



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:00 PM UTC

PDB ID : 3OV6 / pdb_00003ov6
Title : CD1c in complex with MPM (mannosyl-beta1-phosphomycoketide)
Authors : Scharf, L.; Li, N.S.; Hawk, A.J.; Garzon, D.; Zhang, T.; Kazen, A.R.; Shah, S.; Haddadian, E.J.; Saghatelian, A.; Faraldo-Gomez, J.D.; Meredith, S.C.; Piccirilli, J.A.; Adams, E.J.
Deposited on : 2010-09-15
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

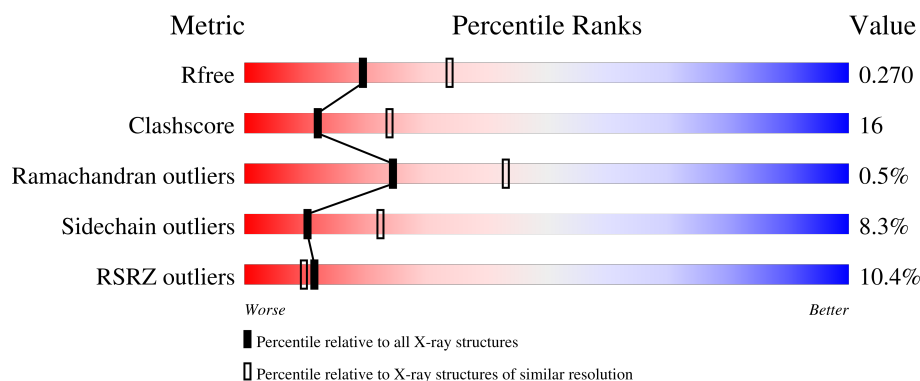
1 Overall quality at a glance

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	397	10% 65% 25% 5%

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
3	D12	A	1104	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3126 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 Beta-2-microglobulin, T-cell surface glycoprotein CD1c, T-cell surface glycoprotein CD1b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	178	0	0
			3014	1926	517	559	12			

There are 26 discrepancies between the modelled and reference sequences:

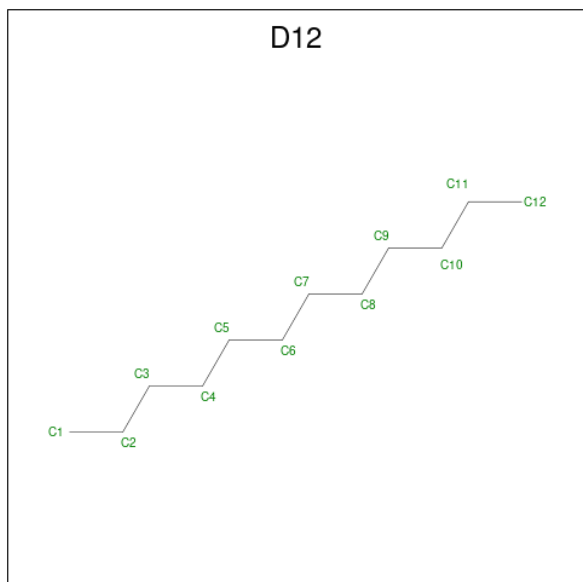
Chain	Residue	Modelled	Actual	Comment	Reference
A	998	ALA	-	expression tag	UNP P61769
A	999	ASP	-	expression tag	UNP P61769
A	1000	PRO	-	expression tag	UNP P61769
A	1100	GLY	-	linker	UNP P61769
A	1101	GLY	-	linker	UNP P61769
A	1102	GLY	-	linker	UNP P61769
A	1103	GLY	-	linker	UNP P61769
A	1104	SER	-	linker	UNP P61769
A	1105	GLY	-	linker	UNP P61769
A	1106	GLY	-	linker	UNP P61769
A	1107	SER	-	linker	UNP P61769
A	1108	GLY	-	linker	UNP P61769
A	1109	SER	-	linker	UNP P61769
A	1110	GLY	-	linker	UNP P61769
A	1111	GLY	-	linker	UNP P61769
A	1112	GLY	-	linker	UNP P61769
A	1113	SER	-	linker	UNP P61769
A	1114	SER	-	linker	UNP P61769
A	52	GLN	ASN	engineered mutation	UNP P29017
A	57	GLN	ASN	engineered mutation	UNP P29017
A	108	GLY	LYS	engineered mutation	UNP P29017
A	128	GLN	ASN	engineered mutation	UNP P29017
A	241	GLN	ASN	engineered mutation	UNP P29016
A	242	GLY	TRP	engineered mutation	UNP P29016
A	279	HIS	-	expression tag	UNP P29016
A	280	HIS	-	expression tag	UNP P29016

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



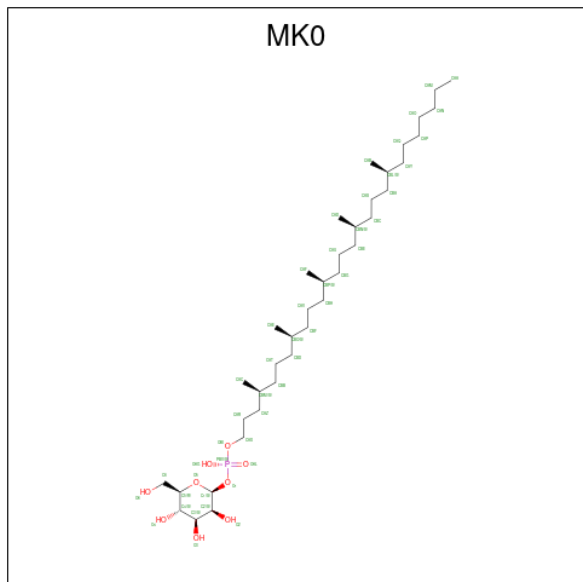
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			12	12		

- 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total	O	1	0
			38	38		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.72Å 87.09Å 88.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.54 – 2.50 43.54 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.54-2.50) 91.3 (43.54-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.240 , 0.273 0.232 , 0.270	Depositor DCC
R_{free} test set	686 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3126	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.59% 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: NAG, MK0, D12

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	0.63	0/3104	1.02	10/4211 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	GLU	N-CA-C	7.10	121.64	113.19
1	A	193	SER	N-CA-C	-6.67	98.58	108.79
1	A	153	GLU	N-CA-C	-6.58	99.75	109.81
1	A	1002	GLN	N-CA-C	6.28	119.13	108.90
1	A	84	HIS	N-CA-C	-6.08	103.79	110.91
1	A	182	VAL	N-CA-C	5.75	115.42	108.06
1	A	33	ASP	N-CA-C	-5.66	99.51	109.02
1	A	1030	PHE	N-CA-C	5.53	118.74	109.95
1	A	150	HIS	N-CA-C	5.25	120.55	114.04
1	A	154	GLY	N-CA-C	-5.03	107.58	114.67

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	3014	0	2858	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	14	0	13	0	0
3	A	12	0	26	10	0
4	A	48	0	76	10	0
5	A	38	0	0	2	0
All	All	3126	0	2973	89	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 16.

All (89) 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:148:LEU:HD21	3:A:1104:D12:H62	1.52	0.88
1:A:69:LEU:HG	4:A:1105:MK0:HACB	1.61	0.83
1:A:73:TYR:HB2	4:A:1105:MK0:HACA	1.60	0.83
1:A:28:GLY:HA3	4:A:1105:MK0:HAOA	1.67	0.75
3:A:1104:D12:H122	4:A:1105:MK0:O6	1.87	0.75
1:A:1096:ASP:H	1:A:1101:GLY:HA2	1.53	0.74
1:A:1033:SER:HB2	1:A:1054:LEU:HD21	1.71	0.72
1:A:218:TRP:HB3	1:A:265:LYS:HB2	1.72	0.72
1:A:73:TYR:CD1	4:A:1105:MK0:HBB	2.28	0.69
1:A:128:GLN:NE2	5:A:1133:HOH:O	2.22	0.68
1:A:165:SER:O	1:A:168:PRO:HD2	1.94	0.68
1:A:215:LYS:N	1:A:216:PRO:HD2	2.10	0.67
1:A:153:GLU:HA	1:A:156:THR:HG23	1.75	0.66
1:A:77:LEU:HD21	3:A:1104:D12:H91	1.78	0.66
1:A:62:GLU:O	1:A:66:LEU:HD22	1.97	0.64
1:A:206:VAL:HG22	1:A:249:THR:HG22	1.81	0.63
1:A:76:GLY:HA3	3:A:1104:D12:H121	1.81	0.62
1:A:1059:ASP:O	1:A:1060:TRP:HB2	1.98	0.62
1:A:175:LEU:O	1:A:179:LYS:HG2	1.98	0.62
1:A:1060:TRP:CE2	1:A:117:ALA:HB2	2.35	0.61
1:A:129:THR:HG22	1:A:129:THR:O	1.99	0.61
1:A:1060:TRP:CD2	1:A:117:ALA:HB2	2.36	0.60
1:A:209:VAL:HG21	1:A:219:VAL:HG21	1.83	0.60
1:A:218:TRP:HH2	1:A:222:MET:HE3	1.67	0.59
1:A:188:PRO:HB3	1:A:212:PHE:HB3	1.86	0.58
1:A:204:GLN:HE21	1:A:249:THR:HB	1.69	0.57
1:A:1095:TRP:CH2	1:A:1097:ARG:HG2	2.39	0.57
1:A:220:MET:HG2	1:A:222:MET:HE2	1.85	0.56
1:A:220:MET:CG	1:A:222:MET:HE2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:CD2	3:A:1104:D12:H91	2.36	0.56
1:A:218:TRP:CH2	1:A:222:MET:HE3	2.41	0.55
1:A:182:VAL:HG22	1:A:183:HIS:HB3	1.88	0.55
1:A:92:TYR:N	1:A:93:PRO:HD3	2.21	0.55
1:A:1001:ILE:HG23	1:A:1002:GLN:N	2.23	0.53
1:A:77:LEU:O	1:A:81:ILE:HG12	2.08	0.53
1:A:161:ASN:O	1:A:165:SER:HB3	2.09	0.52
1:A:209:VAL:HG21	1:A:219:VAL:CG2	2.40	0.52
1:A:92:TYR:H	1:A:93:PRO:HD3	1.76	0.51
1:A:77:LEU:HD22	3:A:1104:D12:H123	1.92	0.51
1:A:182:VAL:HG13	1:A:183:HIS:CG	2.45	0.50
1:A:215:LYS:N	1:A:216:PRO:CD	2.75	0.50
1:A:218:TRP:HH2	1:A:222:MET:CE	2.24	0.49
1:A:76:GLY:HA3	3:A:1104:D12:C12	2.42	0.49
1:A:144:VAL:O	1:A:148:LEU:HD13	2.13	0.49
1:A:205:LEU:HB3	1:A:221:TRP:CZ2	2.47	0.49
1:A:8:VAL:HG21	1:A:175:LEU:HD21	1.94	0.49
1:A:13:ILE:O	1:A:28:GLY:HA2	2.13	0.48
1:A:83:ASP:O	1:A:84:HIS:HB3	2.14	0.48
1:A:1027:VAL:O	1:A:1063:TYR:HA	2.14	0.48
1:A:1015:ALA:HB1	1:A:1097:ARG:HD3	1.95	0.47
1:A:130:THR:O	1:A:132:VAL:HG23	2.15	0.47
1:A:154:GLY:HA2	1:A:157:GLU:HB2	1.97	0.47
1:A:190:ALA:HA	1:A:208:HIS:O	2.14	0.47
1:A:1099:MET:HA	1:A:195:GLY:HA2	1.97	0.46
1:A:73:TYR:CE1	3:A:1104:D12:H91	2.51	0.46
1:A:1055:SER:HB3	1:A:1063:TYR:CZ	2.51	0.46
1:A:160:TYR:O	1:A:164:ARG:HG2	2.16	0.45
1:A:1000:PRO:HA	1:A:1001:ILE:HA	1.76	0.45
1:A:77:LEU:CD2	3:A:1104:D12:H123	2.47	0.45
1:A:140:LEU:O	1:A:144:VAL:HG12	2.17	0.45
1:A:114:PHE:CD2	1:A:114:PHE:C	2.95	0.45
1:A:114:PHE:HE1	4:A:1105:MK0:HBDA	1.81	0.44
1:A:162:LEU:HG	4:A:1105:MK0:HBH	1.99	0.44
1:A:1012:ARG:HH12	1:A:241:GLN:HG2	1.82	0.44
1:A:220:MET:HG3	1:A:221:TRP:N	2.33	0.44
1:A:77:LEU:HD11	3:A:1104:D12:H32	2.00	0.44
1:A:174:LEU:HD12	1:A:174:LEU:HA	1.83	0.43
1:A:126:PHE:CZ	1:A:129:THR:HA	2.53	0.43
1:A:266:HIS:CD2	5:A:1130:HOH:O	2.72	0.43
1:A:1059:ASP:O	1:A:1060:TRP:CB	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LEU:HD12	1:A:162:LEU:HA	1.87	0.42
1:A:197:SER:HA	1:A:198:PRO:HD3	1.88	0.42
1:A:1004:THR:O	1:A:1004:THR:CG2	2.66	0.42
1:A:127:GLN:O	1:A:128:GLN:C	2.63	0.42
1:A:145:CYS:O	1:A:149:ASN:HB2	2.19	0.42
1:A:167:CYS:HB3	1:A:168:PRO:HD3	2.01	0.42
1:A:211:GLY:HA2	1:A:243:THR:OG1	2.20	0.42
1:A:137:CYS:HA	1:A:138:GLY:HA3	1.53	0.42
1:A:40:TRP:HB2	4:A:1105:MK0:HAQA	2.01	0.42
1:A:1096:ASP:O	1:A:1097:ARG:C	2.63	0.42
1:A:1036:GLU:O	1:A:1082:VAL:HA	2.20	0.41
1:A:264:VAL:HB	1:A:274:ILE:HB	2.02	0.41
1:A:8:VAL:HG12	1:A:9:SER:N	2.35	0.41
1:A:83:ASP:O	1:A:84:HIS:CB	2.68	0.41
1:A:171:LEU:HD12	1:A:171:LEU:O	2.20	0.41
4:A:1105:MK0:HBE	4:A:1105:MK0:HBP	1.94	0.40
1:A:153:GLU:HA	1:A:156:THR:CG2	2.46	0.40
4:A:1105:MK0:HACA	4:A:1105:MK0:HARA	1.90	0.40
1:A:40:TRP:CZ2	1:A:45:GLY:HA2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	370/397 (93%)	349 (94%)	19 (5%)	2 (0%)	24 43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1102	GLY
1	A	92	TYR

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	327/339 (96%)	300 (92%)	27 (8%)	10	22

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1001	ILE
1	A	1004	THR
1	A	1019	LYS
1	A	1031	HIS
1	A	1047	GLU
1	A	1088	SER
1	A	1093	VAL
1	A	19	VAL
1	A	23	TRP
1	A	66	LEU
1	A	68	LEU
1	A	137	CYS
1	A	139	SER
1	A	146	HIS
1	A	151	GLN
1	A	156	THR
1	A	162	LEU
1	A	174	LEU
1	A	175	LEU
1	A	176	ASP
1	A	182	VAL
1	A	183	HIS
1	A	194	SER
1	A	205	LEU
1	A	233	LEU
1	A	254	ASP
1	A	270	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1031	HIS
1	A	57	GLN
1	A	105	HIS
1	A	115	GLN
1	A	150	HIS
1	A	161	ASN
1	A	204	GLN
1	A	228	GLN
1	A	232	GLN
1	A	241	GLN

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](#)

3 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	$\# Z > 2$
4	MK0	A	1105	-	47,48,48	0.58	1 (2%)	60,61,61	1.52	11 (18%)
2	NAG	A	1	1	14,14,15	0.70	0	17,19,21	2.14	3 (17%)
3	D12	A	1104	-	11,11,11	0.31	0	10,10,10	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MK0	A	1105	-	-	19/46/66/66	0/1/1/1
2	NAG	A	1	1	-	1/6/23/26	0/1/1/1
3	D12	A	1104	-	-	2/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1105	MK0	PBV-O1	2.37	1.66	1.59

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAG	C2-N2-C7	6.34	131.40	122.90
4	A	1105	MK0	C4-C3-C2	4.39	118.54	110.83
4	A	1105	MK0	C3-C4-C5	4.03	117.54	110.23
2	A	1	NAG	O5-C1-C2	-4.00	105.11	111.29
4	A	1105	MK0	CAV-CBH-CBP	-3.31	104.96	115.97
4	A	1105	MK0	CAS-CBA-CBL	3.24	126.73	115.97
4	A	1105	MK0	PBV-OBI-CAX	-2.88	107.54	121.26
4	A	1105	MK0	C1-C2-C3	2.72	115.73	110.01
4	A	1105	MK0	O5-C5-C4	2.69	114.55	109.70
4	A	1105	MK0	C1-O5-C5	2.54	118.68	113.72
4	A	1105	MK0	OBI-CAX-CAR	2.47	118.04	109.28
4	A	1105	MK0	CAT-CBD-CBO	-2.38	108.06	115.97
2	A	1	NAG	O7-C7-N2	2.37	126.17	121.98
4	A	1105	MK0	O1-C1-C2	2.09	112.21	108.38

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	NAG	C3-C2-N2-C7
4	A	1105	MK0	CAX-OBI-PBV-O1
4	A	1105	MK0	CAX-OBI-PBV-OAG
4	A	1105	MK0	CAQ-CAY-CBL-CAB
4	A	1105	MK0	CAX-CAR-CAZ-CBM
4	A	1105	MK0	CBD-CAT-CBB-CBM

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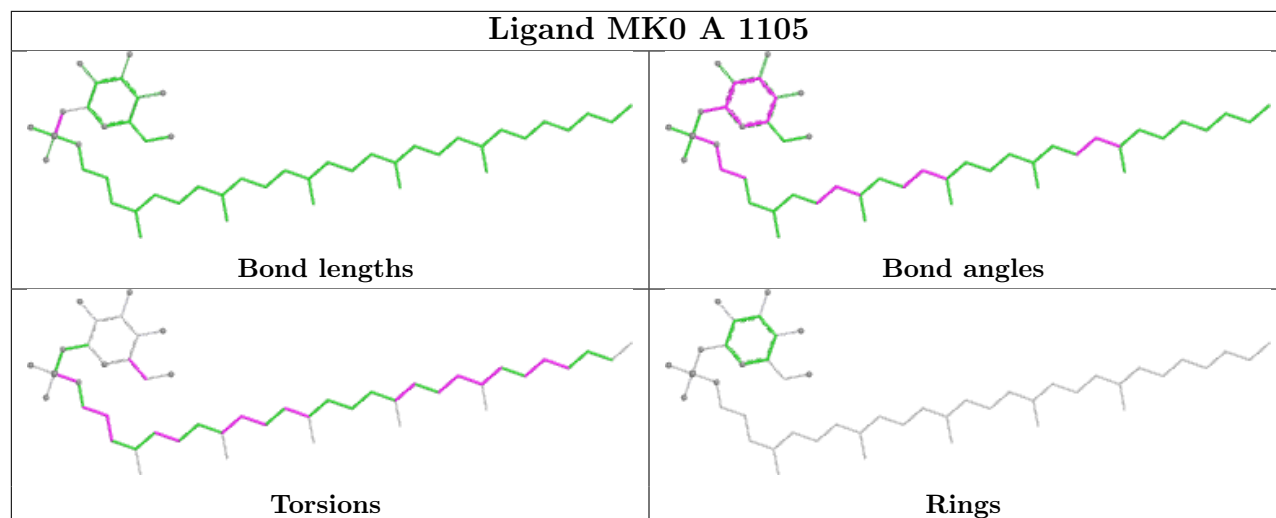
Mol	Chain	Res	Type	Atoms
4	A	1105	MK0	CAN-CAO-CAP-CAQ
3	A	1104	D12	C3-C4-C5-C6
4	A	1105	MK0	CBH-CAV-CBF-CBO
4	A	1105	MK0	CAZ-CAR-CAX-OBI
4	A	1105	MK0	O5-C5-C6-O6
4	A	1105	MK0	CBC-CAS-CBA-CBL
4	A	1105	MK0	CAV-CBH-CBP-CBG
4	A	1105	MK0	CAV-CBH-CBP-CAF
3	A	1104	D12	C9-C10-C11-C12
4	A	1105	MK0	CAX-OBI-PBV-OAL
4	A	1105	MK0	CAS-CBC-CBN-CBE
4	A	1105	MK0	CAS-CBC-CBN-CAD
4	A	1105	MK0	CAV-CBF-CBO-CBD
4	A	1105	MK0	CAS-CBA-CBL-CAB
4	A	1105	MK0	CAO-CAP-CAQ-CAY
4	A	1105	MK0	CAS-CBA-CBL-CAY

There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1105	MK0	10	0
3	A	1104	D12	10	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

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	376/397 (94%)	0.64	39 (10%)	11 10	21, 50, 81, 114	46 (12%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	VAL	6.5
1	A	183	HIS	5.9
1	A	146	HIS	5.2
1	A	152	TYR	4.8
1	A	137	CYS	4.3
1	A	92	TYR	4.3
1	A	1001	ILE	4.1
1	A	180	MET	3.8
1	A	185	GLN	3.7
1	A	164	ARG	3.5
1	A	1102	GLY	3.4
1	A	136	GLY	3.3
1	A	21	GLN	3.1
1	A	59	SER	3.1
1	A	43	GLU	2.8
1	A	91	LYS	2.8
1	A	150	HIS	2.6
1	A	83	ASP	2.6
1	A	140	LEU	2.5
1	A	216	PRO	2.5
1	A	22	SER	2.5
1	A	129	THR	2.4
1	A	153	GLU	2.4
1	A	179	LYS	2.4
1	A	82	GLN	2.4
1	A	1101	GLY	2.3
1	A	101	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	77	LEU	2.3
1	A	113	PHE	2.2
1	A	90	SER	2.2
1	A	270	GLU	2.2
1	A	72	PHE	2.2
1	A	181	TYR	2.2
1	A	18	PHE	2.2
1	A	19	VAL	2.1
1	A	84	HIS	2.1
1	A	111	GLU	2.1
1	A	215	LYS	2.0
1	A	11	HIS	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](#)

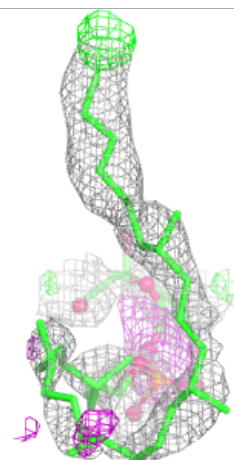
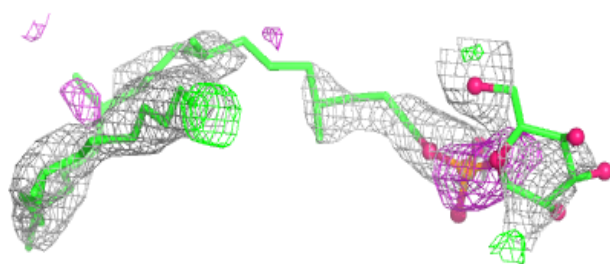
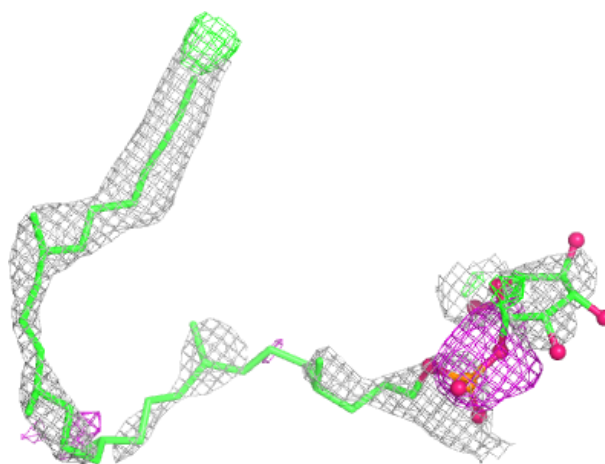
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	NAG	A	1	14/15	0.26	0.23	101,111,114,115	0
4	MK0	A	1105	48/48	0.73	0.20	42,67,114,120	0
3	D12	A	1104	12/12	0.77	0.24	66,72,80,84	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 MK0 A 1105:

$2mF_o-DF_c$ (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.