



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:57 PM UTC

PDB ID : 8FD1 / pdb_00008fd1
Title : Crystal structure of photoactivated rhodopsin in complex with a nanobody
Authors : Salom, D.; Palczewski, K.; Kiser, P.D.
Deposited on : 2022-12-01
Resolution : 4.25 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

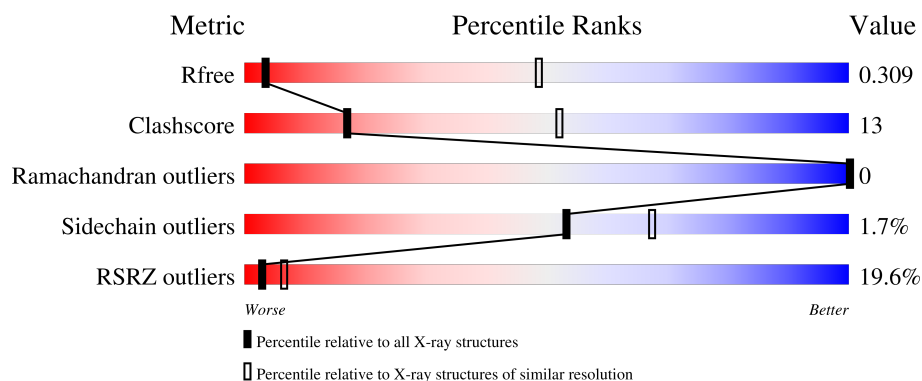
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.25 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.



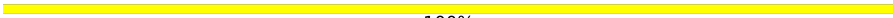
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1029 (4.62-3.90)
Clashscore	190562	1074 (4.62-3.90)
Ramachandran outliers	187476	1001 (4.62-3.88)
Sidechain outliers	187428	1021 (4.66-3.86)
RSRZ outliers	180081	1026 (4.62-3.90)

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	348	
1	B	348	
2	C	126	
2	D	126	
3	E	6	

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Mol	Chain	Length	Quality of chain
4	F	3	 100%
5	G	5	 80%20%
6	H	2	 50%50%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6758 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.

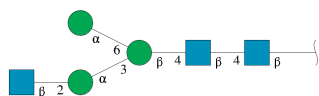
- Molecule 1 is a protein called Rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2415	1619	363	407	26			
1	B	307	Total	C	N	O	S	0	0	0
			2431	1628	368	409	26			

- Molecule 2 is a protein called Nanobody Nb2.

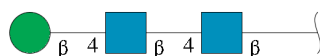
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	114	Total	C	N	O	S	0	0	0
			850	534	143	168	5			
2	D	114	Total	C	N	O	S	0	0	0
			859	539	146	168	6			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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.



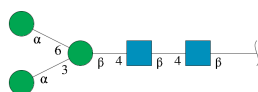
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	0	0	0
			75	42	3	30			

- Molecule 4 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.



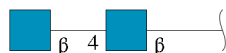
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

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

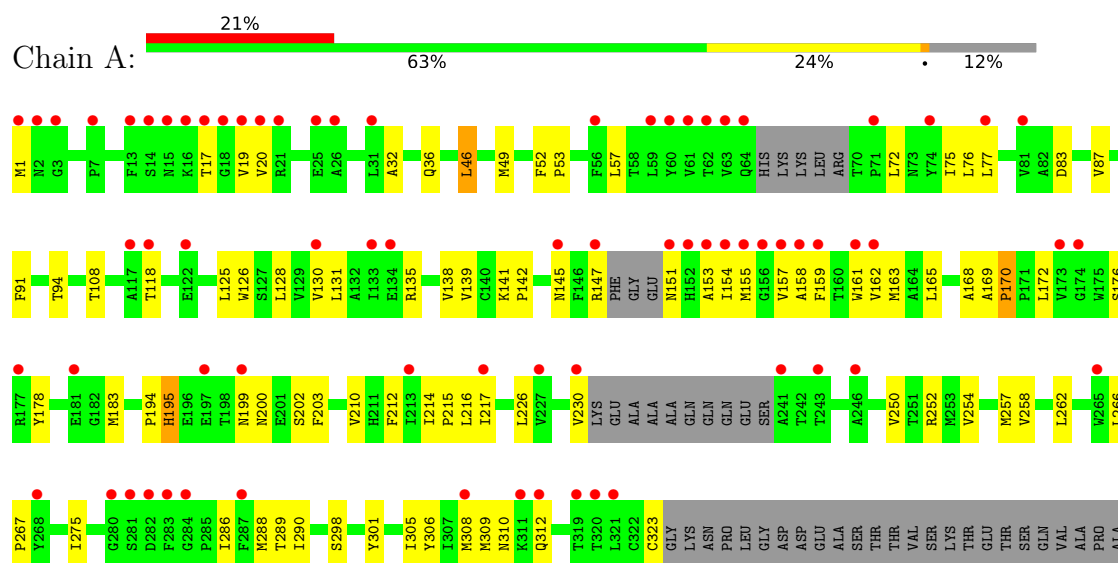


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

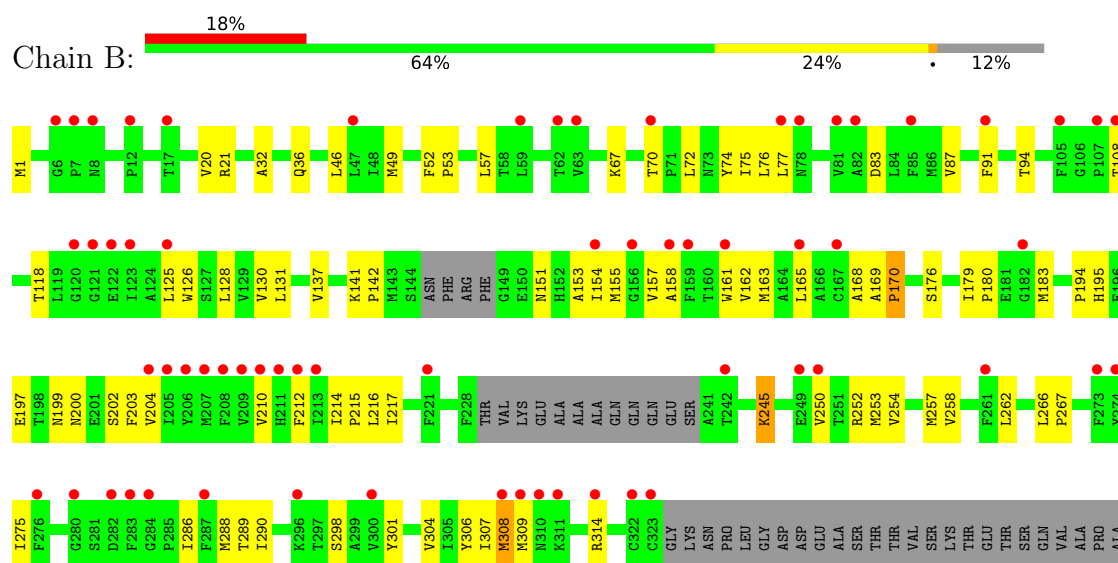
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

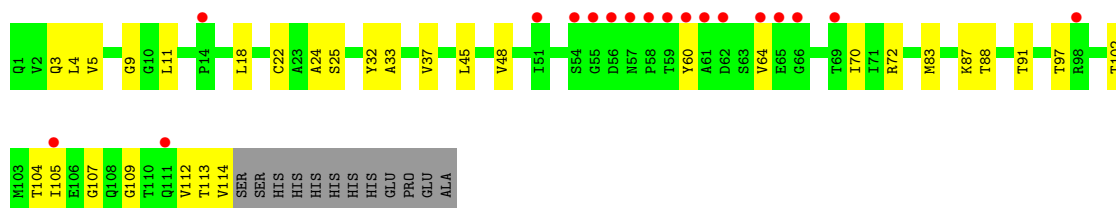
• Molecule 1: Rhodopsin



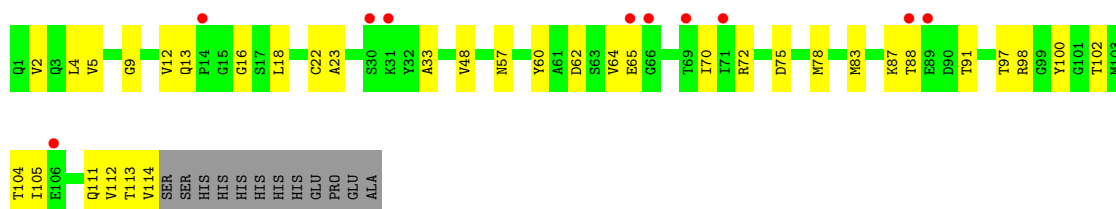
• Molecule 1: Rhodopsin



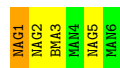
• Molecule 2: Nanobody Nb2



- Molecule 2: Nanobody Nb2



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



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



- 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



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.29Å 120.29Å 227.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.36 – 4.25 47.36 – 4.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.36-4.25) 99.9 (47.36-4.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 4.29Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.279 , 0.295 0.290 , 0.309	Depositor DCC
R_{free} test set	697 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	280.3	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 212.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.095 for -h,-k,l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	6758	wwPDB-VP
Average B, all atoms (Å ²)	304.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.50	1/2492 (0.0%)	0.99	1/3400 (0.0%)
1	B	0.50	0/2509	0.99	2/3421 (0.1%)
2	C	0.49	0/867	0.87	0/1177
2	D	0.49	0/876	0.88	2/1187 (0.2%)
All	All	0.50	1/6744 (0.0%)	0.96	5/9185 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	195	HIS	CE1-NE2	5.13	1.37	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	PRO	N-CA-C	5.48	117.38	110.70
1	B	170	PRO	N-CA-C	5.39	117.27	110.70
2	D	12	VAL	CA-C-N	5.33	127.91	120.65
2	D	12	VAL	C-N-CA	5.33	127.91	120.65
1	B	70	THR	CB-CA-C	5.10	116.06	108.87

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2415	0	2385	69	0
1	B	2431	0	2408	65	0
2	C	850	0	819	20	0
2	D	859	0	837	23	0
3	E	75	0	64	1	0
4	F	39	0	34	0	0
5	G	61	0	52	1	0
6	H	28	0	25	1	0
All	All	6758	0	6624	170	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 (170) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ARG:HA	1:A:138:VAL:HG22	1.62	0.80
1:B:1:MET:HE1	2:D:100:TYR:O	1.83	0.79
1:B:75:ILE:HD13	1:B:157:VAL:HG22	1.66	0.77
1:A:252:ARG:HG3	1:A:309:MET:HE1	1.67	0.76
1:A:75:ILE:HD13	1:A:157:VAL:HG22	1.66	0.76
1:B:252:ARG:HG3	1:B:309:MET:HE1	1.67	0.73
1:B:76:LEU:HD13	1:B:306:TYR:CD1	2.22	0.73
1:A:194:PRO:HG3	2:C:32:TYR:HB3	1.70	0.72
1:B:210:VAL:HA	1:B:214:ILE:HD12	1.71	0.72
1:A:76:LEU:HD23	1:A:306:TYR:CD1	2.24	0.72
1:B:183:MET:HE2	1:B:286:ILE:HD12	1.71	0.72
1:B:125:LEU:HD21	1:B:215:PRO:HG2	1.71	0.72
1:A:183:MET:HE2	1:A:286:ILE:HD12	1.72	0.71
1:A:138:VAL:HG12	1:A:147:ARG:HH11	1.54	0.71
1:A:125:LEU:HD21	1:A:215:PRO:HG2	1.71	0.70
1:A:210:VAL:HA	1:A:214:ILE:HD12	1.71	0.70
1:A:76:LEU:HD11	1:A:257:MET:HE1	1.74	0.69
1:A:131:LEU:HD23	1:A:254:VAL:HG22	1.75	0.69
1:B:131:LEU:HD23	1:B:254:VAL:HG22	1.74	0.68
1:A:49:MET:HE3	1:B:49:MET:HE3	1.77	0.67
2:C:83:MET:HE1	2:C:112:VAL:HG11	1.80	0.64
1:B:75:ILE:CD1	1:B:157:VAL:HG22	2.27	0.64
2:D:88:THR:O	2:D:91:THR:HG22	1.98	0.64
1:A:75:ILE:CD1	1:A:157:VAL:HG22	2.28	0.63
2:C:88:THR:O	2:C:91:THR:HG22	1.99	0.62
2:C:37:VAL:HG11	2:C:102:THR:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ASN:O	1:B:155:MET:HG2	1.99	0.61
1:B:75:ILE:HG21	1:B:131:LEU:CD1	2.33	0.59
1:B:57:LEU:C	1:B:57:LEU:HD23	2.27	0.59
1:A:195:HIS:HB3	1:A:200:ASN:ND2	2.18	0.59
2:C:11:LEU:HG	2:C:113:THR:HG23	1.85	0.58
2:D:13:GLN:HB2	2:D:16:GLY:HA3	1.85	0.58
1:A:57:LEU:C	1:A:57:LEU:HD23	2.28	0.58
1:A:53:PRO:HD3	1:B:49:MET:HE2	1.86	0.57
1:A:305:ILE:HA	1:A:308:MET:HE3	1.86	0.57
1:A:75:ILE:HG21	1:A:131:LEU:CD1	2.33	0.57
2:D:83:MET:HE1	2:D:112:VAL:HG11	1.86	0.57
1:A:17:THR:OG1	1:A:19:VAL:HG12	2.06	0.56
1:A:138:VAL:HG12	1:A:147:ARG:NH1	2.21	0.56
1:A:138:VAL:CG1	1:A:147:ARG:HH11	2.19	0.55
1:A:286:ILE:HA	1:A:289:THR:HG22	1.89	0.55
1:B:307:ILE:O	1:B:314:ARG:NH1	2.36	0.55
1:A:1:MET:HA	1:A:1:MET:HE2	1.89	0.54
1:B:153:ALA:O	1:B:157:VAL:HG23	2.08	0.54
1:B:286:ILE:HA	1:B:289:THR:HG22	1.89	0.54
1:B:67:LYS:HA	1:B:67:LYS:HE2	1.89	0.54
1:B:212:PHE:O	1:B:216:LEU:HD23	2.08	0.54
2:D:111:GLN:HG3	2:D:113:THR:HG23	1.89	0.54
1:A:151:ASN:O	1:A:155:MET:HG2	2.08	0.53
1:B:158:ALA:O	1:B:162:VAL:HG23	2.08	0.53
2:D:87:LYS:O	2:D:114:VAL:HG11	2.08	0.53
1:B:20:VAL:HG12	5:G:1:NAG:H82	1.91	0.53
2:D:2:VAL:HG21	2:D:98:ARG:HH12	1.74	0.53
1:A:20:VAL:HG12	3:E:1:NAG:H82	1.91	0.52
1:B:275:ILE:HD12	1:B:288:MET:HE2	1.91	0.52
1:A:153:ALA:O	1:A:157:VAL:HG23	2.09	0.52
2:C:87:LYS:O	2:C:114:VAL:HG11	2.10	0.52
2:C:97:THR:HG22	2:C:104:THR:HA	1.91	0.52
1:B:304:VAL:O	1:B:308:MET:HB3	2.10	0.52
1:A:212:PHE:O	1:A:216:LEU:HD23	2.10	0.51
1:A:298:SER:HA	1:A:301:TYR:CE2	2.46	0.51
1:B:298:SER:HA	1:B:301:TYR:CE2	2.46	0.51
2:D:97:THR:HG22	2:D:104:THR:HA	1.92	0.51
1:B:32:ALA:HB1	1:B:36:GLN:OE1	2.11	0.51
1:B:77:LEU:C	1:B:77:LEU:HD23	2.36	0.50
1:A:32:ALA:HB1	1:A:36:GLN:OE1	2.11	0.50
1:A:77:LEU:C	1:A:77:LEU:HD23	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:GLU:OE2	2:D:98:ARG:NH1	2.44	0.50
1:A:158:ALA:O	1:A:162:VAL:HG23	2.12	0.50
1:A:262:LEU:HA	1:A:266:LEU:HD13	1.94	0.49
2:D:4:LEU:HD12	2:D:105:ILE:CG2	2.42	0.49
1:A:275:ILE:HD12	1:A:288:MET:HE2	1.93	0.49
1:B:262:LEU:HA	1:B:266:LEU:HD13	1.93	0.49
1:B:266:LEU:N	1:B:267:PRO:HD2	2.28	0.49
1:A:76:LEU:HD23	1:A:306:TYR:CG	2.47	0.48
1:B:72:LEU:HG	1:B:76:LEU:HD12	1.96	0.48
1:A:76:LEU:HD11	1:A:257:MET:CE	2.43	0.48
1:A:301:TYR:C	1:A:301:TYR:CD1	2.91	0.47
1:B:176:SER:HA	1:B:200:ASN:HB3	1.96	0.47
1:B:301:TYR:C	1:B:301:TYR:CD1	2.91	0.47
1:A:310:ASN:OD1	1:A:312:GLN:OE1	2.31	0.47
1:A:266:LEU:N	1:A:267:PRO:HD2	2.28	0.47
2:C:60:TYR:HE1	2:C:70:ILE:HG22	1.80	0.47
1:A:139:VAL:HG11	1:A:226:LEU:HD21	1.96	0.47
1:B:245:LYS:HA	1:B:245:LYS:HE3	1.96	0.47
1:B:250:VAL:O	1:B:254:VAL:HG23	2.14	0.47
1:B:75:ILE:HD11	1:B:130:VAL:HG11	1.97	0.47
1:A:286:ILE:HG22	1:A:290:ILE:HG12	1.97	0.47
1:B:75:ILE:HG21	1:B:131:LEU:HD11	1.97	0.47
2:C:60:TYR:CE1	2:C:70:ILE:HG22	2.50	0.47
1:A:176:SER:HA	1:A:200:ASN:HB3	1.95	0.47
1:B:254:VAL:O	1:B:258:VAL:HG23	2.14	0.47
1:A:118:THR:HG21	1:A:168:ALA:HA	1.97	0.47
1:B:214:ILE:HA	1:B:217:ILE:HD12	1.97	0.47
1:A:52:PHE:CD2	1:B:49:MET:HG2	2.50	0.47
1:A:250:VAL:O	1:A:254:VAL:HG23	2.15	0.47
1:B:72:LEU:HD22	1:B:250:VAL:HG13	1.97	0.47
1:B:118:THR:HG21	1:B:168:ALA:HA	1.97	0.46
1:A:83:ASP:O	1:A:87:VAL:HG23	2.15	0.46
2:C:4:LEU:HD12	2:C:105:ILE:HG23	1.96	0.46
1:B:74:TYR:CE1	1:B:154:ILE:HD11	2.50	0.46
1:B:83:ASP:O	1:B:87:VAL:HG23	2.15	0.46
1:A:169:ALA:N	1:A:170:PRO:CD	2.79	0.46
1:B:286:ILE:HG22	1:B:290:ILE:HG12	1.97	0.46
2:D:60:TYR:CE1	2:D:70:ILE:HG22	2.50	0.46
1:B:169:ALA:N	1:B:170:PRO:CD	2.79	0.46
2:D:62:ASP:HA	2:D:65:GLU:HB2	1.97	0.46
1:A:91:PHE:HA	1:A:94:THR:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LYS:O	1:A:141:LYS:HG3	2.16	0.46
1:B:52:PHE:N	1:B:53:PRO:HD2	2.31	0.46
1:B:214:ILE:HB	1:B:215:PRO:HD3	1.98	0.46
1:A:52:PHE:N	1:A:53:PRO:HD2	2.31	0.45
1:B:195:HIS:HB3	1:B:200:ASN:ND2	2.31	0.45
2:C:88:THR:O	2:C:91:THR:CG2	2.64	0.45
1:A:75:ILE:HD11	1:A:130:VAL:HG11	1.97	0.45
2:D:60:TYR:HE1	2:D:70:ILE:HG22	1.80	0.45
2:C:33:ALA:HA	2:C:72:ARG:HH12	1.81	0.45
1:A:214:ILE:HA	1:A:217:ILE:HD12	1.99	0.45
1:A:176:SER:HA	1:A:200:ASN:CB	2.45	0.45
1:A:262:LEU:O	1:A:266:LEU:HD13	2.16	0.45
2:D:88:THR:O	2:D:91:THR:CG2	2.65	0.45
1:A:75:ILE:HG21	1:A:131:LEU:HD11	1.98	0.45
1:B:262:LEU:O	1:B:266:LEU:HD13	2.17	0.45
1:A:161:TRP:O	1:A:165:LEU:HD23	2.17	0.45
1:A:199:ASN:O	1:A:202:SER:OG	2.35	0.44
1:A:72:LEU:HD22	1:A:250:VAL:HG13	1.99	0.44
1:B:91:PHE:HA	1:B:94:THR:HG22	1.98	0.44
1:A:254:VAL:O	1:A:258:VAL:HG23	2.17	0.44
1:B:161:TRP:O	1:B:165:LEU:HD23	2.18	0.44
1:A:141:LYS:N	1:A:142:PRO:CD	2.81	0.43
1:B:128:LEU:HD21	1:B:257:MET:HB3	2.00	0.43
1:B:128:LEU:HD22	1:B:258:VAL:HG22	2.00	0.43
1:A:46:LEU:HD13	1:A:46:LEU:HA	1.84	0.43
1:B:199:ASN:O	1:B:202:SER:OG	2.35	0.43
1:B:141:LYS:N	1:B:142:PRO:CD	2.81	0.43
1:B:21:ARG:NE	1:B:21:ARG:HA	2.34	0.43
1:B:176:SER:HA	1:B:200:ASN:CB	2.48	0.43
2:C:4:LEU:HD23	2:C:24:ALA:HA	2.00	0.42
1:A:159:PHE:CE1	1:A:163:MET:HG3	2.54	0.42
2:D:33:ALA:HA	2:D:72:ARG:HH12	1.84	0.42
1:A:214:ILE:HB	1:A:215:PRO:HD3	2.00	0.42
2:D:2:VAL:HG21	2:D:98:ARG:NH1	2.35	0.42
1:A:52:PHE:CD2	1:B:49:MET:CG	3.02	0.42
2:C:5:VAL:O	2:C:22:CYS:HA	2.20	0.42
2:C:9:GLY:HA2	2:C:18:LEU:HD21	2.01	0.42
2:D:57:ASN:HB2	6:H:2:NAG:O6	2.20	0.42
2:D:9:GLY:HA2	2:D:18:LEU:HD21	2.00	0.42
1:A:126:TRP:NE1	1:A:163:MET:HB3	2.35	0.41
1:B:194:PRO:O	1:B:195:HIS:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3:GLN:HB3	2:C:25:SER:HB2	2.02	0.41
2:D:5:VAL:O	2:D:22:CYS:HA	2.19	0.41
1:B:203:PHE:CD2	1:B:203:PHE:C	2.99	0.41
1:A:135:ARG:HA	1:A:135:ARG:HD3	1.89	0.41
1:A:128:LEU:HD22	1:A:258:VAL:HG22	2.03	0.41
1:A:154:ILE:HG22	1:A:155:MET:HE2	2.02	0.41
2:D:23:ALA:HB2	2:D:78:MET:SD	2.61	0.41
2:C:48:VAL:HG13	2:C:64:VAL:HG21	2.02	0.41
2:D:91:THR:O	2:D:91:THR:HG23	2.21	0.41
1:A:172:LEU:HD21	1:A:178:TYR:CE2	2.56	0.41
1:B:72:LEU:HD21	1:B:253:MET:CE	2.50	0.41
2:C:91:THR:HA	2:C:112:VAL:O	2.21	0.41
1:A:203:PHE:CD2	1:A:203:PHE:C	2.99	0.41
2:C:91:THR:O	2:C:91:THR:HG23	2.21	0.41
1:B:200:ASN:O	1:B:204:VAL:HG23	2.20	0.40
1:B:126:TRP:NE1	1:B:163:MET:HB3	2.37	0.40
2:C:107:GLY:C	2:C:109:GLY:H	2.28	0.40
2:D:91:THR:HA	2:D:112:VAL:O	2.22	0.40
1:B:137:VAL:HA	1:B:142:PRO:HD2	2.04	0.40
1:B:179:ILE:CG1	1:B:180:PRO:HD2	2.52	0.40
2:D:48:VAL:HG13	2:D:64:VAL:HG21	2.03	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	297/348 (85%)	276 (93%)	21 (7%)	0	100	100
1	B	301/348 (86%)	280 (93%)	21 (7%)	0	100	100
2	C	112/126 (89%)	98 (88%)	14 (12%)	0	100	100
2	D	112/126 (89%)	99 (88%)	13 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	822/948 (87%)	753 (92%)	69 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	260/296 (88%)	255 (98%)	5 (2%)	50	66
1	B	261/296 (88%)	257 (98%)	4 (2%)	57	70
2	C	90/105 (86%)	89 (99%)	1 (1%)	65	73
2	D	92/105 (88%)	90 (98%)	2 (2%)	45	64
All	All	703/802 (88%)	691 (98%)	12 (2%)	53	67

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	108	THR
1	A	145	ASN
1	A	230	VAL
1	A	323	CYS
1	B	46	LEU
1	B	108	THR
1	B	245	LYS
1	B	308	MET
2	C	45	LEU
2	D	75	ASP
2	D	102	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	B	78	ASN
2	C	39	GLN
2	C	108	GLN
2	D	13	GLN
2	D	35	ASN
2	D	39	GLN
2	D	57	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

16 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	$\# Z > 2$
3	NAG	E	1	3,1	14,14,15	0.40	0	17,19,21	0.90	1 (5%)
3	NAG	E	2	3	14,14,15	0.42	0	17,19,21	0.86	1 (5%)
3	BMA	E	3	3	11,11,12	0.43	0	15,15,17	0.90	1 (6%)
3	MAN	E	4	3	11,11,12	0.30	0	15,15,17	0.99	0
3	NAG	E	5	3	14,14,15	0.53	0	17,19,21	1.28	3 (17%)
3	MAN	E	6	3	11,11,12	0.52	0	15,15,17	0.79	0
4	NAG	F	1	4,1	14,14,15	0.46	0	17,19,21	1.12	1 (5%)
4	NAG	F	2	4	14,14,15	0.36	0	17,19,21	0.94	1 (5%)
4	BMA	F	3	4	11,11,12	0.59	0	15,15,17	1.39	3 (20%)
5	NAG	G	1	1,5	14,14,15	0.38	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	G	2	5	14,14,15	0.43	0	17,19,21	0.80	0
5	BMA	G	3	5	11,11,12	0.47	0	15,15,17	0.94	0
5	MAN	G	4	5	11,11,12	0.46	0	15,15,17	0.68	0
5	MAN	G	5	5	11,11,12	0.43	0	15,15,17	0.83	0
6	NAG	H	1	6,1	14,14,15	0.43	0	17,19,21	0.78	0
6	NAG	H	2	6	14,14,15	0.48	0	17,19,21	1.13	2 (11%)

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
3	NAG	E	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	NAG	E	5	3	-	1/6/23/26	0/1/1/1
3	MAN	E	6	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	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
5	NAG	G	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	G	2	5	-	3/6/23/26	0/1/1/1
5	BMA	G	3	5	-	1/2/19/22	0/1/1/1
5	MAN	G	4	5	-	2/2/19/22	0/1/1/1
5	MAN	G	5	5	-	0/2/19/22	0/1/1/1
6	NAG	H	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	H	2	6	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5	NAG	O5-C1-C2	3.59	116.84	111.29
4	F	3	BMA	C1-C2-C3	3.29	114.43	109.64
4	F	1	NAG	C4-C3-C2	3.11	115.58	111.02
6	H	2	NAG	C1-C2-N2	2.78	114.81	110.43
3	E	2	NAG	C1-C2-N2	2.58	114.50	110.43
4	F	2	NAG	C1-C2-N2	2.56	114.47	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3	BMA	C1-C2-C3	2.55	113.36	109.64
6	H	2	NAG	O5-C1-C2	-2.33	107.68	111.29
3	E	1	NAG	O5-C1-C2	2.23	114.74	111.29
3	E	5	NAG	C4-C3-C2	2.22	114.28	111.02
4	F	3	BMA	O5-C1-C2	2.14	115.90	110.79
4	F	3	BMA	C1-O5-C5	2.04	114.92	112.19
3	E	5	NAG	C2-N2-C7	2.01	125.59	122.90

There are no chirality outliers.

All (20) torsion outliers are listed below:

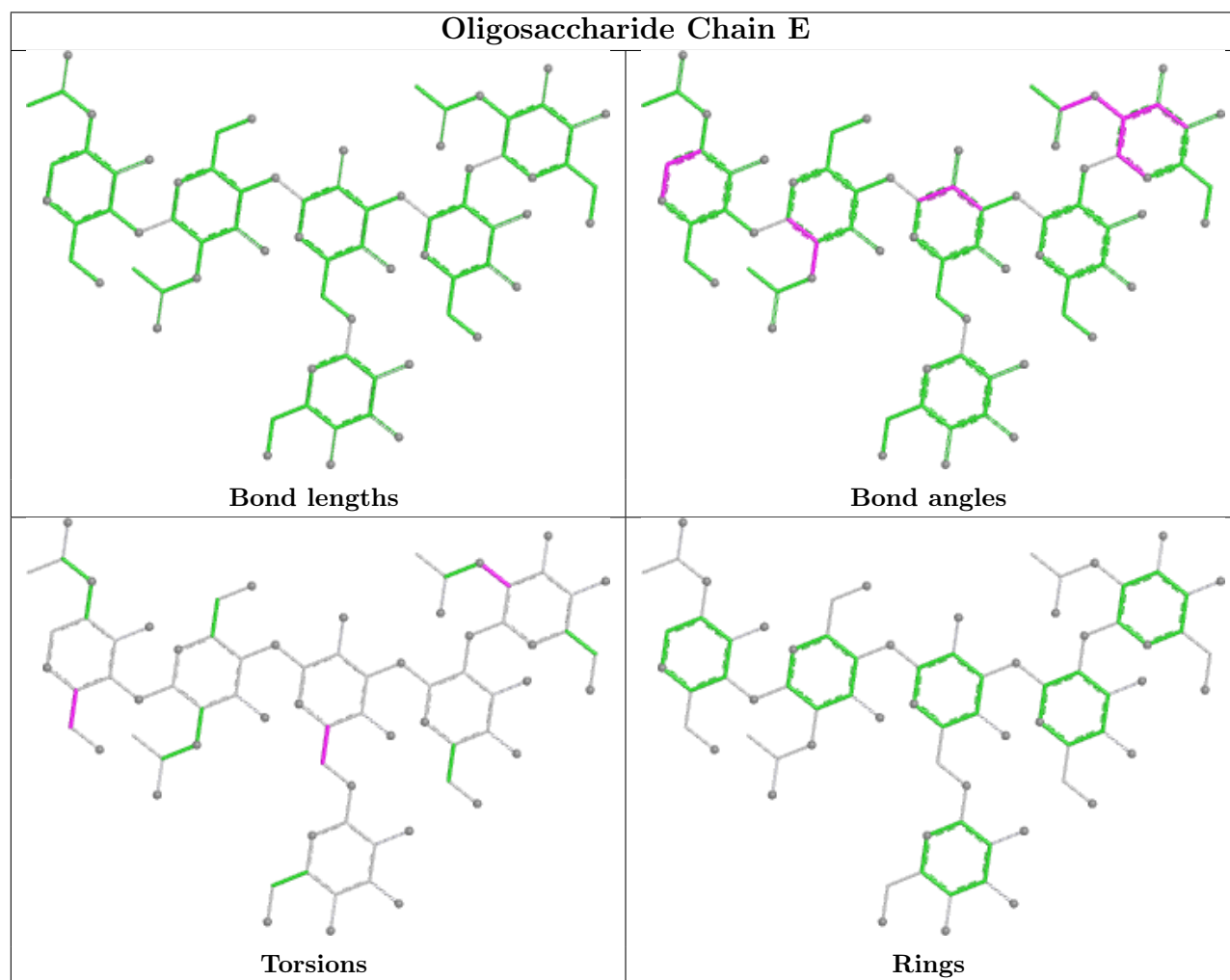
Mol	Chain	Res	Type	Atoms
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
6	H	2	NAG	C8-C7-N2-C2
6	H	2	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
5	G	4	MAN	O5-C5-C6-O6
6	H	1	NAG	C8-C7-N2-C2
6	H	1	NAG	O7-C7-N2-C2
5	G	4	MAN	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6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

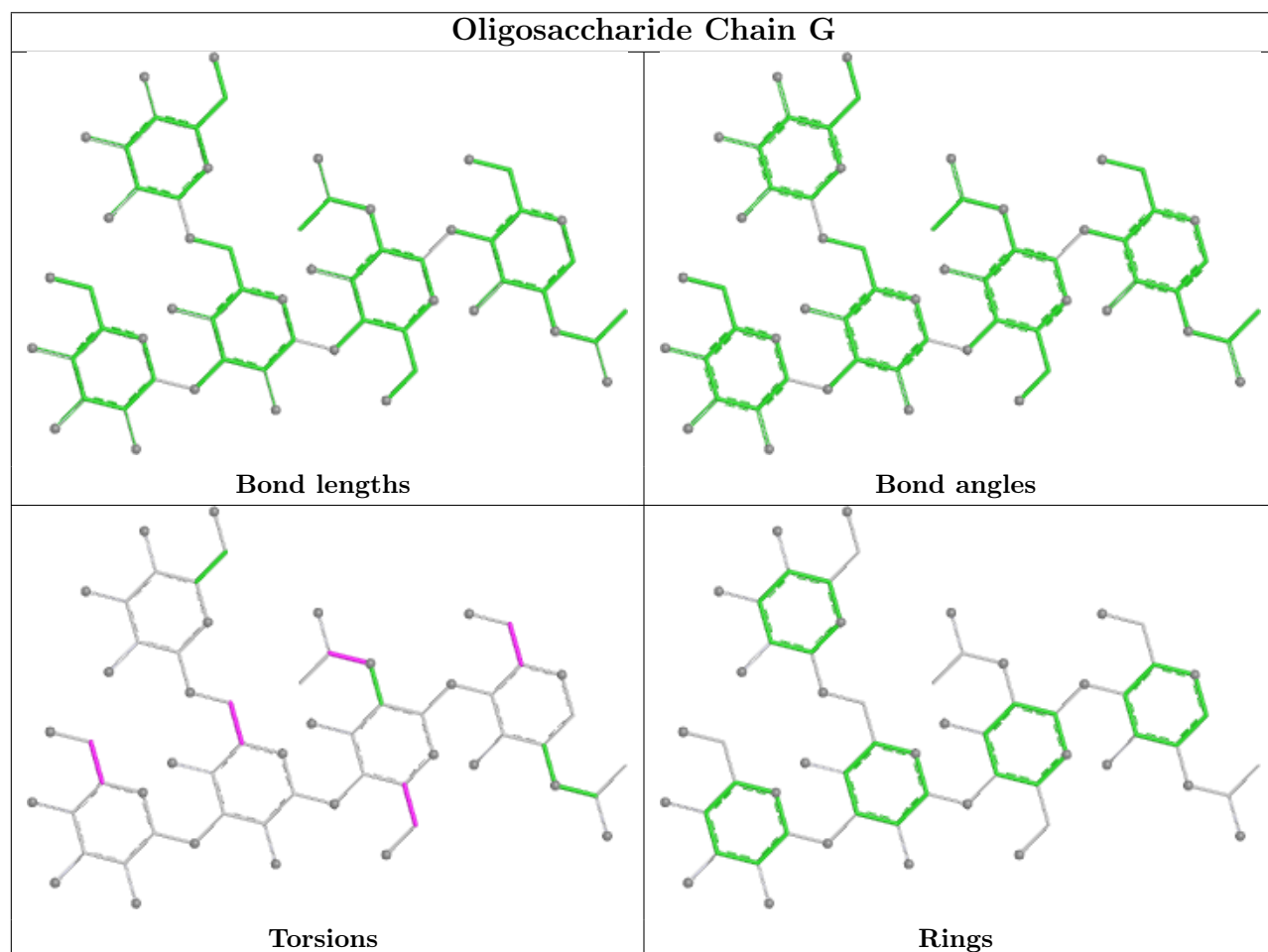
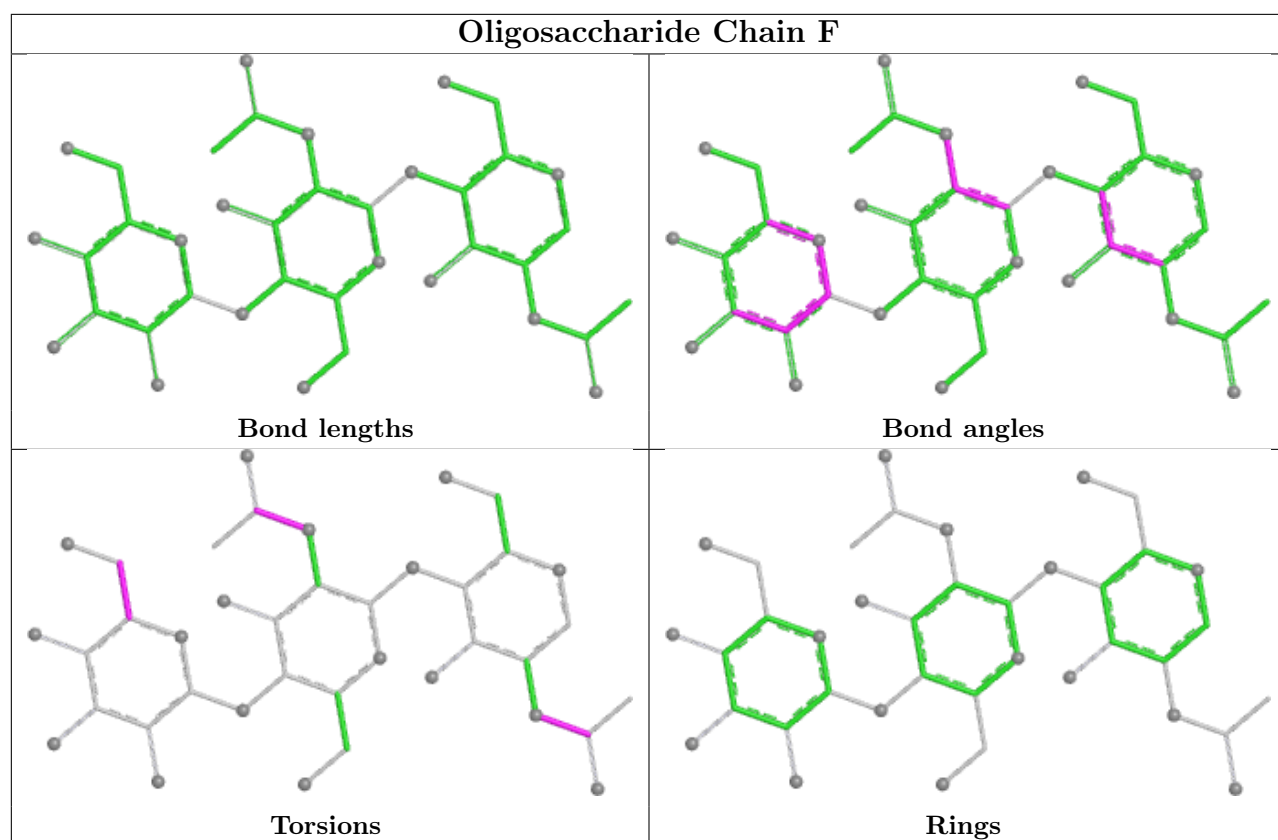
There are no ring outliers.

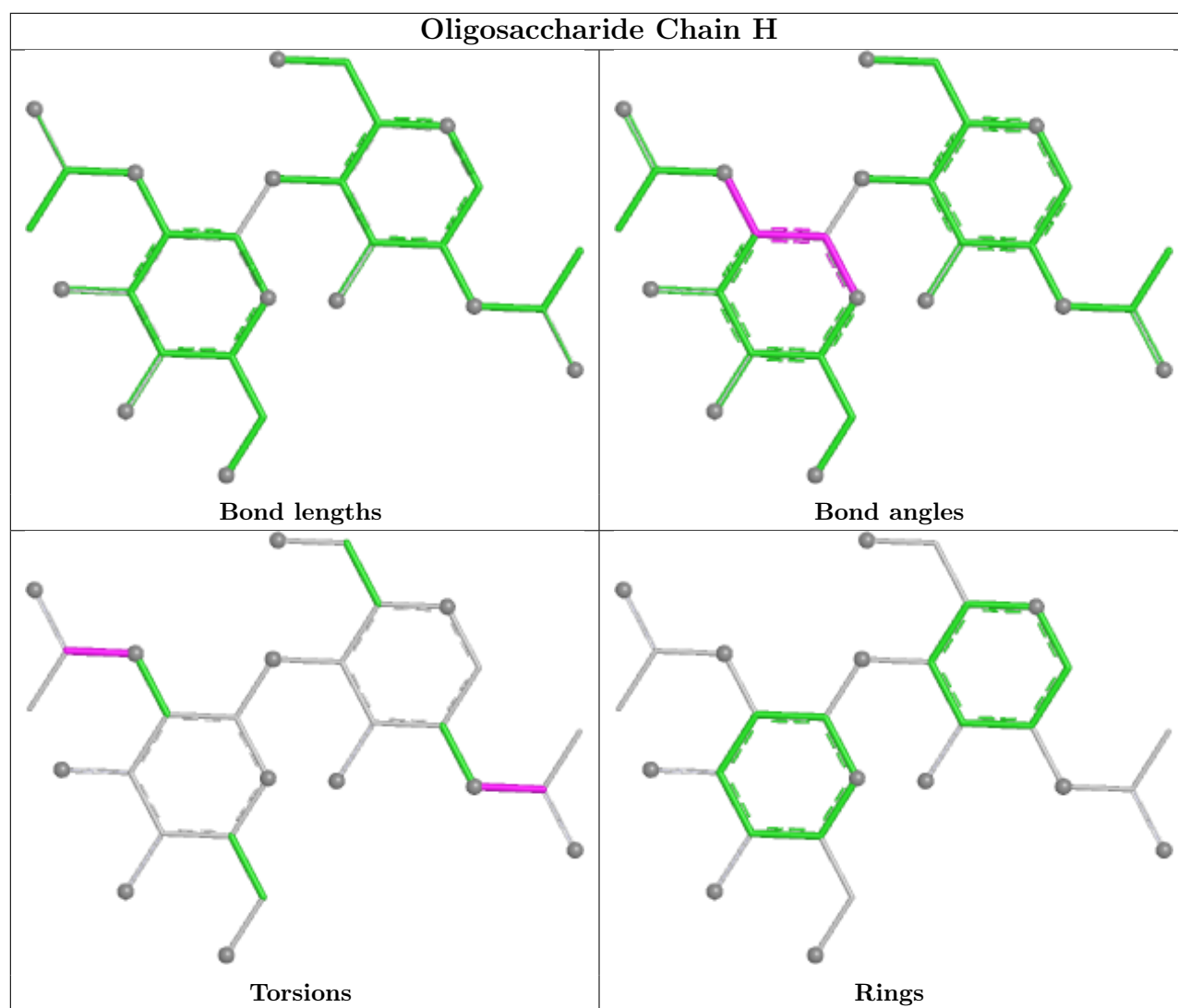
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	1	NAG	1	0
3	E	1	NAG	1	0
6	H	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](#)

There are no ligands in this entry.

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	305/348 (87%)	1.42	73 (23%) 2 5	247, 300, 358, 397	0
1	B	307/348 (88%)	1.06	64 (20%) 2 6	250, 297, 348, 387	0
2	C	114/126 (90%)	0.98	18 (15%) 5 8	262, 302, 331, 352	0
2	D	114/126 (90%)	0.31	10 (8%) 15 19	264, 305, 340, 386	0
All	All	840/948 (88%)	1.07	165 (19%) 3 6	247, 300, 351, 397	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	57	ASN	18.4
1	A	154	ILE	14.0
1	A	282	ASP	13.4
1	A	16	LYS	12.5
1	A	156	GLY	11.1
1	A	153	ALA	10.8
1	A	2	ASN	10.1
2	C	58	PRO	9.7
1	A	1	MET	9.3
2	C	56	ASP	9.3
1	A	62	THR	9.2
1	A	25	GLU	9.2
1	A	155	MET	9.0
1	A	63	VAL	8.7
1	A	14	SER	8.0
1	A	17	THR	7.9
2	C	59	THR	7.8
1	A	283	PHE	7.4
1	B	208	PHE	7.0
1	B	161	TRP	6.8
1	B	207	MET	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	162	VAL	6.5
1	A	13	PHE	6.3
1	B	47	LEU	6.1
1	A	77	LEU	6.1
1	A	64	GLN	6.0
1	B	81	VAL	5.9
1	A	157	VAL	5.8
1	A	130	VAL	5.5
1	B	212	PHE	5.5
1	A	133	ILE	5.5
1	B	323	CYS	5.4
1	A	151	ASN	5.4
1	A	321	LEU	5.2
2	C	66	GLY	5.2
1	A	74	TYR	5.1
1	B	91	PHE	5.1
1	B	284	GLY	5.0
1	B	209	VAL	5.0
1	B	154	ILE	5.0
2	C	54	SER	4.9
1	B	322	CYS	4.9
1	A	21	ARG	4.8
1	B	77	LEU	4.7
1	B	125	LEU	4.6
1	B	308	MET	4.6
1	B	211	HIS	4.5
1	B	7	PRO	4.4
2	C	55	GLY	4.4
1	A	15	ASN	4.3
1	A	311	LYS	4.2
1	A	152	HIS	4.2
1	B	210	VAL	4.2
1	A	19	VAL	4.2
1	A	59	LEU	4.2
1	A	197	GLU	4.2
1	B	206	TYR	4.1
1	A	213	ILE	4.1
1	B	213	ILE	4.1
1	A	158	ALA	4.1
1	B	204	VAL	4.1
1	B	205	ILE	4.0
1	B	287	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	18	GLY	3.9
2	D	88	THR	3.9
1	B	8	ASN	3.8
2	C	65	GLU	3.8
1	A	71	PRO	3.8
1	A	60	TYR	3.8
2	C	60	TYR	3.7
1	A	159	PHE	3.6
2	C	98	ARG	3.5
1	B	158	ALA	3.5
1	B	296	LYS	3.4
1	A	243	THR	3.4
2	D	14	PRO	3.4
1	A	319	THR	3.4
1	B	300	VAL	3.3
2	D	89	GLU	3.3
1	B	108	THR	3.3
1	B	62	THR	3.3
1	B	274	TYR	3.2
1	A	56	PHE	3.2
1	A	174	GLY	3.2
1	A	3	GLY	3.2
2	C	62	ASP	3.2
1	B	17	THR	3.2
1	A	199	ASN	3.2
2	D	71	ILE	3.2
1	A	230	VAL	3.1
1	B	156	GLY	3.1
1	A	134	GLU	3.1
1	A	173	VAL	3.1
1	B	283	PHE	3.0
1	A	217	ILE	3.0
1	B	121	GLY	3.0
1	A	117	ALA	3.0
1	A	118	THR	3.0
1	B	85	PHE	3.0
1	A	265	TRP	2.9
1	B	123	ILE	2.9
1	A	161	TRP	2.9
2	D	66	GLY	2.9
1	B	59	LEU	2.9
2	C	61	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	165	LEU	2.8
1	B	122	GLU	2.8
1	A	241	ALA	2.8
2	D	69	THR	2.8
1	A	281	SER	2.7
1	A	246	ALA	2.7
1	A	31	LEU	2.7
1	A	308	MET	2.7
1	A	284	GLY	2.6
1	B	12	PRO	2.6
1	B	107	PRO	2.6
1	B	120	GLY	2.6
1	B	311	LYS	2.6
1	B	282	ASP	2.6
1	B	314	ARG	2.5
2	C	111	GLN	2.5
1	B	221	PHE	2.5
1	B	105	PHE	2.5
1	A	20	VAL	2.5
1	A	312	GLN	2.5
1	A	81	VAL	2.5
1	A	147	ARG	2.4
1	B	309	MET	2.4
1	B	273	PHE	2.4
1	A	7	PRO	2.4
1	B	242	THR	2.4
1	B	167	CYS	2.4
1	B	250	VAL	2.3
1	B	159	PHE	2.3
2	D	106	GLU	2.3
2	C	51	ILE	2.3
1	A	280	GLY	2.3
2	D	30	SER	2.3
2	C	14	PRO	2.3
1	A	26	ALA	2.3
1	A	287	PHE	2.3
1	B	70	THR	2.2
1	B	63	VAL	2.2
1	A	145	ASN	2.2
1	B	82	ALA	2.2
1	B	276	PHE	2.2
1	A	268	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	177	ARG	2.2
1	A	227	VAL	2.2
1	B	280	GLY	2.2
1	B	261	PHE	2.2
2	C	69	THR	2.2
1	B	182	GLY	2.1
1	A	181	GLU	2.1
1	B	249	GLU	2.1
1	B	6	GLY	2.1
1	B	78	ASN	2.1
2	C	64	VAL	2.1
2	C	105	ILE	2.1
1	A	61	VAL	2.0
1	A	122	GLU	2.0
1	A	320	THR	2.0
2	D	65	GLU	2.0
2	D	31	LYS	2.0
1	B	310	ASN	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.

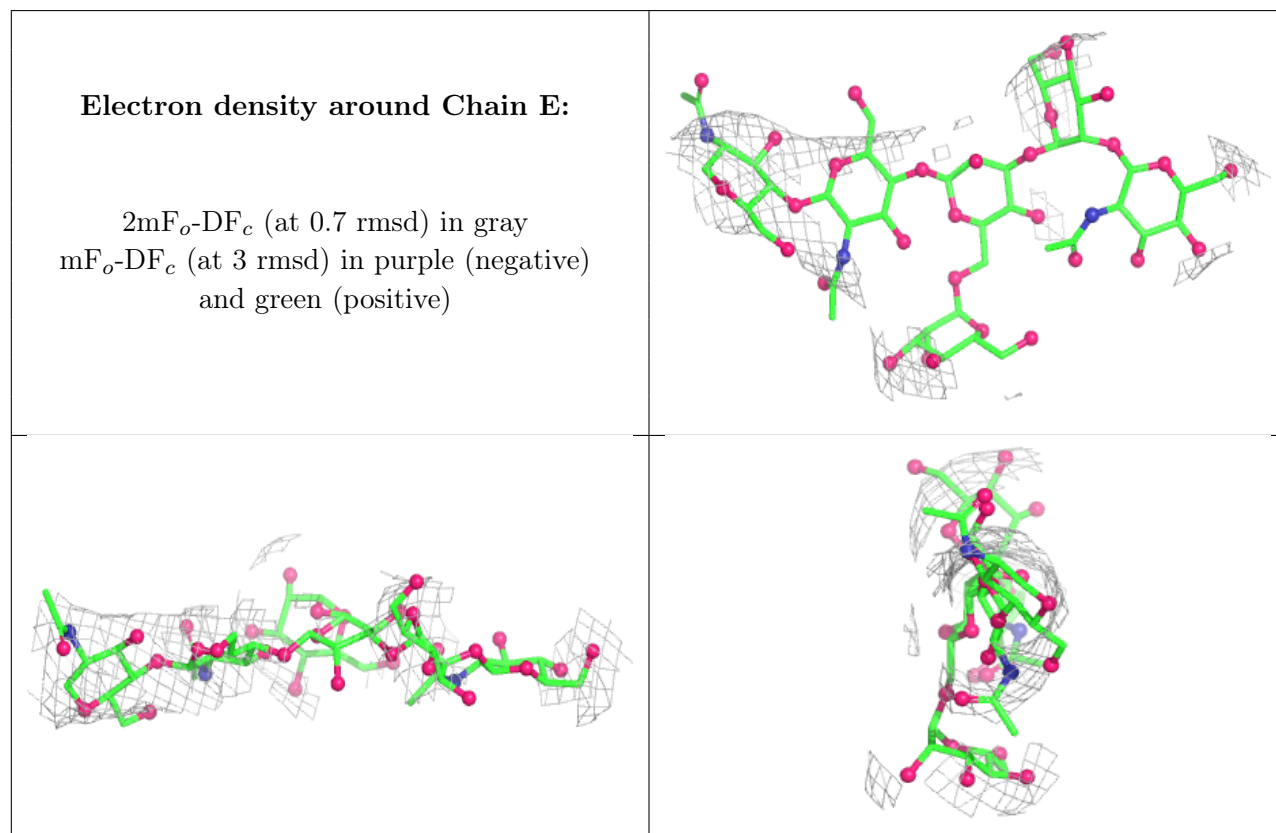
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	H	2	14/15	0.01	0.19	282,349,372,407	0
4	BMA	F	3	11/12	0.12	0.23	263,344,373,374	0
3	NAG	E	5	14/15	0.17	0.14	315,358,391,398	0
4	NAG	F	2	14/15	0.45	0.19	303,324,341,359	0
5	MAN	G	5	11/12	0.61	0.09	302,313,334,357	0
3	MAN	E	4	11/12	0.65	0.18	276,325,365,375	0
3	MAN	E	6	11/12	0.74	0.09	276,337,358,360	0
5	MAN	G	4	11/12	0.79	0.23	252,322,333,334	0
6	NAG	H	1	14/15	0.80	0.12	301,321,329,333	0
4	NAG	F	1	14/15	0.81	0.28	290,318,341,372	0

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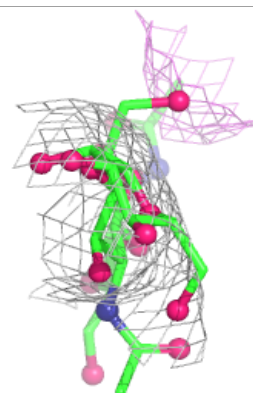
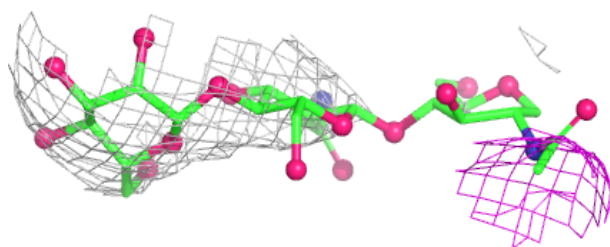
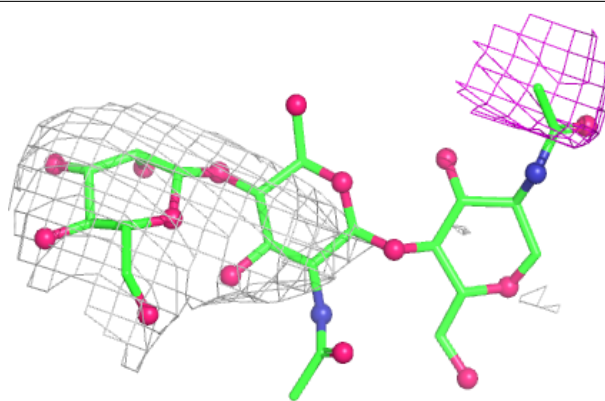
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BMA	G	3	11/12	0.87	0.05	282,306,313,317	0
3	BMA	E	3	11/12	0.89	0.05	295,306,346,375	0
5	NAG	G	2	14/15	0.93	0.07	244,292,310,317	0
5	NAG	G	1	14/15	0.95	0.10	272,293,328,333	0
3	NAG	E	2	14/15	0.96	0.11	264,282,314,317	0
3	NAG	E	1	14/15	0.97	0.22	259,278,328,358	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.

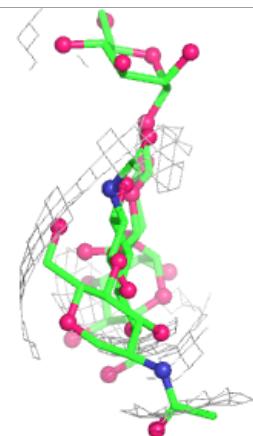
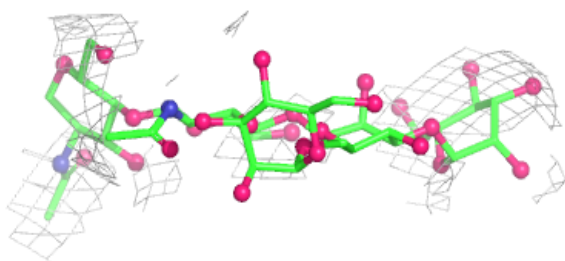
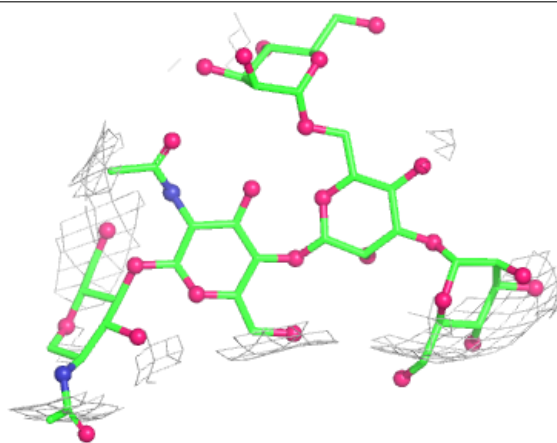


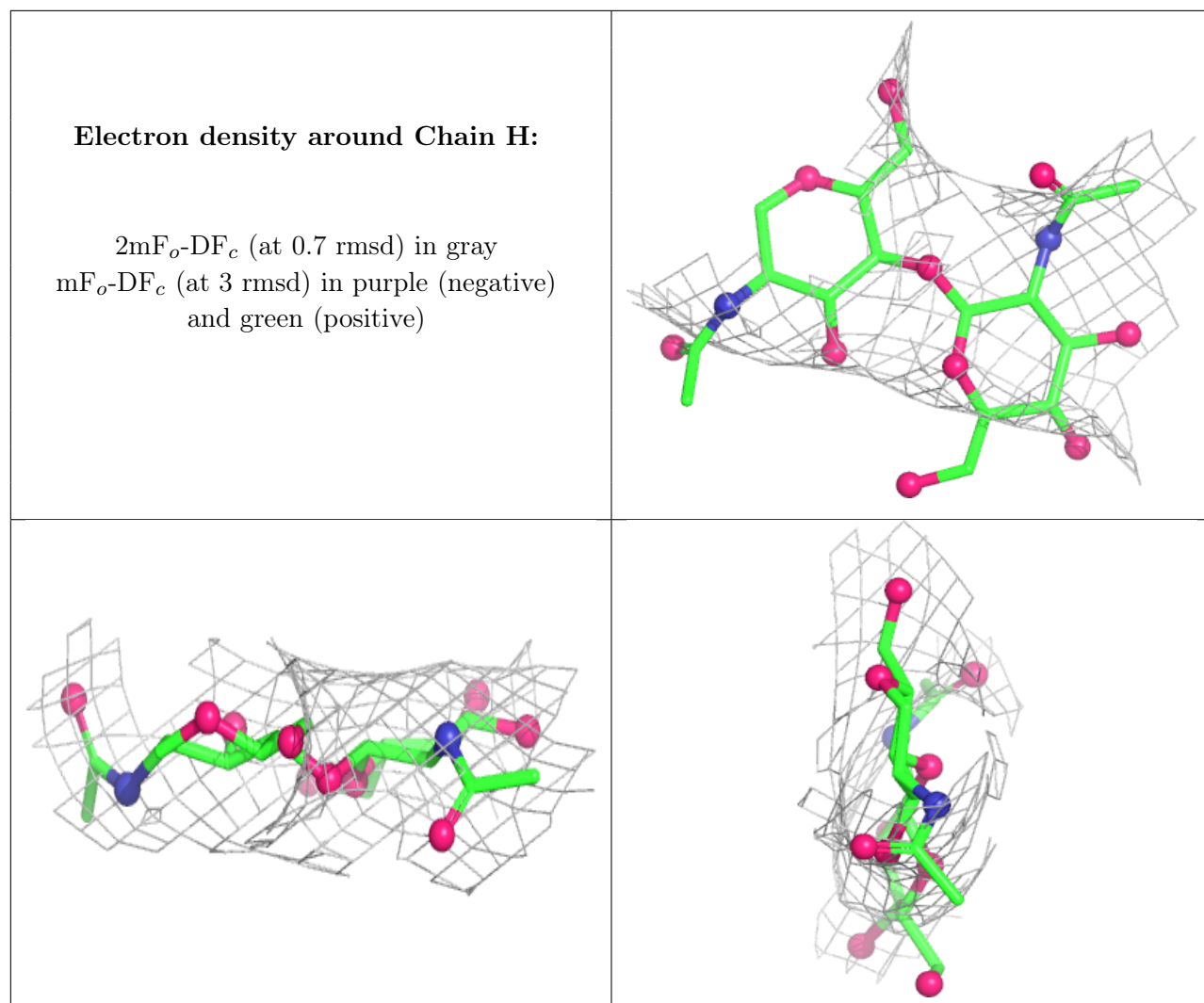
Electron density around Chain F:

$2mF_o-DF_c$ (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)





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.