

wwPDB X-ray Structure Validation Summary Report (i)

Sep 3, 2023 – 04:16 AM EDT

PDB ID : 3RLF

Title: Crystal structure of the maltose-binding protein/maltose transporter complex

in an outward-facing conformation bound to MgAMPPNP

Authors : Oldham, M.L.; Chen, J.

Deposited on : 2011-04-19

Resolution : 2.20 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 (i) 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 (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.35

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

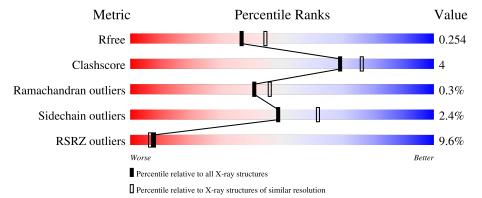
Validation Pipeline (wwPDB-VP) : 2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \ resolution} \\ (\#{\rm Entries, \ resolution \ range(\AA)}) \end{array}$
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	
			12%	
1	\mathbf{E}	380	89%	9% •
			14%	
2	F	514	86%	8% • 5%
			6%	
3	G	296	90%	6% • •
			4%	
4	A	381	86%	11% • •
			8%	
4	В	381	85%	11% • •



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Mol	Chain	Length	Quality of chain
5	С	2	100%



2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 15268 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 Maltose-binding periplasmic protein.

\mathbf{Mol}	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	E	374	Total 2914	C 1875	N 476	O 557	S 6	0	2	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	371	ALA	-	expression tag	UNP P0AEX9
E	372	SER	-	expression tag	UNP P0AEX9
E	373	ALA	-	expression tag	UNP P0AEX9
E	374	SER	-	expression tag	UNP P0AEX9
E	375	HIS	-	expression tag	UNP P0AEX9
E	376	HIS	_	expression tag	UNP P0AEX9
E	377	HIS	-	expression tag	UNP P0AEX9
E	378	HIS	-	expression tag	UNP P0AEX9
E	379	HIS	-	expression tag	UNP P0AEX9
E	380	HIS	-	expression tag	UNP P0AEX9

• Molecule 2 is a protein called Maltose transport system permease protein malF.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	F	490	Total 3832	C 2517	N 612	O 686	S 17	0	1	0

• Molecule 3 is a protein called Maltose transport system permease protein malG.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
3	G	286	Total 2214	C 1484	N 352	O 370	S 8	0	2	0

• Molecule 4 is a protein called Maltose/maltodextrin import ATP-binding protein MalK.



\mathbf{Mol}	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	371	Total 2876	C 1819	- 1	O 529	S 13	0	0	0
4	В	371	Total 2881	C 1822	- 1	O 531	S 13	0	1	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	372	ALA	-	expression tag	UNP P68187
A	373	SER	-	expression tag	UNP P68187
A	374	ALA	-	expression tag	UNP P68187
A	375	SER	-	expression tag	UNP P68187
A	376	HIS	-	expression tag	UNP P68187
A	377	HIS	-	expression tag	UNP P68187
A	378	HIS	-	expression tag	UNP P68187
A	379	HIS	-	expression tag	UNP P68187
A	380	HIS	-	expression tag	UNP P68187
A	381	HIS	-	expression tag	UNP P68187
В	372	ALA	-	expression tag	UNP P68187
В	373	SER	-	expression tag	UNP P68187
В	374	ALA	-	expression tag	UNP P68187
В	375	SER	-	expression tag	UNP P68187
В	376	HIS	-	expression tag	UNP P68187
В	377	HIS	-	expression tag	UNP P68187
В	378	HIS	-	expression tag	UNP P68187
В	379	HIS	-	expression tag	UNP P68187
В	380	HIS		expression tag	UNP P68187
В	381	HIS	-	expression tag	UNP P68187

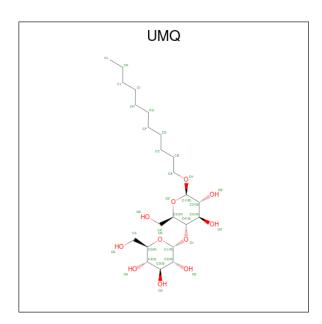
 $\bullet \ \ {\rm Molecule} \ 5 \ {\rm is \ an \ oligosaccharide \ called \ alpha-D-glucopyranose.} \\ (1-4)-{\rm alpha-D-glucopyranose.}$



Mol	Chain	Residues	At	oms		ZeroOcc	AltConf	Trace
5	С	2	Total 23	C 12	O 11	0	0	0

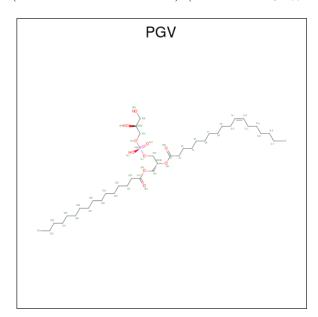
 \bullet Molecule 6 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $\mathrm{C}_{23}\mathrm{H}_{44}\mathrm{O}_{11}).$





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	Е	1	Total 34	C 23	O 11	0	0

• Molecule 7 is (1R)-2-{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHO RYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	Total C O P 51 40 10 1	0	0
7	F	1	Total C 14 14	0	0



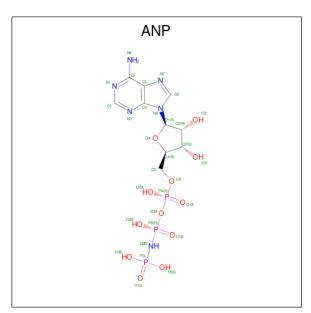
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	1	Total C 14 14	0	0
7	G	1	Total C 12 12	0	0

• Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Mg 1 1	0	0
8	В	1	Total Mg 1 1	0	0

• Molecule 9 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf			
0	٨	1	Total	С	N	О	Р	0	0	
9	A	1	31	10	6	12	3	U	0	
0	D	1	Total	С	N	О	Р	0	0	
9	Б	1	31	10	6	12	3	U	0	

• Molecule 10 is water.



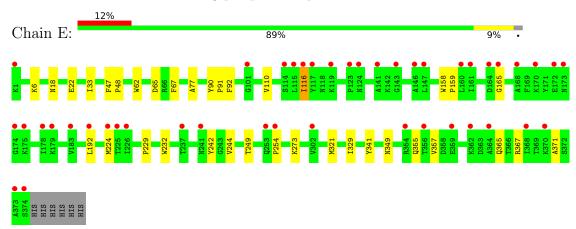
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	E	62	Total O 62 62	0	0
10	F	63	Total O 63 63	0	0
10	G	59	Total O 59 59	0	0
10	A	81	Total O 81 81	0	0
10	В	74	Total O 74 74	0	0



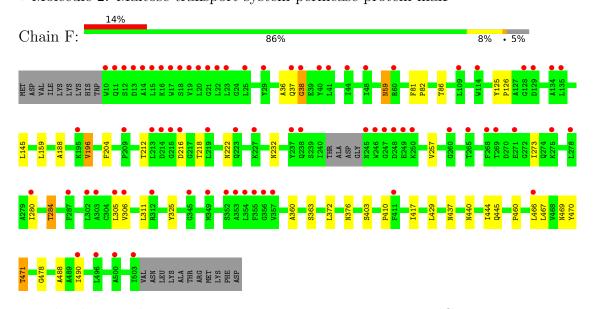
3 Residue-property plots (i)

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: Maltose-binding periplasmic protein



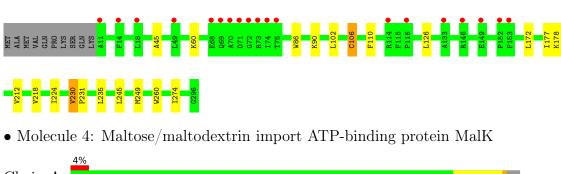
• Molecule 2: Maltose transport system permease protein malF

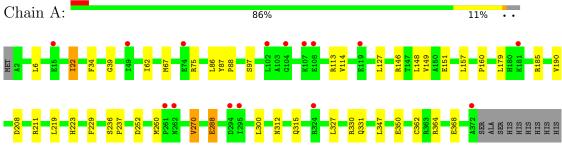


• Molecule 3: Maltose transport system permease protein malG

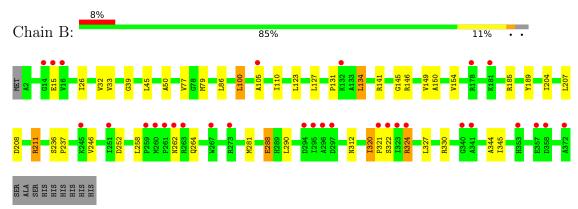








 \bullet Molecule 4: Maltose/maltodextrin import ATP-binding protein MalK



• Molecule 5: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C:

GLC1 GLC2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	72.10Å 95.81Å 109.98Å	Donogitor
a, b, c, α , β , γ	86.70° 82.68° 76.40°	Depositor
Resolution (Å)	20.00 - 2.20	Depositor
rtesolution (A)	19.97 - 2.20	EDS
% Data completeness	86.3 (20.00-2.20)	Depositor
(in resolution range)	86.3 (19.97-2.20)	EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.17 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
P. P.	0.223 , 0.254	Depositor
R, R_{free}	0.223 , 0.254	DCC
R_{free} test set	6209 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.39, 56.1	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15268	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 3.87% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: UMQ, ANP, GLC, MG, PGV

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	
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	Е	0.34	0/2983	0.46	0/4048
2	F	0.36	0/3927	0.50	0/5344
3	G	0.37	0/2278	0.49	0/3115
4	A	0.34	0/2926	0.53	1/3968 (0.0%)
4	В	0.35	0/2932	0.53	0/3974
All	All	0.35	0/15046	0.50	1/20449~(0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
4	A	347	LEU	CA-CB-CG	5.08	126.98	115.30

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	Е	2914	0	2888	19	0
2	F	3832	0	3861	32	0
3	G	2214	0	2302	11	0
4	A	2876	0	2941	26	0
4	В	2881	0	2942	29	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	С	23	0	21	0	0
6	Ε	34	0	44	0	0
7	F	65	0	100	2	0
7	G	26	0	44	1	0
8	A	1	0	0	0	0
8	В	1	0	0	0	0
9	A	31	0	13	2	0
9	В	31	0	13	2	0
10	A	81	0	0	1	0
10	В	74	0	0	2	0
10	Ε	62	0	0	0	0
10	F	63	0	0	0	0
10	G	59	0	0	0	0
All	All	15268	0	15169	111	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 4.

The worst 5 of 111 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}({ m \AA})$	overlap (Å)
2:F:471:THR:HG21	2:F:490:ILE:HG21	1.42	1.01
4:A:39:GLY:H	9:A:2501:ANP:HNB1	1.16	0.94
4:B:39:GLY:H	9:B:2502:ANP:HNB1	1.18	0.88
4:A:223:HIS:CE1	4:A:368:GLU:HG2	2.12	0.85
4:B:344:ALA:N	4:B:344:ALA:CB	2.45	0.80

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	Perce	ntiles
1	E	374/380 (98%)	364 (97%)	9 (2%)	1 (0%)	41	46
2	F	487/514 (95%)	471 (97%)	14 (3%)	2 (0%)	34	37
3	G	286/296 (97%)	283 (99%)	2 (1%)	1 (0%)	41	46
4	A	369/381 (97%)	360 (98%)	9 (2%)	0	100	100
4	В	369/381 (97%)	360 (98%)	8 (2%)	1 (0%)	41	46
All	All	1885/1952~(97%)	1838 (98%)	42 (2%)	5 (0%)	41	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	37	GLN
2	F	38	GLY
1	Е	165	GLY
4	В	105	ALA
3	G	230	VAL

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	E	299/305~(98%)	295 (99%)	4 (1%)	69 81
2	F	403/424 (95%)	395 (98%)	8 (2%)	55 69
3	G	230/237 (97%)	226 (98%)	4 (2%)	60 74
4	A	314/323 (97%)	305 (97%)	9 (3%)	42 54
4	В	315/323 (98%)	303 (96%)	12 (4%)	33 42
All	All	1561/1612 (97%)	1524 (98%)	37 (2%)	49 62

5 of 37 residues with a non-rotameric sidechain are listed below:

\mathbf{Mol}	Chain	Res	\mathbf{Type}
4	В	127	LEU
4	В	320	ILE
4	В	134	LEU



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Mol	Chain	Res	Type
4	В	252	ASP
3	G	106	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	241	ASN
4	В	180	HIS
2	F	222	ASN
2	F	232	ASN
2	F	437	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

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	Bo	Bond lengths			Bond angles		
IVIOI	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
5	GLC	С	1	5	12,12,12	0.51	0	17,17,17	1.08	1 (5%)	
5	GLC	С	2	5	11,11,12	0.35	0	15,15,17	0.98	1 (6%)	

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.

\mathbf{M}	ol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5)	GLC	С	1	5	-	0/2/22/22	0/1/1/1
5)	GLC	С	2	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
5	С	1	GLC	C1-O5-C5	3.08	119.48	113.66
5	С	2	GLC	C1-O5-C5	2.97	116.21	112.19

There are no chirality outliers.

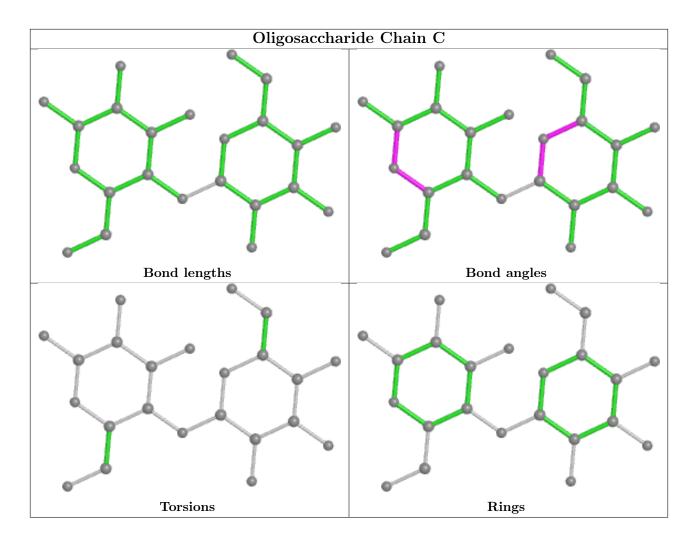
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	ol Type Chain Res		Link	Bo	Bond lengths			Bond angles		
MIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	ANP	A	2501	8	29,33,33	1.88	8 (27%)	31,52,52	2.17	7 (22%)
7	PGV	F	4001	-	50,50,50	1.08	3 (6%)	53,56,56	1.02	3 (5%)
7	PGV	F	4002	-	13,13,50	0.28	0	12,12,56	0.52	0
9	ANP	В	2502	8	29,33,33	1.83	9 (31%)	31,52,52	1.89	6 (19%)
7	PGV	G	4006	-	13,13,50	0.27	0	12,12,56	0.54	0



Mol	True	Chain	Res	Link	Вс	ond leng	ths	Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	UMQ	Е	5004	-	35,35,35	0.44	0	46,46,46	0.84	2 (4%)
7	PGV	G	4009	-	11,11,50	0.27	0	10,10,56	0.53	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
9	ANP	A	2501	8	-	4/14/38/38	0/3/3/3
7	PGV	F	4001	-	-	27/55/55/55	-
7	PGV	F	4002	-	-	9/11/11/55	-
9	ANP	В	2502	8	-	4/14/38/38	0/3/3/3
7	PGV	G	4006	-	-	3/11/11/55	-
6	UMQ	Е	5004	-	-	10/20/60/60	0/2/2/2
7	PGV	G	4009	-	-	7/9/9/55	-

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
9	A	2501	ANP	PB-N3B	4.41	1.74	1.63
7	F	4001	PGV	O03-C19	4.39	1.46	1.33
9	A	2501	ANP	PG-N3B	4.36	1.74	1.63
7	F	4001	PGV	O01-C1	4.29	1.46	1.34
9	В	2502	ANP	PB-N3B	4.25	1.74	1.63

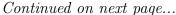
The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
9	A	2501	ANP	O1G-PG-N3B	-7.95	100.06	111.77
9	В	2502	ANP	O1G-PG-N3B	-5.91	103.07	111.77
9	A	2501	ANP	O2B-PB-O1B	4.68	119.74	109.92
7	F	4001	PGV	O01-C1-C2	4.16	120.48	111.50
9	В	2502	ANP	O2B-PB-O1B	4.16	118.64	109.92

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

7 F 4001 PGV C03-O11-P-O12	\mathbf{Mol}	Chain	Res	Type	Atoms
	7	F	4001	PGV	C03-O11-P-O12





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Mol	Chain	Res	Type	Atoms
7	F	4001	PGV	C03-O11-P-O13
7	F	4001	PGV	C03-O11-P-O14
7	F	4001	PGV	C04-C05-C06-O06
7	F	4001	PGV	C2-C1-O01-C02

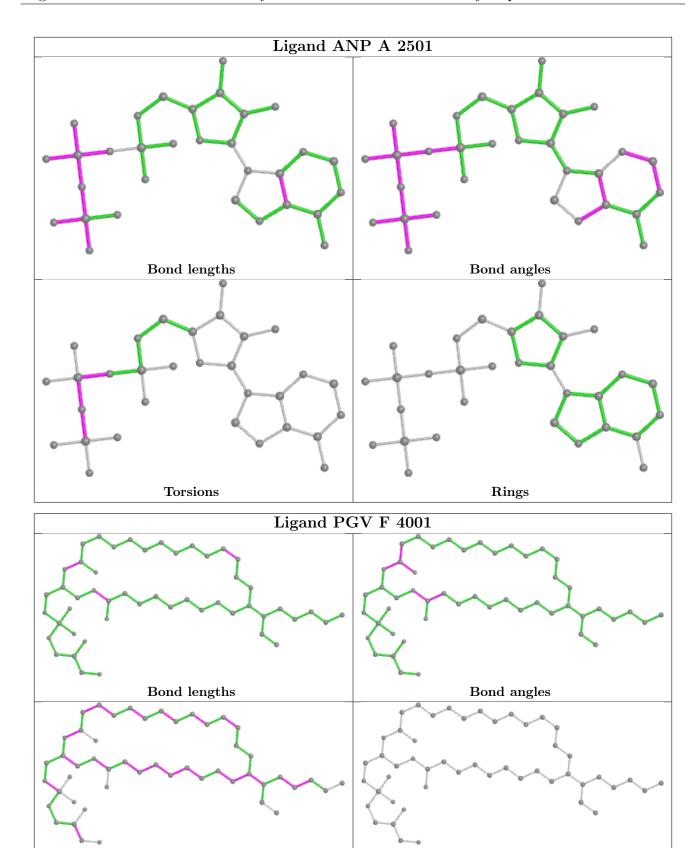
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2501	ANP	2	0
7	F	4001	PGV	2	0
9	В	2502	ANP	2	0
7	G	4006	PGV	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

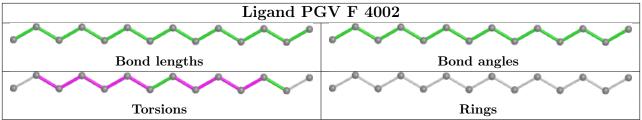


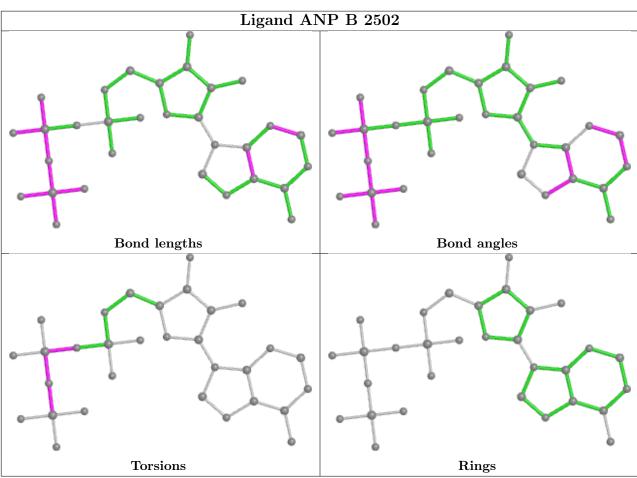


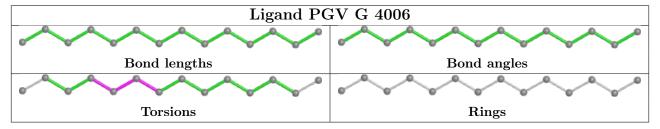


Rings

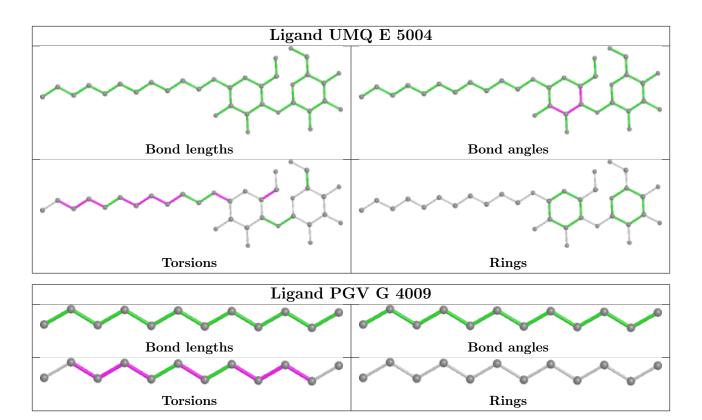
Torsions











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, 95^{th} 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>	$\#\mathrm{RSRZ}{>}2$		Q<0.9
1	E	374/380 (98%)	0.55	44 (11%) 4 4	30, 66, 111, 133	1 (0%)
2	F	490/514 (95%)	0.83	74 (15%) 2 2	32, 61, 127, 188	0
3	G	286/296 (96%)	0.26	19 (6%) 18 17	28, 44, 81, 108	0
4	A	371/381 (97%)	0.18	15 (4%) 38 36	27, 44, 69, 94	0
4	В	371/381 (97%)	0.25	30 (8%) 12 10	25, 46, 84, 112	0
All	All	1892/1952~(96%)	0.45	182 (9%) 8 6	25, 51, 104, 188	1 (0%)

The worst 5 of 182 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	10	TRP	19.4
2	F	37	GLN	11.0
2	F	38	GLY	8.9
2	F	14	ALA	7.6
2	F	29	TYR	7.4

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, 95^{th} 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.

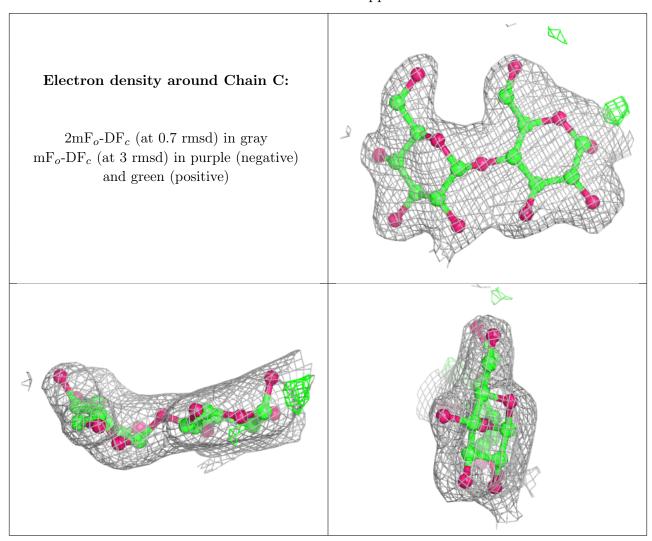
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\mathrm{\AA}^2)$	Q<0.9
5	GLC	С	1	12/12	0.95	0.08	47,49,52,54	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
5	GLC	С	2	11/12	0.95	0.11	46,48,50,51	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 (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, 95^{th} 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.

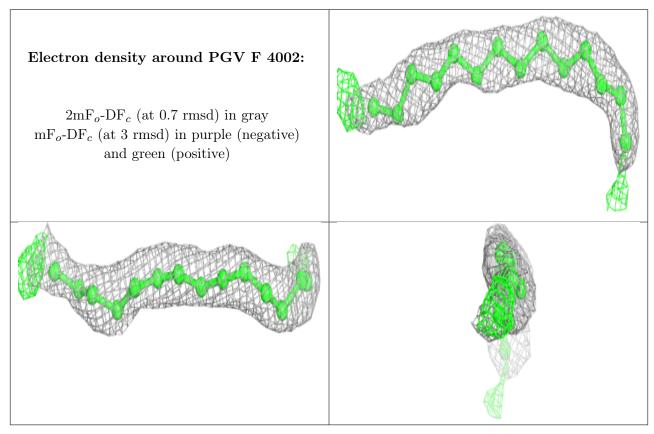
Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B\text{-factors}}({f \AA}^2)$	Q<0.9
7	PGV	F	4002	14/51	0.72	0.25	58,60,65,66	0
7	PGV	G	4009	12/51	0.73	0.23	70,71,74,74	0



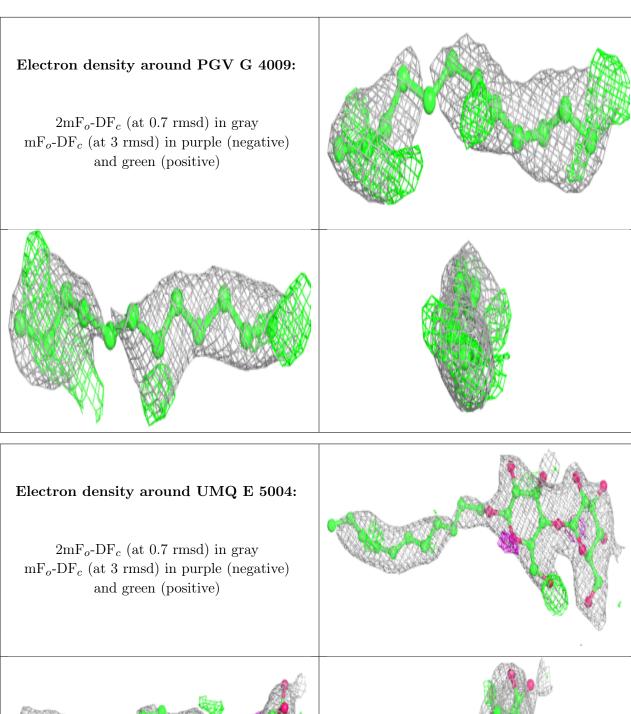
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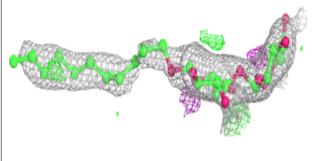
Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B-factors}({f \AA}^2)$	Q<0.9
6	UMQ	Ε	5004	34/34	0.77	0.28	74,80,82,83	0
7	PGV	F	4001	51/51	0.81	0.23	75,83,86,91	0
7	PGV	G	4006	14/51	0.83	0.19	71,75,82,84	0
8	MG	A	1501	1/1	0.98	0.04	28,28,28,28	0
8	MG	В	1502	1/1	0.98	0.11	30,30,30,30	0
9	ANP	A	2501	31/31	0.98	0.09	25,32,41,41	0
9	ANP	В	2502	31/31	0.98	0.10	28,35,41,42	0

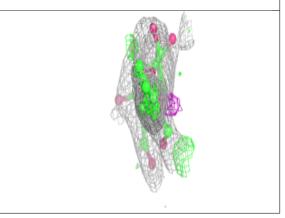
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



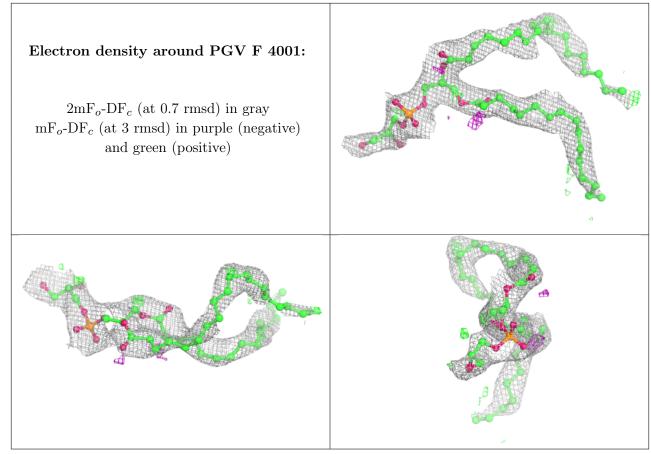


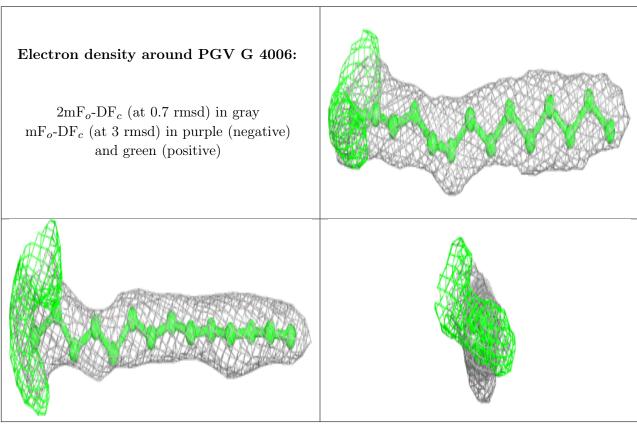








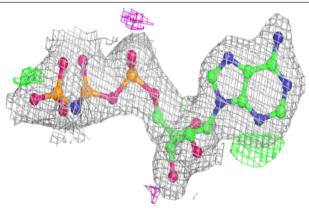


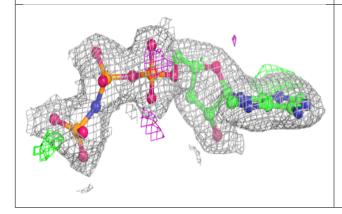


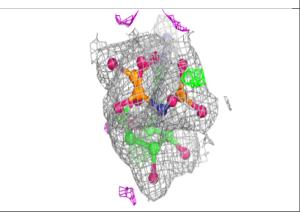


Electron density around ANP A 2501:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

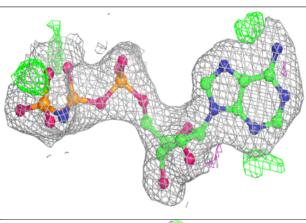


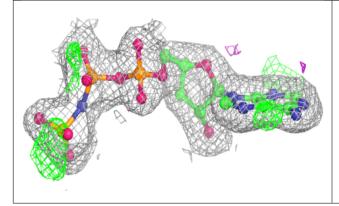


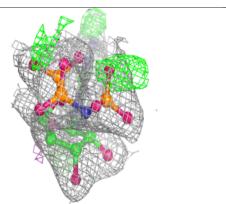


Electron density around ANP B 2502:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)









6.5 Other polymers (i)

There are no such residues in this entry.

