wwPDB X-ray Structure Validation Summary Report (i)

Oct 16, 2023 – 01:22 PM EDT

PDB ID	:	1UHG
Title	:	Crystal Structure of S-Ovalbumin At 1.9 Angstrom Resolution
Authors	:	Yamasaki, M.; Takahashi, N.; Hirose, M.
Deposited on	:	2003-07-03
Resolution	:	1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

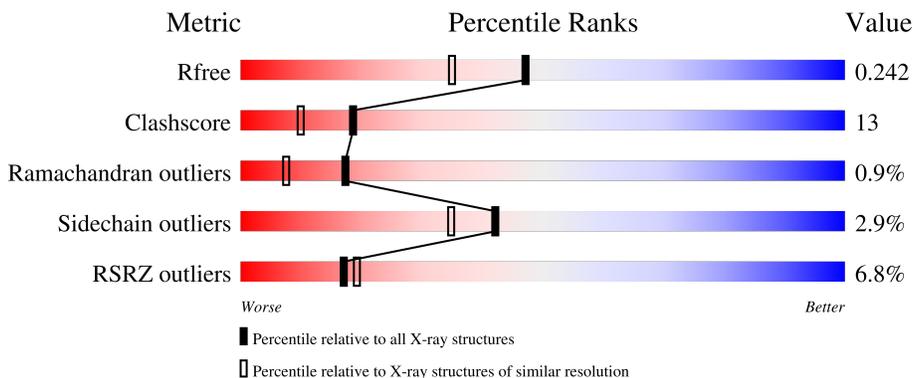|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.242
Clashscore		13
Ramachandran outliers		0.9%
Sidechain outliers		2.9%
RSRZ outliers		6.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	385	7% / 75% / 22% / ..
1	B	385	8% / 76% / 21% / .
1	C	385	8% / 73% / 22% / ..
1	D	385	4% / 77% / 21% / .
2	E	2	50% / 50%

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

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
1	SEP	C	68	-	-	-	X
1	DSN	D	164	X	-	-	-
2	NAG	E	2	-	-	-	X

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 12910 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 Ovalbumin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	383	Total 2987	C 1891	N 496	O 576	P 2	S 22	0	0	0
1	B	385	Total 3001	C 1901	N 499	O 578	P 1	S 22	0	0	0
1	C	374	Total 2933	C 1865	N 488	O 558		S 22	0	0	0
1	D	385	Total 3005	C 1901	N 499	O 581	P 2	S 22	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	SEP	SER	modified residue	UNP P01012
A	164	DSN	SER	modified residue	UNP P01012
A	236	DSN	SER	modified residue	UNP P01012
A	320	DSN	SER	modified residue	UNP P01012
A	344	SEP	SER	modified residue	UNP P01012
B	68	SEP	SER	modified residue	UNP P01012
B	164	DSN	SER	modified residue	UNP P01012
B	236	DSN	SER	modified residue	UNP P01012
B	320	DSN	SER	modified residue	UNP P01012
B	344	SEP	SER	modified residue	UNP P01012
C	68	SEP	SER	modified residue	UNP P01012
C	164	DSN	SER	modified residue	UNP P01012
C	236	DSN	SER	modified residue	UNP P01012
C	320	DSN	SER	modified residue	UNP P01012
C	344	SEP	SER	modified residue	UNP P01012
D	68	SEP	SER	modified residue	UNP P01012
D	164	DSN	SER	modified residue	UNP P01012
D	236	DSN	SER	modified residue	UNP P01012
D	320	DSN	SER	modified residue	UNP P01012
D	344	SEP	SER	modified residue	UNP P01012

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total 28	C 16	N 2	O 10	0	0	0
2	F	2	Total 28	C 16	N 2	O 10	0	0	0
2	G	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
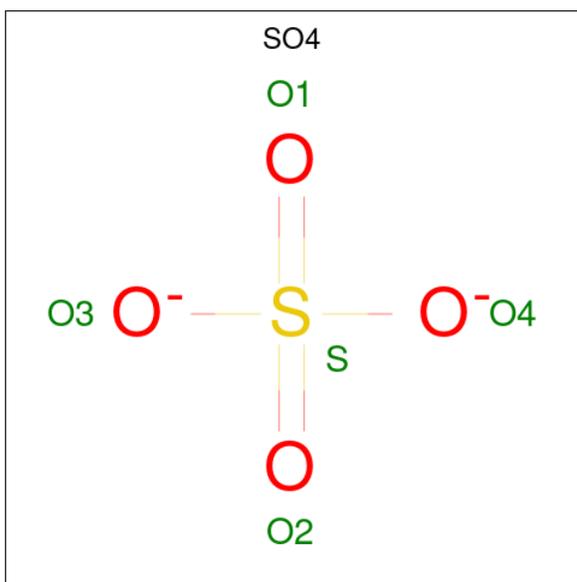
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0

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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
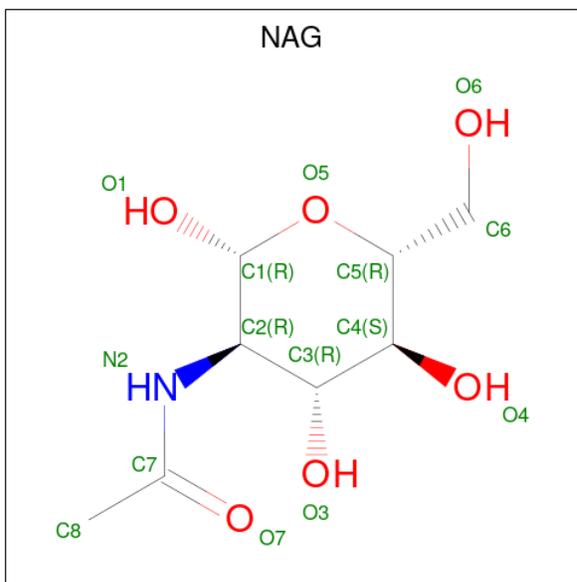
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total C N O 14 8 1 5				0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	218	Total O 218 218		0	0
5	B	219	Total O 219 219		0	0
5	C	206	Total O 206 206		0	0
5	D	208	Total O 208 208		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.
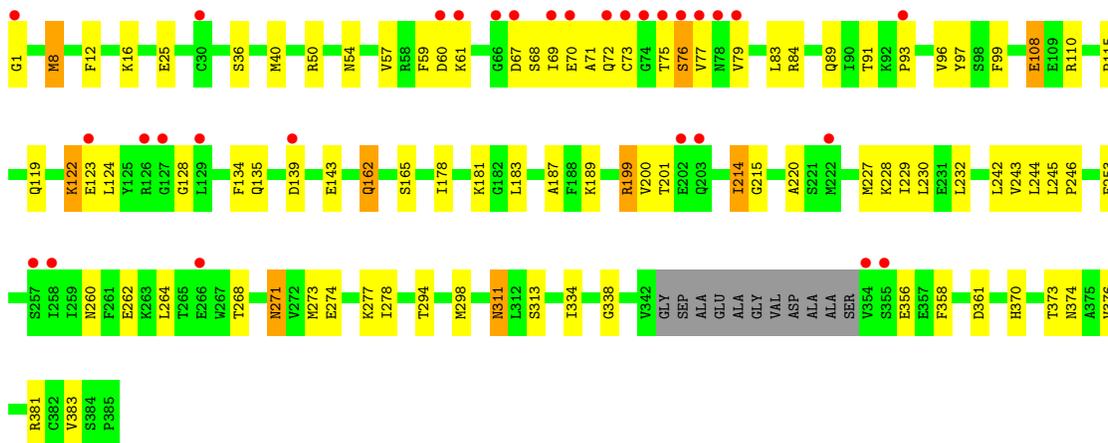
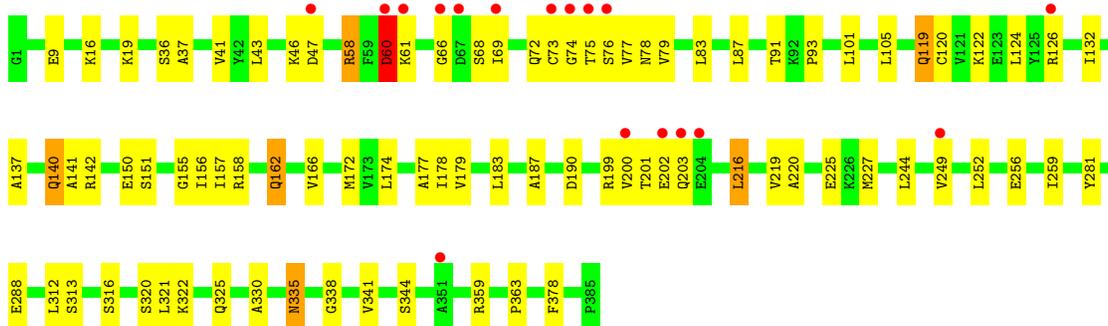- Molecule 1: Ovalbumin
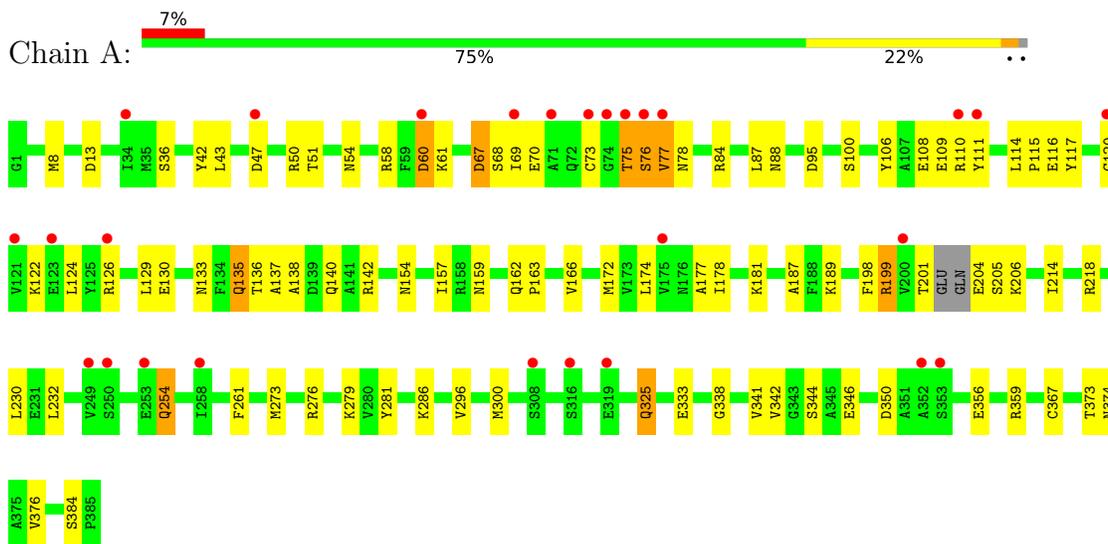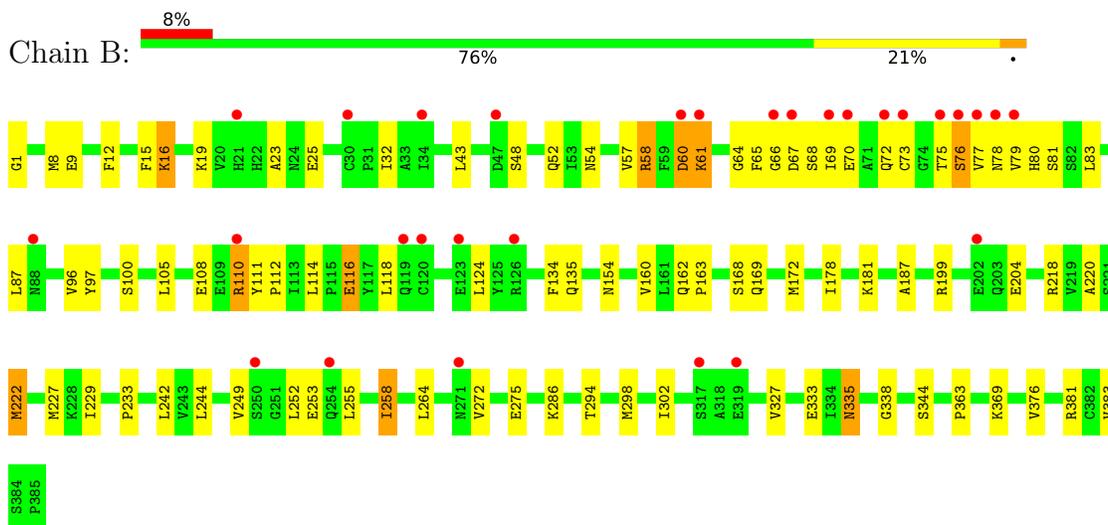
Chain A:

- Molecule 1: Ovalbumin

Chain B:

- Molecule 1: Ovalbumin

Chain C:

• Molecule 1: Ovalbumin

Chain D:

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

Chain E:

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

Chain F:

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

Chain G:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	62.65Å 70.91Å 83.39Å 87.24° 71.73° 75.95°	Depositor
Resolution (Å)	14.89 – 1.90	Depositor
	29.25 – 1.80	EDS
% Data completeness	96.1 (14.89-1.90)	Depositor
(in resolution range)	94.7 (29.25-1.80)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 1.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.196 , 0.247	Depositor
	0.190 , 0.242	DCC
R_{free} test set	10051 reflections (8.66%)	wwPDB-VP
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 58.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12910	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.56% 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: SEP, NAG, DSN, SO4

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	0.51	1/2999 (0.0%)	0.70	0/4043
1	B	0.49	0/3018	0.69	0/4070
1	C	0.51	0/2960	0.69	0/3991
1	D	0.52	0/3018	0.69	2/4070 (0.0%)
All	All	0.51	1/11995 (0.0%)	0.69	2/16174 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	1	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	CYS	CB-SG	-5.30	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	183	LEU	CA-CB-CG	5.35	127.60	115.30
1	D	216	LEU	CA-CB-CG	5.34	127.58	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	164	DSN	CA

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	2987	0	2964	81	0
1	B	3001	0	2978	85	0
1	C	2933	0	2924	84	0
1	D	3005	0	2979	80	0
2	E	28	0	25	1	0
2	F	28	0	25	0	0
2	G	28	0	25	2	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
4	D	14	0	13	3	0
5	A	218	0	0	10	0
5	B	219	0	0	3	0
5	C	206	0	0	1	0
5	D	208	0	0	6	0
All	All	12910	0	11933	316	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 13.

The worst 5 of 316 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:99:PHE:CZ	1:C:178:ILE:HD11	1.92	1.04
1:C:8:MET:HE3	1:C:376:VAL:HG21	1.50	0.93
1:B:199:ARG:HG2	1:B:249:VAL:HG21	1.54	0.89
1:D:162:GLN:H	1:D:162:GLN:NE2	1.72	0.86
1:B:100:SER:O	1:B:178:ILE:HD12	1.76	0.85

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	374/385 (97%)	361 (96%)	9 (2%)	4 (1%)	14	5
1	B	378/385 (98%)	363 (96%)	11 (3%)	4 (1%)	14	5
1	C	366/385 (95%)	347 (95%)	16 (4%)	3 (1%)	19	9
1	D	378/385 (98%)	368 (97%)	8 (2%)	2 (0%)	29	18
All	All	1496/1540 (97%)	1439 (96%)	44 (3%)	13 (1%)	17	7

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASP
1	A	67	ASP
1	B	61	LYS
1	C	60	ASP
1	C	67	ASP

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	324/326 (99%)	316 (98%)	8 (2%)	47	41
1	B	326/326 (100%)	317 (97%)	9 (3%)	43	36
1	C	322/326 (99%)	309 (96%)	13 (4%)	31	22
1	D	326/326 (100%)	318 (98%)	8 (2%)	47	41
All	All	1298/1304 (100%)	1260 (97%)	38 (3%)	42	35

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	274	GLU
1	D	203	GLN
1	C	311	ASN
1	D	119	GLN
1	D	335	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	203	GLN
1	D	140	GLN
1	C	213	GLN
1	C	311	ASN
1	D	162	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

19 non-standard protein/DNA/RNA residues 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	$\#|Z| > 2$
1	SEP	D	344	1	8,9,10	1.02	1 (12%)	8,12,14	2.88	2 (25%)
1	SEP	D	68	1	8,9,10	1.00	0	8,12,14	2.84	2 (25%)
1	SEP	C	68	1	4,5,10	0.68	0	0,5,14	-	-
1	SEP	A	344	1	8,9,10	0.83	0	8,12,14	2.38	2 (25%)
1	SEP	B	344	1	8,9,10	1.02	0	8,12,14	2.33	2 (25%)
1	SEP	B	68	1	4,5,10	0.61	0	0,5,14	-	-
1	SEP	A	68	1	8,9,10	0.98	1 (12%)	8,12,14	2.15	2 (25%)

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
1	SEP	D	344	1	-	1/5/8/10	-
1	SEP	D	68	1	-	0/5/8/10	-
1	DSN	D	164	1	1/1/1/2	-	-
1	SEP	C	68	1	-	0/2/4/10	-
1	SEP	A	344	1	-	4/5/8/10	-
1	SEP	B	344	1	-	1/5/8/10	-
1	SEP	B	68	1	-	0/2/4/10	-
1	SEP	A	68	1	-	1/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	344	SEP	P-O1P	2.05	1.57	1.50
1	A	68	SEP	P-O1P	2.03	1.57	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(º)	Ideal(º)
1	D	68	SEP	P-OG-CB	-7.00	99.00	118.30
1	D	344	SEP	P-OG-CB	-6.43	100.59	118.30
1	A	344	SEP	P-OG-CB	-5.80	102.32	118.30
1	B	344	SEP	P-OG-CB	-5.29	103.73	118.30
1	A	68	SEP	P-OG-CB	-5.09	104.28	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	164	DSN	CA

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	68	SEP	N-CA-CB-OG
1	A	344	SEP	N-CA-CB-OG
1	A	344	SEP	CB-OG-P-O1P
1	A	344	SEP	CB-OG-P-O2P
1	A	344	SEP	CB-OG-P-O3P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	68	SEP	2	0
1	B	68	SEP	1	0

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	E	1	1,2	14,14,15	0.62	0	17,19,21	0.91	1 (5%)
2	NAG	E	2	2	14,14,15	0.56	0	17,19,21	0.63	0
2	NAG	F	1	1,2	14,14,15	0.74	0	17,19,21	0.67	0
2	NAG	F	2	2	14,14,15	0.58	0	17,19,21	1.03	1 (5%)
2	NAG	G	1	1,2	14,14,15	0.65	0	17,19,21	0.70	0
2	NAG	G	2	2	14,14,15	0.77	0	17,19,21	1.03	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
2	NAG	E	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	2	NAG	C2-N2-C7	-3.27	118.25	122.90
2	E	1	NAG	C2-N2-C7	-3.13	118.45	122.90
2	G	2	NAG	C2-N2-C7	-2.19	119.79	122.90
2	G	2	NAG	C1-O5-C5	2.07	114.99	112.19

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
2	G	2	NAG	C8-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	1	0
2	G	2	NAG	1	0
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.

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
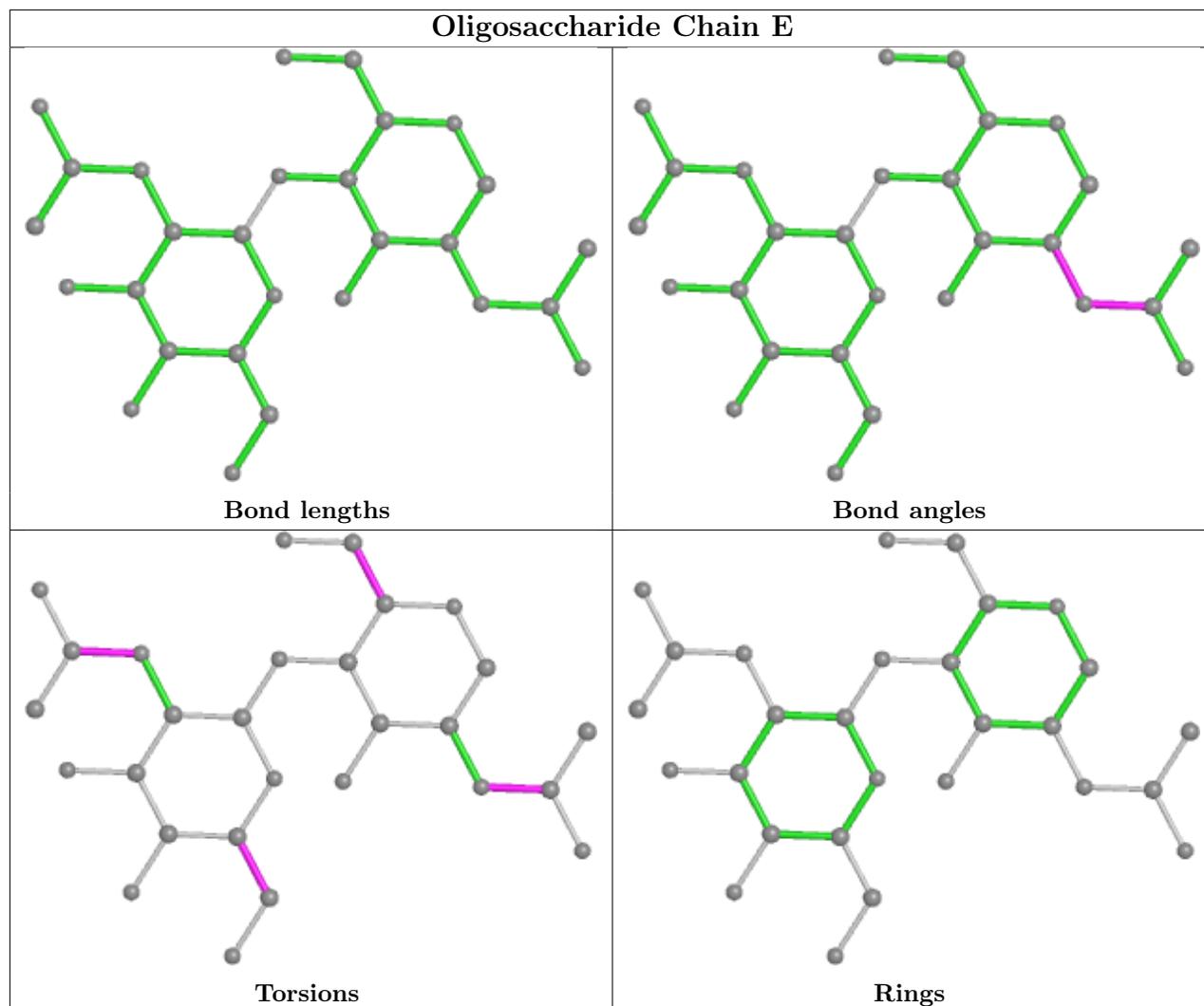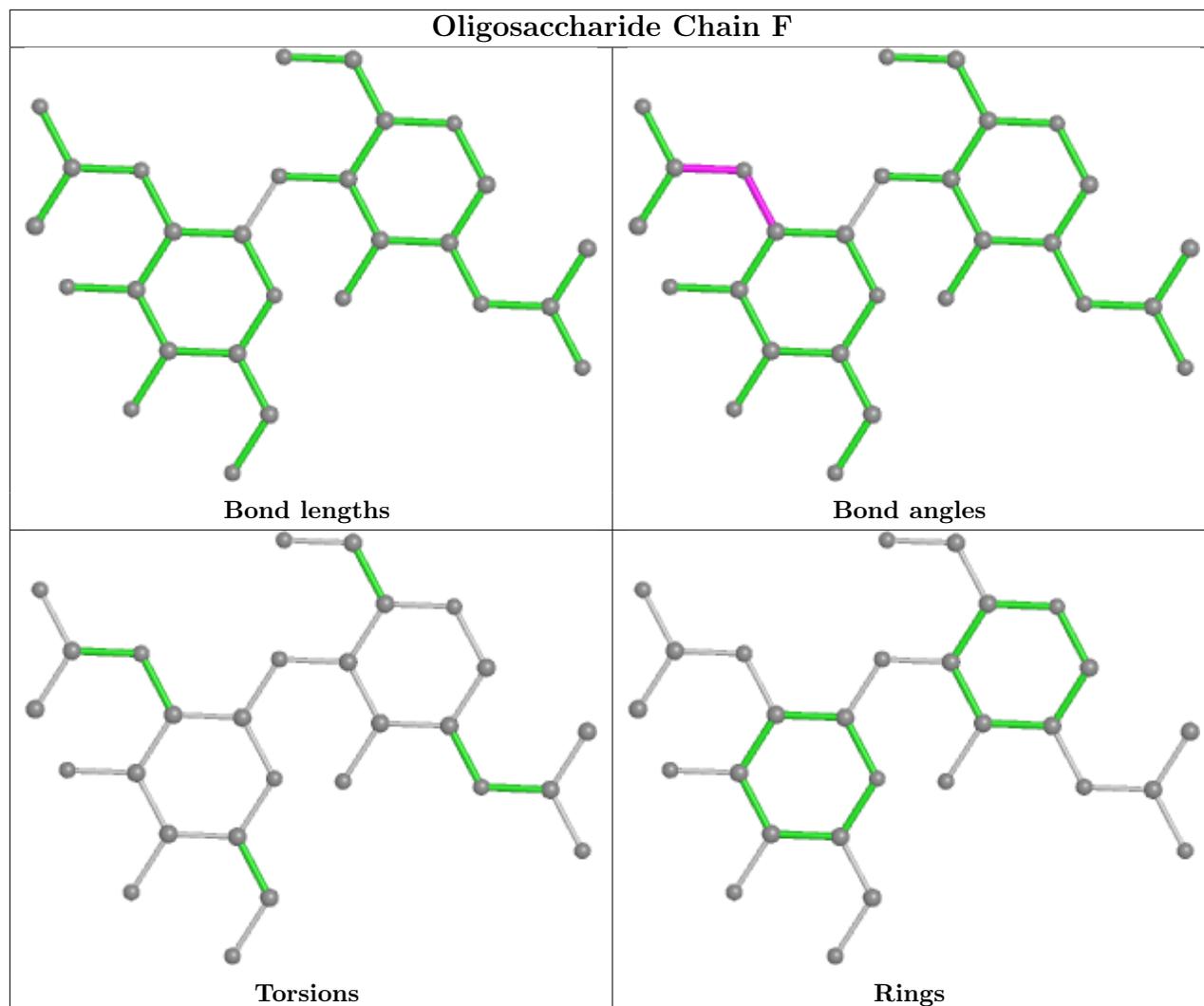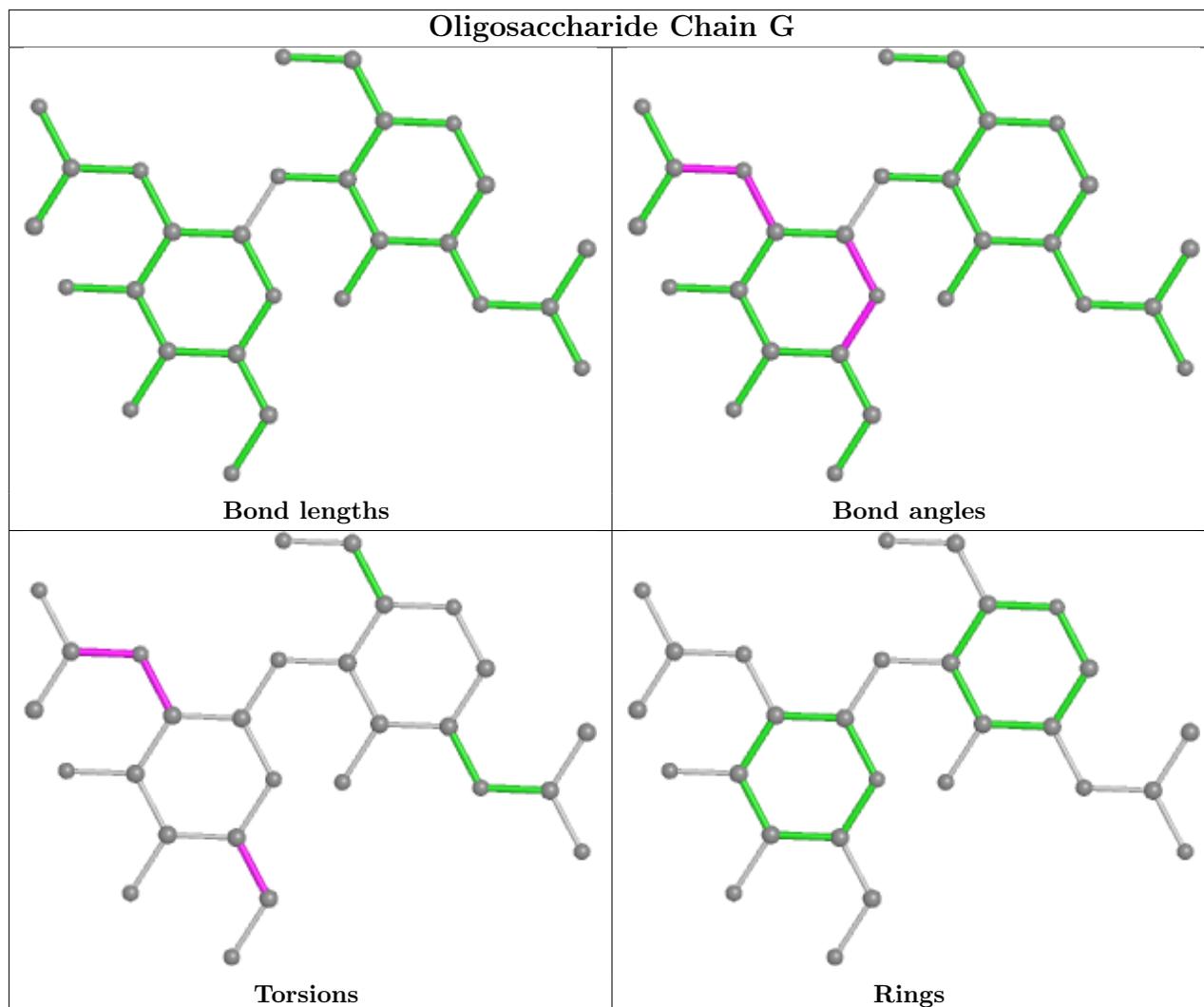
5.6   Ligand geometry ⓘ

8 ligands 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	SO4	D	3401	-	4,4,4	0.28	0	6,6,6	0.06	0
4	NAG	D	386	1	14,14,15	0.70	0	17,19,21	0.79	0
3	SO4	A	401	-	4,4,4	0.28	0	6,6,6	0.14	0
3	SO4	A	402	-	4,4,4	0.28	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	SO4	B	1401	-	4,4,4	0.27	0	6,6,6	0.07	0
3	SO4	B	1402	-	4,4,4	0.22	0	6,6,6	0.08	0
3	SO4	D	3402	-	4,4,4	0.29	0	6,6,6	0.10	0
3	SO4	C	2401	-	4,4,4	0.33	0	6,6,6	0.07	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	386	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
4	D	386	NAG	C8-C7-N2-C2
4	D	386	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	386	NAG	3	0

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(Å^2)	Q<0.9
1	A	378/385 (98%)	0.47	27 (7%)	16	17	13, 28, 50, 62	0
1	B	380/385 (98%)	0.41	29 (7%)	13	15	14, 26, 50, 75	0
1	C	370/385 (96%)	0.45	30 (8%)	12	13	12, 25, 48, 67	0
1	D	380/385 (98%)	0.26	17 (4%)	33	36	14, 26, 43, 56	0
All	All	1508/1540 (97%)	0.39	103 (6%)	17	19	12, 26, 49, 75	0

The worst 5 of 103 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	77	VAL	8.4
1	B	77	VAL	8.1
1	B	75	THR	7.3
1	B	67	ASP	6.6
1	C	75	THR	6.4

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

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
1	SEP	C	68	6/11	0.63	0.54	63,65,65,65	0
1	SEP	B	68	6/11	0.64	0.37	67,68,68,69	0
1	SEP	D	68	10/11	0.65	0.29	53,57,64,64	0
1	SEP	D	344	10/11	0.69	0.22	25,36,52,53	0
1	SEP	A	68	10/11	0.78	0.18	50,55,60,61	0
1	DSN	A	320	6/7	0.81	0.28	45,49,51,53	0
1	DSN	D	164	6/7	0.81	0.25	37,38,41,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	DSN	D	320	6/7	0.81	0.21	34,37,39,42	0
1	DSN	C	320	6/7	0.81	0.18	31,36,38,41	0
1	DSN	B	320	6/7	0.85	0.24	32,37,40,44	0
1	SEP	A	344	10/11	0.92	0.12	40,44,51,51	0
1	SEP	B	344	10/11	0.92	0.13	23,30,46,48	0
1	DSN	B	164	6/7	0.93	0.11	27,30,32,37	0
1	DSN	C	164	6/7	0.94	0.16	29,31,33,36	0
1	DSN	B	236	6/7	0.94	0.14	23,29,31,35	0
1	DSN	A	164	6/7	0.94	0.20	38,39,42,45	0
1	DSN	C	236	6/7	0.95	0.08	20,24,26,28	0
1	DSN	D	236	6/7	0.95	0.11	18,22,25,27	0
1	DSN	A	236	6/7	0.96	0.07	19,20,22,27	0

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.
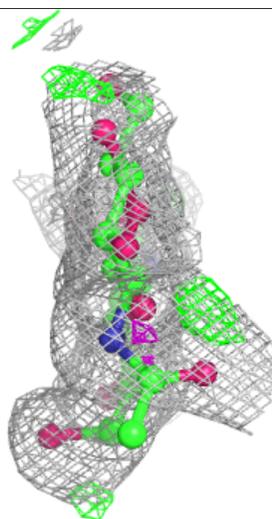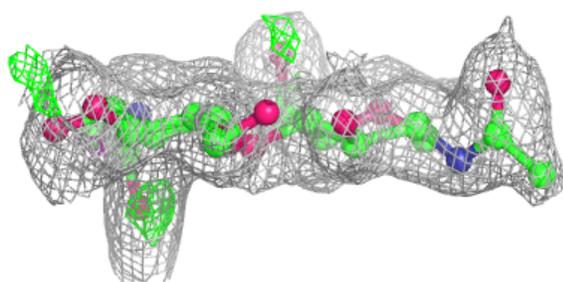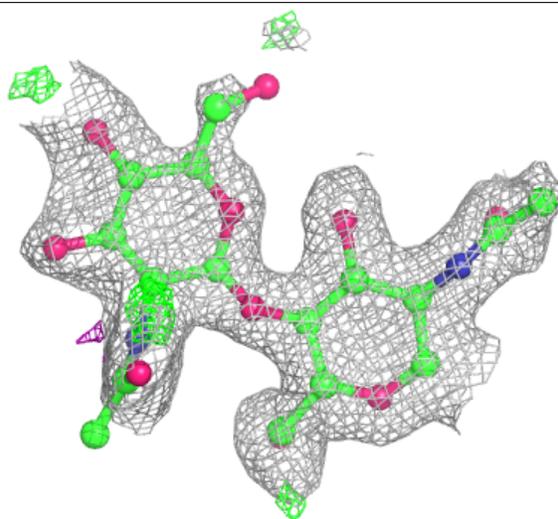
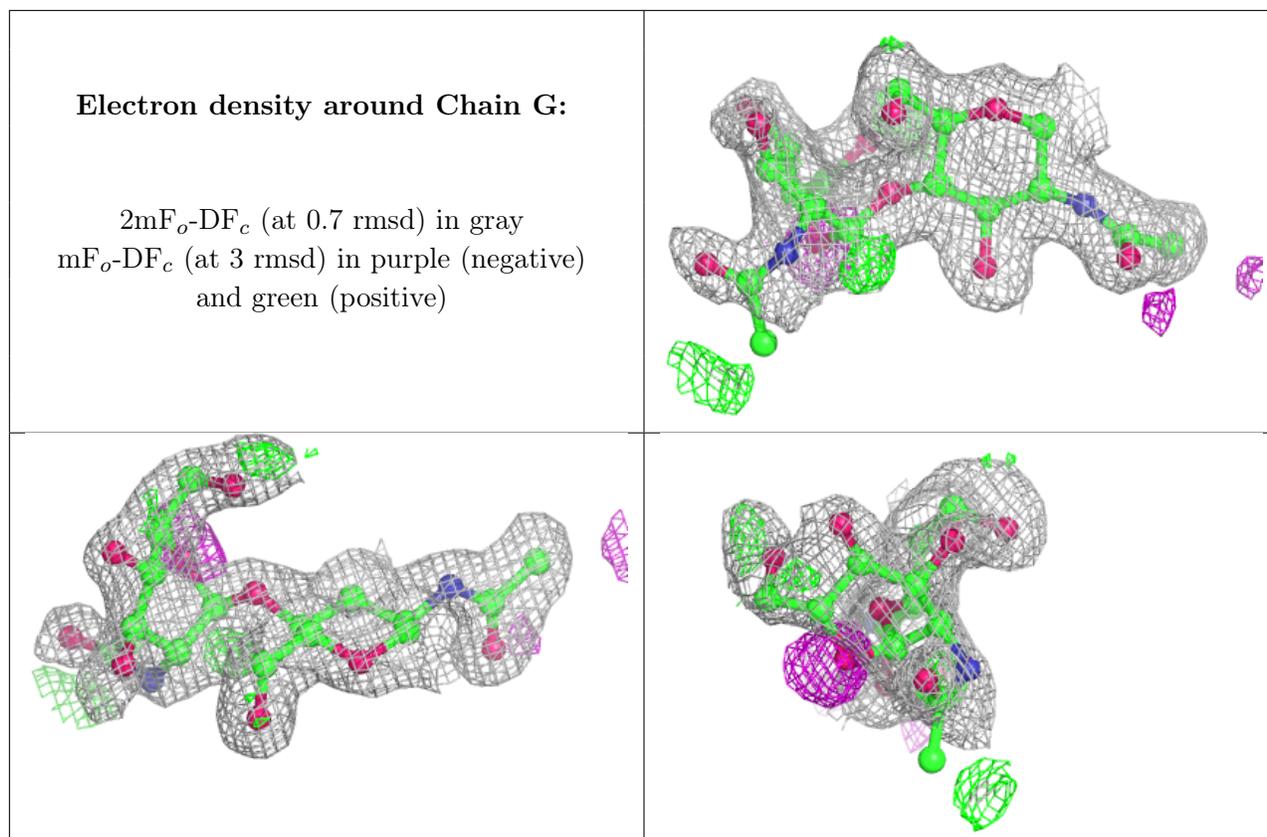| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	E	2	14/15	0.50	0.45	58,61,64,64	0
2	NAG	G	2	14/15	0.64	0.29	40,44,49,49	0
2	NAG	F	2	14/15	0.67	0.25	41,46,47,51	0
2	NAG	E	1	14/15	0.82	0.18	38,42,47,53	0
2	NAG	G	1	14/15	0.93	0.09	19,21,24,31	0
2	NAG	F	1	14/15	0.93	0.10	21,26,30,35	0

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)
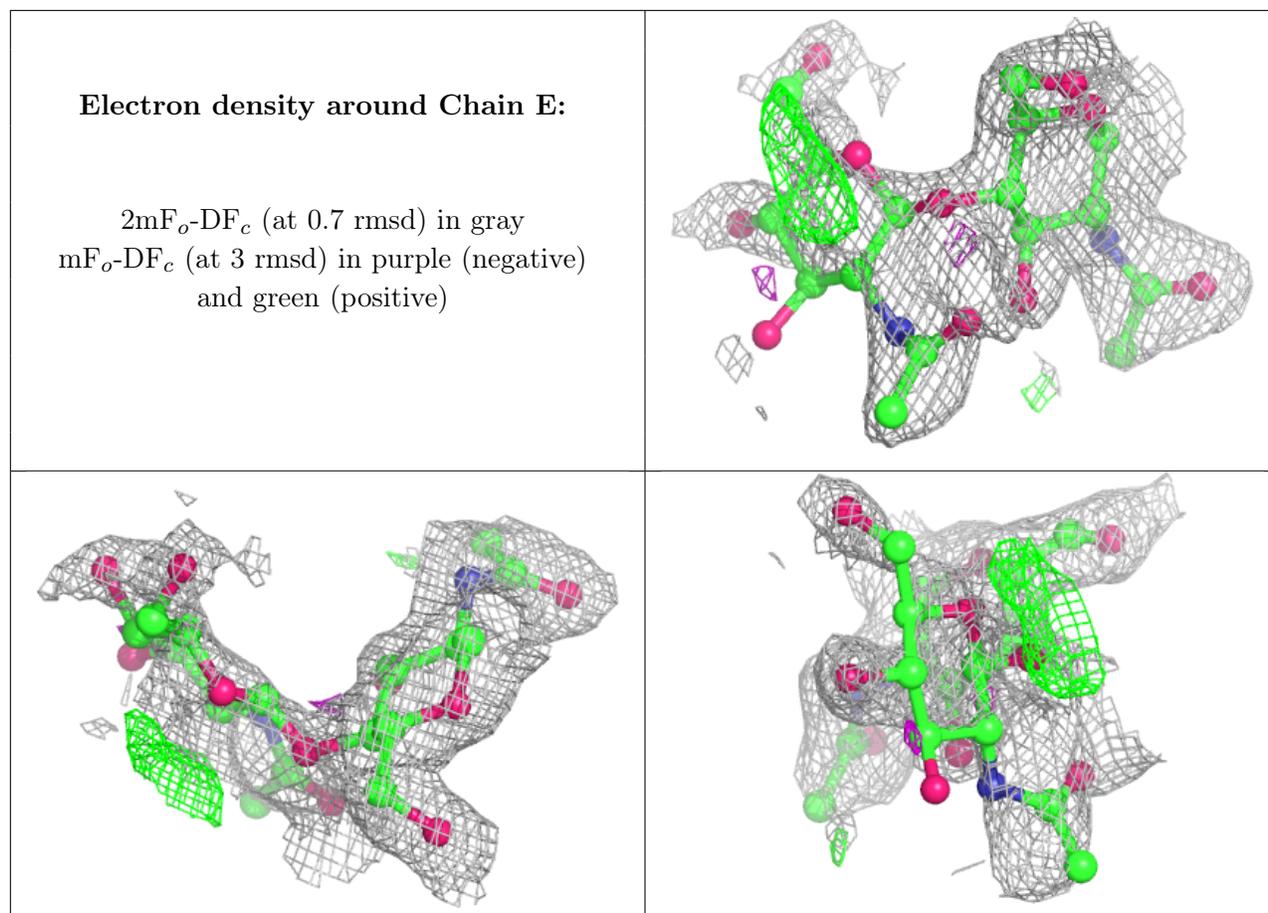
Electron density around Chain F:

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

Electron density around Chain G:

$2mF_o\text{-}DF_c$ (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(Å^2)	Q<0.9
3	SO4	B	1401	5/5	0.80	0.23	99,99,99,99	0
3	SO4	D	3402	5/5	0.84	0.24	74,74,74,74	0
4	NAG	D	386	14/15	0.84	0.18	32,37,41,41	0
3	SO4	D	3401	5/5	0.88	0.23	78,78,79,79	0
3	SO4	A	401	5/5	0.89	0.16	52,52,53,54	0
3	SO4	B	1402	5/5	0.90	0.23	89,89,90,90	0
3	SO4	A	402	5/5	0.90	0.21	56,56,58,58	0
3	SO4	C	2401	5/5	0.95	0.19	52,52,53,53	0

6.5 Other polymers ⓘ

There are no such residues in this entry.