



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:37 PM UTC

PDB ID : 4KHZ / pdb_00004khz
Title : Crystal structure of the maltose-binding protein/maltose transporter complex in an pre-translocation conformation bound to maltoheptaose
Authors : Oldham, M.L.; Chen, S.; Chen, J.
Deposited on : 2013-05-01
Resolution : 2.90 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

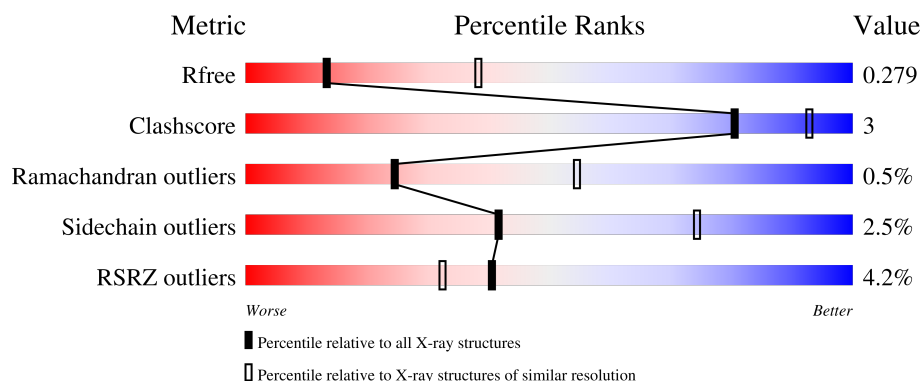
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	E	380	2% 91% 6% • •
2	F	514	6% 87% 6% • 6%
3	G	296	6% 83% 11% • 5%
4	A	381	2% 87% 9% • •
4	B	381	4% 90% 7% •

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Mol	Chain	Length	Quality of chain
5	C	4	75% 25%
6	D	3	33% 33% 33%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14715 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	370	Total	C	N	O	S	0	0	0
			2877	1853	469	549	6			

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	483	Total	C	N	O	S	0	0	0
			3750	2464	597	672	17			

- Molecule 3 is a protein called Binding-protein-dependent transport systems inner membrane component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	282	Total	C	N	O	S	0	0	0
			2182	1461	348	364	9			

- Molecule 4 is a protein called Binding-protein-dependent transport systems inner membrane component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	370	Total	C	N	O	S	0	1	0
			2879	1820	515	531	13			
4	B	368	Total	C	N	O	S	0	0	0
			2855	1806	511	525	13			

There are 20 discrepancies between the modelled and reference sequences:

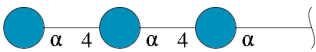
Chain	Residue	Modelled	Actual	Comment	Reference
A	372	ALA	-	expression tag	UNP C9QV42
A	373	SER	-	expression tag	UNP C9QV42
A	374	ALA	-	expression tag	UNP C9QV42
A	375	SER	-	expression tag	UNP C9QV42
A	376	HIS	-	expression tag	UNP C9QV42
A	377	HIS	-	expression tag	UNP C9QV42
A	378	HIS	-	expression tag	UNP C9QV42
A	379	HIS	-	expression tag	UNP C9QV42
A	380	HIS	-	expression tag	UNP C9QV42
A	381	HIS	-	expression tag	UNP C9QV42
B	372	ALA	-	expression tag	UNP C9QV42
B	373	SER	-	expression tag	UNP C9QV42
B	374	ALA	-	expression tag	UNP C9QV42
B	375	SER	-	expression tag	UNP C9QV42
B	376	HIS	-	expression tag	UNP C9QV42
B	377	HIS	-	expression tag	UNP C9QV42
B	378	HIS	-	expression tag	UNP C9QV42
B	379	HIS	-	expression tag	UNP C9QV42
B	380	HIS	-	expression tag	UNP C9QV42
B	381	HIS	-	expression tag	UNP C9QV42

- Molecule 5 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



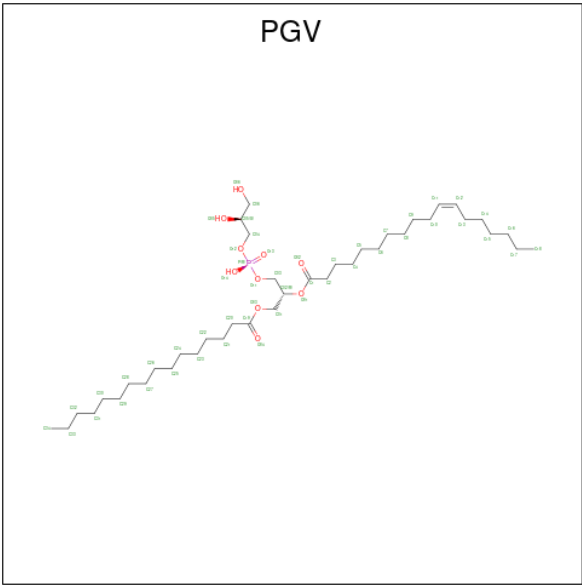
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	C	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 6 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
6	D	3	Total	C	O	0	0	1
			23	12	11			

- Molecule 7 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	21	Total	O	0	0
			21	21		
8	F	11	Total	O	0	0
			11	11		
8	G	5	Total	O	0	0
			5	5		
8	A	9	Total	O	0	0
			9	9		

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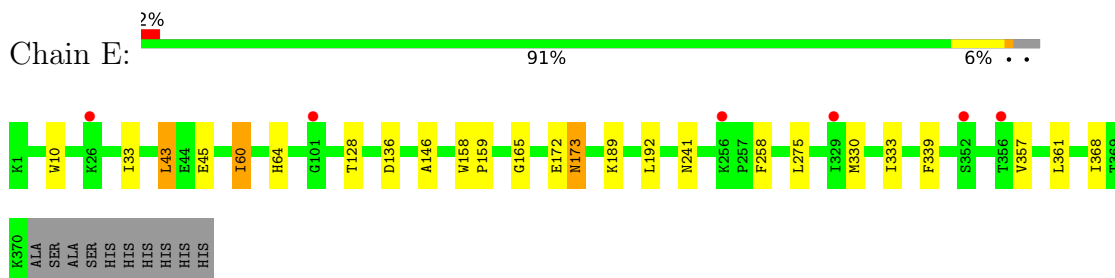
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	7	Total	O	0	0
			7	7		

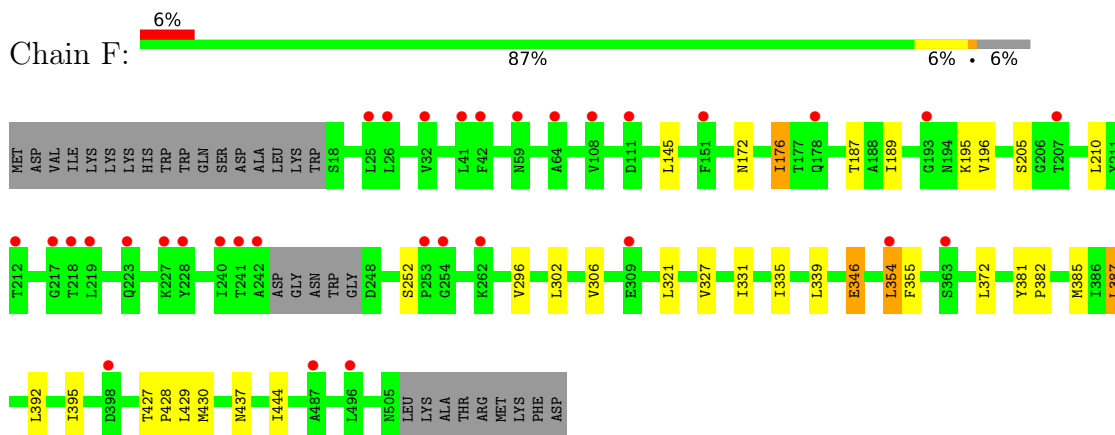
3 Residue-property plots

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.

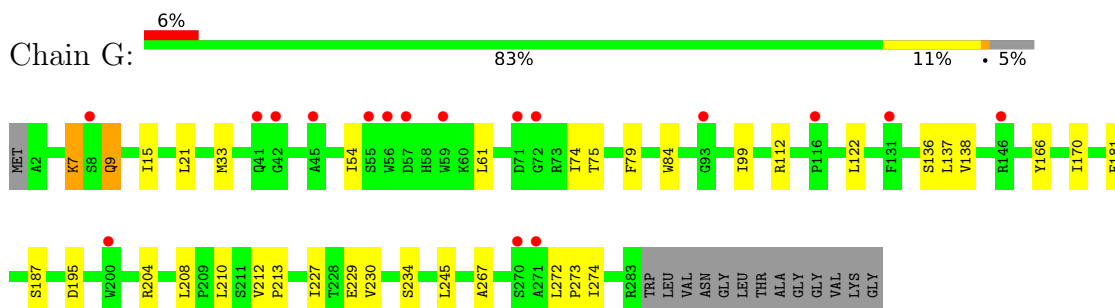
- Molecule 1: Maltose-binding periplasmic protein



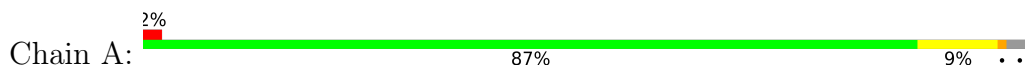
- Molecule 2: Maltose transport system permease protein MalF

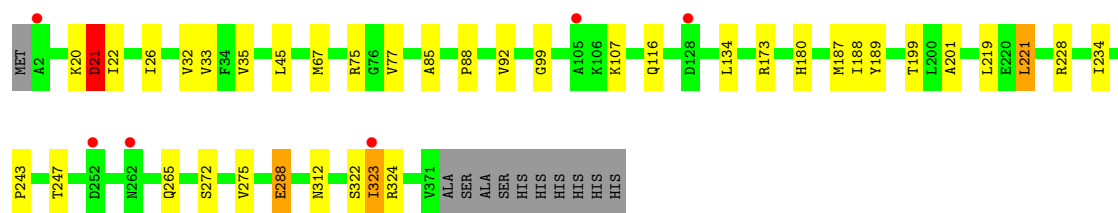


- Molecule 3: Binding-protein-dependent transport systems inner membrane component

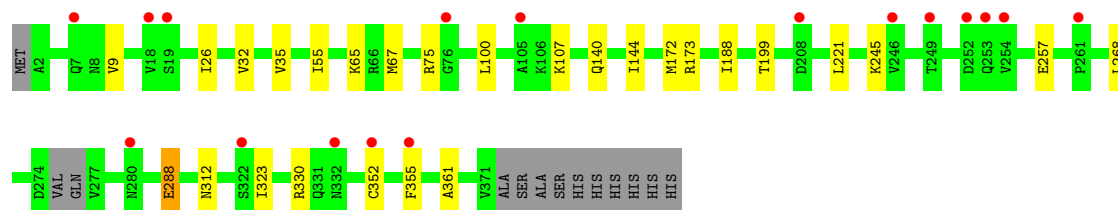
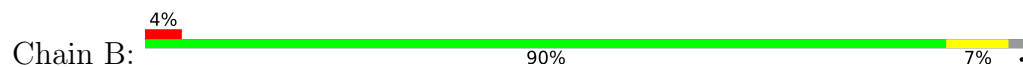


- Molecule 4: Binding-protein-dependent transport systems inner membrane component

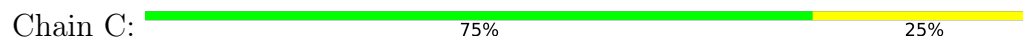




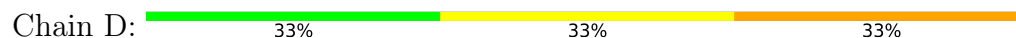
- Molecule 4: Binding-protein-dependent transport systems inner membrane component



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



- Molecule 6: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.25Å 92.22Å 117.81Å 90.73° 101.68° 103.60°	Depositor
Resolution (Å)	19.81 – 2.90 19.81 – 2.90	Depositor EDS
% Data completeness (in resolution range)	71.7 (19.81-2.90) 71.7 (19.81-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.243 , 0.283 0.241 , 0.279	Depositor DCC
R_{free} test set	2438 reflections (3.54%)	wwPDB-VP
Wilson B-factor (Å ²)	76.1	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14715	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: GLC, 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	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	E	0.37	0/2946	0.71	2/3998 (0.1%)
2	F	0.39	0/3841	0.67	0/5228
3	G	0.40	0/2242	0.72	0/3065
4	A	0.37	0/2929	0.65	0/3972
4	B	0.38	0/2904	0.64	0/3936
All	All	0.38	0/14862	0.68	2/20199 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	333	ILE	CA-C-N	5.19	125.23	119.32
1	E	333	ILE	C-N-CA	5.19	125.23	119.32

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	E	2877	0	2859	11	0
2	F	3750	0	3783	20	0
3	G	2182	0	2271	15	0
4	A	2879	0	2940	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2855	0	2919	15	0
5	C	45	0	39	0	0
6	D	23	0	19	1	0
7	F	51	0	76	0	0
8	A	9	0	0	0	0
8	B	7	0	0	0	0
8	E	21	0	0	0	0
8	F	11	0	0	0	0
8	G	5	0	0	0	0
All	All	14715	0	14906	77	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 3.

All (77) 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:F:321:LEU:HB3	2:F:385:MET:HE1	1.78	0.65
1:E:136:ASP:HA	1:E:146:ALA:HB2	1.81	0.61
4:A:247:THR:HG21	4:A:265:GLN:HE21	1.68	0.59
1:E:43:LEU:HD11	1:E:60:ILE:CD1	2.34	0.58
4:A:243:PRO:HD3	4:A:323:ILE:HD12	1.85	0.57
3:G:210:LEU:HD21	4:A:88:PRO:HD2	1.85	0.56
4:B:26:ILE:HG23	4:B:32:VAL:HG21	1.88	0.55
1:E:189:LYS:HG2	1:E:361:LEU:HD12	1.87	0.55
3:G:9:GLN:HE21	3:G:9:GLN:HA	1.72	0.54
2:F:327:VAL:HG13	2:F:331:ILE:HD11	1.88	0.54
1:E:10:TRP:HB3	1:E:43:LEU:HD13	1.91	0.53
3:G:136:SER:O	3:G:138:VAL:N	2.42	0.52
4:B:173:ARG:NH1	4:B:199:THR:HG21	2.25	0.52
2:F:296:VAL:HG21	2:F:430:MET:HE3	1.93	0.50
4:A:22:ILE:HD11	4:A:45:LEU:HD21	1.94	0.50
4:A:247:THR:HG21	4:A:265:GLN:NE2	2.27	0.50
4:A:33:VAL:CG2	4:A:201:ALA:HB2	2.42	0.50
1:E:33:ILE:HD13	1:E:275:LEU:HD13	1.94	0.49
4:A:243:PRO:CD	4:A:323:ILE:HD12	2.42	0.49
3:G:79:PHE:HB3	3:G:84:TRP:CH2	2.48	0.49
2:F:392:LEU:HD12	2:F:395:ILE:HD12	1.93	0.48
2:F:381:TYR:N	2:F:382:PRO:HD2	2.29	0.48
4:A:75:ARG:HB2	4:A:77:VAL:HG12	1.96	0.48
1:E:339:PHE:HA	1:E:368:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:302:LEU:HB3	2:F:385:MET:HE2	1.95	0.47
2:F:331:ILE:HD12	3:G:267:ALA:HB1	1.96	0.47
4:B:67:MET:CE	4:B:75:ARG:HA	2.44	0.47
1:E:172:GLU:O	1:E:173:ASN:C	2.57	0.47
1:E:64:HIS:NE2	1:E:330:MET:O	2.42	0.47
2:F:387:LEU:CD2	2:F:429:LEU:HD13	2.45	0.47
2:F:387:LEU:HD21	2:F:429:LEU:HD13	1.96	0.46
4:B:355:PHE:CE2	4:B:361:ALA:HB2	2.50	0.46
4:A:221:LEU:HB3	4:A:234:ILE:HD12	1.97	0.46
3:G:112:ARG:NH2	3:G:181:PHE:O	2.49	0.46
3:G:166:TYR:CE1	3:G:229:GLU:HG2	2.51	0.46
4:A:92:VAL:HG22	4:A:134:LEU:HD11	1.98	0.46
4:A:272:SER:O	4:A:275:VAL:HG22	2.16	0.46
1:E:258:PHE:HB3	1:E:330:MET:HE2	1.98	0.46
2:F:437:ASN:HD21	6:D:3:GLC:H62	1.80	0.45
3:G:227:ILE:HG21	3:G:274:ILE:HD11	1.97	0.45
1:E:192:LEU:HD23	1:E:357:VAL:HG13	1.97	0.45
1:E:158:TRP:N	1:E:159:PRO:CD	2.80	0.45
2:F:302:LEU:CB	2:F:385:MET:HE2	2.46	0.44
4:A:26:ILE:HG23	4:A:32:VAL:HG21	1.99	0.44
4:A:20:LYS:O	4:A:21:ASP:C	2.59	0.44
4:A:180:HIS:HB2	4:A:187:MET:HE2	1.99	0.44
2:F:189:ILE:HD12	2:F:195:LYS:HG2	1.99	0.44
4:A:67:MET:HE2	4:A:75:ARG:HA	2.00	0.44
4:A:92:VAL:CG2	4:A:134:LEU:HD11	2.48	0.44
4:B:26:ILE:HD13	4:B:188:ILE:HD12	2.00	0.43
3:G:272:LEU:N	3:G:273:PRO:HD2	2.33	0.43
4:B:268:LEU:HD22	4:B:352:CYS:HB2	2.00	0.43
3:G:99:ILE:HG23	3:G:170:ILE:HG22	2.01	0.42
3:G:204:ARG:HA	3:G:208:LEU:HD12	2.01	0.42
4:A:288:GLU:HG2	4:B:312:ASN:HB2	2.02	0.42
2:F:302:LEU:O	2:F:306:VAL:HG23	2.19	0.42
2:F:335:ILE:O	2:F:339:LEU:HG	2.20	0.42
2:F:354:LEU:HD12	2:F:355:PHE:H	1.85	0.42
4:B:288:GLU:HG3	4:B:330:ARG:HD3	2.00	0.42
3:G:195:ASP:HB3	4:A:99:GLY:HA2	2.01	0.42
2:F:196:VAL:HG23	2:F:205:SER:C	2.44	0.42
4:B:140:GLN:NE2	4:B:144:ILE:HD11	2.35	0.42
2:F:346:GLU:HG3	3:G:33:MET:HE2	2.02	0.41
4:B:67:MET:HE3	4:B:75:ARG:HG2	2.02	0.41
4:B:140:GLN:HE22	4:B:144:ILE:HD11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:187:SER:HB3	4:A:85:ALA:HB2	2.01	0.41
2:F:372:LEU:HD11	2:F:444:ILE:HD13	2.03	0.41
4:A:26:ILE:HD13	4:A:188:ILE:HD12	2.01	0.41
4:B:55:ILE:N	4:B:55:ILE:HD12	2.34	0.41
4:B:9:VAL:HG13	4:B:55:ILE:HG23	2.03	0.41
3:G:212:VAL:N	3:G:213:PRO:CD	2.84	0.41
4:A:312:ASN:HB2	4:B:288:GLU:HG2	2.03	0.41
4:A:33:VAL:HG22	4:A:189:TYR:HB3	2.03	0.41
4:A:173:ARG:NH1	4:A:199:THR:HG21	2.36	0.41
2:F:427:THR:N	2:F:428:PRO:HD2	2.37	0.40
2:F:172:ASN:O	2:F:176:ILE:HG23	2.20	0.40
4:B:245:LYS:O	4:B:257:GLU:N	2.51	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	E	368/380 (97%)	353 (96%)	12 (3%)	3 (1%)	16	44
2	F	479/514 (93%)	447 (93%)	31 (6%)	1 (0%)	43	72
3	G	280/296 (95%)	260 (93%)	17 (6%)	3 (1%)	11	36
4	A	369/381 (97%)	348 (94%)	19 (5%)	2 (0%)	24	54
4	B	364/381 (96%)	345 (95%)	18 (5%)	1 (0%)	36	65
All	All	1860/1952 (95%)	1753 (94%)	97 (5%)	10 (0%)	24	54

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	173	ASN
3	G	137	LEU

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Mol	Chain	Res	Type
3	G	7	LYS
4	A	21	ASP
4	A	322	SER
3	G	230	VAL
1	E	241	ASN
4	B	323	ILE
2	F	252	SER
1	E	165	GLY

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	E	297/305 (97%)	293 (99%)	4 (1%)	61	86
2	F	394/424 (93%)	387 (98%)	7 (2%)	51	80
3	G	228/237 (96%)	217 (95%)	11 (5%)	23	55
4	A	315/323 (98%)	305 (97%)	10 (3%)	34	68
4	B	312/323 (97%)	305 (98%)	7 (2%)	45	77
All	All	1546/1612 (96%)	1507 (98%)	39 (2%)	42	74

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	43	LEU
1	E	45	GLU
1	E	60	ILE
1	E	128	THR
2	F	145	LEU
2	F	176	ILE
2	F	187	THR
2	F	210	LEU
2	F	346	GLU
2	F	354	LEU
2	F	387	LEU

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Mol	Chain	Res	Type
3	G	7	LYS
3	G	9	GLN
3	G	15	ILE
3	G	21	LEU
3	G	54	ILE
3	G	61	LEU
3	G	74	ILE
3	G	75	THR
3	G	122	LEU
3	G	234	SER
3	G	245	LEU
4	A	21	ASP
4	A	35	VAL
4	A	107	LYS
4	A	116	GLN
4	A	219	LEU
4	A	221	LEU
4	A	228	ARG
4	A	288	GLU
4	A	323	ILE
4	A	324	ARG
4	B	35	VAL
4	B	65	LYS
4	B	100	LEU
4	B	107	LYS
4	B	172	MET
4	B	221	LEU
4	B	288	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	100	ASN
1	E	282	ASN
1	E	355	GLN
2	F	37	GLN
2	F	98	ASN
2	F	106	GLN
2	F	158	GLN
2	F	222	ASN
2	F	223	GLN
2	F	231	ASN

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Mol	Chain	Res	Type
2	F	376	ASN
2	F	437	ASN
2	F	440	ASN
3	G	9	GLN
3	G	69	GLN
3	G	256	GLN
4	A	116	GLN
4	A	255	GLN
4	A	265	GLN
4	A	305	GLN
4	A	315	GLN
4	B	115	ASN
4	B	312	ASN
4	B	331	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 ⓘ

Of 7 monosaccharides modelled in this entry, 6 were used 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	$\# Z > 2$
5	GLC	C	1	5	12,12,12	0.52	0	17,17,17	0.50	0
5	GLC	C	2	5	11,11,12	0.63	0	15,15,17	0.78	0
5	GLC	C	3	5	11,11,12	0.70	0	15,15,17	0.76	0
5	GLC	C	4	5	11,11,12	0.50	0	15,15,17	1.20	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GLC	D	2	6	11,11,12	0.53	0	15,15,17	1.14	1 (6%)
6	GLC	D	3	6	11,11,12	0.60	0	15,15,17	0.89	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.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GLC	C	1	5	-	0/2/22/22	0/1/1/1
5	GLC	C	2	5	-	0/2/19/22	0/1/1/1
5	GLC	C	3	5	-	0/2/19/22	0/1/1/1
5	GLC	C	4	5	-	2/2/19/22	0/1/1/1
6	GLC	D	2	6	-	2/2/19/22	0/1/1/1
6	GLC	D	3	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	4	GLC	C1-O5-C5	3.97	117.50	112.19
6	D	2	GLC	C1-O5-C5	3.42	116.77	112.19
6	D	3	GLC	C1-O5-C5	2.26	115.22	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	4	GLC	O5-C5-C6-O6
6	D	2	GLC	O5-C5-C6-O6
5	C	4	GLC	C4-C5-C6-O6
6	D	2	GLC	C4-C5-C6-O6

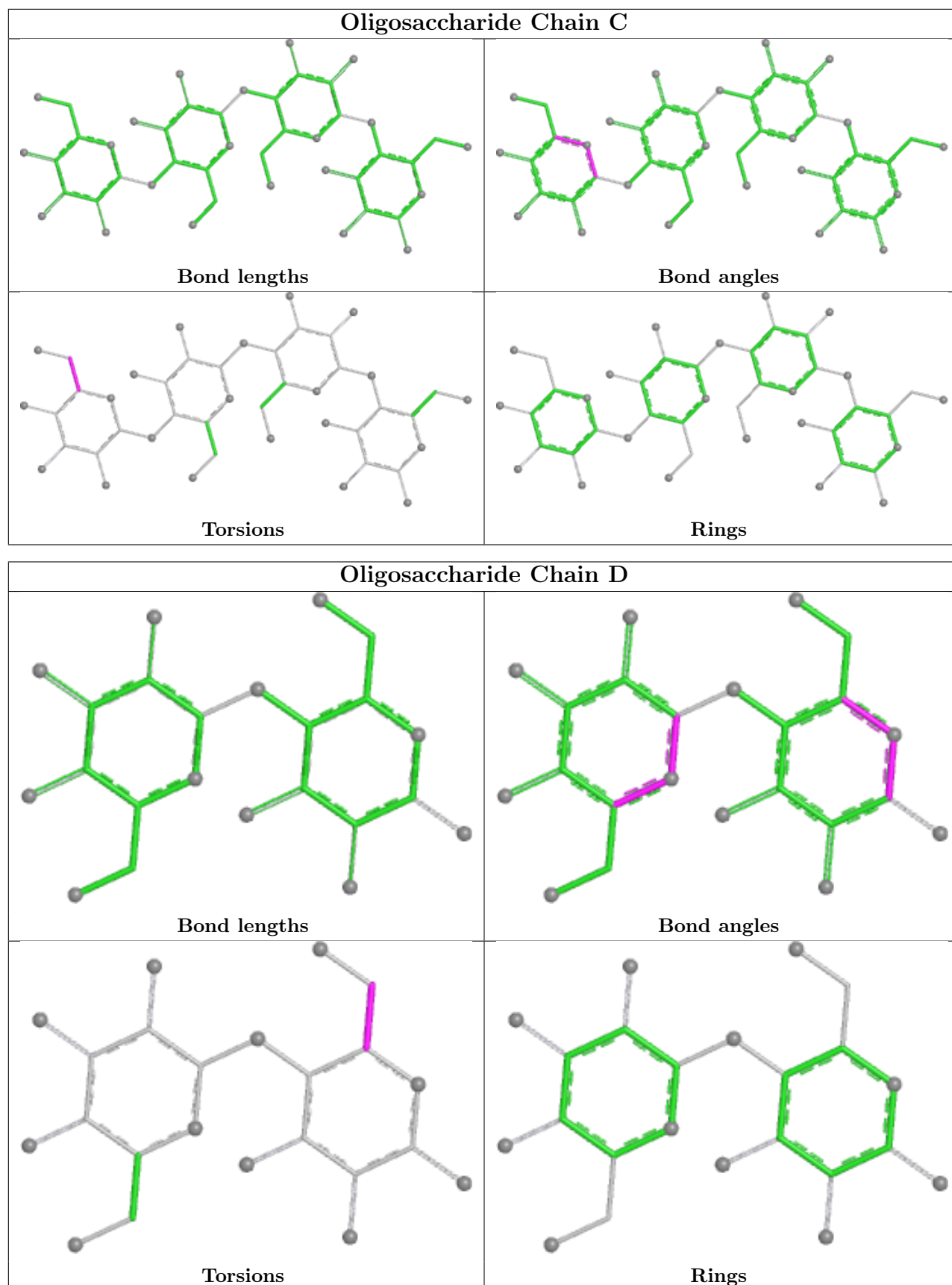
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	3	GLC	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 oligosaccharide.



5.6 Ligand geometry

1 ligand is 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$
7	PGV	F	604	-	50,50,50	1.09	3 (6%)	53,56,56	0.98	3 (5%)

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	PGV	F	604	-	-	22/55/55/55	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	604	PGV	O01-C1	4.24	1.46	1.34
7	F	604	PGV	O03-C19	4.23	1.45	1.33
7	F	604	PGV	C12-C11	3.77	1.53	1.31

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	604	PGV	O01-C1-C2	3.97	120.06	111.48
7	F	604	PGV	O03-C19-C20	2.73	120.17	111.83
7	F	604	PGV	O03-C19-O04	-2.03	118.55	123.63

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	604	PGV	C03-O11-P-O12
7	F	604	PGV	C03-O11-P-O13

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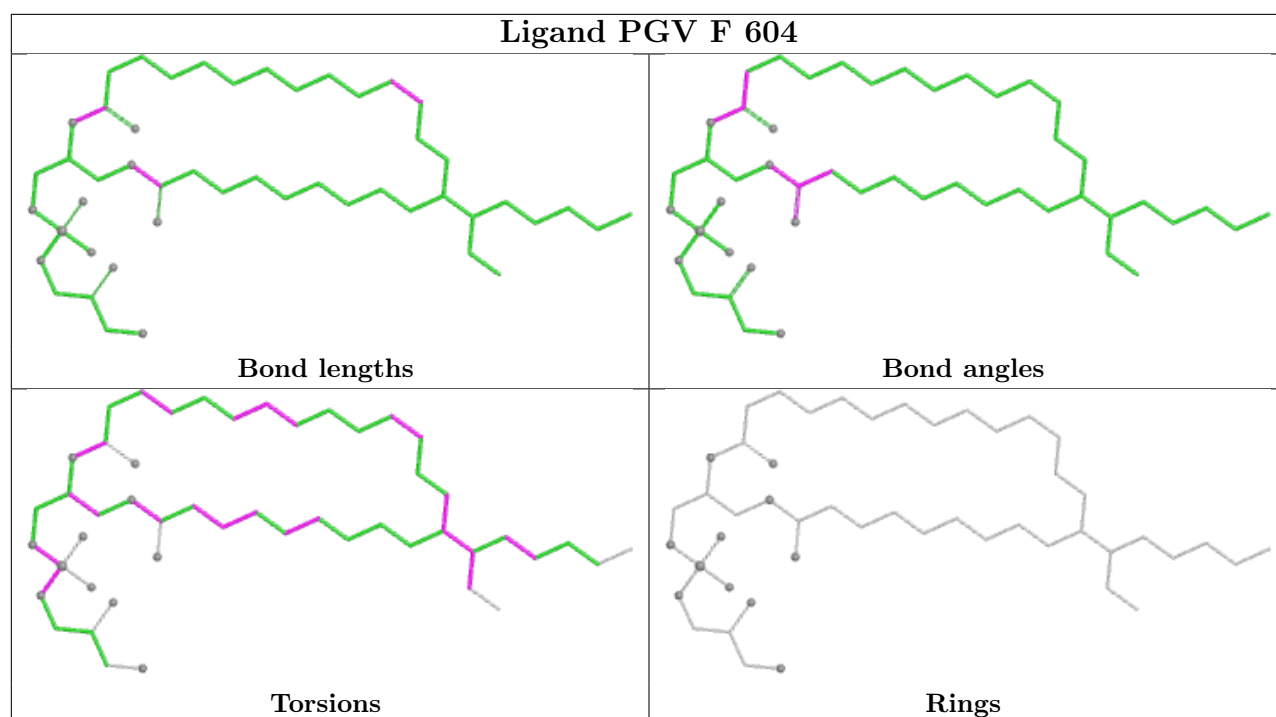
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Mol	Chain	Res	Type	Atoms
7	F	604	PGV	C04-O12-P-O11
7	F	604	PGV	C04-O12-P-O13
7	F	604	PGV	C2-C1-O01-C02
7	F	604	PGV	O02-C1-O01-C02
7	F	604	PGV	C20-C19-O03-C01
7	F	604	PGV	O04-C19-O03-C01
7	F	604	PGV	C10-C11-C12-C13
7	F	604	PGV	C2-C3-C4-C5
7	F	604	PGV	C22-C23-C24-C25
7	F	604	PGV	C27-C28-C29-C30
7	F	604	PGV	C13-C14-C15-C16
7	F	604	PGV	C20-C21-C22-C23
7	F	604	PGV	C19-C20-C21-C22
7	F	604	PGV	C6-C7-C8-C9
7	F	604	PGV	C29-C30-C31-C32
7	F	604	PGV	O03-C01-C02-O01
7	F	604	PGV	C03-O11-P-O14
7	F	604	PGV	O03-C01-C02-C03
7	F	604	PGV	C15-C16-C17-C18
7	F	604	PGV	C5-C6-C7-C8

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 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	E	370/380 (97%)	0.13	6 (1%) 70 62	57, 82, 117, 133	0
2	F	483/514 (93%)	0.56	32 (6%) 24 19	63, 101, 154, 189	0
3	G	282/296 (95%)	0.59	17 (6%) 27 21	58, 86, 145, 170	0
4	A	370/381 (97%)	0.26	6 (1%) 70 62	45, 91, 123, 176	1 (0%)
4	B	368/381 (96%)	0.45	17 (4%) 37 29	66, 100, 170, 218	0
All	All	1873/1952 (95%)	0.40	78 (4%) 40 32	45, 94, 150, 218	1 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	41	LEU	5.1
2	F	207	THR	4.9
2	F	254	GLY	4.8
3	G	71	ASP	4.2
3	G	55	SER	4.1
4	A	2	ALA	4.1
2	F	262	LYS	3.9
4	B	18	VAL	3.7
4	B	249	THR	3.7
2	F	42	PHE	3.6
4	B	7	GLN	3.5
3	G	8	SER	3.5
3	G	72	GLY	3.5
4	A	262	ASN	3.4
3	G	57	ASP	3.3
4	B	252	ASP	3.1
4	A	252[A]	ASP	3.1
4	B	280	ASN	3.1
2	F	253	PRO	3.1
4	A	128	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
3	G	271	ALA	3.0
3	G	131	PHE	2.8
2	F	32	VAL	2.8
2	F	242	ALA	2.7
2	F	241	THR	2.7
4	B	355	PHE	2.7
3	G	270	SER	2.7
2	F	212	THR	2.6
2	F	228	TYR	2.5
3	G	56	TRP	2.5
4	B	352	CYS	2.5
2	F	398	ASP	2.5
4	B	19	SER	2.4
4	B	254	VAL	2.4
2	F	223	GLN	2.4
2	F	219	LEU	2.4
4	B	76	GLY	2.4
2	F	309	GLU	2.4
3	G	42	GLY	2.4
2	F	227	LYS	2.4
1	E	356	THR	2.4
2	F	496	LEU	2.4
3	G	93	GLY	2.4
2	F	64	ALA	2.4
3	G	45	ALA	2.4
4	A	105	ALA	2.3
2	F	354	LEU	2.3
2	F	178	GLN	2.3
2	F	25	LEU	2.3
1	E	256	LYS	2.3
2	F	218	THR	2.3
3	G	116	PRO	2.3
2	F	59	ASN	2.3
2	F	217	GLY	2.3
4	B	332	ASN	2.2
2	F	363	SER	2.2
4	B	322	SER	2.2
1	E	26	LYS	2.2
4	A	323	ILE	2.2
4	B	261	PRO	2.2
1	E	101	GLY	2.2
2	F	26	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	352	SER	2.2
2	F	108	VAL	2.1
3	G	59	TRP	2.1
3	G	200	TRP	2.1
2	F	487	ALA	2.1
4	B	105	ALA	2.1
1	E	329	ILE	2.1
2	F	193	GLY	2.1
2	F	151	PHE	2.1
3	G	41	GLN	2.1
4	B	246	VAL	2.0
2	F	111	ASP	2.0
4	B	208	ASP	2.0
4	B	253	GLN	2.0
3	G	146	ARG	2.0
2	F	240	ILE	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](#)

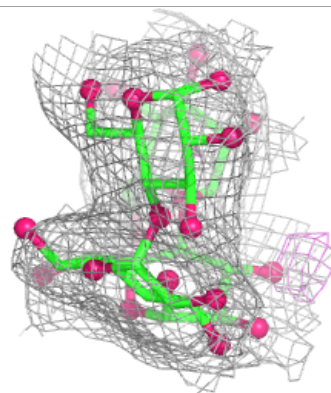
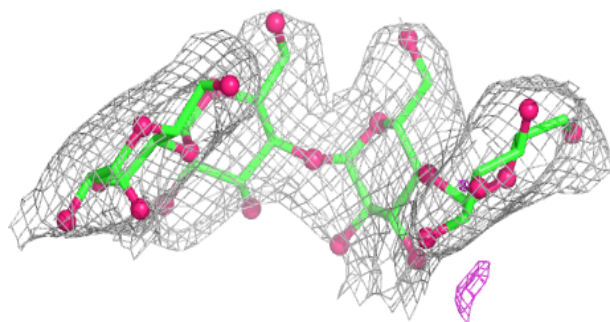
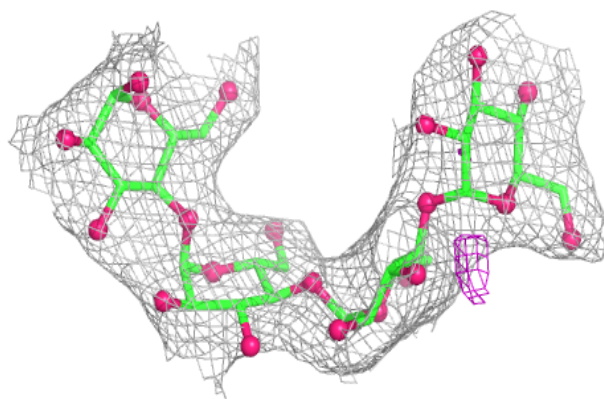
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GLC	C	1	12/12	-	-	59,62,63,65	0
5	GLC	C	2	11/12	-	-	67,70,72,72	0
5	GLC	C	3	11/12	-	-	73,74,77,77	0
5	GLC	C	4	11/12	-	-	78,81,84,84	0
6	GLC	D	1	1/12	-	-	66,66,66,66	0
6	GLC	D	2	11/12	-	-	62,62,64,64	0
6	GLC	D	3	11/12	-	-	61,62,63,63	0

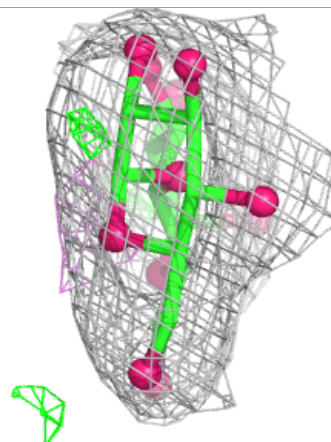
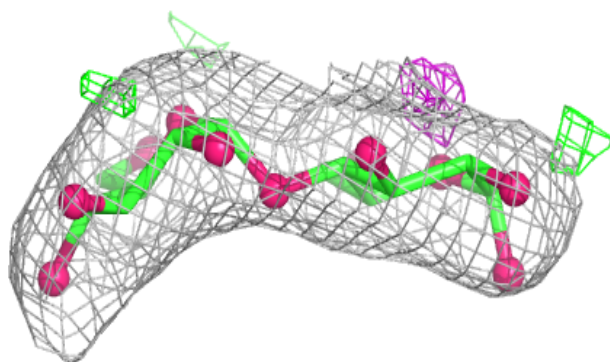
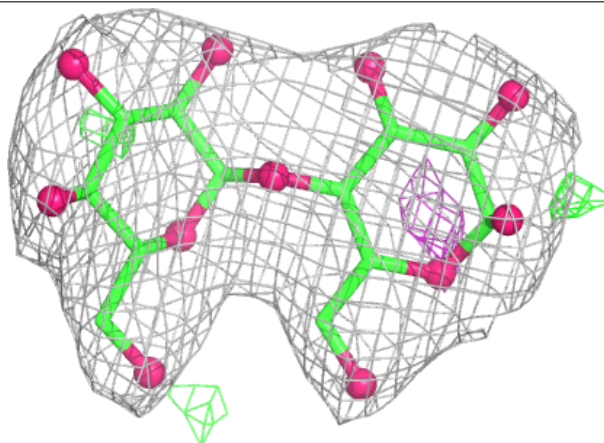
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

**Electron density around Chain D:**

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

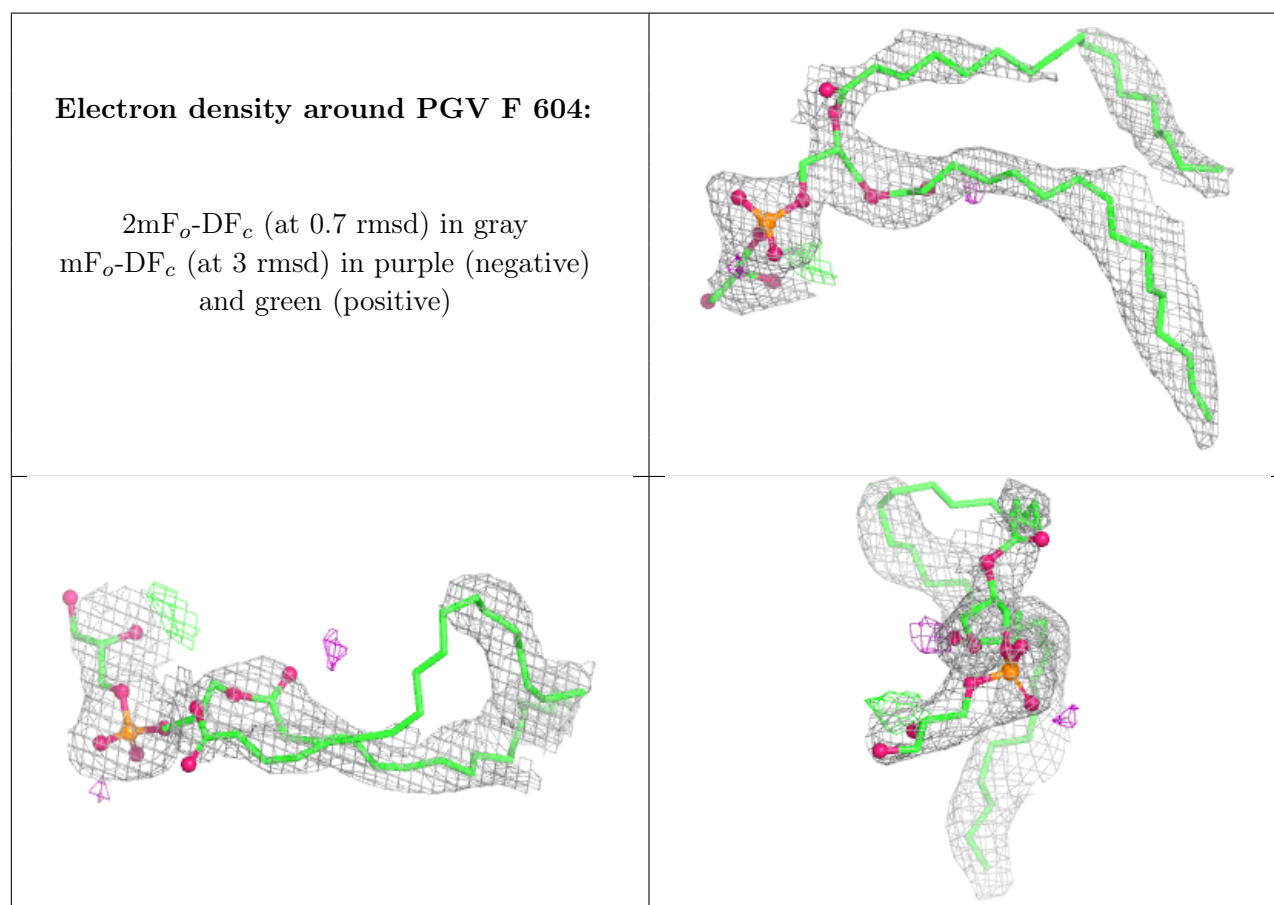


6.4 Ligands [i](#)

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(Å ²)	Q<0.9
7	PGV	F	604	51/51	0.85	0.17	100,108,121,122	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 [i](#)

There are no such residues in this entry.