presenting dual lipids MPM and GD3 ganglioside
Authors : Cao, T.P.; Rossjohn, J.; Shahine, A.
Deposited on : 2025-05-05
Resolution : 2.12 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 : 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) : 2.46

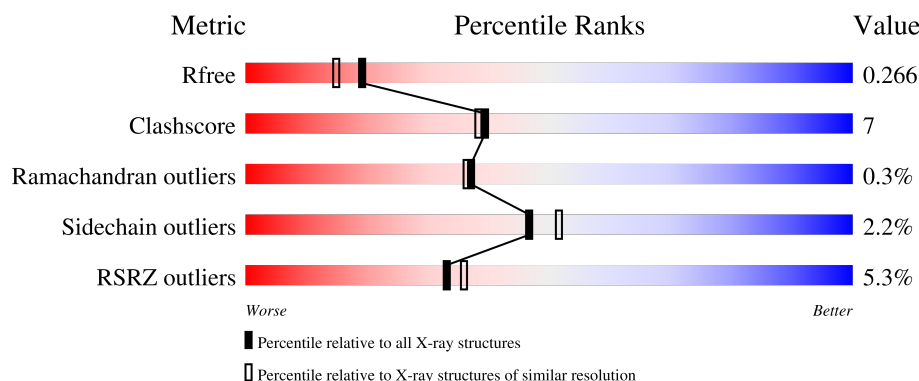
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	7689 (2.14-2.10)
Clashscore	180529	8431 (2.14-2.10)
Ramachandran outliers	177936	8366 (2.14-2.10)
Sidechain outliers	177891	8367 (2.14-2.10)
RSRZ outliers	164620	7689 (2.14-2.10)

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	280	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>.</div> </div> </div>
2	B	98	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>..</div> </div> </div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 3205 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.

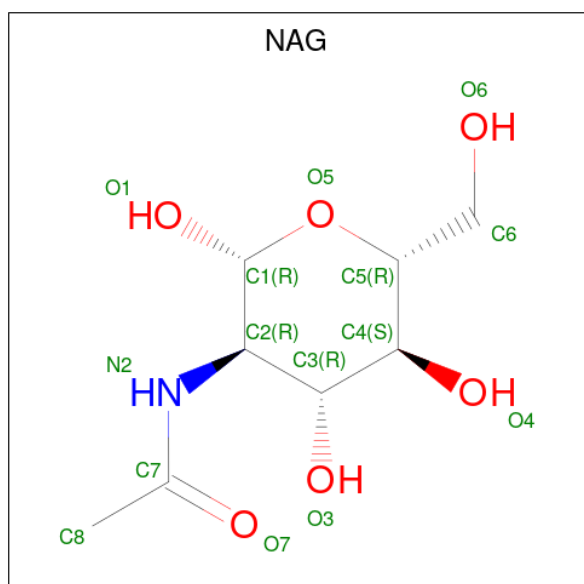
- Molecule 1 is a protein called T-cell surface glycoprotein CD1c/T-cell surface glycoprotein CD1b chimeric protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	1	0
			2216	1421	380	406	9			

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

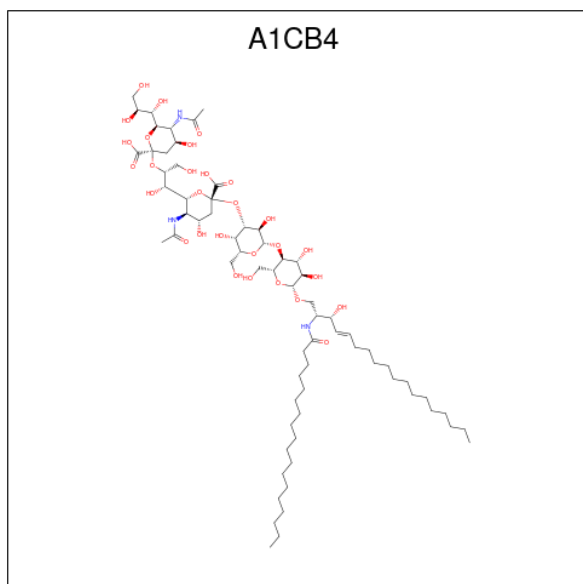
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	95	Total	C	N	O	S	0	0	0
			783	500	133	148	2			

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



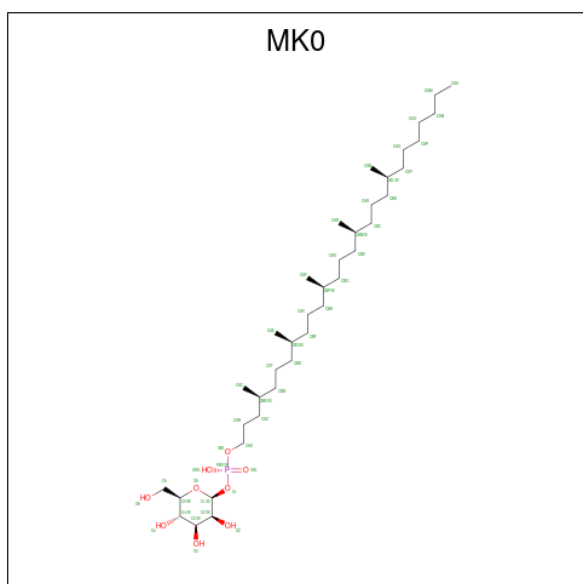
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is (2R,3R,4E)-3-hydroxy-2-octadecanamido-octadec-4-en-1-yl 5-acetamido-3,5-dideoxy-L-glycero-beta-L-altro-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		
4	A	1	102	70	3	29	0	0

- Molecule 5 is 1-O-[(S)-hydroxy{[(4S,8S,16S,20S)-4,8,12,16,20-pentamethylheptacosyl]oxy}phosphoryl]-beta-D-mannopyranose (CCD ID: MK0) (formula: $C_{38}H_{77}O_9P$) (labeled as "Ligand of Interest" by depositor).

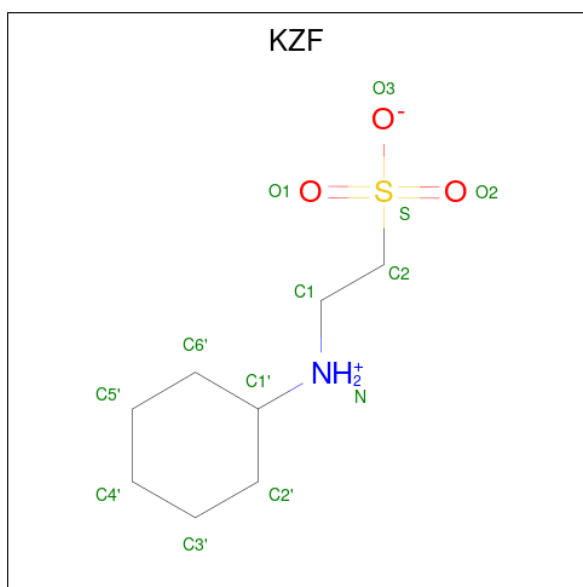


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			48	38	9	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is 2-(cyclohexylazanumyl)ethanesulfonate (CCD ID: KZF) (formula: C₈H₁₇NO₃S).



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

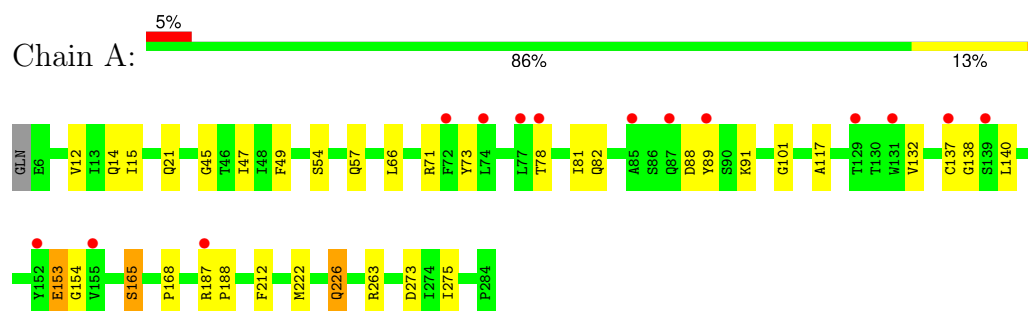
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	18	Total	O	0	0
			18	18		
8	B	10	Total	O	0	0
			10	10		

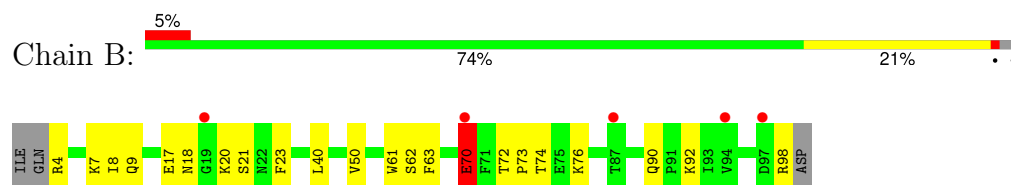
3 Residue-property plots [i](#)

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	54.91Å 84.94Å 93.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.47 – 2.12 42.47 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.4 (42.47-2.12) 99.4 (42.47-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.21.2-5419	Depositor
R, R_{free}	0.218 , 0.260 0.228 , 0.266	Depositor DCC
R_{free} test set	1351 reflections (5.34%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 50.6	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	0.95	EDS
Total number of atoms	3205	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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: KZF, MK0, A1CB4, NAG, CL

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	0.43	0/2287	0.63	0/3110
2	B	0.47	0/806	0.70	1/1095 (0.1%)
All	All	0.44	0/3093	0.65	1/4205 (0.0%)

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
2	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	70	GLU	CB-CA-C	-5.42	100.38	109.65

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	ARG	Sidechain
2	B	98	ARG	Sidechain

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	2216	0	2100	26	1
2	B	783	0	733	13	0
3	A	14	0	13	0	1
4	A	102	0	0	2	0
5	A	48	0	76	7	0
6	A	1	0	0	0	0
7	A	13	0	0	0	0
8	A	18	0	0	0	0
8	B	10	0	0	0	0
All	All	3205	0	2922	40	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 7.

All (40) 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)
2:B:8:ILE:HD12	2:B:92:LYS:HD2	1.63	0.81
1:A:73:TYR:HB2	5:A:303:MK0:HAR	1.64	0.79
2:B:23:PHE:CE1	2:B:70:GLU:HG2	2.21	0.75
2:B:74:THR:HG22	2:B:76:LYS:H	1.59	0.68
2:B:4:ARG:NH1	2:B:62:SER:HB3	2.10	0.67
2:B:4:ARG:HH11	2:B:62:SER:HB3	1.60	0.64
1:A:12:VAL:HG13	5:A:303:MK0:HAO	1.81	0.62
1:A:188:PRO:HB3	1:A:212:PHE:HB3	1.82	0.61
1:A:66:LEU:HD13	5:A:303:MK0:HBC	1.84	0.59
1:A:101:GLY:HA2	5:A:303:MK0:HAFB	1.88	0.56
1:A:88:ASP:OD2	1:A:91:LYS:HD2	2.05	0.55
1:A:263:ARG:NH1	1:A:275:ILE:HD11	2.22	0.54
1:A:81:ILE:HD12	4:A:302:A1CB4:C12	2.38	0.54
1:A:47:ILE:HD13	5:A:303:MK0:HABB	1.91	0.53
1:A:143:SER:O	1:A:147:LEU:HG	2.09	0.53
1:A:153:GLU:HG2	1:A:154:GLY:H	1.75	0.52
4:A:302:A1CB4:O65	4:A:302:A1CB4:O63	2.30	0.49
5:A:303:MK0:HAR	5:A:303:MK0:HBBA	1.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:GLY:O	1:A:71:ARG:NH1	2.47	0.48
1:A:137:CYS:SG	1:A:138:GLY:N	2.87	0.47
1:A:140:LEU:O	1:A:144:VAL:HG23	2.13	0.47
1:A:165:SER:O	1:A:168:PRO:HD2	2.15	0.46
2:B:7:LYS:HZ1	2:B:9:GLN:NE2	2.14	0.45
2:B:17:GLU:HB2	2:B:20:LYS:HB2	1.99	0.45
1:A:117:ALA:HB2	2:B:61:TRP:CE2	2.53	0.44
1:A:263:ARG:NH2	1:A:273:ASP:OD2	2.50	0.44
1:A:153:GLU:HG2	1:A:154:GLY:N	2.32	0.44
1:A:21:GLN:CD	1:A:21:GLN:H	2.26	0.44
1:A:89:TYR:C	1:A:91:LYS:H	2.25	0.43
1:A:78:THR:HG22	1:A:78:THR:O	2.17	0.43
2:B:21:SER:HA	2:B:72:THR:HG22	2.00	0.43
2:B:18:ASN:HA	2:B:73:PRO:O	2.20	0.42
5:A:303:MK0:HAEB	5:A:303:MK0:HAT	1.79	0.41
1:A:222:MET:HE3	1:A:222:MET:HB3	1.95	0.41
1:A:165:SER:C	1:A:168:PRO:HD2	2.45	0.41
2:B:74:THR:HG22	2:B:76:LYS:N	2.32	0.41
2:B:40:LEU:HD12	2:B:50:VAL:HG23	2.02	0.40
1:A:15:ILE:HG12	2:B:63:PHE:HE1	1.86	0.40
1:A:226:GLN:O	1:A:226:GLN:HG3	2.21	0.40
1:A:49:PHE:HB3	1:A:54:SER:HB2	2.04	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:57:GLN:OE1	3:A:301:NAG:O4[3_554]	2.13	0.07

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	278/280 (99%)	265 (95%)	12 (4%)	1 (0%)	30	28
2	B	93/98 (95%)	91 (98%)	2 (2%)	0	100	100
All	All	371/378 (98%)	356 (96%)	14 (4%)	1 (0%)	37	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	GLU

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	237/239 (99%)	232 (98%)	5 (2%)	48	54
2	B	87/93 (94%)	85 (98%)	2 (2%)	45	50
All	All	324/332 (98%)	317 (98%)	7 (2%)	47	51

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

Mol	Chain	Res	Type
1	A	14	GLN
1	A	82	GLN
1	A	132	VAL
1	A	165	SER
1	A	226	GLN
2	B	70	GLU
2	B	90	GLN

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	82	GLN
1	A	87	GLN
1	A	146	HIS

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Mol	Chain	Res	Type
1	A	185	GLN
2	B	9	GLN

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 ⓘ

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	KZF	A	305	-	13,13,13	1.65	3 (23%)	16,17,17	2.36	4 (25%)
3	NAG	A	301	1	14,14,15	0.94	2 (14%)	17,19,21	1.30	1 (5%)
5	MK0	A	303	-	47,48,48	1.28	6 (12%)	60,61,61	0.93	2 (3%)
4	A1CB4	A	302	-	102,105,105	2.09	29 (28%)	130,141,141	1.55	24 (18%)

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	KZF	A	305	-	-	4/7/15/15	0/1/1/1
3	NAG	A	301	1	-	0/6/23/26	0/1/1/1
5	MK0	A	303	-	-	27/46/66/66	0/1/1/1
4	A1CB4	A	302	-	-	41/101/179/179	0/4/4/4

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	302	A1CB4	C18-N20	6.13	1.47	1.34
4	A	302	A1CB4	C45-C46	-5.29	1.48	1.53
4	A	302	A1CB4	C60-C58	5.22	1.59	1.52
4	A	302	A1CB4	C56-C57	-5.10	1.48	1.53
4	A	302	A1CB4	C49-C47	4.86	1.58	1.52
4	A	302	A1CB4	O42-C35	4.77	1.48	1.42
4	A	302	A1CB4	O59-C54	4.75	1.48	1.42
4	A	302	A1CB4	O48-C43	4.38	1.48	1.42
7	A	305	KZF	C2-S	4.37	1.83	1.77
4	A	302	A1CB4	C49-C50	4.32	1.61	1.52
4	A	302	A1CB4	C76-N75	4.23	1.48	1.34
4	A	302	A1CB4	C67-N66	4.00	1.47	1.34
4	A	302	A1CB4	O29-C24	3.82	1.51	1.41
5	A	303	MK0	PBV-O1	3.76	1.70	1.59
5	A	303	MK0	O5-C5	3.60	1.53	1.44
4	A	302	A1CB4	C22-C21	3.15	1.57	1.51
4	A	302	A1CB4	O59-C58	3.09	1.48	1.44
4	A	302	A1CB4	O23-C24	2.76	1.44	1.40
4	A	302	A1CB4	C55-C54	2.73	1.56	1.52
5	A	303	MK0	O5-C1	2.62	1.48	1.41
4	A	302	A1CB4	C44-C45	-2.60	1.49	1.53
4	A	302	A1CB4	C55-C56	-2.58	1.49	1.53
4	A	302	A1CB4	C86-C87	2.58	1.54	1.50
4	A	302	A1CB4	O48-C47	2.58	1.47	1.44
5	A	303	MK0	PBV-OBI	2.49	1.69	1.59
7	A	305	KZF	O1-S	2.45	1.52	1.45
4	A	302	A1CB4	O38-C33	2.38	1.48	1.41
3	A	301	NAG	O5-C1	-2.36	1.39	1.43
7	A	305	KZF	O2-S	2.29	1.51	1.45
4	A	302	A1CB4	O19-C18	-2.27	1.18	1.23
5	A	303	MK0	CAR-CAZ	2.24	1.61	1.52
4	A	302	A1CB4	O68-C67	-2.15	1.18	1.23
4	A	302	A1CB4	C26-C25	-2.10	1.46	1.52
4	A	302	A1CB4	C78-C76	2.09	1.54	1.50
4	A	302	A1CB4	C46-N75	2.09	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	302	A1CB4	O38-C37	2.07	1.49	1.44
4	A	302	A1CB4	O32-C27	2.06	1.49	1.43
4	A	302	A1CB4	O72-C71	2.05	1.28	1.22
3	A	301	NAG	C2-N2	-2.03	1.42	1.46
5	A	303	MK0	CAT-CBD	2.01	1.60	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	305	KZF	O3-S-O1	-5.87	96.70	111.40
4	A	302	A1CB4	C44-C45-C46	5.53	118.26	109.72
7	A	305	KZF	O1-S-C2	5.41	114.91	106.73
4	A	302	A1CB4	O59-C58-C60	4.68	113.96	106.65
4	A	302	A1CB4	C22-C21-N20	-4.63	103.06	109.66
4	A	302	A1CB4	C45-C46-N75	-4.02	102.52	110.44
4	A	302	A1CB4	O48-C47-C46	3.28	112.84	109.84
4	A	302	A1CB4	C17-C18-N20	3.27	121.63	115.86
4	A	302	A1CB4	C36-C35-C34	3.06	115.10	110.86
4	A	302	A1CB4	C33-O32-C27	-2.96	110.96	117.98
4	A	302	A1CB4	C54-C55-C56	2.91	116.62	110.73
3	A	301	NAG	O5-C1-C2	-2.77	107.01	111.29
4	A	302	A1CB4	C78-C76-N75	2.75	120.69	116.12
4	A	302	A1CB4	OA2-C86-C87	-2.61	104.14	110.88
4	A	302	A1CB4	C10-C09-C08	2.61	127.54	114.37
4	A	302	A1CB4	O19-C18-N20	-2.56	118.61	122.95
7	A	305	KZF	C1-N-C1'	-2.53	109.31	114.18
4	A	302	A1CB4	C12-C11-C10	-2.52	101.63	114.37
4	A	302	A1CB4	C55-C56-C57	2.40	113.43	109.72
4	A	302	A1CB4	O29-C24-O23	-2.38	104.43	110.04
4	A	302	A1CB4	C69-C67-N66	2.37	120.04	116.12
4	A	302	A1CB4	C47-C46-N75	2.36	114.66	110.91
4	A	302	A1CB4	C58-C57-N66	-2.28	107.26	110.91
4	A	302	A1CB4	C61-C60-C58	2.24	117.27	113.05
4	A	302	A1CB4	C54-O59-C58	-2.23	109.13	114.36
5	A	303	MK0	CAS-CBA-CBL	-2.22	108.58	115.97
5	A	303	MK0	CAF-CBP-CBG	-2.19	103.45	111.27
4	A	302	A1CB4	C89-C88-C87	-2.18	115.73	125.47
4	A	302	A1CB4	O29-C28-C27	2.10	114.07	109.72
7	A	305	KZF	O3-S-C2	2.10	110.11	106.00
4	A	302	A1CB4	C35-C36-C37	2.02	113.88	109.57

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	302	A1CB4	C86-C21-C22-O23
4	A	302	A1CB4	N20-C21-C22-O23
4	A	302	A1CB4	O29-C24-O23-C22
4	A	302	A1CB4	O74-C49-C50-C51
4	A	302	A1CB4	O74-C49-C50-O53
4	A	302	A1CB4	O53-C50-C51-O52
4	A	302	A1CB4	O53-C54-C71-O73
4	A	302	A1CB4	C21-C86-C87-C88
4	A	302	A1CB4	OA2-C86-C87-C88
5	A	303	MK0	C2-C1-O1-PBV
5	A	303	MK0	O5-C1-O1-PBV
5	A	303	MK0	CAU-CBE-CBN-CAD
5	A	303	MK0	CAX-OBI-PBV-O1
7	A	305	KZF	C2-C1-N-C1'
7	A	305	KZF	C1-C2-S-O3
4	A	302	A1CB4	C17-C18-N20-C21
4	A	302	A1CB4	O29-C28-C30-O31
4	A	302	A1CB4	C36-C37-C39-O40
4	A	302	A1CB4	O19-C18-N20-C21
4	A	302	A1CB4	O38-C37-C39-O40
4	A	302	A1CB4	C47-C49-C50-C51
4	A	302	A1CB4	C11-C12-C13-C14
4	A	302	A1CB4	C94-C95-C96-C97
5	A	303	MK0	CAS-CBA-CBL-CAB
4	A	302	A1CB4	C78-C76-N75-C46
4	A	302	A1CB4	O77-C76-N75-C46
5	A	303	MK0	CAR-CAZ-CBM-CBB
4	A	302	A1CB4	C92-C93-C94-C95
5	A	303	MK0	CBG-CAU-CBE-CBN
4	A	302	A1CB4	C90-C91-C92-C93
4	A	302	A1CB4	C27-C28-C30-O31
5	A	303	MK0	CBF-CAV-CBH-CBP
4	A	302	A1CB4	C05-C06-C07-C08
4	A	302	A1CB4	C07-C08-C09-C10
5	A	303	MK0	CAT-CBD-CBO-CAE
4	A	302	A1CB4	C13-C14-C15-C16
5	A	303	MK0	CAN-CAO-CAP-CAQ
5	A	303	MK0	CAS-CBC-CBN-CBE
5	A	303	MK0	CAV-CBF-CBO-CBD
5	A	303	MK0	CAU-CBG-CBP-CBH
5	A	303	MK0	CAT-CBB-CBM-CAC
5	A	303	MK0	CAV-CBH-CBP-CAF

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Mol	Chain	Res	Type	Atoms
4	A	302	A1CB4	C10-C11-C12-C13
4	A	302	A1CB4	C08-C09-C10-C11
5	A	303	MK0	CAS-CBC-CBN-CAD
4	A	302	A1CB4	C02-C03-C04-C05
5	A	303	MK0	CAU-CBE-CBN-CBC
5	A	303	MK0	CAV-CBH-CBP-CBG
4	A	302	A1CB4	O53-C54-C71-O72
7	A	305	KZF	C1-C2-S-O1
7	A	305	KZF	C1-C2-S-O2
5	A	303	MK0	CAT-CBB-CBM-CAZ
4	A	302	A1CB4	C03-C04-C05-C06
4	A	302	A1CB4	C95-C96-C97-C98
5	A	303	MK0	CBD-CAT-CBB-CBM
5	A	303	MK0	CAS-CBA-CBL-CAY
5	A	303	MK0	CAA-CAM-CAN-CAO
4	A	302	A1CB4	C57-C58-C60-C61
5	A	303	MK0	CAU-CBG-CBP-CAF
5	A	303	MK0	CBE-CAU-CBG-CBP
4	A	302	A1CB4	C14-C15-C16-C17
5	A	303	MK0	CAR-CAZ-CBM-CAC
4	A	302	A1CB4	C47-C49-C50-O53
4	A	302	A1CB4	C57-C58-C60-O65
5	A	303	MK0	C1-O1-PBV-OAL
4	A	302	A1CB4	C87-C88-C89-C90
4	A	302	A1CB4	C89-C90-C91-C92
4	A	302	A1CB4	C06-C07-C08-C09
4	A	302	A1CB4	C04-C05-C06-C07
4	A	302	A1CB4	C56-C57-N66-C67
4	A	302	A1CB4	C55-C54-C71-O72
5	A	303	MK0	CBA-CAS-CBC-CBN

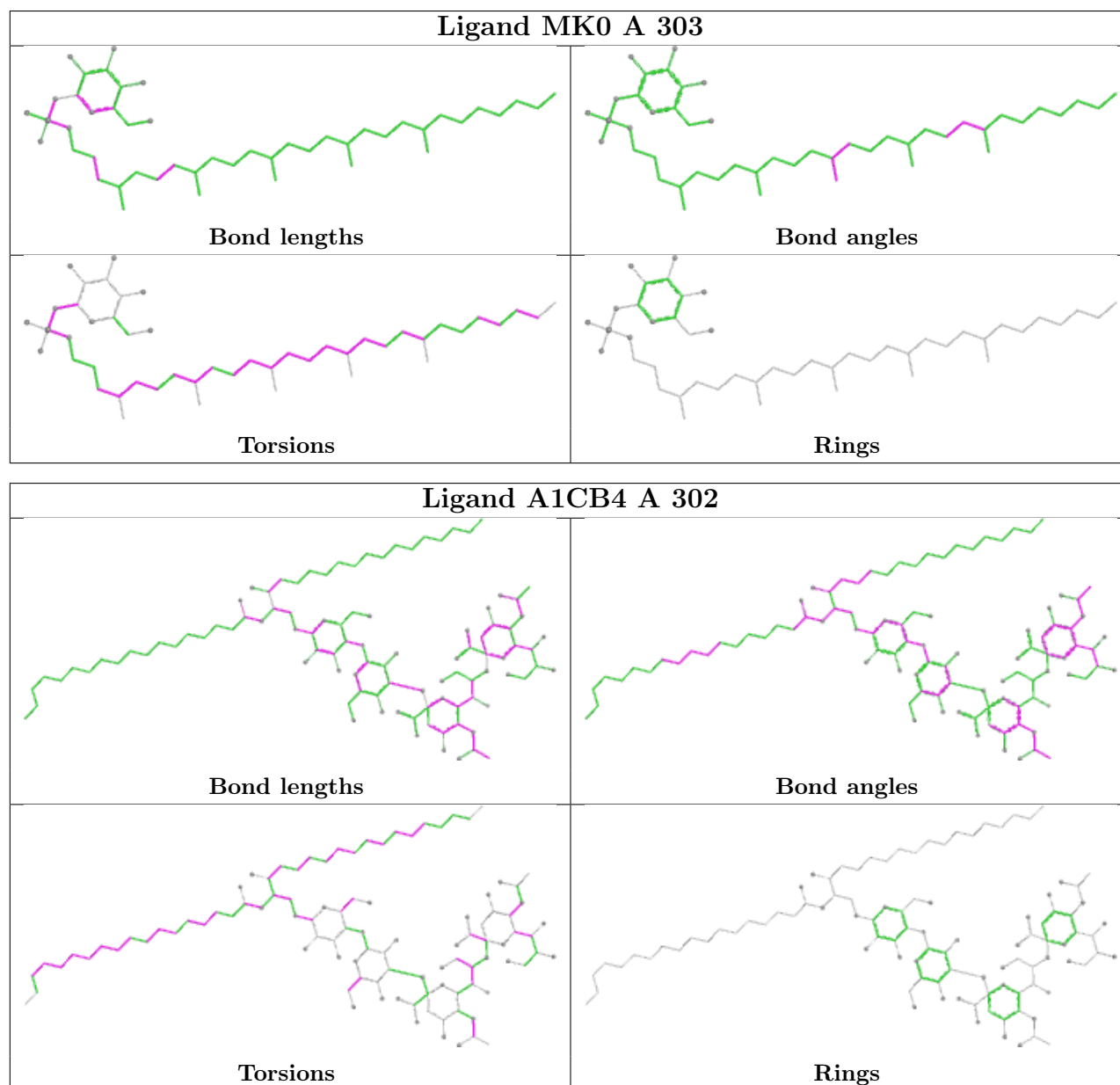
There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	NAG	0	1
5	A	303	MK0	7	0
4	A	302	A1CB4	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 ⓘ

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	279/280 (99%)	0.60	15 (5%) 32 35	34, 51, 88, 103	1 (0%)
2	B	95/98 (96%)	0.59	5 (5%) 33 36	35, 48, 67, 78	0
All	All	374/378 (98%)	0.60	20 (5%) 33 36	34, 50, 87, 103	1 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	78	THR	4.4
2	B	97	ASP	3.3
1	A	87	GLN	3.3
2	B	70	GLU	3.2
1	A	85	ALA	3.1
1	A	137	CYS	3.1
1	A	72[A]	PHE	3.1
1	A	129	THR	3.0
1	A	152	TYR	2.9
1	A	89	TYR	2.7
1	A	187	ARG	2.3
2	B	19	GLY	2.3
1	A	148	LEU	2.3
2	B	94	VAL	2.2
1	A	74	LEU	2.2
1	A	155	VAL	2.2
1	A	131	TRP	2.2
2	B	87	THR	2.1
1	A	77	LEU	2.1
1	A	139	SER	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](#)

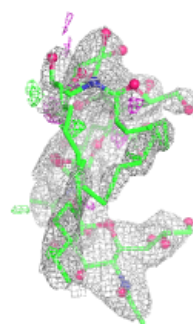
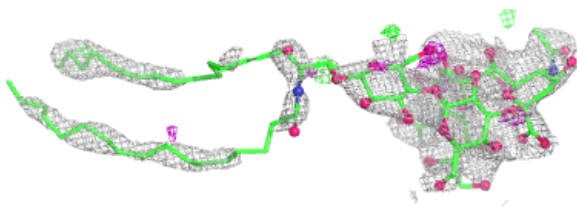
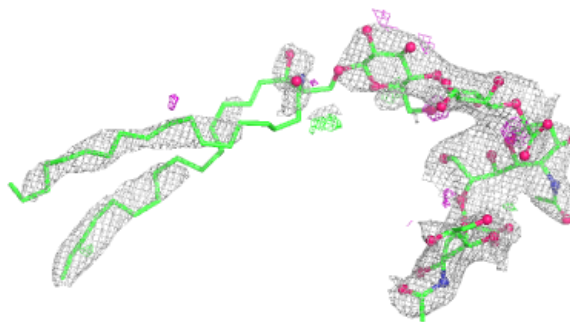
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	A1CB4	A	302	102/102	0.83	0.16	59,95,101,107	0
3	NAG	A	301	14/15	0.85	0.10	63,68,72,72	0
5	MK0	A	303	48/48	0.87	0.16	48,68,106,108	1
7	KZF	A	305	13/13	0.88	0.14	62,66,73,83	0
6	CL	A	304	1/1	0.94	0.09	56,56,56,56	0

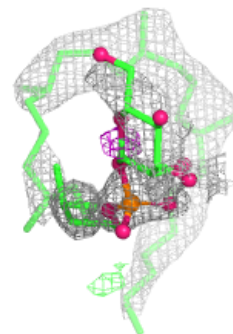
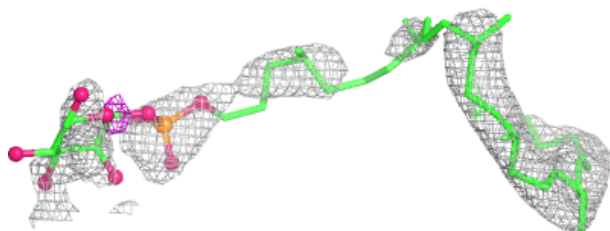
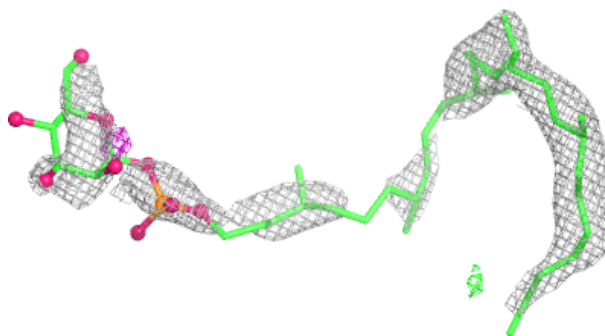
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1CB4 A 302:

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

**Electron density around MK0 A 303:**

$2mF_o-DF_c$ (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.