



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:07 PM UTC

PDB ID : 6BE6 / pdb_00006be6
Title : ADAM10 Extracellular Domain
Authors : Seegar, T.C.M.
Deposited on : 2017-10-24
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

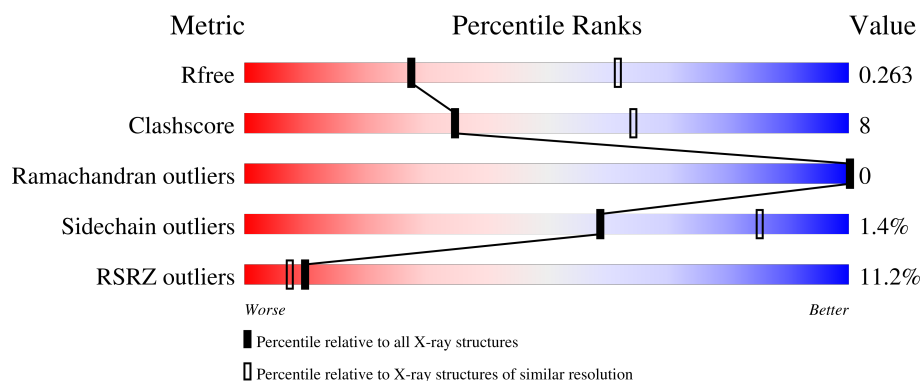
1 Overall quality at a glance

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	449	8% 78% 17% • •
1	B	449	13% 77% 19% •
1	C	449	12% 79% 18% •
1	D	449	9% 82% 15% •
2	E	5	80% 20%

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Mol	Chain	Length	Quality of chain
3	F	7	
4	G	5	
5	H	8	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	SO4	C	704	-	-	X	-
8	SO4	D	704	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13995 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 Disintegrin and metalloproteinase domain-containing protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3311	2033	585	653	40			
1	B	431	Total	C	N	O	S	0	0	0
			3310	2033	585	652	40			
1	C	433	Total	C	N	O	S	0	0	0
			3324	2040	587	657	40			
1	D	433	Total	C	N	O	S	0	0	0
			3325	2040	587	658	40			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	267	GLN	ASN	conflict	UNP O14672
A	439	GLN	ASN	conflict	UNP O14672
A	551	GLN	ASN	conflict	UNP O14672
A	655	GLY	-	expression tag	UNP O14672
A	656	GLY	-	expression tag	UNP O14672
A	657	HIS	-	expression tag	UNP O14672
A	658	HIS	-	expression tag	UNP O14672
A	659	HIS	-	expression tag	UNP O14672
A	660	HIS	-	expression tag	UNP O14672
A	661	HIS	-	expression tag	UNP O14672
A	662	HIS	-	expression tag	UNP O14672
B	267	GLN	ASN	conflict	UNP O14672
B	439	GLN	ASN	conflict	UNP O14672
B	551	GLN	ASN	conflict	UNP O14672
B	655	GLY	-	expression tag	UNP O14672
B	656	GLY	-	expression tag	UNP O14672
B	657	HIS	-	expression tag	UNP O14672
B	658	HIS	-	expression tag	UNP O14672
B	659	HIS	-	expression tag	UNP O14672
B	660	HIS	-	expression tag	UNP O14672

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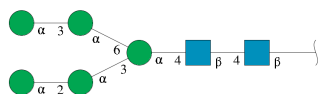
Chain	Residue	Modelled	Actual	Comment	Reference
B	661	HIS	-	expression tag	UNP O14672
B	662	HIS	-	expression tag	UNP O14672
C	267	GLN	ASN	conflict	UNP O14672
C	439	GLN	ASN	conflict	UNP O14672
C	551	GLN	ASN	conflict	UNP O14672
C	655	GLY	-	expression tag	UNP O14672
C	656	GLY	-	expression tag	UNP O14672
C	657	HIS	-	expression tag	UNP O14672
C	658	HIS	-	expression tag	UNP O14672
C	659	HIS	-	expression tag	UNP O14672
C	660	HIS	-	expression tag	UNP O14672
C	661	HIS	-	expression tag	UNP O14672
C	662	HIS	-	expression tag	UNP O14672
D	267	GLN	ASN	conflict	UNP O14672
D	439	GLN	ASN	conflict	UNP O14672
D	551	GLN	ASN	conflict	UNP O14672
D	655	GLY	-	expression tag	UNP O14672
D	656	GLY	-	expression tag	UNP O14672
D	657	HIS	-	expression tag	UNP O14672
D	658	HIS	-	expression tag	UNP O14672
D	659	HIS	-	expression tag	UNP O14672
D	660	HIS	-	expression tag	UNP O14672
D	661	HIS	-	expression tag	UNP O14672
D	662	HIS	-	expression tag	UNP O14672

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



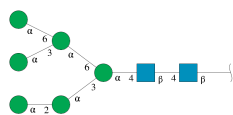
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	7	Total	C	N	O	0	0	0
			83	46	2	35			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	8	Total	C	N	O	0	0	0
			94	52	2	40			

- 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		

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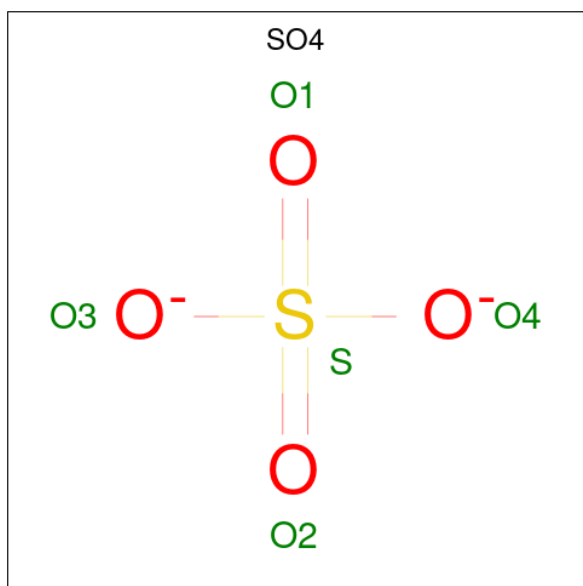
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Zn	0	0
			1	1		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	O	S	0	0
			5	4	1		
8	D	1	Total	O	S	0	0
			5	4	1		
8	D	1	Total	O	S	0	0
			5	4	1		

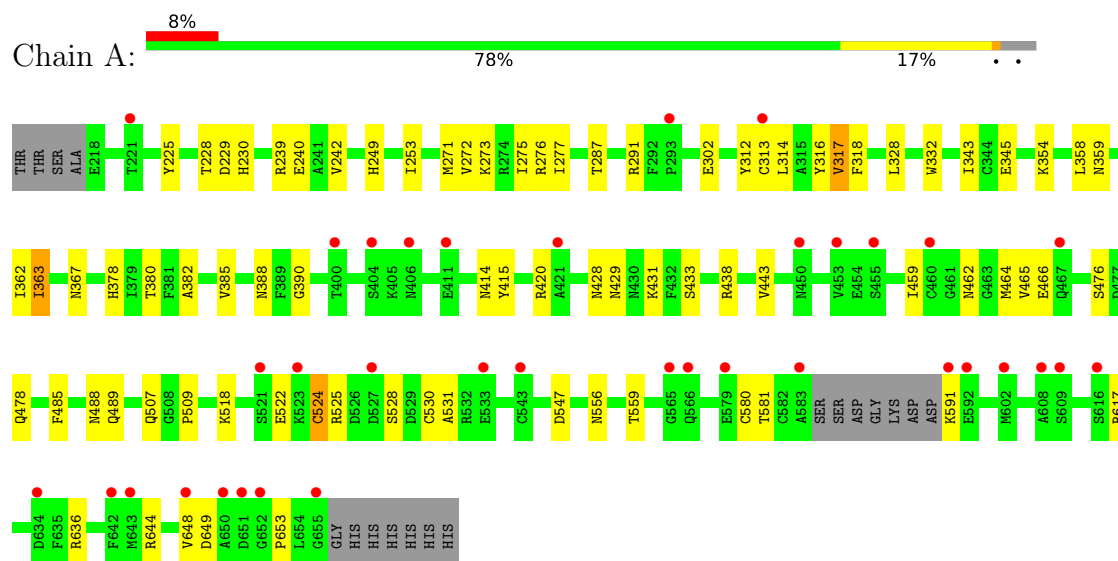
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	100	Total	O	0	0
			100	100		
9	B	90	Total	O	0	0
			90	90		
9	C	87	Total	O	0	0
			87	87		
9	D	106	Total	O	0	0
			106	106		

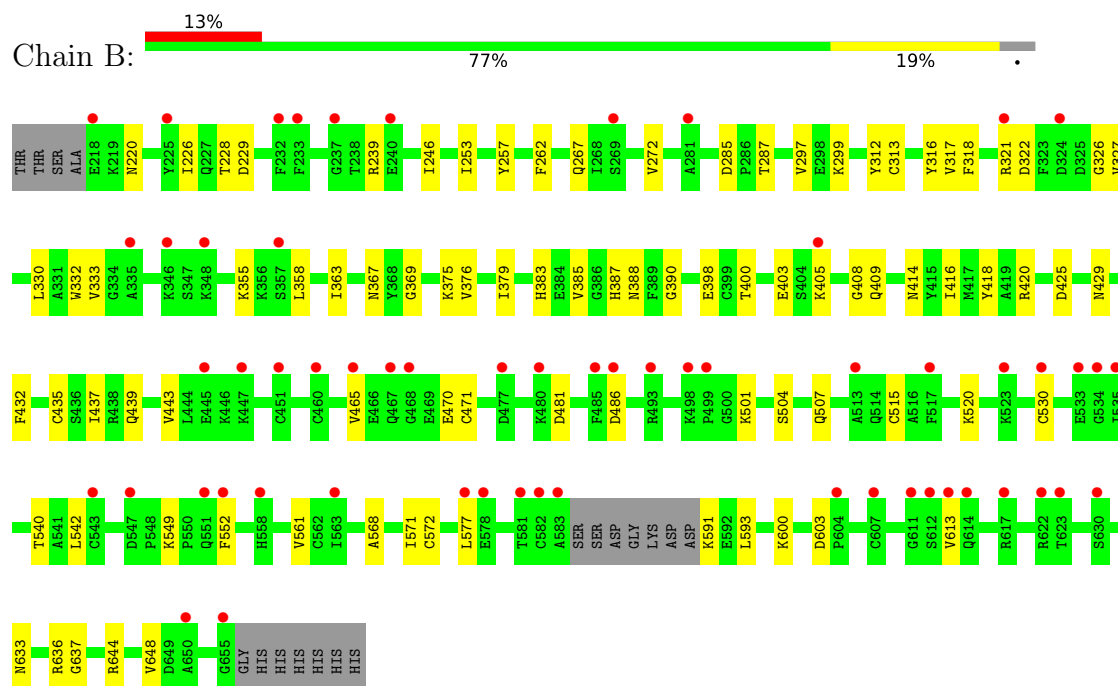
3 Residue-property plots

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.

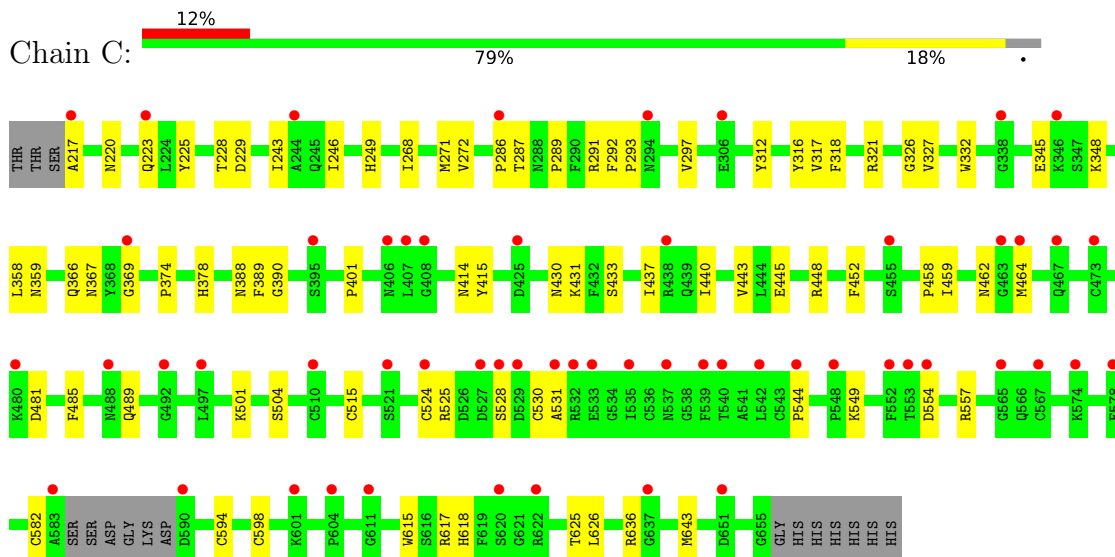
- Molecule 1: Disintegrin and metalloproteinase domain-containing protein 10



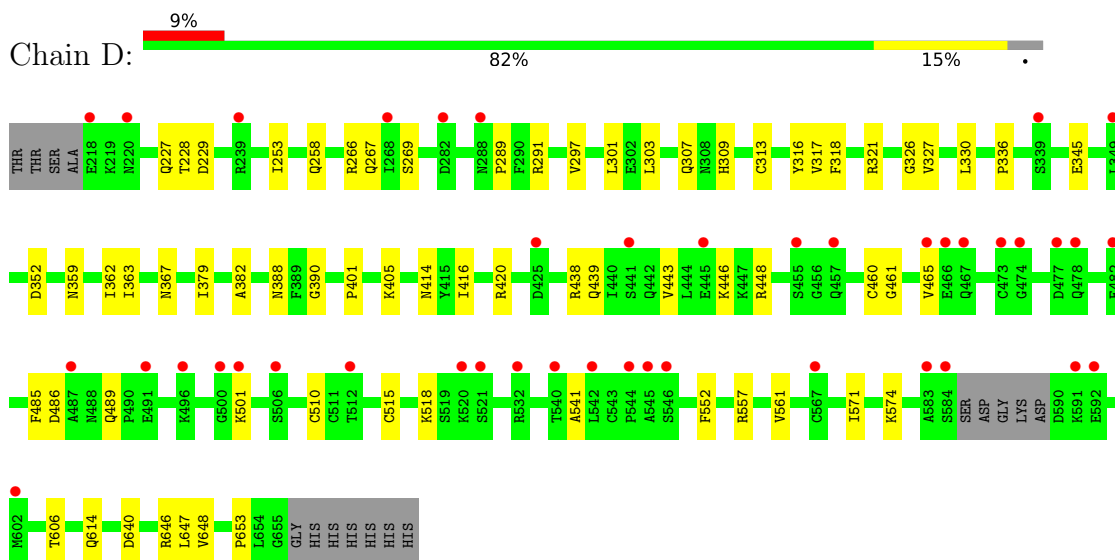
- Molecule 1: Disintegrin and metalloproteinase domain-containing protein 10



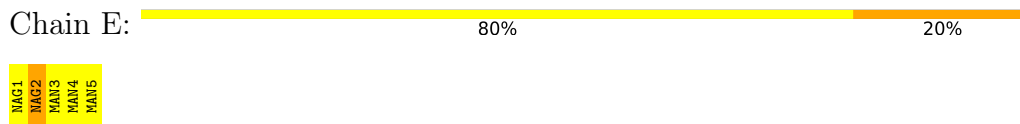
- Molecule 1: Disintegrin and metalloproteinase domain-containing protein 10



- Molecule 1: Disintegrin and metalloproteinase domain-containing protein 10



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



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





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



- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	131.42Å 188.78Å 86.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.48 – 2.80 47.48 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.9 (47.48-2.80) 82.1 (47.48-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.87 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.236 , 0.284 (Not available) , 0.263	Depositor DCC
R_{free} test set	2655 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	13995	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MAN, ZN, SO4, CA

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	0.09	0/3377	0.27	0/4549
1	B	0.12	0/3376	0.30	0/4547
1	C	0.09	0/3390	0.27	0/4567
1	D	0.09	0/3391	0.27	0/4568
All	All	0.10	0/13534	0.27	0/18231

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	3311	0	3125	47	1
1	B	3310	0	3123	54	0
1	C	3324	0	3134	52	0
1	D	3325	0	3134	46	0
2	E	61	0	52	5	0
3	F	83	0	70	4	0
4	G	61	0	52	2	0
5	H	94	0	79	4	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	5	0	0	0	0
8	B	10	0	0	1	0
8	C	10	0	0	3	1
8	D	10	0	0	2	0
9	A	100	0	0	2	0
9	B	90	0	0	4	0
9	C	87	0	0	8	0
9	D	106	0	0	6	0
All	All	13995	0	12769	199	1

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 8.

All (199) 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:C:431:LYS:HE3	9:C:835:HOH:O	1.73	0.89
1:C:229:ASP:OD2	1:C:321:ARG:NH2	2.12	0.81
1:A:302:GLU:OE2	1:A:354:LYS:NZ	2.13	0.78
1:A:390:GLY:HA3	1:A:443:VAL:HG21	1.68	0.75
1:B:400:THR:OG1	1:B:414:ASN:ND2	2.21	0.74
1:C:431:LYS:CE	9:C:835:HOH:O	2.33	0.72
1:C:445:GLU:OE2	9:C:801:HOH:O	2.08	0.72
1:C:272:VAL:HG23	1:C:462:ASN:HD22	1.55	0.71
1:B:540:THR:HG22	1:B:542:LEU:H	1.55	0.71
1:C:326:GLY:HA2	1:C:367:ASN:HD21	1.54	0.71
1:B:400:THR:O	1:B:400:THR:HG23	1.92	0.70
1:A:420:ARG:HH11	1:A:636:ARG:HG2	1.58	0.69
1:A:287:THR:OG1	2:E:2:NAG:H83	1.94	0.68
1:A:363:ILE:HD11	1:A:380:THR:HG22	1.75	0.67
1:B:229:ASP:OD2	1:B:321:ARG:NH2	2.29	0.66
1:C:390:GLY:HA3	1:C:443:VAL:HG21	1.78	0.65
1:C:525:ARG:NH2	1:C:544:PRO:O	2.27	0.65
1:C:228:THR:HG22	1:C:318:PHE:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:THR:OG1	2:E:2:NAG:C8	2.45	0.65
1:B:572:CYS:HB3	1:B:577:LEU:HB2	1.80	0.64
1:C:594:CYS:HA	1:C:626:LEU:HD12	1.80	0.63
1:A:276:ARG:NH1	9:A:801:HOH:O	2.20	0.63
1:A:438:ARG:HD3	1:D:438:ARG:NH1	2.15	0.62
1:A:228:THR:HG22	1:A:318:PHE:HB2	1.80	0.62
1:B:409:GLN:NE2	9:B:805:HOH:O	2.32	0.62
1:B:435:CYS:O	1:B:439:GLN:NE2	2.32	0.62
1:D:420:ARG:HG3	1:D:648:VAL:HB	1.82	0.61
1:C:345:GLU:HB2	1:C:359:ASN:HB3	1.80	0.61
1:C:485:PHE:HB3	1:C:489:GLN:HG3	1.83	0.61
1:B:552:PHE:HA	1:B:561:VAL:HB	1.82	0.61
1:A:591:LYS:HD3	1:A:644:ARG:HA	1.83	0.60
1:A:524:CYS:SG	1:A:525:ARG:N	2.74	0.60
1:B:299:LYS:NZ	9:B:806:HOH:O	2.34	0.60
1:B:420:ARG:HD3	1:B:636:ARG:HA	1.82	0.60
1:D:326:GLY:HA2	1:D:367:ASN:HD21	1.66	0.60
1:C:625:THR:OG1	1:C:643:MET:SD	2.59	0.60
1:C:243:ILE:HD13	1:C:246:ILE:HD11	1.84	0.60
1:B:220:ASN:ND2	1:B:267:GLN:O	2.35	0.59
1:B:228:THR:HG22	1:B:318:PHE:HB2	1.83	0.59
1:A:345:GLU:H	1:A:359:ASN:HB3	1.67	0.59
1:C:367:ASN:ND2	9:C:804:HOH:O	2.27	0.59
1:C:636:ARG:NH1	9:C:803:HOH:O	2.21	0.59
1:B:316:TYR:OH	1:B:388:ASN:ND2	2.35	0.58
1:B:408:GLY:HA3	1:C:217:ALA:HB3	1.85	0.58
1:D:258:GLN:HE21	1:D:269:SER:HB3	1.69	0.58
1:D:552:PHE:HB3	1:D:574:LYS:HG3	1.86	0.58
1:A:420:ARG:NH1	1:A:636:ARG:HG2	2.19	0.57
1:B:561:VAL:HG13	1:B:571:ILE:HA	1.87	0.56
1:B:297:VAL:HG11	1:B:327:VAL:HG11	1.86	0.56
1:C:530:CYS:HA	1:C:549:LYS:HD2	1.88	0.55
1:D:228:THR:HG22	1:D:318:PHE:HB2	1.87	0.55
1:D:291:ARG:NH1	9:D:814:HOH:O	2.38	0.55
1:D:448:ARG:NH2	9:D:808:HOH:O	2.33	0.55
1:B:355:LYS:H	3:F:5:MAN:H61	1.72	0.55
1:C:374:PRO:O	1:C:378:HIS:ND1	2.38	0.55
1:C:271:MET:HE1	1:C:459:ILE:H	1.72	0.55
2:E:2:NAG:H83	2:E:2:NAG:H3	1.88	0.55
1:B:239:ARG:NH1	9:B:808:HOH:O	2.39	0.54
1:C:448:ARG:HG3	1:C:452:PHE:CG	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:SER:HB3	1:A:531:ALA:HB3	1.89	0.54
1:D:253:ILE:HG22	1:D:382:ALA:HB2	1.89	0.54
1:D:557:ARG:NH2	9:D:804:HOH:O	2.27	0.54
1:D:606:THR:HB	1:D:614:GLN:HE22	1.72	0.53
1:D:405:LYS:NZ	8:D:704:SO4:O2	2.40	0.53
1:A:428:ASN:OD1	1:D:266:ARG:NH1	2.41	0.53
1:A:636:ARG:NH2	9:A:803:HOH:O	2.26	0.53
1:D:401:PRO:HD2	1:D:414:ASN:HA	1.91	0.53
1:D:390:GLY:HA3	1:D:443:VAL:HG21	1.89	0.53
1:A:314:LEU:HD21	1:A:343:ILE:HA	1.91	0.52
1:A:580:CYS:SG	1:A:581:THR:N	2.82	0.52
1:C:348:LYS:HD3	1:D:647:LEU:HD22	1.90	0.52
1:A:420:ARG:HA	1:A:648:VAL:HG11	1.92	0.52
1:A:465:VAL:HG21	1:A:507:GLN:HA	1.91	0.52
1:B:520:LYS:HD2	1:B:520:LYS:H	1.74	0.52
1:D:382:ALA:HB3	1:D:416:ILE:HD11	1.92	0.52
1:C:332:TRP:CE2	1:C:358:LEU:HD22	2.45	0.52
1:A:253:ILE:HG22	1:A:382:ALA:HB2	1.93	0.51
1:C:557:ARG:NH2	8:C:703:SO4:O1	2.40	0.51
2:E:1:NAG:H61	2:E:2:NAG:C7	2.42	0.50
1:B:390:GLY:HA3	1:B:443:VAL:HG21	1.94	0.50
1:B:481:ASP:OD2	1:B:504:SER:OG	2.24	0.50
1:D:345:GLU:H	1:D:359:ASN:HB3	1.76	0.50
1:B:322:ASP:OD2	1:B:369:GLY:N	2.44	0.50
1:A:275:ILE:O	1:A:478:GLN:NE2	2.45	0.50
1:B:297:VAL:HG12	1:B:330:LEU:HD22	1.93	0.50
1:C:271:MET:HE1	1:C:458:PRO:HA	1.93	0.50
1:D:316:TYR:OH	1:D:388:ASN:ND2	2.44	0.50
1:A:414:ASN:O	1:A:429:ASN:ND2	2.46	0.49
1:A:225:TYR:HB2	1:A:312:TYR:CD1	2.48	0.49
1:D:486:ASP:OD1	1:D:489:GLN:HG2	2.13	0.49
1:D:501:LYS:HD2	1:D:515:CYS:HB2	1.95	0.49
1:D:510:CYS:HB2	1:D:541:ALA:HA	1.95	0.49
1:D:460:CYS:SG	1:D:461:GLY:N	2.86	0.49
1:C:316:TYR:OH	1:C:388:ASN:ND2	2.46	0.48
1:A:332:TRP:CE2	1:A:358:LEU:HD22	2.47	0.48
1:A:485:PHE:HB3	1:A:489:GLN:HG3	1.95	0.48
1:B:379:ILE:O	1:B:383:HIS:N	2.43	0.48
1:C:430:ASN:OD1	9:C:802:HOH:O	2.19	0.48
1:B:470:GLU:O	1:B:507:GLN:NE2	2.40	0.48
1:C:464:MET:HE1	9:C:868:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:LEU:HD21	1:A:367:ASN:HB2	1.96	0.48
1:B:262:PHE:HD1	1:B:437:ILE:HG23	1.79	0.48
1:C:554:ASP:OD1	1:C:554:ASP:N	2.42	0.48
1:D:227:GLN:HB2	1:D:317:VAL:HG22	1.96	0.48
1:C:617:ARG:NH2	8:C:704:SO4:S	2.87	0.47
1:D:640:ASP:OD2	1:D:646:ARG:NH2	2.46	0.47
1:A:547:ASP:OD1	1:A:547:ASP:N	2.48	0.47
1:A:431:LYS:HD2	1:D:266:ARG:HH12	1.79	0.47
1:D:510:CYS:HA	1:D:518:LYS:HD2	1.95	0.47
1:B:332:TRP:CE2	1:B:358:LEU:HD22	2.50	0.47
1:C:286:PRO:HA	1:C:291:ARG:NH1	2.29	0.47
1:A:518:LYS:HB3	1:A:522:GLU:HG3	1.97	0.47
1:B:285:ASP:OD1	1:B:287:THR:HG22	2.15	0.47
1:C:598:CYS:O	1:C:615:TRP:NE1	2.48	0.47
1:B:405:LYS:HG2	8:B:704:SO4:O2	2.15	0.46
1:B:600:LYS:HB3	1:B:603:ASP:HB3	1.98	0.46
1:C:271:MET:HE3	1:C:271:MET:HB2	1.84	0.46
1:C:433:SER:O	1:C:437:ILE:HG13	2.15	0.46
1:B:403:GLU:OE2	1:B:418:TYR:OH	2.28	0.46
1:B:416:ILE:HG22	1:B:429:ASN:O	2.15	0.46
1:A:229:ASP:HB3	2:E:1:NAG:H81	1.96	0.46
1:B:425:ASP:OD2	1:B:568:ALA:HB2	2.15	0.46
1:B:400:THR:O	1:B:400:THR:CG2	2.63	0.46
1:A:462:ASN:ND2	1:A:466:GLU:OE2	2.42	0.46
1:A:239:ARG:HG3	1:A:277:ILE:HG21	1.97	0.46
1:A:415:TYR:CG	1:A:433:SER:HB3	2.51	0.46
1:C:249:HIS:HA	1:C:378:HIS:HD2	1.81	0.46
1:A:653:PRO:HG3	1:B:332:TRP:CE2	2.51	0.45
1:B:637:GLY:HA2	1:B:648:VAL:HG23	1.98	0.45
1:C:225:TYR:HB2	1:C:312:TYR:CD1	2.51	0.45
1:A:240:GLU:OE2	1:A:509:PRO:HB3	2.16	0.45
1:B:398:GLU:H	1:B:398:GLU:CD	2.23	0.45
1:C:289:PRO:HD3	4:G:2:NAG:H5	1.98	0.45
1:B:465:VAL:HG11	1:B:507:GLN:HG2	1.98	0.45
1:B:501:LYS:HD2	1:B:515:CYS:HB2	1.99	0.45
1:D:318:PHE:CE2	1:D:363:ILE:HD11	2.52	0.45
1:B:530:CYS:HA	1:B:549:LYS:HD2	1.98	0.45
1:A:316:TYR:OH	1:A:388:ASN:ND2	2.50	0.44
1:D:379:ILE:HG23	1:D:416:ILE:HG13	1.99	0.44
1:D:317:VAL:HB	1:D:362:ILE:HG22	1.98	0.44
1:C:501:LYS:HD2	1:C:515:CYS:SG	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:GLN:NE2	9:D:817:HOH:O	2.46	0.44
1:B:333:VAL:HG22	1:B:387:HIS:HB3	1.99	0.44
1:C:401:PRO:HD2	1:C:414:ASN:HA	1.99	0.44
1:A:230:HIS:CE1	1:A:291:ARG:HA	2.52	0.44
1:A:272:VAL:HG21	1:A:464:MET:HE1	1.99	0.44
1:B:385:VAL:HA	1:B:388:ASN:HD22	1.83	0.44
1:D:297:VAL:HG21	1:D:327:VAL:HG11	2.00	0.44
5:H:6:MAN:H62	5:H:8:MAN:H2	1.63	0.44
1:C:481:ASP:OD2	1:C:504:SER:OG	2.36	0.43
3:F:4:MAN:H2	3:F:5:MAN:H2	1.52	0.43
1:B:326:GLY:HA2	1:B:367:ASN:HD21	1.83	0.43
5:H:6:MAN:H3	5:H:7:MAN:H2	1.78	0.43
1:B:416:ILE:HD11	1:B:432:PHE:CE1	2.53	0.43
1:B:465:VAL:HG12	1:B:471:CYS:HA	2.01	0.43
1:D:352:ASP:HB2	9:D:809:HOH:O	2.19	0.43
1:C:415:TYR:CD2	1:C:433:SER:HB3	2.54	0.43
1:B:375:LYS:HG3	1:B:376:VAL:HG23	2.00	0.43
1:C:287:THR:HB	4:G:2:NAG:H3	2.01	0.43
1:A:273:LYS:HA	1:A:459:ILE:HD11	2.00	0.43
1:B:229:ASP:HB3	3:F:1:NAG:H81	2.00	0.43
1:C:332:TRP:CE2	1:D:653:PRO:HG3	2.54	0.43
1:A:249:HIS:HA	1:A:378:HIS:CD2	2.54	0.43
1:B:593:LEU:HD13	1:B:633:ASN:HB2	2.00	0.43
1:B:312:TYR:O	9:B:801:HOH:O	2.21	0.42
1:D:229:ASP:OD2	1:D:321:ARG:NH2	2.52	0.42
1:C:366:GLN:HE21	1:C:369:GLY:HA2	1.83	0.42
1:C:528:SER:HB2	1:C:531:ALA:HB3	2.00	0.42
1:A:225:TYR:HB2	1:A:312:TYR:CG	2.55	0.42
1:C:220:ASN:HB3	1:C:268:ILE:HD13	2.00	0.42
1:D:438:ARG:NH2	9:D:819:HOH:O	2.51	0.42
1:D:465:VAL:HG23	1:D:465:VAL:O	2.19	0.42
1:A:317:VAL:HG13	1:A:362:ILE:HG22	2.00	0.42
1:D:289:PRO:HD3	5:H:2:NAG:H5	2.02	0.42
1:D:485:PHE:HB3	1:D:489:GLN:HG3	2.00	0.42
1:D:297:VAL:HG22	1:D:330:LEU:HD12	2.02	0.41
1:D:301:LEU:HD22	1:D:330:LEU:HB3	2.01	0.41
3:F:1:NAG:H62	3:F:2:NAG:N2	2.36	0.41
1:A:385:VAL:HA	1:A:388:ASN:HD22	1.85	0.41
1:C:292:PHE:HA	1:C:293:PRO:HD3	1.91	0.41
1:C:297:VAL:HG21	1:C:327:VAL:HG11	2.03	0.41
1:A:476:SER:N	1:A:488:ASN:OD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:ASN:O	1:B:636:ARG:HD2	2.20	0.41
1:B:226:ILE:HG21	1:B:246:ILE:HG23	2.02	0.41
1:A:556:ASN:HD22	1:A:559:THR:HB	1.84	0.41
1:C:389:PHE:HB3	1:C:440:ILE:HG23	2.02	0.41
1:C:617:ARG:NH2	8:C:704:SO4:O3	2.54	0.41
1:C:249:HIS:HA	1:C:378:HIS:CD2	2.56	0.41
1:D:336:PRO:HB3	1:D:446:LYS:HD2	2.02	0.41
5:H:4:MAN:H2	5:H:5:MAN:H2	1.71	0.41
1:C:291:ARG:NH2	9:C:816:HOH:O	2.54	0.41
1:D:405:LYS:NZ	8:D:704:SO4:O3	2.54	0.41
1:B:257:TYR:OH	1:B:385:VAL:HG13	2.20	0.41
1:D:330:LEU:HD23	1:D:330:LEU:HA	1.96	0.41
1:A:271:MET:HE3	1:A:271:MET:HB2	1.98	0.40
1:B:486:ASP:N	1:B:486:ASP:OD1	2.54	0.40
1:D:307:GLN:HB2	1:D:309:HIS:NE2	2.37	0.40
1:B:591:LYS:HE3	1:B:644:ARG:CZ	2.51	0.40
1:D:561:VAL:HG13	1:D:571:ILE:HA	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:ARG:NH2	8:C:704:SO4:O2[1_556]	1.30	0.90

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	427/449 (95%)	406 (95%)	21 (5%)	0	100	100
1	B	427/449 (95%)	399 (93%)	28 (7%)	0	100	100
1	C	429/449 (96%)	399 (93%)	30 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	429/449 (96%)	400 (93%)	29 (7%)	0	100	100
All	All	1712/1796 (95%)	1604 (94%)	108 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	373/388 (96%)	366 (98%)	7 (2%)	50	81
1	B	373/388 (96%)	367 (98%)	6 (2%)	55	83
1	C	374/388 (96%)	369 (99%)	5 (1%)	61	86
1	D	375/388 (97%)	372 (99%)	3 (1%)	73	90
All	All	1495/1552 (96%)	1474 (99%)	21 (1%)	59	85

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	VAL
1	A	313	CYS
1	A	317	VAL
1	A	363	ILE
1	A	524	CYS
1	A	530	CYS
1	A	649	ASP
1	B	253	ILE
1	B	272	VAL
1	B	313	CYS
1	B	317	VAL
1	B	363	ILE
1	B	613	VAL
1	C	223	GLN
1	C	317	VAL
1	C	524	CYS

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Mol	Chain	Res	Type
1	C	582	CYS
1	C	618	HIS
1	D	303	LEU
1	D	313	CYS
1	D	439	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	GLN
1	A	378	HIS
1	A	388	ASN
1	A	429	ASN
1	A	467	GLN
1	A	556	ASN
1	A	558	HIS
1	A	618	HIS
1	B	249	HIS
1	B	258	GLN
1	B	367	ASN
1	B	378	HIS
1	B	388	ASN
1	B	414	ASN
1	B	439	GLN
1	B	560	GLN
1	B	566	GLN
1	B	627	GLN
1	C	249	HIS
1	C	366	GLN
1	C	367	ASN
1	C	371	HIS
1	C	388	ASN
1	C	414	ASN
1	C	429	ASN
1	C	430	ASN
1	C	457	GLN
1	C	502	GLN
1	C	566	GLN
1	C	627	GLN
1	C	633	ASN
1	D	258	GLN
1	D	267	GLN

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Mol	Chain	Res	Type
1	D	288	ASN
1	D	304	ASN
1	D	366	GLN
1	D	367	ASN
1	D	388	ASN
1	D	406	ASN
1	D	409	GLN
1	D	478	GLN
1	D	595	HIS
1	D	614	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 ⓘ

25 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	0.43	0	17,19,21	0.45	0
2	NAG	E	2	2	14,14,15	0.34	0	17,19,21	1.45	2 (11%)
2	MAN	E	3	2	11,11,12	0.72	0	15,15,17	0.88	2 (13%)
2	MAN	E	4	2	11,11,12	0.77	0	15,15,17	1.69	2 (13%)
2	MAN	E	5	2	11,11,12	0.86	0	15,15,17	0.85	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.26	0	17,19,21	0.48	0
3	NAG	F	2	3	14,14,15	0.31	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	F	3	3	11,11,12	0.77	0	15,15,17	1.24	2 (13%)
3	MAN	F	4	3	11,11,12	0.56	0	15,15,17	0.98	1 (6%)
3	MAN	F	5	3	11,11,12	0.94	1 (9%)	15,15,17	0.90	1 (6%)
3	MAN	F	6	3	11,11,12	1.01	0	15,15,17	1.17	1 (6%)
3	MAN	F	7	3	11,11,12	0.94	1 (9%)	15,15,17	1.34	2 (13%)
4	NAG	G	1	1,4	14,14,15	0.30	0	17,19,21	0.45	0
4	NAG	G	2	4	14,14,15	0.24	0	17,19,21	0.47	0
4	MAN	G	3	4	11,11,12	0.73	0	15,15,17	1.18	1 (6%)
4	MAN	G	4	4	11,11,12	0.79	1 (9%)	15,15,17	1.15	1 (6%)
4	MAN	G	5	4	11,11,12	0.75	0	15,15,17	0.87	1 (6%)
5	NAG	H	1	5,1	14,14,15	0.38	0	17,19,21	0.44	0
5	NAG	H	2	5	14,14,15	0.21	0	17,19,21	0.45	0
5	MAN	H	3	5	11,11,12	0.86	0	15,15,17	1.06	2 (13%)
5	MAN	H	4	5	11,11,12	0.74	0	15,15,17	1.23	2 (13%)
5	MAN	H	5	5	11,11,12	1.37	2 (18%)	15,15,17	1.62	4 (26%)
5	MAN	H	6	5	11,11,12	1.10	1 (9%)	15,15,17	1.21	3 (20%)
5	MAN	H	7	5	11,11,12	0.79	0	15,15,17	0.96	2 (13%)
5	MAN	H	8	5	11,11,12	0.68	0	15,15,17	1.05	1 (6%)

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	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	6/6/23/26	0/1/1/1
2	MAN	E	3	2	-	2/2/19/22	1/1/1/1
2	MAN	E	4	2	-	1/2/19/22	1/1/1/1
2	MAN	E	5	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	MAN	F	3	3	-	2/2/19/22	1/1/1/1
3	MAN	F	4	3	-	2/2/19/22	0/1/1/1
3	MAN	F	5	3	-	0/2/19/22	0/1/1/1
3	MAN	F	6	3	-	0/2/19/22	1/1/1/1
3	MAN	F	7	3	-	0/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	MAN	G	3	4	-	0/2/19/22	1/1/1/1
4	MAN	G	4	4	-	2/2/19/22	0/1/1/1
4	MAN	G	5	4	-	2/2/19/22	0/1/1/1
5	NAG	H	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	1/6/23/26	0/1/1/1
5	MAN	H	3	5	-	0/2/19/22	1/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	MAN	H	5	5	-	1/2/19/22	0/1/1/1
5	MAN	H	6	5	-	0/2/19/22	0/1/1/1
5	MAN	H	7	5	-	2/2/19/22	0/1/1/1
5	MAN	H	8	5	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	5	MAN	C1-C2	3.55	1.60	1.52
5	H	6	MAN	C1-C2	2.94	1.59	1.52
5	H	5	MAN	C2-C3	2.58	1.56	1.52
4	G	4	MAN	C1-C2	2.20	1.57	1.52
3	F	7	MAN	C1-C2	2.20	1.57	1.52
3	F	5	MAN	C1-C2	2.17	1.57	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4	MAN	C1-O5-C5	4.87	118.71	112.19
2	E	2	NAG	C2-N2-C7	4.67	129.16	122.90
3	F	3	MAN	C1-O5-C5	3.57	116.96	112.19
4	G	3	MAN	C1-O5-C5	3.48	116.85	112.19
3	F	7	MAN	C1-O5-C5	3.31	116.62	112.19
5	H	5	MAN	C1-C2-C3	3.26	114.39	109.64
3	F	6	MAN	C1-O5-C5	3.26	116.55	112.19
5	H	3	MAN	C1-O5-C5	3.16	116.42	112.19
5	H	4	MAN	C1-O5-C5	3.10	116.34	112.19
5	H	5	MAN	C1-O5-C5	3.07	116.30	112.19
4	G	4	MAN	C1-O5-C5	3.03	116.25	112.19
2	E	4	MAN	O3-C3-C2	2.96	116.10	110.05
3	F	4	MAN	O2-C2-C3	-2.77	104.42	110.15
5	H	4	MAN	O2-C2-C3	-2.73	104.49	110.15
5	H	8	MAN	C1-O5-C5	2.70	115.80	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	5	MAN	O2-C2-C3	-2.61	104.74	110.15
2	E	2	NAG	C1-C2-N2	2.57	114.49	110.43
5	H	6	MAN	C1-C2-C3	2.47	113.24	109.64
5	H	6	MAN	C1-O5-C5	2.31	115.28	112.19
2	E	3	MAN	C1-O5-C5	2.23	115.17	112.19
4	G	5	MAN	O2-C2-C3	-2.21	105.58	110.15
2	E	3	MAN	O2-C2-C3	-2.12	105.76	110.15
5	H	7	MAN	O2-C2-C3	-2.09	105.82	110.15
3	F	3	MAN	O2-C2-C3	-2.09	105.83	110.15
5	H	6	MAN	O2-C2-C3	-2.09	105.83	110.15
5	H	7	MAN	C1-O5-C5	2.07	114.97	112.19
3	F	7	MAN	O2-C2-C3	-2.07	105.86	110.15
2	E	5	MAN	O2-C2-C3	-2.03	105.94	110.15
3	F	5	MAN	O2-C2-C3	-2.02	105.96	110.15
5	H	3	MAN	O2-C2-C3	-2.02	105.97	110.15
5	H	5	MAN	O5-C5-C4	-2.01	105.94	110.83

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	E	3	MAN	O5-C5-C6-O6
4	G	5	MAN	O5-C5-C6-O6
3	F	4	MAN	O5-C5-C6-O6
4	G	4	MAN	C4-C5-C6-O6
3	F	3	MAN	O5-C5-C6-O6
4	G	4	MAN	O5-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
2	E	3	MAN	C4-C5-C6-O6
4	G	5	MAN	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	F	3	MAN	C4-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
3	F	4	MAN	C4-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
4	G	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	E	4	MAN	O5-C5-C6-O6
5	H	5	MAN	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
5	H	7	MAN	C4-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
5	H	7	MAN	O5-C5-C6-O6
2	E	2	NAG	C1-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7

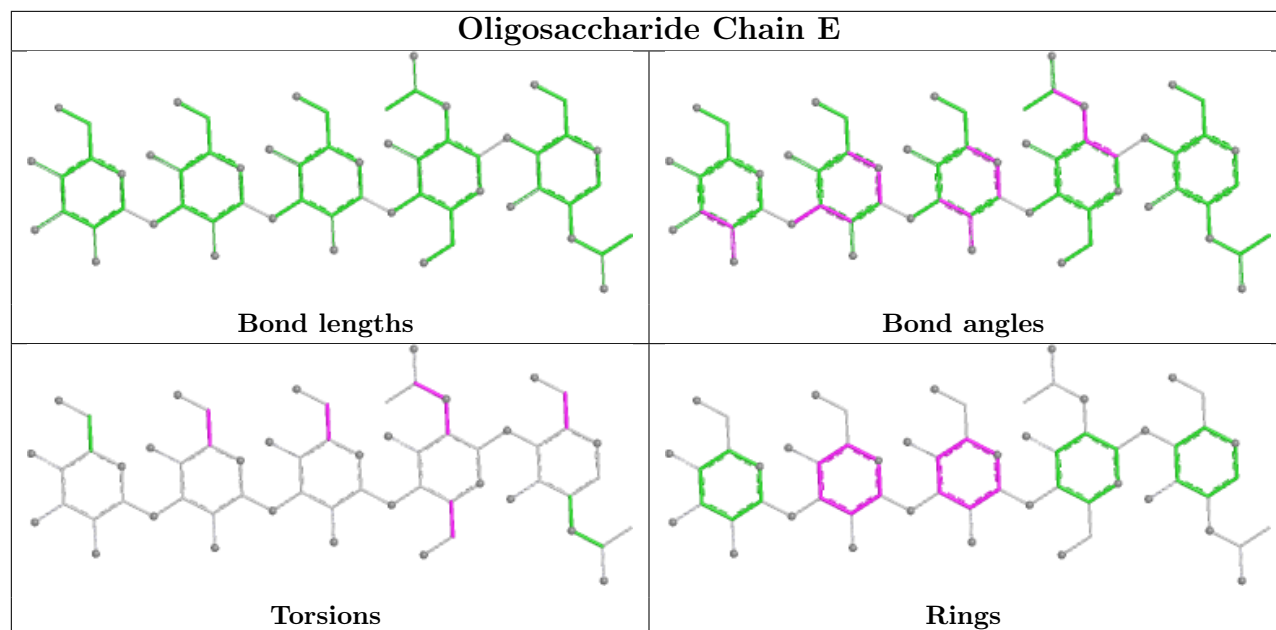
All (6) ring outliers are listed below:

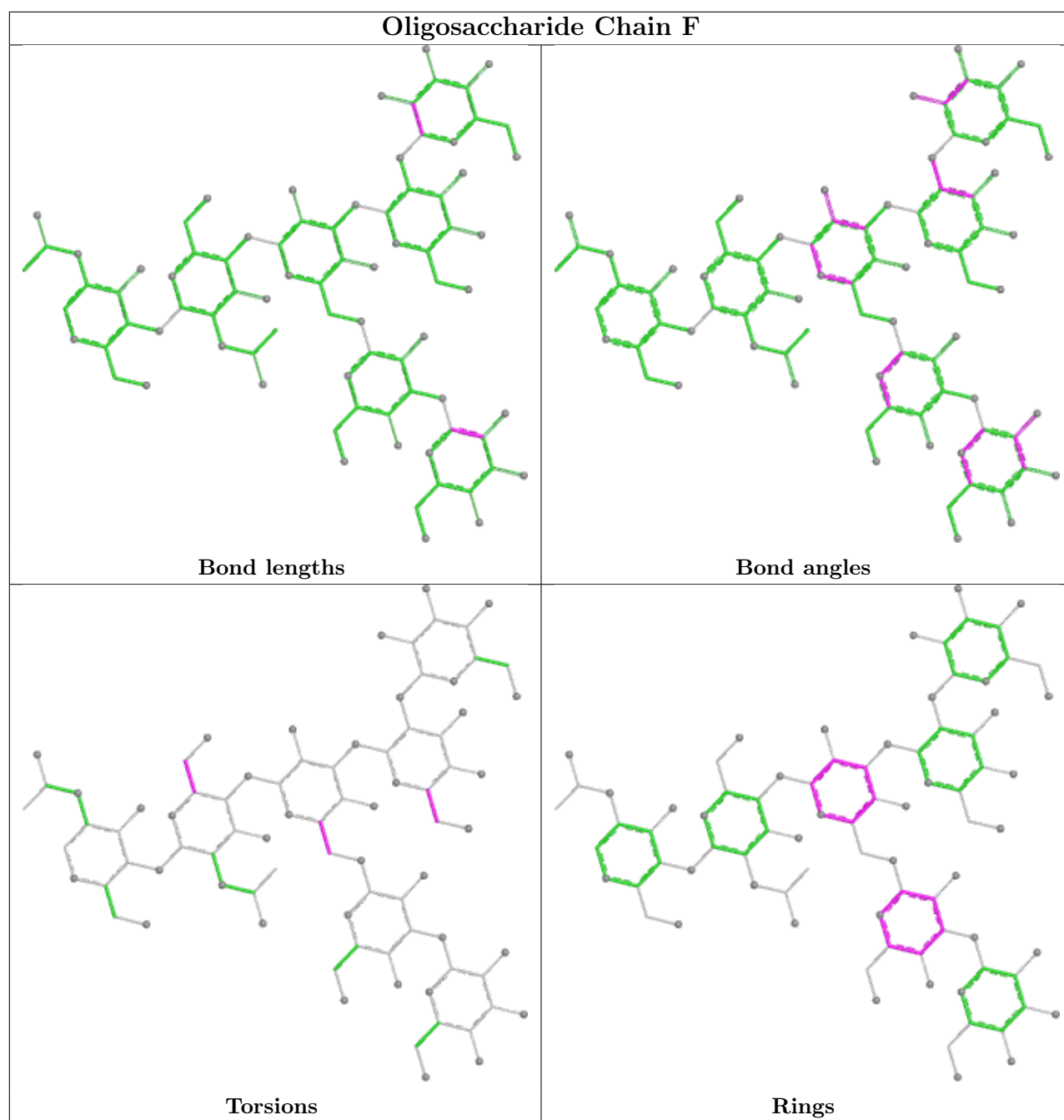
Mol	Chain	Res	Type	Atoms
3	F	3	MAN	C1-C2-C3-C4-C5-O5
2	E	4	MAN	C1-C2-C3-C4-C5-O5
3	F	6	MAN	C1-C2-C3-C4-C5-O5
2	E	3	MAN	C1-C2-C3-C4-C5-O5
4	G	3	MAN	C1-C2-C3-C4-C5-O5
5	H	3	MAN	C1-C2-C3-C4-C5-O5

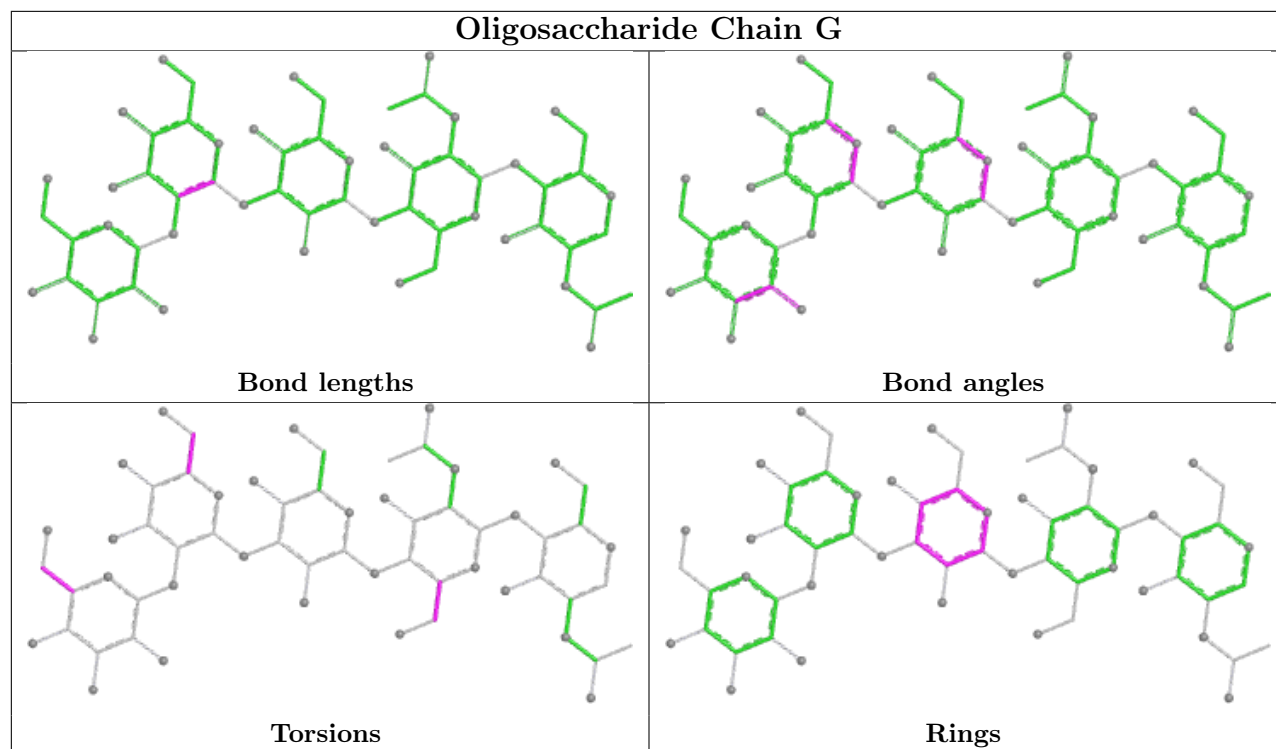
13 monomers are involved in 15 short contacts:

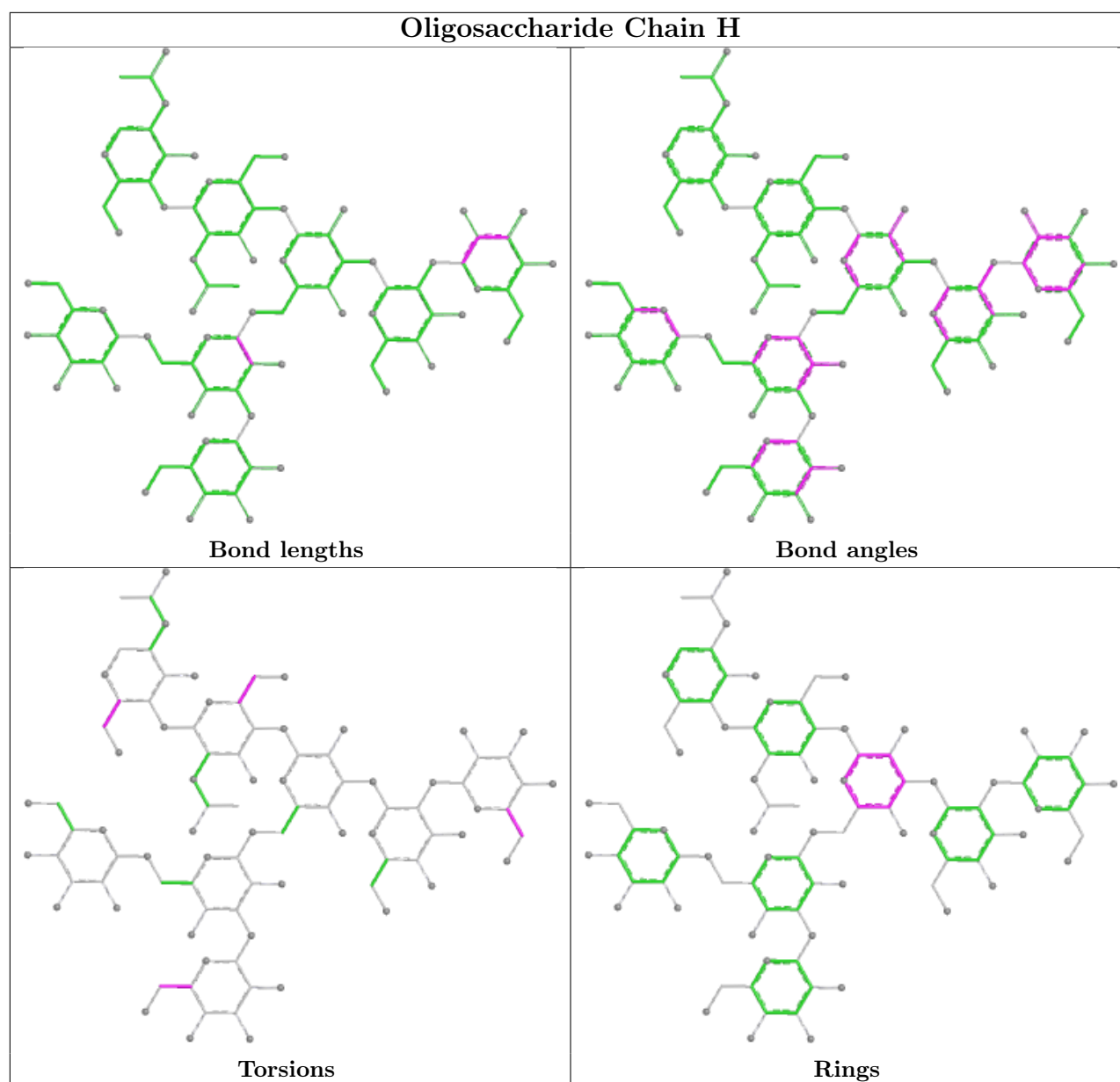
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	NAG	2	0
5	H	7	MAN	1	0
2	E	2	NAG	4	0
5	H	6	MAN	2	0
3	F	4	MAN	1	0
2	E	1	NAG	2	0
5	H	4	MAN	1	0
5	H	5	MAN	1	0
3	F	1	NAG	2	0
3	F	2	NAG	1	0
3	F	5	MAN	2	0
5	H	8	MAN	1	0
5	H	2	NAG	1	0

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 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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	$\# Z > 2$
8	SO4	A	703	-	4,4,4	0.24	0	6,6,6	0.08	0
8	SO4	D	703	-	4,4,4	0.24	0	6,6,6	0.08	0
8	SO4	B	703	-	4,4,4	0.24	0	6,6,6	0.06	0
8	SO4	C	704	-	4,4,4	0.23	0	6,6,6	0.09	0
8	SO4	B	704	-	4,4,4	0.22	0	6,6,6	0.07	0
8	SO4	D	704	-	4,4,4	0.24	0	6,6,6	0.08	0
8	SO4	C	703	-	4,4,4	0.23	0	6,6,6	0.07	0

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.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	704	SO4	2	1
8	B	704	SO4	1	0
8	D	704	SO4	2	0
8	C	703	SO4	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	431/449 (95%)	0.82	36 (8%) 17 12	15, 39, 72, 102	0
1	B	431/449 (95%)	1.08	59 (13%) 6 5	17, 47, 78, 106	0
1	C	433/449 (96%)	1.03	56 (12%) 7 6	14, 47, 82, 104	0
1	D	433/449 (96%)	0.98	42 (9%) 13 10	19, 46, 91, 108	0
All	All	1728/1796 (96%)	0.98	193 (11%) 10 7	14, 45, 82, 108	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	425	ASP	5.8
1	D	583	ALA	4.8
1	A	602	MET	4.3
1	C	527	ASP	4.3
1	D	584	SER	4.2
1	A	655	GLY	3.9
1	C	521	SER	3.7
1	C	480	LYS	3.7
1	D	545	ALA	3.6
1	B	607	CYS	3.6
1	A	521	SER	3.5
1	D	455	SER	3.4
1	D	496	LYS	3.4
1	B	611	GLY	3.4
1	C	217	ALA	3.4
1	A	651	ASP	3.4
1	B	232	PHE	3.3
1	C	369	GLY	3.3
1	A	616	SER	3.2
1	D	512	THR	3.2
1	C	338	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	463	GLY	3.2
1	C	548	PRO	3.1
1	C	407	LEU	3.1
1	C	535	ILE	3.1
1	C	542	LEU	3.1
1	C	408	GLY	3.1
1	D	282	ASP	3.0
1	B	622	ARG	3.0
1	D	506	SER	3.0
1	D	520	LYS	3.0
1	C	539	PHE	3.0
1	D	465	VAL	3.0
1	B	583	ALA	3.0
1	A	523	LYS	3.0
1	B	577	LEU	3.0
1	B	357	SER	2.9
1	A	642	PHE	2.9
1	C	583	ALA	2.9
1	B	493	ARG	2.9
1	D	567	CYS	2.9
1	B	445	GLU	2.8
1	B	321	ARG	2.8
1	C	620	SER	2.8
1	B	563	ILE	2.8
1	B	467	GLN	2.8
1	D	478	GLN	2.8
1	D	592	GLU	2.8
1	C	395	SER	2.8
1	C	492	GLY	2.8
1	C	533	GLU	2.7
1	C	286	PRO	2.7
1	A	404	SER	2.7
1	B	240	GLU	2.7
1	C	565	GLY	2.7
1	C	553	THR	2.7
1	A	527	ASP	2.7
1	B	281	ALA	2.6
1	D	482	GLU	2.6
1	C	637	GLY	2.6
1	D	339	SER	2.6
1	A	565	GLY	2.6
1	B	498	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	574	LYS	2.6
1	C	223	GLN	2.6
1	D	467	GLN	2.6
1	B	655	GLY	2.6
1	D	544	PRO	2.6
1	C	464	MET	2.6
1	C	406	ASN	2.6
1	C	622	ARG	2.5
1	B	582	CYS	2.5
1	B	269	SER	2.5
1	B	346	LYS	2.5
1	A	313	CYS	2.5
1	B	451	CYS	2.5
1	A	592	GLU	2.5
1	D	477	ASP	2.5
1	A	467	GLN	2.5
1	C	651	ASP	2.4
1	A	453	VAL	2.4
1	A	533	GLU	2.4
1	B	233	PHE	2.4
1	A	293	PRO	2.4
1	B	460	CYS	2.4
1	A	652	GLY	2.4
1	B	324	ASP	2.4
1	B	477	ASP	2.4
1	C	306	GLU	2.4
1	B	581	THR	2.4
1	D	540	THR	2.4
1	B	468	GLY	2.4
1	C	552	PHE	2.4
1	C	455	SER	2.4
1	D	268	ILE	2.4
1	A	583	ALA	2.3
1	B	513	ALA	2.3
1	A	591	LYS	2.3
1	A	406	ASN	2.3
1	C	531	ALA	2.3
1	D	473	CYS	2.3
1	A	566	GLN	2.3
1	D	349	LEU	2.3
1	C	540	THR	2.3
1	D	288	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	466	GLU	2.3
1	A	460	CYS	2.3
1	C	467	GLN	2.3
1	C	497	LEU	2.3
1	D	457	GLN	2.3
1	B	612	SER	2.3
1	D	521	SER	2.3
1	A	400	THR	2.3
1	C	578	GLU	2.3
1	B	486	ASP	2.3
1	B	530	CYS	2.3
1	B	623	THR	2.3
1	B	613	VAL	2.3
1	B	552	PHE	2.2
1	B	614	GLN	2.2
1	C	567	CYS	2.2
1	D	602	MET	2.2
1	D	491	GLU	2.2
1	B	480	LYS	2.2
1	C	438	ARG	2.2
1	B	543	CYS	2.2
1	B	604	PRO	2.2
1	D	441	SER	2.2
1	D	500	GLY	2.2
1	B	335	ALA	2.2
1	B	650	ALA	2.2
1	C	601	LYS	2.2
1	D	501	LYS	2.2
1	D	532	ARG	2.2
1	B	499	PRO	2.2
1	C	544	PRO	2.2
1	C	604	PRO	2.2
1	A	221	THR	2.2
1	C	473	CYS	2.2
1	B	630	SER	2.2
1	B	517	PHE	2.2
1	B	533	GLU	2.2
1	C	244	ALA	2.2
1	C	294	ASN	2.2
1	B	447	LYS	2.2
1	A	609	SER	2.2
1	D	487	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	450	ASN	2.1
1	C	488	ASN	2.1
1	C	529	ASP	2.1
1	D	425	ASP	2.1
1	C	611	GLY	2.1
1	D	474	GLY	2.1
1	B	551	GLN	2.1
1	B	558	HIS	2.1
1	B	465	VAL	2.1
1	A	643	MET	2.1
1	B	485	PHE	2.1
1	A	411	GLU	2.1
1	D	218	GLU	2.1
1	D	445	GLU	2.1
1	D	546	SER	2.1
1	C	346	LYS	2.1
1	C	537	ASN	2.1
1	C	554	ASP	2.1
1	B	617	ARG	2.1
1	D	239	ARG	2.1
1	A	543	CYS	2.1
1	C	524	CYS	2.1
1	C	528	SER	2.1
1	B	523	LYS	2.1
1	D	591	LYS	2.1
1	B	237	GLY	2.1
1	C	590	ASP	2.1
1	A	421	ALA	2.1
1	A	579	GLU	2.1
1	A	455	SER	2.0
1	B	348	LYS	2.0
1	B	405	LYS	2.0
1	A	648	VAL	2.0
1	D	542	LEU	2.0
1	B	534	GLY	2.0
1	C	532	ARG	2.0
1	A	634	ASP	2.0
1	B	535	ILE	2.0
1	B	547	ASP	2.0
1	B	578	GLU	2.0
1	B	225	TYR	2.0
1	C	510	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	220	ASN	2.0
1	A	608	ALA	2.0
1	A	650	ALA	2.0
1	B	218	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

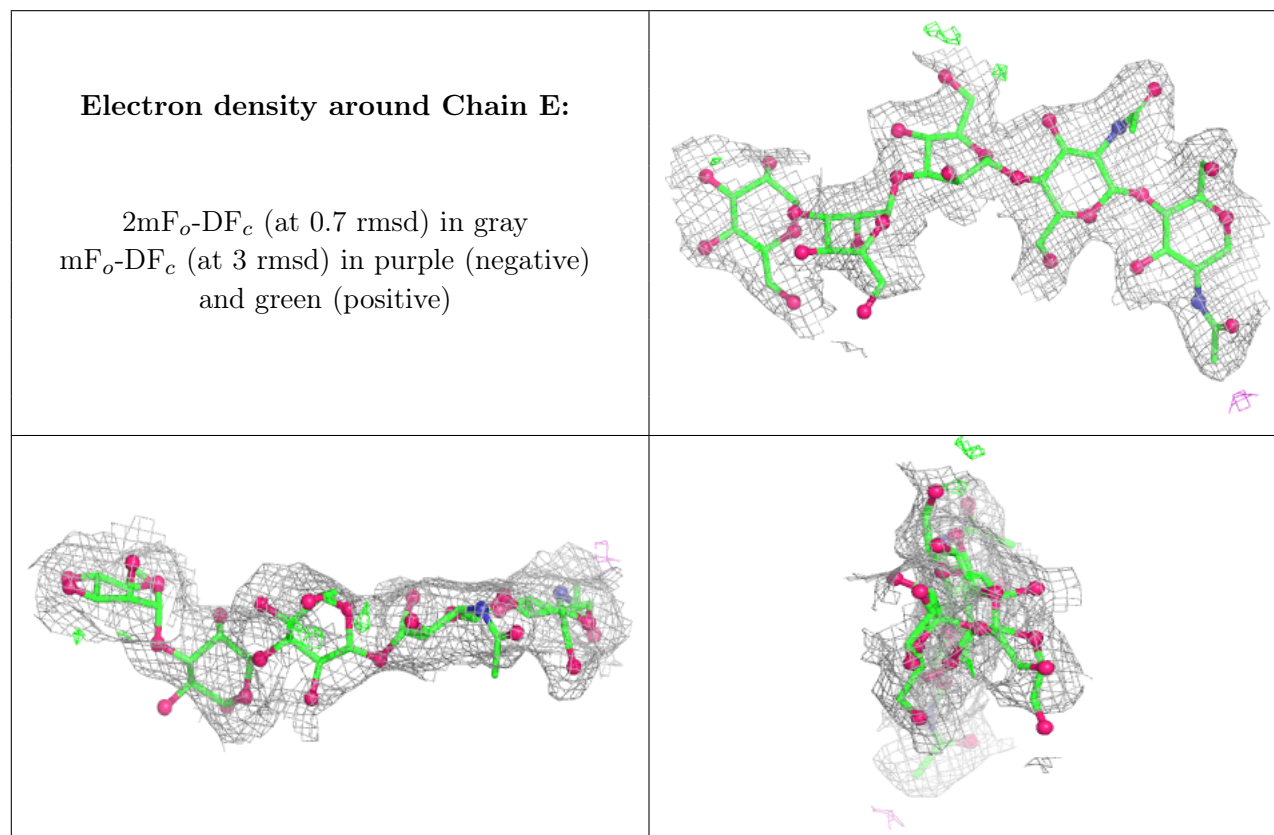
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MAN	H	8	11/12	0.55	0.18	61,78,104,106	0
5	MAN	H	5	11/12	0.57	0.18	50,85,98,104	0
3	MAN	F	5	11/12	0.60	0.16	52,70,81,83	0
3	MAN	F	6	11/12	0.62	0.19	74,80,99,101	0
3	MAN	F	7	11/12	0.68	0.20	53,80,95,104	0
5	MAN	H	7	11/12	0.70	0.19	65,76,82,84	0
5	MAN	H	6	11/12	0.70	0.19	66,77,87,92	0
2	MAN	E	5	11/12	0.71	0.15	52,71,81,82	0
2	MAN	E	4	11/12	0.75	0.20	57,71,92,119	0
4	MAN	G	5	11/12	0.75	0.18	35,49,69,72	0
2	MAN	E	3	11/12	0.76	0.14	34,49,65,70	0
4	MAN	G	4	11/12	0.77	0.14	54,60,66,67	0
3	MAN	F	4	11/12	0.78	0.16	48,62,86,96	0
5	MAN	H	4	11/12	0.78	0.14	53,73,78,89	0
5	MAN	H	3	11/12	0.82	0.15	53,65,85,87	0
3	NAG	F	2	14/15	0.85	0.17	25,42,54,60	0
3	MAN	F	3	11/12	0.85	0.15	32,52,71,71	0
4	NAG	G	2	14/15	0.86	0.13	29,42,53,57	0
4	MAN	G	3	11/12	0.86	0.10	28,42,56,58	0
2	NAG	E	2	14/15	0.89	0.11	29,38,54,55	0
5	NAG	H	2	14/15	0.89	0.13	33,49,68,78	0
3	NAG	F	1	14/15	0.89	0.15	26,34,55,71	0
4	NAG	G	1	14/15	0.89	0.13	27,44,55,58	0
5	NAG	H	1	14/15	0.90	0.10	25,32,38,43	0

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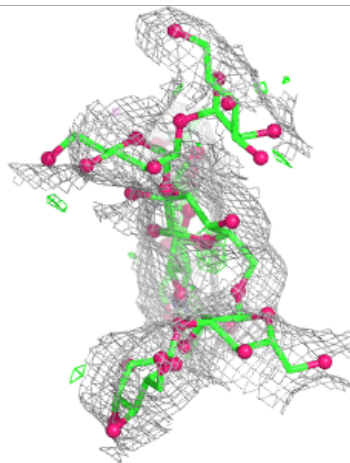
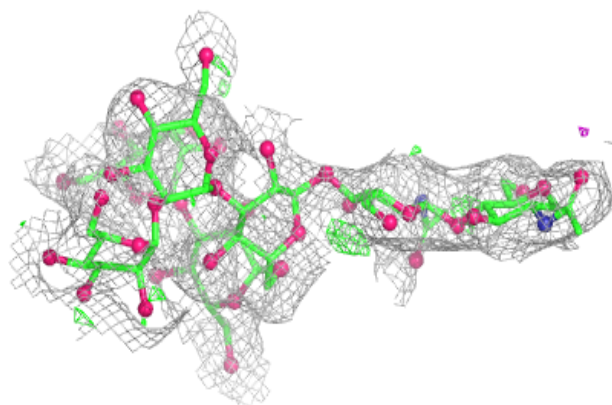
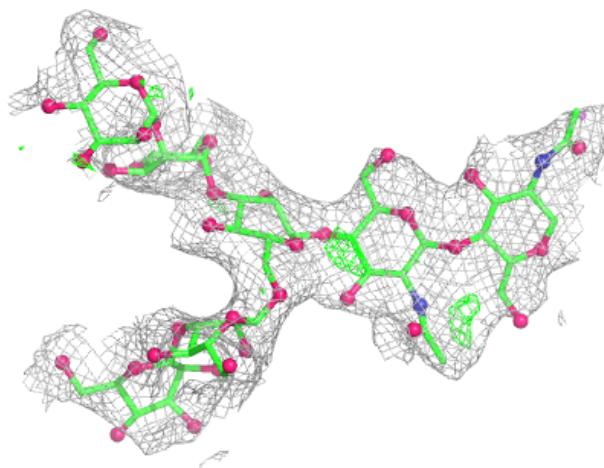
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	E	1	14/15	0.90	0.11	14,29,45,55	0

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.



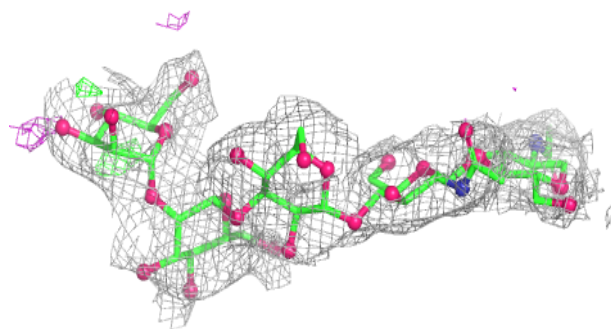
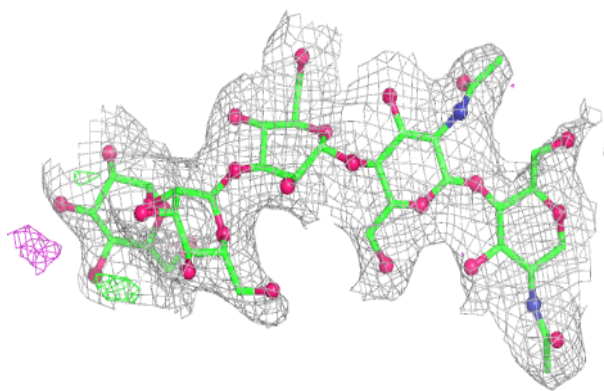
Electron density around Chain F:

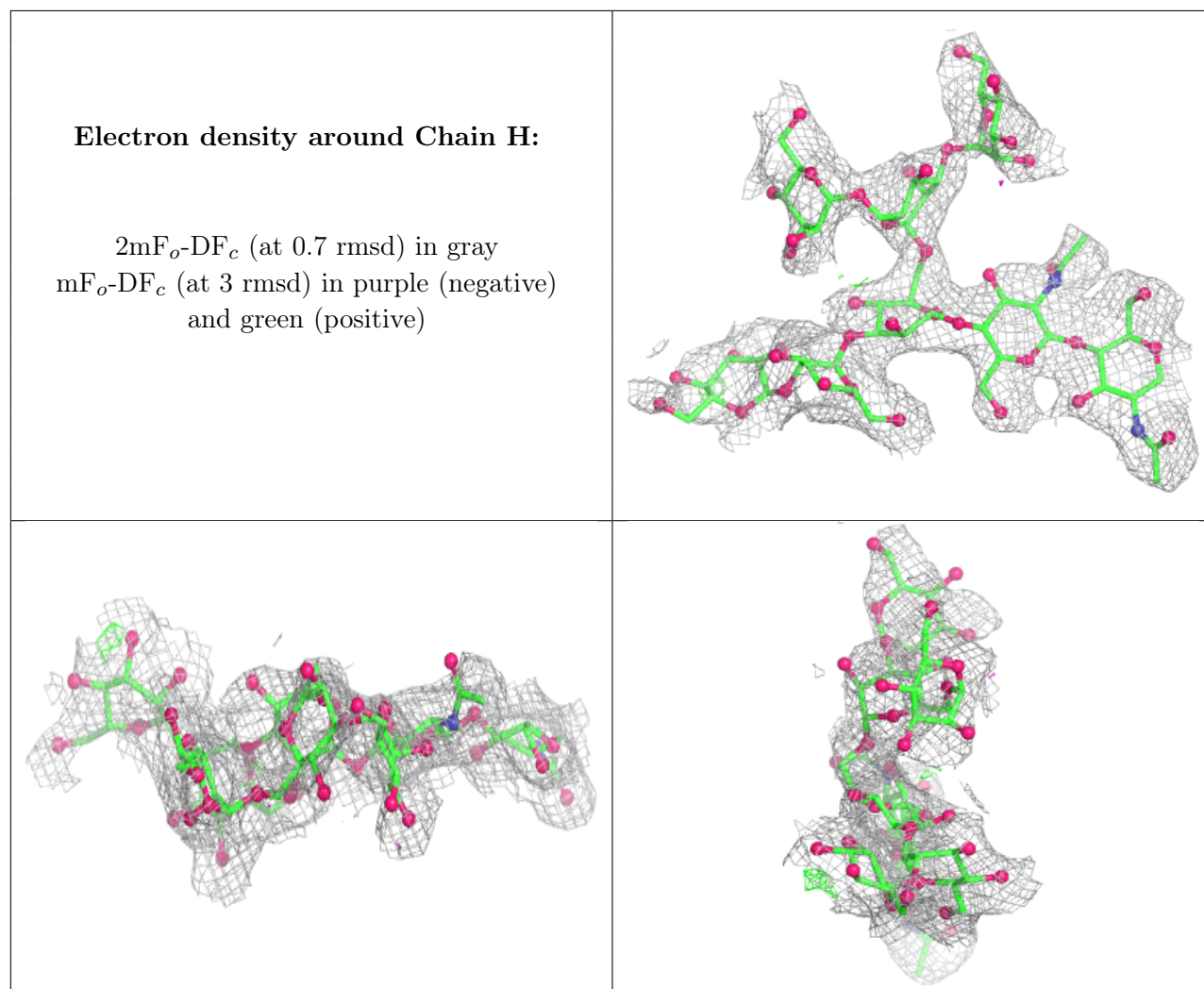
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands ⓘ

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
8	SO4	C	703	5/5	0.47	0.14	106,109,123,124	0
8	SO4	C	704	5/5	0.75	0.19	72,89,99,110	0
8	SO4	D	704	5/5	0.79	0.17	51,84,101,102	0
8	SO4	B	704	5/5	0.82	0.20	50,77,100,118	0
8	SO4	A	703	5/5	0.84	0.12	72,78,81,81	0
7	CA	B	702	1/1	0.91	0.09	40,40,40,40	0
8	SO4	B	703	5/5	0.92	0.07	44,46,52,66	0
8	SO4	D	703	5/5	0.93	0.09	37,45,56,68	0
7	CA	C	702	1/1	0.96	0.05	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	CA	D	702	1/1	0.97	0.06	38,38,38,38	0
6	ZN	A	701	1/1	0.97	0.04	22,22,22,22	0
7	CA	A	702	1/1	0.98	0.04	35,35,35,35	0
6	ZN	D	701	1/1	0.99	0.04	30,30,30,30	0
6	ZN	B	701	1/1	0.99	0.02	20,20,20,20	0
6	ZN	C	701	1/1	0.99	0.03	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.