WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 20, 2023 – 10:03 PM JST

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PDB ID	:	7DMU
Title	:	Structure of SARS-CoV-2 spike receptor-binding domain complexed with high affinity ACE2 mutant 3N39
Authors	:	Arimori, T.; Takagi, J.
Deposited on	:	2020-12-07
Resolution	:	3.20 Å(reported)

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.
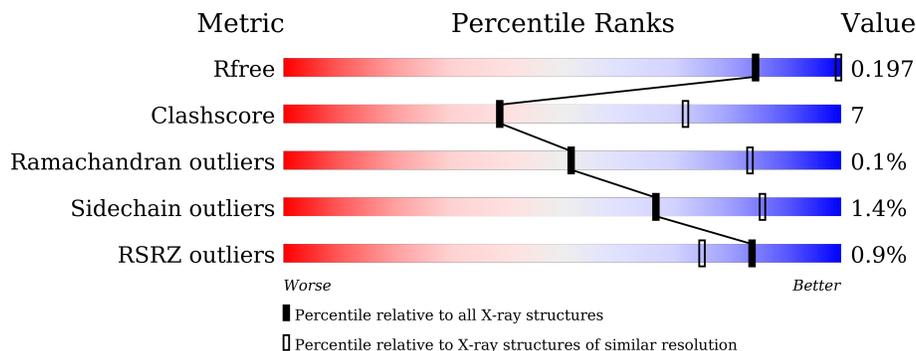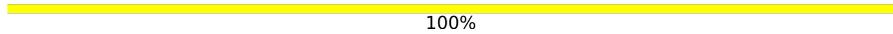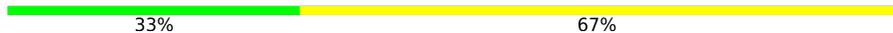

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 <=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	606	80% ... 18% .
1	C	606	% / 81% ... 18% .
2	B	218	3% / 74% ... 15% ... 10%
2	D	218	% / 72% ... 17% ... 11%
3	E	5	100%
4	F	2	50% ... 50%

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Mol	Chain	Length	Quality of chain
4	G	2	50% 50%
4	K	2	100%
4	M	2	50% 50%
5	H	5	20% 80%
5	J	5	20% 80%
5	L	5	20% 80%
6	I	3	33% 67%

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
5	MAN	H	5	-	-	-	X

2 Entry composition ⓘ

There are 10 unique types of molecules in this entry. The entry contains 13306 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total 4876	C 3122	N 806	O 919	S 29	0	0	0
1	C	598	Total 4885	C 3127	N 808	O 921	S 29	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	VAL	ALA	engineered mutation	UNP Q9BYF1
A	26	GLU	LYS	engineered mutation	UNP Q9BYF1
A	31	ASN	LYS	engineered mutation	UNP Q9BYF1
A	35	LYS	GLU	engineered mutation	UNP Q9BYF1
A	64	ILE	ASN	engineered mutation	UNP Q9BYF1
A	79	PHE	LEU	engineered mutation	UNP Q9BYF1
A	90	HIS	ASN	engineered mutation	UNP Q9BYF1
A	616	SER	-	expression tag	UNP Q9BYF1
A	617	SER	-	expression tag	UNP Q9BYF1
A	618	HIS	-	expression tag	UNP Q9BYF1
A	619	HIS	-	expression tag	UNP Q9BYF1
A	620	HIS	-	expression tag	UNP Q9BYF1
A	621	HIS	-	expression tag	UNP Q9BYF1
A	622	HIS	-	expression tag	UNP Q9BYF1
A	623	HIS	-	expression tag	UNP Q9BYF1
C	25	VAL	ALA	engineered mutation	UNP Q9BYF1
C	26	GLU	LYS	engineered mutation	UNP Q9BYF1
C	31	ASN	LYS	engineered mutation	UNP Q9BYF1
C	35	LYS	GLU	engineered mutation	UNP Q9BYF1
C	64	ILE	ASN	engineered mutation	UNP Q9BYF1
C	79	PHE	LEU	engineered mutation	UNP Q9BYF1
C	90	HIS	ASN	engineered mutation	UNP Q9BYF1
C	616	SER	-	expression tag	UNP Q9BYF1
C	617	SER	-	expression tag	UNP Q9BYF1
C	618	HIS	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	619	HIS	-	expression tag	UNP Q9BYF1
C	620	HIS	-	expression tag	UNP Q9BYF1
C	621	HIS	-	expression tag	UNP Q9BYF1
C	622	HIS	-	expression tag	UNP Q9BYF1
C	623	HIS	-	expression tag	UNP Q9BYF1

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	196	Total 1551	C 995	N 258	O 290	S 8	0	0	0
2	D	195	Total 1543	C 989	N 257	O 289	S 8	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	532	GLY	-	expression tag	UNP P0DTC2
B	533	THR	-	expression tag	UNP P0DTC2
B	534	LEU	-	expression tag	UNP P0DTC2
B	535	LEU	-	expression tag	UNP P0DTC2
B	536	GLY	-	expression tag	UNP P0DTC2
D	532	GLY	-	expression tag	UNP P0DTC2
D	533	THR	-	expression tag	UNP P0DTC2
D	534	LEU	-	expression tag	UNP P0DTC2
D	535	LEU	-	expression tag	UNP P0DTC2
D	536	GLY	-	expression tag	UNP P0DTC2

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyran ose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.
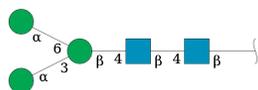

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total 61	C 34	N 2	O 25	0	0	0

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.
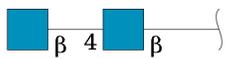
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total 28	C 16	N 2	O 10	0	0	0
4	G	2	Total 28	C 16	N 2	O 10	0	0	0
4	K	2	Total 28	C 16	N 2	O 10	0	0	0
4	M	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran ose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.
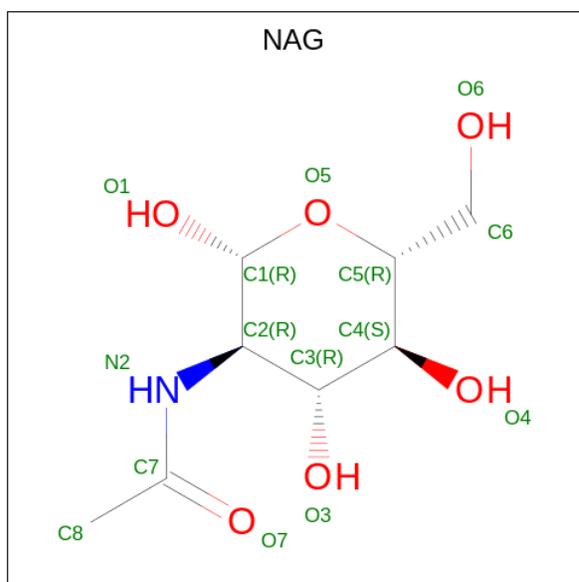
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	5	Total 61	C 34	N 2	O 25	0	0	0
5	J	5	Total 61	C 34	N 2	O 25	0	0	0
5	L	5	Total 61	C 34	N 2	O 25	0	0	0

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	3	Total 39	C 22	N 2	O 15	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total 1	Zn 1	0	0
8	C	1	Total 1	Zn 1	0	0

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O

O3 O⁻ — S — O⁻ O4

S

O

O2
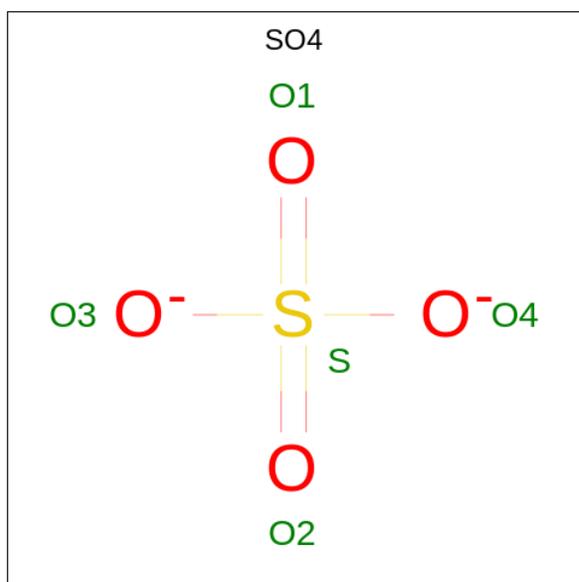
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total 5	O 4	S 1	0	0
9	C	1	Total 5	O 4	S 1	0	0

• Molecule 10 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total 1	O 1	0	0
10	C	1	Total 1	O 1	0	0

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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.

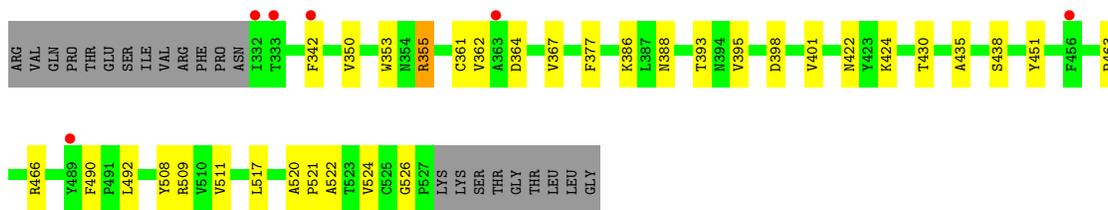• Molecule 1: Angiotensin-converting enzyme 2
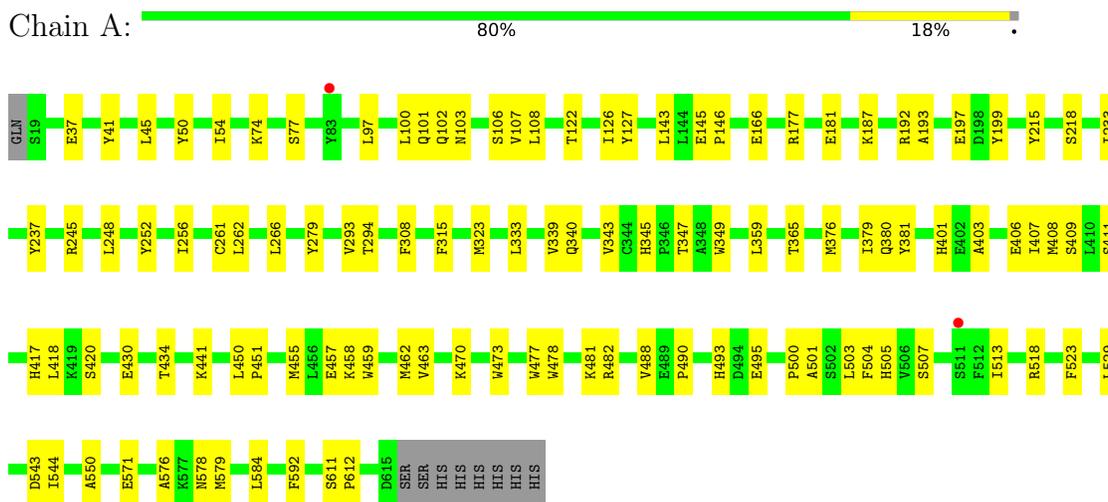
• Molecule 1: Angiotensin-converting enzyme 2
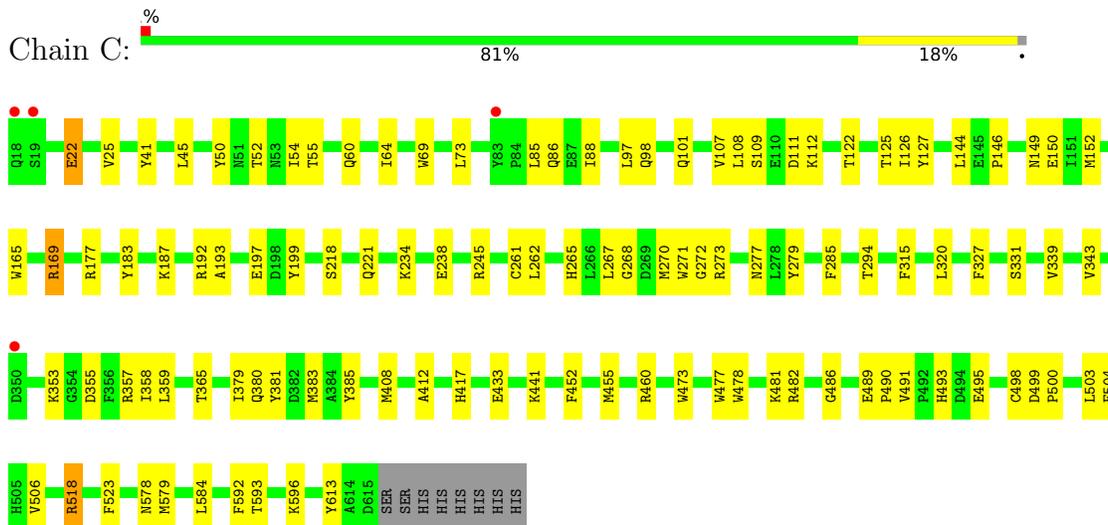
• Molecule 2: Spike protein S1

• Molecule 2: Spike protein S1

Chain D:

• Molecule 3: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyrano
se-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra
nose

Chain E:

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

Chain F:

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

Chain G:

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

Chain K:

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

Chain M:

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

Chain H:

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

Chain J:

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

Chain L:

• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	227.80Å 227.80Å 147.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.91 – 3.20 48.13 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.91-3.20) 99.9 (48.13-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.179 , 0.198 0.179 , 0.197	Depositor DCC
R_{free} test set	6193 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	133.8	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 88.9	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.056 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13306	wwPDB-VP
Average B, all atoms (Å^2)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality   ⓘ

5.1   Standard geometry   ⓘ

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

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	0.39	0/5015	0.54	0/6815
1	C	0.39	0/5024	0.56	2/6827 (0.0%)
2	B	0.41	0/1595	0.57	0/2172
2	D	0.37	0/1587	0.56	0/2161
All	All	0.39	0/13221	0.55	2/17975 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	169	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	C	518	ARG	NE-CZ-NH1	-5.55	117.53	120.30

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	4876	0	4639	68	0
1	C	4885	0	4647	72	0
2	B	1551	0	1470	24	0
2	D	1543	0	1459	26	0
3	E	61	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	28	0	25	2	0
4	G	28	0	25	1	0
4	K	28	0	25	1	0
4	M	28	0	25	1	0
5	H	61	0	52	0	0
5	J	61	0	52	2	0
5	L	61	0	52	0	0
6	I	39	0	34	0	0
7	A	14	0	13	0	0
7	C	28	0	26	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
9	A	5	0	0	0	0
9	C	5	0	0	0	0
10	A	1	0	0	0	0
10	C	1	0	0	0	0
All	All	13306	0	12596	193	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 7.

The worst 5 of 193 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:355:ASP:OD2	1:C:357:ARG:NH1	2.19	0.73
2:D:353:TRP:O	2:D:466:ARG:NH1	2.24	0.71
1:C:109:SER:HB3	1:C:112:LYS:HD2	1.74	0.70
1:A:347:THR:HG1	1:A:349:TRP:HE1	1.37	0.69
1:A:411:SER:HB3	1:A:543:ASP:HA	1.72	0.69

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	595/606 (98%)	574 (96%)	21 (4%)	0	100	100
1	C	596/606 (98%)	577 (97%)	18 (3%)	1 (0%)	47	79
2	B	194/218 (89%)	185 (95%)	9 (5%)	0	100	100
2	D	193/218 (88%)	184 (95%)	9 (5%)	0	100	100
All	All	1578/1648 (96%)	1520 (96%)	57 (4%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	339	VAL

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	528/537 (98%)	522 (99%)	6 (1%)	73	88
1	C	529/537 (98%)	520 (98%)	9 (2%)	60	83
2	B	169/189 (89%)	167 (99%)	2 (1%)	71	88
2	D	168/189 (89%)	165 (98%)	3 (2%)	59	82
All	All	1394/1452 (96%)	1374 (99%)	20 (1%)	67	86

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	518	ARG
2	D	369	TYR
2	D	387	LEU
2	D	377	PHE
2	B	355	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	C	535	HIS
2	D	506	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 ⓘ

31 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	#$|Z| > 2$
3	NAG	E	1	3,1	14,14,15	0.61	1 (7%)	17,19,21	0.50	0
3	NAG	E	2	3	14,14,15	0.96	1 (7%)	17,19,21	0.67	0
3	BMA	E	3	3	11,11,12	0.80	0	15,15,17	1.05	1 (6%)
3	MAN	E	4	3	11,11,12	1.37	1 (9%)	15,15,17	1.68	5 (33%)
3	MAN	E	5	3	11,11,12	0.88	0	15,15,17	1.48	3 (20%)
4	NAG	F	1	4,1	14,14,15	0.57	1 (7%)	17,19,21	0.55	0
4	NAG	F	2	4	14,14,15	0.55	0	17,19,21	0.81	0
4	NAG	G	1	4,1	14,14,15	0.38	0	17,19,21	0.46	0
4	NAG	G	2	4	14,14,15	0.61	0	17,19,21	1.33	2 (11%)
5	NAG	H	1	1,5	14,14,15	0.42	0	17,19,21	0.73	1 (5%)
5	NAG	H	2	5	14,14,15	0.36	0	17,19,21	0.62	0
5	BMA	H	3	5	11,11,12	1.85	2 (18%)	15,15,17	1.61	4 (26%)
5	MAN	H	4	5	11,11,12	1.53	2 (18%)	15,15,17	1.67	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|>2$	Counts	RMSZ	#$\|Z\|>2$
5	MAN	H	5	5	11,11,12	1.89	3 (27%)	15,15,17	2.18	3 (20%)
6	NAG	I	1	6,2	14,14,15	0.30	0	17,19,21	0.70	1 (5%)
6	NAG	I	2	6	14,14,15	0.29	0	17,19,21	0.48	0
6	BMA	I	3	6	11,11,12	1.21	1 (9%)	15,15,17	1.41	2 (13%)
5	NAG	J	1	1,5	14,14,15	0.57	0	17,19,21	0.74	0
5	NAG	J	2	5	14,14,15	0.52	0	17,19,21	0.59	0
5	BMA	J	3	5	11,11,12	0.96	0	15,15,17	1.83	4 (26%)
5	MAN	J	4	5	11,11,12	1.59	3 (27%)	15,15,17	2.11	4 (26%)
5	MAN	J	5	5	11,11,12	1.49	2 (18%)	15,15,17	1.64	3 (20%)
4	NAG	K	1	4,1	14,14,15	0.36	0	17,19,21	0.49	0
4	NAG	K	2	4	14,14,15	0.37	0	17,19,21	0.41	0
5	NAG	L	1	1,5	14,14,15	0.24	0	17,19,21	0.61	0
5	NAG	L	2	5	14,14,15	0.69	1 (7%)	17,19,21	0.62	0
5	BMA	L	3	5	11,11,12	0.75	0	15,15,17	1.06	1 (6%)
5	MAN	L	4	5	11,11,12	1.26	2 (18%)	15,15,17	1.26	1 (6%)
5	MAN	L	5	5	11,11,12	1.23	1 (9%)	15,15,17	0.88	1 (6%)
4	NAG	M	1	2,4	14,14,15	0.28	0	17,19,21	0.88	1 (5%)
4	NAG	M	2	4	14,14,15	0.63	0	17,19,21	1.22	1 (5%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	H	5	5	-	1/2/19/22	0/1/1/1
6	NAG	I	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1
6	BMA	I	3	6	-	1/2/19/22	0/1/1/1
5	NAG	J	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	1/6/23/26	0/1/1/1
5	BMA	J	3	5	-	1/2/19/22	0/1/1/1
5	MAN	J	4	5	-	2/2/19/22	0/1/1/1
5	MAN	J	5	5	-	1/2/19/22	0/1/1/1
4	NAG	K	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
5	NAG	L	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	L	2	5	-	1/6/23/26	0/1/1/1
5	BMA	L	3	5	-	0/2/19/22	0/1/1/1
5	MAN	L	4	5	-	1/2/19/22	1/1/1/1
5	MAN	L	5	5	-	1/2/19/22	0/1/1/1
4	NAG	M	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	5/6/23/26	0/1/1/1

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	3	BMA	C1-C2	4.72	1.63	1.52
5	H	5	MAN	C4-C5	4.12	1.61	1.53
3	E	2	NAG	O5-C1	-3.43	1.38	1.43
5	H	5	MAN	O5-C1	-3.36	1.38	1.43
5	J	5	MAN	C2-C3	3.22	1.57	1.52

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	5	MAN	C1-C2-C3	-6.85	101.25	109.67
5	J	4	MAN	C1-O5-C5	6.16	120.54	112.19
5	H	4	MAN	C1-O5-C5	5.10	119.11	112.19
4	G	2	NAG	C2-N2-C7	4.52	129.33	122.90
4	M	2	NAG	C2-N2-C7	4.37	129.13	122.90

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	2	NAG	C1-C2-N2-C7
5	J	1	NAG	C1-C2-N2-C7
5	H	4	MAN	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	4	MAN	C1-C2-C3-C4-C5-O5
5	L	4	MAN	C1-C2-C3-C4-C5-O5

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1	NAG	1	0
4	K	2	NAG	1	0
5	J	1	NAG	2	0
4	F	2	NAG	1	0
4	F	1	NAG	1	0
4	G	2	NAG	1	0
4	M	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.

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain K

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain M

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain J

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain L

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\#|Z| > 2$
7	NAG	C	802	1	14,14,15	0.39	0	17,19,21	0.49	0
7	NAG	C	801	1	14,14,15	1.05	2 (14%)	17,19,21	0.46	0
9	SO4	A	1003	-	4,4,4	0.17	0	6,6,6	0.36	0
9	SO4	C	804	-	4,4,4	0.12	0	6,6,6	0.25	0
7	NAG	A	1001	1	14,14,15	1.45	1 (7%)	17,19,21	1.27	2 (11%)

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
7	NAG	C	802	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1001	1	-	3/6/23/26	0/1/1/1
7	NAG	C	801	1	-	3/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1001	NAG	C1-C2	4.56	1.59	1.52
7	C	801	NAG	C1-C2	2.93	1.56	1.52
7	C	801	NAG	O5-C1	2.38	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1001	NAG	C4-C3-C2	3.71	116.46	111.02
7	A	1001	NAG	O5-C5-C4	-2.61	104.48	110.83

There are no chirality outliers.

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PROTEIN DATA BANK

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	802	NAG	O5-C5-C6-O6
7	A	1001	NAG	C8-C7-N2-C2
7	A	1001	NAG	O7-C7-N2-C2
7	C	802	NAG	C4-C5-C6-O6
7	C	801	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	597/606 (98%)	-0.12	2 (0%)	94	92	96, 126, 165, 201	0
1	C	598/606 (98%)	-0.11	4 (0%)	87	81	99, 126, 166, 207	0
2	B	196/218 (89%)	0.00	6 (3%)	49	32	110, 139, 182, 222	0
2	D	195/218 (89%)	-0.06	2 (1%)	82	72	105, 138, 179, 225	0
All	All	1586/1648 (96%)	-0.09	14 (0%)	84	75	96, 129, 171, 225	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	18	GLN	4.4
2	D	423	TYR	2.8
2	B	342	PHE	2.5
1	C	83	TYR	2.5
2	B	456	PHE	2.5

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

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

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
5	BMA	J	3	11/12	0.65	0.26	209,267,286,301	0
6	BMA	I	3	11/12	0.69	0.27	194,233,257,261	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
5	MAN	J	5	11/12	0.71	0.28	183,236,248,254	0
5	MAN	J	4	11/12	0.74	0.33	177,246,273,283	0
5	MAN	L	5	11/12	0.79	0.32	221,240,261,263	0
5	MAN	H	5	11/12	0.79	0.47	201,268,279,288	0
3	MAN	E	4	11/12	0.80	0.20	233,268,291,297	0
3	BMA	E	3	11/12	0.81	0.22	225,248,263,264	0
5	MAN	L	4	11/12	0.81	0.32	183,224,246,247	0
4	NAG	K	2	14/15	0.85	0.33	149,225,241,244	0
4	NAG	M	2	14/15	0.88	0.35	174,210,226,232	0
5	BMA	H	3	11/12	0.88	0.39	223,253,260,262	0
3	MAN	E	5	11/12	0.88	0.24	182,228,279,298	0
5	MAN	H	4	11/12	0.90	0.39	174,241,256,259	0
5	BMA	L	3	11/12	0.92	0.24	234,238,246,248	0
4	NAG	F	2	14/15	0.92	0.24	164,228,249,252	0
3	NAG	E	2	14/15	0.93	0.20	171,194,234,258	0
4	NAG	G	2	14/15	0.93	0.34	165,222,234,235	0
4	NAG	F	1	14/15	0.94	0.11	164,173,215,239	0
5	NAG	H	2	14/15	0.94	0.28	175,200,230,253	0
6	NAG	I	1	14/15	0.94	0.34	128,163,201,211	0
6	NAG	I	2	14/15	0.94	0.45	181,211,243,269	0
3	NAG	E	1	14/15	0.94	0.14	143,148,160,183	0
5	NAG	J	2	14/15	0.95	0.14	158,202,235,257	0
4	NAG	M	1	14/15	0.95	0.26	132,157,199,203	0
5	NAG	L	2	14/15	0.95	0.22	172,203,223,241	0
5	NAG	J	1	14/15	0.96	0.14	143,152,172,193	0
5	NAG	L	1	14/15	0.96	0.18	149,174,186,197	0
4	NAG	K	1	14/15	0.96	0.23	143,168,198,216	0
5	NAG	H	1	14/15	0.97	0.18	149,177,186,199	0
4	NAG	G	1	14/15	0.97	0.21	164,184,216,217	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 E:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
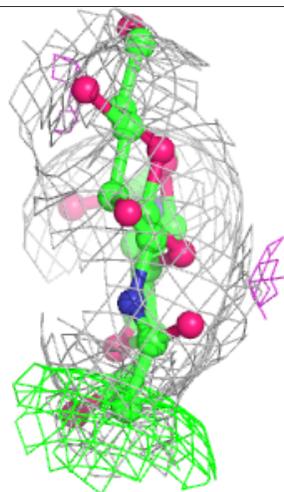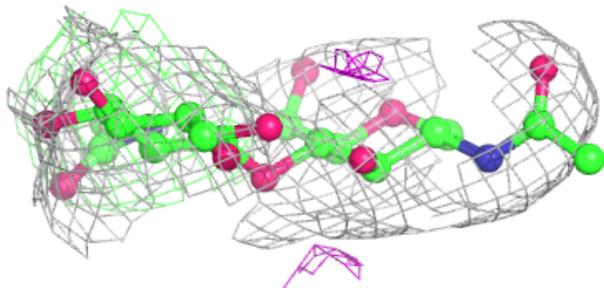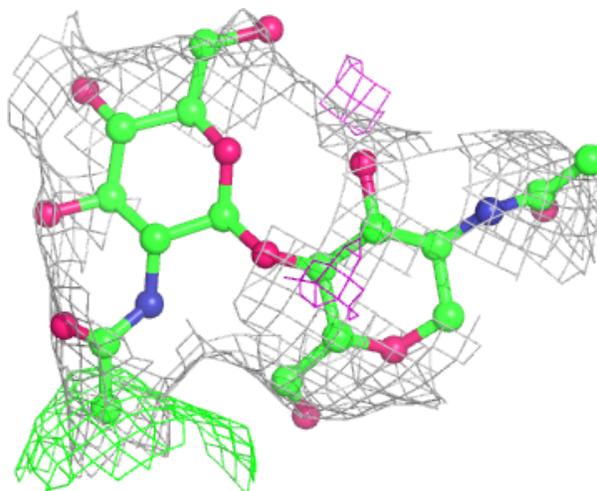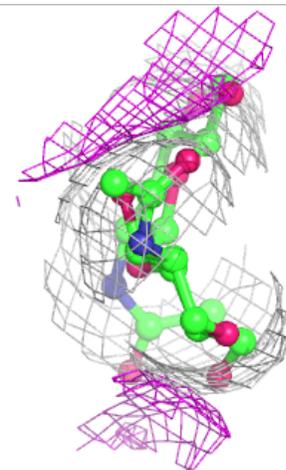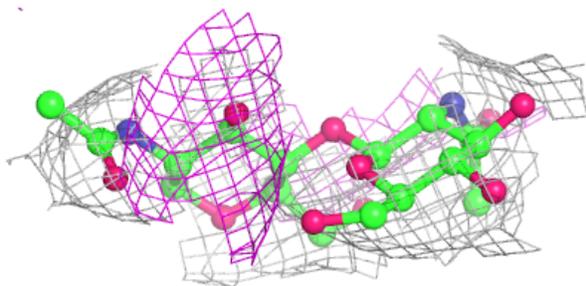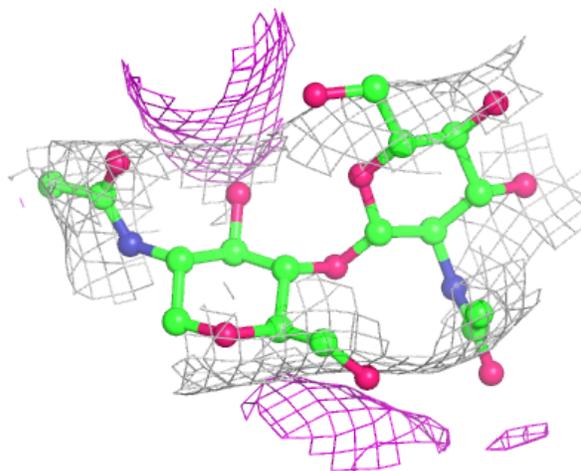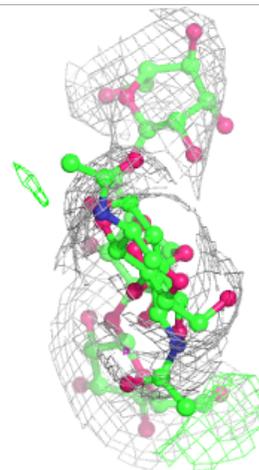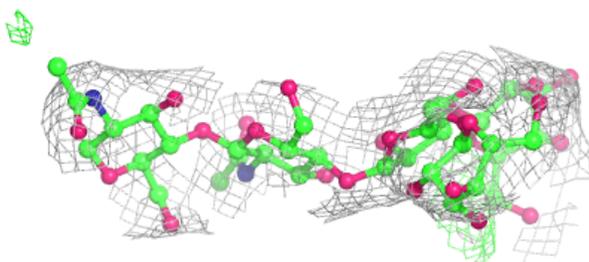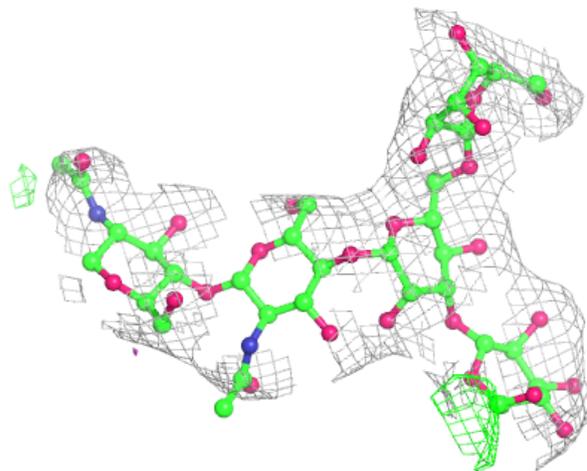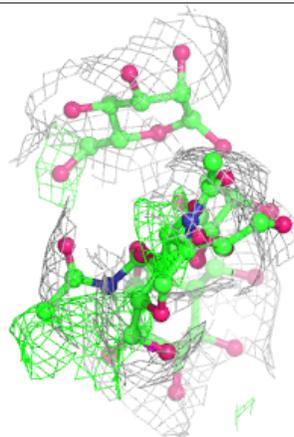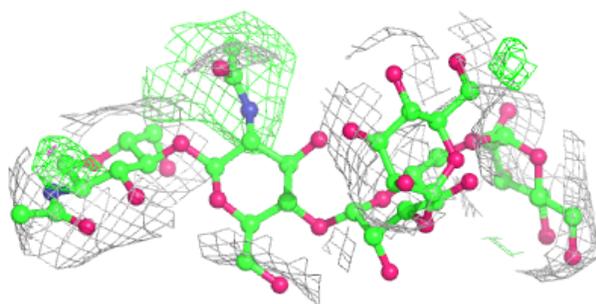and green (positive)
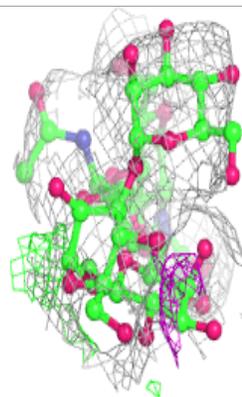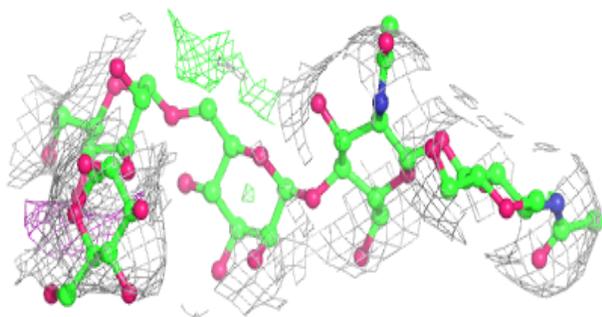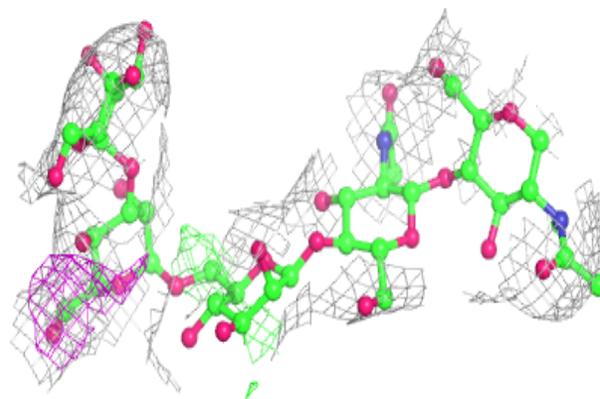
Electron density around Chain F:

$2mF_o$-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
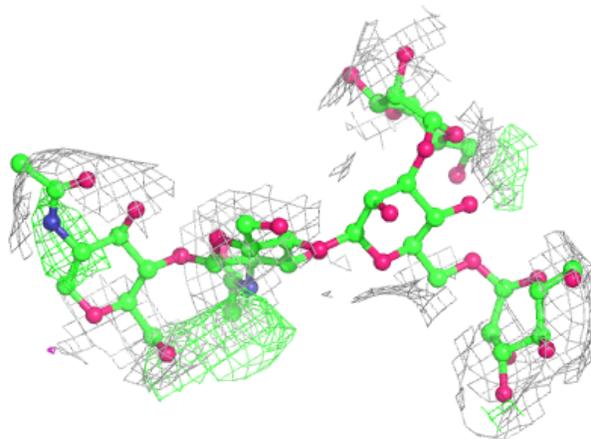mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
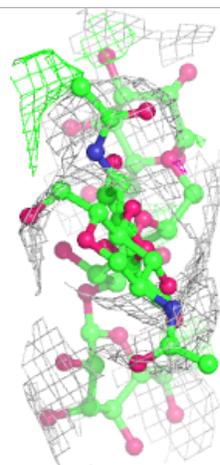and green (positive)
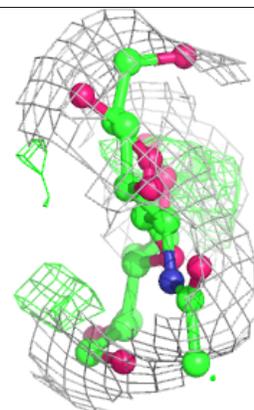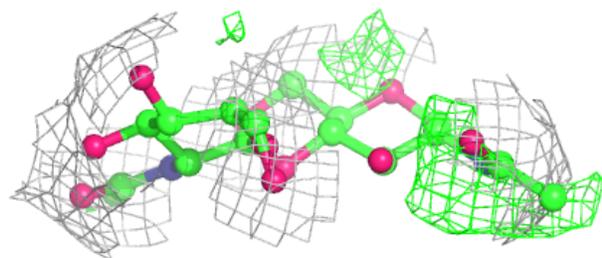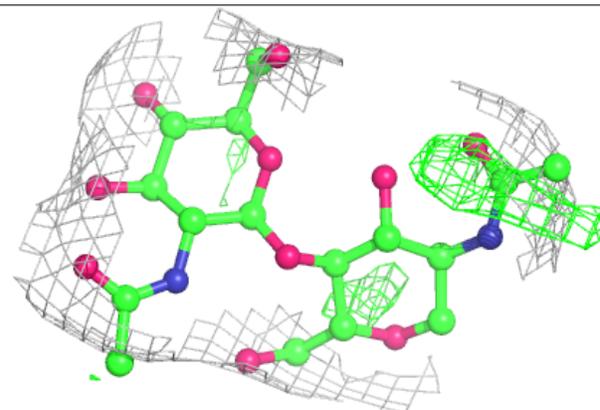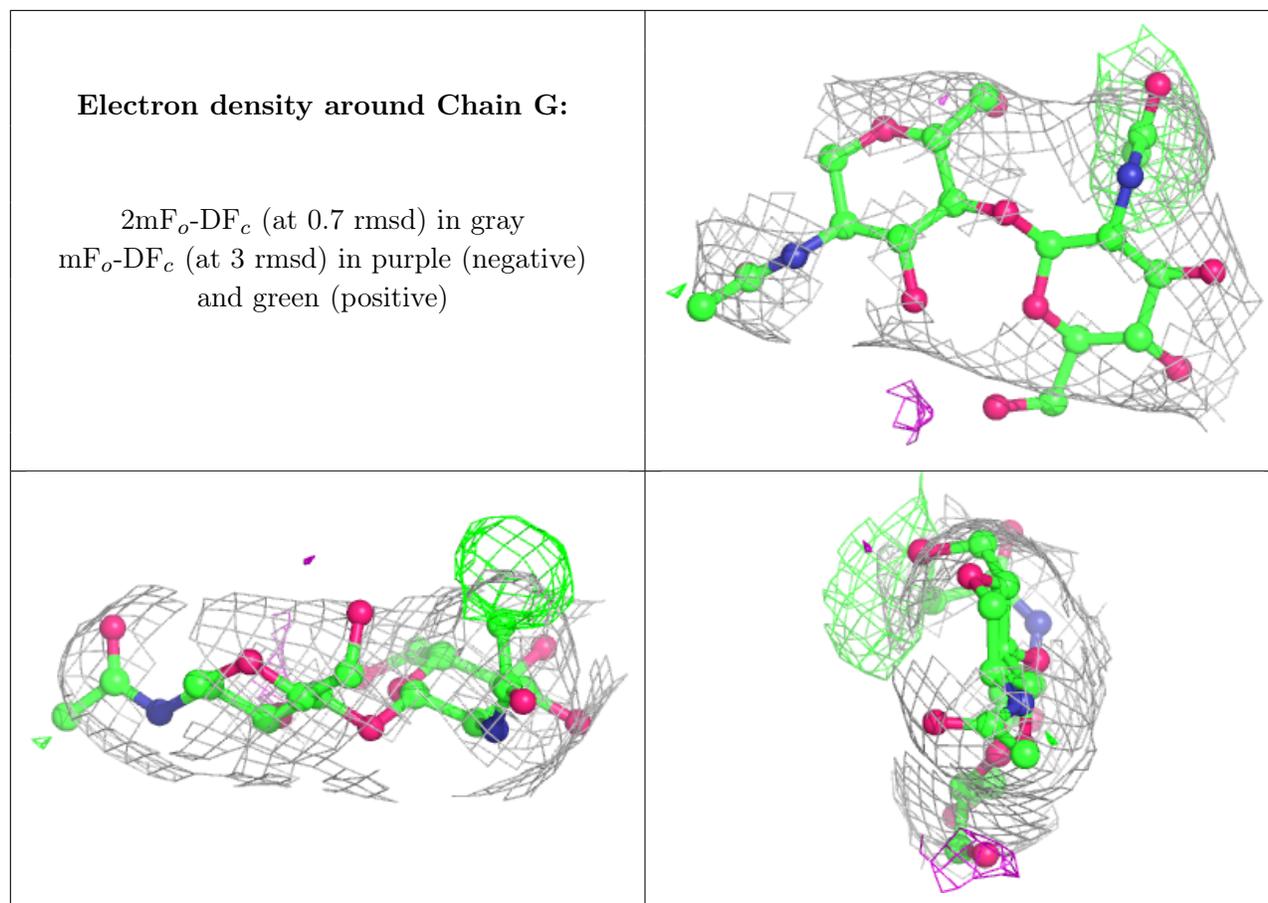
Electron density around Chain K:

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

Electron density around Chain M:

$2mF_o$-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:

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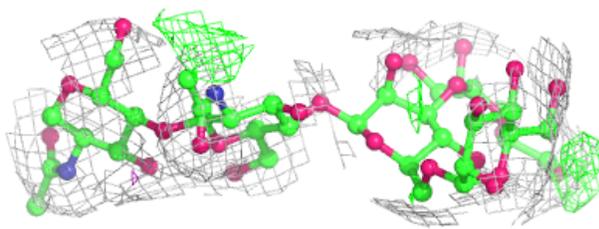and green (positive)

Electron density around Chain J:

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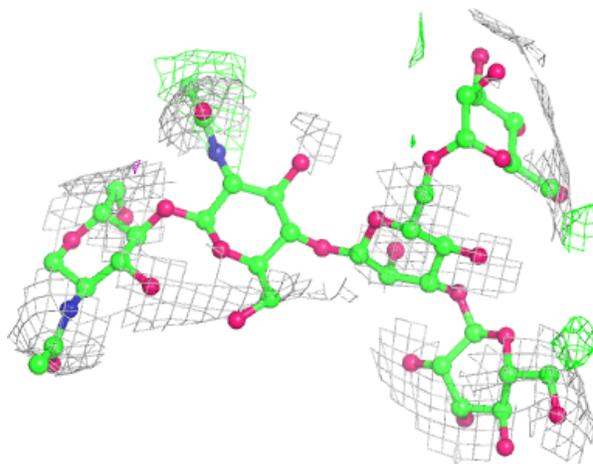and green (positive)

Electron density around Chain L:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
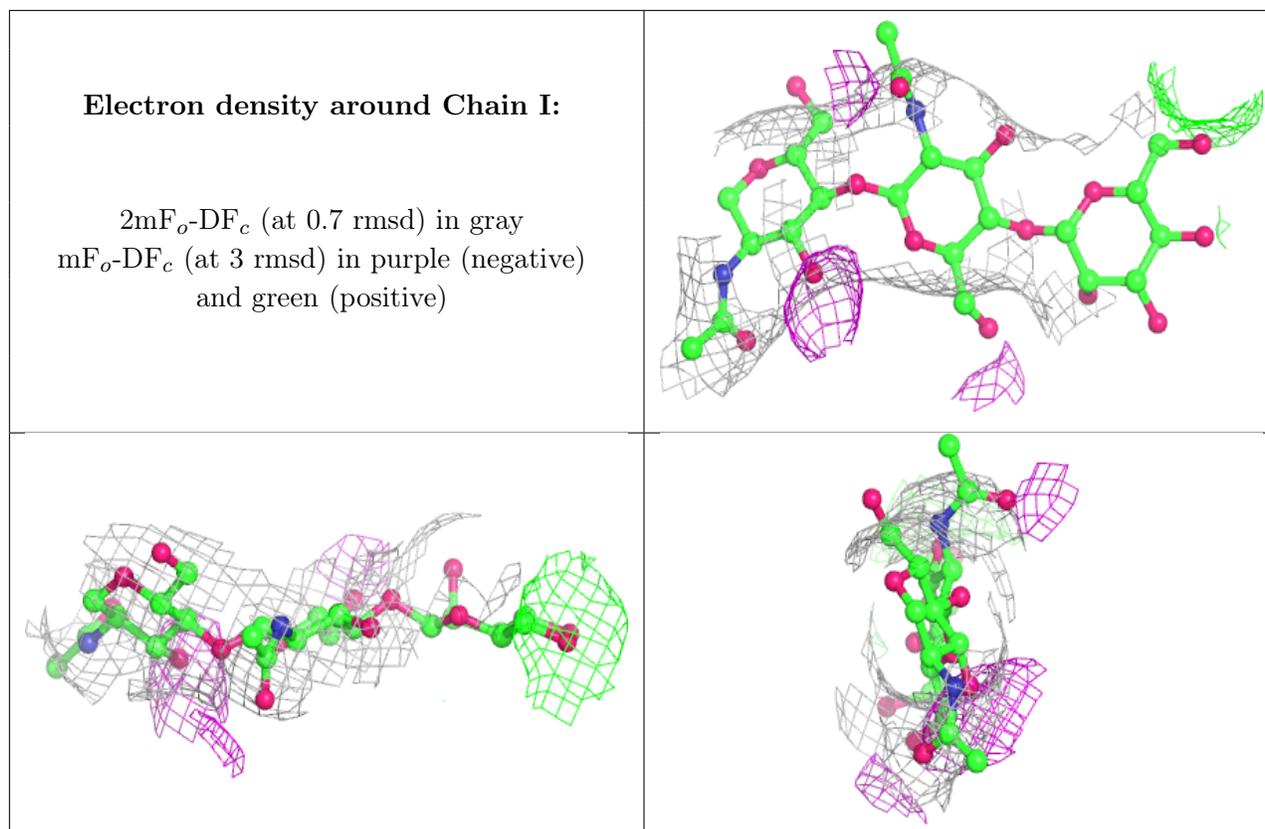
Electron density around Chain I:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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(Å²)	Q<0.9
7	NAG	C	802	14/15	0.87	0.21	170,194,215,224	0
7	NAG	C	801	14/15	0.88	0.11	123,159,193,202	0
7	NAG	A	1001	14/15	0.89	0.20	160,192,215,218	0
9	SO4	A	1003	5/5	0.94	0.46	121,132,142,150	0
9	SO4	C	804	5/5	0.95	0.51	125,136,157,157	0
8	ZN	C	803	1/1	0.96	0.34	167,167,167,167	0
8	ZN	A	1002	1/1	0.99	0.36	144,144,144,144	0

6.5 Other polymers ⓘ

There are no such residues in this entry.