



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:07 PM UTC

PDB ID : 5N0A / pdb_00005n0a
Title : Crystal structure of A259C covalently linked dengue 2 virus envelope glycoprotein dimer in complex with the Fab fragment of the broadly neutralizing human antibody EDE2 A11
Authors : Vaney, M.C.; Rouvinski, A.; Guardado-Calvo, P.; Sharma, A.; Rey, F.A.
Deposited on : 2017-02-02
Resolution : 3.90 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

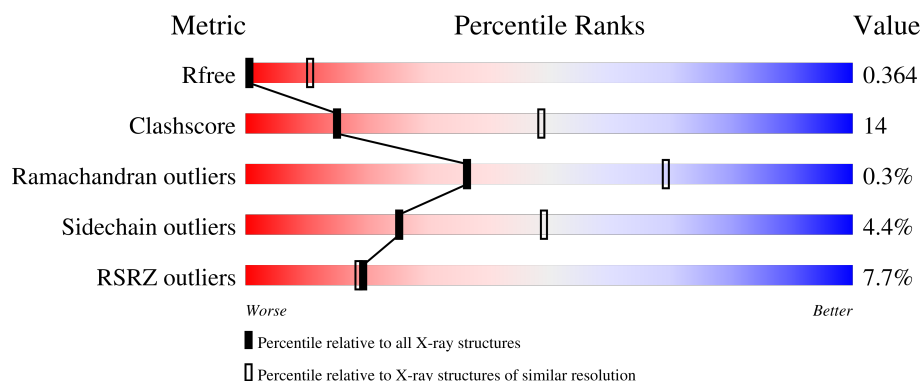
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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 $\leq 5\%$. 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	430	
1	B	430	
2	H	283	
2	I	283	
3	L	218	

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Mol	Chain	Length	Quality of chain
3	M	218	2% 44% 7% 50%
4	C	6	33% 50% 17%
4	D	6	17% 83%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9683 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 Envelope Glycoprotein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2914	1842	497	551	24			
1	B	379	Total	C	N	O	S	0	0	0
			2943	1859	501	558	25			

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	118	LYS	MET	conflict	UNP Q68Y26
A	259	CYS	ALA	engineered mutation	UNP Q68Y26
A	396	LEU	-	expression tag	UNP Q68Y26
A	397	VAL	-	expression tag	UNP Q68Y26
A	398	PRO	-	expression tag	UNP Q68Y26
A	399	ARG	-	expression tag	UNP Q68Y26
A	400	GLY	-	expression tag	UNP Q68Y26
A	401	SER	-	expression tag	UNP Q68Y26
A	402	SER	-	expression tag	UNP Q68Y26
A	403	ALA	-	expression tag	UNP Q68Y26
A	404	TRP	-	expression tag	UNP Q68Y26
A	405	SER	-	expression tag	UNP Q68Y26
A	406	HIS	-	expression tag	UNP Q68Y26
A	407	PRO	-	expression tag	UNP Q68Y26
A	408	GLN	-	expression tag	UNP Q68Y26
A	409	PHE	-	expression tag	UNP Q68Y26
A	410	GLU	-	expression tag	UNP Q68Y26
A	411	LYS	-	expression tag	UNP Q68Y26
A	412	GLY	-	expression tag	UNP Q68Y26
A	413	GLY	-	expression tag	UNP Q68Y26
A	414	SER	-	expression tag	UNP Q68Y26
A	415	GLY	-	expression tag	UNP Q68Y26
A	416	GLY	-	expression tag	UNP Q68Y26
A	417	GLY	-	expression tag	UNP Q68Y26
A	418	SER	-	expression tag	UNP Q68Y26

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Chain	Residue	Modelled	Actual	Comment	Reference
A	419	GLY	-	expression tag	UNP Q68Y26
A	420	GLY	-	expression tag	UNP Q68Y26
A	421	SER	-	expression tag	UNP Q68Y26
A	422	ALA	-	expression tag	UNP Q68Y26
A	423	TRP	-	expression tag	UNP Q68Y26
A	424	SER	-	expression tag	UNP Q68Y26
A	425	HIS	-	expression tag	UNP Q68Y26
A	426	PRO	-	expression tag	UNP Q68Y26
A	427	GLN	-	expression tag	UNP Q68Y26
A	428	PHE	-	expression tag	UNP Q68Y26
A	429	GLU	-	expression tag	UNP Q68Y26
A	430	LYS	-	expression tag	UNP Q68Y26
B	118	LYS	MET	conflict	UNP Q68Y26
B	259	CYS	ALA	engineered mutation	UNP Q68Y26
B	396	LEU	-	expression tag	UNP Q68Y26
B	397	VAL	-	expression tag	UNP Q68Y26
B	398	PRO	-	expression tag	UNP Q68Y26
B	399	ARG	-	expression tag	UNP Q68Y26
B	400	GLY	-	expression tag	UNP Q68Y26
B	401	SER	-	expression tag	UNP Q68Y26
B	402	SER	-	expression tag	UNP Q68Y26
B	403	ALA	-	expression tag	UNP Q68Y26
B	404	TRP	-	expression tag	UNP Q68Y26
B	405	SER	-	expression tag	UNP Q68Y26
B	406	HIS	-	expression tag	UNP Q68Y26
B	407	PRO	-	expression tag	UNP Q68Y26
B	408	GLN	-	expression tag	UNP Q68Y26
B	409	PHE	-	expression tag	UNP Q68Y26
B	410	GLU	-	expression tag	UNP Q68Y26
B	411	LYS	-	expression tag	UNP Q68Y26
B	412	GLY	-	expression tag	UNP Q68Y26
B	413	GLY	-	expression tag	UNP Q68Y26
B	414	SER	-	expression tag	UNP Q68Y26
B	415	GLY	-	expression tag	UNP Q68Y26
B	416	GLY	-	expression tag	UNP Q68Y26
B	417	GLY	-	expression tag	UNP Q68Y26
B	418	SER	-	expression tag	UNP Q68Y26
B	419	GLY	-	expression tag	UNP Q68Y26
B	420	GLY	-	expression tag	UNP Q68Y26
B	421	SER	-	expression tag	UNP Q68Y26
B	422	ALA	-	expression tag	UNP Q68Y26
B	423	TRP	-	expression tag	UNP Q68Y26

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Chain	Residue	Modelled	Actual	Comment	Reference
B	424	SER	-	expression tag	UNP Q68Y26
B	425	HIS	-	expression tag	UNP Q68Y26
B	426	PRO	-	expression tag	UNP Q68Y26
B	427	GLN	-	expression tag	UNP Q68Y26
B	428	PHE	-	expression tag	UNP Q68Y26
B	429	GLU	-	expression tag	UNP Q68Y26
B	430	LYS	-	expression tag	UNP Q68Y26

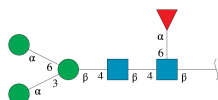
- Molecule 2 is a protein called BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	131	Total	C	N	O	S	0	0	0
			1032	652	178	197	5			
2	I	131	Total	C	N	O	S	0	0	0
			1032	652	178	197	5			

- Molecule 3 is a protein called BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	110	Total	C	N	O	S	0	0	0
			810	502	137	167	4			
3	M	110	Total	C	N	O	S	0	0	0
			810	502	137	167	4			

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

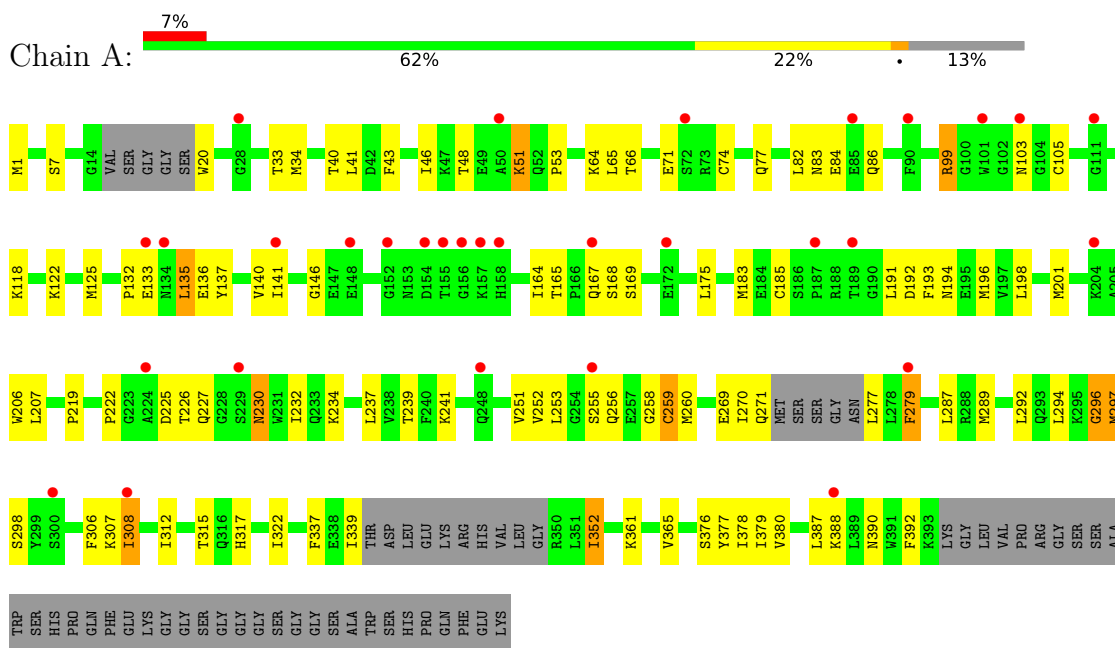


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	6	Total	C	N	O	0	0	0
			71	40	2	29			
4	D	6	Total	C	N	O	0	0	0
			71	40	2	29			

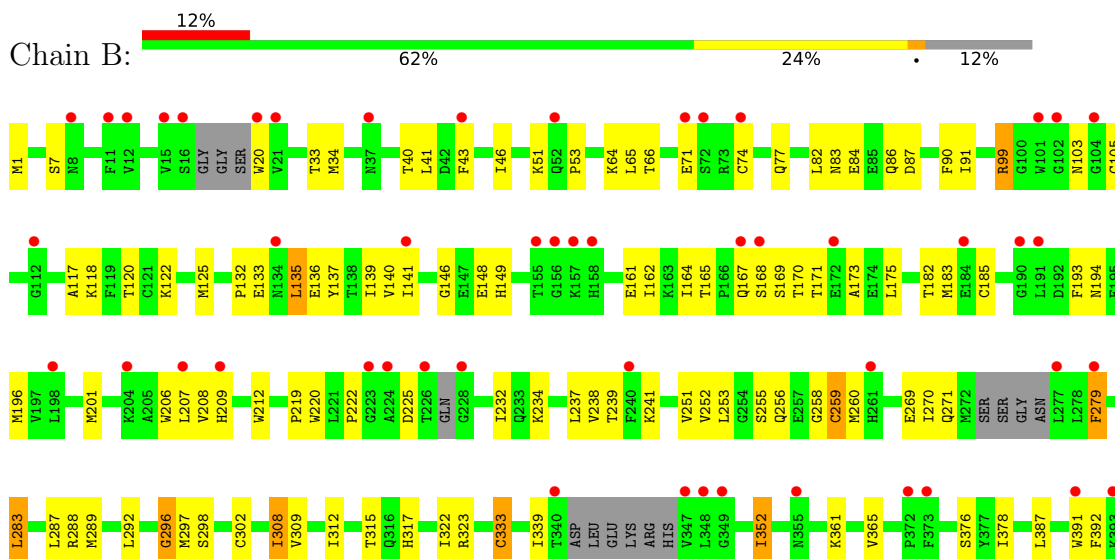
3 Residue-property plots

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: Envelope Glycoprotein E

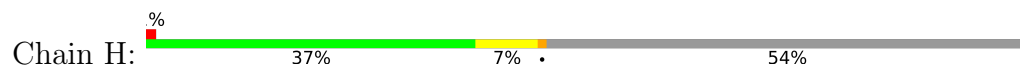


• Molecule 1: Envelope Glycoprotein E



LYS
GLY
LEU
VAL
PRO
ARG
GLY
SER
SER
SER
ALA
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS
GLY
GLY
SER
GLY
GLY
GLY
GLY
GLY
GLY
ALA
ALA
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

● Molecule 2: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11 HEAVY CHAIN



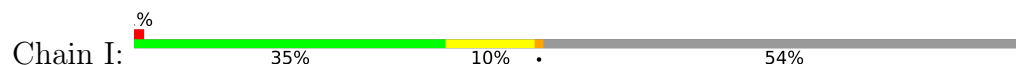
GLU
V2
P14
G15
A40
K43
R50
V63
K64
R66
R66
F67
A74
M62
V93
G96
Y100
Y100A
D100B
S100C
T100D
G100E
Y100F
Y100G
P100H
D100I
S100J
F100K
F100L
K100M
Y100N
G100O
M100P
D101
S112
SER
ALA
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GLY
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GLY
ALA
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Y100N
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GLY
GLY
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

● Molecule 2: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11 HEAVY CHAIN



GLU
V2
P14
C22
A40
K43
R50
I51
R57
V63
K64
G65
R66
F67
T68
I69
S70
R71
L78
M82
V93
G96
Y100
Y100A
D100B
D100C
S100C
T100D
G100E
Y100F
Y100G
P100H
D100I
S100J
F100K
F100L
K100M
Y100N
G100O
M100P
D101
S112
SER
ALA
SER
THR
LYS
GLY

PRO
SER
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PHE
PRO
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ALA
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● Molecule 3: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11

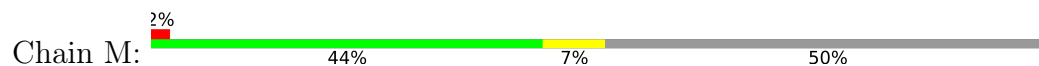


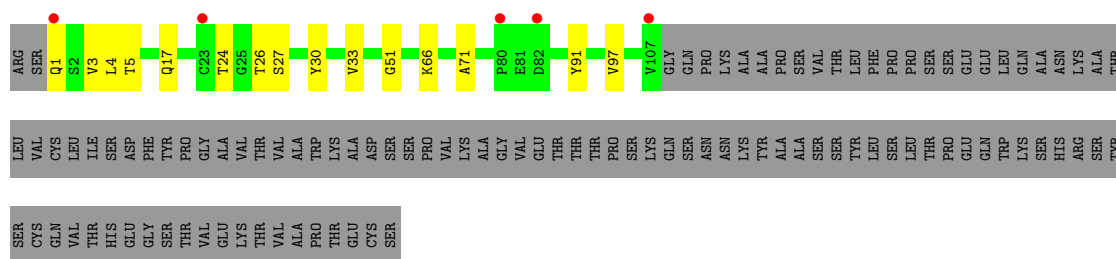
ARG
Q1
S2
V3
L4
C23
T26
S27
Y30
V33
K66
V97
Y107
GLY
GLN
SER
GLN
ASN
LYS
ALA
ALA
PRO
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VAL
SER
THR
LEU
PHE
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PRO
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LEU
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HIS
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TYR
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CYS
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● Molecule 3: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11





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

Chain C: 33% 50% 17%



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

Chain D: 17% 83%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	58.77Å 182.30Å 208.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.90 20.00 – 3.90	Depositor EDS
% Data completeness (in resolution range)	90.7 (20.00-3.90) 89.8 (20.00-3.90)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	0.32	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.88Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.285 , 0.300 0.324 , 0.364	Depositor DCC
R_{free} test set	955 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	78.7	Xtriage
Anisotropy	1.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 122.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	9683	wwPDB-VP
Average B, all atoms (Å ²)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.65% 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, NAG, BMA, FUC

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	0.66	0/2972	1.20	16/4014 (0.4%)
1	B	0.67	0/2998	1.19	15/4047 (0.4%)
2	H	0.57	0/1060	1.01	0/1439
2	I	0.58	0/1060	1.02	0/1439
3	L	0.63	0/825	1.00	3/1122 (0.3%)
3	M	0.63	0/825	0.99	3/1122 (0.3%)
All	All	0.64	0/9740	1.12	37/13183 (0.3%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	PHE	CA-C-N	8.82	132.46	120.38
1	A	279	PHE	C-N-CA	8.82	132.46	120.38
1	B	279	PHE	CA-C-N	8.54	132.08	120.38
1	B	279	PHE	C-N-CA	8.54	132.08	120.38
1	A	296	GLY	CA-C-N	7.10	135.09	121.54
1	A	296	GLY	C-N-CA	7.10	135.09	121.54
3	L	66	LYS	N-CA-C	6.98	120.05	109.23
3	M	66	LYS	N-CA-C	6.61	119.47	109.23
1	B	296	GLY	CA-C-N	6.52	133.99	121.54
1	B	296	GLY	C-N-CA	6.52	133.99	121.54
3	L	1	GLN	CA-C-N	5.92	131.71	121.64
3	L	1	GLN	C-N-CA	5.92	131.71	121.64
3	M	1	GLN	CA-C-N	5.91	131.69	121.64
3	M	1	GLN	C-N-CA	5.91	131.69	121.64
1	A	234	LYS	CA-C-N	5.66	128.64	120.38
1	A	234	LYS	C-N-CA	5.66	128.64	120.38
1	B	83	ASN	CA-C-N	5.64	128.62	120.38
1	B	83	ASN	C-N-CA	5.64	128.62	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	ASN	CA-C-N	5.57	128.51	120.38
1	A	83	ASN	C-N-CA	5.57	128.51	120.38
1	B	352	ILE	N-CA-C	-5.49	106.45	111.67
1	A	352	ILE	N-CA-C	-5.47	106.47	111.67
1	A	361	LYS	CA-C-N	5.43	127.55	120.28
1	A	361	LYS	C-N-CA	5.43	127.55	120.28
1	B	234	LYS	CA-C-N	5.42	128.29	120.38
1	B	234	LYS	C-N-CA	5.42	128.29	120.38
1	A	51	LYS	N-CA-C	5.41	119.83	111.56
1	B	361	LYS	CA-C-N	5.37	127.48	120.28
1	B	361	LYS	C-N-CA	5.37	127.48	120.28
1	B	308	ILE	CA-C-N	5.28	127.70	120.46
1	B	308	ILE	C-N-CA	5.28	127.70	120.46
1	B	168	SER	CA-C-N	5.28	127.88	120.28
1	B	168	SER	C-N-CA	5.28	127.88	120.28
1	A	308	ILE	CA-C-N	5.24	127.63	120.46
1	A	308	ILE	C-N-CA	5.24	127.63	120.46
1	A	168	SER	CA-C-N	5.20	127.77	120.28
1	A	168	SER	C-N-CA	5.20	127.77	120.28

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	2914	0	2907	98	0
1	B	2943	0	2943	106	0
2	H	1032	0	963	11	0
2	I	1032	0	963	41	0
3	L	810	0	798	5	0
3	M	810	0	798	12	0
4	C	71	0	61	1	0
4	D	71	0	61	2	0
All	All	9683	0	9494	262	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 14.

All (262) 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:B:46:ILE:HD12	1:B:140:VAL:CG2	1.28	1.56
1:B:46:ILE:CD1	1:B:140:VAL:CG2	1.85	1.51
2:I:50:ARG:NH1	2:I:100(L):PHE:HE2	1.28	1.31
1:B:46:ILE:CD1	1:B:140:VAL:HG21	1.52	1.24
2:I:67:PHE:CE1	2:I:82:MET:HB3	1.72	1.22
1:A:191:LEU:CD2	1:A:196:MET:HE2	1.73	1.19
2:I:50:ARG:NH1	2:I:100(L):PHE:CE2	2.06	1.19
1:A:219:PRO:HD3	1:A:237:LEU:HD13	1.13	1.11
1:A:219:PRO:CD	1:A:237:LEU:HD13	1.79	1.10
1:B:312:ILE:HG12	1:B:322:ILE:HG12	1.32	1.10
1:A:41:LEU:HD13	1:A:141:ILE:HD11	1.35	1.08
1:A:312:ILE:HG12	1:A:322:ILE:HG12	1.34	1.08
2:I:67:PHE:HE1	2:I:82:MET:HB3	0.90	1.06
2:I:67:PHE:CE1	2:I:82:MET:HE2	1.91	1.04
1:B:41:LEU:HD13	1:B:141:ILE:HD11	1.35	1.04
1:A:219:PRO:HD3	1:A:237:LEU:CD1	1.89	1.02
1:A:191:LEU:HD23	1:A:196:MET:CE	1.90	1.01
1:B:46:ILE:HD13	1:B:140:VAL:HG21	1.41	1.00
1:B:46:ILE:HD11	1:B:140:VAL:CG2	1.97	0.95
2:I:67:PHE:HE1	2:I:82:MET:CB	1.79	0.95
2:I:67:PHE:CZ	2:I:82:MET:HE2	2.02	0.95
1:A:191:LEU:HD23	1:A:196:MET:HE2	0.96	0.94
1:A:191:LEU:CD2	1:A:196:MET:CE	2.47	0.91
1:B:46:ILE:CD1	1:B:140:VAL:HG23	1.70	0.90
1:A:255:SER:OG	1:B:255:SER:CB	2.20	0.89
1:B:46:ILE:CD1	1:B:140:VAL:CB	2.50	0.89
1:B:46:ILE:HD11	1:B:140:VAL:CB	2.02	0.89
1:B:46:ILE:HD11	1:B:140:VAL:HB	1.56	0.88
1:A:169:SER:HB2	1:A:185:CYS:O	1.75	0.87
1:B:169:SER:HB2	1:B:185:CYS:O	1.75	0.87
2:I:67:PHE:CE1	2:I:82:MET:CB	2.55	0.86
2:I:51:ILE:HD11	2:I:78:LEU:CD1	2.06	0.85
1:B:208:VAL:HG11	1:B:212:TRP:CE3	2.11	0.85
1:A:82:LEU:HB3	1:A:84:GLU:OE1	1.78	0.84
1:A:255:SER:OG	1:B:255:SER:HB3	1.77	0.84
1:B:82:LEU:HB3	1:B:84:GLU:OE1	1.77	0.83
3:M:5:THR:HG23	3:M:24:THR:HG23	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:CYS:N	1:B:333:CYS:SG	2.51	0.83
1:B:256:GLN:HA	1:B:259:CYS:SG	2.20	0.82
1:A:256:GLN:HA	1:A:259:CYS:SG	2.19	0.81
1:B:162:ILE:HD12	1:B:173:ALA:HB2	1.62	0.80
2:I:67:PHE:CE1	2:I:82:MET:CE	2.63	0.80
2:I:51:ILE:HG22	2:I:57:ARG:HG2	1.63	0.80
2:I:63:VAL:HG22	2:I:67:PHE:HD2	1.46	0.79
1:B:46:ILE:HD12	1:B:140:VAL:HG23	0.76	0.75
1:B:99:ARG:NH1	1:B:103:ASN:OD1	2.19	0.75
1:B:46:ILE:HD11	1:B:140:VAL:HG21	1.64	0.73
1:A:255:SER:OG	1:B:255:SER:HB2	1.87	0.73
2:I:51:ILE:HG23	2:I:69:ILE:CG2	2.19	0.72
3:L:4:LEU:HD13	3:L:97:VAL:HG13	1.72	0.72
2:H:63:VAL:HG11	2:H:67:PHE:HB2	1.72	0.72
1:A:133:GLU:HB3	1:A:167:GLN:HG2	1.71	0.72
1:B:162:ILE:HD11	1:B:171:THR:CG2	2.20	0.72
3:M:4:LEU:HD13	3:M:97:VAL:HG13	1.72	0.72
2:I:50:ARG:NH1	2:I:100(L):PHE:CZ	2.57	0.71
1:A:201:MET:HE1	1:A:260:MET:HB3	1.73	0.71
2:I:63:VAL:HG22	2:I:67:PHE:CD2	2.25	0.71
1:B:133:GLU:HB3	1:B:167:GLN:HG2	1.72	0.70
1:B:201:MET:HE1	1:B:260:MET:HB3	1.74	0.68
2:I:51:ILE:CG2	2:I:69:ILE:HG23	2.24	0.67
3:L:30:TYR:HA	3:L:33:VAL:HG23	1.77	0.67
1:B:46:ILE:HD12	1:B:140:VAL:CB	2.18	0.67
1:A:51:LYS:O	1:A:53:PRO:HD3	1.95	0.67
1:A:34:MET:HG2	1:A:40:THR:HG22	1.77	0.66
1:B:34:MET:HG2	1:B:40:THR:HG22	1.78	0.65
1:B:64:LYS:HB3	1:B:122:LYS:HD2	1.79	0.65
1:B:51:LYS:O	1:B:53:PRO:HD3	1.97	0.65
1:B:185:CYS:HB3	1:B:283:LEU:HD22	1.77	0.65
2:I:63:VAL:CG2	2:I:67:PHE:HD2	2.09	0.65
2:H:63:VAL:CG1	2:H:67:PHE:HB2	2.27	0.65
1:A:191:LEU:HD21	1:A:196:MET:CE	2.26	0.65
1:B:308:ILE:HD11	1:B:387:LEU:HD13	1.79	0.65
1:A:315:THR:HG23	1:A:317:HIS:H	1.61	0.64
1:B:315:THR:HG23	1:B:317:HIS:H	1.62	0.63
1:B:253:LEU:O	1:B:253:LEU:HG	1.97	0.63
1:A:207:LEU:HG	1:A:270:ILE:HD11	1.81	0.63
1:A:253:LEU:O	1:A:253:LEU:HG	1.98	0.63
1:B:392:PHE:O	1:B:392:PHE:CD1	2.52	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:51:ILE:HG23	2:I:69:ILE:HG21	1.80	0.62
1:B:46:ILE:CD1	1:B:140:VAL:HB	2.22	0.62
2:H:96:GLY:HA3	2:H:101:ASP:OD2	1.99	0.62
2:I:96:GLY:HA3	2:I:101:ASP:OD2	1.99	0.62
1:A:392:PHE:CD1	1:A:392:PHE:O	2.52	0.62
2:I:67:PHE:CZ	2:I:82:MET:CE	2.79	0.62
2:H:50:ARG:HH12	2:H:100(L):PHE:HE2	1.48	0.61
2:I:51:ILE:HD11	2:I:78:LEU:HD12	1.82	0.61
2:I:51:ILE:HG23	2:I:69:ILE:HG23	1.83	0.61
3:M:33:VAL:HG11	3:M:71:ALA:HB1	1.82	0.60
1:B:207:LEU:CD2	1:B:279:PHE:HZ	2.14	0.60
3:M:3:VAL:HB	3:M:26:THR:HG22	1.84	0.60
2:I:51:ILE:HG12	2:I:69:ILE:CD1	2.32	0.60
1:A:277:LEU:HB3	1:A:279:PHE:CE2	2.37	0.59
3:L:3:VAL:HB	3:L:26:THR:HG22	1.84	0.59
3:L:4:LEU:CD1	3:L:97:VAL:HG13	2.33	0.59
1:A:48:THR:CG2	1:A:279:PHE:CD2	2.85	0.59
1:A:337:PHE:CD1	1:A:380:VAL:HG22	2.38	0.59
2:H:50:ARG:NH1	2:H:100(L):PHE:CE2	2.71	0.59
1:A:46:ILE:HG13	1:A:140:VAL:CG2	2.33	0.58
2:H:50:ARG:NH1	2:H:100(L):PHE:HE2	2.01	0.58
3:M:4:LEU:CD1	3:M:97:VAL:HG13	2.33	0.58
1:A:230:ASN:H	1:A:230:ASN:HD22	1.51	0.58
3:L:26:THR:HG23	3:L:27:SER:H	1.69	0.58
1:A:296:GLY:C	1:A:298:SER:H	2.12	0.57
3:M:26:THR:HG23	3:M:27:SER:H	1.69	0.57
1:A:219:PRO:CG	1:A:237:LEU:HD13	2.34	0.57
1:A:241:LYS:HD3	1:B:271:GLN:HE22	1.70	0.57
1:B:296:GLY:C	1:B:298:SER:H	2.13	0.56
1:B:99:ARG:HA	1:B:103:ASN:HD21	1.70	0.56
1:A:48:THR:CG2	1:A:279:PHE:HD2	2.18	0.56
1:A:239:THR:HB	1:A:251:VAL:HG13	1.88	0.56
3:M:33:VAL:HG11	3:M:71:ALA:CB	2.36	0.56
1:A:33:THR:CG2	1:A:43:PHE:HE1	2.19	0.56
1:A:306:PHE:O	1:A:387:LEU:HD11	2.06	0.56
1:B:219:PRO:HD3	1:B:237:LEU:HD13	1.88	0.56
3:M:30:TYR:O	3:M:33:VAL:HG12	2.06	0.56
1:A:230:ASN:HD22	1:A:230:ASN:N	2.03	0.55
1:A:294:LEU:HD12	1:A:297:MET:CE	2.37	0.55
1:A:64:LYS:HB2	1:A:122:LYS:HD2	1.87	0.54
1:B:33:THR:CG2	1:B:43:PHE:HE1	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ILE:HD13	1:B:238:VAL:CB	2.37	0.54
1:B:289:MET:HG2	1:B:292:LEU:HD12	1.90	0.54
1:A:339:ILE:O	1:A:339:ILE:HG22	2.07	0.54
2:H:100(C):SER:HB3	4:D:1:NAG:HN2	1.73	0.54
1:A:289:MET:HG2	1:A:292:LEU:HD12	1.89	0.54
1:B:239:THR:HB	1:B:251:VAL:HG13	1.89	0.54
1:B:43:PHE:CE2	1:B:141:ILE:HD12	2.43	0.54
1:B:65:LEU:HG	1:B:252:VAL:HG12	1.90	0.54
1:A:125:MET:HE1	1:A:260:MET:HE2	1.89	0.53
1:B:339:ILE:HG22	1:B:339:ILE:O	2.07	0.53
2:H:93:VAL:HG11	2:H:100(P):MET:HB3	1.90	0.53
1:A:43:PHE:CE2	1:A:141:ILE:HD12	2.43	0.53
1:A:99:ARG:NH1	1:A:105:CYS:SG	2.82	0.53
1:B:141:ILE:HG23	1:B:175:LEU:HD21	1.90	0.53
2:I:50:ARG:HH12	2:I:100(L):PHE:HE2	0.61	0.53
2:I:93:VAL:HG11	2:I:100(P):MET:HB3	1.90	0.53
3:M:33:VAL:CG1	3:M:51:GLY:HA2	2.39	0.53
1:A:141:ILE:HG23	1:A:175:LEU:HD21	1.90	0.52
1:A:74:CYS:HB2	1:A:77:GLN:HG3	1.91	0.52
1:A:65:LEU:HG	1:A:252:VAL:HG12	1.90	0.52
2:I:67:PHE:HD1	2:I:82:MET:HA	1.75	0.52
1:B:74:CYS:HB2	1:B:77:GLN:HG3	1.92	0.52
2:I:100(L):PHE:CD2	3:M:91:TYR:OH	2.59	0.52
1:A:48:THR:HG22	1:A:279:PHE:CD2	2.45	0.52
1:A:258:GLY:HA3	1:B:256:GLN:OE1	2.10	0.51
1:A:294:LEU:HD12	1:A:297:MET:HE3	1.91	0.51
1:A:207:LEU:HG	1:A:270:ILE:CD1	2.40	0.51
1:A:256:GLN:OE1	1:B:258:GLY:HA3	2.11	0.51
1:A:322:ILE:CD1	1:A:378:ILE:HG21	2.40	0.51
1:A:183:MET:HG2	1:A:185:CYS:SG	2.51	0.51
1:B:99:ARG:NH1	1:B:105:CYS:SG	2.84	0.51
1:A:192:ASP:O	1:A:196:MET:HG3	2.10	0.51
1:A:270:ILE:HD13	1:A:279:PHE:CE1	2.45	0.51
2:I:51:ILE:HD11	2:I:78:LEU:HD11	1.93	0.51
2:I:67:PHE:CD1	2:I:82:MET:CB	2.94	0.51
2:I:51:ILE:HD12	2:I:71:ARG:HD2	1.93	0.50
1:A:377:TYR:CD1	1:A:390:ASN:OD1	2.65	0.50
1:B:376:SER:OG	1:B:391:TRP:HB3	2.11	0.50
1:A:207:LEU:CG	1:A:270:ILE:HD11	2.42	0.50
1:B:133:GLU:HB3	1:B:167:GLN:CG	2.41	0.50
2:I:67:PHE:CE1	2:I:82:MET:CG	2.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:TRP:NE1	1:A:269:GLU:HG2	2.26	0.50
1:B:322:ILE:CD1	1:B:378:ILE:HG21	2.42	0.49
1:B:90:PHE:CE1	1:B:118:LYS:HB2	2.47	0.49
1:B:148:GLU:O	1:B:323:ARG:NH2	2.46	0.49
1:B:220:TRP:CZ2	1:B:232:ILE:HG21	2.47	0.49
1:B:34:MET:HG2	1:B:40:THR:CG2	2.43	0.49
1:B:91:ILE:HD13	1:B:238:VAL:HB	1.94	0.49
2:H:67:PHE:CE1	2:H:82:MET:HB3	2.47	0.49
1:A:192:ASP:O	1:A:196:MET:CG	2.60	0.49
1:B:308:ILE:CD1	1:B:387:LEU:HD13	2.41	0.49
3:M:33:VAL:HG13	3:M:51:GLY:HA2	1.94	0.49
1:A:241:LYS:HD3	1:B:271:GLN:NE2	2.28	0.49
1:B:206:TRP:NE1	1:B:269:GLU:HG2	2.27	0.49
1:A:71:GLU:HB2	1:A:82:LEU:HD21	1.94	0.48
1:B:194:ASN:O	1:B:194:ASN:OD1	2.31	0.48
1:A:194:ASN:OD1	1:A:194:ASN:O	2.30	0.48
1:A:46:ILE:HG13	1:A:140:VAL:HG23	1.95	0.48
1:A:312:ILE:HG12	1:A:322:ILE:CG1	2.25	0.48
1:B:136:GLU:HA	1:B:165:THR:HG22	1.95	0.48
1:B:207:LEU:HD21	1:B:279:PHE:HZ	1.78	0.48
1:A:136:GLU:HA	1:A:165:THR:HG22	1.96	0.47
1:A:230:ASN:H	1:A:230:ASN:ND2	2.12	0.47
1:B:71:GLU:HB2	1:B:82:LEU:HD21	1.95	0.47
2:I:67:PHE:CD1	2:I:82:MET:HA	2.49	0.47
1:B:132:PRO:HG3	1:B:193:PHE:HB2	1.96	0.47
1:B:312:ILE:HG12	1:B:322:ILE:CG1	2.23	0.47
1:A:34:MET:HG2	1:A:40:THR:CG2	2.42	0.47
1:A:103:ASN:OD1	2:H:100(D):THR:HG23	2.14	0.47
1:A:33:THR:HG22	1:A:43:PHE:HE1	1.79	0.47
2:I:67:PHE:CD1	2:I:82:MET:HB3	2.41	0.47
1:A:253:LEU:O	1:A:253:LEU:CG	2.63	0.47
1:B:125:MET:HE1	1:B:260:MET:HE2	1.97	0.47
1:A:271:GLN:HE22	1:B:241:LYS:HD3	1.79	0.47
1:B:208:VAL:HG11	1:B:212:TRP:CZ3	2.49	0.47
1:A:132:PRO:HG3	1:A:193:PHE:HB2	1.97	0.47
1:B:309:VAL:HB	1:B:323:ARG:HG2	1.96	0.47
1:B:207:LEU:HD22	1:B:279:PHE:HZ	1.79	0.46
1:A:137:TYR:HB2	1:A:164:ILE:HG13	1.97	0.46
1:B:64:LYS:HG2	1:B:120:THR:HB	1.98	0.46
1:A:125:MET:HB3	1:A:201:MET:HG3	1.98	0.46
1:B:207:LEU:HD21	1:B:279:PHE:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:THR:O	1:A:227:GLN:HB2	2.16	0.46
1:B:182:THR:HB	1:B:288:ARG:HB2	1.98	0.45
1:B:162:ILE:HD11	1:B:171:THR:HB	1.99	0.45
2:I:51:ILE:HG12	2:I:69:ILE:HD13	1.97	0.45
1:B:33:THR:HG22	1:B:43:PHE:HE1	1.80	0.45
1:A:133:GLU:HB3	1:A:167:GLN:CG	2.41	0.45
1:B:253:LEU:O	1:B:253:LEU:CG	2.63	0.45
1:A:207:LEU:CD1	1:A:270:ILE:HD11	2.47	0.45
1:A:132:PRO:O	1:A:135:LEU:HB2	2.16	0.45
1:B:207:LEU:CD1	1:B:270:ILE:HG13	2.47	0.45
1:A:20:TRP:HA	1:A:287:LEU:O	2.18	0.44
1:A:270:ILE:HD13	1:A:279:PHE:HE1	1.83	0.44
1:B:132:PRO:O	1:B:135:LEU:HB2	2.16	0.44
1:B:162:ILE:HD11	1:B:171:THR:HG22	1.94	0.44
1:B:137:TYR:HB2	1:B:164:ILE:HG13	1.98	0.44
1:B:20:TRP:HA	1:B:287:LEU:O	2.17	0.44
1:B:222:PRO:HD2	1:B:225:ASP:HB3	2.00	0.44
2:I:100:TYR:CE1	4:C:2:NAG:H4	2.53	0.43
1:A:33:THR:HG21	1:A:43:PHE:HE1	1.83	0.43
1:A:146:GLY:O	1:A:365:VAL:HA	2.18	0.43
1:B:208:VAL:CG1	1:B:212:TRP:CE3	2.94	0.43
2:I:67:PHE:HE1	2:I:82:MET:HE2	1.71	0.43
1:A:277:LEU:CB	1:A:279:PHE:CE2	3.01	0.43
1:B:90:PHE:HD1	1:B:117:ALA:C	2.27	0.43
1:A:65:LEU:HG	1:A:252:VAL:CG1	2.49	0.43
1:A:198:LEU:HD13	1:A:207:LEU:HD21	2.00	0.42
2:H:40:ALA:HB3	2:H:43:LYS:HD2	2.00	0.42
1:B:7:SER:O	1:B:317:HIS:HE1	2.02	0.42
1:B:146:GLY:O	1:B:365:VAL:HA	2.19	0.42
1:A:222:PRO:HD2	1:A:225:ASP:HB3	2.01	0.42
1:B:65:LEU:HD12	1:B:252:VAL:HG13	2.01	0.42
1:B:219:PRO:HA	1:B:232:ILE:O	2.19	0.42
2:I:40:ALA:HB3	2:I:43:LYS:HD2	2.00	0.42
1:B:65:LEU:HG	1:B:252:VAL:CG1	2.49	0.42
1:B:207:LEU:HD13	1:B:270:ILE:CG1	2.50	0.42
1:A:41:LEU:HD11	1:A:292:LEU:HD11	2.02	0.42
1:A:219:PRO:HA	1:A:232:ILE:O	2.19	0.42
2:I:51:ILE:HG21	2:I:69:ILE:HG23	2.00	0.42
1:B:87:ASP:HB3	1:B:90:PHE:HD2	1.83	0.42
1:B:208:VAL:HG12	1:B:209:HIS:N	2.35	0.42
1:A:66:THR:HG23	1:A:118:LYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ILE:HG23	1:A:308:ILE:O	2.20	0.42
1:B:66:THR:HG23	1:B:118:LYS:HB3	2.02	0.42
1:B:207:LEU:CD2	1:B:279:PHE:CZ	2.99	0.42
1:A:7:SER:O	1:A:317:HIS:HE1	2.02	0.41
1:A:65:LEU:HD12	1:A:252:VAL:HG13	2.01	0.41
1:A:307:LYS:HZ3	1:A:307:LYS:HB3	1.85	0.41
1:B:170:THR:HA	1:B:183:MET:O	2.20	0.41
1:A:219:PRO:CD	1:A:237:LEU:CD1	2.66	0.41
2:I:100(L):PHE:CE2	3:M:91:TYR:OH	2.72	0.41
1:B:41:LEU:HD11	1:B:292:LEU:HD11	2.02	0.41
1:B:33:THR:HG21	1:B:43:PHE:HE1	1.84	0.41
1:A:40:THR:HG21	1:A:352:ILE:O	2.21	0.41
1:A:230:ASN:N	1:A:230:ASN:ND2	2.69	0.41
1:B:40:THR:HG21	1:B:352:ILE:O	2.20	0.41
2:I:22:CYS:HB3	2:I:78:LEU:HB3	2.03	0.41
2:I:67:PHE:CD1	2:I:82:MET:HG2	2.56	0.41
1:B:149:HIS:HB3	4:D:1:NAG:H2	2.03	0.41
1:A:379:ILE:HG13	1:A:388:LYS:HA	2.04	0.40
1:B:91:ILE:HD13	1:B:238:VAL:HG11	2.03	0.40
1:B:139:ILE:HG21	1:B:183:MET:HE1	2.04	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	365/430 (85%)	346 (95%)	18 (5%)	1 (0%)	36 69
1	B	369/430 (86%)	351 (95%)	17 (5%)	1 (0%)	36 69
2	H	129/283 (46%)	124 (96%)	4 (3%)	1 (1%)	16 50
2	I	129/283 (46%)	124 (96%)	4 (3%)	1 (1%)	16 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	108/218 (50%)	104 (96%)	4 (4%)	0	100	100
3	M	108/218 (50%)	104 (96%)	4 (4%)	0	100	100
All	All	1208/1862 (65%)	1153 (95%)	51 (4%)	4 (0%)	36	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	MET
1	B	297	MET
2	I	65	GLY
2	H	65	GLY

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	326/368 (89%)	319 (98%)	7 (2%)	47	65
1	B	330/368 (90%)	321 (97%)	9 (3%)	39	60
2	H	109/236 (46%)	94 (86%)	15 (14%)	3	18
2	I	109/236 (46%)	94 (86%)	15 (14%)	3	18
3	L	92/185 (50%)	92 (100%)	0	100	100
3	M	92/185 (50%)	91 (99%)	1 (1%)	65	74
All	All	1058/1578 (67%)	1011 (96%)	47 (4%)	25	49

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	86	GLN
1	A	99	ARG
1	A	135	LEU
1	A	230	ASN
1	A	259	CYS

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Mol	Chain	Res	Type
1	A	376	SER
1	B	1	MET
1	B	86	GLN
1	B	99	ARG
1	B	135	LEU
1	B	161	GLU
1	B	196	MET
1	B	259	CYS
1	B	283	LEU
1	B	333	CYS
2	H	100	TYR
2	H	100(A)	TYR
2	H	100(B)	ASP
2	H	100(C)	SER
2	H	100(D)	THR
2	H	100(F)	TYR
2	H	100(G)	TYR
2	H	100(H)	PRO
2	H	100(I)	ASP
2	H	100(J)	SER
2	H	100(K)	PHE
2	H	100(L)	PHE
2	H	100(M)	LYS
2	H	100(N)	TYR
2	H	100(P)	MET
2	I	100	TYR
2	I	100(A)	TYR
2	I	100(B)	ASP
2	I	100(C)	SER
2	I	100(D)	THR
2	I	100(F)	TYR
2	I	100(G)	TYR
2	I	100(H)	PRO
2	I	100(I)	ASP
2	I	100(J)	SER
2	I	100(K)	PHE
2	I	100(L)	PHE
2	I	100(M)	LYS
2	I	100(N)	TYR
2	I	100(P)	MET
3	M	17	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	ASN
1	A	230	ASN
1	A	271	GLN
1	A	316	GLN
1	B	194	ASN
1	B	271	GLN
1	B	366	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 ⓘ

12 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	$\# Z > 2$
4	NAG	C	1	1,4	14,14,15	0.30	0	17,19,21	0.57	0
4	NAG	C	2	4	14,14,15	0.36	0	17,19,21	1.35	3 (17%)
4	BMA	C	3	4	11,11,12	0.39	0	15,15,17	1.10	1 (6%)
4	MAN	C	4	4	11,11,12	0.38	0	15,15,17	0.97	1 (6%)
4	MAN	C	5	4	11,11,12	0.36	0	15,15,17	0.88	1 (6%)
4	FUC	C	6	4	10,10,11	0.44	0	14,14,16	0.88	0
4	NAG	D	1	1,4	14,14,15	0.32	0	17,19,21	0.59	0
4	NAG	D	2	4	14,14,15	0.37	0	17,19,21	1.33	3 (17%)
4	BMA	D	3	4	11,11,12	0.36	0	15,15,17	1.15	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	D	4	4	11,11,12	0.39	0	15,15,17	0.97	1 (6%)
4	MAN	D	5	4	11,11,12	0.36	0	15,15,17	0.83	1 (6%)
4	FUC	D	6	4	10,10,11	0.44	0	14,14,16	0.88	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	C	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	0/1/1/1
4	BMA	C	3	4	-	2/2/19/22	1/1/1/1
4	MAN	C	4	4	-	1/2/19/22	1/1/1/1
4	MAN	C	5	4	-	0/2/19/22	0/1/1/1
4	FUC	C	6	4	-	-	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	1/1/1/1
4	MAN	D	4	4	-	1/2/19/22	1/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
4	FUC	D	6	4	-	-	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3	BMA	C1-O5-C5	3.97	117.51	112.19
4	C	3	BMA	C1-O5-C5	3.73	117.19	112.19
4	D	4	MAN	C1-O5-C5	3.56	116.96	112.19
4	C	4	MAN	C1-O5-C5	3.55	116.94	112.19
4	D	2	NAG	C1-O5-C5	3.51	116.89	112.19
4	C	2	NAG	O5-C1-C2	3.45	116.62	111.29
4	C	2	NAG	C1-O5-C5	3.44	116.79	112.19
4	D	2	NAG	O5-C1-C2	3.30	116.40	111.29
4	C	5	MAN	C1-O5-C5	2.98	116.18	112.19
4	D	5	MAN	C1-O5-C5	2.79	115.93	112.19
4	D	2	NAG	O4-C4-C5	2.16	114.64	109.32
4	C	2	NAG	O4-C4-C5	2.16	114.63	109.32

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	3	BMA	O5-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
4	C	3	BMA	C4-C5-C6-O6
4	D	3	BMA	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
4	C	4	MAN	O5-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6

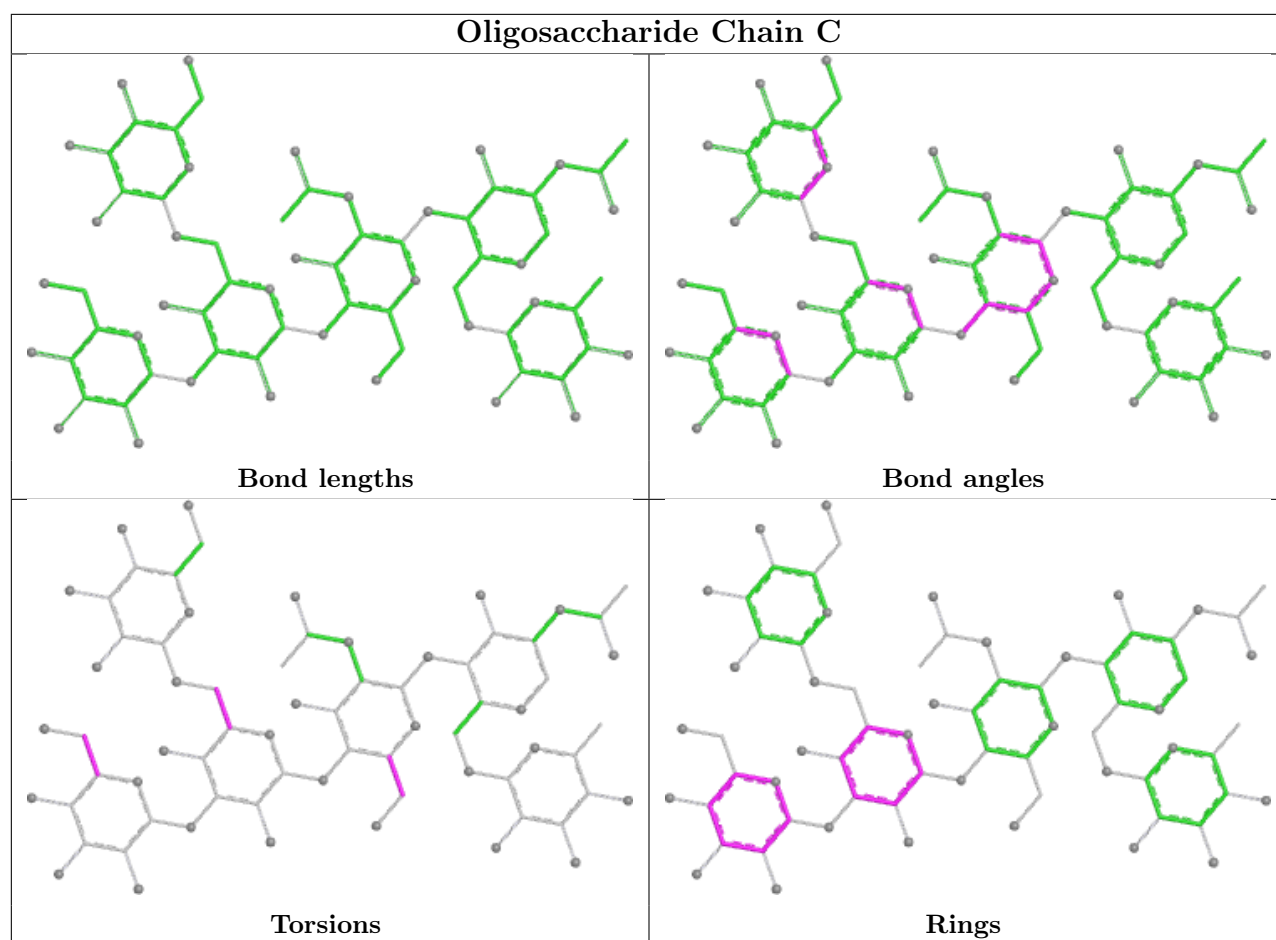
All (4) ring outliers are listed below:

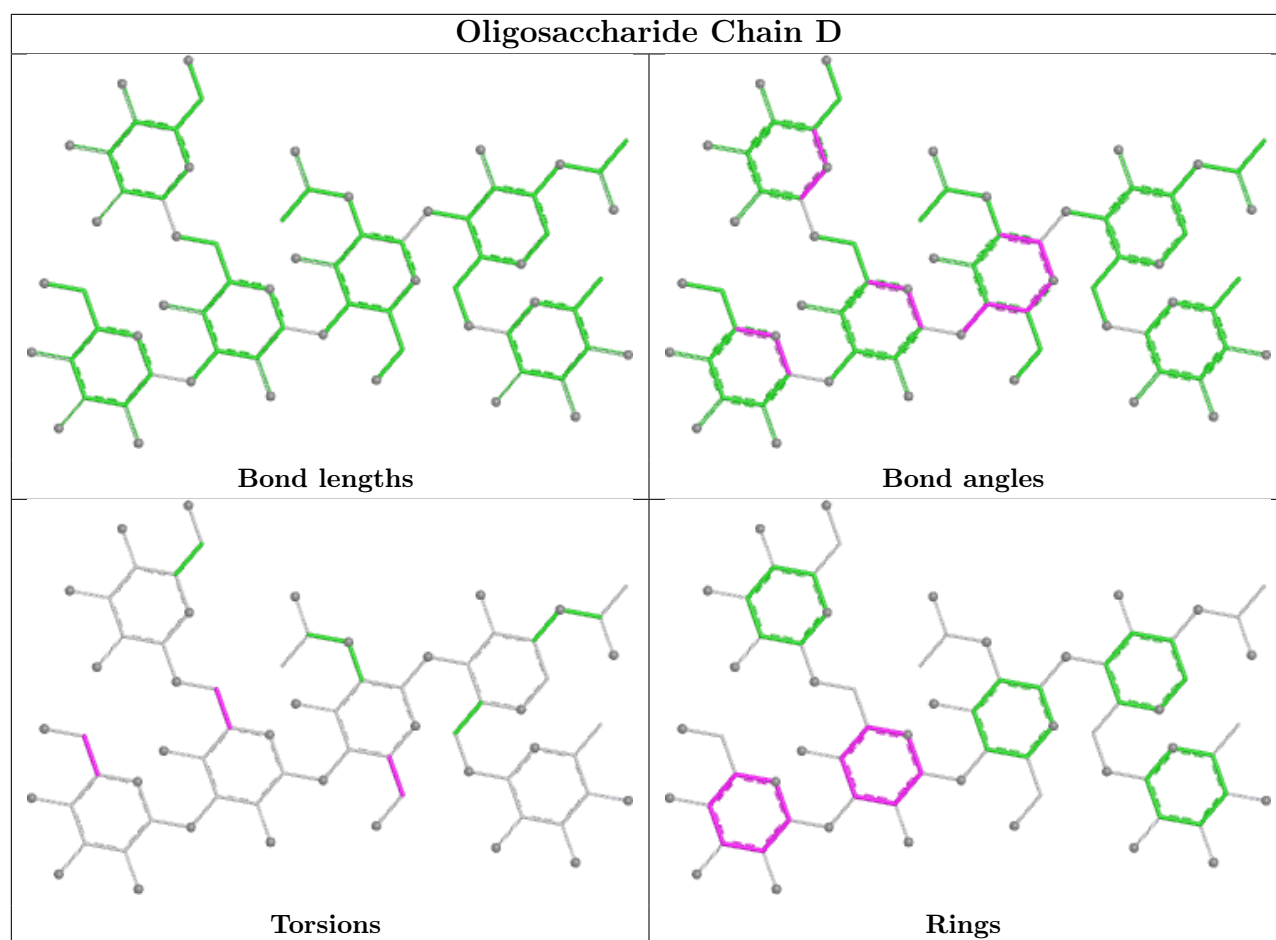
Mol	Chain	Res	Type	Atoms
4	C	3	BMA	C1-C2-C3-C4-C5-O5
4	D	3	BMA	C1-C2-C3-C4-C5-O5
4	C	4	MAN	C1-C2-C3-C4-C5-O5
4	D	4	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 3 short contacts:

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

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





5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	373/430 (86%)	0.80	31 (8%) 17 18	81, 143, 236, 287	0
1	B	379/430 (88%)	0.90	50 (13%) 7 10	68, 142, 233, 287	0
2	H	131/283 (46%)	0.66	3 (2%) 61 43	89, 133, 218, 295	0
2	I	131/283 (46%)	0.56	3 (2%) 61 43	91, 130, 189, 229	0
3	L	110/218 (50%)	0.55	3 (2%) 56 39	83, 121, 163, 204	0
3	M	110/218 (50%)	0.64	5 (4%) 38 28	83, 128, 166, 235	0
All	All	1234/1862 (66%)	0.75	95 (7%) 19 18	68, 138, 218, 295	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	GLY	5.6
1	A	167	GLN	5.4
1	B	372	PRO	4.6
3	M	23	CYS	4.6
3	M	107	VAL	4.3
1	B	15	VAL	4.1
1	A	90	PHE	4.0
1	B	393	LYS	3.9
1	A	152	GLY	3.9
1	B	224	ALA	3.8
1	A	156	GLY	3.8
1	B	72	SER	3.7
1	A	224	ALA	3.6
3	L	23	CYS	3.5
1	B	184	GLU	3.5
2	H	74	ALA	3.4
1	A	103	ASN	3.3
1	B	155	THR	3.3
1	B	198	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	8	ASN	3.2
1	A	158	HIS	3.2
2	I	14	PRO	3.2
1	B	168	SER	3.2
2	H	14	PRO	3.2
1	B	373	PHE	3.2
3	L	2	SER	3.2
1	B	207	LEU	3.2
1	B	340	THR	3.1
1	B	191	LEU	3.1
1	B	141	ILE	2.9
1	B	279	PHE	2.9
1	B	74	CYS	2.9
1	A	72	SER	2.8
1	A	229	SER	2.8
1	B	190	GLY	2.7
1	A	204	LYS	2.7
1	B	101	TRP	2.7
1	A	187	PRO	2.7
1	B	20	TRP	2.7
1	A	134	ASN	2.6
1	B	355	ASN	2.6
1	B	112	GLY	2.6
1	B	43	PHE	2.6
1	B	349	GLY	2.6
1	B	37	ASN	2.6
1	B	167	GLN	2.6
1	B	228	GLY	2.6
1	B	157	LYS	2.5
1	A	101	TRP	2.4
1	B	226	THR	2.4
2	I	112	SER	2.4
1	A	279	PHE	2.4
1	B	21	VAL	2.4
1	B	71	GLU	2.4
1	B	134	ASN	2.4
1	B	348	LEU	2.4
1	B	223	GLY	2.4
1	A	300	SER	2.4
1	A	154	ASP	2.4
1	A	172	GLU	2.4
1	A	50	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	209	HIS	2.3
1	A	148	GLU	2.3
3	M	82	ASP	2.3
1	B	16	SER	2.3
1	A	141	ILE	2.3
1	A	248	GLN	2.3
1	A	85	GLU	2.3
1	A	133	GLU	2.3
3	M	80	PRO	2.3
1	B	261	HIS	2.2
1	B	104	GLY	2.2
1	A	388	LYS	2.2
1	B	156	GLY	2.2
3	L	107	VAL	2.2
1	B	240	PHE	2.2
1	B	391	TRP	2.2
1	B	102	GLY	2.1
1	B	277	LEU	2.1
1	A	155	THR	2.1
1	B	11	PHE	2.1
1	A	157	LYS	2.1
1	B	158	HIS	2.1
1	A	255	SER	2.1
3	M	1	GLN	2.1
1	B	12	VAL	2.1
1	A	111	GLY	2.0
2	H	15	GLY	2.0
2	I	65	GLY	2.0
1	A	308	ILE	2.0
1	B	172	GLU	2.0
1	B	204	LYS	2.0
1	B	347	VAL	2.0
1	B	52	GLN	2.0
1	A	189	THR	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

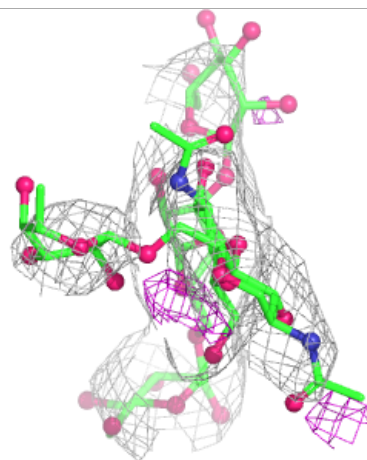
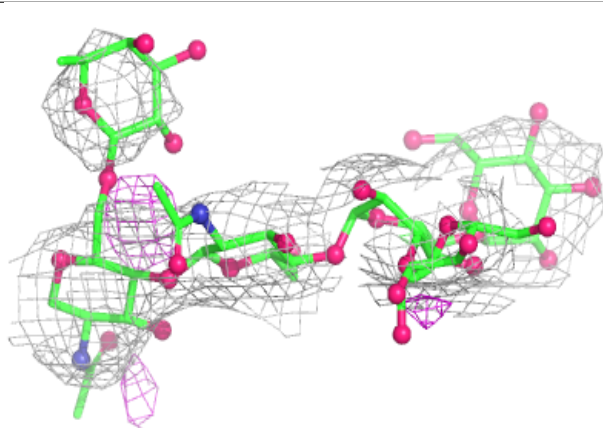
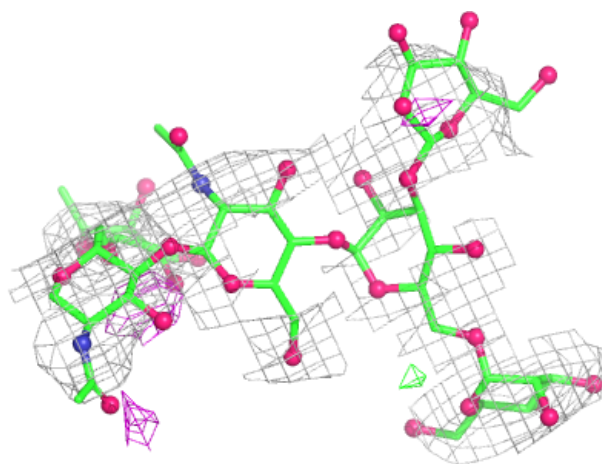
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	C	1	14/15	-	-	96,118,153,167	0
4	NAG	C	2	14/15	-	-	95,113,144,146	0
4	BMA	C	3	11/12	-	-	81,104,118,137	0
4	MAN	C	4	11/12	-	-	162,183,190,199	0
4	MAN	C	5	11/12	-	-	109,116,124,136	0
4	FUC	C	6	10/11	-	-	171,175,183,190	0
4	NAG	D	1	14/15	-	-	87,101,171,184	0
4	NAG	D	2	14/15	-	-	83,99,149,159	0
4	BMA	D	3	11/12	-	-	97,109,131,155	0
4	MAN	D	4	11/12	-	-	172,184,188,190	0
4	MAN	D	5	11/12	-	-	104,125,132,133	0
4	FUC	D	6	10/11	-	-	179,185,188,189	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.

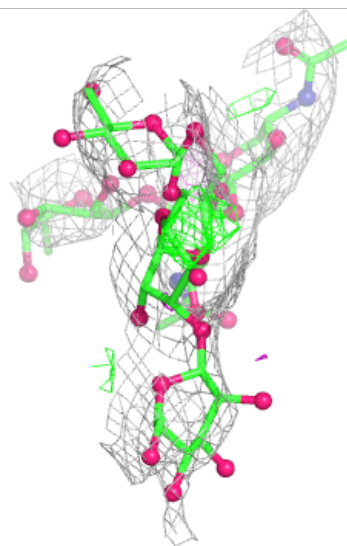
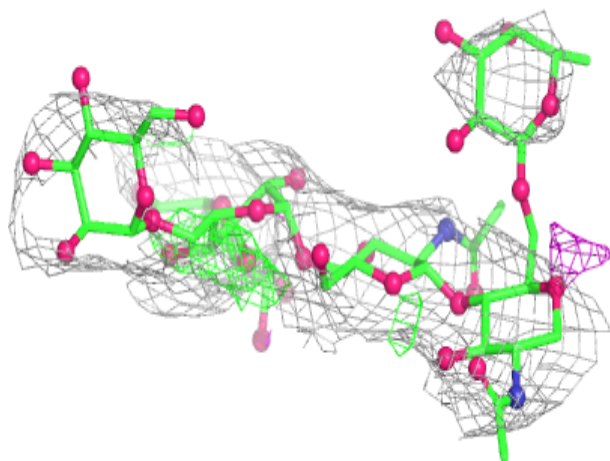
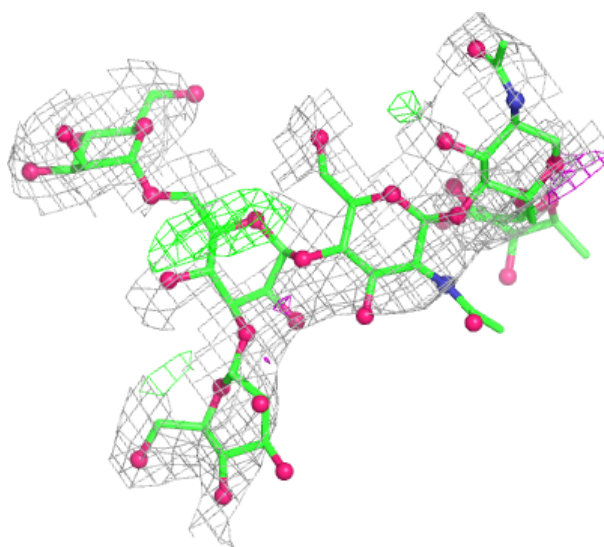
Electron density around Chain C:

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



Electron density around Chain D:

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



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.