



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 07:34 PM EST

PDB ID : 6SKA
Title : Teneurin 2 in complex with Latrophilin 1 Lec-Olf domains
Authors : Chu, A.; Carrasquero, M.A.; Lowe, E.; Seiradake, E.
Deposited on : 2019-08-15
Resolution : 3.86 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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.21
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

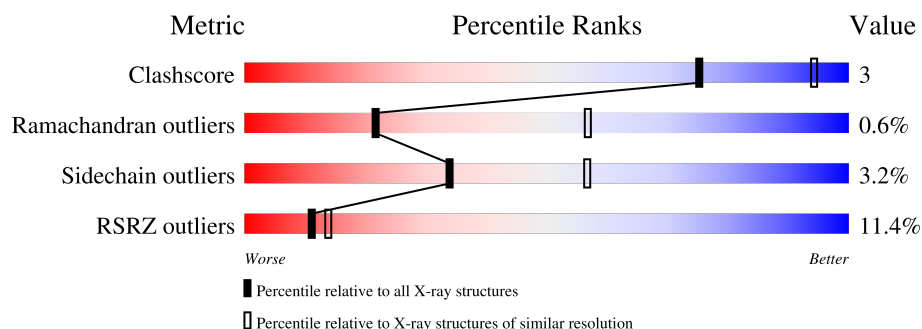
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.86 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	180529	1117 (4.02-3.70)
Ramachandran outliers	177936	1077 (4.02-3.70)
Sidechain outliers	177891	1070 (4.02-3.70)
RSRZ outliers	164620	1056 (4.02-3.70)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1836	<div> <div>10%</div> <div>91%</div> <div>8%</div> </div>
2	D	347	<div> <div>17%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>
3	B	8	<div> <div>25%</div> <div>75%</div> </div>
4	C	2	<div> <div>100%</div> </div>
4	E	2	<div> <div>100%</div> </div>
4	F	2	<div> <div>50%</div> <div>50%</div> </div>
4	G	2	<div> <div>100%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	H	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17628 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 Teneurin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1836	Total	C	N	O	S	0	1	0
			14513	9168	2508	2774	63			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP Q9DER5
A	?	-	THR	deletion	UNP Q9DER5
A	?	-	GLU	deletion	UNP Q9DER5
A	?	-	GLU	deletion	UNP Q9DER5
A	?	-	ASN	deletion	UNP Q9DER5
A	?	-	SER	deletion	UNP Q9DER5
A	?	-	ILE	deletion	UNP Q9DER5

- Molecule 2 is a protein called Adhesion G protein-coupled receptor L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	347	Total	C	N	O	S	0	0	0
			2810	1775	479	539	17			

There are 11 discrepancies between the modelled and reference sequences:

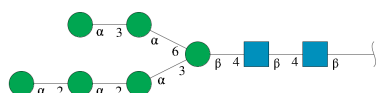
Chain	Residue	Modelled	Actual	Comment	Reference
D	132	VAL	ILE	conflict	UNP Q80TR1
D	?	-	VAL	deletion	UNP Q80TR1
D	?	-	TYR	deletion	UNP Q80TR1
D	?	-	VAL	deletion	UNP Q80TR1
D	?	-	ASP	deletion	UNP Q80TR1
D	?	-	ASP	deletion	UNP Q80TR1
D	?	-	ASP	deletion	UNP Q80TR1
D	?	-	SER	deletion	UNP Q80TR1
D	?	-	GLU	deletion	UNP Q80TR1

Continued on next page...

Continued from previous page...

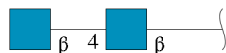
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ALA	deletion	UNP Q80TR1
D	?	-	ALA	deletion	UNP Q80TR1

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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	B	8	Total	C	N	O	0	0	0
			94	52	2	40			

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



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

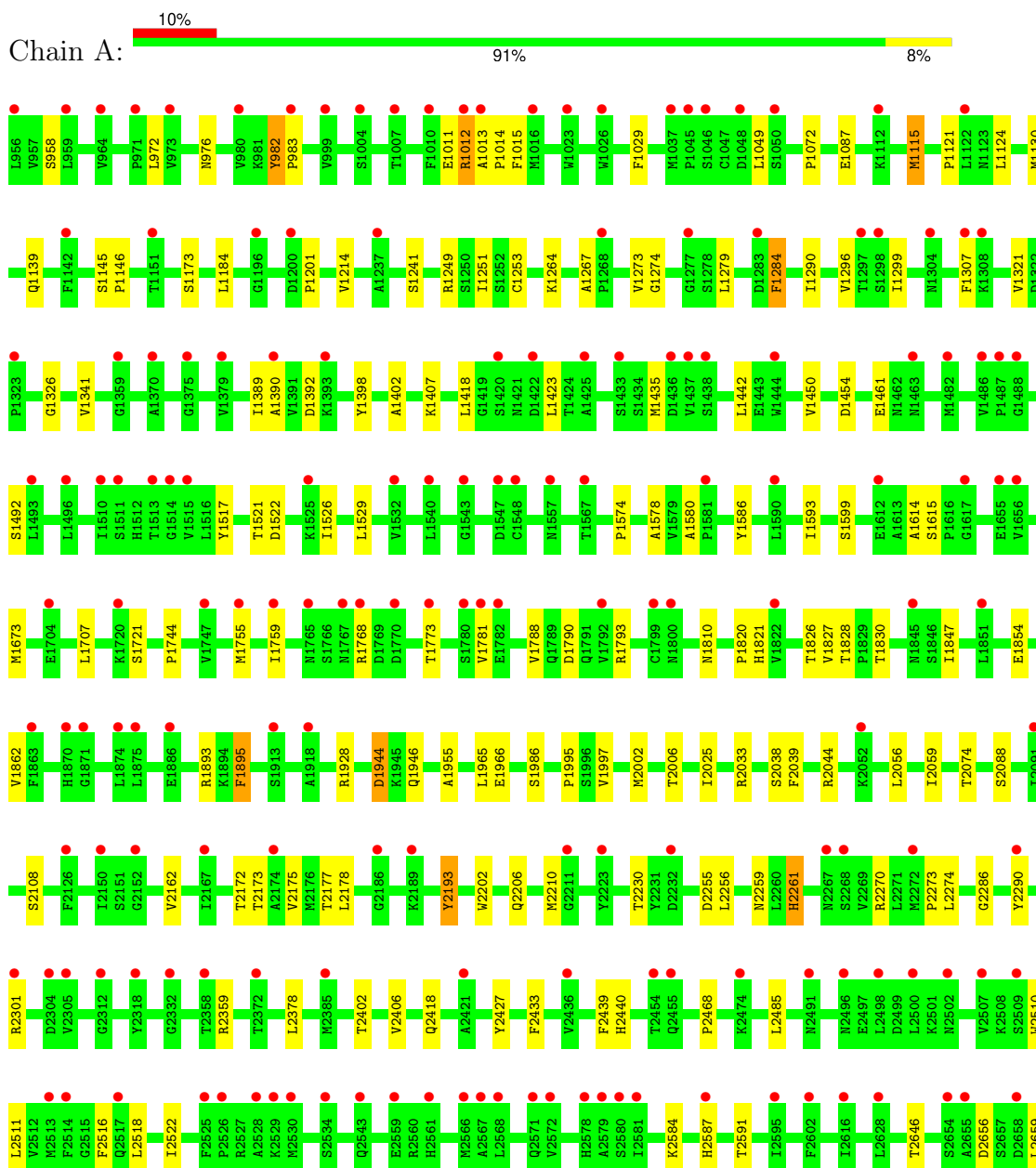
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

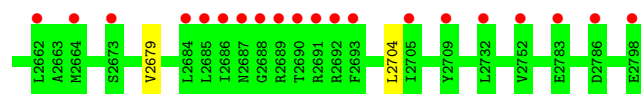
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Ca	0	0
			1	1		

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. 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.

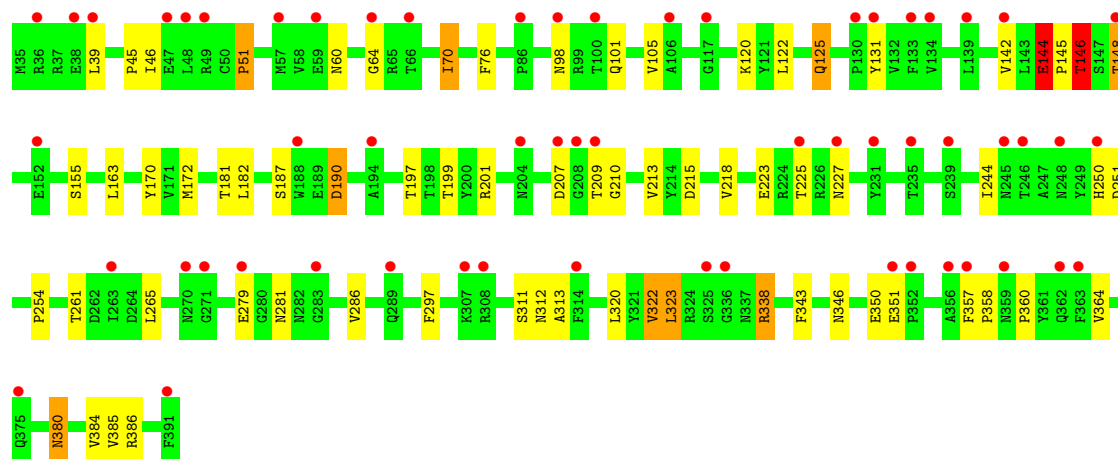
• Molecule 1: Teneurin-2





- Molecule 2: Adhesion G protein-coupled receptor L1

Chain D: 17% 80% 17%



- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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

Chain B: 25% 75%



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

Chain C: 100%



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

Chain E: 100%



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

Chain F:  50% 50%


MAG1
MAG2

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

Chain G:  100%


MAG1
MAG2

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

Chain H:  50% 50%


MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	96.26Å 96.26Å 809.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.09 – 3.86 52.09 – 3.86	Depositor EDS
% Data completeness (in resolution range)	91.0 (52.09-3.86) 91.0 (52.09-3.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.89Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	(Not available) , (Not available) 0.285 , (Not available)	Depositor DCC
R_{free} test set	3362 reflections (0.00%)	wwPDB-VP
Wilson B-factor (Å ²)	104.8	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 112.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	17628	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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, CA

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	0.36	0/14825	0.60	0/20101
2	D	0.37	0/2886	0.57	0/3935
All	All	0.36	0/17711	0.59	0/24036

There are no bond length outliers.

There are no bond angle outliers.

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	14513	0	14252	73	0
2	D	2810	0	2639	28	0
3	B	94	0	79	0	0
4	C	28	0	25	0	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
4	H	28	0	25	0	0
5	A	70	0	65	0	0
6	D	1	0	0	0	0
All	All	17628	0	17160	99	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 3.

All (99) 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:364:VAL:HA	2:D:380:ASN:HB2	1.58	0.85
1:A:1821:HIS:HD2	1:A:1830:THR:HG21	1.44	0.81
1:A:982:TYR:HB3	1:A:983:PRO:HD3	1.63	0.78
1:A:982:TYR:HB3	1:A:983:PRO:CD	2.17	0.74
1:A:2468:PRO:HB3	1:A:2485:LEU:HB3	1.76	0.67
1:A:1821:HIS:CD2	1:A:1830:THR:HG21	2.28	0.66
1:A:2172:THR:HG21	2:D:51:PRO:HA	1.79	0.65
1:A:1201:PRO:HB3	1:A:1214:VAL:HB	1.81	0.63
1:A:1130:MET:HB2	1:A:1173:SER:HB2	1.81	0.62
1:A:1521:THR:HB	1:A:1574:PRO:HD2	1.83	0.59
2:D:148:THR:HB	2:D:384:VAL:HG23	1.84	0.59
2:D:251:ASP:HA	2:D:254:PRO:HG3	1.85	0.58
1:A:972:LEU:HD22	1:A:1012:ARG:HE	1.69	0.57
1:A:1895:PHE:HE1	1:A:2511:LEU:HA	1.68	0.57
1:A:1744:PRO:HB2	1:A:2006:THR:HG21	1.86	0.57
2:D:338:ARG:HA	2:D:357:PHE:HB3	1.86	0.56
1:A:1130:MET:HG2	1:A:1139:GLN:HG2	1.88	0.55
1:A:1773:THR:HG23	1:A:1788:VAL:HB	1.88	0.55
1:A:2406:VAL:HG11	1:A:2433:PHE:HE2	1.71	0.55
1:A:2418:GLN:HB2	1:A:2427:TYR:HB3	1.89	0.55
1:A:2173:THR:HG22	1:A:2175:VAL:H	1.72	0.54
2:D:170:TYR:HB3	2:D:182:LEU:HD11	1.90	0.54
2:D:311:SER:HB2	2:D:323:LEU:HB3	1.89	0.54
2:D:163:LEU:HD13	2:D:215:ASP:H	1.73	0.54
1:A:2511:LEU:HD13	1:A:2518:LEU:HD11	1.91	0.53
1:A:1274:GLY:HA2	1:A:1321:VAL:HG11	1.91	0.53
1:A:1390:ALA:HB1	1:A:1450:VAL:HG23	1.89	0.52
1:A:1279:LEU:HD23	1:A:1290:ILE:HD12	1.92	0.52
1:A:1995:PRO:HB2	1:A:2256:LEU:HB3	1.92	0.52
2:D:144:GLU:H	2:D:145:PRO:HD3	1.75	0.51
2:D:187:SER:H	2:D:190:ASP:HB2	1.76	0.51
1:A:2056:LEU:HD21	1:A:2059:ILE:HD11	1.93	0.51
1:A:1955:ALA:HB3	1:A:2210:MET:HE3	1.94	0.50
1:A:1273:VAL:HG23	1:A:1578:ALA:HB1	1.92	0.50
1:A:2290:TYR:CZ	1:A:2301:ARG:HG3	2.47	0.50
1:A:1290:ILE:HG12	1:A:1296:VAL:HG22	1.94	0.50
2:D:45:PRO:HB3	2:D:105:VAL:HG22	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1827:VAL:HG13	1:A:1828:THR:HG23	1.93	0.49
1:A:1013:ALA:HB3	1:A:1014:PRO:HD3	1.95	0.49
1:A:1299:ILE:HD12	1:A:1341:VAL:HG11	1.94	0.49
2:D:60:ASN:HB3	2:D:125:GLN:HB2	1.95	0.49
2:D:207:ASP:HB2	2:D:223:GLU:HA	1.95	0.49
2:D:343:PHE:HD1	2:D:350:GLU:HB3	1.76	0.49
1:A:1820:PRO:HB3	1:A:1826:THR:HA	1.95	0.48
1:A:2261:HIS:HA	1:A:2274:LEU:HB2	1.95	0.48
2:D:142:VAL:HB	2:D:358:PRO:HD3	1.95	0.48
1:A:2039:PHE:HB2	1:A:2044:ARG:HB2	1.93	0.48
1:A:1854:GLU:HB2	1:A:1862:VAL:HB	1.94	0.48
1:A:2584:LYS:HB3	1:A:2587:HIS:HB2	1.95	0.48
1:A:1895:PHE:HZ	1:A:2510:TRP:HB3	1.78	0.47
2:D:313:ALA:HB2	2:D:322:VAL:HG13	1.97	0.47
1:A:2402:THR:HG23	1:A:2439:PHE:HA	1.96	0.47
2:D:244:ILE:HD12	2:D:297:PHE:HZ	1.80	0.47
1:A:1522:ASP:HB2	1:A:1526:ILE:HB	1.96	0.46
1:A:1755:MET:HG3	1:A:1759:ILE:HG12	1.97	0.46
1:A:1580:ALA:HB2	1:A:1586:TYR:CE2	2.51	0.46
1:A:1517:TYR:HB3	1:A:1529:LEU:HD11	1.98	0.46
2:D:213:VAL:HG22	2:D:218:VAL:HG22	1.97	0.46
1:A:982:TYR:CB	1:A:983:PRO:CD	2.91	0.46
1:A:1893:ARG:HB2	2:D:70:ILE:HD12	1.97	0.46
1:A:2178:LEU:HD13	1:A:2193:TYR:CD2	2.51	0.46
2:D:281:ASN:HD22	2:D:286:VAL:HG22	1.81	0.46
2:D:181:THR:HG22	2:D:201:ARG:HA	1.99	0.45
1:A:1788:VAL:HG22	1:A:1793:ARG:HG2	1.97	0.45
1:A:1121:PRO:HG2	1:A:1124:LEU:HB2	1.98	0.45
2:D:146:THR:HB	2:D:386:ARG:HB2	1.98	0.45
1:A:1249:ARG:HB3	1:A:1264:LYS:HB3	2.00	0.44
1:A:2646:THR:HG22	1:A:2704:LEU:HD22	1.98	0.44
1:A:1012:ARG:HD2	1:A:1015:PHE:HD2	1.82	0.44
2:D:209:THR:H	2:D:261:THR:HG22	1.83	0.44
1:A:1267:ALA:HB3	1:A:1284:PHE:HB2	2.00	0.44
1:A:1442:LEU:HG	1:A:1461:GLU:HG3	2.00	0.43
1:A:2659:LEU:HD21	1:A:2679:VAL:HG11	1.99	0.43
1:A:1072:PRO:HB2	1:A:1087:GLU:HG2	2.00	0.43
1:A:1251:ILE:HB	1:A:1307:PHE:HD2	1.83	0.43
1:A:2088:SER:HB3	1:A:2108:SER:HB3	2.00	0.42
2:D:244:ILE:HD12	2:D:297:PHE:CZ	2.54	0.42
1:A:1115:MET:H	1:A:1115:MET:HG2	1.73	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1707:LEU:HB3	1:A:1721:SER:HB2	2.00	0.42
1:A:2025:ILE:HB	1:A:2038:SER:HB2	2.01	0.42
1:A:976:ASN:HB3	1:A:1011:GLU:HB2	2.01	0.42
1:A:2518:LEU:HB3	1:A:2522:ILE:HD12	2.01	0.42
1:A:2406:VAL:HG11	1:A:2433:PHE:CE2	2.54	0.42
2:D:46:ILE:HG21	2:D:122:LEU:HD23	2.02	0.42
2:D:64:GLY:HA2	2:D:120:LYS:HG2	2.01	0.42
1:A:1614:ALA:HB3	1:A:1828:THR:HG21	2.02	0.42
1:A:2511:LEU:O	1:A:2516:PHE:HB2	2.20	0.42
1:A:1145:SER:C	1:A:1146:PRO:N	2.74	0.41
1:A:1944:ASP:HB3	1:A:1946:GLN:H	1.85	0.41
1:A:1398:TYR:CE1	1:A:1407:LYS:HG2	2.56	0.41
1:A:1049:LEU:HD12	1:A:1184:LEU:HD23	2.03	0.41
2:D:313:ALA:HB1	2:D:320:LEU:HD11	2.03	0.41
1:A:2255:ASP:HB3	1:A:2259:ASN:H	1.86	0.41
2:D:144:GLU:N	2:D:145:PRO:CD	2.84	0.41
1:A:2162:VAL:HG11	1:A:2378:LEU:HD11	2.03	0.40
1:A:1768:ARG:HH22	1:A:2033:ARG:HD2	1.85	0.40
1:A:1810:ASN:HA	1:A:2074:THR:HB	2.03	0.40
1:A:2172:THR:HG22	1:A:2177:THR:HG22	2.02	0.40
1:A:2273:PRO:HD2	1:A:2286:GLY:HA2	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	1829/1836 (100%)	1758 (96%)	63 (3%)	8 (0%)	30	65
2	D	343/347 (99%)	310 (90%)	27 (8%)	6 (2%)	7	36
All	All	2172/2183 (100%)	2068 (95%)	90 (4%)	14 (1%)	22	57

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	982	TYR
2	D	360	PRO
1	A	1284	PHE
2	D	210	GLY
1	A	1966	GLU
1	A	1402	ALA
2	D	250	HIS
1	A	1492	SER
1	A	1790	ASP
1	A	1997	VAL
2	D	146	THR
2	D	144	GLU
1	A	1326	GLY
2	D	51	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1601/1600 (100%)	1567 (98%)	34 (2%)	48 67
2	D	306/306 (100%)	279 (91%)	27 (9%)	8 30
All	All	1907/1906 (100%)	1846 (97%)	61 (3%)	34 57

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	958	SER
1	A	1012	ARG
1	A	1029	PHE
1	A	1115	MET
1	A	1241	SER
1	A	1253	CYS
1	A	1389	ILE
1	A	1392	ASP
1	A	1418	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1423	LEU
1	A	1435	MET
1	A	1454	ASP
1	A	1593	ILE
1	A	1599	SER
1	A	1615	SER
1	A	1673	MET
1	A	1781	VAL
1	A	1847	ILE
1	A	1895	PHE
1	A	1928	ARG
1	A	1944	ASP
1	A	1965	LEU
1	A	1986	SER
1	A	2002	MET
1	A	2193	TYR
1	A	2202	TRP
1	A	2206	GLN
1	A	2230	THR
1	A	2261	HIS
1	A	2270	ARG
1	A	2359	ARG
1	A	2440	HIS
1	A	2591	THR
1	A	2656	ASP
2	D	39	LEU
2	D	70	ILE
2	D	76	PHE
2	D	98	ASN
2	D	101	GLN
2	D	125	GLN
2	D	131	TYR
2	D	144	GLU
2	D	146	THR
2	D	148	THR
2	D	155	SER
2	D	172	MET
2	D	190	ASP
2	D	197	THR
2	D	199	THR
2	D	225	THR
2	D	227	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	265	LEU
2	D	279	GLU
2	D	312	ASN
2	D	322	VAL
2	D	323	LEU
2	D	338	ARG
2	D	346	ASN
2	D	351	GLU
2	D	380	ASN
2	D	385	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1285	ASN
2	D	281	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 ⓘ

18 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	B	1	3,1	14,14,15	0.43	0	17,19,21	0.69	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	2	3	14,14,15	0.42	0	17,19,21	0.54	0
3	BMA	B	3	3	11,11,12	0.50	0	15,15,17	0.51	0
3	MAN	B	4	3	11,11,12	0.52	0	15,15,17	0.95	2 (13%)
3	MAN	B	5	3	11,11,12	0.58	0	15,15,17	0.87	1 (6%)
3	MAN	B	6	3	11,11,12	0.56	0	15,15,17	0.87	1 (6%)
3	MAN	B	7	3	11,11,12	0.56	0	15,15,17	0.88	1 (6%)
3	MAN	B	8	3	11,11,12	0.56	0	15,15,17	0.94	1 (6%)
4	NAG	C	1	4,1	14,14,15	0.44	0	17,19,21	0.70	0
4	NAG	C	2	4	14,14,15	0.45	0	17,19,21	0.60	0
4	NAG	E	1	4,1	14,14,15	0.43	0	17,19,21	0.66	0
4	NAG	E	2	4	14,14,15	0.44	0	17,19,21	0.59	0
4	NAG	F	1	4,1	14,14,15	0.43	0	17,19,21	0.68	1 (5%)
4	NAG	F	2	4	14,14,15	0.45	0	17,19,21	0.60	0
4	NAG	G	1	4,1	14,14,15	0.44	0	17,19,21	0.62	0
4	NAG	G	2	4	14,14,15	0.44	0	17,19,21	0.55	0
4	NAG	H	1	4,1	14,14,15	0.44	0	17,19,21	0.71	1 (5%)
4	NAG	H	2	4	14,14,15	0.43	0	17,19,21	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1
3	BMA	B	3	3	-	0/2/19/22	0/1/1/1
3	MAN	B	4	3	-	2/2/19/22	0/1/1/1
3	MAN	B	5	3	-	1/2/19/22	0/1/1/1
3	MAN	B	6	3	-	0/2/19/22	0/1/1/1
3	MAN	B	7	3	-	0/2/19/22	0/1/1/1
3	MAN	B	8	3	-	0/2/19/22	0/1/1/1
4	NAG	C	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	C	2	4	-	3/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	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	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	H	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	4/6/23/26	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(°)
3	B	5	MAN	C1-O5-C5	2.73	115.85	112.19
3	B	8	MAN	C1-O5-C5	2.61	115.68	112.19
3	B	7	MAN	C1-O5-C5	2.39	115.39	112.19
3	B	4	MAN	C1-C2-C3	2.28	112.96	109.64
3	B	6	MAN	C1-O5-C5	2.24	115.19	112.19
3	B	4	MAN	C1-O5-C5	2.18	115.11	112.19
3	B	1	NAG	C1-O5-C5	2.13	115.04	112.19
4	F	1	NAG	C1-O5-C5	2.12	115.02	112.19
4	H	1	NAG	C1-O5-C5	2.06	114.95	112.19

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1	NAG	C8-C7-N2-C2
3	B	1	NAG	O7-C7-N2-C2
3	B	2	NAG	C8-C7-N2-C2
3	B	2	NAG	O7-C7-N2-C2
4	C	2	NAG	C8-C7-N2-C2
4	C	2	NAG	O7-C7-N2-C2
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2

Continued on next page...

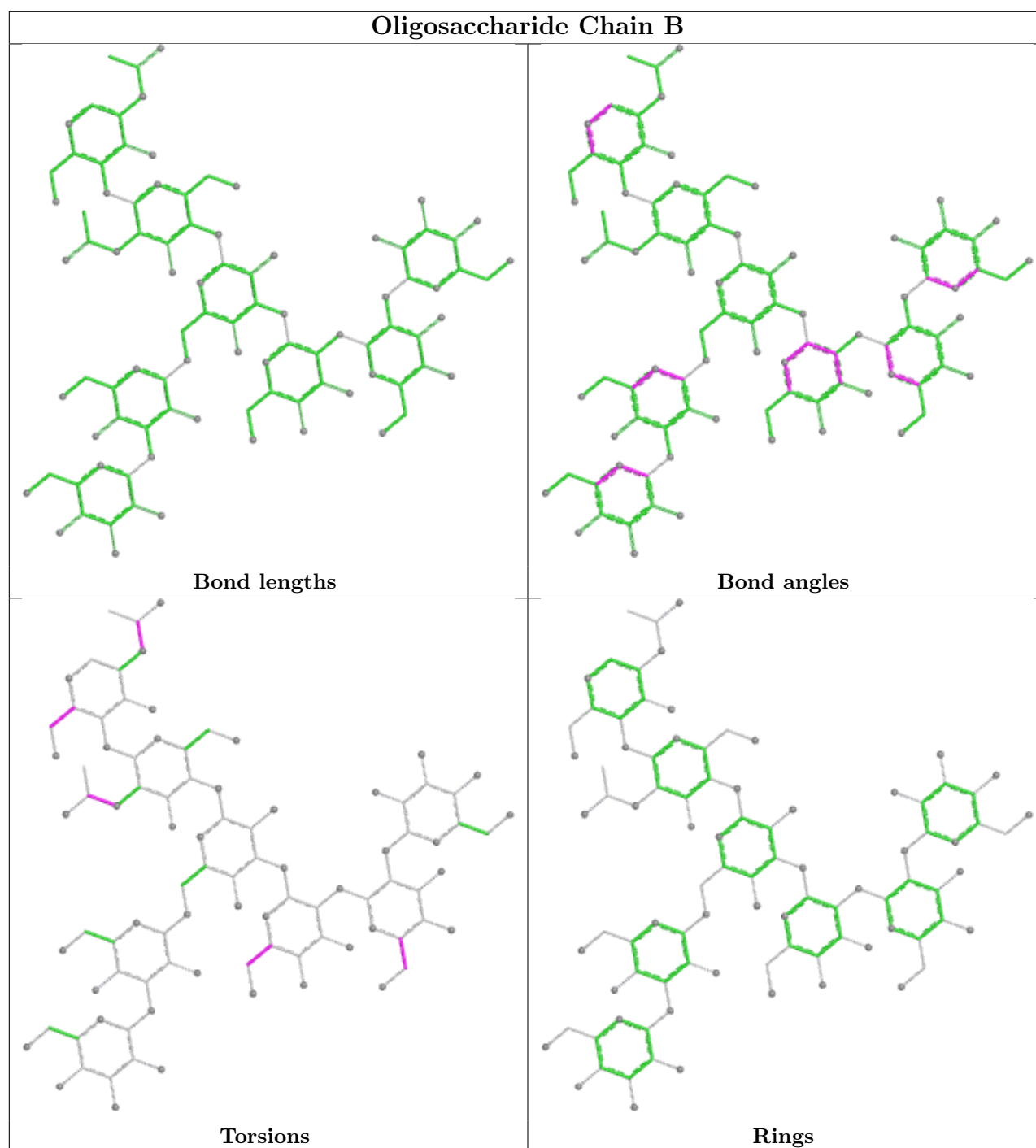
Continued from previous page...

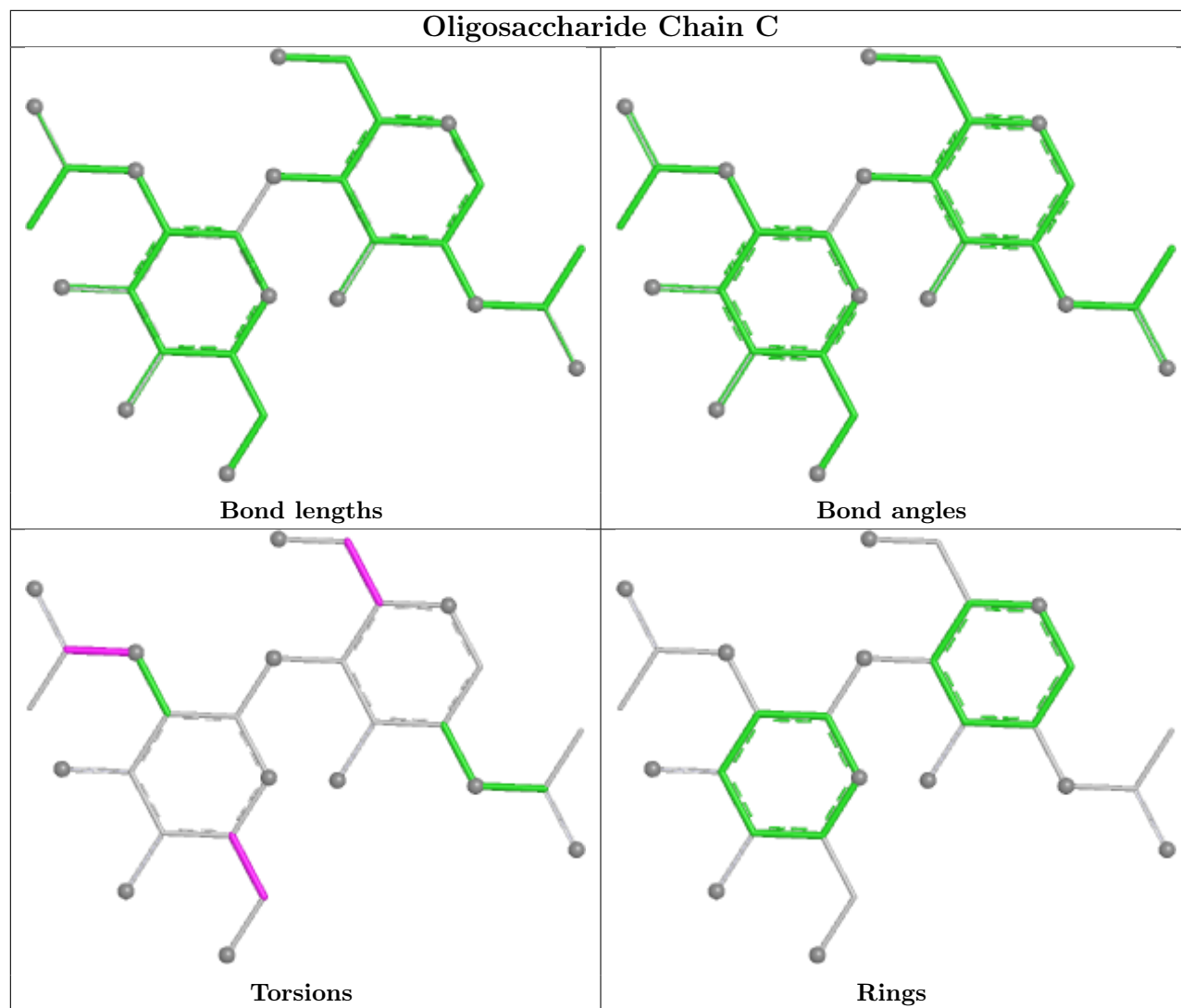
Mol	Chain	Res	Type	Atoms
4	H	1	NAG	O7-C7-N2-C2
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
4	F	1	NAG	C8-C7-N2-C2
3	B	1	NAG	O5-C5-C6-O6
3	B	1	NAG	C4-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6
3	B	4	MAN	C4-C5-C6-O6
4	C	1	NAG	C4-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
3	B	4	MAN	O5-C5-C6-O6
4	E	1	NAG	C1-C2-N2-C7
3	B	5	MAN	C4-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6

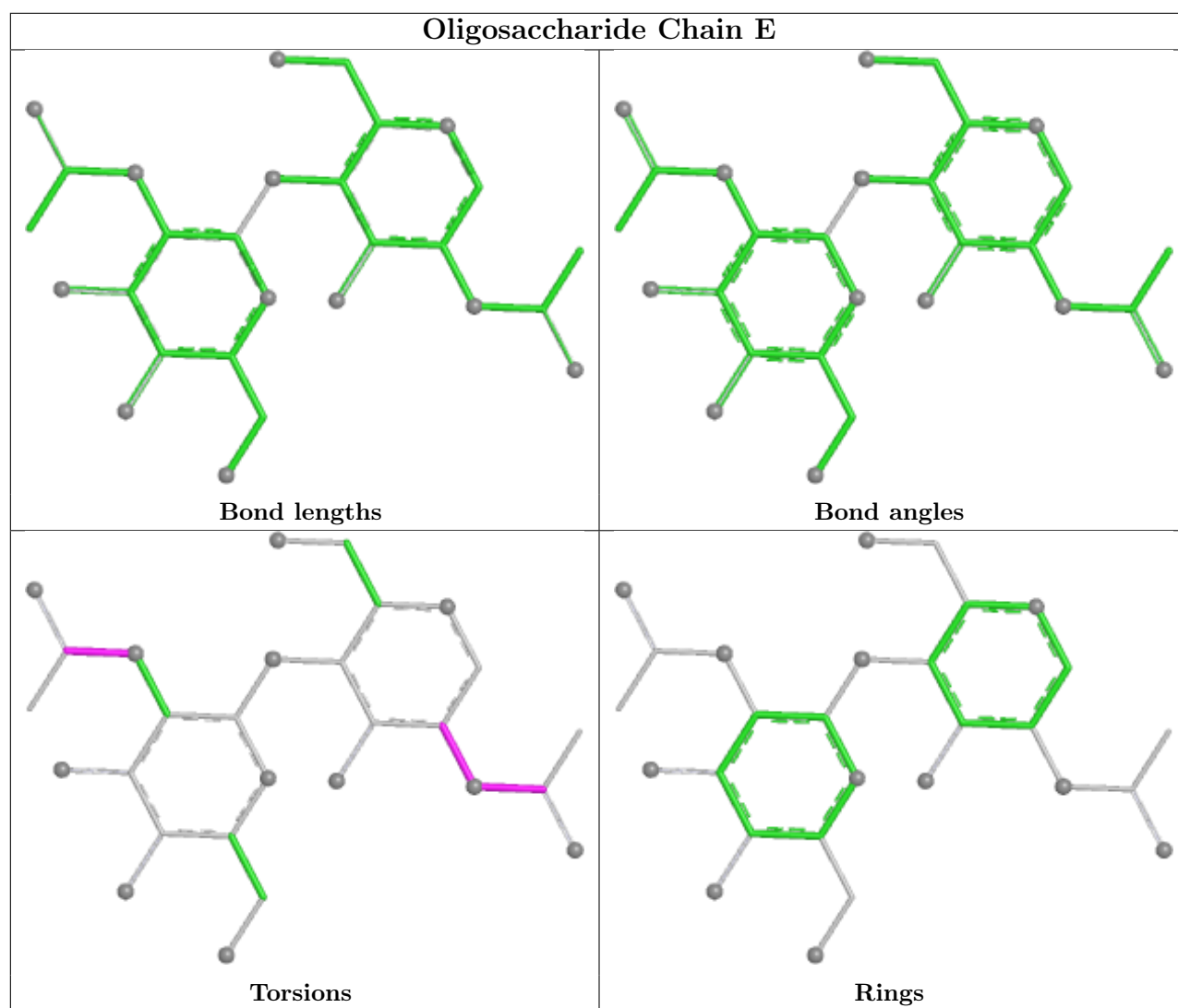
There are no ring outliers.

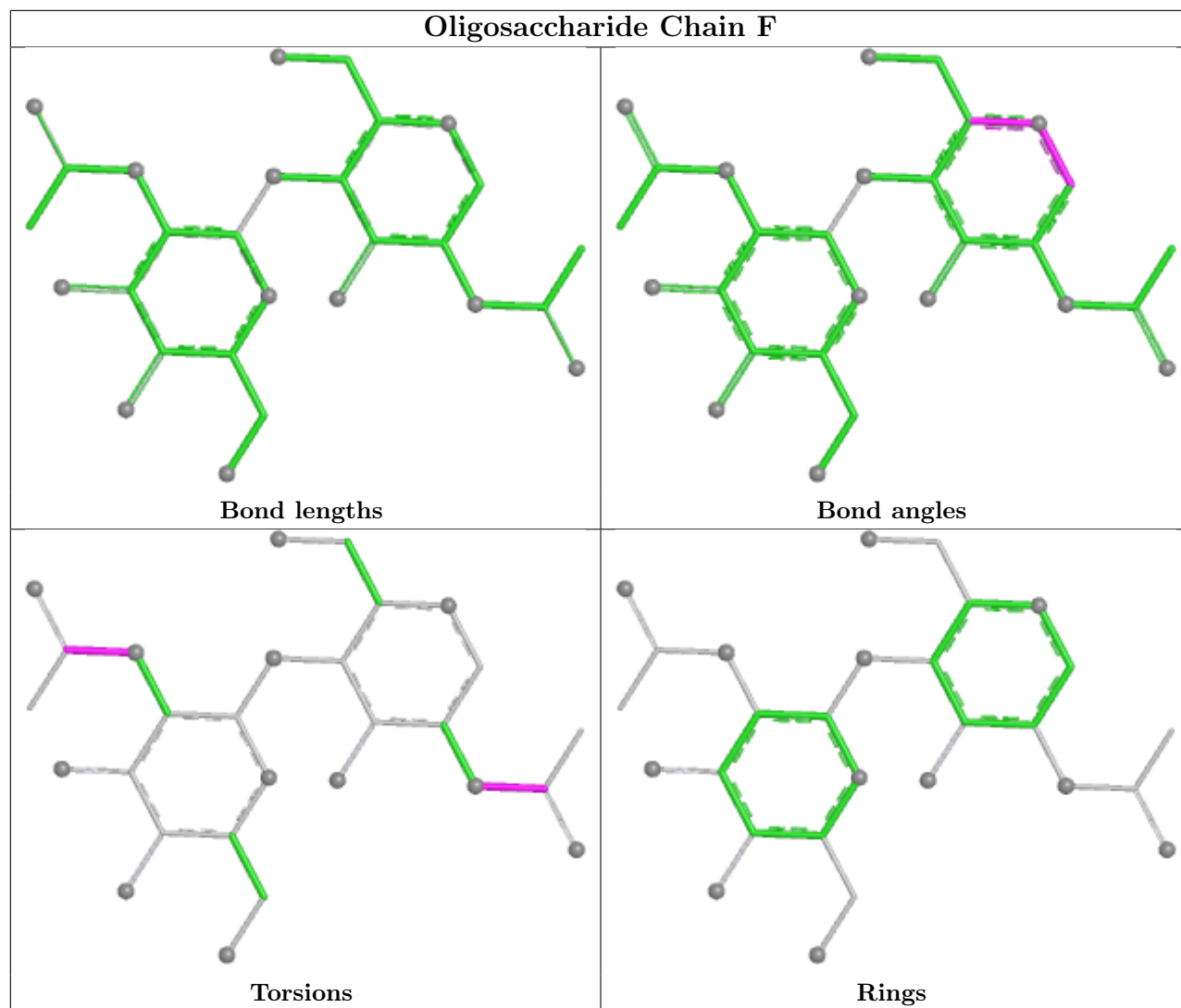
No monomer is involved in short contacts.

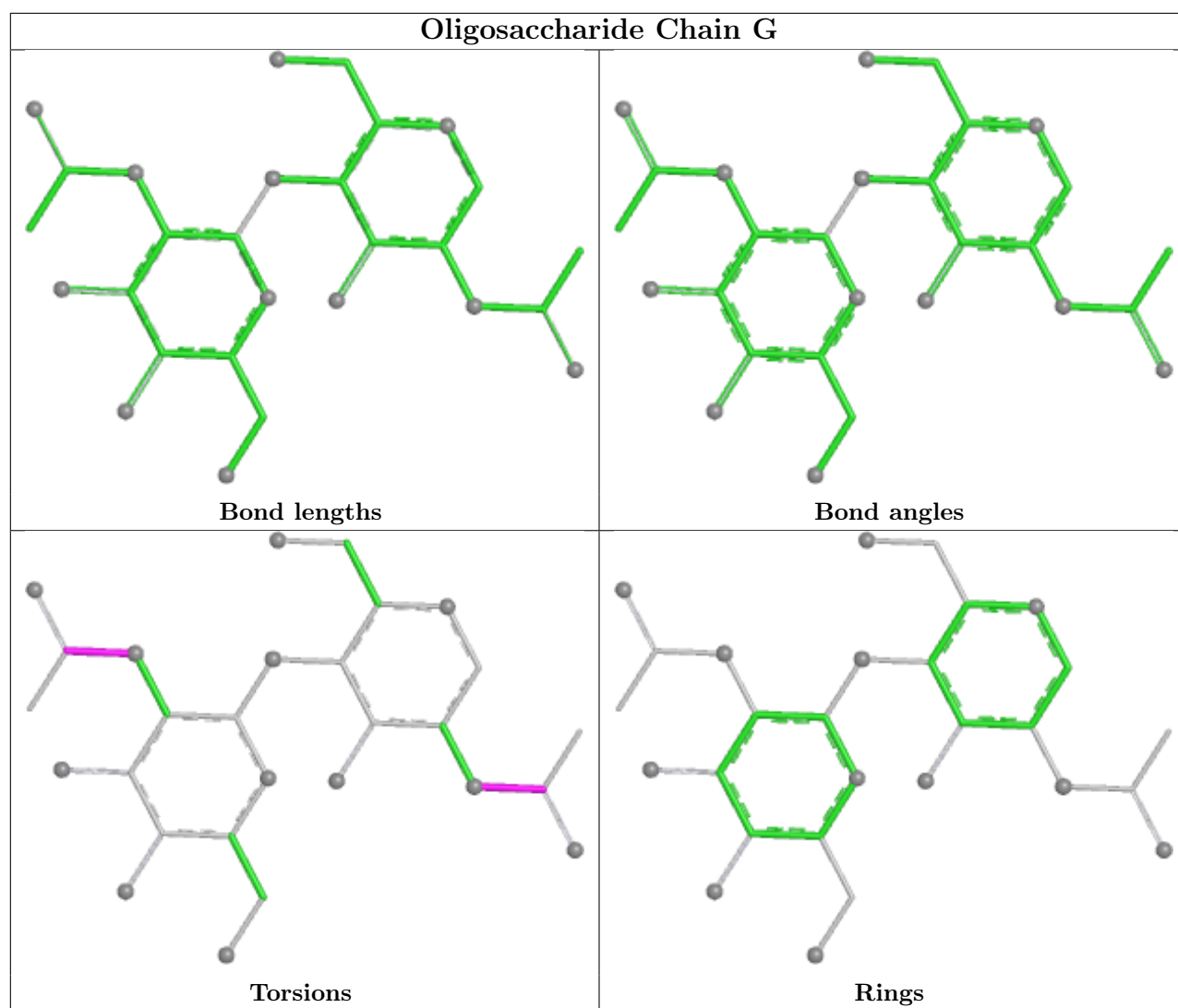
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

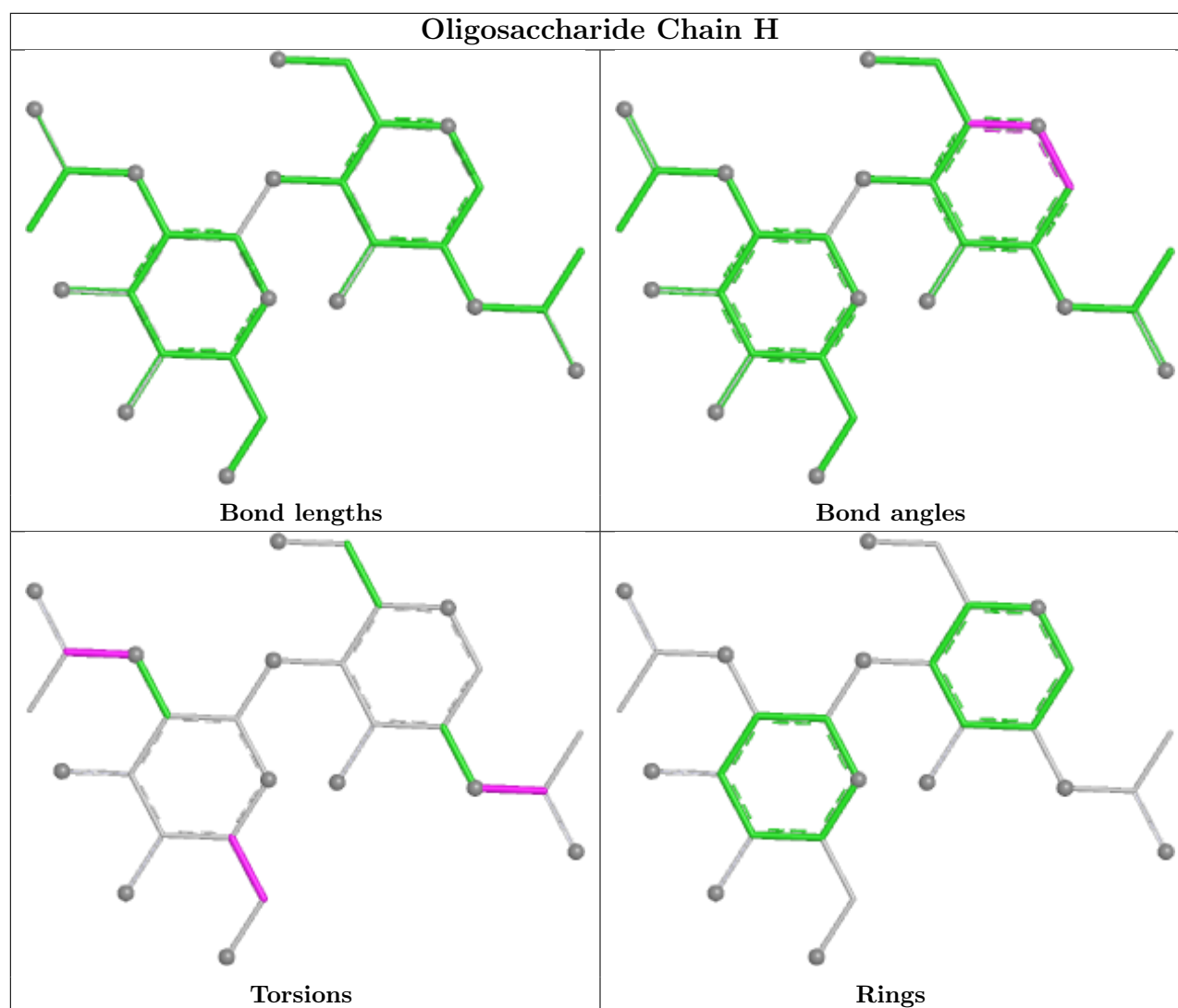












5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z > 2$
5	NAG	A	3011	1	14,14,15	0.44	0	17,19,21	0.65	0
5	NAG	A	3014	1	14,14,15	0.44	0	17,19,21	1.18	2 (11%)
5	NAG	A	3000	1	14,14,15	0.44	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	3022	1	14,14,15	0.44	0	17,19,21	0.69	0
5	NAG	A	3019	1	14,14,15	0.46	0	17,19,21	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	3011	1	-	5/6/23/26	0/1/1/1
5	NAG	A	3014	1	-	4/6/23/26	0/1/1/1
5	NAG	A	3000	1	-	2/6/23/26	0/1/1/1
5	NAG	A	3022	1	-	4/6/23/26	0/1/1/1
5	NAG	A	3019	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3014	NAG	C1-C2-N2	3.27	115.59	110.43
5	A	3014	NAG	C2-N2-C7	3.26	127.27	122.90

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	3000	NAG	C8-C7-N2-C2
5	A	3000	NAG	O7-C7-N2-C2
5	A	3011	NAG	C8-C7-N2-C2
5	A	3011	NAG	O7-C7-N2-C2
5	A	3014	NAG	C1-C2-N2-C7
5	A	3014	NAG	C8-C7-N2-C2
5	A	3014	NAG	O7-C7-N2-C2
5	A	3019	NAG	C8-C7-N2-C2
5	A	3019	NAG	O7-C7-N2-C2
5	A	3011	NAG	O5-C5-C6-O6
5	A	3022	NAG	C8-C7-N2-C2
5	A	3022	NAG	O7-C7-N2-C2
5	A	3022	NAG	O5-C5-C6-O6
5	A	3014	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	3011	NAG	C4-C5-C6-O6
5	A	3022	NAG	C4-C5-C6-O6
5	A	3011	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1037:MET	C	1045:PRO	N	15.82
1	D	325:SER	C	336:GLY	N	7.27
1	A	1891:ASP	C	1892:HIS	N	3.08
1	A	1145:SER	C	1146:PRO	N	2.74

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Warning: The R factor obtained from EDS is 0.318, which does not match the depositor's R factor of 0.0. Please interpret the results in this section carefully.

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	1836/1836 (100%)	0.92	190 (10%)	13 15	45, 123, 188, 241	1 (0%)
2	D	347/347 (100%)	1.06	58 (16%)	5 9	70, 144, 230, 300	0
All	All	2183/2183 (100%)	0.94	248 (11%)	11 14	45, 126, 194, 300	1 (0%)

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2568	LEU	5.8
2	D	263	ILE	5.7
1	A	2684	LEU	5.4
1	A	2571	GLN	5.1
1	A	2530	MET	5.0
1	A	1845	ASN	4.5
1	A	2658	ASP	4.2
1	A	2655	ALA	4.2
2	D	98	ASN	4.1
2	D	130	PRO	4.1
1	A	2616	ILE	4.0
2	D	49	ARG	3.9
2	D	204	ASN	3.9
1	A	2686	ILE	3.9
1	A	2587	HIS	3.9
2	D	325	SER	3.8
2	D	308	ARG	3.8
2	D	362	GLN	3.8
1	A	1425	ALA	3.8
1	A	1045	PRO	3.8
1	A	2690	THR	3.7
1	A	2526	PRO	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	2673	SER	3.7
1	A	2685	LEU	3.7
1	A	2528	ALA	3.7
2	D	194	ALA	3.6
1	A	2305	VAL	3.5
2	D	359	ASN	3.5
1	A	2211	GLY	3.5
1	A	2496	ASN	3.5
2	D	246	THR	3.4
1	A	2052	LYS	3.4
2	D	59	GLU	3.4
1	A	2581	ILE	3.4
1	A	2525	PHE	3.4
1	A	2454	THR	3.4
2	D	271	GLY	3.4
1	A	2688	GLY	3.3
2	D	227	ASN	3.3
1	A	1444	TRP	3.3
1	A	1773	THR	3.3
1	A	956	LEU	3.3
1	A	2567	ALA	3.3
1	A	1196	GLY	3.3
1	A	2513	MET	3.2
1	A	2301	ARG	3.2
2	D	375	GLN	3.2
1	A	973	VAL	3.1
1	A	1486	VAL	3.1
1	A	2752	VAL	3.1
1	A	1016	MET	3.1
2	D	239	SER	3.1
2	D	245	ASN	3.1
1	A	2798	GLU	3.1
1	A	2578	HIS	3.1
1	A	2186	GLY	3.1
1	A	2223	TYR	3.1
1	A	1581	PRO	3.1
1	A	2561	HIS	3.1
1	A	1488	GLY	3.0
1	A	1004	SER	3.0
1	A	2691	ARG	3.0
2	D	208	GLY	3.0
1	A	1782	GLU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	2689	ARG	3.0
1	A	2662	LEU	2.9
2	D	148	THR	2.9
2	D	356	ALA	2.9
1	A	1050	SER	2.9
2	D	352	PRO	2.9
2	D	188	TRP	2.9
1	A	1297	THR	2.9
2	D	131	TYR	2.9
1	A	1759	ILE	2.8
1	A	980	VAL	2.8
1	A	1720	LYS	2.8
1	A	1359	GLY	2.8
1	A	2491	ASN	2.8
1	A	1487	PRO	2.8
2	D	133	PHE	2.8
1	A	1656	VAL	2.8
2	D	235	THR	2.8
1	A	1704	GLU	2.8
2	D	142	VAL	2.8
1	A	2529	LYS	2.8
1	A	2559	GLU	2.8
1	A	1013	ALA	2.8
1	A	2579	ALA	2.8
2	D	36	ARG	2.8
1	A	1875	LEU	2.8
1	A	2566	MET	2.7
2	D	314	PHE	2.7
1	A	1525	LYS	2.7
1	A	1767	ASN	2.7
2	D	134	VAL	2.7
2	D	48	LEU	2.7
1	A	1142	PHE	2.7
1	A	1007	THR	2.7
1	A	1037	MET	2.7
1	A	1755	MET	2.7
2	D	307	LYS	2.7
1	A	1122	LEU	2.7
1	A	1422	ASP	2.7
1	A	1918	ALA	2.6
1	A	1510	ILE	2.6
1	A	2732	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	209	THR	2.6
1	A	1590	LEU	2.6
1	A	1437	VAL	2.6
1	A	1800	ASN	2.6
1	A	2628	LEU	2.6
2	D	47	GLU	2.6
1	A	2436	VAL	2.6
1	A	1557	ASN	2.6
1	A	2705	ILE	2.6
2	D	57	MET	2.6
1	A	1048	ASP	2.6
1	A	2498	LEU	2.6
1	A	2332	GLY	2.6
1	A	2572	VAL	2.5
1	A	1112	LYS	2.5
1	A	1514	GLY	2.5
2	D	250	HIS	2.5
1	A	1655	GLU	2.5
1	A	1747	VAL	2.5
1	A	2150	ILE	2.5
1	A	2152	GLY	2.5
1	A	1781	VAL	2.5
1	A	2474	LYS	2.5
1	A	2507	VAL	2.5
1	A	2372	THR	2.5
1	A	2534	SER	2.5
1	A	2580	SER	2.5
2	D	64	GLY	2.5
1	A	2267	ASN	2.5
1	A	2455	GLN	2.5
2	D	106	ALA	2.5
1	A	1023	TRP	2.5
1	A	1493	LEU	2.5
1	A	2272	MET	2.5
1	A	2174	ALA	2.5
1	A	1874	LEU	2.5
1	A	1792	VAL	2.5
1	A	2358	THR	2.4
1	A	1799	CYS	2.4
1	A	1298	SER	2.4
1	A	1513	THR	2.4
1	A	1436	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1780	SER	2.4
1	A	1308	LYS	2.4
1	A	964	VAL	2.4
1	A	983	PRO	2.4
1	A	1863	PHE	2.4
1	A	2514	PHE	2.4
1	A	1822	VAL	2.4
1	A	1913	SER	2.4
1	A	1770	ASP	2.4
1	A	1617	GLY	2.3
2	D	100	THR	2.3
1	A	1433	SER	2.3
1	A	1438	SER	2.3
1	A	2509	SER	2.3
1	A	2312	GLY	2.3
1	A	2693	PHE	2.3
1	A	999	VAL	2.3
1	A	1420	SER	2.3
1	A	2602	PHE	2.3
2	D	248	ASN	2.3
1	A	1567	THR	2.3
1	A	2290	TYR	2.3
1	A	2500	LEU	2.3
2	D	152	GLU	2.3
1	A	1532	VAL	2.3
1	A	1046	SER	2.3
1	A	1026	TRP	2.3
1	A	1886	GLU	2.3
1	A	2091	ILE	2.3
2	D	279	GLU	2.3
2	D	207	ASP	2.3
1	A	2421	ALA	2.3
1	A	1482	MET	2.2
1	A	1768	ARG	2.2
2	D	39	LEU	2.2
1	A	1370	ALA	2.2
1	A	1283	ASP	2.2
2	D	391	PHE	2.2
1	A	1870	HIS	2.2
1	A	2664	MET	2.2
1	A	2595	ILE	2.2
2	D	66	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	139	LEU	2.2
2	D	283	GLY	2.2
1	A	2126	PHE	2.2
1	A	2502	ASN	2.2
1	A	1375	GLY	2.2
1	A	1871	GLY	2.2
1	A	1307	PHE	2.2
2	D	357	PHE	2.2
1	A	971	PRO	2.2
2	D	225	THR	2.2
1	A	1463	ASN	2.2
1	A	2786	ASP	2.2
1	A	2189	LYS	2.1
1	A	2304	ASP	2.1
2	D	38	GLU	2.1
1	A	1277	GLY	2.1
1	A	2543	GLN	2.1
1	A	1511	SER	2.1
1	A	1547	ASP	2.1
1	A	1765	ASN	2.1
2	D	231	TYR	2.1
1	A	1237	ALA	2.1
1	A	1323	PRO	2.1
1	A	2385	MET	2.1
2	D	336	GLY	2.1
1	A	1010	PHE	2.1
1	A	1390	ALA	2.1
1	A	1151	THR	2.1
1	A	1012	ARG	2.1
1	A	1543	GLY	2.1
1	A	2687	ASN	2.1
1	A	1851	LEU	2.1
1	A	2517	GLN	2.1
1	A	2692	ARG	2.1
1	A	2318	TYR	2.1
2	D	117	GLY	2.1
1	A	1379	VAL	2.1
1	A	1548	CYS	2.1
1	A	1200	ASP	2.0
2	D	86	PRO	2.0
1	A	959	LEU	2.0
1	A	1393	LYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	2709	TYR	2.0
1	A	1515	VAL	2.0
1	A	2783	GLU	2.0
2	D	351	GLU	2.0
1	A	1304	ASN	2.0
1	A	2232	ASP	2.0
1	A	1268	PRO	2.0
1	A	2167	ILE	2.0
1	A	1540	LEU	2.0
2	D	363	PHE	2.0
1	A	1612	GLU	2.0
1	A	2268	SER	2.0
1	A	2654	SER	2.0
2	D	270	ASN	2.0
2	D	289	GLN	2.0
1	A	1496	LEU	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](#)

SUGAR-RSR INFOmissingINFO

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	A	3014	14/15	0.42	0.21	152,156,159,159	0
5	NAG	A	3019	14/15	0.44	0.18	215,217,218,219	0
5	NAG	A	3000	14/15	0.62	0.18	224,225,228,228	0
5	NAG	A	3022	14/15	0.63	0.14	187,190,194,194	0
5	NAG	A	3011	14/15	0.75	0.18	139,144,149,149	0
6	CA	D	1100	1/1	0.99	0.14	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.