



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:20 PM BST

PDB ID : 5FUU  
EMDB ID: : EMD-3308  
Title : Ectodomain of cleaved wild type JR-FL EnvDCT trimer in complex with PGT151 Fab  
Authors : Lee, J.H.; Ward, A.B.  
Deposited on : 2016-01-29  
Resolution : 4.20 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

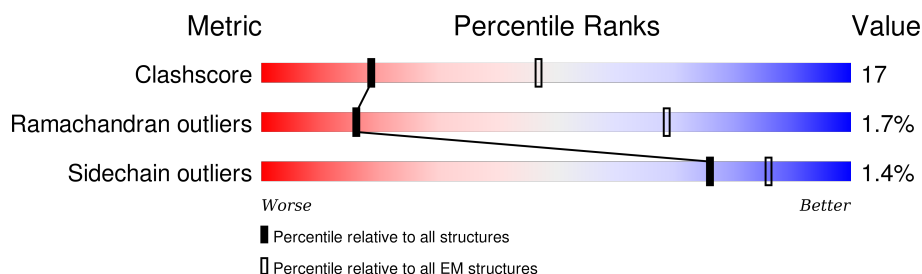
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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  $\geq 3$ , 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	473	
1	C	473	
1	E	473	
2	B	153	
2	D	153	
2	F	153	
3	H	240	
3	M	240	
4	L	219	

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Mol	Chain	Length	Quality of chain
4	N	219	

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
10	NAG	B	1638	-	-	X	-
10	NAG	B	1641	-	-	X	-
11	NAG	C	1241	-	-	X	-
13	FUC	D	1613	-	-	X	-
15	NAG	E	1387	-	-	X	-
16	NAG	F	1638	-	-	X	-
5	NAG	A	1088	-	-	X	-
5	NAG	A	1339	-	-	X	-
5	NAG	C	1156	-	-	X	-
5	NAG	C	1157	-	-	X	-
5	NAG	C	1392	-	-	X	-
5	NAG	E	1160	-	-	X	-
5	NAG	E	1339	-	-	X	-
5	NAG	E	1355	-	-	X	-
6	NAG	E	1397	-	-	X	-
7	NAG	A	1156	-	-	X	-
7	NAG	C	1160	-	-	X	-
7	NAG	C	1301	-	-	X	-

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 20735 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 GP160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	449	Total	C	N	O	S	0	0
			3553	2233	624	671	25		
1	C	444	Total	C	N	O	S	0	0
			3506	2208	613	660	25		
1	E	448	Total	C	N	O	S	0	0
			3537	2224	620	668	25		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	THR	VAL	ENGINEERED MUTATION	UNP Q75760
C	31	THR	VAL	ENGINEERED MUTATION	UNP Q75760
E	31	THR	VAL	ENGINEERED MUTATION	UNP Q75760

- Molecule 2 is a protein called HIV-1 ENVELOPE GLYCOPROTEIN GP160.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	144	Total	C	N	O	S	0	0
			1150	722	200	221	7		
2	D	147	Total	C	N	O	S	0	0
			1159	731	203	218	7		
2	F	153	Total	C	N	O	S	0	0
			1209	763	209	230	7		

- Molecule 3 is a protein called IMMUNOGLOBULIN G PGT151.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	135	Total	C	N	O	S	0	0
			1073	682	188	197	6		
3	M	135	Total	C	N	O	S	0	0
			1067	679	185	197	6		

- Molecule 4 is a protein called IMMUNOGLOBULIN G PGT151.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	114	Total	C	N	O	S	0	0
			881	553	151	173	4		
4	N	112	Total	C	N	O	S	0	0
			866	545	149	168	4		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

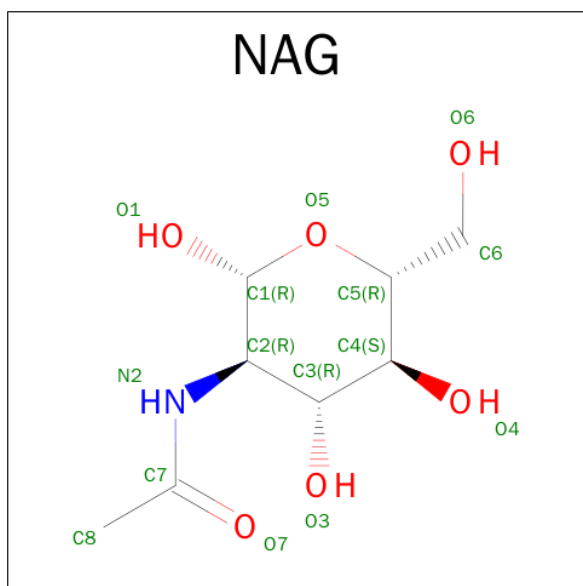
Mol	Chain	Residues	Atoms				AltConf
5	A	2	Total	C	N	O	0
			140	80	10	50	
5	A	2	Total	C	N	O	0
			140	80	10	50	
5	A	2	Total	C	N	O	0
			140	80	10	50	
5	A	2	Total	C	N	O	0
			140	80	10	50	
5	A	2	Total	C	N	O	0
			140	80	10	50	
5	C	2	Total	C	N	O	0
			168	96	12	60	
5	C	2	Total	C	N	O	0
			168	96	12	60	
5	C	2	Total	C	N	O	0
			168	96	12	60	
5	C	2	Total	C	N	O	0
			168	96	12	60	
5	C	2	Total	C	N	O	0
			168	96	12	60	
5	C	2	Total	C	N	O	0
			168	96	12	60	
5	D	2	Total	C	N	O	0
			56	32	4	20	
5	D	2	Total	C	N	O	0
			56	32	4	20	
5	E	2	Total	C	N	O	0
			224	128	16	80	
5	E	2	Total	C	N	O	0
			224	128	16	80	
5	E	2	Total	C	N	O	0
			224	128	16	80	
5	E	2	Total	C	N	O	0
			224	128	16	80	
5	E	2	Total	C	N	O	0
			224	128	16	80	

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Mol	Chain	Residues	Atoms				AltConf
5	E	2	Total	C	N	O	0
			224	128	16	80	
5	E	2	Total	C	N	O	0
			224	128	16	80	
5	E	2	Total	C	N	O	0
			224	128	16	80	
5	F	2	Total	C	N	O	0
			28	16	2	10	

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			42	24	3	15	
6	A	1	Total	C	N	O	0
			42	24	3	15	
6	A	1	Total	C	N	O	0
			42	24	3	15	
6	B	1	Total	C	N	O	0
			28	16	2	10	
6	B	1	Total	C	N	O	0
			28	16	2	10	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	

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

- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				AltConf
7	A	3	Total	C	N	O	0
			312	176	16	120	
7	A	3	Total	C	N	O	0
			312	176	16	120	
7	A	3	Total	C	N	O	0
			312	176	16	120	
7	A	3	Total	C	N	O	0
			312	176	16	120	
7	A	3	Total	C	N	O	0
			312	176	16	120	
7	A	3	Total	C	N	O	0
			312	176	16	120	
7	A	3	Total	C	N	O	0
			312	176	16	120	
7	A	3	Total	C	N	O	0
			312	176	16	120	
7	C	3	Total	C	N	O	0
			273	154	14	105	
7	C	3	Total	C	N	O	0
			273	154	14	105	
7	C	3	Total	C	N	O	0
			273	154	14	105	
7	C	3	Total	C	N	O	0
			273	154	14	105	
7	C	3	Total	C	N	O	0
			273	154	14	105	
7	C	3	Total	C	N	O	0
			273	154	14	105	
7	E	3	Total	C	N	O	0
			156	88	8	60	

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Mol	Chain	Residues	Atoms				AltConf
7	E	3	Total	C	N	O	0
			156	88	8	60	
7	E	3	Total	C	N	O	0
			156	88	8	60	
7	E	3	Total	C	N	O	0
			156	88	8	60	

- Molecule 8 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				AltConf
8	A	7	Total	C	N	O	0
			83	46	2	35	
8	C	7	Total	C	N	O	0
			83	46	2	35	
8	E	7	Total	C	N	O	0
			83	46	2	35	

- Molecule 9 is a polymer of unknown type called SUGAR (11-MER).

Mol	Chain	Residues	Atoms				AltConf
9	B	11	Total	C	N	O	0
			135	76	5	54	
9	F	11	Total	C	N	O	0
			135	76	5	54	

- Molecule 10 is a polymer of unknown type called SUGAR (13-MER).

Mol	Chain	Residues	Atoms				AltConf
10	B	13	Total	C	N	O	0
			160	90	6	64	

- Molecule 11 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				AltConf
11	C	5	Total	C	N	O	0
			61	34	2	25	

- Molecule 12 is a polymer of unknown type called SUGAR (8-MER).



Mol	Chain	Residues	Atoms				AltConf
12	C	8	Total	C	N	O	0
			94	52	2	40	
12	E	8	Total	C	N	O	0
			94	52	2	40	

- Molecule 13 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				AltConf
13	D	3	Total	C	N	O	0
			38	22	2	14	

- Molecule 14 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				AltConf
14	E	6	Total	C	N	O	0
			72	40	2	30	

- Molecule 15 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				AltConf
15	E	4	Total	C	N	O	0
			50	28	2	20	

- Molecule 16 is a polymer of unknown type called SUGAR (12-MER).

Mol	Chain	Residues	Atoms				AltConf
16	F	12	Total	C	N	O	0
			149	84	6	59	



ALA	VAL	GLY	ILE	GLY	ALA	VAL	PHE	LEU	G521	F522	G531	A532	Q540	A541	R542	L543	L544	L545	L556	R564	Q567	L568	T569	V570	W571	G572	L573	G600	K601	L602	S613	M637	E641	D664
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|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|
| A512 | V518 | F519 | S528 | T529 | Q540 | V549 | Q550 | M565 | L568 | T569 | V570 | I573 | K574 | G600 | K601 | T605 | S613 | M616 | Y638 | E641 | Q658 | GIU | LEU | LEU | LEU | LEU | LEU | ASP |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|

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|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| R1 | R2 | Q3 | L4 | P14 | C22 | P28 | F29 | Y32 | P33 | W55 | H56 | V57 | M95 | F96 | Q97 | E98 | Y100M | V111 | S112 | S113 | ALA | SER | SER | THR | THR | LYS | GLY | PRO | SER | VAL | VAL | PHE | PRO | LEU | ALA | ALA | PRO | SER | SER | SER | LYS | THR | THR | SER | GLY | GLY | THR | THR | ALA | ALA | LEU | GLY | CYS | LEU | VAL | LYS |
|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

[illegible]

- [illegible]

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| D1 | T7 | P8 | E60 | M83 | T109 | VAL | ALA | ALA | ALA | PRO | SER | SER | VAL | PRO | PRO | PRO | ASP | GLU | GLN | LEU | LYS | LYS | SER | GLY | THR | ALA | SER | ALA | VAL | VAL | VAL | CYS | LEU | LEU | ASN | ASN | ASN | ASP | PRO | PRO | ARG | GLU | GLU | ALA | ALA | LYS | VAL | VAL | GLN | TRP | LYS | LYS | GLN | SER | GLY | ASN |
|----|----|----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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THR  
LYS  
SER  
PHE  
ASN  
ARG  
GLY  
GLU  
CYS

● Molecule 4: IMMUNOGLOBULIN G PGT151

Chain N: 

47%

49%

ASP  
I2  
V3  
M4  
C23  
N28  
Y36  
L46  
V51  
S52  
N53  
R54  
F55  
R108  
THR  
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ALA  
ALA  
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GLU  
CYS

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	WHOLE MICROGRAPH, Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	32.4	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	22500	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: FUC, GAL, NAG, BMA, 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	0.77	1/3625 (0.0%)	0.69	2/4921 (0.0%)
1	C	0.76	0/3578	0.70	2/4857 (0.0%)
1	E	0.76	1/3609 (0.0%)	0.72	1/4899 (0.0%)
2	B	0.81	0/1168	0.67	0/1583
2	D	0.75	0/1178	0.69	0/1597
2	F	0.81	0/1228	0.71	1/1665 (0.1%)
3	H	0.72	0/1102	0.70	1/1496 (0.1%)
3	M	0.73	0/1096	0.69	0/1489
4	L	0.71	0/899	0.67	0/1213
4	N	0.69	0/884	0.70	0/1192
All	All	0.76	2/18367 (0.0%)	0.70	7/24912 (0.0%)

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	4
1	C	0	2
1	E	0	5
2	B	0	1
2	D	0	3
2	F	0	2
All	All	0	17

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	118	PRO	N-CD	5.63	1.55	1.47
1	A	118	PRO	N-CD	5.33	1.55	1.47

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	353	PHE	N-CA-CB	-6.31	99.24	110.60
2	F	616	ASN	CB-CA-C	5.64	121.68	110.40
1	C	157	CYS	N-CA-CB	-5.41	100.86	110.60
1	A	385	CYS	N-CA-CB	-5.39	100.90	110.60
1	E	54	CYS	N-CA-CB	-5.10	101.42	110.60

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	499	THR	Mainchain
1	A	507	GLN	Mainchain
1	A	81	PRO	Mainchain,Peptide
2	B	600	GLY	Mainchain
1	C	65	VAL	Mainchain

## 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	3553	0	3481	126	0
1	C	3506	0	3441	157	0
1	E	3537	0	3463	149	0
2	B	1150	0	1132	47	0
2	D	1159	0	1148	42	0
2	F	1209	0	1197	35	0
3	H	1073	0	1040	40	0
3	M	1067	0	1029	40	0
4	L	881	0	868	3	0
4	N	866	0	854	14	0
5	A	140	0	125	32	0
5	C	168	0	150	38	0
5	D	56	0	50	3	0
5	E	224	0	200	53	0
5	F	28	0	25	0	0
6	A	42	0	39	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	28	0	26	0	0
6	C	14	0	13	0	0
6	D	14	0	13	0	0
6	E	28	0	26	11	0
6	F	14	0	13	0	0
7	A	312	0	272	43	0
7	C	273	0	238	46	0
7	E	156	0	136	13	0
8	A	83	0	70	2	0
8	C	83	0	70	7	0
8	E	83	0	70	1	0
9	B	135	0	115	8	0
9	F	135	0	115	9	0
10	B	160	0	136	32	0
11	C	61	0	52	15	0
12	C	94	0	79	3	0
12	E	94	0	79	4	0
13	D	38	0	34	14	0
14	E	72	0	61	4	0
15	E	50	0	43	7	0
16	F	149	0	127	19	0
All	All	20735	0	20030	693	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 17.

The worst 5 of 693 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:TYR:CD1	7:A:1156:NAG:H82	1.21	1.65
1:A:173:TYR:CG	7:A:1156:NAG:H82	1.30	1.60
1:A:210:PHE:CD2	1:A:380:GLY:HA2	1.35	1.56
1:E:183:PRO:CA	1:E:191:TYR:CD1	1.87	1.56
1:A:395:TRP:HH2	5:A:1339:NAG:C8	1.20	1.54

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	441/473 (93%)	409 (93%)	28 (6%)	4 (1%)	21	67
1	C	436/473 (92%)	395 (91%)	31 (7%)	10 (2%)	8	50
1	E	440/473 (93%)	405 (92%)	27 (6%)	8 (2%)	11	55
2	B	142/153 (93%)	127 (89%)	8 (6%)	7 (5%)	3	32
2	D	145/153 (95%)	136 (94%)	7 (5%)	2 (1%)	14	59
2	F	151/153 (99%)	137 (91%)	11 (7%)	3 (2%)	9	53
3	H	133/240 (55%)	125 (94%)	7 (5%)	1 (1%)	24	69
3	M	133/240 (55%)	124 (93%)	7 (5%)	2 (2%)	13	58
4	L	112/219 (51%)	105 (94%)	7 (6%)	0	100	100
4	N	110/219 (50%)	104 (94%)	5 (4%)	1 (1%)	21	67
All	All	2243/2796 (80%)	2067 (92%)	138 (6%)	38 (2%)	16	56

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	ALA
2	B	532	ALA
2	B	541	ALA
2	B	545	LEU
2	B	570	VAL

### 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	404/424 (95%)	400 (99%)	4 (1%)	82	91
1	C	398/424 (94%)	389 (98%)	9 (2%)	58	83
1	E	401/424 (95%)	395 (98%)	6 (2%)	72	89
2	B	123/128 (96%)	119 (97%)	4 (3%)	45	78
2	D	122/128 (95%)	121 (99%)	1 (1%)	86	93
2	F	128/128 (100%)	126 (98%)	2 (2%)	70	88
3	H	116/207 (56%)	116 (100%)	0	100	100
3	M	115/207 (56%)	114 (99%)	1 (1%)	84	93
4	L	101/195 (52%)	100 (99%)	1 (1%)	82	91
4	N	99/195 (51%)	98 (99%)	1 (1%)	82	91
All	All	2007/2460 (82%)	1978 (99%)	29 (1%)	76	89

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	301	ASN
1	C	378	CYS
4	L	53	ASN
1	C	332	ASN
2	D	540	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	442	GLN
1	C	389	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

203 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	0.48	0	15,19,21	1.38	2 (13%)
5	NAG	A	1089	5	14,14,15	0.51	0	15,19,21	1.26	3 (20%)
7	NAG	A	1156	1,7	14,14,15	0.49	0	15,19,21	1.39	2 (13%)
7	NAG	A	1157	7	14,14,15	0.48	0	15,19,21	1.26	3 (20%)
7	BMA	A	1158	7	11,11,12	0.62	0	15,15,17	1.49	4 (26%)
7	NAG	A	1160	1,7	14,14,15	0.49	0	15,19,21	1.38	2 (13%)
7	NAG	A	1161	7	14,14,15	0.52	0	15,19,21	1.26	3 (20%)
7	BMA	A	1162	7	11,11,12	0.64	0	15,15,17	1.48	4 (26%)
7	NAG	A	1241	1,7	14,14,15	0.49	0	15,19,21	1.39	2 (13%)
7	NAG	A	1242	7	14,14,15	0.46	0	15,19,21	1.28	2 (13%)
7	BMA	A	1243	7	11,11,12	0.61	0	15,15,17	1.50	4 (26%)
8	NAG	A	1262	1,8	14,14,15	0.60	0	15,19,21	0.66	0
8	NAG	A	1263	8	14,14,15	0.54	0	15,19,21	0.87	0
8	BMA	A	1264	8	11,11,12	0.63	0	15,15,17	0.80	1 (6%)
8	MAN	A	1265	8	11,11,12	0.64	0	15,15,17	0.96	1 (6%)
8	MAN	A	1266	8	11,11,12	0.63	0	15,15,17	0.60	0
8	MAN	A	1267	8	11,11,12	0.58	0	15,15,17	0.67	0
8	MAN	A	1268	8	11,11,12	0.50	0	15,15,17	0.67	0
7	NAG	A	1276	1,7	14,14,15	0.47	0	15,19,21	1.39	2 (13%)
7	NAG	A	1277	7	14,14,15	0.50	0	15,19,21	1.27	3 (20%)
7	BMA	A	1278	7	11,11,12	0.61	0	15,15,17	1.49	4 (26%)
5	NAG	A	1295	1,5	14,14,15	0.47	0	15,19,21	1.38	2 (13%)
5	NAG	A	1296	5	14,14,15	0.48	0	15,19,21	1.26	3 (20%)
5	NAG	A	1301	1,5	14,14,15	0.48	0	15,19,21	1.39	2 (13%)
5	NAG	A	1302	5	14,14,15	0.49	0	15,19,21	1.26	3 (20%)
7	NAG	A	1332	1,7	14,14,15	0.48	0	15,19,21	1.38	2 (13%)
7	NAG	A	1333	7	14,14,15	0.50	0	15,19,21	1.26	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BMA	A	1334	7	11,11,12	0.62	0	15,15,17	1.48	4 (26%)
5	NAG	A	1339	1,5	14,14,15	0.49	0	15,19,21	1.38	2 (13%)
5	NAG	A	1340	5	14,14,15	0.49	0	15,19,21	1.26	3 (20%)
7	NAG	A	1362	1,7	14,14,15	0.48	0	15,19,21	1.37	2 (13%)
7	NAG	A	1363	7	14,14,15	0.48	0	15,19,21	1.27	3 (20%)
7	BMA	A	1364	7	11,11,12	0.61	0	15,15,17	1.48	4 (26%)
7	NAG	A	1386	1,7	14,14,15	0.50	0	15,19,21	1.39	2 (13%)
7	NAG	A	1387	7	14,14,15	0.49	0	15,19,21	1.27	3 (20%)
7	BMA	A	1388	7	11,11,12	0.62	0	15,15,17	1.50	4 (26%)
7	NAG	A	1392	1,7	14,14,15	0.50	0	15,19,21	1.40	2 (13%)
7	NAG	A	1393	7	14,14,15	0.49	0	15,19,21	1.27	3 (20%)
7	BMA	A	1394	7	11,11,12	0.63	0	15,15,17	1.50	4 (26%)
5	NAG	A	1448	1,5	14,14,15	0.47	0	15,19,21	1.39	2 (13%)
5	NAG	A	1449	5	14,14,15	0.51	0	15,19,21	1.27	2 (13%)
9	NAG	B	1611	9,2	14,14,15	1.48	3 (21%)	15,19,21	1.10	1 (6%)
9	NAG	B	1612	9	14,14,15	1.30	1 (7%)	15,19,21	1.33	2 (13%)
9	BMA	B	1613	9	11,11,12	1.32	2 (18%)	15,15,17	1.14	1 (6%)
9	MAN	B	1614	9	11,11,12	1.66	4 (36%)	15,15,17	1.45	2 (13%)
9	NAG	B	1617	9	14,14,15	1.34	3 (21%)	15,19,21	1.19	2 (13%)
9	MAN	B	1619	9	11,11,12	1.48	3 (27%)	15,15,17	1.31	2 (13%)
9	NAG	B	1620	9	14,14,15	1.39	3 (21%)	15,19,21	1.30	2 (13%)
9	GAL	B	1621	9	11,11,12	1.30	2 (18%)	15,15,17	1.08	1 (6%)
9	NAG	B	1622	9	14,14,15	1.39	3 (21%)	15,19,21	1.09	1 (6%)
9	GAL	B	1623	9	11,11,12	1.30	2 (18%)	15,15,17	1.09	1 (6%)
9	FUC	B	1624	9	10,10,11	1.35	1 (10%)	13,14,16	0.94	1 (7%)
10	NAG	B	1637	10,2	14,14,15	1.48	3 (21%)	15,19,21	1.08	1 (6%)
10	NAG	B	1638	10	14,14,15	1.31	2 (14%)	15,19,21	1.33	2 (13%)
10	BMA	B	1639	10	11,11,12	1.33	2 (18%)	15,15,17	1.15	1 (6%)
10	MAN	B	1640	10	11,11,12	1.68	4 (36%)	15,15,17	1.43	2 (13%)
10	NAG	B	1641	10	14,14,15	1.32	2 (14%)	15,19,21	1.25	2 (13%)
10	GAL	B	1642	10	11,11,12	1.29	2 (18%)	15,15,17	1.10	1 (6%)
10	NAG	B	1643	10	14,14,15	1.32	3 (21%)	15,19,21	1.17	2 (13%)
10	GAL	B	1644	10	11,11,12	1.31	2 (18%)	15,15,17	1.07	1 (6%)
10	MAN	B	1645	10	11,11,12	1.50	3 (27%)	15,15,17	1.31	2 (13%)
10	NAG	B	1646	10	14,14,15	1.37	3 (21%)	15,19,21	1.28	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	GAL	B	1647	10	11,11,12	1.30	2 (18%)	15,15,17	1.09	1 (6%)
10	NAG	B	1648	10	14,14,15	1.37	3 (21%)	15,19,21	1.11	1 (6%)
10	FUC	B	1650	10	10,10,11	1.34	1 (10%)	13,14,16	0.96	1 (7%)
7	NAG	C	1088	1,7	14,14,15	0.49	0	15,19,21	1.38	2 (13%)
7	NAG	C	1089	7	14,14,15	0.51	0	15,19,21	1.26	3 (20%)
7	BMA	C	1090	7	11,11,12	0.62	0	15,15,17	1.49	4 (26%)
5	NAG	C	1135	1,5	14,14,15	0.48	0	15,19,21	1.38	2 (13%)
5	NAG	C	1136	5	14,14,15	0.50	0	15,19,21	1.27	3 (20%)
5	NAG	C	1156	1,5	14,14,15	0.50	0	15,19,21	1.39	2 (13%)
5	NAG	C	1157	5	14,14,15	0.49	0	15,19,21	1.26	2 (13%)
7	NAG	C	1160	1,7	14,14,15	0.49	0	15,19,21	1.38	2 (13%)
7	NAG	C	1161	7	14,14,15	0.51	0	15,19,21	1.27	3 (20%)
7	BMA	C	1162	7	11,11,12	0.61	0	15,15,17	1.49	4 (26%)
11	NAG	C	1241	1,11	14,14,15	0.49	0	15,19,21	1.38	2 (13%)
11	NAG	C	1242	11	14,14,15	0.47	0	15,19,21	1.29	2 (13%)
11	BMA	C	1243	11	11,11,12	0.61	0	15,15,17	1.50	4 (26%)
11	MAN	C	1244	11	11,11,12	0.53	0	15,15,17	1.58	4 (26%)
11	MAN	C	1246	11	11,11,12	0.57	0	15,15,17	2.62	4 (26%)
8	NAG	C	1262	1,8	14,14,15	0.59	0	15,19,21	0.66	0
8	NAG	C	1263	8	14,14,15	0.56	0	15,19,21	0.87	0
8	BMA	C	1264	8	11,11,12	0.63	0	15,15,17	0.80	0
8	MAN	C	1265	8	11,11,12	0.64	0	15,15,17	0.96	1 (6%)
8	MAN	C	1266	8	11,11,12	0.63	0	15,15,17	0.58	0
8	MAN	C	1267	8	11,11,12	0.59	0	15,15,17	0.66	0
8	MAN	C	1268	8	11,11,12	0.51	0	15,15,17	0.66	0
7	NAG	C	1276	1,7	14,14,15	0.47	0	15,19,21	1.38	2 (13%)
7	NAG	C	1277	7	14,14,15	0.49	0	15,19,21	1.27	3 (20%)
7	BMA	C	1278	7	11,11,12	0.62	0	15,15,17	1.49	4 (26%)
5	NAG	C	1295	1,5	14,14,15	0.48	0	15,19,21	1.39	2 (13%)
5	NAG	C	1296	5	14,14,15	0.49	0	15,19,21	1.26	3 (20%)
7	NAG	C	1301	1,7	14,14,15	0.48	0	15,19,21	1.38	2 (13%)
7	NAG	C	1302	7	14,14,15	0.49	0	15,19,21	1.25	3 (20%)
7	BMA	C	1303	7	11,11,12	0.62	0	15,15,17	1.49	4 (26%)
7	NAG	C	1332	1,7	14,14,15	0.49	0	15,19,21	1.38	2 (13%)
7	NAG	C	1333	7	14,14,15	0.50	0	15,19,21	1.26	3 (20%)
7	BMA	C	1334	7	11,11,12	0.62	0	15,15,17	1.50	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	C	1339	1,5	14,14,15	0.50	0	15,19,21	1.38	2 (13%)
5	NAG	C	1340	5	14,14,15	0.51	0	15,19,21	1.27	3 (20%)
5	NAG	C	1355	1,5	14,14,15	0.47	0	15,19,21	1.38	2 (13%)
5	NAG	C	1356	5	14,14,15	0.50	0	15,19,21	1.27	3 (20%)
7	NAG	C	1362	1,7	14,14,15	0.49	0	15,19,21	1.38	2 (13%)
7	NAG	C	1363	7	14,14,15	0.49	0	15,19,21	1.27	3 (20%)
7	BMA	C	1364	7	11,11,12	0.60	0	15,15,17	1.48	4 (26%)
7	NAG	C	1386	1,7	14,14,15	0.50	0	15,19,21	1.39	2 (13%)
7	NAG	C	1387	7	14,14,15	0.50	0	15,19,21	1.26	3 (20%)
7	BMA	C	1388	7	11,11,12	0.63	0	15,15,17	1.49	4 (26%)
5	NAG	C	1392	1,5	14,14,15	0.50	0	15,19,21	1.39	2 (13%)
5	NAG	C	1393	5	14,14,15	0.50	0	15,19,21	1.27	3 (20%)
12	NAG	C	1448	1,12	14,14,15	0.47	0	15,19,21	1.37	2 (13%)
12	NAG	C	1449	12	14,14,15	0.51	0	15,19,21	1.26	2 (13%)
12	BMA	C	1450	12	11,11,12	0.61	0	15,15,17	1.49	4 (26%)
12	MAN	C	1451	12	11,11,12	0.52	0	15,15,17	1.57	4 (26%)
12	MAN	C	1452	12	11,11,12	0.57	0	15,15,17	2.40	5 (33%)
12	MAN	C	1453	12	11,11,12	0.60	0	15,15,17	2.62	4 (26%)
12	MAN	C	1454	12	11,11,12	0.57	0	15,15,17	2.03	7 (46%)
12	MAN	C	1455	12	11,11,12	0.57	0	15,15,17	2.38	8 (53%)
13	NAG	D	1611	13,2	14,14,15	1.48	4 (28%)	15,19,21	1.10	1 (6%)
13	NAG	D	1612	13	14,14,15	1.32	1 (7%)	15,19,21	1.32	2 (13%)
13	FUC	D	1613	13	10,10,11	1.35	1 (10%)	13,14,16	0.93	1 (7%)
5	NAG	D	1625	2,5	14,14,15	0.49	0	15,19,21	1.39	2 (13%)
5	NAG	D	1626	5	14,14,15	0.50	0	15,19,21	1.28	3 (20%)
5	NAG	D	1637	2,5	14,14,15	1.49	3 (21%)	15,19,21	1.07	1 (6%)
5	NAG	D	1638	5	14,14,15	1.31	2 (14%)	15,19,21	1.33	2 (13%)
7	NAG	E	1088	1,7	14,14,15	0.47	0	15,19,21	1.37	2 (13%)
7	NAG	E	1089	7	14,14,15	0.51	0	15,19,21	1.26	3 (20%)
7	BMA	E	1090	7	11,11,12	0.59	0	15,15,17	1.49	4 (26%)
5	NAG	E	1135	1,5	14,14,15	0.49	0	15,19,21	1.38	2 (13%)
5	NAG	E	1136	5	14,14,15	0.50	0	15,19,21	1.27	3 (20%)
7	NAG	E	1156	1,7	14,14,15	0.49	0	15,19,21	1.38	2 (13%)
7	NAG	E	1157	7	14,14,15	0.51	0	15,19,21	1.26	3 (20%)
7	BMA	E	1158	7	11,11,12	0.63	0	15,15,17	1.49	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	E	1160	1,5	14,14,15	0.49	0	15,19,21	1.39	2 (13%)
5	NAG	E	1161	5	14,14,15	0.50	0	15,19,21	1.27	3 (20%)
14	NAG	E	1241	1,14	14,14,15	0.50	0	15,19,21	1.39	2 (13%)
14	NAG	E	1242	14	14,14,15	0.48	0	15,19,21	1.28	3 (20%)
14	BMA	E	1243	14	11,11,12	0.62	0	15,15,17	1.51	4 (26%)
14	MAN	E	1244	14	11,11,12	0.52	0	15,15,17	1.60	4 (26%)
14	MAN	E	1245	14	11,11,12	0.56	0	15,15,17	2.42	5 (33%)
14	MAN	E	1246	14	11,11,12	0.58	0	15,15,17	2.61	4 (26%)
8	NAG	E	1262	1,8	14,14,15	0.60	0	15,19,21	0.66	0
8	NAG	E	1263	8	14,14,15	0.55	0	15,19,21	0.87	0
8	BMA	E	1264	8	11,11,12	0.63	0	15,15,17	0.80	1 (6%)
8	MAN	E	1265	8	11,11,12	0.64	0	15,15,17	0.96	1 (6%)
8	MAN	E	1266	8	11,11,12	0.62	0	15,15,17	0.59	0
8	MAN	E	1267	8	11,11,12	0.59	0	15,15,17	0.66	0
8	MAN	E	1268	8	11,11,12	0.51	0	15,15,17	0.67	0
5	NAG	E	1276	1,5	14,14,15	0.48	0	15,19,21	1.39	2 (13%)
5	NAG	E	1277	5	14,14,15	0.50	0	15,19,21	1.27	3 (20%)
5	NAG	E	1295	1,5	14,14,15	0.48	0	15,19,21	1.39	2 (13%)
5	NAG	E	1296	5	14,14,15	0.49	0	15,19,21	1.26	3 (20%)
5	NAG	E	1301	1,5	14,14,15	0.49	0	15,19,21	1.38	2 (13%)
5	NAG	E	1302	5	14,14,15	0.49	0	15,19,21	1.26	3 (20%)
7	NAG	E	1332	1,7	14,14,15	0.48	0	15,19,21	1.38	2 (13%)
7	NAG	E	1333	7	14,14,15	0.50	0	15,19,21	1.26	3 (20%)
7	BMA	E	1334	7	11,11,12	0.62	0	15,15,17	1.48	4 (26%)
5	NAG	E	1339	1,5	14,14,15	0.49	0	15,19,21	1.38	2 (13%)
5	NAG	E	1340	5	14,14,15	0.50	0	15,19,21	1.26	3 (20%)
5	NAG	E	1355	1,5	14,14,15	0.48	0	15,19,21	1.38	2 (13%)
5	NAG	E	1356	5	14,14,15	0.49	0	15,19,21	1.26	3 (20%)
5	NAG	E	1362	1,5	14,14,15	0.49	0	15,19,21	1.39	2 (13%)
5	NAG	E	1363	5	14,14,15	0.47	0	15,19,21	1.27	3 (20%)
15	NAG	E	1386	1,15	14,14,15	0.50	0	15,19,21	1.39	2 (13%)
15	NAG	E	1387	15	14,14,15	0.50	0	15,19,21	1.27	3 (20%)
15	BMA	E	1388	15	11,11,12	0.62	0	15,15,17	1.49	4 (26%)
15	MAN	E	1390	15	11,11,12	0.59	0	15,15,17	2.61	4 (26%)
7	NAG	E	1392	1,7	14,14,15	0.50	0	15,19,21	1.39	2 (13%)
7	NAG	E	1393	7	14,14,15	0.49	0	15,19,21	1.27	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BMA	E	1394	7	11,11,12	0.61	0	15,15,17	1.50	4 (26%)
12	NAG	E	1448	1,12	14,14,15	0.48	0	15,19,21	1.39	2 (13%)
12	NAG	E	1449	12	14,14,15	0.51	0	15,19,21	1.27	2 (13%)
12	BMA	E	1450	12	11,11,12	0.61	0	15,15,17	1.49	4 (26%)
12	MAN	E	1451	12	11,11,12	0.54	0	15,15,17	1.58	4 (26%)
12	MAN	E	1452	12	11,11,12	0.57	0	15,15,17	2.40	5 (33%)
12	MAN	E	1453	12	11,11,12	0.60	0	15,15,17	2.61	4 (26%)
12	MAN	E	1454	12	11,11,12	0.56	0	15,15,17	2.02	7 (46%)
12	MAN	E	1455	12	11,11,12	0.57	0	15,15,17	2.39	8 (53%)
9	NAG	F	1611	9,2	14,14,15	1.48	4 (28%)	15,19,21	1.10	1 (6%)
9	NAG	F	1612	9	14,14,15	1.30	1 (7%)	15,19,21	1.34	2 (13%)
9	BMA	F	1613	9	11,11,12	1.31	2 (18%)	15,15,17	1.14	1 (6%)
9	MAN	F	1614	9	11,11,12	1.67	4 (36%)	15,15,17	1.45	2 (13%)
9	NAG	F	1617	9	14,14,15	1.34	3 (21%)	15,19,21	1.18	2 (13%)
9	MAN	F	1619	9	11,11,12	1.47	3 (27%)	15,15,17	1.30	2 (13%)
9	NAG	F	1620	9	14,14,15	1.40	3 (21%)	15,19,21	1.30	2 (13%)
9	GAL	F	1621	9	11,11,12	1.31	2 (18%)	15,15,17	1.09	1 (6%)
9	NAG	F	1622	9	14,14,15	1.39	3 (21%)	15,19,21	1.10	1 (6%)
9	GAL	F	1623	9	11,11,12	1.32	2 (18%)	15,15,17	1.09	1 (6%)
9	FUC	F	1624	9	10,10,11	1.35	1 (10%)	13,14,16	0.94	1 (7%)
5	NAG	F	1625	2,5	14,14,15	0.49	0	15,19,21	1.38	2 (13%)
5	NAG	F	1626	5	14,14,15	0.49	0	15,19,21	1.27	3 (20%)
16	NAG	F	1637	2,16	14,14,15	1.48	3 (21%)	15,19,21	1.07	1 (6%)
16	NAG	F	1638	16	14,14,15	1.31	2 (14%)	15,19,21	1.33	2 (13%)
16	BMA	F	1639	16	11,11,12	1.32	2 (18%)	15,15,17	1.16	1 (6%)
16	MAN	F	1640	16	11,11,12	1.68	4 (36%)	15,15,17	1.44	2 (13%)
16	NAG	F	1641	16	14,14,15	1.33	2 (14%)	15,19,21	1.25	2 (13%)
16	GAL	F	1642	16	11,11,12	1.28	2 (18%)	15,15,17	1.12	1 (6%)
16	NAG	F	1643	16	14,14,15	1.33	3 (21%)	15,19,21	1.16	2 (13%)
16	GAL	F	1644	16	11,11,12	1.32	2 (18%)	15,15,17	1.07	1 (6%)
16	MAN	F	1645	16	11,11,12	1.49	3 (27%)	15,15,17	1.31	2 (13%)
16	NAG	F	1646	16	14,14,15	1.38	3 (21%)	15,19,21	1.27	2 (13%)
16	NAG	F	1648	16	14,14,15	1.36	3 (21%)	15,19,21	1.10	1 (6%)
16	FUC	F	1650	16	10,10,11	1.33	1 (10%)	13,14,16	0.95	1 (7%)



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
7	NAG	A	1156	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1157	7	-	0/6/23/26	0/1/1/1
7	BMA	A	1158	7	-	0/2/19/22	0/1/1/1
7	NAG	A	1160	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1161	7	-	0/6/23/26	0/1/1/1
7	BMA	A	1162	7	-	0/2/19/22	0/1/1/1
7	NAG	A	1241	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1242	7	-	0/6/23/26	0/1/1/1
7	BMA	A	1243	7	-	0/2/19/22	0/1/1/1
8	NAG	A	1262	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	1263	8	-	0/6/23/26	0/1/1/1
8	BMA	A	1264	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1265	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1266	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1267	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1268	8	-	0/2/19/22	0/1/1/1
7	NAG	A	1276	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1277	7	-	0/6/23/26	0/1/1/1
7	BMA	A	1278	7	-	0/2/19/22	0/1/1/1
5	NAG	A	1295	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1296	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1301	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1302	5	-	0/6/23/26	0/1/1/1
7	NAG	A	1332	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1333	7	-	0/6/23/26	0/1/1/1
7	BMA	A	1334	7	-	0/2/19/22	0/1/1/1
5	NAG	A	1339	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1340	5	-	0/6/23/26	0/1/1/1
7	NAG	A	1362	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1363	7	-	0/6/23/26	0/1/1/1
7	BMA	A	1364	7	-	0/2/19/22	0/1/1/1
7	NAG	A	1386	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1387	7	-	0/6/23/26	0/1/1/1
7	BMA	A	1388	7	-	0/2/19/22	0/1/1/1
7	NAG	A	1392	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1393	7	-	0/6/23/26	0/1/1/1
7	BMA	A	1394	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1448	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1449	5	-	0/6/23/26	0/1/1/1
9	NAG	B	1611	9,2	-	0/6/23/26	0/1/1/1
9	NAG	B	1612	9	-	0/6/23/26	0/1/1/1
9	BMA	B	1613	9	-	0/2/19/22	0/1/1/1
9	MAN	B	1614	9	-	0/2/19/22	0/1/1/1
9	NAG	B	1617	9	-	0/6/23/26	0/1/1/1
9	MAN	B	1619	9	-	0/2/19/22	0/1/1/1
9	NAG	B	1620	9	-	0/6/23/26	0/1/1/1
9	GAL	B	1621	9	-	0/2/19/22	0/1/1/1
9	NAG	B	1622	9	-	0/6/23/26	0/1/1/1
9	GAL	B	1623	9	-	0/2/19/22	0/1/1/1
9	FUC	B	1624	9	-	0/0/17/20	0/1/1/1
10	NAG	B	1637	10,2	-	0/6/23/26	0/1/1/1
10	NAG	B	1638	10	-	0/6/23/26	0/1/1/1
10	BMA	B	1639	10	-	0/2/19/22	0/1/1/1
10	MAN	B	1640	10	-	0/2/19/22	0/1/1/1
10	NAG	B	1641	10	-	0/6/23/26	0/1/1/1
10	GAL	B	1642	10	-	0/2/19/22	0/1/1/1
10	NAG	B	1643	10	-	0/6/23/26	0/1/1/1
10	GAL	B	1644	10	-	0/2/19/22	0/1/1/1
10	MAN	B	1645	10	-	0/2/19/22	0/1/1/1
10	NAG	B	1646	10	-	0/6/23/26	0/1/1/1
10	GAL	B	1647	10	-	0/2/19/22	0/1/1/1
10	NAG	B	1648	10	-	0/6/23/26	0/1/1/1
10	FUC	B	1650	10	-	0/0/17/20	0/1/1/1
7	NAG	C	1088	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	1089	7	-	0/6/23/26	0/1/1/1
7	BMA	C	1090	7	-	0/2/19/22	0/1/1/1
5	NAG	C	1135	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1136	5	-	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
7	NAG	C	1160	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	1161	7	-	0/6/23/26	0/1/1/1
7	BMA	C	1162	7	-	0/2/19/22	0/1/1/1
11	NAG	C	1241	1,11	-	0/6/23/26	0/1/1/1
11	NAG	C	1242	11	-	0/6/23/26	0/1/1/1
11	BMA	C	1243	11	-	0/2/19/22	0/1/1/1
11	MAN	C	1244	11	-	0/2/19/22	0/1/1/1
11	MAN	C	1246	11	-	0/2/19/22	0/1/1/1
8	NAG	C	1262	1,8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	C	1263	8	-	0/6/23/26	0/1/1/1
8	BMA	C	1264	8	-	0/2/19/22	0/1/1/1
8	MAN	C	1265	8	-	0/2/19/22	0/1/1/1
8	MAN	C	1266	8	-	0/2/19/22	0/1/1/1
8	MAN	C	1267	8	-	0/2/19/22	0/1/1/1
8	MAN	C	1268	8	-	0/2/19/22	0/1/1/1
7	NAG	C	1276	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	1277	7	-	0/6/23/26	0/1/1/1
7	BMA	C	1278	7	-	0/2/19/22	0/1/1/1
5	NAG	C	1295	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1296	5	-	0/6/23/26	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	NAG	C	1332	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	1333	7	-	0/6/23/26	0/1/1/1
7	BMA	C	1334	7	-	0/2/19/22	0/1/1/1
5	NAG	C	1339	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1340	5	-	0/6/23/26	0/1/1/1
5	NAG	C	1355	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1356	5	-	0/6/23/26	0/1/1/1
7	NAG	C	1362	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	1363	7	-	0/6/23/26	0/1/1/1
7	BMA	C	1364	7	-	0/2/19/22	0/1/1/1
7	NAG	C	1386	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	1387	7	-	0/6/23/26	0/1/1/1
7	BMA	C	1388	7	-	0/2/19/22	0/1/1/1
5	NAG	C	1392	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1393	5	-	0/6/23/26	0/1/1/1
12	NAG	C	1448	1,12	-	0/6/23/26	0/1/1/1
12	NAG	C	1449	12	-	0/6/23/26	0/1/1/1
12	BMA	C	1450	12	-	0/2/19/22	0/1/1/1
12	MAN	C	1451	12	-	0/2/19/22	0/1/1/1
12	MAN	C	1452	12	-	0/2/19/22	0/1/1/1
12	MAN	C	1453	12	-	0/2/19/22	0/1/1/1
12	MAN	C	1454	12	-	0/2/19/22	0/1/1/1
12	MAN	C	1455	12	-	0/2/19/22	0/1/1/1
13	NAG	D	1611	13,2	-	0/6/23/26	0/1/1/1
13	NAG	D	1612	13	-	0/6/23/26	0/1/1/1
13	FUC	D	1613	13	-	0/0/17/20	0/1/1/1
5	NAG	D	1625	2,5	-	0/6/23/26	0/1/1/1
5	NAG	D	1626	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	D	1637	2,5	-	0/6/23/26	0/1/1/1
5	NAG	D	1638	5	-	0/6/23/26	0/1/1/1
7	NAG	E	1088	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	1089	7	-	0/6/23/26	0/1/1/1
7	BMA	E	1090	7	-	0/2/19/22	0/1/1/1
5	NAG	E	1135	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	1136	5	-	0/6/23/26	0/1/1/1
7	NAG	E	1156	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	1157	7	-	0/6/23/26	0/1/1/1
7	BMA	E	1158	7	-	0/2/19/22	0/1/1/1
5	NAG	E	1160	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	1161	5	-	0/6/23/26	0/1/1/1
14	NAG	E	1241	1,14	-	0/6/23/26	0/1/1/1
14	NAG	E	1242	14	-	0/6/23/26	0/1/1/1
14	BMA	E	1243	14	-	0/2/19/22	0/1/1/1
14	MAN	E	1244	14	-	0/2/19/22	0/1/1/1
14	MAN	E	1245	14	-	0/2/19/22	0/1/1/1
14	MAN	E	1246	14	-	0/2/19/22	0/1/1/1
8	NAG	E	1262	1,8	-	0/6/23/26	0/1/1/1
8	NAG	E	1263	8	-	0/6/23/26	0/1/1/1
8	BMA	E	1264	8	-	0/2/19/22	0/1/1/1
8	MAN	E	1265	8	-	0/2/19/22	0/1/1/1
8	MAN	E	1266	8	-	0/2/19/22	0/1/1/1
8	MAN	E	1267	8	-	0/2/19/22	0/1/1/1
8	MAN	E	1268	8	-	0/2/19/22	0/1/1/1
5	NAG	E	1276	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	1277	5	-	0/6/23/26	0/1/1/1
5	NAG	E	1295	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	1296	5	-	0/6/23/26	0/1/1/1
5	NAG	E	1301	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	1302	5	-	0/6/23/26	0/1/1/1
7	NAG	E	1332	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	1333	7	-	0/6/23/26	0/1/1/1
7	BMA	E	1334	7	-	0/2/19/22	0/1/1/1
5	NAG	E	1339	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	1340	5	-	0/6/23/26	0/1/1/1
5	NAG	E	1355	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	1356	5	-	0/6/23/26	0/1/1/1
5	NAG	E	1362	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	1363	5	-	0/6/23/26	0/1/1/1
15	NAG	E	1386	1,15	-	0/6/23/26	0/1/1/1
15	NAG	E	1387	15	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BMA	E	1388	15	-	0/2/19/22	0/1/1/1
15	MAN	E	1390	15	-	0/2/19/22	0/1/1/1
7	NAG	E	1392	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	1393	7	-	0/6/23/26	0/1/1/1
7	BMA	E	1394	7	-	0/2/19/22	0/1/1/1
12	NAG	E	1448	1,12	-	0/6/23/26	0/1/1/1
12	NAG	E	1449	12	-	0/6/23/26	0/1/1/1
12	BMA	E	1450	12	-	0/2/19/22	0/1/1/1
12	MAN	E	1451	12	-	0/2/19/22	0/1/1/1
12	MAN	E	1452	12	-	0/2/19/22	0/1/1/1
12	MAN	E	1453	12	-	0/2/19/22	0/1/1/1
12	MAN	E	1454	12	-	0/2/19/22	0/1/1/1
12	MAN	E	1455	12	-	0/2/19/22	0/1/1/1
9	NAG	F	1611	9,2	-	0/6/23/26	0/1/1/1
9	NAG	F	1612	9	-	0/6/23/26	0/1/1/1
9	BMA	F	1613	9	-	0/2/19/22	0/1/1/1
9	MAN	F	1614	9	-	0/2/19/22	0/1/1/1
9	NAG	F	1617	9	-	0/6/23/26	0/1/1/1
9	MAN	F	1619	9	-	0/2/19/22	0/1/1/1
9	NAG	F	1620	9	-	0/6/23/26	0/1/1/1
9	GAL	F	1621	9	-	0/2/19/22	0/1/1/1
9	NAG	F	1622	9	-	0/6/23/26	0/1/1/1
9	GAL	F	1623	9	-	0/2/19/22	0/1/1/1
9	FUC	F	1624	9	-	0/0/17/20	0/1/1/1
5	NAG	F	1625	2,5	-	0/6/23/26	0/1/1/1
5	NAG	F	1626	5	-	0/6/23/26	0/1/1/1
16	NAG	F	1637	2,16	-	0/6/23/26	0/1/1/1
16	NAG	F	1638	16	-	0/6/23/26	0/1/1/1
16	BMA	F	1639	16	-	0/2/19/22	0/1/1/1
16	MAN	F	1640	16	-	0/2/19/22	0/1/1/1
16	NAG	F	1641	16	-	0/6/23/26	0/1/1/1
16	GAL	F	1642	16	-	0/2/19/22	0/1/1/1
16	NAG	F	1643	16	-	0/6/23/26	0/1/1/1
16	GAL	F	1644	16	-	0/2/19/22	0/1/1/1
16	MAN	F	1645	16	-	0/2/19/22	0/1/1/1
16	NAG	F	1646	16	-	0/6/23/26	0/1/1/1
16	NAG	F	1648	16	-	0/6/23/26	0/1/1/1
16	FUC	F	1650	16	-	0/0/17/20	0/1/1/1

The worst 5 of 128 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	1646	NAG	O5-C5	2.00	1.47	1.43
16	F	1646	NAG	O5-C5	2.00	1.47	1.43
16	F	1638	NAG	O5-C5	2.00	1.47	1.43
13	D	1611	NAG	C8-C7	2.01	1.54	1.50
9	F	1611	NAG	C8-C7	2.02	1.54	1.50

The worst 5 of 476 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	E	1455	MAN	C6-C5-C4	-4.71	101.19	112.99
12	C	1455	MAN	C6-C5-C4	-4.69	101.24	112.99
14	E	1246	MAN	C2-C3-C4	-4.18	103.75	111.05
11	C	1246	MAN	C2-C3-C4	-4.17	103.77	111.05
12	E	1453	MAN	C2-C3-C4	-4.16	103.79	111.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

95 monomers are involved in 338 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1088	NAG	9	0
5	A	1089	NAG	1	0
7	A	1156	NAG	25	0
7	A	1157	NAG	3	0
7	A	1160	NAG	1	0
7	A	1161	NAG	1	0
7	A	1241	NAG	4	0
8	A	1262	NAG	1	0
8	A	1263	NAG	1	0
8	A	1267	MAN	1	0
7	A	1276	NAG	3	0
7	A	1277	NAG	2	0
5	A	1295	NAG	3	0
5	A	1296	NAG	1	0
5	A	1301	NAG	6	0
5	A	1339	NAG	12	0
7	A	1387	NAG	4	0
7	A	1392	NAG	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1393	NAG	5	0
7	A	1394	BMA	3	0
5	A	1448	NAG	2	0
9	B	1611	NAG	1	0
9	B	1621	GAL	1	0
9	B	1622	NAG	1	0
9	B	1623	GAL	1	0
9	B	1624	FUC	5	0
10	B	1637	NAG	3	0
10	B	1638	NAG	14	0
10	B	1640	MAN	2	0
10	B	1641	NAG	7	0
10	B	1642	GAL	1	0
10	B	1643	NAG	2	0
10	B	1644	GAL	2	0
10	B	1648	NAG	4	0
10	B	1650	FUC	1	0
5	C	1156	NAG	13	0
5	C	1157	NAG	9	0
7	C	1160	NAG	14	0
7	C	1161	NAG	2	0
11	C	1241	NAG	8	0
11	C	1242	NAG	6	0
11	C	1243	BMA	1	0
8	C	1262	NAG	1	0
8	C	1263	NAG	1	0
8	C	1264	BMA	4	0
8	C	1265	MAN	4	0
8	C	1268	MAN	2	0
7	C	1276	NAG	3	0
7	C	1277	NAG	2	0
7	C	1301	NAG	17	0
7	C	1302	NAG	1	0
7	C	1303	BMA	1	0
7	C	1332	NAG	6	0
5	C	1355	NAG	5	0
7	C	1387	NAG	5	0
5	C	1392	NAG	13	0
12	C	1448	NAG	2	0
12	C	1452	MAN	1	0
13	D	1611	NAG	3	0
13	D	1613	FUC	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1625	NAG	1	0
5	D	1626	NAG	1	0
5	D	1637	NAG	2	0
5	D	1638	NAG	1	0
7	E	1156	NAG	6	0
7	E	1157	NAG	2	0
5	E	1160	NAG	14	0
5	E	1161	NAG	2	0
14	E	1242	NAG	1	0
14	E	1243	BMA	2	0
14	E	1246	MAN	1	0
8	E	1262	NAG	1	0
8	E	1263	NAG	1	0
5	E	1276	NAG	3	0
5	E	1277	NAG	2	0
5	E	1301	NAG	2	0
5	E	1339	NAG	13	0
5	E	1355	NAG	16	0
5	E	1362	NAG	5	0
15	E	1387	NAG	7	0
15	E	1388	BMA	1	0
7	E	1392	NAG	6	0
7	E	1393	NAG	1	0
7	E	1394	BMA	1	0
12	E	1448	NAG	2	0
12	E	1452	MAN	2	0
9	F	1612	NAG	1	0
9	F	1621	GAL	3	0
9	F	1624	FUC	5	0
16	F	1637	NAG	2	0
16	F	1638	NAG	12	0
16	F	1639	BMA	3	0
16	F	1640	MAN	2	0
16	F	1641	NAG	3	0
16	F	1642	GAL	1	0

## 5.6 Ligand geometry

10 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	$\# Z  > 2$
6	NAG	A	1135	1	14,14,15	0.49	0	15,19,21	1.38	2 (13%)
6	NAG	A	1355	1	14,14,15	0.47	0	15,19,21	1.39	2 (13%)
6	NAG	A	1397	1	14,14,15	0.49	0	15,19,21	1.39	2 (13%)
6	NAG	B	1600	2	14,14,15	0.50	0	15,19,21	1.39	2 (13%)
6	NAG	B	1625	2	14,14,15	0.48	0	15,19,21	1.39	2 (13%)
6	NAG	C	1397	1	14,14,15	0.49	0	15,19,21	1.39	2 (13%)
6	NAG	D	1600	2	14,14,15	0.50	0	15,19,21	1.40	2 (13%)
6	NAG	E	1187	1	14,14,15	0.49	0	15,19,21	1.39	2 (13%)
6	NAG	E	1397	1	14,14,15	0.48	0	15,19,21	1.39	2 (13%)
6	NAG	F	1600	2	14,14,15	0.50	0	15,19,21	1.38	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
6	NAG	A	1135	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1355	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1397	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1600	2	-	0/6/23/26	0/1/1/1
6	NAG	B	1625	2	-	0/6/23/26	0/1/1/1
6	NAG	C	1397	1	-	0/6/23/26	0/1/1/1
6	NAG	D	1600	2	-	0/6/23/26	0/1/1/1
6	NAG	E	1187	1	-	0/6/23/26	0/1/1/1
6	NAG	E	1397	1	-	0/6/23/26	0/1/1/1
6	NAG	F	1600	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1600	NAG	O7-C7-C8	-2.87	116.79	122.07
6	C	1397	NAG	O7-C7-C8	-2.84	116.84	122.07
6	A	1397	NAG	O7-C7-C8	-2.84	116.84	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	1397	NAG	O7-C7-C8	-2.84	116.85	122.07
6	B	1600	NAG	O7-C7-C8	-2.82	116.87	122.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1355	NAG	2	0
6	A	1397	NAG	3	0
6	E	1397	NAG	11	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.