



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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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

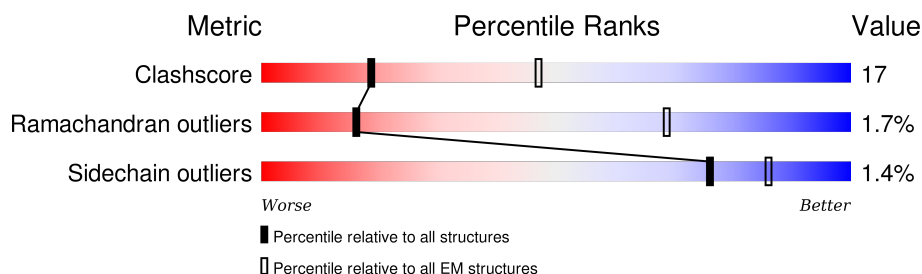
1 Overall quality at a glance

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 ≥ 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
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).

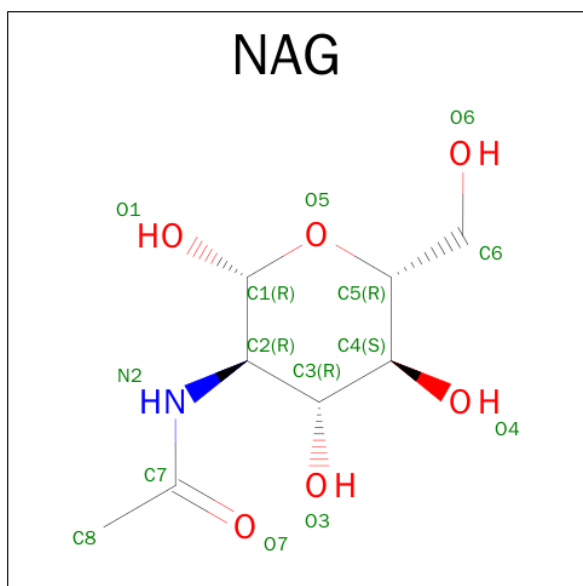
Mol	Chain	Residues	Atoms				AltConf
5	A	2	Total	C	N	O	0
			140	80	10	50	
5	A	2	Total	C	N	O	0
			140	80	10	50	
5	A	2	Total	C	N	O	0
			140	80	10	50	
5	A	2	Total	C	N	O	0
			140	80	10	50	
5	A	2	Total	C	N	O	0
			140	80	10	50	
5	C	2	Total	C	N	O	0
			168	96	12	60	
5	C	2	Total	C	N	O	0
			168	96	12	60	
5	C	2	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	

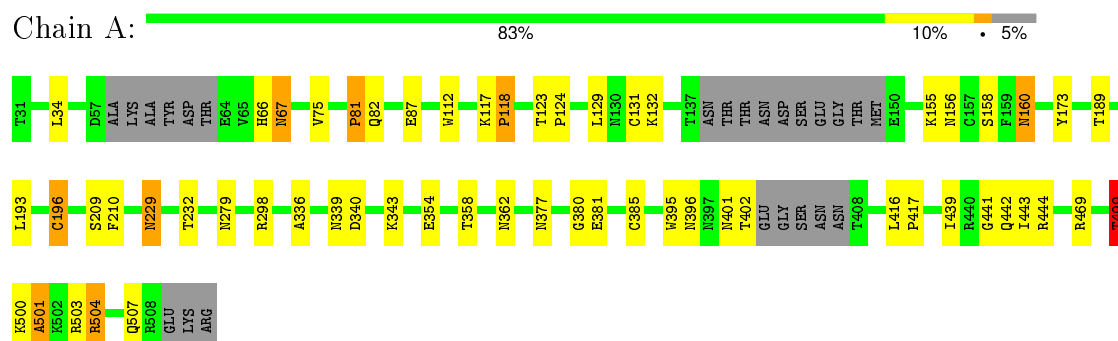
- Molecule 16 is a polymer of unknown type called SUGAR (12-MER).

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

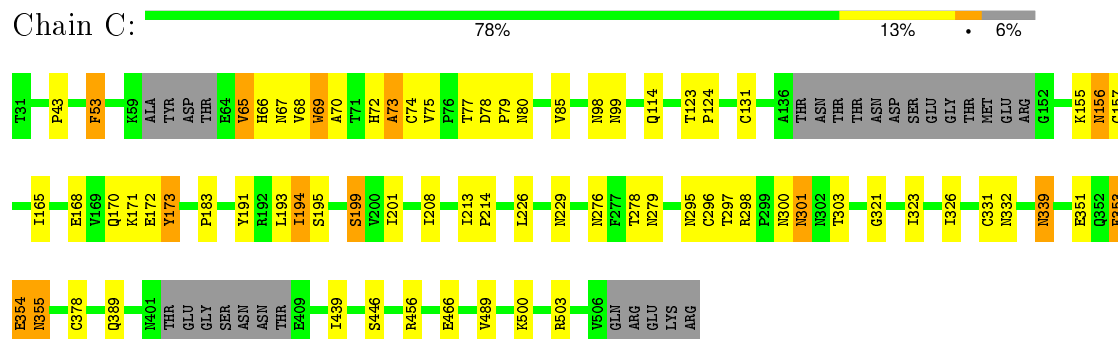
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

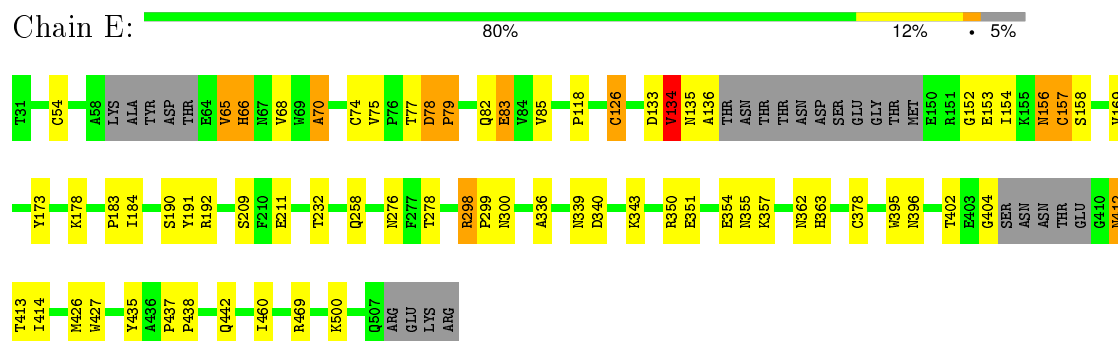
- Molecule 1: HIV-1 ENVELOPE GLYCOPROTEIN GP160



- 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 | K573 | K574 | G600 | K601 | T605 | S613 | N616 | V638 | E641 | Q658 | G6U | L6U | L6U | G6U | L6U | L6U | L6U |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|

-
- | Food Item | Count |
|-----------|-------|
| A512 | 1 |
| A517 | 1 |
| V518 | 1 |
| F519 | 1 |
| L520 | 1 |
| Q551 | 1 |
| Q552 | 1 |
| N553 | 1 |
| Q562 | 1 |
| G600 | 1 |
| K601 | 1 |
| N616 | 1 |
| L619 | 1 |
| N637 | 1 |
| E641 | 1 |
| L663 | 1 |
| D664 | 1 |

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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 | PRO | LEU | ALA | ALA | PRO | PRO | SER | SER | SER | LYS | THR | THR | SER | GLY | GLY | THR | THR | ALA | ALA | LEU | GLY | CYS | LEU | VAL | LYS |
|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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

GLN
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VAL
TYR
ALA
CYS
GLU
VAL
THR
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LEU
SER
SER
PRO
VAL
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
VAL
VAL
ALA
ALA
PRO
SER
SER
PHE
VAL
PHE
ILE
SER
PHE
THR
PRO
PRO
SER
SER
ASP
GLU
GLN
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LYS
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GLY
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ALA
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CYS
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LEU
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ASN
ASN
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GLN
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ASP
ASN
ALA
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GLY
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

All (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
1	A	196	CYS	N-CA-CB	-5.09	101.44	110.60
3	H	22	CYS	N-CA-CB	-5.04	101.53	110.60

There are no chirality outliers.

All (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,Peptide
2	D	518	VAL	Mainchain
2	D	528	SER	Mainchain
2	D	600	GLY	Mainchain
1	E	157	CYS	Mainchain
1	E	412	ASN	Mainchain,Peptide
1	E	65	VAL	Mainchain
1	E	66	HIS	Mainchain
2	F	518	VAL	Mainchain
2	F	600	GLY	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
15:E:1387:NAG:C8	7:E:1392:NAG:H83	1.37	1.52
1:A:210:PHE:CE2	1:A:380:GLY:HA2	1.44	1.52
1:E:183:PRO:HA	1:E:191:TYR:CD1	1.00	1.52
16:F:1638:NAG:H62	3:H:98:GLU:CD	1.31	1.51
2:B:522:PHE:CD1	2:B:544:LEU:HD13	1.47	1.46
1:A:298:ARG:HE	1:A:443:ILE:CD1	1.28	1.43
1:A:395:TRP:CH2	5:A:1339:NAG:H81	1.54	1.40
1:C:323:ILE:CD1	7:C:1301:NAG:H83	1.50	1.39
1:C:297:THR:HG22	7:C:1332:NAG:C8	1.52	1.36
1:E:169:VAL:CG1	5:E:1160:NAG:H82	1.55	1.36
1:A:298:ARG:NE	1:A:443:ILE:CD1	1.86	1.35
1:A:173:TYR:CD1	7:A:1156:NAG:C8	2.10	1.35
2:D:638:TYR:CE1	13:D:1613:FUC:C6	2.11	1.32
1:A:87:GLU:CD	5:A:1088:NAG:H81	1.50	1.32
1:E:351:GLU:CA	5:E:1355:NAG:H81	1.59	1.31
1:A:298:ARG:NE	1:A:443:ILE:HD12	1.00	1.30
1:C:301:ASN:OD1	1:C:323:ILE:HB	1.22	1.30
1:A:173:TYR:CG	7:A:1156:NAG:C8	2.14	1.30
1:E:183:PRO:HA	1:E:191:TYR:CE1	1.67	1.29
1:A:401:ASN:HB2	6:A:1397:NAG:O6	1.15	1.29
1:E:183:PRO:CA	1:E:191:TYR:CE1	2.16	1.28
15:E:1387:NAG:H81	7:E:1392:NAG:C8	1.62	1.28
1:A:395:TRP:CH2	5:A:1339:NAG:C8	2.12	1.27
2:D:638:TYR:CE1	13:D:1613:FUC:H63	1.66	1.27
10:B:1638:NAG:H62	3:M:98:GLU:OE2	1.35	1.25
1:E:134:VAL:HG12	1:E:135:ASN:ND2	1.49	1.25
1:E:183:PRO:HB3	1:E:191:TYR:CE1	1.72	1.23
2:D:638:TYR:CD1	13:D:1613:FUC:C6	2.21	1.22
1:E:169:VAL:HB	5:E:1160:NAG:C8	1.70	1.22
1:A:210:PHE:CD2	1:A:380:GLY:CA	2.23	1.22
10:B:1638:NAG:H62	3:M:98:GLU:CD	1.59	1.22
1:E:134:VAL:CG1	1:E:135:ASN:HD22	1.51	1.22
1:C:173:TYR:CD2	5:C:1156:NAG:H4	1.76	1.20
1:E:355:ASN:HB2	1:E:357:LYS:CG	1.72	1.20
1:E:351:GLU:N	5:E:1355:NAG:H81	1.55	1.20
15:E:1387:NAG:C8	7:E:1392:NAG:C8	2.19	1.19
2:D:638:TYR:CD1	13:D:1613:FUC:H62	1.76	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:ILE:CG1	7:C:1301:NAG:H83	1.73	1.18
1:C:170:GLN:OE1	7:C:1160:NAG:H2	1.40	1.18
1:E:183:PRO:CB	1:E:191:TYR:CE1	2.26	1.18
1:E:183:PRO:HA	1:E:191:TYR:CG	1.80	1.17
1:C:53:PHE:CE1	1:C:75:VAL:HG21	1.80	1.15
1:E:184:ILE:N	1:E:191:TYR:HD1	1.42	1.15
1:A:87:GLU:OE2	5:A:1088:NAG:H81	1.47	1.15
1:E:169:VAL:HG12	5:E:1160:NAG:H82	1.26	1.14
1:C:297:THR:CG2	7:C:1332:NAG:H82	1.76	1.14
1:C:323:ILE:HG13	7:C:1301:NAG:N2	1.61	1.13
1:E:395:TRP:CH2	5:E:1339:NAG:H81	1.84	1.13
1:C:323:ILE:HG13	7:C:1301:NAG:C8	1.77	1.13
1:C:323:ILE:CG1	7:C:1301:NAG:C8	2.28	1.12
1:E:351:GLU:HA	5:E:1355:NAG:H81	1.16	1.12
1:A:210:PHE:CE2	1:A:380:GLY:CA	2.32	1.12
1:A:336:ALA:HB2	5:A:1339:NAG:O6	1.49	1.11
1:A:173:TYR:HB3	7:A:1156:NAG:HN2	1.12	1.11
1:C:323:ILE:HD11	7:C:1301:NAG:H83	1.17	1.10
7:A:1387:NAG:C8	7:A:1392:NAG:H83	1.82	1.09
1:E:355:ASN:HB2	1:E:357:LYS:HG2	1.26	1.09
7:A:1387:NAG:H82	7:A:1392:NAG:H83	1.33	1.09
1:C:168:GLU:CG	7:C:1160:NAG:H82	1.83	1.07
1:E:343:LYS:HE3	5:E:1339:NAG:H82	1.36	1.07
1:E:350:ARG:C	5:E:1355:NAG:C8	2.22	1.07
1:C:85:VAL:CG2	11:C:1242:NAG:H82	1.84	1.07
1:A:87:GLU:CD	5:A:1088:NAG:C8	2.25	1.05
1:C:389:GLN:NE2	5:C:1392:NAG:H81	1.69	1.05
1:C:173:TYR:CE1	5:C:1156:NAG:O3	2.09	1.04
1:E:190:SER:O	1:E:191:TYR:CD1	2.10	1.04
1:E:184:ILE:N	1:E:191:TYR:CD1	2.17	1.04
16:F:1638:NAG:C6	3:H:98:GLU:CD	2.26	1.03
16:F:1638:NAG:H62	3:H:98:GLU:OE1	1.56	1.03
1:A:339:ASN:OD1	1:A:340:ASP:N	1.90	1.02
1:C:323:ILE:HG13	7:C:1301:NAG:C7	1.89	1.02
1:E:169:VAL:CB	5:E:1160:NAG:H82	1.88	1.02
1:A:229:ASN:HB3	7:A:1241:NAG:O6	1.59	1.02
1:A:173:TYR:CD2	7:A:1156:NAG:C7	2.43	1.01
1:A:229:ASN:CB	7:A:1241:NAG:O6	2.08	1.01
1:A:401:ASN:CB	6:A:1397:NAG:O6	2.08	1.01
1:E:357:LYS:HD2	6:E:1397:NAG:C8	1.89	1.01
1:C:53:PHE:HE1	1:C:75:VAL:CG2	1.74	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:522:PHE:CD1	2:B:544:LEU:CD1	2.44	1.00
1:C:173:TYR:CD1	5:C:1156:NAG:H2	1.96	1.00
1:C:173:TYR:CZ	5:C:1156:NAG:O3	2.15	1.00
14:E:1243:BMA:H4	12:E:1452:MAN:O2	1.60	1.00
1:C:53:PHE:CE1	1:C:75:VAL:CG2	2.44	1.00
1:E:169:VAL:CB	5:E:1160:NAG:C8	2.38	1.00
1:C:323:ILE:HD11	7:C:1301:NAG:C8	1.92	0.99
1:E:395:TRP:CH2	5:E:1339:NAG:C8	2.45	0.99
1:A:442:GLN:NE2	5:A:1301:NAG:C8	2.25	0.99
10:B:1638:NAG:H5	3:M:98:GLU:HG3	1.44	0.99
2:B:522:PHE:H	2:B:544:LEU:CD1	1.75	0.99
1:E:500:LYS:HE3	2:F:619:LEU:HD12	1.43	0.99
1:A:395:TRP:HH2	5:A:1339:NAG:H82	1.25	0.99
1:E:350:ARG:C	5:E:1355:NAG:H81	1.82	0.98
1:C:85:VAL:HG21	11:C:1242:NAG:H82	1.44	0.98
1:C:323:ILE:CD1	7:C:1301:NAG:C8	2.42	0.98
1:C:500:LYS:HE3	2:F:663:LEU:HD11	1.42	0.98
1:A:442:GLN:NE2	5:A:1301:NAG:H82	1.79	0.97
1:A:395:TRP:HH2	5:A:1339:NAG:H81	0.81	0.97
8:C:1262:NAG:H61	8:C:1263:NAG:H82	1.47	0.97
1:E:351:GLU:HA	5:E:1355:NAG:C8	1.93	0.96
1:E:158:SER:OG	7:E:1156:NAG:H83	1.63	0.96
1:E:183:PRO:C	1:E:191:TYR:CD1	2.37	0.96
2:D:638:TYR:HE1	13:D:1613:FUC:H63	1.05	0.96
1:A:298:ARG:CZ	1:A:443:ILE:CD1	2.44	0.96
8:A:1262:NAG:H61	8:A:1263:NAG:H82	1.47	0.96
1:E:350:ARG:O	5:E:1355:NAG:C8	2.13	0.95
2:F:641:GLU:OE1	9:F:1624:FUC:H62	1.65	0.95
1:C:301:ASN:OD1	1:C:323:ILE:CB	2.13	0.95
1:C:295:ASN:OD1	1:C:446:SER:HB2	1.66	0.95
1:E:343:LYS:CE	5:E:1339:NAG:H82	1.97	0.95
1:C:168:GLU:HG3	7:C:1160:NAG:H82	1.47	0.94
1:C:323:ILE:HG13	7:C:1301:NAG:HN2	1.17	0.94
2:D:638:TYR:HD1	13:D:1613:FUC:H62	1.30	0.94
1:E:350:ARG:C	5:E:1355:NAG:H82	1.88	0.93
2:B:522:PHE:HD1	2:B:544:LEU:HD13	1.16	0.93
8:E:1262:NAG:H61	8:E:1263:NAG:H82	1.47	0.93
1:A:298:ARG:CZ	1:A:443:ILE:HD12	1.99	0.93
3:M:100(C):ARG:NH1	3:M:100(E):ASP:OD1	2.01	0.93
1:C:354:GLU:O	1:C:355:ASN:ND2	2.02	0.93
7:C:1387:NAG:C8	5:C:1392:NAG:H83	1.98	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:THR:HG22	7:C:1332:NAG:H82	0.95	0.92
1:E:134:VAL:HB	1:E:135:ASN:HB2	1.51	0.92
1:E:395:TRP:HH2	5:E:1339:NAG:C8	1.80	0.92
10:B:1643:NAG:H62	4:N:55:PHE:HZ	1.34	0.92
1:E:169:VAL:O	5:E:1160:NAG:H81	1.69	0.92
2:B:522:PHE:H	2:B:544:LEU:HD12	1.33	0.92
1:A:354:GLU:HB3	6:A:1355:NAG:H82	1.51	0.91
1:A:210:PHE:HD2	1:A:380:GLY:HA2	1.32	0.91
1:C:353:PHE:CZ	1:C:456:ARG:NH1	2.37	0.91
1:C:500:LYS:HG3	2:F:663:LEU:CD1	2.01	0.90
10:B:1641:NAG:O7	3:M:28:PRO:CD	2.19	0.90
16:F:1638:NAG:C6	3:H:98:GLU:OE1	2.17	0.90
10:B:1638:NAG:H62	3:M:98:GLU:CG	2.02	0.90
1:A:173:TYR:CG	7:A:1156:NAG:C7	2.55	0.90
1:A:444:ARG:NH2	5:A:1295:NAG:O6	2.05	0.89
1:A:87:GLU:OE1	5:A:1088:NAG:C7	2.20	0.88
1:A:210:PHE:CD1	1:A:377:ASN:ND2	2.40	0.88
10:B:1640:MAN:H62	10:B:1641:NAG:HN2	1.38	0.88
1:E:357:LYS:CD	6:E:1397:NAG:C8	2.52	0.88
1:E:169:VAL:CG1	5:E:1160:NAG:C8	2.49	0.88
1:A:87:GLU:OE1	5:A:1088:NAG:H81	1.71	0.88
16:F:1638:NAG:H5	3:H:98:GLU:HB2	1.56	0.88
3:H:32:TYR:CE1	3:H:98:GLU:HG2	2.10	0.87
1:C:351:GLU:HA	5:C:1355:NAG:H81	1.53	0.87
1:C:354:GLU:C	1:C:355:ASN:ND2	2.28	0.86
1:A:298:ARG:CD	1:A:443:ILE:HD12	2.05	0.86
16:F:1640:MAN:H62	16:F:1641:NAG:N2	1.90	0.86
1:C:297:THR:CG2	7:C:1332:NAG:C8	2.43	0.86
1:C:295:ASN:OD1	1:C:446:SER:CB	2.23	0.86
1:C:168:GLU:HG3	7:C:1160:NAG:C8	2.04	0.86
1:C:500:LYS:HG3	2:F:663:LEU:HD13	1.55	0.86
10:B:1644:GAL:O2	4:N:55:PHE:HE2	1.58	0.86
3:H:55:TRP:CD1	3:H:100(M):TYR:OH	2.27	0.86
1:E:357:LYS:HD2	6:E:1397:NAG:H83	1.58	0.86
1:E:183:PRO:HB3	1:E:191:TYR:CZ	2.10	0.86
1:C:323:ILE:CG1	7:C:1301:NAG:HN2	1.88	0.86
1:E:357:LYS:CD	6:E:1397:NAG:H83	2.05	0.85
1:C:297:THR:HG22	7:C:1332:NAG:H83	1.56	0.85
1:A:401:ASN:HB2	6:A:1397:NAG:HO6	1.40	0.85
1:A:210:PHE:HD2	1:A:380:GLY:CA	1.86	0.85
15:E:1387:NAG:H82	7:E:1392:NAG:C8	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:GLN:HE22	5:C:1392:NAG:H81	1.39	0.84
1:A:395:TRP:CH2	5:A:1339:NAG:H82	2.03	0.84
1:E:355:ASN:CB	1:E:357:LYS:HG2	2.06	0.84
1:E:183:PRO:C	1:E:191:TYR:HD1	1.75	0.84
16:F:1638:NAG:H62	3:H:98:GLU:OE2	1.76	0.84
2:B:542:ARG:CZ	2:B:542:ARG:HB2	2.06	0.84
2:D:638:TYR:CE1	13:D:1613:FUC:H61	2.09	0.84
1:A:442:GLN:HE21	5:A:1301:NAG:H82	1.42	0.84
1:A:87:GLU:OE1	5:A:1088:NAG:C8	2.23	0.84
1:E:469:ARG:NH2	5:E:1362:NAG:O6	2.11	0.84
10:B:1638:NAG:C5	3:M:98:GLU:HG3	2.08	0.84
1:C:389:GLN:HE22	5:C:1392:NAG:C7	1.90	0.84
3:M:100(N):TYR:HE2	4:N:28:ASN:ND2	1.75	0.83
3:H:2:VAL:HG12	3:H:2:VAL:O	1.76	0.83
1:C:500:LYS:HE3	2:F:663:LEU:CD1	2.09	0.83
1:C:353:PHE:CE1	1:C:456:ARG:NH1	2.47	0.83
10:B:1640:MAN:H62	10:B:1641:NAG:N2	1.93	0.83
1:A:210:PHE:CE1	1:A:377:ASN:ND2	2.46	0.83
1:E:336:ALA:O	1:E:339:ASN:OD1	1.97	0.82
1:C:500:LYS:CE	2:F:663:LEU:HD11	2.10	0.82
3:H:55:TRP:HD1	3:H:100(M):TYR:OH	1.61	0.81
10:B:1641:NAG:O7	3:M:28:PRO:HD3	1.79	0.81
16:F:1640:MAN:H62	16:F:1641:NAG:HN2	1.46	0.81
9:F:1621:GAL:H61	3:H:57:VAL:O	1.80	0.81
1:C:389:GLN:HE22	5:C:1392:NAG:C8	1.92	0.80
1:C:172:GLU:C	1:C:173:TYR:HD1	1.83	0.80
1:A:87:GLU:OE1	5:A:1088:NAG:O7	2.00	0.80
9:F:1612:NAG:O3	3:H:55:TRP:CZ3	2.34	0.80
1:A:298:ARG:NH2	1:A:443:ILE:HD11	1.96	0.80
1:A:173:TYR:CB	7:A:1156:NAG:HN2	1.93	0.80
10:B:1638:NAG:C6	3:M:98:GLU:OE2	2.26	0.80
1:C:389:GLN:NE2	5:C:1392:NAG:C8	2.44	0.79
1:C:173:TYR:CG	5:C:1156:NAG:H2	2.18	0.79
1:C:168:GLU:OE2	7:C:1160:NAG:H82	1.83	0.79
2:B:641:GLU:CD	9:B:1624:FUC:H4	2.02	0.79
1:C:500:LYS:HE3	2:F:663:LEU:HD21	1.65	0.79
1:A:173:TYR:CE1	7:A:1156:NAG:C8	2.66	0.78
10:B:1638:NAG:C6	3:M:98:GLU:CD	2.48	0.78
1:C:173:TYR:OH	5:C:1157:NAG:H5	1.84	0.78
1:A:173:TYR:HB3	7:A:1156:NAG:N2	1.95	0.78
1:E:169:VAL:HB	5:E:1160:NAG:H81	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:TYR:CE1	7:A:1156:NAG:H82	2.11	0.78
1:C:85:VAL:HG13	11:C:1241:NAG:O6	1.85	0.77
1:E:351:GLU:N	5:E:1355:NAG:C8	2.36	0.77
1:C:168:GLU:CD	7:C:1160:NAG:H82	2.04	0.77
3:M:100(G):TRP:CE3	3:M:100(G):TRP:O	2.38	0.76
10:B:1643:NAG:H62	4:N:55:PHE:CZ	2.20	0.76
1:A:298:ARG:CZ	1:A:443:ILE:HD11	2.14	0.76
1:C:173:TYR:CG	5:C:1156:NAG:H4	2.21	0.76
1:E:355:ASN:CB	1:E:357:LYS:CG	2.60	0.75
1:A:298:ARG:NH2	1:A:443:ILE:CD1	2.50	0.75
2:B:522:PHE:N	2:B:544:LEU:CD1	2.50	0.74
1:C:85:VAL:HG23	11:C:1242:NAG:H82	1.69	0.74
1:A:343:LYS:HE3	5:A:1339:NAG:H82	1.68	0.74
1:E:173:TYR:CG	7:E:1156:NAG:H2	2.23	0.74
2:F:641:GLU:OE1	9:F:1624:FUC:C6	2.35	0.74
1:E:190:SER:O	1:E:191:TYR:CG	2.40	0.74
1:E:350:ARG:O	5:E:1355:NAG:H82	1.85	0.74
2:B:641:GLU:OE2	9:B:1624:FUC:H4	1.87	0.74
1:C:173:TYR:CE2	5:C:1156:NAG:H4	2.22	0.74
1:A:156:ASN:OD1	7:A:1156:NAG:O7	2.05	0.74
1:A:173:TYR:CD2	7:A:1156:NAG:C8	2.71	0.74
10:B:1638:NAG:C6	3:M:98:GLU:CG	2.65	0.74
10:B:1638:NAG:C6	3:M:98:GLU:HG3	2.18	0.73
7:A:1387:NAG:H81	7:A:1392:NAG:H83	1.67	0.73
1:A:173:TYR:CD2	7:A:1156:NAG:N2	2.56	0.73
1:A:442:GLN:NE2	5:A:1301:NAG:H81	2.02	0.73
1:C:168:GLU:CG	7:C:1160:NAG:C8	2.62	0.73
1:E:343:LYS:HE3	5:E:1339:NAG:C8	2.17	0.73
1:A:298:ARG:HE	1:A:443:ILE:CG1	2.00	0.73
1:E:500:LYS:HE3	2:F:619:LEU:CD1	2.18	0.73
7:C:1387:NAG:C8	5:C:1392:NAG:C8	2.67	0.73
3:H:55:TRP:HD1	3:H:100(M):TYR:HH	0.78	0.73
9:B:1621:GAL:O3	14:E:1246:MAN:O2	2.00	0.73
1:E:134:VAL:CB	1:E:135:ASN:HB2	2.19	0.72
10:B:1644:GAL:O2	4:N:55:PHE:CE2	2.38	0.72
1:E:442:GLN:OE1	5:E:1301:NAG:C8	2.36	0.72
5:E:1276:NAG:H62	5:E:1277:NAG:H82	1.71	0.72
3:H:1:ARG:HA	3:H:2:VAL:HB	1.71	0.72
1:A:354:GLU:CB	6:A:1355:NAG:H82	2.19	0.72
3:H:32:TYR:CZ	3:H:98:GLU:HG2	2.24	0.72
1:C:85:VAL:CG2	11:C:1242:NAG:C8	2.67	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:ASP:HB2	1:E:79:PRO:HA	1.72	0.72
1:E:134:VAL:HG12	1:E:135:ASN:HD22	0.65	0.72
7:A:1276:NAG:H62	7:A:1277:NAG:H82	1.71	0.72
2:B:522:PHE:HD1	2:B:544:LEU:CD1	1.96	0.71
1:E:339:ASN:OD1	1:E:340:ASP:N	2.23	0.71
7:C:1276:NAG:H62	7:C:1277:NAG:H82	1.71	0.71
1:E:395:TRP:HH2	5:E:1339:NAG:H82	1.56	0.70
1:C:85:VAL:HG22	11:C:1241:NAG:O6	1.91	0.70
1:A:209:SER:OG	8:A:1267:MAN:H61	1.91	0.70
15:E:1387:NAG:H81	7:E:1392:NAG:H83	0.72	0.70
1:E:357:LYS:NZ	6:E:1397:NAG:H83	2.07	0.70
1:C:339:ASN:C	1:C:339:ASN:OD1	2.29	0.70
10:B:1638:NAG:O4	3:M:98:GLU:HG2	1.92	0.69
1:C:389:GLN:HE21	5:C:1392:NAG:H81	1.54	0.69
1:E:355:ASN:HB2	1:E:357:LYS:CA	2.23	0.69
7:A:1387:NAG:H82	7:A:1392:NAG:C8	2.18	0.69
16:F:1638:NAG:C5	3:H:98:GLU:HB2	2.22	0.69
1:C:353:PHE:CE2	1:C:466:GLU:OE2	2.45	0.69
9:F:1621:GAL:H2	3:H:56:HIS:CD2	2.28	0.69
1:E:184:ILE:N	1:E:191:TYR:CE1	2.61	0.69
1:A:343:LYS:CE	5:A:1339:NAG:H82	2.21	0.69
1:E:156:ASN:O	1:E:156:ASN:CG	2.30	0.69
1:C:354:GLU:O	1:C:355:ASN:CG	2.31	0.69
2:F:518:VAL:O	2:F:518:VAL:HG23	1.92	0.69
1:E:395:TRP:CH2	5:E:1339:NAG:H82	2.29	0.68
7:A:1393:NAG:H3	7:A:1394:BMA:O5	1.92	0.68
1:E:173:TYR:CE2	7:E:1156:NAG:H61	2.29	0.68
1:C:500:LYS:CD	2:F:663:LEU:HD11	2.24	0.68
16:F:1638:NAG:H5	3:H:98:GLU:CB	2.24	0.67
7:E:1393:NAG:O3	7:E:1394:BMA:O5	2.11	0.67
1:E:357:LYS:CD	6:E:1397:NAG:H82	2.22	0.67
1:C:172:GLU:O	1:C:173:TYR:HD1	1.77	0.67
1:E:169:VAL:HG11	5:E:1160:NAG:H82	1.72	0.67
1:E:343:LYS:CE	5:E:1339:NAG:C8	2.72	0.67
1:A:336:ALA:HB2	5:A:1339:NAG:HO6	1.59	0.67
1:E:169:VAL:HB	5:E:1160:NAG:H83	1.71	0.67
1:E:395:TRP:CZ3	5:E:1339:NAG:H81	2.30	0.67
1:C:500:LYS:HE3	2:F:663:LEU:CD2	2.25	0.66
1:E:469:ARG:NH2	5:E:1362:NAG:O5	2.27	0.66
1:A:336:ALA:CB	5:A:1339:NAG:O6	2.36	0.66
1:C:303:THR:OG1	7:C:1301:NAG:H82	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:ASP:O	1:E:134:VAL:HG13	1.95	0.66
1:C:351:GLU:OE2	5:C:1355:NAG:C8	2.44	0.66
1:C:354:GLU:C	1:C:355:ASN:HD22	1.97	0.66
2:D:565:MET:O	2:D:565:MET:HG3	1.96	0.65
1:C:65:VAL:HB	1:C:66:HIS:HA	1.78	0.65
1:A:298:ARG:HH21	1:A:443:ILE:HG13	1.60	0.65
1:A:210:PHE:HE2	1:A:380:GLY:CA	2.04	0.65
1:E:133:ASP:C	1:E:134:VAL:HG22	2.16	0.65
1:A:442:GLN:HE21	5:A:1301:NAG:C8	2.00	0.65
1:C:172:GLU:C	1:C:173:TYR:CD1	2.69	0.65
1:E:395:TRP:CZ3	5:E:1339:NAG:C8	2.79	0.65
1:C:439:ILE:CG2	8:C:1268:MAN:O6	2.44	0.65
7:C:1387:NAG:H82	5:C:1392:NAG:C8	2.27	0.65
1:E:169:VAL:HG12	5:E:1160:NAG:C8	2.16	0.65
7:A:1393:NAG:C3	7:A:1394:BMA:O5	2.44	0.65
8:C:1264:BMA:H61	8:C:1265:MAN:C5	2.26	0.65
2:B:540:GLN:O	2:B:542:ARG:N	2.30	0.65
2:D:638:TYR:CD1	13:D:1613:FUC:H63	2.09	0.64
1:A:173:TYR:CG	7:A:1156:NAG:N2	2.65	0.64
16:F:1641:NAG:H62	16:F:1642:GAL:O2	1.97	0.64
1:C:297:THR:HG21	7:C:1332:NAG:HN2	1.61	0.64
1:C:85:VAL:HG21	11:C:1241:NAG:H62	1.79	0.64
1:C:85:VAL:CG2	11:C:1241:NAG:H62	2.28	0.64
7:C:1387:NAG:H82	5:C:1392:NAG:H83	1.79	0.64
10:B:1641:NAG:H62	10:B:1642:GAL:O2	1.97	0.64
1:E:354:GLU:O	1:E:355:ASN:CG	2.36	0.63
1:C:85:VAL:HG21	11:C:1242:NAG:C8	2.24	0.63
1:A:279:ASN:ND2	7:A:1276:NAG:O6	2.32	0.63
10:B:1650:FUC:H4	3:M:100(C):ARG:HD3	1.80	0.63
8:C:1264:BMA:H61	8:C:1265:MAN:H5	1.81	0.63
1:A:81:PRO:HA	1:A:82:GLN:HB2	1.78	0.63
1:E:355:ASN:HB2	1:E:357:LYS:HA	1.80	0.63
1:C:353:PHE:CD2	1:C:466:GLU:OE2	2.52	0.63
2:D:616:ASN:O	2:D:616:ASN:OD1	2.17	0.63
1:A:298:ARG:HH21	1:A:443:ILE:CD1	2.11	0.63
3:M:100(N):TYR:HD1	3:M:100(O):TYR:N	1.95	0.63
1:E:183:PRO:HB3	1:E:191:TYR:HE1	1.56	0.62
1:E:68:VAL:O	1:E:68:VAL:HG12	1.99	0.62
1:E:232:THR:HG22	1:E:232:THR:O	1.98	0.62
16:F:1638:NAG:O6	3:H:98:GLU:OE1	2.17	0.62
1:C:85:VAL:HG22	11:C:1241:NAG:C6	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:HIS:O	1:A:67:ASN:HB2	2.00	0.62
1:E:469:ARG:NH2	5:E:1362:NAG:C6	2.63	0.62
7:A:1393:NAG:O3	7:A:1394:BMA:C1	2.47	0.62
2:F:641:GLU:OE1	9:F:1624:FUC:H4	1.98	0.62
1:A:298:ARG:HH21	1:A:443:ILE:CG1	2.11	0.62
1:E:357:LYS:HD2	6:E:1397:NAG:H82	1.78	0.62
2:B:522:PHE:CE1	2:B:544:LEU:HD22	2.35	0.61
1:E:355:ASN:CB	1:E:357:LYS:HA	2.30	0.61
1:E:82:GLN:O	1:E:83:GLU:CB	2.48	0.61
1:C:170:GLN:HG3	1:C:171:LYS:N	2.14	0.61
2:F:551:GLN:O	2:F:552:GLN:CB	2.48	0.61
1:C:170:GLN:OE1	7:C:1160:NAG:C2	2.34	0.61
1:A:156:ASN:OD1	7:A:1156:NAG:C7	2.49	0.60
15:E:1387:NAG:H82	7:E:1392:NAG:H81	1.83	0.60
1:E:355:ASN:HB2	1:E:357:LYS:CB	2.30	0.60
1:C:156:ASN:OD1	5:C:1156:NAG:O7	2.19	0.60
1:C:323:ILE:CG1	7:C:1301:NAG:H82	2.26	0.60
1:C:173:TYR:CD1	1:C:173:TYR:N	2.69	0.60
1:C:171:LYS:CE	5:C:1157:NAG:H62	2.31	0.60
1:E:65:VAL:HG12	1:E:65:VAL:O	1.99	0.60
2:F:600:GLY:HA2	2:F:601:LYS:HB2	1.84	0.60
1:C:503:ARG:HD2	2:D:605:THR:O	2.01	0.60
2:D:518:VAL:HG23	2:D:518:VAL:O	2.02	0.60
1:C:323:ILE:HG13	7:C:1301:NAG:H83	1.49	0.60
1:E:350:ARG:O	5:E:1355:NAG:C7	2.50	0.60
1:E:355:ASN:HB2	1:E:357:LYS:HG3	1.74	0.60
1:A:173:TYR:CB	7:A:1156:NAG:H82	2.23	0.59
5:E:1160:NAG:O3	5:E:1161:NAG:O5	2.19	0.59
1:C:53:PHE:CZ	1:C:75:VAL:HG21	2.34	0.59
16:F:1639:BMA:H2	3:H:98:GLU:OE2	2.03	0.59
1:A:499:THR:O	1:A:499:THR:CG2	2.50	0.59
1:E:78:ASP:CB	1:E:79:PRO:HA	2.32	0.59
1:C:85:VAL:HG23	11:C:1242:NAG:C8	2.29	0.59
7:C:1160:NAG:O3	7:C:1161:NAG:O5	2.20	0.59
7:C:1387:NAG:H83	5:C:1392:NAG:H83	1.85	0.59
1:A:75:VAL:CG2	2:B:556:LEU:HD13	2.33	0.59
4:L:109:THR:HG22	4:L:109:THR:O	2.02	0.59
1:C:354:GLU:O	5:C:1355:NAG:C7	2.51	0.59
1:A:75:VAL:HG21	2:B:556:LEU:HD13	1.85	0.59
1:C:173:TYR:CD1	5:C:1156:NAG:C2	2.82	0.59
1:E:65:VAL:CG1	1:E:65:VAL:O	2.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:442:GLN:OE1	5:E:1301:NAG:H82	2.03	0.58
2:B:564:ARG:NH1	2:D:574:LYS:NZ	2.50	0.58
1:A:112:TRP:HH2	1:A:210:PHE:CE1	2.20	0.58
2:F:600:GLY:HA2	2:F:601:LYS:O	2.03	0.58
1:C:389:GLN:NE2	5:C:1392:NAG:C7	2.66	0.58
1:A:298:ARG:HH22	1:A:441:GLY:H	1.50	0.58
10:B:1638:NAG:C5	3:M:98:GLU:CG	2.80	0.57
1:C:353:PHE:CD2	1:C:466:GLU:OE1	2.57	0.57
1:C:295:ASN:OD1	1:C:446:SER:HB3	2.02	0.57
1:E:133:ASP:O	1:E:134:VAL:HG22	2.04	0.57
1:C:439:ILE:HG22	8:C:1268:MAN:O6	2.05	0.57
16:F:1639:BMA:O2	3:H:98:GLU:HG3	2.05	0.57
1:E:355:ASN:OD1	1:E:357:LYS:HG3	2.04	0.56
2:B:637:ASN:N	2:B:637:ASN:OD1	2.38	0.56
2:B:542:ARG:NH1	2:B:542:ARG:HB2	2.20	0.56
3:H:1:ARG:HA	3:H:2:VAL:C	2.26	0.56
3:M:100(G):TRP:HE3	3:M:100(G):TRP:O	1.84	0.56
1:A:298:ARG:HH21	1:A:443:ILE:HD11	1.71	0.56
3:M:100(N):TYR:HE2	4:N:28:ASN:HD21	1.49	0.56
1:E:412:ASN:HB2	1:E:413:THR:O	2.06	0.56
1:A:298:ARG:HB2	1:A:443:ILE:HB	1.86	0.56
1:C:173:TYR:CE2	5:C:1157:NAG:C1	2.89	0.56
2:D:528:SER:HA	2:D:529:THR:CB	2.36	0.56
1:A:81:PRO:HA	1:A:82:GLN:CB	2.35	0.56
1:C:170:GLN:HB3	7:C:1160:NAG:O7	2.06	0.56
1:E:82:GLN:O	1:E:83:GLU:HB2	2.05	0.56
7:C:1301:NAG:O7	7:C:1301:NAG:O3	2.24	0.55
1:E:157:CYS:HA	1:E:158:SER:HB2	1.89	0.55
1:C:53:PHE:CE1	1:C:75:VAL:HG23	2.39	0.55
1:E:500:LYS:CE	2:F:619:LEU:HD12	2.27	0.55
3:M:32:TYR:CE1	3:M:98:GLU:HB3	2.41	0.55
1:E:133:ASP:OD1	1:E:134:VAL:N	2.39	0.55
2:B:600:GLY:HA2	2:B:601:LYS:CB	2.35	0.55
3:H:1:ARG:HA	3:H:2:VAL:CB	2.33	0.55
1:E:152:GLY:O	1:E:178:LYS:HD2	2.06	0.55
1:E:357:LYS:HD3	6:E:1397:NAG:H82	1.87	0.55
1:A:499:THR:OG1	1:A:500:LYS:HA	2.06	0.55
1:E:157:CYS:HA	1:E:158:SER:CB	2.37	0.55
2:F:518:VAL:HA	2:F:519:PHE:HB2	1.88	0.55
1:C:68:VAL:HB	1:C:69:TRP:HA	1.89	0.55
2:F:517:ALA:O	2:F:519:PHE:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:CYS:SG	1:C:155:LYS:HB3	2.47	0.55
1:E:343:LYS:HE2	5:E:1339:NAG:H82	1.84	0.55
3:M:100(N):TYR:CD1	3:M:100(O):TYR:N	2.75	0.55
2:B:522:PHE:CE1	2:B:544:LEU:HD13	2.27	0.55
1:C:171:LYS:NZ	5:C:1157:NAG:H61	2.22	0.55
1:C:85:VAL:CG2	11:C:1241:NAG:C6	2.84	0.55
1:C:85:VAL:CG1	11:C:1241:NAG:O6	2.54	0.54
3:H:2:VAL:O	3:H:2:VAL:CG1	2.49	0.54
1:E:65:VAL:HB	1:E:66:HIS:HA	1.88	0.54
1:C:351:GLU:OE2	5:C:1355:NAG:H83	2.07	0.54
1:C:114:GLN:NE2	2:D:568:LEU:HD22	2.22	0.54
1:C:72:HIS:O	1:C:73:ALA:HB2	2.08	0.54
1:E:351:GLU:HA	5:E:1355:NAG:C7	2.38	0.54
1:C:65:VAL:HB	1:C:66:HIS:CA	2.36	0.54
1:A:173:TYR:CE1	7:A:1156:NAG:H81	2.41	0.54
2:B:522:PHE:CD2	2:B:540:GLN:OE1	2.60	0.54
5:C:1156:NAG:O3	5:C:1157:NAG:O5	2.26	0.54
10:B:1648:NAG:HN2	4:N:53:ASN:ND2	2.06	0.54
2:B:564:ARG:HH11	2:D:574:LYS:NZ	2.05	0.54
1:E:413:THR:CG2	1:E:414:ILE:N	2.71	0.53
7:A:1156:NAG:O3	7:A:1157:NAG:O5	2.26	0.53
1:C:173:TYR:OH	5:C:1157:NAG:C5	2.54	0.53
2:B:570:VAL:O	2:B:573:ILE:N	2.42	0.53
1:A:503:ARG:O	1:A:504:ARG:HB3	2.08	0.53
1:C:389:GLN:NE2	5:C:1392:NAG:O7	2.35	0.53
1:A:499:THR:O	1:A:499:THR:HG22	2.09	0.53
2:F:641:GLU:OE1	9:F:1624:FUC:C4	2.56	0.53
10:B:1637:NAG:O7	10:B:1637:NAG:C1	2.57	0.53
1:E:350:ARG:O	5:E:1355:NAG:H81	1.97	0.53
9:F:1621:GAL:H2	3:H:56:HIS:HD2	1.74	0.53
2:D:528:SER:HA	2:D:529:THR:HB	1.91	0.53
2:D:641:GLU:OE2	13:D:1613:FUC:H4	2.09	0.53
2:F:600:GLY:CA	2:F:601:LYS:O	2.57	0.53
2:D:613:SER:OG	13:D:1611:NAG:C5	2.56	0.53
16:F:1637:NAG:O7	16:F:1637:NAG:C1	2.57	0.52
2:B:564:ARG:HG2	2:D:574:LYS:HE2	1.91	0.52
2:D:549:VAL:O	2:D:550:GLN:HB2	2.08	0.52
8:C:1264:BMA:C6	8:C:1265:MAN:C5	2.88	0.52
3:H:28:PRO:O	3:H:29:PHE:HB2	2.10	0.52
1:C:114:GLN:HE22	2:D:568:LEU:HD22	1.74	0.52
1:C:65:VAL:H	1:C:66:HIS:HB3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:518:VAL:HA	2:D:519:PHE:HB2	1.91	0.52
5:D:1637:NAG:O7	5:D:1637:NAG:C1	2.57	0.52
16:F:1637:NAG:O3	16:F:1638:NAG:O5	2.25	0.52
2:F:641:GLU:OE2	9:F:1624:FUC:O4	2.22	0.52
2:D:616:ASN:OD1	2:D:616:ASN:C	2.47	0.52
1:C:276:ASN:OD1	1:C:278:THR:HB	2.09	0.52
2:F:637:ASN:N	2:F:637:ASN:OD1	2.42	0.52
1:A:229:ASN:CG	7:A:1241:NAG:O6	2.48	0.51
1:C:351:GLU:CD	5:C:1355:NAG:C8	2.78	0.51
2:D:613:SER:OG	13:D:1611:NAG:H5	2.10	0.51
1:C:78:ASP:N	1:C:79:PRO:CD	2.73	0.51
1:C:303:THR:OG1	7:C:1301:NAG:C8	2.58	0.51
1:C:500:LYS:CG	2:F:663:LEU:CD1	2.83	0.51
1:C:170:GLN:HG3	1:C:171:LYS:H	1.75	0.51
1:E:460:ILE:C	1:E:460:ILE:HD12	2.31	0.51
2:B:531:GLY:O	2:B:532:ALA:CB	2.58	0.51
1:A:173:TYR:CB	7:A:1156:NAG:C8	2.85	0.51
16:F:1638:NAG:O4	3:H:98:GLU:HB2	2.10	0.51
2:B:542:ARG:NH1	2:B:542:ARG:CB	2.74	0.51
1:E:357:LYS:HD3	6:E:1397:NAG:C8	2.37	0.51
8:C:1264:BMA:C6	8:C:1265:MAN:H5	2.39	0.51
7:E:1156:NAG:O3	7:E:1157:NAG:O5	2.26	0.51
1:E:276:ASN:OD1	1:E:276:ASN:C	2.49	0.51
3:H:111:VAL:O	3:H:112:SER:CB	2.58	0.50
1:E:135:ASN:O	1:E:136:ALA:HB3	2.11	0.50
1:A:503:ARG:O	1:A:504:ARG:CB	2.59	0.50
1:A:117:LYS:CB	1:A:118:PRO:CD	2.90	0.50
2:D:528:SER:HB2	2:D:529:THR:HB	1.93	0.50
1:E:460:ILE:HD12	1:E:460:ILE:O	2.12	0.50
1:C:279:ASN:ND2	7:C:1276:NAG:O6	2.45	0.50
1:C:500:LYS:HG3	2:F:663:LEU:HD11	1.90	0.49
4:L:50:GLU:HB2	4:L:53:ASN:HB3	1.95	0.49
1:E:351:GLU:HA	5:E:1355:NAG:O7	2.12	0.49
14:E:1243:BMA:C4	12:E:1452:MAN:O2	2.49	0.49
1:C:500:LYS:CE	2:F:663:LEU:HD21	2.40	0.49
3:M:100(N):TYR:CD1	3:M:100(N):TYR:C	2.85	0.49
1:E:362:ASN:OD1	1:E:363:HIS:O	2.30	0.49
2:F:552:GLN:N	2:F:553:ASN:HA	2.27	0.49
2:D:613:SER:HB3	13:D:1611:NAG:H62	1.94	0.49
1:A:129:LEU:C	1:A:129:LEU:HD12	2.33	0.49
1:A:358:THR:HG23	1:A:396:ASN:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ARG:CB	1:A:443:ILE:HB	2.43	0.49
10:B:1638:NAG:H5	3:M:98:GLU:CG	2.30	0.49
1:C:173:TYR:HD1	1:C:173:TYR:N	2.10	0.49
1:E:413:THR:HG22	1:E:414:ILE:N	2.27	0.49
1:C:85:VAL:CG2	11:C:1241:NAG:O6	2.59	0.49
7:A:1160:NAG:O3	7:A:1161:NAG:O5	2.26	0.49
1:A:173:TYR:CB	7:A:1156:NAG:N2	2.63	0.49
10:B:1648:NAG:HN2	4:N:53:ASN:CG	2.16	0.49
3:M:100(N):TYR:C	3:M:100(N):TYR:HD1	2.16	0.48
1:E:75:VAL:HA	2:F:562:GLN:HG3	1.95	0.48
1:A:442:GLN:CD	5:A:1301:NAG:H82	2.33	0.48
2:B:641:GLU:OE1	9:B:1624:FUC:H62	2.13	0.48
3:H:1:ARG:CA	3:H:2:VAL:HB	2.43	0.48
2:D:569:THR:O	2:D:570:VAL:HB	2.13	0.48
1:C:53:PHE:C	1:C:53:PHE:CD1	2.85	0.48
1:C:339:ASN:O	1:C:339:ASN:OD1	2.31	0.48
2:D:528:SER:HB2	2:D:529:THR:O	2.13	0.48
3:H:32:TYR:OH	3:H:98:GLU:HG2	2.13	0.48
1:A:34:LEU:HA	1:A:499:THR:HB	1.96	0.48
2:B:542:ARG:CZ	2:B:542:ARG:CB	2.86	0.48
1:E:355:ASN:CB	1:E:357:LYS:HG3	2.39	0.48
2:B:613:SER:OG	9:B:1611:NAG:C1	2.62	0.48
3:H:96:PHE:CD2	3:H:97:GLN:HG3	2.49	0.48
9:B:1622:NAG:H62	9:B:1623:GAL:O2	2.13	0.48
10:B:1638:NAG:O3	3:M:97:GLN:NE2	2.46	0.48
10:B:1637:NAG:O3	10:B:1638:NAG:O5	2.25	0.47
3:M:100(N):TYR:CE2	4:N:28:ASN:ND2	2.67	0.47
7:A:1276:NAG:C6	7:A:1277:NAG:H82	2.44	0.47
1:E:153:GLU:HG3	1:E:154:ILE:HG13	1.96	0.47
1:A:173:TYR:HE2	7:A:1157:NAG:H62	1.79	0.47
1:C:173:TYR:CD1	5:C:1156:NAG:O3	2.63	0.47
2:B:568:LEU:HD13	2:D:573:ILE:HD13	1.96	0.47
1:A:160:ASN:OD1	1:A:160:ASN:N	2.47	0.47
2:F:551:GLN:O	2:F:552:GLN:HB2	2.15	0.47
2:B:564:ARG:NH1	2:D:574:LYS:HZ1	2.11	0.47
3:H:14:PRO:HD3	3:H:112:SER:HA	1.96	0.47
1:A:210:PHE:CD2	1:A:380:GLY:N	2.80	0.47
1:E:412:ASN:CB	1:E:413:THR:HB	2.44	0.47
1:A:117:LYS:CB	1:A:118:PRO:HD3	2.44	0.47
2:B:600:GLY:CA	2:B:601:LYS:O	2.62	0.47
1:A:173:TYR:CE2	7:A:1156:NAG:C7	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:E:1387:NAG:HO3	15:E:1388:BMA:C1	2.28	0.47
1:C:500:LYS:HG3	1:C:500:LYS:O	2.14	0.47
2:D:600:GLY:HA2	2:D:601:LYS:CB	2.43	0.47
1:A:132:LYS:NZ	1:A:189:THR:HG21	2.29	0.47
1:E:426:MET:HB3	1:E:427:TRP:CE3	2.50	0.47
1:E:134:VAL:CG1	1:E:135:ASN:ND2	2.35	0.47
1:C:353:PHE:HE1	1:C:456:ARG:HH12	1.58	0.47
1:C:353:PHE:CD2	1:C:466:GLU:CD	2.87	0.47
2:F:519:PHE:HE2	3:M:100(K):ASN:HD21	1.59	0.47
1:A:173:TYR:HD2	7:A:1156:NAG:O3	1.99	0.46
1:C:170:GLN:HB3	7:C:1160:NAG:C7	2.46	0.46
2:B:568:LEU:HD11	2:B:573:ILE:CG1	2.45	0.46
2:B:521:GLY:HA2	2:B:544:LEU:HD11	1.97	0.46
1:C:53:PHE:HE1	1:C:75:VAL:CB	2.28	0.46
2:B:570:VAL:O	2:B:571:TRP:C	2.54	0.46
1:A:381:GLU:HG3	1:A:443:ILE:HD13	1.97	0.46
1:C:78:ASP:N	1:C:79:PRO:HD3	2.30	0.46
12:E:1448:NAG:C3	12:E:1448:NAG:O7	2.64	0.46
1:A:336:ALA:O	1:A:339:ASN:OD1	2.34	0.46
1:E:357:LYS:CE	6:E:1397:NAG:H83	2.45	0.46
10:B:1648:NAG:H3	4:N:53:ASN:OD1	2.15	0.46
5:A:1295:NAG:H62	5:A:1296:NAG:H82	1.96	0.46
12:C:1448:NAG:O7	12:C:1448:NAG:H3	2.16	0.46
1:E:85:VAL:CG2	14:E:1242:NAG:H82	2.46	0.46
12:E:1448:NAG:O7	12:E:1448:NAG:H3	2.16	0.46
1:C:70:ALA:O	1:C:74:CYS:HB3	2.16	0.46
16:F:1638:NAG:H62	3:H:98:GLU:CG	2.32	0.46
2:B:568:LEU:HD11	2:B:573:ILE:HG12	1.98	0.46
2:B:568:LEU:HD11	2:B:573:ILE:HD11	1.97	0.46
4:N:4:MET:SD	4:N:23:CYS:SG	3.14	0.46
1:E:209:SER:OG	1:E:211:GLU:HG3	2.15	0.46
1:E:412:ASN:HB3	1:E:413:THR:HB	1.97	0.46
1:A:343:LYS:HE2	5:A:1339:NAG:H82	1.95	0.45
2:B:522:PHE:CG	2:B:522:PHE:O	2.69	0.45
10:B:1641:NAG:O7	3:M:28:PRO:CG	2.64	0.45
2:F:551:GLN:C	2:F:553:ASN:HA	2.36	0.45
1:E:126:CYS:SG	1:E:192:ARG:HB2	2.56	0.45
1:C:171:LYS:HE2	5:C:1157:NAG:H62	1.97	0.45
1:C:500:LYS:CG	2:F:663:LEU:HD11	2.45	0.45
1:A:81:PRO:CA	1:A:82:GLN:HB2	2.46	0.45
1:E:396:ASN:O	1:E:404:GLY:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:111:VAL:O	3:M:112:SER:CB	2.64	0.45
1:E:134:VAL:CG1	1:E:135:ASN:HB2	2.46	0.45
1:A:444:ARG:NH2	5:A:1295:NAG:C6	2.79	0.45
2:B:541:ALA:HA	2:B:602:LEU:HD11	1.97	0.45
10:B:1641:NAG:O7	3:M:28:PRO:HD2	2.12	0.45
11:C:1243:BMA:H4	12:C:1452:MAN:O2	2.17	0.45
1:E:343:LYS:HE2	5:E:1339:NAG:C8	2.45	0.45
1:A:381:GLU:HG3	1:A:443:ILE:CD1	2.47	0.45
2:F:518:VAL:O	2:F:518:VAL:CG2	2.60	0.45
1:A:499:THR:CB	1:A:500:LYS:HA	2.47	0.45
5:A:1448:NAG:H3	5:A:1448:NAG:O7	2.16	0.45
5:A:1448:NAG:C3	5:A:1448:NAG:O7	2.64	0.45
3:M:13:GLN:HG2	3:M:113:SER:HA	1.98	0.45
7:C:1276:NAG:C6	7:C:1277:NAG:H82	2.44	0.45
3:M:4:LEU:C	3:M:4:LEU:HD23	2.37	0.45
1:A:339:ASN:OD1	1:A:339:ASN:C	2.51	0.45
12:C:1448:NAG:C3	12:C:1448:NAG:O7	2.64	0.45
3:H:4:LEU:HD12	3:H:4:LEU:N	2.32	0.45
5:E:1276:NAG:C6	5:E:1277:NAG:H82	2.43	0.44
1:C:170:GLN:OE1	7:C:1160:NAG:O7	2.35	0.44
2:D:600:GLY:HA2	2:D:601:LYS:HB2	2.00	0.44
4:N:36:TYR:HB3	4:N:46:LEU:HA	2.00	0.44
1:A:416:LEU:HA	1:A:417:PRO:HD2	1.91	0.44
1:C:226:LEU:HD13	1:C:489:VAL:HG22	1.98	0.44
2:D:638:TYR:HD1	13:D:1613:FUC:C6	1.96	0.44
2:B:600:GLY:HA2	2:B:601:LYS:HB2	1.99	0.44
1:C:68:VAL:HA	1:C:69:TRP:O	2.18	0.44
5:E:1160:NAG:C3	5:E:1161:NAG:O5	2.66	0.44
1:C:199:SER:O	1:C:201:ILE:HG23	2.17	0.44
3:M:100(E):ASP:HB2	3:M:100(I):GLY:HA3	2.00	0.44
1:E:357:LYS:HZ3	6:E:1397:NAG:H83	1.82	0.44
3:M:100(N):TYR:HE2	4:N:28:ASN:HD22	1.60	0.44
3:M:111:VAL:O	3:M:112:SER:HB3	2.17	0.44
1:E:354:GLU:C	1:E:355:ASN:CG	2.76	0.44
1:A:66:HIS:O	1:A:67:ASN:CB	2.66	0.44
1:C:123:THR:HB	1:C:124:PRO:HD3	2.00	0.44
1:C:323:ILE:HG12	7:C:1301:NAG:H82	2.00	0.44
5:A:1088:NAG:O3	5:A:1089:NAG:O5	2.32	0.44
7:C:1160:NAG:C3	7:C:1161:NAG:O5	2.66	0.44
1:C:353:PHE:O	1:C:355:ASN:N	2.51	0.44
2:B:568:LEU:HD22	2:D:573:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:1302:NAG:O3	7:C:1303:BMA:O5	2.31	0.44
7:A:1392:NAG:C6	7:A:1393:NAG:H82	2.48	0.43
1:C:194:ILE:HG22	1:C:195:SER:N	2.33	0.43
1:A:229:ASN:HB2	7:A:1241:NAG:O6	2.10	0.43
1:C:213:ILE:HB	1:C:214:PRO:HD2	2.00	0.43
2:B:564:ARG:NH1	2:D:574:LYS:HZ3	2.15	0.43
1:C:131:CYS:SG	1:C:155:LYS:CB	3.06	0.43
1:C:171:LYS:NZ	5:C:1157:NAG:C6	2.82	0.43
1:C:321:GLY:O	5:C:1156:NAG:O6	2.23	0.43
4:L:7:THR:HB	4:L:8:PRO:HD2	2.00	0.43
7:A:1156:NAG:C3	7:A:1157:NAG:O5	2.67	0.43
5:C:1156:NAG:C3	5:C:1157:NAG:O5	2.67	0.43
1:E:278:THR:OG1	5:E:1276:NAG:C1	2.66	0.43
10:B:1648:NAG:HN2	4:N:53:ASN:HD21	1.66	0.43
1:A:123:THR:N	1:A:124:PRO:CD	2.81	0.43
1:E:183:PRO:C	1:E:191:TYR:CE1	2.77	0.43
1:E:169:VAL:C	5:E:1160:NAG:H81	2.36	0.43
1:A:500:LYS:O	1:A:501:ALA:CB	2.67	0.43
16:F:1639:BMA:C2	3:H:98:GLU:HG3	2.49	0.43
1:A:439:ILE:HD11	1:A:443:ILE:HG12	2.01	0.43
1:E:134:VAL:HG12	1:E:135:ASN:CB	2.48	0.43
1:C:168:GLU:HG3	7:C:1160:NAG:H81	1.95	0.43
7:A:1392:NAG:H61	7:A:1393:NAG:H82	2.00	0.43
3:H:55:TRP:CG	3:H:55:TRP:O	2.71	0.43
2:B:522:PHE:HE1	2:B:544:LEU:HD22	1.83	0.43
1:C:193:LEU:O	1:C:194:ILE:C	2.57	0.43
5:D:1625:NAG:O3	5:D:1626:NAG:O5	2.30	0.43
1:E:350:ARG:HB3	5:E:1355:NAG:H82	2.01	0.42
3:M:33:PRO:HG2	3:M:95:MET:SD	2.59	0.42
3:H:33:PRO:HG2	3:H:95:MET:HE3	2.01	0.42
3:H:1:ARG:CA	3:H:2:VAL:C	2.87	0.42
1:C:183:PRO:HA	1:C:191:TYR:CD2	2.54	0.42
3:H:55:TRP:HD1	3:H:100(M):TYR:CZ	2.37	0.42
1:E:298:ARG:O	1:E:300:ASN:N	2.53	0.42
1:A:131:CYS:SG	1:A:155:LYS:HB3	2.59	0.42
2:B:522:PHE:N	2:B:544:LEU:HD12	2.17	0.42
1:E:469:ARG:HH21	5:E:1362:NAG:C6	2.32	0.42
1:C:300:ASN:HB3	1:C:326:ILE:HA	1.99	0.42
2:F:519:PHE:O	2:F:520:LEU:C	2.57	0.42
1:E:437:PRO:HA	1:E:438:PRO:HD3	1.87	0.42
1:E:134:VAL:HA	1:E:135:ASN:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:THR:O	1:E:78:ASP:HB3	2.20	0.42
1:E:354:GLU:C	1:E:355:ASN:ND2	2.72	0.42
2:B:531:GLY:O	2:B:532:ALA:HB3	2.20	0.42
1:A:87:GLU:OE2	5:A:1088:NAG:C8	2.40	0.42
1:E:350:ARG:CB	5:E:1355:NAG:H82	2.50	0.42
1:C:65:VAL:HB	1:C:66:HIS:HB3	2.02	0.42
2:D:638:TYR:HE1	13:D:1613:FUC:C6	1.78	0.41
1:A:158:SER:HB3	7:A:1156:NAG:C8	2.50	0.41
2:B:564:ARG:HH11	2:D:574:LYS:HZ3	1.67	0.41
3:M:25:SER:O	3:M:26:ASP:HB2	2.19	0.41
2:B:641:GLU:OE1	9:B:1624:FUC:H4	2.21	0.41
1:E:70:ALA:O	1:E:74:CYS:N	2.53	0.41
2:D:565:MET:CG	2:D:565:MET:O	2.68	0.41
1:A:112:TRP:HH2	1:A:210:PHE:HE1	1.65	0.41
1:E:183:PRO:CB	1:E:191:TYR:CZ	2.83	0.41
1:E:133:ASP:C	1:E:134:VAL:CG2	2.85	0.41
7:E:1156:NAG:C3	7:E:1157:NAG:O5	2.67	0.41
1:C:67:ASN:HB3	1:C:208:ILE:HD13	2.02	0.41
10:B:1637:NAG:H2	3:M:100:GLY:HA3	2.03	0.41
2:B:641:GLU:OE2	9:B:1624:FUC:C4	2.64	0.41
2:D:528:SER:CA	2:D:529:THR:HB	2.50	0.41
2:D:528:SER:CA	2:D:529:THR:CB	2.99	0.41
3:M:4:LEU:HD21	3:M:92:CYS:SG	2.61	0.41
1:E:173:TYR:CD2	7:E:1156:NAG:O5	2.74	0.41
1:A:499:THR:HG23	1:A:500:LYS:HA	2.03	0.41
1:A:362:ASN:HB3	1:A:469:ARG:HD3	2.02	0.41
1:E:469:ARG:HH21	5:E:1362:NAG:C5	2.34	0.40
3:H:111:VAL:O	3:H:112:SER:HB3	2.19	0.40
1:C:66:HIS:HB2	1:C:67:ASN:HB2	2.03	0.40
5:D:1637:NAG:O3	5:D:1638:NAG:O5	2.25	0.40
1:C:77:THR:OG1	1:C:79:PRO:HD3	2.22	0.40
1:A:193:LEU:HB2	1:A:196:CYS:SG	2.61	0.40
1:A:210:PHE:CE2	1:A:380:GLY:C	2.92	0.40
2:D:549:VAL:O	2:D:550:GLN:CB	2.70	0.40
1:C:98:ASN:OD1	1:C:98:ASN:C	2.59	0.40
1:C:296:CYS:HA	1:C:331:CYS:HA	2.02	0.40

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

All (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
1	C	73	ALA
1	C	80	ASN
1	C	99	ASN
1	C	194	ILE
1	C	355	ASN
1	E	78	ASP
1	E	83	GLU
1	E	258	GLN
2	F	520	LEU

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Mol	Chain	Res	Type
2	F	552	GLN
3	H	112	SER
3	M	112	SER
2	B	543	LEU
2	B	567	GLN
1	C	69	TRP
2	D	550	GLN
1	E	134	VAL
1	E	402	THR
4	N	51	VAL
1	A	504	ARG
1	C	354	GLU
1	E	70	ALA
2	F	601	LYS
3	M	100(K)	ASN
2	B	601	LYS
1	C	199	SER
1	E	79	PRO
1	A	67	ASN
1	A	232	THR
1	C	165	ILE
1	E	299	PRO
1	C	43	PRO
2	D	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	229	ASN
1	A	402	THR
1	A	499	THR
2	B	522	PHE
2	B	542	ARG
2	B	543	LEU
2	B	637	ASN
1	C	53	PHE
1	C	156	ASN
1	C	173	TYR
1	C	229	ASN
1	C	298	ARG
1	C	301	ASN
1	C	332	ASN
1	C	339	ASN
1	C	378	CYS
2	D	540	GLN
1	E	126	CYS
1	E	134	VAL
1	E	156	ASN
1	E	298	ARG
1	E	378	CYS
1	E	435	TYR
2	F	616	ASN
2	F	637	ASN
4	L	53	ASN
3	M	100(N)	TYR
4	N	36	TYR

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (128) bond length outliers are listed below:

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
10	B	1638	NAG	O5-C5	2.02	1.47	1.43
5	D	1638	NAG	O5-C5	2.03	1.47	1.43
16	F	1644	GAL	O5-C5	2.06	1.48	1.43
9	F	1623	GAL	O5-C5	2.07	1.48	1.43
16	F	1643	NAG	O5-C5	2.08	1.48	1.43
10	B	1644	GAL	O5-C5	2.08	1.48	1.43
9	F	1617	NAG	O5-C5	2.08	1.48	1.43
9	B	1617	NAG	O5-C5	2.09	1.48	1.43
10	B	1643	NAG	O5-C5	2.09	1.48	1.43
9	F	1620	NAG	O5-C5	2.09	1.48	1.43
9	B	1623	GAL	O5-C5	2.10	1.48	1.43
9	B	1620	NAG	O5-C5	2.11	1.48	1.43
16	F	1643	NAG	O4-C4	2.11	1.47	1.43
9	F	1622	NAG	O5-C5	2.12	1.48	1.43
10	B	1643	NAG	O4-C4	2.12	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	F	1642	GAL	O5-C5	2.13	1.48	1.43
10	B	1642	GAL	O5-C5	2.14	1.48	1.43
9	F	1621	GAL	O5-C5	2.15	1.48	1.43
13	D	1611	NAG	O4-C4	2.16	1.48	1.43
9	F	1611	NAG	O4-C4	2.16	1.48	1.43
9	F	1614	MAN	O4-C4	2.16	1.48	1.43
9	F	1613	BMA	O5-C5	2.16	1.48	1.43
9	B	1613	BMA	O5-C5	2.16	1.48	1.43
16	F	1637	NAG	O4-C4	2.17	1.48	1.43
10	B	1647	GAL	O5-C5	2.17	1.48	1.43
9	B	1621	GAL	O5-C5	2.17	1.48	1.43
10	B	1637	NAG	O4-C4	2.17	1.48	1.43
9	B	1614	MAN	O4-C4	2.17	1.48	1.43
10	B	1641	NAG	O4-C4	2.18	1.48	1.43
9	B	1622	NAG	O5-C5	2.18	1.48	1.43
16	F	1648	NAG	O4-C4	2.18	1.48	1.43
16	F	1641	NAG	O4-C4	2.18	1.48	1.43
9	B	1611	NAG	O4-C4	2.18	1.48	1.43
10	B	1648	NAG	O4-C4	2.19	1.48	1.43
10	B	1648	NAG	O5-C5	2.19	1.48	1.43
5	D	1637	NAG	O4-C4	2.20	1.48	1.43
10	B	1639	BMA	O5-C5	2.20	1.48	1.43
16	F	1639	BMA	O5-C5	2.21	1.48	1.43
16	F	1648	NAG	O5-C5	2.21	1.48	1.43
9	F	1614	MAN	O2-C2	2.22	1.48	1.43
10	B	1645	MAN	O2-C2	2.23	1.48	1.43
10	B	1646	NAG	O4-C4	2.23	1.48	1.43
16	F	1646	NAG	O4-C4	2.24	1.48	1.43
9	B	1614	MAN	O2-C2	2.24	1.48	1.43
9	B	1617	NAG	O4-C4	2.24	1.48	1.43
16	F	1640	MAN	O2-C2	2.25	1.48	1.43
9	F	1619	MAN	O2-C2	2.25	1.48	1.43
10	B	1640	MAN	O2-C2	2.25	1.48	1.43
16	F	1645	MAN	O2-C2	2.25	1.48	1.43
9	F	1617	NAG	O4-C4	2.25	1.48	1.43
9	B	1622	NAG	O4-C4	2.26	1.48	1.43
9	B	1619	MAN	O2-C2	2.28	1.48	1.43
9	F	1620	NAG	O4-C4	2.28	1.48	1.43
9	F	1622	NAG	O4-C4	2.30	1.48	1.43
9	B	1620	NAG	O4-C4	2.30	1.48	1.43
9	F	1611	NAG	O5-C5	2.30	1.48	1.43
10	B	1640	MAN	O4-C4	2.31	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1611	NAG	O5-C5	2.32	1.48	1.43
16	F	1640	MAN	O4-C4	2.32	1.48	1.43
16	F	1645	MAN	O5-C5	2.34	1.48	1.43
13	D	1611	NAG	O5-C5	2.34	1.48	1.43
16	F	1637	NAG	O5-C5	2.34	1.48	1.43
10	B	1645	MAN	O5-C5	2.35	1.48	1.43
9	F	1614	MAN	O5-C5	2.35	1.48	1.43
10	B	1637	NAG	O5-C5	2.37	1.48	1.43
9	B	1614	MAN	O5-C5	2.39	1.48	1.43
5	D	1637	NAG	O5-C5	2.40	1.48	1.43
10	B	1640	MAN	O5-C5	2.41	1.48	1.43
16	F	1640	MAN	O5-C5	2.42	1.48	1.43
9	F	1619	MAN	O5-C5	2.46	1.48	1.43
9	B	1619	MAN	O5-C5	2.47	1.48	1.43
9	B	1619	MAN	O5-C1	2.59	1.47	1.43
9	F	1619	MAN	O5-C1	2.60	1.48	1.43
16	F	1639	BMA	O5-C1	2.63	1.48	1.43
9	F	1613	BMA	O5-C1	2.66	1.48	1.43
10	B	1642	GAL	O5-C1	2.68	1.48	1.43
10	B	1639	BMA	O5-C1	2.68	1.48	1.43
9	B	1613	BMA	O5-C1	2.69	1.48	1.43
9	B	1621	GAL	O5-C1	2.70	1.48	1.43
16	F	1642	GAL	O5-C1	2.72	1.48	1.43
10	B	1647	GAL	O5-C1	2.74	1.48	1.43
16	F	1645	MAN	O5-C1	2.74	1.48	1.43
9	F	1621	GAL	O5-C1	2.75	1.48	1.43
10	B	1645	MAN	O5-C1	2.76	1.48	1.43
10	B	1643	NAG	O5-C1	2.77	1.48	1.43
10	B	1644	GAL	O5-C1	2.79	1.48	1.43
5	D	1638	NAG	O5-C1	2.79	1.48	1.43
10	B	1638	NAG	O5-C1	2.79	1.48	1.43
16	F	1641	NAG	O5-C1	2.80	1.48	1.43
9	B	1623	GAL	O5-C1	2.81	1.48	1.43
16	F	1643	NAG	O5-C1	2.81	1.48	1.43
16	F	1638	NAG	O5-C1	2.82	1.48	1.43
16	F	1644	GAL	O5-C1	2.82	1.48	1.43
10	B	1641	NAG	O5-C1	2.82	1.48	1.43
9	B	1617	NAG	O5-C1	2.83	1.48	1.43
9	F	1617	NAG	O5-C1	2.84	1.48	1.43
10	B	1648	NAG	O5-C1	2.84	1.48	1.43
9	B	1622	NAG	O5-C1	2.84	1.48	1.43
16	F	1648	NAG	O5-C1	2.86	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	1613	FUC	O5-C1	2.87	1.48	1.43
9	F	1622	NAG	O5-C1	2.88	1.48	1.43
9	F	1612	NAG	O5-C1	2.88	1.48	1.43
9	F	1623	GAL	O5-C1	2.88	1.48	1.43
9	B	1612	NAG	O5-C1	2.89	1.48	1.43
9	B	1624	FUC	O5-C1	2.91	1.48	1.43
9	B	1620	NAG	O5-C1	2.92	1.48	1.43
16	F	1650	FUC	O5-C1	2.92	1.48	1.43
9	F	1624	FUC	O5-C1	2.93	1.48	1.43
10	B	1650	FUC	O5-C1	2.94	1.48	1.43
13	D	1612	NAG	O5-C1	2.96	1.48	1.43
9	F	1620	NAG	O5-C1	2.97	1.48	1.43
10	B	1646	NAG	O5-C1	2.99	1.48	1.43
16	F	1646	NAG	O5-C1	3.06	1.48	1.43
9	F	1611	NAG	O5-C1	3.07	1.48	1.43
9	B	1611	NAG	O5-C1	3.09	1.48	1.43
13	D	1611	NAG	O5-C1	3.09	1.48	1.43
10	B	1637	NAG	O5-C1	3.14	1.48	1.43
16	F	1637	NAG	O5-C1	3.15	1.48	1.43
5	D	1637	NAG	O5-C1	3.17	1.48	1.43
10	B	1640	MAN	O5-C1	3.42	1.49	1.43
16	F	1640	MAN	O5-C1	3.42	1.49	1.43
9	B	1614	MAN	O5-C1	3.45	1.49	1.43
9	F	1614	MAN	O5-C1	3.52	1.49	1.43

All (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
14	E	1245	MAN	O2-C2-C3	-4.16	101.80	110.19
15	E	1390	MAN	C2-C3-C4	-4.15	103.81	111.05
12	C	1453	MAN	C2-C3-C4	-4.15	103.82	111.05
12	C	1452	MAN	O2-C2-C3	-4.12	101.89	110.19
12	E	1452	MAN	O2-C2-C3	-4.10	101.93	110.19
12	E	1454	MAN	O4-C4-C3	-4.03	101.27	110.36
12	C	1454	MAN	O4-C4-C3	-4.03	101.27	110.36
12	E	1455	MAN	O4-C4-C3	-3.63	102.17	110.36
12	C	1455	MAN	O4-C4-C3	-3.63	102.18	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	1246	MAN	O5-C1-C2	-3.45	105.39	110.89
12	C	1453	MAN	O5-C1-C2	-3.41	105.43	110.89
15	E	1390	MAN	O5-C1-C2	-3.41	105.44	110.89
12	E	1453	MAN	O5-C1-C2	-3.39	105.48	110.89
14	E	1246	MAN	O5-C1-C2	-3.38	105.49	110.89
12	E	1455	MAN	C3-C4-C5	-3.14	104.63	110.23
12	C	1455	MAN	C3-C4-C5	-3.12	104.66	110.23
12	E	1455	MAN	O2-C2-C3	-2.94	104.25	110.19
12	C	1455	MAN	O2-C2-C3	-2.93	104.29	110.19
12	E	1452	MAN	O4-C4-C3	-2.85	103.94	110.36
7	A	1386	NAG	O7-C7-C8	-2.85	116.83	122.07
12	C	1452	MAN	O4-C4-C3	-2.84	103.95	110.36
5	C	1392	NAG	O7-C7-C8	-2.84	116.84	122.07
7	A	1392	NAG	O7-C7-C8	-2.84	116.84	122.07
15	E	1386	NAG	O7-C7-C8	-2.84	116.85	122.07
14	E	1245	MAN	O4-C4-C3	-2.84	103.96	110.36
7	C	1386	NAG	O7-C7-C8	-2.84	116.85	122.07
7	C	1332	NAG	O7-C7-C8	-2.83	116.87	122.07
7	E	1392	NAG	O7-C7-C8	-2.83	116.87	122.07
5	A	1295	NAG	O7-C7-C8	-2.82	116.87	122.07
5	A	1339	NAG	O7-C7-C8	-2.82	116.88	122.07
5	E	1295	NAG	O7-C7-C8	-2.82	116.88	122.07
14	E	1241	NAG	O7-C7-C8	-2.82	116.88	122.07
11	C	1241	NAG	O7-C7-C8	-2.82	116.89	122.07
7	A	1241	NAG	O7-C7-C8	-2.81	116.90	122.07
7	A	1160	NAG	O7-C7-C8	-2.81	116.90	122.07
5	E	1135	NAG	O7-C7-C8	-2.81	116.91	122.07
5	C	1135	NAG	O7-C7-C8	-2.81	116.91	122.07
7	C	1160	NAG	O7-C7-C8	-2.80	116.91	122.07
5	E	1160	NAG	O7-C7-C8	-2.80	116.91	122.07
7	A	1332	NAG	O7-C7-C8	-2.80	116.92	122.07
7	E	1332	NAG	O7-C7-C8	-2.80	116.92	122.07
7	C	1301	NAG	O7-C7-C8	-2.79	116.93	122.07
5	E	1339	NAG	O7-C7-C8	-2.79	116.93	122.07
5	E	1301	NAG	O7-C7-C8	-2.79	116.93	122.07
5	E	1362	NAG	O7-C7-C8	-2.79	116.94	122.07
7	A	1156	NAG	O7-C7-C8	-2.79	116.94	122.07
5	C	1355	NAG	O7-C7-C8	-2.79	116.94	122.07
5	D	1625	NAG	O7-C7-C8	-2.78	116.95	122.07
5	F	1625	NAG	O7-C7-C8	-2.78	116.95	122.07
5	E	1276	NAG	O7-C7-C8	-2.78	116.96	122.07
5	C	1156	NAG	O7-C7-C8	-2.78	116.96	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1295	NAG	O7-C7-C8	-2.77	116.96	122.07
5	C	1156	NAG	C4-C3-C2	-2.77	107.04	111.34
5	A	1448	NAG	O7-C7-C8	-2.77	116.97	122.07
7	E	1156	NAG	O7-C7-C8	-2.77	116.97	122.07
7	A	1392	NAG	C4-C3-C2	-2.77	107.04	111.34
7	A	1276	NAG	O7-C7-C8	-2.77	116.97	122.07
5	E	1355	NAG	O7-C7-C8	-2.77	116.98	122.07
12	E	1448	NAG	O7-C7-C8	-2.77	116.98	122.07
7	E	1156	NAG	C4-C3-C2	-2.76	107.05	111.34
5	C	1339	NAG	O7-C7-C8	-2.76	116.99	122.07
5	A	1301	NAG	O7-C7-C8	-2.76	116.99	122.07
5	A	1301	NAG	C4-C3-C2	-2.76	107.06	111.34
7	A	1156	NAG	C4-C3-C2	-2.76	107.06	111.34
5	A	1088	NAG	O7-C7-C8	-2.75	117.00	122.07
5	E	1362	NAG	C4-C3-C2	-2.75	107.07	111.34
5	C	1392	NAG	C4-C3-C2	-2.75	107.07	111.34
7	C	1362	NAG	O7-C7-C8	-2.75	117.01	122.07
7	C	1276	NAG	O7-C7-C8	-2.75	117.01	122.07
7	E	1088	NAG	O7-C7-C8	-2.75	117.01	122.07
12	C	1448	NAG	O7-C7-C8	-2.75	117.01	122.07
7	E	1392	NAG	C4-C3-C2	-2.74	107.08	111.34
5	C	1295	NAG	C4-C3-C2	-2.74	107.08	111.34
7	C	1362	NAG	C4-C3-C2	-2.74	107.08	111.34
7	C	1088	NAG	O7-C7-C8	-2.74	117.03	122.07
7	A	1362	NAG	O7-C7-C8	-2.73	117.04	122.07
7	E	1088	NAG	C4-C3-C2	-2.73	107.10	111.34
12	E	1448	NAG	C4-C3-C2	-2.73	107.10	111.34
5	E	1135	NAG	C4-C3-C2	-2.73	107.10	111.34
5	E	1355	NAG	C4-C3-C2	-2.73	107.10	111.34
7	A	1386	NAG	C4-C3-C2	-2.73	107.11	111.34
7	C	1386	NAG	C4-C3-C2	-2.72	107.11	111.34
7	C	1088	NAG	C4-C3-C2	-2.72	107.11	111.34
5	E	1295	NAG	C4-C3-C2	-2.72	107.12	111.34
5	A	1088	NAG	C4-C3-C2	-2.72	107.12	111.34
5	C	1355	NAG	C4-C3-C2	-2.72	107.12	111.34
7	A	1362	NAG	C4-C3-C2	-2.72	107.12	111.34
14	E	1241	NAG	C4-C3-C2	-2.72	107.12	111.34
5	C	1339	NAG	C4-C3-C2	-2.72	107.12	111.34
7	A	1276	NAG	C4-C3-C2	-2.71	107.13	111.34
5	F	1625	NAG	C4-C3-C2	-2.71	107.13	111.34
5	E	1276	NAG	C4-C3-C2	-2.71	107.13	111.34
5	E	1301	NAG	C4-C3-C2	-2.71	107.13	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1625	NAG	C4-C3-C2	-2.71	107.13	111.34
5	C	1135	NAG	C4-C3-C2	-2.71	107.14	111.34
7	C	1301	NAG	C4-C3-C2	-2.71	107.14	111.34
5	A	1339	NAG	C4-C3-C2	-2.71	107.14	111.34
5	E	1160	NAG	C4-C3-C2	-2.71	107.14	111.34
15	E	1386	NAG	C4-C3-C2	-2.70	107.14	111.34
5	A	1448	NAG	C4-C3-C2	-2.70	107.15	111.34
7	C	1160	NAG	C4-C3-C2	-2.70	107.15	111.34
5	A	1295	NAG	C4-C3-C2	-2.69	107.16	111.34
7	C	1332	NAG	C4-C3-C2	-2.69	107.16	111.34
12	C	1448	NAG	C4-C3-C2	-2.69	107.16	111.34
5	E	1339	NAG	C4-C3-C2	-2.69	107.16	111.34
11	C	1241	NAG	C4-C3-C2	-2.69	107.17	111.34
7	C	1276	NAG	C4-C3-C2	-2.69	107.17	111.34
7	E	1332	NAG	C4-C3-C2	-2.68	107.18	111.34
5	A	1302	NAG	O5-C5-C6	-2.68	101.60	107.34
7	A	1332	NAG	C4-C3-C2	-2.68	107.18	111.34
5	E	1363	NAG	O5-C5-C6	-2.68	101.61	107.34
7	A	1241	NAG	C4-C3-C2	-2.67	107.19	111.34
5	A	1449	NAG	O5-C5-C6	-2.67	101.62	107.34
7	A	1160	NAG	C4-C3-C2	-2.67	107.19	111.34
12	E	1449	NAG	O5-C5-C6	-2.67	101.62	107.34
5	A	1296	NAG	O5-C5-C6	-2.67	101.63	107.34
7	A	1387	NAG	O5-C5-C6	-2.66	101.64	107.34
12	C	1449	NAG	O5-C5-C6	-2.66	101.65	107.34
7	A	1277	NAG	O5-C5-C6	-2.65	101.67	107.34
5	E	1277	NAG	O5-C5-C6	-2.65	101.67	107.34
5	E	1136	NAG	O5-C5-C6	-2.65	101.67	107.34
5	C	1136	NAG	O5-C5-C6	-2.65	101.67	107.34
7	A	1393	NAG	O5-C5-C6	-2.64	101.68	107.34
7	A	1363	NAG	O5-C5-C6	-2.64	101.68	107.34
5	F	1626	NAG	O5-C5-C6	-2.64	101.68	107.34
5	E	1302	NAG	O5-C5-C6	-2.64	101.68	107.34
7	C	1363	NAG	O5-C5-C6	-2.64	101.68	107.34
7	E	1393	NAG	O5-C5-C6	-2.64	101.69	107.34
7	E	1157	NAG	O5-C5-C6	-2.64	101.69	107.34
5	C	1393	NAG	O5-C5-C6	-2.64	101.69	107.34
5	C	1157	NAG	O5-C5-C6	-2.64	101.69	107.34
7	E	1333	NAG	O5-C5-C6	-2.64	101.69	107.34
5	C	1356	NAG	O5-C5-C6	-2.64	101.70	107.34
5	E	1296	NAG	O5-C5-C6	-2.63	101.70	107.34
5	A	1340	NAG	O5-C5-C6	-2.63	101.71	107.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1277	NAG	O5-C5-C6	-2.63	101.71	107.34
5	E	1356	NAG	O5-C5-C6	-2.63	101.71	107.34
5	C	1296	NAG	O5-C5-C6	-2.63	101.71	107.34
7	A	1333	NAG	O5-C5-C6	-2.63	101.71	107.34
11	C	1242	NAG	O5-C5-C6	-2.63	101.72	107.34
7	C	1333	NAG	O5-C5-C6	-2.63	101.72	107.34
5	D	1626	NAG	O5-C5-C6	-2.63	101.72	107.34
15	E	1387	NAG	O5-C5-C6	-2.63	101.72	107.34
5	E	1161	NAG	O5-C5-C6	-2.62	101.72	107.34
7	C	1302	NAG	O5-C5-C6	-2.62	101.73	107.34
7	A	1161	NAG	O5-C5-C6	-2.62	101.73	107.34
7	A	1242	NAG	O5-C5-C6	-2.62	101.74	107.34
5	C	1340	NAG	O5-C5-C6	-2.61	101.74	107.34
7	A	1157	NAG	O5-C5-C6	-2.61	101.75	107.34
7	C	1161	NAG	O5-C5-C6	-2.61	101.75	107.34
14	E	1242	NAG	O5-C5-C6	-2.61	101.75	107.34
5	E	1340	NAG	O5-C5-C6	-2.61	101.75	107.34
5	A	1089	NAG	O5-C5-C6	-2.60	101.76	107.34
7	E	1089	NAG	O5-C5-C6	-2.60	101.77	107.34
7	C	1387	NAG	O5-C5-C6	-2.60	101.77	107.34
7	C	1089	NAG	O5-C5-C6	-2.58	101.81	107.34
7	E	1090	BMA	O4-C4-C5	-2.49	102.67	109.23
7	E	1334	BMA	O4-C4-C5	-2.48	102.69	109.23
7	A	1162	BMA	O4-C4-C5	-2.47	102.72	109.23
7	A	1334	BMA	O4-C4-C5	-2.46	102.73	109.23
7	C	1334	BMA	O4-C4-C5	-2.46	102.74	109.23
7	A	1394	BMA	O4-C4-C5	-2.46	102.74	109.23
12	E	1450	BMA	O4-C4-C5	-2.46	102.75	109.23
7	C	1090	BMA	O4-C4-C5	-2.46	102.75	109.23
12	C	1450	BMA	O4-C4-C5	-2.46	102.75	109.23
7	A	1388	BMA	O4-C4-C5	-2.45	102.77	109.23
7	C	1162	BMA	O4-C4-C5	-2.45	102.77	109.23
7	E	1394	BMA	O4-C4-C5	-2.45	102.77	109.23
7	C	1303	BMA	O4-C4-C5	-2.45	102.78	109.23
7	C	1278	BMA	O4-C4-C5	-2.45	102.78	109.23
7	A	1158	BMA	O4-C4-C5	-2.45	102.78	109.23
7	C	1364	BMA	O4-C4-C5	-2.44	102.79	109.23
15	E	1388	BMA	O4-C4-C5	-2.44	102.80	109.23
7	E	1158	BMA	O4-C4-C5	-2.44	102.80	109.23
7	C	1388	BMA	O4-C4-C5	-2.44	102.80	109.23
7	A	1278	BMA	O4-C4-C5	-2.43	102.82	109.23
10	B	1638	NAG	O5-C5-C4	-2.43	106.11	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1364	BMA	O4-C4-C5	-2.43	102.83	109.23
11	C	1242	NAG	C4-C3-C2	-2.43	107.57	111.34
9	F	1612	NAG	O5-C5-C4	-2.42	106.13	110.13
5	D	1638	NAG	O5-C5-C4	-2.42	106.13	110.13
7	A	1243	BMA	O4-C4-C5	-2.41	102.87	109.23
14	E	1243	BMA	O4-C4-C5	-2.41	102.87	109.23
16	F	1638	NAG	O5-C5-C4	-2.41	106.14	110.13
11	C	1243	BMA	O4-C4-C5	-2.41	102.89	109.23
9	B	1612	NAG	O5-C5-C4	-2.38	106.20	110.13
13	D	1612	NAG	O5-C5-C4	-2.38	106.20	110.13
12	E	1454	MAN	O3-C3-C2	-2.36	105.67	110.01
7	A	1242	NAG	C4-C3-C2	-2.35	107.69	111.34
5	D	1626	NAG	C4-C3-C2	-2.34	107.70	111.34
14	E	1242	NAG	C4-C3-C2	-2.34	107.70	111.34
12	C	1454	MAN	O3-C3-C2	-2.34	105.73	110.01
7	E	1393	NAG	C4-C3-C2	-2.33	107.72	111.34
5	E	1136	NAG	C4-C3-C2	-2.32	107.75	111.34
5	C	1356	NAG	C4-C3-C2	-2.31	107.75	111.34
7	A	1393	NAG	C4-C3-C2	-2.31	107.76	111.34
5	A	1089	NAG	C4-C3-C2	-2.31	107.76	111.34
7	C	1161	NAG	C4-C3-C2	-2.30	107.77	111.34
5	C	1393	NAG	C4-C3-C2	-2.30	107.77	111.34
7	E	1333	NAG	C4-C3-C2	-2.30	107.78	111.34
7	A	1243	BMA	C6-C5-C4	-2.30	107.23	112.99
14	E	1243	BMA	C6-C5-C4	-2.29	107.24	112.99
5	F	1626	NAG	C4-C3-C2	-2.29	107.78	111.34
5	C	1340	NAG	C4-C3-C2	-2.29	107.79	111.34
7	A	1277	NAG	C4-C3-C2	-2.29	107.79	111.34
5	E	1296	NAG	C4-C3-C2	-2.29	107.79	111.34
15	E	1387	NAG	C4-C3-C2	-2.29	107.79	111.34
7	C	1277	NAG	C4-C3-C2	-2.29	107.79	111.34
5	E	1161	NAG	C4-C3-C2	-2.28	107.79	111.34
11	C	1243	BMA	C6-C5-C4	-2.28	107.27	112.99
5	E	1363	NAG	C4-C3-C2	-2.28	107.80	111.34
5	E	1340	NAG	C4-C3-C2	-2.28	107.80	111.34
5	E	1277	NAG	C4-C3-C2	-2.28	107.80	111.34
7	C	1363	NAG	C4-C3-C2	-2.28	107.80	111.34
5	C	1136	NAG	C4-C3-C2	-2.28	107.80	111.34
7	A	1157	NAG	C4-C3-C2	-2.28	107.80	111.34
5	A	1449	NAG	C4-C3-C2	-2.28	107.81	111.34
12	E	1449	NAG	C4-C3-C2	-2.28	107.81	111.34
5	E	1356	NAG	C4-C3-C2	-2.28	107.81	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1089	NAG	C4-C3-C2	-2.27	107.81	111.34
7	C	1387	NAG	C4-C3-C2	-2.27	107.81	111.34
5	C	1157	NAG	C4-C3-C2	-2.27	107.81	111.34
7	A	1161	NAG	C4-C3-C2	-2.27	107.81	111.34
7	A	1333	NAG	C4-C3-C2	-2.27	107.81	111.34
12	C	1449	NAG	C4-C3-C2	-2.27	107.82	111.34
7	A	1162	BMA	C6-C5-C4	-2.27	107.30	112.99
7	A	1387	NAG	C4-C3-C2	-2.27	107.82	111.34
5	A	1340	NAG	C4-C3-C2	-2.27	107.82	111.34
7	E	1394	BMA	C6-C5-C4	-2.27	107.31	112.99
7	E	1089	NAG	C4-C3-C2	-2.27	107.82	111.34
7	A	1394	BMA	C6-C5-C4	-2.27	107.31	112.99
7	C	1334	BMA	C6-C5-C4	-2.26	107.31	112.99
7	A	1363	NAG	C4-C3-C2	-2.26	107.83	111.34
7	C	1333	NAG	C4-C3-C2	-2.26	107.83	111.34
7	A	1278	BMA	C6-C5-C4	-2.26	107.33	112.99
7	C	1162	BMA	C6-C5-C4	-2.26	107.33	112.99
5	C	1296	NAG	C4-C3-C2	-2.26	107.84	111.34
7	C	1388	BMA	C6-C5-C4	-2.26	107.33	112.99
7	E	1158	BMA	C6-C5-C4	-2.25	107.34	112.99
7	A	1364	BMA	C6-C5-C4	-2.25	107.34	112.99
7	A	1158	BMA	C6-C5-C4	-2.25	107.35	112.99
7	E	1157	NAG	C4-C3-C2	-2.25	107.85	111.34
15	E	1388	BMA	C6-C5-C4	-2.25	107.35	112.99
7	E	1334	BMA	C6-C5-C4	-2.25	107.35	112.99
7	C	1364	BMA	C6-C5-C4	-2.25	107.35	112.99
5	A	1296	NAG	C4-C3-C2	-2.24	107.86	111.34
12	E	1450	BMA	C6-C5-C4	-2.24	107.36	112.99
7	C	1278	BMA	C6-C5-C4	-2.24	107.37	112.99
7	C	1303	BMA	C6-C5-C4	-2.24	107.37	112.99
12	C	1450	BMA	C6-C5-C4	-2.24	107.37	112.99
7	A	1388	BMA	C6-C5-C4	-2.24	107.37	112.99
7	A	1334	BMA	C6-C5-C4	-2.23	107.39	112.99
5	E	1302	NAG	C4-C3-C2	-2.23	107.88	111.34
7	C	1302	NAG	C4-C3-C2	-2.23	107.88	111.34
7	C	1090	BMA	C6-C5-C4	-2.23	107.40	112.99
7	E	1090	BMA	C6-C5-C4	-2.23	107.41	112.99
5	A	1302	NAG	C4-C3-C2	-2.21	107.90	111.34
12	C	1454	MAN	O5-C5-C6	-2.15	102.75	107.34
12	E	1454	MAN	O5-C5-C6	-2.13	102.77	107.34
9	B	1620	NAG	O5-C5-C4	-2.12	106.63	110.13
9	F	1620	NAG	O5-C5-C4	-2.11	106.64	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	E	1244	MAN	O4-C4-C3	-2.11	105.61	110.36
9	B	1617	NAG	O5-C5-C4	-2.09	106.68	110.13
11	C	1244	MAN	O4-C4-C3	-2.08	105.68	110.36
9	F	1617	NAG	O5-C5-C4	-2.08	106.70	110.13
12	E	1451	MAN	O4-C4-C3	-2.06	105.72	110.36
16	F	1641	NAG	O5-C5-C4	-2.06	106.73	110.13
16	F	1643	NAG	O5-C5-C4	-2.05	106.74	110.13
12	C	1451	MAN	O4-C4-C3	-2.04	105.75	110.36
10	B	1641	NAG	O5-C5-C4	-2.04	106.75	110.13
10	B	1643	NAG	O5-C5-C4	-2.04	106.76	110.13
16	F	1646	NAG	O5-C5-C4	-2.00	106.82	110.13
8	C	1265	MAN	C1-C2-C3	2.00	111.98	109.55
5	A	1089	NAG	O5-C5-C4	2.00	113.45	110.13
5	F	1626	NAG	O5-C5-C4	2.01	113.46	110.13
7	C	1277	NAG	O5-C5-C4	2.01	113.46	110.13
8	E	1265	MAN	C1-C2-C3	2.01	111.99	109.55
14	E	1242	NAG	O5-C5-C4	2.01	113.47	110.13
8	A	1265	MAN	C1-C2-C3	2.01	111.99	109.55
7	C	1387	NAG	O5-C5-C4	2.01	113.47	110.13
5	E	1302	NAG	O5-C5-C4	2.02	113.47	110.13
7	E	1393	NAG	O5-C5-C4	2.02	113.48	110.13
7	A	1387	NAG	O5-C5-C4	2.02	113.48	110.13
5	C	1340	NAG	O5-C5-C4	2.02	113.48	110.13
5	E	1340	NAG	O5-C5-C4	2.02	113.48	110.13
5	C	1296	NAG	O5-C5-C4	2.02	113.48	110.13
12	C	1455	MAN	C2-C3-C4	2.02	114.58	111.05
5	A	1340	NAG	O5-C5-C4	2.02	113.48	110.13
8	A	1264	BMA	C1-C2-C3	2.02	112.00	109.55
15	E	1387	NAG	O5-C5-C4	2.03	113.49	110.13
12	E	1455	MAN	C2-C3-C4	2.03	114.58	111.05
7	E	1333	NAG	O5-C5-C4	2.03	113.49	110.13
8	E	1264	BMA	C1-C2-C3	2.03	112.01	109.55
7	E	1089	NAG	O5-C5-C4	2.03	113.49	110.13
5	E	1296	NAG	O5-C5-C4	2.03	113.50	110.13
7	A	1277	NAG	O5-C5-C4	2.03	113.50	110.13
7	C	1333	NAG	O5-C5-C4	2.03	113.50	110.13
5	E	1277	NAG	O5-C5-C4	2.04	113.50	110.13
9	B	1624	FUC	C1-C2-C3	2.04	112.02	109.55
7	A	1393	NAG	O5-C5-C4	2.04	113.51	110.13
7	C	1089	NAG	O5-C5-C4	2.04	113.51	110.13
5	A	1302	NAG	O5-C5-C4	2.04	113.52	110.13
5	A	1296	NAG	O5-C5-C4	2.04	113.52	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1157	NAG	O5-C5-C4	2.04	113.52	110.13
7	A	1333	NAG	O5-C5-C4	2.05	113.53	110.13
7	C	1302	NAG	O5-C5-C4	2.05	113.53	110.13
12	C	1454	MAN	C1-O5-C5	2.05	115.15	112.14
7	A	1363	NAG	O5-C5-C4	2.05	113.53	110.13
7	C	1363	NAG	O5-C5-C4	2.06	113.54	110.13
5	D	1626	NAG	O5-C5-C4	2.06	113.54	110.13
5	C	1356	NAG	O5-C5-C4	2.06	113.54	110.13
13	D	1613	FUC	C1-C2-C3	2.06	112.05	109.55
9	F	1624	FUC	C1-C2-C3	2.06	112.05	109.55
7	E	1157	NAG	O5-C5-C4	2.06	113.55	110.13
12	E	1454	MAN	O3-C3-C4	2.06	115.01	110.36
5	E	1136	NAG	O5-C5-C4	2.07	113.56	110.13
12	E	1454	MAN	C1-O5-C5	2.07	115.18	112.14
7	C	1161	NAG	O5-C5-C4	2.07	113.56	110.13
5	E	1363	NAG	O5-C5-C4	2.07	113.56	110.13
12	C	1454	MAN	O3-C3-C4	2.07	115.03	110.36
5	C	1393	NAG	O5-C5-C4	2.07	113.56	110.13
12	C	1450	BMA	O5-C5-C4	2.07	113.56	110.13
5	E	1356	NAG	O5-C5-C4	2.07	113.56	110.13
5	C	1136	NAG	O5-C5-C4	2.07	113.57	110.13
7	A	1161	NAG	O5-C5-C4	2.08	113.57	110.13
7	E	1090	BMA	O5-C5-C4	2.10	113.61	110.13
7	C	1364	BMA	O5-C5-C4	2.10	113.61	110.13
12	E	1450	BMA	O5-C5-C4	2.11	113.62	110.13
5	E	1161	NAG	O5-C5-C4	2.11	113.64	110.13
7	E	1334	BMA	O5-C5-C4	2.11	113.64	110.13
7	C	1303	BMA	O5-C5-C4	2.12	113.64	110.13
7	C	1278	BMA	O5-C5-C4	2.12	113.64	110.13
7	E	1158	BMA	O5-C5-C4	2.12	113.65	110.13
7	A	1158	BMA	O5-C5-C4	2.13	113.66	110.13
7	A	1162	BMA	O5-C5-C4	2.13	113.66	110.13
7	E	1394	BMA	O5-C5-C4	2.13	113.66	110.13
7	A	1334	BMA	O5-C5-C4	2.13	113.66	110.13
7	A	1394	BMA	O5-C5-C4	2.13	113.66	110.13
7	C	1388	BMA	O5-C5-C4	2.13	113.67	110.13
7	C	1090	BMA	O5-C5-C4	2.14	113.69	110.13
7	C	1162	BMA	O5-C5-C4	2.15	113.70	110.13
7	C	1334	BMA	O5-C5-C4	2.15	113.70	110.13
14	E	1243	BMA	O5-C5-C4	2.16	113.70	110.13
11	C	1243	BMA	O5-C5-C4	2.16	113.72	110.13
12	C	1451	MAN	O3-C3-C4	2.16	115.24	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1364	BMA	O5-C5-C4	2.17	113.72	110.13
15	E	1388	BMA	O5-C5-C4	2.17	113.73	110.13
7	A	1278	BMA	O5-C5-C4	2.17	113.73	110.13
12	E	1451	MAN	O3-C3-C4	2.17	115.26	110.36
7	A	1243	BMA	O5-C5-C4	2.18	113.74	110.13
11	C	1244	MAN	O3-C3-C4	2.19	115.30	110.36
7	A	1388	BMA	O5-C5-C4	2.21	113.79	110.13
10	B	1650	FUC	C1-C2-C3	2.22	112.24	109.55
16	F	1650	FUC	C1-C2-C3	2.23	112.25	109.55
14	E	1244	MAN	O3-C3-C4	2.23	115.39	110.36
12	C	1451	MAN	O5-C1-C2	2.31	114.58	110.89
12	E	1451	MAN	O5-C1-C2	2.32	114.61	110.89
14	E	1245	MAN	O6-C6-C5	2.33	119.09	111.30
11	C	1244	MAN	O5-C5-C6	2.34	112.34	107.34
14	E	1244	MAN	O5-C5-C6	2.34	112.35	107.34
12	C	1452	MAN	O6-C6-C5	2.35	119.14	111.30
12	E	1452	MAN	O6-C6-C5	2.35	119.16	111.30
11	C	1244	MAN	O5-C1-C2	2.36	114.66	110.89
12	C	1451	MAN	O5-C5-C6	2.39	112.45	107.34
14	E	1244	MAN	O5-C1-C2	2.39	114.72	110.89
12	E	1451	MAN	O5-C5-C6	2.41	112.50	107.34
12	C	1455	MAN	O2-C2-C1	2.41	114.07	109.23
12	E	1455	MAN	O5-C5-C6	2.43	112.54	107.34
12	C	1455	MAN	O5-C5-C6	2.43	112.54	107.34
12	E	1455	MAN	O2-C2-C1	2.43	114.10	109.23
12	E	1454	MAN	O5-C5-C4	2.46	114.21	110.13
11	C	1246	MAN	O5-C5-C4	2.49	114.25	110.13
12	C	1454	MAN	O5-C5-C4	2.50	114.27	110.13
14	E	1246	MAN	O5-C5-C4	2.52	114.31	110.13
12	C	1453	MAN	O5-C5-C4	2.56	114.37	110.13
12	E	1453	MAN	O5-C5-C4	2.57	114.39	110.13
15	E	1390	MAN	O5-C5-C4	2.60	114.44	110.13
10	B	1640	MAN	C1-C2-C3	2.65	112.76	109.55
16	F	1640	MAN	C1-C2-C3	2.69	112.81	109.55
9	F	1623	GAL	C1-O5-C5	2.73	116.16	112.14
10	B	1644	GAL	C1-O5-C5	2.74	116.17	112.14
9	B	1623	GAL	C1-O5-C5	2.75	116.18	112.14
16	F	1644	GAL	C1-O5-C5	2.75	116.19	112.14
9	B	1614	MAN	C1-C2-C3	2.81	112.95	109.55
9	B	1621	GAL	C1-O5-C5	2.81	116.27	112.14
9	F	1621	GAL	C1-O5-C5	2.82	116.29	112.14
10	B	1642	GAL	C1-O5-C5	2.83	116.30	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	1614	MAN	C1-C2-C3	2.83	112.98	109.55
10	B	1647	GAL	C1-O5-C5	2.84	116.32	112.14
7	C	1364	BMA	O2-C2-C3	2.86	115.95	110.19
7	A	1364	BMA	O2-C2-C3	2.86	115.96	110.19
16	F	1642	GAL	C1-O5-C5	2.87	116.36	112.14
11	C	1243	BMA	O2-C2-C3	2.88	115.99	110.19
7	A	1334	BMA	O2-C2-C3	2.89	116.01	110.19
7	E	1334	BMA	O2-C2-C3	2.89	116.01	110.19
7	A	1243	BMA	O2-C2-C3	2.89	116.02	110.19
12	C	1450	BMA	O2-C2-C3	2.90	116.03	110.19
12	E	1450	BMA	O2-C2-C3	2.90	116.03	110.19
7	A	1162	BMA	O2-C2-C3	2.90	116.03	110.19
7	A	1388	BMA	O2-C2-C3	2.90	116.03	110.19
14	E	1243	BMA	O2-C2-C3	2.90	116.04	110.19
7	C	1162	BMA	O2-C2-C3	2.91	116.04	110.19
7	C	1388	BMA	O2-C2-C3	2.91	116.06	110.19
7	A	1278	BMA	O2-C2-C3	2.91	116.06	110.19
15	E	1388	BMA	O2-C2-C3	2.92	116.06	110.19
7	C	1303	BMA	O2-C2-C3	2.92	116.06	110.19
7	A	1394	BMA	O2-C2-C3	2.92	116.07	110.19
7	E	1394	BMA	O2-C2-C3	2.92	116.07	110.19
7	C	1278	BMA	O2-C2-C3	2.93	116.09	110.19
7	E	1090	BMA	O2-C2-C3	2.93	116.09	110.19
7	C	1334	BMA	O2-C2-C3	2.94	116.11	110.19
7	E	1158	BMA	O2-C2-C3	2.94	116.11	110.19
7	C	1090	BMA	O2-C2-C3	2.94	116.11	110.19
7	A	1158	BMA	O2-C2-C3	2.96	116.14	110.19
9	B	1622	NAG	C1-O5-C5	2.98	116.53	112.14
9	F	1622	NAG	C1-O5-C5	3.02	116.59	112.14
16	F	1637	NAG	C1-O5-C5	3.03	116.60	112.14
5	D	1637	NAG	C1-O5-C5	3.05	116.62	112.14
12	E	1454	MAN	O4-C4-C5	3.05	117.27	109.23
10	B	1637	NAG	C1-O5-C5	3.07	116.65	112.14
9	B	1619	MAN	C1-C2-C3	3.07	113.27	109.55
9	F	1619	MAN	C1-C2-C3	3.07	113.27	109.55
16	F	1648	NAG	C1-O5-C5	3.07	116.66	112.14
10	B	1645	MAN	C1-C2-C3	3.08	113.28	109.55
12	C	1454	MAN	O4-C4-C5	3.08	117.34	109.23
10	B	1648	NAG	C1-O5-C5	3.08	116.67	112.14
16	F	1645	MAN	C1-C2-C3	3.09	113.30	109.55
9	F	1611	NAG	C1-O5-C5	3.13	116.75	112.14
13	D	1611	NAG	C1-O5-C5	3.14	116.76	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1611	NAG	C1-O5-C5	3.14	116.76	112.14
9	F	1619	MAN	C1-O5-C5	3.20	116.85	112.14
16	F	1643	NAG	C1-O5-C5	3.22	116.88	112.14
12	C	1455	MAN	O5-C5-C4	3.22	115.47	110.13
9	B	1619	MAN	C1-O5-C5	3.23	116.89	112.14
12	E	1455	MAN	O5-C5-C4	3.27	115.54	110.13
10	B	1643	NAG	C1-O5-C5	3.28	116.97	112.14
10	B	1645	MAN	C1-O5-C5	3.28	116.97	112.14
16	F	1645	MAN	C1-O5-C5	3.30	116.99	112.14
9	F	1617	NAG	C1-O5-C5	3.35	117.07	112.14
9	B	1617	NAG	C1-O5-C5	3.37	117.09	112.14
9	B	1613	BMA	C1-O5-C5	3.49	117.28	112.14
9	F	1613	BMA	C1-O5-C5	3.51	117.30	112.14
10	B	1639	BMA	C1-O5-C5	3.56	117.38	112.14
16	F	1639	BMA	C1-O5-C5	3.59	117.42	112.14
16	F	1641	NAG	C1-O5-C5	3.69	117.56	112.14
10	B	1641	NAG	C1-O5-C5	3.69	117.57	112.14
13	D	1612	NAG	C1-O5-C5	3.73	117.63	112.14
5	D	1638	NAG	C1-O5-C5	3.75	117.66	112.14
16	F	1638	NAG	C1-O5-C5	3.76	117.67	112.14
9	B	1612	NAG	C1-O5-C5	3.76	117.68	112.14
10	B	1638	NAG	C1-O5-C5	3.77	117.69	112.14
9	F	1612	NAG	C1-O5-C5	3.80	117.73	112.14
16	F	1646	NAG	C1-O5-C5	3.80	117.73	112.14
10	B	1646	NAG	C1-O5-C5	3.85	117.80	112.14
9	F	1620	NAG	C1-O5-C5	3.89	117.86	112.14
9	B	1620	NAG	C1-O5-C5	3.90	117.87	112.14
10	B	1640	MAN	C1-O5-C5	4.16	118.25	112.14
16	F	1640	MAN	C1-O5-C5	4.19	118.30	112.14
9	F	1614	MAN	C1-O5-C5	4.21	118.33	112.14
9	B	1614	MAN	C1-O5-C5	4.22	118.34	112.14
12	E	1452	MAN	C1-O5-C5	4.45	118.69	112.14
12	C	1452	MAN	C1-O5-C5	4.46	118.70	112.14
14	E	1245	MAN	C1-O5-C5	4.53	118.81	112.14
12	C	1452	MAN	O2-C2-C1	5.14	119.53	109.23
14	E	1245	MAN	O2-C2-C1	5.14	119.53	109.23
12	E	1452	MAN	O2-C2-C1	5.15	119.54	109.23
15	E	1390	MAN	C1-C2-C3	7.15	118.22	109.55
14	E	1246	MAN	C1-C2-C3	7.18	118.25	109.55
12	E	1453	MAN	C1-C2-C3	7.19	118.27	109.55
11	C	1246	MAN	C1-C2-C3	7.22	118.30	109.55
12	C	1453	MAN	C1-C2-C3	7.23	118.31	109.55

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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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 [i](#)

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.

All (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
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
6	E	1187	NAG	O7-C7-C8	-2.81	116.90	122.07
6	F	1600	NAG	O7-C7-C8	-2.80	116.91	122.07
6	B	1625	NAG	O7-C7-C8	-2.80	116.92	122.07
6	A	1135	NAG	O7-C7-C8	-2.80	116.92	122.07
6	A	1355	NAG	O7-C7-C8	-2.78	116.95	122.07
6	D	1600	NAG	C4-C3-C2	-2.78	107.03	111.34
6	A	1355	NAG	C4-C3-C2	-2.74	107.09	111.34
6	A	1135	NAG	C4-C3-C2	-2.73	107.10	111.34
6	B	1600	NAG	C4-C3-C2	-2.73	107.11	111.34
6	F	1600	NAG	C4-C3-C2	-2.72	107.11	111.34
6	B	1625	NAG	C4-C3-C2	-2.72	107.11	111.34
6	E	1187	NAG	C4-C3-C2	-2.72	107.12	111.34
6	C	1397	NAG	C4-C3-C2	-2.72	107.12	111.34
6	A	1397	NAG	C4-C3-C2	-2.69	107.16	111.34
6	E	1397	NAG	C4-C3-C2	-2.68	107.18	111.34

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.