



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:24 AM UTC

PDB ID : 5CXF / pdb_00005cxf
Title : Crystal structure of the extracellular domain of glycoprotein B from Human Cytomegalovirus
Authors : Burke, H.G.; Heldwein, E.E.
Deposited on : 2015-07-28
Resolution : 3.60 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

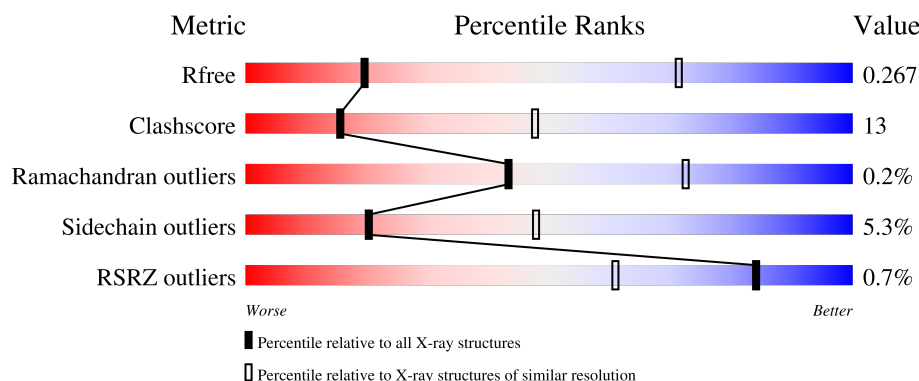
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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 $\leq 5\%$. 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	630	61% 26% 11%
1	B	630	61% 28% 10%
1	C	630	61% 28% 9%
2	D	4	50% 50%
3	E	3	33% 67%

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Mol	Chain	Length	Quality of chain
4	F	2	 100%
4	G	2	 50%50%
4	H	2	 100%
4	J	2	 50%50%
4	K	2	 50%50%
5	I	5	 20%80%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14373 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 Envelope glycoprotein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	562	Total	C	N	O	S	0	0	0
			4561	2894	781	862	24			
1	B	570	Total	C	N	O	S	0	0	0
			4626	2931	794	877	24			
1	C	576	Total	C	N	O	S	0	0	0
			4669	2958	801	886	24			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	GLY	TYR	engineered mutation	UNP P06473
A	156	HIS	ILE	engineered mutation	UNP P06473
A	157	ARG	TYR	engineered mutation	UNP P06473
A	206	HIS	TYR	engineered mutation	UNP P06473
A	240	ALA	TRP	engineered mutation	UNP P06473
A	241	THR	LEU	engineered mutation	UNP P06473
A	242	HIS	TYR	engineered mutation	UNP P06473
A	434V	ASP	-	engineered mutation	UNP P06473
A	434W	ASP	ARG	engineered mutation	UNP P06473
A	434X	ASP	THR	engineered mutation	UNP P06473
A	434Y	ASP	ARG	engineered mutation	UNP P06473
A	434Z	LYS	ARG	engineered mutation	UNP P06473
B	155	GLY	TYR	engineered mutation	UNP P06473
B	156	HIS	ILE	engineered mutation	UNP P06473
B	157	ARG	TYR	engineered mutation	UNP P06473
B	206	HIS	TYR	engineered mutation	UNP P06473
B	240	ALA	TRP	engineered mutation	UNP P06473
B	241	THR	LEU	engineered mutation	UNP P06473
B	242	HIS	TYR	engineered mutation	UNP P06473
B	438R	ASP	-	engineered mutation	UNP P06473
B	438S	ASP	ARG	engineered mutation	UNP P06473
B	438T	ASP	THR	engineered mutation	UNP P06473
B	438U	ASP	ARG	engineered mutation	UNP P06473

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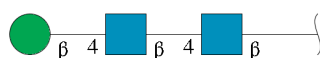
Chain	Residue	Modelled	Actual	Comment	Reference
B	438V	LYS	ARG	engineered mutation	UNP P06473
C	155	GLY	TYR	engineered mutation	UNP P06473
C	156	HIS	ILE	engineered mutation	UNP P06473
C	157	ARG	TYR	engineered mutation	UNP P06473
C	206	HIS	TYR	engineered mutation	UNP P06473
C	240	ALA	TRP	engineered mutation	UNP P06473
C	241	THR	LEU	engineered mutation	UNP P06473
C	242	HIS	TYR	engineered mutation	UNP P06473
C	440P	ASP	-	engineered mutation	UNP P06473
C	440Q	ASP	ARG	engineered mutation	UNP P06473
C	440R	ASP	THR	engineered mutation	UNP P06473
C	440S	ASP	ARG	engineered mutation	UNP P06473
C	440T	LYS	ARG	engineered mutation	UNP P06473

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
2	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 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.



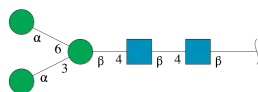
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 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
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
5	I	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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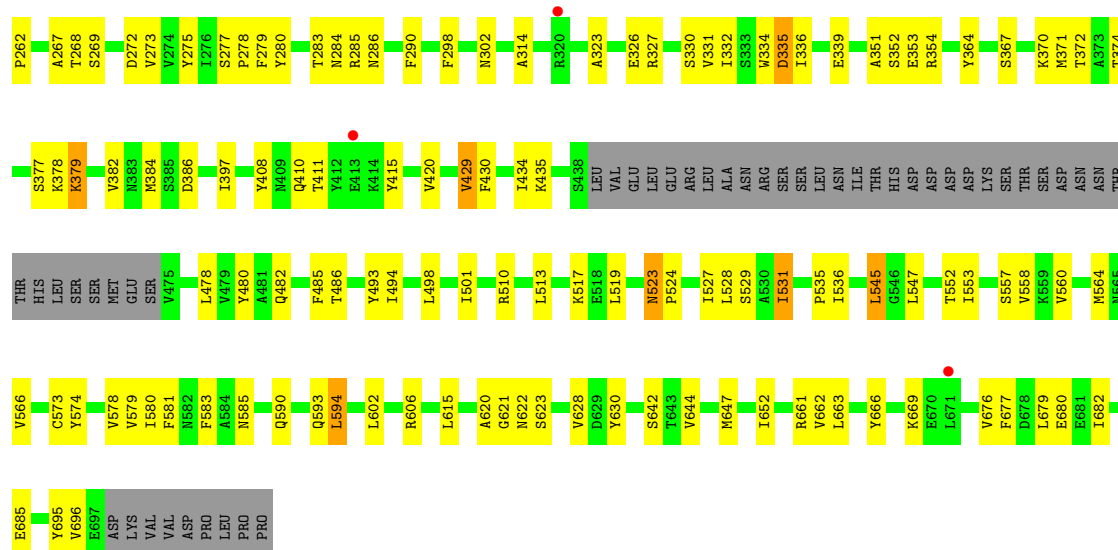
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		

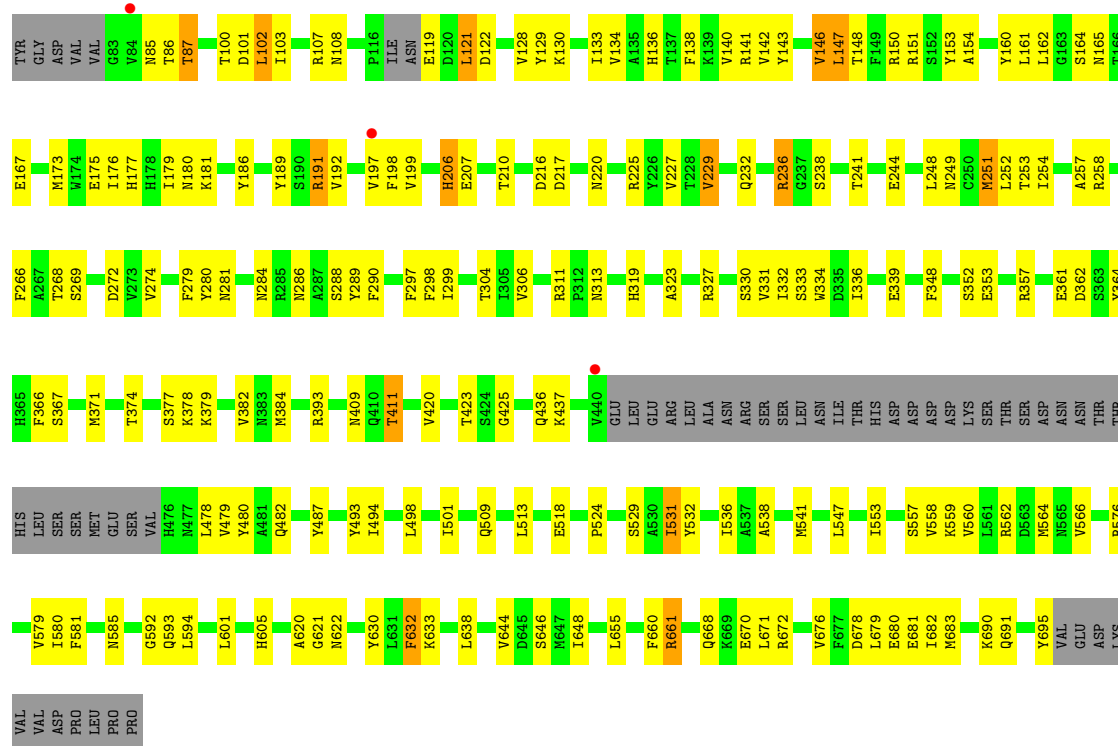
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	O	0	0
			1	1		
8	C	1	Total	O	0	0
			1	1		



• Molecule 1: Envelope glycoprotein B

Chain C: 61% 28% 9%



• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 50% 50%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  33% 67%

MAG1
MAG2
BMA3

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

Chain F:  100%

MAG1
MAG2

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

Chain G:  50% 50%

MAG1
MAG2

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

Chain H:  100%

MAG1
MAG2

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

Chain J:  50% 50%

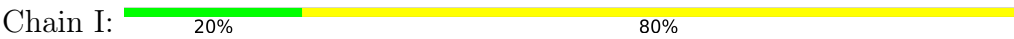
MAG1
MAG2

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

Chain K:  50% 50%

MAG1
MAG2

- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



HA01
HA02
HA03
HA04
HA05

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.18Å 133.93Å 295.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.63 – 3.60 57.63 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (57.63-3.60) 86.7 (57.63-3.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.232 , 0.269 0.235 , 0.267	Depositor DCC
R_{free} test set	1892 reflections (4.22%)	wwPDB-VP
Wilson B-factor (Å ²)	88.4	Xtriage
Anisotropy	0.871	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14373	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.53	0/4663	0.86	2/6314 (0.0%)
1	B	0.55	0/4729	0.91	6/6403 (0.1%)
1	C	0.56	0/4773	0.90	1/6464 (0.0%)
All	All	0.55	0/14165	0.89	9/19181 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	523	ASN	CA-C-N	6.28	126.02	119.05
1	B	523	ASN	C-N-CA	6.28	126.02	119.05
1	B	101	ASP	N-CA-C	6.02	119.53	108.58
1	B	314	ALA	N-CA-C	5.43	116.20	108.54
1	A	155	GLY	N-CA-C	-5.26	103.52	112.51
1	B	429	VAL	N-CA-C	5.24	115.40	107.75
1	A	163	GLY	N-CA-C	5.20	118.05	112.33
1	C	87	THR	N-CA-C	-5.15	106.95	113.18
1	B	171	PRO	O-C-N	5.09	123.65	121.31

There are no chirality outliers.

There are no planarity outliers.

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	4561	0	4417	143	0
1	B	4626	0	4482	149	0
1	C	4669	0	4523	148	0
2	D	50	0	43	0	0
3	E	39	0	34	1	0
4	F	28	0	25	2	0
4	G	28	0	25	0	0
4	H	28	0	25	2	0
4	J	28	0	25	2	0
4	K	28	0	25	2	0
5	I	61	0	52	0	0
6	A	98	0	91	1	0
6	B	56	0	52	3	0
6	C	70	0	65	2	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
All	All	14373	0	13884	379	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 13.

All (379) 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:327:ARG:HH21	1:C:332:ILE:HD11	1.29	0.96
1:B:225:ARG:HD3	1:B:253:THR:HG22	1.56	0.88
1:A:642:SER:HB2	1:B:103:ILE:HG22	1.60	0.83
1:B:103:ILE:HD11	1:B:528:LEU:HD21	1.60	0.83
1:A:559:LYS:HB2	1:A:580:ILE:HG13	1.61	0.83
1:B:524:PRO:HB3	1:B:545:LEU:HD13	1.63	0.80
1:B:198:PHE:HB3	1:C:161:LEU:HB2	1.63	0.79
1:B:124:GLY:HA2	1:B:434:ILE:HG12	1.63	0.79
1:C:191:ARG:HB2	1:C:191:ARG:HH11	1.51	0.76
1:A:382:VAL:HB	1:A:420:VAL:HG23	1.67	0.75
1:A:533:ASN:O	1:A:533:ASN:ND2	2.17	0.74
1:A:124:GLY:HA2	1:A:434:ILE:HG12	1.69	0.74
1:B:382:VAL:HB	1:B:420:VAL:HG23	1.70	0.74
1:C:382:VAL:HB	1:C:420:VAL:HG23	1.69	0.74
1:B:323:ALA:HB2	1:B:336:ILE:HD11	1.70	0.73
1:A:161:LEU:HB3	1:C:198:PHE:HB3	1.72	0.72
1:A:238:SER:O	1:A:241:THR:OG1	2.06	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:HIS:NE2	1:C:160:TYR:OH	2.23	0.71
1:A:594:LEU:HD11	1:A:620:ALA:HB2	1.72	0.71
1:C:384:MET:O	1:C:393:ARG:NH2	2.20	0.71
1:A:327:ARG:HH21	1:A:332:ILE:HD11	1.55	0.71
1:A:560:VAL:HA	1:A:579:VAL:HG22	1.74	0.70
1:C:411:THR:O	1:C:436:GLN:NE2	2.24	0.70
1:C:560:VAL:HA	1:C:579:VAL:HG22	1.74	0.70
1:B:151:ARG:HG2	1:B:244:GLU:HB3	1.74	0.69
1:C:227:VAL:HG12	1:C:251:MET:HB2	1.74	0.69
1:B:408:TYR:CE2	1:B:434:ILE:HD13	2.28	0.69
1:B:165:ASN:ND2	1:C:165:ASN:OD1	2.17	0.69
1:A:554:ASN:HB3	1:A:557:SER:HB3	1.75	0.68
1:C:146:VAL:HG22	1:C:249:ASN:HB3	1.75	0.68
1:A:160:TYR:OH	1:C:206:HIS:NE2	2.23	0.68
1:B:594:LEU:HD11	1:B:620:ALA:HB2	1.77	0.67
1:B:140:VAL:HG23	1:B:334:TRP:HB3	1.76	0.67
1:C:378:LYS:O	1:C:379:LYS:HG2	1.95	0.66
1:A:146:VAL:HG22	1:A:249:ASN:HB3	1.77	0.66
1:C:423:THR:HG22	1:C:425:GLY:H	1.60	0.66
1:C:594:LEU:HD11	1:C:620:ALA:HB2	1.79	0.65
1:B:352:SER:HB2	1:B:371:MET:HE2	1.78	0.65
1:C:189:TYR:OH	1:C:191:ARG:HD3	1.96	0.65
1:B:353:GLU:HG2	1:B:354:ARG:HG2	1.77	0.65
1:A:686:PHE:HE1	1:A:690:LYS:HE2	1.61	0.65
1:B:377:SER:OG	1:B:378:LYS:N	2.25	0.65
1:C:377:SER:OG	1:C:378:LYS:N	2.27	0.65
1:B:105:PHE:HD2	1:B:517:LYS:HA	1.62	0.65
1:B:272:ASP:OD2	1:B:327:ARG:NH2	2.30	0.65
1:B:351:ALA:O	1:B:370:LYS:NZ	2.30	0.64
1:C:478:LEU:HD23	1:C:480:TYR:HE1	1.62	0.64
1:A:191:ARG:HH12	1:A:193:ILE:HD11	1.62	0.64
1:A:593:GLN:HB2	1:A:605:HIS:CD2	2.33	0.64
1:C:564:MET:HB2	1:C:630:TYR:HB3	1.80	0.64
1:B:367:SER:HA	1:B:374:THR:HG22	1.81	0.63
1:A:378:LYS:O	1:A:379:LYS:HG2	1.99	0.63
1:A:593:GLN:HB2	1:A:605:HIS:HD2	1.63	0.63
1:B:144:GLN:NE2	1:B:330:SER:OG	2.31	0.63
1:A:231:ASP:HB3	1:B:696:VAL:HG21	1.81	0.63
1:A:326:GLU:HG2	1:A:331:VAL:HG12	1.80	0.63
1:B:128:VAL:HG12	1:B:429:VAL:HG22	1.81	0.62
1:B:279:PHE:O	1:B:284:ASN:ND2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:MET:HE3	1:C:298:PHE:HD2	1.62	0.62
1:A:650:LEU:HD11	1:C:501:ILE:HD12	1.82	0.62
1:C:672:ARG:NH2	1:C:678:ASP:OD2	2.33	0.61
1:C:323:ALA:HB2	1:C:336:ILE:HD11	1.82	0.61
1:A:202:HIS:CE1	1:A:203:ARG:HG3	2.36	0.61
1:A:216:ASP:OD1	1:A:217:ASP:N	2.33	0.61
1:B:89:TYR:OH	1:C:107:ARG:NH1	2.33	0.60
6:C:808:NAG:H3	6:C:808:NAG:H83	1.83	0.60
1:C:524:PRO:HB2	1:C:538:ALA:HB3	1.84	0.60
1:A:408:TYR:CE2	1:A:434:ILE:HD13	2.37	0.59
1:A:175:GLU:O	1:A:179:ILE:HG13	2.02	0.59
1:B:173:MET:HE2	1:B:298:PHE:HD2	1.67	0.59
1:A:478:LEU:HD23	1:B:663:LEU:HD13	1.84	0.59
1:B:170:ALA:HB1	1:B:331:VAL:HG23	1.85	0.59
4:H:2:NAG:H3	4:H:2:NAG:H83	1.84	0.59
1:A:520:SER:HB2	1:A:545:LEU:HD21	1.83	0.59
1:B:88:LYS:NZ	1:B:535:PRO:HD3	2.18	0.59
1:C:173:MET:HA	1:C:176:ILE:HD12	1.83	0.59
1:C:558:VAL:HG13	1:C:579:VAL:HG11	1.84	0.59
1:B:275:TYR:HE2	1:C:220:ASN:HB2	1.67	0.58
1:C:592:GLY:HA2	1:C:605:HIS:HE1	1.68	0.58
1:A:151:ARG:NH2	1:C:244:GLU:OE2	2.36	0.58
1:A:423:THR:HG22	1:A:425:GLY:H	1.68	0.58
1:B:232:GLN:HB3	1:C:695:TYR:CD2	2.39	0.58
1:C:103:ILE:HD11	1:C:547:LEU:HD11	1.86	0.58
1:B:326:GLU:HA	1:B:331:VAL:HG22	1.86	0.57
1:C:153:TYR:HB3	1:C:160:TYR:HB2	1.87	0.57
1:A:140:VAL:HG23	1:A:334:TRP:HB3	1.87	0.57
1:A:177:HIS:O	1:A:181:LYS:HG2	2.03	0.57
1:B:193:ILE:HB	1:B:198:PHE:HE1	1.68	0.57
1:B:302:ASN:OD1	6:B:805:NAG:N2	2.38	0.57
1:A:126:MET:HG3	1:A:429:VAL:HG13	1.87	0.57
1:C:143:TYR:O	1:C:330:SER:HB3	2.05	0.57
1:C:353:GLU:OE1	1:C:353:GLU:N	2.37	0.57
1:B:126:MET:HG3	1:B:429:VAL:HG13	1.87	0.56
1:B:615:LEU:HD13	1:B:628:VAL:HG22	1.87	0.56
1:C:140:VAL:HG23	1:C:334:TRP:HB3	1.85	0.56
4:H:1:NAG:H83	4:H:1:NAG:H3	1.87	0.56
1:A:143:TYR:OH	1:A:180:ASN:OD1	2.19	0.56
1:B:378:LYS:O	1:B:379:LYS:HG3	2.04	0.56
1:A:279:PHE:O	1:A:284:ASN:ND2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:THR:HB	1:A:316:PRO:HB2	1.86	0.56
1:A:198:PHE:HB3	1:B:161:LEU:HB2	1.87	0.56
1:A:533:ASN:OD1	1:B:510:ARG:NH1	2.39	0.56
1:B:593:GLN:HE21	1:B:606:ARG:H	1.54	0.56
1:A:288:SER:OG	1:A:289:TYR:N	2.39	0.56
1:A:377:SER:OG	1:A:378:LYS:N	2.38	0.56
1:C:280:TYR:O	1:C:336:ILE:HD13	2.06	0.56
1:B:280:TYR:O	1:B:336:ILE:HD13	2.06	0.55
1:B:88:LYS:HZ1	1:B:535:PRO:HD3	1.71	0.55
1:B:105:PHE:CD2	1:B:517:LYS:HA	2.41	0.55
1:C:272:ASP:HB2	1:C:327:ARG:HH22	1.71	0.55
1:A:337:GLN:HG3	1:A:342:VAL:HG21	1.88	0.55
1:A:353:GLU:OE1	1:A:370:LYS:NZ	2.38	0.55
1:A:139:LYS:HG2	1:A:256:THR:HG22	1.88	0.54
1:A:673:SER:HB2	1:C:134:VAL:HG12	1.88	0.54
1:B:529:SER:OG	1:B:536:ILE:N	2.39	0.54
1:B:524:PRO:HB3	1:B:545:LEU:CD1	2.37	0.54
1:C:288:SER:OG	1:C:289:TYR:N	2.40	0.54
1:C:478:LEU:HD23	1:C:480:TYR:CE1	2.42	0.54
1:B:267:ALA:HB2	1:B:273:VAL:HG13	1.88	0.54
1:B:335:ASP:OD1	1:B:335:ASP:N	2.41	0.54
1:B:353:GLU:OE1	1:B:353:GLU:N	2.32	0.54
1:C:225:ARG:HB3	1:C:253:THR:HG22	1.90	0.54
1:A:186:TYR:CE1	1:A:210:THR:HG22	2.43	0.53
1:A:677:PHE:HE2	1:B:680:GLU:HG3	1.72	0.53
1:C:297:PHE:CE1	1:C:323:ALA:HB1	2.43	0.53
1:A:290:PHE:HZ	1:A:294:ALA:HA	1.74	0.53
1:B:144:GLN:HA	1:B:171:PRO:HD3	1.90	0.53
1:A:186:TYR:HE1	1:A:210:THR:HG22	1.73	0.53
1:A:694:LYS:O	1:C:232:GLN:HB2	2.09	0.53
4:F:2:NAG:H3	4:F:2:NAG:H83	1.90	0.53
1:B:111:CYS:HB2	1:B:510:ARG:NH2	2.24	0.53
1:B:327:ARG:HH21	1:B:332:ILE:HD11	1.73	0.53
1:A:167:GLU:OE2	1:B:150:ARG:NH1	2.42	0.52
1:B:142:VAL:HG22	1:B:332:ILE:HG12	1.90	0.52
1:B:372:THR:HG21	1:C:660:PHE:HA	1.91	0.52
1:C:141:ARG:NH1	1:C:333:SER:OG	2.41	0.52
1:C:150:ARG:CZ	1:C:164:SER:HB3	2.39	0.52
1:A:479:VAL:HG11	1:C:479:VAL:HG12	1.92	0.52
1:B:106:GLU:O	1:B:513:LEU:HD21	2.09	0.52
1:A:191:ARG:NH1	1:A:193:ILE:HD11	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:LEU:HD12	1:C:679:LEU:HD12	1.91	0.52
1:B:101:ASP:HB3	1:B:547:LEU:HB2	1.92	0.52
1:C:173:MET:HE3	1:C:298:PHE:CD2	2.44	0.52
1:A:150:ARG:CZ	1:A:164:SER:HB3	2.40	0.51
1:B:243:ARG:HD2	1:B:244:GLU:H	1.75	0.51
1:C:192:VAL:HG22	1:C:197:VAL:HG22	1.92	0.51
1:A:368:SER:HB3	1:A:371:MET:HB3	1.92	0.51
1:A:411:THR:OG1	1:A:412:TYR:N	2.44	0.51
1:C:189:TYR:HE2	1:C:191:ARG:NH1	2.08	0.51
1:A:353:GLU:OE1	1:A:353:GLU:N	2.38	0.51
1:C:100:THR:OG1	1:C:101:ASP:N	2.44	0.51
1:B:677:PHE:CD2	1:C:680:GLU:HA	2.46	0.51
1:B:585:ASN:HA	6:B:811:NAG:H81	1.92	0.51
1:C:529:SER:OG	1:C:536:ILE:N	2.44	0.51
1:A:628:VAL:HG21	1:A:633:LYS:HD2	1.93	0.51
1:C:177:HIS:O	1:C:181:LYS:HG2	2.09	0.51
1:C:181:LYS:NZ	1:C:304:THR:OG1	2.37	0.51
1:A:270:THR:HA	1:B:685:GLU:HG2	1.93	0.51
1:A:367:SER:HA	1:A:374:THR:HG22	1.93	0.51
1:A:130:LYS:HD2	1:B:666:TYR:CE1	2.45	0.50
1:B:652:ILE:HG21	1:C:498:LEU:HD13	1.93	0.50
1:C:180:ASN:O	1:C:306:VAL:HG13	2.11	0.50
1:C:409:ASN:CG	1:C:411:THR:HG1	2.19	0.50
1:A:684:ARG:HD2	1:B:275:TYR:OH	2.12	0.50
1:A:491:ARG:HG3	1:C:655:LEU:HB3	1.94	0.50
1:B:679:LEU:HD12	1:C:679:LEU:HD12	1.93	0.50
1:C:576:ARG:O	1:C:593:GLN:NE2	2.43	0.50
1:B:384:MET:HE3	1:B:397:ILE:HD11	1.92	0.50
1:B:478:LEU:HD23	1:B:480:TYR:HE1	1.77	0.50
1:C:119:GLU:OE2	1:C:121:LEU:HD23	2.11	0.50
1:A:557:SER:O	1:A:557:SER:OG	2.27	0.50
1:A:686:PHE:CE1	1:A:690:LYS:HE2	2.43	0.50
1:B:386:ASP:HA	4:F:1:NAG:H82	1.92	0.50
1:B:557:SER:O	1:B:581:PHE:HA	2.11	0.50
1:C:138:PHE:CZ	1:C:266:PHE:CE1	3.00	0.49
1:A:153:TYR:HB3	1:A:160:TYR:HB2	1.94	0.49
1:B:93:VAL:HG11	1:B:602:LEU:HD12	1.94	0.49
1:B:148:THR:HG22	1:B:166:THR:HG23	1.93	0.49
1:A:148:THR:HG23	1:A:166:THR:HG22	1.94	0.49
1:C:146:VAL:CG2	1:C:249:ASN:HB3	2.41	0.49
1:A:193:ILE:HG21	1:B:234:HIS:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:MET:HB2	1:B:630:TYR:HB3	1.94	0.49
1:C:122:ASP:HB2	1:C:357:ARG:HB3	1.95	0.49
1:A:146:VAL:CG2	1:A:249:ASN:HB3	2.42	0.49
1:B:482:GLN:NE2	1:C:661:ARG:O	2.38	0.49
1:C:334:TRP:CZ3	1:C:336:ILE:HG12	2.47	0.49
1:B:581:PHE:HZ	1:B:602:LEU:HD11	1.77	0.49
1:A:147:LEU:HB3	1:A:248:LEU:HD12	1.94	0.49
1:B:371:MET:HA	1:C:661:ARG:HD3	1.94	0.48
1:A:165:ASN:ND2	1:B:164:SER:O	2.46	0.48
1:B:494:ILE:HG13	1:C:494:ILE:HD11	1.95	0.48
1:B:374:THR:HG23	1:B:485:PHE:HD2	1.78	0.48
1:B:229:VAL:HG22	1:B:249:ASN:HB3	1.95	0.48
1:C:361:GLU:HG2	1:C:362:ASP:OD1	2.14	0.48
1:B:581:PHE:HE2	1:B:583:PHE:CE1	2.31	0.48
1:B:221:THR:OG1	1:B:222:HIS:N	2.47	0.48
1:C:257:ALA:HB2	1:C:268:THR:HG22	1.95	0.48
1:C:173:MET:HG3	1:C:177:HIS:CD2	2.49	0.47
1:C:632:PHE:CD1	1:C:632:PHE:C	2.92	0.47
1:A:234:HIS:HD2	1:C:198:PHE:CZ	2.31	0.47
1:A:679:LEU:HD12	1:B:679:LEU:HD12	1.95	0.47
1:C:367:SER:HA	1:C:374:THR:HG22	1.96	0.47
1:B:177:HIS:O	1:B:181:LYS:HG2	2.14	0.47
1:A:147:LEU:HD13	1:A:149:PHE:CE1	2.49	0.47
1:B:141:ARG:NH1	1:B:143:TYR:OH	2.47	0.47
1:A:661:ARG:O	1:C:482:GLN:NE2	2.34	0.47
1:B:283:THR:C	1:B:285:ARG:H	2.23	0.47
1:C:148:THR:HG21	1:C:232:GLN:NE2	2.30	0.47
1:C:352:SER:HB2	1:C:371:MET:HE3	1.97	0.47
1:A:151:ARG:HB3	1:A:244:GLU:CG	2.44	0.47
1:B:228:THR:HG22	1:B:229:VAL:HG12	1.97	0.47
1:B:244:GLU:OE1	1:C:162:LEU:HD13	2.13	0.47
1:C:136:HIS:O	1:C:258:ARG:HA	2.14	0.47
1:C:286:ASN:OD1	6:C:808:NAG:N2	2.47	0.47
1:A:193:ILE:HB	1:A:198:PHE:CE1	2.50	0.47
1:A:691:GLN:NE2	1:B:327:ARG:HH11	2.12	0.47
1:B:193:ILE:HB	1:B:198:PHE:CE1	2.48	0.47
1:B:279:PHE:CD2	1:B:339:GLU:HB3	2.50	0.47
1:C:290:PHE:HE2	1:C:297:PHE:CD2	2.33	0.47
1:A:231:ASP:CB	1:B:696:VAL:HG21	2.45	0.47
1:A:664:GLU:HG3	1:A:664:GLU:O	2.14	0.47
1:A:676:VAL:HG13	1:C:258:ARG:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ASN:OD1	6:B:804:NAG:N2	2.48	0.47
1:B:560:VAL:HA	1:B:579:VAL:HG22	1.96	0.46
1:B:564:MET:O	1:B:574:TYR:HB2	2.16	0.46
1:A:147:LEU:HD12	1:A:167:GLU:HB2	1.97	0.46
1:B:410:GLN:N	1:B:410:GLN:OE1	2.47	0.46
1:B:621:GLY:HA2	1:B:622:ASN:HA	1.51	0.46
1:C:436:GLN:HE21	1:C:437:LYS:H	1.63	0.46
1:A:206:HIS:CE1	1:B:160:TYR:HH	2.30	0.46
1:A:244:GLU:OE2	1:B:151:ARG:NE	2.49	0.46
1:C:147:LEU:HD23	1:C:248:LEU:HD11	1.97	0.46
1:A:371:MET:HE3	1:A:371:MET:HB2	1.83	0.46
1:B:257:ALA:HB2	1:B:268:THR:HG22	1.98	0.46
1:B:527:ILE:O	1:B:531:ILE:HG23	2.16	0.46
1:B:165:ASN:ND2	1:C:164:SER:O	2.49	0.46
1:C:141:ARG:O	1:C:333:SER:N	2.43	0.46
1:A:232:GLN:H	1:B:696:VAL:HG23	1.81	0.46
1:A:582:ASN:HD21	1:A:589:VAL:HG22	1.81	0.45
1:C:141:ARG:HG2	1:C:254:ILE:HG12	1.98	0.45
1:C:238:SER:O	1:C:241:THR:OG1	2.34	0.45
1:A:257:ALA:HB2	1:A:268:THR:HG22	1.99	0.45
1:A:261:TYR:CG	1:A:262:PRO:HA	2.51	0.45
1:C:186:TYR:HE1	1:C:210:THR:HG22	1.79	0.45
1:A:165:ASN:HD22	1:B:164:SER:N	2.13	0.45
1:A:181:LYS:HB2	1:A:182:PHE:CD2	2.52	0.45
1:C:411:THR:HG22	1:C:436:GLN:NE2	2.31	0.45
1:B:229:VAL:HG13	1:B:249:ASN:HB3	1.98	0.45
1:B:269:SER:OG	1:C:681:GLU:HB3	2.17	0.45
1:A:279:PHE:CD2	1:A:339:GLU:HB3	2.52	0.45
1:C:272:ASP:HB2	1:C:327:ARG:NH2	2.31	0.45
1:C:366:PHE:O	1:C:374:THR:HA	2.16	0.45
1:A:541:MET:HB2	1:A:544:VAL:O	2.17	0.45
1:A:680:GLU:O	1:A:684:ARG:HG2	2.17	0.45
1:B:285:ARG:NE	1:B:290:PHE:HB3	2.32	0.45
1:B:558:VAL:HG13	1:B:579:VAL:HG11	1.98	0.45
1:B:677:PHE:HE2	1:C:680:GLU:HG3	1.82	0.45
1:C:409:ASN:OD1	1:C:411:THR:OG1	2.34	0.45
1:A:372:THR:O	1:A:482:GLN:HG2	2.17	0.45
1:A:425:GLY:HA3	1:A:480:TYR:OH	2.17	0.45
1:B:103:ILE:HD11	1:B:528:LEU:CD2	2.41	0.45
1:A:554:ASN:HD22	6:A:810:NAG:H83	1.82	0.45
1:A:679:LEU:HD23	1:A:679:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:TYR:CD1	1:B:379:LYS:HA	2.51	0.45
1:A:185:CYS:HB3	1:A:228:THR:HG21	1.98	0.44
1:B:223:SER:HB3	1:B:255:THR:HG22	1.99	0.44
1:B:523:ASN:ND2	1:C:518:GLU:OE2	2.50	0.44
1:B:223:SER:CB	1:B:255:THR:HG22	2.47	0.44
1:A:334:TRP:HZ3	1:A:336:ILE:HG12	1.82	0.44
1:B:280:TYR:HE1	1:B:285:ARG:HD3	1.82	0.44
1:B:644:VAL:O	1:C:108:ASN:ND2	2.50	0.44
1:C:279:PHE:CD2	1:C:339:GLU:HB3	2.52	0.44
1:A:547:LEU:HD23	1:A:547:LEU:H	1.81	0.44
1:B:186:TYR:CE1	1:B:210:THR:HG22	2.52	0.44
1:B:573:CYS:HB3	1:B:630:TYR:CE2	2.53	0.44
1:C:143:TYR:HB2	1:C:331:VAL:CG1	2.46	0.44
1:C:621:GLY:HA2	1:C:622:ASN:HA	1.49	0.44
1:A:150:ARG:HH22	1:C:167:GLU:CD	2.25	0.44
1:A:351:ALA:O	1:A:370:LYS:NZ	2.36	0.44
1:A:334:TRP:CZ3	1:A:336:ILE:HG12	2.52	0.44
1:A:509:GLN:OE1	1:C:648:ILE:HG22	2.18	0.44
1:B:415:TYR:CD2	1:B:435:LYS:HE2	2.52	0.44
1:A:147:LEU:HB3	1:A:248:LEU:CD1	2.48	0.44
1:C:85:ASN:C	1:C:87:THR:H	2.26	0.44
1:C:632:PHE:C	1:C:632:PHE:HD1	2.24	0.44
1:A:323:ALA:HB2	1:A:336:ILE:HD11	1.99	0.43
1:B:244:GLU:OE2	1:C:151:ARG:NH2	2.49	0.43
1:B:682:ILE:HD13	1:C:683:MET:HE2	2.00	0.43
1:B:272:ASP:OD2	1:B:332:ILE:HD11	2.17	0.43
1:C:632:PHE:HD1	1:C:633:LYS:N	2.16	0.43
1:A:641:ILE:HG12	1:B:102:LEU:HD13	1.99	0.43
1:B:146:VAL:HG22	1:B:168:TYR:CD1	2.53	0.43
1:B:236:ARG:HD2	1:B:236:ARG:HA	1.73	0.43
1:C:142:VAL:HG22	1:C:332:ILE:HG23	2.00	0.43
4:K:1:NAG:H83	4:K:1:NAG:H3	2.00	0.43
1:A:136:HIS:O	1:A:258:ARG:HA	2.19	0.43
1:A:143:TYR:O	1:A:330:SER:HB2	2.19	0.43
1:C:216:ASP:OD1	1:C:217:ASP:N	2.48	0.43
1:C:531:ILE:HG13	1:C:532:TYR:CD1	2.54	0.43
4:J:1:NAG:O7	4:J:1:NAG:O3	2.31	0.43
1:A:564:MET:O	1:A:574:TYR:HB2	2.18	0.43
1:B:334:TRP:CZ3	1:B:336:ILE:HG12	2.53	0.43
1:B:519:LEU:HD23	1:B:519:LEU:HA	1.81	0.43
1:B:100:THR:HB	1:B:101:ASP:H	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:VAL:HG12	1:B:430:PHE:CD1	2.54	0.43
1:C:229:VAL:O	1:C:249:ASN:ND2	2.51	0.43
1:A:632:PHE:CD1	1:A:632:PHE:C	2.97	0.43
1:C:281:ASN:OD1	1:C:284:ASN:ND2	2.52	0.42
1:B:133:ILE:HD11	1:C:670:GLU:HB3	2.01	0.42
1:A:270:THR:HG22	1:B:685:GLU:HG2	2.00	0.42
1:A:691:GLN:NE2	1:B:327:ARG:NH1	2.68	0.42
1:B:141:ARG:HG2	1:B:254:ILE:HG12	2.00	0.42
1:B:695:TYR:CE1	1:C:191:ARG:NE	2.87	0.42
1:A:151:ARG:HB3	1:A:244:GLU:HG2	2.02	0.42
1:A:486:THR:HG23	1:C:487:TYR:HD2	1.84	0.42
1:C:284:ASN:OD1	4:J:1:NAG:H83	2.20	0.42
1:C:668:GLN:HA	1:C:671:LEU:HG	2.01	0.42
1:A:207:GLU:OE1	1:A:207:GLU:N	2.53	0.42
1:A:403:ILE:O	1:A:407:SER:OG	2.37	0.42
1:A:621:GLY:HA2	1:A:622:ASN:HA	1.43	0.42
1:A:142:VAL:HG22	1:A:332:ILE:HG23	2.02	0.42
1:A:104:ARG:O	1:C:644:VAL:HG23	2.19	0.42
1:B:378:LYS:O	1:B:378:LYS:HD3	2.20	0.42
1:B:647:MET:SD	1:C:509:GLN:HG2	2.59	0.42
1:C:191:ARG:HH11	1:C:191:ARG:CB	2.28	0.42
1:C:311:ARG:HB3	1:C:313:ASN:OD1	2.18	0.42
1:C:690:LYS:HB2	1:C:691:GLN:HE22	1.85	0.42
1:A:228:THR:HG21	1:A:250:CYS:HB3	2.01	0.42
1:B:142:VAL:HB	1:B:253:THR:OG1	2.19	0.42
1:B:261:TYR:CG	1:B:262:PRO:HA	2.53	0.42
1:B:277:SER:HA	1:B:278:PRO:HD3	1.91	0.42
1:A:103:ILE:HG13	1:A:547:LEU:HD22	2.02	0.42
1:B:175:GLU:O	1:B:179:ILE:HG13	2.20	0.42
1:A:487:TYR:HD2	1:B:486:THR:HG23	1.84	0.42
1:A:528:LEU:HD23	1:A:528:LEU:HA	1.86	0.42
1:C:268:THR:OG1	1:C:272:ASP:OD1	2.35	0.42
1:A:478:LEU:HD12	1:A:480:TYR:HE1	1.84	0.41
1:C:585:ASN:N	4:K:1:NAG:O7	2.53	0.41
1:B:372:THR:O	1:B:482:GLN:HG2	2.19	0.41
1:C:236:ARG:HD3	1:C:236:ARG:C	2.45	0.41
1:C:638:LEU:HD23	1:C:638:LEU:HA	1.77	0.41
1:B:580:ILE:HA	1:B:590:GLN:O	2.20	0.41
1:C:189:TYR:CE2	1:C:191:ARG:NH1	2.88	0.41
1:C:357:ARG:NH2	1:C:364:TYR:HE2	2.18	0.41
1:A:160:TYR:HH	1:C:206:HIS:CD2	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:MET:O	1:A:176:ILE:HG12	2.21	0.41
1:A:176:ILE:HA	1:A:179:ILE:HD12	2.03	0.41
1:A:554:ASN:HB3	1:A:557:SER:CB	2.48	0.41
1:C:102:LEU:HD22	1:C:541:MET:HE1	2.03	0.41
1:C:559:LYS:HE2	1:C:580:ILE:HG13	2.03	0.41
1:A:229:VAL:HG22	1:A:231:ASP:H	1.86	0.41
1:A:655:LEU:HD13	1:C:493:TYR:CG	2.55	0.41
1:A:324:PHE:CD1	1:A:333:SER:HB2	2.56	0.41
1:B:187:SER:OG	1:B:211:MET:SD	2.79	0.41
1:C:129:TYR:CZ	1:C:348:PHE:HB2	2.56	0.41
1:C:272:ASP:CB	1:C:327:ARG:HH22	2.34	0.41
1:A:279:PHE:CG	1:A:339:GLU:HB3	2.56	0.41
1:C:85:ASN:O	1:C:86:THR:OG1	2.31	0.41
1:C:297:PHE:HE1	1:C:323:ALA:HB1	1.85	0.41
3:E:2:NAG:H4	3:E:3:BMA:H2	1.78	0.41
1:B:225:ARG:CD	1:B:253:THR:HG22	2.40	0.40
1:C:153:TYR:HD1	1:C:154:ALA:N	2.19	0.40
1:C:266:PHE:HB3	1:C:274:VAL:HB	2.02	0.40
1:A:206:HIS:NE2	1:B:160:TYR:OH	2.39	0.40
1:A:352:SER:HA	1:A:370:LYS:NZ	2.36	0.40
1:A:357:ARG:NH2	1:A:364:TYR:HE1	2.18	0.40
1:B:408:TYR:HE2	1:B:434:ILE:HD13	1.81	0.40
1:A:173:MET:HG3	1:A:177:HIS:CE1	2.56	0.40
1:C:557:SER:O	1:C:581:PHE:HA	2.22	0.40
1:C:576:ARG:H	1:C:593:GLN:HE22	1.69	0.40
1:A:143:TYR:HB2	1:A:331:VAL:CG2	2.52	0.40
1:A:534:LYS:O	1:A:536:ILE:HG13	2.20	0.40
1:A:666:TYR:CE1	1:C:130:LYS:HD2	2.56	0.40
1:B:493:TYR:CG	1:C:655:LEU:HD13	2.56	0.40
1:C:107:ARG:HA	1:C:513:LEU:HD21	2.03	0.40
1:C:175:GLU:O	1:C:179:ILE:HG13	2.21	0.40
1:A:565:ASN:HA	1:A:573:CYS:HA	2.02	0.40
1:A:655:LEU:HA	1:A:655:LEU:HD12	1.93	0.40
1:A:671:LEU:O	1:A:674:SER:OG	2.40	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	554/630 (88%)	541 (98%)	11 (2%)	2 (0%)	30	61
1	B	564/630 (90%)	541 (96%)	22 (4%)	1 (0%)	43	72
1	C	570/630 (90%)	544 (95%)	26 (5%)	0	100	100
All	All	1688/1890 (89%)	1626 (96%)	59 (4%)	3 (0%)	43	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	413	GLU
1	A	284	ASN
1	B	100	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	504/569 (89%)	477 (95%)	27 (5%)	20	47
1	B	512/569 (90%)	485 (95%)	27 (5%)	20	48
1	C	517/569 (91%)	489 (95%)	28 (5%)	20	47
All	All	1533/1707 (90%)	1451 (95%)	82 (5%)	20	48

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	133	ILE
1	A	146	VAL
1	A	147	LEU
1	A	151	ARG
1	A	161	LEU
1	A	191	ARG
1	A	199	VAL
1	A	203	ARG
1	A	206	HIS
1	A	225	ARG
1	A	229	VAL
1	A	325	LEU
1	A	531	ILE
1	A	533	ASN
1	A	534	LYS
1	A	553	ILE
1	A	566	VAL
1	A	578	VAL
1	A	580	ILE
1	A	591	TYR
1	A	631	LEU
1	A	642	SER
1	A	662	VAL
1	A	676	VAL
1	A	693	VAL
1	A	694	LYS
1	B	92	ARG
1	B	100	THR
1	B	131	ARG
1	B	133	ILE
1	B	147	LEU
1	B	148	THR
1	B	169	VAL
1	B	199	VAL
1	B	229	VAL
1	B	335	ASP
1	B	379	LYS
1	B	411	THR
1	B	498	LEU
1	B	501	ILE
1	B	531	ILE
1	B	545	LEU

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Mol	Chain	Res	Type
1	B	552	THR
1	B	553	ILE
1	B	566	VAL
1	B	578	VAL
1	B	594	LEU
1	B	623	SER
1	B	642	SER
1	B	661	ARG
1	B	662	VAL
1	B	669	LYS
1	B	676	VAL
1	C	102	LEU
1	C	121	LEU
1	C	128	VAL
1	C	133	ILE
1	C	146	VAL
1	C	147	LEU
1	C	191	ARG
1	C	199	VAL
1	C	206	HIS
1	C	207	GLU
1	C	229	VAL
1	C	236	ARG
1	C	251	MET
1	C	252	LEU
1	C	269	SER
1	C	299	ILE
1	C	319	HIS
1	C	411	THR
1	C	531	ILE
1	C	553	ILE
1	C	562	ARG
1	C	566	VAL
1	C	601	LEU
1	C	632	PHE
1	C	646	SER
1	C	661	ARG
1	C	676	VAL
1	C	682	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	HIS
1	A	220	ASN
1	A	582	ASN
1	B	108	ASN
1	B	132	ASN
1	B	136	HIS
1	B	144	GLN
1	B	178	HIS
1	B	212	GLN
1	C	284	ASN
1	C	293	ASN
1	C	476	HIS
1	C	605	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

22 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	D	1	2,1	14,14,15	0.31	0	17,19,21	0.61	0
2	NAG	D	2	2	14,14,15	0.32	0	17,19,21	0.65	0
2	BMA	D	3	2	11,11,12	0.92	1 (9%)	15,15,17	1.49	2 (13%)
2	MAN	D	4	2	11,11,12	1.26	2 (18%)	15,15,17	1.33	2 (13%)
3	NAG	E	1	3,1	14,14,15	0.65	1 (7%)	17,19,21	0.77	0
3	NAG	E	2	3	14,14,15	0.19	0	17,19,21	0.79	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	E	3	3	11,11,12	1.40	1 (9%)	15,15,17	0.99	0
4	NAG	F	1	4,1	14,14,15	0.82	1 (7%)	17,19,21	1.00	2 (11%)
4	NAG	F	2	4	14,14,15	0.64	0	17,19,21	1.39	2 (11%)
4	NAG	G	1	4,1	14,14,15	0.47	0	17,19,21	0.70	0
4	NAG	G	2	4	14,14,15	0.64	1 (7%)	17,19,21	0.83	1 (5%)
4	NAG	H	1	4,1	14,14,15	0.50	0	17,19,21	1.51	3 (17%)
4	NAG	H	2	4	14,14,15	1.37	2 (14%)	17,19,21	1.30	1 (5%)
5	NAG	I	1	5,1	14,14,15	0.36	0	17,19,21	0.87	1 (5%)
5	NAG	I	2	5	14,14,15	0.54	0	17,19,21	0.62	0
5	BMA	I	3	5	11,11,12	1.15	0	15,15,17	1.15	2 (13%)
5	MAN	I	4	5	11,11,12	1.46	3 (27%)	15,15,17	1.05	1 (6%)
5	MAN	I	5	5	11,11,12	1.31	1 (9%)	15,15,17	0.88	0
4	NAG	J	1	4,1	14,14,15	0.70	0	17,19,21	1.15	2 (11%)
4	NAG	J	2	4	14,14,15	0.58	0	17,19,21	1.17	1 (5%)
4	NAG	K	1	4,1	14,14,15	0.91	1 (7%)	17,19,21	1.81	2 (11%)
4	NAG	K	2	4	14,14,15	0.40	0	17,19,21	0.40	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	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
4	NAG	F	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	6/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	G	2	4	-	3/6/23/26	0/1/1/1
4	NAG	H	1	4,1	-	6/6/23/26	0/1/1/1
4	NAG	H	2	4	-	4/6/23/26	0/1/1/1
5	NAG	I	1	5,1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	BMA	I	3	5	-	2/2/19/22	0/1/1/1
5	MAN	I	4	5	-	1/2/19/22	0/1/1/1
5	MAN	I	5	5	-	1/2/19/22	0/1/1/1
4	NAG	J	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2	NAG	C1-C2	4.07	1.57	1.52
3	E	3	BMA	C4-C5	3.51	1.60	1.53
5	I	4	MAN	C2-C3	3.31	1.57	1.52
4	F	1	NAG	O5-C1	-2.85	1.38	1.43
4	K	1	NAG	O5-C1	2.81	1.48	1.43
4	H	2	NAG	O5-C1	2.75	1.48	1.43
5	I	5	MAN	O5-C1	-2.61	1.39	1.43
5	I	4	MAN	C1-C2	2.46	1.58	1.52
4	G	2	NAG	C1-C2	2.31	1.55	1.52
2	D	4	MAN	C2-C3	2.29	1.56	1.52
3	E	1	NAG	O5-C1	-2.27	1.39	1.43
2	D	4	MAN	C1-C2	2.25	1.57	1.52
5	I	4	MAN	O5-C5	2.16	1.47	1.43
2	D	3	BMA	C1-C2	2.15	1.57	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	1	NAG	C1-O5-C5	4.95	118.82	112.19
4	F	2	NAG	C2-N2-C7	4.77	129.29	122.90
4	H	1	NAG	C2-N2-C7	4.70	129.20	122.90
4	K	1	NAG	C2-N2-C7	4.68	129.17	122.90
4	H	2	NAG	C2-N2-C7	4.54	128.99	122.90
2	D	4	MAN	C1-O5-C5	3.89	117.40	112.19
4	J	2	NAG	C3-C4-C5	3.78	117.08	110.23
2	D	3	BMA	C1-O5-C5	3.44	116.80	112.19
2	D	3	BMA	C1-C2-C3	3.21	114.32	109.64
4	J	1	NAG	C1-O5-C5	3.11	116.36	112.19
4	H	1	NAG	C1-C2-N2	2.64	114.59	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1	NAG	O4-C4-C5	-2.62	102.86	109.32
4	J	1	NAG	C1-C2-N2	2.43	114.26	110.43
4	F	2	NAG	C1-C2-N2	2.42	114.24	110.43
5	I	3	BMA	O5-C5-C4	-2.27	105.31	110.83
4	F	1	NAG	C3-C4-C5	2.25	114.31	110.23
5	I	4	MAN	C1-O5-C5	2.24	115.19	112.19
3	E	2	NAG	C1-O5-C5	2.23	115.17	112.19
4	H	1	NAG	O4-C4-C3	2.19	115.55	110.38
4	F	1	NAG	C1-O5-C5	-2.14	109.32	112.19
4	G	2	NAG	C1-O5-C5	2.14	115.05	112.19
5	I	3	BMA	C6-C5-C4	2.07	118.11	113.02
2	D	4	MAN	C1-C2-C3	2.00	112.56	109.64

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C4-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
5	I	3	BMA	O5-C5-C6-O6
5	I	3	BMA	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
4	K	1	NAG	C8-C7-N2-C2
4	K	1	NAG	O7-C7-N2-C2
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
5	I	4	MAN	O5-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C3-C2-N2-C7
4	K	1	NAG	C1-C2-N2-C7
4	G	1	NAG	C4-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
4	J	1	NAG	C3-C2-N2-C7
4	K	1	NAG	C3-C2-N2-C7
4	F	1	NAG	C4-C5-C6-O6
4	F	2	NAG	C1-C2-N2-C7
4	H	1	NAG	C1-C2-N2-C7
4	H	2	NAG	C1-C2-N2-C7
4	F	1	NAG	C3-C2-N2-C7
4	F	2	NAG	C3-C2-N2-C7
4	H	1	NAG	C3-C2-N2-C7
4	H	2	NAG	C3-C2-N2-C7
4	K	1	NAG	O5-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6
5	I	5	MAN	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 9 short contacts:

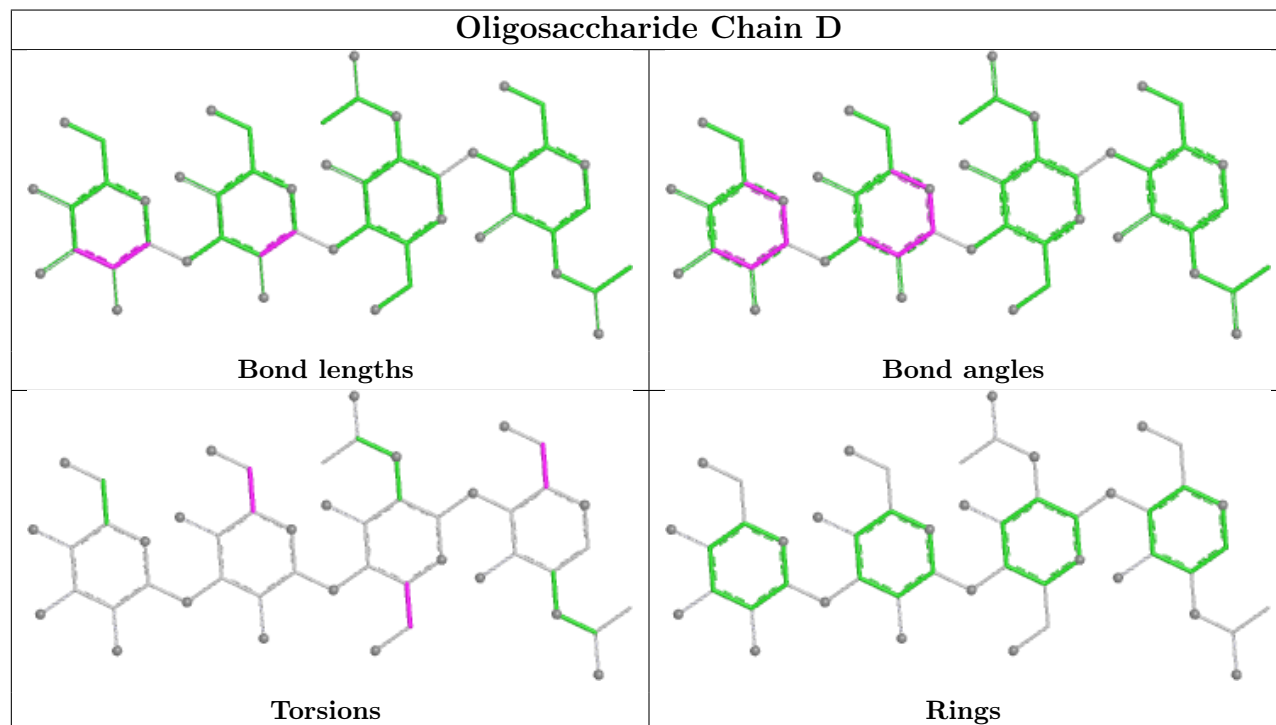
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	1	0
4	J	1	NAG	2	0
3	E	3	BMA	1	0
4	H	1	NAG	1	0
4	H	2	NAG	1	0
4	K	1	NAG	2	0

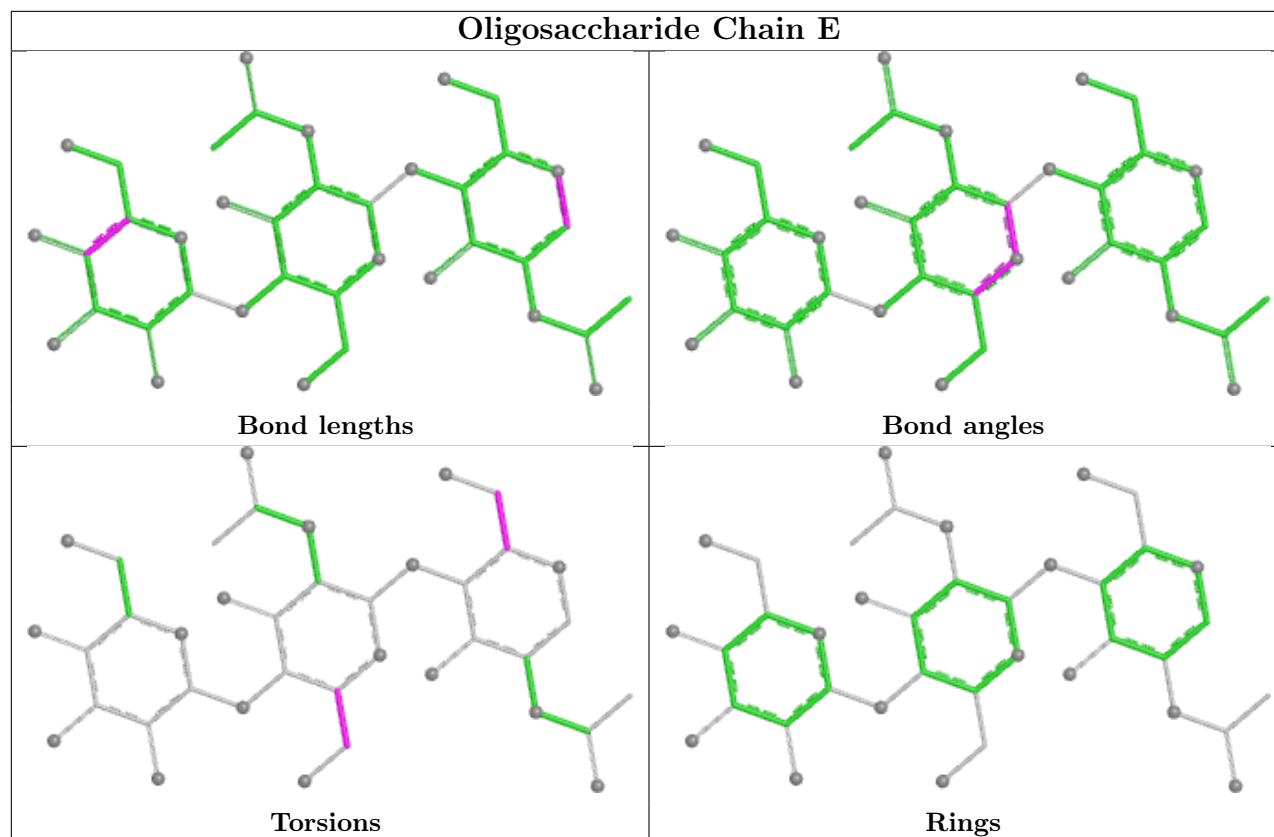
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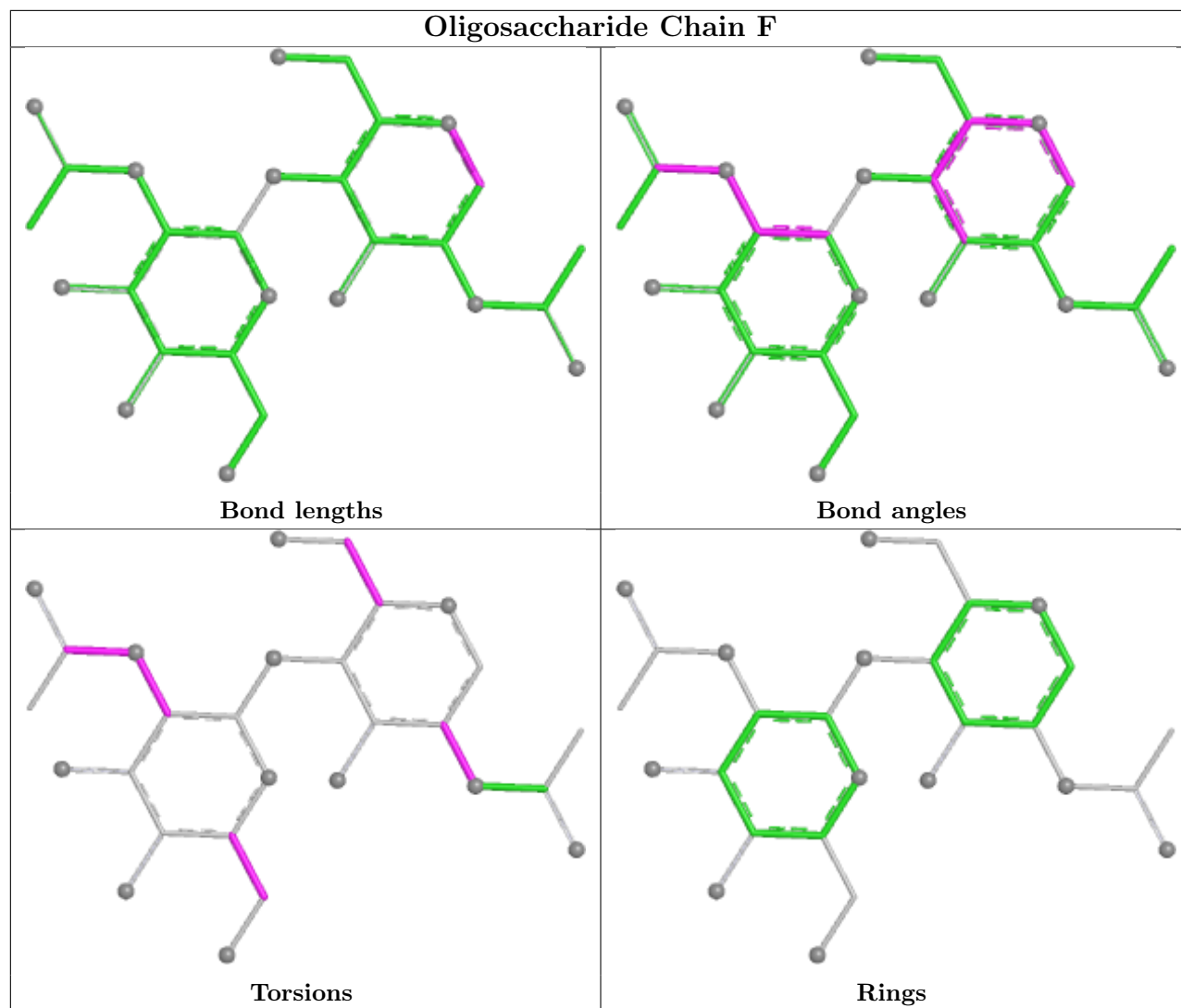
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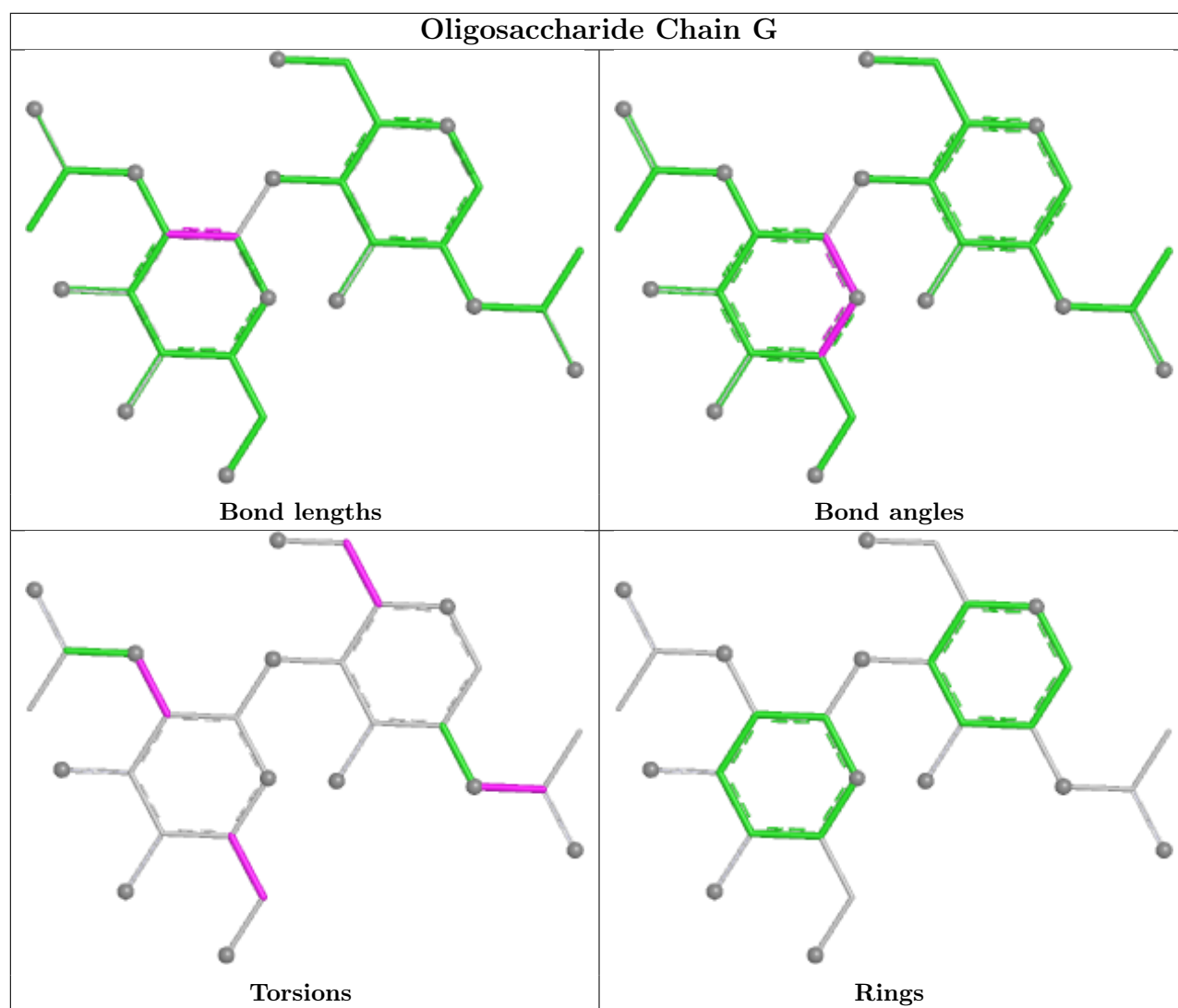
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	NAG	1	0
3	E	2	NAG	1	0

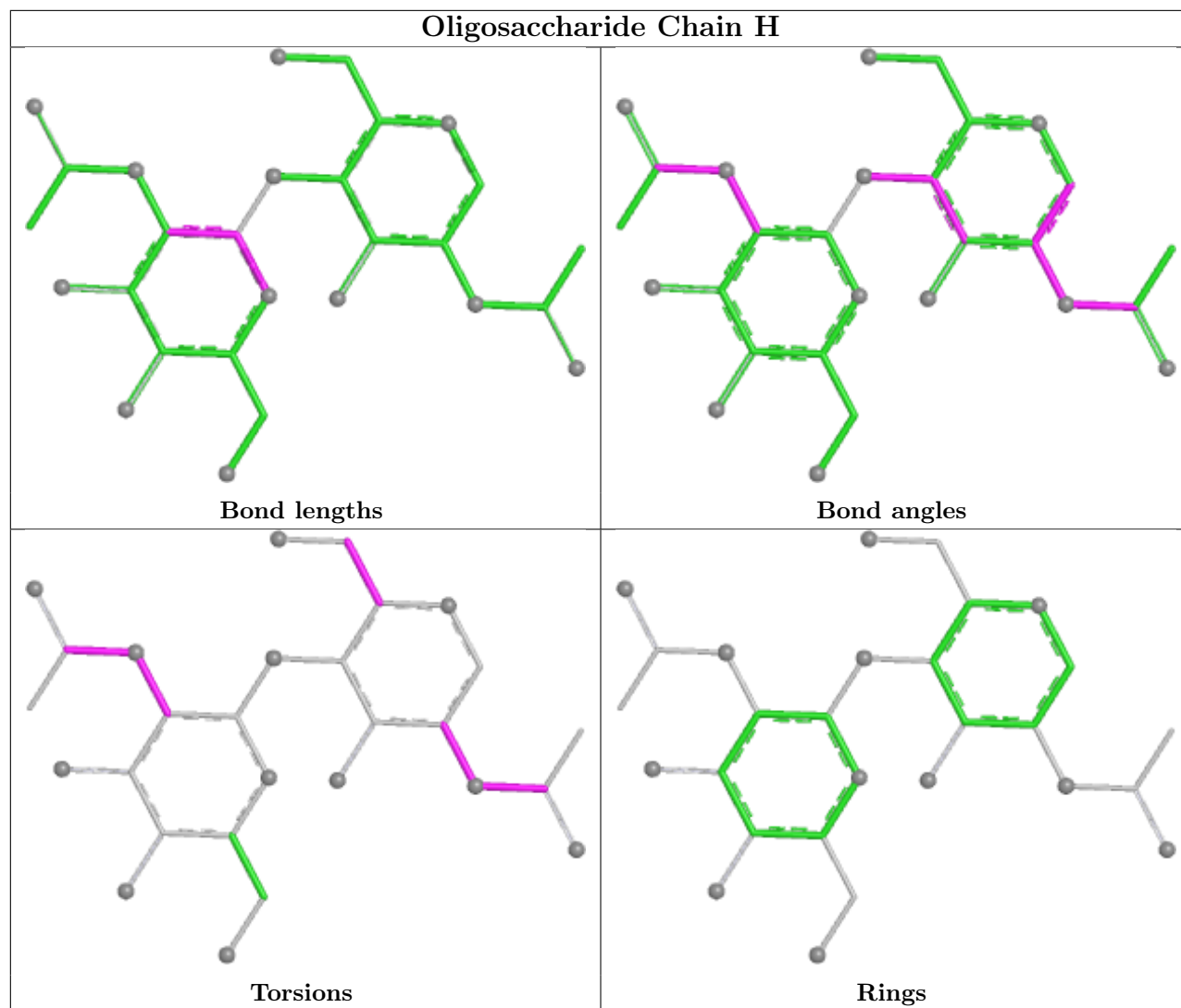
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

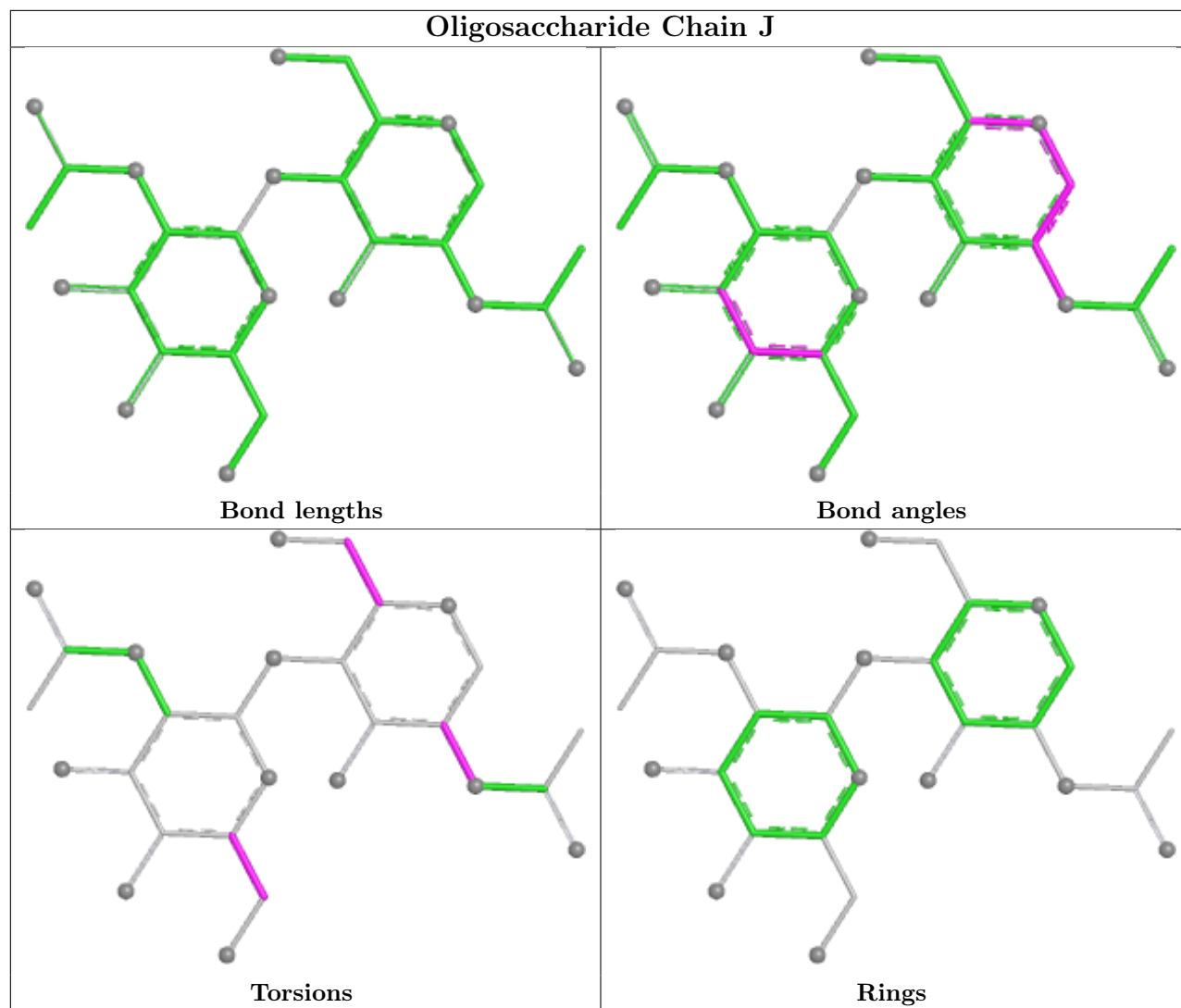


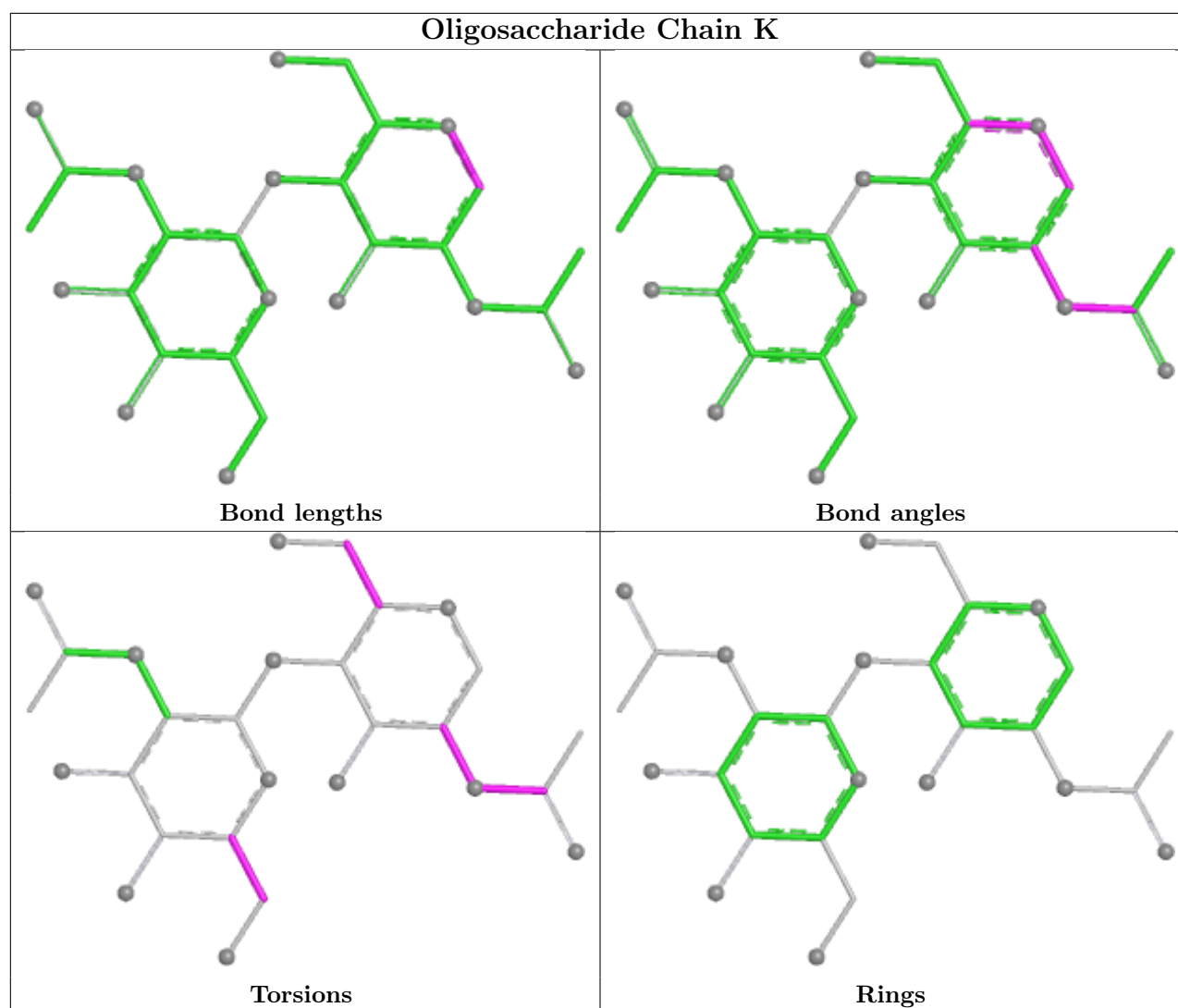


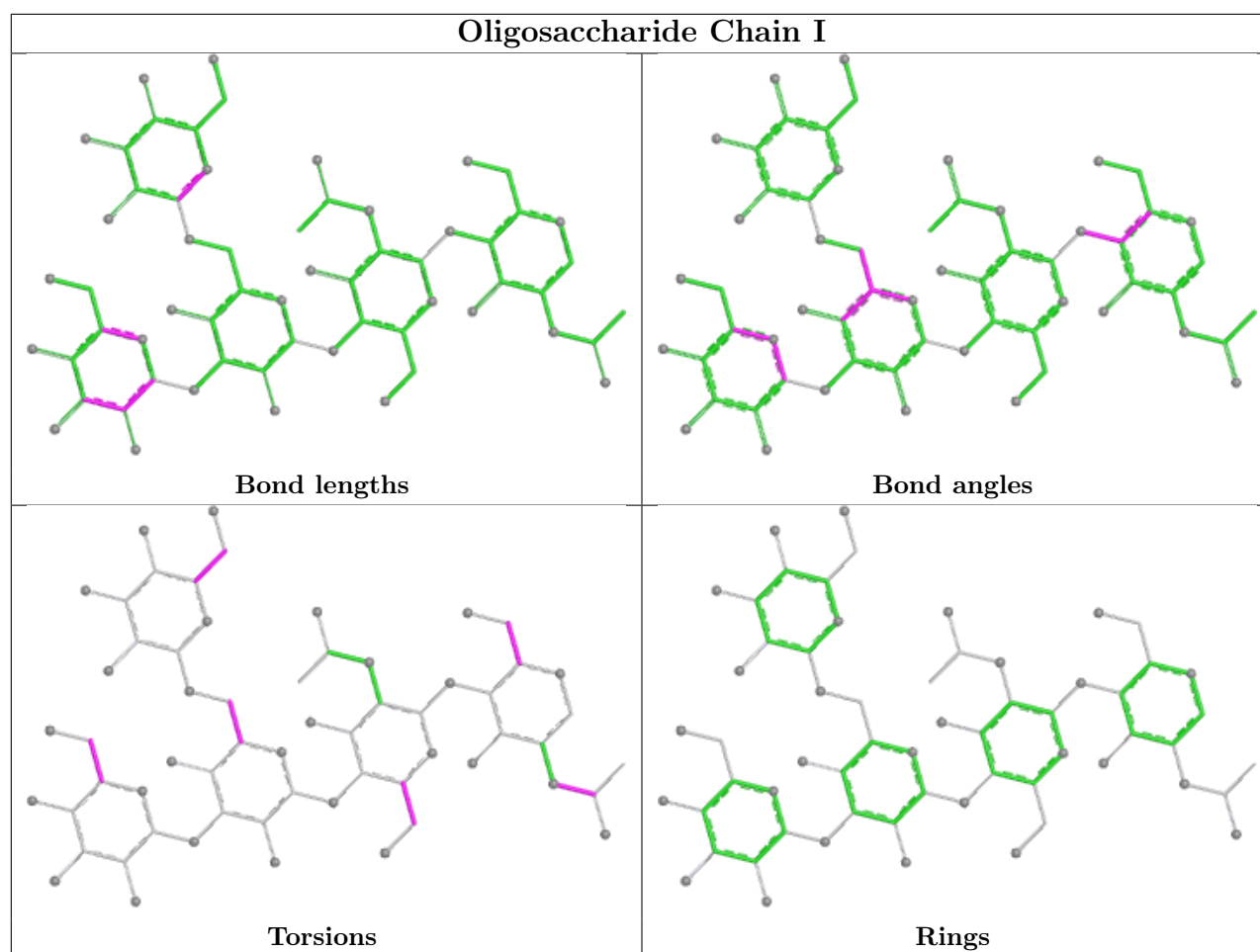












5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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	$\# Z > 2$
6	NAG	C	808	1	14,14,15	1.07	1 (7%)	17,19,21	1.35	2 (11%)
6	NAG	A	811	1	14,14,15	0.77	1 (7%)	17,19,21	0.67	0
6	NAG	C	809	1	14,14,15	0.47	0	17,19,21	0.67	0
6	NAG	A	808	1	14,14,15	0.30	0	17,19,21	0.66	0
6	NAG	C	811	1	14,14,15	0.42	0	17,19,21	0.63	0
6	NAG	B	805	1	14,14,15	0.31	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	810	1	14,14,15	0.38	0	17,19,21	0.82	0
6	NAG	A	805	1	14,14,15	0.24	0	17,19,21	0.52	0
6	NAG	A	810	1	14,14,15	0.38	0	17,19,21	0.36	0
6	NAG	A	809	1	14,14,15	0.57	0	17,19,21	0.58	0
6	NAG	A	807	1	14,14,15	0.64	1 (7%)	17,19,21	0.77	0
6	NAG	B	804	1	14,14,15	0.37	0	17,19,21	0.73	0
6	NAG	C	810	1	14,14,15	0.61	0	17,19,21	0.63	1 (5%)
6	NAG	C	812	1	14,14,15	0.59	0	17,19,21	0.78	1 (5%)
6	NAG	A	806	1	14,14,15	0.45	0	17,19,21	0.44	0
6	NAG	B	811	1	14,14,15	0.30	0	17,19,21	0.58	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
6	NAG	C	808	1	-	6/6/23/26	0/1/1/1
6	NAG	A	811	1	-	3/6/23/26	0/1/1/1
6	NAG	C	809	1	-	0/6/23/26	0/1/1/1
6	NAG	A	808	1	-	0/6/23/26	0/1/1/1
6	NAG	C	811	1	-	3/6/23/26	0/1/1/1
6	NAG	B	805	1	-	2/6/23/26	0/1/1/1
6	NAG	B	810	1	-	2/6/23/26	0/1/1/1
6	NAG	A	805	1	-	2/6/23/26	0/1/1/1
6	NAG	A	810	1	-	3/6/23/26	0/1/1/1
6	NAG	A	809	1	-	4/6/23/26	0/1/1/1
6	NAG	A	807	1	-	2/6/23/26	0/1/1/1
6	NAG	B	804	1	-	3/6/23/26	0/1/1/1
6	NAG	C	810	1	-	2/6/23/26	0/1/1/1
6	NAG	C	812	1	-	2/6/23/26	0/1/1/1
6	NAG	A	806	1	-	3/6/23/26	0/1/1/1
6	NAG	B	811	1	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	808	NAG	C1-C2	3.45	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	811	NAG	O5-C1	2.45	1.47	1.43
6	A	807	NAG	O5-C1	-2.19	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	808	NAG	C2-N2-C7	4.57	129.03	122.90
6	C	812	NAG	C1-O5-C5	-2.67	108.61	112.19
6	C	810	NAG	C1-O5-C5	2.05	114.93	112.19
6	C	808	NAG	C1-C2-N2	2.04	113.65	110.43

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	809	NAG	O5-C5-C6-O6
6	A	809	NAG	C4-C5-C6-O6
6	B	810	NAG	O5-C5-C6-O6
6	C	811	NAG	O5-C5-C6-O6
6	C	808	NAG	C4-C5-C6-O6
6	A	807	NAG	C4-C5-C6-O6
6	B	804	NAG	O5-C5-C6-O6
6	C	808	NAG	O5-C5-C6-O6
6	B	811	NAG	O5-C5-C6-O6
6	B	810	NAG	C4-C5-C6-O6
6	C	811	NAG	C4-C5-C6-O6
6	B	811	NAG	C4-C5-C6-O6
6	A	806	NAG	C8-C7-N2-C2
6	A	806	NAG	O7-C7-N2-C2
6	A	809	NAG	C8-C7-N2-C2
6	A	809	NAG	O7-C7-N2-C2
6	A	810	NAG	C8-C7-N2-C2
6	A	810	NAG	O7-C7-N2-C2
6	B	811	NAG	C8-C7-N2-C2
6	B	811	NAG	O7-C7-N2-C2
6	C	808	NAG	C8-C7-N2-C2
6	C	808	NAG	O7-C7-N2-C2
6	A	807	NAG	O5-C5-C6-O6
6	A	805	NAG	O5-C5-C6-O6
6	B	805	NAG	O5-C5-C6-O6
6	A	805	NAG	C4-C5-C6-O6
6	B	805	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	C	810	NAG	O5-C5-C6-O6
6	C	810	NAG	C4-C5-C6-O6
6	A	811	NAG	O5-C5-C6-O6
6	A	810	NAG	O5-C5-C6-O6
6	B	804	NAG	C4-C5-C6-O6
6	A	811	NAG	C1-C2-N2-C7
6	C	812	NAG	C4-C5-C6-O6
6	A	811	NAG	C3-C2-N2-C7
6	B	804	NAG	C3-C2-N2-C7
6	C	811	NAG	C3-C2-N2-C7
6	A	806	NAG	O5-C5-C6-O6
6	C	808	NAG	C1-C2-N2-C7
6	C	808	NAG	C3-C2-N2-C7
6	C	812	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	808	NAG	2	0
6	B	805	NAG	1	0
6	A	810	NAG	1	0
6	B	804	NAG	1	0
6	B	811	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	562/630 (89%)	0.04	5 (0%) 81 56	66, 116, 152, 183	0
1	B	570/630 (90%)	-0.01	4 (0%) 84 61	65, 108, 149, 166	0
1	C	576/630 (91%)	-0.04	3 (0%) 87 66	64, 102, 145, 176	0
All	All	1708/1890 (90%)	-0.00	12 (0%) 84 61	64, 109, 151, 183	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	671	LEU	3.2
1	A	259	SER	3.2
1	A	696	VAL	3.0
1	B	255	THR	2.9
1	A	261	TYR	2.5
1	C	440	VAL	2.5
1	A	267	ALA	2.4
1	A	543	ASP	2.2
1	B	320	ARG	2.2
1	B	413	GLU	2.2
1	C	197	VAL	2.1
1	C	84	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [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,

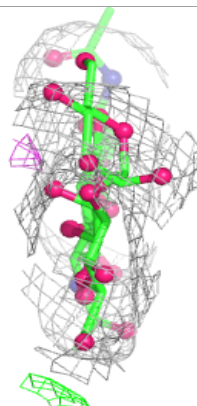
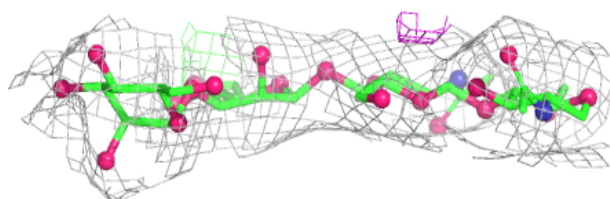
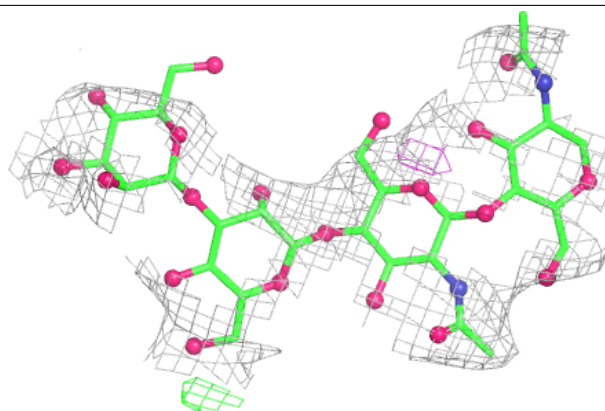
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	H	2	14/15	0.17	0.12	167,181,186,187	0
4	NAG	H	1	14/15	0.29	0.12	141,165,180,182	0
4	NAG	G	1	14/15	0.41	0.11	176,180,186,188	0
4	NAG	J	2	14/15	0.43	0.12	163,176,182,184	0
4	NAG	F	1	14/15	0.46	0.10	155,171,184,190	0
4	NAG	F	2	14/15	0.53	0.11	169,184,193,193	0
5	MAN	I	5	11/12	0.54	0.12	135,143,148,148	0
2	BMA	D	3	11/12	0.56	0.11	133,144,153,158	0
2	MAN	D	4	11/12	0.58	0.10	145,169,176,177	0
5	MAN	I	4	11/12	0.60	0.09	127,135,151,156	0
3	BMA	E	3	11/12	0.61	0.11	120,133,138,139	0
4	NAG	J	1	14/15	0.64	0.11	144,161,172,173	0
4	NAG	G	2	14/15	0.64	0.10	177,188,192,192	0
4	NAG	K	1	14/15	0.67	0.12	153,165,177,180	0
4	NAG	K	2	14/15	0.78	0.09	180,183,188,189	0
2	NAG	D	2	14/15	0.79	0.12	109,114,131,131	0
5	NAG	I	1	14/15	0.79	0.13	80,89,99,105	0
5	NAG	I	2	14/15	0.83	0.09	87,95,106,110	0
5	BMA	I	3	11/12	0.89	0.06	106,117,130,136	0
3	NAG	E	2	14/15	0.90	0.07	109,114,121,122	0
2	NAG	D	1	14/15	0.93	0.07	105,114,124,126	0
3	NAG	E	1	14/15	0.94	0.09	104,111,122,126	0

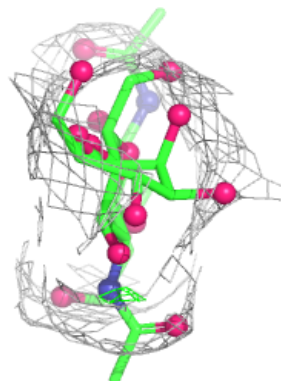
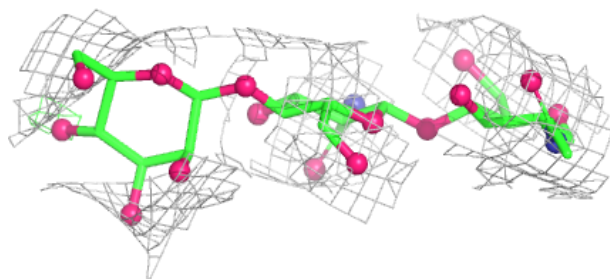
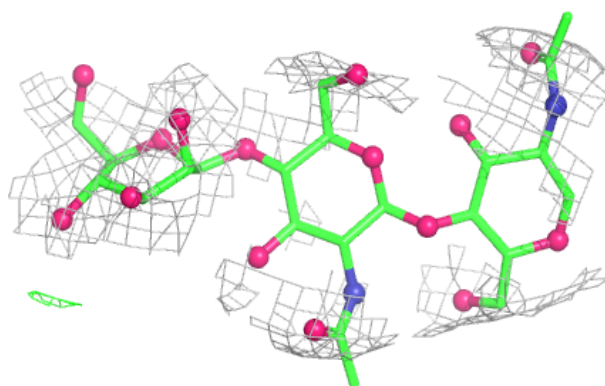
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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

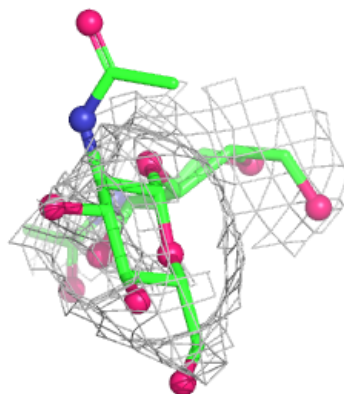
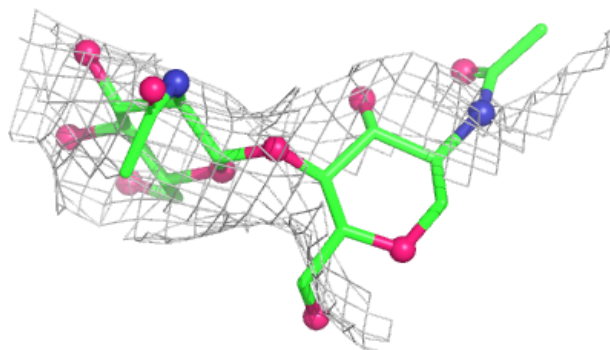
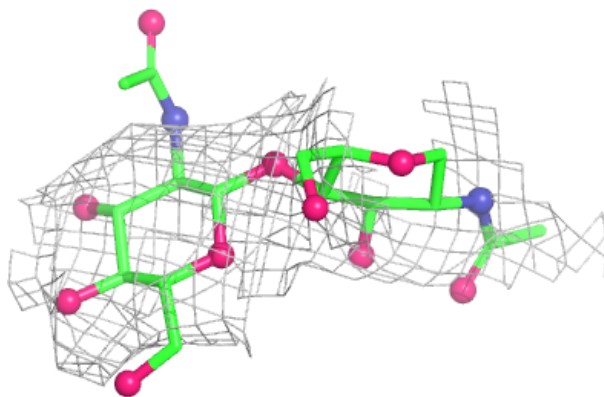
**Electron density around Chain E:**

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



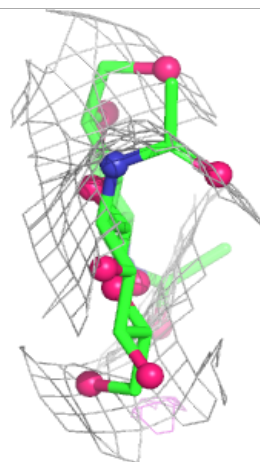
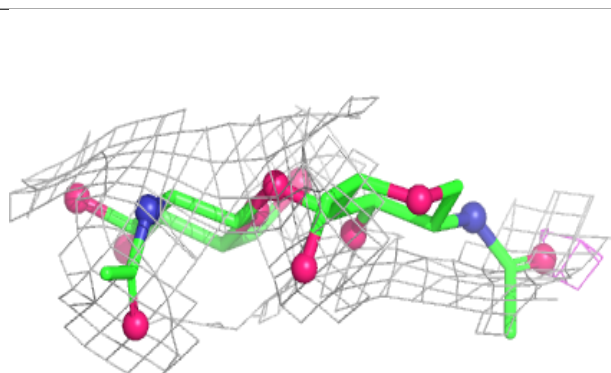
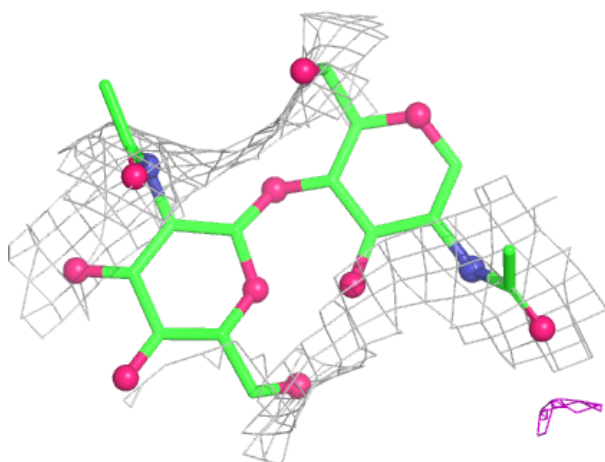
Electron density around Chain F:

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



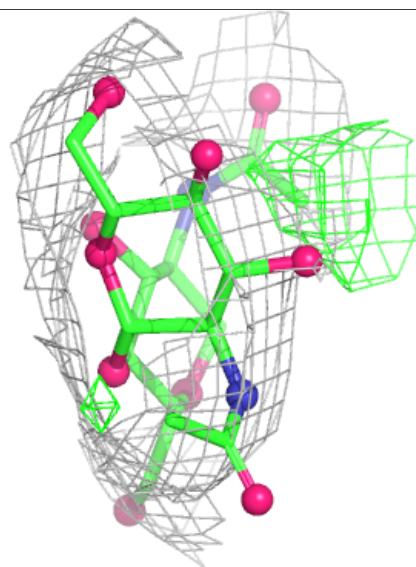
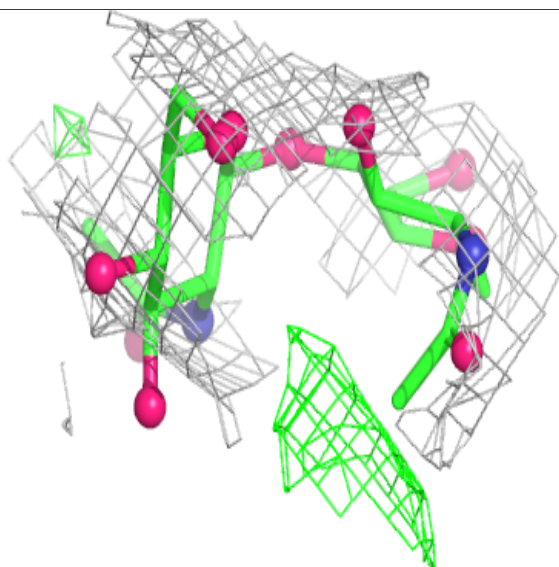
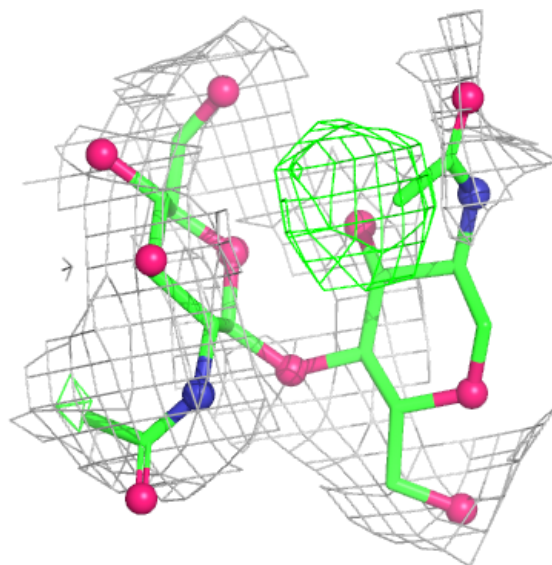
Electron density around Chain G:

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



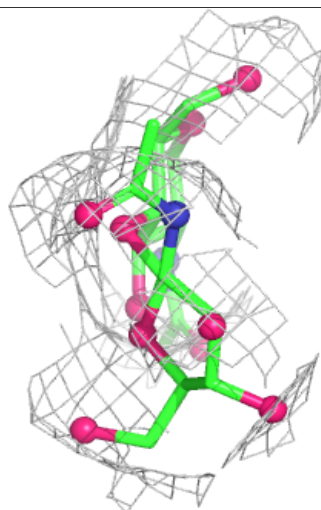
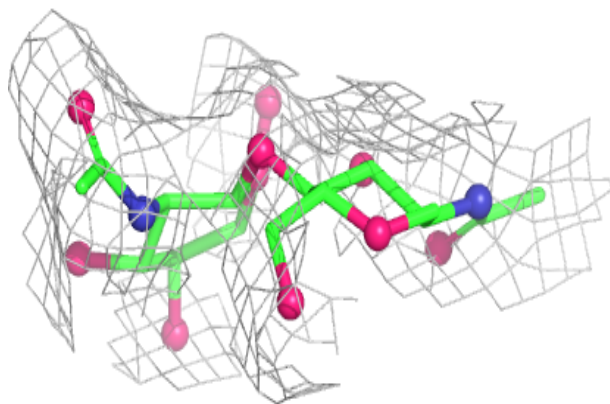
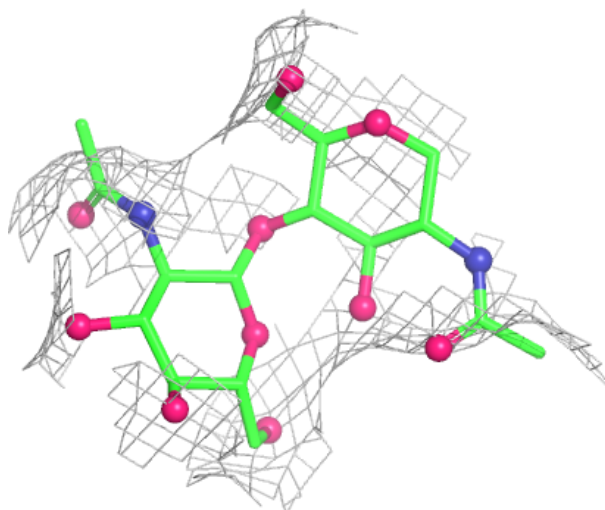
Electron density around Chain H:

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



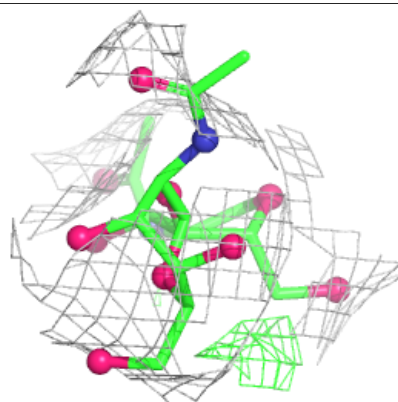
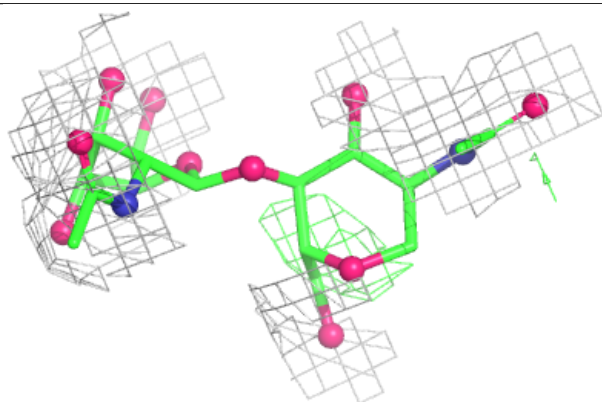
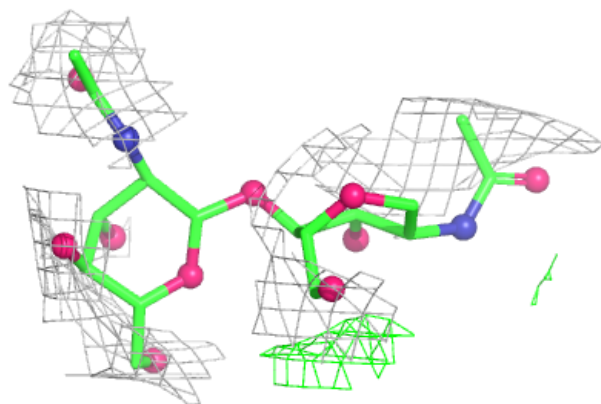
Electron density around Chain J:

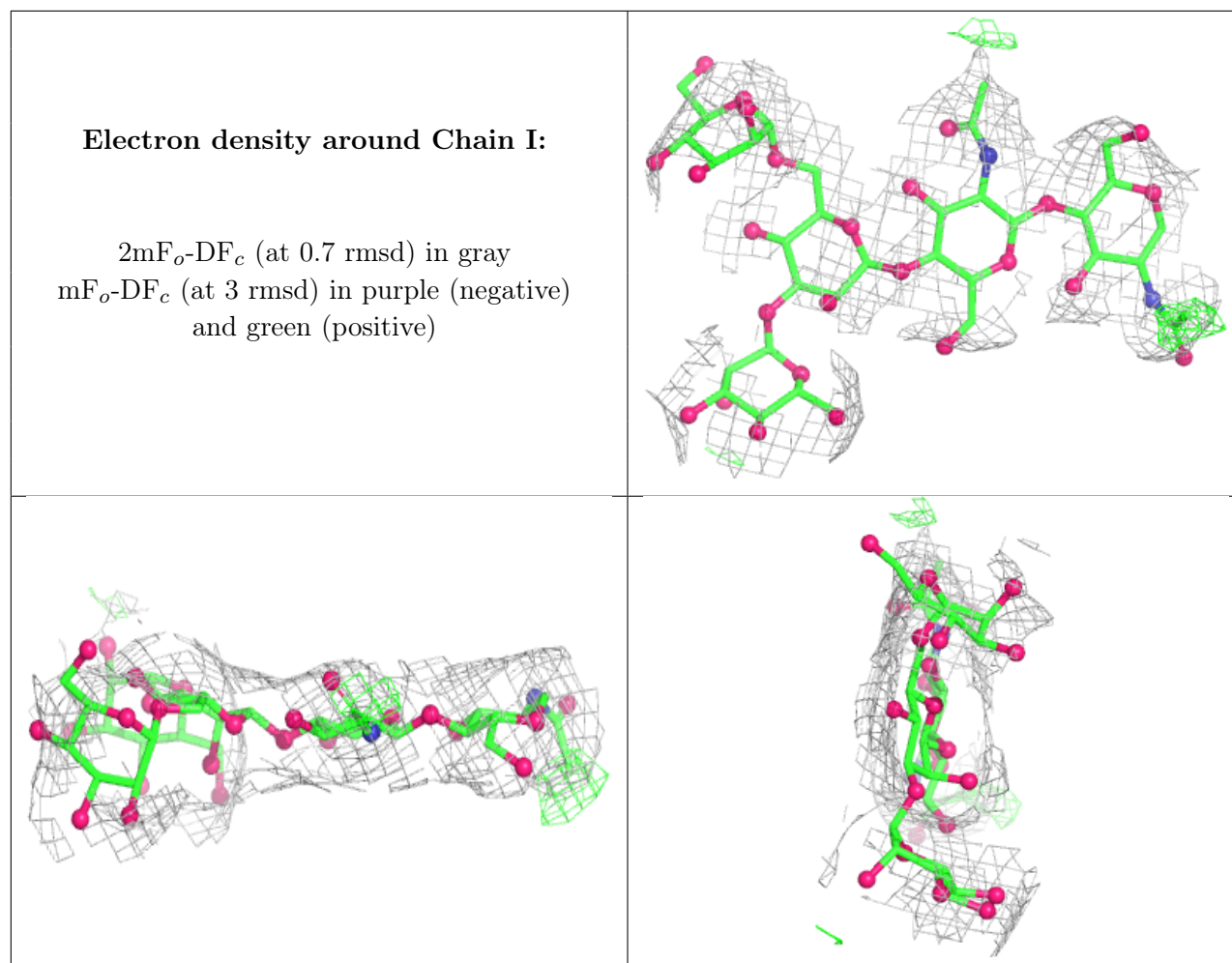
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
6	NAG	B	810	14/15	0.10	0.12	146,166,174,174	0
6	NAG	C	812	14/15	0.28	0.12	163,172,176,178	0
6	NAG	B	804	14/15	0.33	0.11	157,181,185,188	0
6	NAG	C	809	14/15	0.34	0.12	149,162,165,170	0
6	NAG	C	808	14/15	0.45	0.09	143,171,174,176	0
6	NAG	A	811	14/15	0.54	0.12	147,171,175,178	0
6	NAG	B	805	14/15	0.54	0.13	134,145,157,163	0
6	NAG	A	805	14/15	0.59	0.15	162,167,177,185	0
6	NAG	A	807	14/15	0.60	0.09	156,167,171,171	0
6	NAG	A	808	14/15	0.63	0.10	169,175,178,179	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	A	809	14/15	0.63	0.08	164,175,183,184	0
6	NAG	B	811	14/15	0.63	0.10	109,125,134,134	0
6	NAG	C	811	14/15	0.64	0.09	162,169,175,178	0
6	NAG	A	806	14/15	0.65	0.09	160,166,169,176	0
6	NAG	A	810	14/15	0.70	0.11	144,160,170,171	0
6	NAG	C	810	14/15	0.77	0.09	160,163,171,173	0
7	CA	A	812	1/1	0.97	0.04	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.