



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Jul 24, 2017 – 01:14 AM EDT

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 : unknown
Resolution : 4.20 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-20029824

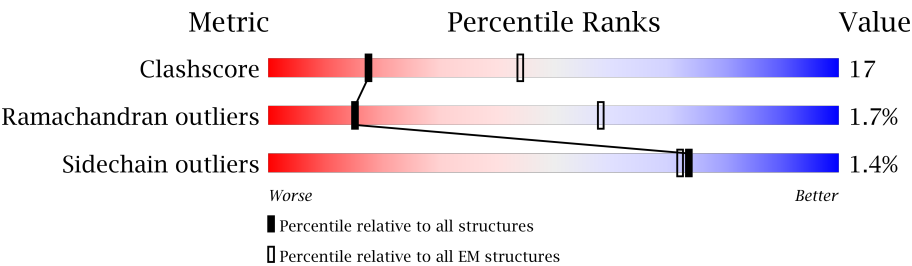
1 Overall quality at a glance i

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	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	473	83% 10% • 5%
1	C	473	78% 13% • 6%
1	E	473	80% 12% • 5%
2	B	153	79% 9% 6% 6%
2	D	153	83% 10% • •
2	F	153	90% 5% 5%
3	H	240	48% 8% 44%
3	M	240	47% 8% • 44%
4	L	219	50% • 48%

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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
5	NAG	A	1088	-	-	X	-
5	NAG	A	1156	-	-	X	-
5	NAG	A	1339	-	-	X	-
5	NAG	B	1638	-	-	X	-
5	NAG	B	1641	-	-	X	-
5	NAG	C	1156	-	-	X	-
5	NAG	C	1157	-	-	X	-
5	NAG	C	1160	-	-	X	-
5	NAG	C	1241	-	-	X	-
5	NAG	C	1301	-	-	X	-
5	NAG	C	1392	-	-	X	-
5	NAG	E	1160	-	-	X	-
5	NAG	E	1339	-	-	X	-
5	NAG	E	1355	-	-	X	-
5	NAG	E	1387	-	-	X	-
5	NAG	E	1397	-	-	X	-
5	NAG	F	1638	-	-	X	-
9	FUC	D	1613	-	-	X	-

2 Entry composition

There are 9 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		

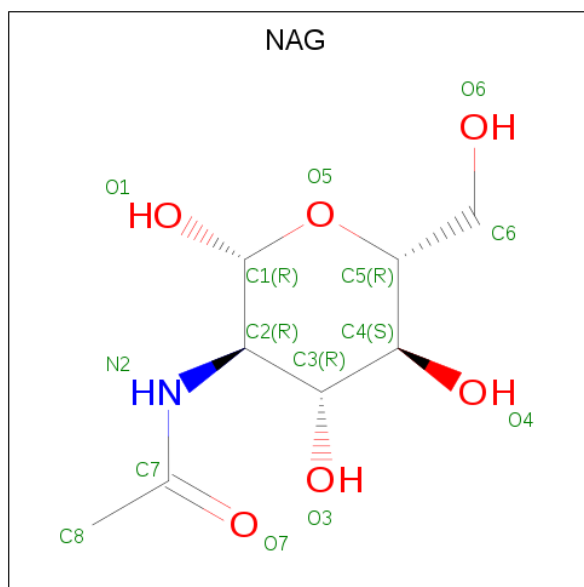
- Molecule 3 is a protein called IMMUNOGLOBULIN G PGT151.

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



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			434	248	31	155	
5	A	1	Total	C	N	O	0
			434	248	31	155	
5	A	1	Total	C	N	O	0
			434	248	31	155	
5	A	1	Total	C	N	O	0
			434	248	31	155	
5	A	1	Total	C	N	O	0
			434	248	31	155	
5	A	1	Total	C	N	O	0
			434	248	31	155	
5	A	1	Total	C	N	O	0
			434	248	31	155	
5	A	1	Total	C	N	O	0
			434	248	31	155	
5	A	1	Total	C	N	O	0
			434	248	31	155	

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Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			182	104	13	65	
5	B	1	Total	C	N	O	0
			182	104	13	65	
5	B	1	Total	C	N	O	0
			182	104	13	65	
5	B	1	Total	C	N	O	0
			182	104	13	65	
5	B	1	Total	C	N	O	0
			182	104	13	65	
5	B	1	Total	C	N	O	0
			182	104	13	65	
5	B	1	Total	C	N	O	0
			182	104	13	65	
5	B	1	Total	C	N	O	0
			182	104	13	65	
5	B	1	Total	C	N	O	0
			182	104	13	65	
5	B	1	Total	C	N	O	0
			182	104	13	65	
5	C	1	Total	C	N	O	0
			462	264	33	165	
5	C	1	Total	C	N	O	0
			462	264	33	165	
5	C	1	Total	C	N	O	0
			462	264	33	165	
5	C	1	Total	C	N	O	0
			462	264	33	165	
5	C	1	Total	C	N	O	0
			462	264	33	165	
5	C	1	Total	C	N	O	0
			462	264	33	165	
5	C	1	Total	C	N	O	0
			462	264	33	165	

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Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			462	264	33	165	
5	C	1	Total	C	N	O	0
			462	264	33	165	
5	C	1	Total	C	N	O	0
			462	264	33	165	
5	C	1	Total	C	N	O	0
			462	264	33	165	
5	D	1	Total	C	N	O	0
			98	56	7	35	
5	D	1	Total	C	N	O	0
			98	56	7	35	
5	D	1	Total	C	N	O	0
			98	56	7	35	
5	D	1	Total	C	N	O	0
			98	56	7	35	
5	D	1	Total	C	N	O	0
			98	56	7	35	
5	D	1	Total	C	N	O	0
			98	56	7	35	
5	D	1	Total	C	N	O	0
			98	56	7	35	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	

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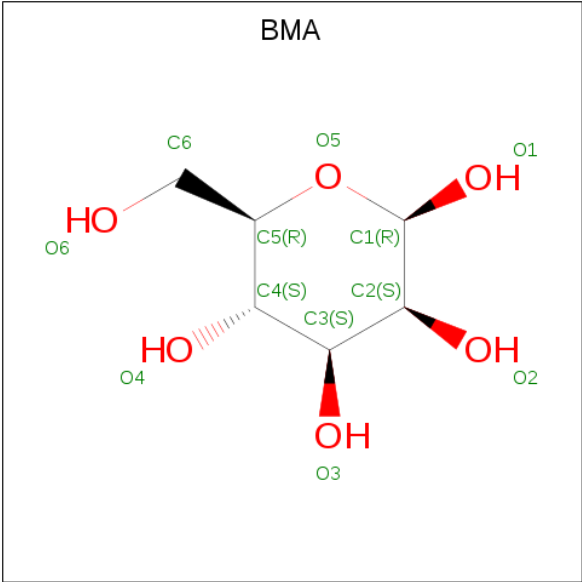
Mol	Chain	Residues	Atoms				AltConf
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	

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Mol	Chain	Residues	Atoms				AltConf
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	E	1	Total	C	N	O	0
			476	272	34	170	
5	F	1	Total	C	N	O	0
			196	112	14	70	
5	F	1	Total	C	N	O	0
			196	112	14	70	
5	F	1	Total	C	N	O	0
			196	112	14	70	
5	F	1	Total	C	N	O	0
			196	112	14	70	
5	F	1	Total	C	N	O	0
			196	112	14	70	
5	F	1	Total	C	N	O	0
			196	112	14	70	
5	F	1	Total	C	N	O	0
			196	112	14	70	
5	F	1	Total	C	N	O	0
			196	112	14	70	
5	F	1	Total	C	N	O	0
			196	112	14	70	
5	F	1	Total	C	N	O	0
			196	112	14	70	
5	F	1	Total	C	N	O	0
			196	112	14	70	
5	F	1	Total	C	N	O	0
			196	112	14	70	

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



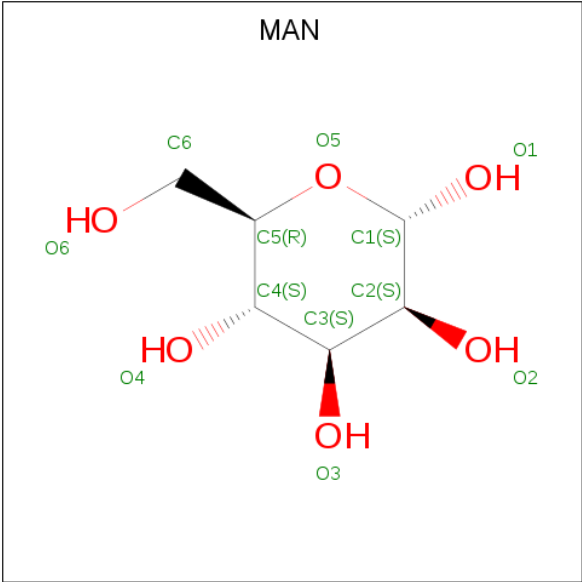
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			99	54	45	
6	A	1	Total	C	O	0
			99	54	45	
6	A	1	Total	C	O	0
			99	54	45	
6	A	1	Total	C	O	0
			99	54	45	
6	A	1	Total	C	O	0
			99	54	45	
6	A	1	Total	C	O	0
			99	54	45	
6	A	1	Total	C	O	0
			99	54	45	
6	A	1	Total	C	O	0
			99	54	45	
6	B	1	Total	C	O	0
			22	12	10	
6	B	1	Total	C	O	0
			22	12	10	
6	C	1	Total	C	O	0
			110	60	50	
6	C	1	Total	C	O	0
			110	60	50	
6	C	1	Total	C	O	0
			110	60	50	

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Mol	Chain	Residues	Atoms			AltConf
6	C	1	Total	C	O	0
			110	60	50	
6	C	1	Total	C	O	0
			110	60	50	
6	C	1	Total	C	O	0
			110	60	50	
6	C	1	Total	C	O	0
			110	60	50	
6	C	1	Total	C	O	0
			110	60	50	
6	C	1	Total	C	O	0
			110	60	50	
6	E	1	Total	C	O	0
			88	48	40	
6	E	1	Total	C	O	0
			88	48	40	
6	E	1	Total	C	O	0
			88	48	40	
6	E	1	Total	C	O	0
			88	48	40	
6	E	1	Total	C	O	0
			88	48	40	
6	E	1	Total	C	O	0
			88	48	40	
6	E	1	Total	C	O	0
			88	48	40	
6	F	1	Total	C	O	0
			22	12	10	
6	F	1	Total	C	O	0
			22	12	10	

- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			44	24	20	
7	A	1	Total	C	O	0
			44	24	20	
7	A	1	Total	C	O	0
			44	24	20	
7	A	1	Total	C	O	0
			44	24	20	
7	B	1	Total	C	O	0
			44	24	20	
7	B	1	Total	C	O	0
			44	24	20	
7	B	1	Total	C	O	0
			44	24	20	
7	B	1	Total	C	O	0
			44	24	20	
7	C	1	Total	C	O	0
			121	66	55	
7	C	1	Total	C	O	0
			121	66	55	
7	C	1	Total	C	O	0
			121	66	55	
7	C	1	Total	C	O	0
			121	66	55	
7	C	1	Total	C	O	0
			121	66	55	
7	C	1	Total	C	O	0
			121	66	55	

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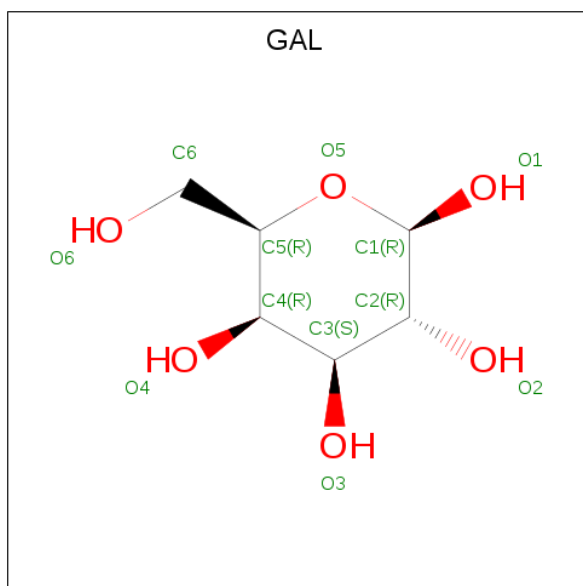
Mol	Chain	Residues	Atoms			AltConf
7	C	1	Total	C	O	0
			121	66	55	
7	C	1	Total	C	O	0
			121	66	55	
7	C	1	Total	C	O	0
			121	66	55	
7	C	1	Total	C	O	0
			121	66	55	
7	C	1	Total	C	O	0
			121	66	55	
7	E	1	Total	C	O	0
			143	78	65	
7	E	1	Total	C	O	0
			143	78	65	
7	E	1	Total	C	O	0
			143	78	65	
7	E	1	Total	C	O	0
			143	78	65	
7	E	1	Total	C	O	0
			143	78	65	
7	E	1	Total	C	O	0
			143	78	65	
7	E	1	Total	C	O	0
			143	78	65	
7	E	1	Total	C	O	0
			143	78	65	
7	E	1	Total	C	O	0
			143	78	65	
7	E	1	Total	C	O	0
			143	78	65	
7	E	1	Total	C	O	0
			143	78	65	
7	F	1	Total	C	O	0
			44	24	20	
7	F	1	Total	C	O	0
			44	24	20	
7	F	1	Total	C	O	0
			44	24	20	

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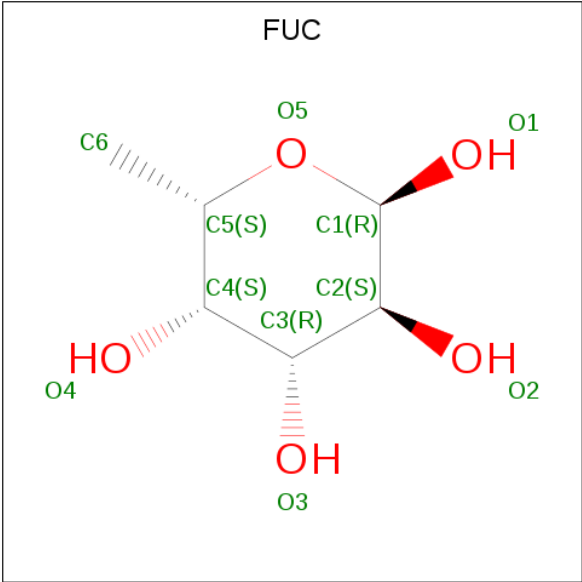
Mol	Chain	Residues	Atoms			AltConf
7	F	1	Total	C	O	0
			44	24	20	

- Molecule 8 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			AltConf
8	B	1	Total	C	O	0
			55	30	25	
8	B	1	Total	C	O	0
			55	30	25	
8	B	1	Total	C	O	0
			55	30	25	
8	B	1	Total	C	O	0
			55	30	25	
8	B	1	Total	C	O	0
			55	30	25	
8	F	1	Total	C	O	0
			44	24	20	
8	F	1	Total	C	O	0
			44	24	20	
8	F	1	Total	C	O	0
			44	24	20	
8	F	1	Total	C	O	0
			44	24	20	

- Molecule 9 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).

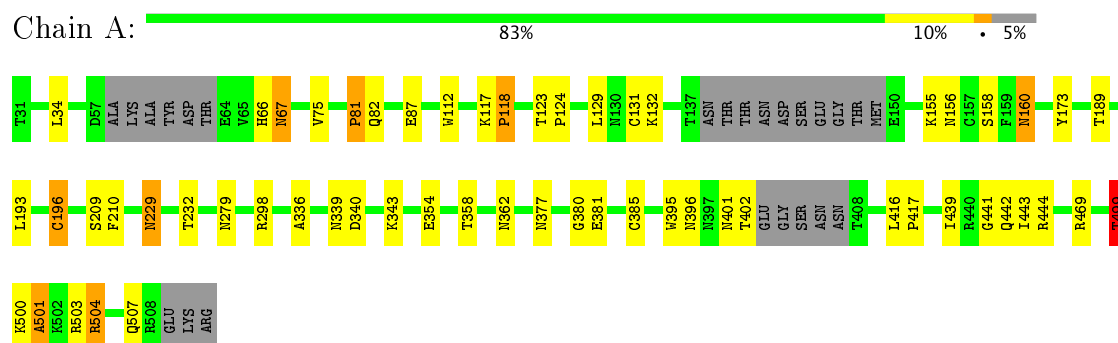


Mol	Chain	Residues	Atoms			AltConf
9	B	1	Total	C	O	0
			20	12	8	
9	B	1	Total	C	O	0
			20	12	8	
9	D	1	Total	C	O	0
			10	6	4	
9	F	1	Total	C	O	0
			20	12	8	
9	F	1	Total	C	O	0
			20	12	8	

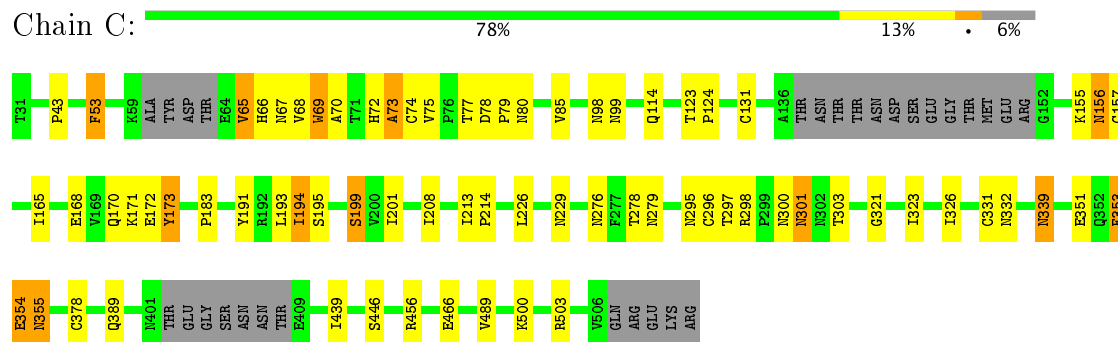
3 Residue-property plots

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.

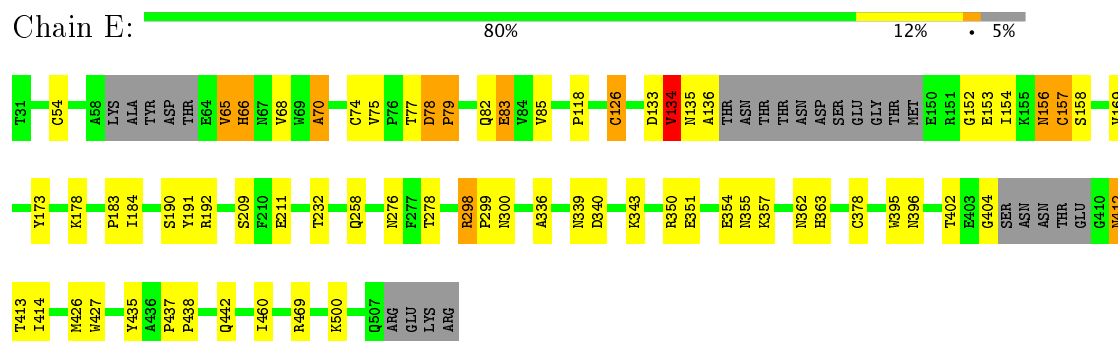
- Molecule 1: HIV-1 ENVELOPE GLYCOPROTEIN GP160



- Molecule 1: HIV-1 ENVELOPE GLYCOPROTEIN GP160



- Molecule 1: HIV-1 ENVELOPE GLYCOPROTEIN GP160



- Molecule 2: HIV-1 ENVELOPE GLYCOPROTEIN GP160

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 | GLU | LEU | LEU | ASP |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|

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| R1 | R2 | R3 | R4 | R5 | R6 | R7 | R8 | R9 | R10 | R11 | R12 | R13 | R14 | R15 | R16 | R17 | R18 | R19 | R20 | R21 | R22 | R23 | R24 | R25 | R26 | R27 | R28 | R29 | R30 | R31 | R32 | R33 | R34 | R35 | R36 | R37 | R38 | R39 | R40 | R41 | R42 | R43 | R44 | R45 | R46 | R47 | R48 | R49 | R50 | R51 | R52 | R53 | R54 | R55 | R56 | R57 | R58 | R59 | R60 | R61 | R62 | R63 | R64 | R65 | R66 | R67 | R68 | R69 | R70 | R71 | R72 | R73 | R74 | R75 | R76 | R77 | R78 | R79 | R80 | R81 | R82 | R83 | R84 | R85 | R86 | R87 | R88 | R89 | R90 | R91 | R92 | R93 | R94 | R95 | R96 | R97 | R98 | R99 | R100 | R101 | R102 | R103 | R104 | R105 | R106 | R107 | R108 | R109 | R110 | R111 | R112 | R113 | R114 | R115 | R116 | R117 | R118 | R119 | R120 | R121 | R122 | R123 | R124 | R125 | R126 | R127 | R128 | R129 | R130 | R131 | R132 | R133 | R134 | R135 | R136 | R137 | R138 | R139 | R140 | R141 | R142 | R143 | R144 | R145 | R146 | R147 | R148 | R149 | R150 | R151 | R152 | R153 | R154 | R155 | R156 | R157 | R158 | R159 | R160 | R161 | R162 | R163 | R164 | R165 | R166 | R167 | R168 | R169 | R170 | R171 | R172 | R173 | R174 | R175 | R176 | R177 | R178 | R179 | R180 | R181 | R182 | R183 | R184 | R185 | R186 | R187 | R188 | R189 | R190 | R191 | R192 | R193 | R194 | R195 | R196 | R197 | R198 | R199 | R200 | R201 | R202 | R203 | R204 | R205 | R206 | R207 | R208 | R209 | R210 | R211 | R212 | R213 | R214 | R215 | R216 | R217 | R218 | R219 | R220 | R221 | R222 | R223 | R224 | R225 | R226 | R227 | R228 | R229 | R230 | R231 | R232 | R233 | R234 | R235 | R236 | R237 | R238 | R239 | R240 | R241 | R242 | R243 | R244 | R245 | R246 | R247 | R248 | R249 | R250 | R251 | R252 | R253 | R254 | R255 | R256 | R257 | R258 | R259 | R260 | R261 | R262 | R263 | R264 | R265 | R266 | R267 | R268 | R269 | R270 | R271 | R272 | R273 | R274 | R275 | R276 | R277 | R278 | R279 | R280 | R281 | R282 | R283 | R284 | R285 | R286 | R287 | R288 | R289 | R290 | R291 | R292 | R293 | R294 | R295 | R296 | R297 | R298 | R299 | R300 | R301 | R302 | R303 | R304 | R305 | R306 | R307 | R308 | R309 | R310 | R311 | R312 | R313 | R314 | R315 | R316 | R317 | R318 | R319 | R320 | R321 | R322 | R323 | R324 | R325 | R326 | R327 | R328 | R329 | R330 | R331 | R332 | R333 | R334 | R335 | R336 | R337 | R338 | R339 | R340 | R341 | R342 | R343 | R344 | R345 | R346 | R347 | R348 | R349 | R350 | R351 | R352 | R353 | R354 | R355 | R356 | R357 | R358 | R359 | R360 | R361 | R362 | R363 | R364 | R365 | R366 | R367 | R368 | R369 | R370 | R371 | R372 | R373 | R374 | R375 | R376 | R377 | R378 | R379 | R380 | R381 | R382 | R383 | R384 | R385 | R386 | R387 | R388 | R389 | R390 | R391 | R392 | R393 | R394 | R395 | R396 | R397 | R398 | R399 | R400 | R401 | R402 | R403 | R404 | R405 | R406 | R407 | R408 | R409 | R410 | R411 | R412 | R413 | R414 | R415 | R416 | R417 | R418 | R419 | R420 | R421 | R422 | R423 | R424 | R425 | R426 | R427 | R428 | R429 | R430 | R431 | R432 | R433 | R434 | R435 | R436 | R437 | R438 | R439 | R440 | R441 | R442 | R443 | R444 | R445 | R446 | R447 | R448 | R449 | R450 | R451 | R452 | R453 | R454 | R455 | R456 | R457 | R458 | R459 | R460 | R461 | R462 | R463 | R464 | R465 | R466 | R467 | R468 | R469 | R470 | R471 | R472 | R473 | R474 | R475 | R476 | R477 | R478 | R479 | R480 | R481 | R482 | R483 | R484 | R485 | R486 | R487 | R488 | R489 | R490 | R491 | R492 | R493 | R494 | R495 | R496 | R497 | R498 | R499 | R500 | R501 | R502 | R503 | R504 | R505 | R506 | R507 | R508 | R509 | R510 | R511 | R512 | R513 | R514 | R515 | R516 | R517 | R518 | R519 | R520 | R521 | R522 | R523 | R524 | R5 |
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| ARG | V2 | Q3 | L4 | | Q13 | S25 | D26 | F27 | P28 | | Y32 | P33 | | G92 | M95 | F96 | Q97 | E98 | S99 | G100 | R100C | L100D | D100E | R100F | W100G | S100H | G100I | R100J | N100K | Y100N | Y100O | V111 | S112 | S113 | A114 | SER | THR | LYS | GLY | PRO | SER | VAL | PHE | PRO | LEU | ALA | PRO | SER | SER | LYS | SER | THR | SER | SER |
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[illegible]

- D1 T7 P8 E50 N63 T109 VAL ALA ALA ALA PRO PRO SER SER VAL PHE ILE PHE PRO PRO ASP ASP GLU GLY LEU LEU SER SER SER THR TRP PRO ARG ARG GLU GLU ALA ALA LYS VAL VAL CYS CYS LEU LEU ASN ASN ASP PHE THR TRP PRO ARG ARG GLU GLU ALA ALA LYS VAL VAL CYS CYS LEU LEU ASN ASN ASP PHE THR TRP PRO ARG ARG GLU GLU ALA ALA LYS VAL VAL CYS CYS LEU LEU ASN ASN ASP PHE THR TRP

GLN	GLU	SER	VAL	THR	GLU	GLN	ASP	SER	LYS	ASP	SER	THR	TYR	SER	LEU	SER	SER	THR	LEU	THR	LEU	THR	LEU	SER	LYS	ALA	LYS	ALA	ASP	TYR	GLU	LYS	HIS	LYS	LYS	VAL	TYR	ALA	CYS	GLU	VAL	THR	HIS	GLN	GLY	LEU	SER	SER	PRO	VAL	THR	LYS	SER	PHE	ASN	ARG	GLY	GLU	CYS
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● Molecule 4: IMMUNOGLOBULIN G PGT151



ASP	I2	V3	M4	G23	N28	Y36	L46	V51	S52	N53	R54	F55	R108	THR	VAL	VAL	ALA	ALA	PRO	SER	SER	VAL	PHE	ILE	SER	PHE	PRO	PRO	SER	ASP	GLU	GLN	GLN	LEU	LYS	SER	GLY	THR	ALA	SER	VAL	VAL	VAL	CYS	LEU	LEU	LEU	ASN	ASN	PHE	TYR	PRO	ARG	GLU	ALA	LYS	VAL	GLN	TRP
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LYS	VAL	ASP	ASN	ALA	LEU	GLN	SER	GLY	ASN	SER	GLN	GLU	SER	VAL	THR	GLU	GLN	ASP	SER	LYS	ASP	SER	ALA	THR	TYR	SER	SER	LEU	SER	THR	LEU	LYS	LYS	ALA	ASP	TYR	GLU	LYS	HIS	LYS	VAL	TYR	ALA	CYS	GLU	VAL	THR	HIS	GLN	GLY	LEU	SER	SER	PRO	VAL	THR	LYS	SER
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PHE	ASN	ARG	GLY	GLU	CYS
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	201386	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	WHOLE MICROGRAPH	Depositor
Microscope	FEI TITAN KRIOS	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

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	434	0	380	81	0
5	B	182	0	158	31	0
5	C	462	0	403	96	0
5	D	98	0	87	6	0
5	E	476	0	418	82	0
5	F	196	0	171	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	99	0	88	3	0
6	B	22	0	16	0	0
6	C	110	0	94	6	0
6	E	88	0	73	4	0
6	F	22	0	16	3	0
7	A	44	0	38	1	0
7	B	44	0	33	2	0
7	C	121	0	105	7	0
7	E	143	0	124	3	0
7	F	44	0	33	2	0
8	B	55	0	50	5	0
8	F	44	0	40	4	0
9	B	20	0	20	6	0
9	D	10	0	10	11	0
9	F	20	0	20	5	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	5:A:1156:NAG:H82	1.21	1.65
1:A:173:TYR:CG	5: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 [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	441/473 (93%)	409 (93%)	28 (6%)	4 (1%)	20	63
1	C	436/473 (92%)	395 (91%)	31 (7%)	10 (2%)	7	45
1	E	440/473 (93%)	405 (92%)	27 (6%)	8 (2%)	10	50
2	B	142/153 (93%)	127 (89%)	8 (6%)	7 (5%)	2	28
2	D	145/153 (95%)	136 (94%)	7 (5%)	2 (1%)	13	54
2	F	151/153 (99%)	137 (91%)	11 (7%)	3 (2%)	9	48
3	H	133/240 (55%)	125 (94%)	7 (5%)	1 (1%)	22	66
3	M	133/240 (55%)	124 (93%)	7 (5%)	2 (2%)	12	53
4	L	112/219 (51%)	105 (94%)	7 (6%)	0	100	100
4	N	110/219 (50%)	104 (94%)	5 (4%)	1 (1%)	20	63
All	All	2243/2796 (80%)	2067 (92%)	138 (6%)	38 (2%)	15	51

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%)	80	90
1	C	398/424 (94%)	389 (98%)	9 (2%)	56	79
1	E	401/424 (95%)	395 (98%)	6 (2%)	70	86
2	B	123/128 (96%)	119 (97%)	4 (3%)	43	72
2	D	122/128 (95%)	121 (99%)	1 (1%)	85	92
2	F	128/128 (100%)	126 (98%)	2 (2%)	68	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	116/207 (56%)	116 (100%)	0	100	100
3	M	115/207 (56%)	114 (99%)	1 (1%)	82	91
4	L	101/195 (52%)	100 (99%)	1 (1%)	80	90
4	N	99/195 (51%)	98 (99%)	1 (1%)	80	90
All	All	2007/2460 (82%)	1978 (99%)	29 (1%)	74	87

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

213 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	$\# Z > 2$
5	NAG	A	1088	1,5	14,14,15	0.48	0	15,19,21	2.61	3 (20%)
5	NAG	A	1089	5	14,14,15	0.51	0	15,19,21	1.21	2 (13%)
5	NAG	A	1135	1	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
5	NAG	A	1156	1,5	14,14,15	0.49	0	15,19,21	2.59	3 (20%)
5	NAG	A	1157	5,6	14,14,15	0.48	0	15,19,21	1.19	2 (13%)
6	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	5,6	14,14,15	0.52	0	15,19,21	1.18	2 (13%)
6	BMA	A	1162	5	11,11,12	0.65	0	13,15,17	1.50	3 (23%)
5	NAG	A	1241	1,5	14,14,15	0.50	0	15,19,21	2.62	3 (20%)
5	NAG	A	1242	5,6	14,14,15	0.47	0	15,19,21	1.25	2 (13%)
6	BMA	A	1243	5	11,11,12	0.62	0	13,15,17	1.52	3 (23%)
5	NAG	A	1262	1,5	14,14,15	0.61	0	15,19,21	0.72	0
5	NAG	A	1263	5,6	14,14,15	0.54	0	15,19,21	0.90	0
6	BMA	A	1264	5,7	11,11,12	0.64	0	13,15,17	0.70	0
7	MAN	A	1265	7,6	11,11,12	0.65	0	13,15,17	0.82	0
7	MAN	A	1266	7	11,11,12	0.64	0	13,15,17	0.58	0
7	MAN	A	1267	7,6	11,11,12	0.58	0	13,15,17	0.65	0
7	MAN	A	1268	7	11,11,12	0.51	0	13,15,17	0.67	0
5	NAG	A	1276	1,5	14,14,15	0.48	0	15,19,21	2.60	3 (20%)
5	NAG	A	1277	5,6	14,14,15	0.51	0	15,19,21	1.19	2 (13%)
6	BMA	A	1278	5	11,11,12	0.62	0	13,15,17	1.50	3 (23%)
5	NAG	A	1295	1,5	14,14,15	0.47	0	15,19,21	2.60	3 (20%)
5	NAG	A	1296	5	14,14,15	0.48	0	15,19,21	1.18	2 (13%)
5	NAG	A	1301	1,5	14,14,15	0.49	0	15,19,21	2.60	3 (20%)
5	NAG	A	1302	5	14,14,15	0.50	0	15,19,21	1.18	2 (13%)
5	NAG	A	1332	1,5	14,14,15	0.48	0	15,19,21	2.60	3 (20%)
5	NAG	A	1333	5,6	14,14,15	0.51	0	15,19,21	1.18	2 (13%)
6	BMA	A	1334	5	11,11,12	0.63	0	13,15,17	1.49	3 (23%)
5	NAG	A	1339	1,5	14,14,15	0.50	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
5	NAG	A	1340	5	14,14,15	0.49	0	15,19,21	1.19	2 (13%)
5	NAG	A	1355	1	14,14,15	0.48	0	15,19,21	2.61	3 (20%)
5	NAG	A	1362	1,5	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
5	NAG	A	1363	5,6	14,14,15	0.48	0	15,19,21	1.19	2 (13%)
6	BMA	A	1364	5	11,11,12	0.62	0	13,15,17	1.48	3 (23%)
5	NAG	A	1386	1,5	14,14,15	0.50	0	15,19,21	2.62	3 (20%)
5	NAG	A	1387	5,6	14,14,15	0.50	0	15,19,21	1.20	2 (13%)
6	BMA	A	1388	5	11,11,12	0.63	0	13,15,17	1.50	3 (23%)
5	NAG	A	1392	1,5	14,14,15	0.50	0	15,19,21	2.61	3 (20%)
5	NAG	A	1393	5,6	14,14,15	0.49	0	15,19,21	1.20	2 (13%)
6	BMA	A	1394	5	11,11,12	0.64	0	13,15,17	1.51	3 (23%)
5	NAG	A	1397	1	14,14,15	0.49	0	15,19,21	2.60	3 (20%)
5	NAG	A	1448	1,5	14,14,15	0.47	0	15,19,21	2.58	3 (20%)
5	NAG	A	1449	5	14,14,15	0.52	0	15,19,21	1.19	2 (13%)
5	NAG	B	1600	2	14,14,15	0.50	0	15,19,21	2.61	3 (20%)
5	NAG	B	1611	9,2,5	14,14,15	1.50	3 (21%)	15,19,21	1.11	1 (6%)
5	NAG	B	1612	5,6	14,14,15	1.32	2 (14%)	15,19,21	1.29	1 (6%)
6	BMA	B	1613	5,7	11,11,12	1.34	2 (18%)	13,15,17	1.26	1 (7%)
7	MAN	B	1614	5,6	11,11,12	1.69	4 (36%)	13,15,17	1.49	2 (15%)
5	NAG	B	1617	7	14,14,15	1.36	3 (21%)	15,19,21	1.24	2 (13%)
7	MAN	B	1619	5,6	11,11,12	1.51	3 (27%)	13,15,17	1.40	2 (15%)
5	NAG	B	1620	8,7	14,14,15	1.41	3 (21%)	15,19,21	1.37	2 (13%)
8	GAL	B	1621	5	11,11,12	1.33	2 (18%)	13,15,17	1.13	1 (7%)
5	NAG	B	1622	8,7	14,14,15	1.42	3 (21%)	15,19,21	1.18	2 (13%)
8	GAL	B	1623	5	11,11,12	1.33	2 (18%)	13,15,17	1.14	1 (7%)
9	FUC	B	1624	5	9,10,11	1.37	1 (11%)	13,14,16	1.01	0
5	NAG	B	1625	2	14,14,15	0.49	0	15,19,21	2.60	3 (20%)
5	NAG	B	1637	9,2,5	14,14,15	1.51	3 (21%)	15,19,21	1.09	1 (6%)
5	NAG	B	1638	5,6	14,14,15	1.33	2 (14%)	15,19,21	1.29	1 (6%)
6	BMA	B	1639	5,7	11,11,12	1.36	2 (18%)	13,15,17	1.27	1 (7%)
7	MAN	B	1640	5,6	11,11,12	1.71	4 (36%)	13,15,17	1.46	2 (15%)
5	NAG	B	1641	8,7	14,14,15	1.34	2 (14%)	15,19,21	1.33	2 (13%)
8	GAL	B	1642	5	11,11,12	1.31	2 (18%)	13,15,17	1.15	1 (7%)
5	NAG	B	1643	8,7	14,14,15	1.34	3 (21%)	15,19,21	1.21	2 (13%)
8	GAL	B	1644	5	11,11,12	1.34	2 (18%)	13,15,17	1.12	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	B	1645	5,6	11,11,12	1.52	3 (27%)	13,15,17	1.40	2 (15%)
5	NAG	B	1646	8,7	14,14,15	1.39	3 (21%)	15,19,21	1.36	2 (13%)
8	GAL	B	1647	5	11,11,12	1.32	2 (18%)	13,15,17	1.14	1 (7%)
5	NAG	B	1648	7	14,14,15	1.39	3 (21%)	15,19,21	1.22	2 (13%)
9	FUC	B	1650	5	9,10,11	1.36	1 (11%)	13,14,16	1.03	1 (7%)
5	NAG	C	1088	1,5	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
5	NAG	C	1089	5,6	14,14,15	0.51	0	15,19,21	1.17	2 (13%)
6	BMA	C	1090	5	11,11,12	0.63	0	13,15,17	1.50	3 (23%)
5	NAG	C	1135	1,5	14,14,15	0.48	0	15,19,21	2.60	3 (20%)
5	NAG	C	1136	5	14,14,15	0.50	0	15,19,21	1.19	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	NAG	C	1160	1,5	14,14,15	0.49	0	15,19,21	2.60	3 (20%)
5	NAG	C	1161	5,6	14,14,15	0.52	0	15,19,21	1.19	2 (13%)
6	BMA	C	1162	5	11,11,12	0.62	0	13,15,17	1.51	3 (23%)
5	NAG	C	1241	1,5	14,14,15	0.49	0	15,19,21	2.60	3 (20%)
5	NAG	C	1242	5,6	14,14,15	0.48	0	15,19,21	1.25	2 (13%)
6	BMA	C	1243	5,7	11,11,12	0.62	0	13,15,17	1.51	3 (23%)
7	MAN	C	1244	6	11,11,12	0.54	0	13,15,17	1.61	3 (23%)
7	MAN	C	1246	6	11,11,12	0.58	0	13,15,17	2.61	3 (23%)
5	NAG	C	1262	1,5	14,14,15	0.60	0	15,19,21	0.72	0
5	NAG	C	1263	5,6	14,14,15	0.57	0	15,19,21	0.90	0
6	BMA	C	1264	5,7	11,11,12	0.64	0	13,15,17	0.70	0
7	MAN	C	1265	7,6	11,11,12	0.65	0	13,15,17	0.82	0
7	MAN	C	1266	7	11,11,12	0.63	0	13,15,17	0.57	0
7	MAN	C	1267	7,6	11,11,12	0.60	0	13,15,17	0.63	0
7	MAN	C	1268	7	11,11,12	0.51	0	13,15,17	0.67	0
5	NAG	C	1276	1,5	14,14,15	0.48	0	15,19,21	2.59	3 (20%)
5	NAG	C	1277	5,6	14,14,15	0.49	0	15,19,21	1.19	2 (13%)
6	BMA	C	1278	5	11,11,12	0.63	0	13,15,17	1.51	3 (23%)
5	NAG	C	1295	1,5	14,14,15	0.48	0	15,19,21	2.59	3 (20%)
5	NAG	C	1296	5	14,14,15	0.50	0	15,19,21	1.19	2 (13%)
5	NAG	C	1301	1,5	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
5	NAG	C	1302	5,6	14,14,15	0.49	0	15,19,21	1.17	2 (13%)
6	BMA	C	1303	5	11,11,12	0.64	0	13,15,17	1.50	3 (23%)
5	NAG	C	1332	1,5	14,14,15	0.50	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	C	1333	5,6	14,14,15	0.50	0	15,19,21	1.17	2 (13%)
6	BMA	C	1334	5	11,11,12	0.63	0	13,15,17	1.51	3 (23%)
5	NAG	C	1339	1,5	14,14,15	0.51	0	15,19,21	2.61	3 (20%)
5	NAG	C	1340	5	14,14,15	0.51	0	15,19,21	1.20	2 (13%)
5	NAG	C	1355	1,5	14,14,15	0.47	0	15,19,21	2.61	3 (20%)
5	NAG	C	1356	5	14,14,15	0.50	0	15,19,21	1.19	2 (13%)
5	NAG	C	1362	1,5	14,14,15	0.50	0	15,19,21	2.60	3 (20%)
5	NAG	C	1363	5,6	14,14,15	0.49	0	15,19,21	1.19	2 (13%)
6	BMA	C	1364	5	11,11,12	0.61	0	13,15,17	1.49	3 (23%)
5	NAG	C	1386	1,5	14,14,15	0.50	0	15,19,21	2.61	3 (20%)
5	NAG	C	1387	5,6	14,14,15	0.50	0	15,19,21	1.20	2 (13%)
6	BMA	C	1388	5	11,11,12	0.64	0	13,15,17	1.51	3 (23%)
5	NAG	C	1392	1,5	14,14,15	0.50	0	15,19,21	2.61	3 (20%)
5	NAG	C	1393	5	14,14,15	0.51	0	15,19,21	1.19	2 (13%)
5	NAG	C	1397	1	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
5	NAG	C	1448	1,5	14,14,15	0.48	0	15,19,21	2.60	3 (20%)
5	NAG	C	1449	5,6	14,14,15	0.51	0	15,19,21	1.19	2 (13%)
6	BMA	C	1450	5,7	11,11,12	0.62	0	13,15,17	1.50	3 (23%)
7	MAN	C	1451	7,6	11,11,12	0.53	0	13,15,17	1.59	3 (23%)
7	MAN	C	1452	7	11,11,12	0.59	0	13,15,17	2.60	5 (38%)
7	MAN	C	1453	7,6	11,11,12	0.61	0	13,15,17	2.60	3 (23%)
7	MAN	C	1454	7	11,11,12	0.58	0	13,15,17	2.05	6 (46%)
7	MAN	C	1455	7	11,11,12	0.58	0	13,15,17	2.39	6 (46%)
5	NAG	D	1600	2	14,14,15	0.51	0	15,19,21	2.62	3 (20%)
5	NAG	D	1611	9,2,5	14,14,15	1.50	3 (21%)	15,19,21	1.11	1 (6%)
5	NAG	D	1612	5	14,14,15	1.34	2 (14%)	15,19,21	1.29	1 (6%)
9	FUC	D	1613	5	9,10,11	1.37	1 (11%)	13,14,16	1.01	0
5	NAG	D	1625	2,5	14,14,15	0.49	0	15,19,21	2.60	3 (20%)
5	NAG	D	1626	5	14,14,15	0.50	0	15,19,21	1.20	2 (13%)
5	NAG	D	1637	2,5	14,14,15	1.51	3 (21%)	15,19,21	1.08	1 (6%)
5	NAG	D	1638	5	14,14,15	1.33	2 (14%)	15,19,21	1.29	1 (6%)
5	NAG	E	1088	1,5	14,14,15	0.48	0	15,19,21	2.61	3 (20%)
5	NAG	E	1089	5,6	14,14,15	0.51	0	15,19,21	1.19	2 (13%)
6	BMA	E	1090	5	11,11,12	0.60	0	13,15,17	1.50	3 (23%)
5	NAG	E	1135	1,5	14,14,15	0.50	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	E	1136	5	14,14,15	0.51	0	15,19,21	1.19	2 (13%)
5	NAG	E	1156	1,5	14,14,15	0.50	0	15,19,21	2.59	3 (20%)
5	NAG	E	1157	5,6	14,14,15	0.51	0	15,19,21	1.17	2 (13%)
6	BMA	E	1158	5	11,11,12	0.65	0	13,15,17	1.51	3 (23%)
5	NAG	E	1160	1,5	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
5	NAG	E	1161	5	14,14,15	0.50	0	15,19,21	1.19	2 (13%)
5	NAG	E	1187	1	14,14,15	0.50	0	15,19,21	2.60	3 (20%)
5	NAG	E	1241	1,5	14,14,15	0.50	0	15,19,21	2.61	3 (20%)
5	NAG	E	1242	5,6	14,14,15	0.48	0	15,19,21	1.23	2 (13%)
6	BMA	E	1243	5,7	11,11,12	0.63	0	13,15,17	1.52	3 (23%)
7	MAN	E	1244	7,6	11,11,12	0.53	0	13,15,17	1.63	3 (23%)
7	MAN	E	1245	7	11,11,12	0.57	0	13,15,17	2.62	5 (38%)
7	MAN	E	1246	6	11,11,12	0.59	0	13,15,17	2.60	3 (23%)
5	NAG	E	1262	1,5	14,14,15	0.60	0	15,19,21	0.72	0
5	NAG	E	1263	5,6	14,14,15	0.56	0	15,19,21	0.90	0
6	BMA	E	1264	5,7	11,11,12	0.64	0	13,15,17	0.70	0
7	MAN	E	1265	7,6	11,11,12	0.64	0	13,15,17	0.83	1 (7%)
7	MAN	E	1266	7	11,11,12	0.62	0	13,15,17	0.57	0
7	MAN	E	1267	7,6	11,11,12	0.60	0	13,15,17	0.63	0
7	MAN	E	1268	7	11,11,12	0.51	0	13,15,17	0.67	0
5	NAG	E	1276	1,5	14,14,15	0.48	0	15,19,21	2.60	3 (20%)
5	NAG	E	1277	5	14,14,15	0.50	0	15,19,21	1.19	2 (13%)
5	NAG	E	1295	1,5	14,14,15	0.48	0	15,19,21	2.60	3 (20%)
5	NAG	E	1296	5	14,14,15	0.50	0	15,19,21	1.19	2 (13%)
5	NAG	E	1301	1,5	14,14,15	0.50	0	15,19,21	2.60	3 (20%)
5	NAG	E	1302	5	14,14,15	0.49	0	15,19,21	1.18	2 (13%)
5	NAG	E	1332	1,5	14,14,15	0.49	0	15,19,21	2.60	3 (20%)
5	NAG	E	1333	5,6	14,14,15	0.51	0	15,19,21	1.18	2 (13%)
6	BMA	E	1334	5	11,11,12	0.63	0	13,15,17	1.50	3 (23%)
5	NAG	E	1339	1,5	14,14,15	0.50	0	15,19,21	2.60	3 (20%)
5	NAG	E	1340	5	14,14,15	0.50	0	15,19,21	1.20	2 (13%)
5	NAG	E	1355	1,5	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
5	NAG	E	1356	5	14,14,15	0.49	0	15,19,21	1.18	2 (13%)
5	NAG	E	1362	1,5	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
5	NAG	E	1363	5	14,14,15	0.47	0	15,19,21	1.19	2 (13%)
5	NAG	E	1386	1,5	14,14,15	0.50	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
5	NAG	E	1387	5,6	14,14,15	0.50	0	15,19,21	1.20	2 (13%)
6	BMA	E	1388	5,7	11,11,12	0.63	0	13,15,17	1.50	3 (23%)
7	MAN	E	1390	6	11,11,12	0.60	0	13,15,17	2.59	3 (23%)
5	NAG	E	1392	1,5	14,14,15	0.50	0	15,19,21	2.60	3 (20%)
5	NAG	E	1393	5,6	14,14,15	0.50	0	15,19,21	1.20	2 (13%)
6	BMA	E	1394	5	11,11,12	0.63	0	13,15,17	1.51	3 (23%)
5	NAG	E	1397	1	14,14,15	0.49	0	15,19,21	2.60	3 (20%)
5	NAG	E	1448	1,5	14,14,15	0.48	0	15,19,21	2.61	3 (20%)
5	NAG	E	1449	5,6	14,14,15	0.51	0	15,19,21	1.19	2 (13%)
6	BMA	E	1450	5,7	11,11,12	0.62	0	13,15,17	1.50	3 (23%)
7	MAN	E	1451	7,6	11,11,12	0.55	0	13,15,17	1.60	3 (23%)
7	MAN	E	1452	7	11,11,12	0.58	0	13,15,17	2.60	5 (38%)
7	MAN	E	1453	7,6	11,11,12	0.61	0	13,15,17	2.60	3 (23%)
7	MAN	E	1454	7	11,11,12	0.57	0	13,15,17	2.05	6 (46%)
7	MAN	E	1455	7	11,11,12	0.58	0	13,15,17	2.40	6 (46%)
5	NAG	F	1600	2	14,14,15	0.51	0	15,19,21	2.61	3 (20%)
5	NAG	F	1611	9,2,5	14,14,15	1.50	3 (21%)	15,19,21	1.11	1 (6%)
5	NAG	F	1612	5,6	14,14,15	1.32	2 (14%)	15,19,21	1.30	1 (6%)
6	BMA	F	1613	5,7	11,11,12	1.34	2 (18%)	13,15,17	1.26	1 (7%)
7	MAN	F	1614	5,6	11,11,12	1.69	4 (36%)	13,15,17	1.50	2 (15%)
5	NAG	F	1617	7	14,14,15	1.36	3 (21%)	15,19,21	1.24	2 (13%)
7	MAN	F	1619	5,6	11,11,12	1.50	3 (27%)	13,15,17	1.39	2 (15%)
5	NAG	F	1620	8,7	14,14,15	1.42	3 (21%)	15,19,21	1.37	2 (13%)
8	GAL	F	1621	5	11,11,12	1.33	2 (18%)	13,15,17	1.14	1 (7%)
5	NAG	F	1622	8,7	14,14,15	1.42	3 (21%)	15,19,21	1.19	2 (13%)
8	GAL	F	1623	5	11,11,12	1.34	2 (18%)	13,15,17	1.14	1 (7%)
9	FUC	F	1624	5	9,10,11	1.37	1 (11%)	13,14,16	1.02	0
5	NAG	F	1625	2,5	14,14,15	0.50	0	15,19,21	2.59	3 (20%)
5	NAG	F	1626	5	14,14,15	0.50	0	15,19,21	1.19	2 (13%)
5	NAG	F	1637	9,2,5	14,14,15	1.51	3 (21%)	15,19,21	1.08	1 (6%)
5	NAG	F	1638	5,6	14,14,15	1.33	2 (14%)	15,19,21	1.29	1 (6%)
6	BMA	F	1639	5,7	11,11,12	1.34	2 (18%)	13,15,17	1.28	1 (7%)
7	MAN	F	1640	5,6	11,11,12	1.70	4 (36%)	13,15,17	1.47	2 (15%)
5	NAG	F	1641	8,7	14,14,15	1.35	3 (21%)	15,19,21	1.33	2 (13%)
8	GAL	F	1642	5	11,11,12	1.30	2 (18%)	13,15,17	1.17	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	F	1643	8,7	14,14,15	1.35	3 (21%)	15,19,21	1.21	2 (13%)
8	GAL	F	1644	5	11,11,12	1.34	2 (18%)	13,15,17	1.13	1 (7%)
7	MAN	F	1645	5,6	11,11,12	1.51	3 (27%)	13,15,17	1.41	2 (15%)
5	NAG	F	1646	7	14,14,15	1.40	3 (21%)	15,19,21	1.35	2 (13%)
5	NAG	F	1648	7	14,14,15	1.38	3 (21%)	15,19,21	1.21	2 (13%)
9	FUC	F	1650	5	9,10,11	1.36	1 (11%)	13,14,16	1.02	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
5	NAG	A	1135	1	-	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	5,6	-	0/6/23/26	0/1/1/1
6	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	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	1162	5	-	0/2/19/22	0/1/1/1
5	NAG	A	1241	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1242	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	1243	5	-	0/2/19/22	0/1/1/1
5	NAG	A	1262	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1263	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	1264	5,7	-	0/2/19/22	0/1/1/1
7	MAN	A	1265	7,6	-	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	7,6	-	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	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	1278	5	-	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
5	NAG	A	1332	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1333	5,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	A	1334	5	-	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
5	NAG	A	1355	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1362	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1363	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	1364	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	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	1388	5	-	0/2/19/22	0/1/1/1
5	NAG	A	1392	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1393	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	1394	5	-	0/2/19/22	0/1/1/1
5	NAG	A	1397	1	-	0/6/23/26	0/1/1/1
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
5	NAG	B	1600	2	-	0/6/23/26	0/1/1/1
5	NAG	B	1611	9,2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1612	5,6	-	0/6/23/26	0/1/1/1
6	BMA	B	1613	5,7	-	0/2/19/22	0/1/1/1
7	MAN	B	1614	5,6	-	0/2/19/22	0/1/1/1
5	NAG	B	1617	7	-	0/6/23/26	0/1/1/1
7	MAN	B	1619	5,6	-	0/2/19/22	0/1/1/1
5	NAG	B	1620	8,7	-	0/6/23/26	0/1/1/1
8	GAL	B	1621	5	-	0/2/19/22	0/1/1/1
5	NAG	B	1622	8,7	-	0/6/23/26	0/1/1/1
8	GAL	B	1623	5	-	0/2/19/22	0/1/1/1
9	FUC	B	1624	5	-	0/0/17/20	0/1/1/1
5	NAG	B	1625	2	-	0/6/23/26	0/1/1/1
5	NAG	B	1637	9,2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1638	5,6	-	0/6/23/26	0/1/1/1
6	BMA	B	1639	5,7	-	0/2/19/22	0/1/1/1
7	MAN	B	1640	5,6	-	0/2/19/22	0/1/1/1
5	NAG	B	1641	8,7	-	0/6/23/26	0/1/1/1
8	GAL	B	1642	5	-	0/2/19/22	0/1/1/1
5	NAG	B	1643	8,7	-	0/6/23/26	0/1/1/1
8	GAL	B	1644	5	-	0/2/19/22	0/1/1/1
7	MAN	B	1645	5,6	-	0/2/19/22	0/1/1/1
5	NAG	B	1646	8,7	-	0/6/23/26	0/1/1/1
8	GAL	B	1647	5	-	0/2/19/22	0/1/1/1
5	NAG	B	1648	7	-	0/6/23/26	0/1/1/1
9	FUC	B	1650	5	-	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1088	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1089	5,6	-	0/6/23/26	0/1/1/1
6	BMA	C	1090	5	-	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
5	NAG	C	1160	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1161	5,6	-	0/6/23/26	0/1/1/1
6	BMA	C	1162	5	-	0/2/19/22	0/1/1/1
5	NAG	C	1241	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1242	5,6	-	0/6/23/26	0/1/1/1
6	BMA	C	1243	5,7	-	0/2/19/22	0/1/1/1
7	MAN	C	1244	6	-	0/2/19/22	0/1/1/1
7	MAN	C	1246	6	-	0/2/19/22	0/1/1/1
5	NAG	C	1262	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1263	5,6	-	0/6/23/26	0/1/1/1
6	BMA	C	1264	5,7	-	0/2/19/22	0/1/1/1
7	MAN	C	1265	7,6	-	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	7,6	-	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	5,6	-	0/6/23/26	0/1/1/1
6	BMA	C	1278	5	-	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
5	NAG	C	1301	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1302	5,6	-	0/6/23/26	0/1/1/1
6	BMA	C	1303	5	-	0/2/19/22	0/1/1/1
5	NAG	C	1332	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1333	5,6	-	0/6/23/26	0/1/1/1
6	BMA	C	1334	5	-	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
5	NAG	C	1362	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1363	5,6	-	0/6/23/26	0/1/1/1
6	BMA	C	1364	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	5,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	C	1388	5	-	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
5	NAG	C	1397	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1448	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1449	5,6	-	0/6/23/26	0/1/1/1
6	BMA	C	1450	5,7	-	0/2/19/22	0/1/1/1
7	MAN	C	1451	7,6	-	0/2/19/22	0/1/1/1
7	MAN	C	1452	7	-	0/2/19/22	0/1/1/1
7	MAN	C	1453	7,6	-	0/2/19/22	0/1/1/1
7	MAN	C	1454	7	-	0/2/19/22	0/1/1/1
7	MAN	C	1455	7	-	0/2/19/22	0/1/1/1
5	NAG	D	1600	2	-	0/6/23/26	0/1/1/1
5	NAG	D	1611	9,2,5	-	0/6/23/26	0/1/1/1
5	NAG	D	1612	5	-	0/6/23/26	0/1/1/1
9	FUC	D	1613	5	-	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
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
5	NAG	E	1088	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	1089	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	1090	5	-	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
5	NAG	E	1156	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	1157	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	1158	5	-	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
5	NAG	E	1187	1	-	0/6/23/26	0/1/1/1
5	NAG	E	1241	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	1242	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	1243	5,7	-	0/2/19/22	0/1/1/1
7	MAN	E	1244	7,6	-	0/2/19/22	0/1/1/1
7	MAN	E	1245	7	-	0/2/19/22	0/1/1/1
7	MAN	E	1246	6	-	0/2/19/22	0/1/1/1
5	NAG	E	1262	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	1263	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	1264	5,7	-	0/2/19/22	0/1/1/1
7	MAN	E	1265	7,6	-	0/2/19/22	0/1/1/1
7	MAN	E	1266	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	E	1267	7,6	-	0/2/19/22	0/1/1/1
7	MAN	E	1268	7	-	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
5	NAG	E	1332	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	1333	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	1334	5	-	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
5	NAG	E	1386	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	1387	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	1388	5,7	-	0/2/19/22	0/1/1/1
7	MAN	E	1390	6	-	0/2/19/22	0/1/1/1
5	NAG	E	1392	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	1393	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	1394	5	-	0/2/19/22	0/1/1/1
5	NAG	E	1397	1	-	0/6/23/26	0/1/1/1
5	NAG	E	1448	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	1449	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	1450	5,7	-	0/2/19/22	0/1/1/1
7	MAN	E	1451	7,6	-	0/2/19/22	0/1/1/1
7	MAN	E	1452	7	-	0/2/19/22	0/1/1/1
7	MAN	E	1453	7,6	-	0/2/19/22	0/1/1/1
7	MAN	E	1454	7	-	0/2/19/22	0/1/1/1
7	MAN	E	1455	7	-	0/2/19/22	0/1/1/1
5	NAG	F	1600	2	-	0/6/23/26	0/1/1/1
5	NAG	F	1611	9,2,5	-	0/6/23/26	0/1/1/1
5	NAG	F	1612	5,6	-	0/6/23/26	0/1/1/1
6	BMA	F	1613	5,7	-	0/2/19/22	0/1/1/1
7	MAN	F	1614	5,6	-	0/2/19/22	0/1/1/1
5	NAG	F	1617	7	-	0/6/23/26	0/1/1/1
7	MAN	F	1619	5,6	-	0/2/19/22	0/1/1/1
5	NAG	F	1620	8,7	-	0/6/23/26	0/1/1/1
8	GAL	F	1621	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	F	1622	8,7	-	0/6/23/26	0/1/1/1
8	GAL	F	1623	5	-	0/2/19/22	0/1/1/1
9	FUC	F	1624	5	-	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
5	NAG	F	1637	9,2,5	-	0/6/23/26	0/1/1/1
5	NAG	F	1638	5,6	-	0/6/23/26	0/1/1/1
6	BMA	F	1639	5,7	-	0/2/19/22	0/1/1/1
7	MAN	F	1640	5,6	-	0/2/19/22	0/1/1/1
5	NAG	F	1641	8,7	-	0/6/23/26	0/1/1/1
8	GAL	F	1642	5	-	0/2/19/22	0/1/1/1
5	NAG	F	1643	8,7	-	0/6/23/26	0/1/1/1
8	GAL	F	1644	5	-	0/2/19/22	0/1/1/1
7	MAN	F	1645	5,6	-	0/2/19/22	0/1/1/1
5	NAG	F	1646	7	-	0/6/23/26	0/1/1/1
5	NAG	F	1648	7	-	0/6/23/26	0/1/1/1
9	FUC	F	1650	5	-	0/0/17/20	0/1/1/1

The worst 5 of 130 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1612	NAG	O5-C5	2.03	1.47	1.43
5	F	1612	NAG	O5-C5	2.03	1.47	1.43
5	F	1641	NAG	O5-C5	2.04	1.47	1.43
5	D	1612	NAG	O5-C5	2.06	1.47	1.43
5	B	1646	NAG	O5-C5	2.09	1.47	1.43

The worst 5 of 465 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1241	NAG	O5-C1-C2	-8.56	99.56	111.47
5	E	1088	NAG	O5-C1-C2	-8.55	99.57	111.47
5	A	1386	NAG	O5-C1-C2	-8.54	99.59	111.47
5	C	1088	NAG	O5-C1-C2	-8.54	99.59	111.47
5	A	1088	NAG	O5-C1-C2	-8.54	99.59	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

98 monomers are involved in 354 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1088	NAG	9	0
5	A	1089	NAG	1	0
5	A	1156	NAG	25	0
5	A	1157	NAG	3	0
5	A	1160	NAG	1	0
5	A	1161	NAG	1	0
5	A	1241	NAG	4	0
5	A	1262	NAG	1	0
5	A	1263	NAG	1	0
7	A	1267	MAN	1	0
5	A	1276	NAG	3	0
5	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
5	A	1355	NAG	2	0
5	A	1387	NAG	4	0
5	A	1392	NAG	6	0
5	A	1393	NAG	5	0
6	A	1394	BMA	3	0
5	A	1397	NAG	3	0
5	A	1448	NAG	2	0
5	B	1611	NAG	1	0
8	B	1621	GAL	1	0
5	B	1622	NAG	1	0
8	B	1623	GAL	1	0
9	B	1624	FUC	5	0
5	B	1637	NAG	3	0
5	B	1638	NAG	14	0
7	B	1640	MAN	2	0
5	B	1641	NAG	7	0
8	B	1642	GAL	1	0
5	B	1643	NAG	2	0
8	B	1644	GAL	2	0
5	B	1648	NAG	4	0
9	B	1650	FUC	1	0
5	C	1156	NAG	13	0
5	C	1157	NAG	9	0
5	C	1160	NAG	14	0
5	C	1161	NAG	2	0
5	C	1241	NAG	8	0
5	C	1242	NAG	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1243	BMA	1	0
5	C	1262	NAG	1	0
5	C	1263	NAG	1	0
6	C	1264	BMA	4	0
7	C	1265	MAN	4	0
7	C	1268	MAN	2	0
5	C	1276	NAG	3	0
5	C	1277	NAG	2	0
5	C	1301	NAG	17	0
5	C	1302	NAG	1	0
6	C	1303	BMA	1	0
5	C	1332	NAG	6	0
5	C	1355	NAG	5	0
5	C	1387	NAG	5	0
5	C	1392	NAG	13	0
5	C	1448	NAG	2	0
7	C	1452	MAN	1	0
5	D	1611	NAG	3	0
9	D	1613	FUC	11	0
5	D	1625	NAG	1	0
5	D	1626	NAG	1	0
5	D	1637	NAG	2	0
5	D	1638	NAG	1	0
5	E	1156	NAG	6	0
5	E	1157	NAG	2	0
5	E	1160	NAG	14	0
5	E	1161	NAG	2	0
5	E	1242	NAG	1	0
6	E	1243	BMA	2	0
7	E	1246	MAN	1	0
5	E	1262	NAG	1	0
5	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
5	E	1387	NAG	7	0
6	E	1388	BMA	1	0
5	E	1392	NAG	6	0
5	E	1393	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1394	BMA	1	0
5	E	1397	NAG	11	0
5	E	1448	NAG	2	0
7	E	1452	MAN	2	0
5	F	1612	NAG	1	0
8	F	1621	GAL	3	0
9	F	1624	FUC	5	0
5	F	1637	NAG	2	0
5	F	1638	NAG	12	0
6	F	1639	BMA	3	0
7	F	1640	MAN	2	0
5	F	1641	NAG	3	0
8	F	1642	GAL	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.