



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 26, 2018 – 02:47 PM EST

PDB ID : 6C26
EMDB ID: : EMD-7336
Title : The Cryo-EM structure of a eukaryotic oligosaccharyl transferase complex
Authors : Bai, L.; Li, H.
Deposited on : 2018-01-06
Resolution : 3.50 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

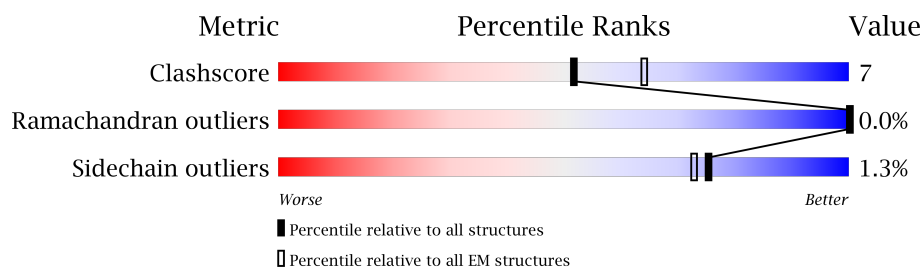
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	718	81% 9% • 10%
2	1	476	80% 10% • 9%
3	5	86	98% •
4	4	36	86% 8% 6%
5	2	130	69% 12% • 17%
6	3	350	34% • 64%
7	C	286	74% 13% 13%
8	B	430	74% 17% • 8%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17188 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	648	Total	C	N	O	S	0	0
			5225	3456	839	907	23		

- Molecule 2 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	432	Total	C	N	O	S	0	0
			3496	2267	560	662	7		

- Molecule 3 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	84	Total	C	N	O	S	0	0
			659	443	98	117	1		

- Molecule 4 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	34	Total	C	N	O	S	0	0
			259	167	39	50	3		

- Molecule 5 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	2	108	Total	C	N	O	S	0	0
			883	598	139	140	6		

- Molecule 6 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	3	126	Total	C	N	O	S	0	0
			1028	700	154	167	7		

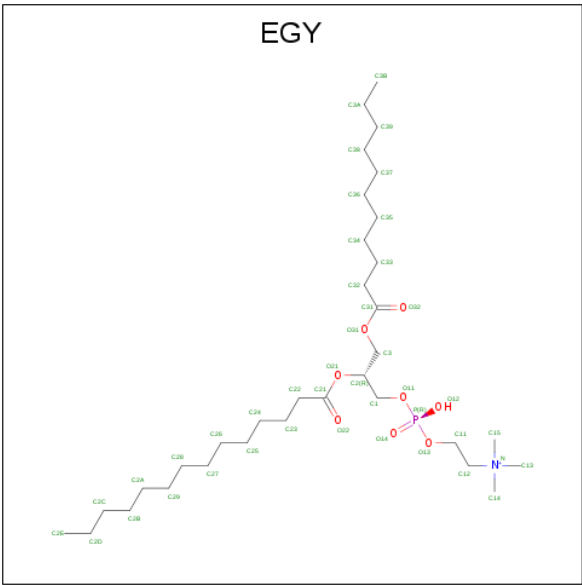
- Molecule 7 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit SWP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	248	Total	C	N	O	S	0	0
			1940	1272	311	353	4		

- Molecule 8 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit WBP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	397	Total	C	N	O	S	0	0
			3218	2063	531	620	4		

- Molecule 9 is (4R,7R)-4-hydroxy-N,N,N-trimethyl-4,9-dioxo-7-[(undecanoyloxy)methyl]-3,5,8-trioxa-4lambda 5 -phosphadocosan-1-aminium (three-letter code: EGY) (formula: C₃₃H₆₇NO₈P).



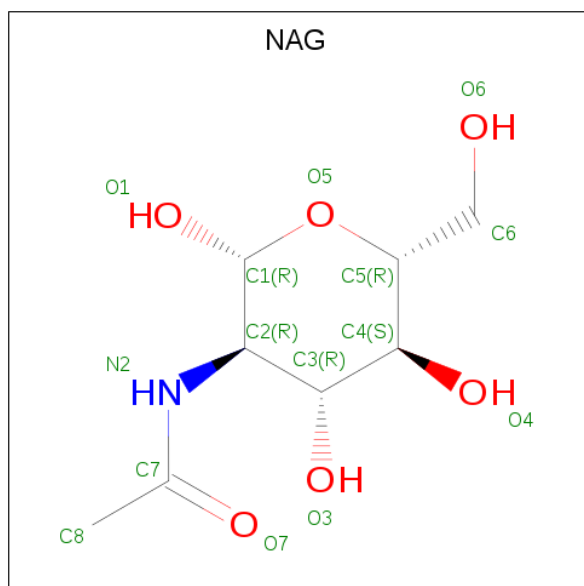
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			129	99	3	24	3	
9	A	1	Total	C	N	O	P	0
			129	99	3	24	3	
9	A	1	Total	C	N	O	P	0
			129	99	3	24	3	

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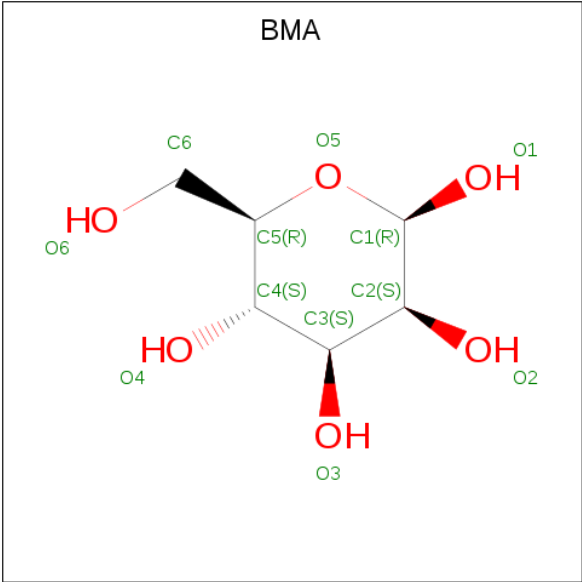
Mol	Chain	Residues	Atoms					AltConf
9	1	1	Total	C	N	O	P	0
			86	66	2	16	2	
9	1	1	Total	C	N	O	P	0
			86	66	2	16	2	
9	4	1	Total	C	N	O	P	0
			43	33	1	8	1	
9	3	1	Total	C	N	O	P	0
			43	33	1	8	1	
9	C	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 10 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
10	A	1	Total	C	N	O	0
			28	16	2	10	
10	A	1	Total	C	N	O	0
			28	16	2	10	
10	1	1	Total	C	N	O	0
			28	16	2	10	
10	1	1	Total	C	N	O	0
			28	16	2	10	
10	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 11 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).

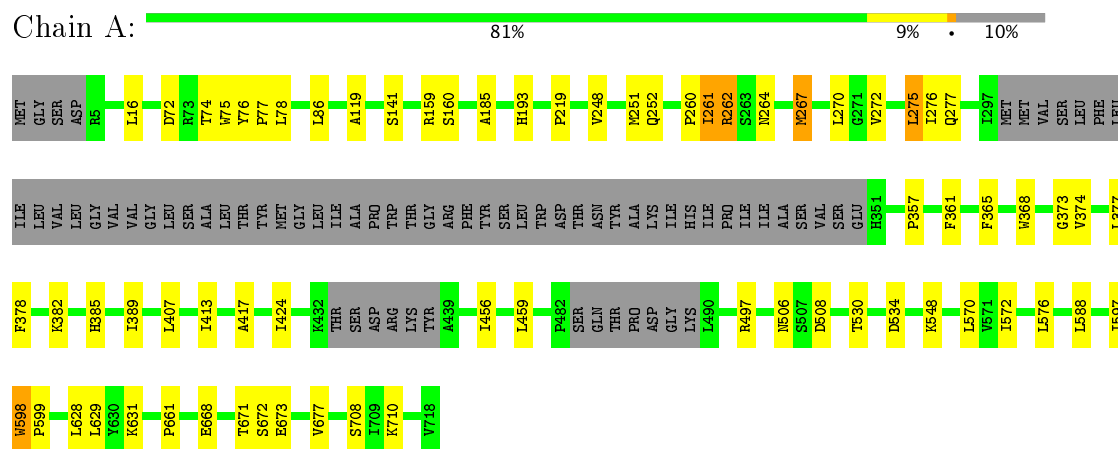


Mol	Chain	Residues	Atoms			AltConf
11	A	1	Total	C	O	0
			55	30	25	
11	A	1	Total	C	O	0
			55	30	25	
11	A	1	Total	C	O	0
			55	30	25	
11	A	1	Total	C	O	0
			55	30	25	
11	A	1	Total	C	O	0
			55	30	25	
11	1	1	Total	C	O	0
			11	6	5	

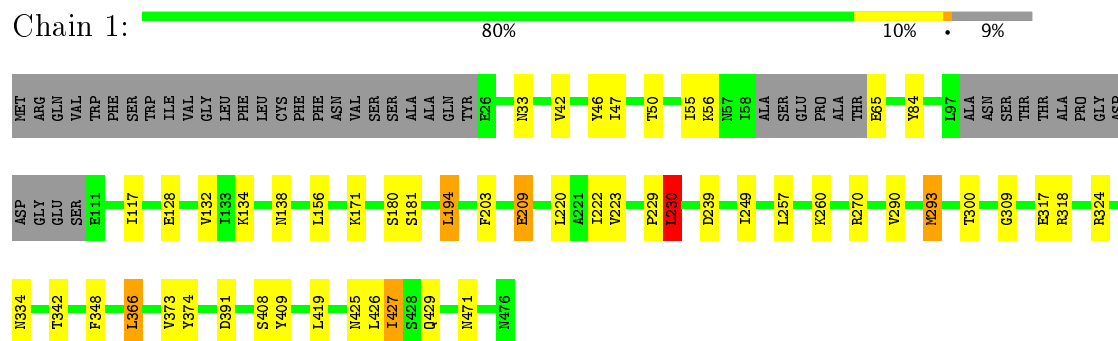
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

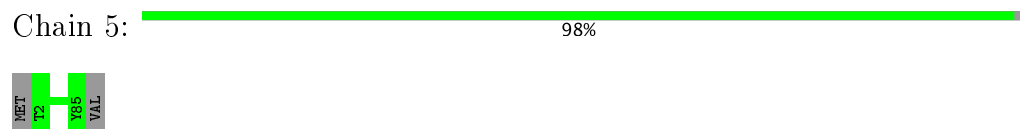
- Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3



- Molecule 2: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1



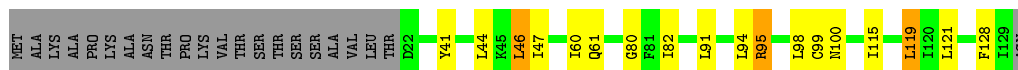
- Molecule 3: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST5



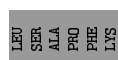
- Molecule 4: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST4



- Molecule 5: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit OST2



- Molecule 6: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 3



- Molecule 7: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit SWP1



- Molecule 8: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit WBP1



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	282202	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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: EGY, BMA, NAG

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.55	0/5377	0.70	6/7309 (0.1%)
2	1	0.53	0/3595	0.70	7/4891 (0.1%)
3	5	0.41	0/677	0.58	0/916
4	4	0.41	0/262	0.57	0/355
5	2	0.46	0/906	0.66	3/1222 (0.2%)
6	3	0.38	0/1057	0.63	0/1435
7	C	0.35	0/1981	0.66	1/2690 (0.0%)
8	B	0.47	0/3300	0.64	1/4482 (0.0%)
All	All	0.49	0/17155	0.67	18/23300 (0.1%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	230	LEU	CA-CB-CG	10.39	139.20	115.30
1	A	76	TYR	C-N-CD	8.57	146.41	128.40
2	1	194	LEU	CA-CB-CG	7.53	132.62	115.30
1	A	459	LEU	CA-CB-CG	7.03	131.46	115.30
5	2	119	LEU	CA-CB-CG	6.17	129.48	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	A	5225	0	5201	58	0
2	1	3496	0	3376	36	0
3	5	659	0	668	0	0
4	4	259	0	268	6	0
5	2	883	0	914	16	0
6	3	1028	0	1062	4	0
7	C	1940	0	1991	25	0
8	B	3218	0	3120	95	0
9	1	86	0	0	0	0
9	3	43	0	0	0	0
9	4	43	0	0	0	0
9	A	129	0	0	1	0
9	C	43	0	0	0	0
10	1	28	0	24	0	0
10	A	28	0	24	1	0
10	B	14	0	13	0	0
11	1	11	0	10	0	0
11	A	55	0	45	1	0
All	All	17188	0	16716	222	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 7.

The worst 5 of 222 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)
8:B:69:TYR:CE1	8:B:74:ARG:HB3	1.48	1.48
8:B:69:TYR:HE1	8:B:74:ARG:CB	1.39	1.33
8:B:279:TYR:HD1	8:B:284:TYR:CE2	1.48	1.31
8:B:291:ILE:HG22	8:B:342:GLY:O	1.17	1.31
8:B:279:TYR:CD1	8:B:284:TYR:CE2	2.32	1.16

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	640/718 (89%)	592 (92%)	47 (7%)	1 (0%)	51	85
2	1	426/476 (90%)	368 (86%)	58 (14%)	0	100	100
3	5	82/86 (95%)	82 (100%)	0	0	100	100
4	4	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
5	2	106/130 (82%)	100 (94%)	6 (6%)	0	100	100
6	3	122/350 (35%)	107 (88%)	15 (12%)	0	100	100
7	C	240/286 (84%)	201 (84%)	39 (16%)	0	100	100
8	B	395/430 (92%)	361 (91%)	34 (9%)	0	100	100
All	All	2043/2512 (81%)	1842 (90%)	200 (10%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	598	TRP

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 PDB entries followed by that with respect to all EM entries.

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	552/613 (90%)	542 (98%)	10 (2%)	64	86
2	1	391/426 (92%)	386 (99%)	5 (1%)	73	90
3	5	73/75 (97%)	73 (100%)	0	100	100
4	4	31/33 (94%)	31 (100%)	0	100	100
5	2	97/115 (84%)	96 (99%)	1 (1%)	80	91
6	3	112/316 (35%)	111 (99%)	1 (1%)	82	93
7	C	216/249 (87%)	214 (99%)	2 (1%)	82	93
8	B	361/392 (92%)	356 (99%)	5 (1%)	71	89
All	All	1833/2219 (83%)	1809 (99%)	24 (1%)	75	90

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

Mol	Chain	Res	Type
2	1	194	LEU
2	1	230	LEU
8	B	74	ARG
2	1	203	PHE
2	1	209	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
5	2	61	GLN
8	B	78	ASN
8	B	259	ASN
2	1	429	GLN
8	B	243	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

19 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
9	EGY	1	501	-	42,42,42	1.23	3 (7%)	47,50,50	1.15	3 (6%)
9	EGY	1	502	-	42,42,42	1.23	3 (7%)	47,50,50	1.12	2 (4%)
10	NAG	1	503	10,2	14,14,15	0.58	0	15,19,21	2.40	4 (26%)
10	NAG	1	504	11,10	14,14,15	1.31	2 (14%)	15,19,21	2.68	4 (26%)
11	BMA	1	505	10	11,11,12	1.02	1 (9%)	13,15,17	0.92	0
9	EGY	3	401	-	42,42,42	1.23	3 (7%)	47,50,50	1.11	2 (4%)
9	EGY	4	101	-	42,42,42	1.23	3 (7%)	47,50,50	1.08	3 (6%)
9	EGY	A	801	-	42,42,42	1.22	3 (7%)	47,50,50	1.13	2 (4%)
9	EGY	A	802	-	42,42,42	1.23	5 (11%)	47,50,50	1.17	3 (6%)
9	EGY	A	803	-	42,42,42	1.24	4 (9%)	47,50,50	1.08	2 (4%)
10	NAG	A	804	1,10	14,14,15	0.33	0	15,19,21	0.79	0
10	NAG	A	805	11,10	14,14,15	0.50	0	15,19,21	0.82	1 (6%)
11	BMA	A	806	11,10	9,10,12	1.76	1 (11%)	13,14,17	2.17	4 (30%)
11	BMA	A	807	11	11,11,12	2.92	5 (45%)	13,15,17	2.71	6 (46%)
11	BMA	A	808	11	11,11,12	2.13	3 (27%)	13,15,17	1.88	4 (30%)
11	BMA	A	809	11	11,11,12	0.91	0	13,15,17	0.93	1 (7%)
11	BMA	A	810	11	12,12,12	0.66	0	17,17,17	0.96	0
10	NAG	B	601	8	14,14,15	0.62	0	15,19,21	1.05	2 (13%)
9	EGY	C	301	-	42,42,42	1.27	4 (9%)	47,50,50	1.16	2 (4%)

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	EGY	1	501	-	-	0/46/46/46	0/0/0/0
9	EGY	1	502	-	-	0/46/46/46	0/0/0/0
10	NAG	1	503	10,2	-	0/6/23/26	0/1/1/1
10	NAG	1	504	11,10	-	0/6/23/26	0/1/1/1
11	BMA	1	505	10	-	0/2/19/22	0/1/1/1
9	EGY	3	401	-	-	0/46/46/46	0/0/0/0
9	EGY	4	101	-	-	0/46/46/46	0/0/0/0
9	EGY	A	801	-	-	0/46/46/46	0/0/0/0
9	EGY	A	802	-	-	0/46/46/46	0/0/0/0
9	EGY	A	803	-	-	0/46/46/46	0/0/0/0
10	NAG	A	804	1,10	-	0/6/23/26	0/1/1/1
10	NAG	A	805	11,10	-	0/6/23/26	0/1/1/1
11	BMA	A	806	11,10	-	0/0/17/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BMA	A	807	11	-	0/2/19/22	0/1/1/1
11	BMA	A	808	11	-	0/2/19/22	0/1/1/1
11	BMA	A	809	11	-	0/2/19/22	0/1/1/1
11	BMA	A	810	11	-	0/2/22/22	0/1/1/1
10	NAG	B	601	8	-	0/6/23/26	0/1/1/1
9	EGY	C	301	-	-	0/46/46/46	0/0/0/0

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	803	EGY	O21-C2	-2.32	1.40	1.46
9	3	401	EGY	O21-C2	-2.29	1.40	1.46
9	1	501	EGY	O21-C2	-2.22	1.40	1.46
9	A	801	EGY	O21-C2	-2.21	1.40	1.46
9	A	802	EGY	O21-C2	-2.18	1.40	1.46

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	806	BMA	O2-C2-C3	-5.31	99.74	110.17
11	A	807	BMA	C1-C2-C3	-4.16	104.38	109.65
11	A	807	BMA	O5-C1-C2	-3.94	104.62	110.79
11	A	806	BMA	C1-C2-C3	-3.88	104.73	109.65
11	A	808	BMA	O5-C1-C2	-2.50	106.88	110.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	803	EGY	1	0
10	A	804	NAG	1	0
11	A	807	BMA	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.