W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2024 – 01:15 PM EDT

PDB ID	:	4GEZ
Title	:	Structure of a neuraminidase-like protein from A/bat/Guatemala/164/2009
Authors	:	Yang, H.; Carney, P.J.; Donis, R.O.; Stevens, J.
Deposited on	:	2012-08-02
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

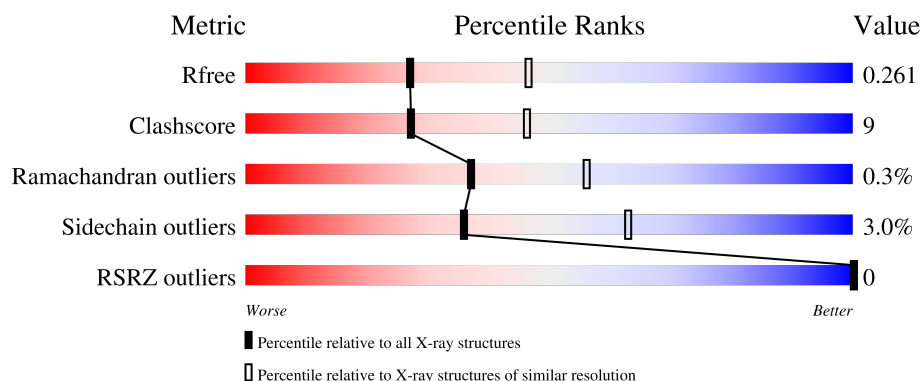|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
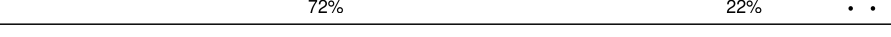*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.261
Clashscore		9
Ramachandran outliers		0.3%
Sidechain outliers		3.0%
RSRZ outliers		0

Worse *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
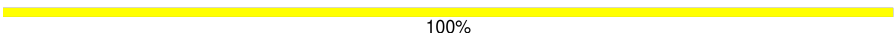
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	378	76% 20% • •
1	B	378	75% 20% • •
1	C	378	79% 16% • •
1	D	378	72% 22% • •
1	E	378	78% 17% • •

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Mol	Chain	Length	Quality of chain
1	F	378	79% 16%
1	G	378	75% 20%
1	H	378	79% 17%
1	I	378	79% 16%
1	J	378	71% 24%
1	K	378	71% 24%
1	L	378	71% 25%
2	M	2	50% 50%
2	O	2	100%
2	Q	2	100%
3	N	3	33% 67%
3	P	3	33% 67%

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 35035 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total 2858	C 1804	N 487	O 547	S 20	0	0	0
1	B	365	Total 2858	C 1804	N 487	O 547	S 20	0	0	0
1	C	365	Total 2858	C 1804	N 487	O 547	S 20	0	0	0
1	D	365	Total 2858	C 1804	N 487	O 547	S 20	0	0	0
1	E	365	Total 2858	C 1804	N 487	O 547	S 20	0	0	0
1	F	365	Total 2858	C 1804	N 487	O 547	S 20	0	0	0
1	G	365	Total 2858	C 1804	N 487	O 547	S 20	0	0	0
1	H	365	Total 2858	C 1804	N 487	O 547	S 20	0	0	0
1	I	365	Total 2858	C 1804	N 487	O 547	S 20	0	0	0
1	J	363	Total 2832	C 1784	N 484	O 544	S 20	0	0	0
1	K	364	Total 2846	C 1795	N 486	O 545	S 20	0	0	0
1	L	365	Total 2858	C 1804	N 487	O 547	S 20	0	0	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	GLY	-	expression tag	UNP H6QM85
A	66	SER	-	expression tag	UNP H6QM85
A	67	GLY	-	expression tag	UNP H6QM85
A	68	ASP	-	expression tag	UNP H6QM85
A	69	SER	-	expression tag	UNP H6QM85

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Chain	Residue	Modelled	Actual	Comment	Reference
A	70	GLY	-	expression tag	UNP H6QM85
A	71	SER	-	expression tag	UNP H6QM85
A	72	PRO	-	expression tag	UNP H6QM85
A	73	GLY	-	expression tag	UNP H6QM85
B	65	GLY	-	expression tag	UNP H6QM85
B	66	SER	-	expression tag	UNP H6QM85
B	67	GLY	-	expression tag	UNP H6QM85
B	68	ASP	-	expression tag	UNP H6QM85
B	69	SER	-	expression tag	UNP H6QM85
B	70	GLY	-	expression tag	UNP H6QM85
B	71	SER	-	expression tag	UNP H6QM85
B	72	PRO	-	expression tag	UNP H6QM85
B	73	GLY	-	expression tag	UNP H6QM85
C	65	GLY	-	expression tag	UNP H6QM85
C	66	SER	-	expression tag	UNP H6QM85
C	67	GLY	-	expression tag	UNP H6QM85
C	68	ASP	-	expression tag	UNP H6QM85
C	69	SER	-	expression tag	UNP H6QM85
C	70	GLY	-	expression tag	UNP H6QM85
C	71	SER	-	expression tag	UNP H6QM85
C	72	PRO	-	expression tag	UNP H6QM85
C	73	GLY	-	expression tag	UNP H6QM85
D	65	GLY	-	expression tag	UNP H6QM85
D	66	SER	-	expression tag	UNP H6QM85
D	67	GLY	-	expression tag	UNP H6QM85
D	68	ASP	-	expression tag	UNP H6QM85
D	69	SER	-	expression tag	UNP H6QM85
D	70	GLY	-	expression tag	UNP H6QM85
D	71	SER	-	expression tag	UNP H6QM85
D	72	PRO	-	expression tag	UNP H6QM85
D	73	GLY	-	expression tag	UNP H6QM85
E	65	GLY	-	expression tag	UNP H6QM85
E	66	SER	-	expression tag	UNP H6QM85
E	67	GLY	-	expression tag	UNP H6QM85
E	68	ASP	-	expression tag	UNP H6QM85
E	69	SER	-	expression tag	UNP H6QM85
E	70	GLY	-	expression tag	UNP H6QM85
E	71	SER	-	expression tag	UNP H6QM85
E	72	PRO	-	expression tag	UNP H6QM85
E	73	GLY	-	expression tag	UNP H6QM85
F	65	GLY	-	expression tag	UNP H6QM85
F	66	SER	-	expression tag	UNP H6QM85

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Chain	Residue	Modelled	Actual	Comment	Reference
F	67	GLY	-	expression tag	UNP H6QM85
F	68	ASP	-	expression tag	UNP H6QM85
F	69	SER	-	expression tag	UNP H6QM85
F	70	GLY	-	expression tag	UNP H6QM85
F	71	SER	-	expression tag	UNP H6QM85
F	72	PRO	-	expression tag	UNP H6QM85
F	73	GLY	-	expression tag	UNP H6QM85
G	65	GLY	-	expression tag	UNP H6QM85
G	66	SER	-	expression tag	UNP H6QM85
G	67	GLY	-	expression tag	UNP H6QM85
G	68	ASP	-	expression tag	UNP H6QM85
G	69	SER	-	expression tag	UNP H6QM85
G	70	GLY	-	expression tag	UNP H6QM85
G	71	SER	-	expression tag	UNP H6QM85
G	72	PRO	-	expression tag	UNP H6QM85
G	73	GLY	-	expression tag	UNP H6QM85
H	65	GLY	-	expression tag	UNP H6QM85
H	66	SER	-	expression tag	UNP H6QM85
H	67	GLY	-	expression tag	UNP H6QM85
H	68	ASP	-	expression tag	UNP H6QM85
H	69	SER	-	expression tag	UNP H6QM85
H	70	GLY	-	expression tag	UNP H6QM85
H	71	SER	-	expression tag	UNP H6QM85
H	72	PRO	-	expression tag	UNP H6QM85
H	73	GLY	-	expression tag	UNP H6QM85
I	65	GLY	-	expression tag	UNP H6QM85
I	66	SER	-	expression tag	UNP H6QM85
I	67	GLY	-	expression tag	UNP H6QM85
I	68	ASP	-	expression tag	UNP H6QM85
I	69	SER	-	expression tag	UNP H6QM85
I	70	GLY	-	expression tag	UNP H6QM85
I	71	SER	-	expression tag	UNP H6QM85
I	72	PRO	-	expression tag	UNP H6QM85
I	73	GLY	-	expression tag	UNP H6QM85
J	65	GLY	-	expression tag	UNP H6QM85
J	66	SER	-	expression tag	UNP H6QM85
J	67	GLY	-	expression tag	UNP H6QM85
J	68	ASP	-	expression tag	UNP H6QM85
J	69	SER	-	expression tag	UNP H6QM85
J	70	GLY	-	expression tag	UNP H6QM85
J	71	SER	-	expression tag	UNP H6QM85
J	72	PRO	-	expression tag	UNP H6QM85

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Chain	Residue	Modelled	Actual	Comment	Reference
J	73	GLY	-	expression tag	UNP H6QM85
K	65	GLY	-	expression tag	UNP H6QM85
K	66	SER	-	expression tag	UNP H6QM85
K	67	GLY	-	expression tag	UNP H6QM85
K	68	ASP	-	expression tag	UNP H6QM85
K	69	SER	-	expression tag	UNP H6QM85
K	70	GLY	-	expression tag	UNP H6QM85
K	71	SER	-	expression tag	UNP H6QM85
K	72	PRO	-	expression tag	UNP H6QM85
K	73	GLY	-	expression tag	UNP H6QM85
L	65	GLY	-	expression tag	UNP H6QM85
L	66	SER	-	expression tag	UNP H6QM85
L	67	GLY	-	expression tag	UNP H6QM85
L	68	ASP	-	expression tag	UNP H6QM85
L	69	SER	-	expression tag	UNP H6QM85
L	70	GLY	-	expression tag	UNP H6QM85
L	71	SER	-	expression tag	UNP H6QM85
L	72	PRO	-	expression tag	UNP H6QM85
L	73	GLY	-	expression tag	UNP H6QM85

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	2	Total 24	C 14	N 1	O 9	0	0	0
2	O	2	Total 24	C 14	N 1	O 9	0	0	0
2	Q	2	Total 24	C 14	N 1	O 9	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.
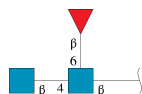
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	N	3	Total 38	C 22	N 2	O 14	0	0	0
3	P	3	Total 38	C 22	N 2	O 14	0	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Ca 1	0	0
4	B	1	Total 1	Ca 1	0	0
4	C	1	Total 1	Ca 1	0	0
4	D	1	Total 1	Ca 1	0	0
4	E	1	Total 1	Ca 1	0	0
4	F	1	Total 1	Ca 1	0	0
4	G	1	Total 1	Ca 1	0	0
4	H	1	Total 1	Ca 1	0	0
4	I	1	Total 1	Ca 1	0	0
4	J	1	Total 1	Ca 1	0	0
4	K	1	Total 1	Ca 1	0	0
4	L	1	Total 1	Ca 1	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 14	C 8	N 1	O 5	0	0
5	A	1	Total 14	C 8	N 1	O 5	0	0
5	B	1	Total 14	C 8	N 1	O 5	0	0
5	C	1	Total 14	C 8	N 1	O 5	0	0
5	D	1	Total 14	C 8	N 1	O 5	0	0
5	D	1	Total 14	C 8	N 1	O 5	0	0
5	D	1	Total 14	C 8	N 1	O 5	0	0
5	E	1	Total 14	C 8	N 1	O 5	0	0
5	F	1	Total 14	C 8	N 1	O 5	0	0
5	G	1	Total 14	C 8	N 1	O 5	0	0
5	H	1	Total 14	C 8	N 1	O 5	0	0
5	I	1	Total 14	C 8	N 1	O 5	0	0
5	K	1	Total 14	C 8	N 1	O 5	0	0
5	L	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 6 is alpha-L-fucopyranose (three-letter code: FUC) (formula: $C_6H_{12}O_5$).

FUC
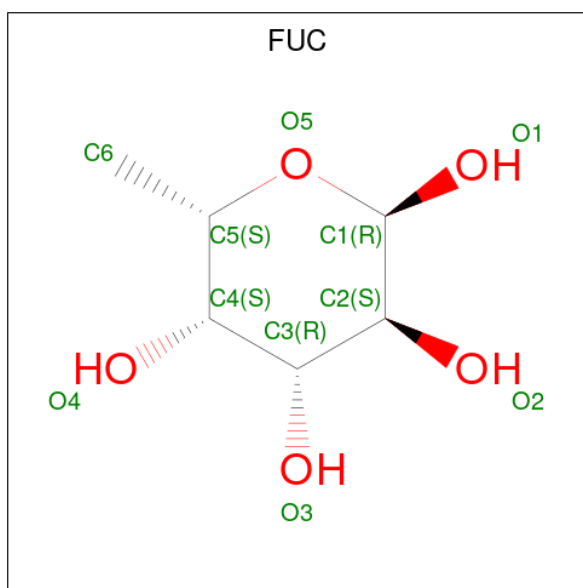
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	55	Total	O	0	0
			55	55		
7	B	54	Total	O	0	0
			54	54		
7	C	45	Total	O	0	0
			45	45		
7	D	46	Total	O	0	0
			46	46		
7	E	60	Total	O	0	0
			60	60		
7	F	41	Total	O	0	0
			41	41		
7	G	31	Total	O	0	0
			31	31		
7	H	15	Total	O	0	0
			15	15		
7	I	14	Total	O	0	0
			14	14		
7	J	25	Total	O	0	0
			25	25		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	K	17	Total 17	O 17	0	0
7	L	8	Total 8	O 8	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: Neuraminidase

Chain A:
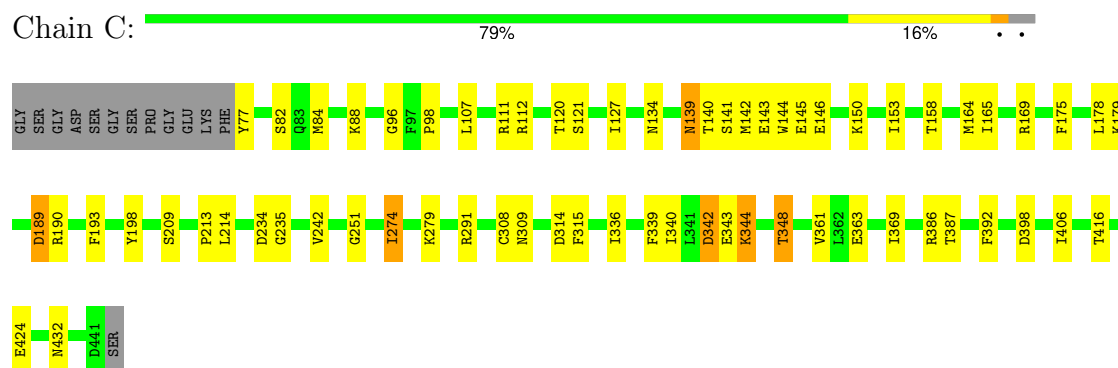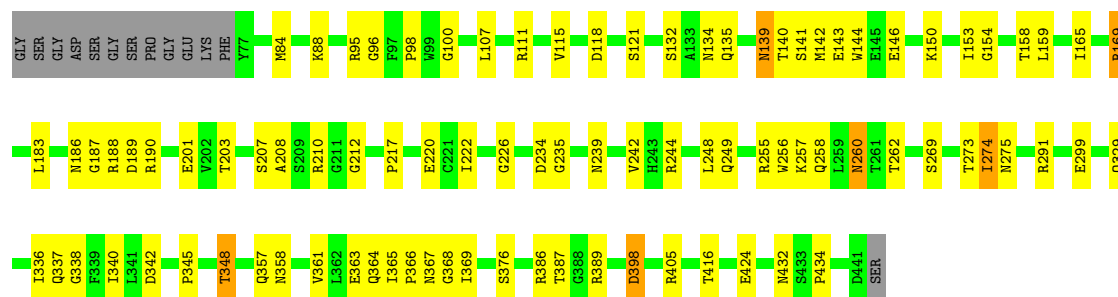

- Molecule 1: Neuraminidase

Chain B:

- Molecule 1: Neuraminidase

Chain C:
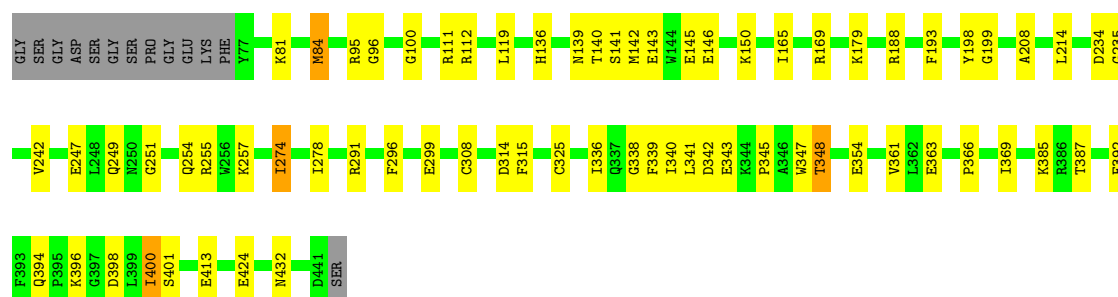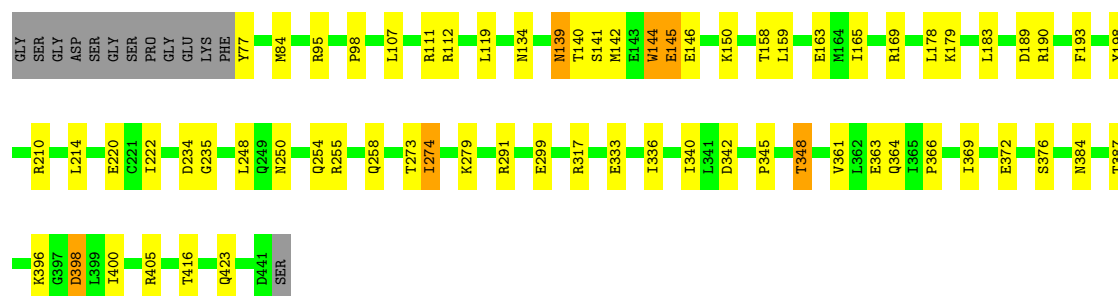
• Molecule 1: Neuraminidase

Chain D:

• Molecule 1: Neuraminidase

Chain E:

• Molecule 1: Neuraminidase

Chain F:

• Molecule 1: Neuraminidase

Chain G:

D342 E343 K344 W347 T348 V361 L362 E363 I369 E372 G373 T374 T387 F392 K396 G397 D398 L399 I400 Q404 T416 N432 D441 SER

• Molecule 1: Neuraminidase

Chain H:

79% 17%

GLY SER GLY ASP SER GLY SER PRO GLY GLU LYS PHE Y77 M84 V87 W90 V91 R95 P98 L107 R111 R112 C117 C122 N134 L138 N139 T140 S141 M142 E146 K150 T158 I165 L166 R169 L178 L183 K197 T203

N218 I222 C223 C228 F229 D234 G235 L248 R255 E267 I274 L285 R291 K298 E299 N309 D314 F315 I336 I340 L341 D342 E343 K344 P345 A346 W347 T348 V361 L362 E363 P366 I369 G373 T387 D398 L399 I400 S401

G402 C403 T416 V417 I422 D441 SER

• Molecule 1: Neuraminidase

Chain I:

79% 16%

GLY SER GLY ASP SER GLY SER PRO GLY GLU LYS PHE Y77 W78 R79 A80 K81 S82 Q83 M84 R95 G100 L107 R111 R112 C117 C122 N134 L137 L138 N139 W144 E145 E146 K150 T158 L159 S160 I165 R169 L178 K179 L183 R190

F193 I196 K197 Y198 V202 T203 D204 R210 L214 P217 D234 Q240 S241 V242 L248 Q249 N250 G251 R255 Q258 Y268 S269 I274 N275 N276 T281 R291 P292 L293 E299 D314 F315 P316 R317 I336 I340 K344 T348

T351 V361 L362 E363 I369 T387 D398 R405 N432 D441 SER

• Molecule 1: Neuraminidase

Chain J:

71% 24%

GLY SER GLY ASP SER GLY SER PRO GLY GLU LYS PHE TYR TRP R79 A80 K81 M84 V87 W90 V91 R95 G96 F97 P98 W99 G100 D106 L107 R111 R112 S116 C117 D118 L119 T120 S121 C122 F125 F126 Q135 H136 L137 L138 N139 T140 S141 M142 E145 E146

K150 T151 T158 E163 M164 I165 R169 K179 V182 F193 Y198 T203 A208 S209 R210 L214 P217 E220 F229 D234 G235 V242 H243 R244 N250 R255 Q258 S269 I274 T283 K290 R291 P292 E299 L300

T313 D314 F315 S324 I336 I340 L341 K344 P345 A346 W347 T348 S349 K350 V361 L362 E363 Q364 I369 G373 S376 T387 G388 R389 Q394 P395 K396 G397 D398 L399 I400 Q404 R405 E411 I412 E413 T416 E424 I438 D441 SER

• Molecule 1: Neuraminidase

Chain K:

71% 24%

GLY SER GLY ASP SER GLY SER PRO GLY GLU LYS PHE TYR W78 K81 M84 R95 P98 L107 R111 S116 C122 S132 A133 N134 L137 L138 N139 T140 S141 M142 E143 W144 E145 E146 K150 I153 T158 I165 R169 D176 R188

F193 I196 K197 Y198 G199 E200 E201 D204 S209 R210 L214 P217 E220 C223 S227 I245 T252 K257 I264 S269 I274 I278 K279 T283 D288 A289 K290 R291 P292 L293 F296 E299 L300 N301 Y302 C308 N309 P312 T313

D314 F315 P316 R317 S324 M327 A328 K331 I336 F339 I340 L341 D342 E343 K344 P345 A346 W347 T348 V361 L362 E363 Q364 I365 I369 G373 S376 T387 F392 D398 L399 I400 S401 G402 R405 T416 C429 N432 I438 N439 W440 D441 SER

• Molecule 1: Neuraminidase

Chain L:

71%   25%

GLY SER GLY ASP SER GLY SER PRO GLY GLU LYS PHE Y77 P104 G105 D106 L107 R111 S116 C117 D118 L119 T120 S121 C122 F125 N134 N139 T140 S141 M142 E143 W144 E145 K150 I153 T158 I165 G168 R169 S172 K179 L183 N186

R190 N191 S192 K197 Y198 G199 E200 R210 G211 G212 P217 I222 C223 I224 E225 C228 F229 D234 G235 V242 H243 R244 L248 R255 W256 T261 N265 F266 S269 T273 I274 N284 K290 R291 P292 K298 E299 C308 N309 G310 T313 D314

F315 C325 A328 G338 F339 I340 L341 D342 A346 W347 T348 S349 V361 I365 I369 E370 S371 E380 S383 R386 T387 P395 K396 G397 D398 L399 I400 R405 E413 C429 N432 N439 W440 D441 SER

• Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

50%   50%

NAG1 FUC2

• Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

100%

NAG1 FUC2

• Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

100%

NAG1 FUC2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

33%   67%

NAG1 NAG2 FUL3

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

33%   67%

NAG1 NAG2 FUL3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	113.33Å 113.33Å 114.31Å 81.47° 81.55° 67.72°	Depositor
Resolution (Å)	29.88 – 2.50 29.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.2 (29.88-2.50) 91.9 (29.88-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.218 , 0.262 0.219 , 0.261	Depositor DCC
R_{free} test set	8258 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	47.7	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 26.0	EDS
L-test for twinning[2]	$< |L| > = 0.44, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.369 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	35035	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FUL, NAG, CA, FUC

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	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.30	0/2926	0.53	0/3966
1	B	0.29	0/2926	0.51	0/3966
1	C	0.29	0/2926	0.52	0/3966
1	D	0.29	0/2926	0.53	0/3966
1	E	0.29	0/2926	0.52	0/3966
1	F	0.30	0/2926	0.53	0/3966
1	G	0.29	0/2926	0.52	0/3966
1	H	0.28	0/2926	0.54	0/3966
1	I	0.28	0/2926	0.54	0/3966
1	J	0.27	0/2897	0.52	0/3925
1	K	0.27	0/2913	0.53	1/3948 (0.0%)
1	L	0.27	0/2926	0.53	0/3966
All	All	0.29	0/35070	0.53	1/47533 (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	1
1	C	0	1
1	G	0	1
1	I	0	1
1	J	0	1
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	293	LEU	CA-CB-CG	5.86	128.77	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	344	LYS	Peptide
1	C	344	LYS	Peptide
1	G	344	LYS	Peptide
1	I	344	LYS	Peptide
1	J	344	LYS	Peptide

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	2858	0	2762	49	2
1	B	2858	0	2764	54	2
1	C	2858	0	2764	51	1
1	D	2858	0	2765	67	0
1	E	2858	0	2763	47	2
1	F	2858	0	2764	43	1
1	G	2858	0	2764	51	1
1	H	2858	0	2764	38	0
1	I	2858	0	2763	51	0
1	J	2832	0	2746	64	0
1	K	2846	0	2755	60	0
1	L	2858	0	2763	60	0
2	M	24	0	22	0	0
2	O	24	0	22	0	1
2	Q	24	0	22	0	0
3	N	38	0	34	2	0
3	P	38	0	34	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	A	28	0	26	2	0
5	B	14	0	13	2	0
5	C	14	0	13	1	0
5	D	42	0	39	2	0
5	E	14	0	13	1	0
5	F	14	0	13	1	0
5	G	14	0	13	0	0
5	H	14	0	13	0	0
5	I	14	0	13	2	0
5	K	14	0	13	0	0
5	L	14	0	12	1	0
6	D	10	0	10	0	0
7	A	55	0	0	9	0
7	B	54	0	0	11	0
7	C	45	0	0	12	0
7	D	46	0	0	16	0
7	E	60	0	0	7	0
7	F	41	0	0	6	0
7	G	31	0	0	7	0
7	H	15	0	0	1	0
7	I	14	0	0	9	0
7	J	25	0	0	14	0
7	K	17	0	0	8	0
7	L	8	0	0	1	0
All	All	35035	0	33462	610	5

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 9.

All (610) 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:D:187:GLY:O	7:D:612:HOH:O	1.83	0.96
1:C:309:ASN:OD1	7:C:645:HOH:O	1.85	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:GLY:O	7:D:626:HOH:O	1.84	0.93
1:B:314:ASP:OD2	7:B:645:HOH:O	1.87	0.93
1:I:291:ARG:NH2	1:I:336:ILE:O	2.02	0.92
1:K:78:TRP:N	7:K:612:HOH:O	2.00	0.92
1:C:82:SER:OG	7:C:616:HOH:O	1.87	0.92
1:D:358:ASN:O	7:D:644:HOH:O	1.88	0.92
1:B:398:ASP:OD2	7:B:617:HOH:O	1.87	0.91
1:I:160:SER:O	7:I:603:HOH:O	1.88	0.91
1:J:220:GLU:OE2	7:J:601:HOH:O	1.89	0.89
1:E:394:GLN:O	7:E:645:HOH:O	1.91	0.88
1:H:291:ARG:NH2	1:H:336:ILE:O	2.07	0.88
1:A:102:GLU:OE2	7:A:612:HOH:O	1.91	0.88
1:G:239:ASN:ND2	7:G:626:HOH:O	1.89	0.87
1:I:340:ILE:HG21	1:I:369:ILE:HD12	1.55	0.87
1:D:345:PRO:HB3	1:D:366:PRO:HA	1.56	0.86
1:I:179:LYS:O	7:I:604:HOH:O	1.91	0.86
1:I:84:MET:HG2	1:I:274:ILE:HG13	1.59	0.85
1:A:291:ARG:NH2	1:A:336:ILE:O	2.10	0.85
1:G:291:ARG:NH2	1:G:336:ILE:O	2.09	0.85
1:J:140:THR:OG1	7:J:622:HOH:O	1.94	0.84
1:B:291:ARG:NH2	1:B:336:ILE:O	2.09	0.84
1:F:291:ARG:NH2	1:F:336:ILE:O	2.11	0.83
1:A:411:GLU:OE2	7:A:646:HOH:O	1.95	0.83
1:D:220:GLU:OE2	7:D:617:HOH:O	1.95	0.83
1:J:106:ASP:OD2	7:J:612:HOH:O	1.95	0.82
1:F:139:ASN:OD1	7:F:625:HOH:O	1.95	0.82
1:E:343:GLU:O	7:E:605:HOH:O	1.97	0.82
1:J:84:MET:HG2	1:J:274:ILE:HG13	1.61	0.82
1:A:340:ILE:HG21	1:A:369:ILE:HD12	1.60	0.82
1:E:340:ILE:HG21	1:E:369:ILE:HD12	1.63	0.81
1:K:220:GLU:OE1	7:K:613:HOH:O	1.97	0.81
1:C:308:CYS:SG	7:C:626:HOH:O	2.38	0.81
1:H:340:ILE:HG21	1:H:369:ILE:HD12	1.62	0.81
1:B:411:GLU:OE2	7:B:608:HOH:O	1.98	0.80
1:F:340:ILE:HG21	1:F:369:ILE:HD12	1.64	0.79
1:H:84:MET:HG2	1:H:274:ILE:HG13	1.64	0.79
1:C:340:ILE:HG21	1:C:369:ILE:HD12	1.61	0.79
1:C:291:ARG:NH2	1:C:336:ILE:O	2.15	0.79
1:E:291:ARG:NH2	1:E:336:ILE:O	2.14	0.78
1:B:259:LEU:O	7:B:640:HOH:O	2.02	0.78
1:D:340:ILE:HG21	1:D:369:ILE:HD12	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:MET:HG2	1:B:274:ILE:HG13	1.65	0.77
1:D:115:VAL:O	7:D:604:HOH:O	2.02	0.77
1:F:255:ARG:NH2	1:F:299:GLU:OE1	2.18	0.77
1:B:414:ASP:OD2	7:B:626:HOH:O	2.03	0.77
1:B:417:VAL:O	7:B:634:HOH:O	2.02	0.77
1:C:111:ARG:NH1	1:C:146:GLU:OE1	2.18	0.76
1:K:399:LEU:O	7:K:617:HOH:O	2.03	0.76
1:F:345:PRO:HB3	1:F:366:PRO:HA	1.68	0.76
1:G:340:ILE:HG21	1:G:369:ILE:HD12	1.68	0.76
1:C:363:GLU:OE1	7:C:628:HOH:O	2.03	0.76
1:J:117:CYS:O	7:J:604:HOH:O	2.04	0.74
1:A:249:GLN:NE2	5:A:503:NAG:O7	2.21	0.73
1:E:249:GLN:NE2	5:E:502:NAG:O7	2.20	0.73
1:B:111:ARG:NH1	1:B:146:GLU:OE1	2.21	0.73
1:K:291:ARG:NH2	1:K:336:ILE:O	2.17	0.73
1:J:121:SER:HB2	7:J:620:HOH:O	1.87	0.72
1:C:121:SER:OG	7:C:640:HOH:O	2.05	0.72
1:J:340:ILE:HG21	1:J:369:ILE:HD12	1.70	0.72
1:G:372:GLU:O	7:G:610:HOH:O	2.08	0.72
1:K:432:ASN:OD1	1:K:432:ASN:N	2.23	0.72
1:E:81:LYS:NZ	1:E:401:SER:O	2.23	0.71
1:C:84:MET:HG2	1:C:274:ILE:HG13	1.72	0.71
1:I:178:LEU:O	7:I:605:HOH:O	2.08	0.70
1:E:255:ARG:HH22	1:E:299:GLU:HA	1.57	0.70
1:C:150:LYS:HB3	1:C:165:ILE:HD11	1.73	0.70
1:G:432:ASN:ND2	7:G:624:HOH:O	1.83	0.69
1:G:150:LYS:HB3	1:G:165:ILE:HD11	1.73	0.69
1:I:77:TYR:OH	7:I:614:HOH:O	2.11	0.69
1:K:150:LYS:HB3	1:K:165:ILE:HD11	1.73	0.69
1:D:255:ARG:HH22	1:D:299:GLU:HA	1.58	0.69
1:K:143:GLU:OE2	1:K:188:ARG:NH1	2.25	0.68
1:D:291:ARG:NH2	1:D:336:ILE:O	2.26	0.68
1:B:340:ILE:HG21	1:B:369:ILE:HD12	1.76	0.68
1:H:111:ARG:HH22	1:H:142:MET:H	1.42	0.68
1:G:112:ARG:O	7:G:602:HOH:O	2.11	0.68
1:D:365:ILE:HG22	7:D:636:HOH:O	1.94	0.67
1:D:153:ILE:O	7:D:622:HOH:O	2.12	0.67
1:E:354:GLU:OE1	7:E:639:HOH:O	2.13	0.67
1:I:111:ARG:NH1	1:I:146:GLU:OE1	2.22	0.67
1:G:81:LYS:HB2	1:G:404:GLN:HB2	1.76	0.67
1:I:281:THR:O	7:I:611:HOH:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:176:ASP:OD2	1:K:198:TYR:OH	2.07	0.67
1:E:396:LYS:NZ	7:E:651:HOH:O	2.28	0.66
1:C:153:ILE:O	7:C:634:HOH:O	2.13	0.66
5:I:502:NAG:O4	7:I:614:HOH:O	2.12	0.66
1:A:350:LYS:NZ	7:A:629:HOH:O	2.27	0.66
1:B:398:ASP:OD1	1:B:405:ARG:NH1	2.29	0.66
1:L:291:ARG:NH1	7:L:606:HOH:O	2.01	0.66
1:A:400:ILE:HG21	1:D:203:THR:HG22	1.78	0.65
1:D:368:GLY:N	7:D:636:HOH:O	2.27	0.65
1:F:144:TRP:O	1:F:169:ARG:NH2	2.24	0.65
1:J:413:GLU:OE2	7:J:615:HOH:O	2.15	0.65
1:A:143:GLU:OE2	1:A:188:ARG:NH1	2.28	0.65
1:G:84:MET:HG2	1:G:274:ILE:HG13	1.78	0.65
1:I:107:LEU:HD23	1:I:158:THR:HG22	1.78	0.65
1:D:234:ASP:OD1	7:D:646:HOH:O	2.14	0.65
1:E:413:GLU:OE2	7:E:659:HOH:O	2.14	0.65
1:I:255:ARG:NH2	1:I:299:GLU:OE1	2.28	0.65
1:J:283:THR:OG1	7:J:617:HOH:O	2.13	0.65
1:K:340:ILE:HG21	1:K:369:ILE:HD12	1.78	0.64
1:F:220:GLU:OE2	7:F:618:HOH:O	2.14	0.64
1:D:220:GLU:HB2	7:D:604:HOH:O	1.96	0.64
1:D:84:MET:HG2	1:D:274:ILE:HG13	1.79	0.63
1:G:145:GLU:OE2	1:H:95:ARG:NH2	2.26	0.63
1:E:179:LYS:HD3	1:E:199:GLY:HA3	1.79	0.63
1:F:398:ASP:OD2	1:F:405:ARG:NH1	2.29	0.62
1:B:77:TYR:N	7:B:648:HOH:O	2.32	0.62
1:K:346:ALA:HB3	1:K:365:ILE:HB	1.81	0.62
5:A:503:NAG:O4	5:A:503:NAG:N2	2.32	0.62
1:D:398:ASP:OD1	1:D:405:ARG:NH1	2.31	0.62
1:L:405:ARG:NH2	1:L:429:CYS:SG	2.73	0.62
1:H:345:PRO:HB3	1:H:366:PRO:HA	1.81	0.62
1:L:340:ILE:HG21	1:L:369:ILE:HD12	1.81	0.62
1:F:84:MET:HG2	1:F:274:ILE:HG13	1.81	0.61
1:J:341:LEU:HB3	1:J:347:TRP:HB2	1.82	0.61
1:B:143:GLU:OE2	1:B:188:ARG:NH1	2.33	0.61
1:C:279:LYS:HD3	1:C:342:ASP:OD1	2.01	0.61
1:B:112:ARG:NH1	1:B:169:ARG:O	2.34	0.61
1:H:150:LYS:NZ	7:H:612:HOH:O	2.07	0.61
1:K:283:THR:OG1	1:K:291:ARG:NH2	2.31	0.61
1:K:312:PRO:HB2	1:K:317:ARG:HD2	1.83	0.61
1:A:269:SER:OG	7:A:614:HOH:O	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:179:LYS:HD3	1:L:199:GLY:HA3	1.83	0.60
1:I:112:ARG:NH1	1:I:169:ARG:O	2.35	0.60
1:C:84:MET:HE1	1:C:406:ILE:HB	1.83	0.60
1:F:150:LYS:HB3	1:F:165:ILE:HD11	1.84	0.60
1:G:112:ARG:NH1	1:G:169:ARG:O	2.35	0.59
1:B:250:ASN:ND2	5:B:505:NAG:O7	2.36	0.59
1:G:209:SER:O	1:G:210:ARG:NH1	2.36	0.59
1:I:183:LEU:HD21	1:I:248:LEU:HD11	1.84	0.59
1:C:213:PRO:O	7:C:613:HOH:O	2.16	0.59
1:J:255:ARG:NH2	1:J:299:GLU:OE1	2.33	0.59
1:L:106:ASP:OD1	1:L:106:ASP:N	2.36	0.59
1:A:405:ARG:NE	7:A:654:HOH:O	2.19	0.59
1:I:249:GLN:NE2	5:I:502:NAG:O7	2.36	0.59
1:E:143:GLU:OE2	1:E:188:ARG:NH1	2.26	0.58
1:H:223:CYS:HA	1:H:228:CYS:HA	1.85	0.58
1:F:111:ARG:NH1	1:F:142:MET:O	2.37	0.58
1:B:255:ARG:NH2	1:B:299:GLU:OE1	2.36	0.58
1:D:111:ARG:NH1	1:D:146:GLU:OE1	2.37	0.58
1:H:348:THR:HG22	1:H:363:GLU:HB2	1.86	0.58
1:K:289:ALA:N	1:K:328:ALA:O	2.35	0.58
1:D:210:ARG:HG3	1:D:242:VAL:HG21	1.85	0.58
1:G:210:ARG:HG3	1:G:242:VAL:HG21	1.86	0.58
1:E:95:ARG:HH22	1:E:385:LYS:HE3	1.68	0.58
1:G:279:LYS:NZ	1:G:343:GLU:OE2	2.31	0.58
1:D:348:THR:HG22	1:D:363:GLU:HB2	1.86	0.57
1:D:139:ASN:HB2	1:D:142:MET:HG3	1.86	0.57
1:I:268:TYR:O	7:I:611:HOH:O	2.17	0.57
1:C:111:ARG:NH2	1:C:141:SER:HB3	2.20	0.57
1:D:118:ASP:OD2	7:D:629:HOH:O	2.17	0.57
1:I:398:ASP:OD1	1:I:405:ARG:NH1	2.38	0.57
1:K:107:LEU:HD23	1:K:158:THR:HG22	1.85	0.57
1:D:208:ALA:HB1	7:D:646:HOH:O	2.03	0.57
1:H:98:PRO:HB3	1:H:416:THR:HG21	1.86	0.57
1:J:81:LYS:HB2	1:J:404:GLN:HB2	1.87	0.57
1:E:143:GLU:HG2	1:E:188:ARG:HH22	1.70	0.56
1:F:250:ASN:ND2	5:F:505:NAG:O5	2.38	0.56
1:H:255:ARG:HH22	1:H:299:GLU:HA	1.71	0.56
1:L:168:GLY:HA2	1:L:186:ASN:ND2	2.20	0.56
1:D:190:ARG:HH22	1:I:144:TRP:HZ3	1.54	0.56
1:A:315:PHE:O	7:A:608:HOH:O	2.18	0.56
1:K:348:THR:HG22	1:K:363:GLU:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:LEU:HD23	1:C:158:THR:HG22	1.87	0.56
1:J:179:LYS:HD2	1:J:198:TYR:CE2	2.41	0.56
1:J:258:GLN:NE2	7:J:611:HOH:O	2.38	0.56
1:E:150:LYS:HB3	1:E:165:ILE:HD11	1.86	0.56
1:G:107:LEU:HD23	1:G:158:THR:HG22	1.87	0.56
1:A:208:ALA:HB1	7:A:649:HOH:O	2.05	0.55
1:B:357:GLN:OE1	1:B:386:ARG:NH2	2.38	0.55
1:D:150:LYS:HB3	1:D:165:ILE:HD11	1.88	0.55
1:E:111:ARG:NH2	1:E:141:SER:HB3	2.21	0.55
1:A:179:LYS:HD2	1:A:198:TYR:CE2	2.42	0.55
1:A:348:THR:HG22	1:A:363:GLU:HB2	1.87	0.55
1:B:111:ARG:NH2	1:B:141:SER:HB3	2.21	0.55
1:B:126:PHE:HE1	1:B:151:THR:HG1	1.54	0.55
1:A:255:ARG:HH22	1:A:299:GLU:HA	1.71	0.55
1:J:394:GLN:HG2	7:J:619:HOH:O	2.06	0.55
1:L:172:SER:HB2	1:L:217:PRO:HD2	1.88	0.55
1:L:107:LEU:HD23	1:L:158:THR:HG22	1.89	0.55
1:H:84:MET:HG3	1:H:343:GLU:HG3	1.88	0.55
1:J:193:PHE:HA	1:J:214:LEU:HD12	1.88	0.55
1:L:222:ILE:HG21	1:L:273:THR:HB	1.88	0.55
1:K:193:PHE:HA	1:K:214:LEU:HD12	1.88	0.54
1:L:266:PHE:HE1	1:L:269:SER:HG	1.54	0.54
1:D:107:LEU:HD23	1:D:158:THR:HG22	1.89	0.54
1:B:250:ASN:HD21	5:B:505:NAG:C1	2.21	0.54
1:B:81:LYS:NZ	1:B:401:SER:O	2.33	0.54
1:F:210:ARG:HH21	1:F:258:GLN:HE22	1.55	0.54
1:B:348:THR:HG22	1:B:363:GLU:HB2	1.88	0.54
5:C:502:NAG:O4	7:C:629:HOH:O	2.19	0.54
1:J:150:LYS:HB3	1:J:165:ILE:HD11	1.89	0.54
1:J:208:ALA:HB1	7:J:610:HOH:O	2.06	0.54
1:B:220:GLU:OE2	7:B:625:HOH:O	2.17	0.54
1:A:112:ARG:NH1	1:A:169:ARG:O	2.41	0.54
1:E:234:ASP:OD1	7:E:631:HOH:O	2.19	0.54
1:L:291:ARG:CZ	1:L:338:GLY:HA3	2.38	0.54
1:G:279:LYS:HD3	1:G:342:ASP:OD1	2.07	0.53
1:I:95:ARG:NH2	1:L:145:GLU:OE2	2.38	0.53
1:L:255:ARG:NH2	1:L:299:GLU:OE1	2.42	0.53
1:I:234:ASP:HB3	1:I:242:VAL:HG22	1.90	0.53
1:A:357:GLN:HB2	7:A:610:HOH:O	2.07	0.53
1:K:299:GLU:HB2	7:K:614:HOH:O	2.08	0.53
1:I:179:LYS:HD2	1:I:198:TYR:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:196:ILE:HD12	1:I:204:ASP:HB3	1.90	0.53
1:I:117:CYS:HA	1:I:122:CYS:HA	1.91	0.52
1:J:138:LEU:O	7:J:622:HOH:O	2.19	0.52
1:J:341:LEU:HD23	1:J:347:TRP:HD1	1.74	0.52
1:G:175:PHE:N	7:G:615:HOH:O	2.12	0.52
1:G:314:ASP:OD1	1:G:315:PHE:N	2.41	0.52
1:F:189:ASP:OD1	1:F:190:ARG:N	2.42	0.52
1:I:348:THR:HG22	1:I:363:GLU:HB2	1.91	0.52
1:K:196:ILE:HD12	1:K:204:ASP:HB3	1.91	0.52
1:C:348:THR:HG22	1:C:363:GLU:HB2	1.91	0.52
1:D:88:LYS:HD3	1:D:434:PRO:HG3	1.89	0.52
1:H:111:ARG:NH1	1:H:146:GLU:OE1	2.39	0.52
1:F:372:GLU:CD	1:F:372:GLU:H	2.13	0.52
1:J:145:GLU:OE2	1:K:95:ARG:NH2	2.39	0.52
1:L:119:LEU:HA	1:L:396:LYS:O	2.09	0.52
1:C:279:LYS:NZ	1:C:343:GLU:OE2	2.28	0.52
1:F:396:LYS:NZ	7:F:604:HOH:O	2.32	0.52
1:H:166:LEU:HD11	1:H:197:LYS:HB2	1.92	0.52
1:A:225:GLU:OE2	1:A:298:LYS:NZ	2.31	0.52
1:D:226:GLY:O	1:D:249:GLN:HG3	2.09	0.52
1:G:111:ARG:NH2	1:G:141:SER:HB3	2.25	0.52
1:L:168:GLY:HA2	1:L:186:ASN:HD21	1.75	0.52
1:B:183:LEU:HD21	1:B:248:LEU:HD11	1.92	0.52
1:G:98:PRO:HB3	1:G:416:THR:HG21	1.92	0.52
1:J:112:ARG:NH1	1:J:169:ARG:O	2.43	0.52
1:L:223:CYS:HA	1:L:228:CYS:HA	1.90	0.52
1:D:432:ASN:OD1	1:D:432:ASN:N	2.43	0.51
1:F:111:ARG:HH22	1:F:142:MET:H	1.58	0.51
1:G:179:LYS:HD2	1:G:198:TYR:CE2	2.45	0.51
1:H:341:LEU:HB3	1:H:347:TRP:HB2	1.92	0.51
1:J:165:ILE:HG21	1:J:182:VAL:HG11	1.91	0.51
1:C:143:GLU:HG2	1:C:169:ARG:HH11	1.75	0.51
1:G:217:PRO:HB2	1:G:269:SER:O	2.11	0.51
1:J:107:LEU:HD23	1:J:158:THR:HG22	1.91	0.51
1:B:197:LYS:HE2	1:B:200:GLU:HA	1.92	0.51
1:G:341:LEU:HD23	1:G:347:TRP:HD1	1.74	0.51
1:C:198:TYR:HB2	1:C:251:GLY:HA3	1.92	0.51
1:H:77:TYR:CE1	1:H:178:LEU:HD13	2.46	0.51
1:J:135:GLN:HG2	1:J:136:HIS:ND1	2.26	0.51
1:L:183:LEU:HD21	1:L:248:LEU:HD11	1.93	0.51
1:B:222:ILE:HG21	1:B:273:THR:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:292:PRO:HG3	7:J:606:HOH:O	2.11	0.51
1:K:98:PRO:HB3	1:K:416:THR:HG21	1.92	0.51
1:A:139:ASN:OD1	1:A:139:ASN:N	2.44	0.50
1:D:364:GLN:OE1	1:D:376:SER:OG	2.26	0.50
1:E:345:PRO:HB3	1:E:366:PRO:HA	1.92	0.50
1:J:348:THR:HG22	1:J:363:GLU:HB2	1.93	0.50
1:K:146:GLU:OE2	1:K:169:ARG:NH1	2.45	0.50
1:C:193:PHE:HA	1:C:214:LEU:HD12	1.94	0.50
1:F:139:ASN:O	1:F:142:MET:HG3	2.11	0.50
1:E:208:ALA:HB1	7:E:631:HOH:O	2.11	0.50
1:G:111:ARG:NH1	1:G:146:GLU:OE1	2.44	0.50
1:K:314:ASP:OD1	1:K:315:PHE:N	2.43	0.50
1:H:255:ARG:NH2	1:H:298:LYS:O	2.44	0.50
1:A:107:LEU:HD23	1:A:158:THR:HG22	1.94	0.50
1:A:193:PHE:HA	1:A:214:LEU:HD12	1.94	0.50
1:B:150:LYS:HB3	1:B:165:ILE:HD11	1.93	0.50
1:G:179:LYS:HD3	1:G:199:GLY:HA3	1.94	0.50
1:J:234:ASP:HB3	1:J:242:VAL:HG22	1.94	0.50
1:L:380:GLU:OE1	1:L:383:SER:OG	2.15	0.50
1:D:207:SER:O	7:D:632:HOH:O	2.20	0.50
1:J:234:ASP:OD1	1:J:235:GLY:N	2.42	0.50
1:K:217:PRO:HB2	1:K:269:SER:O	2.12	0.50
5:L:502:NAG:O6	5:L:502:NAG:O4	2.30	0.50
1:H:107:LEU:HD23	1:H:158:THR:HG22	1.94	0.49
1:J:373:GLY:N	7:J:625:HOH:O	1.90	0.49
1:L:234:ASP:OD1	1:L:235:GLY:N	2.43	0.49
1:D:186:ASN:ND2	7:D:641:HOH:O	2.25	0.49
1:E:100:GLY:HA3	1:H:134:ASN:ND2	2.27	0.49
5:D:503:NAG:H61	5:D:504:NAG:H82	1.94	0.49
1:F:364:GLN:OE1	1:F:376:SER:OG	2.27	0.49
1:G:257:LYS:HB2	1:G:300:LEU:HD13	1.95	0.49
1:I:193:PHE:HA	1:I:214:LEU:HD12	1.93	0.49
1:J:291:ARG:NH2	1:J:336:ILE:O	2.45	0.49
1:J:364:GLN:OE1	1:J:376:SER:OG	2.30	0.49
1:J:87:VAL:HG11	1:J:90:TRP:CZ2	2.48	0.49
1:J:126:PHE:HE1	1:J:151:THR:HG1	1.58	0.49
1:B:98:PRO:HB3	1:B:416:THR:HG21	1.94	0.49
1:D:357:GLN:OE1	1:D:386:ARG:NH2	2.45	0.49
1:H:134:ASN:O	1:H:138:LEU:HG	2.13	0.49
1:B:111:ARG:HH21	1:B:141:SER:HB3	1.77	0.49
1:B:119:LEU:HA	1:B:396:LYS:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:210:ARG:NH2	1:F:258:GLN:HE22	2.10	0.49
1:I:276:ASN:N	1:I:276:ASN:OD1	2.46	0.49
1:C:112:ARG:NH1	1:C:169:ARG:O	2.46	0.49
1:J:314:ASP:OD1	1:J:315:PHE:N	2.44	0.49
1:L:439:ASN:OD1	1:L:441:ASP:HB2	2.13	0.49
1:G:396:LYS:NZ	7:G:615:HOH:O	2.45	0.48
1:I:139:ASN:OD1	7:I:609:HOH:O	2.20	0.48
1:K:209:SER:HB3	1:K:210:ARG:NH2	2.28	0.48
1:E:234:ASP:OD1	1:E:235:GLY:N	2.45	0.48
1:J:341:LEU:HD23	1:J:347:TRP:CD1	2.48	0.48
1:L:234:ASP:HB3	1:L:242:VAL:HG22	1.95	0.48
1:A:411:GLU:OE1	7:A:632:HOH:O	2.20	0.48
1:H:111:ARG:NH2	1:H:142:MET:H	2.09	0.48
1:B:140:THR:HA	1:B:141:SER:HA	1.58	0.48
1:C:111:ARG:HH22	1:C:142:MET:H	1.62	0.48
1:F:112:ARG:NH1	1:F:169:ARG:O	2.47	0.48
1:J:140:THR:HA	1:J:141:SER:HA	1.61	0.48
1:L:210:ARG:HG3	1:L:242:VAL:HG21	1.95	0.48
1:L:222:ILE:O	1:L:229:PHE:N	2.42	0.48
1:H:234:ASP:OD1	1:H:235:GLY:N	2.45	0.48
1:J:98:PRO:HB3	1:J:416:THR:HG21	1.96	0.48
1:D:258:GLN:H	1:I:240:GLN:NE2	2.12	0.48
1:B:190:ARG:HG3	1:B:211:GLY:HA2	1.95	0.48
1:H:140:THR:HA	1:H:141:SER:HA	1.60	0.48
1:F:183:LEU:HD21	1:F:248:LEU:HD11	1.96	0.48
1:K:122:CYS:HB2	1:K:153:ILE:HG21	1.96	0.48
1:K:144:TRP:O	1:K:169:ARG:NH2	2.42	0.48
1:L:118:ASP:OD1	1:L:121:SER:N	2.28	0.48
1:E:119:LEU:HA	1:E:396:LYS:O	2.14	0.47
1:J:116:SER:HB3	1:J:125:PHE:CE1	2.49	0.47
1:L:243:HIS:CD2	1:L:261:THR:HG21	2.49	0.47
1:E:341:LEU:HB3	1:E:347:TRP:HB2	1.96	0.47
1:F:107:LEU:HD23	1:F:158:THR:HG22	1.94	0.47
1:F:348:THR:HG22	1:F:363:GLU:HB2	1.95	0.47
1:H:150:LYS:HB3	1:H:165:ILE:HD11	1.96	0.47
1:K:279:LYS:HD3	1:K:342:ASP:OD1	2.14	0.47
1:B:217:PRO:HB2	1:B:269:SER:O	2.14	0.47
1:C:98:PRO:HB3	1:C:416:THR:HG21	1.95	0.47
1:F:384:ASN:ND2	7:F:615:HOH:O	2.47	0.47
1:I:202:VAL:HG11	1:J:91:VAL:HG21	1.95	0.47
1:D:234:ASP:OD1	1:D:235:GLY:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:ARG:NH2	1:E:385:LYS:HE3	2.29	0.47
1:F:145:GLU:OE2	1:G:95:ARG:NH2	2.38	0.47
1:J:79:ARG:N	7:J:618:HOH:O	2.47	0.47
1:J:290:LYS:NZ	1:J:324:SER:O	2.48	0.47
7:B:637:HOH:O	3:N:2:NAG:N2	2.35	0.47
1:D:96:GLY:N	1:D:424:GLU:OE2	2.34	0.47
1:E:193:PHE:HA	1:E:214:LEU:HD12	1.96	0.47
1:K:257:LYS:HZ1	1:K:302:TYR:HE1	1.63	0.47
1:K:369:ILE:HG22	7:K:611:HOH:O	2.13	0.47
1:C:144:TRP:O	1:C:169:ARG:NH2	2.33	0.47
1:C:164:MET:HB3	1:D:154:GLY:HA2	1.96	0.47
1:A:111:ARG:HH22	1:A:142:MET:H	1.62	0.47
1:A:417:VAL:HG11	1:A:422:ILE:HG12	1.96	0.47
1:C:140:THR:HA	1:C:141:SER:HA	1.52	0.47
1:C:146:GLU:OE2	1:C:169:ARG:HG3	2.15	0.47
1:D:244:ARG:HD3	1:D:256:TRP:CE3	2.49	0.47
1:D:260:ASN:ND2	1:D:262:THR:OG1	2.44	0.47
1:E:348:THR:HG22	1:E:363:GLU:HB2	1.95	0.47
3:P:1:NAG:H61	3:P:3:FUL:O2	2.15	0.47
1:B:234:ASP:OD1	1:B:235:GLY:N	2.44	0.47
1:F:317:ARG:NH1	7:F:606:HOH:O	2.44	0.47
1:K:111:ARG:NH1	1:K:142:MET:O	2.44	0.47
1:K:140:THR:HA	1:K:141:SER:HA	1.55	0.47
1:K:341:LEU:HD23	1:K:347:TRP:CD1	2.50	0.47
1:K:364:GLN:OE1	1:K:376:SER:OG	2.32	0.47
1:D:118:ASP:OD1	1:D:121:SER:N	2.34	0.47
1:H:417:VAL:HG11	1:H:422:ILE:HG12	1.97	0.47
1:K:293:LEU:HD21	1:K:369:ILE:HG21	1.97	0.47
1:H:139:ASN:OD1	1:H:139:ASN:N	2.48	0.47
1:I:82:SER:O	1:I:275:ASN:HB2	2.15	0.47
1:K:288:ASP:OD1	1:K:328:ALA:N	2.47	0.47
1:L:314:ASP:OD1	1:L:315:PHE:N	2.48	0.47
1:E:145:GLU:OE2	1:F:95:ARG:NH2	2.26	0.46
1:E:234:ASP:HB3	1:E:242:VAL:HG22	1.96	0.46
1:I:145:GLU:OE2	1:J:95:ARG:NH2	2.32	0.46
1:L:143:GLU:HG2	1:L:169:ARG:NH1	2.30	0.46
1:I:150:LYS:HB3	1:I:165:ILE:HD11	1.97	0.46
1:L:210:ARG:CZ	1:L:244:ARG:HH21	2.27	0.46
1:J:117:CYS:HA	1:J:122:CYS:HA	1.97	0.46
1:L:117:CYS:HA	1:L:122:CYS:HA	1.97	0.46
1:K:341:LEU:HD23	1:K:347:TRP:HD1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:398:ASP:OD2	1:K:405:ARG:NH1	2.48	0.46
1:B:81:LYS:NZ	1:B:398:ASP:O	2.47	0.46
1:D:239:ASN:HD21	5:D:502:NAG:C1	2.29	0.46
1:E:339:PHE:HB2	1:E:392:PHE:CE2	2.50	0.46
1:E:432:ASN:OD1	1:E:432:ASN:N	2.49	0.46
1:G:341:LEU:HB3	1:G:347:TRP:HB2	1.97	0.46
1:H:183:LEU:HD21	1:H:248:LEU:HD11	1.96	0.46
1:J:398:ASP:OD2	1:J:405:ARG:HD3	2.16	0.46
1:K:438:ILE:HD13	1:K:440:TRP:CZ2	2.51	0.46
1:L:142:MET:HB3	1:L:144:TRP:CD1	2.51	0.46
1:A:210:ARG:HG3	1:A:242:VAL:HG21	1.98	0.46
1:D:275:ASN:ND2	1:D:275:ASN:O	2.49	0.46
1:K:309:ASN:OD1	1:K:373:GLY:HA3	2.15	0.46
1:L:308:CYS:HB2	1:L:371:SER:O	2.16	0.46
1:E:84:MET:HG2	1:E:274:ILE:HG13	1.97	0.46
1:D:132:SER:O	1:D:135:GLN:HB2	2.16	0.46
1:K:317:ARG:O	1:K:331:LYS:HD2	2.16	0.46
1:K:405:ARG:HH21	1:K:429:CYS:HB3	1.81	0.46
1:D:217:PRO:HB2	1:D:269:SER:O	2.15	0.46
1:F:222:ILE:HG21	1:F:273:THR:HB	1.97	0.46
1:I:134:ASN:HA	1:I:137:LEU:HD12	1.97	0.46
1:B:110:SER:HB2	1:B:126:PHE:HB2	1.97	0.45
1:J:119:LEU:HA	1:J:396:LYS:O	2.16	0.45
1:L:190:ARG:HG3	1:L:211:GLY:O	2.16	0.45
1:C:139:ASN:O	1:C:142:MET:HG3	2.15	0.45
1:D:139:ASN:OD1	1:D:139:ASN:N	2.49	0.45
1:G:234:ASP:OD1	1:G:235:GLY:N	2.48	0.45
1:B:244:ARG:HD3	1:B:256:TRP:CD1	2.51	0.45
1:D:210:ARG:NH2	1:D:258:GLN:HE22	2.15	0.45
1:A:400:ILE:HG22	1:D:201:GLU:OE1	2.16	0.45
1:A:432:ASN:OD1	1:A:432:ASN:N	2.47	0.45
1:C:175:PHE:N	7:C:601:HOH:O	2.36	0.45
1:A:136:HIS:CD2	1:E:136:HIS:CD2	3.05	0.45
1:C:189:ASP:OD1	1:C:190:ARG:N	2.50	0.45
1:D:98:PRO:HB3	1:D:416:THR:HG21	1.99	0.45
1:D:367:ASN:N	7:D:636:HOH:O	2.50	0.45
1:F:119:LEU:HA	1:F:396:LYS:O	2.17	0.45
1:G:126:PHE:HE1	1:G:151:THR:HG1	1.63	0.45
1:J:145:GLU:OE1	1:K:98:PRO:HG3	2.17	0.45
1:L:111:ARG:NH2	1:L:141:SER:OG	2.49	0.45
1:A:234:ASP:OD1	1:A:235:GLY:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:ILE:HG21	1:D:273:THR:HB	1.98	0.45
1:F:98:PRO:HB3	1:F:416:THR:HG21	1.97	0.45
1:C:314:ASP:OD1	1:C:315:PHE:N	2.49	0.45
1:D:212:GLY:O	7:D:646:HOH:O	2.21	0.45
1:F:134:ASN:ND2	1:G:100:GLY:HA3	2.32	0.45
1:G:146:GLU:OE2	1:G:169:ARG:HG3	2.17	0.45
1:I:100:GLY:HA3	1:L:134:ASN:ND2	2.32	0.45
1:J:96:GLY:N	1:J:424:GLU:OE2	2.39	0.45
1:J:138:LEU:HD13	1:J:142:MET:SD	2.57	0.45
1:J:146:GLU:OE2	1:J:169:ARG:HG3	2.16	0.45
1:J:234:ASP:HB3	1:J:242:VAL:CG2	2.47	0.45
1:A:100:GLY:HA3	1:D:134:ASN:ND2	2.32	0.45
1:I:314:ASP:OD1	1:I:315:PHE:N	2.50	0.45
1:J:111:ARG:NH1	1:J:142:MET:O	2.44	0.45
1:L:290:LYS:HE3	1:L:328:ALA:HB2	1.97	0.45
1:L:150:LYS:HB3	1:L:165:ILE:HD11	1.99	0.45
1:A:389:ARG:NH1	1:A:411:GLU:OE1	2.44	0.45
1:G:432:ASN:OD1	1:G:432:ASN:N	2.46	0.45
1:I:198:TYR:HB2	1:I:251:GLY:HA3	1.98	0.45
1:I:317:ARG:NH2	1:I:351:THR:OG1	2.47	0.45
1:I:432:ASN:OD1	1:I:432:ASN:N	2.48	0.45
1:K:279:LYS:NZ	1:K:342:ASP:O	2.44	0.45
1:L:122:CYS:HB2	1:L:153:ILE:HG21	1.98	0.45
1:K:252:THR:OG1	7:K:604:HOH:O	2.21	0.44
1:L:346:ALA:HB3	1:L:365:ILE:HB	1.99	0.44
1:A:198:TYR:HB2	1:A:251:GLY:HA3	1.98	0.44
1:G:341:LEU:HD23	1:G:347:TRP:CD1	2.52	0.44
1:C:386:ARG:NH1	7:C:638:HOH:O	2.51	0.44
1:F:234:ASP:OD1	1:F:235:GLY:N	2.44	0.44
1:C:234:ASP:OD1	1:C:235:GLY:N	2.45	0.44
1:G:117:CYS:HA	1:G:122:CYS:HA	1.99	0.44
1:C:432:ASN:OD1	1:C:432:ASN:N	2.46	0.44
1:G:222:ILE:HG21	1:G:273:THR:HB	2.00	0.44
1:J:313:THR:HG22	1:J:350:LYS:HD3	2.00	0.44
1:E:278:ILE:HD13	1:E:296:PHE:CE2	2.53	0.44
1:J:217:PRO:HB2	1:J:269:SER:O	2.17	0.44
1:A:111:ARG:NH1	1:A:146:GLU:OE1	2.46	0.44
1:K:341:LEU:HB3	1:K:347:TRP:HB2	2.00	0.44
1:D:143:GLU:O	1:D:188:ARG:NH2	2.51	0.44
1:J:198:TYR:HB3	1:J:203:THR:HG21	2.00	0.44
1:L:197:LYS:HE2	1:L:200:GLU:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ILE:O	3:N:3:FUL:H62	2.18	0.44
1:C:190:ARG:H	1:C:190:ARG:HG3	1.33	0.43
1:D:144:TRP:O	1:D:169:ARG:NH2	2.44	0.43
1:J:229:PHE:CE2	1:J:300:LEU:HD21	2.53	0.43
1:L:140:THR:HA	1:L:141:SER:HA	1.40	0.43
1:L:212:GLY:HA3	1:L:235:GLY:C	2.38	0.43
1:A:96:GLY:N	1:A:424:GLU:OE2	2.43	0.43
1:A:150:LYS:HB3	1:A:165:ILE:HD11	2.00	0.43
1:D:183:LEU:HD21	1:D:248:LEU:HD11	2.00	0.43
1:B:220:GLU:HG2	1:B:221:CYS:O	2.18	0.43
1:I:144:TRP:HA	1:I:144:TRP:CE3	2.52	0.43
1:A:140:THR:HA	1:A:141:SER:HA	1.54	0.43
1:E:140:THR:HA	1:E:141:SER:HA	1.46	0.43
1:B:159:LEU:HD13	1:C:107:LEU:HD21	2.00	0.43
1:G:197:LYS:HE2	1:G:200:GLU:HA	2.00	0.43
1:H:117:CYS:HA	1:H:122:CYS:HA	2.01	0.43
1:K:146:GLU:OE2	1:K:169:ARG:HG3	2.18	0.43
1:K:291:ARG:HA	1:K:292:PRO:HD2	1.88	0.43
1:L:265:ASN:HB3	1:L:284:ASN:OD1	2.19	0.43
1:E:84:MET:HE3	1:E:84:MET:HB3	1.93	0.43
1:K:278:ILE:HD13	1:K:296:PHE:CE2	2.54	0.43
1:L:243:HIS:HD2	1:L:261:THR:HG21	1.82	0.43
1:C:145:GLU:OE2	1:D:95:ARG:NH2	2.32	0.43
1:K:116:SER:OG	1:K:220:GLU:HG3	2.18	0.43
1:L:432:ASN:N	1:L:432:ASN:OD1	2.46	0.43
1:A:117:CYS:HA	1:A:122:CYS:HA	2.00	0.43
1:C:143:GLU:HG2	1:C:169:ARG:NH1	2.34	0.43
1:H:112:ARG:HD3	1:H:218:ASN:ND2	2.34	0.43
1:F:146:GLU:OE2	1:F:169:ARG:HG3	2.19	0.43
1:F:423:GLN:OE1	7:F:621:HOH:O	2.21	0.43
1:G:198:TYR:HB2	1:G:251:GLY:HA3	2.01	0.43
1:L:186:ASN:O	1:L:192:SER:HA	2.18	0.43
1:E:111:ARG:HH22	1:E:142:MET:H	1.67	0.43
1:J:274:ILE:HD13	1:J:274:ILE:HA	1.92	0.43
1:K:134:ASN:HA	1:K:137:LEU:HD12	2.00	0.43
1:L:244:ARG:HD3	1:L:256:TRP:CE3	2.53	0.43
1:A:134:ASN:ND2	1:B:100:GLY:HA3	2.34	0.42
1:D:291:ARG:CZ	1:D:338:GLY:HA3	2.48	0.42
1:L:119:LEU:HD23	1:L:396:LYS:O	2.19	0.42
1:C:120:THR:OG1	7:C:640:HOH:O	2.20	0.42
1:G:348:THR:HG22	1:G:363:GLU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:274:ILE:HD13	1:I:274:ILE:HA	1.93	0.42
1:A:107:LEU:HD21	1:D:159:LEU:HD13	2.02	0.42
1:A:257:LYS:HB2	1:A:300:LEU:HD13	2.00	0.42
1:C:77:TYR:CE1	1:C:178:LEU:HD13	2.54	0.42
1:E:314:ASP:OD1	1:E:315:PHE:N	2.52	0.42
1:G:139:ASN:OD1	1:G:139:ASN:N	2.51	0.42
1:G:220:GLU:O	7:G:623:HOH:O	2.22	0.42
1:D:146:GLU:OE2	1:D:169:ARG:HG3	2.20	0.42
1:L:143:GLU:HG2	1:L:169:ARG:HH12	1.84	0.42
1:C:339:PHE:HB2	1:C:392:PHE:CE2	2.55	0.42
1:I:144:TRP:HA	1:I:144:TRP:HE3	1.84	0.42
1:I:193:PHE:HE1	1:J:438:ILE:HG21	1.85	0.42
1:D:190:ARG:H	1:D:190:ARG:HG3	1.57	0.42
1:I:255:ARG:HH22	1:I:299:GLU:HA	1.84	0.42
1:K:107:LEU:HB2	1:K:132:SER:HB3	2.02	0.42
1:L:309:ASN:OD1	1:L:310:GLY:N	2.49	0.42
1:B:107:LEU:HD23	1:B:158:THR:HG22	2.02	0.42
1:C:77:TYR:CD1	1:C:178:LEU:HD13	2.55	0.42
1:C:179:LYS:HD2	1:C:198:TYR:CE2	2.55	0.42
1:E:96:GLY:N	1:E:424:GLU:OE2	2.49	0.42
1:E:341:LEU:HD23	1:E:347:TRP:CD1	2.54	0.42
1:F:77:TYR:CE1	1:F:178:LEU:HD13	2.55	0.42
1:G:259:LEU:HB2	1:G:261:THR:HG23	2.01	0.42
1:H:314:ASP:OD1	1:H:315:PHE:N	2.53	0.42
1:K:81:LYS:HD2	1:K:402:GLY:O	2.19	0.42
1:G:278:ILE:HD13	1:G:296:PHE:CE2	2.55	0.42
1:F:193:PHE:HA	1:F:214:LEU:HD12	2.01	0.42
1:L:308:CYS:HA	1:L:325:CYS:HA	2.01	0.42
1:D:337:GLN:OE1	1:D:389:ARG:NH2	2.53	0.42
1:G:87:VAL:HG11	1:G:90:TRP:CZ2	2.55	0.42
1:K:200:GLU:N	7:K:602:HOH:O	2.37	0.42
1:L:139:ASN:OD1	1:L:139:ASN:N	2.52	0.42
1:L:225:GLU:OE2	1:L:298:LYS:NZ	2.32	0.42
1:B:127:ILE:CG2	1:B:146:GLU:HB3	2.50	0.41
1:B:239:ASN:OD1	1:B:240:GLN:HG2	2.20	0.41
1:B:383:SER:OG	1:B:439:ASN:ND2	2.53	0.41
1:F:179:LYS:HD2	1:F:198:TYR:CE2	2.55	0.41
1:I:134:ASN:ND2	1:J:100:GLY:HA3	2.34	0.41
1:I:210:ARG:HG3	1:I:242:VAL:HG21	2.02	0.41
1:L:313:THR:HB	1:L:349:SER:O	2.20	0.41
1:I:293:LEU:HD21	1:I:369:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:301:ASN:ND2	7:K:614:HOH:O	2.49	0.41
1:C:96:GLY:N	1:C:424:GLU:OE2	2.52	0.41
1:D:84:MET:CG	1:D:274:ILE:HG13	2.49	0.41
1:E:247:GLU:OE1	1:E:255:ARG:NE	2.45	0.41
1:E:341:LEU:HD23	1:E:347:TRP:HD1	1.85	0.41
1:E:400:ILE:HG21	1:H:203:THR:HG22	2.02	0.41
1:F:145:GLU:HG2	1:G:98:PRO:HD3	2.02	0.41
1:H:417:VAL:HG21	1:H:422:ILE:HG13	2.01	0.41
1:I:79:ARG:HG3	1:I:80:ALA:O	2.20	0.41
1:A:222:ILE:O	1:A:229:PHE:N	2.47	0.41
1:C:111:ARG:HH21	1:C:141:SER:HB3	1.86	0.41
1:E:198:TYR:HB2	1:E:251:GLY:HA3	2.00	0.41
1:E:291:ARG:CZ	1:E:338:GLY:HA3	2.50	0.41
1:G:113:ALA:HA	1:G:125:PHE:O	2.20	0.41
1:I:159:LEU:HD13	1:J:107:LEU:HD21	2.02	0.41
1:I:217:PRO:HB2	1:I:269:SER:O	2.21	0.41
1:K:201:GLU:OE2	1:L:400:ILE:HG22	2.20	0.41
1:L:386:ARG:HD3	1:L:413:GLU:OE1	2.20	0.41
1:A:217:PRO:HB2	1:A:269:SER:O	2.21	0.41
1:B:274:ILE:HD13	1:B:274:ILE:HA	1.91	0.41
1:C:291:ARG:N	7:C:602:HOH:O	2.34	0.41
1:D:398:ASP:CG	1:D:405:ARG:HH11	2.23	0.41
1:F:140:THR:HA	1:F:141:SER:HA	1.43	0.41
1:A:339:PHE:HB2	1:A:392:PHE:CE2	2.56	0.41
1:B:291:ARG:NH1	7:B:636:HOH:O	2.54	0.41
1:I:240:GLN:OE1	7:I:607:HOH:O	2.22	0.41
1:K:264:ILE:HG22	1:K:327:MET:SD	2.61	0.41
1:L:104:PRO:HG2	1:L:107:LEU:HG	2.03	0.41
1:B:77:TYR:HD1	1:B:77:TYR:HA	1.72	0.41
1:C:139:ASN:N	1:C:139:ASN:OD1	2.53	0.41
1:E:112:ARG:NH1	1:E:169:ARG:O	2.54	0.41
1:G:140:THR:HA	1:G:141:SER:HA	1.42	0.41
1:G:339:PHE:HB2	1:G:392:PHE:CE2	2.56	0.41
1:H:267:GLU:HG3	1:H:285:LEU:HD12	2.03	0.41
1:H:309:ASN:OD1	1:H:373:GLY:HA3	2.19	0.41
1:I:210:ARG:NH2	1:I:258:GLN:HE22	2.19	0.41
1:C:127:ILE:CG2	1:C:146:GLU:HB3	2.51	0.41
1:D:140:THR:HA	1:D:141:SER:HA	1.49	0.41
1:G:195:MET:SD	1:H:91:VAL:HB	2.60	0.41
1:H:222:ILE:O	1:H:229:PHE:N	2.43	0.41
1:H:401:SER:HB2	1:H:403:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:116:SER:HB3	1:L:125:PHE:CE1	2.56	0.41
1:E:146:GLU:OE2	1:E:169:ARG:HG3	2.21	0.41
1:J:210:ARG:HE	1:J:244:ARG:NH2	2.19	0.41
1:K:339:PHE:HB2	1:K:392:PHE:CE2	2.56	0.41
1:B:121:SER:HB2	7:B:650:HOH:O	2.20	0.41
1:B:139:ASN:OD1	1:B:139:ASN:N	2.53	0.41
1:D:244:ARG:HG2	1:D:258:GLN:HA	2.03	0.41
1:F:84:MET:CG	1:F:274:ILE:HG13	2.49	0.41
1:K:245:ILE:HB	1:K:257:LYS:HB3	2.02	0.41
1:L:291:ARG:NH2	1:L:338:GLY:HA3	2.35	0.41
1:A:77:TYR:CE1	1:A:178:LEU:HD13	2.55	0.40
1:A:372:GLU:HG2	1:A:374:THR:HG23	2.03	0.40
1:E:308:CYS:HA	1:E:325:CYS:HA	2.03	0.40
1:J:198:TYR:CZ	1:J:250:ASN:HA	2.55	0.40
1:A:111:ARG:NH1	1:A:142:MET:O	2.48	0.40
1:A:234:ASP:HB3	1:A:242:VAL:HG22	2.02	0.40
1:F:159:LEU:HD13	1:G:107:LEU:HD21	2.03	0.40
1:F:279:LYS:HD3	1:F:342:ASP:OD1	2.21	0.40
1:L:291:ARG:HA	1:L:292:PRO:HD2	1.87	0.40
1:B:267:GLU:HG3	1:B:285:LEU:HD12	2.03	0.40
1:B:314:ASP:OD1	1:B:315:PHE:N	2.55	0.40
1:C:134:ASN:ND2	1:D:100:GLY:HA3	2.36	0.40
1:J:210:ARG:HG3	1:J:242:VAL:HG21	2.03	0.40
1:J:389:ARG:HD3	1:J:411:GLU:OE1	2.20	0.40
1:K:308:CYS:HA	1:K:324:SER:O	2.21	0.40
1:L:395:PRO:HG2	1:L:405:ARG:NH1	2.37	0.40
1:A:313:THR:HG21	1:A:348:THR:OG1	2.21	0.40
1:A:341:LEU:HD23	1:A:347:TRP:HD1	1.86	0.40
1:B:341:LEU:HB3	1:B:347:TRP:HB2	2.04	0.40
1:D:190:ARG:NH2	1:I:144:TRP:HZ3	2.17	0.40
1:K:223:CYS:HA	1:K:227:SER:O	2.22	0.40
1:B:344:LYS:HE3	1:B:344:LYS:HB3	1.88	0.40
1:C:234:ASP:HB3	1:C:242:VAL:HG22	2.03	0.40
1:H:87:VAL:HG11	1:H:90:TRP:CZ2	2.56	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLN:OE1	1:G:88:LYS:NZ[1_455]	2.12	0.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LYS:NZ	1:F:254:GLN:O[1_455]	2.15	0.05
1:B:299:GLU:OE2	2:O:2:FUC:O3[1_545]	2.15	0.05
1:C:88:LYS:NZ	1:E:254:GLN:OE1[1_545]	2.17	0.03
1:B:254:GLN:O	1:E:257:LYS:NZ[1_545]	2.19	0.01

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 X-ray entries followed by that with respect to entries of similar resolution.

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	363/378 (96%)	340 (94%)	22 (6%)	1 (0%)	37	56
1	B	363/378 (96%)	339 (93%)	22 (6%)	2 (1%)	22	39
1	C	363/378 (96%)	342 (94%)	20 (6%)	1 (0%)	37	56
1	D	363/378 (96%)	344 (95%)	18 (5%)	1 (0%)	37	56
1	E	363/378 (96%)	343 (94%)	19 (5%)	1 (0%)	37	56
1	F	363/378 (96%)	342 (94%)	20 (6%)	1 (0%)	37	56
1	G	363/378 (96%)	340 (94%)	22 (6%)	1 (0%)	37	56
1	H	363/378 (96%)	341 (94%)	21 (6%)	1 (0%)	37	56
1	I	363/378 (96%)	338 (93%)	24 (7%)	1 (0%)	37	56
1	J	361/378 (96%)	338 (94%)	21 (6%)	2 (1%)	22	39
1	K	362/378 (96%)	339 (94%)	22 (6%)	1 (0%)	37	56
1	L	363/378 (96%)	344 (95%)	18 (5%)	1 (0%)	37	56
All	All	4353/4536 (96%)	4090 (94%)	249 (6%)	14 (0%)	37	56

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	ASP
1	E	398	ASP
1	F	398	ASP

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Mol	Chain	Res	Type
1	B	398	ASP
1	C	398	ASP
1	G	398	ASP
1	H	398	ASP
1	J	398	ASP
1	K	398	ASP
1	D	398	ASP
1	I	398	ASP
1	L	398	ASP
1	J	345	PRO
1	B	397	GLY

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 X-ray entries followed by that with respect to entries of similar resolution.

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	318/327 (97%)	310 (98%)	8 (2%)	42	69
1	B	318/327 (97%)	308 (97%)	10 (3%)	35	62
1	C	318/327 (97%)	309 (97%)	9 (3%)	38	65
1	D	318/327 (97%)	307 (96%)	11 (4%)	31	57
1	E	318/327 (97%)	310 (98%)	8 (2%)	42	69
1	F	318/327 (97%)	308 (97%)	10 (3%)	35	62
1	G	318/327 (97%)	304 (96%)	14 (4%)	24	47
1	H	318/327 (97%)	310 (98%)	8 (2%)	42	69
1	I	318/327 (97%)	307 (96%)	11 (4%)	31	57
1	J	316/327 (97%)	308 (98%)	8 (2%)	42	69
1	K	317/327 (97%)	306 (96%)	11 (4%)	31	57
1	L	318/327 (97%)	311 (98%)	7 (2%)	47	73
All	All	3813/3924 (97%)	3698 (97%)	115 (3%)	36	63

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	209	SER
1	A	274	ILE
1	A	275	ASN
1	A	342	ASP
1	A	348	THR
1	A	361	VAL
1	A	387	THR
1	B	139	ASN
1	B	169	ARG
1	B	209	SER
1	B	274	ILE
1	B	275	ASN
1	B	333	GLU
1	B	348	THR
1	B	361	VAL
1	B	387	THR
1	B	400	ILE
1	C	139	ASN
1	C	189	ASP
1	C	209	SER
1	C	274	ILE
1	C	342	ASP
1	C	344	LYS
1	C	348	THR
1	C	361	VAL
1	C	387	THR
1	D	139	ASN
1	D	169	ARG
1	D	189	ASP
1	D	257	LYS
1	D	260	ASN
1	D	274	ILE
1	D	329	GLN
1	D	342	ASP
1	D	348	THR
1	D	361	VAL
1	D	387	THR
1	E	84	MET
1	E	139	ASN
1	E	274	ILE
1	E	342	ASP
1	E	348	THR

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Mol	Chain	Res	Type
1	E	361	VAL
1	E	387	THR
1	E	400	ILE
1	F	139	ASN
1	F	144	TRP
1	F	145	GLU
1	F	163	GLU
1	F	274	ILE
1	F	333	GLU
1	F	348	THR
1	F	361	VAL
1	F	387	THR
1	F	400	ILE
1	G	79	ARG
1	G	139	ASN
1	G	169	ARG
1	G	188	ARG
1	G	209	SER
1	G	257	LYS
1	G	274	ILE
1	G	301	ASN
1	G	344	LYS
1	G	348	THR
1	G	361	VAL
1	G	374	THR
1	G	387	THR
1	G	400	ILE
1	H	139	ASN
1	H	169	ARG
1	H	274	ILE
1	H	344	LYS
1	H	348	THR
1	H	361	VAL
1	H	387	THR
1	H	400	ILE
1	I	79	ARG
1	I	139	ASN
1	I	144	TRP
1	I	169	ARG
1	I	190	ARG
1	I	274	ILE
1	I	276	ASN

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Mol	Chain	Res	Type
1	I	344	LYS
1	I	348	THR
1	I	361	VAL
1	I	387	THR
1	J	139	ASN
1	J	163	GLU
1	J	274	ILE
1	J	344	LYS
1	J	348	THR
1	J	361	VAL
1	J	387	THR
1	J	400	ILE
1	K	84	MET
1	K	139	ASN
1	K	169	ARG
1	K	274	ILE
1	K	293	LEU
1	K	344	LYS
1	K	348	THR
1	K	361	VAL
1	K	387	THR
1	K	400	ILE
1	K	432	ASN
1	L	106	ASP
1	L	139	ASN
1	L	274	ILE
1	L	342	ASP
1	L	348	THR
1	L	361	VAL
1	L	387	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	HIS
1	A	258	GLN
1	B	250	ASN
1	C	136	HIS
1	D	260	ASN
1	D	275	ASN
1	E	136	HIS
1	F	250	ASN

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Mol	Chain	Res	Type
1	G	136	HIS
1	I	240	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 ⓘ

12 monosaccharides 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	$\#|Z| > 2$
2	NAG	M	1	1,2	14,14,15	0.50	0	17,19,21	1.00	1 (5%)
2	FUC	M	2	2	10,10,11	0.77	0	14,14,16	0.78	0
3	NAG	N	1	1,3	14,14,15	0.51	0	17,19,21	1.26	2 (11%)
3	NAG	N	2	3	14,14,15	0.43	0	17,19,21	1.69	4 (23%)
3	FUL	N	3	3	10,10,11	1.55	3 (30%)	14,14,16	1.54	3 (21%)
2	NAG	O	1	1,2	14,14,15	0.70	0	17,19,21	1.53	2 (11%)
2	FUC	O	2	2	10,10,11	0.90	0	14,14,16	0.74	0
3	NAG	P	1	1,3	14,14,15	0.48	0	17,19,21	1.33	2 (11%)
3	NAG	P	2	3	14,14,15	0.51	0	17,19,21	1.54	3 (17%)
3	FUL	P	3	3	10,10,11	1.45	2 (20%)	14,14,16	1.79	4 (28%)
2	NAG	Q	1	1,2	14,14,15	0.52	0	17,19,21	1.92	3 (17%)
2	FUC	Q	2	2	10,10,11	1.11	1 (10%)	14,14,16	0.61	0

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
2	NAG	M	1	1,2	-	2/6/23/26	0/1/1/1
2	FUC	M	2	2	-	-	0/1/1/1
3	NAG	N	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	N	2	3	-	3/6/23/26	0/1/1/1
3	FUL	N	3	3	-	-	0/1/1/1
2	NAG	O	1	1,2	-	1/6/23/26	0/1/1/1
2	FUC	O	2	2	-	-	0/1/1/1
3	NAG	P	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	P	2	3	-	4/6/23/26	0/1/1/1
3	FUL	P	3	3	-	-	0/1/1/1
2	NAG	Q	1	1,2	-	0/6/23/26	0/1/1/1
2	FUC	Q	2	2	-	-	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	3	FUL	C4-C5	2.75	1.58	1.52
3	P	3	FUL	C4-C5	2.47	1.58	1.52
2	Q	2	FUC	O5-C1	-2.44	1.39	1.43
3	N	3	FUL	O5-C5	2.37	1.48	1.43
3	N	3	FUL	C4-C3	2.12	1.57	1.52
3	P	3	FUL	C4-C3	2.04	1.57	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	1	NAG	C1-O5-C5	6.00	120.23	112.19
3	N	2	NAG	C1-O5-C5	4.21	117.83	112.19
3	P	3	FUL	O5-C5-C4	3.89	116.56	109.55
2	O	1	NAG	C4-C3-C2	3.57	116.25	111.02
3	P	1	NAG	O5-C5-C6	3.50	114.48	107.66
3	P	3	FUL	C3-C4-C5	3.48	115.10	109.81
2	M	1	NAG	C1-O5-C5	3.33	116.65	112.19
3	N	3	FUL	O5-C5-C4	3.32	115.53	109.55
3	P	2	NAG	C3-C4-C5	3.32	116.26	110.23
2	Q	1	NAG	O5-C1-C2	3.26	116.34	111.29
3	N	1	NAG	O5-C5-C6	3.03	113.57	107.66
3	P	3	FUL	O2-C2-C1	2.97	116.02	109.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	2	NAG	C4-C3-C2	2.95	115.34	111.02
3	P	2	NAG	C1-O5-C5	2.83	115.97	112.19
3	N	3	FUL	O2-C2-C1	2.69	115.39	109.22
3	P	1	NAG	C1-O5-C5	2.65	115.73	112.19
3	N	3	FUL	C3-C4-C5	2.64	113.83	109.81
3	N	1	NAG	C1-O5-C5	2.59	115.65	112.19
3	N	2	NAG	C3-C4-C5	2.53	114.81	110.23
3	N	2	NAG	C2-N2-C7	2.48	126.23	122.90
2	O	1	NAG	C3-C4-C5	2.46	114.70	110.23
2	Q	1	NAG	C6-C5-C4	-2.29	107.39	113.02
3	P	3	FUL	C1-O5-C5	2.18	118.10	112.97
3	N	2	NAG	O5-C5-C4	2.09	115.92	110.83

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	N	1	NAG	C8-C7-N2-C2
3	N	1	NAG	O7-C7-N2-C2
3	P	2	NAG	C8-C7-N2-C2
3	P	2	NAG	O7-C7-N2-C2
3	P	1	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
3	P	1	NAG	C8-C7-N2-C2
3	N	2	NAG	O5-C5-C6-O6
3	P	1	NAG	O7-C7-N2-C2
3	P	2	NAG	O5-C5-C6-O6
3	N	2	NAG	C3-C2-N2-C7
2	O	1	NAG	O5-C5-C6-O6
3	N	2	NAG	C1-C2-N2-C7
3	P	2	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 4 short contacts:

| Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	3	FUL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	3	FUL	1	0
2	O	2	FUC	0	1
3	N	2	NAG	1	0
3	P	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain M

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain O

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain Q

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain N

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain P

Bond lengths

Bond angles

Torsions

Rings
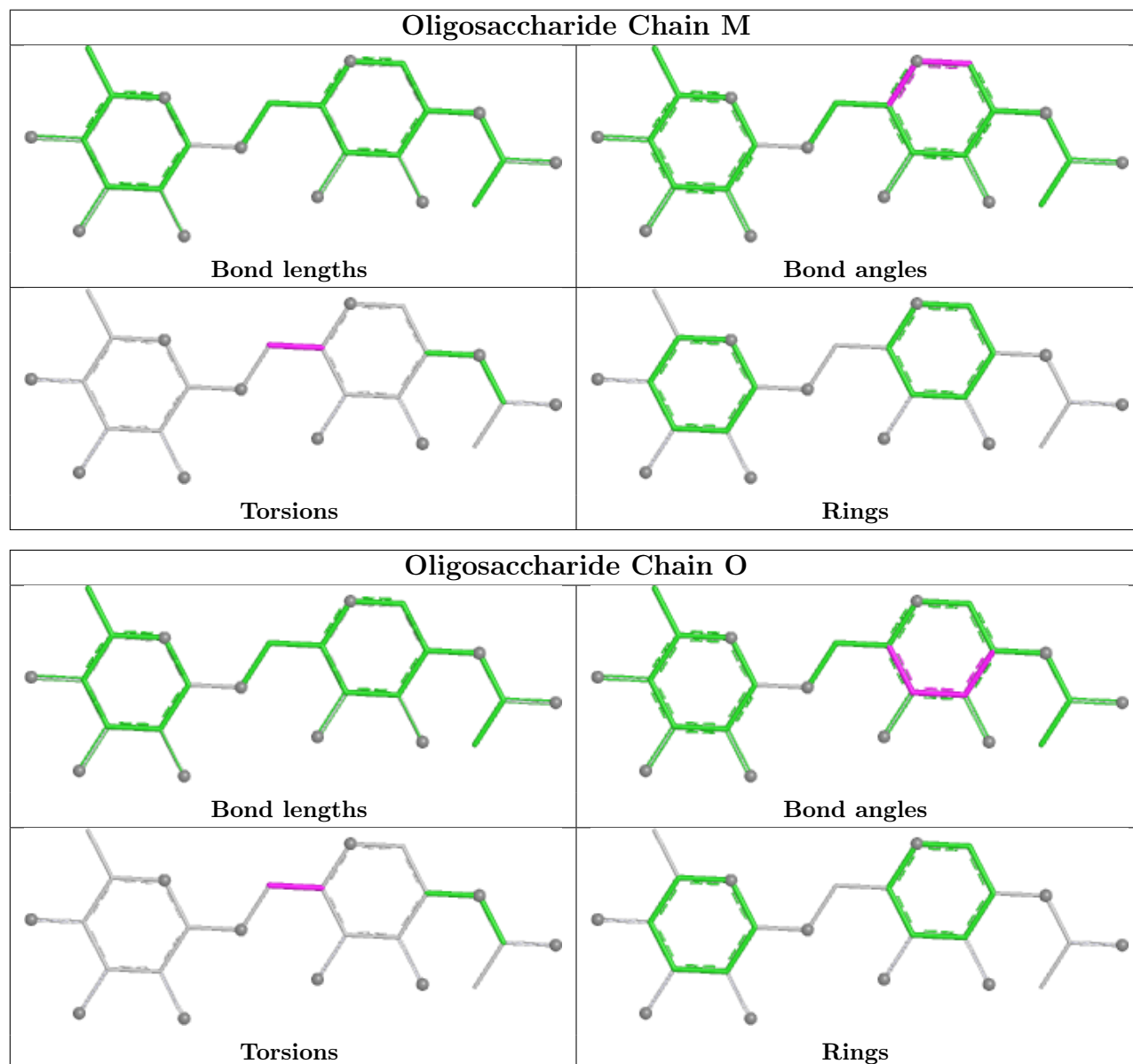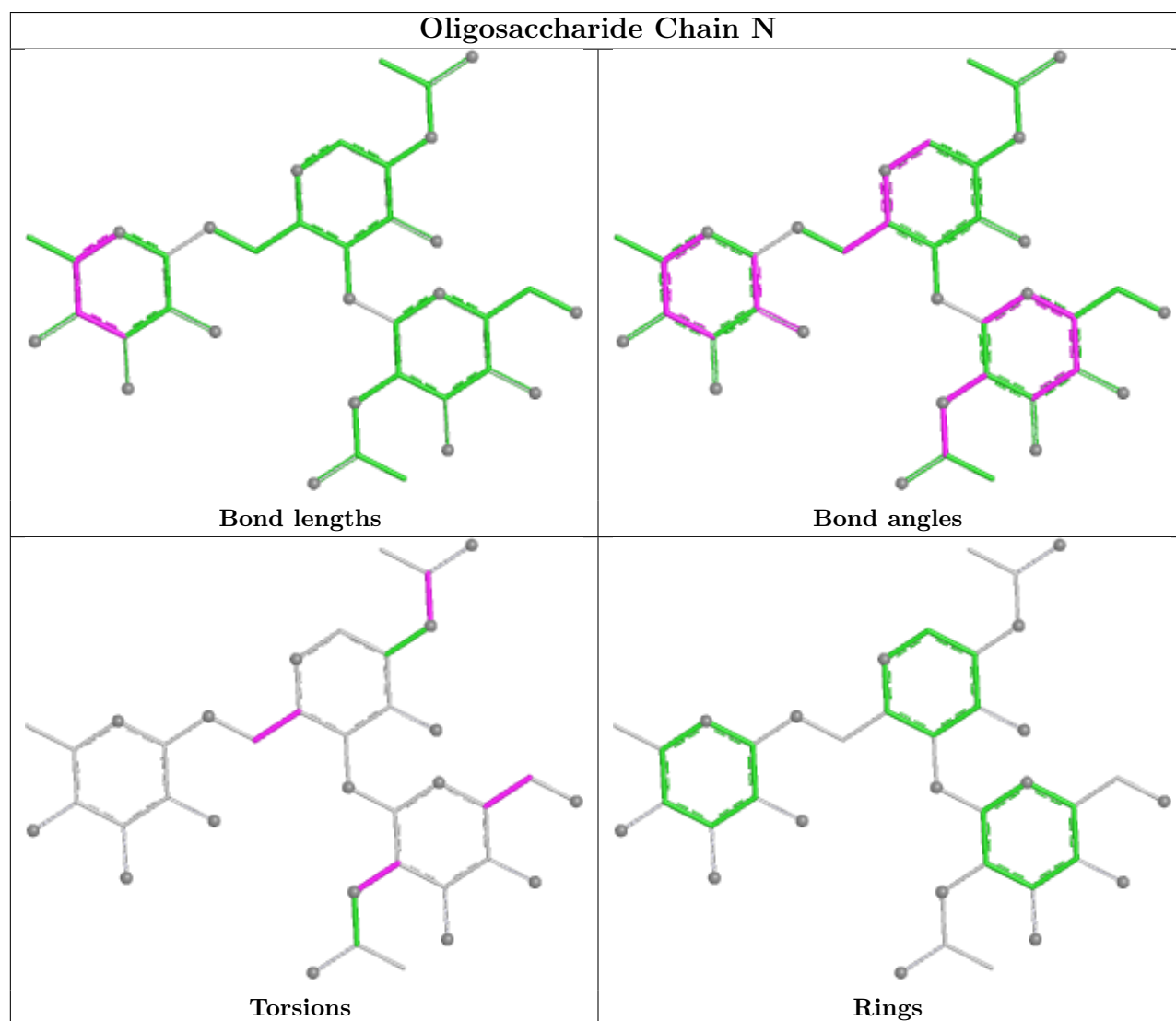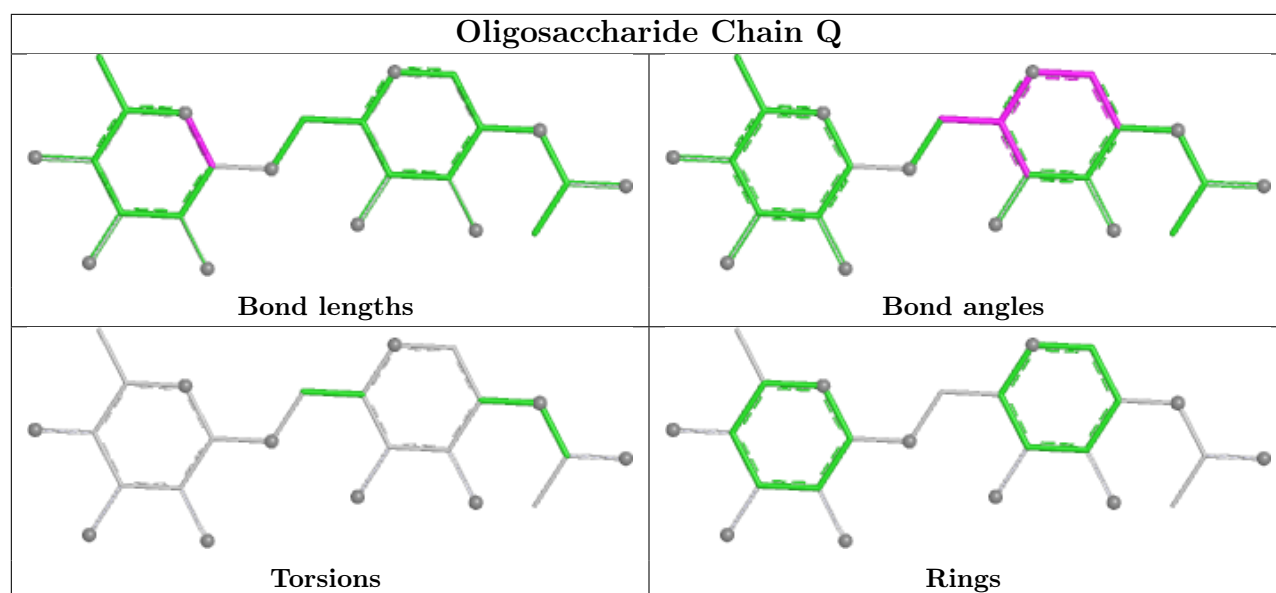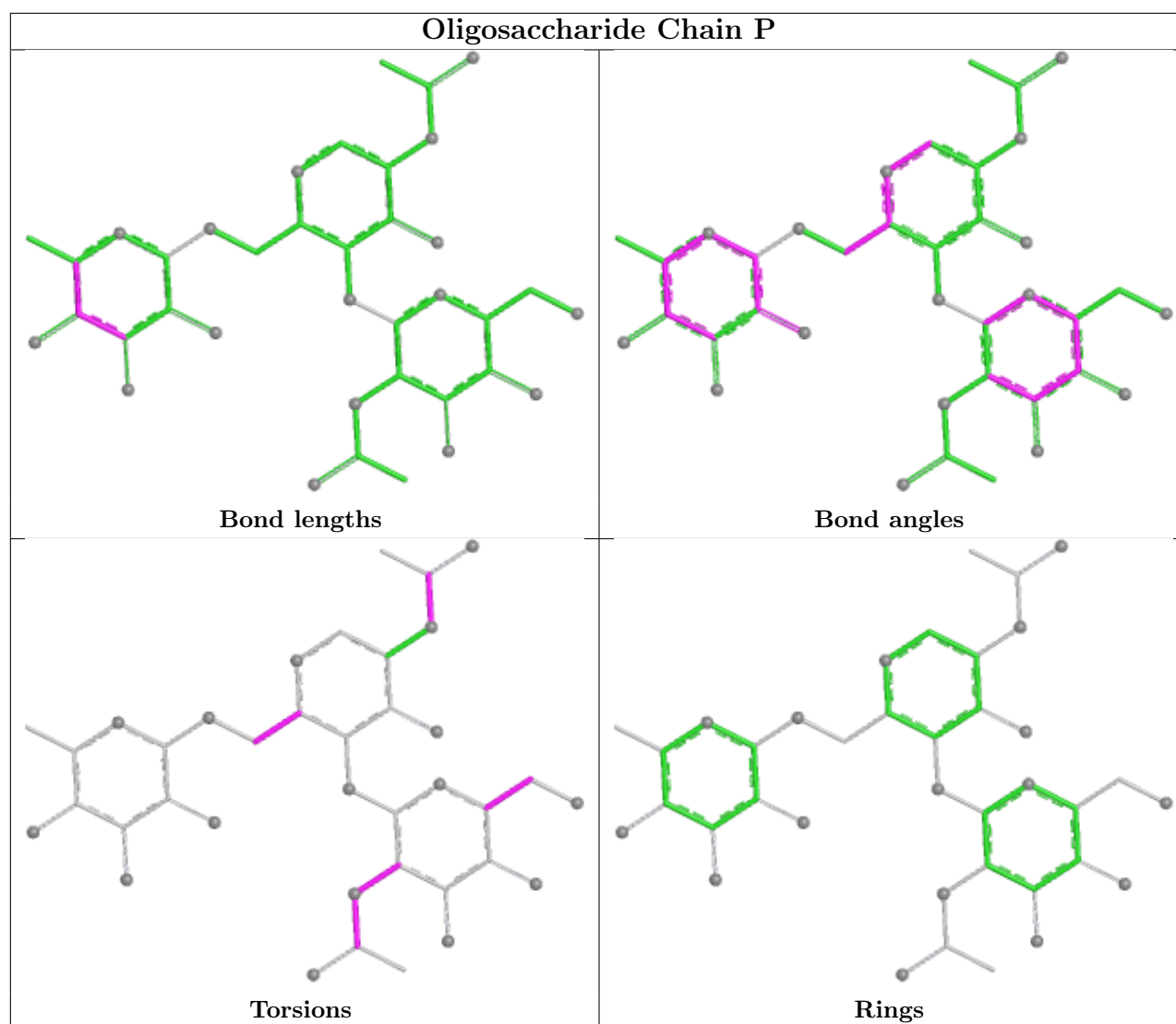
5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 12 are monoatomic - leaving 15 for Mogul analysis.

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	E	502	1	14,14,15	0.45	0	17,19,21	0.74	0
5	NAG	D	504	-	14,14,15	0.43	0	17,19,21	4.50	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
5	NAG	G	502	1	14,14,15	0.50	0	17,19,21	0.90	1 (5%)
6	FUC	D	505	-	10,10,11	1.97	2 (20%)	14,14,16	3.23	3 (21%)
5	NAG	D	503	-	14,14,15	0.63	0	17,19,21	1.58	2 (11%)
5	NAG	D	502	-	14,14,15	0.49	0	17,19,21	1.23	1 (5%)
5	NAG	H	502	1	14,14,15	0.52	0	17,19,21	0.96	1 (5%)
5	NAG	C	502	1	14,14,15	0.60	0	17,19,21	1.03	1 (5%)
5	NAG	B	505	-	14,14,15	0.54	0	17,19,21	1.06	1 (5%)
5	NAG	A	502	1	14,14,15	0.46	0	17,19,21	1.00	1 (5%)
5	NAG	F	505	-	14,14,15	0.50	0	17,19,21	0.66	0
5	NAG	I	502	1	14,14,15	0.52	0	17,19,21	1.40	1 (5%)
5	NAG	L	502	1	14,14,15	0.53	0	17,19,21	1.19	2 (11%)
5	NAG	K	502	1	14,14,15	0.56	0	17,19,21	1.25	3 (17%)
5	NAG	A	503	1	14,14,15	0.44	0	17,19,21	1.65	3 (17%)

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	E	502	1	-	2/6/23/26	0/1/1/1
5	NAG	D	504	-	-	2/6/23/26	0/1/1/1
5	NAG	G	502	1	-	4/6/23/26	0/1/1/1
6	FUC	D	505	-	-	-	0/1/1/1
5	NAG	D	503	-	-	0/6/23/26	0/1/1/1
5	NAG	D	502	-	-	2/6/23/26	0/1/1/1
5	NAG	H	502	1	-	2/6/23/26	0/1/1/1
5	NAG	C	502	1	-	2/6/23/26	0/1/1/1
5	NAG	B	505	-	-	1/6/23/26	0/1/1/1
5	NAG	A	502	1	-	3/6/23/26	0/1/1/1
5	NAG	F	505	-	-	2/6/23/26	0/1/1/1
5	NAG	I	502	1	-	3/6/23/26	0/1/1/1
5	NAG	L	502	1	-	2/6/23/26	0/1/1/1
5	NAG	K	502	1	-	5/6/23/26	0/1/1/1
5	NAG	A	503	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	505	FUC	C2-C3	4.36	1.59	1.52
6	D	505	FUC	C1-C2	3.91	1.61	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	504	NAG	C1-O5-C5	12.78	129.32	112.19
5	D	504	NAG	O5-C1-C2	-12.19	92.44	111.29
6	D	505	FUC	O5-C1-C2	-10.85	84.91	110.79
5	I	502	NAG	C1-O5-C5	4.26	117.90	112.19
5	D	503	NAG	O5-C1-C2	4.19	117.78	111.29
6	D	505	FUC	C1-C2-C3	4.08	115.59	109.64
5	A	503	NAG	C1-O5-C5	3.92	117.44	112.19
5	A	503	NAG	C2-N2-C7	3.89	128.12	122.90
5	D	504	NAG	O5-C5-C6	3.79	115.04	107.66
5	L	502	NAG	C1-O5-C5	3.69	117.13	112.19
5	D	502	NAG	C1-O5-C5	3.25	116.55	112.19
5	D	503	NAG	C1-O5-C5	3.20	116.47	112.19
5	H	502	NAG	C1-O5-C5	3.16	116.42	112.19
5	K	502	NAG	C1-O5-C5	3.10	116.34	112.19
5	A	502	NAG	C1-O5-C5	2.88	116.04	112.19
5	G	502	NAG	C1-O5-C5	2.82	115.96	112.19
5	K	502	NAG	O5-C1-C2	2.73	115.52	111.29
5	A	503	NAG	C4-C3-C2	-2.59	107.22	111.02
5	C	502	NAG	C1-O5-C5	2.43	115.45	112.19
5	B	505	NAG	O5-C1-C2	-2.41	107.57	111.29
5	D	504	NAG	C3-C4-C5	-2.28	106.10	110.23
5	L	502	NAG	O5-C1-C2	2.23	114.75	111.29
5	D	504	NAG	C4-C3-C2	-2.15	107.87	111.02
5	K	502	NAG	C2-N2-C7	2.11	125.73	122.90
6	D	505	FUC	C3-C4-C5	-2.07	106.67	109.81

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	NAG	C3-C2-N2-C7
5	A	502	NAG	C8-C7-N2-C2
5	A	502	NAG	O7-C7-N2-C2
5	E	502	NAG	C8-C7-N2-C2
5	E	502	NAG	O7-C7-N2-C2
5	H	502	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	H	502	NAG	O7-C7-N2-C2
5	I	502	NAG	C1-C2-N2-C7
5	I	502	NAG	C8-C7-N2-C2
5	I	502	NAG	O7-C7-N2-C2
5	K	502	NAG	C3-C2-N2-C7
5	K	502	NAG	C8-C7-N2-C2
5	K	502	NAG	O7-C7-N2-C2
5	D	504	NAG	O5-C5-C6-O6
5	K	502	NAG	O5-C5-C6-O6
5	G	502	NAG	O5-C5-C6-O6
5	L	502	NAG	O5-C5-C6-O6
5	D	504	NAG	C4-C5-C6-O6
5	F	505	NAG	C8-C7-N2-C2
5	G	502	NAG	C4-C5-C6-O6
5	K	502	NAG	C4-C5-C6-O6
5	F	505	NAG	O7-C7-N2-C2
5	C	502	NAG	O5-C5-C6-O6
5	D	502	NAG	C8-C7-N2-C2
5	C	502	NAG	C4-C5-C6-O6
5	D	502	NAG	O7-C7-N2-C2
5	B	505	NAG	O5-C5-C6-O6
5	L	502	NAG	C4-C5-C6-O6
5	A	503	NAG	C3-C2-N2-C7
5	G	502	NAG	C8-C7-N2-C2
5	G	502	NAG	O7-C7-N2-C2

There are no ring outliers.

10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	502	NAG	1	0
5	D	504	NAG	1	0
5	D	503	NAG	1	0
5	D	502	NAG	1	0
5	C	502	NAG	1	0
5	B	505	NAG	2	0
5	F	505	NAG	1	0
5	I	502	NAG	2	0
5	L	502	NAG	1	0
5	A	503	NAG	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	365/378 (96%)	-1.62	0	100	100	10, 33, 79, 133	0
1	B	365/378 (96%)	-1.67	0	100	100	11, 34, 71, 137	0
1	C	365/378 (96%)	-1.65	0	100	100	12, 39, 81, 141	0
1	D	365/378 (96%)	-1.62	0	100	100	11, 38, 88, 148	0
1	E	365/378 (96%)	-1.65	0	100	100	11, 34, 82, 133	0
1	F	365/378 (96%)	-1.65	0	100	100	12, 34, 69, 140	0
1	G	365/378 (96%)	-1.51	0	100	100	14, 46, 93, 135	0
1	H	365/378 (96%)	-1.54	0	100	100	13, 45, 96, 139	0
1	I	365/378 (96%)	-1.44	0	100	100	39, 65, 106, 137	0
1	J	363/378 (96%)	-1.33	0	100	100	47, 75, 104, 146	0
1	K	364/378 (96%)	-1.13	0	100	100	45, 87, 112, 149	0
1	L	365/378 (96%)	-1.07	0	100	100	45, 84, 116, 145	0
All	All	4377/4536 (96%)	-1.49	0	100	100	10, 51, 104, 149	0

There are no RSRZ outliers to report.

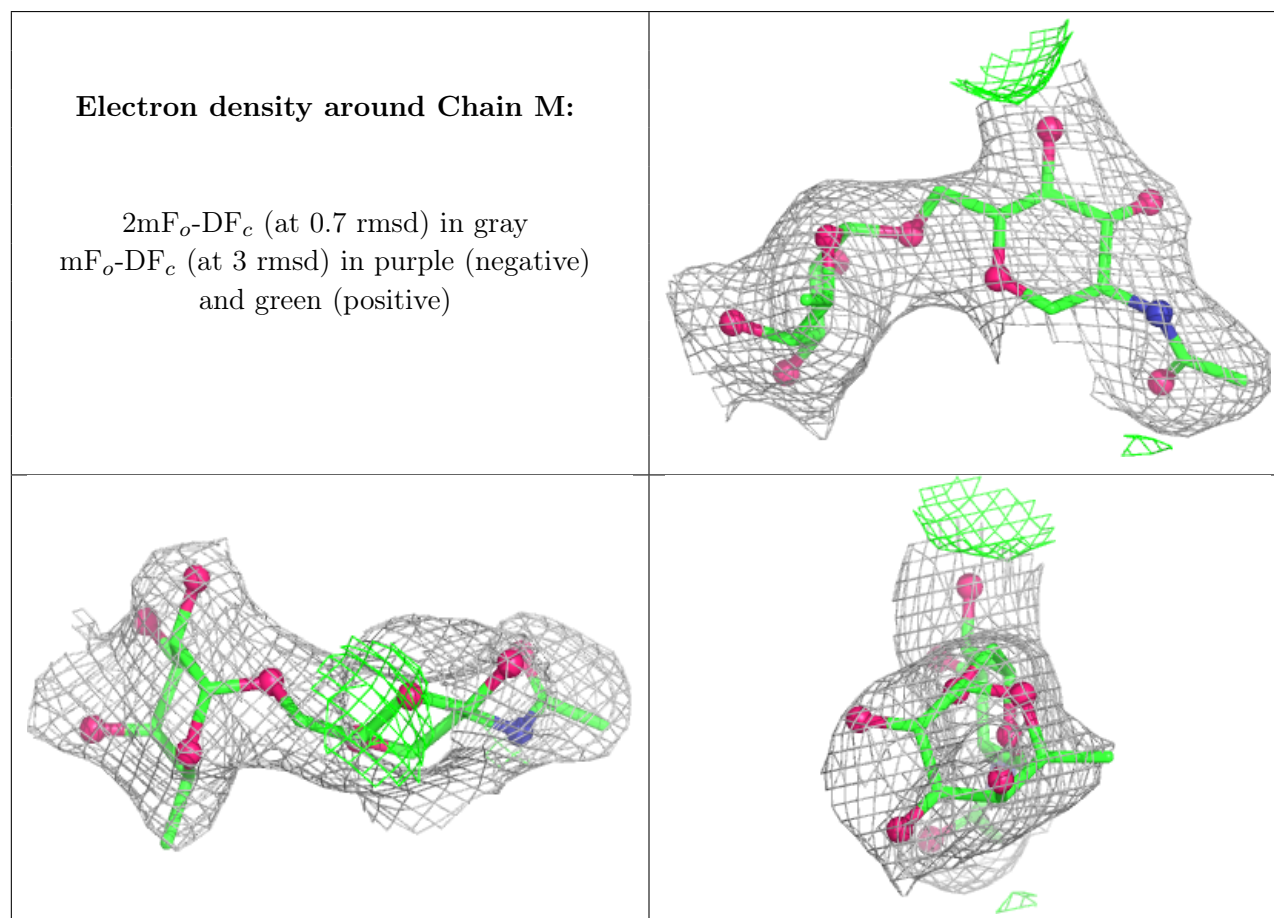## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	NAG	N	2	14/15	0.97	0.04	86,92,96,96	0
3	NAG	P	2	14/15	0.97	0.04	89,95,101,102	0
3	FUL	N	3	10/11	0.98	0.05	68,80,83,84	0
3	NAG	P	1	14/15	0.98	0.03	55,67,75,82	0
2	FUC	M	2	10/11	0.98	0.04	26,46,53,63	0
3	FUL	P	3	10/11	0.98	0.04	54,61,69,70	0
3	NAG	N	1	14/15	0.99	0.03	60,69,80,83	0
2	NAG	M	1	14/15	0.99	0.03	38,48,52,52	0
2	NAG	O	1	14/15	0.99	0.03	45,48,54,55	0
2	FUC	O	2	10/11	0.99	0.03	54,57,61,63	0
2	NAG	Q	1	14/15	0.99	0.03	35,55,67,68	0
2	FUC	Q	2	10/11	0.99	0.03	74,79,86,87	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.
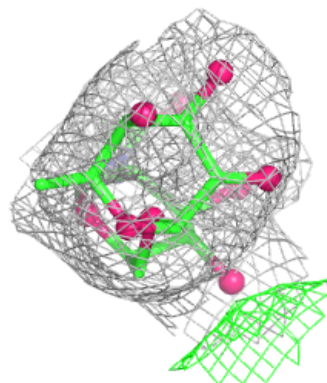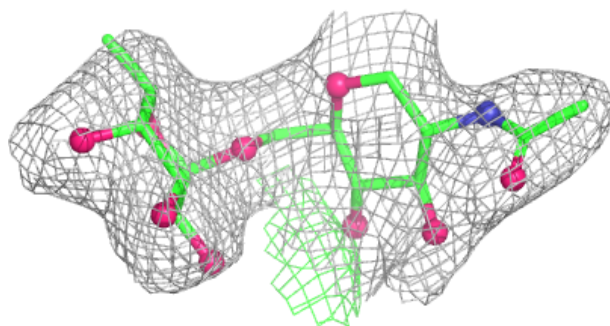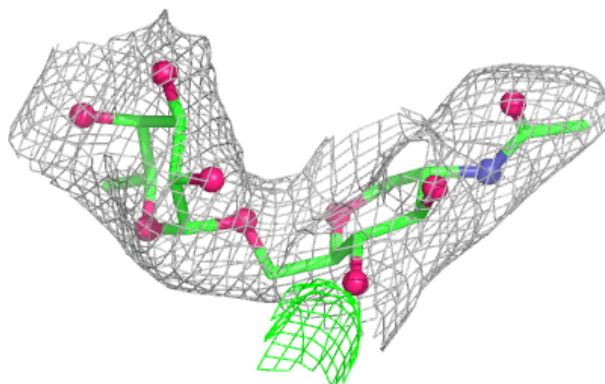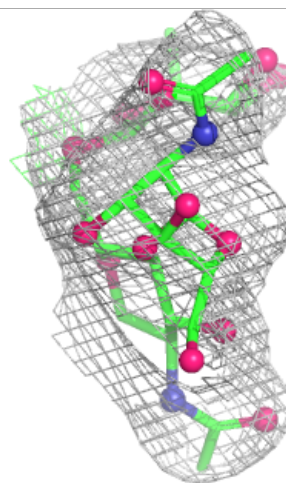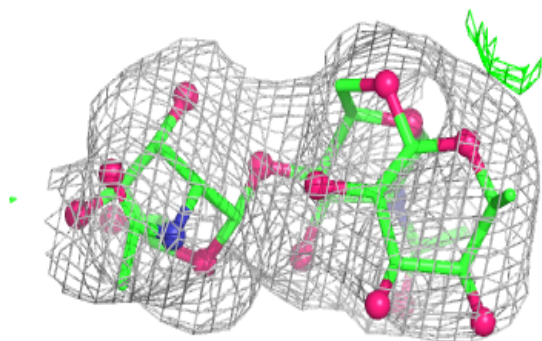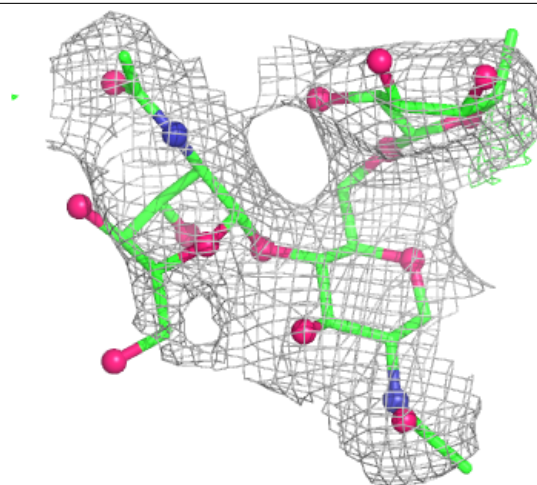

Electron density around Chain M:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around Chain O:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
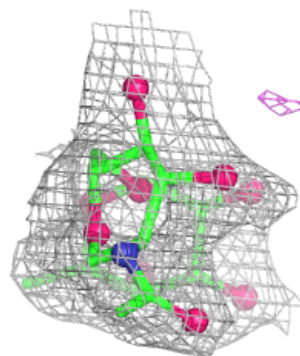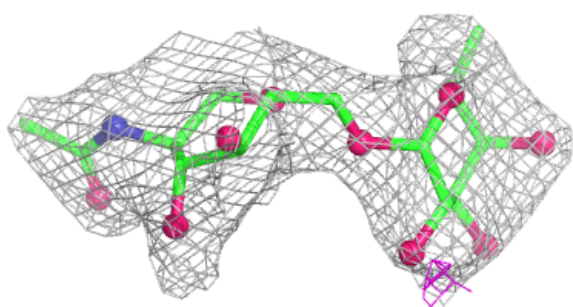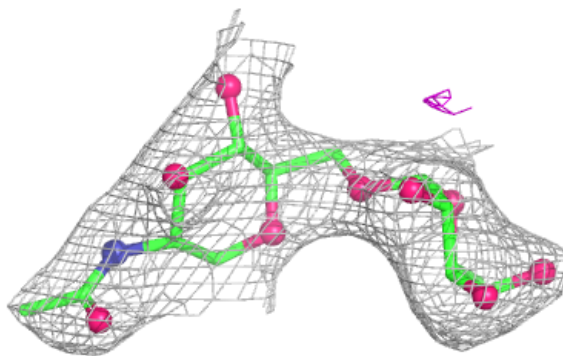
Electron density around Chain Q:
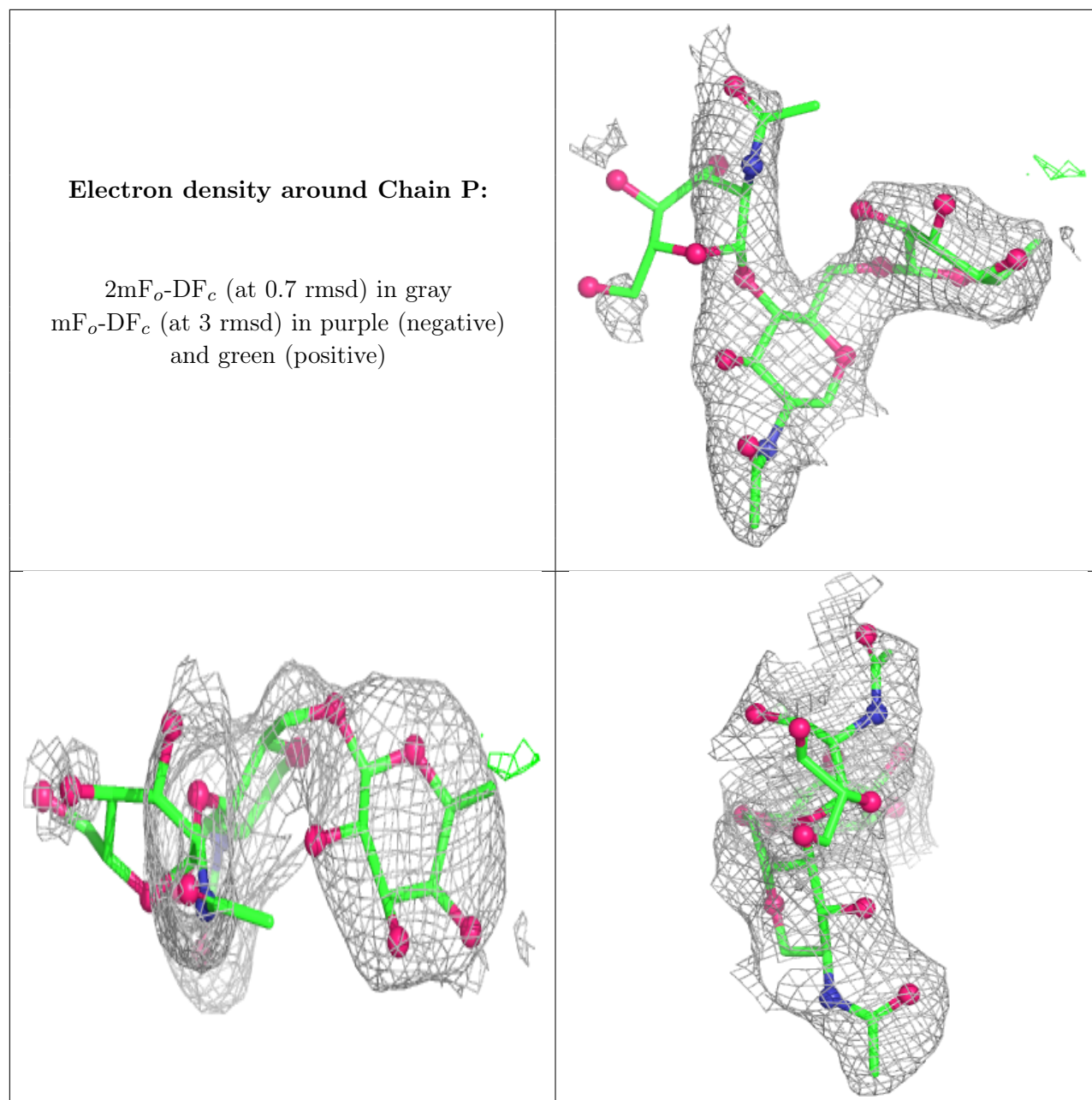
$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around Chain N:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around Chain P:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
5	NAG	K	502	14/15	0.94	0.06	73,86,92,93	0
5	NAG	A	502	14/15	0.95	0.05	82,102,105,105	0
5	NAG	G	502	14/15	0.96	0.04	64,72,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
5	NAG	L	502	14/15	0.96	0.04	75,86,94,96	0
5	NAG	I	502	14/15	0.97	0.04	79,85,89,91	0
5	NAG	E	502	14/15	0.97	0.06	83,97,100,101	0
5	NAG	B	505	14/15	0.97	0.07	64,76,81,83	0
5	NAG	H	502	14/15	0.98	0.03	54,67,82,84	0
5	NAG	D	503	14/15	0.98	0.04	49,73,79,83	0
5	NAG	A	503	14/15	0.98	0.05	83,99,103,104	0
5	NAG	D	502	14/15	0.98	0.03	75,87,90,91	0
5	NAG	F	505	14/15	0.99	0.05	63,81,85,86	0
5	NAG	D	504	14/15	0.99	0.03	30,81,85,85	0
5	NAG	C	502	14/15	0.99	0.03	44,53,61,64	0
6	FUC	D	505	10/11	0.99	0.04	46,59,84,86	0
4	CA	D	501	1/1	1.00	0.01	33,33,33,33	0
4	CA	E	501	1/1	1.00	0.03	41,41,41,41	0
4	CA	F	501	1/1	1.00	0.01	45,45,45,45	0
4	CA	G	501	1/1	1.00	0.02	28,28,28,28	0
4	CA	H	501	1/1	1.00	0.02	37,37,37,37	0
4	CA	I	501	1/1	1.00	0.02	51,51,51,51	0
4	CA	J	501	1/1	1.00	0.01	65,65,65,65	0
4	CA	K	501	1/1	1.00	0.02	51,51,51,51	0
4	CA	L	501	1/1	1.00	0.03	84,84,84,84	0
4	CA	A	501	1/1	1.00	0.01	34,34,34,34	0
4	CA	B	501	1/1	1.00	0.02	42,42,42,42	0
4	CA	C	501	1/1	1.00	0.02	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.