



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 12:24 pm GMT

PDB ID : 5ACO
EMDB ID: : EMD-3121
Title : Cryo-EM structure of PGT128 Fab in complex with BG505 SOSIP.664 Env trimer
Authors : Lee, J.H.; Ward, A.B.
Deposited on : 2015-08-17
Resolution : 4.36 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) : recalc29047

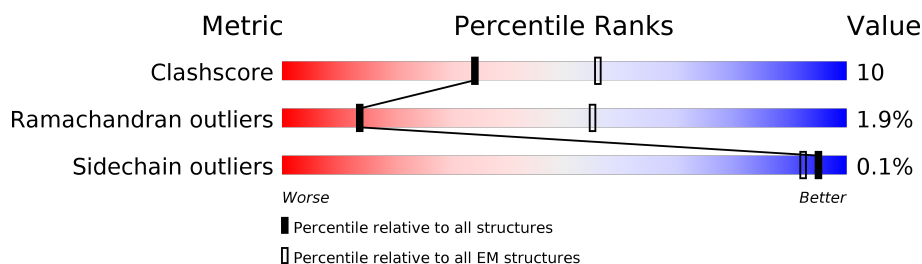
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.36 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	476	81% 9% • 8%
1	C	476	80% 10% • 8%
1	D	476	80% 10% • 8%
2	B	153	70% 15% • 14%
2	E	153	69% 16% • 14%
2	F	153	69% 16% • 14%
3	G	239	50% 5% 45%
3	H	239	50% 5% 45%
3	I	239	50% 5% 45%

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Mol	Chain	Length	Quality of chain
4	J	211	
4	K	211	
4	L	211	

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
5	NAG	A	1088	-	-	X	-
5	NAG	C	1088	-	-	X	-
5	NAG	D	1088	-	-	X	-
6	NAG	C	1448	-	-	X	-
9	NAG	A	1332	-	-	X	-
9	MAN	A	1340	-	-	X	-
9	NAG	C	1332	-	-	X	-
9	MAN	C	1340	-	-	X	-
9	NAG	D	1332	-	-	X	-
9	MAN	D	1340	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 21297 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 HIV-1 ENVELOPE GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	438	Total	C	N	O	S	0	0
			3453	2170	610	645	28		
1	C	438	Total	C	N	O	S	0	0
			3453	2170	610	645	28		
1	D	438	Total	C	N	O	S	0	0
			3453	2170	610	645	28		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ASN	THR	ENGINEERED MUTATION	UNP Q2N0S6
A	501	CYS	ALA	ENGINEERED MUTATION	UNP Q2N0S6
C	332	ASN	THR	ENGINEERED MUTATION	UNP Q2N0S6
C	501	CYS	ALA	ENGINEERED MUTATION	UNP Q2N0S6
D	332	ASN	THR	ENGINEERED MUTATION	UNP Q2N0S6
D	501	CYS	ALA	ENGINEERED MUTATION	UNP Q2N0S6

- Molecule 2 is a protein called HIV-1 ENVELOPE GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	132	Total	C	N	O	S	0	0
			1051	667	180	198	6		
2	E	132	Total	C	N	O	S	0	0
			1051	667	180	198	6		
2	F	132	Total	C	N	O	S	0	0
			1051	667	180	198	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	ENGINEERED MUTATION	UNP Q2N0S6
B	605	CYS	THR	ENGINEERED MUTATION	UNP Q2N0S6
E	559	PRO	ILE	ENGINEERED MUTATION	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	605	CYS	THR	ENGINEERED MUTATION	UNP Q2N0S6
F	559	PRO	ILE	ENGINEERED MUTATION	UNP Q2N0S6
F	605	CYS	THR	ENGINEERED MUTATION	UNP Q2N0S6

- Molecule 3 is a protein called PGT128 FAB.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	132	Total 1028	C 659	N 175	O 190	S 4	0	0
3	H	132	Total 1028	C 659	N 175	O 190	S 4	0	0
3	I	132	Total 1028	C 659	N 175	O 190	S 4	0	0

- Molecule 4 is a protein called PGT128 FAB.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	103	Total 752	C 469	N 128	O 153	S 2	0	0
4	K	103	Total 752	C 469	N 128	O 153	S 2	0	0
4	L	103	Total 752	C 469	N 128	O 153	S 2	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				AltConf
5	A	3	Total	C	N	O	0
			234	132	12	90	
5	A	3	Total	C	N	O	0
			234	132	12	90	
5	A	3	Total	C	N	O	0
			234	132	12	90	
5	A	3	Total	C	N	O	0
			234	132	12	90	
5	A	3	Total	C	N	O	0
			234	132	12	90	
5	C	3	Total	C	N	O	0
			234	132	12	90	

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Mol	Chain	Residues	Atoms				AltConf
5	C	3	Total	C	N	O	0
			234	132	12	90	
5	C	3	Total	C	N	O	0
			234	132	12	90	
5	C	3	Total	C	N	O	0
			234	132	12	90	
5	C	3	Total	C	N	O	0
			234	132	12	90	
5	C	3	Total	C	N	O	0
			234	132	12	90	
5	D	3	Total	C	N	O	0
			234	132	12	90	
5	D	3	Total	C	N	O	0
			234	132	12	90	
5	D	3	Total	C	N	O	0
			234	132	12	90	
5	D	3	Total	C	N	O	0
			234	132	12	90	
5	D	3	Total	C	N	O	0
			234	132	12	90	

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				AltConf
6	A	2	Total	C	N	O	0
			168	96	12	60	
6	A	2	Total	C	N	O	0
			168	96	12	60	
6	A	2	Total	C	N	O	0
			168	96	12	60	
6	A	2	Total	C	N	O	0
			168	96	12	60	
6	A	2	Total	C	N	O	0
			168	96	12	60	
6	B	2	Total	C	N	O	0
			28	16	2	10	
6	C	2	Total	C	N	O	0
			168	96	12	60	

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Mol	Chain	Residues	Atoms				AltConf
6	C	2	Total	C	N	O	0
			168	96	12	60	
6	C	2	Total	C	N	O	0
			168	96	12	60	
6	C	2	Total	C	N	O	0
			168	96	12	60	
6	C	2	Total	C	N	O	0
			168	96	12	60	
6	C	2	Total	C	N	O	0
			168	96	12	60	
6	D	2	Total	C	N	O	0
			168	96	12	60	
6	D	2	Total	C	N	O	0
			168	96	12	60	
6	D	2	Total	C	N	O	0
			168	96	12	60	
6	D	2	Total	C	N	O	0
			168	96	12	60	
6	D	2	Total	C	N	O	0
			168	96	12	60	
6	E	2	Total	C	N	O	0
			28	16	2	10	
6	F	2	Total	C	N	O	0
			28	16	2	10	

- Molecule 7 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				AltConf
7	A	7	Total	C	N	O	0
			166	92	4	70	
7	A	7	Total	C	N	O	0
			166	92	4	70	
7	C	7	Total	C	N	O	0
			166	92	4	70	
7	C	7	Total	C	N	O	0
			166	92	4	70	
7	D	7	Total	C	N	O	0
			166	92	4	70	
7	D	7	Total	C	N	O	0
			166	92	4	70	

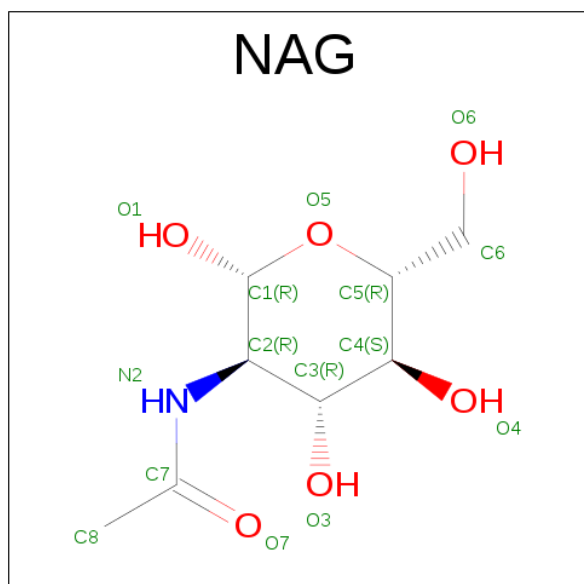
- Molecule 8 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				AltConf
8	A	5	Total	C	N	O	0
			61	34	2	25	
8	C	5	Total	C	N	O	0
			61	34	2	25	
8	D	5	Total	C	N	O	0
			61	34	2	25	

- Molecule 9 is a polymer of unknown type called SUGAR (10-MER).

Mol	Chain	Residues	Atoms				AltConf
9	A	10	Total	C	N	O	0
			116	64	2	50	
9	C	10	Total	C	N	O	0
			116	64	2	50	
9	D	10	Total	C	N	O	0
			116	64	2	50	

- Molecule 10 is SUGAR (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
			14	8	1	5	
10	B	1	Total	C	N	O	0
			28	16	2	10	

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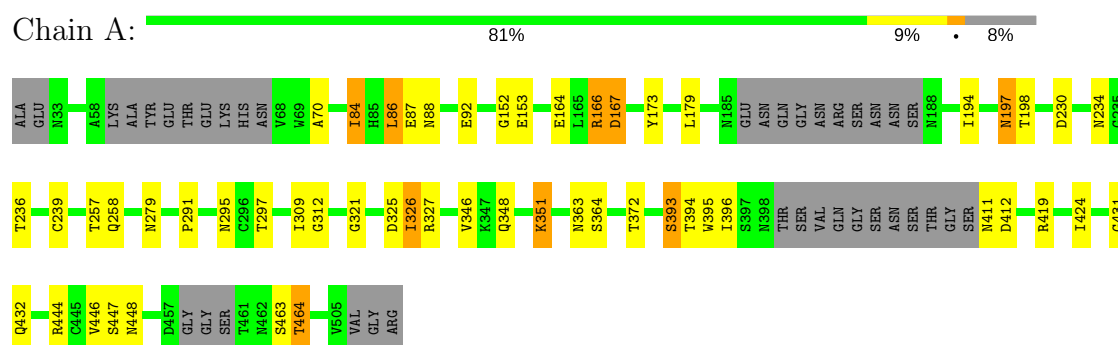
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Mol	Chain	Residues	Atoms				AltConf
10	B	1	Total	C	N	O	0
			28	16	2	10	
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	D	1	Total	C	N	O	0
			14	8	1	5	
10	E	1	Total	C	N	O	0
			28	16	2	10	
10	E	1	Total	C	N	O	0
			28	16	2	10	
10	F	1	Total	C	N	O	0
			28	16	2	10	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

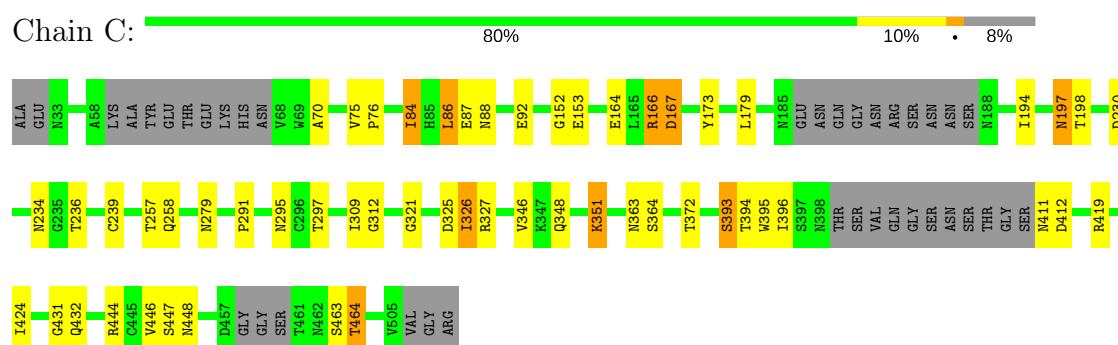
3 Residue-property plots

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.

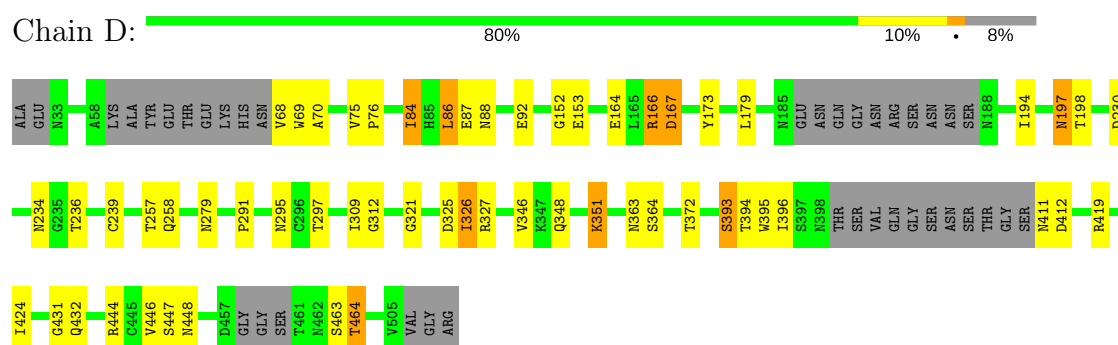
• Molecule 1: HIV-1 ENVELOPE GLYCOPROTEIN



• Molecule 1: HIV-1 ENVELOPE GLYCOPROTEIN

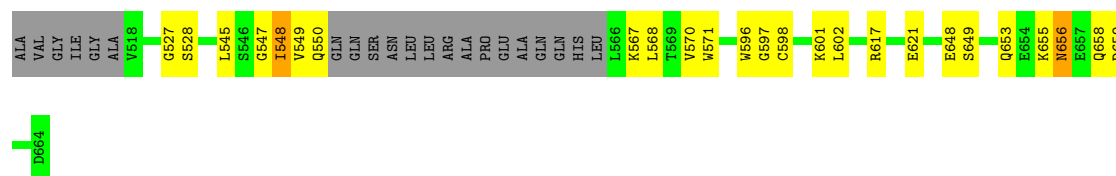


• Molecule 1: HIV-1 ENVELOPE GLYCOPROTEIN



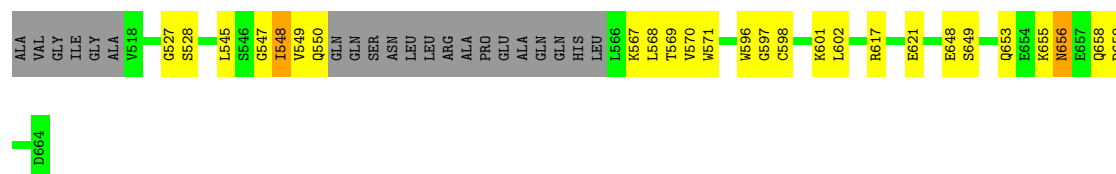
• Molecule 2: HIV-1 ENVELOPE GLYCOPROTEIN

Chain B:  70% 15% • 14%



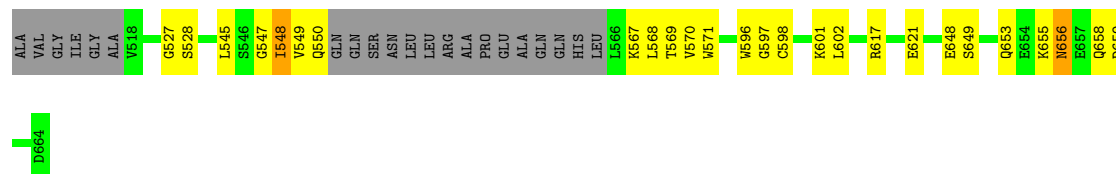
- Molecule 2: HIV-1 ENVELOPE GLYCOPROTEIN

Chain E:  69% 16% • 14%



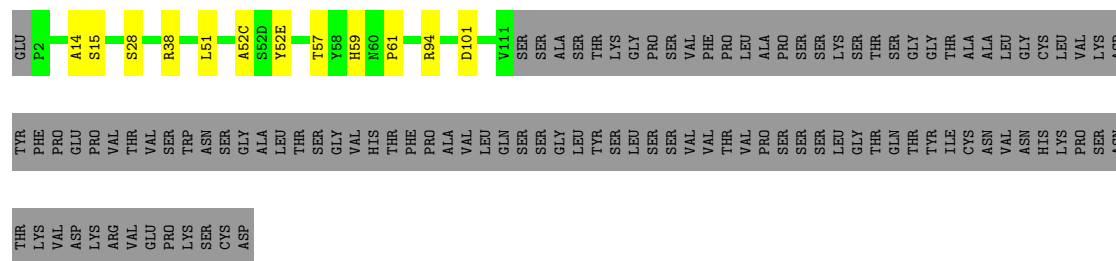
- Molecule 2: HIV-1 ENVELOPE GLYCOPROTEIN

Chain F:  69% 16% • 14%



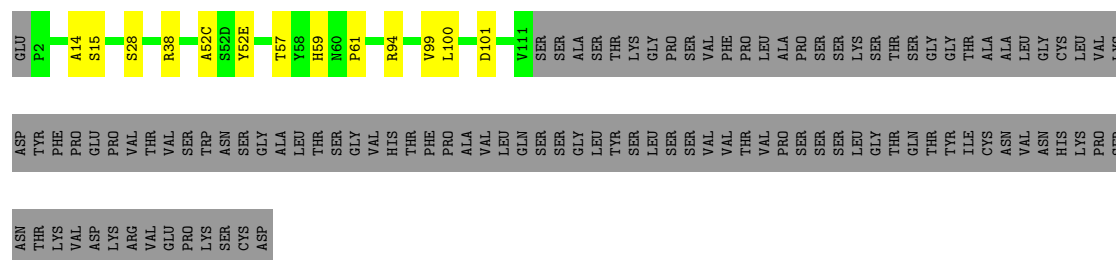
- Molecule 3: PGT128 FAB

Chain G:  50% 5% 45%

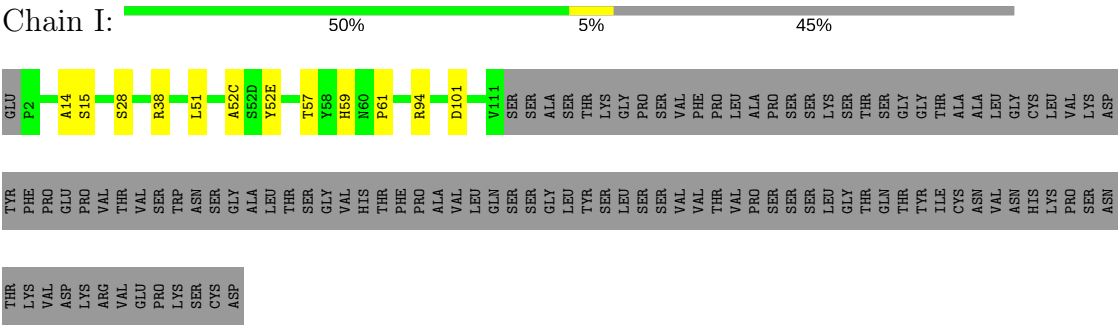


- Molecule 3: PGT128 FAB

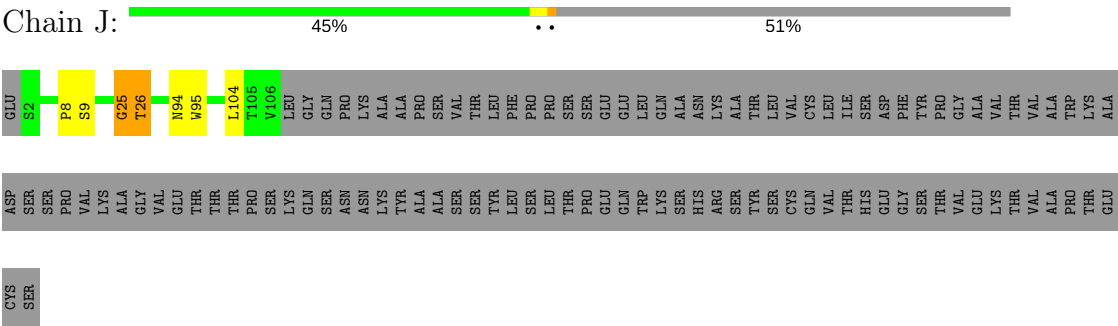
Chain H:  50% 5% 45%



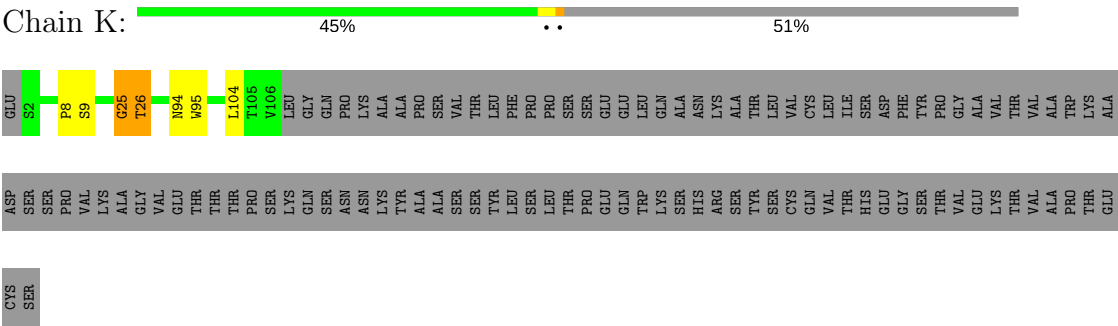
● Molecule 3: PGT128 FAB



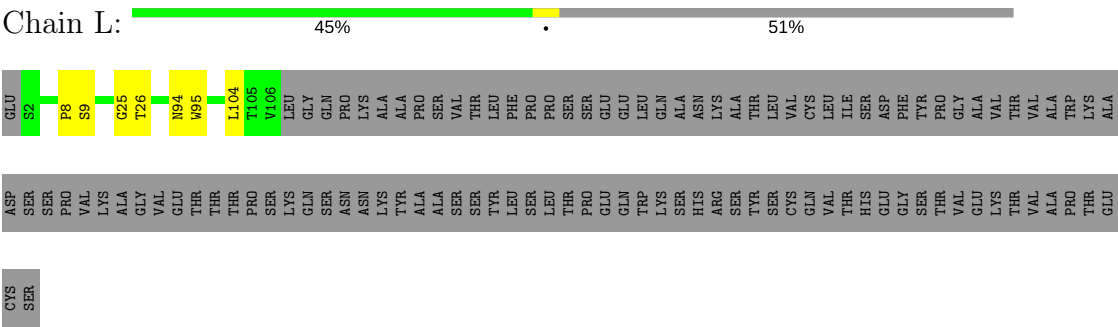
● Molecule 4: PGT128 FAB



● Molecule 4: PGT128 FAB



● Molecule 4: PGT128 FAB



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	WHOLE MICROGRAPH	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	22500	Depositor
Image detector	DIRECT ELECTRON DETECTOR	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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	0.64	2/3523 (0.1%)	0.73	15/4783 (0.3%)
1	C	0.64	2/3523 (0.1%)	0.73	15/4783 (0.3%)
1	D	0.64	2/3523 (0.1%)	0.73	15/4783 (0.3%)
2	B	0.72	1/1069 (0.1%)	0.81	5/1448 (0.3%)
2	E	0.72	1/1069 (0.1%)	0.81	5/1448 (0.3%)
2	F	0.72	1/1069 (0.1%)	0.81	5/1448 (0.3%)
3	G	0.66	0/1061	0.72	0/1455
3	H	0.65	0/1061	0.72	0/1455
3	I	0.65	0/1061	0.72	0/1455
4	J	0.75	2/769 (0.3%)	0.92	3/1048 (0.3%)
4	K	0.75	2/769 (0.3%)	0.92	3/1048 (0.3%)
4	L	0.75	2/769 (0.3%)	0.92	3/1048 (0.3%)
All	All	0.67	15/19266 (0.1%)	0.77	69/26202 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	658	GLN	C-N	12.04	1.61	1.34
2	F	658	GLN	C-N	12.04	1.61	1.34
2	E	658	GLN	C-N	12.00	1.61	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	8	PRO	C-N	10.79	1.58	1.34
4	J	8	PRO	C-N	10.77	1.58	1.34

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	648	GLU	N-CA-C	14.16	149.23	111.00
2	B	648	GLU	N-CA-C	14.16	149.22	111.00
2	F	648	GLU	N-CA-C	14.14	149.18	111.00
1	C	84	ILE	O-C-N	12.71	143.04	122.70
1	D	84	ILE	O-C-N	12.70	143.01	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	86	LEU	Mainchain
1	C	86	LEU	Mainchain
1	D	86	LEU	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3453	0	3390	72	0
1	C	3453	0	3390	77	0
1	D	3453	0	3390	72	0
2	B	1051	0	1037	34	0
2	E	1051	0	1037	34	0
2	F	1051	0	1037	34	0
3	G	1028	0	990	26	0
3	H	1028	0	990	26	0
3	I	1028	0	990	27	0
4	J	752	0	724	9	0
4	K	752	0	724	9	0
4	L	752	0	724	8	0
5	A	234	0	204	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	234	0	204	15	0
5	D	234	0	204	15	0
6	A	168	0	150	11	0
6	B	28	0	25	0	0
6	C	168	0	150	12	0
6	D	168	0	150	10	0
6	E	28	0	25	0	0
6	F	28	0	25	0	0
7	A	166	0	140	4	0
7	C	166	0	140	5	0
7	D	166	0	140	4	0
8	A	61	0	52	0	0
8	C	61	0	52	0	0
8	D	61	0	52	0	0
9	A	116	0	97	39	0
9	C	116	0	97	40	0
9	D	116	0	97	41	0
10	A	14	0	13	0	0
10	B	28	0	26	1	0
10	C	14	0	13	0	0
10	D	14	0	13	0	0
10	E	28	0	26	1	0
10	F	28	0	26	0	0
All	All	21297	0	20544	427	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 10.

The worst 5 of 427 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)
5:A:1088:NAG:H81	2:B:528:SER:HB3	1.24	1.15
5:D:1088:NAG:H81	2:F:528:SER:HB3	1.25	1.14
1:D:194:ILE:HD11	6:D:1197:NAG:O6	1.48	1.14
1:A:194:ILE:HD11	6:A:1197:NAG:O6	1.48	1.14
5:C:1088:NAG:H81	2:E:528:SER:HB3	1.24	1.10

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 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	428/476 (90%)	386 (90%)	33 (8%)	9 (2%)	8	47
1	C	428/476 (90%)	386 (90%)	33 (8%)	9 (2%)	8	47
1	D	428/476 (90%)	386 (90%)	33 (8%)	9 (2%)	8	47
2	B	128/153 (84%)	102 (80%)	22 (17%)	4 (3%)	5	39
2	E	128/153 (84%)	102 (80%)	22 (17%)	4 (3%)	5	39
2	F	128/153 (84%)	102 (80%)	22 (17%)	4 (3%)	5	39
3	G	130/239 (54%)	121 (93%)	9 (7%)	0	100	100
3	H	130/239 (54%)	121 (93%)	9 (7%)	0	100	100
3	I	130/239 (54%)	121 (93%)	9 (7%)	0	100	100
4	J	101/211 (48%)	91 (90%)	8 (8%)	2 (2%)	9	48
4	K	101/211 (48%)	91 (90%)	8 (8%)	2 (2%)	9	48
4	L	101/211 (48%)	91 (90%)	8 (8%)	2 (2%)	9	48
All	All	2361/3237 (73%)	2100 (89%)	216 (9%)	45 (2%)	14	49

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	ASP
1	A	396	ILE
1	C	167	ASP
1	C	396	ILE
1	D	167	ASP

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 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	393/423 (93%)	392 (100%)	1 (0%)	94	96
1	C	393/423 (93%)	392 (100%)	1 (0%)	94	96
1	D	393/423 (93%)	392 (100%)	1 (0%)	94	96
2	B	114/129 (88%)	114 (100%)	0	100	100
2	E	114/129 (88%)	114 (100%)	0	100	100
2	F	114/129 (88%)	114 (100%)	0	100	100
3	G	110/203 (54%)	110 (100%)	0	100	100
3	H	110/203 (54%)	110 (100%)	0	100	100
3	I	110/203 (54%)	110 (100%)	0	100	100
4	J	84/177 (48%)	84 (100%)	0	100	100
4	K	84/177 (48%)	84 (100%)	0	100	100
4	L	84/177 (48%)	84 (100%)	0	100	100
All	All	2103/2796 (75%)	2100 (100%)	3 (0%)	95	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	ASN
1	C	197	ASN
1	D	197	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	279	ASN
3	I	59	HIS
3	G	59	HIS
1	C	279	ASN
3	H	59	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 ⓘ

183 carbohydrates 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$
5	NAG	A	1088	1,5	14,14,15	0.49	0	15,19,21	2.60	3 (20%)
5	NAG	A	1089	5	14,14,15	0.50	0	15,19,21	1.19	2 (13%)
5	BMA	A	1090	5	11,11,12	0.62	0	13,15,17	1.50	3 (23%)
6	NAG	A	1133	1,6	14,14,15	0.49	0	15,19,21	2.60	3 (20%)
6	NAG	A	1134	6	14,14,15	0.50	0	15,19,21	1.19	2 (13%)
5	NAG	A	1156	1,5	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
5	NAG	A	1157	5	14,14,15	0.50	0	15,19,21	1.20	2 (13%)
5	BMA	A	1158	5	11,11,12	0.63	0	13,15,17	1.50	3 (23%)
5	NAG	A	1160	1,5	14,14,15	0.49	0	15,19,21	2.60	3 (20%)
5	NAG	A	1161	5	14,14,15	0.50	0	15,19,21	1.17	2 (13%)
5	BMA	A	1162	5	11,11,12	0.64	0	13,15,17	1.51	3 (23%)
6	NAG	A	1197	1,6	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
6	NAG	A	1198	6	14,14,15	0.51	0	15,19,21	1.17	2 (13%)
6	NAG	A	1234	1,6	14,14,15	0.50	0	15,19,21	2.61	3 (20%)
6	NAG	A	1235	6	14,14,15	0.49	0	15,19,21	1.20	2 (13%)
7	NAG	A	1262	1,7	14,14,15	0.58	0	15,19,21	0.74	0
7	NAG	A	1263	7	14,14,15	0.56	0	15,19,21	0.89	0
7	BMA	A	1264	7	11,11,12	0.64	0	13,15,17	0.70	0
7	MAN	A	1265	7	11,11,12	0.65	0	13,15,17	0.82	0
7	MAN	A	1266	7	11,11,12	0.60	0	13,15,17	0.56	0
7	MAN	A	1267	7	11,11,12	0.60	0	13,15,17	0.62	0
7	MAN	A	1268	7	11,11,12	0.52	0	13,15,17	0.68	0
5	NAG	A	1276	1,5	14,14,15	0.48	0	15,19,21	2.60	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1277	5	14,14,15	0.50	0	15,19,21	1.18	2 (13%)
5	BMA	A	1278	5	11,11,12	0.62	0	13,15,17	1.50	3 (23%)
8	NAG	A	1295	1,8	14,14,15	0.49	0	15,19,21	2.60	3 (20%)
8	NAG	A	1296	8	14,14,15	0.50	0	15,19,21	1.19	2 (13%)
8	BMA	A	1297	8	11,11,12	0.63	0	13,15,17	1.50	3 (23%)
8	MAN	A	1298	8	11,11,12	0.54	0	13,15,17	1.62	3 (23%)
8	MAN	A	1299	8	11,11,12	0.61	0	13,15,17	2.58	3 (23%)
7	NAG	A	1301	1,7	14,14,15	0.31	0	15,19,21	0.95	1 (6%)
7	NAG	A	1302	7	14,14,15	0.31	0	15,19,21	2.58	4 (26%)
7	BMA	A	1303	7	11,11,12	0.44	0	13,15,17	1.34	2 (15%)
7	MAN	A	1304	7	11,11,12	0.32	0	13,15,17	1.35	2 (15%)
7	MAN	A	1305	7	11,11,12	0.44	0	13,15,17	0.96	1 (7%)
7	MAN	A	1306	7	11,11,12	0.44	0	13,15,17	0.89	1 (7%)
7	MAN	A	1308	7	11,11,12	0.48	0	13,15,17	0.86	1 (7%)
9	NAG	A	1332	1,9	14,14,15	0.30	0	15,19,21	0.96	2 (13%)
9	NAG	A	1333	9	14,14,15	0.32	0	15,19,21	1.03	1 (6%)
9	BMA	A	1334	9	11,11,12	0.41	0	13,15,17	0.64	0
9	MAN	A	1335	9	11,11,12	0.42	0	13,15,17	1.11	1 (7%)
9	MAN	A	1336	9	11,11,12	0.28	0	13,15,17	1.16	1 (7%)
9	MAN	A	1337	9	11,11,12	0.33	0	13,15,17	0.95	2 (15%)
9	MAN	A	1339	9	11,11,12	0.46	0	13,15,17	1.11	2 (15%)
9	MAN	A	1340	9	11,11,12	0.49	0	13,15,17	1.24	1 (7%)
9	MAN	A	1341	9	11,11,12	0.37	0	13,15,17	1.33	1 (7%)
9	MAN	A	1342	9	11,11,12	0.33	0	13,15,17	0.82	0
6	NAG	A	1355	1,6	14,14,15	0.50	0	15,19,21	2.61	3 (20%)
6	NAG	A	1356	6	14,14,15	0.50	0	15,19,21	1.19	2 (13%)
5	NAG	A	1363	1,5	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
5	NAG	A	1364	5	14,14,15	0.50	0	15,19,21	1.19	2 (13%)
5	BMA	A	1365	5	11,11,12	0.63	0	13,15,17	1.51	3 (23%)
5	NAG	A	1386	1,5	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
5	NAG	A	1387	5	14,14,15	0.49	0	15,19,21	1.19	2 (13%)
5	BMA	A	1388	5	11,11,12	0.63	0	13,15,17	1.51	3 (23%)
6	NAG	A	1392	1,6	14,14,15	0.49	0	15,19,21	2.60	3 (20%)
6	NAG	A	1393	6	14,14,15	0.50	0	15,19,21	1.20	2 (13%)
6	NAG	A	1448	1,6	14,14,15	0.49	0	15,19,21	2.61	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	1449	6	14,14,15	0.51	0	15,19,21	1.19	2 (13%)
6	NAG	B	1611	2,6	14,14,15	0.50	0	15,19,21	2.61	3 (20%)
6	NAG	B	1612	6	14,14,15	0.51	0	15,19,21	1.19	2 (13%)
5	NAG	C	1088	1,5	14,14,15	0.48	0	15,19,21	2.60	3 (20%)
5	NAG	C	1089	5	14,14,15	0.50	0	15,19,21	1.20	2 (13%)
5	BMA	C	1090	5	11,11,12	0.62	0	13,15,17	1.51	3 (23%)
6	NAG	C	1133	1,6	14,14,15	0.49	0	15,19,21	2.60	3 (20%)
6	NAG	C	1134	6	14,14,15	0.50	0	15,19,21	1.20	2 (13%)
5	NAG	C	1156	1,5	14,14,15	0.50	0	15,19,21	2.61	3 (20%)
5	NAG	C	1157	5	14,14,15	0.50	0	15,19,21	1.19	2 (13%)
5	BMA	C	1158	5	11,11,12	0.62	0	13,15,17	1.49	3 (23%)
5	NAG	C	1160	1,5	14,14,15	0.49	0	15,19,21	2.60	3 (20%)
5	NAG	C	1161	5	14,14,15	0.50	0	15,19,21	1.18	2 (13%)
5	BMA	C	1162	5	11,11,12	0.64	0	13,15,17	1.50	3 (23%)
6	NAG	C	1197	1,6	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
6	NAG	C	1198	6	14,14,15	0.53	0	15,19,21	1.17	2 (13%)
6	NAG	C	1234	1,6	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
6	NAG	C	1235	6	14,14,15	0.48	0	15,19,21	1.20	2 (13%)
7	NAG	C	1262	1,7	14,14,15	0.58	0	15,19,21	0.73	0
7	NAG	C	1263	7	14,14,15	0.55	0	15,19,21	0.90	0
7	BMA	C	1264	7	11,11,12	0.64	0	13,15,17	0.71	0
7	MAN	C	1265	7	11,11,12	0.64	0	13,15,17	0.82	0
7	MAN	C	1266	7	11,11,12	0.62	0	13,15,17	0.57	0
7	MAN	C	1267	7	11,11,12	0.60	0	13,15,17	0.61	0
7	MAN	C	1268	7	11,11,12	0.52	0	13,15,17	0.67	0
5	NAG	C	1276	1,5	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
5	NAG	C	1277	5	14,14,15	0.50	0	15,19,21	1.19	2 (13%)
5	BMA	C	1278	5	11,11,12	0.62	0	13,15,17	1.50	3 (23%)
8	NAG	C	1295	1,8	14,14,15	0.48	0	15,19,21	2.60	3 (20%)
8	NAG	C	1296	8	14,14,15	0.51	0	15,19,21	1.18	2 (13%)
8	BMA	C	1297	8	11,11,12	0.64	0	13,15,17	1.50	3 (23%)
8	MAN	C	1298	8	11,11,12	0.54	0	13,15,17	1.61	3 (23%)
8	MAN	C	1299	8	11,11,12	0.63	0	13,15,17	2.57	3 (23%)
7	NAG	C	1301	1,7	14,14,15	0.31	0	15,19,21	0.95	1 (6%)
7	NAG	C	1302	7	14,14,15	0.31	0	15,19,21	2.58	4 (26%)
7	BMA	C	1303	7	11,11,12	0.44	0	13,15,17	1.34	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	C	1304	7	11,11,12	0.32	0	13,15,17	1.36	2 (15%)
7	MAN	C	1305	7	11,11,12	0.44	0	13,15,17	0.95	1 (7%)
7	MAN	C	1306	7	11,11,12	0.45	0	13,15,17	0.88	1 (7%)
7	MAN	C	1308	7	11,11,12	0.47	0	13,15,17	0.86	1 (7%)
9	NAG	C	1332	1,9	14,14,15	0.31	0	15,19,21	0.97	2 (13%)
9	NAG	C	1333	9	14,14,15	0.33	0	15,19,21	1.02	1 (6%)
9	BMA	C	1334	9	11,11,12	0.41	0	13,15,17	0.63	0
9	MAN	C	1335	9	11,11,12	0.42	0	13,15,17	1.12	1 (7%)
9	MAN	C	1336	9	11,11,12	0.28	0	13,15,17	1.16	1 (7%)
9	MAN	C	1337	9	11,11,12	0.33	0	13,15,17	0.96	2 (15%)
9	MAN	C	1339	9	11,11,12	0.46	0	13,15,17	1.11	2 (15%)
9	MAN	C	1340	9	11,11,12	0.49	0	13,15,17	1.24	1 (7%)
9	MAN	C	1341	9	11,11,12	0.38	0	13,15,17	1.33	1 (7%)
9	MAN	C	1342	9	11,11,12	0.33	0	13,15,17	0.83	0
6	NAG	C	1355	1,6	14,14,15	0.50	0	15,19,21	2.61	3 (20%)
6	NAG	C	1356	6	14,14,15	0.50	0	15,19,21	1.20	2 (13%)
5	NAG	C	1363	1,5	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
5	NAG	C	1364	5	14,14,15	0.51	0	15,19,21	1.19	2 (13%)
5	BMA	C	1365	5	11,11,12	0.63	0	13,15,17	1.50	3 (23%)
5	NAG	C	1386	1,5	14,14,15	0.48	0	15,19,21	2.61	3 (20%)
5	NAG	C	1387	5	14,14,15	0.49	0	15,19,21	1.20	2 (13%)
5	BMA	C	1388	5	11,11,12	0.63	0	13,15,17	1.51	3 (23%)
6	NAG	C	1392	1,6	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
6	NAG	C	1393	6	14,14,15	0.50	0	15,19,21	1.20	2 (13%)
6	NAG	C	1448	1,6	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
6	NAG	C	1449	6	14,14,15	0.50	0	15,19,21	1.19	2 (13%)
5	NAG	D	1088	1,5	14,14,15	0.48	0	15,19,21	2.60	3 (20%)
5	NAG	D	1089	5	14,14,15	0.50	0	15,19,21	1.19	2 (13%)
5	BMA	D	1090	5	11,11,12	0.62	0	13,15,17	1.51	3 (23%)
6	NAG	D	1133	1,6	14,14,15	0.48	0	15,19,21	2.61	3 (20%)
6	NAG	D	1134	6	14,14,15	0.50	0	15,19,21	1.19	2 (13%)
5	NAG	D	1156	1,5	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
5	NAG	D	1157	5	14,14,15	0.50	0	15,19,21	1.20	2 (13%)
5	BMA	D	1158	5	11,11,12	0.63	0	13,15,17	1.50	3 (23%)
5	NAG	D	1160	1,5	14,14,15	0.49	0	15,19,21	2.60	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	D	1161	5	14,14,15	0.49	0	15,19,21	1.17	2 (13%)
5	BMA	D	1162	5	11,11,12	0.64	0	13,15,17	1.51	3 (23%)
6	NAG	D	1197	1,6	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
6	NAG	D	1198	6	14,14,15	0.51	0	15,19,21	1.18	2 (13%)
6	NAG	D	1234	1,6	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
6	NAG	D	1235	6	14,14,15	0.49	0	15,19,21	1.19	2 (13%)
7	NAG	D	1262	1,7	14,14,15	0.58	0	15,19,21	0.74	0
7	NAG	D	1263	7	14,14,15	0.56	0	15,19,21	0.89	0
7	BMA	D	1264	7	11,11,12	0.65	0	13,15,17	0.69	0
7	MAN	D	1265	7	11,11,12	0.65	0	13,15,17	0.83	0
7	MAN	D	1266	7	11,11,12	0.61	0	13,15,17	0.57	0
7	MAN	D	1267	7	11,11,12	0.59	0	13,15,17	0.62	0
7	MAN	D	1268	7	11,11,12	0.52	0	13,15,17	0.68	0
5	NAG	D	1276	1,5	14,14,15	0.48	0	15,19,21	2.61	3 (20%)
5	NAG	D	1277	5	14,14,15	0.50	0	15,19,21	1.18	2 (13%)
5	BMA	D	1278	5	11,11,12	0.62	0	13,15,17	1.51	3 (23%)
8	NAG	D	1295	1,8	14,14,15	0.47	0	15,19,21	2.61	3 (20%)
8	NAG	D	1296	8	14,14,15	0.50	0	15,19,21	1.18	2 (13%)
8	BMA	D	1297	8	11,11,12	0.62	0	13,15,17	1.50	3 (23%)
8	MAN	D	1298	8	11,11,12	0.54	0	13,15,17	1.61	3 (23%)
8	MAN	D	1299	8	11,11,12	0.61	0	13,15,17	2.58	3 (23%)
7	NAG	D	1301	1,7	14,14,15	0.30	0	15,19,21	0.95	1 (6%)
7	NAG	D	1302	7	14,14,15	0.31	0	15,19,21	2.58	4 (26%)
7	BMA	D	1303	7	11,11,12	0.44	0	13,15,17	1.34	2 (15%)
7	MAN	D	1304	7	11,11,12	0.33	0	13,15,17	1.36	2 (15%)
7	MAN	D	1305	7	11,11,12	0.44	0	13,15,17	0.96	1 (7%)
7	MAN	D	1306	7	11,11,12	0.43	0	13,15,17	0.90	1 (7%)
7	MAN	D	1308	7	11,11,12	0.48	0	13,15,17	0.85	1 (7%)
9	NAG	D	1332	1,9	14,14,15	0.31	0	15,19,21	0.96	1 (6%)
9	NAG	D	1333	9	14,14,15	0.33	0	15,19,21	1.03	1 (6%)
9	BMA	D	1334	9	11,11,12	0.41	0	13,15,17	0.64	0
9	MAN	D	1335	9	11,11,12	0.42	0	13,15,17	1.11	1 (7%)
9	MAN	D	1336	9	11,11,12	0.28	0	13,15,17	1.16	1 (7%)
9	MAN	D	1337	9	11,11,12	0.33	0	13,15,17	0.95	2 (15%)
9	MAN	D	1339	9	11,11,12	0.46	0	13,15,17	1.11	2 (15%)
9	MAN	D	1340	9	11,11,12	0.49	0	13,15,17	1.24	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MAN	D	1341	9	11,11,12	0.37	0	13,15,17	1.33	1 (7%)
9	MAN	D	1342	9	11,11,12	0.34	0	13,15,17	0.82	0
6	NAG	D	1355	1,6	14,14,15	0.50	0	15,19,21	2.61	3 (20%)
6	NAG	D	1356	6	14,14,15	0.50	0	15,19,21	1.19	2 (13%)
5	NAG	D	1363	1,5	14,14,15	0.48	0	15,19,21	2.61	3 (20%)
5	NAG	D	1364	5	14,14,15	0.50	0	15,19,21	1.18	2 (13%)
5	BMA	D	1365	5	11,11,12	0.63	0	13,15,17	1.51	3 (23%)
5	NAG	D	1386	1,5	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
5	NAG	D	1387	5	14,14,15	0.50	0	15,19,21	1.19	2 (13%)
5	BMA	D	1388	5	11,11,12	0.64	0	13,15,17	1.51	3 (23%)
6	NAG	D	1392	1,6	14,14,15	0.50	0	15,19,21	2.60	3 (20%)
6	NAG	D	1393	6	14,14,15	0.51	0	15,19,21	1.20	2 (13%)
6	NAG	D	1448	1,6	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
6	NAG	D	1449	6	14,14,15	0.50	0	15,19,21	1.19	2 (13%)
6	NAG	E	1611	2,6	14,14,15	0.51	0	15,19,21	2.60	3 (20%)
6	NAG	E	1612	6	14,14,15	0.51	0	15,19,21	1.19	2 (13%)
6	NAG	F	1611	2,6	14,14,15	0.50	0	15,19,21	2.60	3 (20%)
6	NAG	F	1612	6	14,14,15	0.51	0	15,19,21	1.18	2 (13%)

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	NAG	A	1088	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1089	5	-	0/6/23/26	0/1/1/1
5	BMA	A	1090	5	-	0/2/19/22	0/1/1/1
6	NAG	A	1133	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1134	6	-	0/6/23/26	0/1/1/1
5	NAG	A	1156	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1157	5	-	0/6/23/26	0/1/1/1
5	BMA	A	1158	5	-	0/2/19/22	0/1/1/1
5	NAG	A	1160	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1161	5	-	0/6/23/26	0/1/1/1
5	BMA	A	1162	5	-	0/2/19/22	0/1/1/1
6	NAG	A	1197	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1198	6	-	0/6/23/26	0/1/1/1
6	NAG	A	1234	1,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1235	6	-	0/6/23/26	0/1/1/1
7	NAG	A	1262	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1263	7	-	0/6/23/26	0/1/1/1
7	BMA	A	1264	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1265	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1266	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1267	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1268	7	-	0/2/19/22	0/1/1/1
5	NAG	A	1276	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1277	5	-	0/6/23/26	0/1/1/1
5	BMA	A	1278	5	-	0/2/19/22	0/1/1/1
8	NAG	A	1295	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	1296	8	-	0/6/23/26	0/1/1/1
8	BMA	A	1297	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1298	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1299	8	-	0/2/19/22	0/1/1/1
7	NAG	A	1301	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1302	7	-	0/6/23/26	0/1/1/1
7	BMA	A	1303	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1304	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1305	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1306	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1308	7	-	0/2/19/22	0/1/1/1
9	NAG	A	1332	1,9	-	0/6/23/26	0/1/1/1
9	NAG	A	1333	9	-	0/6/23/26	0/1/1/1
9	BMA	A	1334	9	-	0/2/19/22	0/1/1/1
9	MAN	A	1335	9	-	0/2/19/22	0/1/1/1
9	MAN	A	1336	9	-	0/2/19/22	0/1/1/1
9	MAN	A	1337	9	-	0/2/19/22	0/1/1/1
9	MAN	A	1339	9	-	0/2/19/22	0/1/1/1
9	MAN	A	1340	9	-	0/2/19/22	0/1/1/1
9	MAN	A	1341	9	-	0/2/19/22	0/1/1/1
9	MAN	A	1342	9	-	0/2/19/22	0/1/1/1
6	NAG	A	1355	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1356	6	-	0/6/23/26	0/1/1/1
5	NAG	A	1363	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1364	5	-	0/6/23/26	0/1/1/1
5	BMA	A	1365	5	-	0/2/19/22	0/1/1/1
5	NAG	A	1386	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1387	5	-	0/6/23/26	0/1/1/1
5	BMA	A	1388	5	-	0/2/19/22	0/1/1/1
6	NAG	A	1392	1,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1393	6	-	0/6/23/26	0/1/1/1
6	NAG	A	1448	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1449	6	-	0/6/23/26	0/1/1/1
6	NAG	B	1611	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1612	6	-	0/6/23/26	0/1/1/1
5	NAG	C	1088	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1089	5	-	0/6/23/26	0/1/1/1
5	BMA	C	1090	5	-	0/2/19/22	0/1/1/1
6	NAG	C	1133	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	1134	6	-	0/6/23/26	0/1/1/1
5	NAG	C	1156	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1157	5	-	0/6/23/26	0/1/1/1
5	BMA	C	1158	5	-	0/2/19/22	0/1/1/1
5	NAG	C	1160	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1161	5	-	0/6/23/26	0/1/1/1
5	BMA	C	1162	5	-	0/2/19/22	0/1/1/1
6	NAG	C	1197	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	1198	6	-	0/6/23/26	0/1/1/1
6	NAG	C	1234	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	1235	6	-	0/6/23/26	0/1/1/1
7	NAG	C	1262	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	1263	7	-	0/6/23/26	0/1/1/1
7	BMA	C	1264	7	-	0/2/19/22	0/1/1/1
7	MAN	C	1265	7	-	0/2/19/22	0/1/1/1
7	MAN	C	1266	7	-	0/2/19/22	0/1/1/1
7	MAN	C	1267	7	-	0/2/19/22	0/1/1/1
7	MAN	C	1268	7	-	0/2/19/22	0/1/1/1
5	NAG	C	1276	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1277	5	-	0/6/23/26	0/1/1/1
5	BMA	C	1278	5	-	0/2/19/22	0/1/1/1
8	NAG	C	1295	1,8	-	0/6/23/26	0/1/1/1
8	NAG	C	1296	8	-	0/6/23/26	0/1/1/1
8	BMA	C	1297	8	-	0/2/19/22	0/1/1/1
8	MAN	C	1298	8	-	0/2/19/22	0/1/1/1
8	MAN	C	1299	8	-	0/2/19/22	0/1/1/1
7	NAG	C	1301	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	1302	7	-	0/6/23/26	0/1/1/1
7	BMA	C	1303	7	-	0/2/19/22	0/1/1/1
7	MAN	C	1304	7	-	0/2/19/22	0/1/1/1
7	MAN	C	1305	7	-	0/2/19/22	0/1/1/1
7	MAN	C	1306	7	-	0/2/19/22	0/1/1/1
7	MAN	C	1308	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	C	1332	1,9	-	0/6/23/26	0/1/1/1
9	NAG	C	1333	9	-	0/6/23/26	0/1/1/1
9	BMA	C	1334	9	-	0/2/19/22	0/1/1/1
9	MAN	C	1335	9	-	0/2/19/22	0/1/1/1
9	MAN	C	1336	9	-	0/2/19/22	0/1/1/1
9	MAN	C	1337	9	-	0/2/19/22	0/1/1/1
9	MAN	C	1339	9	-	0/2/19/22	0/1/1/1
9	MAN	C	1340	9	-	0/2/19/22	0/1/1/1
9	MAN	C	1341	9	-	0/2/19/22	0/1/1/1
9	MAN	C	1342	9	-	0/2/19/22	0/1/1/1
6	NAG	C	1355	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	1356	6	-	0/6/23/26	0/1/1/1
5	NAG	C	1363	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1364	5	-	0/6/23/26	0/1/1/1
5	BMA	C	1365	5	-	0/2/19/22	0/1/1/1
5	NAG	C	1386	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1387	5	-	0/6/23/26	0/1/1/1
5	BMA	C	1388	5	-	0/2/19/22	0/1/1/1
6	NAG	C	1392	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	1393	6	-	0/6/23/26	0/1/1/1
6	NAG	C	1448	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	1449	6	-	0/6/23/26	0/1/1/1
5	NAG	D	1088	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	1089	5	-	0/6/23/26	0/1/1/1
5	BMA	D	1090	5	-	0/2/19/22	0/1/1/1
6	NAG	D	1133	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	1134	6	-	0/6/23/26	0/1/1/1
5	NAG	D	1156	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	1157	5	-	0/6/23/26	0/1/1/1
5	BMA	D	1158	5	-	0/2/19/22	0/1/1/1
5	NAG	D	1160	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	1161	5	-	0/6/23/26	0/1/1/1
5	BMA	D	1162	5	-	0/2/19/22	0/1/1/1
6	NAG	D	1197	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	1198	6	-	0/6/23/26	0/1/1/1
6	NAG	D	1234	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	1235	6	-	0/6/23/26	0/1/1/1
7	NAG	D	1262	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	1263	7	-	0/6/23/26	0/1/1/1
7	BMA	D	1264	7	-	0/2/19/22	0/1/1/1
7	MAN	D	1265	7	-	0/2/19/22	0/1/1/1
7	MAN	D	1266	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	D	1267	7	-	0/2/19/22	0/1/1/1
7	MAN	D	1268	7	-	0/2/19/22	0/1/1/1
5	NAG	D	1276	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	1277	5	-	0/6/23/26	0/1/1/1
5	BMA	D	1278	5	-	0/2/19/22	0/1/1/1
8	NAG	D	1295	1,8	-	0/6/23/26	0/1/1/1
8	NAG	D	1296	8	-	0/6/23/26	0/1/1/1
8	BMA	D	1297	8	-	0/2/19/22	0/1/1/1
8	MAN	D	1298	8	-	0/2/19/22	0/1/1/1
8	MAN	D	1299	8	-	0/2/19/22	0/1/1/1
7	NAG	D	1301	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	1302	7	-	0/6/23/26	0/1/1/1
7	BMA	D	1303	7	-	0/2/19/22	0/1/1/1
7	MAN	D	1304	7	-	0/2/19/22	0/1/1/1
7	MAN	D	1305	7	-	0/2/19/22	0/1/1/1
7	MAN	D	1306	7	-	0/2/19/22	0/1/1/1
7	MAN	D	1308	7	-	0/2/19/22	0/1/1/1
9	NAG	D	1332	1,9	-	0/6/23/26	0/1/1/1
9	NAG	D	1333	9	-	0/6/23/26	0/1/1/1
9	BMA	D	1334	9	-	0/2/19/22	0/1/1/1
9	MAN	D	1335	9	-	0/2/19/22	0/1/1/1
9	MAN	D	1336	9	-	0/2/19/22	0/1/1/1
9	MAN	D	1337	9	-	0/2/19/22	0/1/1/1
9	MAN	D	1339	9	-	0/2/19/22	0/1/1/1
9	MAN	D	1340	9	-	0/2/19/22	0/1/1/1
9	MAN	D	1341	9	-	0/2/19/22	0/1/1/1
9	MAN	D	1342	9	-	0/2/19/22	0/1/1/1
6	NAG	D	1355	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	1356	6	-	0/6/23/26	0/1/1/1
5	NAG	D	1363	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	1364	5	-	0/6/23/26	0/1/1/1
5	BMA	D	1365	5	-	0/2/19/22	0/1/1/1
5	NAG	D	1386	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	1387	5	-	0/6/23/26	0/1/1/1
5	BMA	D	1388	5	-	0/2/19/22	0/1/1/1
6	NAG	D	1392	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	1393	6	-	0/6/23/26	0/1/1/1
6	NAG	D	1448	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	1449	6	-	0/6/23/26	0/1/1/1
6	NAG	E	1611	2,6	-	0/6/23/26	0/1/1/1
6	NAG	E	1612	6	-	0/6/23/26	0/1/1/1
6	NAG	F	1611	2,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	F	1612	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 359 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1133	NAG	O5-C1-C2	-8.53	99.60	111.47
5	C	1386	NAG	O5-C1-C2	-8.52	99.62	111.47
5	D	1156	NAG	O5-C1-C2	-8.51	99.63	111.47
5	A	1386	NAG	O5-C1-C2	-8.51	99.63	111.47
5	D	1386	NAG	O5-C1-C2	-8.51	99.64	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

54 monomers are involved in 211 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1088	NAG	8	0
5	A	1156	NAG	1	0
6	A	1197	NAG	4	0
6	A	1198	NAG	1	0
6	A	1234	NAG	1	0
6	A	1235	NAG	1	0
7	A	1262	NAG	2	0
7	A	1263	NAG	1	0
5	A	1276	NAG	5	0
5	A	1277	NAG	2	0
7	A	1301	NAG	1	0
7	A	1308	MAN	1	0
9	A	1332	NAG	14	0
9	A	1339	MAN	4	0
9	A	1340	MAN	17	0
9	A	1342	MAN	4	0
5	A	1363	NAG	1	0
6	A	1448	NAG	6	0
5	C	1088	NAG	8	0
5	C	1156	NAG	1	0
6	C	1197	NAG	4	0
6	C	1198	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1234	NAG	1	0
6	C	1235	NAG	1	0
7	C	1262	NAG	3	0
7	C	1263	NAG	1	0
5	C	1276	NAG	5	0
5	C	1277	NAG	2	0
7	C	1301	NAG	1	0
7	C	1308	MAN	1	0
9	C	1332	NAG	15	0
9	C	1339	MAN	4	0
9	C	1340	MAN	17	0
9	C	1342	MAN	4	0
5	C	1363	NAG	1	0
6	C	1448	NAG	7	0
5	D	1088	NAG	8	0
5	D	1156	NAG	1	0
6	D	1197	NAG	3	0
6	D	1198	NAG	1	0
6	D	1234	NAG	1	0
6	D	1235	NAG	1	0
7	D	1262	NAG	2	0
7	D	1263	NAG	1	0
5	D	1276	NAG	5	0
5	D	1277	NAG	2	0
7	D	1301	NAG	1	0
7	D	1308	MAN	1	0
9	D	1332	NAG	15	0
9	D	1339	MAN	4	0
9	D	1340	MAN	18	0
9	D	1342	MAN	4	0
5	D	1363	NAG	1	0
6	D	1448	NAG	6	0

5.6 Ligand geometry

9 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
10	NAG	A	1343	1	14,14,15	0.50	0	15,19,21	2.61	3 (20%)
10	NAG	B	1618	2	14,14,15	0.50	0	15,19,21	2.62	3 (20%)
10	NAG	B	1637	2	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
10	NAG	C	1343	1	14,14,15	0.49	0	15,19,21	2.62	3 (20%)
10	NAG	D	1343	1	14,14,15	0.51	0	15,19,21	2.60	3 (20%)
10	NAG	E	1618	2	14,14,15	0.50	0	15,19,21	2.61	3 (20%)
10	NAG	E	1637	2	14,14,15	0.48	0	15,19,21	2.61	3 (20%)
10	NAG	F	1618	2	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
10	NAG	F	1637	2	14,14,15	0.49	0	15,19,21	2.61	3 (20%)

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
10	NAG	A	1343	1	-	0/6/23/26	0/1/1/1
10	NAG	B	1618	2	-	0/6/23/26	0/1/1/1
10	NAG	B	1637	2	-	0/6/23/26	0/1/1/1
10	NAG	C	1343	1	-	0/6/23/26	0/1/1/1
10	NAG	D	1343	1	-	0/6/23/26	0/1/1/1
10	NAG	E	1618	2	-	0/6/23/26	0/1/1/1
10	NAG	E	1637	2	-	0/6/23/26	0/1/1/1
10	NAG	F	1618	2	-	0/6/23/26	0/1/1/1
10	NAG	F	1637	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1343	NAG	O5-C1-C2	-8.52	99.61	111.47
10	B	1618	NAG	O5-C1-C2	-8.52	99.62	111.47
10	E	1637	NAG	O5-C1-C2	-8.51	99.63	111.47
10	F	1618	NAG	O5-C1-C2	-8.51	99.64	111.47
10	A	1343	NAG	O5-C1-C2	-8.50	99.64	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1618	NAG	1	0
10	E	1618	NAG	1	0

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.