



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:55 PM UTC

PDB ID : 1O7D / pdb_00001o7d
Title : The structure of the bovine lysosomal α -mannosidase suggests a novel mechanism for low pH activation
Authors : Heikinheimo, P.; Helland, R.; Leiros, H.S.; Leiros, I.; Karlsen, S.; Evjen, G.; Ravelli, R.; Schoehn, G.; Ruigrok, R.; Tollersrud, O.-K.; Mcsweeney, S.; Hough, E.
Deposited on : 2002-10-30
Resolution : 2.70 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

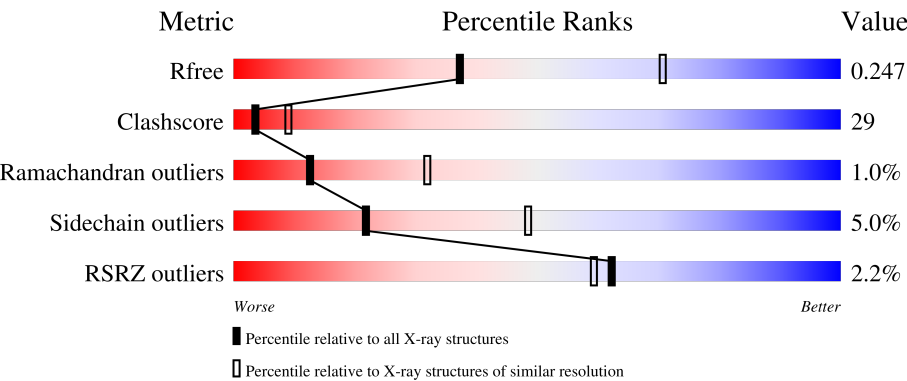
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 $\leq 5\%$. 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	298	<div><div>%</div><div><div></div><div>54%</div><div>39%</div><div>6%</div><div>.</div></div></div>
2	B	84	<div><div>6%</div><div><div></div><div>44%</div><div>40%</div><div>6%</div><div>10%</div></div></div>
3	C	159	<div><div>%</div><div><div></div><div>45%</div><div>45%</div><div>5%</div><div>5%</div></div></div>
4	D	282	<div><div>3%</div><div><div></div><div>44%</div><div>47%</div><div>5%</div><div>.</div></div></div>

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Mol	Chain	Length	Quality of chain
5	E	126	
6	F	9	
7	G	2	
7	H	2	
7	I	2	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	F	1	X	-	-	-
7	NAG	G	2	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 7385 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 Lysosomal alpha-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	1
			2365	1520	408	426	11			

- Molecule 2 is a protein called Lysosomal alpha-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total	C	N	O	S	0	0	1
			622	409	101	109	3			

- Molecule 3 is a protein called Lysosomal alpha-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	151	Total	C	N	O	S	0	0	1
			1136	722	194	214	6			

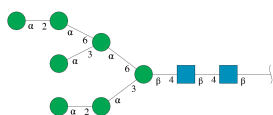
- Molecule 4 is a protein called Lysosomal alpha-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	270	Total	C	N	O	S	0	0	1
			2150	1356	397	392	5			

- Molecule 5 is a protein called Lysosomal alpha-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	109	Total	C	N	O	S	0	0	1
			851	543	148	159	1			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



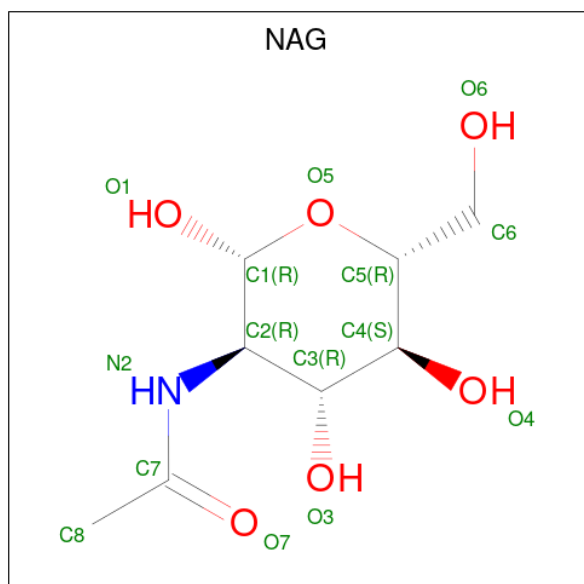
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



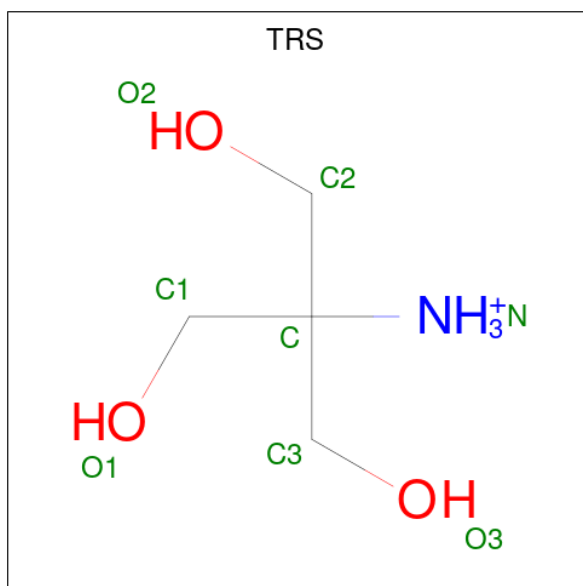
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 9 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	Zn	0	0
			1	1		

- Molecule 11 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	O	S	0	0
			5	4	1		
11	E	1	Total	O	S	0	0
			5	4	1		

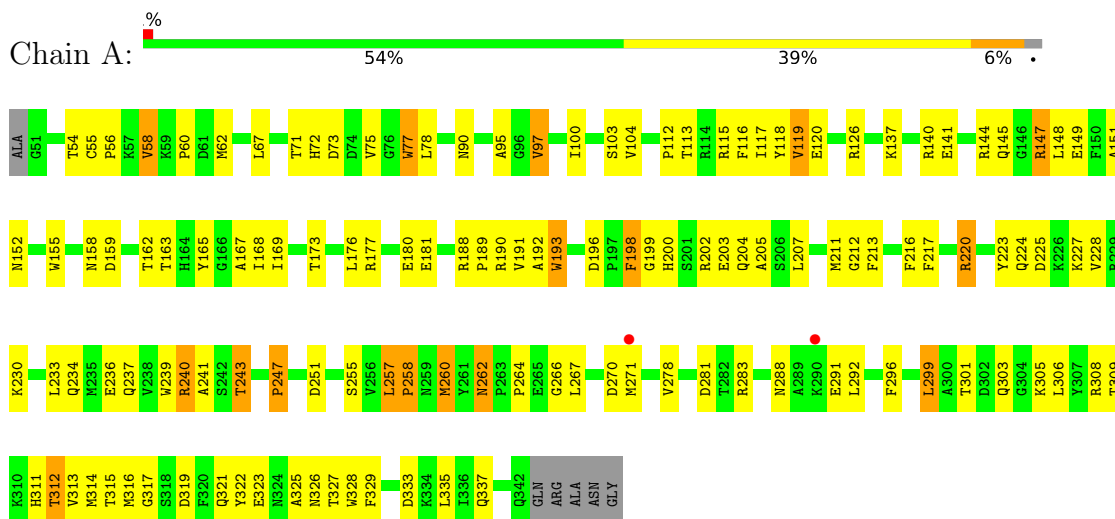
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	14	Total	O	0	0
			14	14		
12	B	2	Total	O	0	0
			2	2		
12	C	3	Total	O	0	0
			3	3		
12	D	14	Total	O	0	0
			14	14		
12	E	6	Total	O	0	0
			6	6		

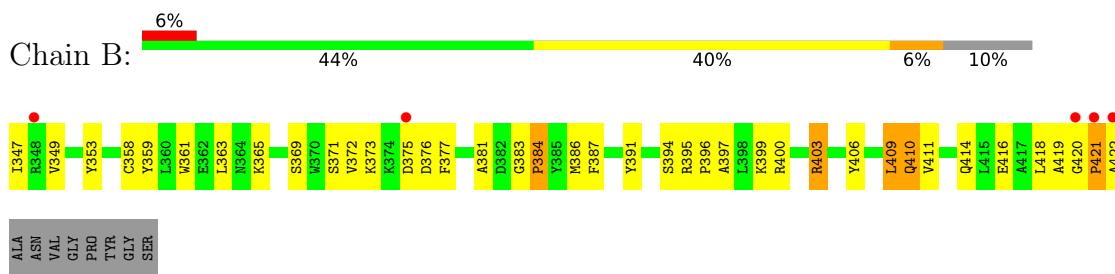
3 Residue-property plots

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.

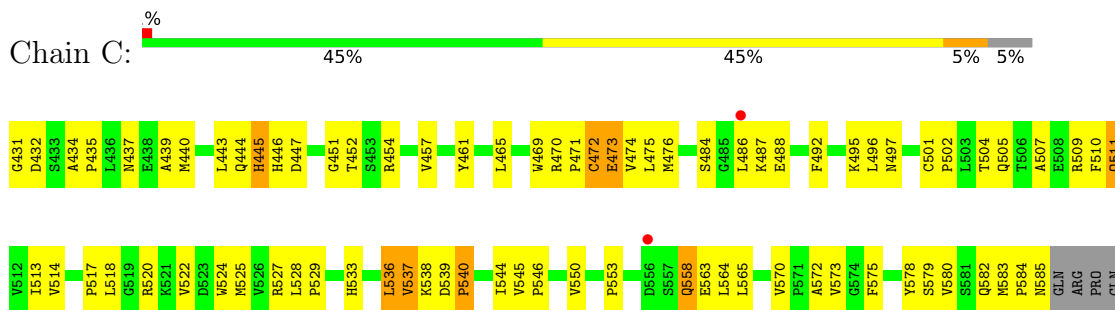
• Molecule 1: Lysosomal alpha-mannosidase



• Molecule 2: Lysosomal alpha-mannosidase

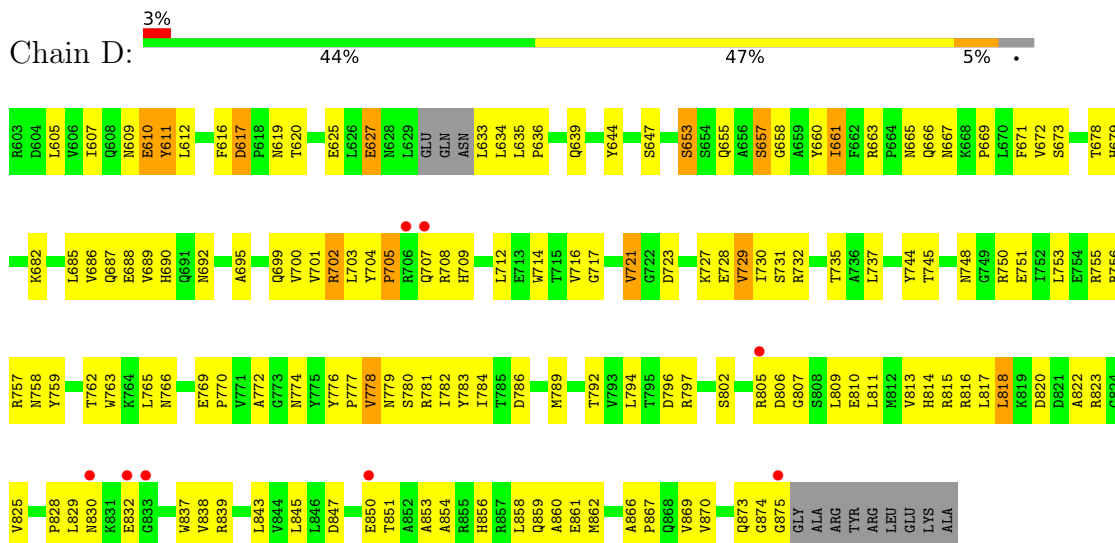


• Molecule 3: Lysosomal alpha-mannosidase

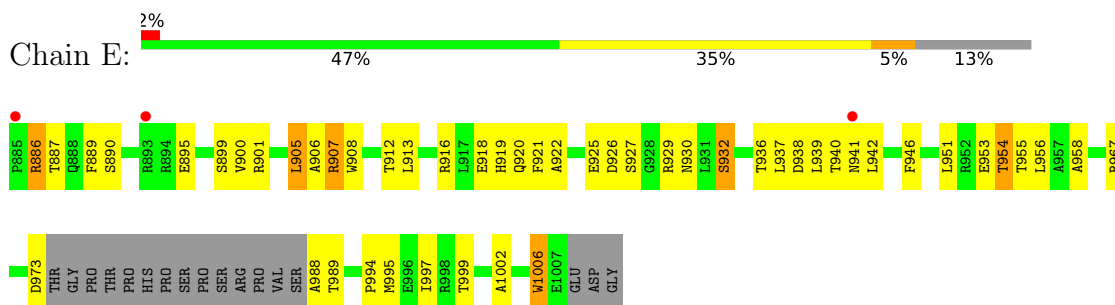


LYS
SER
TRP
SER

• Molecule 4: Lysosomal alpha-mannosidase



• Molecule 5: Lysosomal alpha-mannosidase



• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 

MAG1
MAG2
EMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 

MAG1
MAG2

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  50% 50%

MAG1
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	117.88Å 117.88Å 582.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.70 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.4 (30.00-2.70) 89.3 (30.00-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.257 , 0.289 0.252 , 0.247	Depositor DCC
R_{free} test set	3584 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	7385	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, SO4, TRS, BMA, 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	0.55	0/2431	1.11	19/3302 (0.6%)
2	B	0.67	0/644	1.00	2/879 (0.2%)
3	C	0.64	1/1163 (0.1%)	1.10	7/1589 (0.4%)
4	D	0.58	0/2198	1.11	15/2986 (0.5%)
5	E	0.66	1/868 (0.1%)	1.08	3/1186 (0.3%)
All	All	0.60	2/7304 (0.0%)	1.10	46/9942 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	584	PRO	C-N	-5.31	1.25	1.33
5	E	1006	TRP	C-N	-5.02	1.26	1.33

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	PRO	C-N-CD	-13.16	91.66	120.60
1	A	119	VAL	N-CA-C	12.72	122.20	111.90
1	A	193	TRP	N-CA-C	8.84	121.01	108.54
3	C	474	VAL	N-CA-C	-8.25	102.77	110.53
1	A	308	ARG	N-CA-C	8.15	121.08	111.71
4	D	765	LEU	N-CA-C	7.63	121.40	109.96
1	A	323	GLU	N-CA-C	-7.19	103.44	111.28
4	D	661	ILE	N-CA-C	7.13	118.91	109.21
1	A	55	CYS	CA-C-N	6.83	126.76	120.21
1	A	55	CYS	C-N-CA	6.83	126.76	120.21
1	A	329	PHE	N-CA-C	6.79	118.68	111.28
1	A	247	PRO	CA-C-N	6.76	143.23	127.00
1	A	247	PRO	C-N-CA	6.76	143.23	127.00
1	A	220	ARG	N-CA-C	6.75	119.70	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	905	LEU	N-CA-C	-6.60	97.30	108.26
1	A	257	LEU	CA-C-N	6.55	128.03	119.84
1	A	257	LEU	C-N-CA	6.55	128.03	119.84
4	D	672	VAL	N-CA-C	-6.48	102.97	112.04
4	D	610	GLU	N-CA-C	6.46	118.86	111.11
4	D	762	THR	N-CA-C	6.41	120.30	112.23
1	A	199	GLY	N-CA-C	-6.16	106.10	111.95
4	D	702	ARG	N-CA-C	6.12	119.52	109.85
4	D	611	TYR	N-CA-C	5.99	120.72	113.41
1	A	155	TRP	N-CA-C	-5.74	105.11	111.71
4	D	729	VAL	N-CA-C	5.73	117.46	109.55
3	C	487	LYS	N-CA-C	5.71	119.42	112.23
3	C	570	VAL	N-CA-C	5.68	114.37	107.61
3	C	432	ASP	N-CA-C	5.67	117.65	108.34
2	B	372	VAL	N-CA-C	5.67	116.74	108.53
5	E	942	LEU	N-CA-C	-5.66	104.48	111.33
3	C	496	LEU	N-CA-C	-5.63	105.03	112.34
3	C	537	VAL	N-CA-C	5.55	115.84	107.80
1	A	55	CYS	N-CA-C	5.53	117.52	109.84
1	A	119	VAL	CB-CA-C	-5.49	106.03	111.30
3	C	558	GLN	N-CA-C	5.48	117.74	109.41
1	A	147	ARG	N-CA-C	-5.47	106.11	112.89
4	D	627	GLU	N-CA-C	5.39	117.46	108.99
4	D	858	LEU	N-CA-C	5.38	117.15	111.28
1	A	97	VAL	N-CA-C	5.34	119.58	111.89
4	D	731	SER	N-CA-C	-5.26	100.16	108.73
4	D	617	ASP	CA-C-N	5.16	125.20	119.32
4	D	617	ASP	C-N-CA	5.16	125.20	119.32
4	D	786	ASP	N-CA-C	-5.11	107.33	113.21
5	E	895	GLU	N-CA-C	5.09	117.25	110.53
2	B	349	VAL	N-CA-C	5.06	115.56	108.17
4	D	721	VAL	N-CA-C	-5.00	107.42	112.17

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	2365	0	2290	134	0
2	B	622	0	587	51	0
3	C	1136	0	1106	96	0
4	D	2150	0	2110	152	0
5	E	851	0	853	64	0
6	F	105	0	88	8	0
7	G	28	0	25	3	0
7	H	28	0	25	6	0
7	I	28	0	25	1	0
8	A	14	0	13	1	0
9	A	8	0	11	1	0
10	A	1	0	0	0	0
11	A	5	0	0	0	0
11	E	5	0	0	0	0
12	A	14	0	0	2	0
12	B	2	0	0	0	0
12	C	3	0	0	1	0
12	D	14	0	0	0	0
12	E	6	0	0	0	0
All	All	7385	0	7133	425	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 29.

All (425) 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)
3:C:540:PRO:CA	5:E:887:THR:HG21	1.81	1.10
1:A:237:GLN:NE2	2:B:373:LYS:HB2	1.69	1.07
3:C:540:PRO:HA	5:E:887:THR:HG21	1.12	1.06
4:D:839:ARG:H	6:F:1:NAG:H81	1.20	1.04
2:B:403:ARG:HG3	2:B:403:ARG:HH11	1.14	1.02
4:D:748:ASN:HA	4:D:779:ASN:HD22	1.24	0.98
4:D:657:SER:HB3	4:D:817:LEU:HD23	1.49	0.94
1:A:167:ALA:HB1	3:C:444:GLN:NE2	1.82	0.94
4:D:839:ARG:N	6:F:1:NAG:H81	1.86	0.90
1:A:237:GLN:HE21	2:B:373:LYS:HB2	1.35	0.90
1:A:119:VAL:HG22	1:A:151:ALA:HB3	1.52	0.89
1:A:167:ALA:HB1	3:C:444:GLN:HE21	1.35	0.88
4:D:717:GLY:HA2	4:D:837:TRP:HD1	1.39	0.88
1:A:314:MET:HB3	1:A:316:MET:HE3	1.56	0.85
1:A:264:PRO:HD3	1:A:316:MET:HE1	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:644:TYR:CZ	4:D:669:PRO:HG3	2.12	0.84
1:A:271:MET:SD	1:A:327:THR:HG21	2.17	0.84
5:E:954:THR:HG22	5:E:999:THR:HB	1.59	0.82
5:E:886:ARG:HG2	5:E:886:ARG:HH11	1.44	0.81
1:A:204:GLN:HA	1:A:204:GLN:HE21	1.44	0.81
3:C:540:PRO:HA	5:E:887:THR:CG2	2.05	0.80
1:A:141:GLU:OE2	1:A:144:ARG:NH2	2.11	0.80
3:C:585:ASN:N	12:C:2003:HOH:O	2.15	0.80
4:D:657:SER:HB3	4:D:817:LEU:CD2	2.12	0.79
3:C:525:MET:HE1	3:C:565:LEU:HB3	1.65	0.79
3:C:564:LEU:HD23	3:C:565:LEU:N	1.98	0.78
3:C:488:GLU:HG2	4:D:873:GLN:O	1.81	0.78
4:D:716:VAL:HG21	4:D:813:VAL:HG11	1.66	0.78
4:D:714:TRP:CZ3	4:D:813:VAL:HG13	2.20	0.77
1:A:212:GLY:HA2	5:E:967:ARG:HD2	1.67	0.77
4:D:633:LEU:HD21	4:D:789:MET:HB2	1.66	0.77
1:A:303:GLN:HE21	1:A:312:THR:CG2	1.98	0.77
4:D:755:ARG:HG2	4:D:755:ARG:HH11	1.50	0.76
3:C:440:MET:O	3:C:444:GLN:HG2	1.86	0.76
3:C:469:TRP:O	3:C:473:GLU:HG2	1.84	0.76
3:C:573:VAL:HG12	3:C:573:VAL:O	1.84	0.76
4:D:783:TYR:HB3	4:D:792:THR:HG23	1.68	0.76
1:A:71:THR:HG22	1:A:73:ASP:OD1	1.86	0.75
5:E:937:LEU:O	5:E:989:THR:HA	1.86	0.75
1:A:56:PRO:HG3	1:A:115:ARG:NH2	2.02	0.75
2:B:403:ARG:HG3	2:B:403:ARG:NH1	1.94	0.75
2:B:416:GLU:HB2	3:C:475:LEU:HD21	1.70	0.74
4:D:853:ALA:HB1	5:E:925:GLU:HB3	1.68	0.73
3:C:536:LEU:HD21	3:C:544:ILE:HG12	1.69	0.73
3:C:443:LEU:HD11	3:C:465:LEU:HG	1.69	0.72
2:B:383:GLY:O	2:B:386:MET:HG2	1.89	0.72
1:A:167:ALA:CB	3:C:444:GLN:NE2	2.52	0.72
3:C:522:VAL:CG1	3:C:524:TRP:HB2	2.19	0.72
4:D:686:VAL:HG12	4:D:687:GLN:N	2.05	0.71
5:E:886:ARG:HG2	5:E:886:ARG:NH1	2.02	0.71
4:D:627:GLU:HB2	4:D:634:LEU:HD12	1.72	0.71
4:D:644:TYR:CE1	4:D:669:PRO:HG3	2.26	0.71
3:C:444:GLN:OE1	3:C:444:GLN:HA	1.90	0.70
4:D:688:GLU:HB3	4:D:702:ARG:HG2	1.73	0.70
1:A:173:THR:O	1:A:177:ARG:HB2	1.92	0.70
4:D:699:GLN:NE2	4:D:712:LEU:HD22	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:472:CYS:O	3:C:476:MET:HG3	1.91	0.69
2:B:373:LYS:HE3	2:B:375:ASP:O	1.92	0.69
3:C:445:HIS:CD2	3:C:447:ASP:H	2.10	0.69
1:A:237:GLN:HE21	2:B:373:LYS:CB	2.04	0.69
3:C:539:ASP:HB2	3:C:540:PRO:CD	2.23	0.69
3:C:539:ASP:HB2	3:C:540:PRO:HD2	1.73	0.69
1:A:240:ARG:HG2	1:A:251:ASP:OD1	1.93	0.69
1:A:317:GLY:HA2	1:A:321:GLN:OE1	1.92	0.68
4:D:716:VAL:CG2	4:D:813:VAL:HG11	2.23	0.68
4:D:861:GLU:HB3	5:E:901:ARG:NH2	2.09	0.68
1:A:204:GLN:HA	1:A:204:GLN:NE2	2.07	0.68
2:B:369:SER:OG	5:E:973:ASP:HB3	1.93	0.68
4:D:717:GLY:HA2	4:D:837:TRP:CD1	2.26	0.68
1:A:270:ASP:HB2	1:A:328:TRP:HE1	1.59	0.68
3:C:540:PRO:CB	5:E:887:THR:HG21	2.24	0.67
1:A:71:THR:HG23	1:A:321:GLN:H	1.59	0.67
6:F:1:NAG:H62	6:F:2:NAG:O5	1.93	0.67
2:B:361:TRP:O	2:B:365:LYS:HG3	1.94	0.67
4:D:704:TYR:HB2	4:D:707:GLN:CD	2.19	0.67
3:C:443:LEU:HD11	3:C:465:LEU:CG	2.24	0.67
4:D:817:LEU:N	4:D:817:LEU:HD12	2.11	0.66
1:A:237:GLN:NE2	2:B:373:LYS:CB	2.55	0.66
2:B:411:VAL:HG22	3:C:517:PRO:HG3	1.76	0.66
1:A:278:VAL:HG22	1:A:292:LEU:HD11	1.78	0.66
4:D:737:LEU:HD11	4:D:784:ILE:HD12	1.77	0.65
4:D:695:ALA:CB	7:H:2:NAG:H83	2.27	0.65
3:C:513:ILE:HB	4:D:870:VAL:CG1	2.27	0.65
3:C:443:LEU:CD1	3:C:465:LEU:HD11	2.27	0.65
4:D:756:ARG:HB3	4:D:759:TYR:HB3	1.77	0.65
4:D:828:PRO:O	4:D:830:ASN:N	2.30	0.65
3:C:527:ARG:HG3	3:C:565:LEU:HD11	1.78	0.64
4:D:748:ASN:HA	4:D:779:ASN:ND2	2.05	0.64
4:D:647:SER:HB3	4:D:663:ARG:O	1.98	0.64
1:A:315:THR:C	1:A:316:MET:HE2	2.23	0.63
3:C:518:LEU:HD11	4:D:862:MET:HA	1.80	0.63
1:A:78:LEU:HD21	4:D:825:VAL:HA	1.80	0.63
1:A:303:GLN:HG2	1:A:312:THR:HG21	1.80	0.63
3:C:501:CYS:O	3:C:505:GLN:HG2	1.99	0.63
4:D:612:LEU:HD11	4:D:708:ARG:O	1.99	0.63
4:D:695:ALA:HB1	7:H:2:NAG:H83	1.81	0.63
1:A:240:ARG:HE	1:A:247:PRO:HG3	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:1:NAG:C6	7:G:2:NAG:C1	2.77	0.62
1:A:97:VAL:HA	1:A:100:ILE:HD12	1.81	0.62
1:A:278:VAL:HG22	1:A:292:LEU:CD1	2.29	0.62
2:B:403:ARG:HH11	2:B:403:ARG:CG	2.00	0.62
4:D:686:VAL:HG22	4:D:704:TYR:CE1	2.34	0.62
5:E:907:ARG:HG3	5:E:907:ARG:HH11	1.64	0.62
1:A:58:VAL:O	1:A:60:PRO:HD3	2.00	0.61
4:D:751:GLU:HG3	5:E:995:MET:HE2	1.80	0.61
1:A:234:GLN:NE2	2:B:371:SER:OG	2.34	0.61
1:A:213:PHE:O	5:E:967:ARG:NH1	2.34	0.60
1:A:117:ILE:HG13	1:A:117:ILE:O	2.00	0.60
5:E:954:THR:HG23	5:E:955:THR:O	2.01	0.60
1:A:112:PRO:HA	1:A:147:ARG:HH11	1.67	0.60
3:C:514:VAL:HG22	4:D:869:VAL:HG22	1.84	0.60
4:D:748:ASN:CA	4:D:779:ASN:HD22	2.08	0.60
1:A:203:GLU:OE1	4:D:750:ARG:HB2	2.00	0.59
3:C:443:LEU:HD11	3:C:465:LEU:CD1	2.31	0.59
3:C:564:LEU:O	3:C:565:LEU:HD12	2.03	0.59
4:D:625:GLU:CD	4:D:634:LEU:HD11	2.28	0.59
4:D:692:ASN:ND2	7:H:1:NAG:H83	2.17	0.59
4:D:737:LEU:HD12	4:D:737:LEU:O	2.02	0.59
4:D:809:LEU:HD23	4:D:810:GLU:N	2.18	0.59
4:D:704:TYR:H	4:D:707:GLN:NE2	2.01	0.59
3:C:553:PRO:HD2	4:D:690:HIS:CE1	2.37	0.59
2:B:359:TYR:O	2:B:363:LEU:HG	2.03	0.58
4:D:644:TYR:CZ	4:D:669:PRO:CG	2.86	0.58
1:A:189:PRO:HB2	1:A:213:PHE:HE1	1.68	0.58
1:A:270:ASP:HB2	1:A:328:TRP:NE1	2.19	0.58
4:D:686:VAL:HG22	4:D:704:TYR:CD1	2.38	0.58
1:A:303:GLN:HE21	1:A:312:THR:HG21	1.68	0.58
1:A:141:GLU:O	1:A:145:GLN:HG2	2.02	0.58
1:A:223:TYR:CE2	2:B:384:PRO:HD3	2.38	0.58
3:C:582:GLN:O	3:C:582:GLN:HG3	2.03	0.58
5:E:919:HIS:ND1	5:E:994:PRO:HA	2.18	0.58
5:E:938:ASP:HA	5:E:988:ALA:O	2.03	0.58
3:C:484:SER:HA	5:E:886:ARG:HB3	1.86	0.57
4:D:611:TYR:O	4:D:612:LEU:HD23	2.04	0.57
4:D:721:VAL:CG1	4:D:816:ARG:HD3	2.34	0.57
1:A:159:ASP:HB2	3:C:446:HIS:HA	1.86	0.57
1:A:224:GLN:O	1:A:228:VAL:HG23	2.04	0.57
2:B:420:GLY:O	2:B:422:ALA:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:LEU:HD21	1:A:305:LYS:O	2.04	0.57
4:D:692:ASN:HD22	7:H:1:NAG:H83	1.70	0.57
4:D:709:HIS:HB3	4:D:845:LEU:CD2	2.34	0.57
1:A:335:LEU:C	1:A:335:LEU:HD13	2.29	0.56
3:C:513:ILE:HD12	3:C:513:ILE:N	2.19	0.56
4:D:839:ARG:H	6:F:1:NAG:C8	2.05	0.56
4:D:745:THR:HG21	4:D:777:PRO:O	2.06	0.56
3:C:495:LYS:C	3:C:497:ASN:N	2.61	0.56
1:A:162:THR:HG21	2:B:399:LYS:HE3	1.87	0.56
3:C:434:ALA:N	3:C:435:PRO:HD2	2.21	0.56
4:D:850:GLU:O	5:E:927:SER:HA	2.06	0.56
4:D:755:ARG:HD3	4:D:776:TYR:CG	2.42	0.55
4:D:854:ALA:CB	5:E:929:ARG:HH21	2.18	0.55
7:G:1:NAG:H61	7:G:2:NAG:C1	2.36	0.55
1:A:188:ARG:O	1:A:190:ARG:NH1	2.40	0.55
1:A:56:PRO:HD3	2:B:358:CYS:SG	2.47	0.55
1:A:112:PRO:HA	1:A:147:ARG:NH1	2.21	0.55
3:C:527:ARG:HG2	3:C:563:GLU:OE1	2.07	0.55
3:C:540:PRO:HB3	5:E:887:THR:CG2	2.37	0.55
1:A:309:THR:C	1:A:311:HIS:H	2.15	0.55
3:C:540:PRO:CB	5:E:887:THR:CG2	2.85	0.55
4:D:794:LEU:HB2	4:D:843:LEU:HB2	1.88	0.55
3:C:553:PRO:HG2	4:D:690:HIS:CD2	2.42	0.55
1:A:240:ARG:HG3	1:A:240:ARG:HH11	1.71	0.55
5:E:926:ASP:CG	5:E:932:SER:HB2	2.31	0.55
4:D:610:GLU:CD	4:D:610:GLU:H	2.13	0.55
4:D:692:ASN:HD22	7:H:1:NAG:C8	2.20	0.54
4:D:682:LYS:HE3	4:D:687:GLN:NE2	2.22	0.54
4:D:755:ARG:HG2	4:D:755:ARG:NH1	2.19	0.54
5:E:916:ARG:HG2	5:E:999:THR:HG23	1.88	0.54
3:C:564:LEU:C	3:C:565:LEU:HD12	2.33	0.54
1:A:119:VAL:HG21	1:A:193:TRP:CD1	2.43	0.54
3:C:522:VAL:HG11	3:C:524:TRP:HB2	1.90	0.54
1:A:313:VAL:HG22	1:A:314:MET:N	2.23	0.54
1:A:220:ARG:NH1	1:A:260:MET:CE	2.71	0.54
4:D:686:VAL:CG1	4:D:687:GLN:N	2.71	0.53
5:E:907:ARG:HG3	5:E:907:ARG:NH1	2.22	0.53
1:A:243:THR:HG22	1:A:243:THR:O	2.07	0.53
4:D:658:GLY:N	4:D:817:LEU:HD22	2.24	0.53
4:D:660:TYR:CE2	4:D:825:VAL:HG23	2.43	0.53
4:D:774:ASN:O	4:D:802:SER:CB	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:653:SER:OG	4:D:663:ARG:NH1	2.41	0.53
4:D:854:ALA:HA	5:E:921:PHE:HE1	1.73	0.53
2:B:400:ARG:HB2	4:D:797:ARG:CZ	2.38	0.53
3:C:513:ILE:HB	4:D:870:VAL:HG13	1.90	0.53
3:C:539:ASP:HA	3:C:578:TYR:CD2	2.43	0.53
4:D:854:ALA:HB1	5:E:929:ARG:HH21	1.74	0.53
5:E:918:GLU:HB2	5:E:997:ILE:HG12	1.90	0.53
5:E:932:SER:O	5:E:994:PRO:HG3	2.08	0.53
5:E:951:LEU:HD12	5:E:1002:ALA:HB2	1.90	0.53
1:A:240:ARG:CG	1:A:251:ASP:OD1	2.57	0.53
1:A:257:LEU:CD2	1:A:313:VAL:HG11	2.39	0.52
3:C:527:ARG:HG3	3:C:565:LEU:CD1	2.39	0.52
1:A:220:ARG:NH1	1:A:260:MET:HE1	2.25	0.52
4:D:616:PHE:CE1	4:D:689:VAL:HG21	2.45	0.52
4:D:817:LEU:HD12	4:D:817:LEU:H	1.73	0.52
5:E:886:ARG:HH11	5:E:886:ARG:CG	2.18	0.52
1:A:71:THR:HG23	1:A:321:GLN:N	2.24	0.52
8:A:1:NAG:O3	8:A:1:NAG:C7	2.58	0.52
4:D:721:VAL:HG13	4:D:816:ARG:HD3	1.91	0.52
2:B:381:ALA:HB2	2:B:387:PHE:CD1	2.45	0.52
5:E:938:ASP:C	5:E:939:LEU:HD23	2.35	0.52
4:D:784:ILE:HG13	4:D:784:ILE:O	2.10	0.52
1:A:230:LYS:HD2	1:A:306:LEU:HD13	1.92	0.52
1:A:321:GLN:O	1:A:322:TYR:HB2	2.09	0.51
3:C:488:GLU:OE1	3:C:488:GLU:N	2.42	0.51
3:C:457:VAL:HG12	3:C:461:TYR:CE2	2.46	0.51
4:D:822:ALA:O	4:D:823:ARG:HD3	2.10	0.51
1:A:54:THR:O	1:A:54:THR:HG22	2.09	0.51
1:A:220:ARG:HG2	1:A:260:MET:HE1	1.93	0.51
4:D:692:ASN:ND2	7:H:1:NAG:C8	2.74	0.51
4:D:716:VAL:HG21	4:D:813:VAL:CG1	2.39	0.51
1:A:230:LYS:HB3	1:A:306:LEU:HD22	1.93	0.51
5:E:889:PHE:CG	5:E:890:SER:N	2.78	0.51
1:A:117:ILE:HA	1:A:149:GLU:O	2.11	0.51
1:A:223:TYR:CZ	2:B:384:PRO:HD3	2.46	0.51
4:D:774:ASN:O	4:D:802:SER:HB2	2.11	0.51
1:A:198:PHE:N	1:A:198:PHE:CD2	2.76	0.51
2:B:386:MET:HB3	4:D:655:GLN:HG2	1.91	0.51
4:D:757:ARG:HH22	4:D:806:ASP:CG	2.18	0.51
3:C:522:VAL:HG12	3:C:524:TRP:HB2	1.92	0.51
1:A:240:ARG:NH2	1:A:247:PRO:HB3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:900:VAL:HG12	5:E:901:ARG:N	2.24	0.50
5:E:929:ARG:O	5:E:930:ASN:C	2.53	0.50
1:A:220:ARG:CZ	1:A:260:MET:HE3	2.41	0.50
1:A:243:THR:O	1:A:243:THR:CG2	2.58	0.50
3:C:513:ILE:HB	4:D:870:VAL:HG12	1.93	0.50
4:D:699:GLN:HE22	4:D:712:LEU:HD22	1.77	0.50
4:D:859:GLN:HA	4:D:862:MET:HE3	1.94	0.50
3:C:473:GLU:HB2	3:C:492:PHE:CE1	2.46	0.50
3:C:507:ALA:HB3	3:C:510:PHE:HD2	1.77	0.50
1:A:165:TYR:O	1:A:169:ILE:HG13	2.11	0.50
4:D:709:HIS:CD2	4:D:843:LEU:HD22	2.47	0.50
1:A:56:PRO:HG3	1:A:115:ARG:HH22	1.73	0.50
3:C:488:GLU:CG	4:D:873:GLN:O	2.57	0.50
3:C:518:LEU:CD1	4:D:862:MET:HG2	2.42	0.50
3:C:564:LEU:HD23	3:C:565:LEU:H	1.75	0.50
4:D:660:TYR:CE2	4:D:823:ARG:HB2	2.47	0.50
1:A:204:GLN:HE21	1:A:204:GLN:CA	2.10	0.49
3:C:443:LEU:CD2	3:C:461:TYR:HB3	2.42	0.49
3:C:504:THR:HG21	3:C:528:LEU:HD13	1.94	0.49
4:D:751:GLU:CG	5:E:995:MET:HE2	2.42	0.49
1:A:196:ASP:O	1:A:220:ARG:HD2	2.11	0.49
4:D:709:HIS:HB3	4:D:845:LEU:HD23	1.93	0.49
1:A:113:THR:HG22	2:B:353:TYR:HD2	1.78	0.49
1:A:202:ARG:O	1:A:241:ALA:HB1	2.13	0.49
4:D:607:ILE:HG21	4:D:689:VAL:HG23	1.95	0.49
5:E:899:SER:HA	5:E:921:PHE:CE2	2.46	0.49
4:D:744:TYR:N	4:D:744:TYR:CD1	2.80	0.49
4:D:866:ALA:HB1	4:D:867:PRO:HD2	1.95	0.49
1:A:237:GLN:HB2	2:B:371:SER:O	2.13	0.49
1:A:291:GLU:HA	1:A:291:GLU:OE1	2.13	0.49
4:D:839:ARG:CA	6:F:1:NAG:H81	2.42	0.49
5:E:954:THR:CG2	5:E:958:ALA:HA	2.43	0.49
7:G:1:NAG:H61	7:G:2:NAG:O5	2.13	0.49
1:A:158:ASN:HA	3:C:444:GLN:O	2.13	0.49
4:D:780:SER:HB2	4:D:781:ARG:HE	1.78	0.49
2:B:395:ARG:HD2	3:C:451:GLY:HA2	1.95	0.48
1:A:224:GLN:HE22	4:D:766:ASN:HB3	1.78	0.48
4:D:750:ARG:HB3	5:E:995:MET:HE1	1.96	0.48
1:A:56:PRO:HG3	1:A:115:ARG:CZ	2.42	0.48
5:E:900:VAL:CG1	5:E:901:ARG:N	2.77	0.48
2:B:396:PRO:HG2	4:D:814:HIS:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:443:LEU:HD11	3:C:465:LEU:HD11	1.91	0.48
4:D:805:ARG:HG3	4:D:805:ARG:HH11	1.78	0.48
4:D:607:ILE:O	4:D:607:ILE:HG13	2.12	0.48
4:D:817:LEU:C	4:D:818:LEU:HD23	2.38	0.48
2:B:391:TYR:HA	2:B:394:SER:OG	2.14	0.48
2:B:411:VAL:HG22	3:C:517:PRO:CG	2.41	0.48
3:C:558:GLN:N	3:C:558:GLN:CD	2.72	0.48
1:A:240:ARG:HG3	1:A:240:ARG:NH1	2.29	0.47
4:D:732:ARG:HG3	4:D:809:LEU:O	2.14	0.47
2:B:403:ARG:NH1	2:B:403:ARG:CG	2.67	0.47
3:C:550:VAL:HG21	3:C:565:LEU:HD22	1.95	0.47
2:B:397:ALA:HB1	6:F:2:NAG:C8	2.45	0.47
2:B:414:GLN:O	2:B:418:LEU:HG	2.14	0.47
1:A:54:THR:HG21	1:A:145:GLN:O	2.14	0.47
2:B:397:ALA:HB1	6:F:2:NAG:H82	1.96	0.47
4:D:723:ASP:OD2	4:D:727:LYS:NZ	2.47	0.47
4:D:820:ASP:OD1	4:D:822:ALA:N	2.46	0.47
3:C:447:ASP:HA	3:C:452:THR:OG1	2.15	0.47
1:A:126:ARG:HE	1:A:126:ARG:HB2	1.53	0.47
1:A:288:ASN:O	1:A:292:LEU:HB2	2.15	0.47
3:C:537:VAL:HG22	3:C:580:VAL:HG22	1.96	0.47
4:D:635:LEU:HD13	4:D:789:MET:SD	2.54	0.47
4:D:658:GLY:CA	4:D:817:LEU:HD22	2.44	0.47
1:A:151:ALA:O	1:A:191:VAL:O	2.33	0.47
4:D:667:ASN:ND2	4:D:770:PRO:CG	2.78	0.47
4:D:769:GLU:HB3	4:D:772:ALA:HB3	1.97	0.47
5:E:908:TRP:HB3	5:E:912:THR:HG22	1.97	0.47
1:A:72:HIS:HD2	1:A:319:ASP:OD1	1.98	0.46
1:A:303:GLN:HE21	1:A:312:THR:HG22	1.76	0.46
3:C:575:PHE:CD1	3:C:575:PHE:C	2.93	0.46
5:E:939:LEU:HD23	5:E:939:LEU:N	2.30	0.46
5:E:918:GLU:CB	5:E:997:ILE:HG12	2.45	0.46
4:D:678:THR:HA	4:D:690:HIS:O	2.16	0.46
1:A:77:TRP:CE2	9:A:2:TRS:H12	2.51	0.46
1:A:119:VAL:HG13	1:A:152:ASN:CB	2.46	0.46
3:C:520:ARG:CA	3:C:572:ALA:HB2	2.46	0.46
1:A:333:ASP:OD1	2:B:353:TYR:OH	2.31	0.46
1:A:77:TRP:CD2	1:A:78:LEU:HG	2.51	0.46
1:A:78:LEU:HD23	3:C:454:ARG:HG3	1.98	0.46
1:A:314:MET:HB3	1:A:316:MET:CE	2.39	0.46
2:B:400:ARG:NH1	4:D:796:ASP:HB2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:MET:HE1	12:A:2014:HOH:O	2.15	0.46
4:D:609:ASN:C	4:D:609:ASN:OD1	2.59	0.46
7:I:1:NAG:H61	7:I:2:NAG:C1	2.45	0.45
1:A:240:ARG:HH21	1:A:247:PRO:CG	2.29	0.45
2:B:414:GLN:HG2	5:E:905:LEU:HB3	1.98	0.45
1:A:335:LEU:HD13	1:A:335:LEU:O	2.17	0.45
1:A:202:ARG:CZ	4:D:753:LEU:HD21	2.46	0.45
1:A:223:TYR:HD1	2:B:381:ALA:O	2.00	0.45
4:D:644:TYR:CE2	4:D:669:PRO:HG3	2.50	0.45
4:D:686:VAL:CG2	4:D:704:TYR:CE1	2.99	0.45
1:A:200:HIS:H	2:B:377:PHE:HB2	1.82	0.45
4:D:814:HIS:CD2	4:D:815:ARG:H	2.35	0.45
5:E:954:THR:HG23	5:E:955:THR:N	2.32	0.45
5:E:936:THR:CG2	5:E:989:THR:CG2	2.95	0.45
2:B:369:SER:OG	5:E:973:ASP:CB	2.63	0.45
3:C:539:ASP:HB3	3:C:545:VAL:HG21	1.99	0.45
1:A:163:THR:OG1	1:A:168:ILE:HD11	2.17	0.44
1:A:225:ASP:HB2	4:D:763:TRP:CZ3	2.52	0.44
3:C:431:GLY:O	3:C:475:LEU:HD13	2.18	0.44
3:C:465:LEU:O	3:C:469:TRP:HD1	2.00	0.44
3:C:564:LEU:HD23	3:C:564:LEU:C	2.42	0.44
4:D:703:LEU:HD23	4:D:703:LEU:HA	1.76	0.44
1:A:176:LEU:O	1:A:180:GLU:HB2	2.17	0.44
4:D:730:ILE:O	4:D:730:ILE:HG13	2.17	0.44
4:D:774:ASN:O	4:D:802:SER:OG	2.31	0.44
2:B:403:ARG:NH2	4:D:779:ASN:O	2.50	0.44
4:D:854:ALA:HB1	5:E:929:ARG:NH2	2.32	0.44
5:E:953:GLU:OE1	5:E:953:GLU:HA	2.17	0.44
4:D:688:GLU:HA	4:D:701:VAL:O	2.17	0.44
1:A:301:THR:O	1:A:305:LYS:HG3	2.17	0.44
3:C:486:LEU:HD11	3:C:511:GLN:NE2	2.32	0.44
4:D:699:GLN:HG2	4:D:700:VAL:N	2.33	0.44
4:D:735:THR:N	4:D:807:GLY:O	2.50	0.44
5:E:946:PHE:HB3	5:E:1006:TRP:CD1	2.52	0.44
1:A:315:THR:O	1:A:316:MET:HE2	2.18	0.43
4:D:778:VAL:HG11	4:D:811:LEU:CD2	2.48	0.43
1:A:202:ARG:CG	1:A:241:ALA:HA	2.49	0.43
3:C:510:PHE:CD1	3:C:510:PHE:C	2.96	0.43
3:C:533:HIS:HD1	3:C:582:GLN:CD	2.24	0.43
5:E:936:THR:HG23	5:E:989:THR:CG2	2.49	0.43
1:A:103:SER:HB3	1:A:325:ALA:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ALA:CB	3:C:444:GLN:HE22	2.27	0.43
4:D:750:ARG:NH1	5:E:997:ILE:HD11	2.33	0.43
1:A:240:ARG:HH21	1:A:247:PRO:CB	2.32	0.43
3:C:445:HIS:CG	3:C:446:HIS:N	2.86	0.43
4:D:686:VAL:HG12	4:D:687:GLN:H	1.79	0.43
5:E:936:THR:CG2	5:E:989:THR:HG23	2.49	0.43
1:A:202:ARG:HA	1:A:239:TRP:CZ2	2.53	0.43
1:A:257:LEU:HD22	1:A:313:VAL:HG11	2.01	0.43
4:D:665:ASN:OD1	4:D:666:GLN:CD	2.61	0.43
1:A:103:SER:O	1:A:104:VAL:C	2.62	0.43
4:D:605:LEU:HB3	4:D:616:PHE:HB2	2.01	0.43
4:D:728:GLU:OE2	4:D:815:ARG:NH2	2.49	0.43
4:D:660:TYR:CZ	4:D:825:VAL:HG23	2.54	0.43
1:A:137:LYS:HA	1:A:140:ARG:HH21	1.84	0.43
4:D:660:TYR:OH	4:D:825:VAL:HG23	2.19	0.42
4:D:699:GLN:HE21	4:D:701:VAL:HG22	1.84	0.42
4:D:728:GLU:HG2	4:D:815:ARG:HB2	2.01	0.42
5:E:926:ASP:OD1	5:E:932:SER:HB2	2.18	0.42
4:D:617:ASP:HB3	4:D:620:THR:OG1	2.19	0.42
5:E:919:HIS:CE1	5:E:994:PRO:HA	2.54	0.42
1:A:75:VAL:HG12	1:A:75:VAL:O	2.20	0.42
4:D:856:HIS:O	4:D:860:ALA:HB2	2.19	0.42
1:A:73:ASP:O	1:A:120:GLU:HG2	2.20	0.42
1:A:177:ARG:O	1:A:181:GLU:HG2	2.19	0.42
3:C:510:PHE:CE1	3:C:580:VAL:HB	2.53	0.42
3:C:528:LEU:HA	3:C:529:PRO:HD3	1.89	0.42
1:A:326:ASN:ND2	12:A:2013:HOH:O	2.51	0.42
3:C:443:LEU:HD21	3:C:461:TYR:HB3	2.01	0.42
5:E:922:ALA:HA	5:E:995:MET:HG2	2.01	0.42
2:B:403:ARG:O	2:B:403:ARG:HG2	2.20	0.42
2:B:406:TYR:CZ	2:B:410:GLN:NE2	2.87	0.42
2:B:406:TYR:OH	2:B:410:GLN:NE2	2.53	0.42
3:C:445:HIS:CE1	3:C:446:HIS:CE1	3.08	0.42
4:D:838:VAL:HG12	4:D:839:ARG:N	2.34	0.42
5:E:899:SER:HA	5:E:921:PHE:HE2	1.85	0.42
5:E:906:ALA:O	5:E:913:LEU:HD22	2.19	0.42
3:C:536:LEU:HB2	3:C:583:MET:HE3	2.02	0.42
4:D:851:THR:O	4:D:851:THR:HG22	2.20	0.42
2:B:386:MET:HE2	4:D:655:GLN:HB2	2.02	0.42
1:A:257:LEU:HA	1:A:258:PRO:HD3	1.82	0.41
3:C:495:LYS:C	3:C:497:ASN:H	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:PHE:HE1	1:A:322:TYR:CE2	2.38	0.41
3:C:439:ALA:HB1	3:C:465:LEU:HD23	2.02	0.41
4:D:692:ASN:OD1	4:D:692:ASN:C	2.63	0.41
3:C:470:ARG:CB	3:C:471:PRO:HD3	2.50	0.41
1:A:180:GLU:C	1:A:180:GLU:CD	2.89	0.41
1:A:192:ALA:HB3	1:A:216:PHE:HD1	1.85	0.41
1:A:217:PHE:CD2	1:A:255:SER:HB3	2.55	0.41
1:A:296:PHE:O	1:A:299:LEU:N	2.53	0.41
2:B:376:ASP:CG	4:D:755:ARG:HH22	2.29	0.41
3:C:545:VAL:HG13	3:C:546:PRO:HD2	2.01	0.41
5:E:940:THR:O	5:E:941:ASN:HB3	2.20	0.41
5:E:941:ASN:CG	5:E:941:ASN:O	2.63	0.41
1:A:90:ASN:ND2	1:A:95:ALA:H	2.18	0.41
5:E:887:THR:O	5:E:887:THR:HG22	2.20	0.41
1:A:118:TYR:HE2	1:A:120:GLU:O	2.04	0.41
2:B:416:GLU:CB	3:C:475:LEU:HD21	2.46	0.41
3:C:538:LYS:HB2	3:C:579:SER:OG	2.20	0.41
4:D:744:TYR:O	4:D:782:ILE:HA	2.20	0.41
1:A:167:ALA:CB	3:C:444:GLN:HE21	2.16	0.41
1:A:211:MET:HG2	5:E:956:LEU:HB3	2.03	0.41
1:A:266:GLY:C	1:A:267:LEU:HD23	2.46	0.41
1:A:281:ASP:OD1	1:A:283:ARG:HG3	2.21	0.41
3:C:524:TRP:CD2	4:D:867:PRO:HG3	2.55	0.41
4:D:671:PHE:C	4:D:673:SER:N	2.79	0.41
1:A:67:LEU:HD23	1:A:314:MET:HB2	2.03	0.41
1:A:90:ASN:HD22	1:A:90:ASN:HA	1.72	0.41
1:A:205:ALA:HB3	1:A:241:ALA:HB2	2.03	0.41
1:A:262:ASN:ND2	1:A:262:ASN:N	2.69	0.41
2:B:409:LEU:HD11	3:C:437:ASN:HA	2.02	0.40
3:C:509:ARG:HB3	4:D:875:GLY:N	2.36	0.40
3:C:536:LEU:HD23	3:C:537:VAL:N	2.36	0.40
4:D:714:TRP:CZ3	4:D:813:VAL:CG1	2.98	0.40
4:D:757:ARG:HG2	4:D:758:ASN:ND2	2.36	0.40
4:D:685:LEU:O	4:D:705:PRO:HD3	2.21	0.40
4:D:704:TYR:O	4:D:707:GLN:HG2	2.21	0.40
2:B:397:ALA:CB	6:F:2:NAG:H82	2.51	0.40
4:D:611:TYR:CD1	4:D:611:TYR:N	2.88	0.40
5:E:954:THR:HG21	5:E:958:ALA:HA	2.03	0.40
1:A:200:HIS:HB2	2:B:377:PHE:CD2	2.56	0.40
2:B:387:PHE:O	4:D:661:ILE:HA	2.22	0.40
2:B:419:ALA:C	2:B:421:PRO:HD3	2.46	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	290/298 (97%)	262 (90%)	25 (9%)	3 (1%)	12	32
2	B	74/84 (88%)	68 (92%)	5 (7%)	1 (1%)	9	23
3	C	149/159 (94%)	133 (89%)	15 (10%)	1 (1%)	18	41
4	D	266/282 (94%)	247 (93%)	16 (6%)	3 (1%)	11	29
5	E	105/126 (83%)	98 (93%)	6 (6%)	1 (1%)	12	32
All	All	884/949 (93%)	808 (91%)	67 (8%)	9 (1%)	12	32

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	920	GLN
1	A	77	TRP
2	B	421	PRO
4	D	874	GLY
1	A	260	MET
3	C	445	HIS
1	A	258	PRO
4	D	653	SER
4	D	829	LEU

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	251/260 (96%)	239 (95%)	12 (5%)	23	50
2	B	65/71 (92%)	60 (92%)	5 (8%)	12	30
3	C	125/139 (90%)	119 (95%)	6 (5%)	23	50
4	D	227/240 (95%)	216 (95%)	11 (5%)	23	50
5	E	93/111 (84%)	89 (96%)	4 (4%)	26	54
All	All	761/821 (93%)	723 (95%)	38 (5%)	22	48

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	VAL
1	A	148	LEU
1	A	198	PHE
1	A	207	LEU
1	A	227	LYS
1	A	236	GLU
1	A	240	ARG
1	A	243	THR
1	A	262	ASN
1	A	299	LEU
1	A	312	THR
1	A	337	GLN
2	B	347	ILE
2	B	384	PRO
2	B	403	ARG
2	B	409	LEU
2	B	410	GLN
3	C	472	CYS
3	C	473	GLU
3	C	502	PRO
3	C	511	GLN
3	C	536	LEU
3	C	540	PRO
4	D	619	ASN
4	D	636	PRO
4	D	639	GLN
4	D	657	SER
4	D	679	HIS
4	D	705	PRO
4	D	729	VAL
4	D	778	VAL

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Mol	Chain	Res	Type
4	D	818	LEU
4	D	832	GLU
4	D	847	ASP
5	E	886	ARG
5	E	907	ARG
5	E	932	SER
5	E	954	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	93	GLN
1	A	145	GLN
1	A	158	ASN
1	A	234	GLN
1	A	237	GLN
1	A	303	GLN
1	A	326	ASN
2	B	350	ASN
3	C	445	HIS
3	C	511	GLN
4	D	628	ASN
4	D	639	GLN
4	D	699	GLN
4	D	707	GLN
4	D	748	ASN
4	D	779	ASN
4	D	814	HIS
4	D	873	GLN
5	E	950	ASN
5	E	960	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 ⓘ

15 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
6	NAG	F	1	3,6	14,14,15	0.62	0	17,19,21	1.27	1 (5%)
6	NAG	F	2	6	14,14,15	0.57	0	17,19,21	0.90	1 (5%)
6	BMA	F	3	6	11,11,12	0.42	0	15,15,17	0.60	0
6	MAN	F	4	6	11,11,12	0.47	0	15,15,17	0.85	1 (6%)
6	MAN	F	5	6	11,11,12	0.53	0	15,15,17	0.68	0
6	MAN	F	6	6	11,11,12	0.40	0	15,15,17	0.71	1 (6%)
6	MAN	F	7	6	11,11,12	0.56	0	15,15,17	0.42	0
6	MAN	F	8	6	11,11,12	0.81	1 (9%)	15,15,17	0.86	0
6	MAN	F	9	6	11,11,12	1.64	2 (18%)	15,15,17	2.78	4 (26%)
7	NAG	G	1	4,7	14,14,15	0.77	0	17,19,21	0.99	1 (5%)
7	NAG	G	2	7	14,14,15	0.84	0	17,19,21	1.18	2 (11%)
7	NAG	H	1	4,7	14,14,15	0.54	0	17,19,21	0.96	1 (5%)
7	NAG	H	2	7	14,14,15	0.60	0	17,19,21	0.76	0
7	NAG	I	1	4,7	14,14,15	0.76	0	17,19,21	1.07	1 (5%)
7	NAG	I	2	7	14,14,15	0.64	0	17,19,21	0.88	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
6	NAG	F	1	3,6	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
6	BMA	F	3	6	-	0/2/19/22	0/1/1/1
6	MAN	F	4	6	-	0/2/19/22	0/1/1/1
6	MAN	F	5	6	-	1/2/19/22	0/1/1/1
6	MAN	F	6	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	F	7	6	-	2/2/19/22	0/1/1/1
6	MAN	F	8	6	-	2/2/19/22	0/1/1/1
6	MAN	F	9	6	-	1/2/19/22	0/1/1/1
7	NAG	G	1	4,7	-	2/6/23/26	0/1/1/1
7	NAG	G	2	7	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	H	1	4,7	-	4/6/23/26	0/1/1/1
7	NAG	H	2	7	-	4/6/23/26	0/1/1/1
7	NAG	I	1	4,7	-	5/6/23/26	0/1/1/1
7	NAG	I	2	7	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	9	MAN	C1-C2	-3.16	1.44	1.52
6	F	9	MAN	O5-C1	2.97	1.48	1.43
6	F	8	MAN	C2-C3	2.18	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	9	MAN	C6-C5-C4	6.27	128.42	113.02
6	F	9	MAN	C1-C2-C3	6.01	118.39	109.64
6	F	9	MAN	C1-O5-C5	3.83	117.31	112.19
6	F	9	MAN	O3-C3-C2	-3.69	102.52	110.05
6	F	1	NAG	O5-C1-C2	3.46	116.65	111.29
7	G	2	NAG	O5-C1-C2	2.87	115.73	111.29
6	F	2	NAG	C2-N2-C7	-2.86	119.06	122.90
7	G	2	NAG	C2-N2-C7	-2.60	119.41	122.90
6	F	4	MAN	C1-O5-C5	2.55	115.60	112.19
7	I	2	NAG	C2-N2-C7	-2.35	119.75	122.90
7	I	1	NAG	C2-N2-C7	-2.25	119.89	122.90
7	H	1	NAG	C2-N2-C7	-2.24	119.89	122.90
7	G	1	NAG	C1-C2-N2	-2.14	107.07	110.43
6	F	6	MAN	C1-O5-C5	2.09	114.99	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	F	1	NAG	C1
7	G	2	NAG	C1

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	1	NAG	C8-C7-N2-C2
6	F	1	NAG	O7-C7-N2-C2
7	G	2	NAG	C8-C7-N2-C2
7	G	2	NAG	O7-C7-N2-C2
7	H	1	NAG	C8-C7-N2-C2
7	H	1	NAG	O7-C7-N2-C2
7	H	2	NAG	C8-C7-N2-C2
7	H	2	NAG	O7-C7-N2-C2
7	I	1	NAG	C8-C7-N2-C2
7	I	1	NAG	O7-C7-N2-C2
7	I	2	NAG	C8-C7-N2-C2
7	I	2	NAG	O7-C7-N2-C2
7	G	1	NAG	O7-C7-N2-C2
7	H	1	NAG	O5-C5-C6-O6
7	H	2	NAG	O5-C5-C6-O6
6	F	7	MAN	O5-C5-C6-O6
7	G	1	NAG	C8-C7-N2-C2
7	H	1	NAG	C4-C5-C6-O6
6	F	7	MAN	C4-C5-C6-O6
7	I	2	NAG	O5-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
7	H	2	NAG	C4-C5-C6-O6
6	F	9	MAN	O5-C5-C6-O6
7	G	2	NAG	O5-C5-C6-O6
7	I	2	NAG	C4-C5-C6-O6
6	F	8	MAN	O5-C5-C6-O6
6	F	2	NAG	C4-C5-C6-O6
6	F	5	MAN	O5-C5-C6-O6
7	I	1	NAG	C4-C5-C6-O6
7	I	1	NAG	O5-C5-C6-O6
7	G	2	NAG	C4-C5-C6-O6
6	F	8	MAN	C4-C5-C6-O6
7	I	1	NAG	C3-C2-N2-C7

There are no ring outliers.

8 monomers are involved in 18 short contacts:

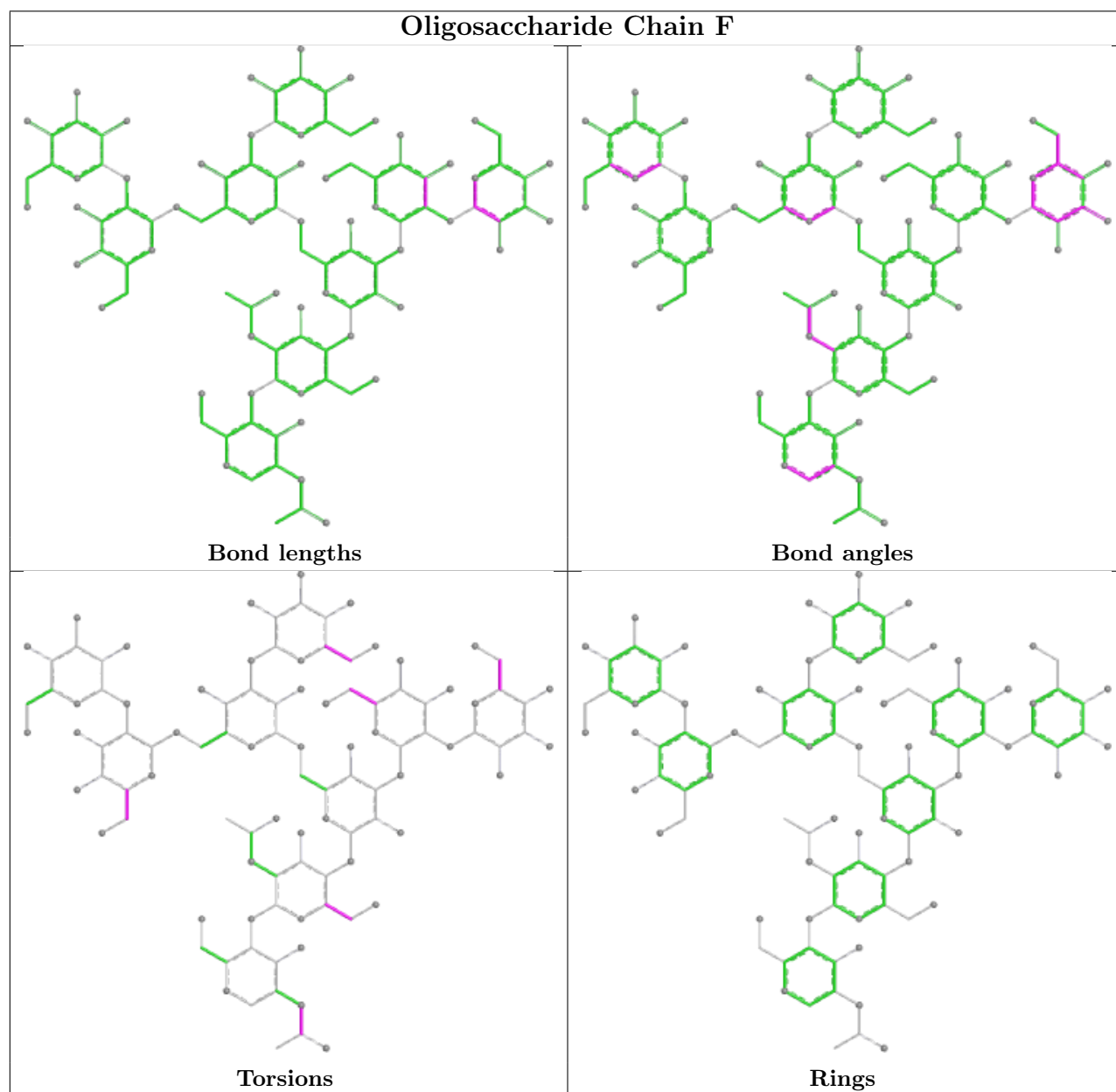
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	2	NAG	1	0
7	G	1	NAG	3	0
6	F	2	NAG	4	0

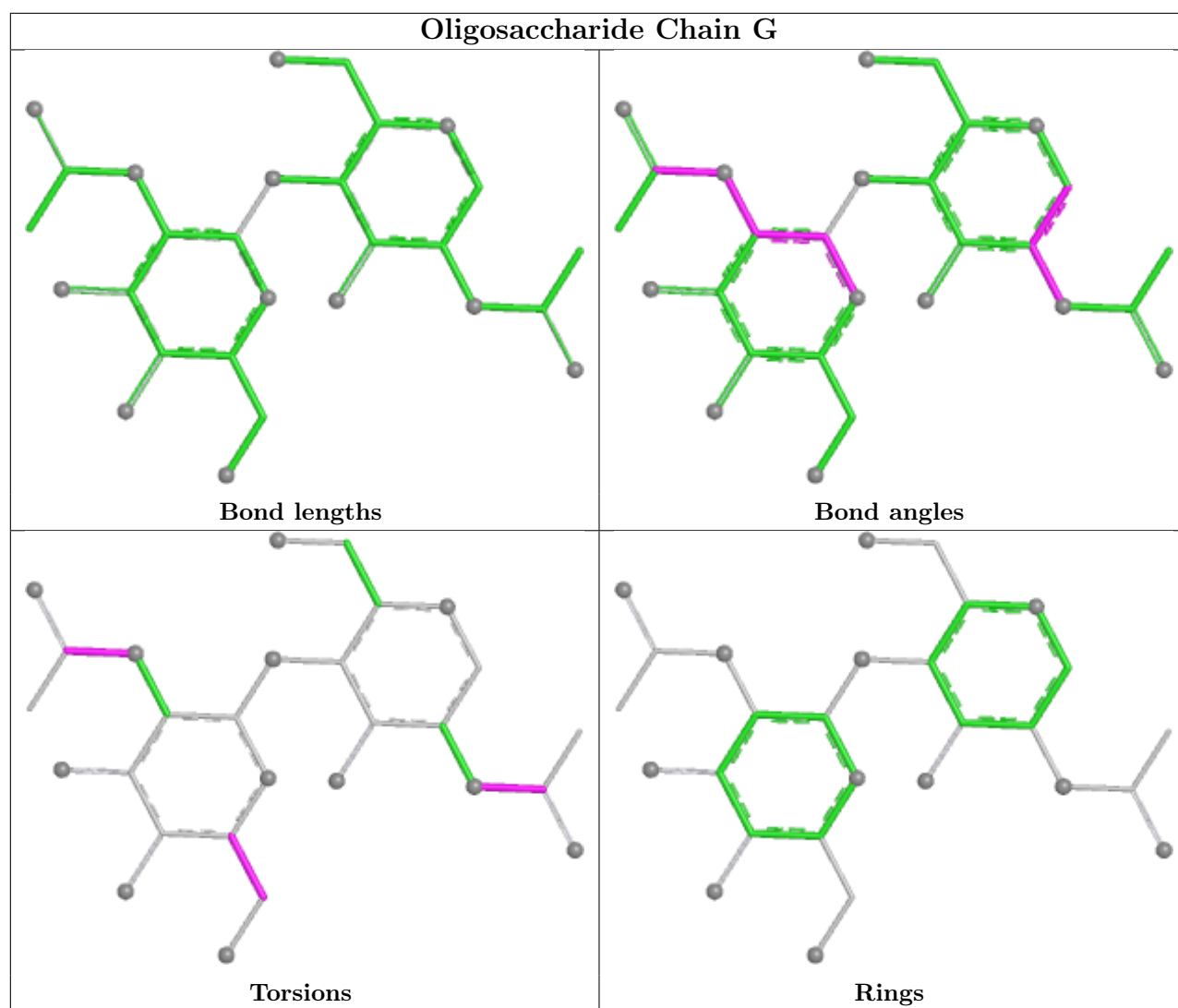
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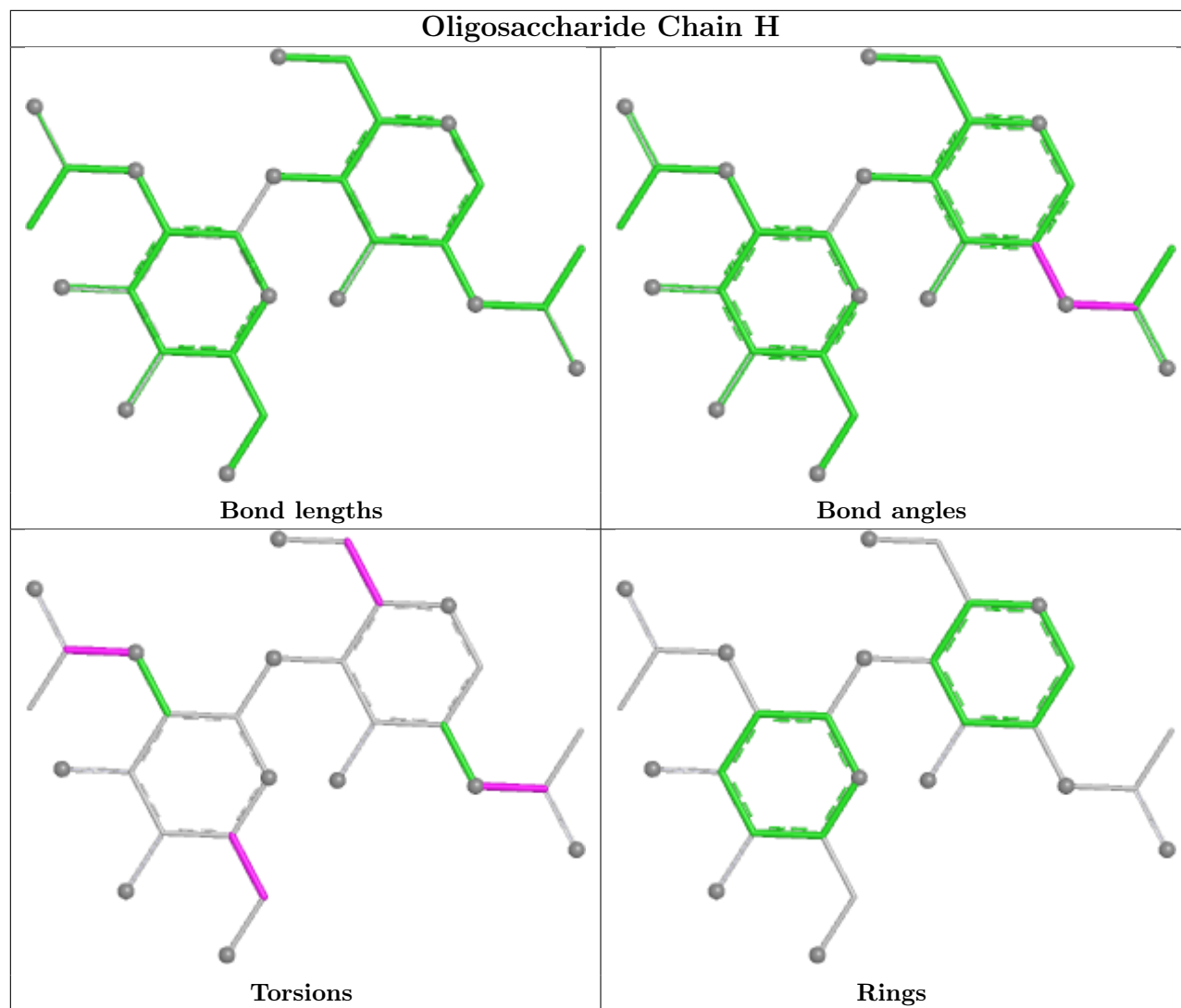
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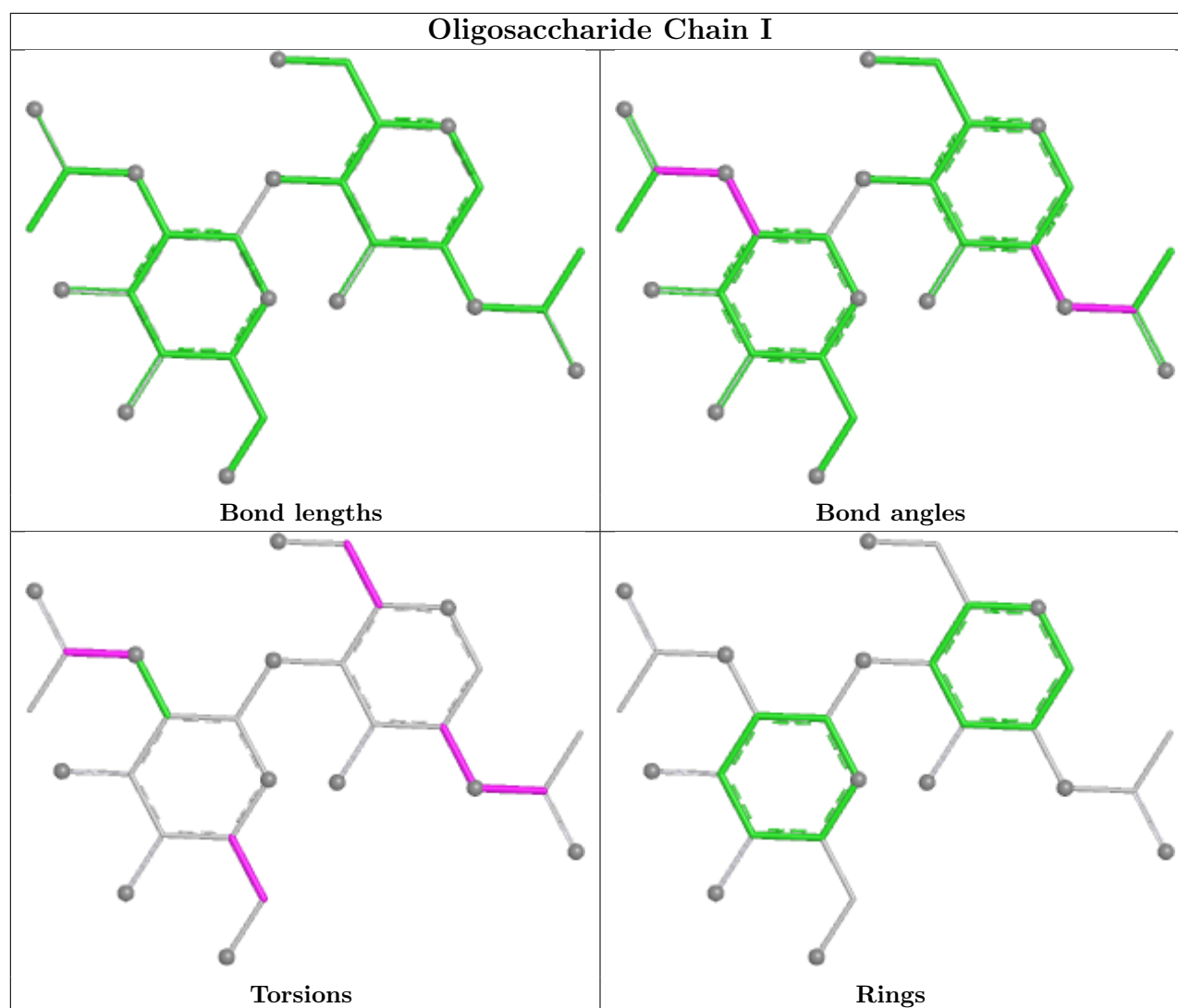
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	1	NAG	1	0
7	H	1	NAG	4	0
7	G	2	NAG	3	0
6	F	1	NAG	5	0
7	H	2	NAG	2	0

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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
9	TRS	A	2	10	7,7,7	1.69	3 (42%)	9,9,9	1.08	0
11	SO4	A	3001	-	4,4,4	0.61	0	6,6,6	0.22	0
8	NAG	A	1	1	14,14,15	0.72	0	17,19,21	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	SO4	E	3002	-	4,4,4	0.72	0	6,6,6	0.15	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
9	TRS	A	2	10	-	0/9/9/9	-
8	NAG	A	1	1	-	5/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2	TRS	C2-C	2.58	1.60	1.53
9	A	2	TRS	C3-C	2.28	1.59	1.53
9	A	2	TRS	C-N	-2.14	1.42	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1	NAG	C3-C2-N2-C7
8	A	1	NAG	C8-C7-N2-C2
8	A	1	NAG	O7-C7-N2-C2
8	A	1	NAG	C4-C5-C6-O6
8	A	1	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2	TRS	1	0
8	A	1	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	292/298 (97%)	-0.02	2 (0%) 84 83	22, 36, 54, 76	0
2	B	76/84 (90%)	0.14	5 (6%) 24 21	18, 35, 70, 87	0
3	C	151/159 (94%)	0.06	2 (1%) 75 73	22, 36, 56, 95	0
4	D	270/282 (95%)	0.22	8 (2%) 52 49	21, 38, 58, 94	0
5	E	109/126 (86%)	0.15	3 (2%) 55 51	16, 38, 59, 92	0
All	All	898/949 (94%)	0.10	20 (2%) 62 59	16, 37, 58, 95	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	421	PRO	4.9
4	D	830	ASN	4.7
5	E	885	PRO	4.2
1	A	271	MET	4.1
3	C	556	ASP	4.0
4	D	875	GLY	3.6
5	E	941	ASN	3.4
4	D	707	GLN	3.1
2	B	348	ARG	3.0
2	B	420	GLY	3.0
1	A	290	LYS	2.9
4	D	832	GLU	2.9
4	D	850	GLU	2.5
2	B	422	ALA	2.4
3	C	486	LEU	2.3
2	B	375	ASP	2.3
5	E	893	ARG	2.2
4	D	833	GLY	2.2
4	D	706	ARG	2.2
4	D	805	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

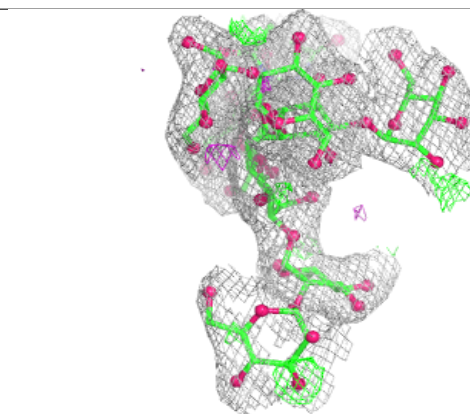
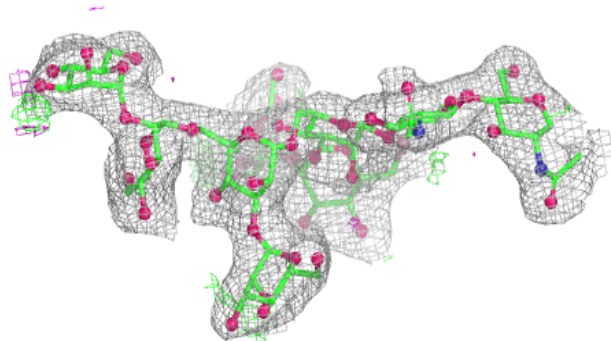
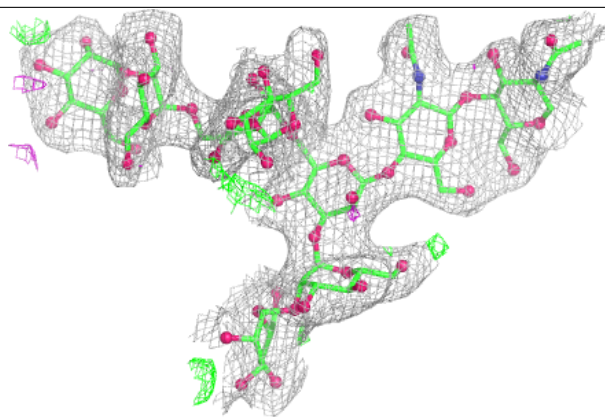
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	G	2	14/15	0.77	0.18	79,79,79,79	0
6	MAN	F	9	11/12	0.81	0.16	72,72,72,72	0
7	NAG	H	2	14/15	0.82	0.14	67,67,67,67	0
7	NAG	I	2	14/15	0.83	0.15	75,75,75,75	0
6	MAN	F	7	11/12	0.84	0.12	57,57,57,57	0
7	NAG	G	1	14/15	0.88	0.12	50,50,50,50	0
7	NAG	H	1	14/15	0.89	0.10	46,46,46,46	0
6	MAN	F	8	11/12	0.91	0.09	44,44,44,44	0
6	MAN	F	5	11/12	0.92	0.10	32,32,32,32	0
7	NAG	I	1	14/15	0.94	0.09	44,44,44,44	0
6	NAG	F	1	14/15	0.94	0.10	31,31,31,31	0
6	BMA	F	3	11/12	0.95	0.08	33,33,33,33	0
6	MAN	F	4	11/12	0.96	0.07	33,33,33,33	0
6	NAG	F	2	14/15	0.96	0.08	25,25,25,25	0
6	MAN	F	6	11/12	0.96	0.07	27,27,27,27	0

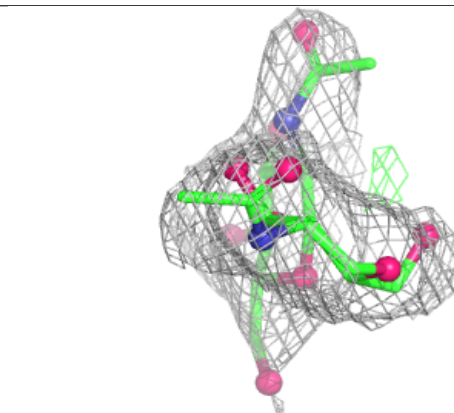
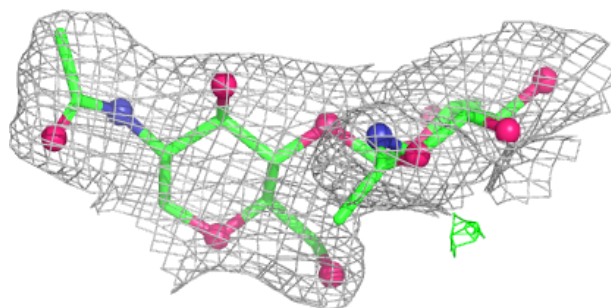
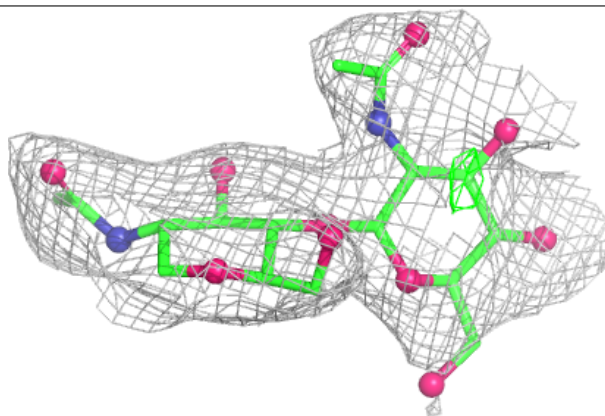
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain F:

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

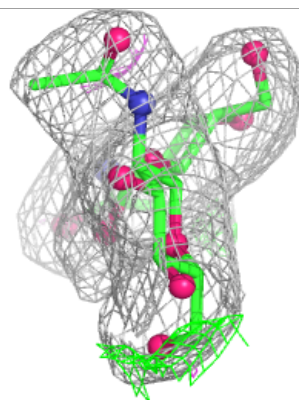
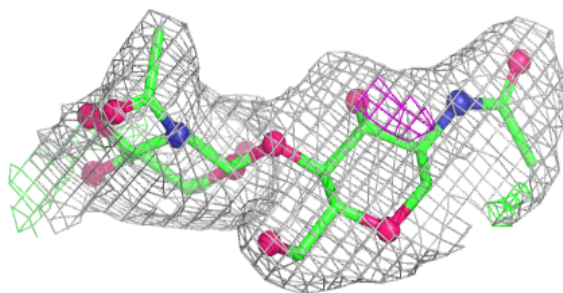
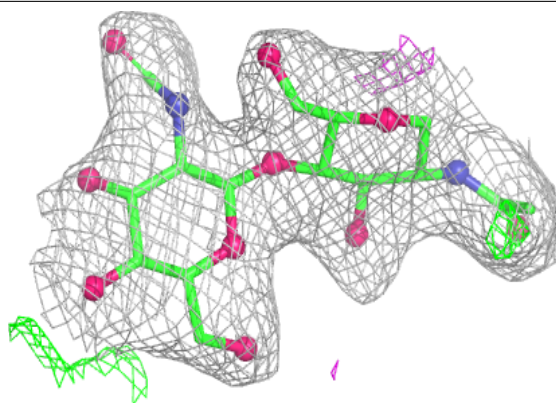
**Electron density around Chain G:**

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

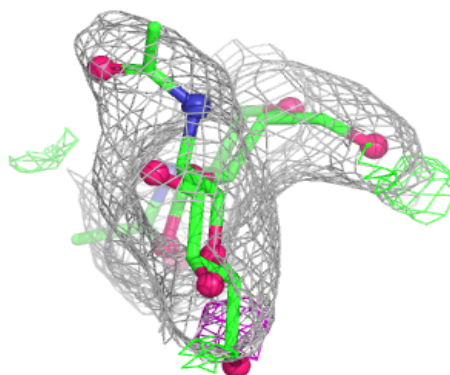
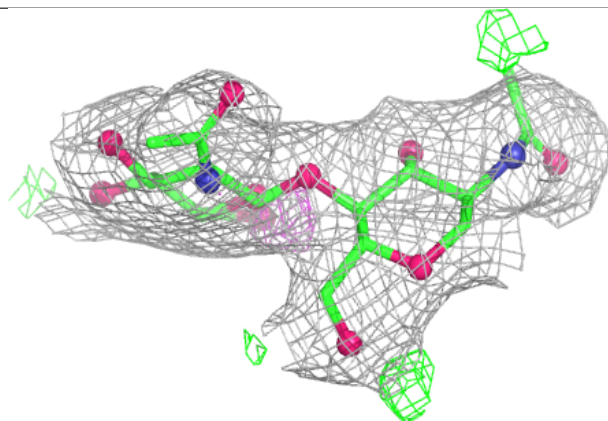
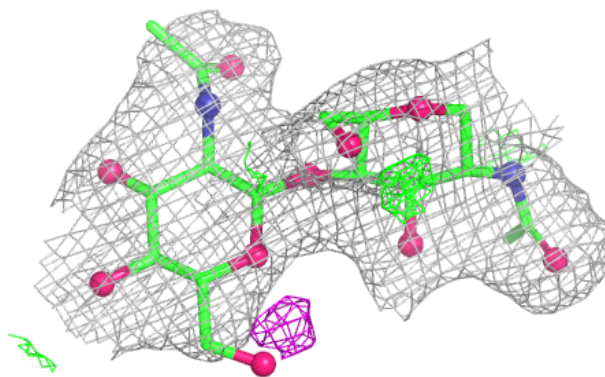


Electron density around Chain H:

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

**Electron density around Chain I:**

$2mF_o-DF_c$ (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(\AA^2)	Q<0.9
8	NAG	A	1	14/15	0.82	0.13	57,57,57,57	0
9	TRS	A	2	8/8	0.86	0.19	35,35,35,35	0
11	SO4	A	3001	5/5	0.96	0.16	36,36,36,36	0
11	SO4	E	3002	5/5	0.98	0.11	36,36,36,36	0
10	ZN	A	3	1/1	0.99	0.04	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.