



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:17 PM EDT

PDB ID : 5N09 / pdb_00005n09
Title : Crystal structure of L107C/A313C covalently linked dengue 2 virus envelope glycoprotein dimer in complex with the Fab fragment of the broadly neutralizing human antibody EDE2 A11
Authors : Duquerroy, S.; Rouvinski, A.; Guardado-Calvo, P.; Vaney, M.-C.; Sharma, A.; Rey, F.
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

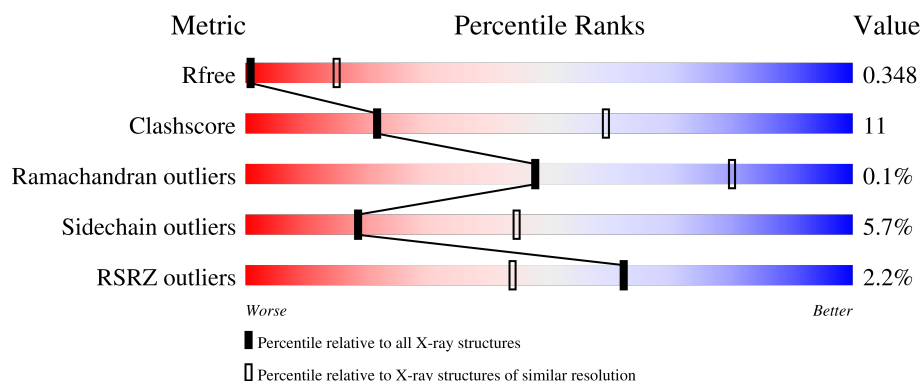
1 Overall quality at a glance

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	 2% 56% 32% 9%
1	B	430	 2% 58% 29% 10%
2	H	283	 2% 64% 15% 20%
2	I	283	 % 65% 14% 20%

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Mol	Chain	Length	Quality of chain
3	L	218	% 79% 18%
3	M	218	3% 85% 12%
4	C	6	17% 50% 33%
4	D	6	17% 67% 17%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12841 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	391	Total	C	N	O	S	0	0	0
			3047	1920	523	578	26			
1	B	388	Total	C	N	O	S	0	0	0
			3020	1903	517	574	26			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	CYS	LEU	engineered mutation	UNP C3VXD1
A	118	LYS	MET	conflict	UNP C3VXD1
A	313	CYS	ALA	engineered mutation	UNP C3VXD1
A	396	LEU	-	expression tag	UNP C3VXD1
A	397	VAL	-	expression tag	UNP C3VXD1
A	398	PRO	-	expression tag	UNP C3VXD1
A	399	ARG	-	expression tag	UNP C3VXD1
A	400	GLY	-	expression tag	UNP C3VXD1
A	401	SER	-	expression tag	UNP C3VXD1
A	402	SER	-	expression tag	UNP C3VXD1
A	403	ALA	-	expression tag	UNP C3VXD1
A	404	TRP	-	expression tag	UNP C3VXD1
A	405	SER	-	expression tag	UNP C3VXD1
A	406	HIS	-	expression tag	UNP C3VXD1
A	407	PRO	-	expression tag	UNP C3VXD1
A	408	GLN	-	expression tag	UNP C3VXD1
A	409	PHE	-	expression tag	UNP C3VXD1
A	410	GLU	-	expression tag	UNP C3VXD1
A	411	LYS	-	expression tag	UNP C3VXD1
A	412	GLY	-	expression tag	UNP C3VXD1
A	413	GLY	-	expression tag	UNP C3VXD1
A	414	SER	-	expression tag	UNP C3VXD1
A	415	GLY	-	expression tag	UNP C3VXD1
A	416	GLY	-	expression tag	UNP C3VXD1
A	417	GLY	-	expression tag	UNP C3VXD1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	418	SER	-	expression tag	UNP C3VXD1
A	419	GLY	-	expression tag	UNP C3VXD1
A	420	GLY	-	expression tag	UNP C3VXD1
A	421	SER	-	expression tag	UNP C3VXD1
A	422	ALA	-	expression tag	UNP C3VXD1
A	423	TRP	-	expression tag	UNP C3VXD1
A	424	SER	-	expression tag	UNP C3VXD1
A	425	HIS	-	expression tag	UNP C3VXD1
A	426	PRO	-	expression tag	UNP C3VXD1
A	427	GLN	-	expression tag	UNP C3VXD1
A	428	PHE	-	expression tag	UNP C3VXD1
A	429	GLU	-	expression tag	UNP C3VXD1
A	430	LYS	-	expression tag	UNP C3VXD1
B	107	CYS	LEU	engineered mutation	UNP C3VXD1
B	118	LYS	MET	conflict	UNP C3VXD1
B	313	CYS	ALA	engineered mutation	UNP C3VXD1
B	396	LEU	-	expression tag	UNP C3VXD1
B	397	VAL	-	expression tag	UNP C3VXD1
B	398	PRO	-	expression tag	UNP C3VXD1
B	399	ARG	-	expression tag	UNP C3VXD1
B	400	GLY	-	expression tag	UNP C3VXD1
B	401	SER	-	expression tag	UNP C3VXD1
B	402	SER	-	expression tag	UNP C3VXD1
B	403	ALA	-	expression tag	UNP C3VXD1
B	404	TRP	-	expression tag	UNP C3VXD1
B	405	SER	-	expression tag	UNP C3VXD1
B	406	HIS	-	expression tag	UNP C3VXD1
B	407	PRO	-	expression tag	UNP C3VXD1
B	408	GLN	-	expression tag	UNP C3VXD1
B	409	PHE	-	expression tag	UNP C3VXD1
B	410	GLU	-	expression tag	UNP C3VXD1
B	411	LYS	-	expression tag	UNP C3VXD1
B	412	GLY	-	expression tag	UNP C3VXD1
B	413	GLY	-	expression tag	UNP C3VXD1
B	414	SER	-	expression tag	UNP C3VXD1
B	415	GLY	-	expression tag	UNP C3VXD1
B	416	GLY	-	expression tag	UNP C3VXD1
B	417	GLY	-	expression tag	UNP C3VXD1
B	418	SER	-	expression tag	UNP C3VXD1
B	419	GLY	-	expression tag	UNP C3VXD1
B	420	GLY	-	expression tag	UNP C3VXD1
B	421	SER	-	expression tag	UNP C3VXD1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	422	ALA	-	expression tag	UNP C3VXD1
B	423	TRP	-	expression tag	UNP C3VXD1
B	424	SER	-	expression tag	UNP C3VXD1
B	425	HIS	-	expression tag	UNP C3VXD1
B	426	PRO	-	expression tag	UNP C3VXD1
B	427	GLN	-	expression tag	UNP C3VXD1
B	428	PHE	-	expression tag	UNP C3VXD1
B	429	GLU	-	expression tag	UNP C3VXD1
B	430	LYS	-	expression tag	UNP C3VXD1

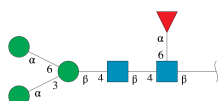
- Molecule 2 is a protein called BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11 - Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	226	Total	C	N	O	S	0	0	0
			1728	1093	292	336	7			
2	I	226	Total	C	N	O	S	0	0	0
			1724	1091	292	334	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1582	987	265	324	6			
3	M	213	Total	C	N	O	S	0	0	0
			1582	987	265	324	6			

- 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				

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

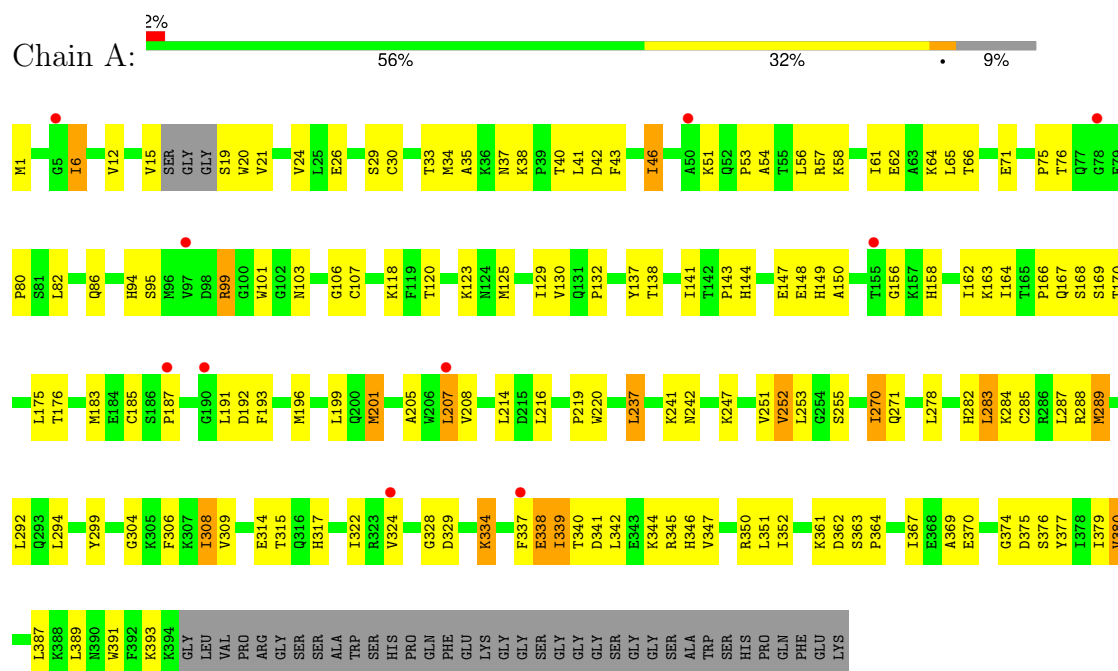
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		
6	H	1	Total	O	0	0
			1	1		

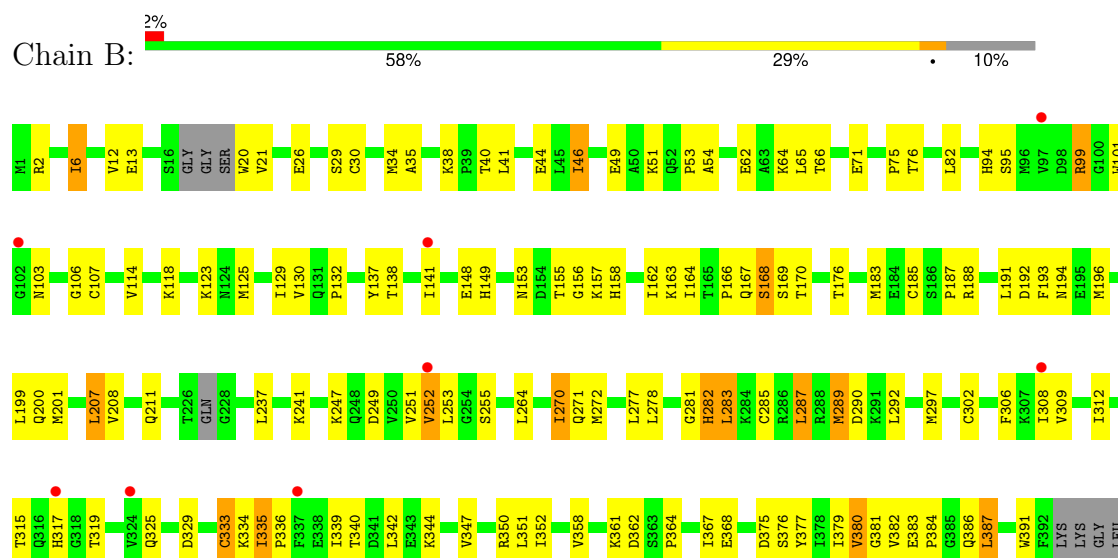
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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

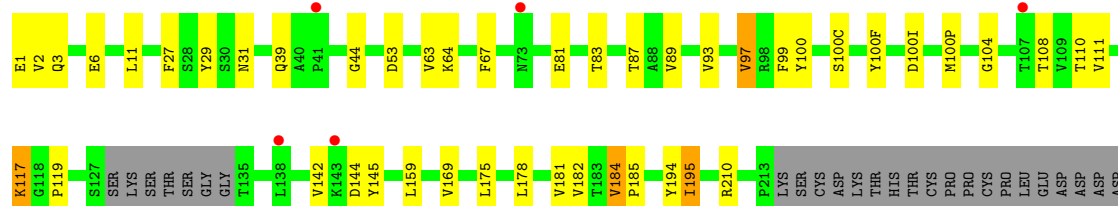


• Molecule 1: Envelope Glycoprotein E



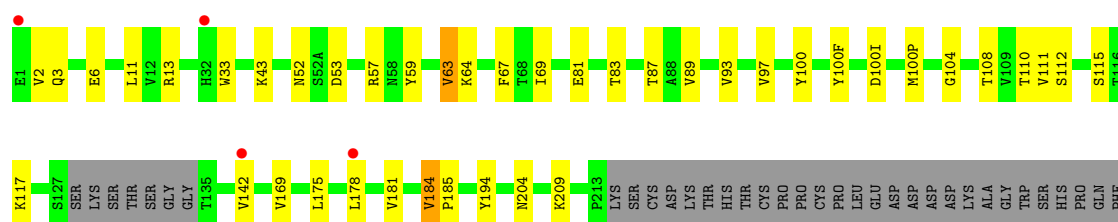
VAL PRO ARG GLY SER SER ALA TRP SER HIS PRO GLN PHE GLU LYS GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS

● Molecule 2: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11 - Heavy chain



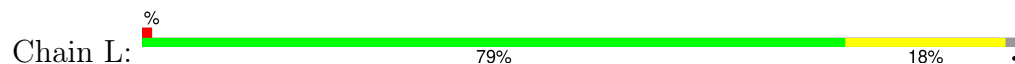
LYS ALA TRP HIS PRO GLN PHE GLU LYS GLY GLY SER GLY GLY SER GLY GLY TRP HIS PRO GLN PHE GLU LYS

● Molecule 2: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11 - Heavy chain

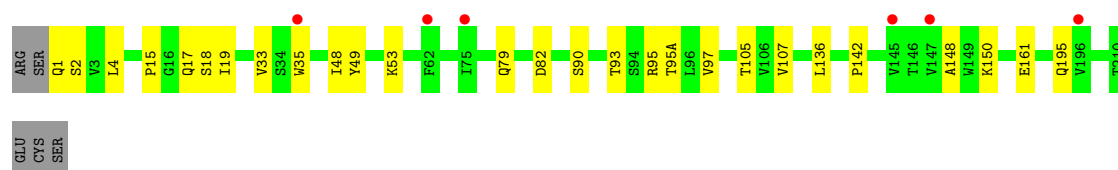


GLU LYS GLY GLY SER GLY GLY GLY GLY GLY SER TRP HIS PRO GLN PHE GLU LYS

● Molecule 3: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11 - Light chain

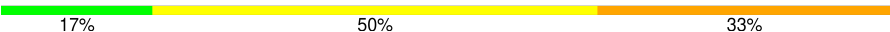


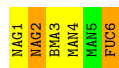
● Molecule 3: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11 - Light chain



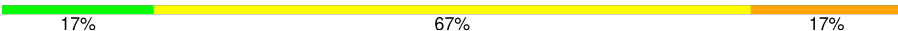
GLU CYS SER

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

Chain C: 



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

Chain D: 



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	58.90Å 180.60Å 205.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.99 – 3.90 39.99 – 3.90	Depositor EDS
% Data completeness (in resolution range)	93.1 (39.99-3.90) 93.0 (39.99-3.90)	Depositor EDS
R_{merge}	0.69	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 3.87Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.304 , 0.347 0.302 , 0.348	Depositor DCC
R_{free} test set	950 reflections (3.27%)	wwPDB-VP
Wilson B-factor (Å ²)	88.8	Xtriage
Anisotropy	0.863	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	12841	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.75% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, FUC, MAN

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	0.34	1/3108 (0.0%)	0.87	0/4198
1	B	0.33	0/3080	0.89	5/4161 (0.1%)
2	H	0.21	0/1774	0.64	0/2419
2	I	0.20	0/1770	0.66	0/2414
3	L	0.23	0/1618	0.64	0/2209
3	M	0.21	0/1618	0.62	0/2209
All	All	0.28	1/12968 (0.0%)	0.76	5/17610 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	LEU	C-N	8.57	1.53	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	281	GLY	CA-C-N	7.04	131.49	121.42
1	B	281	GLY	C-N-CA	7.04	131.49	121.42
1	B	168	SER	CA-C-N	5.19	127.75	120.28
1	B	168	SER	C-N-CA	5.19	127.75	120.28
1	B	287	LEU	CA-CB-CG	5.04	133.94	116.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3047	0	3041	94	0
1	B	3020	0	3005	93	0
2	H	1728	0	1656	31	0
2	I	1724	0	1652	28	0
3	L	1582	0	1553	28	0
3	M	1582	0	1553	15	0
4	C	71	0	61	3	0
4	D	71	0	61	4	0
5	B	14	0	13	0	0
6	A	1	0	0	1	0
6	H	1	0	0	0	0
All	All	12841	0	12595	274	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 11.

All (274) 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:99:ARG:NH1	1:B:103:ASN:O	1.83	1.10
1:A:99:ARG:NH1	1:A:103:ASN:O	1.89	1.04
1:B:99:ARG:NH1	1:B:103:ASN:OD1	1.95	0.97
1:A:99:ARG:NH1	1:A:103:ASN:OD1	2.03	0.92
2:H:117:LYS:HZ1	2:I:115:SER:H	1.21	0.88
1:B:380:VAL:HG13	1:B:387:LEU:HB2	1.57	0.87
1:A:315:THR:HG23	1:A:317:HIS:H	1.46	0.79
1:B:132:PRO:HG3	1:B:193:PHE:HB2	1.66	0.76
2:H:181:VAL:HG21	3:L:136:LEU:HD21	1.68	0.75
1:B:329:ASP:HA	1:B:361:LYS:HE2	1.69	0.75
1:B:315:THR:HG23	1:B:317:HIS:H	1.52	0.74
2:H:117:LYS:NZ	2:I:115:SER:H	1.85	0.74
1:B:306:PHE:O	1:B:387:LEU:HD11	1.89	0.72
1:A:219:PRO:HD3	1:A:237:LEU:HD13	1.71	0.72
3:L:105:THR:HG21	3:L:142:PRO:HB3	1.71	0.71
1:B:166:PRO:HB3	1:B:187:PRO:HG3	1.72	0.71
2:H:169:VAL:HG21	3:L:161:GLU:HB3	1.74	0.69
1:A:125:MET:HG2	1:A:199:LEU:HD11	1.73	0.69
1:B:125:MET:HG2	1:B:199:LEU:HD11	1.76	0.67
1:A:306:PHE:O	1:A:387:LEU:HD11	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:PHE:CD2	1:A:141:ILE:HD12	2.31	0.66
1:A:341:ASP:OD2	1:A:346:HIS:CE1	2.50	0.64
1:B:297:MET:O	1:B:334:LYS:NZ	2.30	0.64
3:L:18:SER:HA	3:L:75:ILE:O	1.97	0.64
2:I:169:VAL:HG21	3:M:161:GLU:HB3	1.78	0.64
1:B:297:MET:C	1:B:334:LYS:HZ1	2.06	0.63
3:L:62:PHE:HZ	3:L:82:ASP:OD2	1.81	0.63
2:I:59:TYR:H	3:M:95:ARG:HH21	1.47	0.63
1:A:164:ILE:HD11	1:A:283:LEU:HD11	1.80	0.63
1:A:132:PRO:HG3	1:A:193:PHE:HB2	1.81	0.62
1:A:34:MET:HG2	1:A:40:THR:HG22	1.81	0.62
1:B:148:GLU:HB3	1:B:364:PRO:HD2	1.81	0.62
1:A:247:LYS:HB2	2:H:100(F):TYR:CZ	2.34	0.62
1:A:380:VAL:HG13	1:A:387:LEU:HB2	1.82	0.62
3:L:105:THR:HG21	3:L:142:PRO:CB	2.30	0.62
2:I:83:THR:O	2:I:111:VAL:HG11	2.00	0.62
1:A:125:MET:HG3	1:A:201:MET:HG3	1.80	0.61
2:I:181:VAL:HG21	3:M:136:LEU:HD21	1.80	0.61
1:A:26:GLU:HG2	1:A:29:SER:HB3	1.82	0.61
1:B:335:ILE:HG13	1:B:335:ILE:O	2.01	0.61
2:H:184:VAL:HG22	2:H:185:PRO:HD2	1.82	0.61
1:A:241:LYS:HE3	1:A:251:VAL:HG11	1.82	0.61
1:B:382:VAL:C	1:B:386:GLN:HB2	2.26	0.61
2:I:117:LYS:HZ2	2:I:175:LEU:HD11	1.65	0.61
1:A:65:LEU:HD12	1:A:252:VAL:HG22	1.82	0.60
1:B:241:LYS:HE3	1:B:251:VAL:HG11	1.81	0.60
2:H:83:THR:O	2:H:111:VAL:HG11	2.01	0.60
1:A:24:VAL:HG22	1:A:284:LYS:HG2	1.82	0.60
1:B:99:ARG:NH2	2:I:100(I):ASP:OD2	2.34	0.60
1:A:156:GLY:C	1:A:158:HIS:H	2.10	0.59
2:I:6:GLU:OE2	2:I:104:GLY:HA3	2.01	0.59
1:B:65:LEU:HD12	1:B:252:VAL:HG22	1.83	0.59
2:I:204:ASN:HB2	3:L:128:ALA:HA	1.84	0.59
1:B:26:GLU:HG2	1:B:29:SER:HB3	1.85	0.59
1:B:302:CYS:N	1:B:333:CYS:SG	2.77	0.58
1:B:2:ARG:HD3	1:B:44:GLU:OE1	2.03	0.58
1:A:41:LEU:HD11	1:A:292:LEU:HD11	1.86	0.58
1:A:341:ASP:OD1	1:A:344:LYS:N	2.37	0.57
1:A:196:MET:HB3	1:A:207:LEU:HG	1.85	0.57
1:B:53:PRO:HB3	1:B:130:VAL:HG22	1.87	0.57
1:B:185:CYS:HA	1:B:285:CYS:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:1:GLN:O	3:M:2:SER:OG	2.22	0.57
1:A:62:GLU:HB3	1:A:123:LYS:HB2	1.86	0.57
2:I:89:VAL:HG22	2:I:108:THR:HG22	1.87	0.57
1:A:101:TRP:NE1	1:A:106:GLY:O	2.36	0.57
2:I:184:VAL:HG22	2:I:185:PRO:HD2	1.87	0.56
1:A:170:THR:HA	1:A:183:MET:O	2.05	0.56
1:B:54:ALA:O	1:B:129:ILE:HG22	2.05	0.56
3:M:105:THR:HG21	3:M:142:PRO:HB3	1.88	0.56
1:B:247:LYS:HE3	1:B:249:ASP:OD2	2.06	0.55
1:B:383:GLU:HG3	1:B:384:PRO:HA	1.88	0.55
1:B:192:ASP:HB3	1:B:194:ASN:OD1	2.07	0.55
2:H:195:ILE:HG22	2:H:210:ARG:HG2	1.89	0.55
2:H:67:PHE:HA	2:H:81:GLU:O	2.08	0.54
2:I:93:VAL:HG11	2:I:100(P):MET:HB3	1.89	0.54
3:M:95:ARG:HG3	3:M:95(A):THR:HG23	1.90	0.54
1:A:149:HIS:HB3	4:C:1:NAG:H2	1.89	0.53
1:A:185:CYS:HA	1:A:285:CYS:HA	1.88	0.53
3:M:49:TYR:HE1	3:M:53:LYS:HE3	1.73	0.53
1:B:41:LEU:HD11	1:B:292:LEU:HD11	1.90	0.53
1:A:61:ILE:HD13	1:A:201:MET:HE2	1.89	0.53
2:H:89:VAL:HG22	2:H:108:THR:HG22	1.89	0.53
1:B:191:LEU:HD23	1:B:192:ASP:H	1.73	0.53
2:I:100:TYR:CE1	4:C:2:NAG:H4	2.44	0.53
1:B:40:THR:HG21	1:B:352:ILE:O	2.09	0.53
1:A:40:THR:HG21	1:A:352:ILE:O	2.09	0.52
1:A:308:ILE:HD13	1:A:389:LEU:HD21	1.92	0.52
1:A:329:ASP:HA	1:A:361:LYS:HE2	1.90	0.52
1:A:191:LEU:HD21	1:A:196:MET:HE3	1.90	0.52
1:B:342:LEU:HD11	1:B:375:ASP:HB2	1.91	0.52
1:A:35:ALA:HB3	1:A:38:LYS:HB2	1.90	0.52
1:A:143:PRO:HG3	1:A:175:LEU:HD22	1.92	0.52
2:I:2:VAL:C	2:I:3:GLN:HG3	2.35	0.52
1:A:304:GLY:HA3	1:A:328:GLY:HA3	1.90	0.52
1:A:299:TYR:O	1:A:334:LYS:NZ	2.25	0.52
2:I:67:PHE:HA	2:I:81:GLU:O	2.10	0.52
2:H:39:GLN:HE22	3:L:38:GLN:HE22	1.58	0.52
1:A:19:SER:C	1:A:20:TRP:HD1	2.17	0.51
1:A:166:PRO:HB3	1:A:187:PRO:HG3	1.93	0.51
1:B:149:HIS:HB3	4:D:1:NAG:H2	1.92	0.51
1:A:345:ARG:HD2	1:A:346:HIS:CD2	2.45	0.51
1:B:153:ASN:ND2	4:D:1:NAG:O7	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:PRO:HD2	1:B:381:GLY:HA2	1.91	0.51
2:I:117:LYS:NZ	2:I:175:LEU:HD11	2.25	0.51
1:B:297:MET:HA	1:B:334:LYS:HZ3	1.74	0.51
2:H:93:VAL:HG11	2:H:100(P):MET:HB3	1.93	0.51
1:B:188:ARG:HB2	1:B:282:HIS:O	2.10	0.51
1:B:51:LYS:C	1:B:53:PRO:HD3	2.36	0.51
1:A:51:LYS:C	1:A:53:PRO:HD3	2.37	0.50
1:B:387:LEU:N	1:B:387:LEU:HD12	2.26	0.50
1:A:80:PRO:O	1:A:94:HIS:HE1	1.94	0.50
1:B:62:GLU:HB3	1:B:123:LYS:HB2	1.92	0.50
1:A:71:GLU:HB2	1:A:82:LEU:HD21	1.93	0.50
1:B:34:MET:HG2	1:B:40:THR:HG22	1.92	0.50
1:A:64:LYS:N	1:A:120:THR:O	2.39	0.50
1:B:49:GLU:CD	1:B:51:LYS:HD3	2.36	0.50
1:B:335:ILE:HG22	1:B:358:VAL:HG23	1.94	0.50
2:I:11:LEU:HD11	2:I:112:SER:HB3	1.94	0.50
1:B:169:SER:HB2	1:B:185:CYS:O	2.12	0.49
1:B:137:TYR:O	1:B:163:LYS:HA	2.12	0.49
1:A:137:TYR:O	1:A:163:LYS:HA	2.12	0.49
3:L:95:ARG:HG3	3:L:95(A):THR:HG23	1.93	0.49
1:A:6:ILE:HD13	1:A:30:CYS:HB2	1.94	0.49
1:B:46:ILE:HG22	1:B:138:THR:O	2.12	0.49
1:B:13:GLU:OE1	1:B:350:ARG:NH2	2.46	0.49
1:A:340:THR:HG22	1:A:347:VAL:HA	1.94	0.49
1:A:337:PHE:O	1:A:338:GLU:OE2	2.30	0.49
4:C:1:NAG:H61	4:C:6:FUC:H2	1.68	0.48
1:A:167:GLN:C	1:A:169:SER:H	2.21	0.48
3:L:109:GLN:HB2	3:L:110:PRO:HD2	1.95	0.48
1:A:46:ILE:HG22	1:A:138:THR:O	2.12	0.48
1:A:255:SER:HB2	1:B:255:SER:HB2	1.94	0.48
2:I:87:THR:OG1	2:I:111:VAL:HG12	2.13	0.48
1:B:191:LEU:HD22	1:B:196:MET:HG3	1.95	0.48
1:A:34:MET:HG2	1:A:40:THR:CG2	2.44	0.48
1:B:71:GLU:HB2	1:B:82:LEU:HD21	1.95	0.48
2:H:87:THR:OG1	2:H:111:VAL:HG12	2.14	0.48
3:L:111:LYS:HE2	3:L:111:LYS:HB3	1.54	0.48
1:A:374:GLY:H	1:A:393:LYS:HB3	1.79	0.48
1:B:6:ILE:HD13	1:B:30:CYS:HB2	1.95	0.48
3:L:39:ARG:HG2	3:L:84:ALA:HB2	1.97	0.47
2:H:100:TYR:CE1	4:D:2:NAG:H4	2.49	0.47
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1:GLN:O	3:L:2:SER:OG	2.25	0.47
3:L:103:LYS:HE2	3:L:143:GLY:O	2.14	0.47
1:A:1:MET:HG3	1:A:144:HIS:HA	1.96	0.47
1:A:54:ALA:O	1:A:129:ILE:HG22	2.13	0.47
1:A:351:LEU:HD23	1:A:369:ALA:HB2	1.95	0.47
2:H:27:PHE:O	2:H:29:TYR:N	2.48	0.47
3:L:62:PHE:CZ	3:L:82:ASP:OD2	2.64	0.47
3:L:81:GLU:HG3	3:L:82:ASP:OD1	2.15	0.47
1:A:141:ILE:HD11	1:A:183:MET:HE1	1.96	0.46
1:B:340:THR:HG22	1:B:347:VAL:HA	1.96	0.46
1:B:375:ASP:HA	1:B:391:TRP:O	2.15	0.46
3:M:150:LYS:HE3	3:M:195:GLN:CD	2.40	0.46
1:A:169:SER:HB2	1:A:185:CYS:O	2.16	0.46
1:B:101:TRP:NE1	1:B:106:GLY:O	2.46	0.46
1:A:205:ALA:HB3	1:A:270:ILE:HG22	1.98	0.46
1:A:58:LYS:O	1:A:220:TRP:HA	2.16	0.46
1:A:342:LEU:HA	1:A:377:TYR:CE1	2.50	0.46
1:A:166:PRO:HG3	1:A:187:PRO:HG3	1.98	0.46
1:B:185:CYS:HB3	1:B:283:LEU:CD2	2.46	0.46
1:A:66:THR:CG2	1:A:118:LYS:HE2	2.45	0.46
1:A:147:GLU:HB3	1:A:150:ALA:HB2	1.97	0.46
1:B:297:MET:C	1:B:334:LYS:NZ	2.72	0.45
1:A:162:ILE:O	1:A:162:ILE:HG13	2.16	0.45
1:A:99:ARG:NH2	2:H:100(I):ASP:OD2	2.49	0.45
1:A:147:GLU:OE1	1:A:148:GLU:N	2.49	0.45
1:A:53:PRO:HB3	1:A:130:VAL:HG22	1.98	0.45
1:B:270:ILE:HG21	1:B:277:LEU:HD22	1.98	0.45
1:A:314:GLU:OE2	1:A:391:TRP:HH2	1.99	0.45
2:I:11:LEU:HD12	2:I:110:THR:O	2.16	0.45
1:B:94:HIS:CD2	1:B:114:VAL:HB	2.51	0.45
1:B:156:GLY:C	1:B:158:HIS:H	2.24	0.45
2:H:1:GLU:HB3	2:H:2:VAL:H	1.53	0.45
3:L:150:LYS:HE3	3:L:195:GLN:CD	2.42	0.45
1:A:379:ILE:HA	1:A:387:LEU:O	2.17	0.45
1:B:191:LEU:HD13	1:B:207:LEU:HD23	1.99	0.45
1:B:351:LEU:HD23	1:B:351:LEU:HA	1.86	0.45
1:B:339:ILE:HA	1:B:377:TYR:O	2.17	0.44
1:B:155:THR:HG21	2:H:99:PHE:CZ	2.52	0.44
1:A:191:LEU:HD22	1:A:196:MET:HG3	1.98	0.44
2:H:184:VAL:HG21	2:H:194:TYR:OH	2.18	0.44
3:M:15:PRO:HD3	3:M:107:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:GLN:HG3	1:B:364:PRO:HG3	1.98	0.44
1:A:342:LEU:HA	1:A:377:TYR:CD1	2.52	0.44
1:B:6:ILE:CD1	1:B:30:CYS:HB2	2.48	0.44
1:B:211:GLN:H	1:B:211:GLN:CD	2.26	0.44
1:B:278:LEU:HD23	1:B:278:LEU:HA	1.80	0.44
3:L:61:ARG:NH1	3:L:79:GLN:OE1	2.50	0.44
1:A:56:LEU:HD21	1:A:214:LEU:HD21	2.00	0.44
1:B:319:THR:CG2	1:B:368:GLU:HG2	2.48	0.44
3:L:35:TRP:HB2	3:L:48:ILE:HB	1.99	0.44
3:M:35:TRP:HB2	3:M:48:ILE:HB	2.00	0.44
1:B:35:ALA:HB3	1:B:38:LYS:HB2	2.00	0.44
2:H:53:ASP:HB2	2:H:100(F):TYR:HD1	1.83	0.43
1:A:191:LEU:HD23	1:A:192:ASP:H	1.83	0.43
1:A:242:ASN:ND2	6:A:601:HOH:O	2.50	0.43
1:B:148:GLU:HG3	1:B:149:HIS:CE1	2.53	0.43
1:A:322:ILE:HG12	1:A:324:VAL:HG13	1.99	0.43
1:B:170:THR:HA	1:B:183:MET:O	2.19	0.43
2:H:159:LEU:HD21	2:H:182:VAL:HG21	2.00	0.43
1:B:162:ILE:O	1:B:162:ILE:HG13	2.19	0.43
3:L:150:LYS:HE3	3:L:195:GLN:OE1	2.18	0.43
1:A:168:SER:O	1:A:168:SER:OG	2.34	0.43
1:A:191:LEU:HD23	1:A:192:ASP:N	2.34	0.43
1:A:342:LEU:HD11	1:A:375:ASP:HB2	2.01	0.43
1:B:237:LEU:HD12	1:B:253:LEU:HB3	2.00	0.43
1:B:253:LEU:HD23	1:B:253:LEU:O	2.18	0.43
1:B:290:ASP:OD1	1:B:290:ASP:N	2.50	0.43
2:H:2:VAL:C	2:H:3:GLN:HG3	2.44	0.43
2:I:53:ASP:HB2	2:I:100(F):TYR:HD1	1.83	0.43
1:B:75:PRO:O	1:B:76:THR:OG1	2.29	0.43
1:B:149:HIS:CB	4:D:1:NAG:H2	2.48	0.43
2:H:6:GLU:OE2	2:H:104:GLY:HA3	2.19	0.43
2:I:209:LYS:HD3	2:I:209:LYS:HA	1.79	0.43
3:L:93:THR:OG1	3:L:95(A):THR:OG1	2.26	0.43
1:A:271:GLN:HB2	1:A:278:LEU:HB2	2.01	0.43
1:B:196:MET:HB3	1:B:207:LEU:HG	2.01	0.43
1:A:37:ASN:HA	1:A:294:LEU:HD11	2.00	0.42
2:I:57:ARG:NH1	2:I:69:ILE:O	2.50	0.42
3:L:144:ALA:O	3:L:198:HIS:HD2	2.02	0.42
1:A:1:MET:H2	1:A:42:ASP:CG	2.27	0.42
1:A:363:SER:HA	1:A:364:PRO:HD3	1.90	0.42
3:M:79:GLN:HB2	3:M:82:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:148:ALA:O	3:M:195:GLN:HG3	2.19	0.42
1:B:387:LEU:H	1:B:387:LEU:CD1	2.32	0.42
2:I:33:TRP:CH2	2:I:52:ASN:HB3	2.55	0.42
1:A:75:PRO:O	1:A:76:THR:OG1	2.33	0.42
1:A:339:ILE:HA	1:A:377:TYR:O	2.20	0.42
1:B:155:THR:HG21	2:H:99:PHE:HZ	1.84	0.42
1:B:387:LEU:HD12	1:B:387:LEU:H	1.83	0.42
1:B:157:LYS:HB3	1:B:157:LYS:HE3	1.75	0.42
2:H:44:GLY:HA2	3:L:87:TYR:OH	2.20	0.42
1:B:12:VAL:HG12	1:B:21:VAL:HG21	2.02	0.41
1:B:200:GLN:HG3	1:B:272:MET:SD	2.60	0.41
2:H:11:LEU:HD12	2:H:110:THR:O	2.20	0.41
2:H:142:VAL:O	2:H:142:VAL:HG23	2.20	0.41
3:L:61:ARG:CD	3:L:79:GLN:HE22	2.33	0.41
1:A:57:ARG:NH1	1:A:220:TRP:CZ3	2.88	0.41
2:H:31:ASN:HB3	2:H:100(C):SER:O	2.20	0.41
1:B:66:THR:CG2	1:B:118:LYS:HE2	2.51	0.41
1:B:168:SER:O	1:B:168:SER:OG	2.37	0.41
2:I:184:VAL:HG21	2:I:194:TYR:OH	2.21	0.41
1:A:220:TRP:CD1	1:A:220:TRP:C	2.98	0.41
1:B:167:GLN:C	1:B:169:SER:H	2.28	0.41
2:H:97:VAL:HA	2:H:100:TYR:CD2	2.55	0.41
3:L:17:GLN:HG2	3:L:18:SER:N	2.36	0.41
3:M:93:THR:OG1	3:M:95(A):THR:OG1	2.27	0.41
1:A:6:ILE:CD1	1:A:30:CYS:HB2	2.50	0.41
1:A:156:GLY:C	1:A:158:HIS:N	2.77	0.41
1:A:350:ARG:HB3	1:A:370:GLU:HB3	2.03	0.41
1:B:164:ILE:HD11	1:B:169:SER:HA	2.02	0.41
3:L:17:GLN:HG2	3:L:18:SER:H	1.84	0.41
3:M:17:GLN:HG2	3:M:18:SER:H	1.86	0.41
1:B:99:ARG:HA	1:B:99:ARG:HD2	1.94	0.41
1:B:199:LEU:HD23	1:B:264:LEU:HD21	2.02	0.41
2:I:59:TYR:HB3	2:I:63:VAL:HG13	2.03	0.41
1:A:289:MET:CG	1:A:292:LEU:HD12	2.51	0.41
1:B:289:MET:HG3	1:B:292:LEU:HD12	2.03	0.41
2:I:142:VAL:O	2:I:142:VAL:HG23	2.20	0.41
3:L:13:GLY:O	3:L:107:VAL:HG23	2.20	0.41
1:A:352:ILE:HG12	1:A:369:ALA:HA	2.03	0.40
1:B:34:MET:HG2	1:B:40:THR:CG2	2.50	0.40
1:A:242:ASN:HD22	1:A:247:LYS:C	2.27	0.40
2:H:144:ASP:HB3	2:H:175:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:VAL:O	1:A:33:THR:HA	2.21	0.40
1:B:211:GLN:OE1	1:B:211:GLN:N	2.49	0.40
1:A:19:SER:C	1:A:20:TRP:CD1	2.99	0.40
1:B:148:GLU:HG3	1:B:149:HIS:ND1	2.36	0.40
2:I:184:VAL:HG22	2:I:185:PRO:CD	2.52	0.40
1:B:125:MET:HG2	1:B:199:LEU:CD1	2.49	0.40
3:L:104:LEU:HD23	3:L:104:LEU:C	2.45	0.40
3:M:4:LEU:HD21	3:M:90:SER:OG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	387/430 (90%)	368 (95%)	19 (5%)	0	100	100
1	B	382/430 (89%)	365 (96%)	17 (4%)	0	100	100
2	H	222/283 (78%)	214 (96%)	7 (3%)	1 (0%)	24	59
2	I	222/283 (78%)	212 (96%)	9 (4%)	1 (0%)	24	59
3	L	211/218 (97%)	205 (97%)	6 (3%)	0	100	100
3	M	211/218 (97%)	207 (98%)	4 (2%)	0	100	100
All	All	1635/1862 (88%)	1571 (96%)	62 (4%)	2 (0%)	48	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	64	LYS
2	I	64	LYS

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	342/368 (93%)	312 (91%)	30 (9%)	9	32
1	B	339/368 (92%)	308 (91%)	31 (9%)	9	31
2	H	192/236 (81%)	186 (97%)	6 (3%)	35	57
2	I	191/236 (81%)	185 (97%)	6 (3%)	35	57
3	L	180/185 (97%)	175 (97%)	5 (3%)	38	59
3	M	180/185 (97%)	177 (98%)	3 (2%)	53	68
All	All	1424/1578 (90%)	1343 (94%)	81 (6%)	18	44

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	15	VAL
1	A	21	VAL
1	A	46	ILE
1	A	86	GLN
1	A	95	SER
1	A	99	ARG
1	A	107	CYS
1	A	176	THR
1	A	201	MET
1	A	207	LEU
1	A	208	VAL
1	A	237	LEU
1	A	252	VAL
1	A	253	LEU
1	A	270	ILE
1	A	282	HIS
1	A	283	LEU
1	A	287	LEU
1	A	288	ARG
1	A	289	MET
1	A	308	ILE

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Mol	Chain	Res	Type
1	A	309	VAL
1	A	334	LYS
1	A	338	GLU
1	A	339	ILE
1	A	362	ASP
1	A	367	ILE
1	A	376	SER
1	A	380	VAL
1	B	6	ILE
1	B	20	TRP
1	B	46	ILE
1	B	64	LYS
1	B	95	SER
1	B	99	ARG
1	B	107	CYS
1	B	141	ILE
1	B	176	THR
1	B	201	MET
1	B	207	LEU
1	B	208	VAL
1	B	252	VAL
1	B	270	ILE
1	B	271	GLN
1	B	282	HIS
1	B	283	LEU
1	B	287	LEU
1	B	289	MET
1	B	308	ILE
1	B	309	VAL
1	B	312	ILE
1	B	333	CYS
1	B	335	ILE
1	B	344	LYS
1	B	362	ASP
1	B	367	ILE
1	B	376	SER
1	B	379	ILE
1	B	380	VAL
1	B	387	LEU
2	H	63	VAL
2	H	97	VAL
2	H	117	LYS

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Mol	Chain	Res	Type
2	H	178	LEU
2	H	184	VAL
2	H	195	ILE
2	I	13	ARG
2	I	43	LYS
2	I	63	VAL
2	I	97	VAL
2	I	178	LEU
2	I	184	VAL
3	L	19	ILE
3	L	33	VAL
3	L	74	THR
3	L	97	VAL
3	L	195	GLN
3	M	19	ILE
3	M	33	VAL
3	M	97	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	HIS
1	A	233	GLN
1	A	244	HIS
1	A	346	HIS
1	B	149	HIS
1	B	244	HIS
1	B	256	GLN
1	B	276	ASN
1	B	325	GLN
1	B	346	HIS
1	B	386	GLN
2	H	31	ASN
2	H	39	GLN
2	H	192	GLN
2	H	199	ASN
2	I	199	ASN
2	I	204	ASN
3	L	109	GLN
3	L	195	GLN
3	M	195	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 ⓘ

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	0.35	0	17,19,21	0.59	0
4	NAG	C	2	4	14,14,15	0.58	0	17,19,21	1.55	2 (11%)
4	BMA	C	3	4	11,11,12	1.06	1 (9%)	15,15,17	1.03	1 (6%)
4	MAN	C	4	4	11,11,12	0.80	0	15,15,17	1.26	2 (13%)
4	MAN	C	5	4	11,11,12	0.81	0	15,15,17	0.83	0
4	FUC	C	6	4	10,10,11	1.01	1 (10%)	14,14,16	1.05	1 (7%)
4	NAG	D	1	1,4	14,14,15	0.36	0	17,19,21	0.66	0
4	NAG	D	2	4	14,14,15	0.48	0	17,19,21	1.59	2 (11%)
4	BMA	D	3	4	11,11,12	1.08	1 (9%)	15,15,17	1.01	1 (6%)
4	MAN	D	4	4	11,11,12	0.83	0	15,15,17	1.23	2 (13%)
4	MAN	D	5	4	11,11,12	0.60	0	15,15,17	0.87	1 (6%)
4	FUC	D	6	4	10,10,11	0.89	0	14,14,16	0.96	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	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	2	4	-	0/6/23/26	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	-	4/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3	BMA	O5-C5	2.49	1.48	1.43
4	D	3	BMA	O5-C5	2.20	1.47	1.43
4	C	6	FUC	C2-C3	2.16	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	NAG	C1-O5-C5	4.51	118.23	112.19
4	C	2	NAG	C1-O5-C5	4.37	118.04	112.19
4	D	4	MAN	C1-O5-C5	3.88	117.39	112.19
4	C	4	MAN	C1-O5-C5	3.83	117.32	112.19
4	C	3	BMA	C1-O5-C5	3.19	116.46	112.19
4	D	2	NAG	O4-C4-C5	3.18	117.16	109.32
4	D	3	BMA	C1-O5-C5	3.12	116.37	112.19
4	C	2	NAG	O4-C4-C5	3.12	117.01	109.32
4	C	4	MAN	O2-C2-C3	-2.24	105.50	110.15
4	D	5	MAN	O2-C2-C3	-2.15	105.69	110.15
4	D	4	MAN	O2-C2-C3	-2.11	105.78	110.15
4	C	6	FUC	C1-O5-C5	2.05	117.81	112.97

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	D	3	BMA	C4-C5-C6-O6
4	C	3	BMA	C4-C5-C6-O6
4	C	3	BMA	O5-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
4	C	1	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
4	C	4	MAN	O5-C5-C6-O6
4	D	1	NAG	C1-C2-N2-C7
4	D	1	NAG	C3-C2-N2-C7

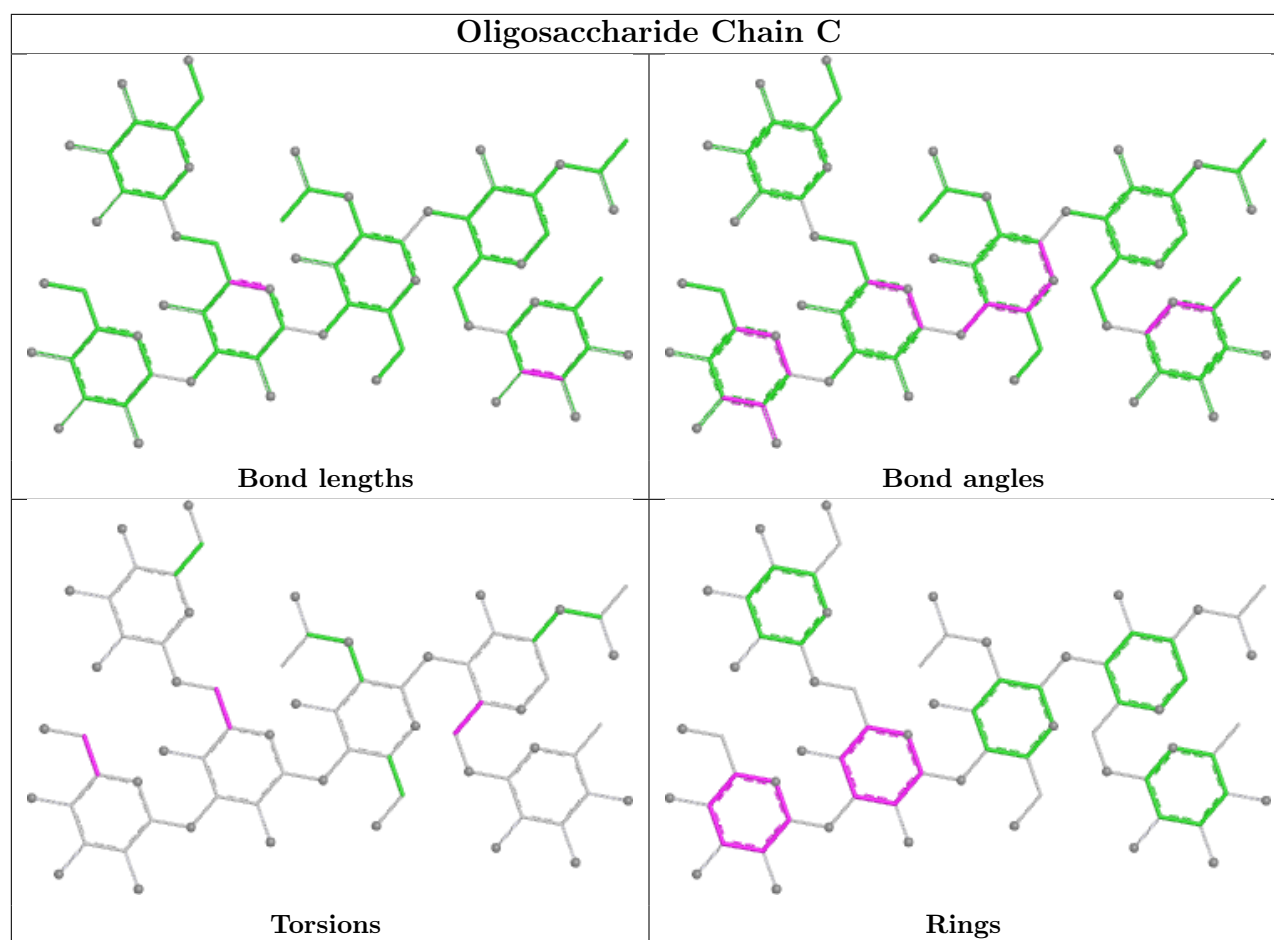
All (4) ring outliers are listed below:

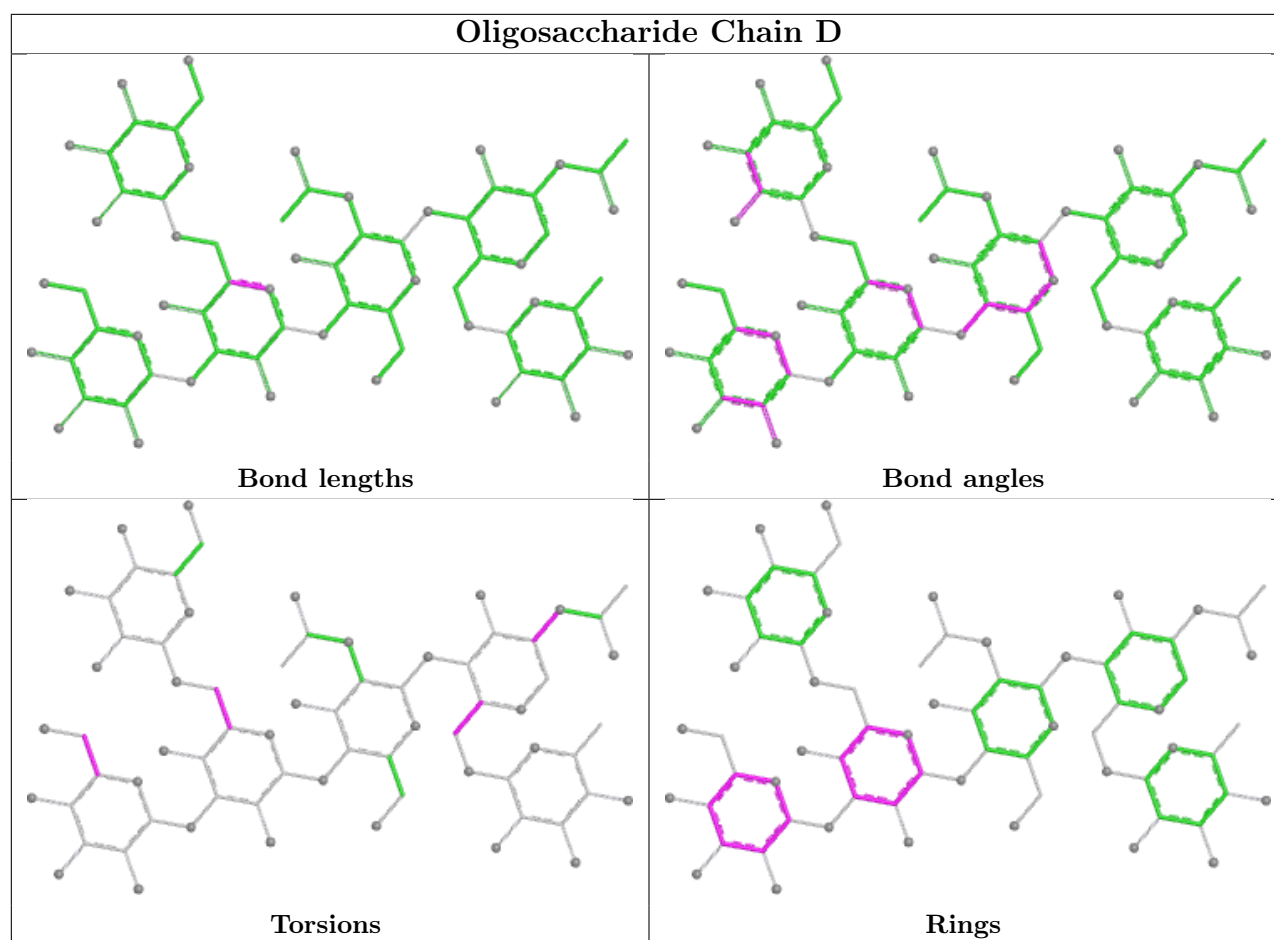
Mol	Chain	Res	Type	Atoms
4	D	3	BMA	C1-C2-C3-C4-C5-O5
4	C	3	BMA	C1-C2-C3-C4-C5-O5
4	C	4	MAN	C1-C2-C3-C4-C5-O5
4	D	4	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1	NAG	2	0
4	D	2	NAG	1	0
4	C	6	FUC	1	0
4	C	2	NAG	1	0
4	D	1	NAG	3	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](#)

1 ligand is 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	$\# Z > 2$
5	NAG	B	507	1	14,14,15	0.28	0	17,19,21	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	507	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	391/430 (90%)	0.31	10 (2%) 57 40	59, 80, 145, 246	0
1	B	388/430 (90%)	0.34	8 (2%) 63 44	59, 85, 161, 262	0
2	H	226/283 (79%)	0.50	5 (2%) 62 44	67, 117, 203, 324	0
2	I	226/283 (79%)	0.40	4 (1%) 67 47	62, 127, 253, 380	0
3	L	213/218 (97%)	0.38	3 (1%) 73 52	72, 128, 207, 288	0
3	M	213/218 (97%)	0.49	6 (2%) 55 38	67, 126, 252, 315	0
All	All	1657/1862 (88%)	0.39	36 (2%) 62 44	59, 96, 209, 380	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	196	VAL	4.7
3	M	147	VAL	3.7
1	B	324	VAL	3.5
3	M	145	VAL	3.4
1	A	324	VAL	3.1
3	M	62	PHE	3.0
1	A	337	PHE	2.9
1	B	102	GLY	2.8
1	A	207	LEU	2.7
1	A	155	THR	2.7
3	M	75	ILE	2.6
3	L	38	GLN	2.5
2	I	1	GLU	2.5
1	A	190	GLY	2.4
2	H	107	THR	2.4
1	A	5	GLY	2.3
3	L	75	ILE	2.3
1	B	252	VAL	2.3
2	I	142	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	138	LEU	2.3
3	L	110	PRO	2.3
1	B	308	ILE	2.3
3	M	35	TRP	2.2
2	I	32	HIS	2.2
1	A	97	VAL	2.2
1	B	97	VAL	2.2
2	H	41	PRO	2.1
1	A	50	ALA	2.1
2	H	143	LYS	2.1
2	H	73	ASN	2.1
1	A	187	PRO	2.1
1	B	317	HIS	2.0
1	B	337	PHE	2.0
1	A	78	GLY	2.0
1	B	141	ILE	2.0
2	I	178	LEU	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.

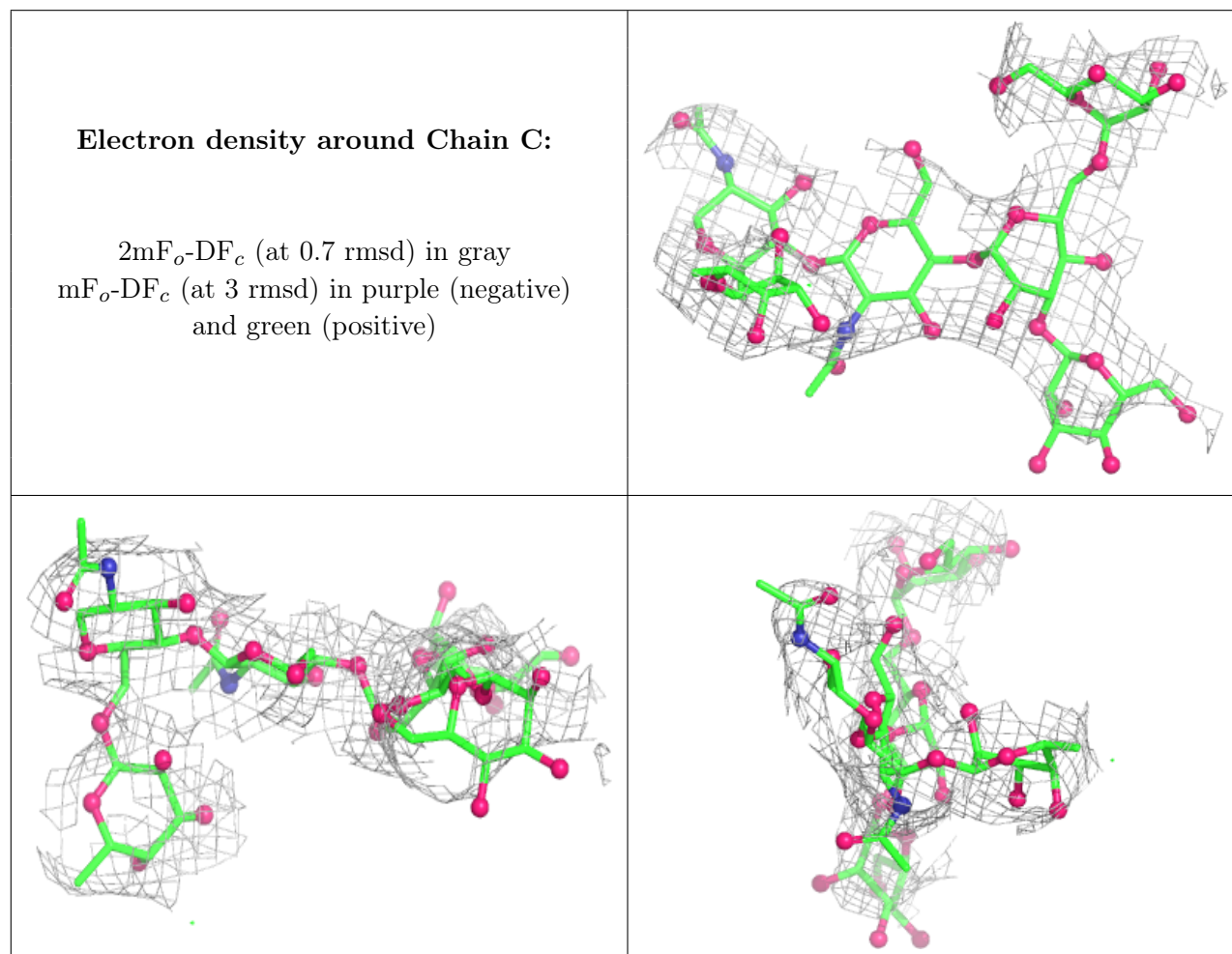
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	C	1	14/15	-	-	66,68,106,109	0
4	NAG	C	2	14/15	-	-	70,72,98,104	0
4	BMA	C	3	11/12	-	-	86,91,116,138	0
4	MAN	C	4	11/12	-	-	115,125,146,175	0
4	MAN	C	5	11/12	-	-	100,104,137,141	0
4	FUC	C	6	10/11	-	-	70,70,114,115	0
4	NAG	D	1	14/15	-	-	75,78,114,130	0
4	NAG	D	2	14/15	-	-	89,102,130,137	0
4	BMA	D	3	11/12	-	-	81,83,103,170	0
4	MAN	D	4	11/12	-	-	206,210,215,216	0
4	MAN	D	5	11/12	-	-	79,81,84,87	0

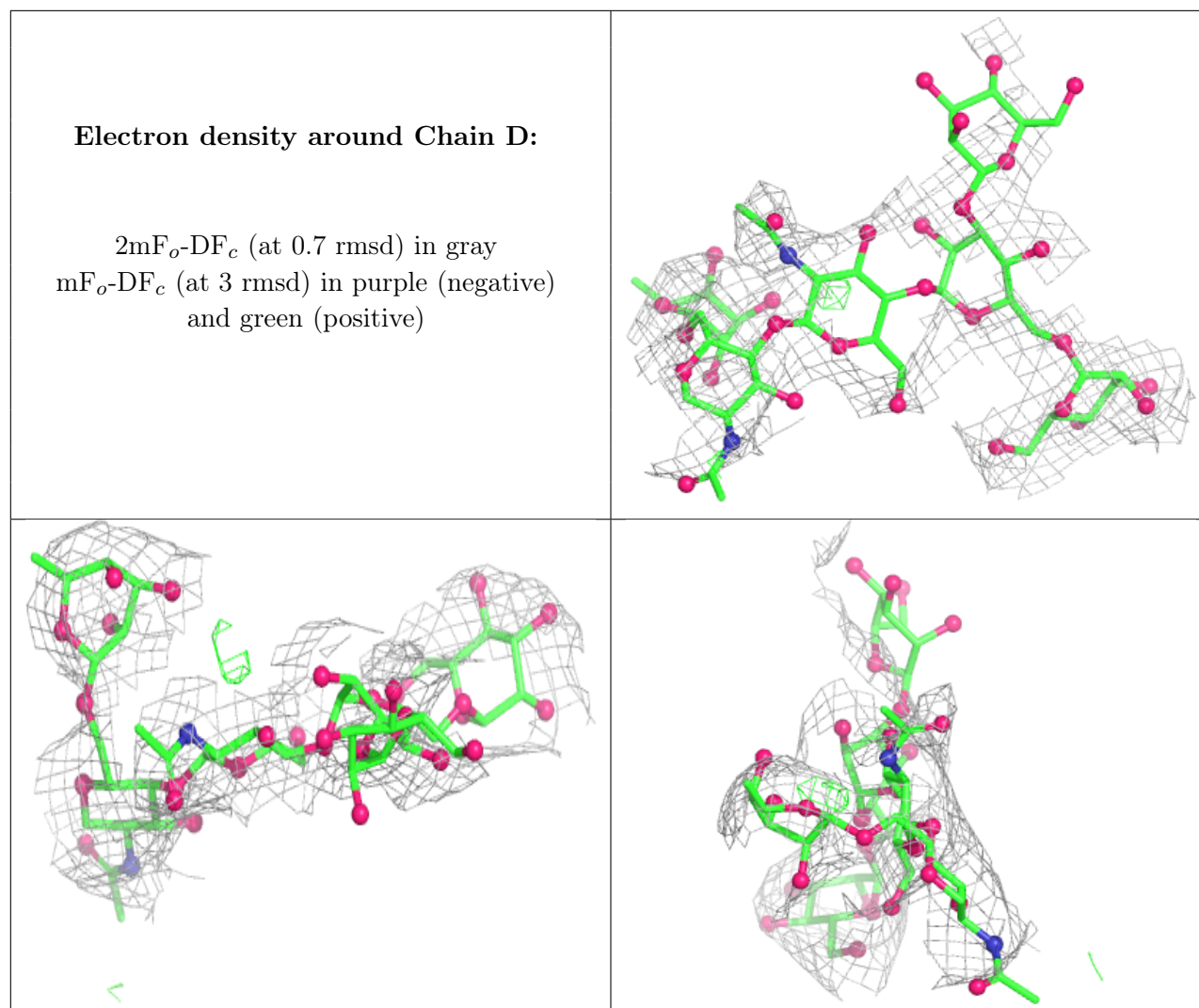
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FUC	D	6	10/11	-	-	99,103,119,136	0

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.





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	B	507	14/15	0.56	0.11	107,126,139,142	0

6.5 Other polymers [i](#)

There are no such residues in this entry.