



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:36 PM UTC

PDB ID : 4FQK / pdb_00004fqk
Title : Influenza B/Brisbane/60/2008 hemagglutinin Fab CR8059 complex
Authors : Dreyfus, C.; Laursen, N.S.; Wilson, I.A.
Deposited on : 2012-06-25
Resolution : 5.65 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

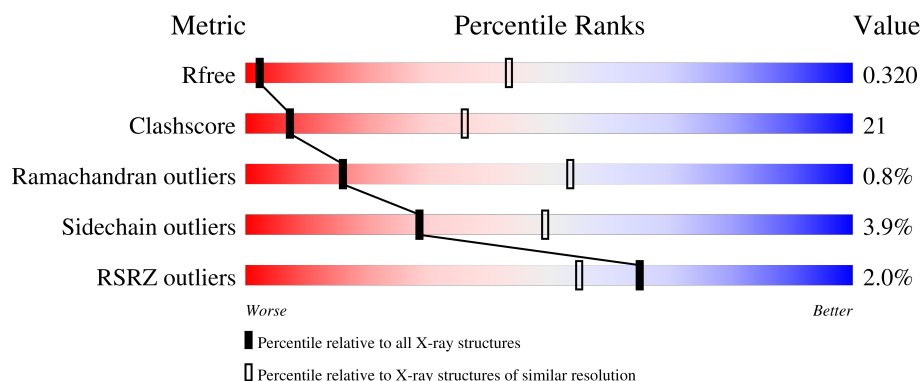
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.65 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1104 (7.32-4.00)
Clashscore	190562	1165 (7.32-4.00)
Ramachandran outliers	187476	1000 (7.32-4.00)
Sidechain outliers	187428	1031 (7.36-3.96)
RSRZ outliers	180081	1097 (7.32-4.00)

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 $\leq 5\%$. 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	347	
1	C	347	
2	B	179	
2	D	179	
3	E	234	

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Mol	Chain	Length	Quality of chain
3	H	234	 % 71% 23% 6%
4	F	216	 3% 79% 19% ..
4	L	216	 % 82% 15% ..
5	G	2	 50% 50%
5	I	2	 100%
5	J	2	 100%
5	N	2	 100%
5	O	2	 100%
5	P	2	 50% 50%
6	K	3	 67% 33%
6	M	3	 33% 33% 33%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14080 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 Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2560	1607	458	480	15			
1	C	337	Total	C	N	O	S	0	0	0
			2560	1607	458	480	15			

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	139	Total	C	N	O	S	0	0	0
			1054	652	182	215	5			
2	D	140	Total	C	N	O	S	0	0	0
			1062	658	183	216	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	524	SER	-	linker	UNP C0LT38
B	525	GLY	-	linker	UNP C0LT38
B	526	ARG	-	linker	UNP C0LT38
D	524	SER	-	linker	UNP C0LT38
D	525	GLY	-	linker	UNP C0LT38
D	526	ARG	-	linker	UNP C0LT38

- Molecule 3 is a protein called Antibody CR8059 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	220	Total	C	N	O	S	0	0	0
			1673	1061	278	327	7			
3	H	221	Total	C	N	O	S	0	0	0
			1679	1064	279	328	8			

- Molecule 4 is a protein called Antibody CR8059 Light Chain.

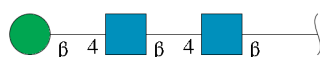
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	213	Total	C	N	O	S	0	0	0
			1606	1006	269	327	4			
4	L	214	Total	C	N	O	S	0	0	0
			1612	1009	270	328	5			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



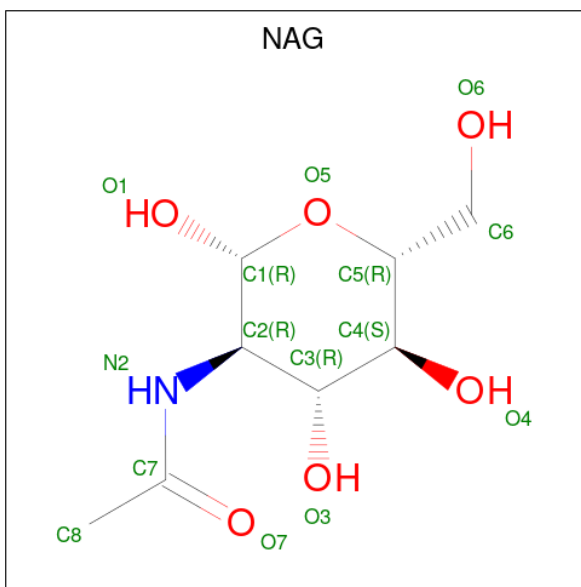
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

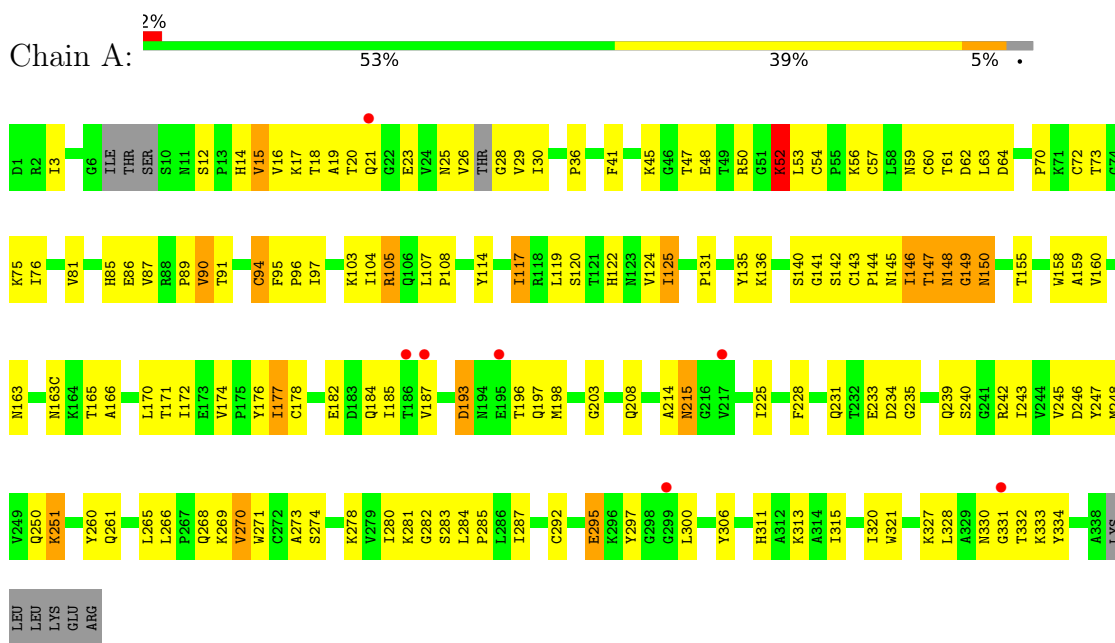


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		

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: Hemagglutinin HA1



LYS
LEU
LEU
LYS
GLU
ARG

• Molecule 2: Hemagglutinin HA2



GLY PHE PHE GLY ALA ILE ALA GLY PHE LEU LEU GLY GLY TRP GLU MET ILE ILE ALA GLY TRP H369 H373 A380 S387 A391 ILE ASN LYS I395 N398 L405 E406 V407 K408 N409 L410 Q411 R412 A416 M417 D418 H421 N422 I424 L425 E426 L427 V431 D432

R435 I439 S440 I443 E444 L448 L449 S450 N451 E452 G453 I454 E458 ASP GLU HIS TRP L463 A464 L465 S476 E479 G483 C484 F485 L496 I499 E508 F509 S510 L511 F514 ASP SER LEU ILE THR ALA ALA SER SER GLY ARG

• Molecule 2: Hemagglutinin HA2



GLY PHE PHE GLY ALA ILE ALA GLY PHE LEU LEU GLY GLY TRP GLU MET ILE ILE ALA GLY TRP H369 H373 A376 A380 S387 A391 ILE ASN LYS I395 N398 L405 E406 V407 K408 N409 L410 Q411 R412 A416 M417 D418 H421 N422 I424 L425 E426

L427 V431 D432 R435 I439 S440 I443 E444 L448 L449 S450 N451 E452 G453 I454 E458 ASP GLU HIS L462 L463 L465 M472 S476 E479 G483 C484 F485 L496 I499 E508 F509 S510 L511 F514 ASP SER LEU ILE THR ALA ALA SER SER

GLY
ARG

• Molecule 3: Antibody CR8059 Heavy Chain



Q1 V2 Q3 Q6 K12 S17 C22 S25 T30 T35 W36 A40 Q43 W50 I51 Y53 T57 K62 K71 D72 T73 M80 B82A S82B L82C D86 R94 D95 Y98 S99 G100 S100A Y100B Y100F Y100G S104 V111 SER

S113 A114 T116 K117 P123 L124 S127 SER LYS SER THR SER GLY G134 T135 G140 K143 F146 T151 V163 F166 P167 A168 V169 L170 Q171 L178 V182 T183 G190 T191 Q192 T193 H200 K201 P202 G205 R210 V211 E212 P213 K214 S215 CYS S104 V111 SER HIS

HIS
HIS
HIS

• Molecule 3: Antibody CR8059 Heavy Chain

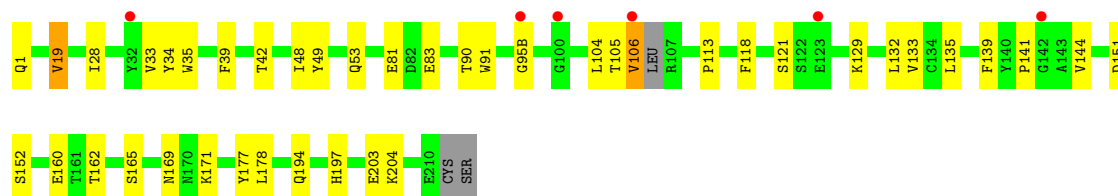
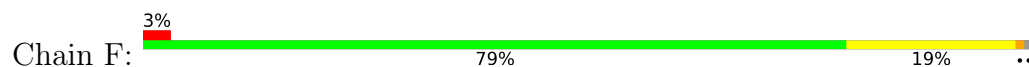


Q1 V2 Q3 Q6 K12 S17 S25 T30 T35 W36 A40 Q43 W50 I51 S52 G52A Y53 T57 K62 K71 D72 T73 M80 B82A S82B L82C D86 R94 D95 V96 Q97 Y98 S99 G100 S100A Y100B Y100F Y100G S104 V111 SER

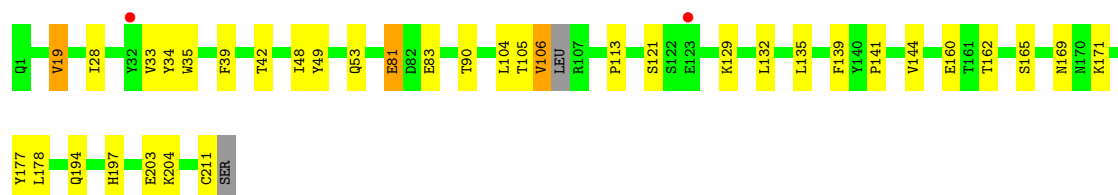
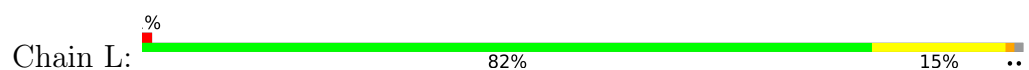
S113 A114 T116 K117 P123 S127 SER LYS SER THR SER GLY G134 T135 G139 G140 K143 F146 T151 V163 F166 P167 A168 V169 L170 Q171 S172 L178 V182 T183 T193 H200 K201 P202 T205 R210 V211 E212 P213 K214 S215 C216 S104 V111 SER HIS HIS



- Molecule 4: Antibody CR8059 Light Chain



- Molecule 4: Antibody CR8059 Light Chain



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  50% 50%

MAG1
MAG2

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  67% 33%

MAG1
MAG2
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  33% 33% 33%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	189.20Å 189.20Å 319.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.93 – 5.65 48.93 – 5.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.93-5.65) 99.9 (48.93-5.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 5.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.306 , 0.324 0.303 , 0.320	Depositor DCC
R_{free} test set	1275 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	243.5	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 995.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.429 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	14080	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: NAG, BMA

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	0.84	0/2618	1.34	22/3553 (0.6%)
1	C	0.84	0/2618	1.34	23/3553 (0.6%)
2	B	0.56	0/1063	1.03	4/1429 (0.3%)
2	D	0.56	0/1071	1.03	4/1440 (0.3%)
3	E	0.53	0/1714	0.88	0/2335
3	H	0.53	0/1720	0.88	1/2343 (0.0%)
4	F	0.52	0/1648	0.88	0/2250
4	L	0.52	0/1654	0.88	0/2258
All	All	0.66	0/14106	1.09	54/19161 (0.3%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	409	ASN	N-CA-C	8.63	122.31	111.69
2	D	409	ASN	N-CA-C	8.59	122.26	111.69
1	C	90	VAL	N-CA-C	7.86	121.25	108.99
1	A	90	VAL	N-CA-C	7.82	121.19	108.99
1	C	50	ARG	N-CA-C	7.74	120.67	108.67
1	A	50	ARG	N-CA-C	7.72	120.63	108.67
1	C	174	VAL	CA-C-N	7.51	127.96	119.92
1	C	174	VAL	C-N-CA	7.51	127.96	119.92
1	A	174	VAL	CA-C-N	7.48	127.93	119.92
1	A	174	VAL	C-N-CA	7.48	127.93	119.92
1	A	3	ILE	N-CA-C	6.81	117.69	107.75
1	C	3	ILE	N-CA-C	6.81	117.69	107.75
1	C	149	GLY	N-CA-C	-6.67	105.24	112.04
1	A	149	GLY	N-CA-C	-6.67	105.24	112.04
1	A	150	ASN	N-CA-C	6.63	119.99	110.24
1	C	150	ASN	N-CA-C	6.61	119.96	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	ASN	N-CA-C	-6.60	99.69	108.34
1	C	163	ASN	N-CA-C	-6.59	99.70	108.34
1	A	160	VAL	CA-C-N	-6.54	111.66	119.84
1	A	160	VAL	C-N-CA	-6.54	111.66	119.84
1	C	160	VAL	CA-C-N	-6.53	111.68	119.84
1	C	160	VAL	C-N-CA	-6.53	111.68	119.84
1	A	228	PHE	CA-C-N	5.78	125.78	119.89
1	A	228	PHE	C-N-CA	5.78	125.78	119.89
1	C	228	PHE	CA-C-N	5.74	125.74	119.89
1	C	228	PHE	C-N-CA	5.74	125.74	119.89
1	C	117	ILE	N-CA-C	5.70	117.63	108.85
1	A	117	ILE	N-CA-C	5.69	117.61	108.85
1	A	15	VAL	N-CA-C	5.67	116.75	108.53
1	C	15	VAL	N-CA-C	5.63	116.70	108.53
2	B	509	PHE	N-CA-C	-5.43	100.25	108.67
2	D	509	PHE	N-CA-C	-5.43	100.26	108.67
2	D	410	LEU	N-CA-C	5.42	117.25	110.91
1	A	331	GLY	N-CA-C	5.38	117.44	110.45
1	C	331	GLY	N-CA-C	5.38	117.44	110.45
2	B	410	LEU	N-CA-C	5.36	117.18	110.91
1	A	52	LYS	N-CA-C	-5.35	100.97	109.59
1	C	52	LYS	N-CA-C	-5.34	100.99	109.59
1	C	47	THR	N-CA-C	5.31	117.89	109.50
1	A	47	THR	N-CA-C	5.28	117.83	109.50
1	A	94	CYS	CA-C-N	5.23	127.91	120.49
1	A	94	CYS	C-N-CA	5.23	127.91	120.49
1	C	94	CYS	CA-C-N	5.17	127.84	120.49
1	C	94	CYS	C-N-CA	5.17	127.84	120.49
1	A	90	VAL	N-CA-CB	-5.17	103.79	112.47
2	B	483	GLY	N-CA-C	-5.14	107.71	115.32
2	D	483	GLY	N-CA-C	-5.14	107.71	115.32
1	C	90	VAL	N-CA-CB	-5.13	103.85	112.47
1	C	287	ILE	O-C-N	-5.08	117.16	123.10
1	A	193	ASP	N-CA-C	5.04	114.89	108.24
1	C	193	ASP	N-CA-C	5.02	114.87	108.24
3	H	139	GLY	N-CA-C	5.02	118.60	111.12
1	A	287	ILE	O-C-N	-5.02	117.22	123.10
1	C	304	LYS	N-CA-C	-5.01	102.89	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2560	0	2559	206	0
1	C	2560	0	2559	197	0
2	B	1054	0	1043	66	0
2	D	1062	0	1054	59	0
3	E	1673	0	1633	52	0
3	H	1679	0	1638	53	0
4	F	1606	0	1541	33	0
4	L	1612	0	1546	31	0
5	G	28	0	25	1	0
5	I	28	0	25	0	0
5	J	28	0	25	0	0
5	N	28	0	25	0	0
5	O	28	0	25	0	0
5	P	28	0	25	5	0
6	K	39	0	34	3	0
6	M	39	0	34	1	0
7	A	14	0	13	0	0
7	C	14	0	13	0	0
All	All	14080	0	13817	575	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 21.

All (575) 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:C:214:ALA:HB2	1:C:248:MET:CE	1.62	1.29
1:A:214:ALA:HB2	1:A:248:MET:CE	1.62	1.27
1:A:214:ALA:HB2	1:A:248:MET:HE3	1.16	1.15
1:C:214:ALA:HB2	1:C:248:MET:HE3	1.16	1.14
1:A:20:THR:CG2	2:B:452:GLU:HG3	1.78	1.13
1:A:320:ILE:CD1	2:B:405:LEU:HD22	1.78	1.12
1:C:320:ILE:CD1	2:D:405:LEU:HD22	1.80	1.11
1:C:131:PRO:HG2	1:C:172:ILE:HD11	1.33	1.11
1:A:280:ILE:HD11	1:A:315:ILE:HG23	1.25	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:ILE:HD11	1:C:315:ILE:HG23	1.25	1.10
1:A:20:THR:CG2	2:B:452:GLU:CG	2.31	1.08
1:A:124:VAL:HG12	1:A:177:ILE:HG13	1.38	1.06
1:A:56:LYS:NZ	1:A:75:LYS:HE3	1.72	1.05
1:C:124:VAL:HG12	1:C:177:ILE:HG13	1.38	1.04
1:A:280:ILE:CD1	1:A:315:ILE:HG12	1.87	1.04
1:C:56:LYS:NZ	1:C:75:LYS:HE3	1.72	1.04
1:A:131:PRO:HG2	1:A:172:ILE:HD11	1.33	1.03
1:C:280:ILE:CD1	1:C:315:ILE:HG12	1.87	1.03
1:C:96:PRO:O	1:C:243:ILE:HG22	1.59	1.02
1:C:283:SER:HB2	3:E:99:SER:O	1.57	1.02
1:A:96:PRO:O	1:A:243:ILE:HG22	1.59	1.01
1:A:20:THR:HG22	2:B:452:GLU:CG	1.91	1.01
1:A:119:LEU:HD21	1:A:269:LYS:HB3	1.43	1.01
4:F:105:THR:HG21	4:F:141:PRO:HB3	1.43	1.01
1:C:131:PRO:HG2	1:C:172:ILE:CD1	1.91	1.00
2:D:416:ALA:HB1	2:D:425:LEU:HD21	1.42	1.00
1:A:328:LEU:HD12	2:B:451:ASN:OD1	1.62	1.00
1:A:214:ALA:CB	1:A:248:MET:HE3	1.92	1.00
1:C:214:ALA:CB	1:C:248:MET:HE3	1.92	0.99
1:C:328:LEU:HD12	2:D:451:ASN:OD1	1.62	0.99
1:A:131:PRO:HG2	1:A:172:ILE:CD1	1.91	0.99
2:B:416:ALA:HB1	2:B:425:LEU:HD21	1.42	0.99
1:C:119:LEU:HD21	1:C:269:LYS:HB3	1.43	0.98
1:A:283:SER:HB2	3:H:99:SER:O	1.63	0.97
1:A:20:THR:HG21	2:B:452:GLU:CG	1.93	0.97
1:A:215:ASN:OD1	1:A:251:LYS:HG2	1.65	0.97
1:C:215:ASN:OD1	1:C:251:LYS:HG2	1.65	0.96
1:C:283:SER:HB3	3:E:100:GLY:HA3	1.48	0.96
1:A:280:ILE:HD12	1:A:315:ILE:HG12	1.48	0.94
1:A:281:LYS:HD2	2:B:412:ARG:CZ	1.98	0.94
1:C:280:ILE:HD12	1:C:315:ILE:HG12	1.48	0.94
4:L:105:THR:HG21	4:L:141:PRO:HB3	1.50	0.94
2:D:421:HIS:O	2:D:425:LEU:HG	1.68	0.93
2:B:421:HIS:O	2:B:425:LEU:HG	1.68	0.93
1:A:240:SER:OG	6:K:1:NAG:H82	1.69	0.93
1:A:280:ILE:HD11	1:A:315:ILE:CG2	1.99	0.92
1:A:285:PRO:HD2	3:H:100(F):TYR:CE2	2.04	0.92
1:C:280:ILE:HD11	1:C:315:ILE:CG2	1.99	0.92
1:C:240:SER:OG	5:P:1:NAG:H82	1.69	0.92
1:A:171:THR:O	1:A:172:ILE:HD13	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LEU:HD23	1:A:120:SER:N	1.86	0.91
1:C:171:THR:O	1:C:172:ILE:HD13	1.71	0.90
1:A:20:THR:HG21	2:B:452:GLU:HG3	1.50	0.90
1:C:278:LYS:HD2	2:D:411:GLN:NE2	1.87	0.89
1:C:285:PRO:HD2	3:E:100(F):TYR:CE2	2.07	0.89
1:A:131:PRO:CG	1:A:172:ILE:HD11	2.01	0.89
1:C:119:LEU:HD23	1:C:120:SER:N	1.87	0.89
1:C:131:PRO:CG	1:C:172:ILE:HD11	2.01	0.89
3:E:167:PRO:HG2	4:F:165:SER:OG	1.70	0.89
1:A:20:THR:CG2	2:B:452:GLU:HG2	2.03	0.89
1:C:281:LYS:HD2	2:D:412:ARG:NH2	1.87	0.89
1:C:320:ILE:HD11	2:D:405:LEU:HD22	1.54	0.88
3:H:167:PRO:HG2	4:L:165:SER:OG	1.73	0.88
1:A:320:ILE:HD11	2:B:405:LEU:HD22	1.54	0.86
1:C:155:THR:CG2	1:C:187:VAL:HB	2.05	0.86
1:C:215:ASN:O	1:C:215:ASN:ND2	2.09	0.86
1:A:155:THR:CG2	1:A:187:VAL:HB	2.05	0.86
1:A:18:THR:HG22	2:B:451:ASN:HB2	1.58	0.85
1:A:215:ASN:ND2	1:A:215:ASN:O	2.09	0.85
1:C:281:LYS:HD2	2:D:412:ARG:CZ	2.07	0.84
1:A:56:LYS:NZ	1:A:75:LYS:CE	2.40	0.84
1:A:283:SER:HB3	3:H:100:GLY:HA3	1.58	0.84
1:C:56:LYS:NZ	1:C:75:LYS:CE	2.40	0.84
1:C:26:VAL:HG12	1:C:28:GLY:O	1.78	0.83
1:A:281:LYS:HD2	2:B:412:ARG:NH2	1.92	0.82
1:A:320:ILE:CD1	2:B:405:LEU:CD2	2.58	0.82
2:B:416:ALA:HB1	2:B:425:LEU:CD2	2.09	0.82
1:C:18:THR:HG22	2:D:451:ASN:HB2	1.61	0.81
2:D:416:ALA:HB1	2:D:425:LEU:CD2	2.09	0.81
1:A:18:THR:HG22	2:B:451:ASN:CB	2.11	0.80
1:C:52:LYS:HE3	3:E:53:TYR:CE1	2.17	0.79
1:A:20:THR:HG22	2:B:452:GLU:HG3	1.50	0.79
1:A:215:ASN:C	1:A:215:ASN:HD22	1.91	0.79
1:C:215:ASN:C	1:C:215:ASN:HD22	1.91	0.78
1:C:18:THR:HG22	2:D:451:ASN:CB	2.13	0.78
1:A:26:VAL:HG12	1:A:28:GLY:O	1.84	0.77
1:A:320:ILE:HD11	2:B:405:LEU:CD2	2.15	0.77
1:A:52:LYS:HE3	3:H:53:TYR:CE1	2.21	0.76
1:A:284:LEU:HB3	1:A:285:PRO:HA	1.67	0.76
1:C:56:LYS:HZ3	1:C:75:LYS:HE3	1.47	0.76
1:A:59:ASN:OD1	3:H:30:THR:HG21	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ILE:CD1	2:D:405:LEU:CD2	2.64	0.75
1:C:52:LYS:CE	3:E:53:TYR:CE1	2.70	0.75
1:A:278:LYS:HD2	2:B:411:GLN:NE2	2.01	0.74
1:C:284:LEU:HB3	1:C:285:PRO:HA	1.67	0.74
1:A:56:LYS:HZ3	1:A:75:LYS:HE3	1.48	0.74
1:C:20:THR:HB	2:D:452:GLU:HG3	1.69	0.74
1:C:59:ASN:OD1	3:E:30:THR:HG21	1.88	0.74
1:A:119:LEU:HD21	1:A:269:LYS:CB	2.18	0.73
1:C:36:PRO:HB2	1:C:297:TYR:CD1	2.24	0.73
1:C:283:SER:CB	3:E:99:SER:O	2.35	0.73
1:A:52:LYS:CE	3:H:53:TYR:CE1	2.72	0.73
1:C:283:SER:CB	3:E:100:GLY:HA3	2.18	0.73
1:A:56:LYS:HZ3	1:A:75:LYS:CE	2.01	0.73
1:A:36:PRO:HB2	1:A:297:TYR:CD1	2.24	0.73
1:C:193:ASP:OD1	1:C:198:MET:SD	2.46	0.73
1:A:193:ASP:OD1	1:A:198:MET:SD	2.46	0.72
1:A:158:TRP:HA	1:A:265:LEU:HD23	1.70	0.72
1:A:280:ILE:HG23	1:A:295:GLU:HG3	1.71	0.72
4:F:106:VAL:O	4:F:106:VAL:HG22	1.89	0.72
1:C:119:LEU:HD23	1:C:120:SER:H	1.54	0.72
1:C:119:LEU:HD21	1:C:269:LYS:CB	2.18	0.72
1:A:292:CYS:HB3	1:A:300:LEU:HB3	1.72	0.72
1:C:158:TRP:HA	1:C:265:LEU:HD23	1.70	0.71
1:C:280:ILE:HD11	1:C:315:ILE:HG12	1.73	0.71
1:C:292:CYS:HB3	1:C:300:LEU:HB3	1.72	0.71
4:L:106:VAL:HG22	4:L:106:VAL:O	1.89	0.71
1:A:56:LYS:HZ1	1:A:75:LYS:HE3	1.54	0.71
2:B:479:GLU:OE1	2:B:485:PHE:CE2	2.44	0.71
1:A:16:VAL:CG2	1:A:29:VAL:CG1	2.69	0.70
1:C:320:ILE:HD11	2:D:405:LEU:CD2	2.20	0.70
1:A:19:ALA:H	2:B:448:LEU:HB3	1.57	0.70
1:C:280:ILE:HG23	1:C:295:GLU:HG3	1.72	0.70
1:A:119:LEU:HD23	1:A:120:SER:H	1.54	0.70
2:B:479:GLU:OE1	2:B:485:PHE:CZ	2.45	0.70
1:C:172:ILE:HG13	1:C:260:TYR:HE2	1.56	0.70
2:D:479:GLU:OE1	2:D:485:PHE:CE2	2.44	0.70
1:A:85:HIS:HB2	3:H:99:SER:HB3	1.74	0.70
2:D:479:GLU:OE1	2:D:485:PHE:CZ	2.45	0.69
1:C:56:LYS:HZ3	1:C:75:LYS:CE	2.01	0.69
1:C:56:LYS:HZ1	1:C:75:LYS:HE3	1.55	0.69
1:A:243:ILE:HD11	1:A:265:LEU:HD11	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:VAL:HG13	1:A:327:LYS:O	1.93	0.69
1:A:280:ILE:HD11	1:A:315:ILE:HG12	1.73	0.69
1:A:85:HIS:HB2	3:H:99:SER:CB	2.23	0.69
1:A:172:ILE:HG13	1:A:260:TYR:HE2	1.56	0.69
1:A:283:SER:CB	3:H:99:SER:O	2.40	0.68
1:C:14:HIS:CD2	1:C:28:GLY:HA2	2.28	0.68
1:C:85:HIS:HB2	3:E:99:SER:CB	2.24	0.68
1:C:243:ILE:HD11	1:C:265:LEU:HD11	1.73	0.68
1:A:147:THR:O	1:A:148:ASN:CG	2.37	0.68
1:A:284:LEU:HD13	3:H:98:TYR:OH	1.93	0.68
1:C:147:THR:O	1:C:148:ASN:CG	2.37	0.68
1:A:16:VAL:CG2	1:A:29:VAL:HG12	2.24	0.68
1:A:214:ALA:HB2	1:A:248:MET:HE2	1.71	0.68
1:C:214:ALA:HB2	1:C:248:MET:HE2	1.71	0.68
1:A:56:LYS:HZ3	1:A:75:LYS:NZ	1.92	0.67
1:A:19:ALA:N	2:B:448:LEU:HB3	2.09	0.67
1:A:26:VAL:HA	1:A:332:THR:O	1.93	0.67
1:C:36:PRO:HB2	1:C:297:TYR:HD1	1.58	0.67
1:C:53:LEU:CD1	1:C:62:ASP:HB3	2.25	0.67
1:A:52:LYS:HE2	3:H:53:TYR:HE1	1.60	0.67
1:C:284:LEU:HD13	3:E:98:TYR:OH	1.95	0.67
1:A:16:VAL:HG23	1:A:29:VAL:CG1	2.25	0.66
1:C:85:HIS:HB2	3:E:99:SER:HB3	1.77	0.66
1:A:53:LEU:CD1	1:A:62:ASP:HB3	2.25	0.66
1:C:52:LYS:HE2	3:E:53:TYR:HE1	1.59	0.66
1:C:56:LYS:NZ	1:C:75:LYS:NZ	2.44	0.66
4:F:83:GLU:HG2	4:F:106:VAL:HG13	1.77	0.66
1:A:56:LYS:NZ	1:A:75:LYS:NZ	2.44	0.66
1:A:36:PRO:HB2	1:A:297:TYR:HD1	1.58	0.66
1:A:85:HIS:HD2	1:A:86:GLU:HG3	1.61	0.66
3:H:166:PHE:CZ	4:L:135:LEU:HB3	2.29	0.66
2:D:373:SER:HB2	2:D:380:ALA:HB3	1.77	0.66
3:E:3:GLN:HB2	3:E:25:SER:HB2	1.78	0.66
2:B:373:SER:HB2	2:B:380:ALA:HB3	1.78	0.65
1:C:89:PRO:HG2	1:C:105:ARG:O	1.96	0.65
3:H:3:GLN:HB2	3:H:25:SER:HB2	1.78	0.65
1:A:14:HIS:CD2	1:A:28:GLY:HA2	2.31	0.65
4:F:33:VAL:HA	4:F:90:THR:HG22	1.78	0.65
1:A:214:ALA:O	1:A:215:ASN:ND2	2.30	0.65
1:C:16:VAL:HG13	1:C:327:LYS:O	1.97	0.65
1:C:85:HIS:HD2	1:C:86:GLU:HG3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:33:VAL:HA	4:L:90:THR:HG22	1.78	0.65
1:A:306:TYR:CE2	2:B:443:ILE:HD13	2.32	0.65
4:L:83:GLU:HG2	4:L:106:VAL:HG13	1.77	0.65
1:A:89:PRO:HG2	1:A:105:ARG:O	1.96	0.65
1:C:56:LYS:HZ3	1:C:75:LYS:NZ	1.95	0.65
1:A:20:THR:HG23	1:A:21:GLN:HG2	1.78	0.64
1:C:214:ALA:O	1:C:215:ASN:ND2	2.30	0.64
2:D:508:GLU:HG3	2:D:509:PHE:H	1.63	0.64
3:E:169:VAL:HA	4:F:162:THR:HG22	1.79	0.64
2:B:427:LEU:O	2:B:431:VAL:HG23	1.97	0.64
1:C:172:ILE:CG1	1:C:260:TYR:HE2	2.11	0.64
2:D:427:LEU:O	2:D:431:VAL:HG23	1.97	0.64
3:H:212:GLU:CG	3:H:213:PRO:HD2	2.28	0.64
3:E:212:GLU:CG	3:E:213:PRO:HD2	2.28	0.63
2:B:508:GLU:HG3	2:B:509:PHE:H	1.63	0.63
1:C:26:VAL:CG1	1:C:28:GLY:O	2.46	0.63
1:C:26:VAL:HA	1:C:332:THR:O	1.98	0.63
1:A:16:VAL:HG23	1:A:29:VAL:HG11	1.80	0.63
1:C:94:CYS:HA	1:C:142:SER:O	1.99	0.63
1:A:172:ILE:CG1	1:A:260:TYR:HE2	2.10	0.62
1:C:171:THR:O	1:C:172:ILE:CD1	2.46	0.62
1:A:94:CYS:HA	1:A:142:SER:O	1.99	0.62
4:F:106:VAL:O	4:F:106:VAL:CG2	2.48	0.61
1:A:16:VAL:CG2	1:A:29:VAL:HG11	2.30	0.61
1:A:171:THR:O	1:A:172:ILE:CD1	2.46	0.61
1:C:85:HIS:HB2	3:E:99:SER:OG	2.01	0.61
1:C:311:HIS:HB2	1:C:321:TRP:CD1	2.36	0.61
2:D:435:ARG:HD3	2:D:439:ILE:CG1	2.31	0.61
1:A:311:HIS:HB2	1:A:321:TRP:CD1	2.36	0.61
1:C:320:ILE:HD13	2:D:405:LEU:HD22	1.78	0.61
1:A:283:SER:CB	3:H:100:GLY:HA3	2.28	0.60
2:D:398:ASN:HD21	2:D:450:SER:HB3	1.66	0.60
2:B:398:ASN:HD21	2:B:450:SER:HB3	1.66	0.60
3:H:169:VAL:HA	4:L:162:THR:HG22	1.82	0.60
4:L:106:VAL:O	4:L:106:VAL:CG2	2.48	0.60
3:E:163:VAL:HG22	3:E:182:VAL:HG22	1.83	0.60
1:A:41:PHE:CZ	1:A:282:GLY:HA2	2.37	0.60
2:B:435:ARG:HD3	2:B:439:ILE:CG1	2.31	0.60
1:C:280:ILE:CD1	1:C:315:ILE:CG1	2.73	0.60
1:A:119:LEU:CD2	1:A:269:LYS:HB3	2.27	0.59
1:C:70:PRO:HB2	1:C:144:PRO:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:83:GLU:CG	4:L:106:VAL:HG13	2.32	0.59
1:A:16:VAL:HG21	1:A:29:VAL:HG12	1.82	0.59
1:A:26:VAL:CG1	1:A:28:GLY:O	2.48	0.59
1:A:280:ILE:CD1	1:A:315:ILE:CG1	2.73	0.59
2:B:418:ASP:O	2:B:422:ASN:ND2	2.36	0.59
2:D:418:ASP:O	2:D:422:ASN:ND2	2.35	0.59
3:H:163:VAL:HG22	3:H:182:VAL:HG22	1.83	0.59
1:A:70:PRO:HB2	1:A:144:PRO:O	2.01	0.59
1:C:41:PHE:CZ	1:C:282:GLY:HA2	2.37	0.59
4:F:83:GLU:CG	4:F:106:VAL:HG13	2.32	0.59
2:B:421:HIS:HB3	2:B:424:ILE:HD12	1.84	0.59
1:A:56:LYS:HZ3	1:A:75:LYS:HZ2	1.51	0.59
2:D:421:HIS:HB3	2:D:424:ILE:HD12	1.84	0.59
1:A:283:SER:O	3:H:100(F):TYR:OH	2.20	0.58
1:C:25:ASN:O	1:C:333:LYS:HA	2.02	0.58
3:H:212:GLU:HG3	3:H:213:PRO:HD2	1.85	0.58
1:C:281:LYS:CD	2:D:412:ARG:NH2	2.65	0.58
2:B:421:HIS:O	2:B:425:LEU:CG	2.48	0.58
3:E:193:THR:HG22	3:E:210:ARG:HH22	1.69	0.58
1:C:16:VAL:CG2	1:C:29:VAL:CG1	2.81	0.58
1:A:155:THR:HG23	1:A:187:VAL:HB	1.84	0.58
1:C:119:LEU:CD2	1:C:269:LYS:HB3	2.26	0.58
1:A:281:LYS:CD	2:B:412:ARG:NH2	2.65	0.58
1:C:292:CYS:SG	1:C:300:LEU:HD23	2.44	0.58
1:A:131:PRO:CD	1:A:172:ILE:HD11	2.34	0.57
1:C:131:PRO:CD	1:C:172:ILE:HD11	2.34	0.57
1:C:328:LEU:HD11	2:D:454:ILE:HD12	1.87	0.57
1:A:85:HIS:HB2	3:H:99:SER:OG	2.05	0.57
3:E:212:GLU:HG3	3:E:213:PRO:HD2	1.85	0.57
3:H:193:THR:HG22	3:H:210:ARG:HH22	1.69	0.57
1:A:18:THR:HG22	2:B:451:ASN:HB3	1.86	0.56
1:A:104:ILE:HD13	1:A:245:VAL:HG12	1.87	0.56
1:A:320:ILE:HD12	2:B:405:LEU:HD22	1.81	0.56
1:C:155:THR:HG23	1:C:187:VAL:HB	1.84	0.56
1:C:131:PRO:CG	1:C:172:ILE:CD1	2.71	0.56
3:H:214:LYS:HZ3	4:L:211:CYS:C	2.13	0.56
1:A:292:CYS:SG	1:A:300:LEU:HD23	2.44	0.56
1:C:19:ALA:N	2:D:448:LEU:HB3	2.20	0.56
1:A:197:GLN:HA	1:A:197:GLN:OE1	2.06	0.56
1:C:197:GLN:OE1	1:C:197:GLN:HA	2.06	0.56
1:C:280:ILE:HD12	1:C:315:ILE:CG1	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:VAL:HG23	1:C:29:VAL:CG1	2.35	0.56
1:C:104:ILE:HD13	1:C:245:VAL:HG12	1.87	0.56
1:C:59:ASN:OD1	3:E:73:THR:CG2	2.53	0.56
3:H:36:TRP:CE2	3:H:80:MET:HB2	2.41	0.56
1:A:25:ASN:O	1:A:333:LYS:HA	2.05	0.56
3:E:166:PHE:CZ	4:F:135:LEU:HB3	2.41	0.56
1:C:16:VAL:CG2	1:C:29:VAL:HG12	2.36	0.55
2:D:508:GLU:HG3	2:D:509:PHE:CD1	2.42	0.55
3:E:36:TRP:CE2	3:E:80:MET:HB2	2.41	0.55
1:C:19:ALA:H	2:D:448:LEU:HB3	1.71	0.55
2:D:421:HIS:O	2:D:425:LEU:CG	2.48	0.55
2:D:476:SER:HB3	2:D:511:LEU:HD13	1.89	0.55
1:C:145:ASN:O	1:C:146:ILE:C	2.50	0.55
4:L:83:GLU:HG2	4:L:106:VAL:CG1	2.37	0.55
2:B:435:ARG:HD3	2:B:439:ILE:HG13	1.89	0.55
3:E:200:HIS:NE2	3:E:202:PRO:HG2	2.22	0.55
1:A:145:ASN:O	1:A:146:ILE:C	2.50	0.55
1:C:103:LYS:NZ	1:C:246:ASP:OD1	2.38	0.55
1:C:26:VAL:O	1:C:28:GLY:N	2.41	0.54
3:H:200:HIS:NE2	3:H:202:PRO:HG2	2.22	0.54
2:B:476:SER:HB3	2:B:511:LEU:HD13	1.89	0.54
1:C:280:ILE:HD11	1:C:315:ILE:CG1	2.37	0.54
1:C:278:LYS:HD2	2:D:411:GLN:HE21	1.67	0.54
1:C:16:VAL:HG23	1:C:29:VAL:HG11	1.89	0.54
1:A:59:ASN:OD1	3:H:73:THR:CG2	2.56	0.54
2:D:410:LEU:HG	2:D:432:ASP:OD2	2.08	0.54
2:D:435:ARG:HD3	2:D:439:ILE:HG13	1.89	0.54
4:F:83:GLU:HG2	4:F:106:VAL:CG1	2.37	0.54
3:H:35:THR:HG22	3:H:50:TRP:HB2	1.88	0.54
2:B:508:GLU:HG3	2:B:509:PHE:CD1	2.42	0.54
1:A:20:THR:HG21	2:B:452:GLU:HG2	1.76	0.53
1:C:283:SER:O	3:E:100(F):TYR:OH	2.26	0.53
3:E:35:THR:HG22	3:E:50:TRP:HB2	1.89	0.53
1:A:284:LEU:CB	1:A:285:PRO:HA	2.36	0.53
2:B:410:LEU:HG	2:B:432:ASP:OD2	2.08	0.53
2:D:422:ASN:HA	2:D:425:LEU:HD12	1.90	0.53
1:C:124:VAL:HG12	1:C:177:ILE:CG1	2.26	0.53
2:D:508:GLU:HG3	2:D:509:PHE:N	2.24	0.53
1:C:85:HIS:CD2	1:C:86:GLU:HG3	2.42	0.53
1:A:18:THR:CG2	2:B:451:ASN:HB3	2.39	0.53
1:A:240:SER:OG	6:K:1:NAG:C8	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ILE:HD12	1:A:315:ILE:CG1	2.30	0.53
1:C:18:THR:HG22	2:D:451:ASN:HB3	1.89	0.53
1:C:306:TYR:CE2	2:D:443:ILE:HD13	2.44	0.53
2:B:408:LYS:O	2:B:435:ARG:NH2	2.42	0.52
2:B:422:ASN:HA	2:B:425:LEU:HD12	1.90	0.52
1:C:16:VAL:CG1	1:C:327:LYS:O	2.58	0.52
3:H:123:PRO:O	4:L:121:SER:HB3	2.10	0.52
1:A:280:ILE:CG2	1:A:295:GLU:HG3	2.39	0.52
2:B:508:GLU:CG	2:B:509:PHE:H	2.22	0.52
1:C:26:VAL:C	1:C:28:GLY:N	2.67	0.52
1:A:16:VAL:CG1	1:A:327:LYS:O	2.57	0.52
1:A:208:GLN:HB3	1:A:261:GLN:HB2	1.92	0.52
1:C:53:LEU:HD11	1:C:62:ASP:HB3	1.91	0.52
1:A:20:THR:HG22	2:B:452:GLU:HG2	1.71	0.52
2:D:508:GLU:CG	2:D:509:PHE:H	2.22	0.52
1:A:85:HIS:CD2	1:A:86:GLU:HG3	2.42	0.52
1:A:53:LEU:HD11	1:A:62:ASP:HB3	1.91	0.52
1:A:103:LYS:NZ	1:A:246:ASP:OD1	2.38	0.52
1:C:208:GLN:HB3	1:C:261:GLN:HB2	1.92	0.52
3:H:115:SER:O	3:H:115:SER:OG	2.23	0.52
1:A:52:LYS:HE2	3:H:53:TYR:CE1	2.38	0.51
2:B:439:ILE:O	2:B:443:ILE:HG13	2.10	0.51
4:L:28:ILE:HG12	4:L:90:THR:HG21	1.92	0.51
1:A:197:GLN:CD	6:K:1:NAG:O7	2.54	0.51
1:A:280:ILE:HD11	1:A:315:ILE:CG1	2.37	0.51
2:B:508:GLU:HG3	2:B:509:PHE:N	2.24	0.51
1:C:285:PRO:O	3:E:100(F):TYR:OH	2.21	0.51
3:E:115:SER:O	3:E:115:SER:OG	2.23	0.51
1:C:16:VAL:HG22	1:C:327:LYS:HB2	1.92	0.51
1:A:94:CYS:O	1:A:235:GLY:N	2.43	0.51
1:A:320:ILE:HD13	2:B:405:LEU:HD22	1.81	0.51
1:A:26:VAL:O	1:A:28:GLY:N	2.44	0.51
1:C:56:LYS:HZ3	1:C:75:LYS:HZ2	1.58	0.51
2:D:408:LYS:O	2:D:435:ARG:NH2	2.42	0.51
1:C:131:PRO:O	1:C:170:LEU:HD13	2.11	0.51
1:C:197:GLN:CD	5:P:1:NAG:O7	2.54	0.51
1:C:97:ILE:HA	1:C:243:ILE:HG23	1.93	0.51
1:A:26:VAL:C	1:A:28:GLY:N	2.69	0.51
2:D:416:ALA:O	2:D:421:HIS:ND1	2.43	0.51
2:D:439:ILE:O	2:D:443:ILE:HG13	2.10	0.51
4:F:28:ILE:HG12	4:F:90:THR:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:167:PRO:CG	4:L:165:SER:OG	2.55	0.51
1:A:285:PRO:O	3:H:100(F):TYR:OH	2.22	0.50
2:B:416:ALA:O	2:B:421:HIS:ND1	2.43	0.50
1:A:105:ARG:NH2	1:A:233:GLU:OE1	2.45	0.50
1:C:59:ASN:OD1	3:E:73:THR:HG23	2.11	0.50
1:A:59:ASN:OD1	3:H:73:THR:HG23	2.12	0.50
1:A:131:PRO:O	1:A:170:LEU:HD13	2.11	0.50
1:C:94:CYS:O	1:C:235:GLY:N	2.43	0.50
1:A:149:GLY:HA3	5:G:1:NAG:O6	2.11	0.50
1:C:16:VAL:CG2	1:C:29:VAL:HG11	2.41	0.50
1:C:105:ARG:NH2	1:C:233:GLU:OE1	2.44	0.50
1:C:18:THR:CG2	2:D:451:ASN:HB3	2.41	0.50
1:C:149:GLY:HA3	6:M:1:NAG:O6	2.11	0.50
1:C:240:SER:OG	5:P:1:NAG:C8	2.51	0.50
4:F:144:VAL:HG12	4:F:197:HIS:HB2	1.94	0.50
3:E:95:ASP:OD2	3:E:100(B):TYR:OH	2.30	0.50
3:H:212:GLU:HG2	3:H:213:PRO:HD2	1.93	0.50
1:A:124:VAL:HG12	1:A:177:ILE:CG1	2.26	0.49
3:E:167:PRO:CG	4:F:165:SER:OG	2.53	0.49
3:H:6:GLN:OE1	3:H:104:SER:OG	2.29	0.49
3:H:171:GLN:HG3	4:L:160:GLU:HG3	1.93	0.49
1:C:215:ASN:ND2	1:C:215:ASN:C	2.63	0.49
3:E:171:GLN:HG3	4:F:160:GLU:HG3	1.93	0.49
1:A:131:PRO:HD2	1:A:172:ILE:HD11	1.94	0.49
3:H:169:VAL:HG11	4:L:177:TYR:CD1	2.47	0.49
1:C:131:PRO:HD2	1:C:172:ILE:HD11	1.94	0.49
4:F:105:THR:CG2	4:F:141:PRO:HB3	2.28	0.49
1:A:97:ILE:HA	1:A:243:ILE:HG23	1.93	0.49
1:A:172:ILE:HG13	1:A:260:TYR:CE2	2.44	0.49
3:E:12:LYS:HE2	3:E:17:SER:O	2.12	0.49
4:L:144:VAL:HG12	4:L:197:HIS:HB2	1.94	0.49
1:C:16:VAL:HG22	1:C:327:LYS:CB	2.42	0.49
3:E:6:GLN:OE1	3:E:104:SER:OG	2.29	0.49
1:C:53:LEU:HG	1:C:62:ASP:CG	2.38	0.49
1:C:97:ILE:HA	1:C:243:ILE:CG2	2.43	0.49
1:C:280:ILE:CG2	1:C:295:GLU:HG3	2.39	0.48
3:H:12:LYS:HE2	3:H:17:SER:O	2.12	0.48
1:C:36:PRO:HB2	1:C:297:TYR:CE1	2.48	0.48
3:E:212:GLU:HG2	3:E:213:PRO:HD2	1.94	0.48
3:H:214:LYS:HG3	4:L:211:CYS:SG	2.52	0.48
1:A:53:LEU:HG	1:A:62:ASP:CG	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PRO:CG	1:A:172:ILE:CD1	2.72	0.48
1:A:163(C):ASN:O	1:A:165:THR:HG22	2.14	0.48
1:C:172:ILE:HG13	1:C:260:TYR:CE2	2.44	0.48
1:A:36:PRO:HB2	1:A:297:TYR:CE1	2.48	0.48
3:H:100(G):TYR:HB3	4:L:34:TYR:CZ	2.49	0.47
1:C:52:LYS:HD3	1:C:62:ASP:OD1	2.14	0.47
1:A:16:VAL:HG22	1:A:327:LYS:CB	2.44	0.47
1:C:163(C):ASN:O	1:C:165:THR:HG22	2.14	0.47
1:C:16:VAL:HG21	1:C:29:VAL:HG12	1.95	0.47
1:C:63:LEU:HA	1:C:108:PRO:HG3	1.96	0.47
1:C:182:GLU:HG2	1:C:274:SER:HB3	1.96	0.47
1:A:63:LEU:HA	1:A:108:PRO:HG3	1.95	0.47
1:C:30:ILE:HG13	1:C:330:ASN:HB2	1.97	0.47
1:A:52:LYS:HD3	1:A:62:ASP:OD1	2.14	0.47
1:A:122:HIS:O	1:A:269:LYS:HD3	2.15	0.47
2:B:435:ARG:HD3	2:B:439:ILE:HG12	1.96	0.47
1:C:193:ASP:OD1	1:C:198:MET:HB2	2.14	0.47
1:A:81:VAL:CG1	1:A:315:ILE:HD11	2.45	0.47
1:A:193:ASP:OD1	1:A:198:MET:HB2	2.14	0.47
2:D:435:ARG:HD3	2:D:439:ILE:HG12	1.96	0.47
1:C:141:GLY:C	1:C:143:CYS:H	2.23	0.47
1:A:97:ILE:HA	1:A:243:ILE:CG2	2.44	0.47
1:C:122:HIS:O	1:C:269:LYS:HD3	2.15	0.47
1:C:178:CYS:SG	1:C:184:GLN:HG3	2.55	0.47
3:E:100(G):TYR:HB3	4:F:34:TYR:CZ	2.50	0.47
1:A:313:LYS:HB3	2:B:411:GLN:HA	1.98	0.46
1:C:81:VAL:CG1	1:C:315:ILE:HD11	2.45	0.46
3:H:95:ASP:OD2	3:H:100(B):TYR:OH	2.30	0.46
1:A:215:ASN:ND2	1:A:215:ASN:C	2.63	0.46
1:C:114:TYR:CG	1:C:273:ALA:HB1	2.51	0.46
1:C:158:TRP:CD1	1:C:158:TRP:C	2.92	0.46
1:A:12:SER:HB2	1:A:334:TYR:HB2	1.96	0.46
1:A:292:CYS:HB3	1:A:300:LEU:HD23	1.98	0.46
1:C:103:LYS:HG3	1:C:247:TYR:CE1	2.50	0.46
1:C:197:GLN:HE21	5:P:1:NAG:H81	1.81	0.46
1:A:30:ILE:HG13	1:A:330:ASN:HB2	1.97	0.46
1:A:103:LYS:HG3	1:A:247:TYR:CE1	2.50	0.46
1:A:182:GLU:HG2	1:A:274:SER:HB3	1.96	0.46
1:C:135:TYR:CD1	1:C:159:ALA:HB1	2.50	0.46
1:C:278:LYS:HD2	2:D:411:GLN:CD	2.39	0.46
4:L:204:LYS:HD3	4:L:204:LYS:HA	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLY:C	1:A:143:CYS:H	2.23	0.46
1:A:250:GLN:O	1:A:251:LYS:O	2.33	0.46
1:C:184:GLN:NE2	1:C:270:VAL:HG11	2.31	0.46
3:E:169:VAL:HG11	4:F:177:TYR:CD1	2.50	0.46
1:A:114:TYR:CG	1:A:273:ALA:HB1	2.51	0.46
1:A:158:TRP:CD1	1:A:158:TRP:C	2.92	0.46
1:A:184:GLN:NE2	1:A:270:VAL:HG11	2.31	0.46
1:A:231:GLN:HG2	1:A:242:ARG:NH2	2.31	0.46
1:C:231:GLN:HG2	1:C:242:ARG:NH2	2.31	0.46
1:C:250:GLN:O	1:C:251:LYS:O	2.33	0.46
1:A:178:CYS:SG	1:A:184:GLN:HG3	2.55	0.46
1:A:16:VAL:HG22	1:A:327:LYS:HB2	1.98	0.45
1:A:135:TYR:CD1	1:A:159:ALA:HB1	2.50	0.45
2:B:407:VAL:HG12	2:B:435:ARG:HH21	1.82	0.45
1:C:61:THR:O	1:C:64:ASP:HB2	2.16	0.45
3:E:116:THR:HA	3:E:146:PHE:O	2.17	0.45
1:C:292:CYS:HB3	1:C:300:LEU:HD23	1.98	0.45
2:D:407:VAL:HG12	2:D:435:ARG:HH21	1.82	0.45
1:A:59:ASN:OD1	3:H:30:THR:CG2	2.62	0.45
1:C:131:PRO:CD	1:C:172:ILE:CD1	2.95	0.45
1:A:61:THR:O	1:A:64:ASP:HB2	2.16	0.45
1:A:313:LYS:HD3	2:B:412:ARG:N	2.32	0.45
1:C:140:SER:C	1:C:141:GLY:O	2.60	0.45
1:A:131:PRO:CD	1:A:172:ILE:CD1	2.95	0.45
1:C:176:TYR:OH	1:C:182:GLU:O	2.35	0.45
1:C:26:VAL:HG21	1:C:329:ALA:HB1	1.99	0.45
1:C:131:PRO:HD2	1:C:172:ILE:CD1	2.47	0.45
1:C:72:CYS:O	1:C:73:THR:HG23	2.17	0.44
1:C:165:THR:HA	1:C:203:GLY:HA3	1.99	0.44
1:C:231:GLN:HB3	1:C:234:ASP:OD2	2.18	0.44
3:E:51:ILE:HB	3:E:57:THR:HG22	1.99	0.44
1:A:147:THR:O	1:A:148:ASN:OD1	2.36	0.44
1:A:165:THR:HA	1:A:203:GLY:HA3	1.98	0.44
1:A:72:CYS:O	1:A:73:THR:HG23	2.17	0.44
1:C:20:THR:HB	2:D:452:GLU:CG	2.45	0.44
4:F:49:TYR:CE1	4:F:53:GLN:HB3	2.52	0.44
4:L:39:PHE:O	4:L:42:THR:OG1	2.33	0.44
3:H:17:SER:HB3	3:H:82(A):ARG:HA	2.00	0.44
1:C:165:THR:OG1	1:C:166:ALA:N	2.51	0.44
4:F:194:GLN:HB3	4:F:203:GLU:HG3	2.00	0.44
3:H:51:ILE:HB	3:H:57:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PRO:HD2	1:A:172:ILE:CD1	2.47	0.44
1:C:185:ILE:HB	1:C:271:TRP:HB2	2.00	0.44
3:H:117:LYS:HB3	3:H:117:LYS:HE2	1.86	0.44
2:B:444:GLU:O	2:B:448:LEU:HG	2.17	0.43
3:E:123:PRO:O	4:F:121:SER:HB3	2.18	0.43
4:L:169:ASN:OD1	4:L:171:LYS:HB2	2.18	0.43
1:A:140:SER:C	1:A:141:GLY:O	2.60	0.43
1:A:185:ILE:HB	1:A:271:TRP:HB2	2.00	0.43
4:L:49:TYR:CE1	4:L:53:GLN:HB3	2.52	0.43
1:C:17:LYS:O	2:D:448:LEU:HD23	2.18	0.43
1:C:95:PHE:CD1	1:C:96:PRO:HD2	2.53	0.43
4:L:105:THR:CG2	4:L:141:PRO:HB3	2.36	0.43
1:C:320:ILE:HD13	2:D:405:LEU:CD2	2.44	0.43
1:A:95:PHE:CD1	1:A:96:PRO:HD2	2.53	0.43
1:C:59:ASN:CG	3:E:73:THR:CG2	2.92	0.43
1:C:125:ILE:O	1:C:268:GLN:NE2	2.47	0.43
1:C:131:PRO:C	1:C:170:LEU:HD13	2.44	0.43
1:C:320:ILE:HG21	2:D:443:ILE:HD11	2.01	0.43
3:E:117:LYS:HB3	3:E:117:LYS:HE2	1.86	0.43
1:A:165:THR:OG1	1:A:166:ALA:N	2.51	0.43
2:D:444:GLU:O	2:D:448:LEU:HG	2.17	0.43
4:F:169:ASN:OD1	4:F:171:LYS:HB2	2.18	0.43
3:H:116:THR:HA	3:H:146:PHE:O	2.17	0.43
3:H:135:THR:OG1	3:H:183:THR:HG23	2.19	0.43
2:D:496:LEU:HD12	2:D:499:ILE:HD12	2.01	0.43
4:L:35:TRP:HB2	4:L:48:ILE:HB	2.00	0.43
1:A:48:GLU:H	1:A:48:GLU:HG2	1.69	0.43
1:A:328:LEU:HD11	2:B:454:ILE:HD12	2.00	0.43
2:B:496:LEU:HD12	2:B:499:ILE:HD12	2.01	0.43
1:C:81:VAL:HG13	1:C:315:ILE:CD1	2.49	0.43
3:E:17:SER:HB3	3:E:82(A):ARG:HA	2.00	0.43
1:A:231:GLN:HB3	1:A:234:ASP:OD2	2.18	0.43
3:E:135:THR:OG1	3:E:183:THR:HG23	2.19	0.43
4:F:204:LYS:HD3	4:F:204:LYS:HA	1.77	0.43
2:D:508:GLU:CG	2:D:509:PHE:N	2.81	0.43
1:A:90:VAL:HG12	1:A:91:THR:O	2.19	0.42
1:A:131:PRO:C	1:A:170:LEU:HD13	2.43	0.42
2:B:508:GLU:CG	2:B:509:PHE:N	2.82	0.42
1:C:147:THR:O	1:C:148:ASN:OD1	2.36	0.42
1:C:292:CYS:CB	1:C:300:LEU:HD23	2.49	0.42
2:D:387:SER:HB2	2:D:465:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ASN:OD1	1:A:150:ASN:N	2.50	0.42
1:A:155:THR:HG21	1:A:187:VAL:HB	1.97	0.42
2:B:387:SER:HB2	2:B:465:LEU:HD11	2.01	0.42
1:C:12:SER:HB2	1:C:334:TYR:HB2	2.01	0.42
1:C:329:ALA:N	2:D:451:ASN:OD1	2.43	0.42
1:A:17:LYS:O	2:B:448:LEU:HD23	2.18	0.42
1:A:59:ASN:CG	3:H:73:THR:CG2	2.93	0.42
4:L:113:PRO:HB3	4:L:139:PHE:HB3	2.01	0.42
4:L:194:GLN:HB3	4:L:203:GLU:HG3	2.00	0.42
1:C:57:CYS:O	1:C:60:CYS:HB2	2.20	0.42
1:C:107:LEU:HB3	1:C:108:PRO:HD3	2.01	0.42
1:C:150:ASN:OD1	1:C:150:ASN:N	2.50	0.42
4:F:39:PHE:O	4:F:42:THR:OG1	2.33	0.42
3:H:212:GLU:CG	3:H:213:PRO:CD	2.97	0.42
1:A:320:ILE:HD13	2:B:405:LEU:CD2	2.42	0.42
1:C:284:LEU:CB	1:C:285:PRO:HA	2.36	0.42
4:L:132:LEU:HD12	4:L:178:LEU:HD23	2.02	0.42
1:A:292:CYS:CB	1:A:300:LEU:HD23	2.49	0.42
4:F:35:TRP:HB2	4:F:48:ILE:HB	2.00	0.42
1:A:81:VAL:HG13	1:A:315:ILE:CD1	2.49	0.42
1:C:90:VAL:HG12	1:C:91:THR:O	2.19	0.42
2:D:435:ARG:CD	2:D:439:ILE:HG13	2.50	0.42
1:A:145:ASN:O	1:A:147:THR:N	2.52	0.42
1:C:15:VAL:HG22	1:C:23:GLU:HG2	2.02	0.42
1:C:59:ASN:OD1	3:E:30:THR:CG2	2.65	0.42
1:C:81:VAL:HG11	1:C:315:ILE:HD11	2.02	0.42
3:H:82(C):LEU:HA	3:H:86:ASP:OD2	2.20	0.42
2:D:440:SER:O	2:D:444:GLU:HG3	2.20	0.41
3:E:169:VAL:CA	4:F:162:THR:HG22	2.47	0.41
3:H:214:LYS:NZ	4:L:211:CYS:C	2.78	0.41
1:C:281:LYS:HB2	1:C:295:GLU:HG2	2.02	0.41
4:F:132:LEU:HD12	4:F:178:LEU:HD23	2.02	0.41
1:A:176:TYR:OH	1:A:182:GLU:O	2.35	0.41
1:A:20:THR:CG2	1:A:21:GLN:HG2	2.47	0.41
1:A:81:VAL:HG11	1:A:315:ILE:HD11	2.02	0.41
1:A:107:LEU:HB3	1:A:108:PRO:HD3	2.01	0.41
2:B:440:SER:O	2:B:444:GLU:HG3	2.20	0.41
1:C:145:ASN:O	1:C:147:THR:N	2.53	0.41
3:E:82(C):LEU:HA	3:E:86:ASP:OD2	2.19	0.41
4:F:113:PRO:HB3	4:F:139:PHE:HB3	2.02	0.41
1:A:57:CYS:O	1:A:60:CYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ILE:HD11	1:A:265:LEU:CD1	2.47	0.41
1:A:285:PRO:HD3	3:H:96:VAL:O	2.21	0.41
1:C:171:THR:C	1:C:172:ILE:HG12	2.46	0.41
2:D:472:MET:H	2:D:472:MET:HG2	1.70	0.41
3:E:169:VAL:HG11	4:F:177:TYR:CE1	2.56	0.41
1:A:53:LEU:O	1:A:76:ILE:HG23	2.21	0.41
1:A:225:ILE:HA	1:A:225:ILE:HD13	1.71	0.41
3:E:212:GLU:CG	3:E:213:PRO:CD	2.97	0.41
1:A:172:ILE:CG1	1:A:260:TYR:CE2	2.97	0.41
1:C:41:PHE:CE1	1:C:282:GLY:HA2	2.56	0.41
1:C:53:LEU:O	1:C:76:ILE:HG23	2.21	0.41
4:F:118:PHE:HB2	4:F:133:VAL:HB	2.03	0.41
1:A:15:VAL:HG22	1:A:23:GLU:HG2	2.02	0.41
1:A:17:LYS:C	2:B:448:LEU:HD23	2.46	0.41
1:A:125:ILE:O	1:A:268:GLN:NE2	2.47	0.41
2:B:409:ASN:O	2:B:410:LEU:HB2	2.21	0.41
2:B:435:ARG:CD	2:B:439:ILE:HG13	2.50	0.41
1:C:197:GLN:NE2	5:P:1:NAG:H81	2.35	0.41
4:F:91:TRP:CZ3	4:F:95(B):GLY:HA2	2.56	0.41
4:L:81:GLU:CD	4:L:81:GLU:H	2.29	0.41
1:C:16:VAL:HG12	1:C:17:LYS:N	2.36	0.41
1:C:52:LYS:HE2	3:E:53:TYR:CE1	2.39	0.41
3:E:124:LEU:HB3	4:F:118:PHE:CD1	2.56	0.41
3:E:40:ALA:HB3	3:E:43:GLN:HG3	2.03	0.40
3:H:40:ALA:HB3	3:H:43:GLN:HG3	2.03	0.40
1:C:93:GLY:HA2	1:C:234:ASP:C	2.46	0.40
4:F:19:VAL:HG21	4:F:104:LEU:CD1	2.52	0.40
4:L:19:VAL:HG21	4:L:104:LEU:CD1	2.52	0.40
1:A:16:VAL:HG12	1:A:17:LYS:N	2.36	0.40
2:B:418:ASP:HA	2:B:425:LEU:HD11	2.03	0.40
2:D:418:ASP:HA	2:D:425:LEU:HD11	2.03	0.40
1:A:281:LYS:HB2	1:A:295:GLU:HG2	2.02	0.40
4:F:151:ASP:HB2	4:F:152:SER:H	1.71	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 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	331/347 (95%)	303 (92%)	22 (7%)	6 (2%)	6	33
1	C	331/347 (95%)	303 (92%)	22 (7%)	6 (2%)	6	33
2	B	133/179 (74%)	128 (96%)	5 (4%)	0	100	100
2	D	134/179 (75%)	129 (96%)	5 (4%)	0	100	100
3	E	214/234 (92%)	202 (94%)	11 (5%)	1 (0%)	24	63
3	H	215/234 (92%)	203 (94%)	11 (5%)	1 (0%)	24	63
4	F	209/216 (97%)	202 (97%)	7 (3%)	0	100	100
4	L	210/216 (97%)	203 (97%)	7 (3%)	0	100	100
All	All	1777/1952 (91%)	1673 (94%)	90 (5%)	14 (1%)	16	53

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	ILE
1	A	251	LYS
1	C	177	ILE
1	C	251	LYS
1	A	148	ASN
1	C	148	ASN
3	E	116	THR
3	H	116	THR
1	A	45	LYS
1	A	146	ILE
1	A	147	THR
1	C	45	LYS
1	C	146	ILE
1	C	147	THR

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	284/294 (97%)	271 (95%)	13 (5%)	24	45
1	C	284/294 (97%)	272 (96%)	12 (4%)	26	48
2	B	116/143 (81%)	112 (97%)	4 (3%)	32	54
2	D	117/143 (82%)	113 (97%)	4 (3%)	32	54
3	E	185/198 (93%)	176 (95%)	9 (5%)	22	43
3	H	186/198 (94%)	177 (95%)	9 (5%)	23	44
4	F	180/183 (98%)	175 (97%)	5 (3%)	38	59
4	L	181/183 (99%)	177 (98%)	4 (2%)	45	64
All	All	1533/1636 (94%)	1473 (96%)	60 (4%)	28	49

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	54	CYS
1	A	87	VAL
1	A	105	ARG
1	A	117	ILE
1	A	125	ILE
1	A	136	LYS
1	A	196	THR
1	A	215	ASN
1	A	239	GLN
1	A	266	LEU
1	A	270	VAL
1	A	295	GLU
2	B	421	HIS
2	B	431	VAL
2	B	435	ARG
2	B	463	LEU
1	C	52	LYS
1	C	54	CYS

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Mol	Chain	Res	Type
1	C	87	VAL
1	C	105	ARG
1	C	117	ILE
1	C	125	ILE
1	C	136	LYS
1	C	215	ASN
1	C	239	GLN
1	C	266	LEU
1	C	270	VAL
1	C	295	GLU
2	D	421	HIS
2	D	431	VAL
2	D	435	ARG
2	D	463	LEU
3	E	62	LYS
3	E	71	LYS
3	E	94	ARG
3	E	140	CYS
3	E	143	LYS
3	E	151	THR
3	E	171	GLN
3	E	178	LEU
3	E	183	THR
4	F	1	GLN
4	F	19	VAL
4	F	81	GLU
4	F	106	VAL
4	F	129	LYS
3	H	62	LYS
3	H	71	LYS
3	H	94	ARG
3	H	140	CYS
3	H	143	LYS
3	H	151	THR
3	H	171	GLN
3	H	178	LEU
3	H	183	THR
4	L	19	VAL
4	L	81	GLU
4	L	106	VAL
4	L	129	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	40	HIS
1	A	85	HIS
1	A	126	ASN
1	A	129	ASN
1	A	220	HIS
2	B	398	ASN
2	B	409	ASN
2	B	422	ASN
1	C	14	HIS
1	C	40	HIS
1	C	126	ASN
1	C	129	ASN
1	C	220	HIS
2	D	398	ASN
2	D	409	ASN
2	D	422	ASN
3	E	39	GLN
3	E	171	GLN
4	F	38	GLN
3	H	39	GLN
3	H	171	GLN
4	L	38	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 ⓘ

18 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	$\# Z > 2$
5	NAG	G	1	1,5	14,14,15	0.53	0	17,19,21	0.96	1 (5%)
5	NAG	G	2	5	14,14,15	0.48	0	17,19,21	0.88	1 (5%)
5	NAG	I	1	1,5	14,14,15	0.39	0	17,19,21	1.82	3 (17%)
5	NAG	I	2	5	14,14,15	0.43	0	17,19,21	1.29	3 (17%)
5	NAG	J	1	1,5	14,14,15	0.54	0	17,19,21	0.97	1 (5%)
5	NAG	J	2	5	14,14,15	0.48	0	17,19,21	0.88	1 (5%)
6	NAG	K	1	6,1	14,14,15	0.50	0	17,19,21	2.28	3 (17%)
6	NAG	K	2	6	14,14,15	0.50	0	17,19,21	1.35	3 (17%)
6	BMA	K	3	6	11,11,12	0.66	0	15,15,17	1.43	3 (20%)
6	NAG	M	1	6,1	14,14,15	0.53	0	17,19,21	0.95	1 (5%)
6	NAG	M	2	6	14,14,15	0.48	0	17,19,21	0.88	1 (5%)
6	BMA	M	3	6	11,11,12	0.57	0	15,15,17	0.75	0
5	NAG	N	1	1,5	14,14,15	0.39	0	17,19,21	1.82	3 (17%)
5	NAG	N	2	5	14,14,15	0.42	0	17,19,21	1.29	3 (17%)
5	NAG	O	1	1,5	14,14,15	0.52	0	17,19,21	0.96	1 (5%)
5	NAG	O	2	5	14,14,15	0.48	0	17,19,21	0.87	1 (5%)
5	NAG	P	1	1,5	14,14,15	0.51	0	17,19,21	2.28	3 (17%)
5	NAG	P	2	5	14,14,15	0.49	0	17,19,21	1.34	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	G	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	G	2	5	-	3/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	NAG	J	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	J	2	5	-	3/6/23/26	0/1/1/1
6	NAG	K	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
6	BMA	K	3	6	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	M	1	6,1	-	3/6/23/26	0/1/1/1
6	NAG	M	2	6	-	3/6/23/26	0/1/1/1
6	BMA	M	3	6	-	0/2/19/22	0/1/1/1
5	NAG	N	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
5	NAG	O	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	O	2	5	-	3/6/23/26	0/1/1/1
5	NAG	P	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	1	NAG	O5-C1-C2	-7.54	99.63	111.29
6	K	1	NAG	O5-C1-C2	-7.53	99.64	111.29
5	I	1	NAG	C1-O5-C5	6.01	120.24	112.19
5	N	1	NAG	C1-O5-C5	5.99	120.21	112.19
5	J	1	NAG	C1-O5-C5	3.23	116.52	112.19
5	O	1	NAG	C1-O5-C5	3.21	116.48	112.19
6	M	1	NAG	C1-O5-C5	3.19	116.46	112.19
5	G	1	NAG	C1-O5-C5	3.18	116.44	112.19
6	K	2	NAG	O5-C5-C6	-3.12	101.59	107.66
5	P	2	NAG	O5-C5-C6	-3.09	101.66	107.66
6	K	1	NAG	O7-C7-C8	-2.90	116.88	122.05
5	P	1	NAG	O7-C7-C8	-2.89	116.91	122.05
6	K	3	BMA	O2-C2-C3	2.84	116.02	110.15
5	N	2	NAG	C2-N2-C7	-2.67	119.32	122.90
6	K	1	NAG	C4-C3-C2	-2.66	107.12	111.02
6	K	3	BMA	O4-C4-C5	-2.66	102.77	109.32
5	P	1	NAG	C4-C3-C2	-2.64	107.15	111.02
5	I	2	NAG	C2-N2-C7	-2.62	119.39	122.90
5	N	1	NAG	O5-C5-C4	2.44	116.75	110.83
5	I	1	NAG	O5-C5-C4	2.41	116.70	110.83
5	N	2	NAG	O5-C1-C2	-2.40	107.58	111.29
5	J	2	NAG	C2-N2-C7	-2.37	119.72	122.90
5	P	2	NAG	O5-C1-C2	-2.37	107.63	111.29
6	K	2	NAG	O5-C1-C2	-2.37	107.63	111.29
5	I	2	NAG	O5-C1-C2	-2.33	107.69	111.29
5	O	2	NAG	C2-N2-C7	-2.31	119.80	122.90
6	K	3	BMA	C6-C5-C4	-2.31	107.34	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	2	NAG	C2-N2-C7	-2.27	119.86	122.90
5	I	1	NAG	C3-C4-C5	2.24	114.29	110.23
6	M	2	NAG	C2-N2-C7	-2.23	119.91	122.90
6	K	2	NAG	C4-C3-C2	-2.23	107.75	111.02
5	P	2	NAG	C4-C3-C2	-2.22	107.76	111.02
5	N	1	NAG	C3-C4-C5	2.21	114.24	110.23
5	I	2	NAG	C4-C3-C2	-2.06	108.00	111.02
5	N	2	NAG	C4-C3-C2	-2.01	108.08	111.02

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	1	NAG	C8-C7-N2-C2
5	N	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
5	N	1	NAG	O7-C7-N2-C2
5	N	1	NAG	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
5	G	2	NAG	C8-C7-N2-C2
5	J	2	NAG	C8-C7-N2-C2
5	O	2	NAG	C8-C7-N2-C2
6	M	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2
5	O	2	NAG	O7-C7-N2-C2
6	M	2	NAG	O7-C7-N2-C2
6	K	3	BMA	C4-C5-C6-O6
5	G	1	NAG	C8-C7-N2-C2
5	J	1	NAG	C8-C7-N2-C2
5	O	1	NAG	C8-C7-N2-C2
6	M	1	NAG	C8-C7-N2-C2
6	K	3	BMA	O5-C5-C6-O6
5	G	1	NAG	O7-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2
5	O	1	NAG	O7-C7-N2-C2
6	M	1	NAG	O7-C7-N2-C2
5	G	2	NAG	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
6	M	2	NAG	O5-C5-C6-O6
5	P	1	NAG	O7-C7-N2-C2

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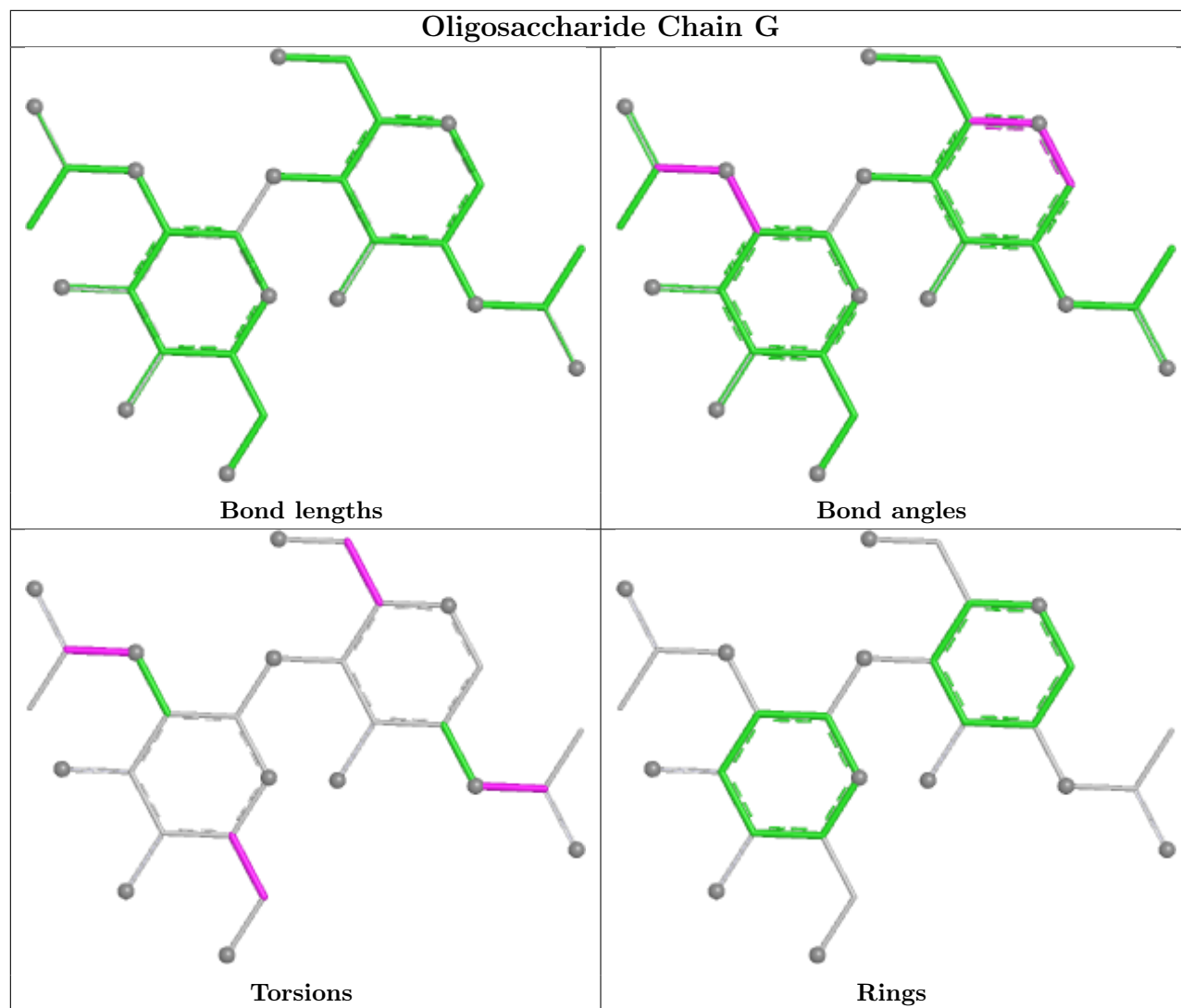
Mol	Chain	Res	Type	Atoms
6	K	1	NAG	O7-C7-N2-C2
5	J	1	NAG	O5-C5-C6-O6
5	O	1	NAG	O5-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
6	M	1	NAG	O5-C5-C6-O6

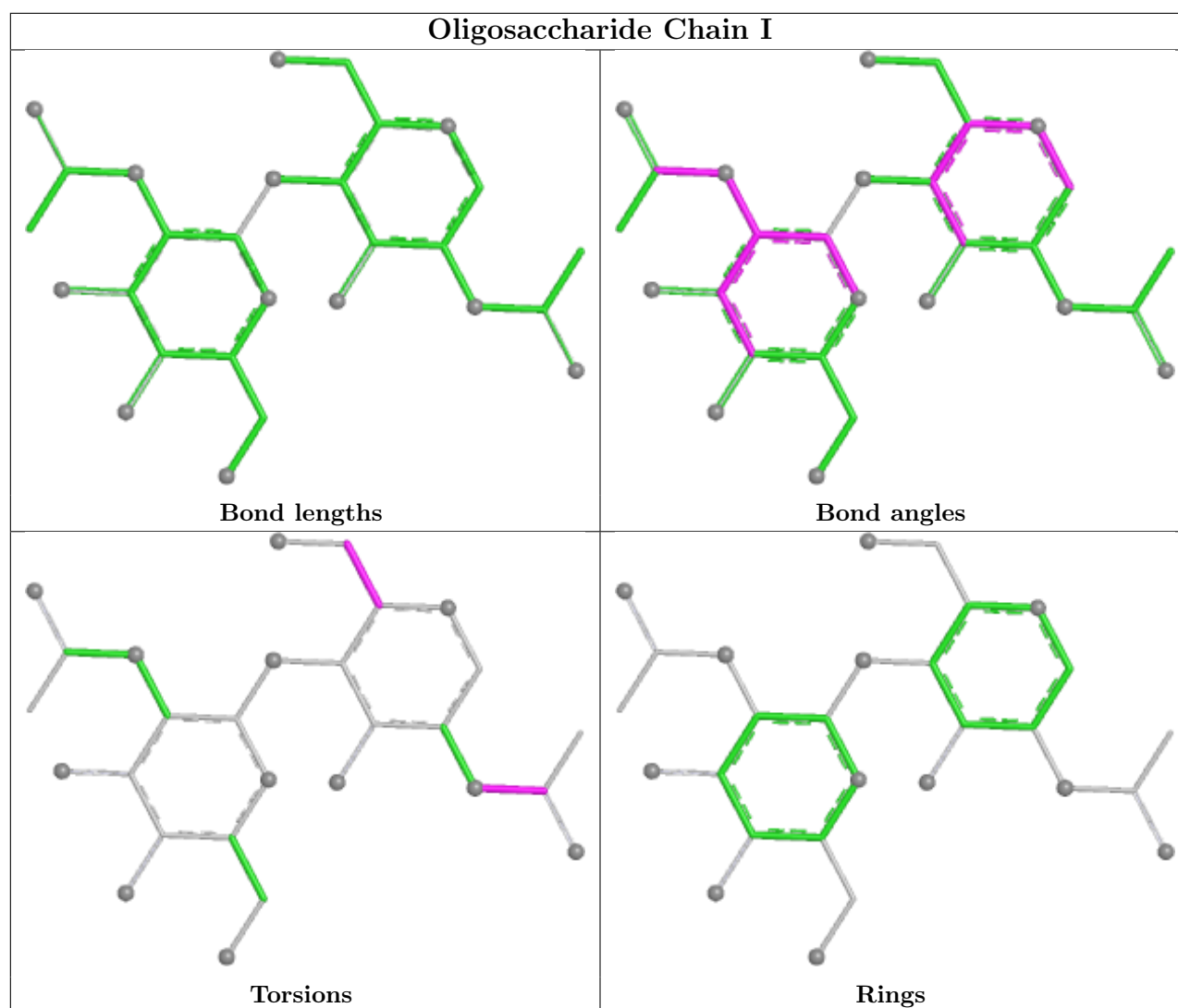
There are no ring outliers.

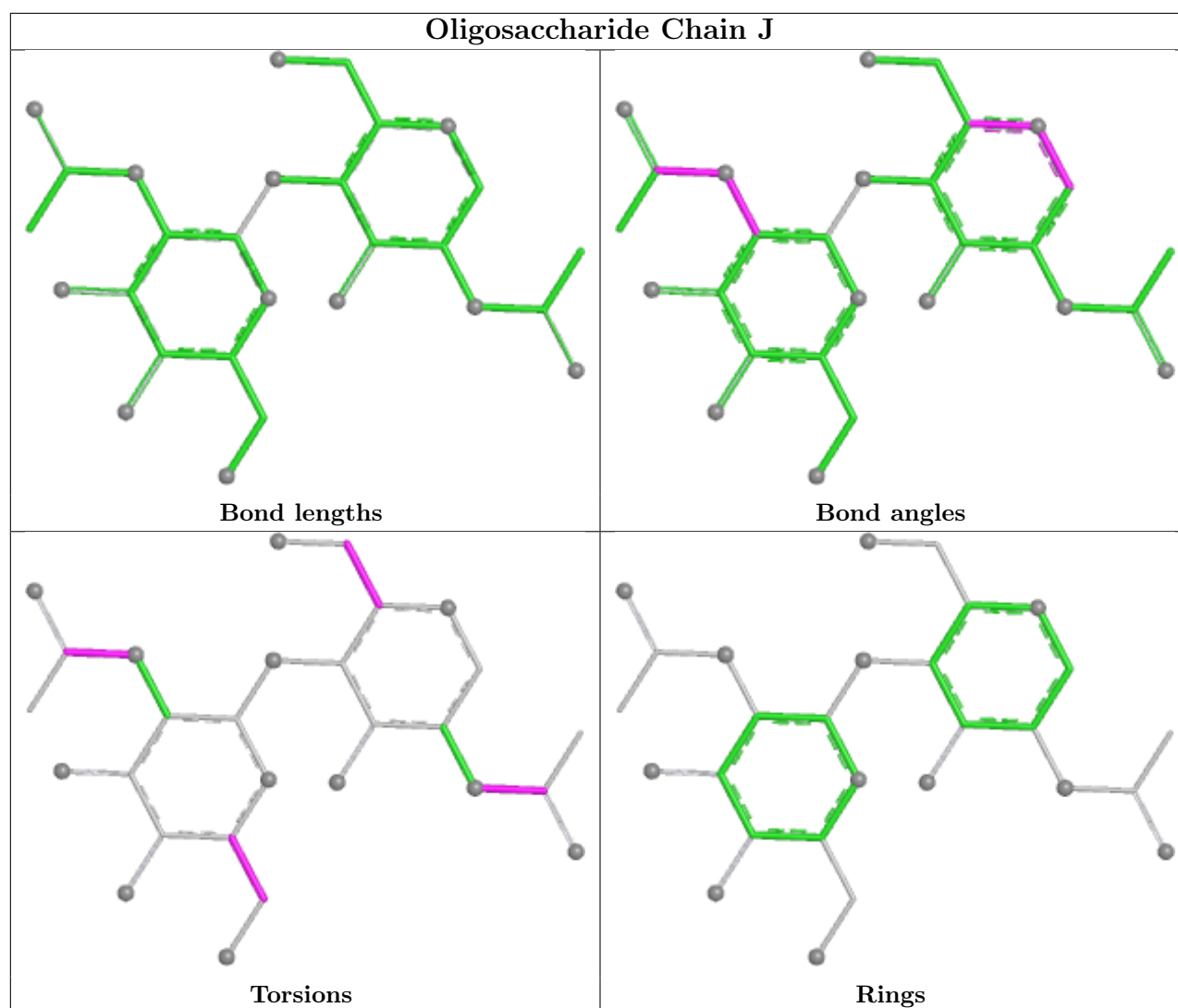
4 monomers are involved in 10 short contacts:

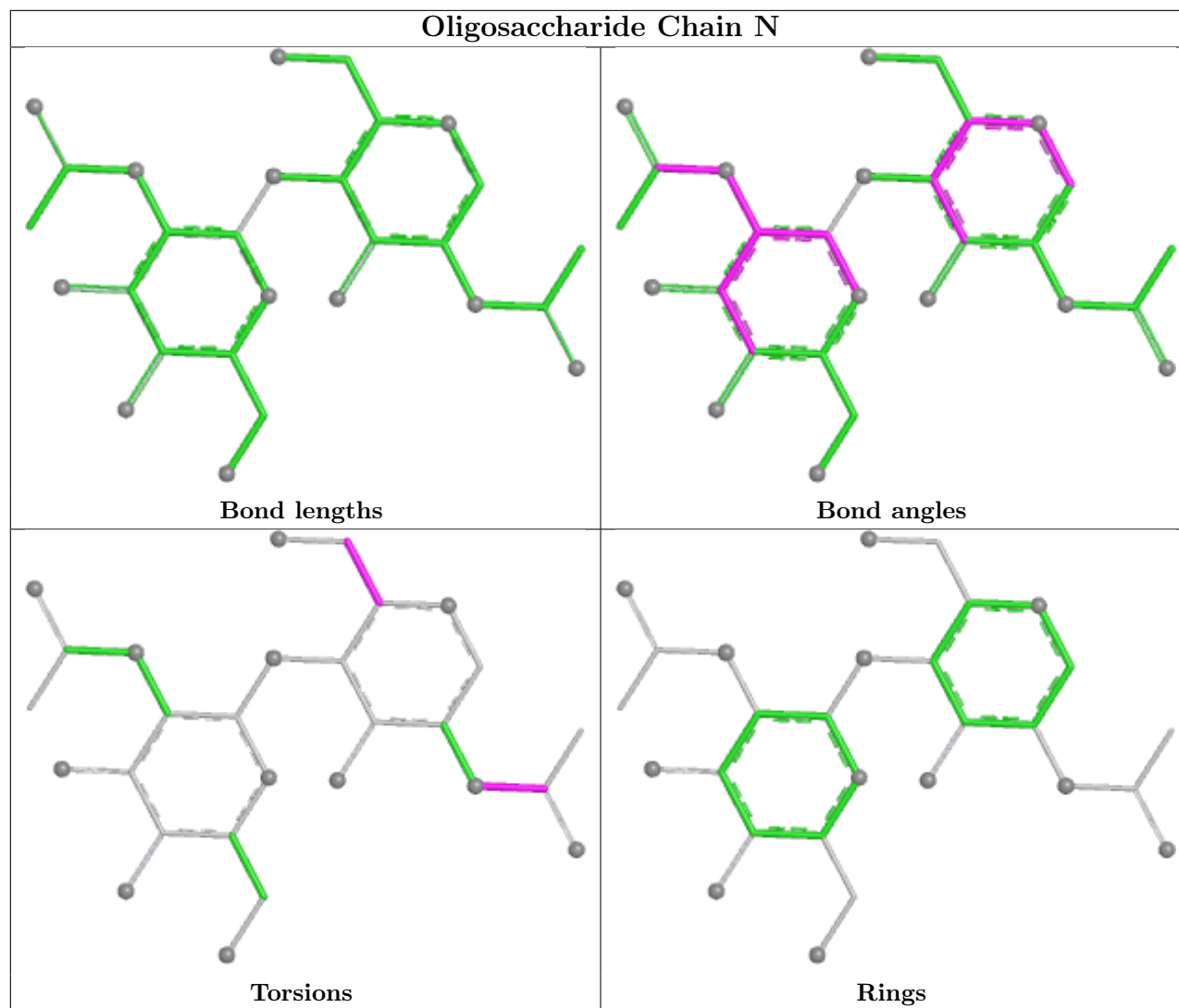
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	1	NAG	3	0
6	M	1	NAG	1	0
5	G	1	NAG	1	0
5	P	1	NAG	5	0

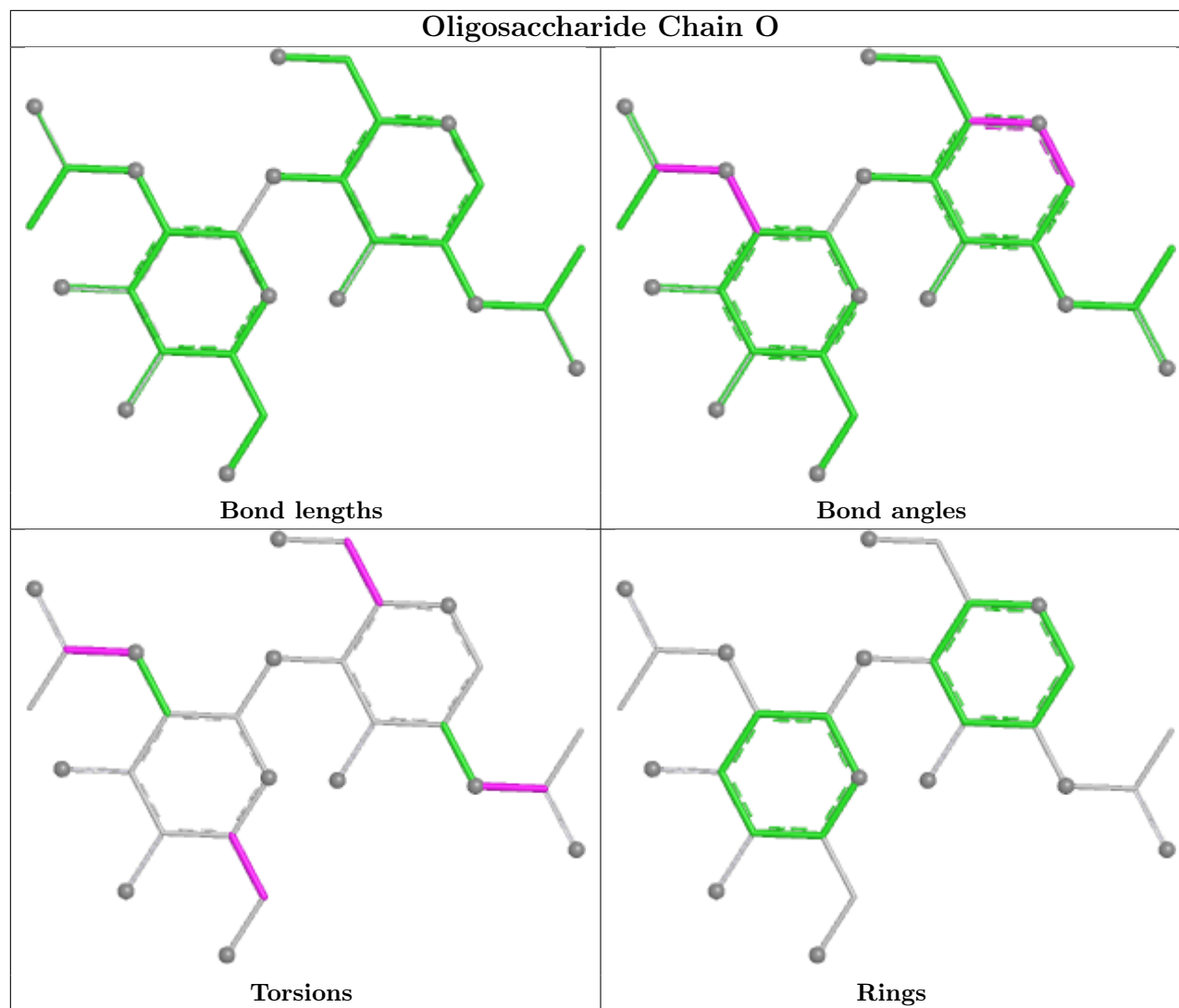
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

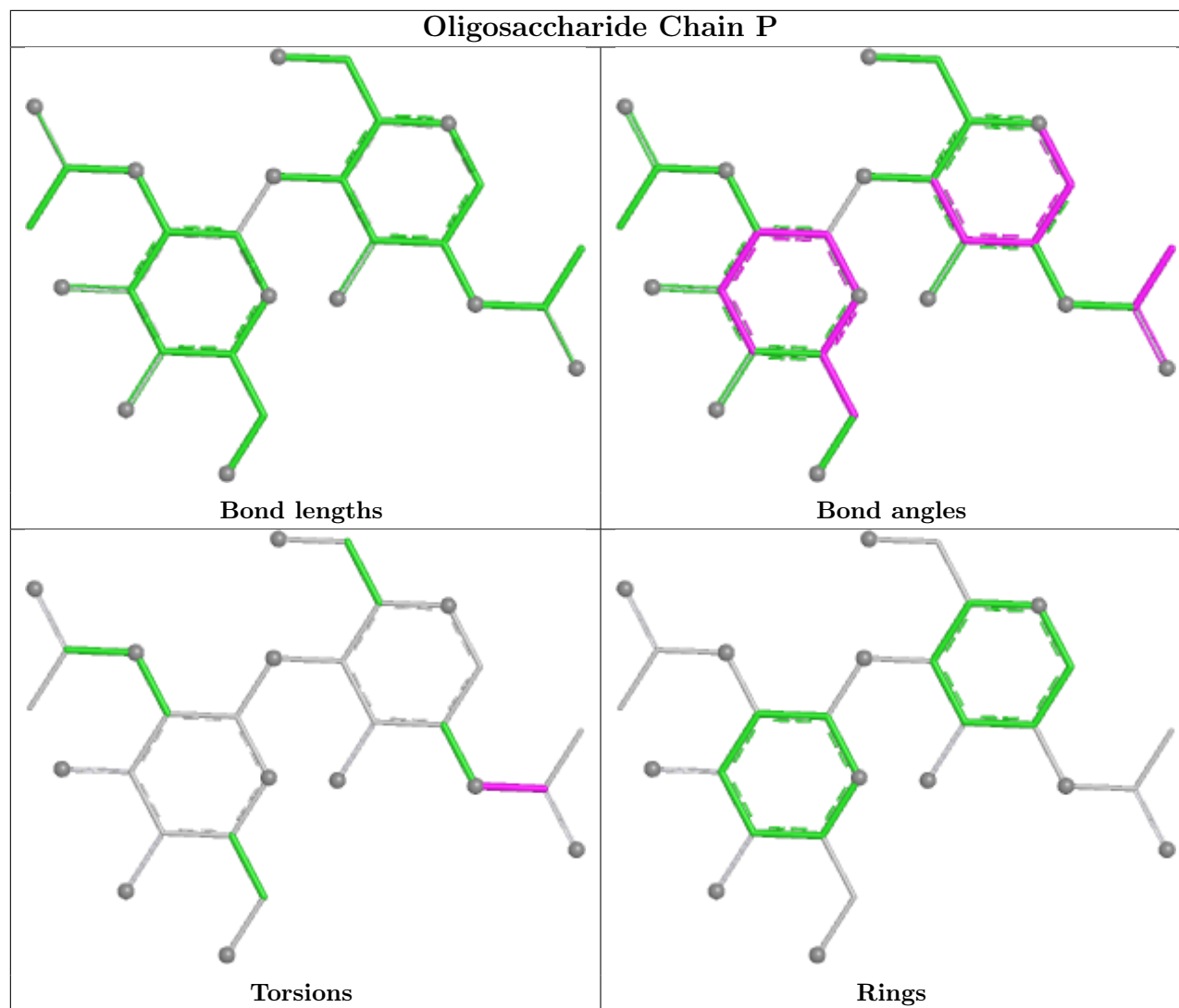


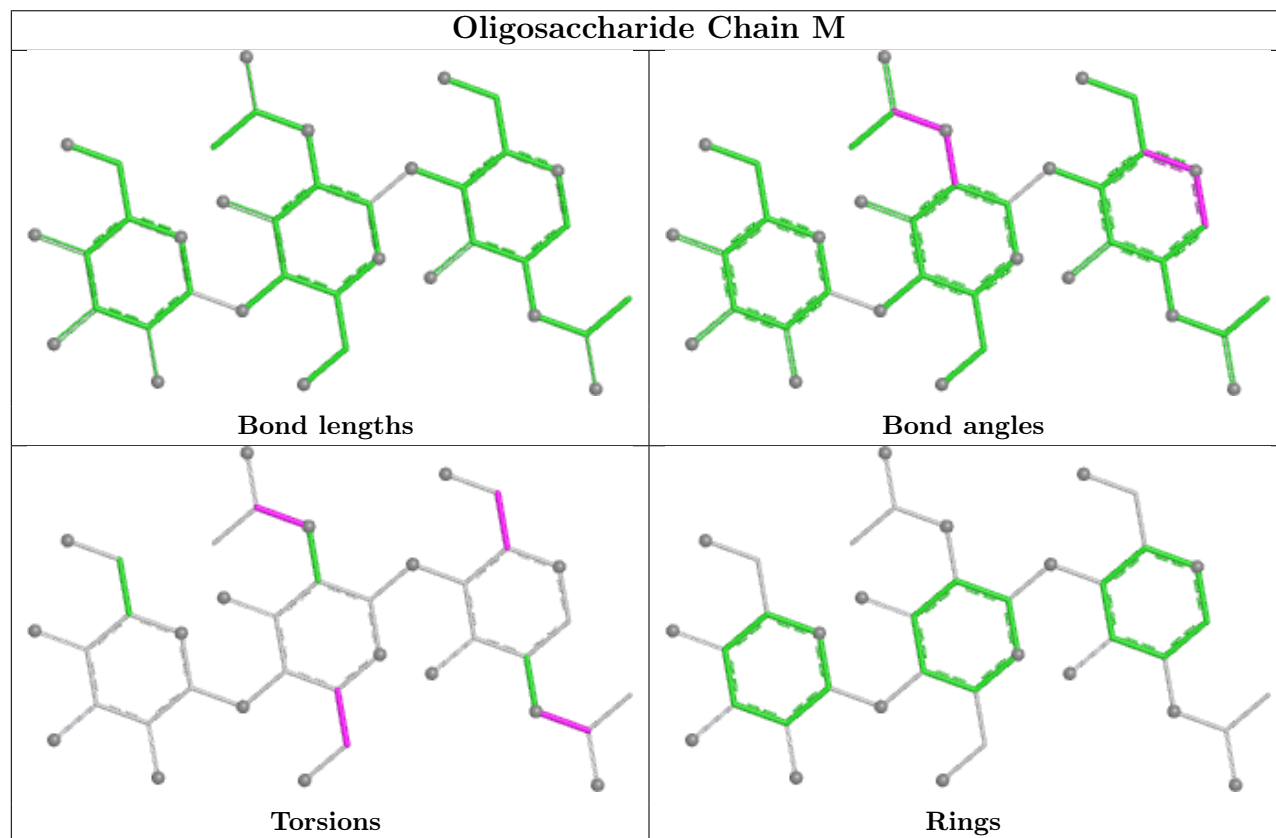
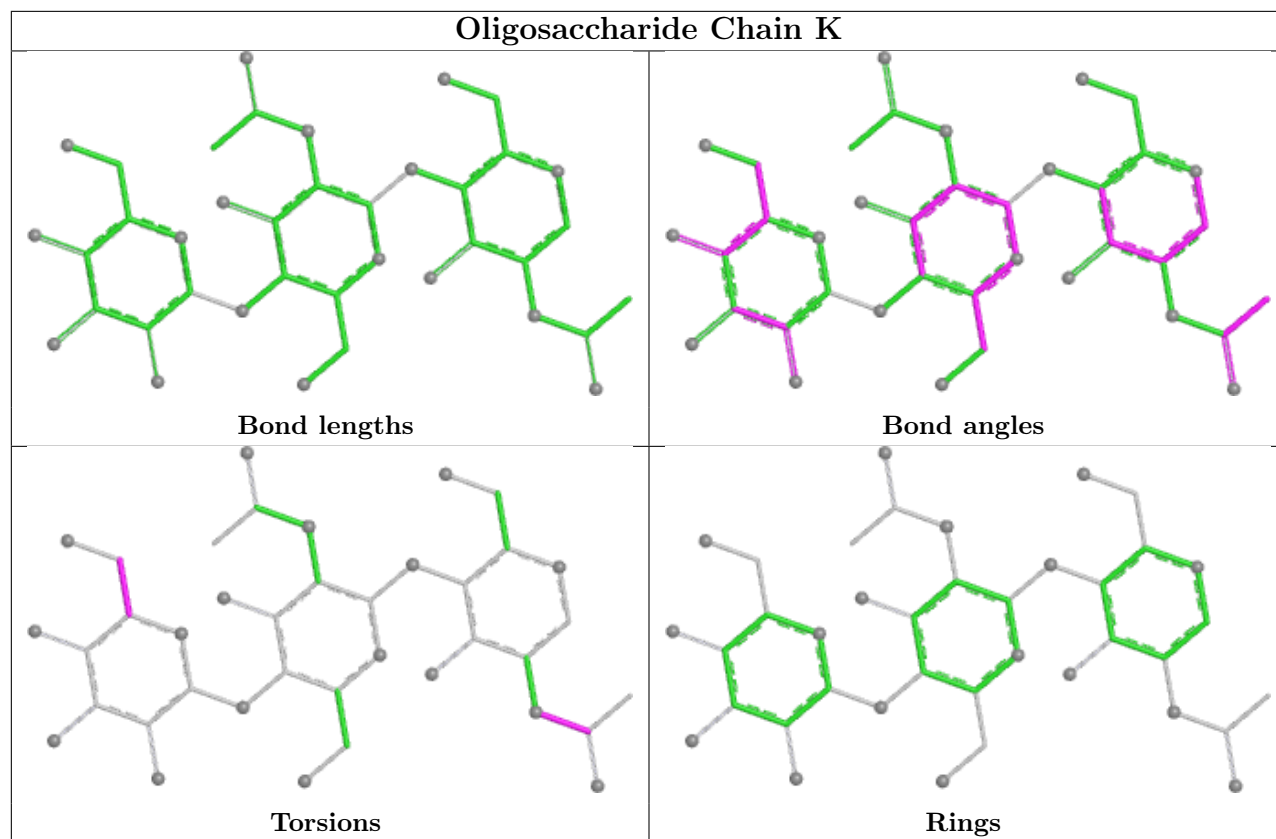












5.6 Ligand geometry

2 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
7	NAG	C	410	1	14,14,15	0.49	0	17,19,21	0.93	1 (5%)
7	NAG	A	410	1	14,14,15	0.48	0	17,19,21	0.93	1 (5%)

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
7	NAG	C	410	1	-	2/6/23/26	0/1/1/1
7	NAG	A	410	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	410	NAG	C1-O5-C5	2.49	115.53	112.19
7	C	410	NAG	C1-O5-C5	2.49	115.52	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	410	NAG	C8-C7-N2-C2
7	C	410	NAG	C8-C7-N2-C2
7	C	410	NAG	O7-C7-N2-C2
7	A	410	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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.

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	337/347 (97%)	-0.03	7 (2%) 63 54	100, 100, 100, 100	0
1	C	337/347 (97%)	0.07	9 (2%) 56 48	100, 100, 100, 100	0
2	B	139/179 (77%)	-0.12	2 (1%) 73 62	100, 100, 100, 100	0
2	D	140/179 (78%)	-0.12	5 (3%) 46 42	100, 100, 100, 100	0
3	E	220/234 (94%)	-0.04	3 (1%) 73 62	100, 100, 100, 100	0
3	H	221/234 (94%)	-0.04	3 (1%) 73 62	100, 100, 100, 100	0
4	F	213/216 (98%)	-0.17	6 (2%) 55 47	100, 100, 100, 100	0
4	L	214/216 (99%)	-0.20	2 (0%) 81 69	100, 100, 100, 100	0
All	All	1821/1952 (93%)	-0.06	37 (2%) 65 55	100, 100, 100, 100	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	190	GLY	8.2
4	L	123	GLU	5.2
1	A	299	GLY	4.2
3	E	191	THR	3.8
1	C	222	VAL	3.6
4	F	100	GLY	3.5
4	L	32	TYR	3.3
1	C	218	THR	3.3
3	E	22	CYS	3.1
1	C	331	GLY	3.0
1	A	187	VAL	2.9
4	F	142	GLY	2.9
3	H	52(A)	GLY	2.7
2	D	510	SER	2.7
2	B	458	GLU	2.7
1	C	199	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
4	F	32	TYR	2.6
2	D	508	GLU	2.6
1	A	331	GLY	2.6
4	F	106	VAL	2.5
4	F	123	GLU	2.4
1	C	200	LYS	2.4
2	D	376	ALA	2.4
2	B	510	SER	2.4
3	H	172	SER	2.4
4	F	95(B)	GLY	2.3
2	D	418	ASP	2.3
1	C	30	ILE	2.2
1	C	299	GLY	2.2
3	H	205	THR	2.2
1	C	227	GLY	2.1
1	A	186	THR	2.1
2	D	401	SER	2.1
1	A	217	VAL	2.1
1	C	204	ASP	2.0
1	A	195	GLU	2.0
1	A	21	GLN	2.0

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.

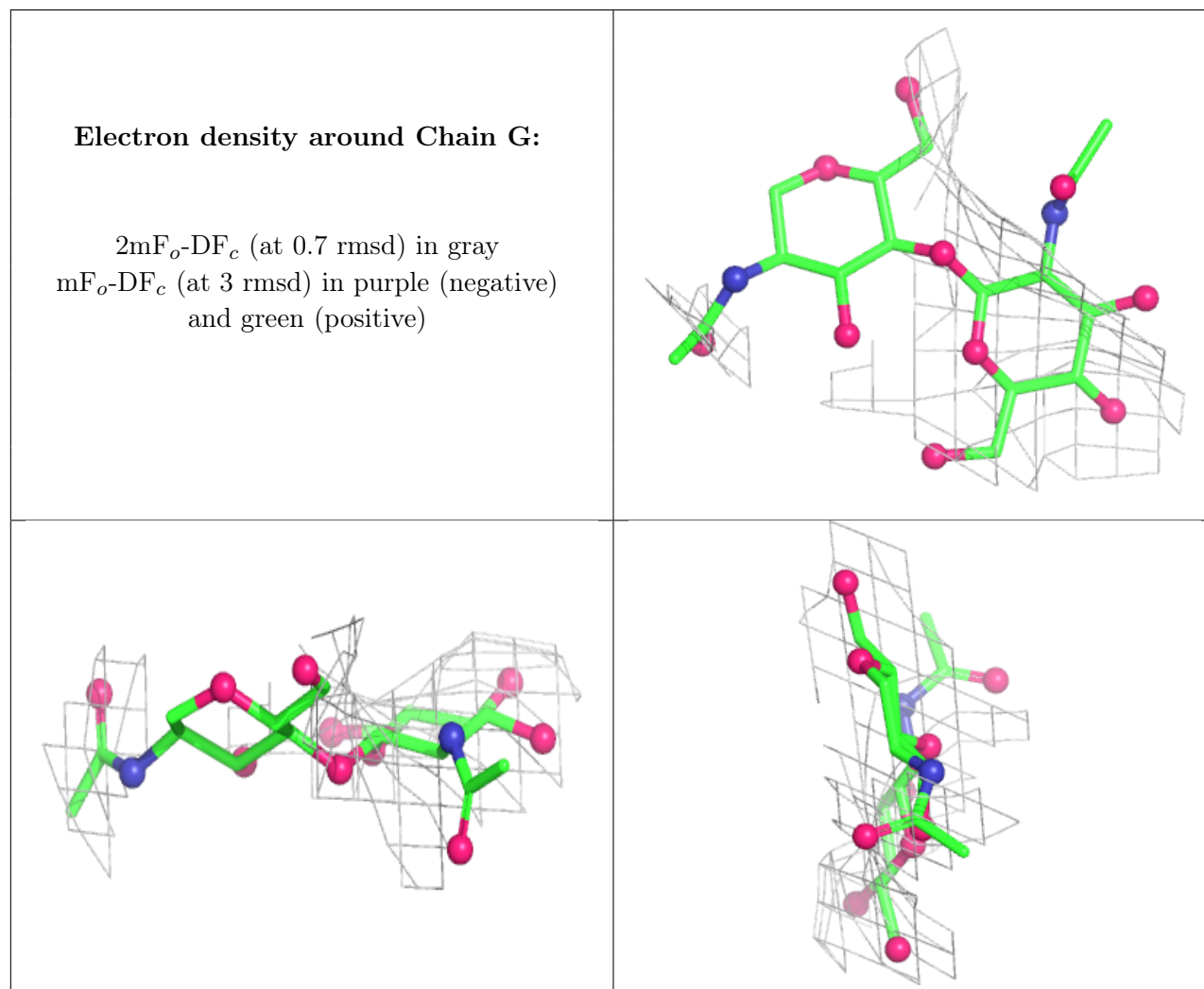
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	G	1	14/15	-	-	100,100,100,100	0
5	NAG	G	2	14/15	-	-	100,100,100,100	0
5	NAG	P	2	14/15	0.91	0.07	100,100,100,100	0
6	NAG	K	2	14/15	0.94	0.08	100,100,100,100	0
5	NAG	O	2	14/15	0.95	0.10	100,100,100,100	0
5	NAG	P	1	14/15	0.95	0.09	100,100,100,100	0
6	BMA	M	3	11/12	0.96	0.07	100,100,100,100	0

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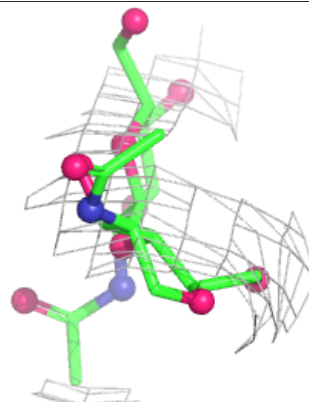
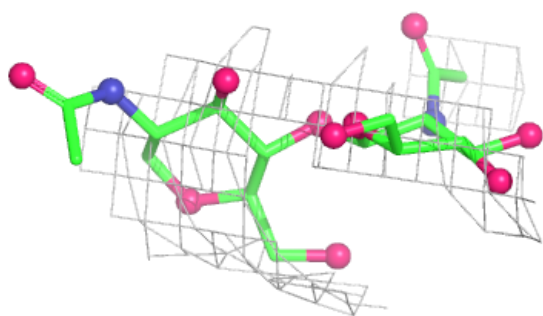
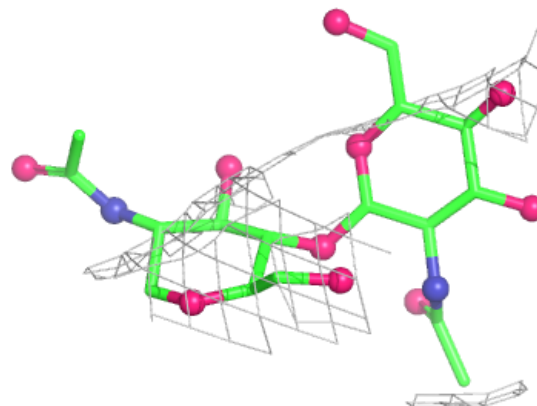
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	N	2	14/15	0.97	0.07	100,100,100,100	0
5	NAG	N	1	14/15	0.97	0.07	100,100,100,100	0
5	NAG	O	1	14/15	0.98	0.09	100,100,100,100	0
6	NAG	K	1	14/15	0.98	0.07	100,100,100,100	0
5	NAG	I	2	14/15	0.98	0.10	100,100,100,100	0
6	NAG	M	2	14/15	0.98	0.11	100,100,100,100	0
5	NAG	J	1	14/15	0.98	0.11	100,100,100,100	0
6	BMA	K	3	11/12	-	-	100,100,100,100	0
6	NAG	M	1	14/15	0.99	0.05	100,100,100,100	0
5	NAG	I	1	14/15	0.99	0.05	100,100,100,100	0
5	NAG	J	2	14/15	0.99	0.06	100,100,100,100	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.

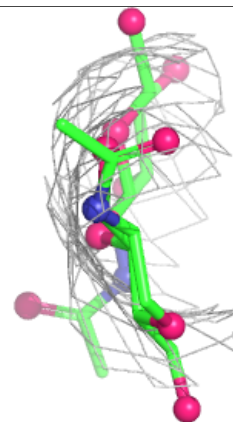
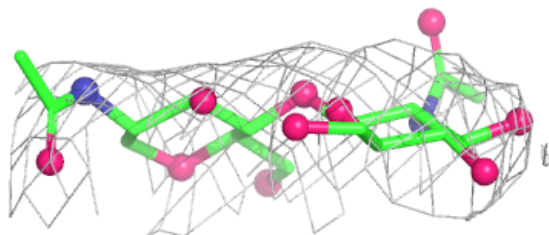
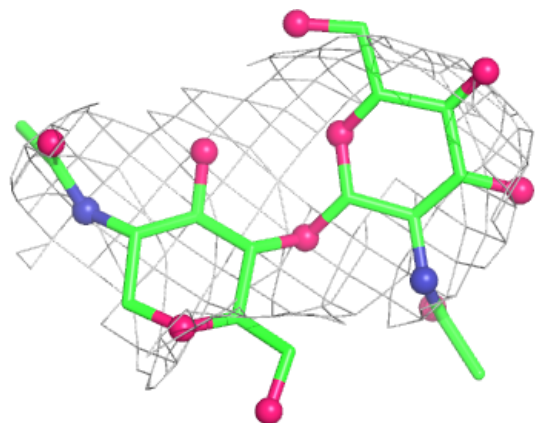


Electron density around Chain I:

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

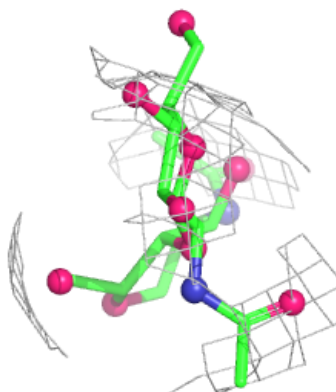
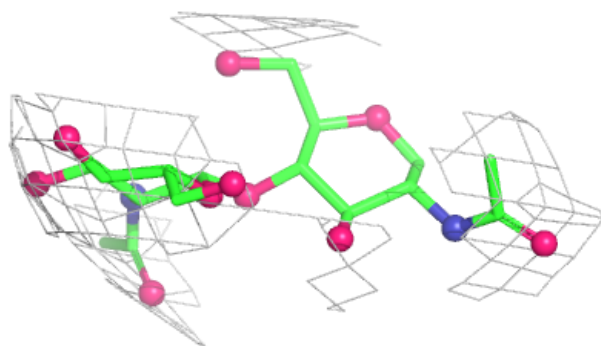
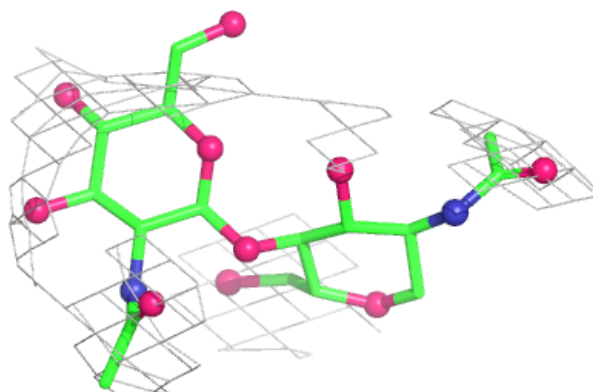
**Electron density around Chain J:**

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

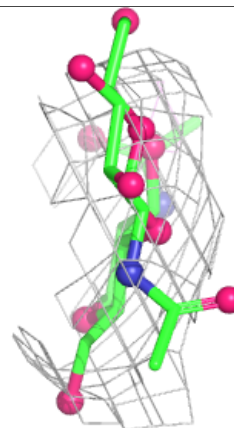
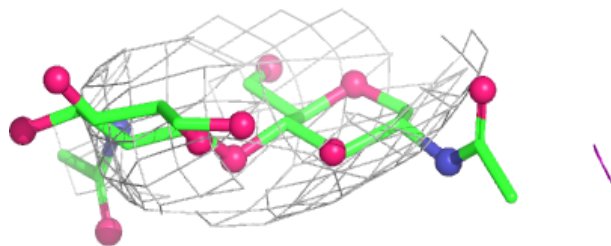
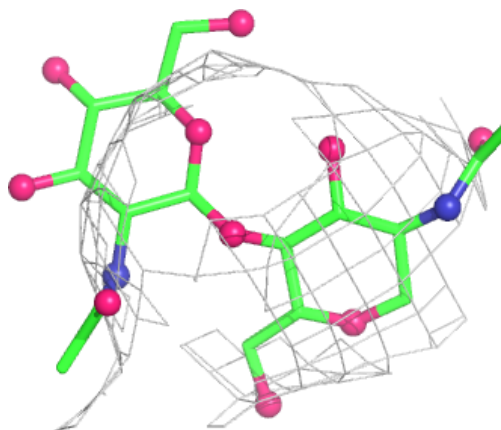


Electron density around Chain N:

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

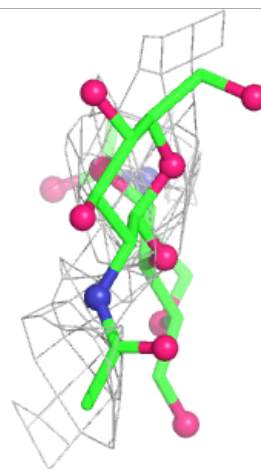
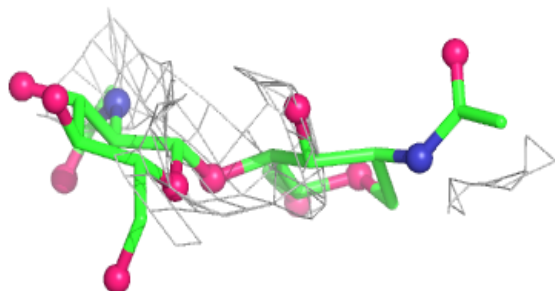
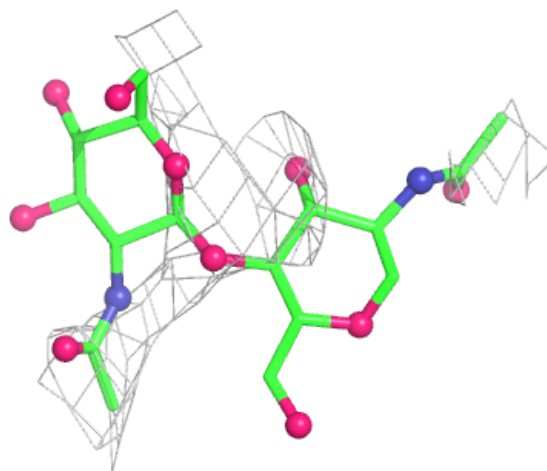
**Electron density around Chain O:**

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



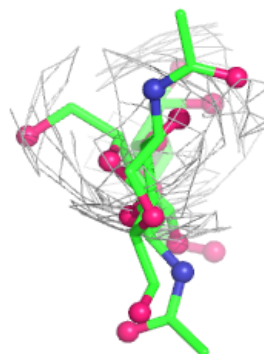
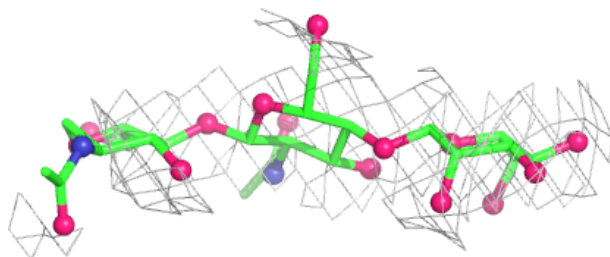
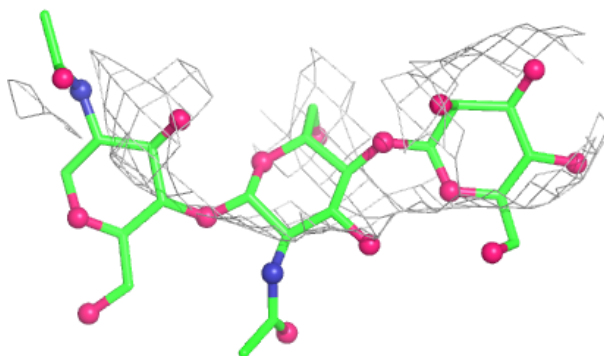
Electron density around Chain P:

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

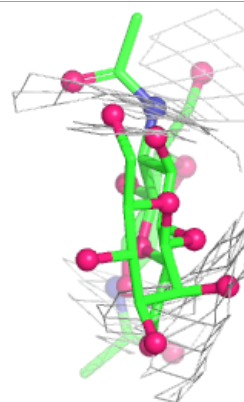
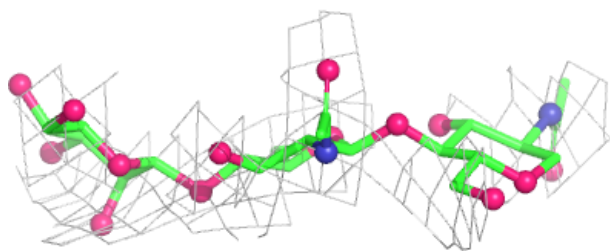
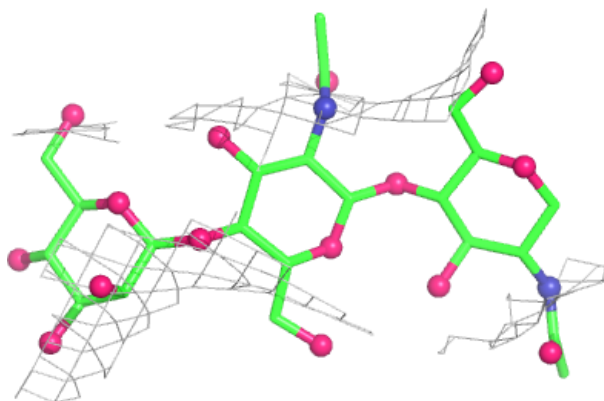


Electron density around Chain K:

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

**Electron density around Chain M:**

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



6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
7	NAG	A	410	14/15	0.96	0.11	100,100,100,100	0
7	NAG	C	410	14/15	0.98	0.09	100,100,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.