



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 06:30 AM BST

PDB ID : 5VL3
Title : CD22 d1-d3 in complex with therapeutic Fab Epratuzumab
Authors : Sicard, T.; Ereno-Orbea, J.; Julien, J.P.
Deposited on : 2017-04-24
Resolution : 3.10 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

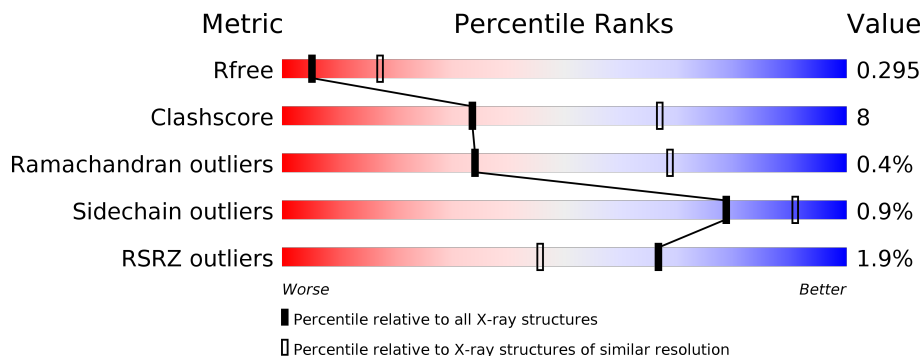
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	Q	323	
1	R	323	
1	S	323	
1	T	323	
2	A	222	
2	C	222	

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Mol	Chain	Length	Quality of chain
2	E	222	 4% 70% 22% 7%
2	H	222	 2% 79% 17%
3	B	222	 % 86% 10%
3	D	222	 86% 11%
3	F	222	 2% 83% 13%
3	L	222	 85% 11%
4	G	2	 100%
4	J	2	 100%
4	M	2	 100%
4	O	2	 100%
5	I	5	 60% 40%
6	K	4	 100%
6	P	4	 75% 25%
7	N	3	 33% 67%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 22912 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 B-cell receptor CD22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	303	2439	1544	415	467	13	0	0	0
1	R	290	2332	1478	393	448	13	0	0	0
1	S	299	2401	1518	409	461	13	0	0	0
1	T	289	2324	1471	395	445	13	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	18	THR	-	expression tag	UNP P20273
Q	19	GLY	-	expression tag	UNP P20273
Q	20	ASP	-	expression tag	UNP P20273
Q	21	SER	-	expression tag	UNP P20273
Q	67	GLN	ASN	engineered mutation	UNP P20273
Q	112	GLN	ASN	engineered mutation	UNP P20273
Q	135	GLN	ASN	engineered mutation	UNP P20273
Q	164	GLN	ASN	engineered mutation	UNP P20273
Q	331	GLY	-	expression tag	UNP P20273
Q	332	GLY	-	expression tag	UNP P20273
Q	333	THR	-	expression tag	UNP P20273
Q	334	LYS	-	expression tag	UNP P20273
Q	335	HIS	-	expression tag	UNP P20273
Q	336	HIS	-	expression tag	UNP P20273
Q	337	HIS	-	expression tag	UNP P20273
Q	338	HIS	-	expression tag	UNP P20273
Q	339	HIS	-	expression tag	UNP P20273
Q	340	HIS	-	expression tag	UNP P20273
R	18	THR	-	expression tag	UNP P20273
R	19	GLY	-	expression tag	UNP P20273
R	20	ASP	-	expression tag	UNP P20273

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Chain	Residue	Modelled	Actual	Comment	Reference
R	21	SER	-	expression tag	UNP P20273
R	67	GLN	ASN	engineered mutation	UNP P20273
R	112	GLN	ASN	engineered mutation	UNP P20273
R	135	GLN	ASN	engineered mutation	UNP P20273
R	164	GLN	ASN	engineered mutation	UNP P20273
R	331	GLY	-	expression tag	UNP P20273
R	332	GLY	-	expression tag	UNP P20273
R	333	THR	-	expression tag	UNP P20273
R	334	LYS	-	expression tag	UNP P20273
R	335	HIS	-	expression tag	UNP P20273
R	336	HIS	-	expression tag	UNP P20273
R	337	HIS	-	expression tag	UNP P20273
R	338	HIS	-	expression tag	UNP P20273
R	339	HIS	-	expression tag	UNP P20273
R	340	HIS	-	expression tag	UNP P20273
S	18	THR	-	expression tag	UNP P20273
S	19	GLY	-	expression tag	UNP P20273
S	20	ASP	-	expression tag	UNP P20273
S	21	SER	-	expression tag	UNP P20273
S	67	GLN	ASN	engineered mutation	UNP P20273
S	112	GLN	ASN	engineered mutation	UNP P20273
S	135	GLN	ASN	engineered mutation	UNP P20273
S	164	GLN	ASN	engineered mutation	UNP P20273
S	331	GLY	-	expression tag	UNP P20273
S	332	GLY	-	expression tag	UNP P20273
S	333	THR	-	expression tag	UNP P20273
S	334	LYS	-	expression tag	UNP P20273
S	335	HIS	-	expression tag	UNP P20273
S	336	HIS	-	expression tag	UNP P20273
S	337	HIS	-	expression tag	UNP P20273
S	338	HIS	-	expression tag	UNP P20273
S	339	HIS	-	expression tag	UNP P20273
S	340	HIS	-	expression tag	UNP P20273
T	18	THR	-	expression tag	UNP P20273
T	19	GLY	-	expression tag	UNP P20273
T	20	ASP	-	expression tag	UNP P20273
T	21	SER	-	expression tag	UNP P20273
T	67	GLN	ASN	engineered mutation	UNP P20273
T	112	GLN	ASN	engineered mutation	UNP P20273
T	135	GLN	ASN	engineered mutation	UNP P20273
T	164	GLN	ASN	engineered mutation	UNP P20273
T	331	GLY	-	expression tag	UNP P20273

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Chain	Residue	Modelled	Actual	Comment	Reference
T	332	GLY	-	expression tag	UNP P20273
T	333	THR	-	expression tag	UNP P20273
T	334	LYS	-	expression tag	UNP P20273
T	335	HIS	-	expression tag	UNP P20273
T	336	HIS	-	expression tag	UNP P20273
T	337	HIS	-	expression tag	UNP P20273
T	338	HIS	-	expression tag	UNP P20273
T	339	HIS	-	expression tag	UNP P20273
T	340	HIS	-	expression tag	UNP P20273

- Molecule 2 is a protein called Epratuzumab Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	214	Total 1640	C 1038	N 274	O 323	S 5	0	0	0
2	C	212	Total 1625	C 1029	N 271	O 320	S 5	0	0	0
2	E	207	Total 1595	C 1012	N 266	O 312	S 5	0	0	0
2	H	214	Total 1640	C 1038	N 274	O 323	S 5	0	0	0

- Molecule 3 is a protein called Epratuzumab Fab Light Chain.

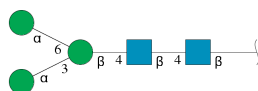
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	213	Total 1642	C 1031	N 274	O 332	S 5	0	0	0
3	D	216	Total 1672	C 1050	N 281	O 336	S 5	0	0	0
3	F	213	Total 1642	C 1031	N 274	O 332	S 5	0	0	0
3	L	213	Total 1642	C 1031	N 274	O 332	S 5	0	0	0

- Molecule 4 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
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	O	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called 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.



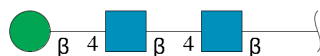
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 is an oligosaccharide called 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.



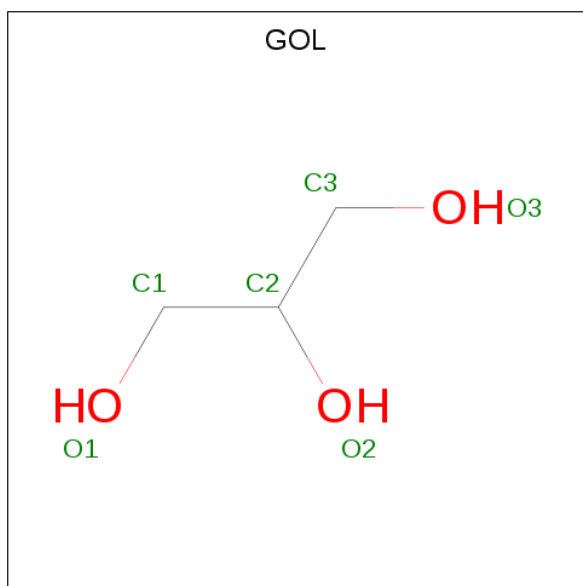
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	K	4	Total	C	N	O	0	0	0
			50	28	2	20			
6	P	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 is an oligosaccharide called 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
			Total	C	N	O			
7	N	3	39	22	2	15	0	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

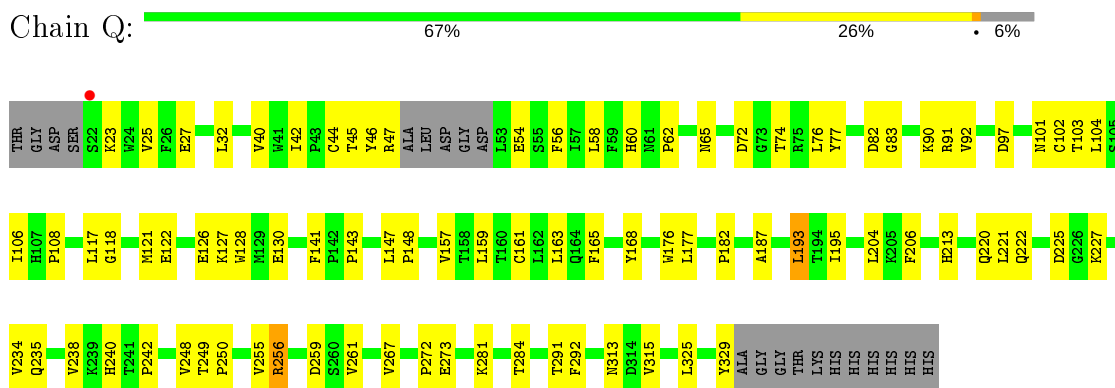


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	S	1	6	3	3	0	0

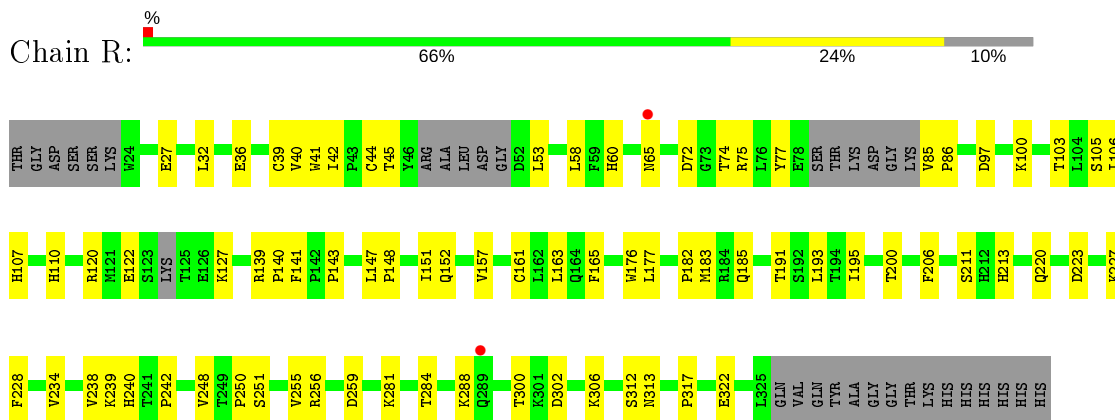
3 Residue-property plots [i](#)

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.

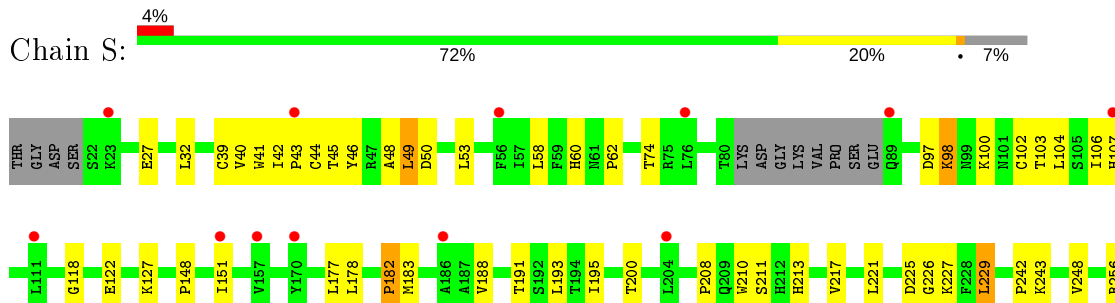
- Molecule 1: B-cell receptor CD22

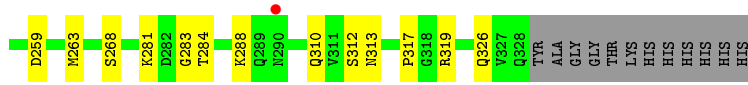


- Molecule 1: B-cell receptor CD22

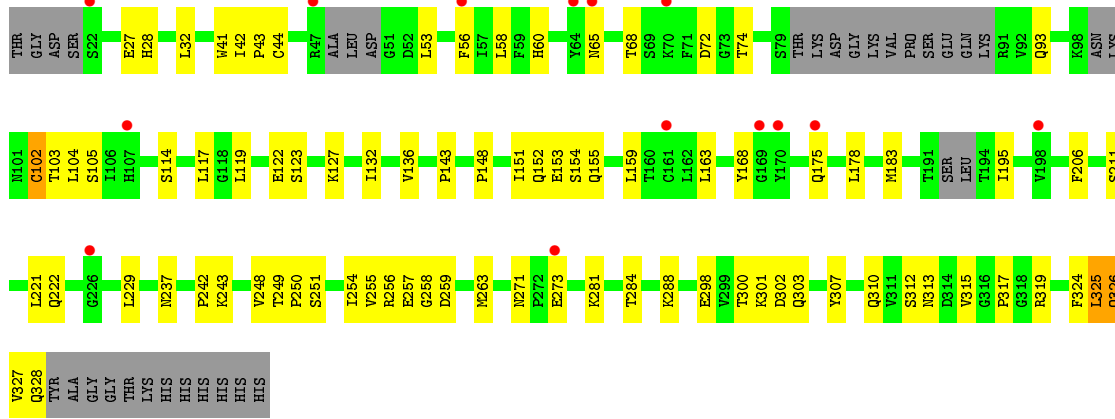


- Molecule 1: B-cell receptor CD22

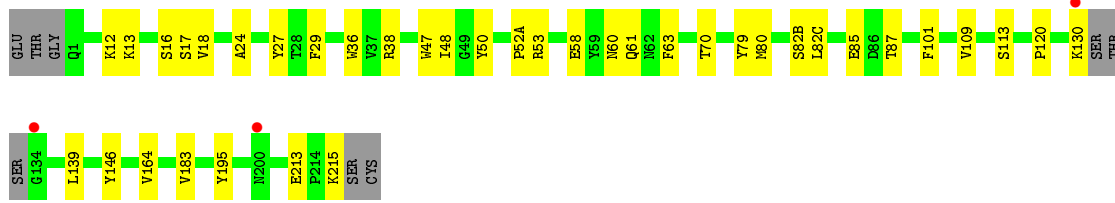
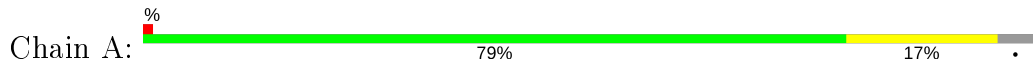




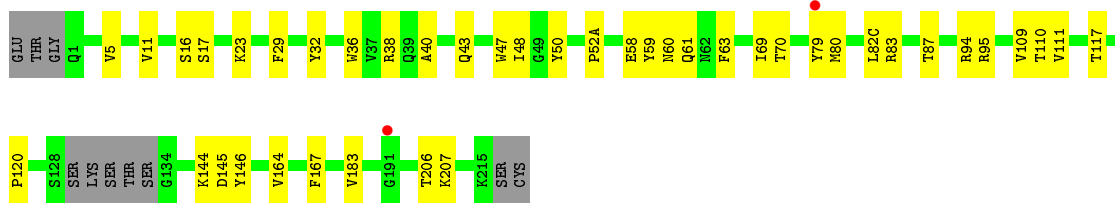
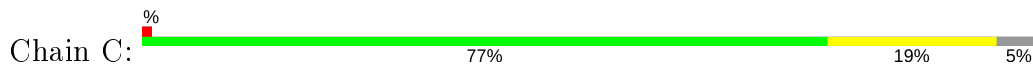
• Molecule 1: B-cell receptor CD22



• Molecule 2: Epratuzumab Fab Heavy Chain

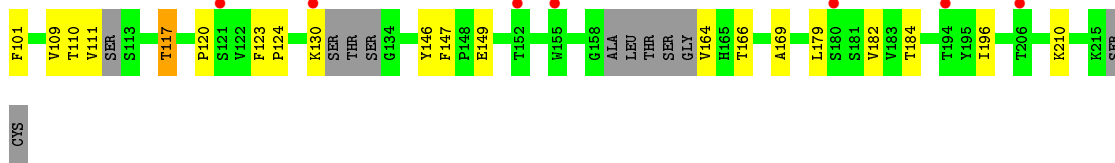


• Molecule 2: Epratuzumab Fab Heavy Chain

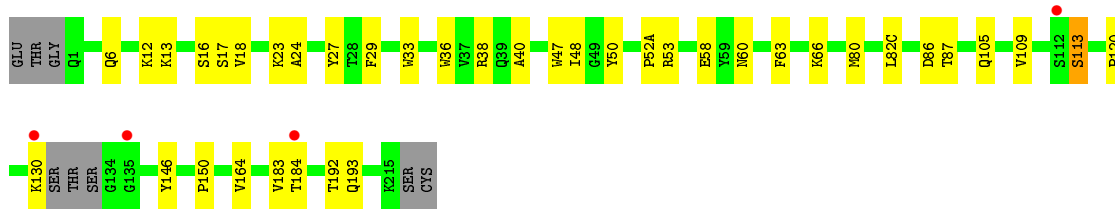
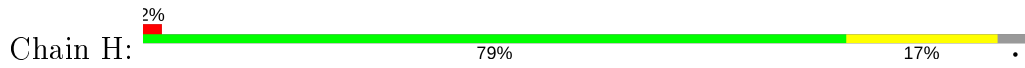


• Molecule 2: Epratuzumab Fab Heavy Chain

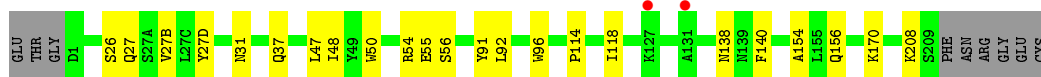
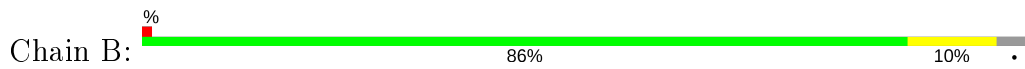




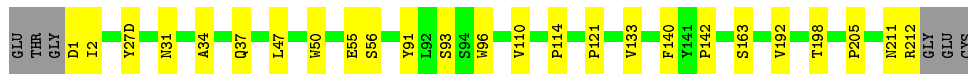
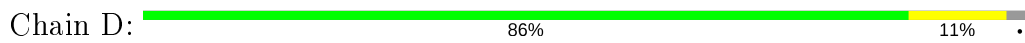
• Molecule 2: Epratuzumab Fab Heavy Chain



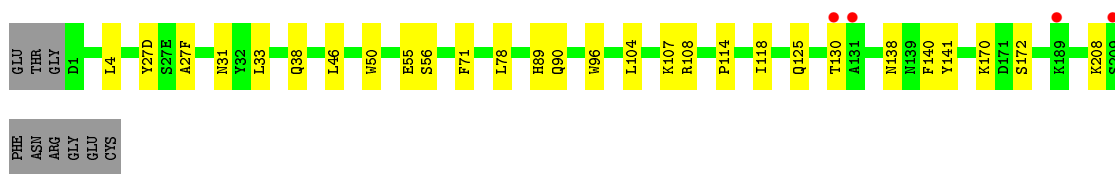
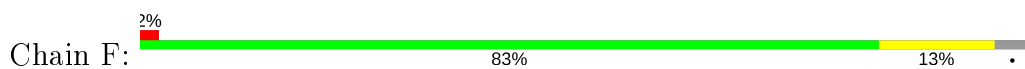
• Molecule 3: Epratuzumab Fab Light Chain



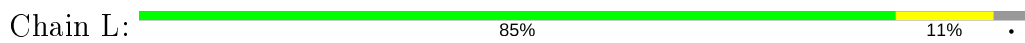
• Molecule 3: Epratuzumab Fab Light Chain



• Molecule 3: Epratuzumab Fab Light Chain



• Molecule 3: Epratuzumab Fab Light Chain



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

Chain G:  100%


NAG1
NAG2

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

Chain J:  100%

NAG1
NAG2

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

Chain M:  100%

NAG1
NAG2

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

Chain O:  100%


NAG1
NAG2

- 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 I:  60% 40%

NAG1
NAG2
BMA3
MAN4
MAN5

- Molecule 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

Chain K:  100%

NAG1
NAG2
BMA3
MAN4

- Molecule 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

Chain P:  75% 25%



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	87.11Å 90.22Å 136.63Å 70.83° 80.81° 80.99°	Depositor
Resolution (Å)	39.34 – 3.10 39.34 – 3.10	Depositor EDS
% Data completeness (in resolution range)	94.2 (39.34-3.10) 94.2 (39.34-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.12Å)	Xtrriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.280 , 0.295 0.280 , 0.295	Depositor DCC
R_{free} test set	2000 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å ²)	65.7	Xtrriage
Anisotropy	0.442	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	22912	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	Q	0.31	0/2498	0.58	0/3388
1	R	0.28	0/2388	0.58	0/3241
1	S	0.29	0/2458	0.58	1/3335 (0.0%)
1	T	0.29	0/2378	0.57	0/3223
2	A	0.28	0/1682	0.52	0/2293
2	C	0.28	0/1667	0.54	0/2274
2	E	0.28	0/1635	0.55	0/2226
2	H	0.28	0/1682	0.54	0/2293
3	B	0.27	0/1680	0.52	0/2282
3	D	0.26	0/1711	0.50	0/2323
3	F	0.26	0/1680	0.50	1/2282 (0.0%)
3	L	0.28	0/1680	0.52	0/2282
All	All	0.28	0/23139	0.55	2/31442 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	38	GLN	C-N-CA	5.33	135.03	121.70
1	S	229	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	2439	0	2387	62	1
1	R	2332	0	2266	51	0
1	S	2401	0	2345	42	2
1	T	2324	0	2259	65	1
2	A	1640	0	1591	27	0
2	C	1625	0	1573	22	0
2	E	1595	0	1542	45	0
2	H	1640	0	1591	26	0
3	B	1642	0	1598	18	0
3	D	1672	0	1626	17	0
3	F	1642	0	1598	22	0
3	L	1642	0	1598	17	0
4	G	28	0	25	0	0
4	J	28	0	25	0	0
4	M	28	0	25	1	0
4	O	28	0	25	0	0
5	I	61	0	52	4	0
6	K	50	0	43	2	0
6	P	50	0	43	4	0
7	N	39	0	34	2	0
8	S	6	0	8	1	0
All	All	22912	0	22254	382	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 382 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:Q:65:ASN:ND2	1:Q:72:ASP:OD2	1.95	1.00
1:R:65:ASN:ND2	1:R:72:ASP:OD2	1.99	0.95
1:R:147:LEU:HD11	1:R:234:VAL:HG11	1.52	0.89
2:E:50:TYR:HE2	2:E:58:GLU:HB2	1.47	0.78
2:H:130:LYS:HB3	3:L:208:LYS:NZ	1.99	0.78

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:127:LYS:NZ	1:S:122:GLU:OE2[1_556]	1.93	0.27
1:S:283:GLY:O	1:T:154:SER:OG[1_655]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	299/323 (93%)	287 (96%)	11 (4%)	1 (0%)	41	73
1	R	282/323 (87%)	271 (96%)	10 (4%)	1 (0%)	34	69
1	S	295/323 (91%)	280 (95%)	13 (4%)	2 (1%)	22	57
1	T	279/323 (86%)	266 (95%)	11 (4%)	2 (1%)	22	57
2	A	210/222 (95%)	201 (96%)	8 (4%)	1 (0%)	29	64
2	C	208/222 (94%)	198 (95%)	9 (4%)	1 (0%)	29	64
2	E	199/222 (90%)	191 (96%)	7 (4%)	1 (0%)	29	64
2	H	210/222 (95%)	203 (97%)	6 (3%)	1 (0%)	29	64
3	B	211/222 (95%)	202 (96%)	9 (4%)	0	100	100
3	D	214/222 (96%)	203 (95%)	11 (5%)	0	100	100
3	F	211/222 (95%)	203 (96%)	8 (4%)	0	100	100
3	L	211/222 (95%)	203 (96%)	8 (4%)	0	100	100
All	All	2829/3068 (92%)	2708 (96%)	111 (4%)	10 (0%)	34	69

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	226	GLY
2	C	117	THR
2	A	82(B)	SER
2	E	117	THR
1	T	326	GLN

5.3.2 Protein sidechains [i](#)

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	Q	282/296 (95%)	278 (99%)	4 (1%)	67	86
1	R	270/296 (91%)	270 (100%)	0	100	100
1	S	277/296 (94%)	271 (98%)	6 (2%)	52	78
1	T	268/296 (90%)	265 (99%)	3 (1%)	73	89
2	A	184/191 (96%)	183 (100%)	1 (0%)	88	94
2	C	182/191 (95%)	180 (99%)	2 (1%)	73	89
2	E	179/191 (94%)	177 (99%)	2 (1%)	73	89
2	H	184/191 (96%)	182 (99%)	2 (1%)	73	89
3	B	188/195 (96%)	187 (100%)	1 (0%)	88	94
3	D	191/195 (98%)	191 (100%)	0	100	100
3	F	188/195 (96%)	188 (100%)	0	100	100
3	L	188/195 (96%)	187 (100%)	1 (0%)	88	94
All	All	2581/2728 (95%)	2559 (99%)	22 (1%)	78	91

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	326	GLN
1	T	325	LEU
3	B	138	ASN
1	T	102	CYS
1	T	254	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	T	222	GLN
3	L	138	ASN
2	H	165	HIS
1	T	173	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	138	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

24 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
4	NAG	G	1	1,4	14,14,15	0.25	0	17,19,21	0.59	0
4	NAG	G	2	4	14,14,15	0.22	0	17,19,21	0.44	0
5	NAG	I	1	1,5	14,14,15	0.27	0	17,19,21	0.46	0
5	NAG	I	2	5	14,14,15	0.62	0	17,19,21	0.49	0
5	BMA	I	3	5	11,11,12	1.21	2 (18%)	15,15,17	1.44	2 (13%)
5	MAN	I	4	5	11,11,12	0.71	0	15,15,17	1.27	2 (13%)
5	MAN	I	5	5	11,11,12	0.71	0	15,15,17	0.98	2 (13%)
4	NAG	J	1	1,4	14,14,15	0.24	0	17,19,21	0.54	0
4	NAG	J	2	4	14,14,15	0.24	0	17,19,21	0.49	0
6	NAG	K	1	1,6	14,14,15	0.28	0	17,19,21	0.50	0
6	NAG	K	2	6	14,14,15	0.42	0	17,19,21	0.40	0
6	BMA	K	3	6	11,11,12	0.93	1 (9%)	15,15,17	1.13	2 (13%)
6	MAN	K	4	6	11,11,12	0.62	0	15,15,17	1.19	2 (13%)
4	NAG	M	1	1,4	14,14,15	0.53	0	17,19,21	0.47	0
4	NAG	M	2	4	14,14,15	0.21	0	17,19,21	0.52	0
7	NAG	N	1	1,7	14,14,15	0.24	0	17,19,21	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	N	2	7	14,14,15	0.27	0	17,19,21	0.53	0
7	BMA	N	3	7	11,11,12	0.69	0	15,15,17	0.77	0
4	NAG	O	1	1,4	14,14,15	0.27	0	17,19,21	0.72	0
4	NAG	O	2	4	14,14,15	0.26	0	17,19,21	0.41	0
6	NAG	P	1	1,6	14,14,15	0.21	0	17,19,21	0.46	0
6	NAG	P	2	6	14,14,15	0.32	0	17,19,21	0.42	0
6	BMA	P	3	6	11,11,12	0.84	0	15,15,17	1.10	1 (6%)
6	MAN	P	4	6	11,11,12	0.64	0	15,15,17	1.07	2 (13%)

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	G	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	I	2	5	-	4/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
5	MAN	I	4	5	-	2/2/19/22	0/1/1/1
5	MAN	I	5	5	-	0/2/19/22	1/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
6	NAG	K	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1
6	BMA	K	3	6	-	0/2/19/22	0/1/1/1
6	MAN	K	4	6	-	2/2/19/22	0/1/1/1
4	NAG	M	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
7	NAG	N	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	N	2	7	-	2/6/23/26	0/1/1/1
7	BMA	N	3	7	-	0/2/19/22	0/1/1/1
4	NAG	O	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
6	NAG	P	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	P	2	6	-	2/6/23/26	0/1/1/1
6	BMA	P	3	6	-	0/2/19/22	0/1/1/1
6	MAN	P	4	6	-	1/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	3	BMA	O5-C1	-2.71	1.39	1.43
5	I	3	BMA	C4-C5	2.19	1.57	1.53
6	K	3	BMA	O5-C1	-2.17	1.40	1.43

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	4	MAN	C1-O5-C5	3.60	117.08	112.19
6	K	4	MAN	C1-O5-C5	3.51	116.95	112.19
5	I	3	BMA	C3-C4-C5	3.21	115.96	110.24
6	P	4	MAN	C1-O5-C5	2.97	116.21	112.19
5	I	3	BMA	C1-O5-C5	2.59	115.70	112.19

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	4	MAN	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
5	I	4	MAN	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	5	MAN	C1-C2-C3-C4-C5-O5

13 monomers are involved in 13 short contacts:

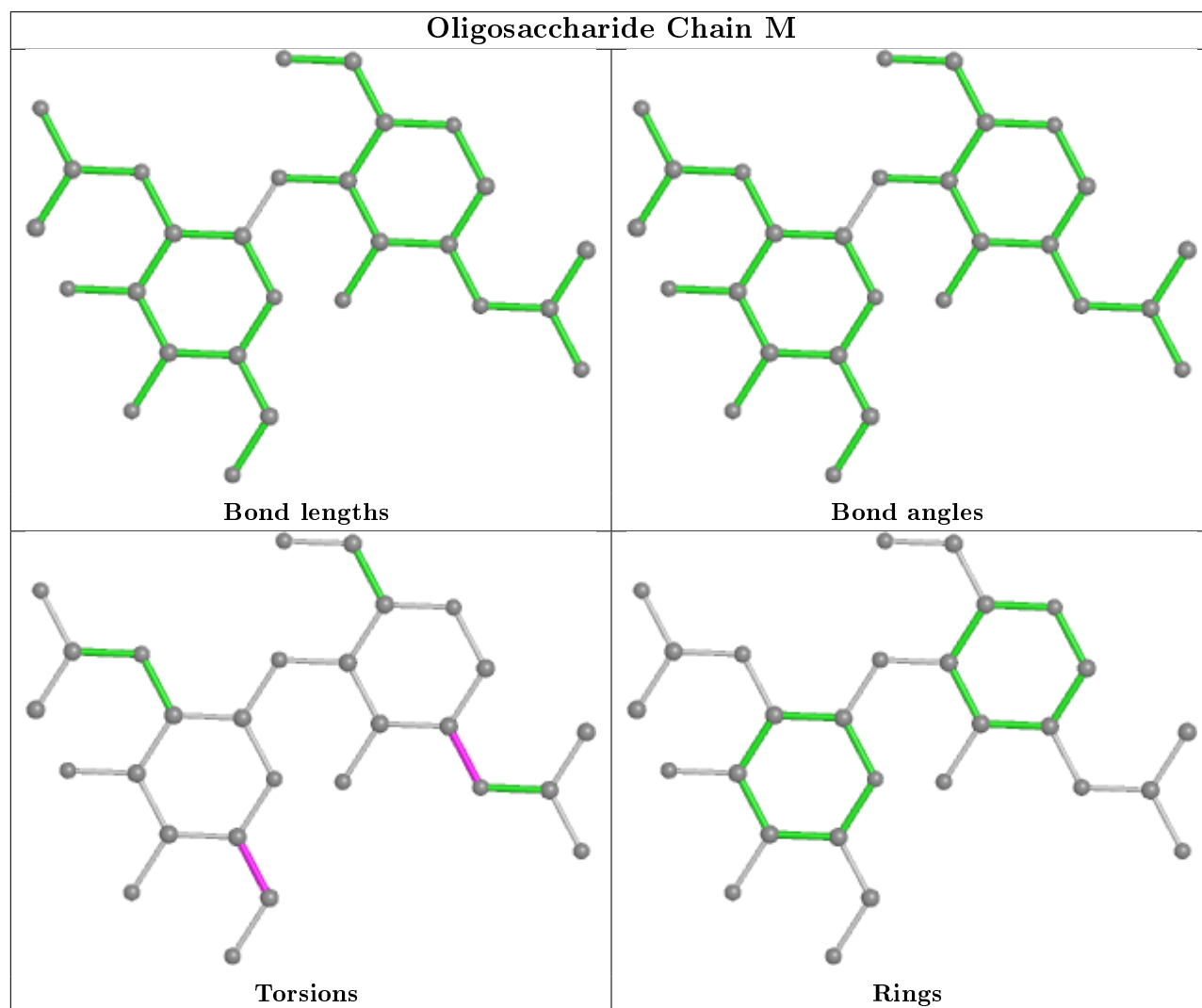
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	N	2	NAG	1	0
6	P	3	BMA	1	0
6	K	2	NAG	1	0
6	K	1	NAG	2	0
4	M	2	NAG	1	0
4	M	1	NAG	1	0
6	P	1	NAG	2	0
5	I	5	MAN	1	0
7	N	1	NAG	2	0
5	I	3	BMA	1	0

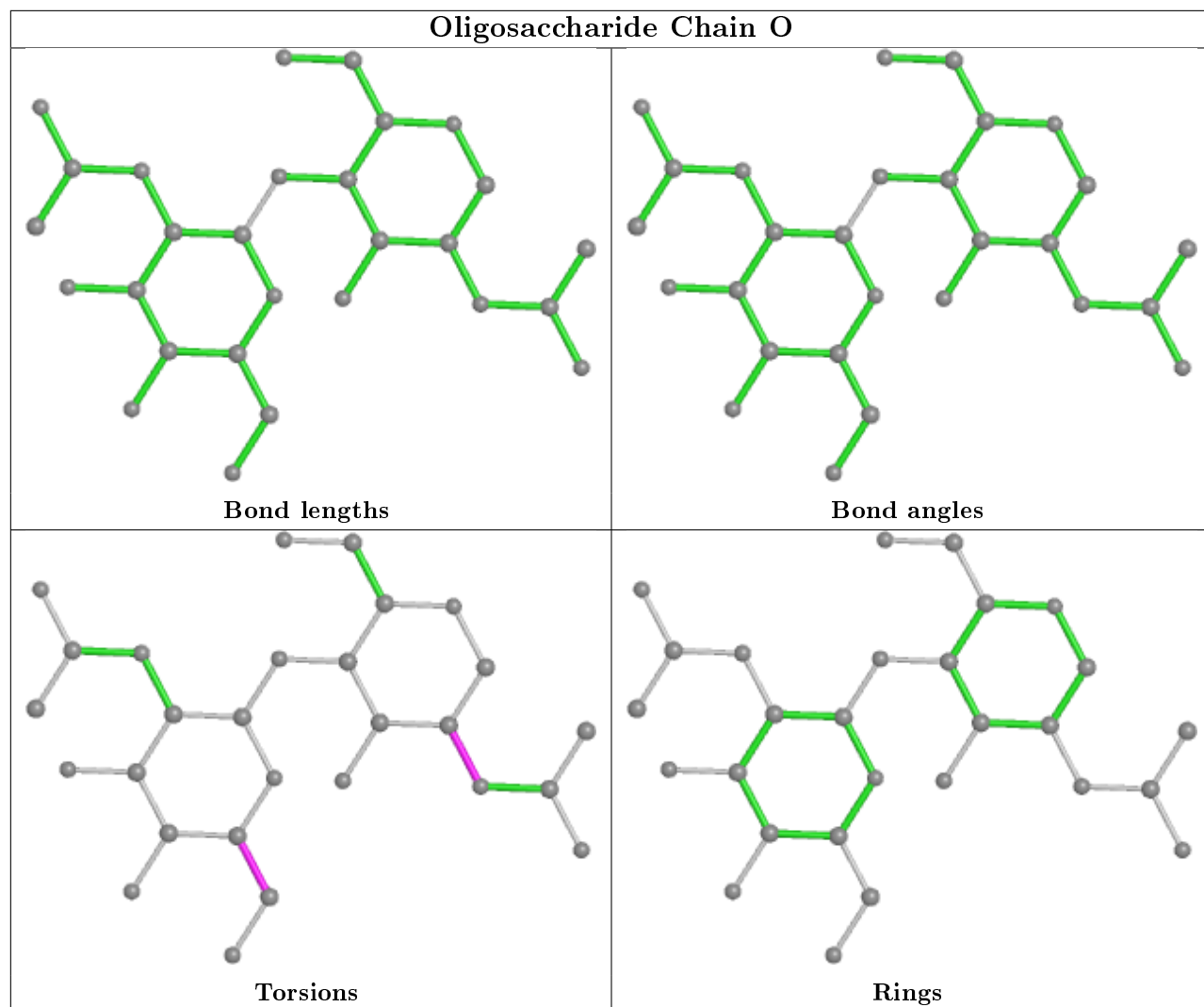
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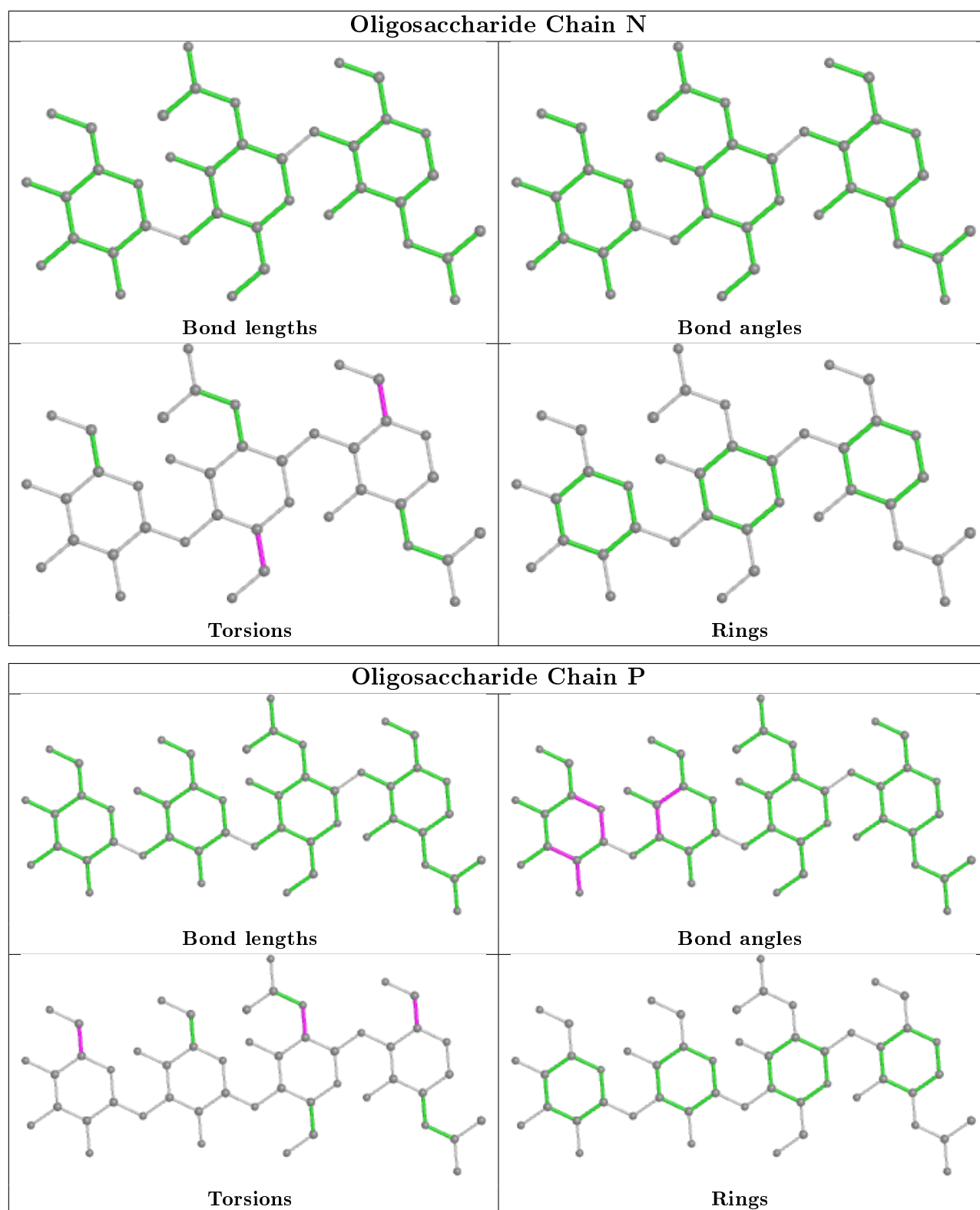
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	P	2	NAG	1	0
5	I	2	NAG	1	0
5	I	1	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







5.6 Ligand geometry [i](#)

1 ligand is 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
8	GOL	S	1006	-	5,5,5	0.91	0	5,5,5	0.98	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
8	GOL	S	1006	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	S	1006	GOL	O1-C1-C2-C3
8	S	1006	GOL	C1-C2-C3-O3
8	S	1006	GOL	O2-C2-C3-O3
8	S	1006	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	S	1006	GOL	1	0

5.7 Other polymers [\(i\)](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	Q	303/323 (93%)	-0.19	1 (0%) 94 88	34, 58, 81, 95	0
1	R	290/323 (89%)	-0.10	2 (0%) 87 75	31, 63, 99, 112	0
1	S	299/323 (92%)	0.35	13 (4%) 35 17	65, 97, 114, 125	0
1	T	289/323 (89%)	0.42	14 (4%) 30 14	64, 97, 118, 144	0
2	A	214/222 (96%)	-0.16	3 (1%) 75 56	30, 62, 101, 118	0
2	C	212/222 (95%)	0.11	2 (0%) 84 69	51, 75, 91, 107	0
2	E	207/222 (93%)	0.42	9 (4%) 35 17	68, 101, 119, 127	0
2	H	214/222 (96%)	-0.17	4 (1%) 66 46	30, 53, 99, 116	0
3	B	213/222 (95%)	-0.19	2 (0%) 84 69	26, 50, 91, 106	0
3	D	216/222 (97%)	-0.08	0 100 100	54, 66, 80, 98	0
3	F	213/222 (95%)	0.16	4 (1%) 66 46	57, 78, 111, 126	0
3	L	213/222 (95%)	-0.35	0 100 100	26, 49, 86, 98	0
All	All	2883/3068 (93%)	0.03	54 (1%) 66 46	26, 71, 109, 144	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	169	GLY	6.2
2	E	130	LYS	5.8
2	E	206	THR	4.0
2	E	155	TRP	3.8
2	H	112	SER	3.6

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

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

6.3 Carbohydrates i

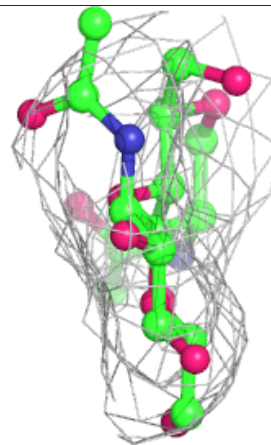
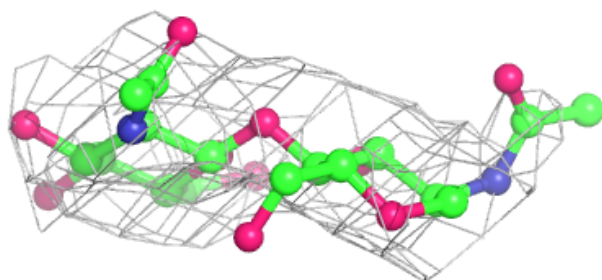
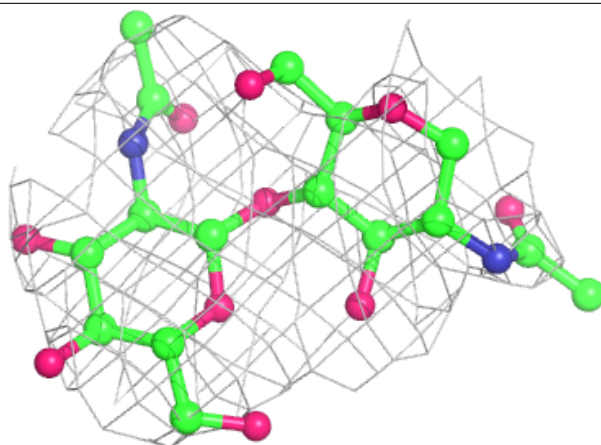
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	BMA	N	3	11/12	0.50	0.25	108,117,122,125	0
5	MAN	I	5	11/12	0.59	0.23	89,106,114,116	0
6	NAG	P	2	14/15	0.63	0.25	89,113,120,129	0
4	NAG	O	2	14/15	0.69	0.28	101,123,133,142	0
7	NAG	N	2	14/15	0.70	0.17	88,113,121,128	0
6	MAN	P	4	11/12	0.71	0.40	103,122,130,141	0
4	NAG	O	1	14/15	0.72	0.31	100,115,121,123	0
4	NAG	M	1	14/15	0.77	0.27	99,113,119,121	0
6	NAG	K	2	14/15	0.78	0.18	59,86,94,99	0
5	MAN	I	4	11/12	0.79	0.28	83,98,106,119	0
6	NAG	P	1	14/15	0.80	0.17	91,102,107,108	0
5	NAG	I	2	14/15	0.81	0.20	58,83,91,99	0
4	NAG	J	2	14/15	0.82	0.19	49,70,78,90	0
6	BMA	P	3	11/12	0.83	0.16	110,119,125,128	0
6	MAN	K	4	11/12	0.85	0.26	86,104,112,124	0
4	NAG	G	2	14/15	0.86	0.22	48,71,81,90	0
4	NAG	J	1	14/15	0.86	0.16	54,68,73,76	0
4	NAG	M	2	14/15	0.86	0.17	94,116,125,135	0
7	NAG	N	1	14/15	0.87	0.17	90,101,106,108	0
5	BMA	I	3	11/12	0.89	0.14	86,96,101,105	0
6	NAG	K	1	14/15	0.90	0.15	66,75,79,81	0
5	NAG	I	1	14/15	0.92	0.15	57,68,73,76	0
4	NAG	G	1	14/15	0.93	0.13	57,71,78,79	0
6	BMA	K	3	11/12	0.93	0.13	86,95,101,105	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.

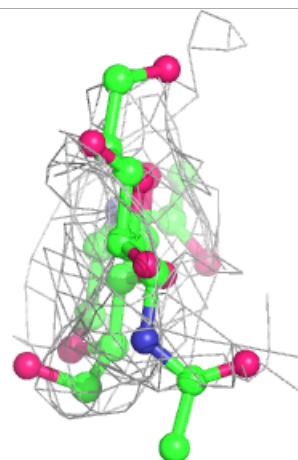
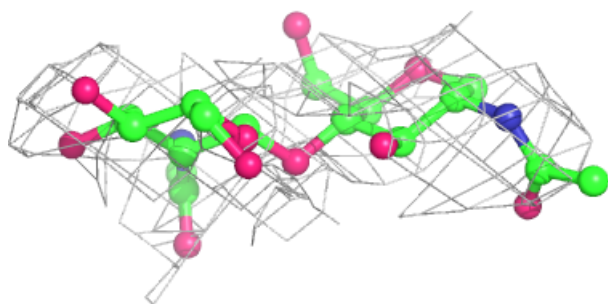
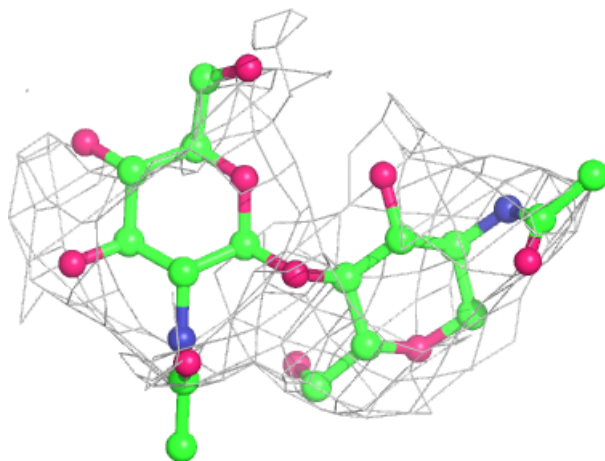
Electron density around Chain M:

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



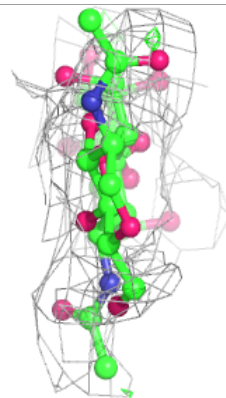
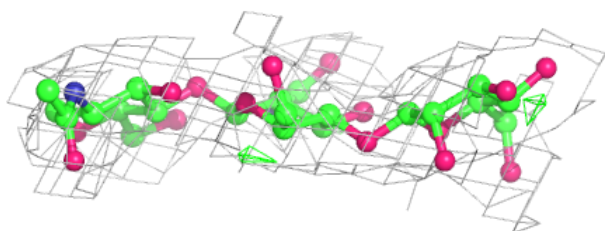
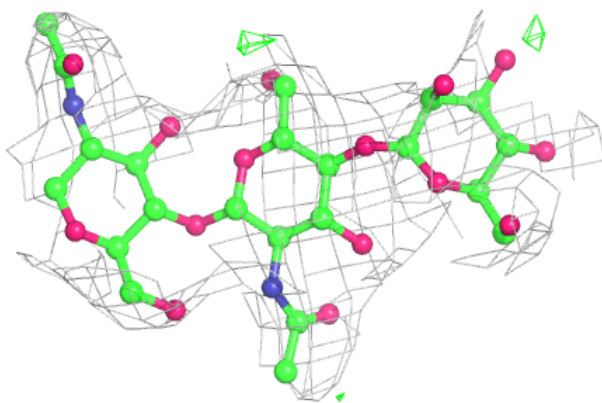
Electron density around Chain O:

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

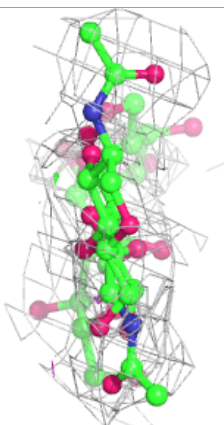
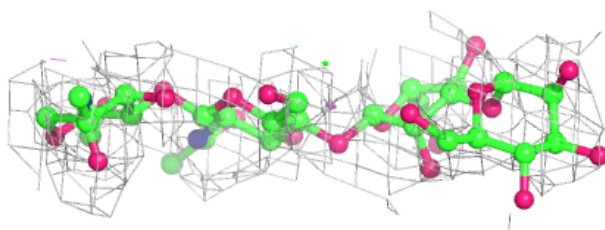
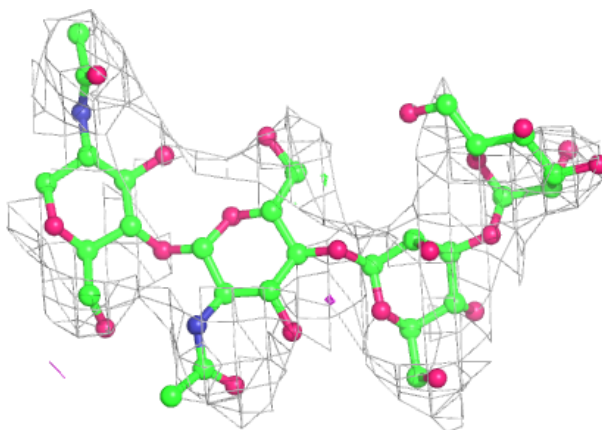


Electron density around Chain N:

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

**Electron density around Chain P:**

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



6.4 Ligands [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(\AA^2)	Q<0.9
8	GOL	S	1006	6/6	0.87	0.16	82,82,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.