



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:43 AM UTC

PDB ID : 4P8Q / pdb_00004p8q
Title : Crystal Structure of Human Insulin Regulated Aminopeptidase with Alanine
in Active Site
Authors : Hermans, S.J.; Ascher, D.B.; Hancock, N.C.; Holien, J.K.; Michell, B.; Morton,
C.J.; Parker, M.W.
Deposited on : 2014-03-31
Resolution : 3.02 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

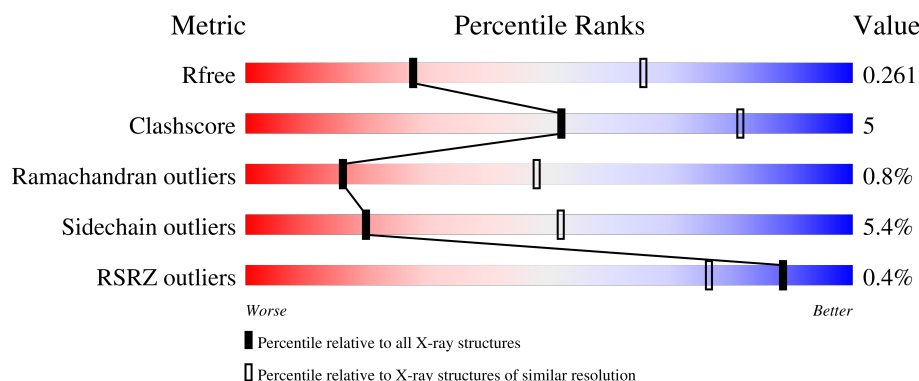
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	872	75% 22% ..
1	B	872	77% 18% ..
2	C	2	100%
2	D	2	100%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	F	2	 100%
2	G	2	 50%50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14164 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 Leucyl-cystinyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	860	Total	C	N	O	S	0	3	0
			6965	4505	1127	1304	29			
1	B	848	Total	C	N	O	S	0	1	0
			6838	4432	1099	1282	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	154	SER	-	expression tag	UNP Q9UIQ6
B	154	SER	-	expression tag	UNP Q9UIQ6

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

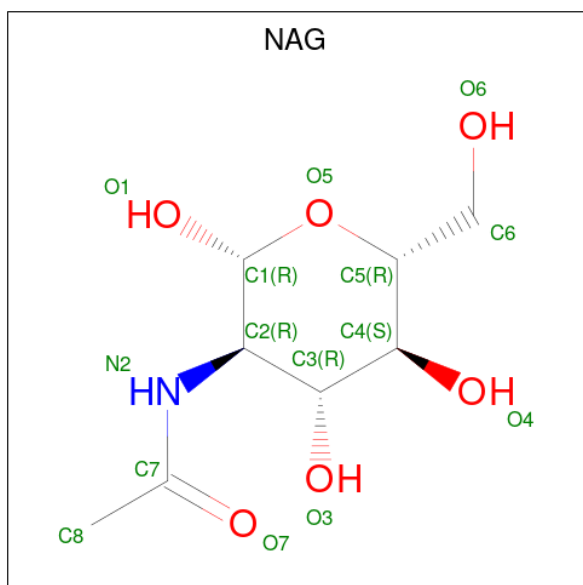


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 5 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			5	3	1	1		
5	B	1	Total	C	N	O	0	0
			5	3	1	1		

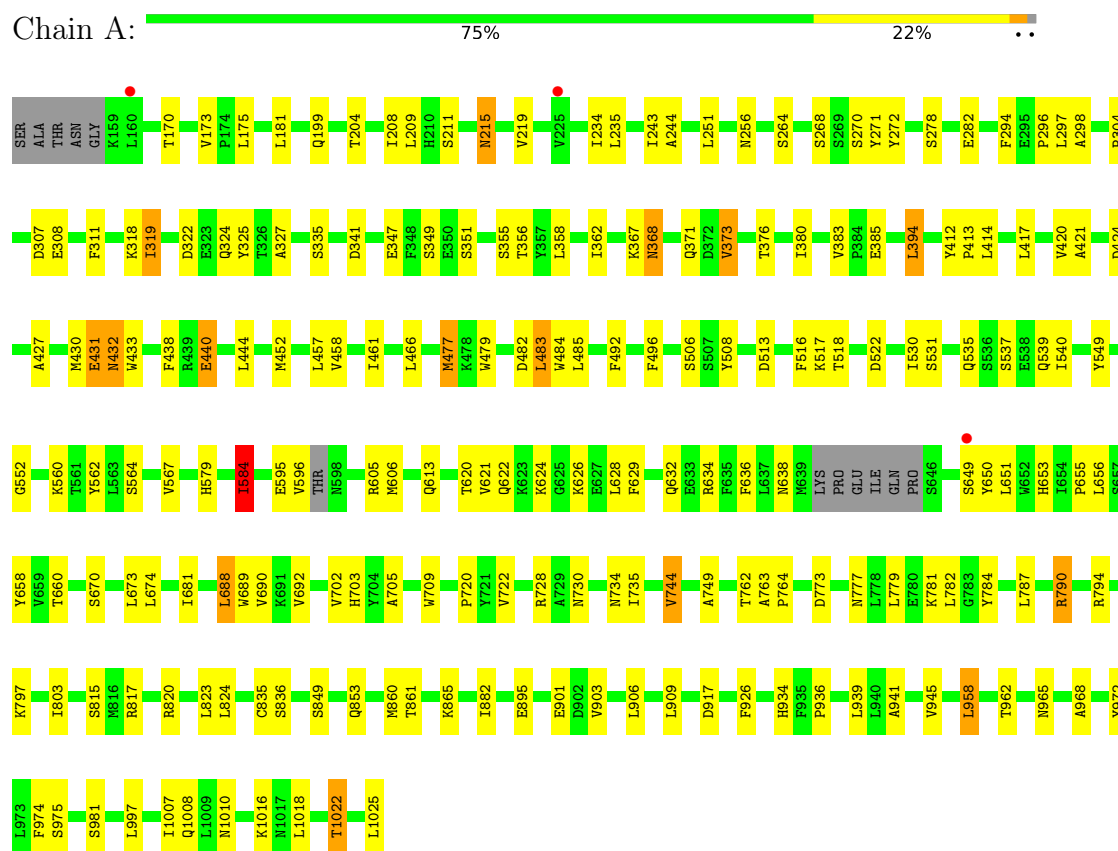
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	45	Total	O	0	0
			45	45		
6	B	10	Total	O	0	0
			10	10		

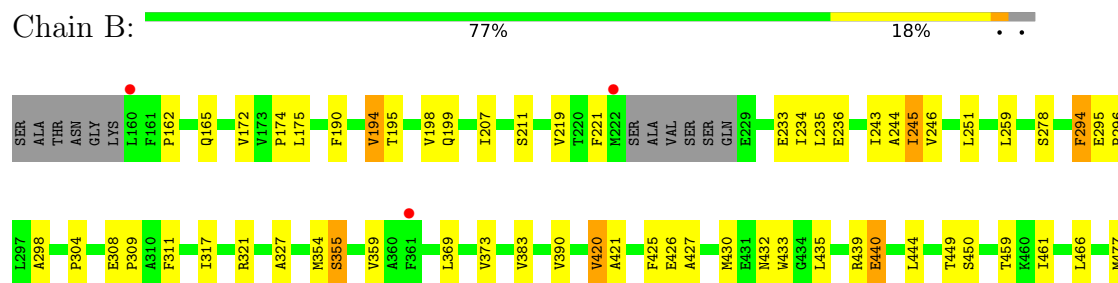
3 Residue-property plots

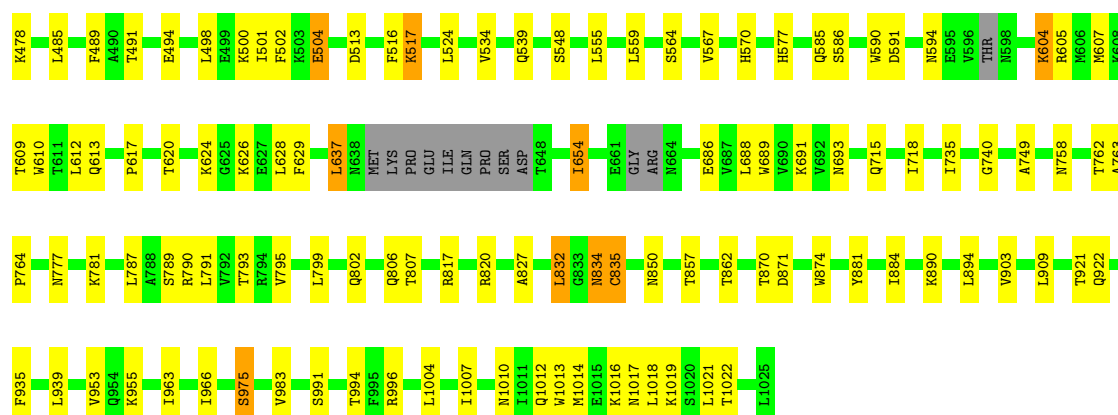
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Leucyl-cystinyl aminopeptidase



• Molecule 1: Leucyl-cystinyl aminopeptidase





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

Chain C:  100%



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

Chain D:  100%



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

Chain E:  100%



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

Chain F:  100%



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

Chain G:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.32Å 256.05Å 71.13Å 90.00° 115.12° 90.00°	Depositor
Resolution (Å)	48.42 – 3.02 48.42 – 3.02	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.42-3.02) 99.4 (48.42-3.02)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.190 , 0.250 0.200 , 0.261	Depositor DCC
R_{free} test set	2157 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.1	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 67.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.046 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14164	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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: UNL, NAG, ZN

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	0.79	0/7144	1.43	47/9690 (0.5%)
1	B	0.78	0/7009	1.40	40/9517 (0.4%)
All	All	0.79	0/14153	1.42	87/19207 (0.5%)

There are no bond length outliers.

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	654	ILE	N-CA-C	8.80	117.76	107.73
1	A	215	ASN	CA-CB-CG	8.70	121.30	112.60
1	A	605	ARG	N-CA-C	-8.12	103.37	113.28
1	A	438	PHE	CA-CB-CG	7.62	121.42	113.80
1	B	1017	ASN	N-CA-C	7.45	122.54	113.38
1	A	649	SER	N-CA-C	-7.45	104.04	113.72
1	A	939	LEU	CA-C-N	7.31	130.07	120.28
1	A	939	LEU	C-N-CA	7.31	130.07	120.28
1	A	268	SER	CA-C-N	7.28	130.63	120.29
1	A	268	SER	C-N-CA	7.28	130.63	120.29
1	B	501	ILE	N-CA-C	7.06	117.88	111.81
1	A	282	GLU	N-CA-C	-6.99	104.73	113.18
1	B	605	ARG	N-CA-C	-6.95	104.61	113.23
1	A	430	MET	N-CA-C	6.64	117.90	108.74
1	A	605	ARG	CA-C-N	6.60	129.41	120.44
1	A	605	ARG	C-N-CA	6.60	129.41	120.44
1	B	548	SER	CA-C-N	6.48	128.86	120.44
1	B	548	SER	C-N-CA	6.48	128.86	120.44
1	A	268	SER	N-CA-C	6.41	119.66	110.24
1	A	440	GLU	CA-C-N	6.36	130.36	120.82
1	A	440	GLU	C-N-CA	6.36	130.36	120.82
1	B	850	ASN	CA-CB-CG	6.36	118.96	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	516	PHE	CA-CB-CG	6.35	120.15	113.80
1	A	981	SER	CA-C-N	6.33	129.09	120.54
1	A	981	SER	C-N-CA	6.33	129.09	120.54
1	B	799	LEU	CA-C-N	6.27	128.59	120.44
1	B	799	LEU	C-N-CA	6.27	128.59	120.44
1	B	612	LEU	N-CA-C	6.25	118.90	111.71
1	B	420	VAL	N-CA-C	6.15	116.87	107.77
1	A	860	MET	N-CA-C	6.03	117.55	110.97
1	A	170	THR	CA-C-N	5.99	128.63	120.54
1	A	170	THR	C-N-CA	5.99	128.63	120.54
1	A	319	ILE	N-CA-C	5.96	116.45	108.11
1	A	516	PHE	CA-CB-CG	5.87	119.67	113.80
1	B	1021	LEU	CA-C-N	5.78	129.49	120.82
1	B	1021	LEU	C-N-CA	5.78	129.49	120.82
1	B	762	THR	N-CA-C	5.63	118.14	111.33
1	A	782	LEU	N-CA-C	-5.62	102.44	110.59
1	A	368	ASN	CA-CB-CG	5.57	118.17	112.60
1	A	595	GLU	N-CA-C	-5.54	102.98	110.68
1	A	431	GLU	N-CA-C	5.51	119.63	113.02
1	B	383	VAL	CB-CA-C	5.49	116.38	111.00
1	B	440	GLU	CA-C-N	5.48	127.88	120.38
1	B	440	GLU	C-N-CA	5.48	127.88	120.38
1	B	294	PHE	CA-CB-CG	5.42	119.22	113.80
1	B	835	CYS	N-CA-C	5.41	122.31	110.80
1	B	1019	LYS	CA-C-N	5.39	127.82	120.54
1	B	1019	LYS	C-N-CA	5.39	127.82	120.54
1	B	832	LEU	N-CA-C	5.39	118.23	107.62
1	A	496	PHE	CA-C-N	5.37	127.73	120.38
1	A	496	PHE	C-N-CA	5.37	127.73	120.38
1	A	508	TYR	CA-C-N	5.35	127.89	120.29
1	A	508	TYR	C-N-CA	5.35	127.89	120.29
1	A	413	PRO	N-CA-C	5.35	120.55	113.86
1	A	584	ILE	N-CA-C	5.35	117.33	108.99
1	A	730	ASN	CA-CB-CG	5.34	117.94	112.60
1	A	518	THR	CA-C-N	5.33	127.69	120.38
1	A	518	THR	C-N-CA	5.33	127.69	120.38
1	A	335	SER	N-CA-C	5.33	117.10	108.26
1	B	787	LEU	CA-C-N	5.25	127.32	120.28
1	B	787	LEU	C-N-CA	5.25	127.32	120.28
1	A	522	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	483	LEU	CA-C-N	5.21	127.79	120.28
1	A	483	LEU	C-N-CA	5.21	127.79	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	502	PHE	CA-C-N	5.21	127.51	120.38
1	B	502	PHE	C-N-CA	5.21	127.51	120.38
1	B	461	ILE	N-CA-C	5.20	115.41	110.42
1	A	552	GLY	CA-C-N	5.19	127.23	120.28
1	A	552	GLY	C-N-CA	5.19	127.23	120.28
1	A	722	VAL	N-CA-C	-5.19	106.26	113.00
1	B	834	ASN	CA-CB-CG	5.18	117.78	112.60
1	B	871	ASP	CA-C-N	5.17	127.16	120.44
1	B	871	ASP	C-N-CA	5.17	127.16	120.44
1	B	939	LEU	CA-C-N	5.17	127.15	120.44
1	B	939	LEU	C-N-CA	5.17	127.15	120.44
1	B	983	VAL	CA-C-N	5.16	127.15	120.44
1	B	983	VAL	C-N-CA	5.16	127.15	120.44
1	A	968	ALA	CA-C-N	5.14	125.80	119.99
1	A	968	ALA	C-N-CA	5.14	125.80	119.99
1	A	373	VAL	N-CA-CB	5.13	116.95	111.46
1	A	709	TRP	N-CA-C	-5.11	105.63	111.14
1	B	862	THR	CA-C-N	5.09	127.43	120.46
1	B	862	THR	C-N-CA	5.09	127.43	120.46
1	A	1018	LEU	N-CA-C	5.05	116.79	111.28
1	B	190	PHE	CA-CB-CG	5.04	118.83	113.80
1	B	894	LEU	CA-C-N	5.03	127.27	120.38
1	B	894	LEU	C-N-CA	5.03	127.27	120.38

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	6965	0	6824	83	0
1	B	6838	0	6660	61	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	28	0	25	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	84	0	78	1	0
4	B	70	0	65	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	45	0	0	0	0
6	B	10	0	0	0	0
All	All	14164	0	13752	142	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 5.

All (142) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ASP:HA	1:A:356:THR:HG21	1.63	0.81
1:A:936:PRO:HA	1:B:903:VAL:HG21	1.64	0.78
1:A:579:HIS:CG	1:A:584:ILE:HD11	2.23	0.74
1:A:564:SER:HB3	1:A:567:VAL:HG23	1.69	0.73
1:B:689:TRP:CD1	1:B:715:GLN:HG3	2.26	0.69
1:B:425:PHE:HB3	1:B:922:GLN:HE22	1.59	0.67
1:A:975:SER:HB3	1:A:1010:ASN:HB3	1.76	0.66
1:A:803:ILE:HG13	1:A:823:LEU:HD22	1.78	0.66
1:A:621:VAL:HG21	1:A:692:VAL:HG21	1.79	0.65
1:A:294:PHE:HA	1:A:298:ALA:HB3	1.76	0.65
1:A:477[B]:MET:HE2	1:A:482:ASP:HB3	1.79	0.64
1:A:535:GLN:HE21	1:A:539:GLN:HE22	1.45	0.64
1:B:421:ALA:HB1	1:B:440:GLU:HA	1.80	0.64
1:B:1014:MET:HE3	1:B:1018:LEU:HB2	1.81	0.62
1:A:204:THR:HG23	1:A:251:LEU:HD12	1.82	0.62
1:B:427:ALA:HB3	1:B:439:ARG:HG2	1.83	0.61
1:A:181:LEU:HB2	1:A:319:ILE:HG22	1.83	0.61
1:B:235:LEU:HB2	1:B:244:ALA:HB3	1.83	0.60
1:A:318:LYS:HB3	1:A:347:GLU:HG3	1.83	0.60
1:A:421:ALA:HB1	1:A:440:GLU:HA	1.82	0.60
1:B:219:VAL:HG11	1:B:234:ILE:HG12	1.83	0.60
1:B:559:LEU:HD22	1:B:607:MET:HE2	1.84	0.60
1:A:861:THR:O	1:A:865:LYS:HG3	2.02	0.60
1:B:432:ASN:HB2	1:B:435:LEU:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:GLU:HB2	1:B:311:PHE:HD2	1.67	0.59
1:B:827:ALA:HA	1:B:832:LEU:HD12	1.83	0.59
1:A:362:ILE:CD1	1:A:420:VAL:HG11	2.34	0.56
1:B:817:ARG:HB3	1:B:820:ARG:HH21	1.71	0.56
1:A:452:MET:HE3	1:A:817:ARG:NH1	2.20	0.56
1:A:703:HIS:HE1	1:A:744:VAL:HG23	1.71	0.56
1:A:895:GLU:HB2	1:A:926:PHE:HZ	1.71	0.56
1:A:613:GLN:OE1	1:A:650:TYR:HA	2.05	0.55
1:B:626:LYS:HG3	1:B:686:GLU:HG2	1.88	0.55
1:B:534:VAL:HG13	1:B:539:GLN:HB3	1.89	0.55
1:A:211:SER:HB3	1:A:243:ILE:HG12	1.89	0.54
1:B:975:SER:HB3	1:B:1010:ASN:HB3	1.88	0.54
1:B:369:LEU:HD22	1:B:390:VAL:HG23	1.90	0.53
1:A:606:MET:HG3	1:A:653:HIS:HB2	1.90	0.53
1:A:720:PRO:HB2	1:A:728:ARG:HD3	1.90	0.53
1:A:492:PHE:HZ	1:A:560:LYS:HD3	1.74	0.53
1:B:294:PHE:HA	1:B:298:ALA:HB3	1.91	0.53
1:B:354:MET:HE3	1:B:359:VAL:HG22	1.90	0.53
1:A:308:GLU:HB2	1:A:311:PHE:HD2	1.73	0.52
1:A:622:GLN:HG3	1:A:705:ALA:HB2	1.90	0.52
1:A:562:TYR:CD1	1:A:655:PRO:HB3	2.44	0.52
1:B:440:GLU:HG2	1:B:444:LEU:HD11	1.90	0.52
1:A:735:ILE:HG12	1:A:749:ALA:HA	1.91	0.52
1:A:688:LEU:HD12	1:A:689:TRP:HD1	1.73	0.52
1:B:321:ARG:HG2	1:B:327:ALA:HB2	1.92	0.51
1:A:656:LEU:HD11	1:A:674:LEU:HB2	1.93	0.51
1:A:941:ALA:O	1:A:945:VAL:HG23	2.10	0.51
1:B:449:THR:O	1:B:857:THR:HG21	2.10	0.51
1:A:934[A]:HIS:HD2	1:A:936:PRO:HD2	1.75	0.51
1:B:309:PRO:HA	1:B:355:SER:HB3	1.93	0.51
1:A:355:SER:HB2	1:A:358:LEU:HD12	1.92	0.51
1:A:934[A]:HIS:CD2	1:A:936:PRO:HD2	2.45	0.51
1:A:958:LEU:HG	1:A:997:LEU:HD11	1.93	0.51
1:B:740:GLY:HA2	1:B:1013:TRP:CD1	2.46	0.50
1:A:215:ASN:OD1	4:A:1104:NAG:H2	2.11	0.50
1:B:777:ASN:O	1:B:781:LYS:HG2	2.12	0.50
1:B:478:LYS:HD2	1:B:585:GLN:HE21	1.76	0.50
1:B:564:SER:HB3	1:B:567:VAL:HG23	1.94	0.49
1:A:901:GLU:HG2	1:A:936:PRO:HG2	1.94	0.49
1:A:417:LEU:HD21	1:A:466:LEU:HD11	1.95	0.49
1:B:221:PHE:HE2	1:B:251:LEU:HD21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:VAL:H	1:A:734:ASN:ND2	2.11	0.48
1:B:610:TRP:HZ3	1:B:617:PRO:HD3	1.78	0.48
1:B:789:SER:O	1:B:793:THR:HG23	2.13	0.48
1:A:628:LEU:HB3	1:A:681:ILE:HB	1.94	0.48
1:B:921:THR:HG21	1:B:955:LYS:HD3	1.96	0.48
1:A:634:ARG:HD3	1:A:636:PHE:HB2	1.95	0.48
1:A:537:SER:HA	1:A:540:ILE:HD12	1.96	0.48
1:A:513:ASP:O	1:A:517:LYS:HG2	2.14	0.47
1:A:371:GLN:HB2	1:A:394:LEU:HD21	1.96	0.47
1:A:380:ILE:HG12	1:A:394:LEU:HB2	1.97	0.47
1:B:1004:LEU:HA	1:B:1007:ILE:HD12	1.96	0.47
1:B:624:LYS:HB2	1:B:629:PHE:HE2	1.79	0.46
1:A:777:ASN:O	1:A:781:LYS:HG2	2.15	0.46
1:B:881:TYR:O	1:B:890:LYS:HE2	2.15	0.46
1:B:524:LEU:HA	1:B:637:LEU:HD11	1.96	0.46
1:A:362:ILE:HD13	1:A:420:VAL:HG11	1.97	0.46
1:A:794:ARG:HH11	1:A:1025:LEU:HA	1.80	0.46
1:A:272:TYR:CZ	1:A:298:ALA:HB2	2.51	0.46
1:A:906:LEU:HA	1:A:909:LEU:HD12	1.98	0.46
1:A:849:SER:OG	1:A:853:GLN:HB2	2.16	0.45
1:A:790:ARG:HH22	1:A:1022:THR:HA	1.82	0.45
1:B:211:SER:HB3	1:B:243:ILE:HG12	1.97	0.45
1:B:245:ILE:HD13	1:B:259:LEU:HD21	1.98	0.45
1:A:688:LEU:HD12	1:A:689:TRP:CD1	2.51	0.45
1:B:735:ILE:HG12	1:B:749:ALA:HA	1.98	0.45
1:B:807:THR:O	1:B:820:ARG:HD3	2.17	0.45
1:A:412:TYR:CE2	1:A:414:LEU:HB2	2.53	0.44
1:A:270:SER:OG	1:A:271:TYR:N	2.39	0.44
1:B:513:ASP:O	1:B:517:LYS:HG2	2.16	0.44
1:A:762:THR:HG22	1:A:815:SER:OG	2.16	0.44
1:A:297:LEU:HD11	1:A:540:ILE:HD13	1.98	0.44
1:B:174:PRO:HA	1:B:198:VAL:HG12	1.99	0.44
1:B:874:TRP:HZ2	1:B:909:LEU:HD11	1.83	0.44
1:A:440:GLU:HG2	1:A:444:LEU:HD11	1.99	0.44
1:B:504:GLU:H	1:B:504:GLU:CD	2.25	0.44
1:A:820:ARG:HG3	1:A:824:LEU:HD12	1.99	0.43
1:B:459:THR:HG22	1:B:498:LEU:HD11	2.01	0.43
1:A:477[B]:MET:SD	1:A:584:ILE:HG22	2.58	0.43
1:A:624:LYS:HB2	1:A:629:PHE:HE2	1.83	0.43
1:B:791:LEU:O	1:B:795:VAL:HG23	2.18	0.43
1:A:319:ILE:HD11	1:A:327:ALA:HB1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:GLU:HA	1:B:296:PRO:HA	1.84	0.43
1:A:211:SER:HB2	1:A:304:PRO:HB3	2.01	0.42
1:A:479:TRP:HA	1:A:479:TRP:CE3	2.54	0.42
1:A:620:THR:HG23	1:A:703:HIS:HD2	1.83	0.42
1:A:763:ALA:HB3	1:A:764:PRO:HD3	2.01	0.42
1:B:591:ASP:HA	1:B:594:ASN:HD22	1.83	0.42
1:B:604:LYS:HD3	1:B:604:LYS:HA	1.80	0.42
1:A:380:ILE:CG1	1:A:394:LEU:HB2	2.50	0.42
1:A:383:VAL:HG22	1:A:385:GLU:HG2	2.01	0.42
1:B:763:ALA:HB3	1:B:764:PRO:HD3	2.01	0.42
1:B:194:VAL:HG21	1:B:304:PRO:HD2	2.01	0.42
1:B:1012:GLN:HG2	1:B:1016:LYS:HE3	2.01	0.42
1:A:424:ASP:HB3	1:A:427:ALA:HB2	2.02	0.42
1:B:802:GLN:O	1:B:806:GLN:HG2	2.20	0.42
1:A:458:VAL:HA	1:A:461:ILE:HG22	2.02	0.42
1:A:484:TRP:CE3	1:A:530:ILE:HD12	2.55	0.42
1:A:779:LEU:HD13	1:A:787:LEU:HB3	2.02	0.42
1:A:974:PHE:HB2	1:A:1007:ILE:HG12	2.02	0.41
1:B:609:THR:O	1:B:613:GLN:HG2	2.21	0.41
1:B:172:VAL:HG21	1:B:207:ILE:HG23	2.02	0.41
1:B:485:LEU:HD22	1:B:586:SER:HA	2.02	0.41
1:B:991:SER:HB2	1:B:994:THR:H	1.85	0.41
1:A:579:HIS:CD2	1:A:584:ILE:HD11	2.55	0.41
1:A:660:THR:HG22	1:A:690:VAL:HA	2.03	0.41
1:A:235:LEU:HB2	1:A:244:ALA:HB3	2.01	0.41
1:A:322:ASP:HB2	1:A:325:TYR:CD2	2.56	0.41
1:A:431:GLU:O	1:A:432:ASN:C	2.64	0.41
1:A:175:LEU:HD11	1:A:199:GLN:HB2	2.01	0.41
1:A:477[B]:MET:CE	1:A:584:ILE:HG22	2.51	0.41
1:B:590:TRP:HB3	1:B:604:LYS:CB	2.51	0.41
1:A:903:VAL:HG12	1:B:935:PHE:CE1	2.56	0.40
1:B:491:THR:O	1:B:494:GLU:HB3	2.21	0.40
1:B:295:GLU:HB2	1:B:430:MET:SD	2.61	0.40
1:A:658:TYR:CZ	1:A:670:SER:HB3	2.57	0.40
1:B:175:LEU:HD11	1:B:199:GLN:HB2	2.04	0.40
1:A:322:ASP:HB3	1:A:324:GLN:OE1	2.22	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	857/872 (98%)	794 (93%)	57 (7%)	6 (1%)	18	51
1	B	839/872 (96%)	770 (92%)	61 (7%)	8 (1%)	12	43
All	All	1696/1744 (97%)	1564 (92%)	118 (7%)	14 (1%)	16	48

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	835	CYS
1	A	638	ASN
1	A	972	TYR
1	B	433	TRP
1	B	693	ASN
1	B	835	CYS
1	A	784	TYR
1	A	917	ASP
1	B	162	PRO
1	B	450	SER
1	B	718	ILE
1	B	373	VAL
1	B	884	ILE
1	A	296	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	765/781 (98%)	720 (94%)	45 (6%)	18	49
1	B	746/781 (96%)	708 (95%)	38 (5%)	21	54
All	All	1511/1562 (97%)	1428 (94%)	83 (6%)	20	51

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	VAL
1	A	208	ILE
1	A	209	LEU
1	A	219	VAL
1	A	234	ILE
1	A	256	ASN
1	A	264	SER
1	A	278	SER
1	A	341	ASP
1	A	349	SER
1	A	351	SER
1	A	367	LYS
1	A	368	ASN
1	A	373	VAL
1	A	376	THR
1	A	394	LEU
1	A	432	ASN
1	A	433	TRP
1	A	457	LEU
1	A	477[A]	MET
1	A	477[B]	MET
1	A	483	LEU
1	A	485	LEU
1	A	506	SER
1	A	531	SER
1	A	549	TYR
1	A	584	ILE
1	A	596	VAL
1	A	626	LYS
1	A	632	GLN
1	A	651	LEU
1	A	673	LEU
1	A	688	LEU
1	A	744	VAL
1	A	773	ASP

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Mol	Chain	Res	Type
1	A	790	ARG
1	A	797	LYS
1	A	836	SER
1	A	882	ILE
1	A	958	LEU
1	A	962	THR
1	A	965	ASN
1	A	1008	GLN
1	A	1016	LYS
1	A	1022	THR
1	B	165	GLN
1	B	194	VAL
1	B	195	THR
1	B	233	GLU
1	B	236	GLU
1	B	245	ILE
1	B	246	VAL
1	B	278	SER
1	B	317	ILE
1	B	355	SER
1	B	420	VAL
1	B	426	GLU
1	B	466	LEU
1	B	477	MET
1	B	489	PHE
1	B	500	LYS
1	B	504	GLU
1	B	517	LYS
1	B	555	LEU
1	B	570	HIS
1	B	577	HIS
1	B	604	LYS
1	B	620	THR
1	B	628	LEU
1	B	637	LEU
1	B	654	ILE
1	B	688	LEU
1	B	691	LYS
1	B	758	ASN
1	B	790	ARG
1	B	834	ASN
1	B	870	THR

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Mol	Chain	Res	Type
1	B	953	VAL
1	B	963	ILE
1	B	966	ILE
1	B	975	SER
1	B	996	ARG
1	B	1022	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	HIS
1	A	293	GLN
1	A	345	GLN
1	A	389	GLN
1	A	469	GLN
1	A	481	ASN
1	A	486	ASN
1	A	535	GLN
1	A	578	ASN
1	A	632	GLN
1	A	653	HIS
1	A	853	GLN
1	A	915	ASN
1	A	1017	ASN
1	B	345	GLN
1	B	486	ASN
1	B	577	HIS
1	B	585	GLN
1	B	715	GLN
1	B	733	ASN
1	B	771	GLN
1	B	806	GLN
1	B	922	GLN
1	B	948	ASN
1	B	1008	GLN
1	B	1012	GLN

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 ⓘ

10 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	0.30	0	17,19,21	1.14	1 (5%)
2	NAG	C	2	2	14,14,15	0.30	0	17,19,21	0.79	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.29	0	17,19,21	0.87	1 (5%)
2	NAG	D	2	2	14,14,15	0.32	0	17,19,21	0.60	1 (5%)
2	NAG	E	1	1,2	14,14,15	0.33	0	17,19,21	1.23	1 (5%)
2	NAG	E	2	2	14,14,15	0.30	0	17,19,21	0.62	1 (5%)
2	NAG	F	1	1,2	14,14,15	0.32	0	17,19,21	1.02	1 (5%)
2	NAG	F	2	2	14,14,15	0.32	0	17,19,21	1.11	3 (17%)
2	NAG	G	1	1,2	14,14,15	0.28	0	17,19,21	0.68	1 (5%)
2	NAG	G	2	2	14,14,15	0.31	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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	O5-C1-C2	-4.52	104.29	111.29
2	C	1	NAG	O5-C1-C2	-4.06	105.02	111.29
2	F	1	NAG	C1-O5-C5	3.54	116.93	112.19
2	F	2	NAG	C1-C2-N2	2.85	114.92	110.43
2	F	2	NAG	O5-C1-C2	-2.59	107.28	111.29
2	C	2	NAG	C1-O5-C5	2.27	115.22	112.19
2	D	1	NAG	O5-C1-C2	-2.20	107.89	111.29
2	F	2	NAG	C1-O5-C5	2.17	115.09	112.19
2	G	1	NAG	C1-O5-C5	2.16	115.08	112.19
2	D	2	NAG	C1-O5-C5	2.15	115.06	112.19
2	E	2	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

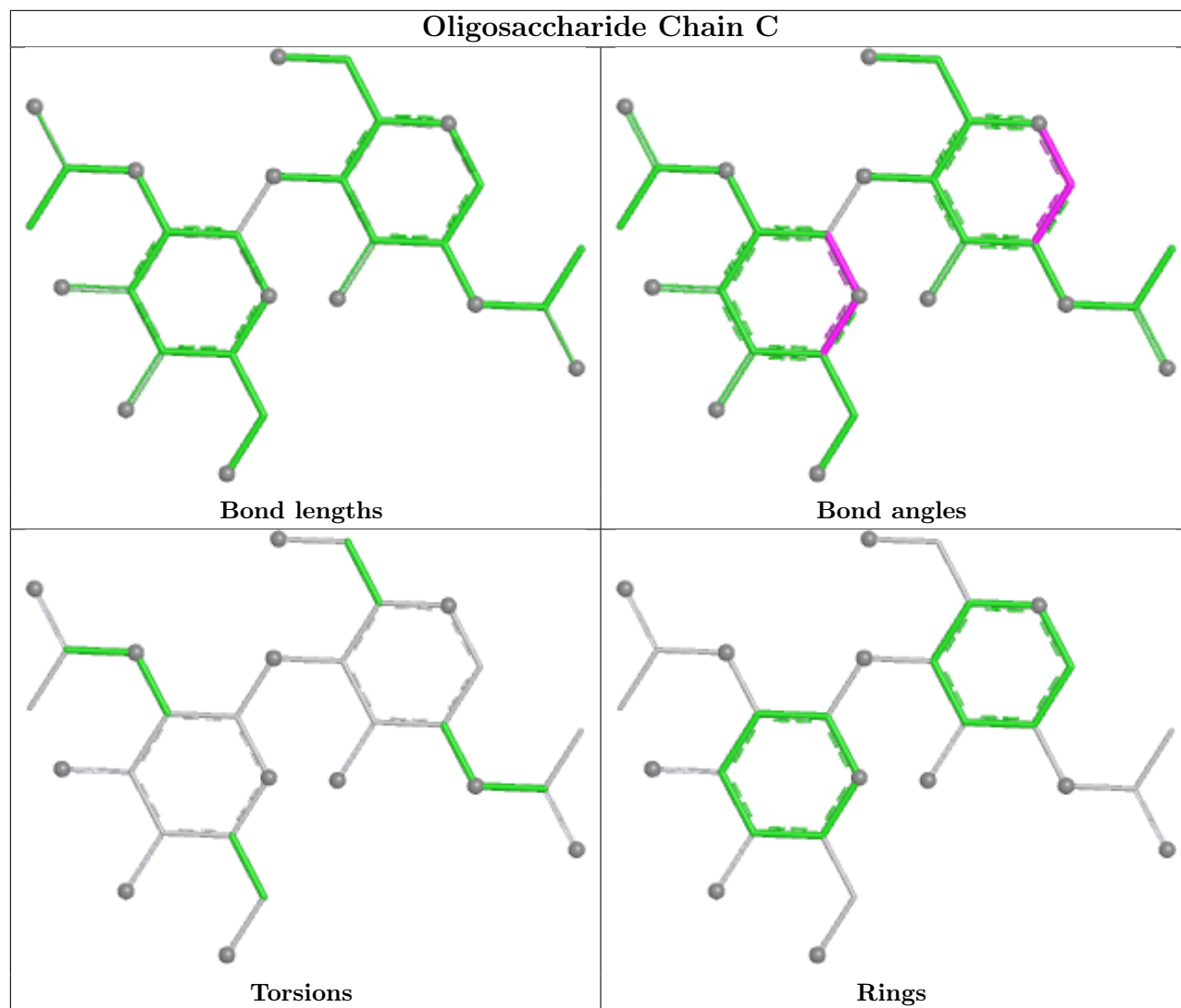
All (5) torsion outliers are listed below:

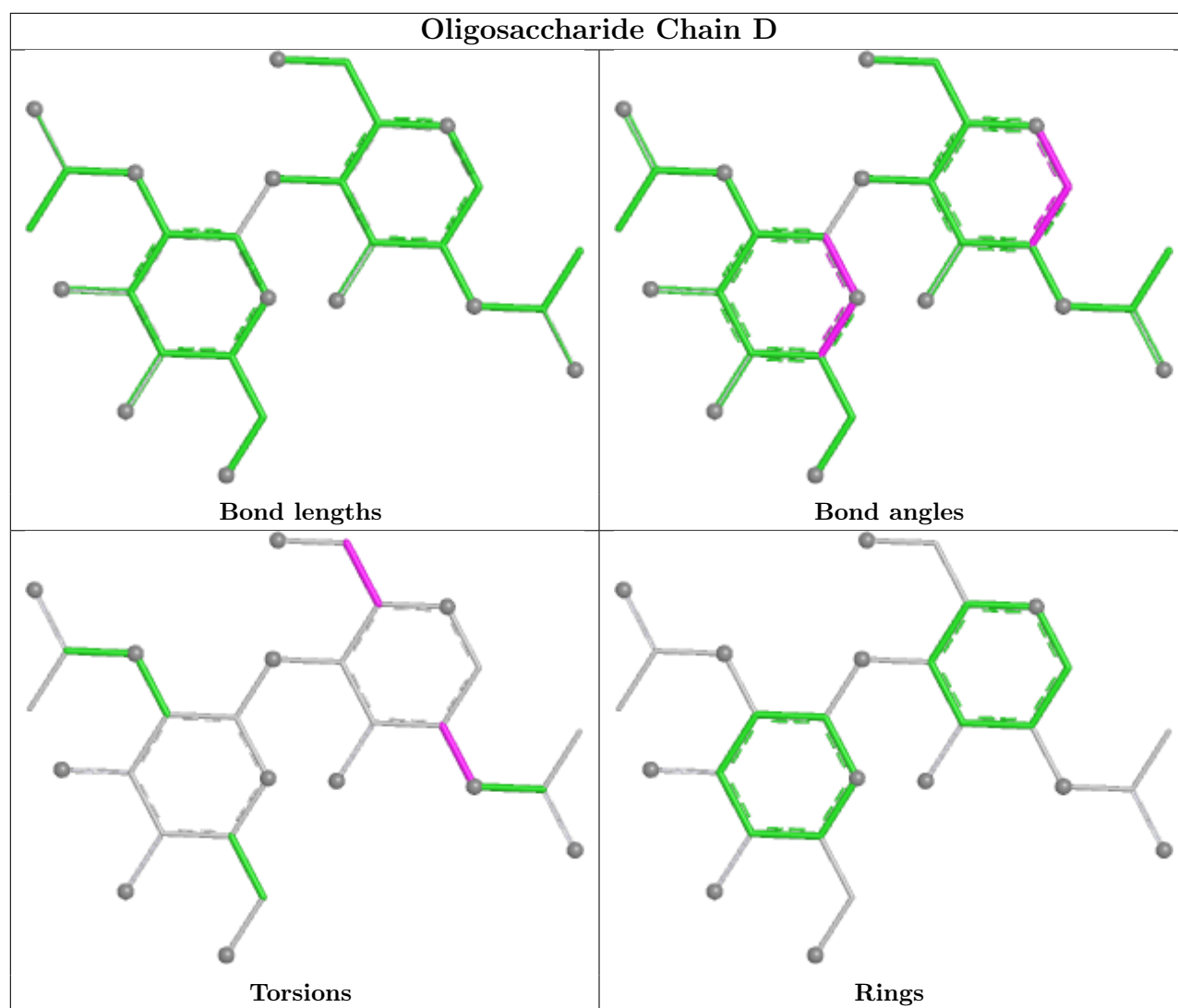
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C1-C2-N2-C7

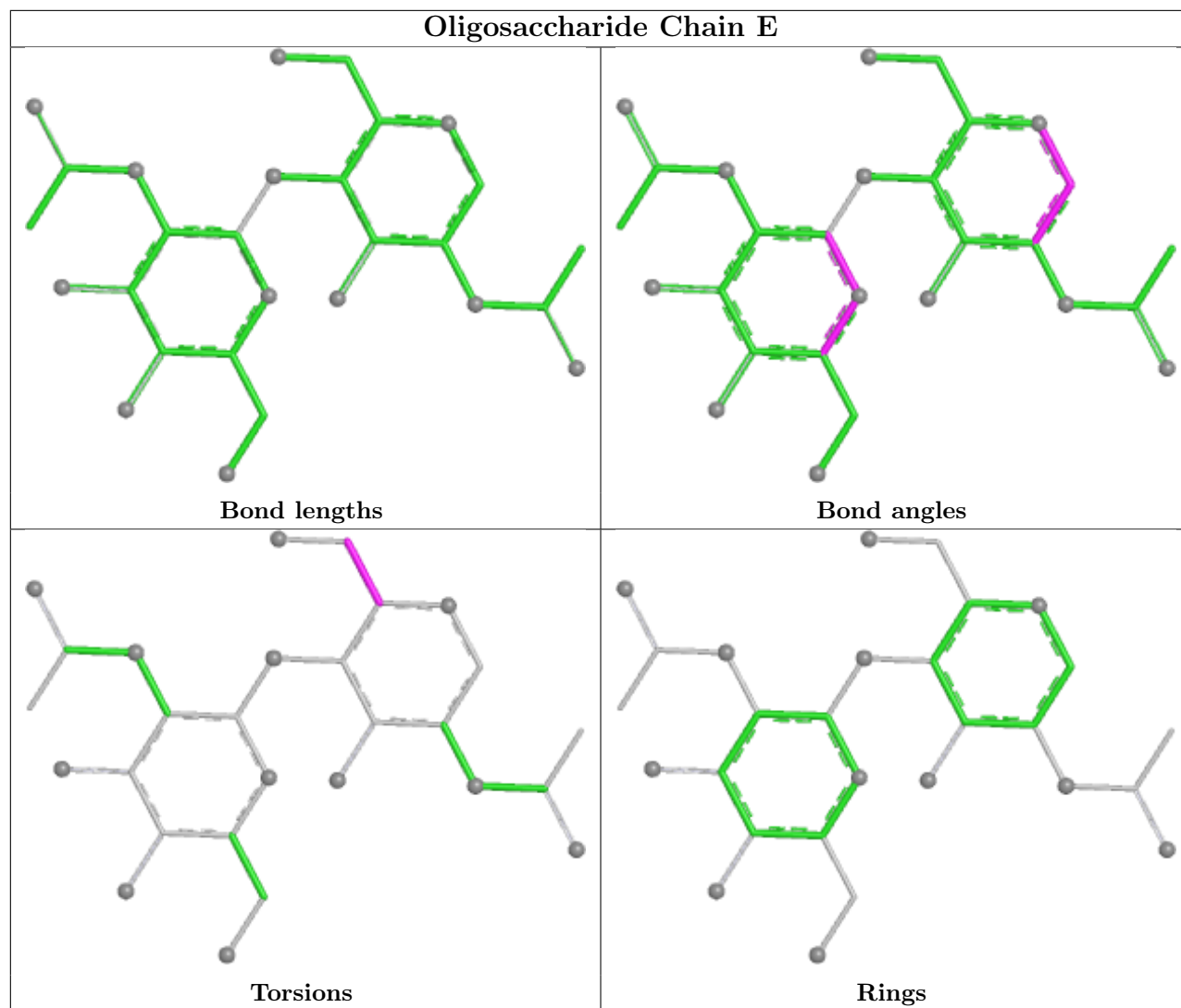
There are no ring outliers.

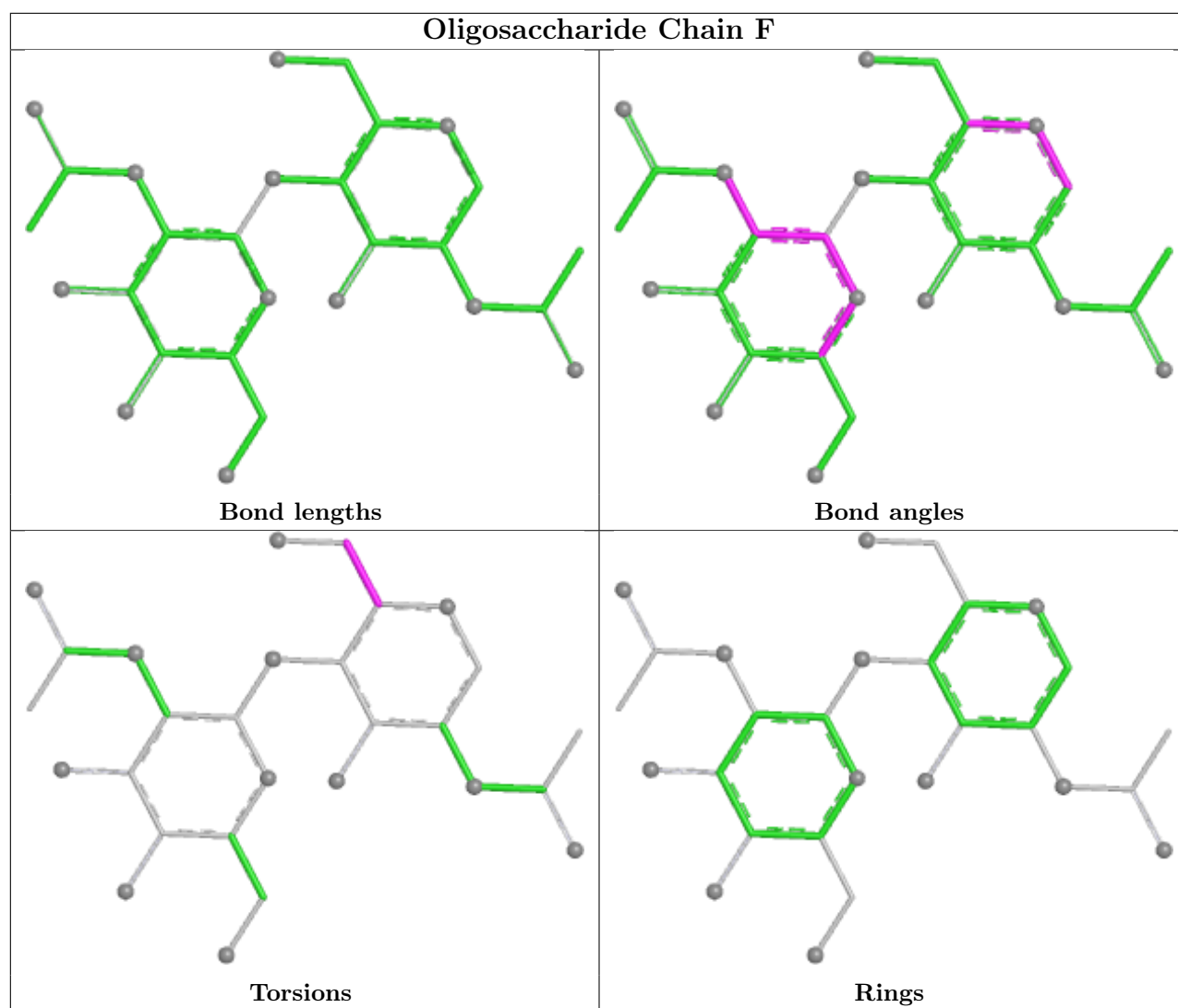
No monomer is involved in short contacts.

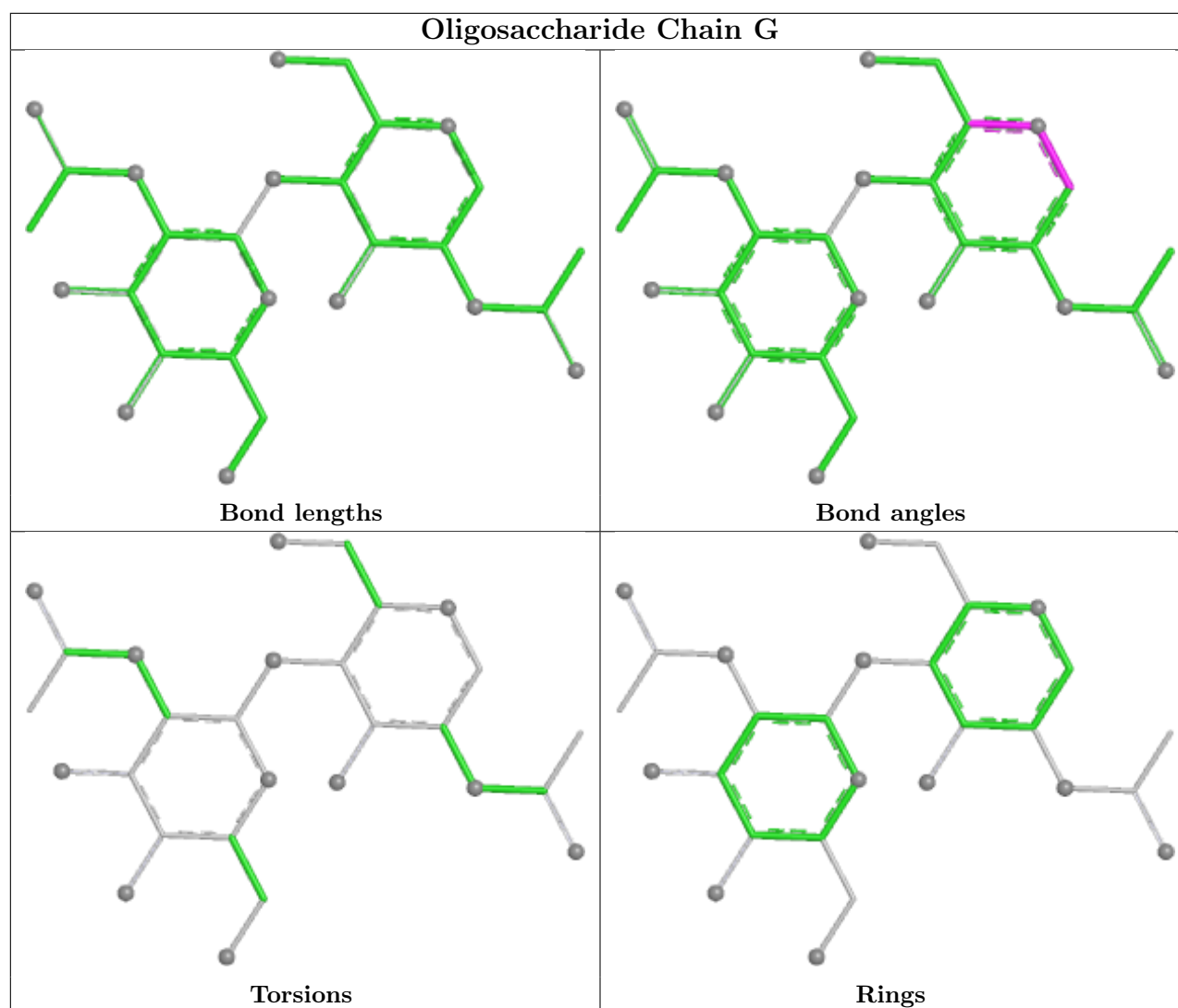
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 2 are monoatomic and 2 are unknown - leaving 11 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	$\# Z > 2$
4	NAG	B	1107	1	14,14,15	0.29	0	17,19,21	0.78	1 (5%)
4	NAG	A	1106	1	14,14,15	0.34	0	17,19,21	0.76	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1104	1	14,14,15	0.32	0	17,19,21	0.77	1 (5%)
4	NAG	B	1110	1	14,14,15	0.28	0	17,19,21	0.96	1 (5%)
4	NAG	B	1111	1	14,14,15	0.29	0	17,19,21	0.69	0
4	NAG	B	1112	1	14,14,15	0.37	0	17,19,21	1.01	2 (11%)
4	NAG	A	1105	1	14,14,15	0.32	0	17,19,21	1.44	3 (17%)
4	NAG	A	1110	1	14,14,15	0.36	0	17,19,21	1.74	2 (11%)
4	NAG	A	1104	1	14,14,15	0.37	0	17,19,21	2.07	2 (11%)
4	NAG	A	1111	1	14,14,15	0.31	0	17,19,21	1.30	3 (17%)
4	NAG	A	1109	1	14,14,15	0.35	0	17,19,21	0.72	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
4	NAG	B	1107	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1106	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1104	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1110	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1111	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1112	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1105	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1110	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1104	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1111	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1109	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1104	NAG	O5-C1-C2	5.91	120.44	111.29
4	A	1104	NAG	C1-O5-C5	5.74	119.88	112.19
4	A	1110	NAG	C1-O5-C5	5.69	119.82	112.19
4	A	1110	NAG	O5-C1-C2	4.01	117.50	111.29
4	A	1105	NAG	O5-C1-C2	3.81	117.18	111.29
4	A	1105	NAG	C1-O5-C5	3.61	117.02	112.19
4	A	1111	NAG	C1-C2-N2	3.42	115.82	110.43
4	B	1110	NAG	O5-C1-C2	-3.08	106.52	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1107	NAG	C1-O5-C5	2.94	116.13	112.19
4	A	1111	NAG	C1-O5-C5	2.90	116.08	112.19
4	B	1112	NAG	O5-C1-C2	2.69	115.45	111.29
4	A	1111	NAG	O5-C1-C2	-2.65	107.19	111.29
4	A	1106	NAG	C1-O5-C5	2.37	115.37	112.19
4	B	1112	NAG	C1-C2-N2	-2.33	106.75	110.43
4	A	1105	NAG	C1-C2-N2	-2.24	106.91	110.43
4	B	1104	NAG	C1-O5-C5	2.04	114.91	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1104	NAG	O5-C5-C6-O6
4	A	1105	NAG	O5-C5-C6-O6
4	B	1111	NAG	O5-C5-C6-O6
4	A	1109	NAG	C4-C5-C6-O6
4	A	1105	NAG	C4-C5-C6-O6
4	B	1104	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1104	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	860/872 (98%)	-0.11	3 (0%)	90 79	24, 60, 93, 124	3 (0%)
1	B	848/872 (97%)	0.04	3 (0%)	88 76	29, 71, 100, 126	1 (0%)
All	All	1708/1744 (97%)	-0.03	6 (0%)	88 76	24, 66, 97, 126	4 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	649	SER	2.7
1	B	160	LEU	2.4
1	B	222	MET	2.2
1	B	361	PHE	2.1
1	A	225	VAL	2.1
1	A	160	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](#)

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

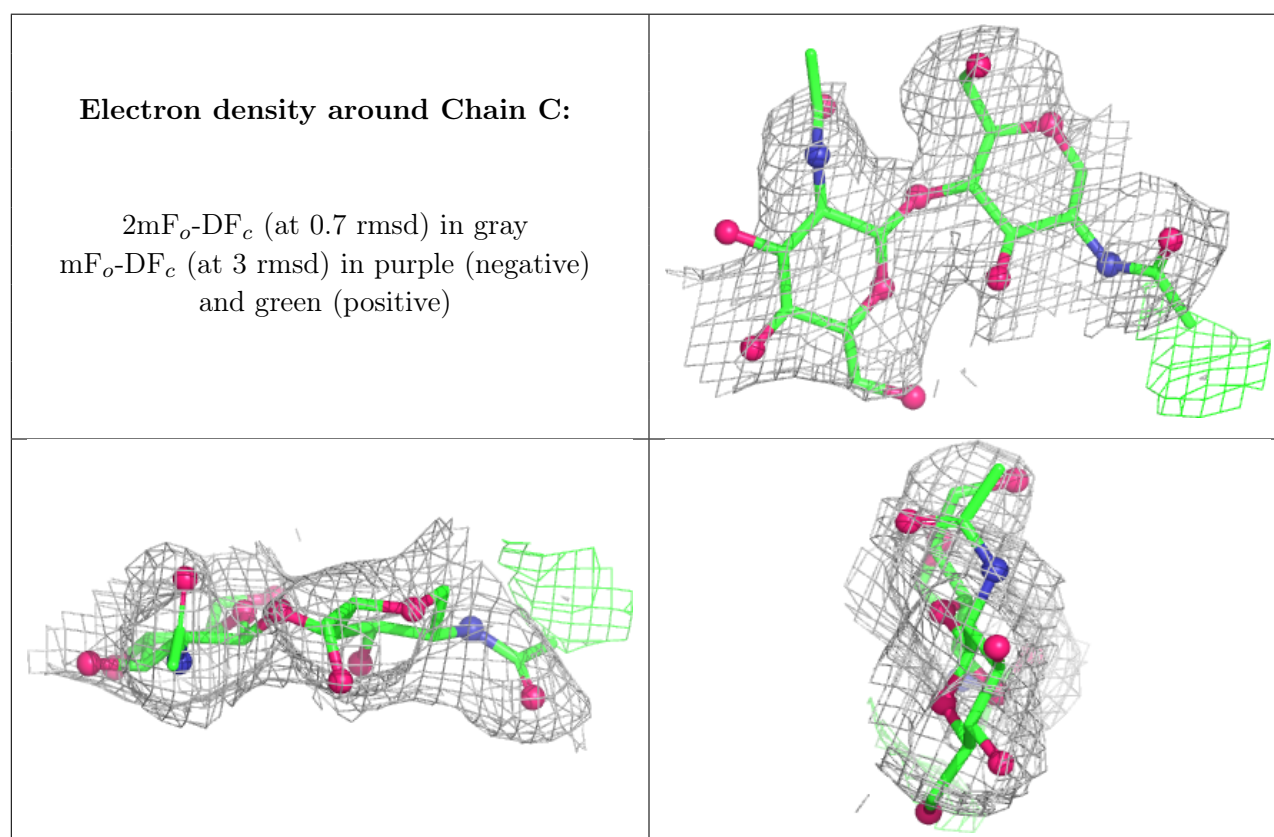
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
2	NAG	D	2	14/15	0.39	0.15	133,138,139,139	0
2	NAG	E	2	14/15	0.53	0.13	139,140,140,140	0
2	NAG	D	1	14/15	0.55	0.16	119,127,132,134	0

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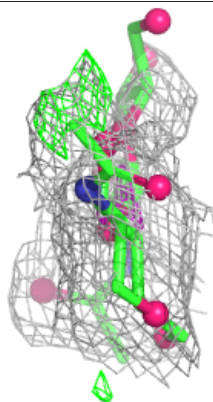
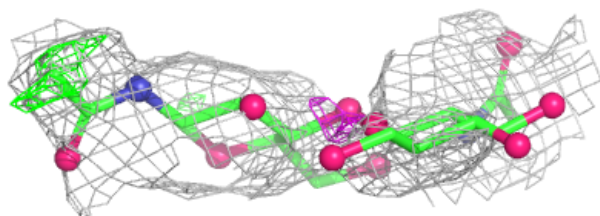
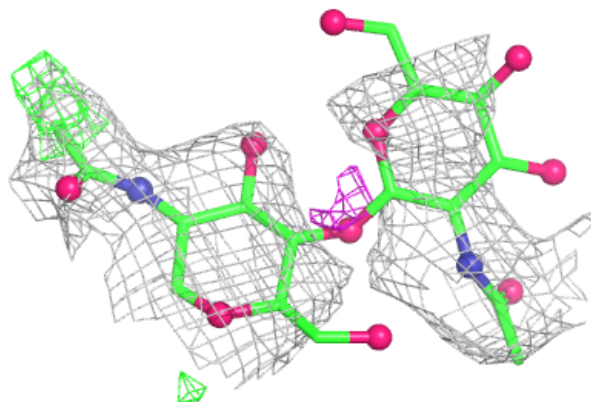
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	E	1	14/15	0.59	0.18	133,135,138,139	0
2	NAG	C	2	14/15	0.61	0.12	122,123,124,125	0
2	NAG	C	1	14/15	0.63	0.15	107,113,117,120	0
2	NAG	F	2	14/15	0.66	0.13	106,108,109,109	0
2	NAG	G	2	14/15	0.68	0.12	109,115,116,117	0
2	NAG	F	1	14/15	0.80	0.12	94,98,103,103	0
2	NAG	G	1	14/15	0.84	0.11	92,98,102,107	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

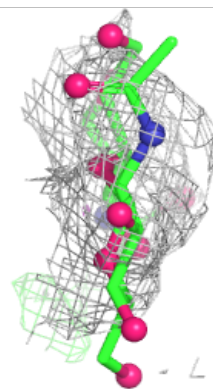
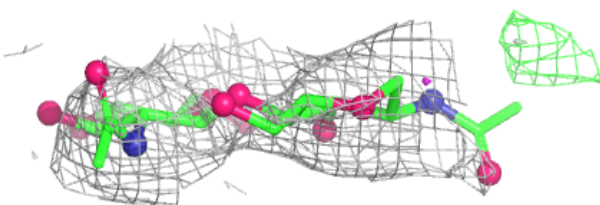
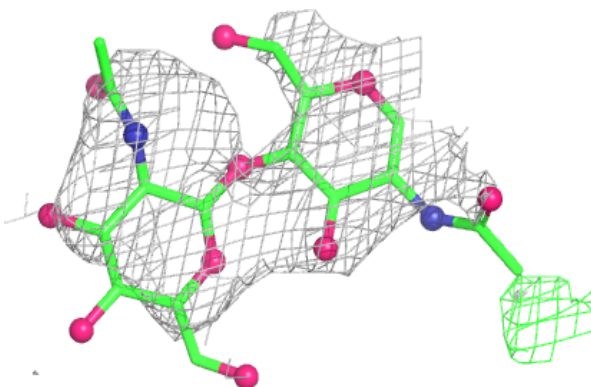


Electron density around Chain D:

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

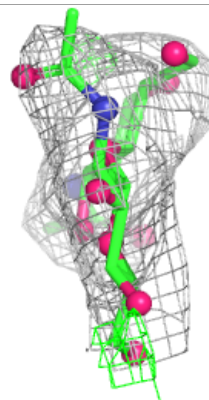
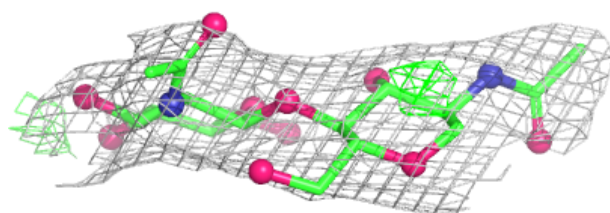
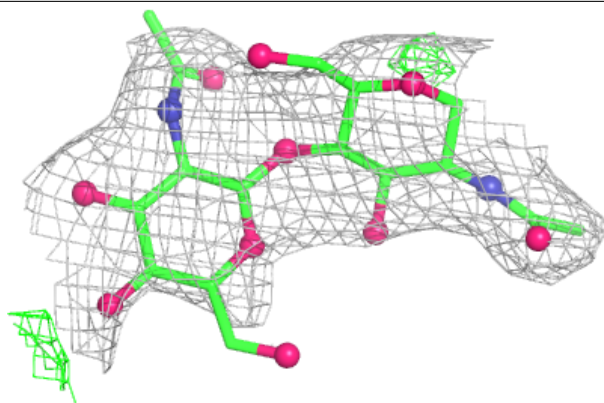
**Electron density around Chain E:**

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

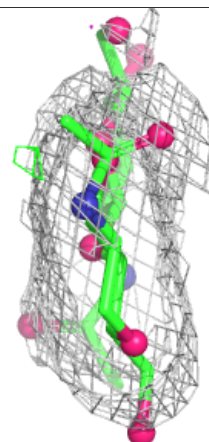
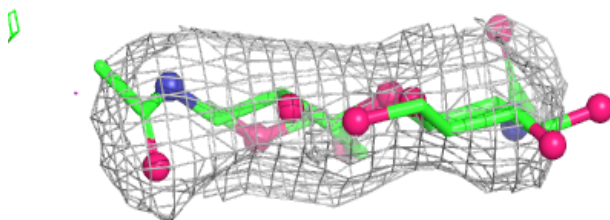
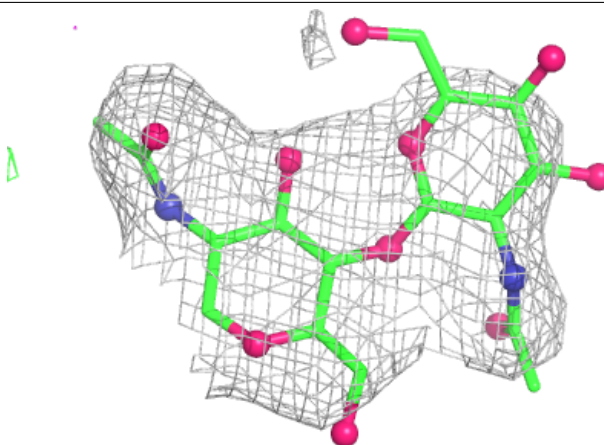


Electron density around Chain F:

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

**Electron density around Chain G:**

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	B	1104	14/15	0.40	0.16	124,127,130,131	0
4	NAG	B	1112	14/15	0.42	0.17	118,121,123,123	0
4	NAG	A	1111	14/15	0.50	0.17	95,96,101,101	0
4	NAG	A	1104	14/15	0.55	0.16	123,130,131,131	0
4	NAG	A	1109	14/15	0.64	0.12	101,106,108,109	0
4	NAG	A	1105	14/15	0.66	0.13	110,116,118,118	0
4	NAG	B	1107	14/15	0.70	0.11	89,95,98,98	0
4	NAG	B	1110	14/15	0.71	0.12	119,121,122,123	0
4	NAG	A	1106	14/15	0.74	0.13	110,112,114,115	0
4	NAG	A	1110	14/15	0.75	0.12	107,111,112,112	0
4	NAG	B	1111	14/15	0.80	0.13	112,113,114,114	0
5	UNL	B	1113	5/-	0.83	0.28	36,57,66,85	5
5	UNL	A	1112	5/-	0.84	0.31	53,59,80,82	5
3	ZN	B	1101	1/1	0.99	0.06	54,54,54,54	1
3	ZN	A	1101	1/1	0.99	0.07	53,53,53,53	1

6.5 Other polymers [i](#)

There are no such residues in this entry.