



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:29 AM UTC

PDB ID : 3S3W / pdb_00003s3w
Title : Structure of chicken acid-sensing ion channel 1 at 2.6 a resolution and ph 7.5
Authors : Dawson, R.J.P.; Benz, J.; Stohler, P.; Tetaz, T.; Joseph, C.; Huber, S.; Schmid, G.; Huegin, D.; Pflimlin, P.; Trube, G.; Rudolph, M.G.; Hennig, M.; Ruf, A.
Deposited on : 2011-05-18
Resolution : 2.60 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

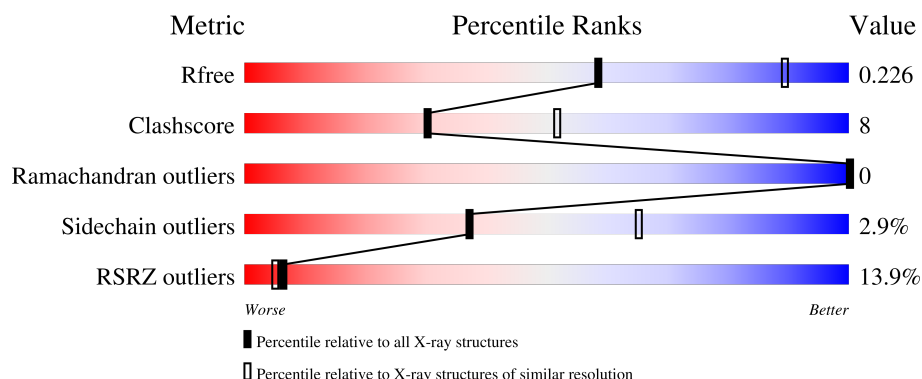
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	459	11% 70% 15% • 14%
1	B	459	14% 69% 16% • 14%
1	C	459	11% 70% 16% • 13%
2	D	2	100%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9925 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 Amiloride-sensitive cation channel 2, neuronal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3162	2022	515	598	27			
1	B	397	Total	C	N	O	S	0	0	0
			3177	2032	516	603	26			
1	C	401	Total	C	N	O	S	0	0	0
			3209	2058	521	603	27			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	MET	-	expression tag	UNP Q1XA76
A	6	SER	-	expression tag	UNP Q1XA76
A	7	TYR	-	expression tag	UNP Q1XA76
A	8	TYR	-	expression tag	UNP Q1XA76
A	9	HIS	-	expression tag	UNP Q1XA76
A	10	HIS	-	expression tag	UNP Q1XA76
A	11	HIS	-	expression tag	UNP Q1XA76
A	12	HIS	-	expression tag	UNP Q1XA76
A	13	HIS	-	expression tag	UNP Q1XA76
A	14	HIS	-	expression tag	UNP Q1XA76
A	15	GLY	-	expression tag	UNP Q1XA76
A	16	ALA	-	expression tag	UNP Q1XA76
A	17	SER	-	expression tag	UNP Q1XA76
A	18	LEU	-	expression tag	UNP Q1XA76
A	19	VAL	-	expression tag	UNP Q1XA76
A	20	PRO	-	expression tag	UNP Q1XA76
A	21	ARG	-	expression tag	UNP Q1XA76
A	22	GLY	-	expression tag	UNP Q1XA76
A	23	SER	-	expression tag	UNP Q1XA76
A	24	HIS	-	expression tag	UNP Q1XA76
A	25	MET	-	expression tag	UNP Q1XA76
B	5	MET	-	expression tag	UNP Q1XA76
B	6	SER	-	expression tag	UNP Q1XA76

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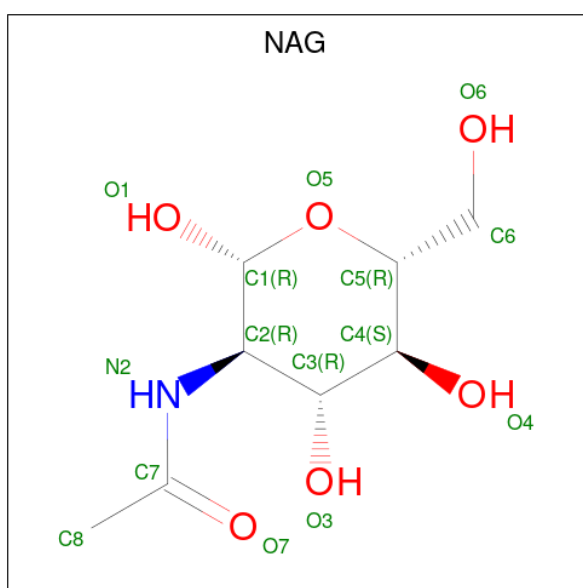
Chain	Residue	Modelled	Actual	Comment	Reference
B	7	TYR	-	expression tag	UNP Q1XA76
B	8	TYR	-	expression tag	UNP Q1XA76
B	9	HIS	-	expression tag	UNP Q1XA76
B	10	HIS	-	expression tag	UNP Q1XA76
B	11	HIS	-	expression tag	UNP Q1XA76
B	12	HIS	-	expression tag	UNP Q1XA76
B	13	HIS	-	expression tag	UNP Q1XA76
B	14	HIS	-	expression tag	UNP Q1XA76
B	15	GLY	-	expression tag	UNP Q1XA76
B	16	ALA	-	expression tag	UNP Q1XA76
B	17	SER	-	expression tag	UNP Q1XA76
B	18	LEU	-	expression tag	UNP Q1XA76
B	19	VAL	-	expression tag	UNP Q1XA76
B	20	PRO	-	expression tag	UNP Q1XA76
B	21	ARG	-	expression tag	UNP Q1XA76
B	22	GLY	-	expression tag	UNP Q1XA76
B	23	SER	-	expression tag	UNP Q1XA76
B	24	HIS	-	expression tag	UNP Q1XA76
B	25	MET	-	expression tag	UNP Q1XA76
C	5	MET	-	expression tag	UNP Q1XA76
C	6	SER	-	expression tag	UNP Q1XA76
C	7	TYR	-	expression tag	UNP Q1XA76
C	8	TYR	-	expression tag	UNP Q1XA76
C	9	HIS	-	expression tag	UNP Q1XA76
C	10	HIS	-	expression tag	UNP Q1XA76
C	11	HIS	-	expression tag	UNP Q1XA76
C	12	HIS	-	expression tag	UNP Q1XA76
C	13	HIS	-	expression tag	UNP Q1XA76
C	14	HIS	-	expression tag	UNP Q1XA76
C	15	GLY	-	expression tag	UNP Q1XA76
C	16	ALA	-	expression tag	UNP Q1XA76
C	17	SER	-	expression tag	UNP Q1XA76
C	18	LEU	-	expression tag	UNP Q1XA76
C	19	VAL	-	expression tag	UNP Q1XA76
C	20	PRO	-	expression tag	UNP Q1XA76
C	21	ARG	-	expression tag	UNP Q1XA76
C	22	GLY	-	expression tag	UNP Q1XA76
C	23	SER	-	expression tag	UNP Q1XA76
C	24	HIS	-	expression tag	UNP Q1XA76
C	25	MET	-	expression tag	UNP Q1XA76

- 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	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0
4	C	1	Total 1	Cl 1	0	0

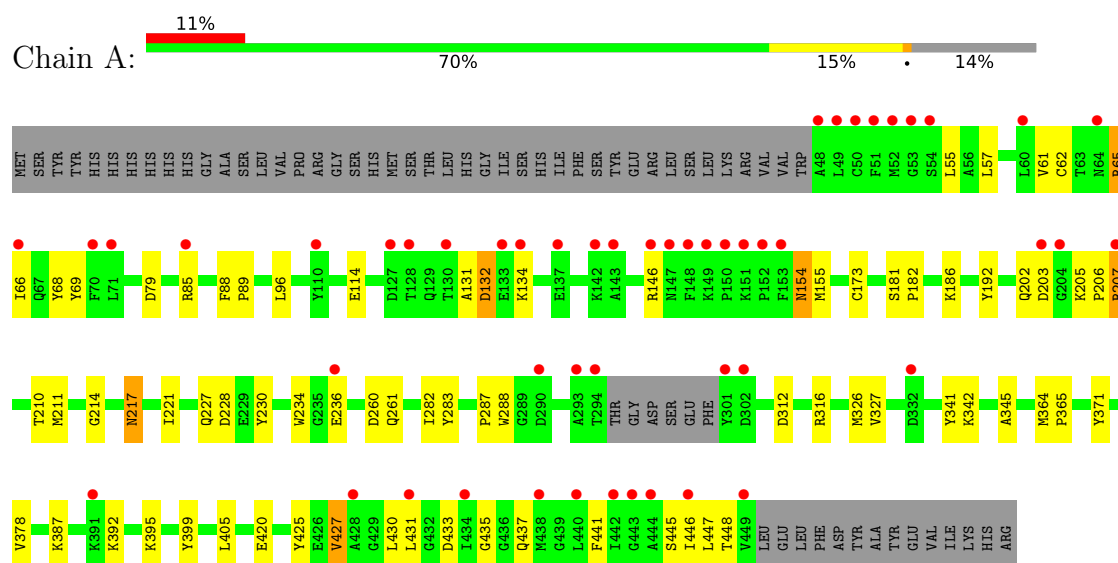
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	85	Total 85	O 85	0	0
5	B	87	Total 87	O 87	0	0
5	C	76	Total 76	O 76	0	0

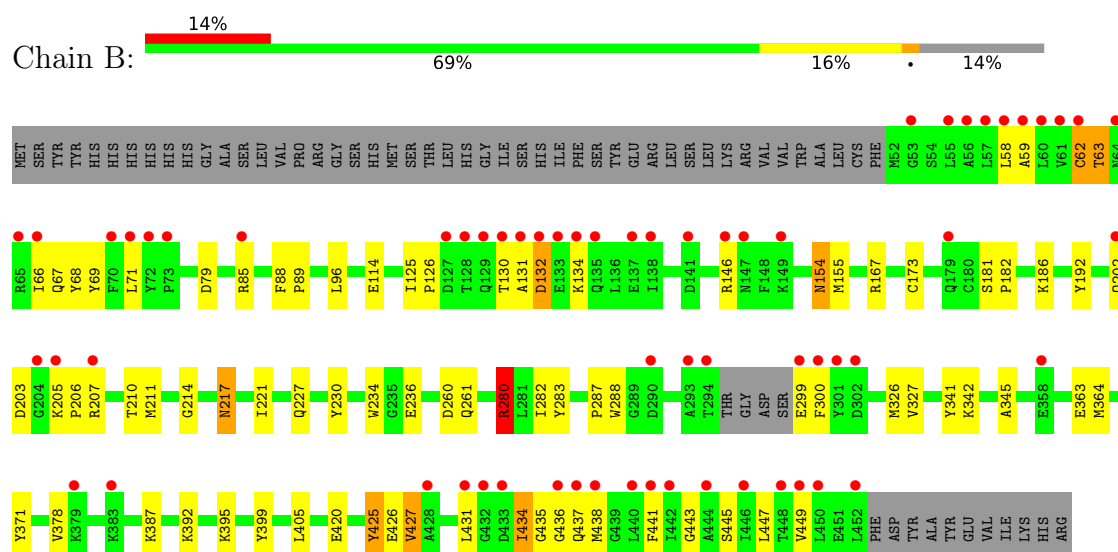
3 Residue-property plots

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: Amiloride-sensitive cation channel 2, neuronal

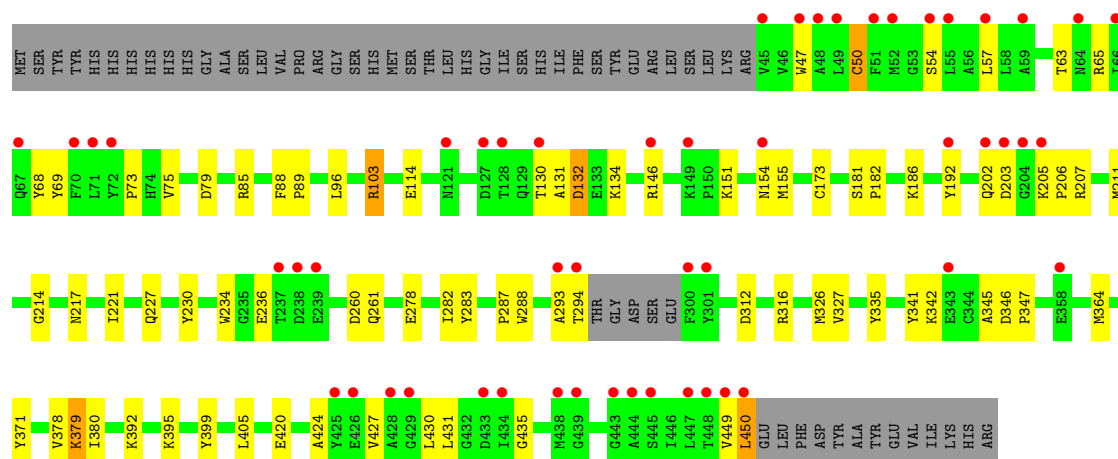


- Molecule 1: Amiloride-sensitive cation channel 2, neuronal



- Molecule 1: Amiloride-sensitive cation channel 2, neuronal





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

Chain D: 100%



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

Chain E: 50%



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

Chain F: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.47Å 142.69Å 159.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.94 – 2.60 47.94 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.94-2.60) 95.6 (47.94-2.60)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.212 , 0.236 0.203 , 0.226	Depositor DCC
R_{free} test set	3924 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9925	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	0/3234	0.70	4/4377 (0.1%)
1	B	0.28	0/3249	0.77	9/4397 (0.2%)
1	C	0.28	0/3284	0.78	9/4447 (0.2%)
All	All	0.27	0/9767	0.75	22/13221 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	103	ARG	NE-CZ-NH2	13.95	131.75	119.20
1	C	103	ARG	NE-CZ-NH1	-12.41	109.09	121.50
1	C	103	ARG	CD-NE-CZ	10.24	138.73	124.40
1	B	280	ARG	NE-CZ-NH2	9.96	128.17	119.20
1	B	280	ARG	NE-CZ-NH1	-9.92	111.58	121.50
1	B	167	ARG	NE-CZ-NH2	9.32	127.59	119.20
1	B	167	ARG	NE-CZ-NH1	-8.72	112.78	121.50
1	C	207	ARG	NE-CZ-NH2	-8.38	111.65	119.20
1	B	146	ARG	NE-CZ-NH2	-7.42	112.52	119.20
1	B	280	ARG	CD-NE-CZ	7.32	134.65	124.40
1	B	146	ARG	CD-NE-CZ	7.02	134.23	124.40
1	C	207	ARG	NE-CZ-NH1	6.91	128.41	121.50
1	C	207	ARG	CD-NE-CZ	6.69	133.76	124.40
1	B	167	ARG	CD-NE-CZ	6.53	133.54	124.40
1	B	146	ARG	NE-CZ-NH1	6.34	127.84	121.50
1	C	146	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	C	103	ARG	CB-CG-CD	5.39	123.69	111.30
1	A	146	ARG	NE-CZ-NH2	5.38	124.05	119.20
1	A	207	ARG	NE-CZ-NH2	5.18	123.87	119.20
1	A	146	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	C	146	ARG	NE-CZ-NH1	-5.11	116.39	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	ARG	NE-CZ-NH1	-5.05	116.45	121.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3162	0	3068	60	0
1	B	3177	0	3081	62	1
1	C	3209	0	3116	54	1
2	D	28	0	25	0	0
2	E	28	0	25	1	0
2	F	28	0	25	0	0
3	A	14	0	13	0	0
3	C	28	0	26	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	85	0	0	1	0
5	B	87	0	0	0	0
5	C	76	0	0	2	0
All	All	9925	0	9379	160	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 (160) 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:A:68:TYR:HD2	1:A:425:TYR:HD2	1.03	0.95
1:A:68:TYR:CD2	1:A:425:TYR:HD2	1.85	0.94
1:A:68:TYR:HD2	1:A:425:TYR:CD2	1.86	0.93
1:B:436:GLY:HA2	1:C:57:LEU:HD22	1.59	0.83
1:A:447:LEU:HD12	1:C:450:LEU:HD23	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ALA:O	1:B:63:THR:OG1	2.07	0.72
1:A:392:LYS:NZ	1:B:236:GLU:OE2	2.23	0.71
1:B:392:LYS:NZ	1:C:236:GLU:OE2	2.23	0.70
1:B:299:GLU:HG2	1:B:300:PHE:H	1.57	0.70
1:B:299:GLU:HG2	1:B:300:PHE:N	2.08	0.68
1:C:395:LYS:HG2	1:C:399:TYR:CD1	2.31	0.66
1:A:395:LYS:HG2	1:A:399:TYR:CD1	2.31	0.65
1:B:58:LEU:O	1:B:62:CYS:HB2	1.97	0.65
1:B:395:LYS:HG2	1:B:399:TYR:CD1	2.31	0.65
1:B:443:GLY:HA3	1:C:50:CYS:SG	2.38	0.64
1:A:68:TYR:CD2	1:A:425:TYR:CD2	2.74	0.61
1:A:441:PHE:O	1:A:445:SER:OG	2.11	0.61
1:C:75:VAL:HG13	1:C:424:ALA:HB2	1.84	0.59
1:A:228:ASP:HB3	5:A:492:HOH:O	2.02	0.59
1:B:68:TYR:HA	1:B:71:LEU:HD12	1.82	0.59
1:C:54:SER:O	1:C:57:LEU:HG	2.02	0.58
1:A:62:CYS:O	1:A:66:ILE:HG12	2.04	0.58
1:B:447:LEU:HD21	1:C:47:TRP:CZ2	2.39	0.57
1:B:186:LYS:HE2	1:B:202:GLN:OE1	2.05	0.57
1:A:186:LYS:HE2	1:A:202:GLN:OE1	2.05	0.57
1:C:186:LYS:HE2	1:C:202:GLN:OE1	2.04	0.57
1:C:326:MET:HE3	1:C:341:TYR:CE2	2.41	0.56
1:C:131:ALA:HB2	1:C:234:TRP:HE1	1.70	0.56
1:B:326:MET:HE3	1:B:341:TYR:CE2	2.41	0.56
1:A:326:MET:HE3	1:A:341:TYR:CE2	2.40	0.56
1:B:62:CYS:O	1:B:434:ILE:HD11	2.06	0.56
1:B:447:LEU:HD11	1:C:47:TRP:NE1	2.21	0.56
1:A:131:ALA:HB2	1:A:234:TRP:HE1	1.70	0.55
1:A:425:TYR:HE1	1:A:430:LEU:N	2.04	0.55
1:A:425:TYR:CE1	1:A:430:LEU:HA	2.42	0.55
1:C:283:TYR:CZ	1:C:364:MET:HE1	2.42	0.55
1:A:154:ASN:C	1:A:154:ASN:OD1	2.50	0.55
1:C:312:ASP:OD2	1:C:316:ARG:NH1	2.40	0.55
1:A:283:TYR:CZ	1:A:364:MET:HE1	2.42	0.54
1:C:181:SER:HB2	1:C:182:PRO:HD2	1.90	0.54
1:B:181:SER:HB2	1:B:182:PRO:HD2	1.90	0.54
1:B:131:ALA:HB2	1:B:234:TRP:HE1	1.71	0.54
1:B:283:TYR:CZ	1:B:364:MET:HE1	2.42	0.54
1:C:203:ASP:HB3	1:C:205:LYS:HG3	1.90	0.53
1:B:405:LEU:HD12	1:B:405:LEU:C	2.33	0.53
1:B:203:ASP:HB3	1:B:205:LYS:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:LYS:HG2	1:B:130:THR:HB	1.91	0.53
1:B:85:ARG:HG2	1:B:211:MET:HE2	1.92	0.52
1:A:181:SER:HB2	1:A:182:PRO:HD2	1.90	0.52
1:A:203:ASP:HB3	1:A:205:LYS:HG3	1.91	0.52
1:A:85:ARG:HG2	1:A:211:MET:HE2	1.92	0.52
1:A:236:GLU:OE2	1:C:392:LYS:NZ	2.43	0.52
1:A:405:LEU:C	1:A:405:LEU:HD12	2.33	0.52
1:C:405:LEU:C	1:C:405:LEU:HD12	2.34	0.52
1:A:425:TYR:OH	1:A:430:LEU:HA	2.10	0.52
1:A:65:ARG:HD3	1:A:433:ASP:HB3	1.93	0.51
1:C:85:ARG:HG2	1:C:211:MET:HE2	1.92	0.51
1:A:69:TYR:CE2	1:A:427:VAL:HG23	2.46	0.51
1:C:395:LYS:HG2	1:C:399:TYR:CE1	2.46	0.51
1:A:341:TYR:HA	1:A:345:ALA:HB3	1.94	0.50
1:A:155:MET:HB2	1:A:327:VAL:HG11	1.94	0.50
1:A:395:LYS:HG2	1:A:399:TYR:CE1	2.46	0.50
1:B:154:ASN:OD1	1:B:154:ASN:C	2.55	0.50
1:A:173:CYS:SG	1:A:221:ILE:HG22	2.52	0.50
1:B:395:LYS:HG2	1:B:399:TYR:CE1	2.46	0.50
1:B:173:CYS:SG	1:B:221:ILE:HG22	2.51	0.50
1:C:173:CYS:SG	1:C:221:ILE:HG22	2.52	0.50
1:B:437:GLN:N	1:B:437:GLN:OE1	2.45	0.50
1:B:434:ILE:CG2	1:B:438:MET:HE3	2.42	0.49
1:C:427:VAL:HG23	5:C:524:HOH:O	2.11	0.49
1:C:132:ASP:OD1	1:C:132:ASP:C	2.55	0.49
1:B:341:TYR:HA	1:B:345:ALA:HB3	1.94	0.49
1:B:132:ASP:OD1	1:B:132:ASP:C	2.55	0.49
1:C:341:TYR:HA	1:C:345:ALA:HB3	1.94	0.49
1:B:155:MET:HB2	1:B:327:VAL:HG11	1.95	0.48
1:C:68:TYR:CE1	1:C:73:PRO:HG3	2.48	0.48
1:B:88:PHE:CG	1:B:89:PRO:HD2	2.49	0.48
1:A:57:LEU:HB3	1:A:437:GLN:OE1	2.14	0.48
1:A:88:PHE:CG	1:A:89:PRO:HD2	2.48	0.48
1:C:278:GLU:OE1	5:C:507:HOH:O	2.20	0.48
1:B:431:LEU:O	1:B:435:GLY:N	2.44	0.48
1:A:132:ASP:OD1	1:A:132:ASP:C	2.56	0.48
1:A:55:LEU:HD13	1:A:441:PHE:CE1	2.49	0.48
1:C:88:PHE:CG	1:C:89:PRO:HD2	2.48	0.47
1:B:68:TYR:HD2	1:B:425:TYR:CD2	2.32	0.47
1:C:155:MET:HB2	1:C:327:VAL:HG11	1.96	0.47
1:C:131:ALA:HB2	1:C:234:TRP:NE1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:PRO:HD2	1:C:288:TRP:CZ3	2.50	0.47
1:A:227:GLN:HA	1:A:230:TYR:CD1	2.49	0.47
1:B:69:TYR:CE2	1:B:427:VAL:HG22	2.50	0.47
1:B:434:ILE:HG21	1:B:438:MET:HE3	1.96	0.47
1:A:287:PRO:HD2	1:A:288:TRP:CZ3	2.50	0.47
1:B:67:GLN:O	1:B:71:LEU:HG	2.14	0.47
1:C:89:PRO:HB3	1:C:371:TYR:CZ	2.51	0.47
1:C:132:ASP:OD1	1:C:134:LYS:N	2.48	0.47
1:C:227:GLN:HA	1:C:230:TYR:CD1	2.50	0.46
1:B:89:PRO:HB3	1:B:371:TYR:CZ	2.51	0.46
1:B:443:GLY:O	1:B:447:LEU:HB2	2.15	0.46
1:B:227:GLN:HA	1:B:230:TYR:CD1	2.50	0.46
1:A:131:ALA:HB2	1:A:234:TRP:NE1	2.30	0.46
1:A:431:LEU:O	1:A:435:GLY:N	2.23	0.46
1:B:287:PRO:HD2	1:B:288:TRP:CZ3	2.50	0.46
1:A:132:ASP:OD1	1:A:134:LYS:N	2.48	0.46
1:B:132:ASP:OD1	1:B:134:LYS:N	2.48	0.46
1:A:89:PRO:HB3	1:A:371:TYR:CZ	2.51	0.46
1:B:387:LYS:HG2	1:C:130:THR:HB	1.97	0.46
1:B:131:ALA:HB2	1:B:234:TRP:NE1	2.30	0.45
1:B:445:SER:O	1:B:449:VAL:HG23	2.17	0.45
1:C:431:LEU:O	1:C:435:GLY:N	2.46	0.45
1:C:192:TYR:CE2	1:C:260:ASP:HA	2.52	0.45
1:A:326:MET:HE3	1:A:341:TYR:HE2	1.82	0.45
1:A:425:TYR:HE1	1:A:430:LEU:CA	2.30	0.45
1:A:214:GLY:HA2	1:B:261:GLN:O	2.17	0.45
1:B:181:SER:HB2	1:B:182:PRO:CD	2.47	0.45
1:C:54:SER:HA	1:C:57:LEU:HD23	1.99	0.45
1:A:192:TYR:CE2	1:A:260:ASP:HA	2.52	0.44
1:A:261:GLN:O	1:C:214:GLY:HA2	2.17	0.44
1:B:58:LEU:HD13	1:B:441:PHE:HB2	1.99	0.44
1:C:181:SER:HB2	1:C:182:PRO:CD	2.47	0.44
1:B:114:GLU:HG2	1:B:342:LYS:HE3	1.99	0.44
1:C:379:LYS:HG3	1:C:380:ILE:N	2.32	0.44
1:A:205:LYS:HB3	1:A:206:PRO:HD2	2.00	0.44
1:A:114:GLU:HG2	1:A:342:LYS:HE3	1.99	0.43
1:B:192:TYR:CE2	1:B:260:ASP:HA	2.52	0.43
1:B:211:MET:HE3	1:B:211:MET:HB2	1.84	0.43
1:A:425:TYR:CE1	1:A:430:LEU:CA	3.01	0.43
1:A:446:ILE:O	1:A:446:ILE:HG22	2.19	0.43
1:B:214:GLY:HA2	1:C:261:GLN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:GLU:HG2	1:C:342:LYS:HE3	1.99	0.43
1:A:57:LEU:HD23	1:A:57:LEU:HA	1.86	0.43
1:A:364:MET:HA	1:A:365:PRO:HD3	1.90	0.43
1:C:450:LEU:HD12	1:C:450:LEU:HA	1.83	0.43
1:B:378:VAL:HG11	1:C:96:LEU:HD11	2.01	0.43
1:A:181:SER:HB2	1:A:182:PRO:CD	2.48	0.42
1:B:205:LYS:HB3	1:B:206:PRO:HD2	2.01	0.42
1:C:205:LYS:HB3	1:C:206:PRO:HD2	2.01	0.42
1:A:378:VAL:HG11	1:B:96:LEU:HD11	2.00	0.42
1:B:280:ARG:HH11	2:E:1:NAG:H3	1.84	0.42
1:C:282:ILE:HB	1:C:420:GLU:HG3	2.02	0.42
1:A:282:ILE:HB	1:A:420:GLU:HG3	2.02	0.41
1:B:282:ILE:HB	1:B:420:GLU:HG3	2.02	0.41
1:B:427:VAL:O	1:B:431:LEU:HG	2.20	0.41
1:B:62:CYS:O	1:B:66:ILE:HG13	2.20	0.41
1:B:326:MET:HE3	1:B:341:TYR:HE2	1.82	0.41
1:C:154:ASN:HD21	1:C:335:TYR:HD2	1.66	0.41
1:A:312:ASP:OD2	1:A:316:ARG:NH2	2.53	0.41
1:A:210:THR:HG23	1:A:217:ASN:HB3	2.03	0.41
1:C:65:ARG:HB3	1:C:430:LEU:CD1	2.51	0.41
1:A:65:ARG:HB3	1:A:430:LEU:HD11	2.02	0.41
1:B:280:ARG:HA	1:B:280:ARG:HD3	1.79	0.41
1:C:57:LEU:C	1:C:57:LEU:HD12	2.46	0.41
1:C:326:MET:HE3	1:C:341:TYR:HE2	1.82	0.41
1:A:425:TYR:CZ	1:A:430:LEU:HA	2.56	0.40
1:C:293:ALA:O	1:C:294:THR:C	2.64	0.40
1:C:346:ASP:HB2	1:C:347:PRO:HD3	2.03	0.40
1:A:96:LEU:HD11	1:C:378:VAL:HG11	2.02	0.40
1:A:211:MET:HE3	1:A:211:MET:HB2	1.83	0.40
1:B:210:THR:HG23	1:B:217:ASN:HB3	2.04	0.40
1:B:125:ILE:HA	1:B:126:PRO:HD3	1.89	0.40
1:C:69:TYR:OH	1:C:427:VAL:HG22	2.21	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:B:363:GLU:OE1	1:C:151:LYS:NZ[3_555]	2.09	0.11

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	392/459 (85%)	383 (98%)	9 (2%)	0	100	100
1	B	393/459 (86%)	384 (98%)	9 (2%)	0	100	100
1	C	397/459 (86%)	390 (98%)	7 (2%)	0	100	100
All	All	1182/1377 (86%)	1157 (98%)	25 (2%)	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	344/401 (86%)	335 (97%)	9 (3%)	40	68
1	B	346/401 (86%)	334 (96%)	12 (4%)	32	59
1	C	349/401 (87%)	340 (97%)	9 (3%)	40	68
All	All	1039/1203 (86%)	1009 (97%)	30 (3%)	37	65

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	VAL
1	A	65	ARG
1	A	79	ASP
1	A	132	ASP
1	A	154	ASN

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Mol	Chain	Res	Type
1	A	207	ARG
1	A	217	ASN
1	A	427	VAL
1	A	448	THR
1	B	62	CYS
1	B	63	THR
1	B	79	ASP
1	B	132	ASP
1	B	154	ASN
1	B	207	ARG
1	B	217	ASN
1	B	280	ARG
1	B	425	TYR
1	B	426	GLU
1	B	427	VAL
1	B	434	ILE
1	C	50	CYS
1	C	63	THR
1	C	79	ASP
1	C	103	ARG
1	C	132	ASP
1	C	217	ASN
1	C	379	LYS
1	C	449	VAL
1	C	450	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	GLN
1	A	321	ASN
1	A	437	GLN
1	B	67	GLN
1	B	179	GLN
1	B	321	ASN
1	C	179	GLN
1	C	321	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 ⓘ

6 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	D	1	2,1	14,14,15	0.55	0	17,19,21	0.75	0
2	NAG	D	2	2	14,14,15	0.49	0	17,19,21	0.76	0
2	NAG	E	1	2,1	14,14,15	0.50	0	17,19,21	0.77	0
2	NAG	E	2	2	14,14,15	0.49	0	17,19,21	0.76	0
2	NAG	F	1	2,1	14,14,15	0.53	0	17,19,21	0.57	0
2	NAG	F	2	2	14,14,15	0.52	0	17,19,21	0.60	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
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	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.

All (8) torsion outliers are listed below:

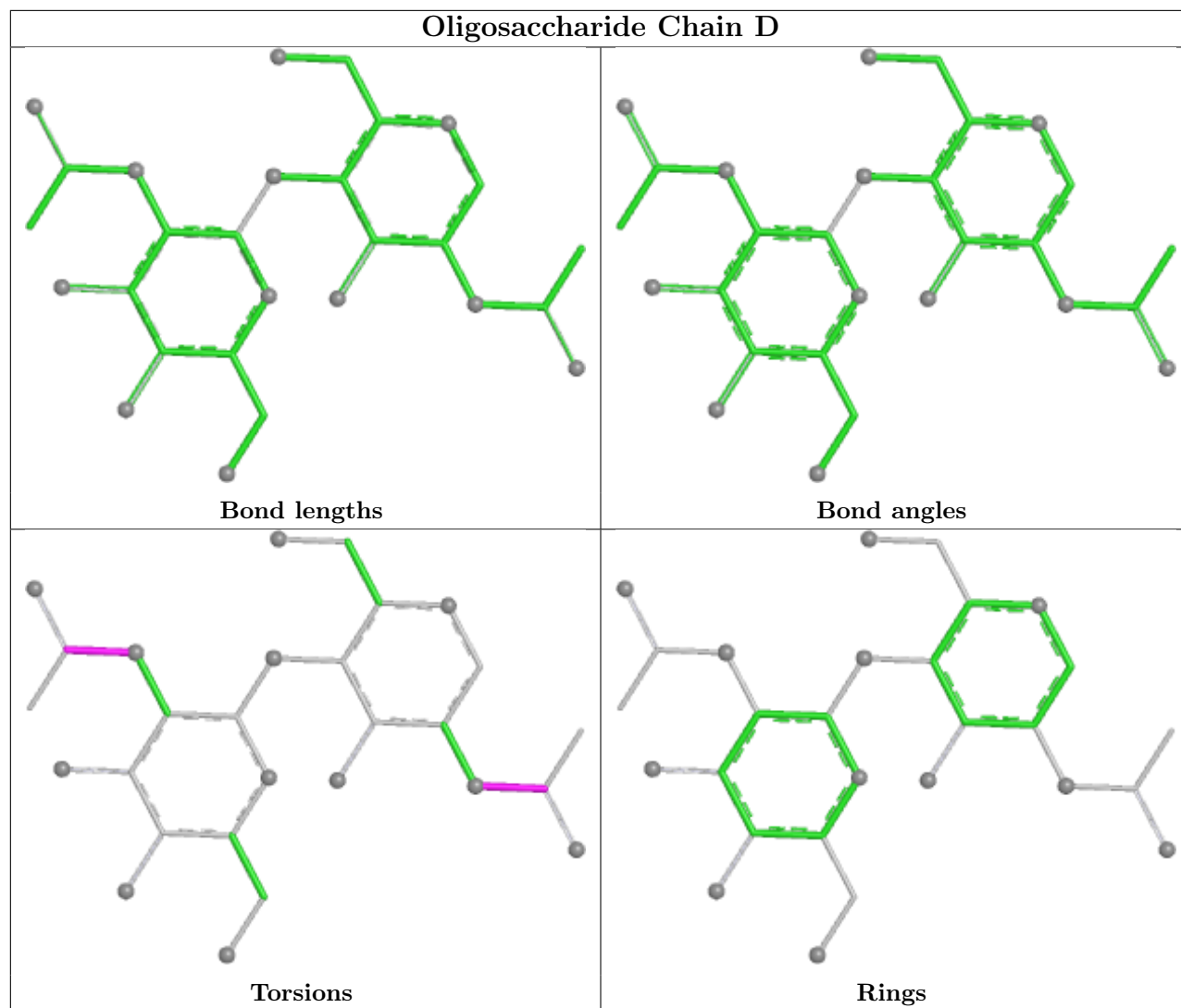
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2

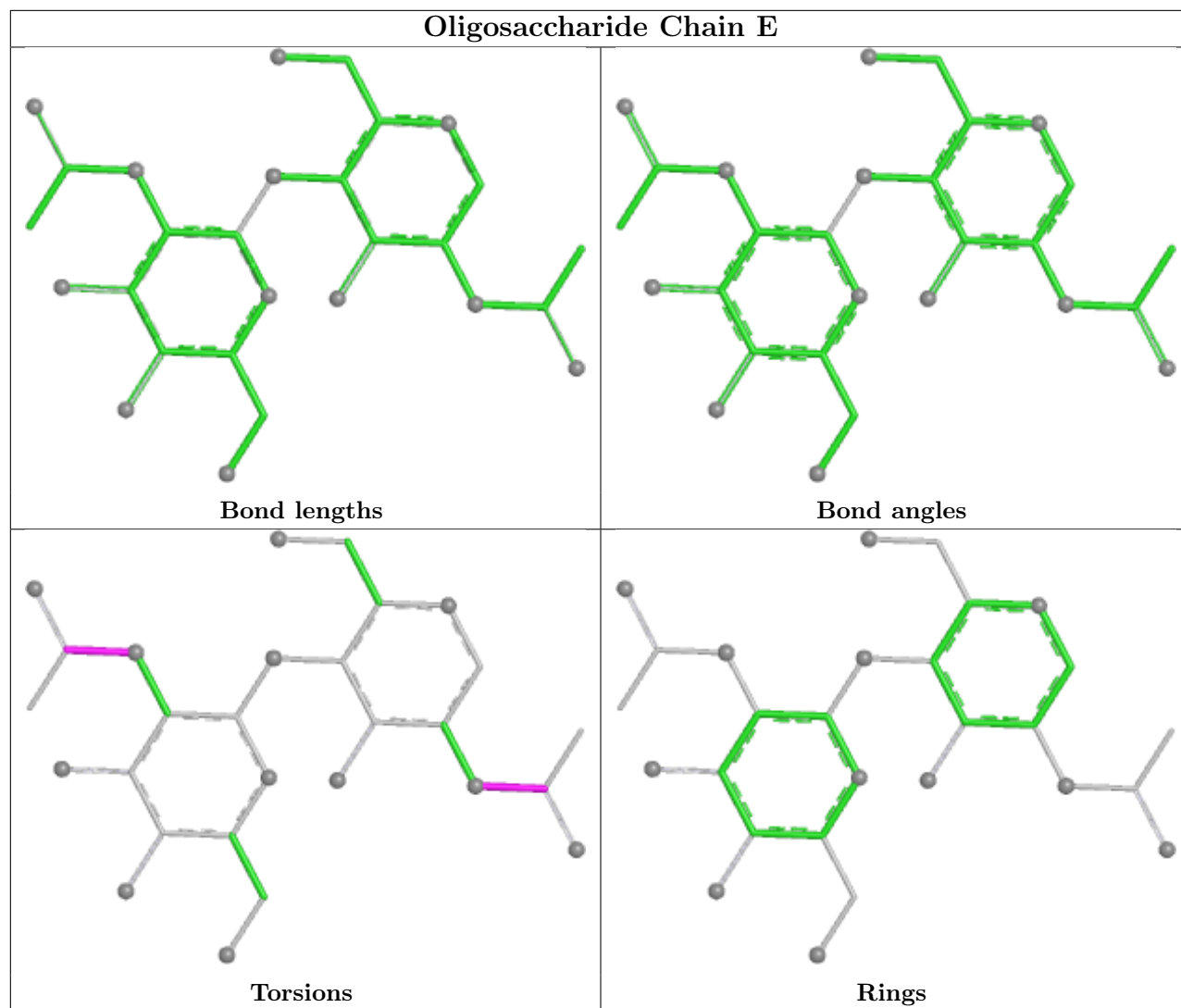
There are no ring outliers.

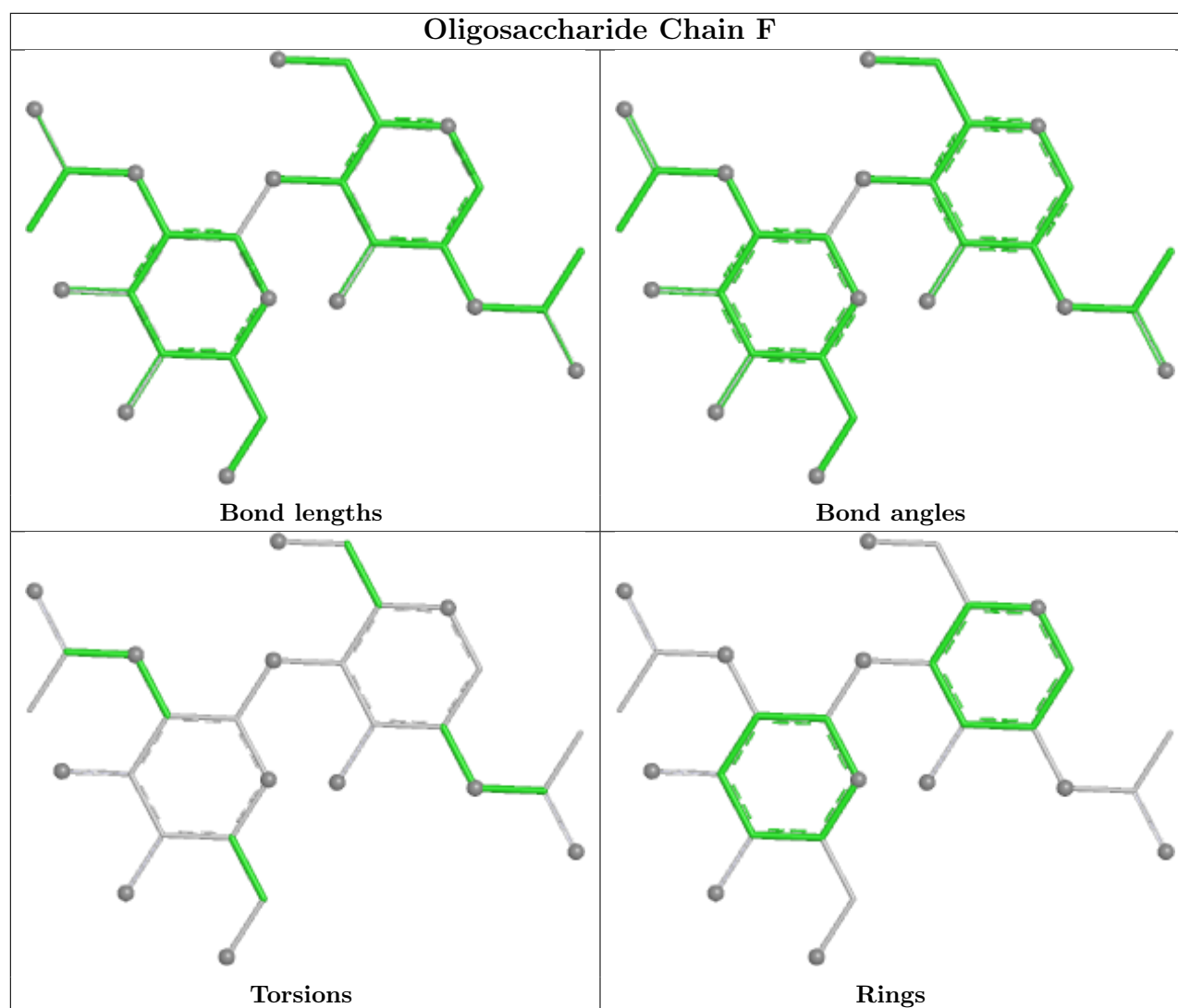
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	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 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\# Z > 2$
3	NAG	A	700	1	14,14,15	0.51	0	17,19,21	0.62	0
3	NAG	C	700	1	14,14,15	0.52	0	17,19,21	0.60	0
3	NAG	C	600	1	14,14,15	0.50	0	17,19,21	0.74	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
3	NAG	A	700	1	-	0/6/23/26	0/1/1/1
3	NAG	C	700	1	-	0/6/23/26	0/1/1/1
3	NAG	C	600	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	600	NAG	C8-C7-N2-C2
3	C	600	NAG	O7-C7-N2-C2

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	396/459 (86%)	0.47	51 (12%) 7 6	27, 51, 149, 229	0
1	B	397/459 (86%)	0.50	63 (15%) 5 4	26, 50, 177, 233	0
1	C	401/459 (87%)	0.45	52 (12%) 7 5	27, 51, 142, 216	0
All	All	1194/1377 (86%)	0.47	166 (13%) 6 5	26, 51, 156, 233	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	294	THR	6.3
1	C	300	PHE	6.0
1	C	45	VAL	5.8
1	C	449	VAL	5.4
1	A	236	GLU	5.3
1	B	300	PHE	5.1
1	B	132	ASP	5.1
1	B	301	TYR	4.8
1	C	434	ILE	4.8
1	C	70	PHE	4.8
1	B	293	ALA	4.8
1	A	301	TYR	4.8
1	B	133	GLU	4.7
1	B	299	GLU	4.7
1	B	134	LYS	4.7
1	C	66	ILE	4.6
1	A	294	THR	4.5
1	B	59	ALA	4.5
1	B	137	GLU	4.4
1	C	450	LEU	4.3
1	A	70	PHE	4.3
1	C	49	LEU	4.2
1	C	447	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	302	ASP	4.0
1	B	85	ARG	4.0
1	A	446	ILE	4.0
1	B	452	LEU	4.0
1	A	51	PHE	4.0
1	C	202	GLN	4.0
1	B	127	ASP	3.9
1	A	150	PRO	3.9
1	B	207	ARG	3.9
1	A	128	THR	3.8
1	A	293	ALA	3.8
1	B	444	ALA	3.8
1	A	60	LEU	3.8
1	B	55	LEU	3.8
1	C	127	ASP	3.7
1	C	72	TYR	3.7
1	B	53	GLY	3.7
1	B	65	ARG	3.7
1	B	450	LEU	3.7
1	C	51	PHE	3.7
1	B	358	GLU	3.7
1	C	55	LEU	3.6
1	C	57	LEU	3.6
1	B	442	ILE	3.6
1	B	446	ILE	3.6
1	B	71	LEU	3.6
1	C	293	ALA	3.6
1	A	449	VAL	3.6
1	B	290	ASP	3.5
1	B	62	CYS	3.5
1	B	57	LEU	3.5
1	B	66	ILE	3.5
1	B	449	VAL	3.5
1	C	445	SER	3.4
1	B	436	GLY	3.4
1	B	70	PHE	3.4
1	A	130	THR	3.3
1	C	294	THR	3.3
1	B	438	MET	3.3
1	A	203	ASP	3.3
1	A	50	CYS	3.3
1	B	138	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	52	MET	3.2
1	B	205	LYS	3.2
1	C	343	GLU	3.2
1	C	128	THR	3.2
1	C	444	ALA	3.2
1	A	391	LYS	3.1
1	A	49	LEU	3.1
1	A	204	GLY	3.1
1	C	439	GLY	3.1
1	C	47	TRP	3.1
1	C	301	TYR	3.1
1	B	64	ASN	3.1
1	B	204	GLY	3.0
1	C	448	THR	3.0
1	C	121	ASN	3.0
1	B	440	LEU	3.0
1	A	66	ILE	2.9
1	A	149	LYS	2.9
1	A	146	ARG	2.9
1	B	72	TYR	2.9
1	C	130	THR	2.9
1	A	147	ASN	2.9
1	A	440	LEU	2.8
1	C	71	LEU	2.8
1	B	433	ASP	2.8
1	B	146	ARG	2.8
1	A	151	LYS	2.8
1	C	238	ASP	2.8
1	B	131	ALA	2.8
1	C	48	ALA	2.8
1	C	443	GLY	2.7
1	B	149	LYS	2.7
1	C	426	GLU	2.7
1	C	203	ASP	2.7
1	A	137	GLU	2.7
1	C	52	MET	2.6
1	A	443	GLY	2.6
1	C	204	GLY	2.6
1	A	54	SER	2.6
1	A	143	ALA	2.6
1	A	148	PHE	2.6
1	B	448	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	431	LEU	2.6
1	A	110	TYR	2.6
1	C	192	TYR	2.6
1	A	53	GLY	2.6
1	B	135	GLN	2.6
1	C	239	GLU	2.5
1	B	432	GLY	2.5
1	C	237	THR	2.5
1	A	153	PHE	2.5
1	C	67	GLN	2.5
1	B	61	VAL	2.5
1	C	64	ASN	2.5
1	C	54	SER	2.5
1	A	444	ALA	2.5
1	A	127	ASP	2.4
1	A	142	LYS	2.4
1	B	379	LYS	2.4
1	B	383	LYS	2.4
1	C	205	LYS	2.4
1	A	134	LYS	2.4
1	B	129	GLN	2.4
1	B	437	GLN	2.4
1	A	302	ASP	2.3
1	C	149	LYS	2.3
1	A	48	ALA	2.3
1	C	358	GLU	2.3
1	B	141	ASP	2.3
1	A	64	ASN	2.3
1	B	58	LEU	2.3
1	B	60	LEU	2.3
1	C	59	ALA	2.3
1	C	425	TYR	2.3
1	A	332	ASP	2.3
1	B	73	PRO	2.3
1	B	428	ALA	2.2
1	B	128	THR	2.2
1	C	154	ASN	2.2
1	A	428	ALA	2.2
1	C	433	ASP	2.2
1	C	146	ARG	2.2
1	A	71	LEU	2.2
1	B	130	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	152	PRO	2.1
1	B	147	ASN	2.1
1	A	442	ILE	2.1
1	B	441	PHE	2.1
1	A	207	ARG	2.1
1	A	438	MET	2.1
1	A	434	ILE	2.1
1	A	290	ASP	2.1
1	B	56	ALA	2.1
1	C	428	ALA	2.1
1	A	431	LEU	2.1
1	C	438	MET	2.0
1	B	179	GLN	2.0
1	B	202	GLN	2.0
1	C	429	GLY	2.0
1	A	133	GLU	2.0
1	A	85	ARG	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](#)

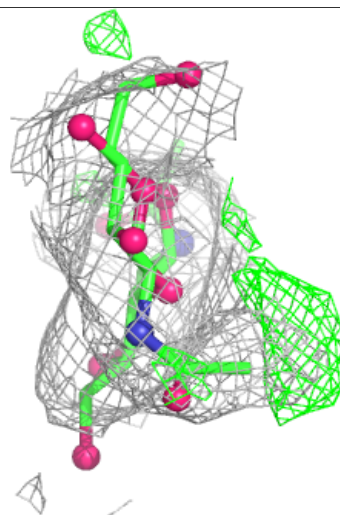
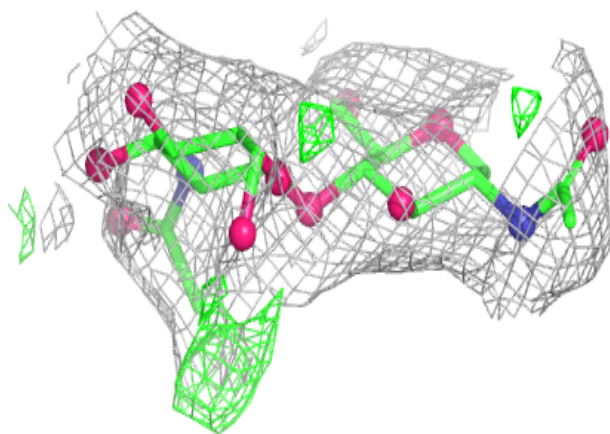
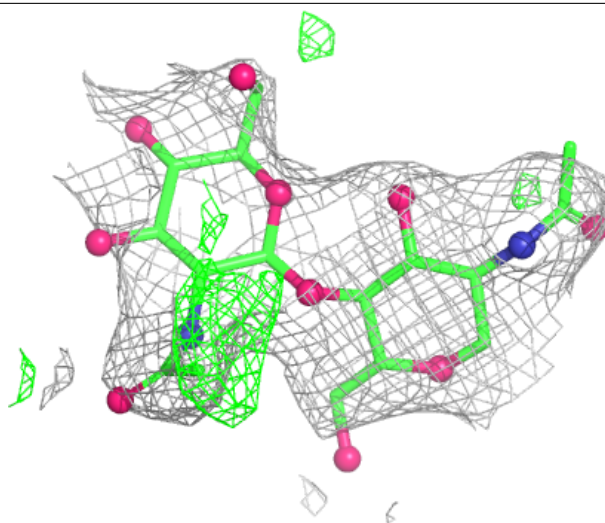
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	D	2	14/15	0.59	0.21	96,136,147,162	0
2	NAG	E	2	14/15	0.70	0.22	93,138,147,164	0
2	NAG	F	2	14/15	0.71	0.16	114,155,167,169	0
2	NAG	F	1	14/15	0.74	0.15	100,121,134,150	0
2	NAG	D	1	14/15	0.89	0.15	58,73,103,106	0
2	NAG	E	1	14/15	0.91	0.11	61,71,101,104	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.

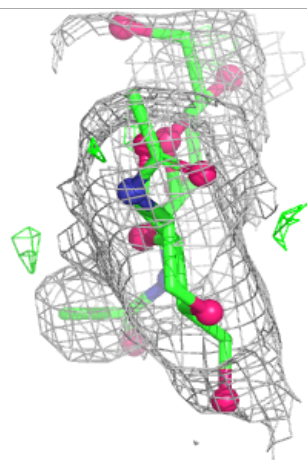
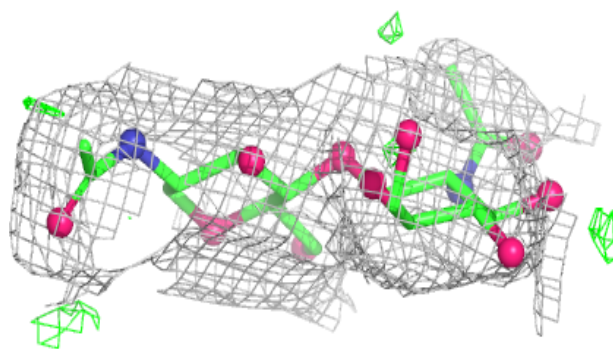
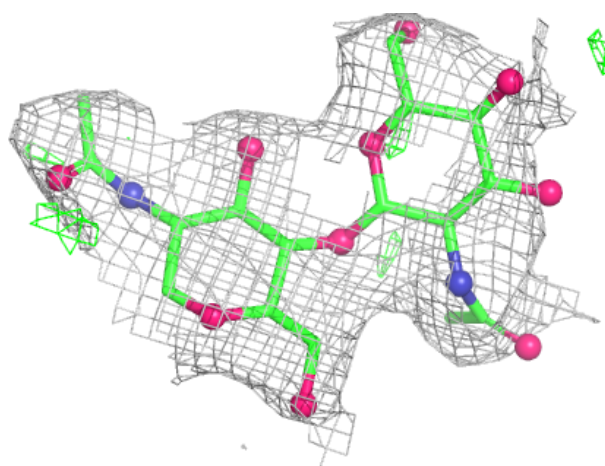
Electron density around Chain D:

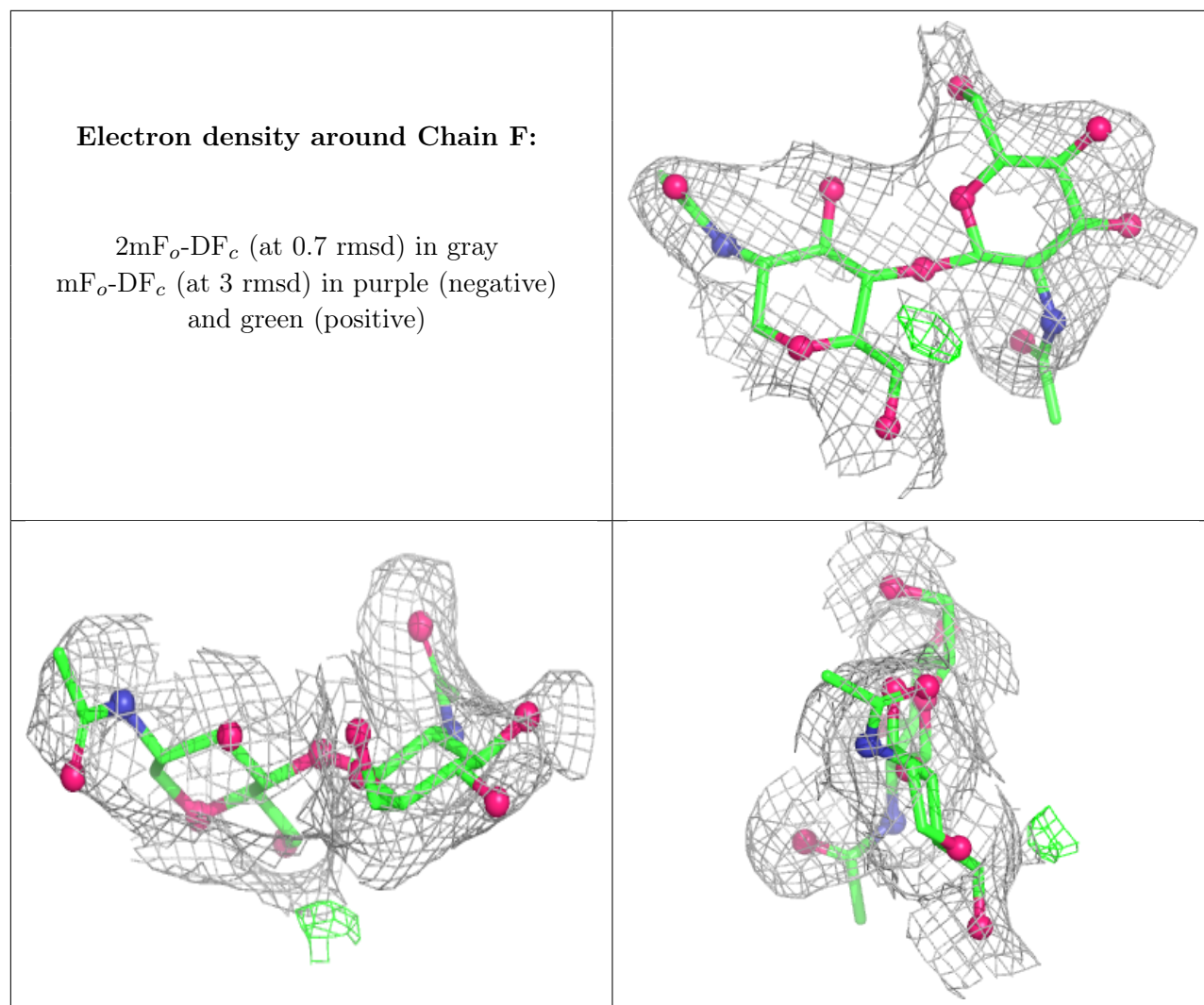
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain E:

$2mF_o-DF_c$ (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
3	NAG	C	700	14/15	0.42	0.20	102,121,137,154	0
3	NAG	A	700	14/15	0.70	0.18	103,120,135,151	0
3	NAG	C	600	14/15	0.76	0.17	69,77,103,106	0
4	CL	B	464	1/1	0.98	0.11	51,51,51,51	0
4	CL	C	464	1/1	0.98	0.06	55,55,55,55	0
4	CL	A	464	1/1	0.99	0.05	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.