



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:22 PM UTC

PDB ID : 1F88 / pdb_00001f88
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

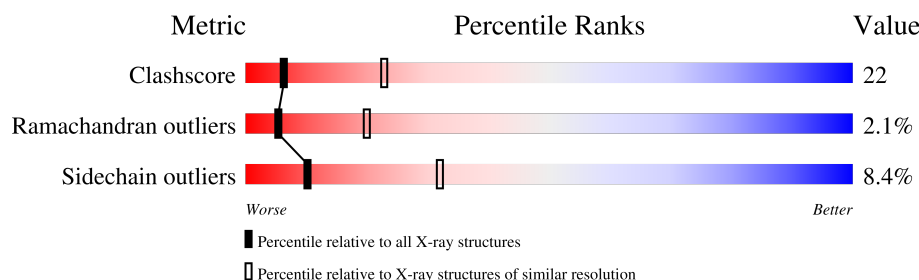
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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	52% 37% 7% ..
1	B	348	44% 36% 7% 12%
2	C	2	50% 50%
2	D	2	100%
2	F	2	100%
3	E	3	33% 67%

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.

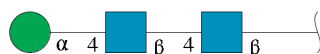
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2638	1754	409	449	26			
1	B	305	Total	C	N	O	S	0	0	0
			2429	1625	371	408	25			

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

- 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
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

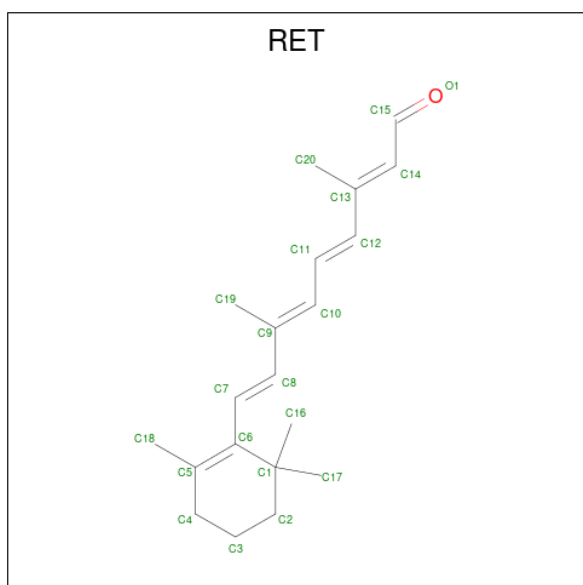
- Molecule 4 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

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 (CCD ID: 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 (CCD ID: 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

Continued on next page...

Continued from previous page...

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



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

Chain C:  50% 50%

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

Xtriage (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.	Xtriage
Total number of atoms	5267	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HG, RET, MAN, ZN, 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	0.64	1/2719 (0.0%)	1.13	20/3704 (0.5%)
1	B	0.57	0/2507	1.10	16/3415 (0.5%)
All	All	0.61	1/5226 (0.0%)	1.12	36/7119 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86	MET	SD-CE	-5.73	1.65	1.79

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	VAL	N-CA-C	10.07	119.90	110.74
1	B	192	TYR	N-CA-C	9.54	121.68	111.28
1	B	301	TYR	N-CA-C	8.10	120.10	111.28
1	A	146	PHE	N-CA-C	8.09	120.76	110.24
1	A	301	TYR	N-CA-C	7.67	120.72	111.82
1	A	77	LEU	N-CA-C	-7.64	102.89	112.90
1	A	9	PHE	N-CA-C	7.46	118.11	108.34
1	A	227	VAL	N-CA-C	-7.42	105.34	113.43
1	B	87	VAL	N-CA-C	7.37	117.50	110.42
1	A	66	LYS	N-CA-C	6.95	121.38	112.34
1	A	192	TYR	N-CA-C	6.78	118.75	111.36
1	B	170	PRO	N-CA-C	6.76	118.95	110.70
1	B	119	LEU	N-CA-C	-6.63	103.97	111.07
1	A	347	PRO	N-CA-CB	6.61	110.19	103.25
1	A	106	GLY	CA-C-N	6.35	126.56	119.32
1	A	106	GLY	C-N-CA	6.35	126.56	119.32
1	B	136	TYR	N-CA-C	-6.31	105.59	113.28
1	A	123	ILE	N-CA-C	-6.23	103.26	111.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	THR	N-CA-C	-6.14	105.77	113.20
1	B	54	ILE	N-CA-C	6.10	116.88	110.72
1	A	69	ARG	N-CA-C	5.99	119.82	111.56
1	A	300	VAL	N-CA-C	5.92	121.65	109.34
1	A	170	PRO	N-CA-C	5.79	117.77	110.70
1	A	26	ALA	N-CA-C	5.74	115.51	108.11
1	B	200	ASN	N-CA-C	-5.64	106.37	113.20
1	B	77	LEU	N-CA-C	-5.62	104.78	111.69
1	B	265	TRP	N-CA-C	5.58	120.37	113.50
1	B	250	VAL	N-CA-C	-5.56	103.98	111.44
1	A	168	ALA	N-CA-C	5.50	119.17	112.23
1	B	65	HIS	N-CA-C	5.42	117.14	108.41
1	B	304	VAL	N-CA-C	-5.37	107.19	111.81
1	A	323	CYS	N-CA-C	5.21	119.47	113.38
1	B	11	VAL	N-CA-C	5.14	112.95	107.76
1	B	156	GLY	N-CA-C	-5.06	106.30	112.77
1	B	197	GLU	N-CA-C	5.04	117.50	111.71
1	A	191	TYR	N-CA-C	-5.01	107.15	114.12

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	2638	0	2573	114	0
1	B	2429	0	2407	106	0
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	20	0	27	7	0
7	A	16	0	0	0	0
7	B	11	0	0	0	0
All	All	5267	0	5143	227	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 22.

All (227) 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:338:SER:C	1:A:340:THR:H	1.88	0.77
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:151:ASN:HD22	1:A:151:ASN:N	1.85	0.73
1:A:44:MET:HE2	1:A:94:THR:HG21	1.72	0.72
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:15:ASN:C	1:A:17:THR:H	2.02	0.65
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:83:ASP:HA	1:A:86:MET:HE3	1.80	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:A:44:MET:HE2	1:A:94:THR:CG2	2.30	0.61
1:B:132:ALA:O	1:B:222:CYS:SG	2.58	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:338:SER:C	1:A:340:THR:N	2.58	0.55
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:A:308:MET:HE3	1:B:99:LEU:HD21	1.89	0.53
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: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: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
1:A:88:PHE:HA	1:A:92:THR:HG23	1.93	0.50
1:B:182:GLY:C	1:B:184:GLN:H	2.19	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:A:271:VAL:HG13	1:A:288:MET:HE1	1.92	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:338:SER:O	1:A:340:THR:N	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HD22	1:A:285:PRO:HG3	1.95	0.49
1:B:149:GLY:C	1:B:151:ASN:H	2.20	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: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:151:ASN:H	1:A:151:ASN:ND2	1.96	0.47
1:A:155:MET:HE3	1:A:155:MET:HA	1.96	0.47
1:A:307:ILE:HG12	1:A:313:PHE:HE1	1.80	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:B:207:MET:HE3	6:B:978:RET:H161	1.96	0.47
1:A:74:TYR:HE2	1:A:150:GLU:HG2	1.80	0.47
1:A:136:TYR:C	1:A:142:PRO:HG2	2.40	0.47
1:B:36:GLN:O	1:B:40:LEU:HG	2.15	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
1:A:303:PRO:O	1:A:307:ILE:HG13	2.15	0.46
1:A:15:ASN:C	1:A:17:THR:N	2.68	0.45
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:22:SER:C	1:A:24:PHE:H	2.24	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:1:MET:C	1:B:3:GLY:H	2.23	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:11:VAL:C	1:A:13:PHE:H	2.25	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: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:308:MET:HE1	1:B:95:LEU:HD11	1.99	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:A:317:MET:HE3	1:A:318:VAL:HG23	2.00	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:225:GLN:C	1:A:227:VAL:H	2.25	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:91:PHE:C	1:A:94:THR:HG22	2.43	0.43
1:A:187:CYS:O	6:A:977:RET:H12	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:MET:HE1	1:B:296:LYS:HD3	2.00	0.43
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:B:62:THR:HA	1:B:68:LEU:HD23	2.02	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: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:194:PRO:O	1:B:195:HIS:C	2.62	0.42
1:B:19:VAL:O	1:B:19:VAL:HG22	2.20	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:A:308:MET:HE2	1:B:41:ALA:HB1	2.03	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:B:199:ASN:C	1:B:201:GLU:H	2.27	0.41
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:A:341:GLU:O	1:A:342:THR:C	2.64	0.40
1:A:194:PRO:O	1:A:195:HIS:C	2.64	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%)	4	15
1	B	299/348 (86%)	262 (88%)	33 (11%)	4 (1%)	9	31
All	All	631/696 (91%)	547 (87%)	71 (11%)	13 (2%)	5	20

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%)	252 (92%)	23 (8%)	10	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	261/296 (88%)	239 (92%)	22 (8%)	10	32
All	All	536/592 (90%)	491 (92%)	45 (8%)	10	32

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	46	LEU
1	A	59	LEU
1	A	68	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	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	A	318	VAL
1	A	319	THR
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	68	LEU
1	B	73	ASN
1	B	76	LEU
1	B	81	VAL
1	B	94	THR
1	B	125	LEU
1	B	152	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	154	ILE
1	B	157	VAL
1	B	185	CYS
1	B	199	ASN
1	B	200	ASN
1	B	221	PHE
1	B	245	LYS
1	B	278	HIS
1	B	308	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	28	GLN
1	A	64	GLN
1	A	111	ASN
1	A	145	ASN
1	A	151	ASN
1	A	211	HIS
1	A	244	GLN
1	A	312	GLN
1	B	8	ASN
1	B	28	GLN
1	B	73	ASN
1	B	100	HIS
1	B	200	ASN
1	B	225	GLN
1	B	279	GLN
1	B	315	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 ⓘ

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	0.62	0	17,19,21	0.75	0
2	NAG	C	2	2	14,14,15	0.72	0	17,19,21	0.77	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.57	0	17,19,21	0.84	1 (5%)
2	NAG	D	2	2	14,14,15	1.01	1 (7%)	17,19,21	0.78	0
3	NAG	E	1	3,1	14,14,15	0.66	0	17,19,21	0.84	1 (5%)
3	NAG	E	2	3	14,14,15	0.54	0	17,19,21	0.90	1 (5%)
3	MAN	E	3	3	11,11,12	0.54	0	15,15,17	0.26	0
2	NAG	F	1	1,2	14,14,15	0.58	0	17,19,21	0.97	1 (5%)
2	NAG	F	2	2	14,14,15	0.54	0	17,19,21	0.82	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	3,1	-	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	3.14	1.56	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C2-N2-C7	-3.25	118.54	122.90
3	E	2	NAG	C2-N2-C7	-2.60	119.41	122.90
3	E	1	NAG	C2-N2-C7	-2.45	119.61	122.90
2	D	1	NAG	C2-N2-C7	-2.39	119.69	122.90
2	F	2	NAG	C2-N2-C7	-2.28	119.85	122.90
2	C	2	NAG	C2-N2-C7	-2.07	120.12	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	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

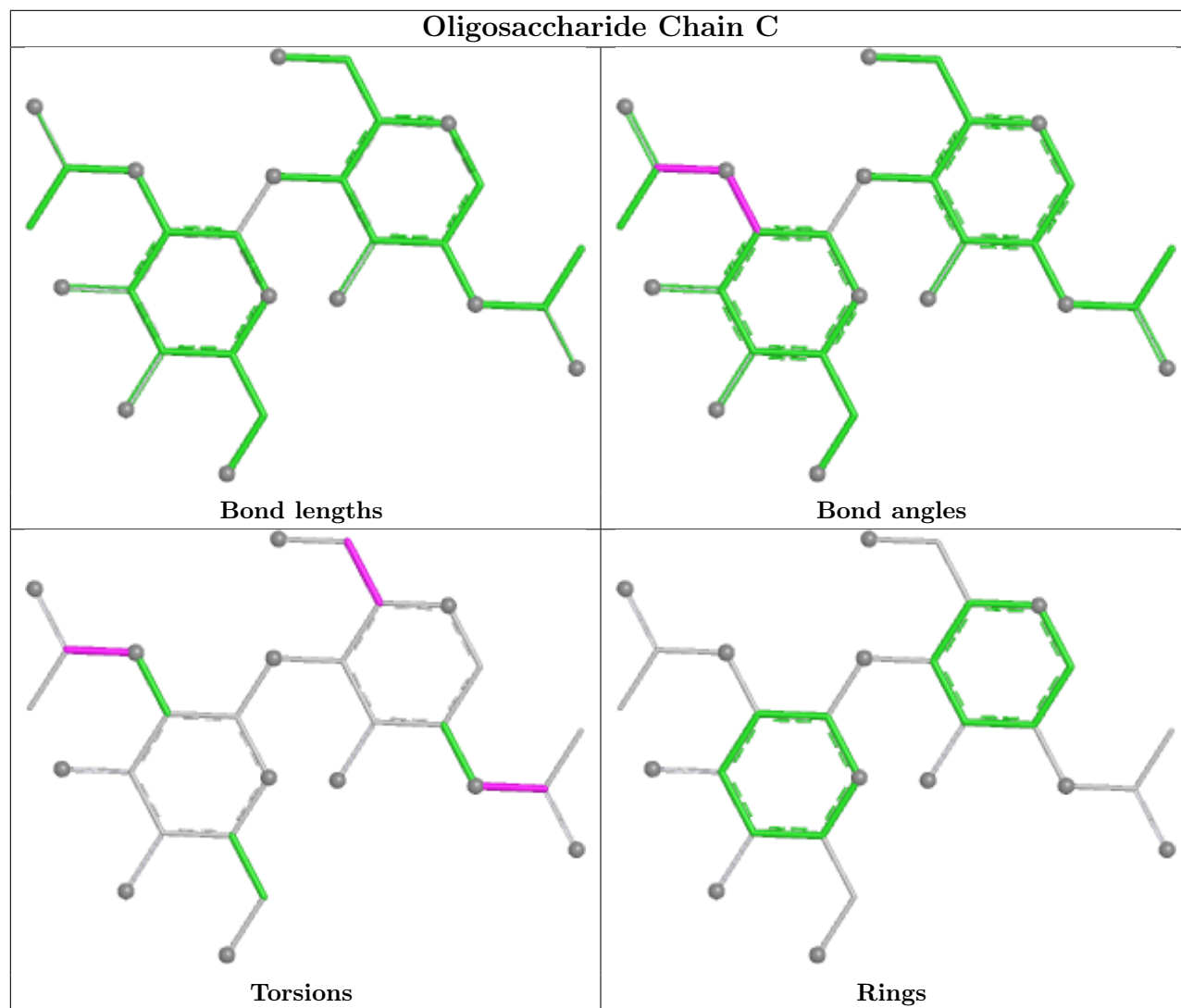
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

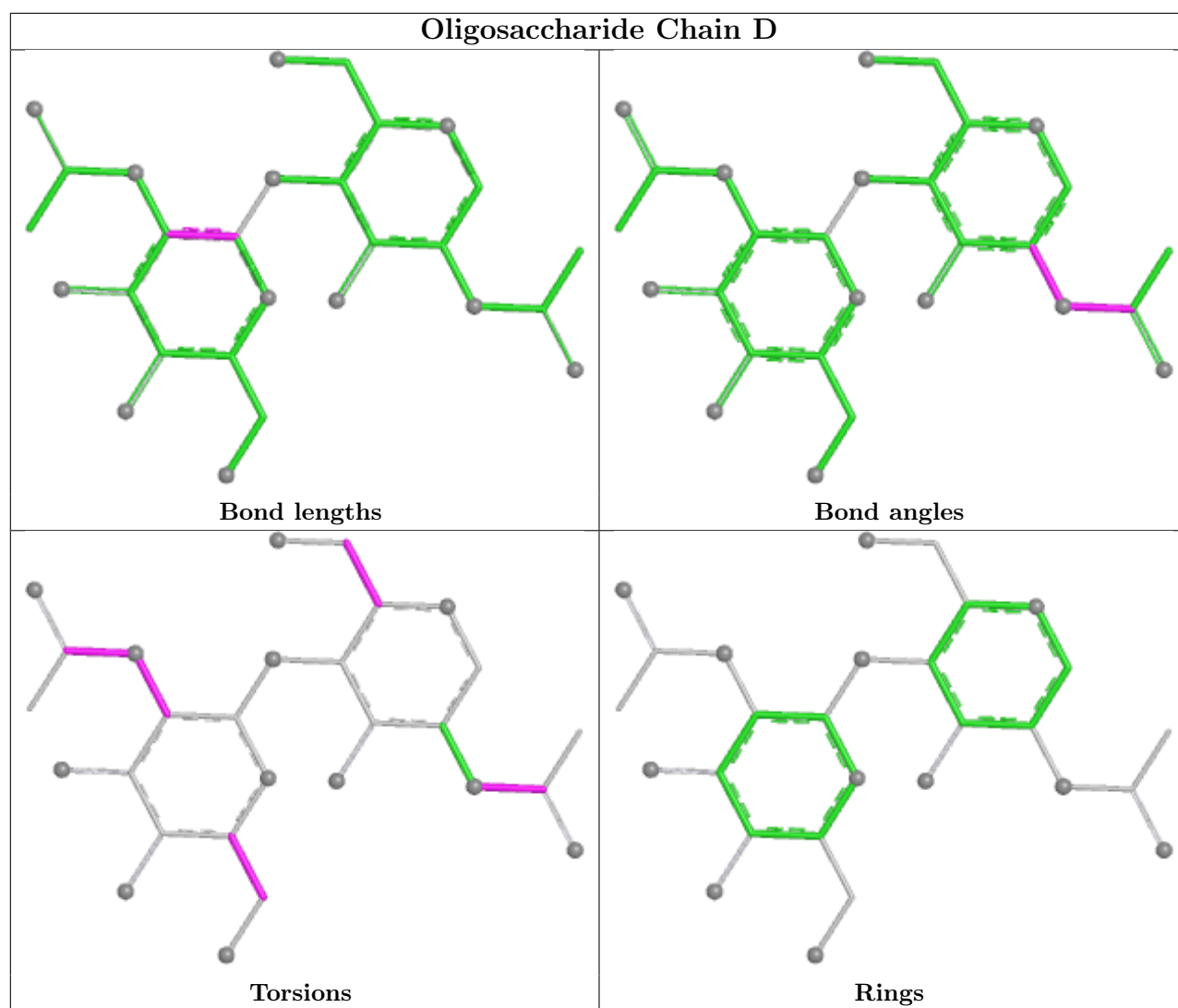
There are no ring outliers.

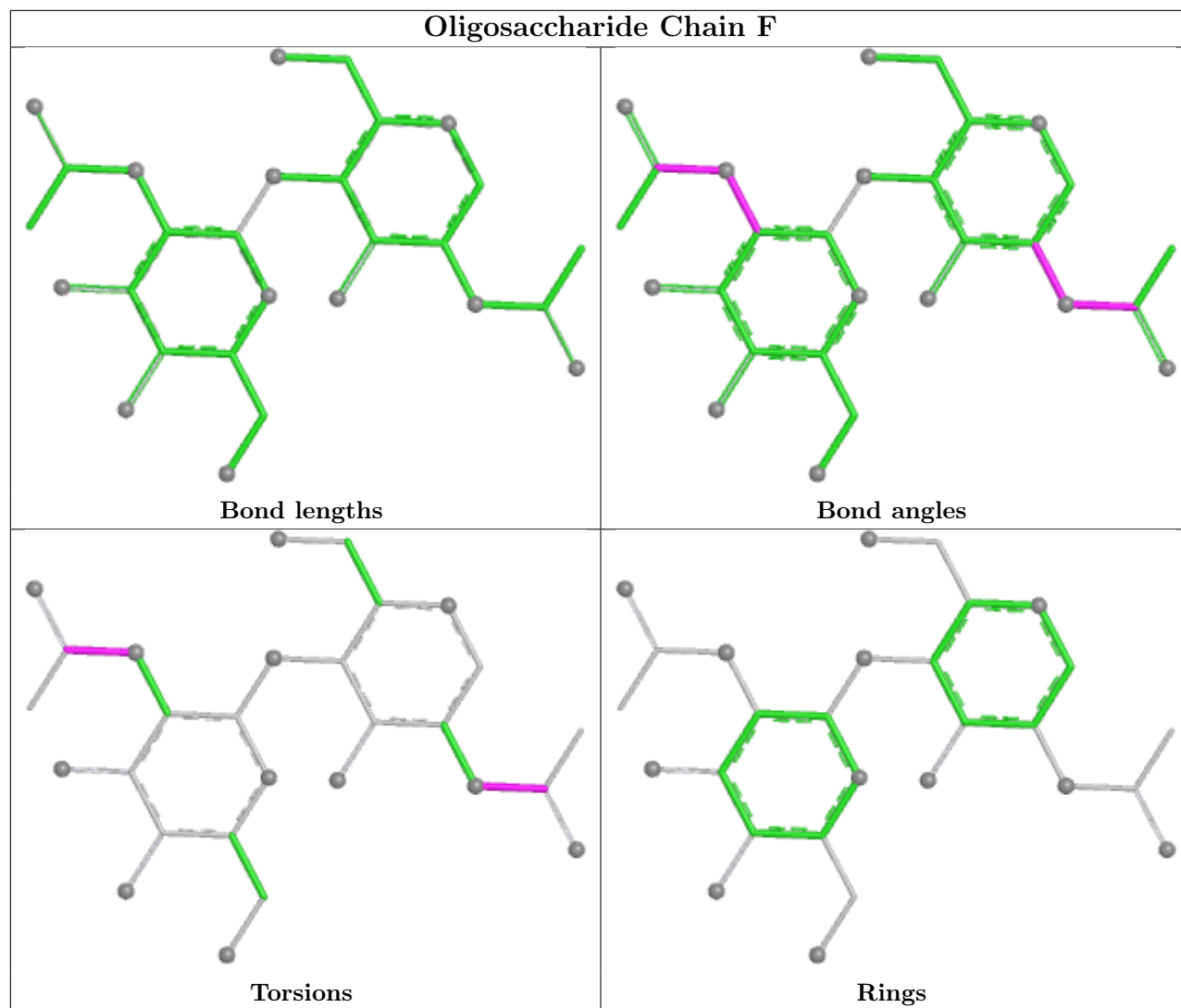
6 monomers are involved in 10 short contacts:

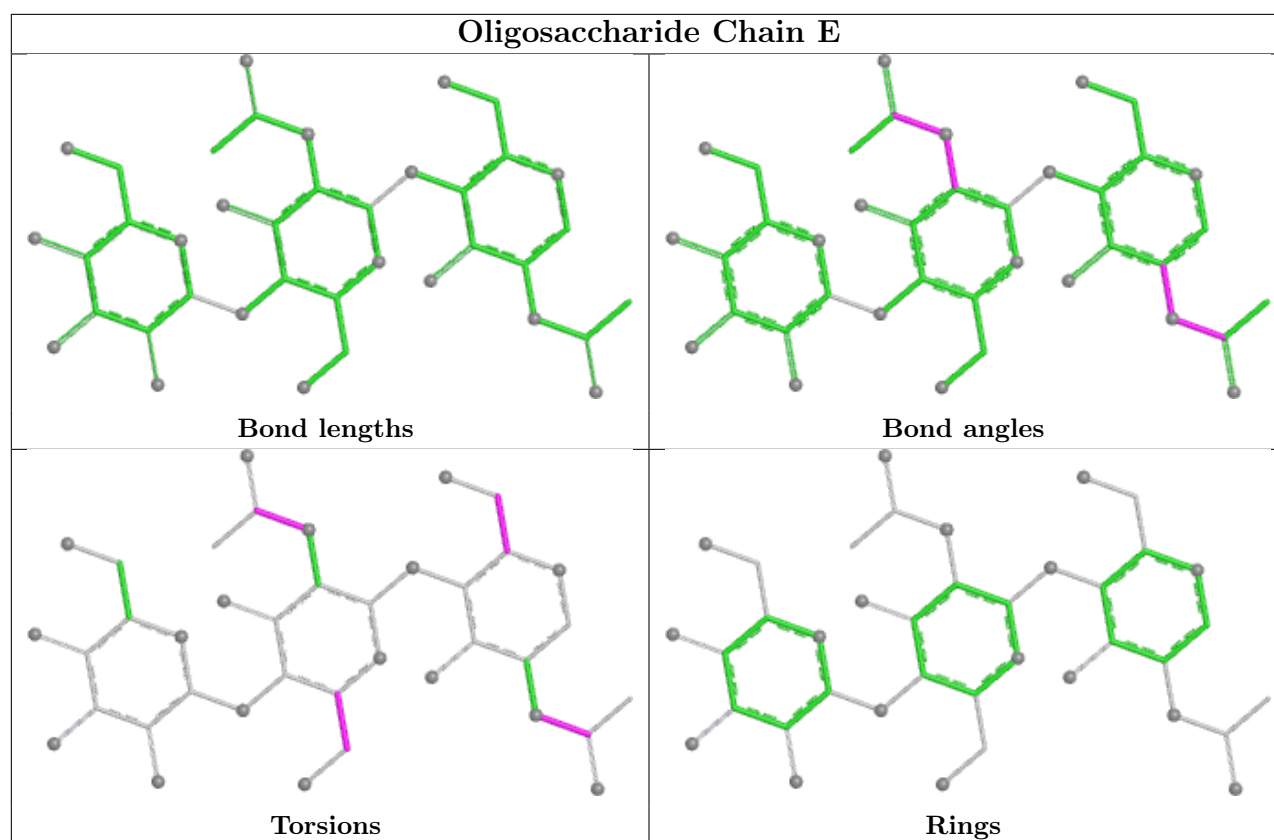
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	4	0
3	E	2	NAG	2	0
3	E	1	NAG	3	0
2	C	2	NAG	1	0
2	D	1	NAG	4	0
2	C	1	NAG	2	0

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	1.05	0	27,27,28	1.66	6 (22%)
6	RET	A	977	1	20,20,21	1.07	0	27,27,28	1.43	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 (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	978	RET	C8-C7-C6	-4.12	115.98	127.00
6	B	978	RET	C19-C9-C8	-3.59	112.60	118.09
6	A	977	RET	C19-C9-C8	-3.57	112.63	118.09
6	A	977	RET	C11-C12-C13	3.34	135.53	126.36
6	B	978	RET	C11-C12-C13	3.33	135.50	126.36
6	B	978	RET	C8-C9-C10	3.11	123.90	119.01
6	A	977	RET	C8-C7-C6	-3.07	118.80	127.00
6	B	978	RET	C7-C8-C9	3.04	130.73	126.23
6	A	977	RET	C8-C9-C10	2.88	123.54	119.01
6	B	978	RET	C10-C11-C12	2.12	129.35	123.20

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

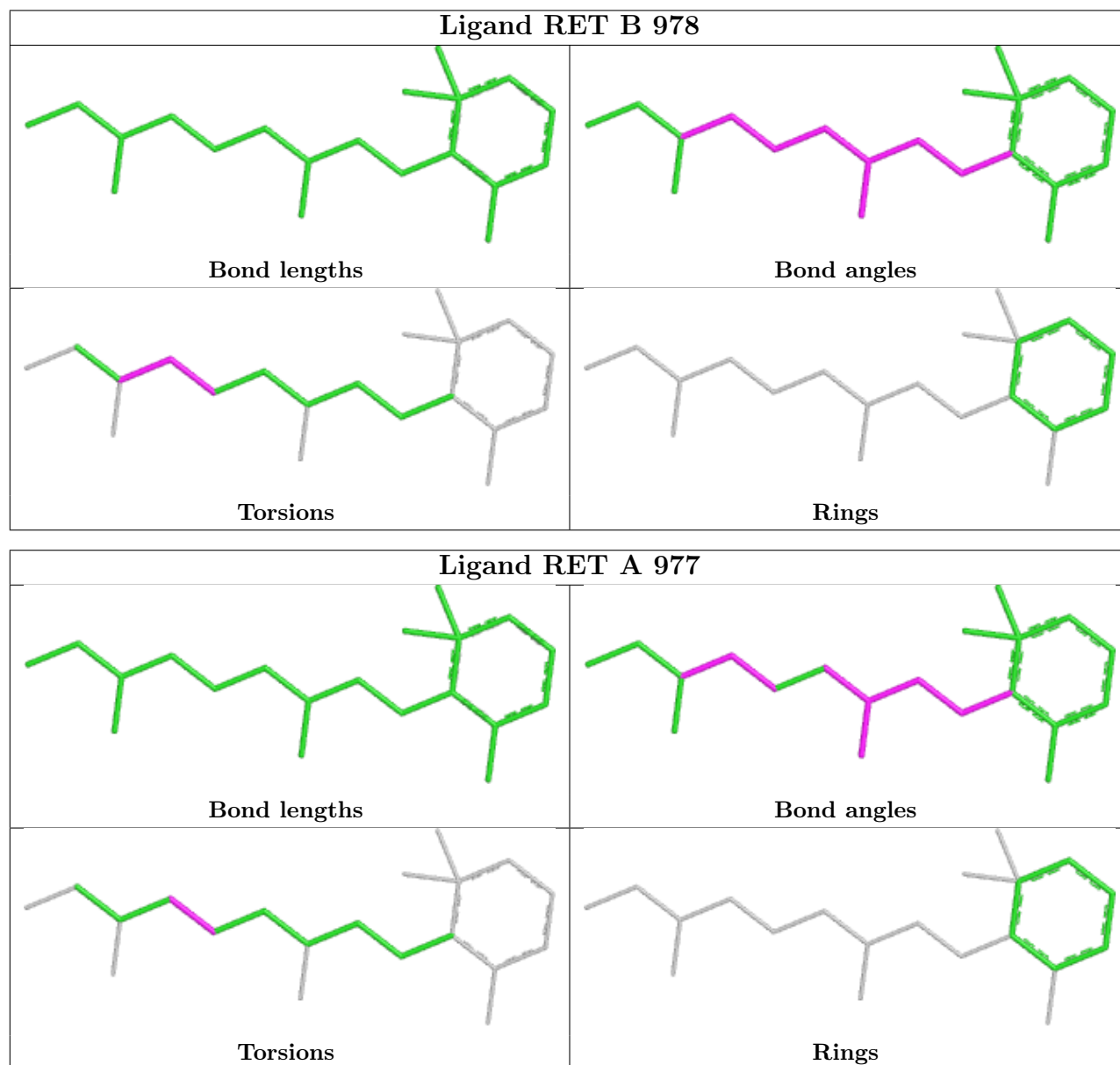
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	978	RET	7	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.