



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 05:26 PM EDT

PDB ID : 1F88
Title : CRYSTAL STRUCTURE OF BOVINE RHODOPSIN
Authors : Okada, T.; Palczewski, K.; Stenkamp, R.E.; Miyano, M.
Deposited on : 2000-06-29
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

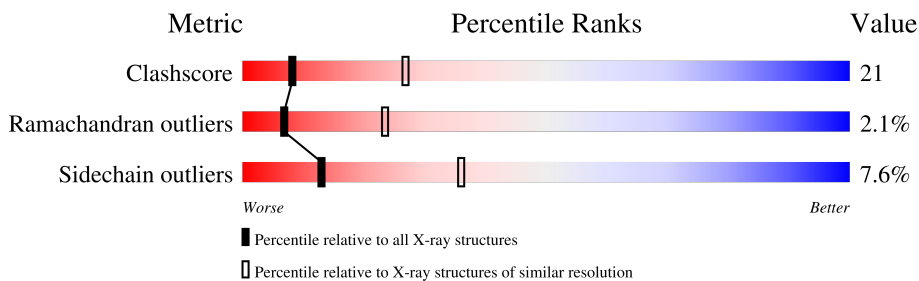
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	348	55% (green), 38% (yellow), . (orange), . (red), . (grey)
1	B	348	47% (green), 36% (yellow), . (orange), 12% (grey)
2	C	2	100% (yellow)
2	D	2	100% (orange)
2	F	2	100% (yellow)
3	E	3	33% (green), 67% (orange)

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	E	3	X	-	-	-

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 5267 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.

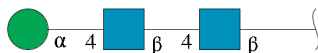
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	338	Total 2638	C 1754	N 409	O 449	S 26	0	0	0
1	B	305	Total 2429	C 1625	N 371	O 408	S 25	0	0	0

- Molecule 2 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
			Total	C	N	O			
2	C	2	Total 28	C 16	N 2	O 10	0	0	0
2	D	2	Total 28	C 16	N 2	O 10	0	0	0
2	F	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 3 is an oligosaccharide called alpha-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
			Total	C	N	O			
3	E	3	Total 39	C 22	N 2	O 15	0	0	0

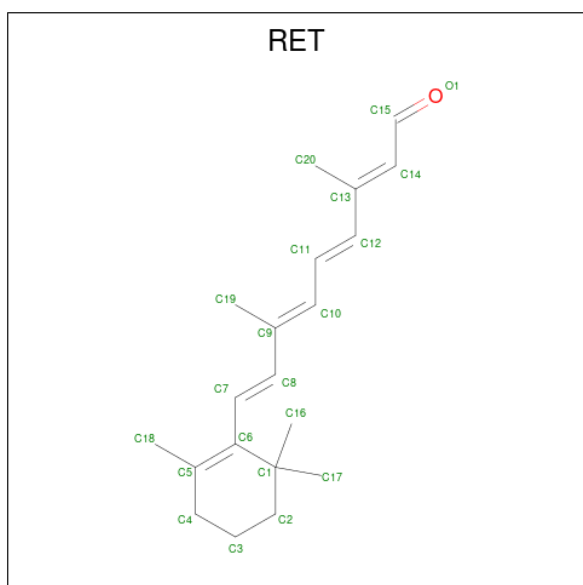
- Molecule 4 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Hg 3 3	0	0
4	B	3	Total Hg 3 3	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Zn 2 2	0	0
5	B	2	Total Zn 2 2	0	0

- Molecule 6 is RETINAL (three-letter code: RET) (formula: C₂₀H₂₈O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 20 20	0	0
6	B	1	Total C 20 20	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	16	Total O 16 16	0	0

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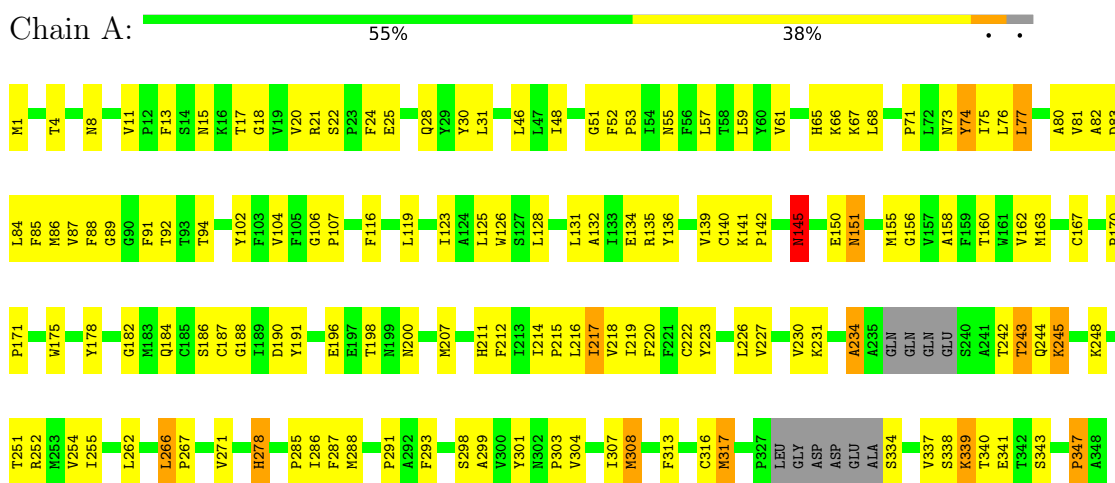
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	11	Total	O	0	0
			11	11		

3 Residue-property plots [i](#)

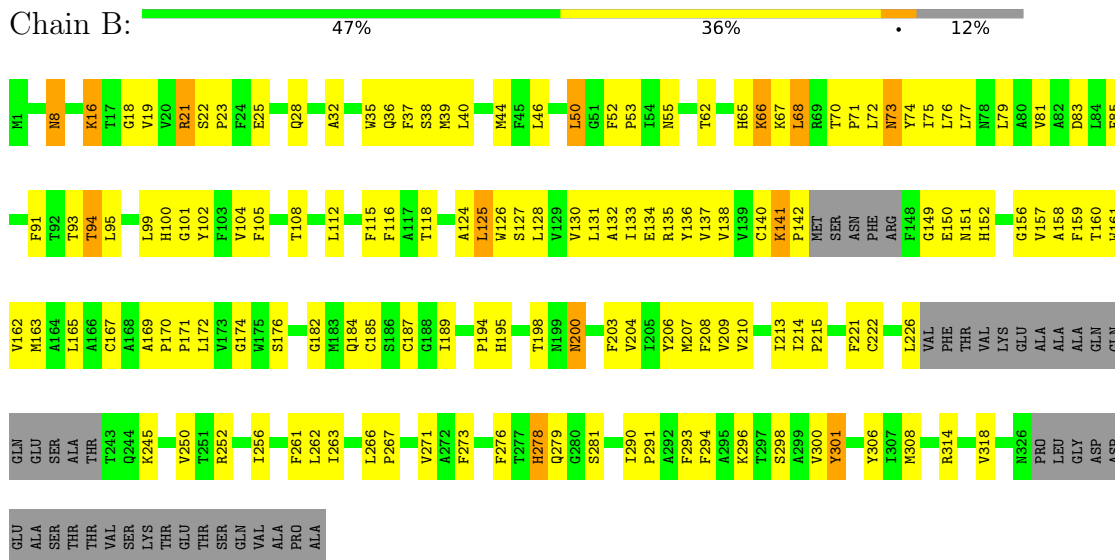
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

- Molecule 1: RHODOPSIN



- Molecule 1: RHODOPSIN



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

Chain C:  100%


MAG1
MAG2

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

Chain D:  100%

MAG1
MAG2

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

Chain F:  100%

MAG1
MAG2

- Molecule 3: alpha-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
MAG3

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	97.25Å 97.25Å 149.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80	Depositor
% Data completeness (in resolution range)	88.0 (30.00-2.80)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.186 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5267	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

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: HG, ZN, NAG, MAN, RET

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	1/2719 (0.0%)	0.69	1/3704 (0.0%)
1	B	0.51	1/2507 (0.0%)	0.65	1/3415 (0.0%)
All	All	0.52	2/5226 (0.0%)	0.67	2/7119 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	25	GLU	CD-OE2	7.59	1.33	1.25
1	A	25	GLU	CD-OE2	7.17	1.33	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	PRO	N-CA-CB	5.75	110.19	103.30
1	B	125	LEU	CA-CB-CG	5.25	127.39	115.30

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	2638	0	2573	107	0
1	B	2429	0	2407	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	28	0	25	3	0
2	D	28	0	25	4	0
2	F	28	0	25	0	0
3	E	39	0	34	3	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	20	0	27	2	0
6	B	20	0	27	6	0
7	A	16	0	0	0	0
7	B	11	0	0	0	0
All	All	5267	0	5143	217	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (217) 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:D:1:NAG:H61	2:D:2:NAG:HN2	1.02	1.06
2:D:1:NAG:H61	2:D:2:NAG:N2	1.70	1.06
2:D:1:NAG:C6	2:D:2:NAG:HN2	1.78	0.96
3:E:1:NAG:H62	3:E:2:NAG:H82	1.50	0.94
1:A:243:THR:HG22	1:A:244:GLN:HE21	1.34	0.92
1:A:151:ASN:HD22	1:A:151:ASN:H	1.19	0.91
1:A:234:ALA:HB3	1:A:252:ARG:HD2	1.50	0.90
1:A:91:PHE:HA	1:A:94:THR:HG22	1.55	0.89
1:B:271:VAL:HG21	1:B:291:PRO:HG2	1.61	0.81
1:B:137:VAL:HA	1:B:142:PRO:HD3	1.64	0.79
1:A:52:PHE:HB3	1:A:53:PRO:HD3	1.65	0.77
1:B:75:ILE:HD13	1:B:131:LEU:HG	1.65	0.76
1:A:230:VAL:HG22	1:A:248:LYS:HE2	1.66	0.76
1:B:72:LEU:HD22	1:B:250:VAL:HG13	1.68	0.76
1:B:8:ASN:HD22	1:B:8:ASN:H	1.31	0.75
1:A:298:SER:HA	1:A:301:TYR:CE1	2.22	0.74
1:A:271:VAL:HG11	1:A:291:PRO:HG2	1.68	0.74
1:A:338:SER:C	1:A:340:THR:H	1.88	0.74
1:A:151:ASN:HD22	1:A:151:ASN:N	1.85	0.73
1:A:251:THR:O	1:A:255:ILE:HG12	1.88	0.72
1:B:156:GLY:O	1:B:160:THR:HG23	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:SER:HA	1:A:301:TYR:HE1	1.55	0.70
1:B:118:THR:HG23	6:B:978:RET:H193	1.72	0.70
1:B:73:ASN:N	1:B:73:ASN:HD22	1.90	0.70
1:B:91:PHE:HA	1:B:94:THR:CG2	2.22	0.69
1:A:190:ASP:HB3	1:A:200:ASN:ND2	2.08	0.68
1:B:126:TRP:CH2	1:B:215:PRO:HG3	2.29	0.68
1:A:91:PHE:HA	1:A:94:THR:CG2	2.22	0.67
1:B:125:LEU:HB2	1:B:261:PHE:CZ	2.30	0.67
1:A:135:ARG:HB3	1:A:226:LEU:HD11	1.76	0.67
1:A:119:LEU:O	1:A:123:ILE:HG12	1.94	0.66
1:A:267:PRO:O	1:A:271:VAL:HG12	1.96	0.66
1:A:156:GLY:O	1:A:160:THR:HG23	1.96	0.65
1:A:167:CYS:HB2	1:A:211:HIS:CE1	2.31	0.65
1:A:167:CYS:HB2	1:A:211:HIS:ND1	2.12	0.65
1:B:200:ASN:O	1:B:204:VAL:HG23	1.96	0.65
1:B:74:TYR:OH	1:B:150:GLU:HG2	1.95	0.65
1:A:136:TYR:O	1:A:142:PRO:HG2	1.97	0.64
1:A:141:LYS:N	1:A:142:PRO:HD3	2.13	0.64
1:B:167:CYS:SG	1:B:207:MET:HG3	2.38	0.64
2:D:1:NAG:H61	2:D:2:NAG:C2	2.28	0.63
1:B:75:ILE:HG23	1:B:127:SER:HB3	1.80	0.63
1:B:75:ILE:HD11	1:B:130:VAL:HG12	1.80	0.63
1:B:290:ILE:HB	1:B:291:PRO:HD3	1.82	0.62
1:B:298:SER:HA	1:B:301:TYR:CD1	2.34	0.62
1:A:214:ILE:HB	1:A:215:PRO:HD3	1.82	0.62
1:B:102:TYR:CZ	1:B:104:VAL:HG12	2.34	0.62
1:B:52:PHE:HB3	1:B:53:PRO:HD3	1.81	0.62
1:B:77:LEU:O	1:B:81:VAL:HG23	1.99	0.61
1:B:8:ASN:HD22	1:B:8:ASN:N	1.94	0.61
1:B:132:ALA:O	1:B:222:CYS:SG	2.58	0.61
1:A:15:ASN:C	1:A:17:THR:H	2.02	0.61
1:B:75:ILE:CD1	1:B:131:LEU:HG	2.30	0.61
1:B:298:SER:HA	1:B:301:TYR:HD1	1.63	0.61
1:B:136:TYR:O	1:B:140:CYS:HB3	2.00	0.60
1:B:32:ALA:HB1	1:B:36:GLN:OE1	2.00	0.60
1:A:262:LEU:HB3	1:A:266:LEU:HD22	1.82	0.60
1:B:76:LEU:HD13	1:B:79:LEU:HD12	1.83	0.60
1:A:51:GLY:O	1:A:55:ASN:HB2	2.01	0.60
1:A:145:ASN:N	1:A:145:ASN:HD22	2.00	0.59
1:B:137:VAL:HA	1:B:142:PRO:CD	2.32	0.59
1:A:28:GLN:HB3	1:A:31:LEU:HD12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ALA:O	1:A:222:CYS:SG	2.57	0.59
1:B:187:CYS:O	6:B:978:RET:H12	2.03	0.59
1:B:124:ALA:O	1:B:128:LEU:HG	2.02	0.59
1:A:65:HIS:HA	1:A:339:LYS:H	1.66	0.59
1:B:158:ALA:O	1:B:162:VAL:HG23	2.03	0.58
1:B:214:ILE:HB	1:B:215:PRO:HD3	1.84	0.58
1:A:151:ASN:H	1:A:151:ASN:ND2	1.96	0.58
1:A:65:HIS:HB3	1:A:338:SER:HA	1.86	0.57
1:A:80:ALA:O	1:A:84:LEU:HG	2.03	0.57
2:C:1:NAG:H83	2:C:1:NAG:O3	2.04	0.57
1:A:158:ALA:O	1:A:162:VAL:HG23	2.04	0.57
1:B:314:ARG:O	1:B:318:VAL:HG23	2.04	0.57
1:A:66:LYS:H	1:A:339:LYS:CB	2.18	0.57
1:B:134:GLU:O	1:B:138:VAL:HG22	2.04	0.57
1:A:91:PHE:CA	1:A:94:THR:HG22	2.33	0.56
1:A:18:GLY:HA2	2:C:1:NAG:C1	2.36	0.56
1:A:308:MET:HE2	1:B:99:LEU:HD21	1.86	0.56
1:A:338:SER:C	1:A:340:THR:N	2.58	0.56
1:A:304:VAL:O	1:A:308:MET:HB2	2.06	0.55
1:B:209:VAL:HG23	1:B:210:VAL:HG23	1.88	0.55
1:A:28:GLN:HG3	1:A:184:GLN:HB2	1.88	0.55
1:A:215:PRO:O	1:A:219:ILE:HG13	2.07	0.55
1:A:75:ILE:HG21	1:A:131:LEU:HD11	1.88	0.55
1:A:339:LYS:HA	1:A:343:SER:CB	2.37	0.54
1:A:4:THR:OG1	1:A:15:ASN:HB2	2.08	0.54
1:B:28:GLN:HG3	1:B:184:GLN:HB2	1.90	0.54
1:B:125:LEU:HB2	1:B:261:PHE:HZ	1.71	0.53
1:B:278:HIS:ND1	1:B:278:HIS:N	2.57	0.53
1:B:263:ILE:O	1:B:294:PHE:HE2	1.92	0.53
1:B:70:THR:HG22	1:B:71:PRO:HD2	1.91	0.53
2:C:2:NAG:O3	2:C:2:NAG:H83	2.08	0.53
1:B:194:PRO:HG3	1:B:279:GLN:HE22	1.75	0.52
1:B:276:PHE:O	1:B:279:GLN:HG3	2.09	0.52
1:A:83:ASP:HA	1:A:86:MET:HE3	1.92	0.52
1:B:75:ILE:HD11	1:B:130:VAL:CG1	2.40	0.52
1:A:86:MET:HG2	1:A:116:PHE:O	2.09	0.52
1:B:267:PRO:O	1:B:271:VAL:HG23	2.09	0.52
1:A:308:MET:HE1	1:B:95:LEU:HD11	1.93	0.51
1:A:151:ASN:N	1:A:151:ASN:ND2	2.54	0.51
1:B:293:PHE:HA	1:B:296:LYS:HD2	1.93	0.51
1:A:170:PRO:HB2	1:A:171:PRO:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:PHE:HA	1:A:92:THR:HG23	1.93	0.50
1:A:82:ALA:O	1:A:86:MET:HG3	2.10	0.50
1:B:140:CYS:HB2	1:B:226:LEU:CD2	2.41	0.50
1:B:23:PRO:HB3	1:B:184:GLN:HB3	1.93	0.50
1:B:115:PHE:CD2	1:B:172:LEU:HD11	2.47	0.50
1:B:66:LYS:HD3	1:B:66:LYS:N	2.27	0.49
1:A:242:THR:HG1	1:A:334:SER:N	2.09	0.49
1:A:338:SER:O	1:A:340:THR:N	2.46	0.49
1:A:31:LEU:HD22	1:A:285:PRO:HG3	1.95	0.49
1:A:308:MET:CE	1:B:99:LEU:HD21	2.42	0.49
1:B:131:LEU:O	1:B:135:ARG:HG2	2.12	0.49
1:A:178:TYR:HA	1:A:188:GLY:O	2.13	0.49
1:A:288:MET:O	1:A:291:PRO:HD2	2.12	0.49
1:A:171:PRO:HA	1:A:175:TRP:O	2.12	0.49
1:B:161:TRP:O	1:B:165:LEU:HB2	2.13	0.49
1:B:262:LEU:O	1:B:266:LEU:HB2	2.13	0.49
1:A:20:VAL:HA	1:A:30:TYR:CZ	2.48	0.49
1:A:68:LEU:HG	1:A:73:ASN:ND2	2.28	0.48
1:B:118:THR:CG2	6:B:978:RET:H193	2.41	0.48
1:B:133:ILE:O	1:B:137:VAL:HG23	2.13	0.48
1:B:73:ASN:HD22	1:B:73:ASN:H	1.61	0.48
1:A:57:LEU:O	1:A:61:VAL:HG23	2.13	0.48
1:A:75:ILE:HG21	1:A:131:LEU:CD1	2.43	0.48
6:B:978:RET:C8	6:B:978:RET:H181	2.43	0.48
1:B:66:LYS:HG2	1:B:67:LYS:HG3	1.96	0.48
1:A:15:ASN:C	1:A:17:THR:N	2.68	0.47
1:B:85:PHE:HB3	1:B:116:PHE:HD1	1.79	0.47
1:B:50:LEU:HD13	1:B:300:VAL:HG11	1.95	0.47
1:B:176:SER:HA	1:B:200:ASN:HB3	1.95	0.47
1:B:137:VAL:HG13	1:B:142:PRO:HD2	1.97	0.47
1:A:307:ILE:HG12	1:A:313:PHE:HE1	1.80	0.47
1:B:73:ASN:N	1:B:73:ASN:ND2	2.60	0.47
1:B:93:THR:HG23	1:B:105:PHE:HD1	1.80	0.47
1:B:157:VAL:O	1:B:161:TRP:HD1	1.97	0.47
1:B:252:ARG:O	1:B:256:ILE:HD13	2.14	0.47
1:A:74:TYR:HE2	1:A:150:GLU:HG2	1.80	0.47
1:B:36:GLN:O	1:B:40:LEU:HG	2.15	0.46
1:A:11:VAL:HG11	1:A:30:TYR:HH	1.81	0.46
1:A:52:PHE:CB	1:A:53:PRO:HD3	2.40	0.46
1:B:108:THR:O	1:B:112:LEU:HG	2.15	0.46
1:B:208:PHE:O	1:B:213:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:PRO:O	1:A:307:ILE:HG13	2.15	0.46
1:B:182:GLY:C	1:B:184:GLN:H	2.19	0.46
1:A:106:GLY:HA3	1:A:107:PRO:HD2	1.78	0.45
1:B:198:THR:OG1	1:B:200:ASN:ND2	2.49	0.45
1:B:35:TRP:O	1:B:39:MET:HB2	2.17	0.45
1:A:271:VAL:HG23	1:A:287:PHE:CZ	2.51	0.45
1:B:189:ILE:HD13	6:B:978:RET:C19	2.46	0.45
1:A:83:ASP:O	1:A:87:VAL:HG23	2.16	0.45
1:B:91:PHE:HA	1:B:94:THR:HG23	1.95	0.45
6:B:978:RET:H10	6:B:978:RET:H202	1.98	0.45
1:A:13:PHE:HB2	1:A:31:LEU:HD21	1.98	0.45
1:A:68:LEU:HG	1:A:73:ASN:HD22	1.82	0.45
1:A:91:PHE:HD2	1:A:91:PHE:N	2.15	0.45
1:B:55:ASN:ND2	1:B:83:ASP:HB3	2.32	0.45
1:A:307:ILE:HG22	1:A:307:ILE:O	2.17	0.45
1:B:85:PHE:HB3	1:B:116:PHE:CD1	2.51	0.45
1:A:91:PHE:N	1:A:91:PHE:CD2	2.84	0.45
1:A:77:LEU:O	1:A:81:VAL:HG23	2.17	0.44
1:B:65:HIS:HB2	1:B:68:LEU:HD22	1.99	0.44
1:B:149:GLY:C	1:B:151:ASN:H	2.20	0.44
1:A:59:LEU:HD23	1:A:84:LEU:HD11	1.98	0.44
1:A:102:TYR:CZ	1:A:104:VAL:HG22	2.53	0.44
1:B:126:TRP:CE2	1:B:163:MET:HB3	2.52	0.44
1:A:67:LYS:HB2	1:A:337:VAL:O	2.17	0.44
1:A:140:CYS:HB2	1:A:226:LEU:HD23	1.98	0.44
1:A:278:HIS:ND1	1:A:278:HIS:N	2.66	0.44
1:B:135:ARG:HD2	1:B:135:ARG:N	2.32	0.44
1:A:216:LEU:O	1:A:220:PHE:HB2	2.17	0.44
1:B:170:PRO:HB2	1:B:171:PRO:HD3	1.99	0.44
1:B:18:GLY:O	1:B:21:ARG:NH2	2.50	0.44
1:A:307:ILE:HG21	1:A:317:MET:SD	2.58	0.43
1:B:76:LEU:HD13	1:B:76:LEU:HA	1.87	0.43
1:B:100:HIS:CG	1:B:104:VAL:HG11	2.53	0.43
1:A:126:TRP:CE2	1:A:163:MET:HB3	2.54	0.43
1:A:307:ILE:HG12	1:A:313:PHE:CE1	2.53	0.43
1:A:316:CYS:SG	1:A:338:SER:CB	3.07	0.43
1:A:163:MET:O	1:A:211:HIS:HE1	2.01	0.43
1:A:223:TYR:O	1:A:227:VAL:HG23	2.18	0.43
1:B:21:ARG:HH22	3:E:1:NAG:H5	1.84	0.43
1:B:37:PHE:CD1	1:B:101:GLY:HA2	2.54	0.43
1:A:187:CYS:O	6:A:977:RET:H12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:MET:O	1:A:211:HIS:CE1	2.72	0.42
1:A:217:ILE:HG22	1:A:218:VAL:N	2.34	0.42
1:A:271:VAL:HG13	1:A:288:MET:HE1	2.01	0.42
1:B:62:THR:HA	1:B:68:LEU:HD23	2.02	0.42
1:B:19:VAL:HG22	1:B:19:VAL:O	2.20	0.42
1:B:189:ILE:HG12	1:B:203:PHE:HE1	1.83	0.42
1:A:135:ARG:HD3	1:A:254:VAL:HG21	2.01	0.42
1:B:152:HIS:ND1	1:B:152:HIS:N	2.67	0.42
1:A:136:TYR:C	1:A:142:PRO:HG2	2.40	0.42
1:B:22:SER:HA	1:B:23:PRO:HD3	1.86	0.42
1:B:35:TRP:CE2	1:B:36:GLN:HG3	2.55	0.42
1:B:8:ASN:N	1:B:8:ASN:ND2	2.64	0.42
1:A:86:MET:HE3	1:A:299:ALA:HA	2.02	0.42
1:A:139:VAL:HB	1:A:226:LEU:HD22	2.01	0.41
1:B:165:LEU:O	1:B:169:ALA:HB3	2.20	0.41
3:E:1:NAG:C3	3:E:2:NAG:O5	2.68	0.41
1:A:245:LYS:HE3	1:A:245:LYS:HA	2.02	0.41
1:A:75:ILE:CG2	1:A:131:LEU:HD11	2.49	0.41
1:B:137:VAL:O	1:B:141:LYS:HA	2.20	0.41
1:B:16:LYS:HB3	1:B:16:LYS:HE2	1.85	0.41
1:A:128:LEU:HD23	1:A:128:LEU:HA	1.89	0.41
6:A:977:RET:H10	6:A:977:RET:H202	2.01	0.41
1:B:208:PHE:CE1	1:B:273:PHE:HB2	2.55	0.41
1:B:159:PHE:O	1:B:163:MET:HG2	2.21	0.41
1:A:85:PHE:O	1:A:89:GLY:N	2.50	0.41
1:B:46:LEU:HA	1:B:46:LEU:HD23	1.85	0.41
1:A:22:SER:C	1:A:24:PHE:H	2.24	0.40
1:A:167:CYS:SG	1:A:207:MET:HG3	2.61	0.40
1:A:48:ILE:HD11	1:A:91:PHE:O	2.21	0.40
1:A:186:SER:HB2	1:A:293:PHE:HE2	1.86	0.40
1:A:182:GLY:HA2	1:A:285:PRO:O	2.21	0.40
1:B:70:THR:CG2	1:B:71:PRO:HD2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	332/348 (95%)	285 (86%)	38 (11%)	9 (3%)	5	17
1	B	299/348 (86%)	262 (88%)	33 (11%)	4 (1%)	12	36
All	All	631/696 (91%)	547 (87%)	71 (11%)	13 (2%)	7	23

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	ALA
1	A	341	GLU
1	A	198	THR
1	A	212	PHE
1	A	231	LYS
1	A	339	LYS
1	B	281	SER
1	A	145	ASN
1	A	347	PRO
1	B	174	GLY
1	B	195	HIS
1	A	196	GLU
1	B	141	LYS

5.3.2 Protein sidechains [i](#)

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	275/296 (93%)	253 (92%)	22 (8%)	12	34
1	B	261/296 (88%)	242 (93%)	19 (7%)	14	38
All	All	536/592 (90%)	495 (92%)	41 (8%)	13	36

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	ASN
1	A	21	ARG
1	A	46	LEU
1	A	71	PRO
1	A	74	TYR
1	A	76	LEU
1	A	77	LEU
1	A	125	LEU
1	A	134	GLU
1	A	145	ASN
1	A	151	ASN
1	A	155	MET
1	A	191	TYR
1	A	217	ILE
1	A	243	THR
1	A	245	LYS
1	A	266	LEU
1	A	278	HIS
1	A	286	ILE
1	A	308	MET
1	A	317	MET
1	B	8	ASN
1	B	16	LYS
1	B	21	ARG
1	B	38	SER
1	B	44	MET
1	B	50	LEU
1	B	66	LYS
1	B	68	LEU
1	B	73	ASN
1	B	94	THR
1	B	185	CYS
1	B	200	ASN
1	B	206	TYR
1	B	221	PHE
1	B	245	LYS
1	B	278	HIS
1	B	301	TYR
1	B	306	TYR
1	B	308	MET

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	8	ASN
1	A	28	GLN
1	A	64	GLN
1	A	145	ASN
1	A	151	ASN
1	A	211	HIS
1	A	244	GLN
1	B	8	ASN
1	B	28	GLN
1	B	73	ASN
1	B	100	HIS
1	B	200	ASN
1	B	279	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](#)

9 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	C	1	1,2	14,14,15	0.63	0	17,19,21	0.72	0
2	NAG	C	2	2	14,14,15	0.69	0	17,19,21	0.76	0
2	NAG	D	1	1,2	14,14,15	0.57	0	17,19,21	0.81	1 (5%)
2	NAG	D	2	2	14,14,15	0.95	1 (7%)	17,19,21	0.78	0
3	NAG	E	1	1,3	14,14,15	0.67	0	17,19,21	0.81	1 (5%)
3	NAG	E	2	3	14,14,15	0.55	0	17,19,21	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	E	3	3	11,11,12	0.54	0	15,15,17	0.30	0
2	NAG	F	1	1,2	14,14,15	0.57	0	17,19,21	0.93	1 (5%)
2	NAG	F	2	2	14,14,15	0.53	0	17,19,21	0.79	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
3	MAN	E	3	3	1/1/4/5	0/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	C1-C2	2.87	1.56	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C2-N2-C7	-3.06	118.54	122.90
3	E	2	NAG	C2-N2-C7	-2.45	119.41	122.90
3	E	1	NAG	C2-N2-C7	-2.31	119.61	122.90
2	D	1	NAG	C2-N2-C7	-2.25	119.69	122.90
2	F	2	NAG	C2-N2-C7	-2.14	119.85	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	3	MAN	C1

All (25) torsion outliers are listed below:

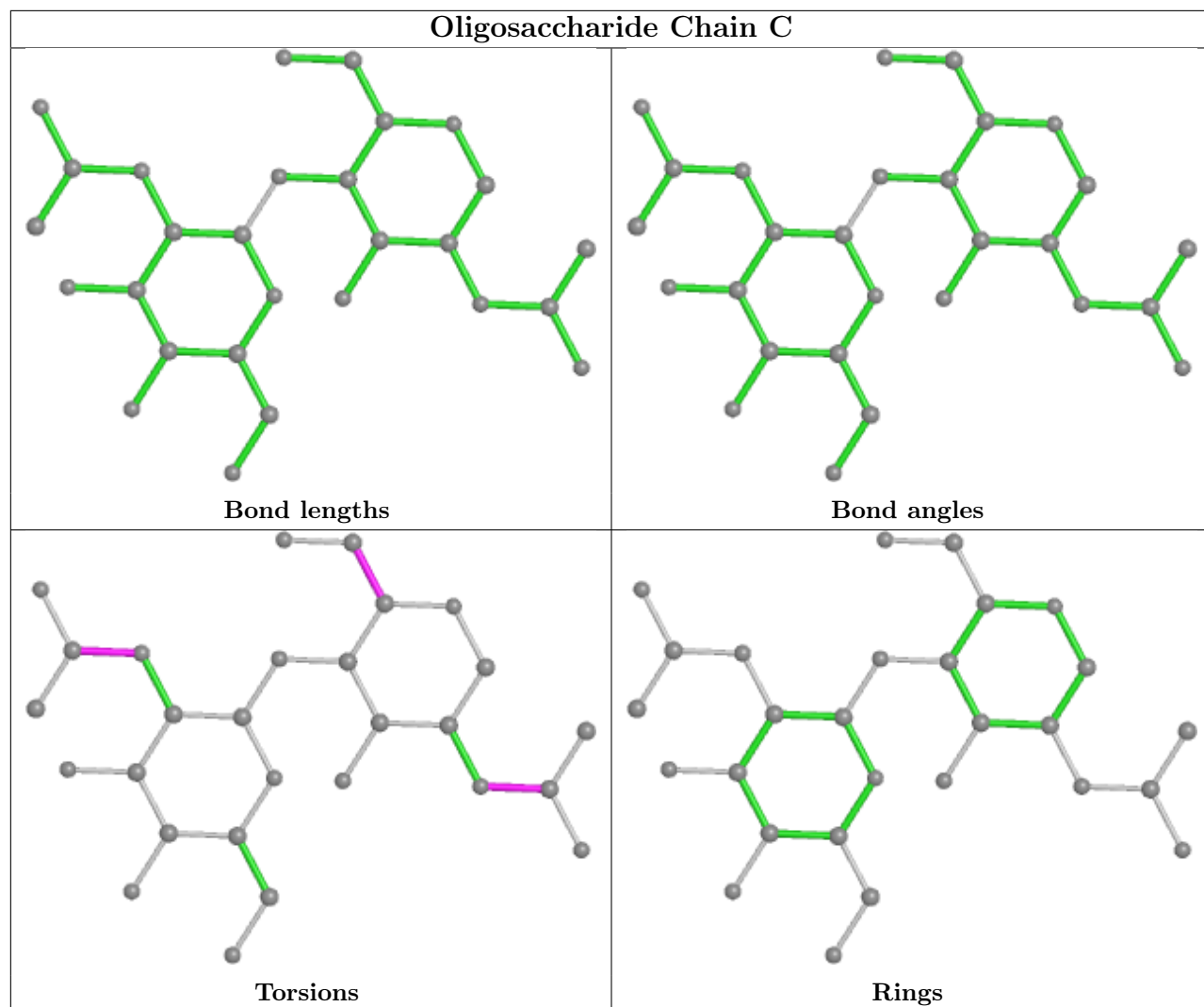
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C3-C2-N2-C7
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	E	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

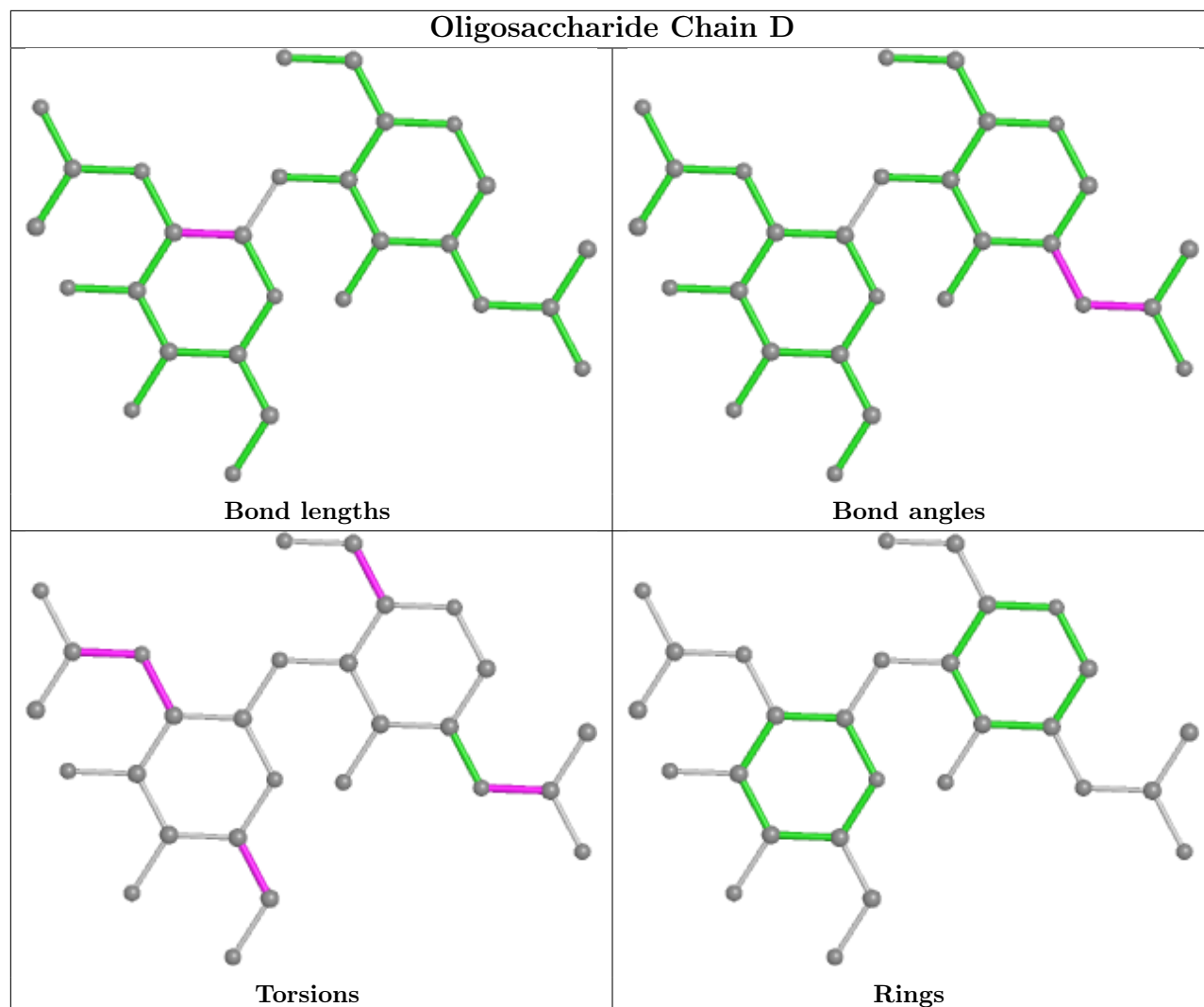
There are no ring outliers.

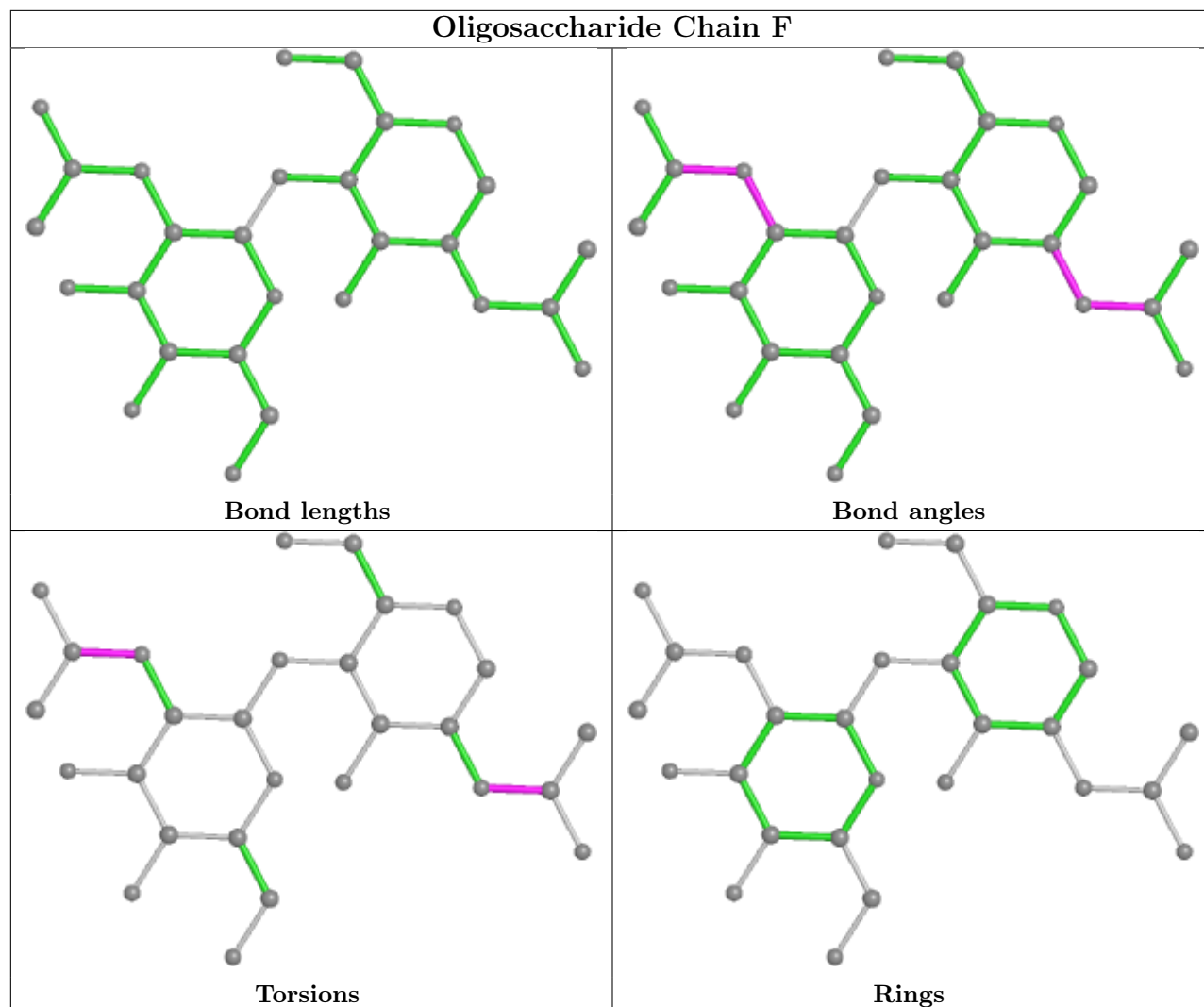
6 monomers are involved in 10 short contacts:

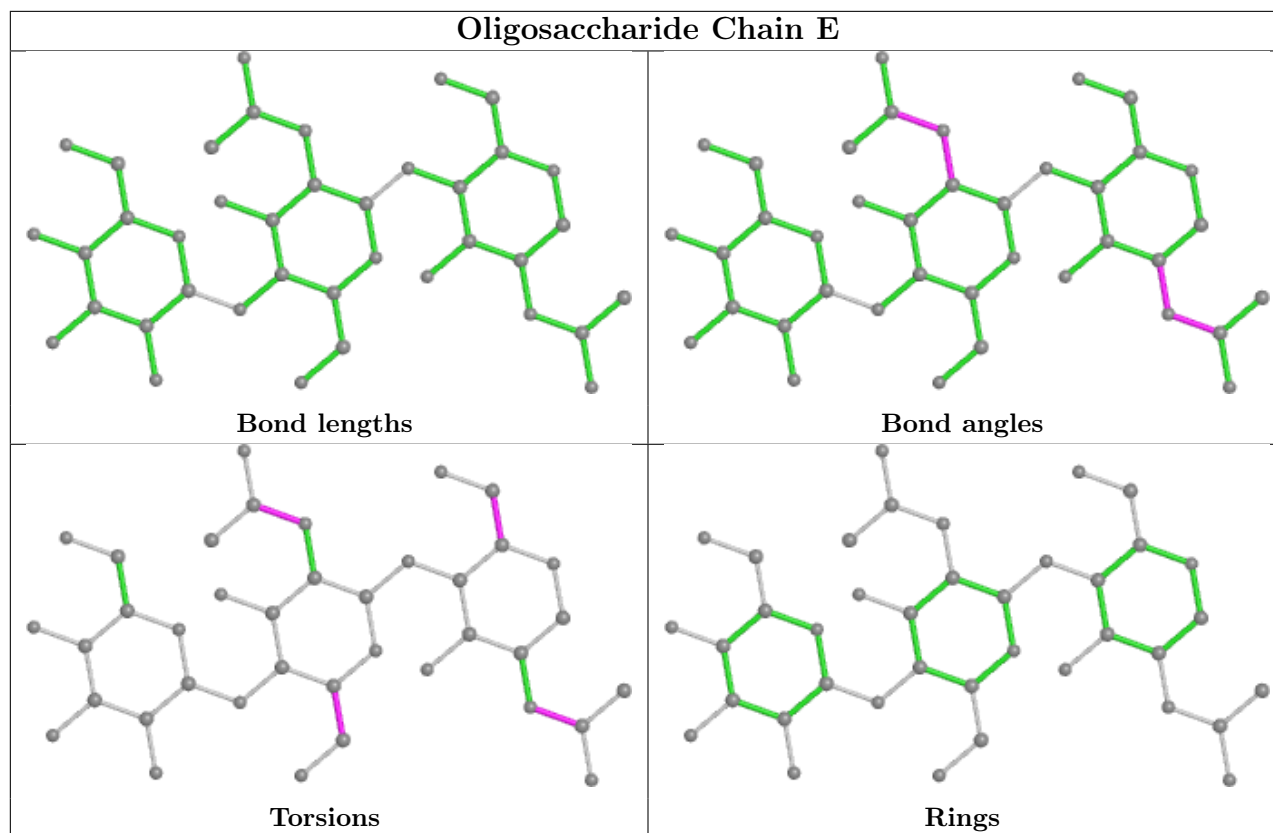
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	1	0
2	D	1	NAG	4	0
3	E	2	NAG	2	0
3	E	1	NAG	3	0
2	D	2	NAG	4	0
2	C	1	NAG	2	0

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](#)

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 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	RET	B	978	1	20,20,21	1.04	0	27,27,28	1.61	5 (18%)
6	RET	A	977	1	20,20,21	1.05	0	27,27,28	1.40	4 (14%)

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	RET	B	978	1	-	3/13/30/31	0/1/1/1
6	RET	A	977	1	-	1/13/30/31	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	978	RET	C8-C7-C6	-3.99	115.98	127.20
6	B	978	RET	C19-C9-C8	-3.47	112.60	118.08
6	A	977	RET	C19-C9-C8	-3.46	112.63	118.08
6	A	977	RET	C11-C12-C13	3.24	135.53	126.42
6	B	978	RET	C11-C12-C13	3.23	135.50	126.42
6	B	978	RET	C8-C9-C10	3.23	123.90	118.94
6	A	977	RET	C8-C9-C10	3.00	123.54	118.94
6	A	977	RET	C8-C7-C6	-2.99	118.80	127.20
6	B	978	RET	C7-C8-C9	2.97	130.73	126.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	978	RET	C11-C12-C13-C20
6	A	977	RET	C10-C11-C12-C13
6	B	978	RET	C10-C11-C12-C13
6	B	978	RET	C11-C12-C13-C14

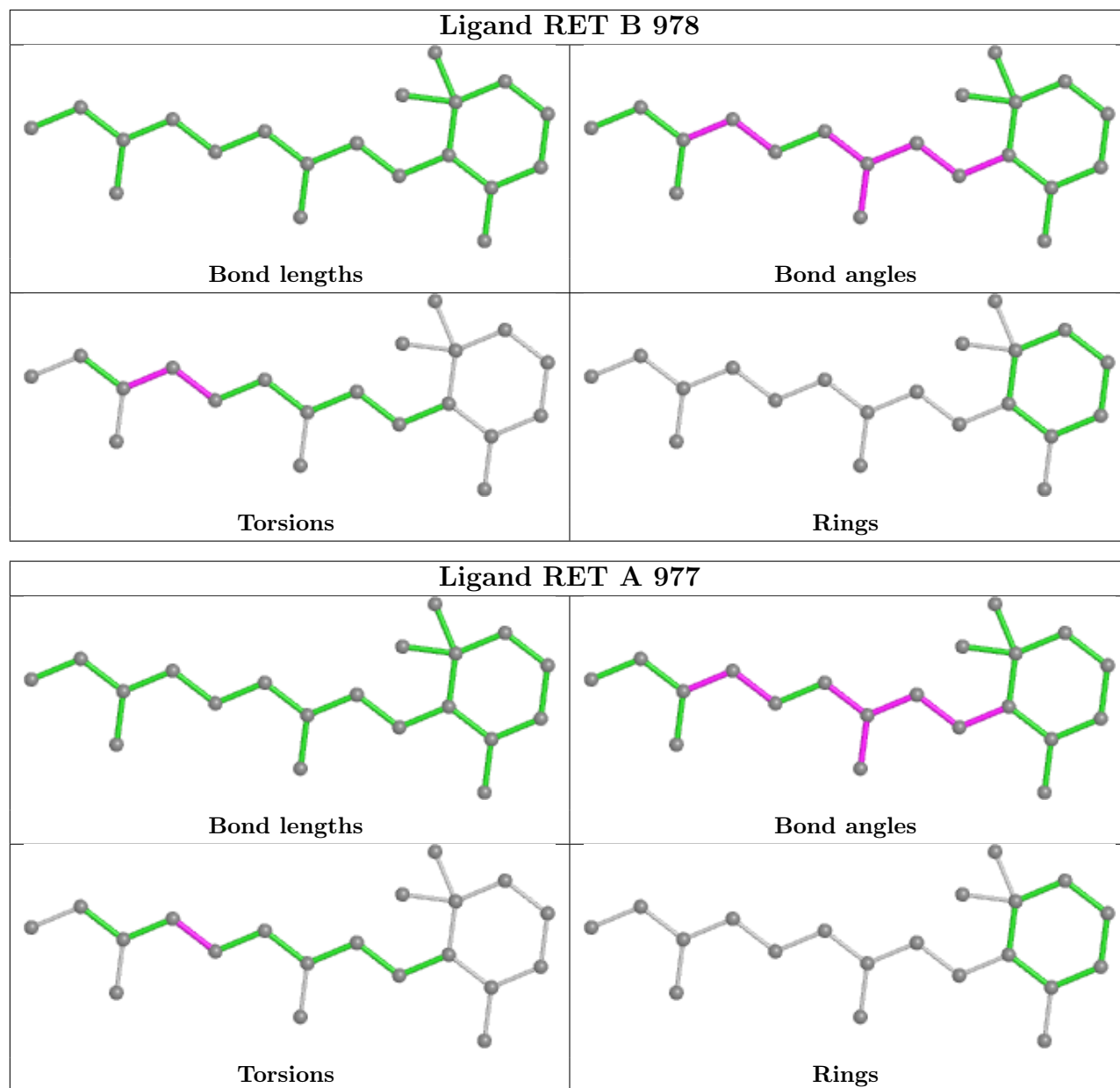
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	978	RET	6	0
6	A	977	RET	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.