W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Jun 18, 2024 – 10:11 PM EDT

PDB ID	:	3ZE2
Title	:	Integrin alphaIIB beta3 headpiece and RGD peptide complex
Authors	:	Zhu, J.H.; Zhu, J.Q.; Springer, T.A.
Deposited on	:	2012-12-03
Resolution	:	2.35 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

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 2.35 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		0.202
Clashscore		2
Ramachandran outliers		0.3%
Sidechain outliers		1.0%
RSRZ outliers		17.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
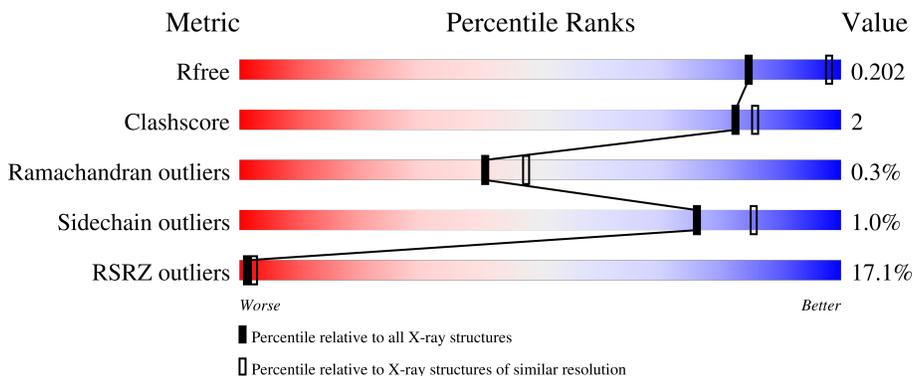
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	457	93% 6% ·
1	C	457	2% 94% 5% ·
2	B	472	15% 89% 10% ·
2	D	472	25% 74% · 22%
3	E	221	2% 93% 5% ·

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Mol	Chain	Length	Quality of chain
3	H	221	51% ... 94%
4	F	214	6% ... 95% ... 5%
4	L	214	55% ... 97%
5	I	6	33% ... 50% 17% 17% 17%
5	J	6	100%
6	G	6	100%
7	K	2	100%
8	M	4	75% 25%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	MAN	M	4	-	-	-	X

2 Entry composition ⓘ

There are 14 unique types of molecules in this entry. The entry contains 41569 atoms, of which 19764 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 INTEGRIN ALPHA-IIB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	454	Total 6845	C 2228	H 3341	N 600	O 668	S 8	2	5	0
1	C	453	Total 6840	C 2227	H 3337	N 602	O 666	S 8	1	6	0

- Molecule 2 is a protein called INTEGRIN BETA-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	469	Total 7218	C 2275	H 3569	N 619	O 721	S 34	0	7	0
2	D	367	Total 5806	C 1834	H 2896	N 487	O 570	S 19	0	6	0

- Molecule 3 is a protein called 10E5 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	216	Total 3239	C 1041	H 1597	N 266	O 329	S 6	0	0	0
3	H	216	Total 3239	C 1041	H 1597	N 266	O 329	S 6	0	0	0

- Molecule 4 is a protein called 10E5 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	214	Total 3222	C 1028	H 1569	N 273	O 343	S 9	0	2	0
4	L	214	Total 3187	C 1019	H 1550	N 268	O 341	S 9	0	0	0

- Molecule 5 is a protein called RGD PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	6	Total	C	H	N	O	0	3	0
			111	32	52	15	12			
5	J	6	Total	C	H	N	O	0	0	0
			74	22	34	9	9			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyran ose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy- beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
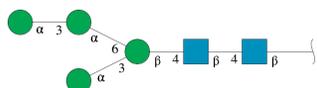
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	6	Total	C	H	N	O	0	0	0
			133	40	61	2	30			

- Molecule 7 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
7	K	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluco pyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	M	4	Total	C	H	N	O	0	0	0
			93	28	43	2	20			

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total 14	C 3	H 8	O 3	0	0
9	A	1	Total 14	C 3	H 8	O 3	0	0
9	C	1	Total 14	C 3	H 8	O 3	0	0
9	C	1	Total 14	C 3	H 8	O 3	0	0
9	C	1	Total 14	C 3	H 8	O 3	0	0
9	C	1	Total 14	C 3	H 8	O 3	0	0
9	E	1	Total 14	C 3	H 8	O 3	0	0
9	F	1	Total 14	C 3	H 8	O 3	0	0
9	F	1	Total 14	C 3	H 8	O 3	0	0
9	J	1	Total 14	C 3	H 8	O 3	0	0

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
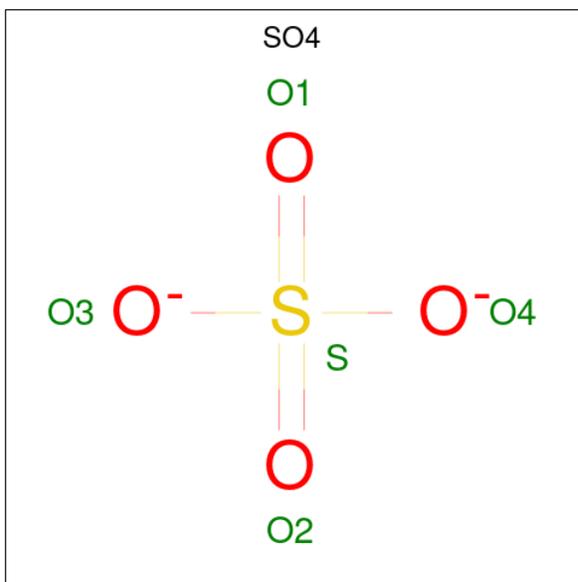
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total 5	O 4	S 1	0	0
10	A	1	Total 5	O 4	S 1	0	0

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	4	Total 4	Ca 4	0	0
11	C	4	Total 4	Ca 4	0	0

- Molecule 12 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	3	Total 3	Mn 3	0	0
12	D	3	Total 3	Mn 3	0	0

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

O6
OH

O1
HO

O5
O

C6

C1(R)   C5(R)

C2(R)   C4(S)
C3(R)

N2
HN

OH
O4

C7

OH
O3

C8

O
O7
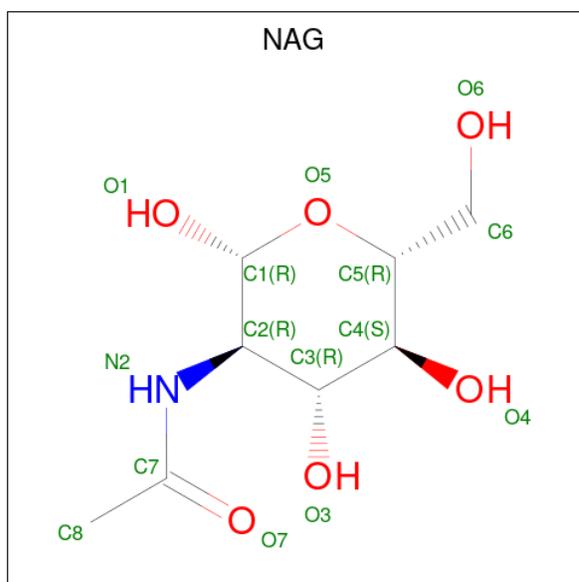
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	483	Total	O	0	0
			483	483		
14	B	211	Total	O	0	0
			211	211		
14	C	283	Total	O	0	0
			283	283		
14	D	107	Total	O	0	0
			107	107		
14	E	129	Total	O	0	0
			129	129		
14	F	68	Total	O	0	0
			68	68		
14	H	18	Total	O	0	0
			18	18		
14	I	2	Total	O	0	0
			2	2		
14	J	2	Total	O	0	0
			2	2		
14	L	15	Total	O	0	0
			15	15		

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: INTEGRIN ALPHA-IIB
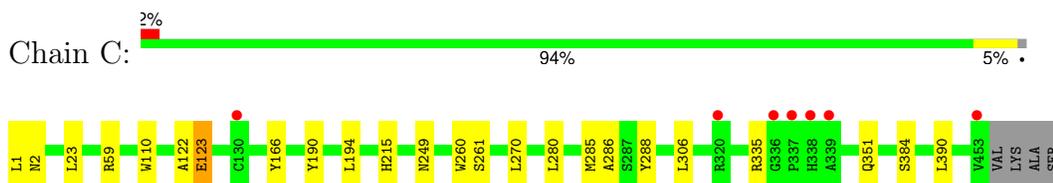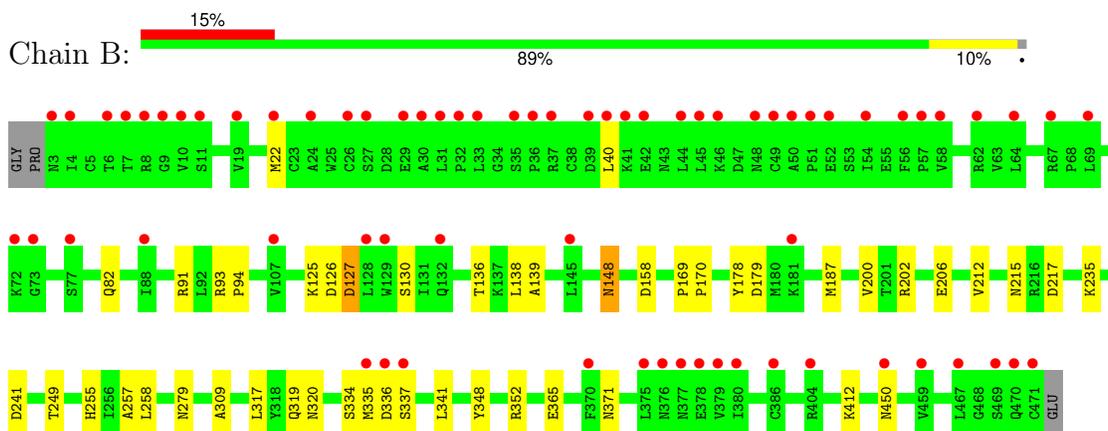
Chain A:

- Molecule 1: INTEGRIN ALPHA-IIB

Chain C:

- Molecule 2: INTEGRIN BETA-3

Chain B:

- Molecule 2: INTEGRIN BETA-3

Chain D:

• Molecule 3: 10E5 FAB HEAVY CHAIN
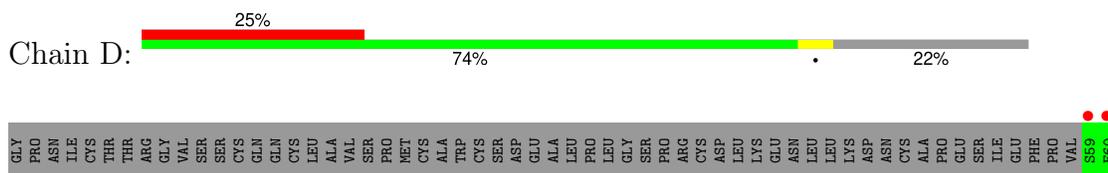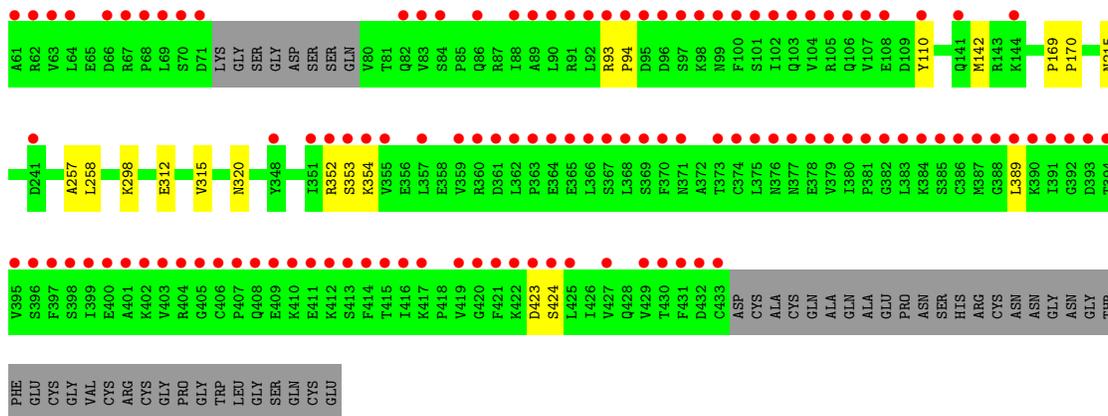
Chain E:

• Molecule 3: 10E5 FAB HEAVY CHAIN
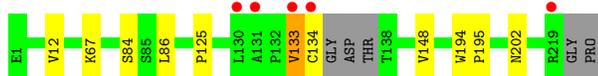
Chain H:

• Molecule 4: 10E5 FAB LIGHT CHAIN
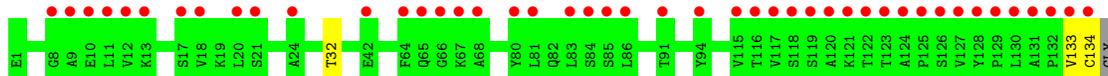
Chain F:

• Molecule 4: 10E5 FAB LIGHT CHAIN

Chain L:
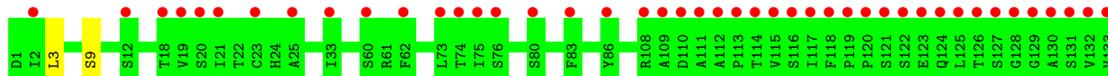
• Molecule 5: RGD PEPTIDE

Chain I:

• Molecule 5: RGD PEPTIDE

Chain J:

There are no outlier residues recorded for this chain.

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

Chain G:

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain K:

• Molecule 8: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	233.21Å 143.56Å 104.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.02 – 2.35 54.02 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.02-2.35) 100.0 (54.02-2.35)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 2.34Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.175 , 0.204 0.174 , 0.202	Depositor DCC
R_{free} test set	1017 reflections (0.69%)	wwPDB-VP
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 56.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	41569	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 2.18% 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: BMA, CA, MN, SO4, MAN, NAG, GOL

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	0.24	0/3612	0.44	0/4923
1	C	0.23	0/3615	0.41	0/4927
2	B	0.22	0/3737	0.40	0/5066
2	D	0.22	0/2976	0.39	0/4031
3	E	0.23	0/1684	0.42	0/2305
3	H	0.21	0/1684	0.38	0/2305
4	F	0.23	0/1692	0.41	0/2294
4	L	0.22	0/1673	0.37	0/2269
5	I	0.20	0/59	0.40	0/76
5	J	0.18	0/40	0.39	0/52
All	All	0.23	0/20772	0.41	0/28248

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3504	3341	3348	20	0
1	C	3503	3337	3345	18	0
2	B	3649	3569	3575	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2910	2896	2900	11	0
3	E	1642	1597	1600	5	0
3	H	1642	1597	1600	5	0
4	F	1653	1569	1571	6	0
4	L	1637	1550	1553	4	0
5	I	59	52	51	6	0
5	J	40	34	34	0	0
6	G	72	61	61	0	0
7	K	28	25	25	2	0
8	M	50	43	43	0	0
9	A	12	16	16	0	0
9	C	24	32	32	1	0
9	E	6	8	8	0	0
9	F	12	16	16	0	0
9	J	6	8	8	0	0
10	A	10	0	0	1	0
11	A	4	0	0	0	0
11	C	4	0	0	0	0
12	B	3	0	0	0	0
12	D	3	0	0	0	0
13	C	14	13	13	0	0
14	A	483	0	0	6	1
14	B	211	0	0	6	0
14	C	283	0	0	6	1
14	D	107	0	0	1	0
14	E	129	0	0	0	0
14	F	68	0	0	0	0
14	H	18	0	0	0	0
14	I	2	0	0	0	0
14	J	2	0	0	0	0
14	L	15	0	0	1	0
All	All	21805	19764	19799	99	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 2.

The worst 5 of 99 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)
14:A:3238:HOH:O	5:I:492[B]:GLY:N	2.03	0.90
14:A:3222:HOH:O	5:I:493[A]:ARG:NH2	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:SER:OG	14:C:3243:HOH:O	2.05	0.74
1:A:384:SER:OG	14:A:3430:HOH:O	2.06	0.73
10:A:1457:SO4:O3	14:A:3482:HOH:O	2.09	0.70

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)
14:A:3480:HOH:O	14:C:3252:HOH:O[1_554]	2.18	0.02

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	457/457 (100%)	445 (97%)	11 (2%)	1 (0%)	47	56
1	C	457/457 (100%)	440 (96%)	16 (4%)	1 (0%)	47	56
2	B	474/472 (100%)	460 (97%)	13 (3%)	1 (0%)	47	56
2	D	369/472 (78%)	355 (96%)	13 (4%)	1 (0%)	41	47
3	E	212/221 (96%)	202 (95%)	9 (4%)	1 (0%)	29	32
3	H	212/221 (96%)	200 (94%)	12 (6%)	0	100	100
4	F	214/214 (100%)	206 (96%)	8 (4%)	0	100	100
4	L	212/214 (99%)	200 (94%)	12 (6%)	0	100	100
5	I	6/6 (100%)	2 (33%)	0	4 (67%)	0	0
5	J	4/6 (67%)	4 (100%)	0	0	100	100
All	All	2617/2740 (96%)	2514 (96%)	94 (4%)	9 (0%)	41	47

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	D	142	MET
1	C	123	GLU
5	I	493[A]	ARG
5	I	493[B]	ARG

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	367/364 (101%)	361 (98%)	6 (2%)	62	75
1	C	367/364 (101%)	362 (99%)	5 (1%)	67	78
2	B	422/417 (101%)	416 (99%)	6 (1%)	67	78
2	D	336/417 (81%)	335 (100%)	1 (0%)	92	96
3	E	187/190 (98%)	186 (100%)	1 (0%)	88	94
3	H	187/190 (98%)	187 (100%)	0	100	100
4	F	190/188 (101%)	188 (99%)	2 (1%)	73	84
4	L	188/188 (100%)	187 (100%)	1 (0%)	88	94
5	I	5/4 (125%)	3 (60%)	2 (40%)	0	0
5	J	4/4 (100%)	4 (100%)	0	100	100
All	All	2253/2326 (97%)	2229 (99%)	24 (1%)	76	84

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	190	TYR
2	D	215	ASN
1	C	288	TYR
3	E	202	ASN
2	B	91	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	275	GLN
2	B	450	ASN
1	C	338	HIS
2	D	316	ASN
3	E	202	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 ⓘ

12 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	$\#|Z| > 2$
6	NAG	G	1	2,6	14,14,15	0.61	0	17,19,21	0.62	0
6	NAG	G	2	6	14,14,15	0.55	0	17,19,21	0.76	0
6	BMA	G	3	6	11,11,12	0.62	0	15,15,17	0.63	0
6	MAN	G	4	6	11,11,12	0.63	0	15,15,17	0.62	0
6	MAN	G	5	6	11,11,12	0.63	0	15,15,17	0.53	0
6	MAN	G	6	6	11,11,12	0.63	0	15,15,17	0.55	0
7	NAG	K	1	7	14,14,15	0.51	0	17,19,21	0.75	0
7	NAG	K	2	7	14,14,15	0.54	0	17,19,21	0.56	0
8	NAG	M	1	2,8	14,14,15	0.46	0	17,19,21	0.80	1 (5%)
8	NAG	M	2	8	14,14,15	0.61	0	17,19,21	0.84	0
8	BMA	M	3	8	11,11,12	0.62	0	15,15,17	0.63	0
8	MAN	M	4	8	11,11,12	0.60	0	15,15,17	0.57	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
6	NAG	G	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1
6	BMA	G	3	6	-	0/2/19/22	0/1/1/1
6	MAN	G	4	6	-	0/2/19/22	0/1/1/1
6	MAN	G	5	6	-	0/2/19/22	0/1/1/1
6	MAN	G	6	6	-	0/2/19/22	0/1/1/1
7	NAG	K	1	7	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	2/6/23/26	0/1/1/1
8	NAG	M	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	M	2	8	-	0/6/23/26	0/1/1/1
8	BMA	M	3	8	-	2/2/19/22	0/1/1/1
8	MAN	M	4	8	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	1	NAG	C1-O5-C5	2.13	115.05	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	K	1	NAG	C8-C7-N2-C2
7	K	1	NAG	O7-C7-N2-C2
8	M	3	BMA	O5-C5-C6-O6
8	M	3	BMA	C4-C5-C6-O6
7	K	2	NAG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	K	1	NAG	2	0
7	K	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 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
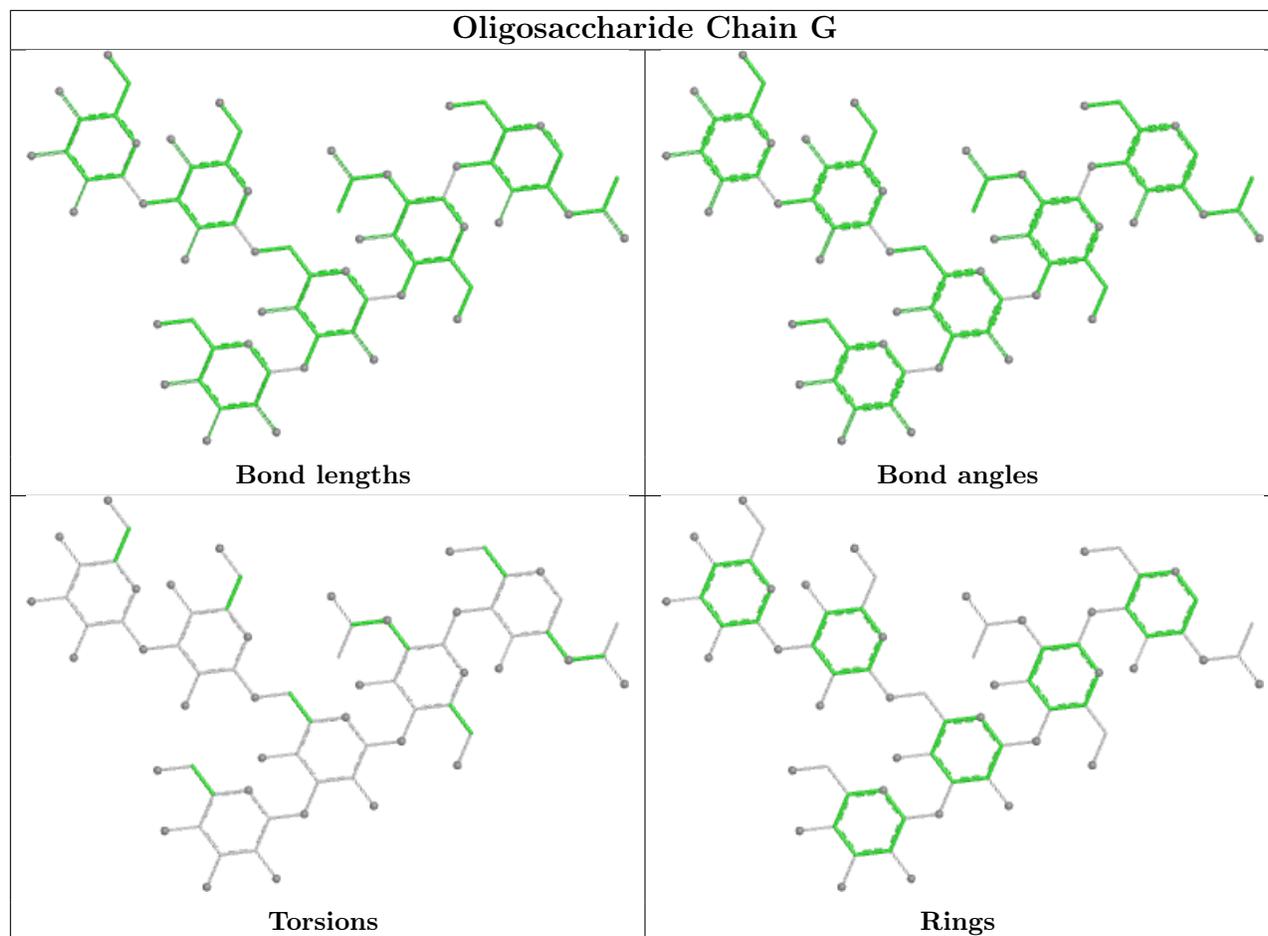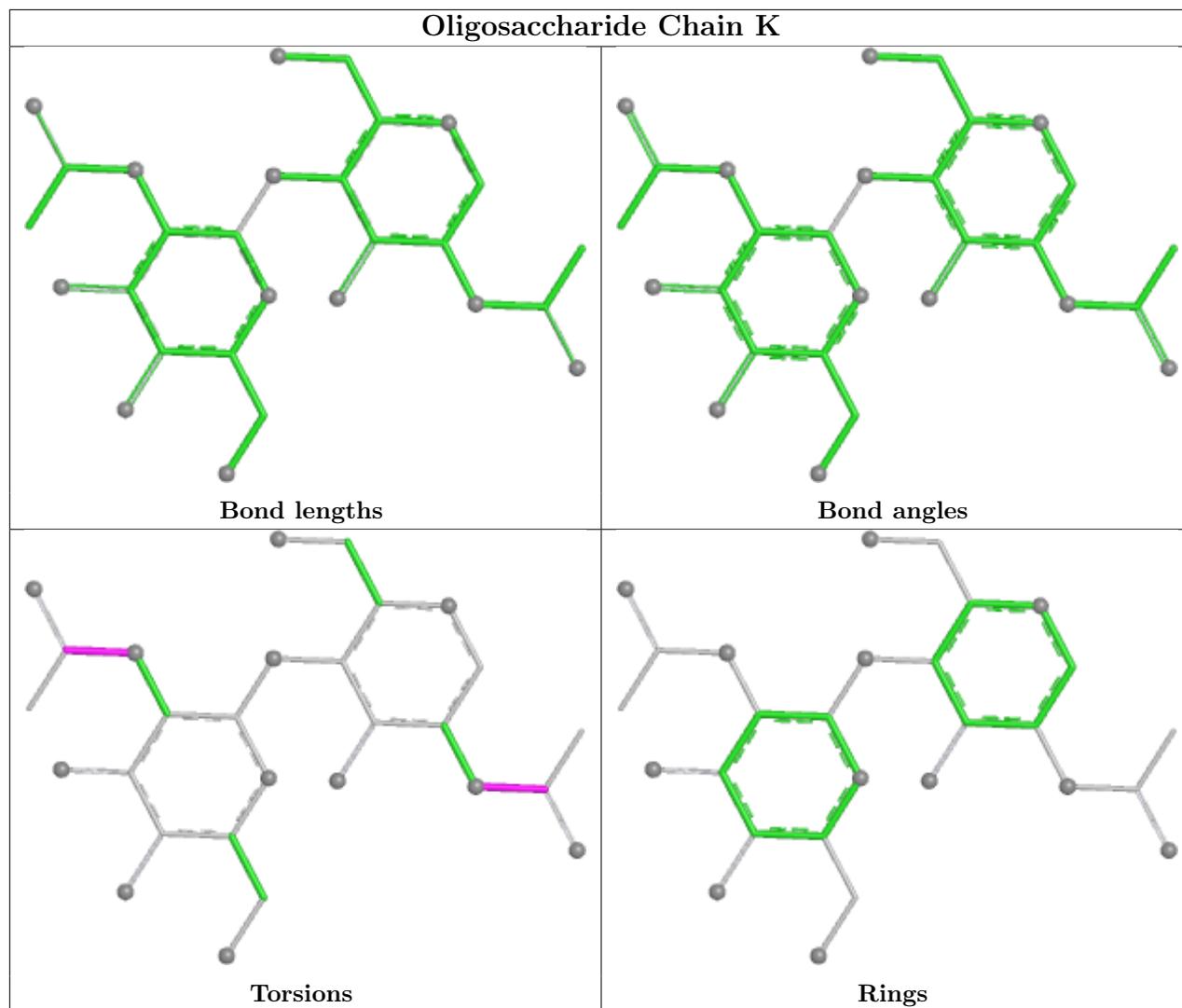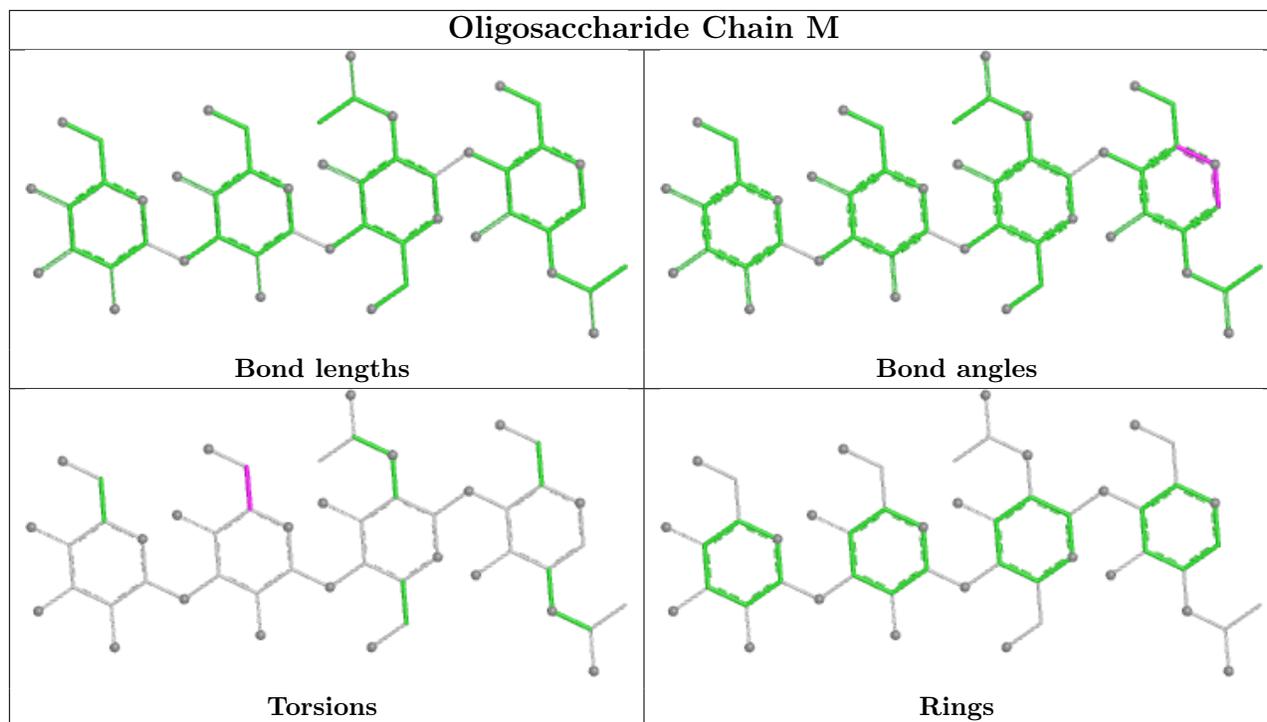
5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 14 are monoatomic - leaving 13 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	#$|Z| > 2$
9	GOL	C	1454	-	5,5,5	0.38	0	5,5,5	0.31	0
9	GOL	A	1455	-	5,5,5	0.39	0	5,5,5	0.11	0
9	GOL	C	1455	-	5,5,5	0.37	0	5,5,5	0.27	0
9	GOL	J	1498	-	5,5,5	0.37	0	5,5,5	0.29	0
9	GOL	A	1456	-	5,5,5	0.38	0	5,5,5	0.20	0
9	GOL	C	1457	-	5,5,5	0.38	0	5,5,5	0.19	0
9	GOL	C	1456	-	5,5,5	0.37	0	5,5,5	0.33	0
9	GOL	E	1220	-	5,5,5	0.39	0	5,5,5	0.24	0
10	SO4	A	1457	-	4,4,4	0.23	0	6,6,6	0.13	0
9	GOL	F	1216	-	5,5,5	0.36	0	5,5,5	0.27	0
10	SO4	A	1458	-	4,4,4	0.24	0	6,6,6	0.06	0
13	NAG	C	2015	1	14,14,15	0.54	0	17,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
9	GOL	F	1215	-	5,5,5	0.40	0	5,5,5	0.25	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
9	GOL	C	1454	-	-	2/4/4/4	-
9	GOL	A	1455	-	-	3/4/4/4	-
9	GOL	C	1455	-	-	2/4/4/4	-
9	GOL	J	1498	-	-	1/4/4/4	-
9	GOL	A	1456	-	-	2/4/4/4	-
9	GOL	C	1457	-	-	2/4/4/4	-
9	GOL	C	1456	-	-	2/4/4/4	-
9	GOL	E	1220	-	-	4/4/4/4	-
9	GOL	F	1216	-	-	2/4/4/4	-
13	NAG	C	2015	1	-	3/6/23/26	0/1/1/1
9	GOL	F	1215	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1455	GOL	O1-C1-C2-C3
9	C	1456	GOL	O1-C1-C2-C3
9	C	1457	GOL	O1-C1-C2-C3
9	E	1220	GOL	C1-C2-C3-O3
9	F	1215	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1457	GOL	1	0
10	A	1457	SO4	1	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(Å²)	Q<0.9
1	A	454/457 (99%)	0.33	2 (0%)	92	96	15, 26, 52, 116	4 (0%)
1	C	453/457 (99%)	0.25	7 (1%)	73	81	22, 38, 72, 130	1 (0%)
2	B	469/472 (99%)	0.87	69 (14%)	2	3	16, 48, 118, 193	127 (27%)
2	D	367/472 (77%)	2.08	119 (32%)	0	0	23, 53, 179, 217	76 (20%)
3	E	216/221 (97%)	0.02	5 (2%)	60	70	26, 42, 70, 107	0
3	H	216/221 (97%)	2.69	113 (52%)	0	0	49, 107, 160, 211	0
4	F	214/214 (100%)	0.42	13 (6%)	21	31	30, 48, 86, 192	2 (0%)
4	L	214/214 (100%)	3.07	117 (54%)	0	0	59, 114, 205, 233	1 (0%)
5	I	6/6 (100%)	1.55	2 (33%)	0	0	27, 33, 51, 56	0
5	J	6/6 (100%)	0.68	0	100	100	31, 38, 70, 72	0
All	All	2615/2740 (95%)	1.06	447 (17%)	1	2	15, 45, 157, 233	211 (8%)

The worst 5 of 447 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	409	GLU	24.2
4	L	181	LEU	21.2
4	L	214	CYS	15.6
4	L	130	ALA	15.2
2	D	395	VAL	13.7

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
7	NAG	K	2	14/15	0.60	0.38	112,122,145,150	0
8	MAN	M	4	11/12	0.70	0.43	106,115,138,138	0
8	BMA	M	3	11/12	0.74	0.29	103,113,135,136	0
6	BMA	G	3	11/12	0.82	0.16	58,74,92,95	0
6	MAN	G	4	11/12	0.85	0.13	65,72,87,89	0
8	NAG	M	2	14/15	0.85	0.23	66,86,99,105	0
6	MAN	G	6	11/12	0.85	0.15	71,78,92,95	0
7	NAG	K	1	14/15	0.85	0.24	77,95,114,119	0
6	MAN	G	5	11/12	0.89	0.15	73,78,93,95	0
8	NAG	M	1	14/15	0.92	0.12	41,55,74,79	0
6	NAG	G	2	14/15	0.96	0.14	34,48,64,68	0
6	NAG	G	1	14/15	0.97	0.16	16,30,47,55	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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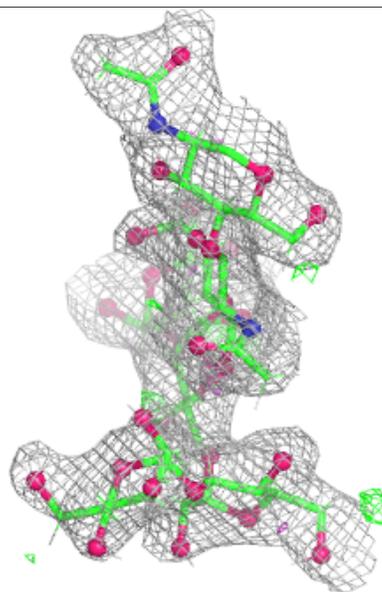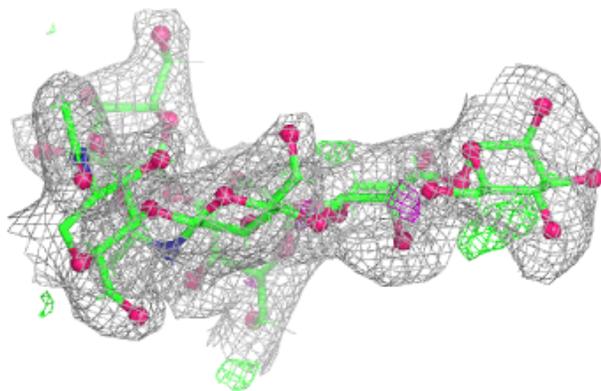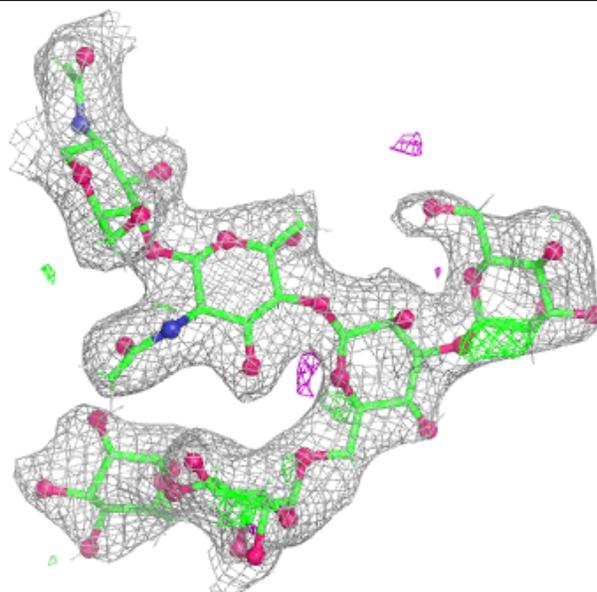
Electron density around Chain K:

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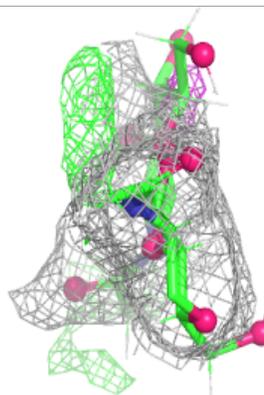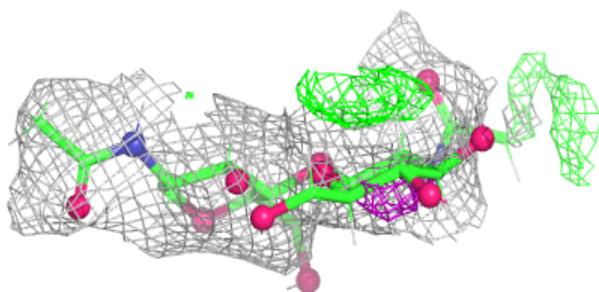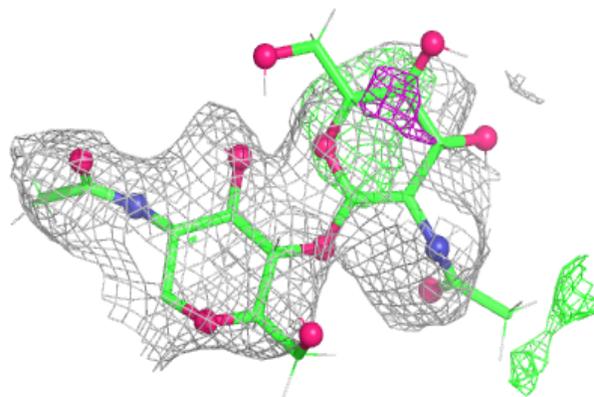
Electron density around Chain M:

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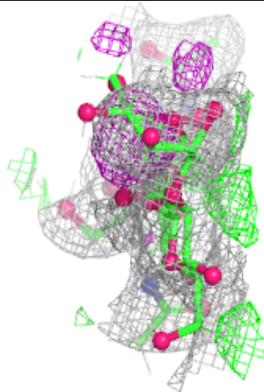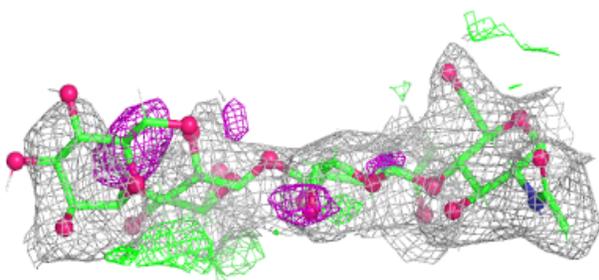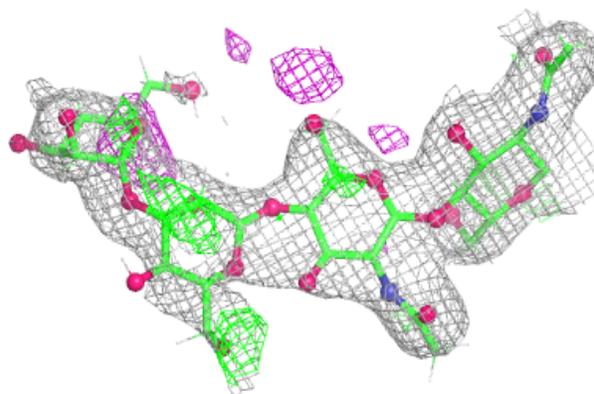
6.4 Ligands ⓘ

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
9	GOL	C	1454	6/6	0.65	0.39	86,104,110,114	0
13	NAG	C	2015	14/15	0.66	0.35	86,102,119,129	0
9	GOL	A	1456	6/6	0.69	0.29	64,84,100,103	0
9	GOL	C	1457	6/6	0.73	0.35	65,78,87,92	0
9	GOL	C	1455	6/6	0.81	0.20	85,102,105,107	0
9	GOL	E	1220	6/6	0.83	0.18	67,81,85,85	0
9	GOL	J	1498	6/6	0.84	0.29	68,82,86,88	0
9	GOL	F	1216	6/6	0.86	0.18	58,70,80,83	0
10	SO4	A	1458	5/5	0.87	0.23	95,97,98,102	0
9	GOL	F	1215	6/6	0.88	0.18	70,84,86,86	0
10	SO4	A	1457	5/5	0.88	0.22	72,79,82,82	0
9	GOL	A	1455	6/6	0.89	0.26	56,67,77,79	0
9	GOL	C	1456	6/6	0.92	0.23	62,79,89,95	0
12	MN	B	2002	1/1	0.97	0.17	52,52,52,52	0
11	CA	C	2007	1/1	0.98	0.14	41,41,41,41	0
11	CA	C	2004	1/1	0.98	0.11	53,53,53,53	0
11	CA	C	2005	1/1	0.98	0.15	46,46,46,46	0
11	CA	C	2006	1/1	0.99	0.12	42,42,42,42	0
12	MN	D	2003	1/1	0.99	0.12	33,33,33,33	0
11	CA	A	2006	1/1	0.99	0.17	19,19,19,19	0
12	MN	B	2001	1/1	1.00	0.20	23,23,23,23	0
11	CA	A	2004	1/1	1.00	0.14	27,27,27,27	0
12	MN	B	2003	1/1	1.00	0.13	28,28,28,28	0
12	MN	D	2001	1/1	1.00	0.20	25,25,25,25	0
12	MN	D	2002	1/1	1.00	0.18	30,30,30,30	0
11	CA	A	2007	1/1	1.00	0.17	23,23,23,23	0
11	CA	A	2005	1/1	1.00	0.16	23,23,23,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.