



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:30 AM UTC

PDB ID : 6ZPT / pdb_00006zpt
Title : Crystal structure of the open conformation of S2_S'-mutant human Angiotensin-1 converting enzyme N-domain.
Authors : Cozier, G.E.; Acharya, K.R.
Deposited on : 2020-07-09
Resolution : 2.80 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

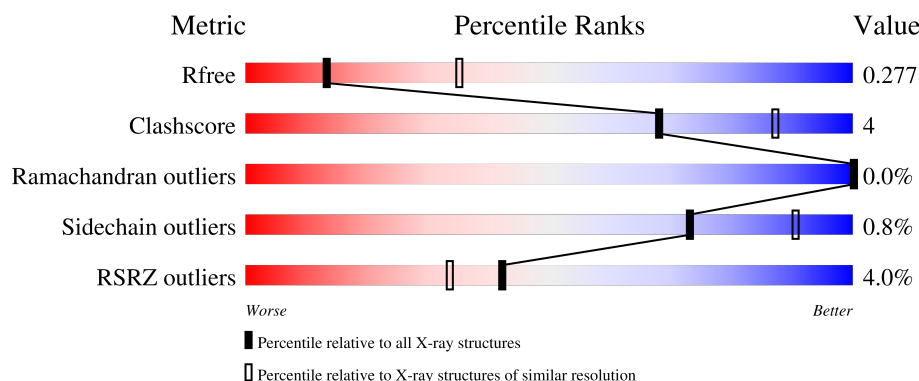
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	629	4% 86% 10% .
1	B	629	4% 89% 7% .
1	C	629	3% 85% 9% 6%
1	D	629	4% 87% 9% .
2	E	2	100%

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Mol	Chain	Length	Quality of chain
3	F	2	 50%50%
3	G	2	 50%50%
3	H	2	 50%50%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 38972 atoms, of which 19031 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 Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	601	Total	C	H	N	O	S	0	4	0
			9642	3171	4708	844	900	19			
1	B	601	Total	C	H	N	O	S	0	0	0
			9611	3161	4695	842	894	19			
1	C	593	Total	C	H	N	O	S	0	2	0
			9479	3111	4633	832	884	19			
1	D	601	Total	C	H	N	O	S	0	4	0
			9638	3169	4710	843	897	19			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	engineered mutation	UNP P12821
A	25	GLN	ASN	engineered mutation	UNP P12821
A	82	GLN	ASN	engineered mutation	UNP P12821
A	117	GLN	ASN	engineered mutation	UNP P12821
A	131	GLN	ASN	engineered mutation	UNP P12821
A	260	THR	SER	engineered mutation	UNP P12821
A	262	SER	GLU	engineered mutation	UNP P12821
A	289	GLN	ASN	engineered mutation	UNP P12821
A	354	GLU	ASP	engineered mutation	UNP P12821
A	357	VAL	SER	engineered mutation	UNP P12821
A	358	VAL	THR	engineered mutation	UNP P12821
A	369	PHE	TYR	engineered mutation	UNP P12821
A	381	GLU	ARG	engineered mutation	UNP P12821
A	431	ASP	GLU	engineered mutation	UNP P12821
A	545	ARG	GLN	engineered mutation	UNP P12821
A	576	LEU	PRO	engineered mutation	UNP P12821
A	629	LEU	-	expression tag	UNP P12821
B	9	GLN	ASN	engineered mutation	UNP P12821
B	25	GLN	ASN	engineered mutation	UNP P12821
B	82	GLN	ASN	engineered mutation	UNP P12821
B	117	GLN	ASN	engineered mutation	UNP P12821

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Chain	Residue	Modelled	Actual	Comment	Reference
B	131	GLN	ASN	engineered mutation	UNP P12821
B	260	THR	SER	engineered mutation	UNP P12821
B	262	SER	GLU	engineered mutation	UNP P12821
B	289	GLN	ASN	engineered mutation	UNP P12821
B	354	GLU	ASP	engineered mutation	UNP P12821
B	357	VAL	SER	engineered mutation	UNP P12821
B	358	VAL	THR	engineered mutation	UNP P12821
B	369	PHE	TYR	engineered mutation	UNP P12821
B	381	GLU	ARG	engineered mutation	UNP P12821
B	431	ASP	GLU	engineered mutation	UNP P12821
B	545	ARG	GLN	engineered mutation	UNP P12821
B	576	LEU	PRO	engineered mutation	UNP P12821
B	629	LEU	-	expression tag	UNP P12821
C	9	GLN	ASN	engineered mutation	UNP P12821
C	25	GLN	ASN	engineered mutation	UNP P12821
C	82	GLN	ASN	engineered mutation	UNP P12821
C	117	GLN	ASN	engineered mutation	UNP P12821
C	131	GLN	ASN	engineered mutation	UNP P12821
C	260	THR	SER	engineered mutation	UNP P12821
C	262	SER	GLU	engineered mutation	UNP P12821
C	289	GLN	ASN	engineered mutation	UNP P12821
C	354	GLU	ASP	engineered mutation	UNP P12821
C	357	VAL	SER	engineered mutation	UNP P12821
C	358	VAL	THR	engineered mutation	UNP P12821
C	369	PHE	TYR	engineered mutation	UNP P12821
C	381	GLU	ARG	engineered mutation	UNP P12821
C	431	ASP	GLU	engineered mutation	UNP P12821
C	545	ARG	GLN	engineered mutation	UNP P12821
C	576	LEU	PRO	engineered mutation	UNP P12821
C	629	LEU	-	expression tag	UNP P12821
D	9	GLN	ASN	engineered mutation	UNP P12821
D	25	GLN	ASN	engineered mutation	UNP P12821
D	82	GLN	ASN	engineered mutation	UNP P12821
D	117	GLN	ASN	engineered mutation	UNP P12821
D	131	GLN	ASN	engineered mutation	UNP P12821
D	260	THR	SER	engineered mutation	UNP P12821
D	262	SER	GLU	engineered mutation	UNP P12821
D	289	GLN	ASN	engineered mutation	UNP P12821
D	354	GLU	ASP	engineered mutation	UNP P12821
D	357	VAL	SER	engineered mutation	UNP P12821
D	358	VAL	THR	engineered mutation	UNP P12821
D	369	PHE	TYR	engineered mutation	UNP P12821

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Chain	Residue	Modelled	Actual	Comment	Reference
D	381	GLU	ARG	engineered mutation	UNP P12821
D	431	ASP	GLU	engineered mutation	UNP P12821
D	545	ARG	GLN	engineered mutation	UNP P12821
D	576	LEU	PRO	engineered mutation	UNP P12821
D	629	LEU	-	expression tag	UNP P12821

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



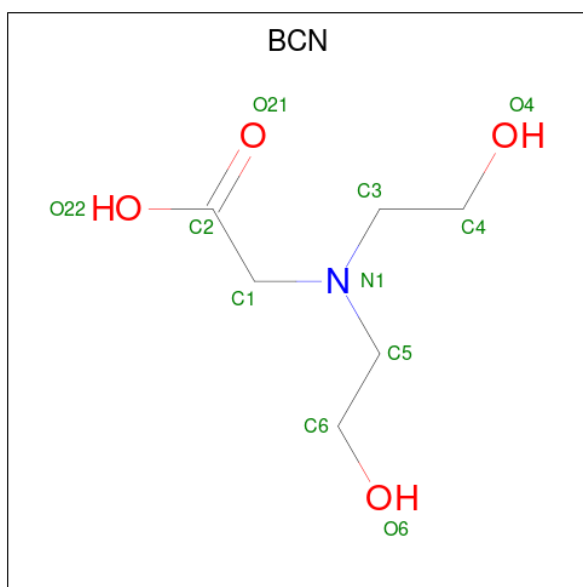
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

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



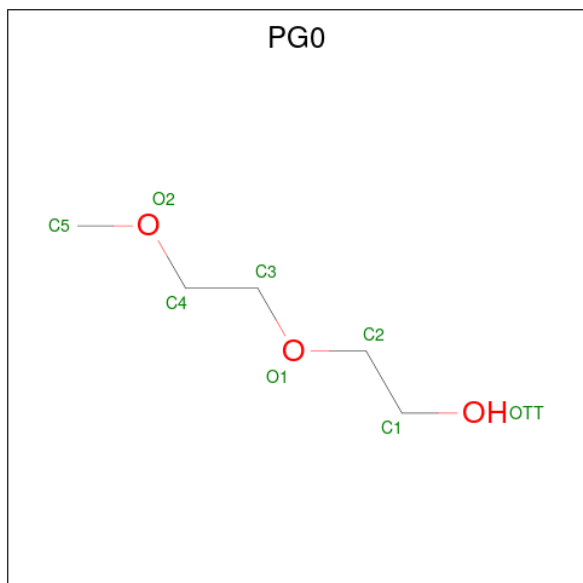
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	2	Total	C	H	N	O	0	0	0
			48	14	24	1	9			
3	G	2	Total	C	H	N	O	0	0	0
			48	14	24	1	9			
3	H	2	Total	C	H	N	O	0	0	0
			48	14	24	1	9			

- Molecule 4 is BICINE (CCD ID: BCN) (formula: C₆H₁₃NO₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 23	C 6	H 12	N 1	O 4	0	0
4	B	1	Total 23	C 6	H 12	N 1	O 4	0	0
4	C	1	Total 23	C 6	H 12	N 1	O 4	0	0
4	D	1	Total 23	C 6	H 12	N 1	O 4	0	0

- Molecule 5 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula: C₅H₁₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			20	5	12	3		
5	A	1	Total	C	H	O	0	1
			40	10	24	6		
5	B	1	Total	C	H	O	0	0
			20	5	12	3		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		
6	B	1	Total	Zn	0	0
			1	1		
6	C	1	Total	Zn	0	0
			1	1		
6	D	1	Total	Zn	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	B	1	Total	Cl	0	0
			1	1		
7	C	1	Total	Cl	0	0
			1	1		
7	D	1	Total	Cl	0	0
			1	1		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

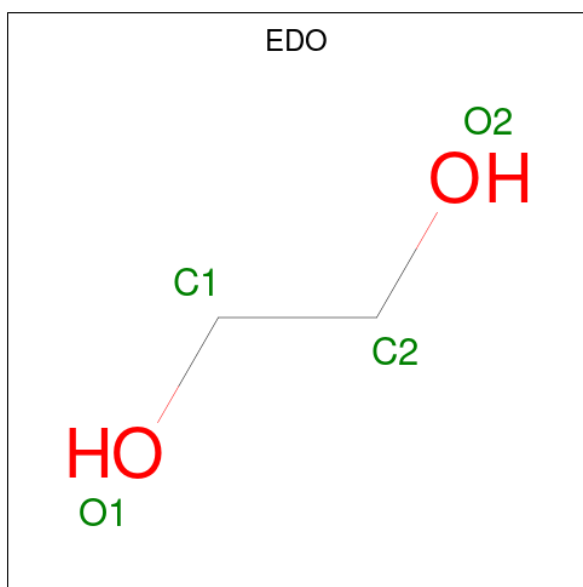
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca	0	0
			1	1		
8	B	1	Total	Ca	0	0
			1	1		
8	C	1	Total	Ca	0	0
			1	1		
8	D	1	Total	Ca	0	0
			1	1		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
9	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
9	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C H O 10 2 6 2	0	0
10	C	1	Total C H O 10 2 6 2	0	0
10	C	1	Total C H O 10 2 6 2	0	0
10	C	1	Total C H O 10 2 6 2	0	0
10	C	1	Total C H O 10 2 6 2	0	0
10	D	1	Total C H O 10 2 6 2	0	0
10	D	1	Total C H O 10 2 6 2	0	0
10	D	1	Total C H O 10 2 6 2	0	0

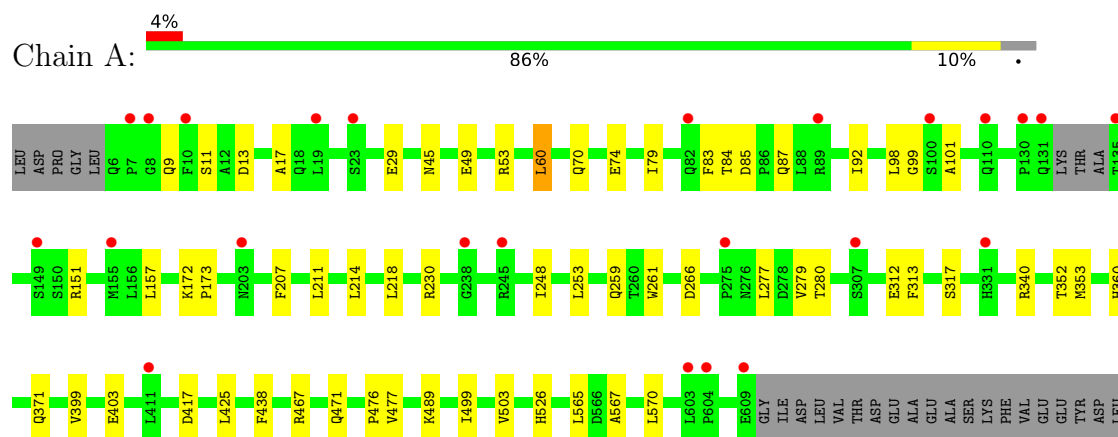
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	21	Total O 21 21	0	0
11	B	10	Total O 10 10	0	0
11	C	16	Total O 16 16	0	0
11	D	8	Total O 8 8	0	0

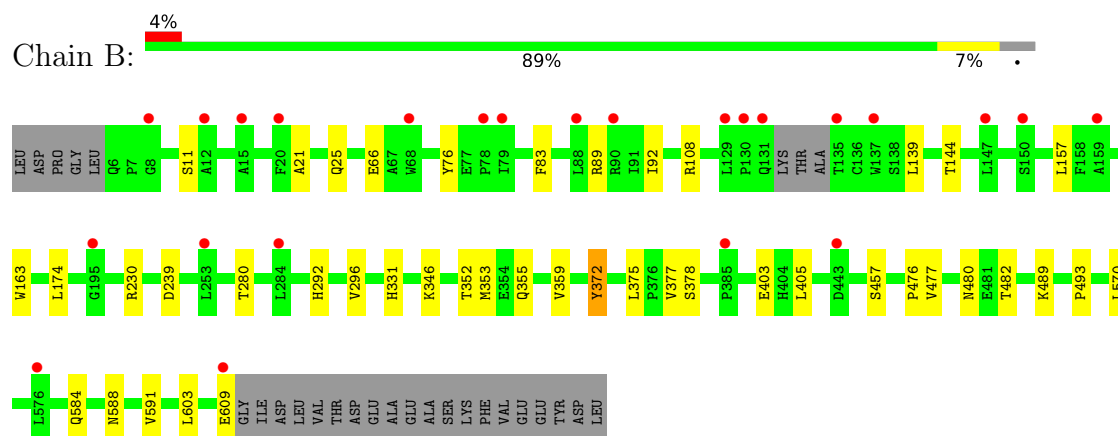
3 Residue-property plots [i](#)

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.

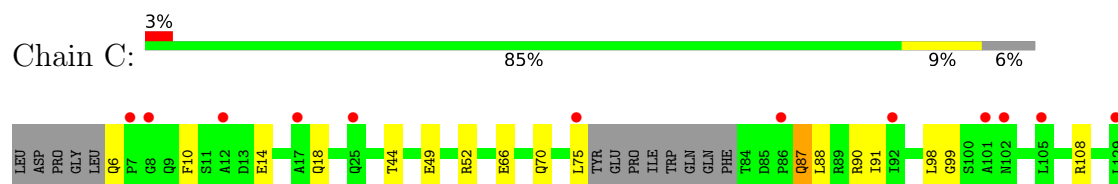
• Molecule 1: Angiotensin-converting enzyme



• Molecule 1: Angiotensin-converting enzyme

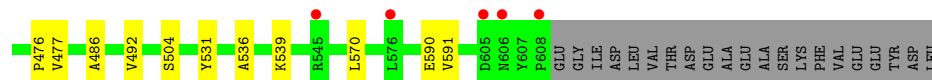
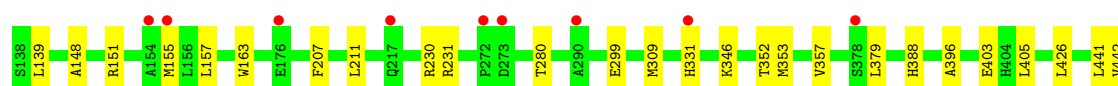
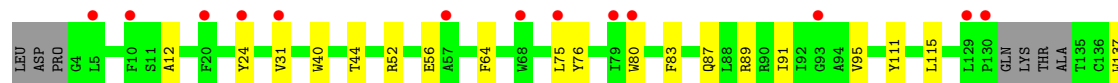
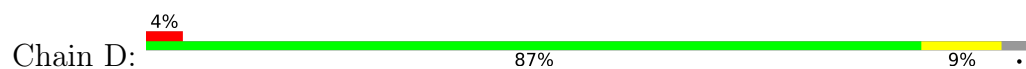


• Molecule 1: Angiotensin-converting enzyme





• Molecule 1: Angiotensin-converting enzyme



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



• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.65Å 99.26Å 127.98Å 98.63° 89.63° 111.15°	Depositor
Resolution (Å)	69.05 – 2.80 69.05 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (69.05-2.80) 98.8 (69.05-2.80)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.224 , 0.278 0.225 , 0.277	Depositor DCC
R_{free} test set	2051 reflections (2.49%)	wwPDB-VP
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.804	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.059 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	38972	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: BCN, FUC, PG0, ZN, CA, NAG, CL, EDO

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	0.11	0/5102	0.28	0/6950
1	B	0.11	0/5071	0.28	0/6908
1	C	0.11	0/5000	0.29	0/6808
1	D	0.10	0/5096	0.27	0/6942
All	All	0.11	0/20269	0.28	0/27608

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	4934	4708	4698	40	0
1	B	4916	4695	4695	26	0
1	C	4846	4633	4627	41	0
1	D	4928	4710	4699	35	0
2	E	28	27	25	0	0
3	F	24	24	22	2	0
3	G	24	24	22	1	0
3	H	24	24	22	0	0
4	A	11	12	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	11	12	10	0	0
4	C	11	12	11	0	0
4	D	11	12	11	0	0
5	A	24	36	36	1	0
5	B	8	12	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	B	28	28	26	0	0
9	C	14	14	13	0	0
10	B	4	6	6	0	0
10	C	16	24	24	0	0
10	D	12	18	18	0	0
11	A	21	0	0	1	0
11	B	10	0	0	0	0
11	C	16	0	0	1	0
11	D	8	0	0	0	0
All	All	19941	19031	18987	141	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 4.

All (141) 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:331:HIS:O	1:B:346:LYS:NZ	2.07	0.87
1:D:157:LEU:HD11	1:D:477:VAL:HG13	1.66	0.78
1:D:40:TRP:O	1:D:44:THR:OG1	2.01	0.78
1:C:157:LEU:HD11	1:C:477:VAL:HG13	1.66	0.78
1:C:371:GLN:OE1	1:C:545:ARG:NH1	2.16	0.77
1:C:6:GLN:N	11:C:801:HOH:O	2.19	0.75
1:C:90:ARG:HG2	1:C:91:ILE:HD12	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.72	0.71
1:A:9:GLN:OE1	1:A:9:GLN:N	2.25	0.70
1:C:10:PHE:O	1:C:75:LEU:HD11	1.93	0.69
1:A:11:SER:OG	1:A:13:ASP:OD1	2.11	0.68
1:C:49:GLU:OE1	1:C:52:ARG:NH1	2.26	0.68
1:C:482:THR:HG21	3:G:1:NAG:O7	1.95	0.66
1:B:609:GLU:OE1	1:B:609:GLU:N	2.29	0.65
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.80	0.63
1:A:74:GLU:OE1	11:A:801:HOH:O	2.16	0.63
1:C:157:LEU:HD13	1:C:476:PRO:HB2	1.81	0.63
1:A:313:PHE:O	1:A:317:SER:OG	2.13	0.62
1:A:214:LEU:HD11	1:A:565:LEU:HB2	1.82	0.61
1:B:403:GLU:N	1:B:403:GLU:OE2	2.32	0.60
1:A:49:GLU:OE1	1:A:53:ARG:NE	2.34	0.59
1:C:137:TRP:CH2	1:C:155:MET:HE1	2.37	0.59
1:B:353:MET:HE3	1:B:405:LEU:HD11	1.85	0.59
1:B:25:GLN:OE1	1:B:378:SER:OG	2.21	0.58
1:D:12:ALA:HB2	1:D:75:LEU:HD22	1.86	0.58
1:D:353:MET:HE3	1:D:405:LEU:HD11	1.87	0.57
1:D:230:ARG:NH2	1:D:591:VAL:O	2.38	0.56
1:B:372:TYR:HB2	1:B:375:LEU:HD12	1.87	0.56
1:B:230:ARG:NH2	1:B:591:VAL:O	2.38	0.56
1:A:17:ALA:HB1	1:A:92:ILE:CD1	2.36	0.56
1:A:17:ALA:HB1	1:A:92:ILE:HD11	1.89	0.55
1:C:277:LEU:HD22	1:C:353:MET:HE1	1.88	0.55
1:C:87:GLN:O	1:C:90:ARG:N	2.39	0.55
1:D:40:TRP:CE2	1:D:44:THR:HG21	2.42	0.55
1:C:10:PHE:HB2	1:C:75:LEU:HD21	1.89	0.54
1:C:360:HIS:ND1	1:C:399:VAL:HG21	2.22	0.54
1:C:221:LEU:HD11	1:C:571:LEU:HD22	1.90	0.54
1:D:31:VAL:HG21	1:D:64:PHE:CG	2.42	0.54
1:A:70:GLN:HG3	1:A:98:LEU:HD21	1.90	0.54
1:B:480:ASN:OD1	1:B:482:THR:OG1	2.25	0.54
1:C:70:GLN:HG3	1:C:98:LEU:HD21	1.90	0.53
1:D:299:GLU:OE1	1:D:531:TYR:OH	2.21	0.53
1:A:340:ARG:NH2	1:C:305:GLU:OE2	2.40	0.52
1:A:403:GLU:OE2	1:A:403:GLU:N	2.38	0.52
1:C:218:LEU:HD13	1:C:436:LEU:HD13	1.90	0.52
1:B:157:LEU:HD13	1:B:476:PRO:HB2	1.92	0.51
1:A:259:GLN:OE1	1:A:489:LYS:NZ	2.31	0.51
1:C:426:LEU:HD13	1:C:430:LEU:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LEU:HD21	1:A:567:ALA:HB1	1.92	0.51
1:A:157:LEU:HD13	1:A:476:PRO:HB2	1.93	0.51
1:B:139:LEU:HD22	1:B:163:TRP:CZ2	2.45	0.51
1:D:91:ILE:HD11	1:D:379:LEU:HD21	1.91	0.51
1:A:280:THR:HG23	1:A:352:THR:HA	1.93	0.51
1:A:214:LEU:HD11	1:A:565:LEU:CB	2.40	0.51
1:D:353:MET:HE3	1:D:405:LEU:CD1	2.41	0.50
1:C:441:LEU:C	1:C:441:LEU:HD12	2.36	0.50
1:A:277:LEU:HG	1:A:353:MET:HE1	1.92	0.50
1:C:221:LEU:CD1	1:C:571:LEU:HD22	2.41	0.50
1:B:280:THR:HG23	1:B:352:THR:HA	1.93	0.50
1:A:312:GLU:N	1:A:312:GLU:OE2	2.43	0.50
1:D:148:ALA:O	1:D:151:ARG:NH2	2.45	0.49
1:C:426:LEU:HD13	1:C:430:LEU:CD1	2.42	0.49
1:B:66:GLU:OE1	1:B:108:ARG:NH1	2.45	0.49
1:D:83:PHE:O	1:D:89:ARG:NH2	2.43	0.49
1:B:157:LEU:HD11	1:B:477:VAL:CG1	2.41	0.48
1:D:91:ILE:O	1:D:95:VAL:HG23	2.13	0.48
1:A:29:GLU:OE1	1:A:340:ARG:NH1	2.46	0.48
1:B:11:SER:O	1:B:76:TYR:OH	2.29	0.48
1:D:87:GLN:O	1:D:91:ILE:HD13	2.13	0.48
1:D:137:TRP:HH2	1:D:155:MET:HE1	1.79	0.48
1:D:441:LEU:C	1:D:441:LEU:HD12	2.38	0.48
1:C:137:TRP:HH2	1:C:155:MET:HE1	1.76	0.48
1:A:84:THR:OG1	1:A:85:ASP:N	2.46	0.47
1:A:467:ARG:NH1	1:A:471:GLN:OE1	2.47	0.47
1:C:432:LYS:NZ	1:C:508:GLN:OE1	2.44	0.47
1:B:584:GLN:O	1:B:588:ASN:ND2	2.44	0.47
1:D:157:LEU:HD13	1:D:476:PRO:HB2	1.96	0.47
1:C:172:LYS:NZ	1:C:481:GLU:O	2.45	0.47
1:D:441:LEU:HD12	1:D:442:VAL:N	2.29	0.47
1:D:76:TYR:O	1:D:80:TRP:N	2.48	0.46
3:F:1:NAG:H83	3:F:1:NAG:H3	1.97	0.46
1:A:570:LEU:C	1:A:570:LEU:HD23	2.40	0.46
3:F:1:NAG:C1	3:F:1:NAG:H82	2.46	0.46
1:A:151:ARG:NH1	1:A:266:ASP:OD1	2.48	0.46
1:C:66:GLU:OE1	1:C:108:ARG:NH1	2.48	0.46
1:B:477:VAL:HG12	1:B:603:LEU:HD21	1.98	0.46
1:D:309:MET:HA	1:D:309:MET:HE2	1.98	0.45
1:C:280:THR:HG23	1:C:352:THR:HA	1.99	0.45
1:B:21:ALA:HB2	1:B:92:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ASP:OD1	1:A:417:ASP:N	2.50	0.44
1:D:207:PHE:CZ	1:D:211:LEU:HD11	2.52	0.44
1:D:331:HIS:O	1:D:346:LYS:NZ	2.49	0.44
1:D:357:VAL:CG1	1:D:396:ALA:HB1	2.47	0.44
1:A:360:HIS:CD2	1:A:399:VAL:HG21	2.53	0.44
1:B:489:LYS:O	1:B:493:PRO:HD2	2.18	0.44
1:A:98:LEU:HB3	1:A:101:ALA:HB3	2.00	0.44
1:A:207:PHE:CZ	1:A:211:LEU:HD11	2.53	0.44
1:A:371:GLN:O	1:C:535:LYS:NZ	2.43	0.43
1:C:273:ASP:OD1	1:C:274:LYS:N	2.51	0.43
1:A:60:LEU:HD23	1:A:60:LEU:O	2.18	0.43
1:A:211:LEU:HD13	1:A:499:ILE:HD11	2.00	0.43
1:D:52:ARG:NH1	1:D:56:GLU:OE2	2.51	0.43
1:D:231:ARG:NE	1:D:590:GLU:OE2	2.39	0.43
1:A:49:GLU:O	1:A:53:ARG:HG3	2.19	0.43
1:A:172:LYS:HB3	1:A:173:PRO:HD3	2.01	0.43
1:A:230:ARG:HB2	1:A:248:ILE:HD11	2.00	0.43
5:A:703[A]:PG0:H12	1:C:307:SER:HB2	2.01	0.42
1:D:24:TYR:CE2	1:D:95:VAL:HG13	2.54	0.42
1:C:44:THR:O	1:C:328:VAL:HG12	2.20	0.42
1:D:139:LEU:HD22	1:D:163:TRP:CZ2	2.54	0.42
1:B:355:GLN:O	1:B:359:VAL:HG23	2.20	0.42
1:C:312:GLU:OE2	1:C:312:GLU:N	2.45	0.42
1:C:570:LEU:C	1:C:570:LEU:HD23	2.45	0.42
1:D:536:ALA:O	1:D:539:LYS:N	2.52	0.42
1:D:137:TRP:CH2	1:D:155:MET:HE1	2.55	0.42
1:C:88:LEU:HD13	1:C:88:LEU:O	2.20	0.41
1:D:280:THR:HG23	1:D:352:THR:HA	2.02	0.41
1:D:486:ALA:O	1:D:492:VAL:HG21	2.20	0.41
1:C:88:LEU:HD13	1:C:88:LEU:C	2.45	0.41
1:A:499:ILE:O	1:A:503:VAL:HG23	2.20	0.41
1:D:111:TYR:CE1	1:D:115:LEU:HD11	2.56	0.41
1:A:340:ARG:HE	1:C:534:THR:HG21	1.84	0.41
1:C:425:LEU:HD21	1:C:526:HIS:CB	2.51	0.41
1:D:570:LEU:HD23	1:D:570:LEU:C	2.46	0.41
1:A:253:LEU:HD22	1:A:261:TRP:CD2	2.55	0.41
1:D:403:GLU:OE2	1:D:403:GLU:N	2.50	0.41
1:B:25:GLN:HB3	1:B:377:VAL:HG22	2.03	0.40
1:B:292:HIS:O	1:B:296:VAL:HG23	2.21	0.40
1:B:372:TYR:CD1	1:B:372:TYR:C	3.00	0.40
1:C:277:LEU:HD22	1:C:353:MET:CE	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:GLN:HG2	1:A:438:PHE:CD2	2.57	0.40
1:B:83:PHE:HB2	1:B:89:ARG:HG2	2.03	0.40
1:C:14:GLU:O	1:C:18:GLN:HG3	2.22	0.40
1:C:283:MET:HE1	1:C:293:MET:HE3	2.03	0.40
1:B:174:LEU:HD12	1:B:174:LEU:N	2.36	0.40
1:A:425:LEU:HD21	1:A:526:HIS:CB	2.52	0.40
1:B:570:LEU:C	1:B:570:LEU:HD23	2.47	0.40
1:D:426:LEU:HD13	1:D:426:LEU:C	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	601/629 (96%)	578 (96%)	22 (4%)	1 (0%)	43	72
1	B	597/629 (95%)	575 (96%)	22 (4%)	0	100	100
1	C	589/629 (94%)	572 (97%)	17 (3%)	0	100	100
1	D	601/629 (96%)	575 (96%)	26 (4%)	0	100	100
All	All	2388/2516 (95%)	2300 (96%)	87 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ASN

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	521/541 (96%)	516 (99%)	5 (1%)	68	88
1	B	518/541 (96%)	514 (99%)	4 (1%)	73	90
1	C	511/541 (94%)	505 (99%)	6 (1%)	63	87
1	D	520/541 (96%)	518 (100%)	2 (0%)	84	94
All	All	2070/2164 (96%)	2053 (99%)	17 (1%)	73	90

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LEU
1	A	79	ILE
1	A	83	PHE
1	A	87	GLN
1	A	279	VAL
1	B	144	THR
1	B	239	ASP
1	B	372	TYR
1	B	457	SER
1	C	87	GLN
1	C	276	ASN
1	C	372	TYR
1	C	388	HIS
1	C	426	LEU
1	C	460	ASN
1	D	388	HIS
1	D	504	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	292	HIS
1	A	331	HIS
1	A	371	GLN
1	A	404	HIS
1	A	598	GLN
1	B	34	GLN
1	B	102	ASN

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Mol	Chain	Res	Type
1	B	213	HIS
1	B	217	GLN
1	B	224	ASN
1	B	585	ASN
1	B	598	GLN
1	C	42	HIS
1	C	276	ASN
1	D	224	ASN
1	D	512	HIS
1	D	585	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 ⓘ

8 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	E	1	2,1	14,14,15	0.28	0	17,19,21	0.55	0
2	NAG	E	2	2	14,14,15	0.25	0	17,19,21	0.50	0
3	NAG	F	1	3,1	14,14,15	0.32	0	17,19,21	1.13	2 (11%)
3	FUC	F	2	3	10,10,11	0.65	0	14,14,16	0.72	0
3	NAG	G	1	3,1	14,14,15	0.20	0	17,19,21	0.57	0
3	FUC	G	2	3	10,10,11	0.70	0	14,14,16	0.87	0
3	NAG	H	1	3,1	14,14,15	0.50	0	17,19,21	0.37	0
3	FUC	H	2	3	10,10,11	0.92	0	14,14,16	0.76	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	4/6/23/26	0/1/1/1
3	FUC	F	2	3	-	-	0/1/1/1
3	NAG	G	1	3,1	-	4/6/23/26	0/1/1/1
3	FUC	G	2	3	-	-	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	FUC	H	2	3	-	-	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	C2-N2-C7	3.44	127.50	122.90
3	F	1	NAG	C1-C2-N2	2.30	114.06	110.43
3	H	2	FUC	O2-C2-C1	2.03	113.87	109.22

There are no chirality outliers.

All (8) torsion outliers are listed below:

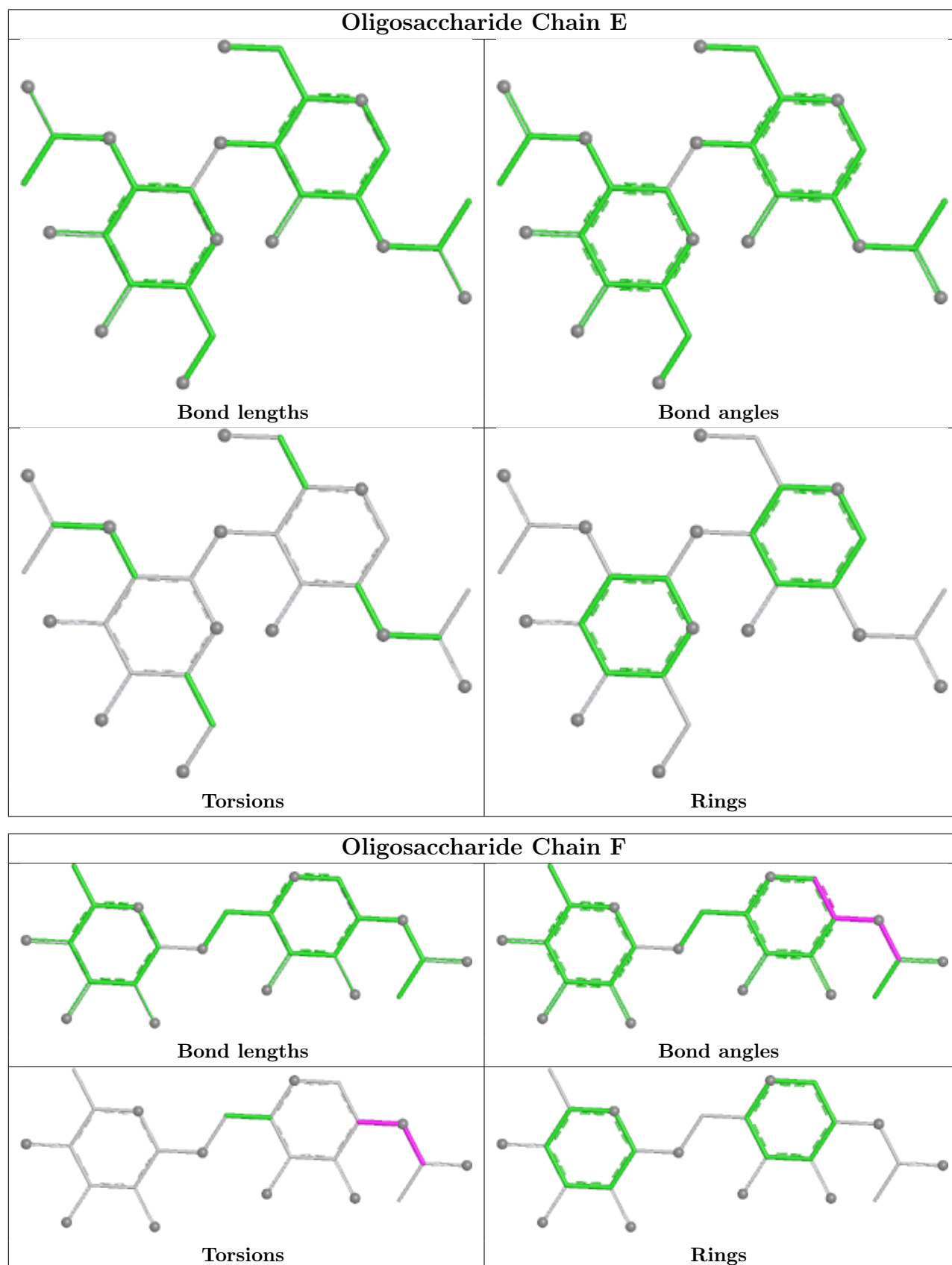
Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C1-C2-N2-C7
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	G	1	NAG	C4-C5-C6-O6
3	G	1	NAG	C3-C2-N2-C7
3	G	1	NAG	C1-C2-N2-C7
3	F	1	NAG	C3-C2-N2-C7
3	G	1	NAG	O5-C5-C6-O6

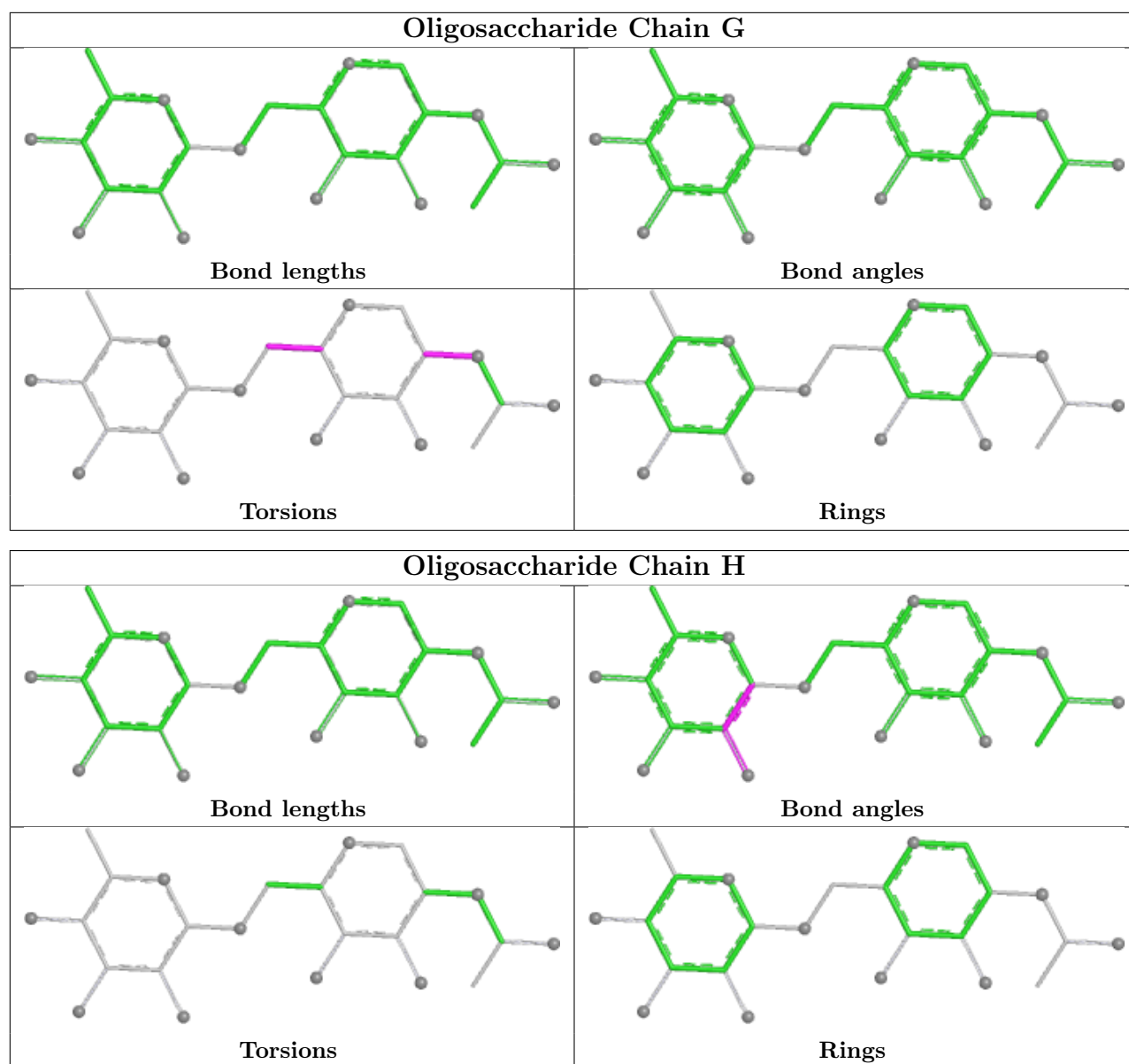
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	2	0
3	G	1	NAG	1	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 31 ligands modelled in this entry, 12 are monoatomic - leaving 19 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PG0	A	703[B]	-	7,7,7	0.50	0	6,6,6	0.15	0
9	NAG	B	702	1	14,14,15	0.36	0	17,19,21	0.47	0
9	NAG	C	701	1	14,14,15	0.30	0	17,19,21	0.49	0
4	BCN	C	706	8	10,10,10	0.96	0	11,11,11	1.03	0
4	BCN	D	703	8	10,10,10	0.99	0	11,11,11	1.01	0
5	PG0	A	702	-	7,7,7	0.48	0	6,6,6	0.23	0
5	PG0	A	703[A]	-	7,7,7	0.50	0	6,6,6	0.23	0
10	EDO	C	703	-	3,3,3	0.44	0	2,2,2	0.30	0
4	BCN	A	701	8	10,10,10	0.99	0	11,11,11	0.93	0
10	EDO	D	702	-	3,3,3	0.43	0	2,2,2	0.41	0
10	EDO	B	704	-	3,3,3	0.43	0	2,2,2	0.49	0
4	BCN	B	703	8	10,10,10	0.96	0	11,11,11	1.02	0
10	EDO	C	705	-	3,3,3	0.45	0	2,2,2	0.29	0
5	PG0	B	705	-	7,7,7	0.50	0	6,6,6	0.30	0
10	EDO	C	704	-	3,3,3	0.45	0	2,2,2	0.32	0
10	EDO	C	702	-	3,3,3	0.39	0	2,2,2	0.49	0
9	NAG	B	701	1	14,14,15	0.31	0	17,19,21	0.72	1 (5%)
10	EDO	D	704	-	3,3,3	0.38	0	2,2,2	0.53	0
10	EDO	D	701	-	3,3,3	0.44	0	2,2,2	0.32	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	PG0	A	703[B]	-	-	0/5/5/5	-
9	NAG	B	702	1	-	2/6/23/26	0/1/1/1
9	NAG	C	701	1	-	4/6/23/26	0/1/1/1
4	BCN	C	706	8	-	0/10/10/10	-
4	BCN	D	703	8	-	1/10/10/10	-
5	PG0	A	702	-	-	2/5/5/5	-
5	PG0	A	703[A]	-	-	2/5/5/5	-
10	EDO	C	703	-	-	0/1/1/1	-
4	BCN	A	701	8	-	0/10/10/10	-
10	EDO	D	702	-	-	0/1/1/1	-
10	EDO	B	704	-	-	1/1/1/1	-
4	BCN	B	703	8	-	0/10/10/10	-
10	EDO	C	705	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PG0	B	705	-	-	3/5/5/5	-
10	EDO	C	704	-	-	0/1/1/1	-
10	EDO	C	702	-	-	0/1/1/1	-
9	NAG	B	701	1	-	2/6/23/26	0/1/1/1
10	EDO	D	704	-	-	0/1/1/1	-
10	EDO	D	701	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	701	NAG	C1-O5-C5	2.52	115.57	112.19

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	701	NAG	O5-C5-C6-O6
9	C	701	NAG	C4-C5-C6-O6
9	B	702	NAG	O5-C5-C6-O6
9	B	702	NAG	C4-C5-C6-O6
5	B	705	PG0	OTT-C1-C2-O1
5	A	702	PG0	OTT-C1-C2-O1
5	A	703[A]	PG0	C3-C4-O2-C5
9	B	701	NAG	C4-C5-C6-O6
9	B	701	NAG	O5-C5-C6-O6
9	C	701	NAG	C1-C2-N2-C7
9	C	701	NAG	C3-C2-N2-C7
5	A	702	PG0	C3-C4-O2-C5
5	A	703[A]	PG0	O1-C3-C4-O2
10	B	704	EDO	O1-C1-C2-O2
5	B	705	PG0	C4-C3-O1-C2
5	B	705	PG0	O1-C3-C4-O2
4	D	703	BCN	C6-C5-N1-C1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	703[A]	PG0	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	601/629 (95%)	0.53	24 (3%)	42 33	29, 64, 99, 124	2 (0%)
1	B	601/629 (95%)	0.66	24 (3%)	42 33	42, 68, 105, 126	0
1	C	593/629 (94%)	0.55	21 (3%)	47 38	37, 66, 105, 126	1 (0%)
1	D	601/629 (95%)	0.63	27 (4%)	38 30	28, 68, 114, 136	2 (0%)
All	All	2396/2516 (95%)	0.59	96 (4%)	42 33	28, 66, 106, 136	5 (0%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	603	LEU	4.3
1	A	135	THR	3.9
1	D	79	ILE	3.9
1	B	135	THR	3.9
1	C	75	LEU	3.8
1	C	273	ASP	3.6
1	B	8	GLY	3.5
1	B	576	LEU	3.4
1	C	92	ILE	3.3
1	A	238	GLY	3.2
1	A	131	GLN	3.2
1	B	130	PRO	3.2
1	A	23	SER	3.1
1	A	130	PRO	3.1
1	B	385	PRO	3.1
1	C	130	PRO	3.0
1	C	7	PRO	3.0
1	C	25	GLN	2.9
1	D	5	LEU	2.8
1	D	31	VAL	2.8
1	A	307	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	130	PRO	2.7
1	A	10	PHE	2.7
1	D	24	TYR	2.7
1	A	245	ARG	2.7
1	C	135	THR	2.7
1	B	12	ALA	2.6
1	C	12	ALA	2.6
1	D	608	PRO	2.6
1	D	129	LEU	2.6
1	B	284	LEU	2.6
1	B	131	GLN	2.6
1	C	101	ALA	2.5
1	D	57	ALA	2.5
1	D	605	ASP	2.5
1	A	100	SER	2.5
1	D	378	SER	2.5
1	D	75	LEU	2.5
1	B	79	ILE	2.5
1	C	102	ASN	2.5
1	C	497	PRO	2.5
1	D	20	PHE	2.4
1	A	82	GLN	2.4
1	C	17	ALA	2.4
1	A	203	ASN	2.4
1	C	8	GLY	2.4
1	C	149	SER	2.4
1	C	86	PRO	2.4
1	D	576	LEU	2.4
1	D	290	ALA	2.4
1	C	350	ARG	2.3
1	D	93	GLY	2.3
1	D	176[A]	GLU	2.3
1	D	606	ASN	2.3
1	B	68	TRP	2.3
1	B	150	SER	2.3
1	C	129	LEU	2.3
1	A	604	PRO	2.3
1	B	90	ARG	2.3
1	C	603	LEU	2.2
1	B	443	ASP	2.2
1	A	155	MET	2.2
1	A	609	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	129	LEU	2.2
1	B	159	ALA	2.2
1	A	7	PRO	2.2
1	A	275	PRO	2.2
1	A	8	GLY	2.2
1	C	105	LEU	2.2
1	C	608	PRO	2.2
1	B	137	TRP	2.2
1	A	149	SER	2.2
1	D	273	ASP	2.1
1	A	110	GLN	2.1
1	D	155	MET	2.1
1	D	154	ALA	2.1
1	A	331	HIS	2.1
1	B	78	PRO	2.1
1	A	19	LEU	2.1
1	B	253	LEU	2.1
1	B	88	LEU	2.1
1	B	20	PHE	2.1
1	B	195	GLY	2.1
1	A	89	ARG	2.1
1	B	15	ALA	2.1
1	D	272	PRO	2.0
1	A	411	LEU	2.0
1	D	10	PHE	2.0
1	B	609	GLU	2.0
1	D	217	GLN	2.0
1	D	331	HIS	2.0
1	B	147	LEU	2.0
1	D	545	ARG	2.0
1	C	343	PHE	2.0
1	D	68	TRP	2.0
1	D	80	TRP	2.0

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

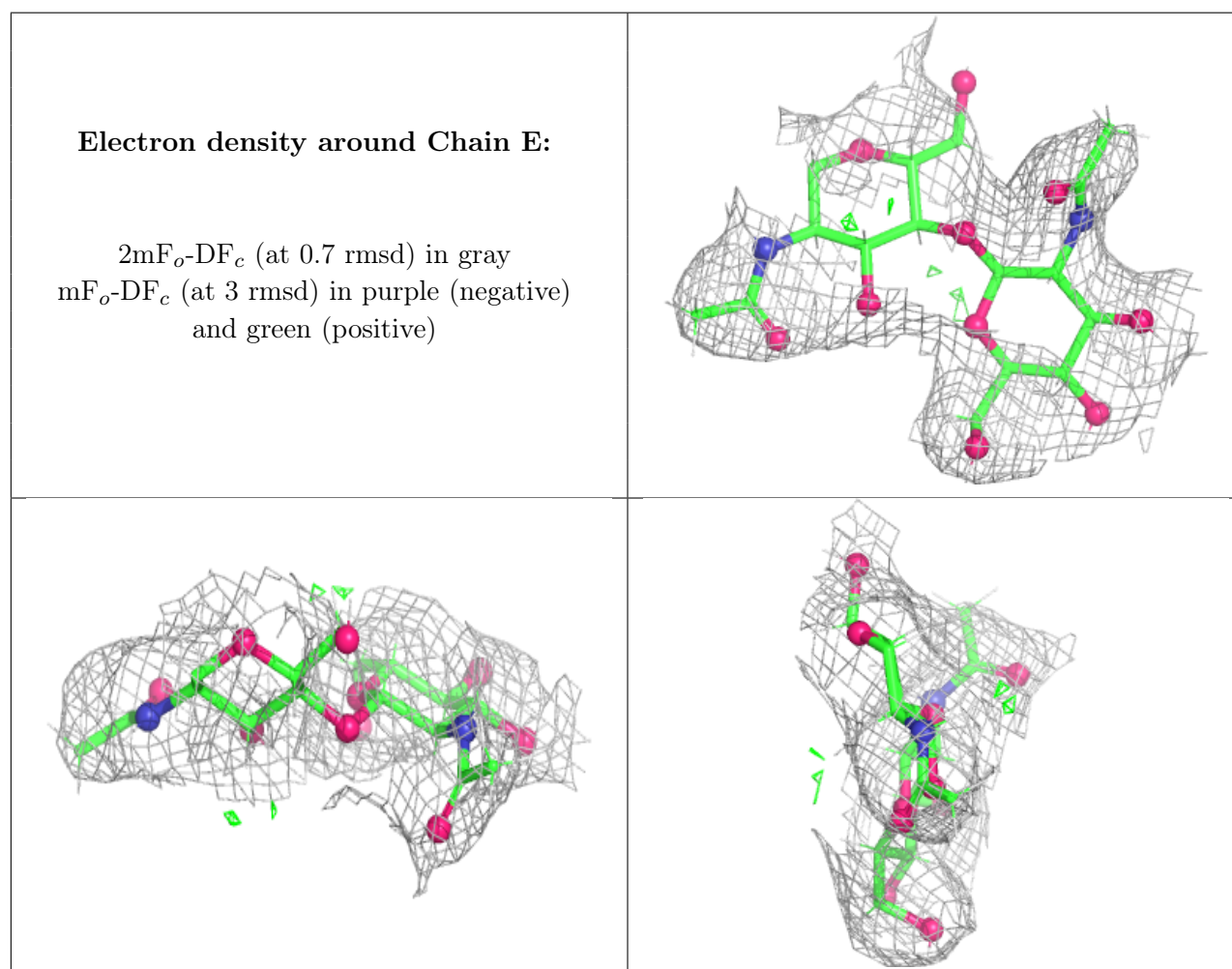
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

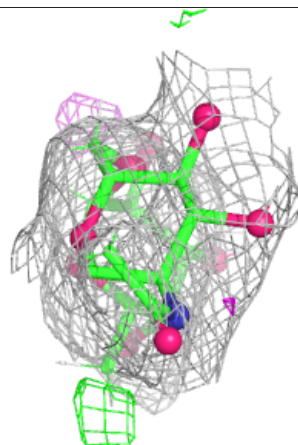
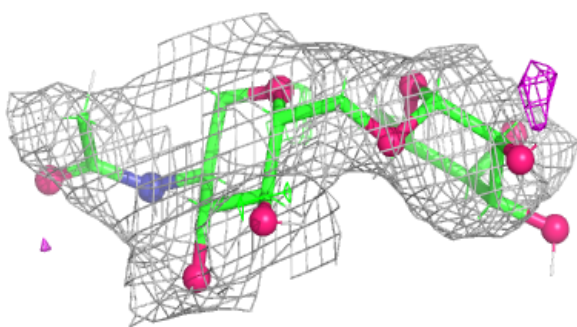
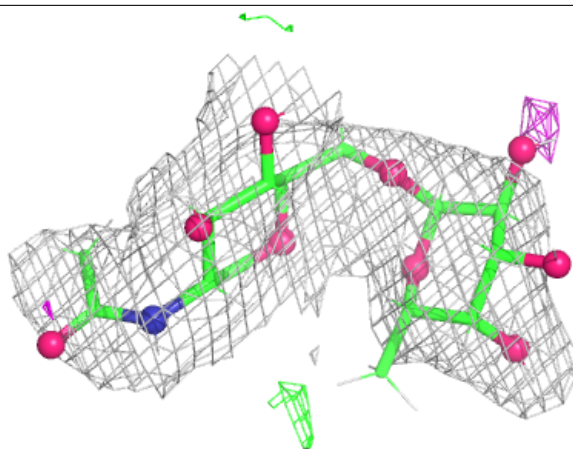
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	E	2	14/15	0.64	0.13	94,114,136,137	0
3	NAG	G	1	14/15	0.73	0.14	68,82,98,101	0
3	FUC	F	2	10/11	0.75	0.16	68,85,101,116	0
3	FUC	G	2	10/11	0.75	0.13	79,95,108,115	0
3	FUC	H	2	10/11	0.76	0.15	67,85,102,106	0
3	NAG	H	1	14/15	0.78	0.13	51,69,92,111	0
2	NAG	E	1	14/15	0.80	0.12	72,92,113,117	0
3	NAG	F	1	14/15	0.82	0.13	58,71,82,86	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.



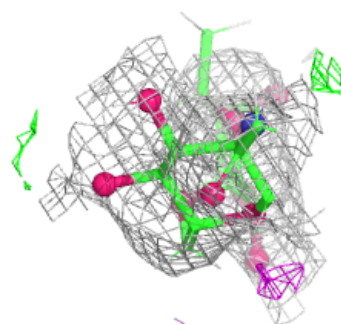
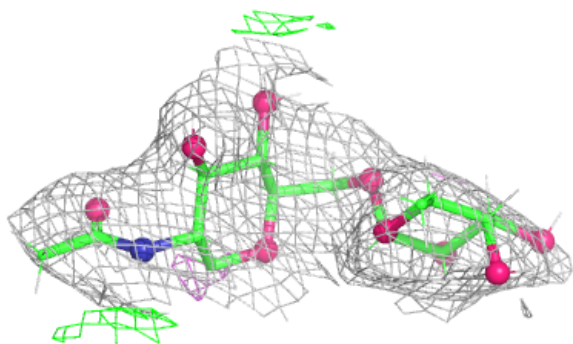
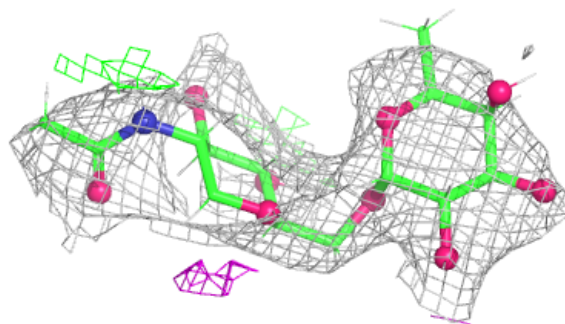
Electron density around Chain F:

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

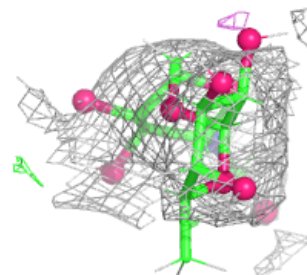
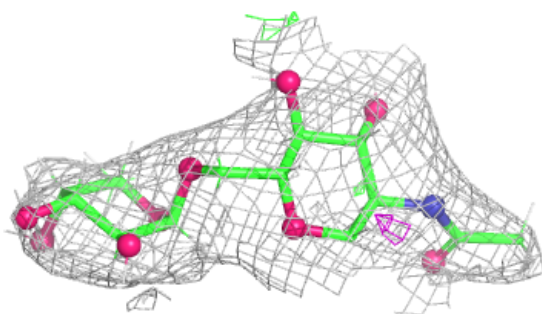
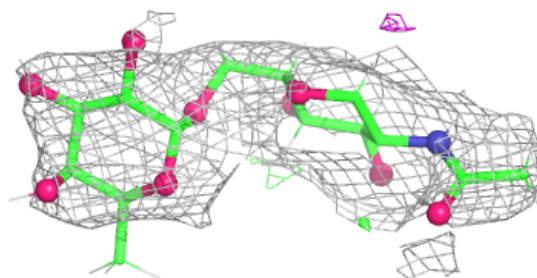


Electron density around Chain G:

$2mF_o-DF_c$ (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)



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(Å ²)	Q<0.9
5	PG0	A	703[A]	8/8	0.49	0.34	52,63,74,75	20
5	PG0	A	703[B]	8/8	0.49	0.34	52,62,74,76	20
9	NAG	C	701	14/15	0.58	0.16	96,112,132,134	0
10	EDO	C	705	4/4	0.64	0.18	59,71,82,82	0
9	NAG	B	701	14/15	0.68	0.16	85,99,116,119	0
5	PG0	B	705	8/8	0.70	0.17	58,76,87,87	0
10	EDO	C	703	4/4	0.73	0.17	61,73,88,88	0
10	EDO	B	704	4/4	0.74	0.22	67,80,83,93	0
10	EDO	D	702	4/4	0.75	0.23	57,70,84,84	0
9	NAG	B	702	14/15	0.78	0.12	56,76,98,104	0
10	EDO	C	704	4/4	0.78	0.19	60,72,87,87	0
10	EDO	D	701	4/4	0.83	0.13	58,70,80,83	0
5	PG0	A	702	8/8	0.83	0.18	58,75,77,77	0
10	EDO	D	704	4/4	0.83	0.15	57,68,77,84	0
10	EDO	C	702	4/4	0.84	0.12	60,72,75,84	0
7	CL	B	707	1/1	0.86	0.15	60,60,60,60	0
4	BCN	A	701	11/11	0.89	0.12	48,64,70,83	0
4	BCN	D	703	11/11	0.89	0.12	49,59,73,76	0
7	CL	C	708	1/1	0.90	0.15	44,44,44,44	0
4	BCN	B	703	11/11	0.90	0.09	50,61,69,73	0
8	CA	C	709	1/1	0.91	0.11	69,69,69,69	0
7	CL	D	706	1/1	0.91	0.10	50,50,50,50	0
4	BCN	C	706	11/11	0.93	0.12	57,69,80,85	0
8	CA	D	707	1/1	0.94	0.11	58,58,58,58	0
7	CL	A	705	1/1	0.94	0.06	54,54,54,54	0
8	CA	B	708	1/1	0.97	0.05	60,60,60,60	0
8	CA	A	706	1/1	0.97	0.04	55,55,55,55	0
6	ZN	A	704	1/1	0.98	0.04	37,37,37,37	0
6	ZN	C	707	1/1	0.99	0.03	44,44,44,44	0
6	ZN	D	705	1/1	0.99	0.06	57,57,57,57	0
6	ZN	B	706	1/1	0.99	0.05	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.