



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 2, 2024 – 07:18 PM EST

PDB ID : 4ONO
Title : CD1c in complex with PM (phosphomycoketide)
Authors : Roy, S.; Adams, E.J.
Deposited on : 2014-01-28
Resolution : 2.71 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.21
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

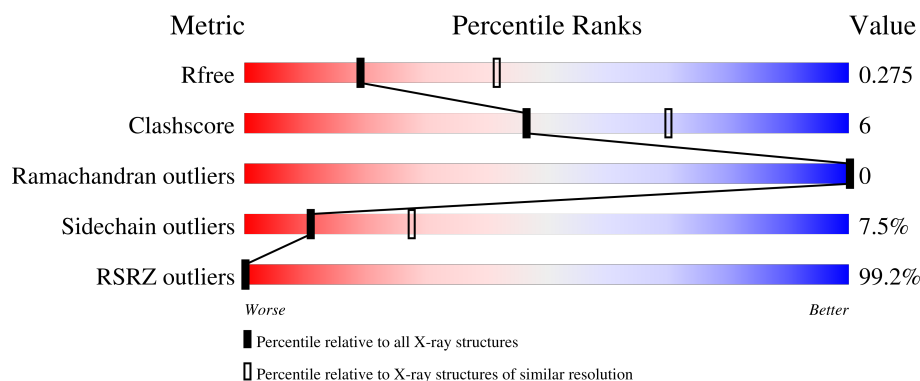
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	395	<div> <div>92%</div> <div>81%</div> <div>12%</div> <div>5%</div> </div>
2	B	2	<div> <div>50%</div> <div>50%</div> </div>

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
2	NAG	B	1	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5909 atoms, of which 2840 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 chimeric protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	374	Total	C	H	N	O	S	539	0	0
			5738	1896	2769	509	552	12			

There are 29 discrepancies between the modelled and reference sequences:

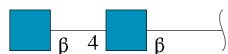
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	PRO	-	expression tag	UNP P61769
A	100	GLY	-	linker	UNP P29017
A	101	GLY	-	linker	UNP P29017
A	102	GLY	-	linker	UNP P29017
A	103	GLY	-	linker	UNP P29017
A	105	SER	-	linker	UNP P29017
A	106	GLY	-	linker	UNP P29017
A	107	GLY	-	linker	UNP P29017
A	108	SER	-	linker	UNP P29017
A	109	GLY	-	linker	UNP P29017
A	110	SER	-	linker	UNP P29017
A	111	GLY	-	linker	UNP P29017
A	112	GLY	-	linker	UNP P29017
A	113	GLY	-	linker	UNP P29017
A	114	SER	-	linker	UNP P29017
A	115	SER	-	linker	UNP P29017
A	116	ALA	-	linker	UNP P29017
A	117	ASP	-	linker	UNP P29017
A	118	ALA	-	linker	UNP P29017
A	119	SER	-	linker	UNP P29017
A	120	GLN	-	linker	UNP P29017
A	167	GLN	ASN	engineered mutation	UNP P29017
A	172	GLN	ASN	engineered mutation	UNP P29017
A	223	GLY	LYS	engineered mutation	UNP P29017
A	243	GLN	ASN	engineered mutation	UNP P29017
A	356	GLN	ASN	engineered mutation	UNP P29016

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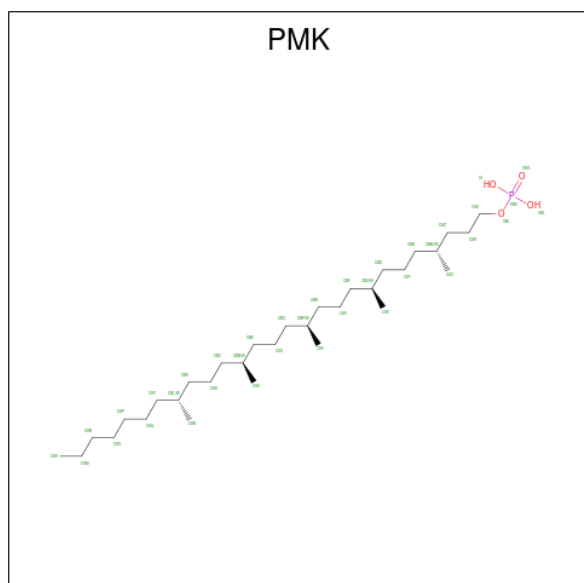
Chain	Residue	Modelled	Actual	Comment	Reference
A	357	GLY	TRP	engineered mutation	UNP P29016
A	394	HIS	ARG	expression tag	UNP P29016
A	395	HIS	ASN	expression tag	UNP P29016

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is (4R,8S,16S,20R)-4,8,12,16,20-pentamethylheptacosyl dihydrogen phosphate (three-letter code: PMK) (formula: C₃₂H₆₇O₄P).

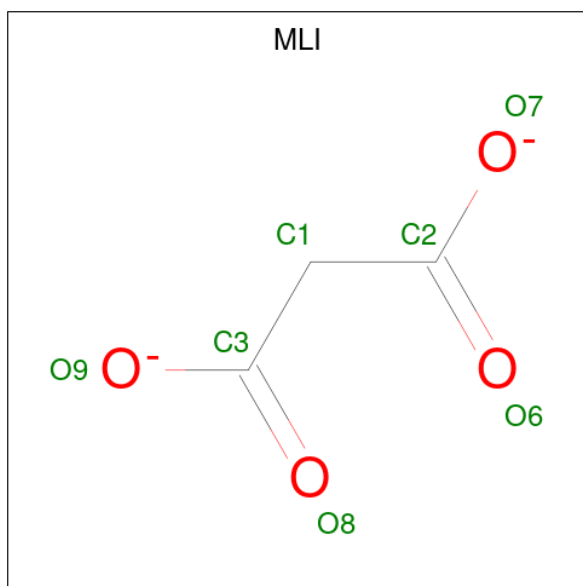


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	O	P	30	0
			102	32	65	4	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 9 3 2 4	0	0
5	A	1	Total C H O 9 3 2 4	0	0
5	A	1	Total C H O 9 3 2 4	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	8	Total O 8 8	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.31Å 86.98Å 89.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.55 – 2.71 34.55 – 2.71	Depositor EDS
% Data completeness (in resolution range)	96.2 (34.55-2.71) 95.5 (34.55-2.71)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.219 , 0.271 0.226 , 0.275	Depositor DCC
R_{free} test set	556 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.51 , 396.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o, F_c correlation	0.46	EDS
Total number of atoms	5909	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.71% 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: MLI, CL, NAG, PMK

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	0.27	0/3058	0.48	0/4153

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	2969	2769	2786	22	0
2	B	28	0	25	7	0
3	A	37	65	67	3	0
4	A	6	0	0	1	0
5	A	21	6	6	0	0
6	A	8	0	0	1	0
All	All	3069	2840	2884	30	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 6.

The worst 5 of 30 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:228:PHE:N	1:A:278:ILE:HD11	1.83	0.94
2:B:1:NAG:C8	2:B:1:NAG:H3	2.03	0.88
2:B:1:NAG:H83	2:B:1:NAG:C3	2.10	0.80
2:B:1:NAG:C8	2:B:1:NAG:C3	2.61	0.78
2:B:1:NAG:H3	2:B:1:NAG:H83	1.64	0.76

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	368/395 (93%)	354 (96%)	14 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	318/338 (94%)	294 (92%)	24 (8%)	11	28

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	LEU
1	A	298	HIS

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Mol	Chain	Res	Type
1	A	291	ASP
1	A	320	LEU
1	A	126	HIS

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

Mol	Chain	Res	Type
1	A	31	HIS

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 ⓘ

2 monosaccharides 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	$\# Z > 2$
2	NAG	B	1	2,1	14,14,15	0.41	0	17,19,21	1.79	2 (11%)
2	NAG	B	2	2	14,14,15	0.34	0	17,19,21	0.47	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
2	NAG	B	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C2-N2-C7	4.46	128.88	122.90
2	B	1	NAG	C1-O5-C5	3.92	117.44	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

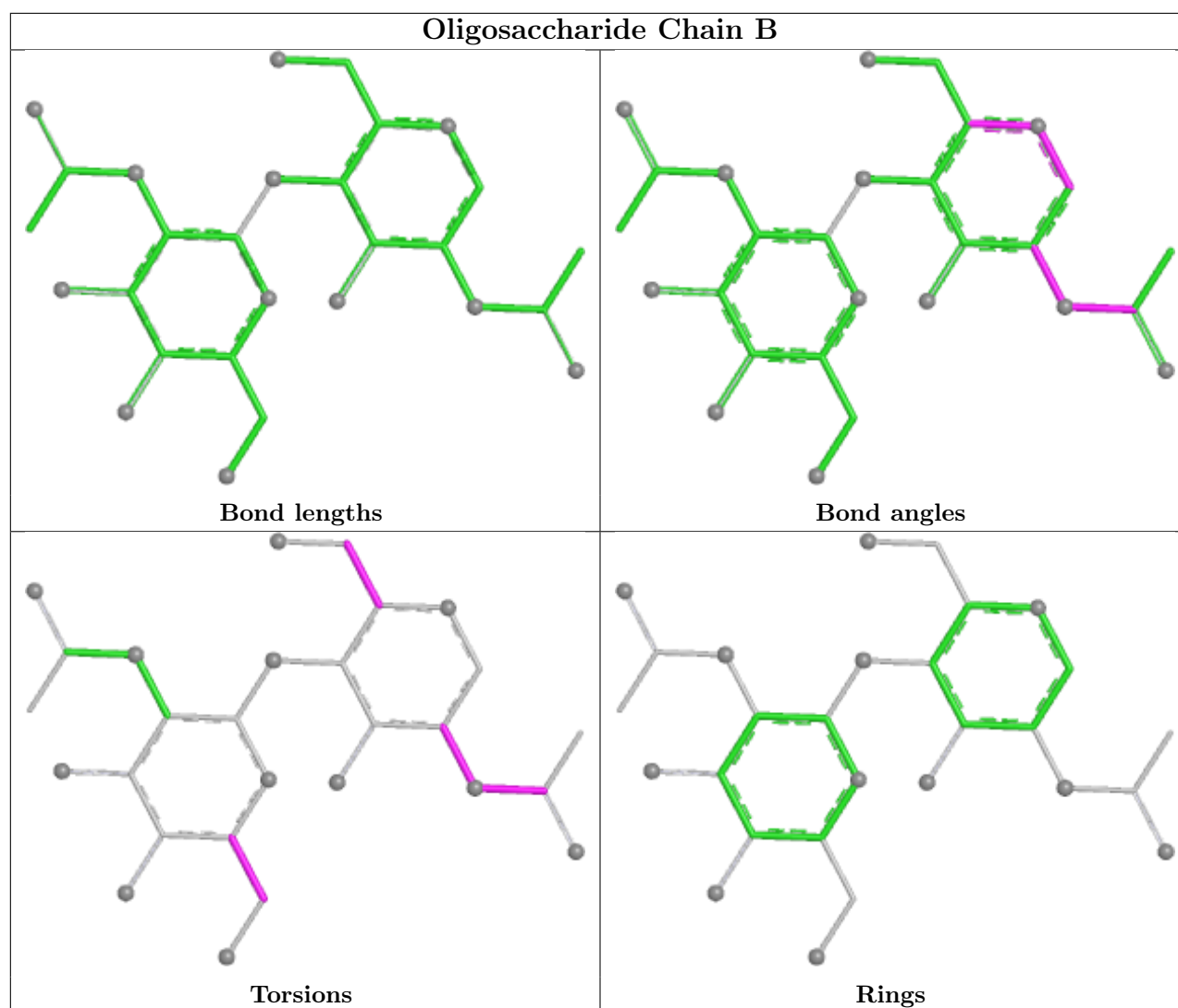
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C3-C2-N2-C7
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are 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	$\# Z > 2$
3	PMK	A	401	-	36,36,36	0.71	0	43,43,43	1.32	5 (11%)
5	MLI	A	409	-	6,6,6	1.09	0	7,7,7	1.32	0
5	MLI	A	410	-	6,6,6	1.19	0	7,7,7	1.36	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MLI	A	408	-	6,6,6	1.23	0	7,7,7	1.24	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
3	PMK	A	401	-	-	16/39/39/39	-
5	MLI	A	409	-	-	0/4/4/4	-
5	MLI	A	410	-	-	2/4/4/4	-
5	MLI	A	408	-	-	2/4/4/4	-

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	PMK	OAL-PBV-OB1	3.29	115.23	106.67
3	A	401	PMK	OB1-PBV-OAG	2.97	114.48	106.44
3	A	401	PMK	O1-PBV-OB1	2.77	113.90	106.67
3	A	401	PMK	CAU-CBE-CBN	-2.58	107.39	115.97
3	A	401	PMK	CAU-CBG-CBP	-2.42	107.92	115.97

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	PMK	CAS-CBA-CBL-CAB
3	A	401	PMK	CAV-CBF-CBO-CAE
3	A	401	PMK	CBD-CAT-CBB-CBM
3	A	401	PMK	CBC-CAS-CBA-CBL
3	A	401	PMK	CAN-CAO-CAP-CAQ

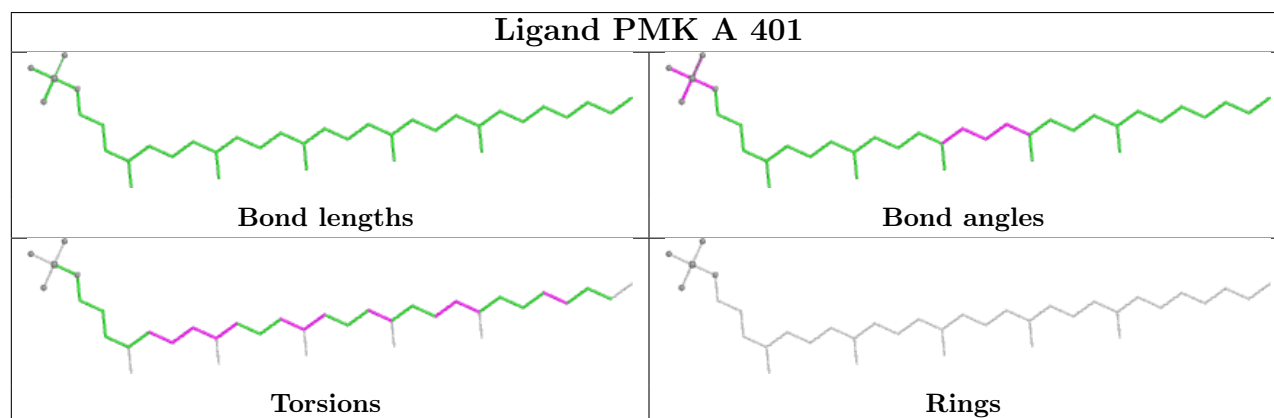
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	PMK	3	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](#)

Warning: The R factor obtained from EDS is 0.5295, which does not match the depositor's R factor of 0.2188. Please interpret the results in this section carefully.

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	367/395 (92%)	9.22	364 (99%) 0 0	11, 53, 92, 138	59 (16%)

The worst 5 of 364 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	GLN	27.7
1	A	263	LEU	26.5
1	A	297	VAL	25.8
1	A	272	GLU	25.7
1	A	257	GLN	25.3

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

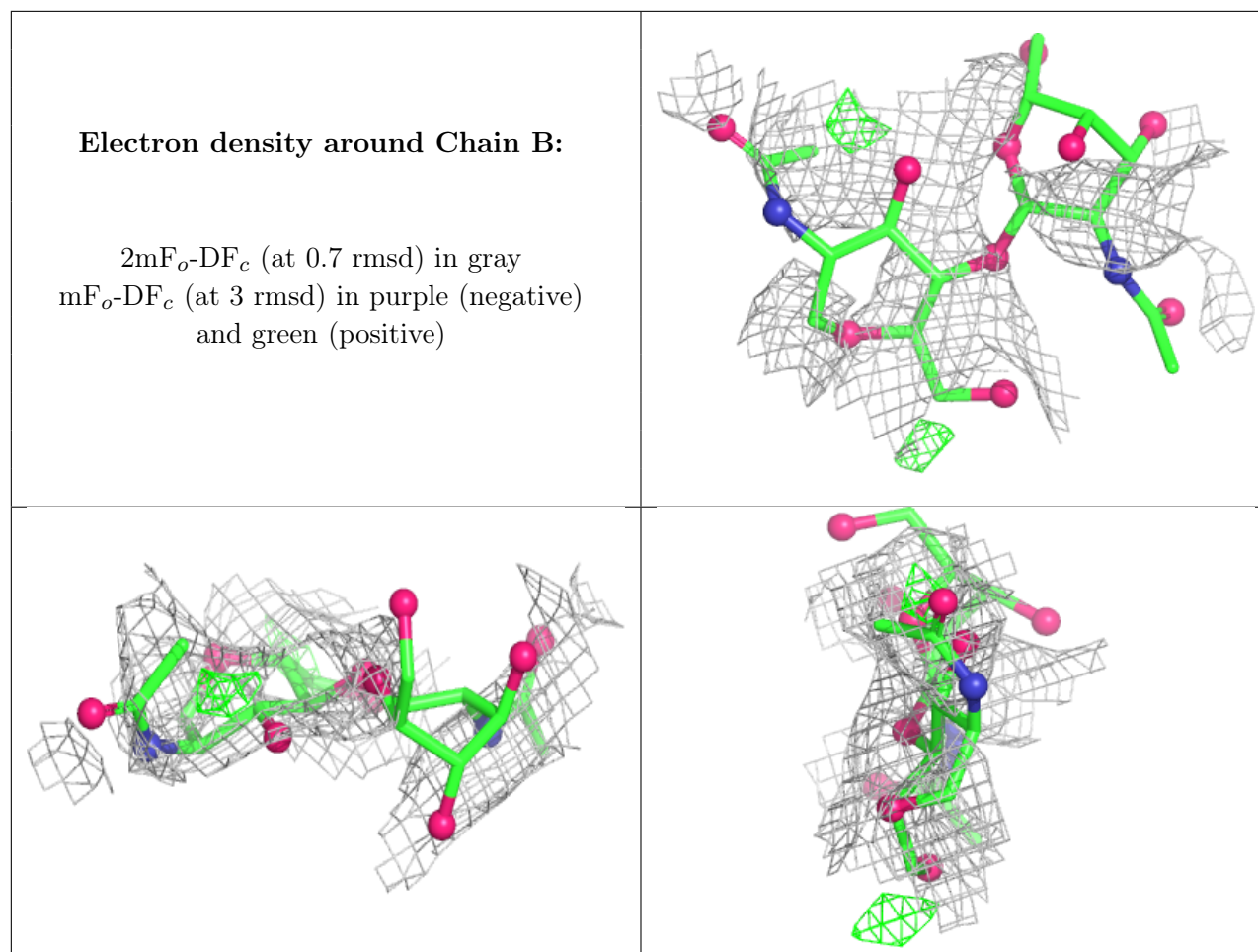
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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
2	NAG	B	1	14/15	0.51	0.82	89,102,111,116	0
2	NAG	B	2	14/15	0.57	0.85	92,107,111,115	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

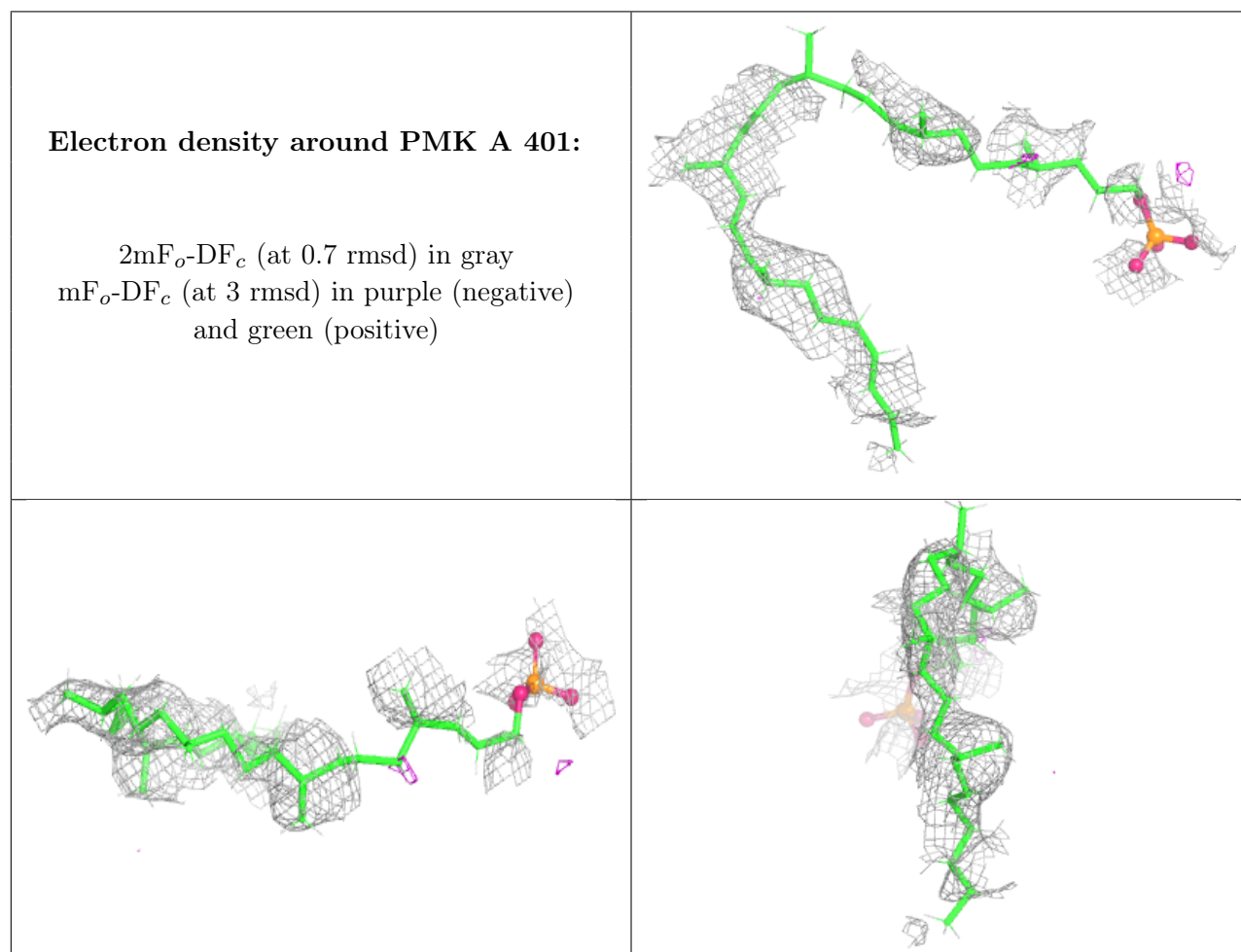


6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
4	CL	A	405	1/1	0.26	0.52	75,75,75,75	0
4	CL	A	402	1/1	0.29	0.37	71,71,71,71	0
5	MLI	A	408	7/7	0.42	0.59	41,62,75,75	0
3	PMK	A	401	37/37	0.44	0.35	50,73,103,119	30
4	CL	A	406	1/1	0.59	0.50	70,70,70,70	0
5	MLI	A	410	7/7	0.60	0.53	57,66,78,78	0
4	CL	A	403	1/1	0.73	0.22	47,47,47,47	0
5	MLI	A	409	7/7	0.75	0.40	63,69,81,81	0
4	CL	A	407	1/1	0.77	0.29	63,63,63,63	0
4	CL	A	404	1/1	0.80	0.20	75,75,75,75	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.