



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:04 PM UTC

PDB ID : 9B2W / pdb_00009b2w
Title : PIV3 HN with Fab 13
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Deposited on : 2024-03-17
Resolution : 2.51 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

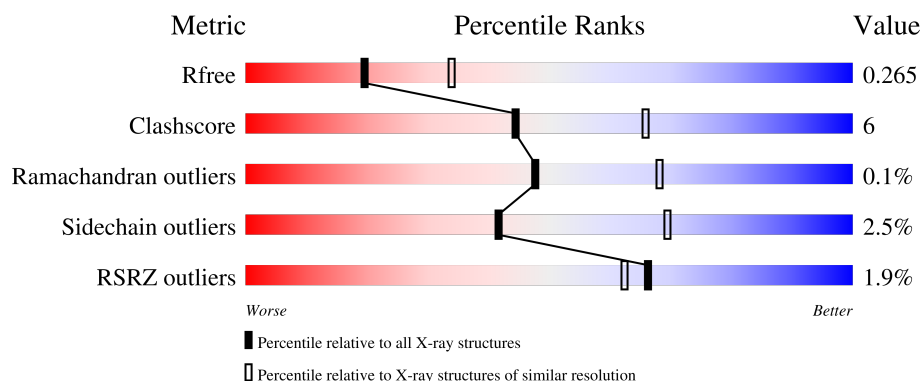
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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.



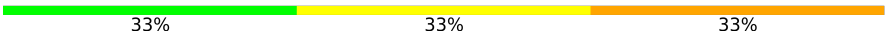
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	461	
1	D	461	
2	B	222	
2	E	222	
3	C	219	

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Mol	Chain	Length	Quality of chain
3	F	219	 84% 15%
4	H	2	 100%
5	G	3	 67% 33%
5	J	3	 33% 33% 33%
6	I	4	 50% 50%
7	K	3	 100%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13578 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-neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	430	Total	C	N	O	S	0	0	0
			3375	2134	581	640	20			
1	A	429	Total	C	N	O	S	0	0	0
			3367	2130	579	638	20			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	HIS	-	expression tag	UNP Q81080
D	2	HIS	-	expression tag	UNP Q81080
D	3	HIS	-	expression tag	UNP Q81080
D	4	HIS	-	expression tag	UNP Q81080
D	5	HIS	-	expression tag	UNP Q81080
D	6	HIS	-	expression tag	UNP Q81080
D	7	SER	-	expression tag	UNP Q81080
D	8	LEU	-	expression tag	UNP Q81080
D	9	VAL	-	expression tag	UNP Q81080
D	10	PRO	-	expression tag	UNP Q81080
D	11	ARG	-	expression tag	UNP Q81080
D	12	GLY	-	expression tag	UNP Q81080
D	13	SER	-	expression tag	UNP Q81080
A	1	HIS	-	expression tag	UNP Q81080
A	2	HIS	-	expression tag	UNP Q81080
A	3	HIS	-	expression tag	UNP Q81080
A	4	HIS	-	expression tag	UNP Q81080
A	5	HIS	-	expression tag	UNP Q81080
A	6	HIS	-	expression tag	UNP Q81080
A	7	SER	-	expression tag	UNP Q81080
A	8	LEU	-	expression tag	UNP Q81080
A	9	VAL	-	expression tag	UNP Q81080
A	10	PRO	-	expression tag	UNP Q81080
A	11	ARG	-	expression tag	UNP Q81080
A	12	GLY	-	expression tag	UNP Q81080

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Chain	Residue	Modelled	Actual	Comment	Reference
A	13	SER	-	expression tag	UNP Q81080

- Molecule 2 is a protein called Fab 13 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	222	Total	C	N	O	S	0	0	0
			1653	1045	277	325	6			
2	E	215	Total	C	N	O	S	0	0	0
			1611	1022	269	314	6			

- Molecule 3 is a protein called Fab 13 Light Chain.

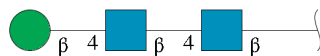
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	218	Total	C	N	O	S	0	0	0
			1669	1039	284	339	7			
3	F	217	Total	C	N	O	S	0	0	0
			1663	1036	283	338	6			

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



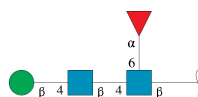
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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.



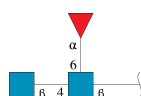
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	J	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



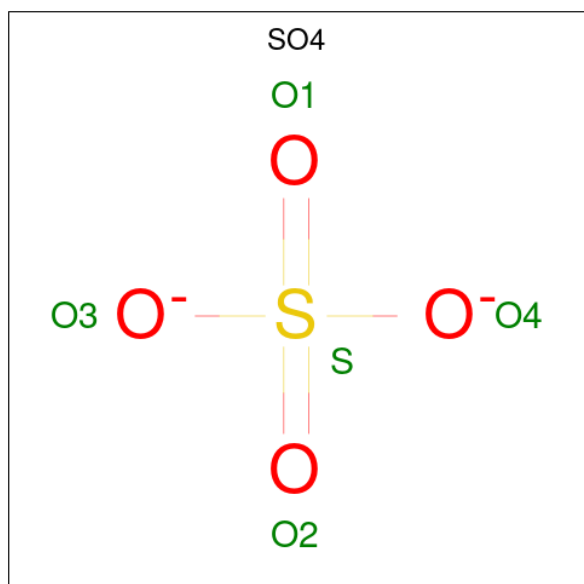
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	K	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

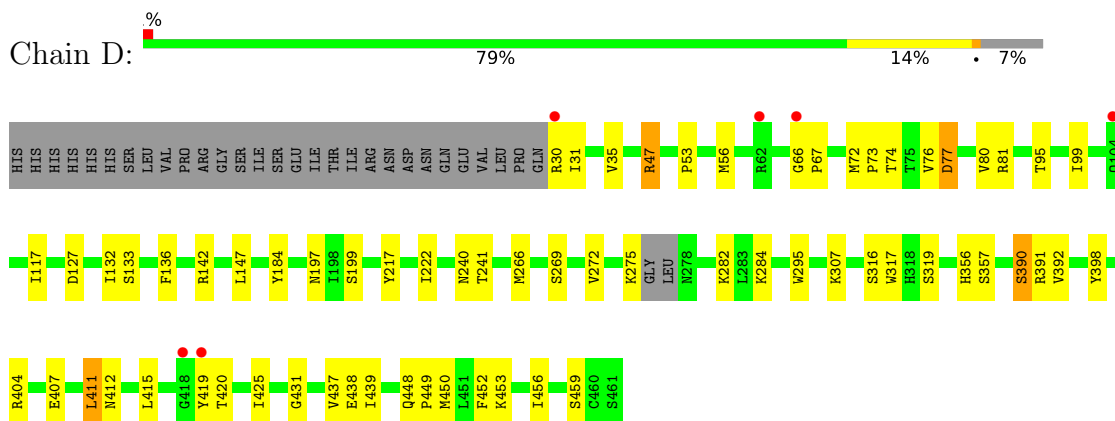
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	3	Total	O	0	0
			3	3		
10	A	5	Total	O	0	0
			5	5		
10	B	1	Total	O	0	0
			1	1		
10	C	1	Total	O	0	0
			1	1		
10	E	3	Total	O	0	0
			3	3		

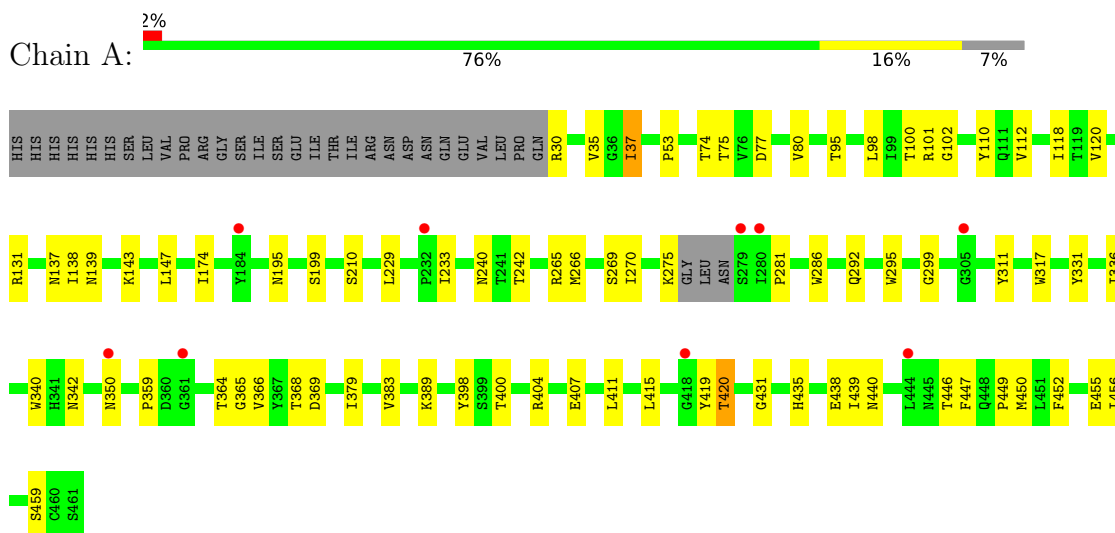
3 Residue-property plots [i](#)

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.

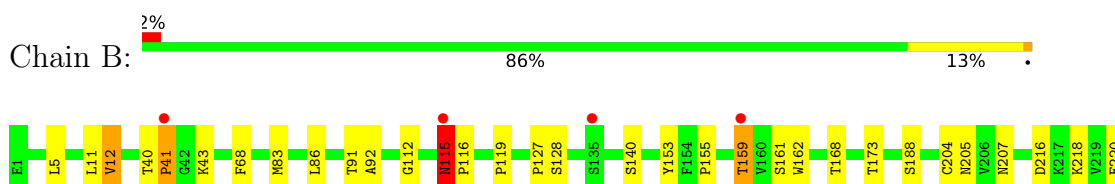
- Molecule 1: Hemagglutinin-neuraminidase



- Molecule 1: Hemagglutinin-neuraminidase



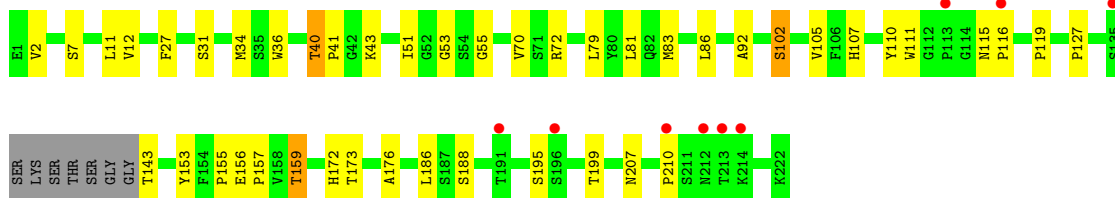
- Molecule 2: Fab 13 Heavy Chain



P221
K222

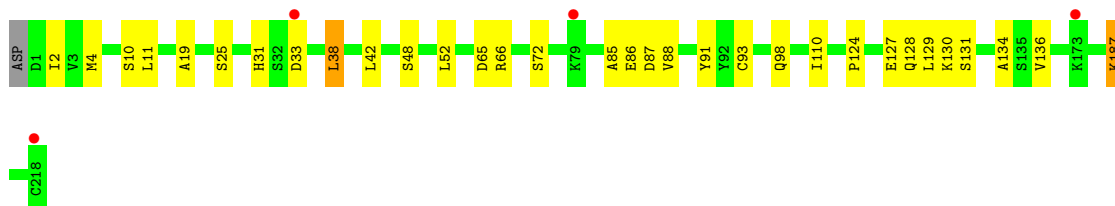
- Molecule 2: Fab 13 Heavy Chain

Chain E:  4% 77% 19% ..



- Molecule 3: Fab 13 Light Chain

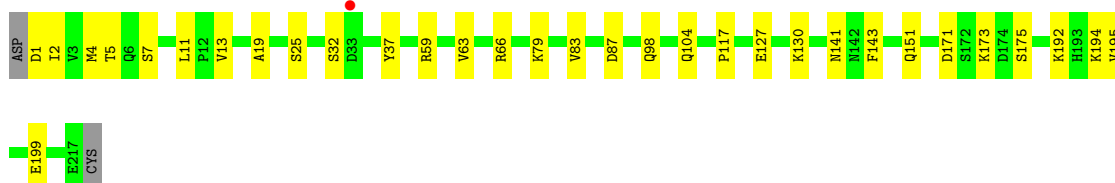
Chain C:  2% 85% 14% .



C218

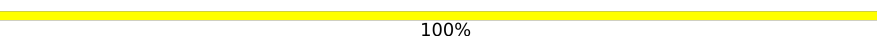
- Molecule 3: Fab 13 Light Chain

Chain F:  84% 15% .



E199
E217
CYS

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

Chain H:  100%

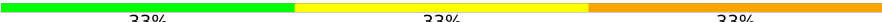
NAG1
NAG2

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

Chain G:  67% 33%

NAG1
NAG2
BMA3

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

Chain J:  33% 33% 33%

NAG1
NAG2
BMA3

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

Chain I:  50% 50%

NAG1
NAG2
BMA3
FUC4

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

NAG1
NAG2
FUC3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.27Å 129.35Å 89.45Å 90.00° 93.57° 90.00°	Depositor
Resolution (Å)	34.76 – 2.51 34.76 – 2.51	Depositor EDS
% Data completeness (in resolution range)	96.8 (34.76-2.51) 98.0 (34.76-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.219 , 0.264 0.220 , 0.265	Depositor DCC
R_{free} test set	3131 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 20.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13578	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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: SO4, BMA, NAG, FUC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/3447	0.41	0/4696
1	D	0.16	0/3455	0.40	0/4707
2	B	0.19	0/1699	0.35	0/2314
2	E	0.20	0/1656	0.40	0/2256
3	C	0.15	0/1704	0.36	0/2313
3	F	0.16	0/1698	0.34	0/2305
All	All	0.17	0/13659	0.39	0/18591

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	115	ASN	Mainchain

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3367	0	3328	52	0
1	D	3375	0	3334	42	0
2	B	1653	0	1594	18	0
2	E	1611	0	1552	24	0
3	C	1669	0	1622	16	0
3	F	1663	0	1617	18	0
4	H	28	0	25	1	0
5	G	39	0	34	0	0
5	J	39	0	34	2	0
6	I	49	0	43	2	0
7	K	38	0	34	0	0
8	A	10	0	0	1	0
8	D	5	0	0	1	0
8	F	5	0	0	0	0
9	A	14	0	13	0	0
10	A	5	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	3	0	0	0	0
10	E	3	0	0	0	0
All	All	13578	0	13230	160	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 6.

All (160) 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)
2:B:40:THR:HG23	2:B:43:LYS:HB2	1.63	0.79
2:E:40:THR:HG23	2:E:43:LYS:HB2	1.68	0.75
1:A:411:LEU:HD23	1:A:415:LEU:HB2	1.68	0.75
1:A:229:LEU:HD13	1:A:233:ILE:HD11	1.70	0.73
1:D:76:VAL:HA	1:A:450:MET:HE1	1.73	0.70
3:F:5:THR:HA	3:F:104:GLN:HE22	1.54	0.70
3:C:31:HIS:ND1	3:C:33:ASP:OD1	2.24	0.69
1:D:73:PRO:HD3	1:D:448:GLN:HE22	1.57	0.69
1:D:419:TYR:HB3	1:D:438:GLU:HG3	1.75	0.68
2:E:172:HIS:HD2	3:F:141:ASN:HD21	1.42	0.68
3:C:85:ALA:HA	3:C:110:ILE:HG13	1.75	0.67
1:D:391:ARG:NH2	8:D:501:SO4:O3	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:SER:HB2	1:A:299:GLY:H	1.61	0.66
2:B:41:PRO:HD3	2:B:92:ALA:HA	1.79	0.65
2:B:205:ASN:ND2	2:B:216:ASP:OD1	2.22	0.65
2:E:159:THR:HG22	2:E:207:ASN:HB3	1.78	0.65
2:E:41:PRO:HD3	2:E:92:ALA:HA	1.78	0.65
1:D:74:THR:HG23	1:A:452:PHE:HA	1.78	0.64
2:E:36:TRP:HE1	2:E:70:VAL:HG23	1.63	0.63
1:D:452:PHE:HA	1:A:74:THR:HG23	1.83	0.61
1:A:404:ARG:NE	1:A:407:GLU:OE2	2.30	0.61
1:A:110:TYR:HD1	1:A:138:ILE:HD13	1.65	0.61
1:D:316:SER:OG	1:D:317:TRP:N	2.33	0.60
2:B:127:PRO:HB3	2:B:153:TYR:HB3	1.84	0.59
3:F:127:GLU:HA	3:F:130:LYS:HE3	1.84	0.58
1:D:420:THR:HG22	1:D:437:VAL:HG13	1.85	0.57
1:A:75:THR:OG1	1:A:100:THR:O	2.21	0.57
1:A:100:THR:HG22	1:A:101:ARG:HD2	1.86	0.57
1:A:174:ILE:HG12	1:A:195:ASN:HD22	1.69	0.57
1:D:80:VAL:HB	1:D:449:PRO:HD3	1.87	0.57
3:C:128:GLN:O	3:C:131:SER:OG	2.23	0.57
3:F:104:GLN:H	3:F:104:GLN:CD	2.12	0.56
2:E:11:LEU:HD13	2:E:155:PRO:HG3	1.88	0.56
1:D:30:ARG:N	1:D:184:TYR:HH	2.02	0.56
2:B:91:THR:OG1	2:B:119:PRO:HD2	2.06	0.56
1:A:37:ILE:HD11	1:A:120:VAL:HG23	1.88	0.55
2:B:83:MET:HB3	2:B:86:LEU:HD21	1.89	0.54
3:C:4:MET:HE1	3:C:25:SER:HB3	1.89	0.54
1:A:77:ASP:OD1	1:A:101:ARG:NH2	2.40	0.54
2:B:159:THR:HG22	2:B:207:ASN:HB3	1.91	0.53
1:D:217:TYR:HB3	1:D:222:ILE:HD12	1.91	0.52
3:F:151:GLN:HB2	3:F:199:GLU:HG2	1.91	0.52
1:A:350:ASN:HA	1:A:389:LYS:NZ	2.24	0.52
2:E:12:VAL:O	2:E:119:PRO:HA	2.10	0.52
2:B:83:MET:HE3	2:B:86:LEU:HD21	1.91	0.51
3:C:11:LEU:HD21	3:C:19:ALA:HB1	1.92	0.51
1:D:47:ARG:NH2	3:F:1:ASP:OD1	2.44	0.50
1:A:286:TRP:CD2	1:A:331:TYR:HB3	2.46	0.50
2:B:173:THR:HG23	2:B:188:SER:HB2	1.93	0.50
3:F:171:ASP:OD1	3:F:173:LYS:N	2.41	0.50
1:A:368:THR:HG22	1:A:420:THR:HG23	1.94	0.50
2:E:2:VAL:HG22	2:E:27:PHE:HB3	1.93	0.50
3:F:171:ASP:O	3:F:175:SER:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PRO:HA	1:A:459:SER:O	2.11	0.49
3:C:38:LEU:HD21	3:C:93:CYS:HB2	1.94	0.49
1:D:404:ARG:NE	1:D:407:GLU:OE2	2.46	0.49
3:F:66:ARG:NH2	3:F:87:ASP:OD1	2.45	0.49
3:F:117:PRO:HB3	3:F:143:PHE:HB3	1.94	0.49
1:D:56:MET:CG	1:D:459:SER:HB2	2.43	0.49
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.95	0.49
2:E:172:HIS:CD2	3:F:141:ASN:HD21	2.26	0.49
1:A:266:MET:HG3	1:A:295:TRP:CZ2	2.48	0.49
1:A:419:TYR:HB3	1:A:438:GLU:HG3	1.94	0.48
1:D:240:ASN:O	1:D:241:THR:OG1	2.29	0.48
1:D:132:ILE:HG13	1:D:133:SER:N	2.29	0.48
1:D:266:MET:HG3	1:D:295:TRP:CZ2	2.49	0.48
2:E:36:TRP:CE2	2:E:81:LEU:HB2	2.49	0.48
3:F:13:VAL:HG21	3:F:83:VAL:HG21	1.96	0.48
1:D:72:MET:HE1	1:A:450:MET:HG2	1.96	0.48
1:A:137:ASN:OD1	1:A:139:ASN:HB2	2.13	0.47
3:F:59:ARG:HG3	3:F:63:VAL:HB	1.95	0.47
1:A:350:ASN:HA	1:A:389:LYS:HZ1	1.80	0.47
3:C:66:ARG:NH2	3:C:87:ASP:OD1	2.42	0.47
1:A:398:TYR:HE2	1:A:456:ILE:HG12	1.79	0.47
3:C:86:GLU:O	3:C:88:VAL:N	2.48	0.47
1:A:383:VAL:HG21	1:A:435:HIS:HB3	1.97	0.46
3:C:2:ILE:HD12	3:C:98:GLN:HB2	1.98	0.46
3:C:124:PRO:HG3	3:C:134:ALA:HB1	1.97	0.46
1:D:81:ARG:CZ	1:D:99:ILE:HD11	2.45	0.46
1:D:222:ILE:HG12	1:D:272:VAL:HG22	1.98	0.46
1:A:440:ASN:HB2	1:A:447:PHE:CE2	2.49	0.46
1:D:307:LYS:HB2	1:D:307:LYS:HE2	1.76	0.46
1:D:412:ASN:HD22	6:I:1:NAG:H83	1.81	0.46
1:A:110:TYR:CD1	1:A:138:ILE:HD13	2.49	0.46
2:E:110:TYR:C	2:E:111:TRP:HD1	2.24	0.46
2:E:156:GLU:HG3	2:E:157:PRO:HA	1.98	0.45
1:A:431:GLY:HA3	1:A:456:ILE:HD12	1.98	0.45
1:A:364:THR:OG1	1:A:365:GLY:N	2.48	0.45
3:F:4:MET:HE1	3:F:25:SER:HB3	1.99	0.45
2:E:105:VAL:HB	2:E:107:HIS:CE1	2.51	0.45
1:A:80:VAL:HG22	1:A:98:LEU:HG	1.98	0.45
1:A:77:ASP:O	1:A:102:GLY:N	2.48	0.44
1:A:340:TRP:CE2	5:J:2:NAG:H5	2.51	0.44
2:E:36:TRP:CZ2	2:E:79:LEU:HG	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:VAL:O	2:B:119:PRO:HA	2.17	0.44
2:E:83:MET:HB3	2:E:86:LEU:HD21	1.99	0.44
3:C:42:LEU:HB2	3:C:52:LEU:HD11	2.00	0.44
2:B:68:PHE:CE2	2:B:83:MET:HG2	2.53	0.44
2:B:162:TRP:CH2	2:B:204:CYS:HB3	2.53	0.44
1:D:77:ASP:OD1	1:D:77:ASP:N	2.41	0.44
1:D:127:ASP:OD1	1:D:453:LYS:NZ	2.45	0.44
3:C:66:ARG:NH1	3:C:87:ASP:OD2	2.46	0.44
1:D:319:SER:HB2	1:D:356:HIS:O	2.18	0.43
1:D:390:SER:HB2	1:D:392:VAL:HG22	1.98	0.43
1:D:411:LEU:HD11	6:I:1:NAG:H62	2.00	0.43
1:A:143:LYS:HB3	1:A:143:LYS:HE2	1.63	0.43
2:B:11:LEU:HD13	2:B:155:PRO:HG3	2.00	0.43
1:D:53:PRO:HA	1:D:459:SER:O	2.18	0.43
1:A:340:TRP:CH2	1:A:342:ASN:HB2	2.53	0.43
1:A:317:TRP:CG	1:A:359:PRO:HA	2.54	0.43
2:E:53:GLY:HA2	2:E:72:ARG:NH1	2.33	0.43
2:E:127:PRO:HB3	2:E:153:TYR:HB3	2.01	0.43
1:D:35:VAL:HG21	3:F:37:TYR:CZ	2.54	0.43
2:B:112:GLY:O	3:C:48:SER:OG	2.30	0.43
2:E:51:ILE:HD11	2:E:55:GLY:HA2	2.00	0.43
2:E:176:ALA:HA	2:E:186:LEU:HB3	2.01	0.43
1:D:95:THR:HB	1:D:147:LEU:HD11	2.00	0.43
1:D:450:MET:HE3	1:D:450:MET:HB2	1.66	0.43
1:A:240:ASN:OD1	1:A:242:THR:HG23	2.19	0.43
3:F:2:ILE:HD12	3:F:98:GLN:HB2	2.01	0.43
2:B:40:THR:CG2	2:B:43:LYS:HB2	2.40	0.43
2:B:115:ASN:HA	2:B:116:PRO:HD3	1.83	0.43
1:D:31:ILE:HG22	1:D:117:ILE:HD13	2.01	0.42
1:A:398:TYR:CE2	1:A:456:ILE:HG12	2.54	0.42
1:D:67:PRO:HB3	1:A:112:VAL:HG21	2.01	0.42
3:C:127:GLU:O	3:C:130:LYS:HG2	2.19	0.42
1:A:174:ILE:HG12	1:A:195:ASN:ND2	2.33	0.42
1:A:292:GLN:HG3	1:A:336:ILE:HB	2.01	0.42
1:A:37:ILE:HD13	1:A:118:ILE:HG22	2.02	0.42
3:F:11:LEU:HD21	3:F:19:ALA:HB1	2.01	0.42
1:D:415:LEU:HD11	1:D:439:ILE:HG23	2.02	0.42
1:A:35:VAL:HG13	8:A:501:SO4:O2	2.19	0.42
1:A:95:THR:HB	1:A:147:LEU:HD11	2.02	0.42
2:E:173:THR:HG23	2:E:188:SER:HB2	2.02	0.42
1:A:80:VAL:HB	1:A:449:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:2:NAG:H4	5:J:3:BMA:H2	1.63	0.41
1:A:270:ILE:O	1:A:270:ILE:HG13	2.18	0.41
1:A:275:LYS:HE2	1:A:281:PRO:HD3	2.02	0.41
3:C:129:LEU:O	3:C:187:LYS:HD3	2.20	0.41
1:D:66:GLY:O	1:A:74:THR:OG1	2.36	0.41
1:A:30:ARG:NH1	1:A:131:ARG:HH22	2.19	0.41
2:B:161:SER:HB2	2:B:205:ASN:HB2	2.02	0.41
3:C:42:LEU:HD13	3:C:91:TYR:CZ	2.56	0.41
2:E:115:ASN:HA	2:E:116:PRO:HD3	1.78	0.41
1:D:136:PHE:HB3	1:D:142:ARG:NH1	2.35	0.41
2:E:155:PRO:HD2	2:E:210:PRO:HB2	2.01	0.41
3:F:192:LYS:HE3	3:F:192:LYS:HB3	1.68	0.41
1:D:398:TYR:HE2	1:D:456:ILE:HG12	1.86	0.41
1:D:431:GLY:HA3	1:D:456:ILE:HD12	2.03	0.41
1:D:266:MET:HG3	1:D:295:TRP:CH2	2.56	0.41
2:E:31:SER:O	2:E:102:SER:OG	2.28	0.41
1:D:197:ASN:HD22	4:H:1:NAG:C7	2.34	0.40
1:A:77:ASP:HA	1:A:446:THR:HG21	2.03	0.40
1:D:199:SER:HB2	1:D:284:LYS:HG2	2.02	0.40
1:A:415:LEU:HD11	1:A:439:ILE:HG23	2.03	0.40
2:B:218:LYS:HD3	2:B:220:GLU:OE2	2.21	0.40
1:A:379:ILE:HG12	1:A:400:THR:HG22	2.02	0.40
1:D:275:LYS:HD3	1:D:282:LYS:NZ	2.36	0.40
1:A:74:THR:O	1:A:74:THR:HG22	2.21	0.40
1:A:311:TYR:CE2	1:A:369:ASP:HA	2.57	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	425/461 (92%)	407 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	426/461 (92%)	404 (95%)	21 (5%)	1 (0%)	43	63
2	B	220/222 (99%)	212 (96%)	7 (3%)	1 (0%)	24	43
2	E	211/222 (95%)	205 (97%)	6 (3%)	0	100	100
3	C	216/219 (99%)	207 (96%)	9 (4%)	0	100	100
3	F	215/219 (98%)	210 (98%)	5 (2%)	0	100	100
All	All	1713/1804 (95%)	1645 (96%)	66 (4%)	2 (0%)	48	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	411	LEU
2	B	41	PRO

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	388/418 (93%)	381 (98%)	7 (2%)	51	77
1	D	389/418 (93%)	383 (98%)	6 (2%)	57	80
2	B	184/184 (100%)	177 (96%)	7 (4%)	29	56
2	E	179/184 (97%)	172 (96%)	7 (4%)	28	55
3	C	192/193 (100%)	186 (97%)	6 (3%)	35	62
3	F	191/193 (99%)	186 (97%)	5 (3%)	40	68
All	All	1523/1590 (96%)	1485 (98%)	38 (2%)	42	69

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	47	ARG
1	D	77	ASP
1	D	269	SER
1	D	357	SER

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Mol	Chain	Res	Type
1	D	390	SER
1	D	425	ILE
1	A	37	ILE
1	A	199	SER
1	A	265	ARG
1	A	269	SER
1	A	366	VAL
1	A	420	THR
1	A	455	GLU
2	B	5	LEU
2	B	12	VAL
2	B	115	ASN
2	B	128	SER
2	B	140	SER
2	B	159	THR
2	B	168	THR
3	C	10	SER
3	C	38	LEU
3	C	65	ASP
3	C	72	SER
3	C	136	VAL
3	C	187	LYS
2	E	7	SER
2	E	40	THR
2	E	102	SER
2	E	143	THR
2	E	159	THR
2	E	195	SER
2	E	199	THR
3	F	7	SER
3	F	32	SER
3	F	79	LYS
3	F	194	LYS
3	F	195	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	448	GLN
1	A	183	ASN
1	A	195	ASN
1	A	293	ASN

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Mol	Chain	Res	Type
1	A	440	ASN
1	A	448	GLN
2	B	13	GLN
3	C	58	ASN
3	C	203	GLN
3	F	35	ASN
3	F	141	ASN
3	F	164	GLN

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](#)

15 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	0.18	0	17,19,21	0.39	0
5	NAG	G	2	5	14,14,15	0.25	0	17,19,21	0.67	0
5	BMA	G	3	5	11,11,12	0.69	0	15,15,17	0.88	1 (6%)
4	NAG	H	1	4,1	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	H	2	4	14,14,15	0.27	0	17,19,21	0.60	1 (5%)
6	NAG	I	1	6,1	14,14,15	0.23	0	17,19,21	0.39	0
6	NAG	I	2	6	14,14,15	0.30	0	17,19,21	0.36	0
6	BMA	I	3	6	11,11,12	0.68	0	15,15,17	0.69	0
6	FUC	I	4	6	10,10,11	0.92	0	14,14,16	1.05	1 (7%)
5	NAG	J	1	1,5	14,14,15	0.30	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	J	2	5	14,14,15	0.23	0	17,19,21	0.55	0
5	BMA	J	3	5	11,11,12	1.10	1 (9%)	15,15,17	1.09	2 (13%)
7	NAG	K	1	1,7	14,14,15	0.48	0	17,19,21	0.44	0
7	NAG	K	2	7	14,14,15	0.34	0	17,19,21	0.57	0
7	FUC	K	3	7	10,10,11	0.64	0	14,14,16	0.68	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
5	NAG	G	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	1/2/19/22	0/1/1/1
4	NAG	H	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
6	NAG	I	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	3/6/23/26	0/1/1/1
6	BMA	I	3	6	-	1/2/19/22	0/1/1/1
6	FUC	I	4	6	-	-	0/1/1/1
5	NAG	J	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	BMA	J	3	5	-	0/2/19/22	0/1/1/1
7	NAG	K	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	2/6/23/26	0/1/1/1
7	FUC	K	3	7	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	3	BMA	C4-C5	2.62	1.58	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	3	BMA	C3-C4-C5	2.49	114.75	110.23
5	G	3	BMA	C1-O5-C5	2.08	114.97	112.19
4	H	2	NAG	C1-O5-C5	2.06	114.95	112.19
6	I	4	FUC	O5-C5-C4	2.05	113.24	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	3	BMA	C1-C2-C3	-2.03	106.69	109.64

There are no chirality outliers.

All (15) torsion outliers are listed below:

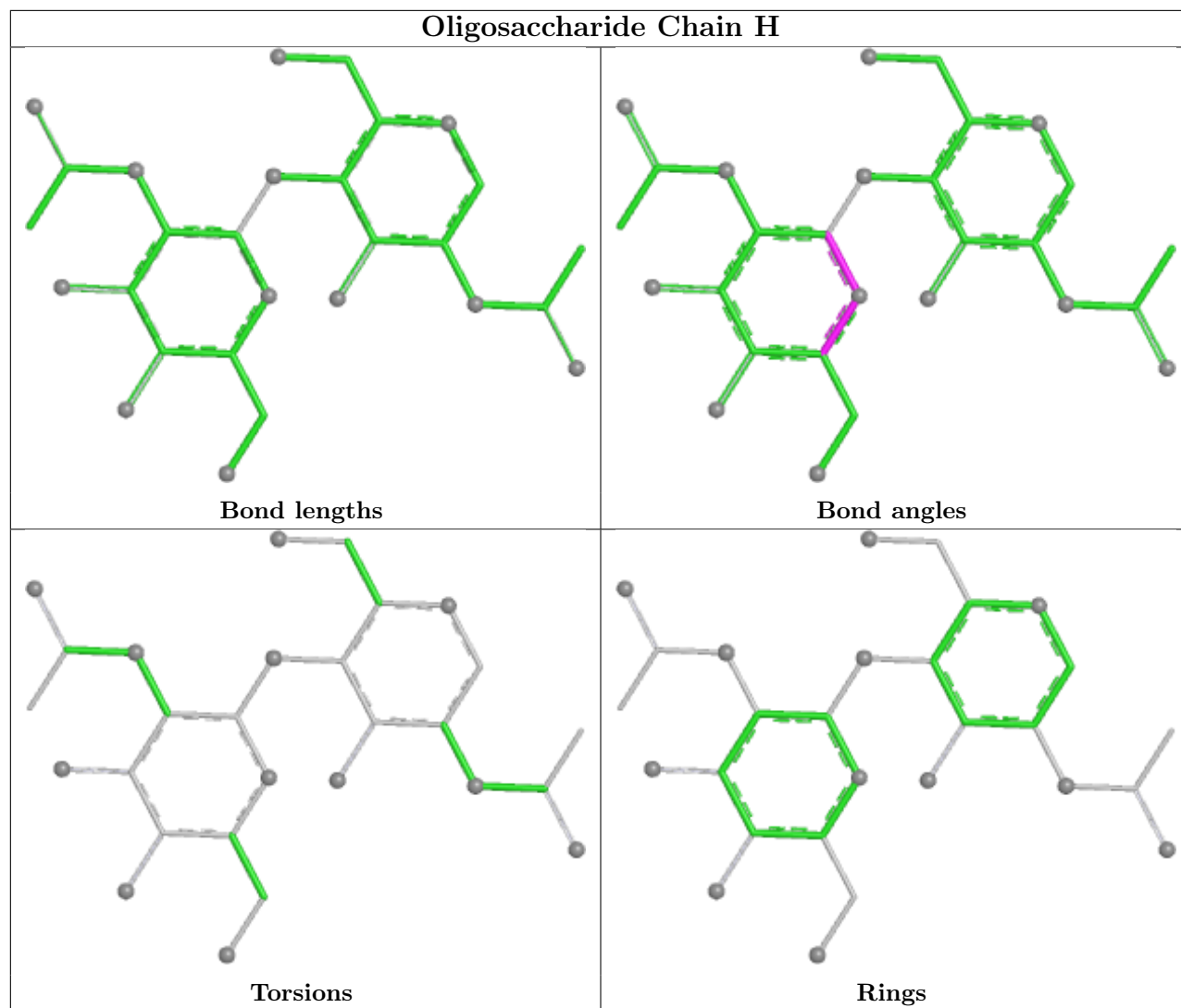
Mol	Chain	Res	Type	Atoms
5	J	2	NAG	C8-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2
6	I	1	NAG	C8-C7-N2-C2
6	I	1	NAG	O7-C7-N2-C2
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
7	K	2	NAG	C8-C7-N2-C2
7	K	2	NAG	O7-C7-N2-C2
5	G	3	BMA	O5-C5-C6-O6
6	I	3	BMA	O5-C5-C6-O6
7	K	1	NAG	C4-C5-C6-O6
5	G	2	NAG	C3-C2-N2-C7
5	G	2	NAG	C1-C2-N2-C7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

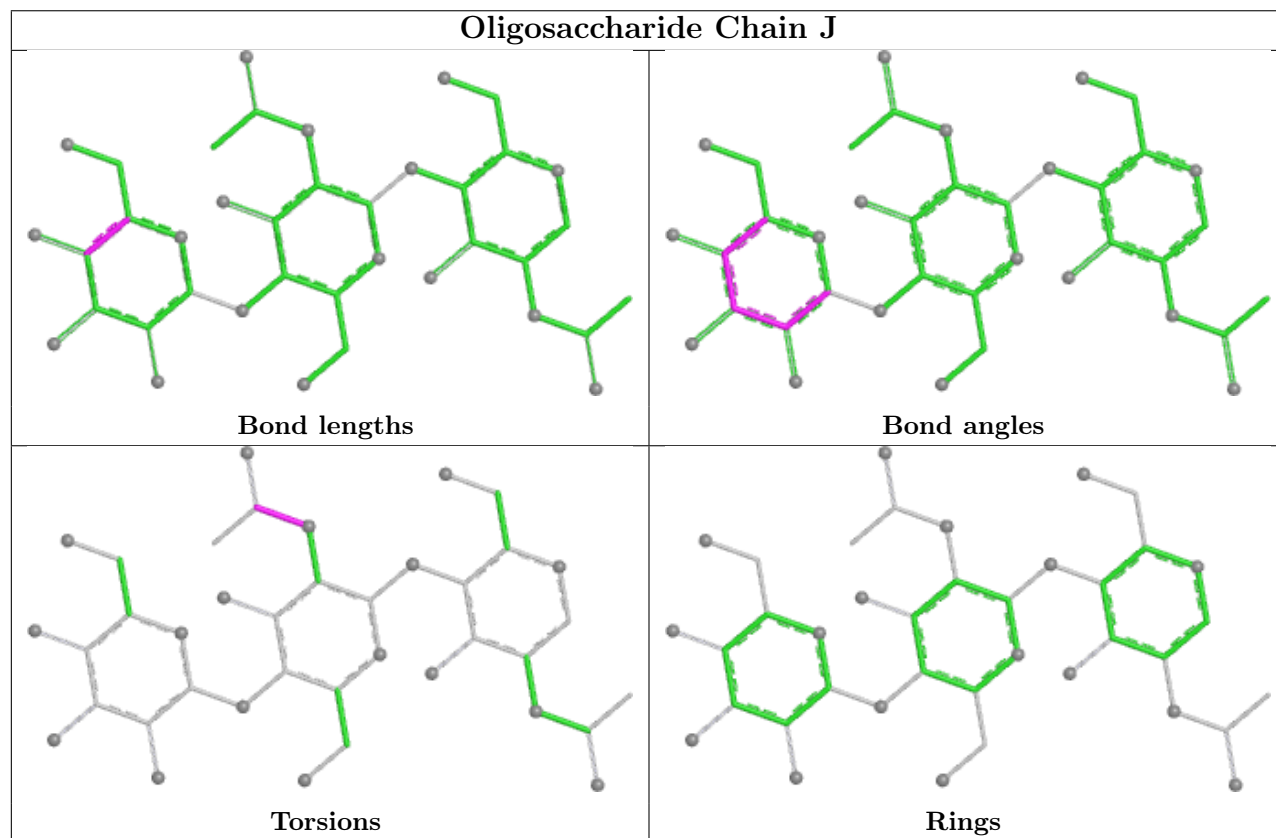
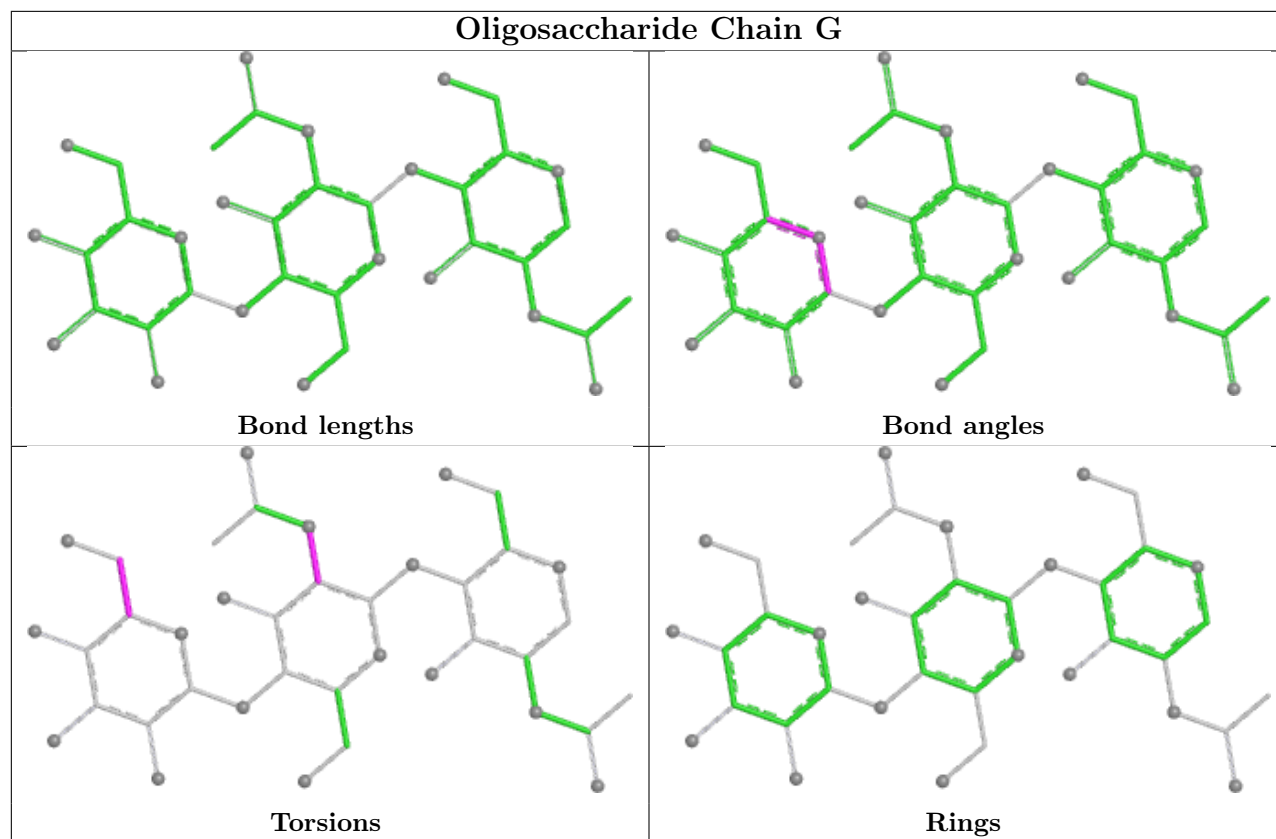
There are no ring outliers.

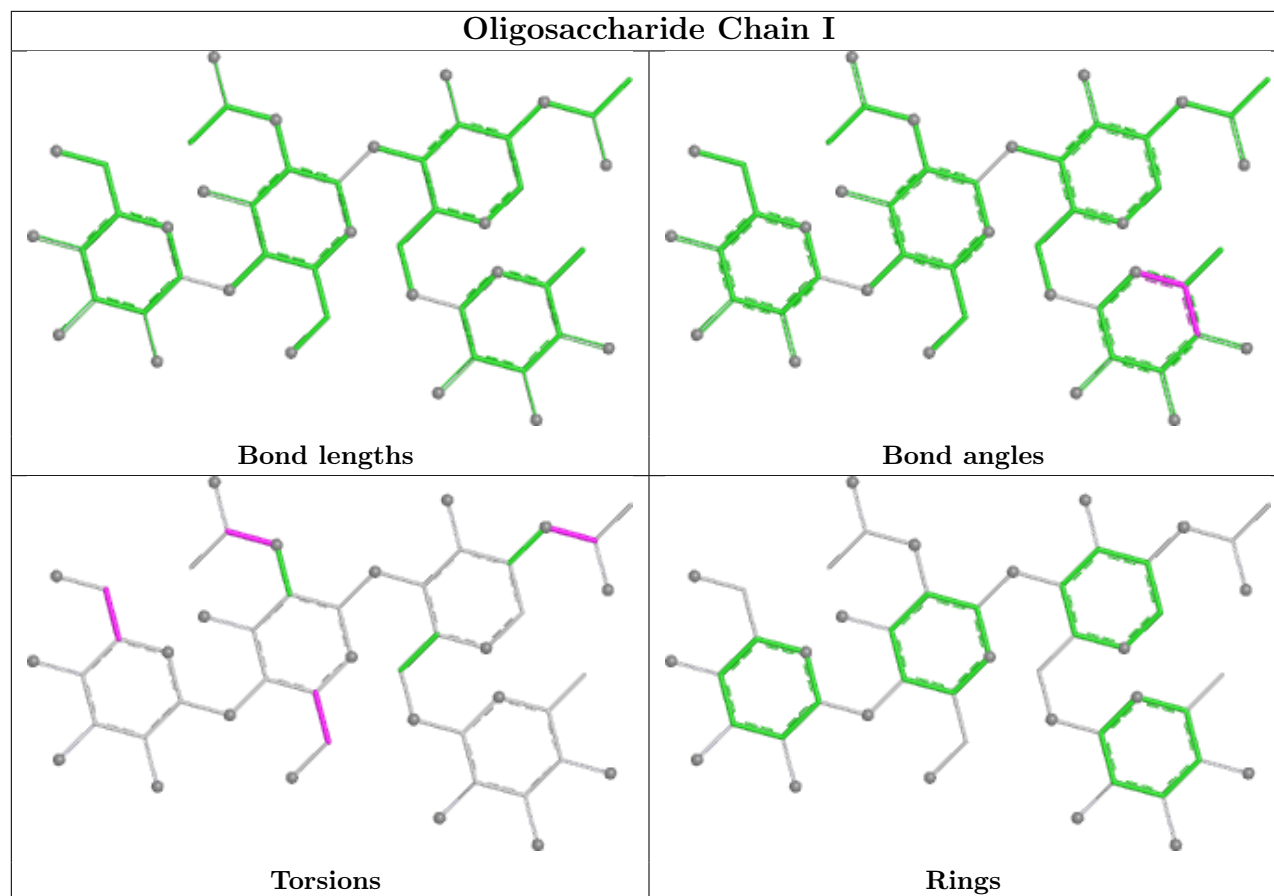
4 monomers are involved in 5 short contacts:

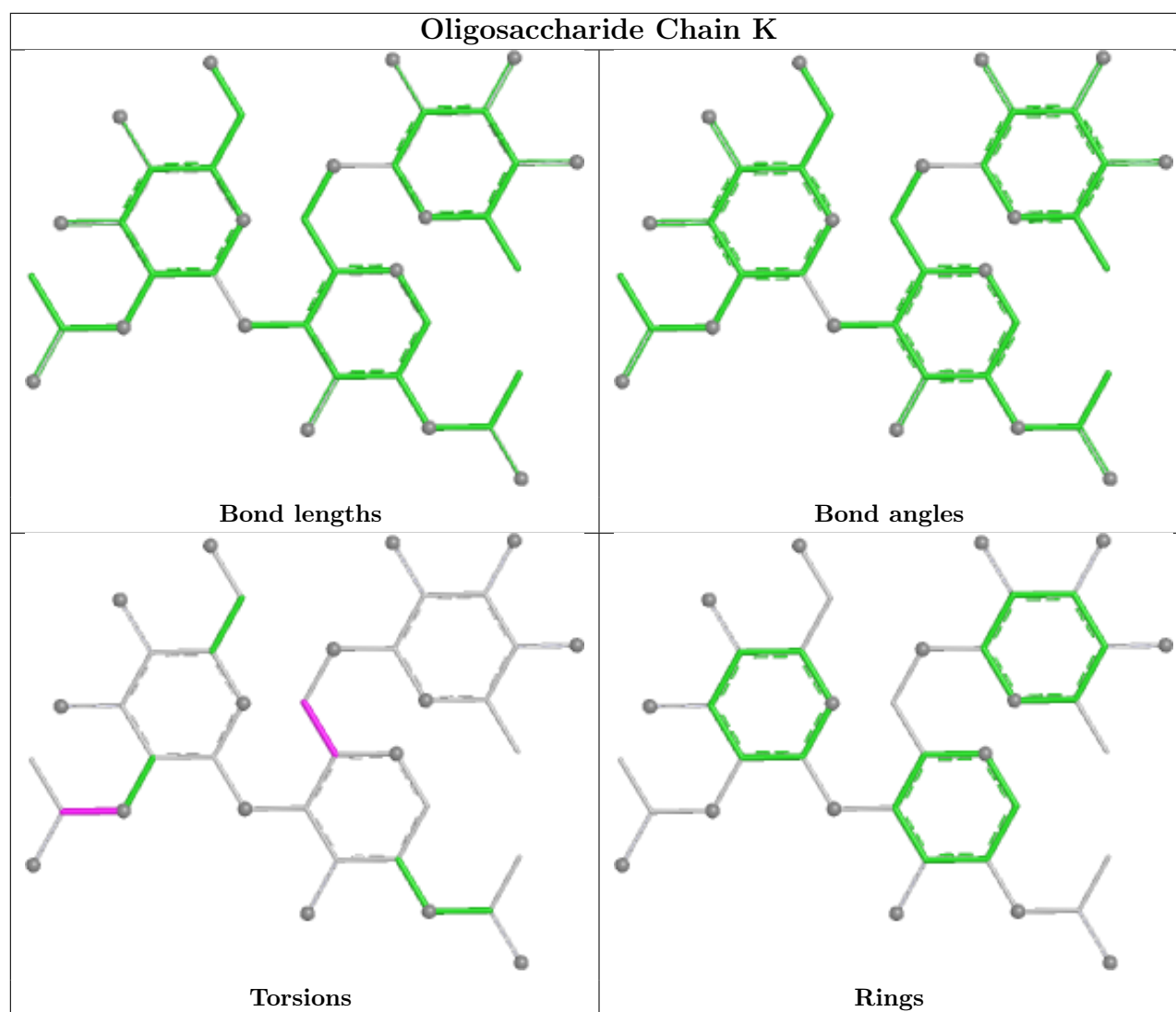
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	1	NAG	2	0
4	H	1	NAG	1	0
5	J	3	BMA	1	0
5	J	2	NAG	2	0

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](#)

5 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	$\# Z > 2$
8	SO4	A	501	-	4,4,4	0.23	0	6,6,6	0.11	0
8	SO4	A	502	-	4,4,4	0.23	0	6,6,6	0.06	0
8	SO4	D	501	-	4,4,4	0.24	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SO4	F	301	-	4,4,4	0.24	0	6,6,6	0.09	0
9	NAG	A	503	1	14,14,15	0.23	0	17,19,21	0.36	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
9	NAG	A	503	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	503	NAG	C8-C7-N2-C2
9	A	503	NAG	O7-C7-N2-C2
9	A	503	NAG	C4-C5-C6-O6
9	A	503	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	501	SO4	1	0
8	D	501	SO4	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

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	429/461 (93%)	0.21	9 (2%) 63 59	27, 38, 53, 61	0
1	D	430/461 (93%)	0.11	6 (1%) 73 70	25, 35, 50, 69	0
2	B	222/222 (100%)	0.32	4 (1%) 67 64	30, 40, 58, 68	0
2	E	215/222 (96%)	0.46	9 (4%) 40 36	28, 38, 55, 64	0
3	C	218/219 (99%)	0.29	4 (1%) 67 64	33, 43, 57, 73	0
3	F	217/219 (99%)	0.23	1 (0%) 87 85	29, 40, 51, 60	0
All	All	1731/1804 (95%)	0.24	33 (1%) 66 62	25, 39, 54, 73	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	212	ASN	6.7
2	E	113	PRO	3.9
2	B	115	ASN	3.8
1	D	418	GLY	3.7
1	D	104	GLN	3.6
1	A	305	GLY	3.4
1	A	350	ASN	3.2
1	A	184	TYR	3.1
2	B	41	PRO	3.0
2	E	116	PRO	2.9
1	D	66	GLY	2.9
2	E	135	SER	2.8
2	E	214	LYS	2.8
3	C	218	CYS	2.7
1	A	418	GLY	2.6
1	A	444	LEU	2.6
2	E	213	THR	2.5
1	D	419	TYR	2.4
1	D	30	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	196	SER	2.4
1	A	361	GLY	2.3
1	A	279	SER	2.3
3	F	33	ASP	2.3
1	D	62	ARG	2.2
3	C	33	ASP	2.1
1	A	232	PRO	2.1
2	E	210	PRO	2.1
2	B	159	THR	2.1
3	C	173	LYS	2.1
2	B	135	SER	2.1
2	E	191	THR	2.1
3	C	79	LYS	2.1
1	A	280	ILE	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.

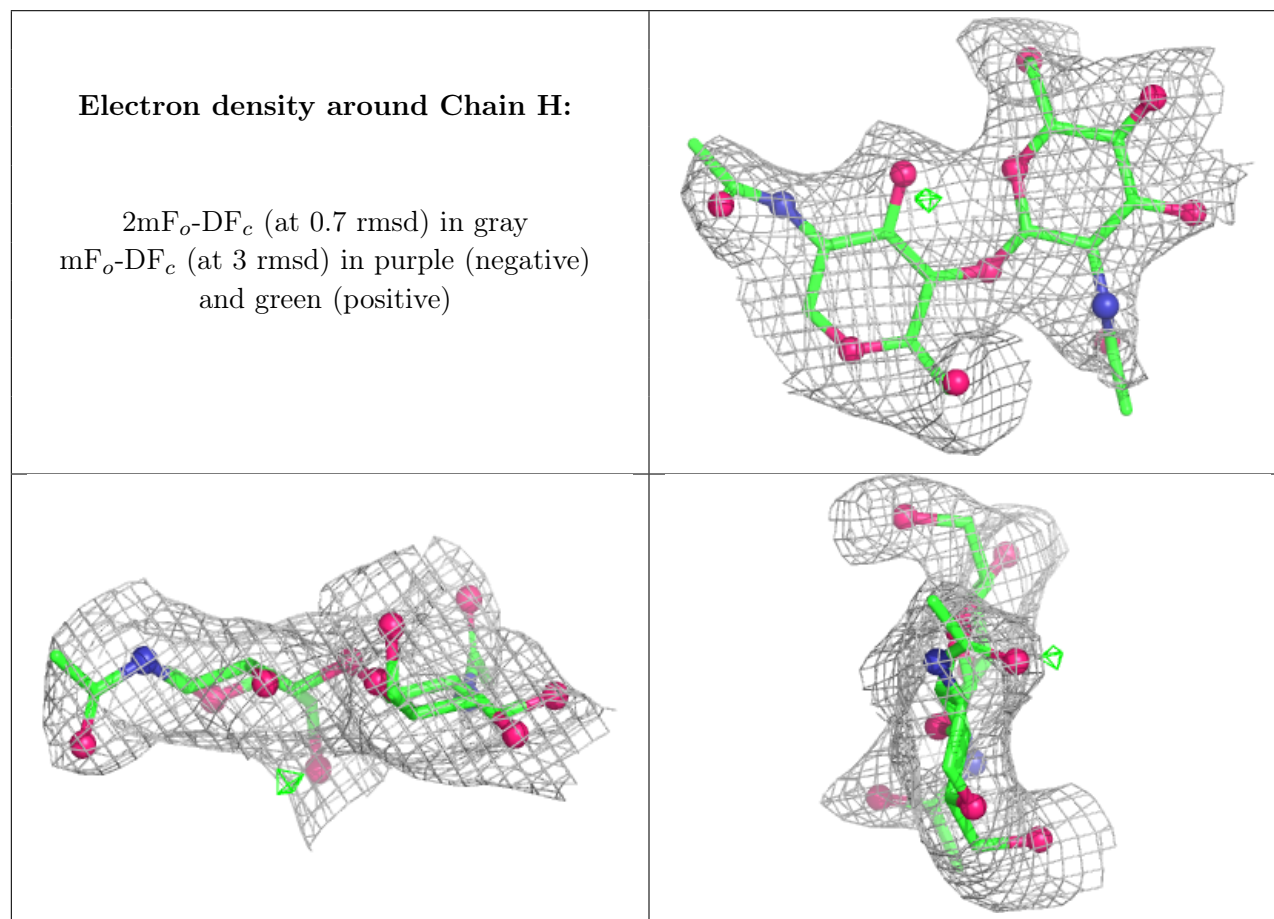
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	J	3	11/12	0.42	0.15	67,76,81,81	0
5	NAG	J	1	14/15	0.46	0.19	66,72,76,77	0
7	NAG	K	2	14/15	0.48	0.18	65,74,77,79	0
7	FUC	K	3	10/11	0.50	0.17	72,74,77,78	0
5	BMA	G	3	11/12	-	-	67,70,73,73	0
5	NAG	J	2	14/15	0.54	0.19	63,74,81,81	0
6	FUC	I	4	10/11	0.56	0.18	68,71,75,81	0
6	BMA	I	3	11/12	0.58	0.13	77,82,85,85	0
6	NAG	I	2	14/15	0.64	0.14	65,75,82,83	0
5	NAG	G	2	14/15	0.66	0.14	54,59,64,66	0
4	NAG	H	2	14/15	0.77	0.13	59,63,68,68	0
4	NAG	H	1	14/15	0.77	0.12	45,50,57,62	0
6	NAG	I	1	14/15	0.79	0.12	57,62,68,72	0
7	NAG	K	1	14/15	0.81	0.11	56,61,70,73	0

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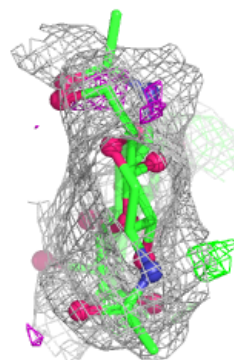
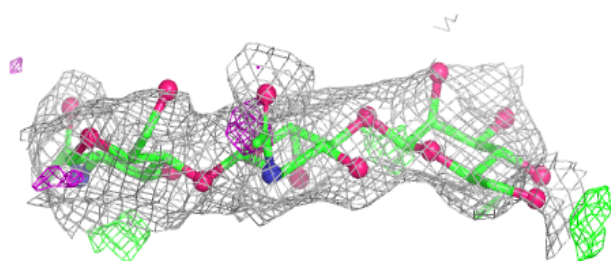
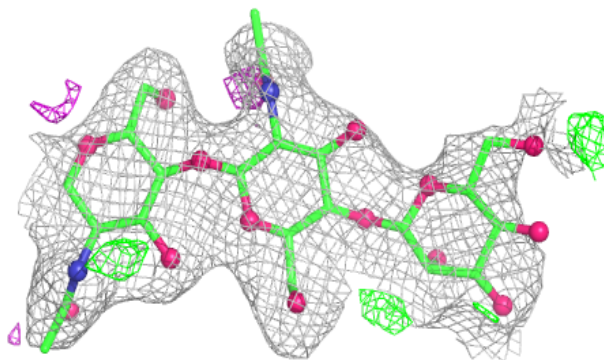
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	G	1	14/15	0.82	0.11	54,58,62,62	0

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.

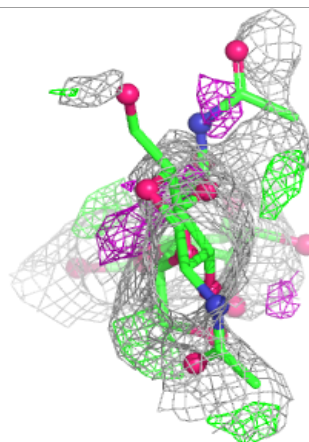
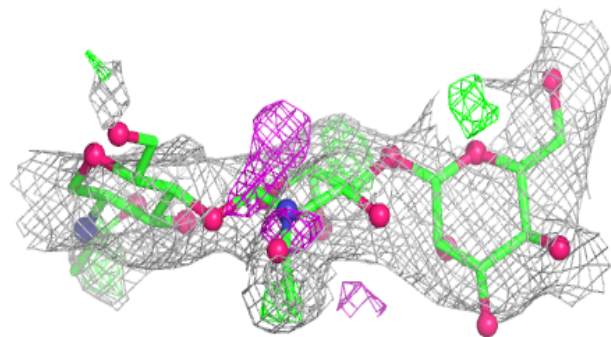
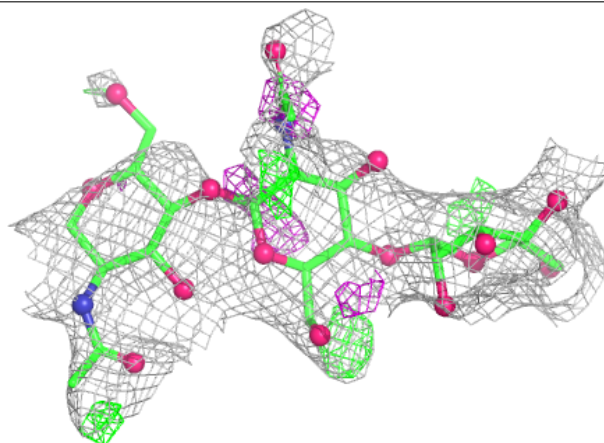


Electron density around Chain G:

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

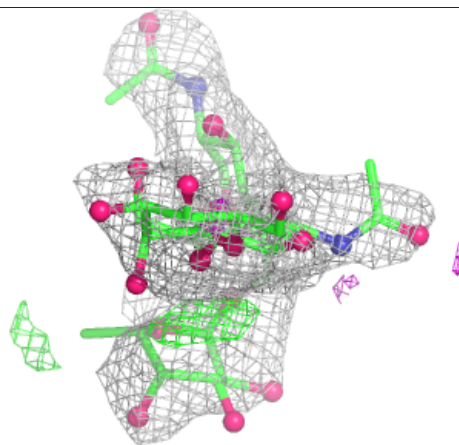
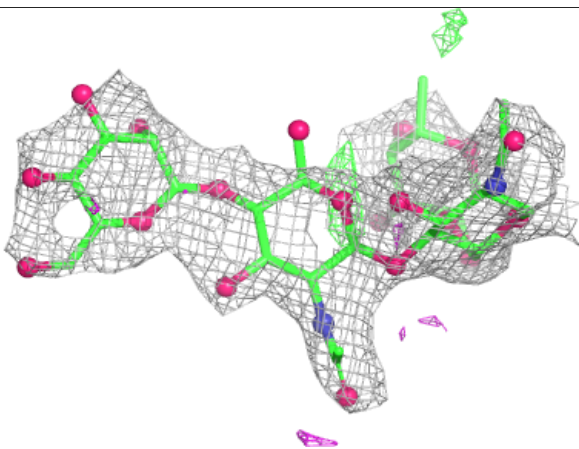
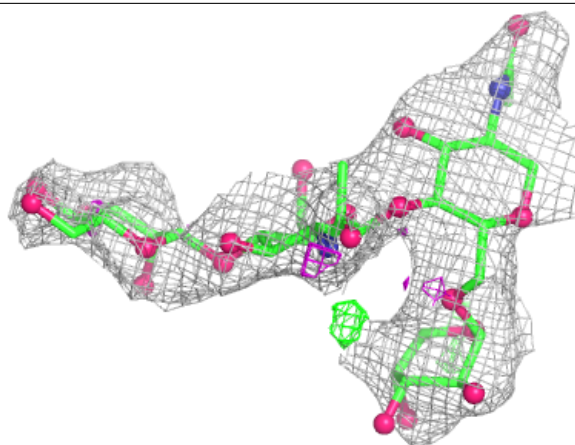
**Electron density around Chain J:**

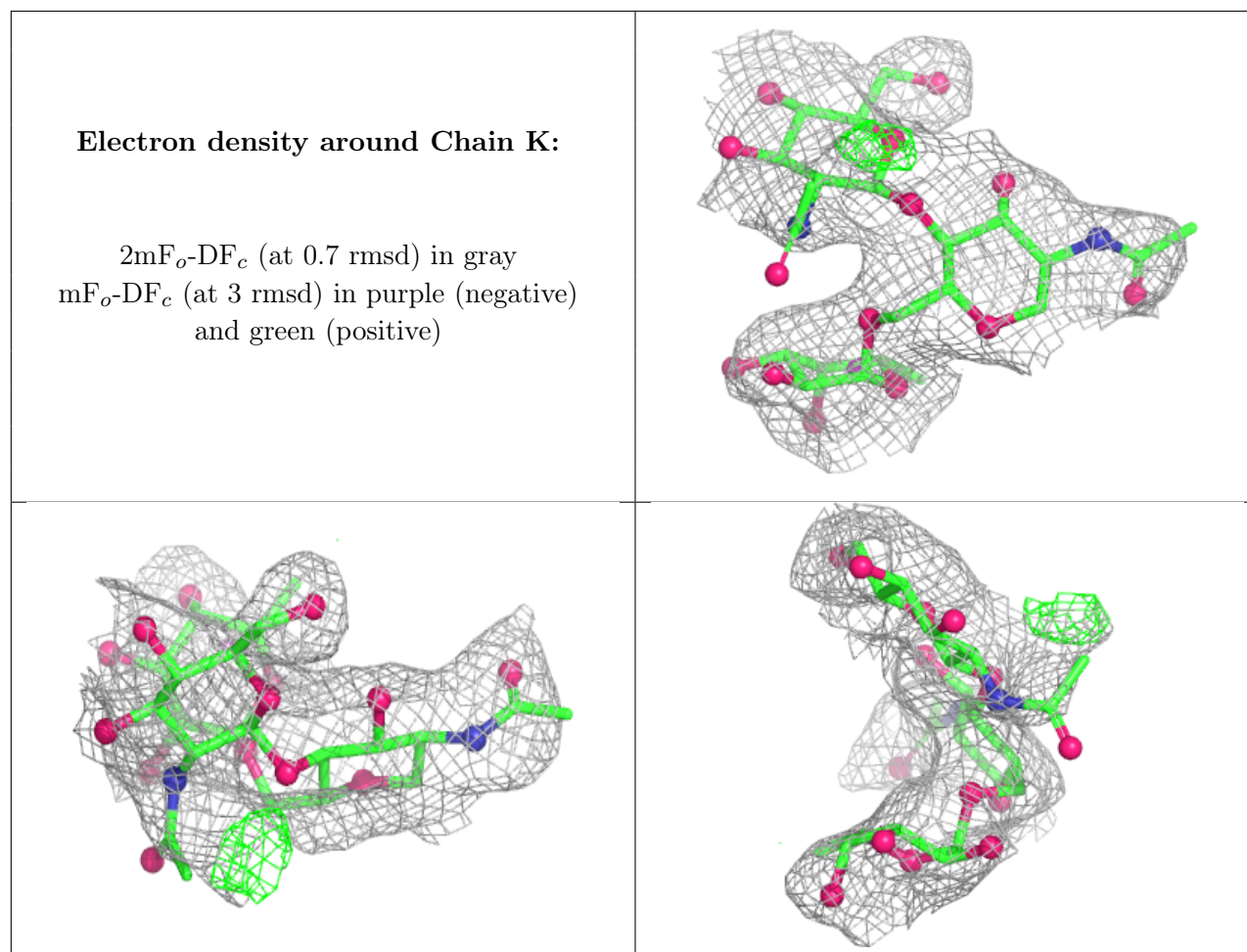
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain I:

$2mF_o-DF_c$ (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
9	NAG	A	503	14/15	0.59	0.16	60,67,71,72	0
8	SO4	D	501	5/5	0.72	0.19	61,68,76,79	0
8	SO4	A	501	5/5	0.86	0.29	57,58,62,66	0
8	SO4	A	502	5/5	0.88	0.11	51,56,59,61	0
8	SO4	F	301	5/5	0.90	0.11	47,54,58,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.