



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:25 AM UTC

PDB ID : 4UFA / pdb_00004ufa
Title : Crystal structure of the Angiotensin-1 converting enzyme N-domain in complex with Ac-SD
Authors : Masuyer, G.; Douglas, R.G.; Sturrock, E.D.; Acharya, K.R.
Deposited on : 2015-03-16
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

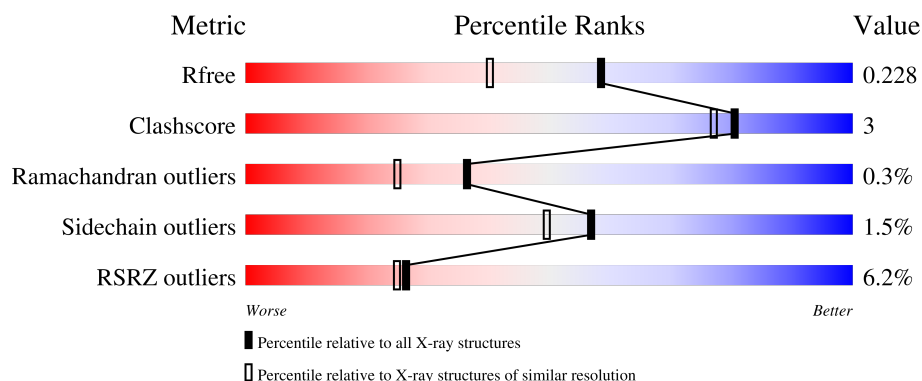
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



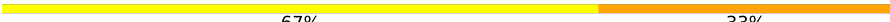
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	629	4% 90% 6%
1	B	629	8% 89% 7%
2	C	2	100%
3	D	4	25% 75%
4	E	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	3	 67% 33%

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
11	SAC	A	1301	-	-	X	-
11	SAC	B	1301	-	-	X	-
12	ASP	A	1302	-	-	X	-
12	ASP	B	1302	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 10977 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ANGIOTENSIN-CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	607	Total	C	N	O	S	0	2	0
			4967	3190	854	904	19			
1	B	607	Total	C	N	O	S	0	0	0
			4941	3175	847	900	19			

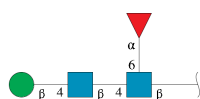
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	629	LEU	-	expression tag	UNP P12821
A	9	GLN	ASN	engineered mutation	UNP P12821
A	25	GLN	ASN	engineered mutation	UNP P12821
A	82	GLN	ASN	engineered mutation	UNP P12821
A	117	GLN	ASN	engineered mutation	UNP P12821
A	131	GLN	ASN	engineered mutation	UNP P12821
A	289	GLN	ASN	engineered mutation	UNP P12821
A	545	ARG	GLN	engineered mutation	UNP P12821
A	576	LEU	PRO	engineered mutation	UNP P12821
B	629	LEU	-	expression tag	UNP P12821
B	9	GLN	ASN	engineered mutation	UNP P12821
B	25	GLN	ASN	engineered mutation	UNP P12821
B					



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

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			24</						

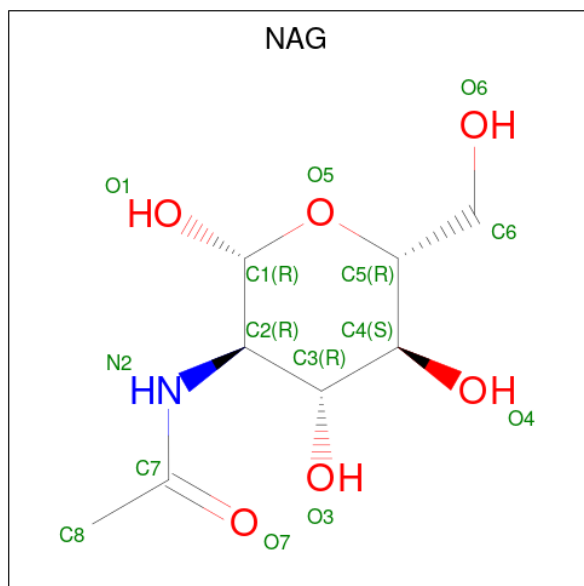
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		
6	B	1	Total	Zn	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

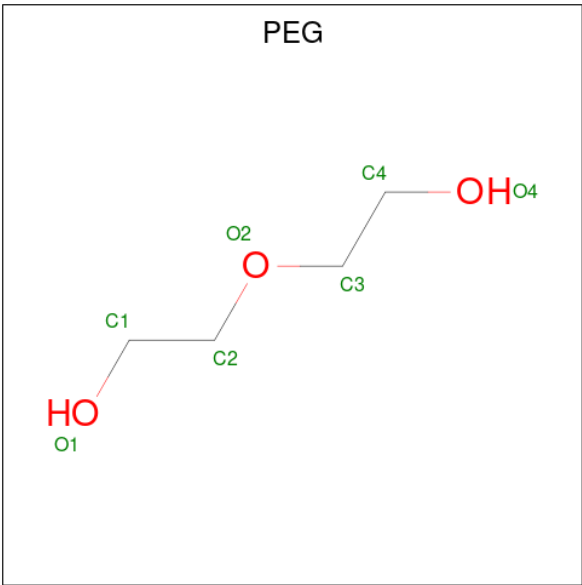
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	B	1	Total	Cl	0	0
			1	1		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



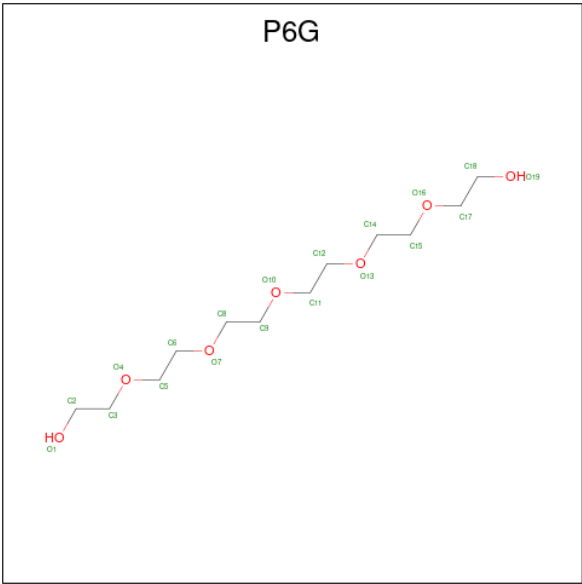
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



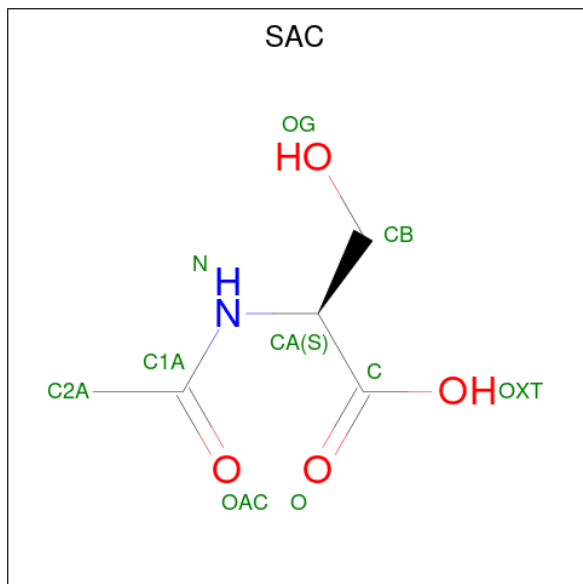
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



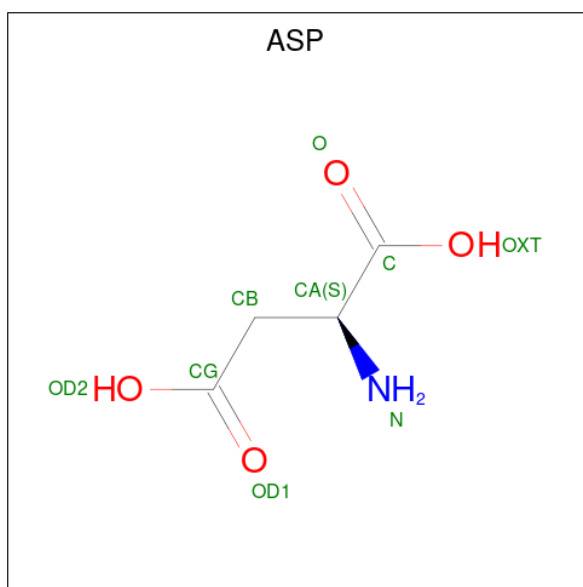
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			19	12	7		
10	B	1	Total	C	O	0	0
			19	12	7		
10	B	1	Total	C	O	0	0
			19	12	7		

- Molecule 11 is N-ACETYL-SERINE (CCD ID: SAC) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	0	0
			9	5	1	3		
11	B	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 12 is ASPARTIC ACID (CCD ID: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	N	O	0	0
			9	4	1	4		
12	B	1	Total	C	N	O	0	0
			9	4	1	4		

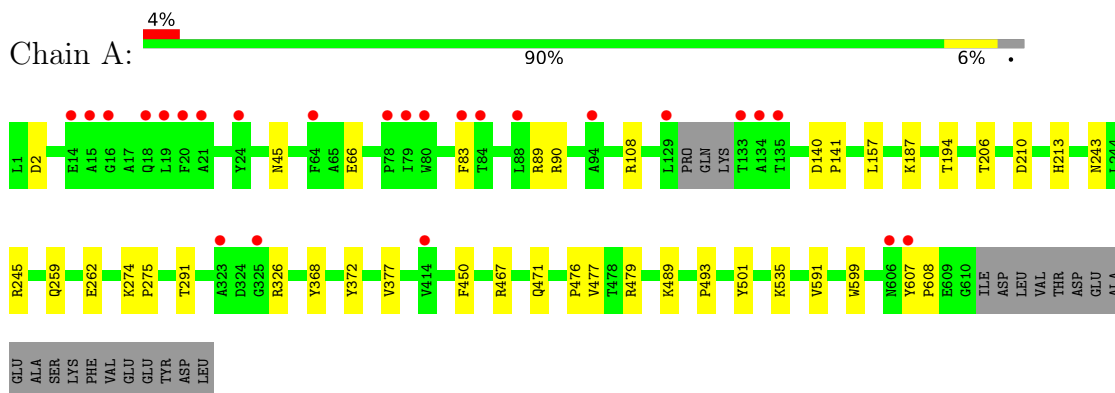
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	443	Total	O	0	0
			443	443		
13	B	333	Total	O	0	0
			333	333		

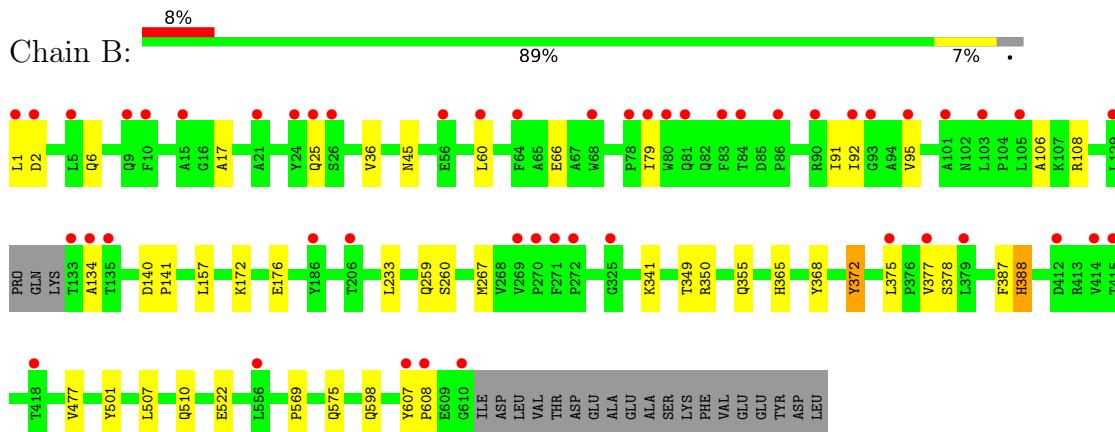
3 Residue-property plots [i](#)

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: ANGIOTENSIN-CONVERTING ENZYME



- Molecule 1: ANGIOTENSIN-CONVERTING ENZYME



Chain D:  25% 75%

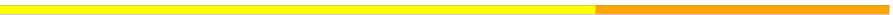
MAG1
MAG2
BMA3
FUC4

- Molecule 4: α -L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

MAG1
FUC2

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  67% 33%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.87Å 76.72Å 82.80Å 88.65° 64.31° 75.22°	Depositor
Resolution (Å)	74.24 – 1.80 74.24 – 1.80	Depositor EDS
% Data completeness (in resolution range)	90.4 (74.24-1.80) 90.4 (74.24-1.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.202 , 0.228 0.202 , 0.228	Depositor DCC
R_{free} test set	6455 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10977	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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: NAG, CL, FUC, SAC, PEG, ZN, BMA, P6G

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	0.66	0/5126	0.89	0/6981
1	B	0.65	0/5096	0.94	3/6942 (0.0%)
All	All	0.65	0/10222	0.92	3/13923 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2	ASP	CA-C-N	6.74	126.25	119.24
1	B	2	ASP	C-N-CA	6.74	126.25	119.24
1	B	79	ILE	N-CA-C	5.63	119.05	113.53

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	A	4967	0	4737	21	0
1	B	4941	0	4707	26	0
2	C	28	0	25	0	0
3	D	49	0	43	0	0</

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	14	0	13	0	0
8	B	14	0	13	0	0
9	A	14	0	20	0	0
9	B	14	0	20	0	0
10	A	19	0	26	0	0
10	B	38	0	52	1	0
11	A	9	0	8	4	0
11	B	9	0	8	4	0
12	A	9	0	4	4	0
12	B	9	0	4	4	0
13	A	443	0	0	3	0
13	B	333	0	0	2	0
All	All	10977	0	9736	52	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 3.

All (52) 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:B:365:HIS:HD1	1:B:388:HIS:HD2	1.18	0.89
1:B:259:GLN:NE2	12:B:1302:ASP:HB2	1.87	0.88
1:B:259:GLN:HE21	12:B:1302:ASP:HB2	1.41	0.85
1:A:467:ARG:HH11	1:A:471:GLN:HE22	1.29	0.80
11:A:1301:SAC:HA	12:A:1302:ASP:OXT	1.81	0.78
1:A:259:GLN:NE2	12:A:1302:ASP:HB2	1.99	0.78
1:B:365:HIS:HD1	1:B:388:HIS:CD2	2.02	0.78
1:B:350:ARG:H	1:B:355:GLN:HE21	1.31	0.77
1:A:259:GLN:HE21	12:A:1302:ASP:HB2		

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:PHE:HB2	1:A:89:ARG:HG2	1.86	0.57
11:A:1301:SAC:HB3	13:A:2301:HOH:O	2.03	0.57
11:B:1301:SAC:HB3	13:B:2234:HOH:O	2.04	0.56
11:B:1301:SAC:HA	12:B:1302:ASP:C	2.30	0.55
1:A:213[B]:HIS:HD2	13:A:2196:HOH:O	1.91	0.53
1:B:66:GLU:CD	1:B:108:ARG:HH22	2.16	0.53
1:B:17:ALA:HB1	1:B:92:ILE:HD11	1.91	0.53
1:A:206:THR:HG23	1:A:210:ASP:OD2	2.09	0.52
1:A:467:ARG:NH1	1:A:471:GLN:HE22	2.04	0.51
1:B:372:TYR:HB2	1:B:375:LEU:HD12	1.93	0.51
1:B:106:ALA:HB1	13:B:2056:HOH:O	2.10	0.51
1:B:91:ILE:O	1:B:95:VAL:HG23	2.12	0.50
1:A:90:ARG:NH2	13:A:2064:HOH:O	2.45	0.50
1:B:501:TYR:CE1	11:B:1301:SAC:HB2	2.47	0.49
1:A:501:TYR:CE1	11:A:1301:SAC:HB2	2.48	0.48
1:A:66:GLU:CD	1:A:108:ARG:HH22	2.22	0.48
1:A:489:LYS:O	1:A:493:PRO:HD2	2.16	0.46
1:B:510:GLN:HG2	1:B:569:PRO:HG2	1.97	0.46
1:B:350:ARG:H	1:B:355:GLN:NE2	2.07	0.46
1:A:157:LEU:HD13	1:A:476:PRO:HB2	1.96	0.46
1:B:36:VAL:HG22	10:B:1204:P6G:H31	1.99	0.44
1:B:607:TYR:HA	1:B:608:PRO:HA	1.75	0.43
1:A:245:ARG:HG2	1:A:591:VAL:CG1	2.48	0.43
1:A:140:ASP:HA	1:A:141:PRO:HA	1.83	0.43
1:B:25:GLN:HE21	1:B:378:SER:H	1.66	0.43
1:A:479:ARG:H	1:B:598:GLN:NE2		

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	605/629 (96%)	593 (98%)	11 (2%)	1 (0%)	43	31
1	B	603/629 (96%)	592 (98%)	8 (1%)	3 (0%)	24	14
All	All	1208/1258 (96%)	1185 (98%)	19 (2%)	4 (0%)	36	25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	45	ASN
1	B	575	GLN
1	A	45	ASN
1	B	134	ALA

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	521/541 (96%)	512 (98%)	9 (2%)	53	45
1	B	517/541 (96%)	510 (99%)	7 (1%)	59	52
All	All	1038/1082 (96%)	1022 (98%)	16 (2%)	57	49

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	187	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	262	GLU
1	A	291	THR
1	A	326	ARG
1	A	368	TYR
1	A	372	TYR
1	A	377	VAL
1	A	535	LYS
1	B	60	LEU
1	B	260	SER
1	B	341	LYS
1	B	368	TYR
1	B	372	TYR
1	B	377	VAL
1	B	388	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	9	GLN
1	A	22	GLN
1	A	188	GLN
1	A	371	GLN
1	A	471	GLN
1	A	491	HIS
1	A	527	GLN
1	A	568	GLN
1	A	600	HIS
1	B	109	GLN
1	B	117	GLN
1	B	276	ASN
1	B	355	GLN
1	B	388	HIS
1	B	491	HIS
1	B	527	GLN
1	B	582	GLN
1	B	598	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

11 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	C	1	1,2	14,14,15	0.59	0	17,19,21	1.31	1 (5%)
2	NAG	C	2	2	14,14,15	0.70	0	17,19,21	1.22	1 (5%)
3	NAG	D	1	1,3	14,14,15	0.46	0	17,19,21	0.99	1 (5%)
3	NAG	D	2	3	14,14,15	0.47	0	17,19,21	1.17	2 (11%)
3	BMA	D	3	3	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
3	FUC	D	4	3	10,10,11	0.76	0	14,14,16	0.58	0
4	NAG	E	1	1,4	14,14,15	0.62	0	17,19,21	1.51	4 (23%)
4	FUC	E	2	4	10,10,11	0.82	0	14,14,16	1.77	4 (28%)
5	NAG	F	1	1,5	14,14,15	0.67	0	17,19,21	1.43	2 (11%)
5	NAG	F	2	5	14,14,15	0.62	0	17,19,21	1.84	3 (17%)

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	FUC	E	2	4	-	-	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	2	NAG	C1-O5-C5	5.33	119.33	112.19
5	F	1	NAG	C1-O5-C5	4.57	118.31	112.19
2	C	1	NAG	C1-O5-C5	4.10	117.68	112.19
4	E	2	FUC	C1-C2-C3	3.12	114.19	109.64
4	E	2	FUC	C1-O5-C5	3.03	120.11	112.97
4	E	2	FUC	C3-C4-C5	3.01	114.38	109.81
2	C	2	NAG	C4-C3-C2	3.00	115.42	111.02
5	F	2	NAG	C4-C3-C2	2.87	115.23	111.02
4	E	1	NAG	C1-O5-C5	2.79	115.93	112.19
3	D	2	NAG	C2-N2-C7	2.74	126.57	122.90
4	E	1	NAG	C4-C3-C2	2.70	114.98	111.02
3	D	3	BMA	C1-O5-C5	2.70	115.81	112.19
5	F	1	NAG	C2-N2-C7	2.55	126.31	122.90
5	F	3	BMA	C1-C2-C3	2.54	113.35	109.64
3	D	2	NAG	C4-C3-C			

Continued from previous page...

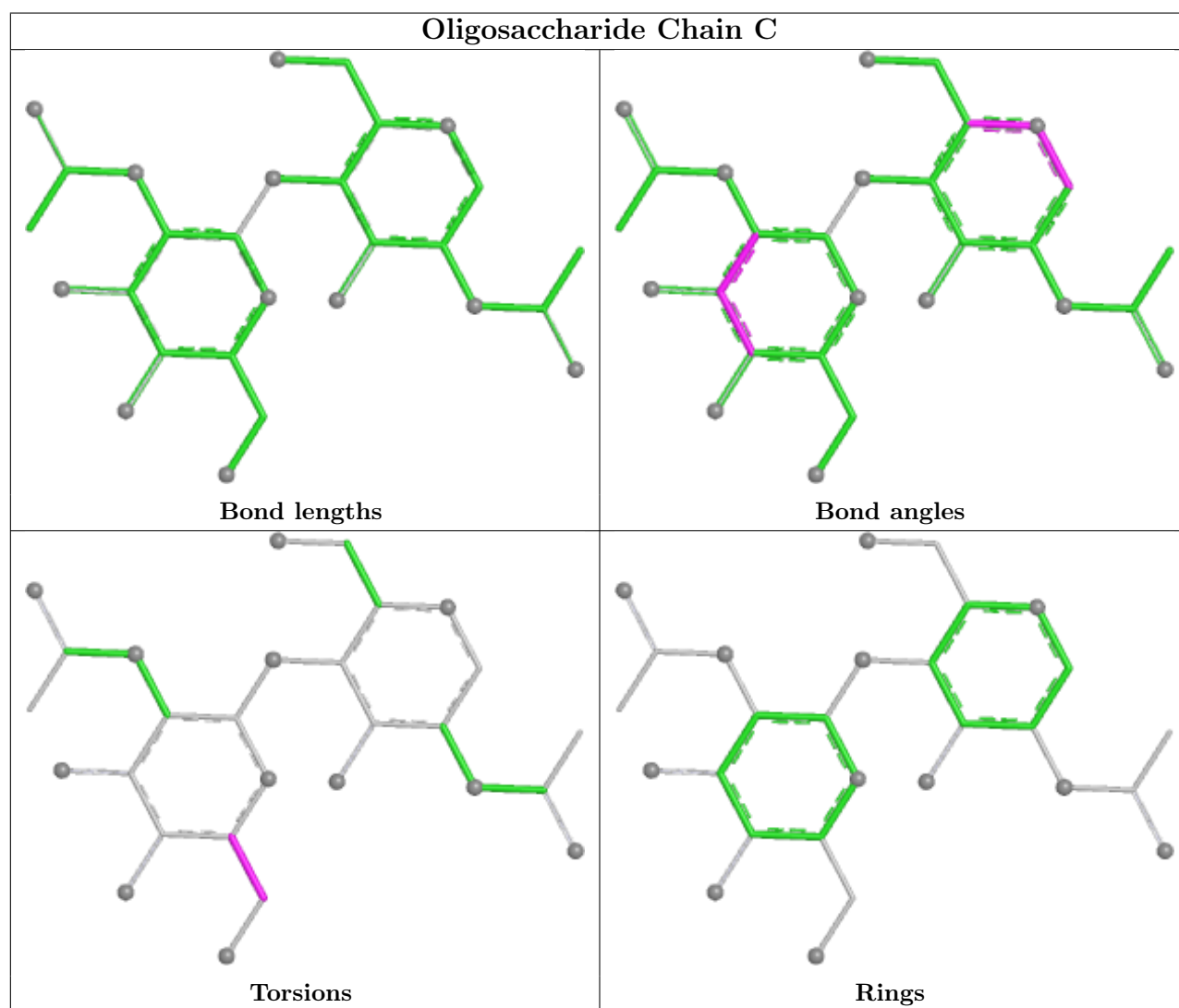
Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C1-C2-N2-C7

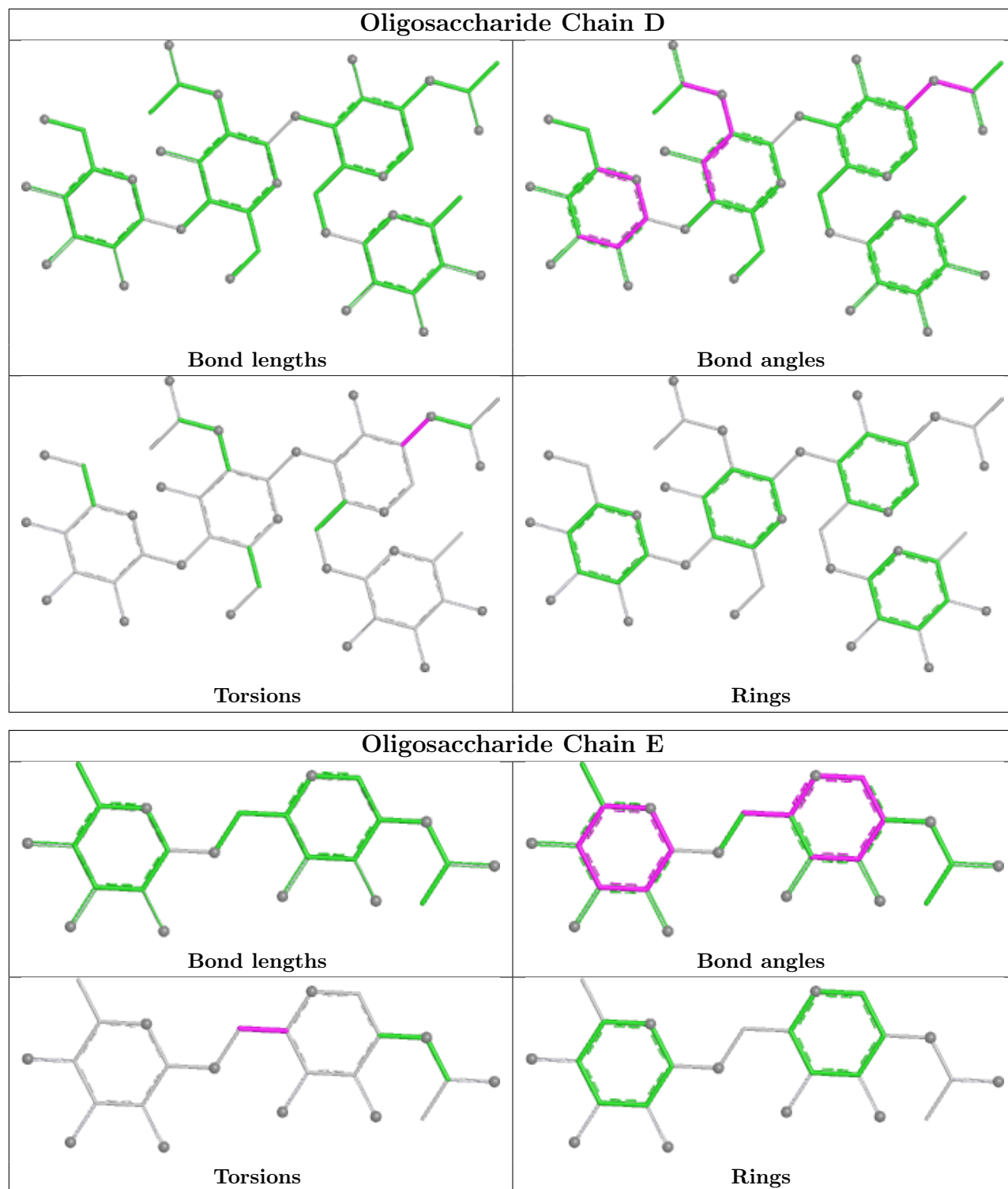
There are no ring outliers.

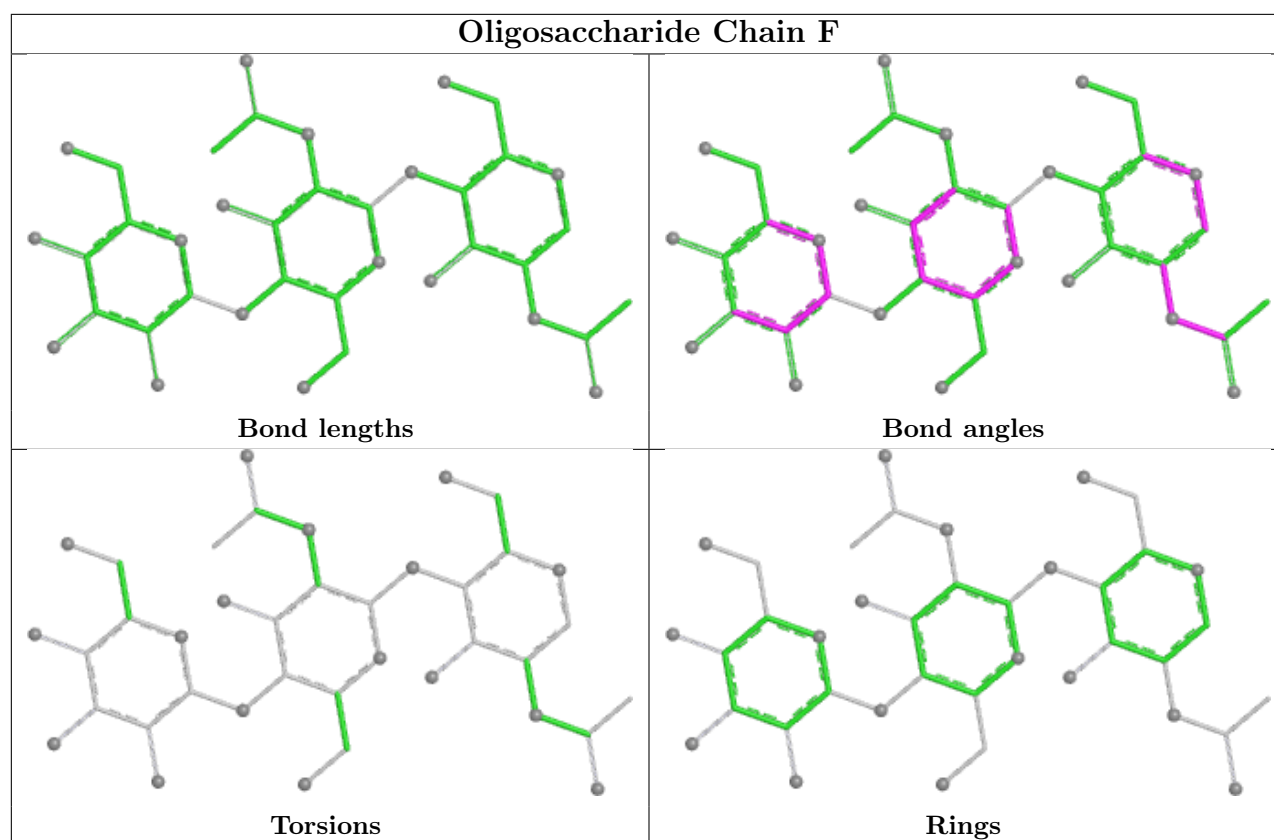
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	3	BMA	1	0

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







5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 4 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	$\# Z > 2$
11	SAC	B	1301	12	7,8,9	1.16	1 (14%)	7,9,11	1.72	1 (14%)
9	PEG	B	1201	-	6,6,6	0.50	0	5,5,5	0.24	0
8	NAG	B	1102	1	14,14,15	0.66	0	17,19,21	1.09	1 (5%)
8	NAG	A	1100	1	14,14,15	0.65	0	17,19,21	1.50	4 (23%)
9	PEG	A	1200	-	6,6,6	0.41	0	5,5,5	0.32	0
10	P6G	B	1204	-	18,18,18	0.50	0	17,17,17	0.26	0
9	PEG	A	1201	-	6,6,6	0.43	0	5,5,5	0.34	0
10	P6G	A	1202	-	18,18,18	0.49	0	17,17,17	0.25	0
10	P6G	B	1203	-	18,18,18	0.58	0	17,17,17	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	SAC	A	1301	12	7,8,9	1.13	1 (14%)	7,9,11	1.60	2 (28%)
12	ASP	B	1302	11	7,8,8	1.39	1 (14%)	6,10,10	2.03	1 (16%)
9	PEG	B	1202	-	6,6,6	0.41	0	5,5,5	0.36	0
12	ASP	A	1302	11	7,8,8	1.43	1 (14%)	6,10,10	2.07	1 (16%)

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
11	SAC	B	1301	12	-	6/7/8/10	-
9	PEG	B	1201	-	-	2/4/4/4	-
8	NAG	B	1102	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1100	1	-	2/6/23/26	0/1/1/1
9	PEG	A	1200	-	-	2/4/4/4	-
10	P6G	B	1204	-	-	7/16/16/16	-
9	PEG	A	1201	-	-	2/4/4/4	-
10	P6G	A	1202	-	-	12/16/16/16	-
10	P6G	B	1203	-	-	11/16/16/16	-
11	SAC	A	1301	12	-	4/7/8/10	-
12	ASP	B	1302	11	-	3/8/8/8	-
9	PEG	B	1202	-	-	1/4/4/4	-
12	ASP	A	1302				

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1301	SAC	C-CA-N	4.07	117.36	109.50
8	A	1100	NAG	C1-O5-C5	3.99	117.54	112.19
11	A	1301	SAC	C-CA-N	3.60	116.44	109.50
8	A	1100	NAG	C4-C3-C2	2.69	114.95	111.02
8	B	1102	NAG	O5-C1-C2	-2.61	107.25	111.29
8	A	1100	NAG	O5-C1-C2	2.29	114.84	111.29
8	A	1100	NAG	O5-C5-C6	2.11	111.76	107.66
11	A	1301	SAC	O-C-CA	-2.09	119.38	124.77

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	1301	SAC	C2A-C1A-N-CA
11	A	1301	SAC	OAC-C1A-N-CA
11	A	1301	SAC	C-CA-CB-OG
11	B	1301	SAC	C2A-C1A-N-CA
11	B	1301	SAC	OAC-C1A-N-CA
11	B	1301	SAC	C-CA-N-C1A
11	B	1301	SAC	C-CA-CB-OG
12	B	1302	ASP	O-C-CA-N
8	A	1100	NAG	O5-C5-C6-O6
10	A	1202	P6G	O4-C5-C6-O7
10	B	1203	P6G	O13-C14-C15-O16
10	B	1203	P6G	O4-C5-C6-O7
12	A	1302	ASP	OXT-C-CA-N
10	B	1203	P6G	O7-C8-C9-O10
10	A	1202	P6G	O10-C11-C12-O13
10	B	1203	P6G	O10-C11-C12-O13
8	A	1100	NAG	

Continued from previous page...

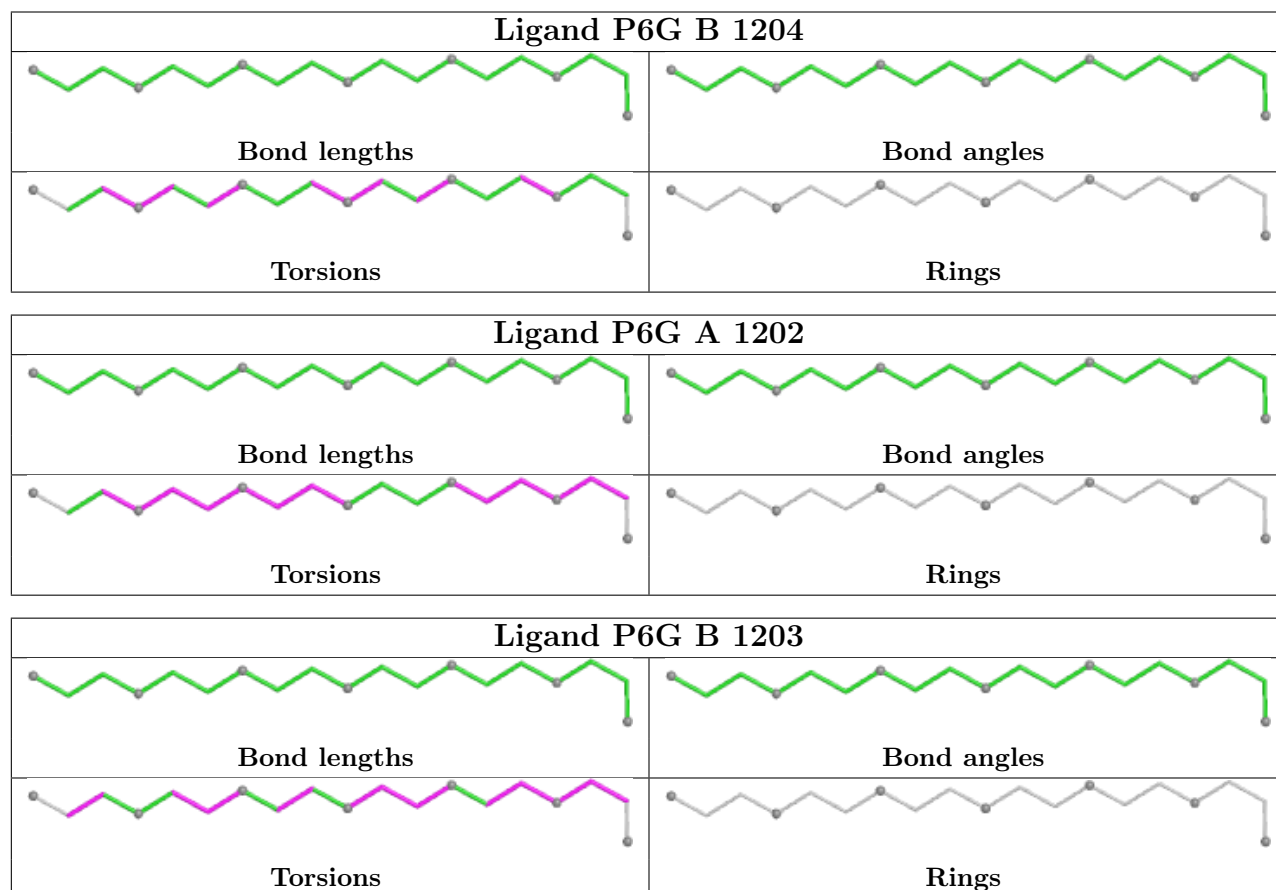
Mol	Chain	Res	Type	Atoms
10	B	1203	P6G	C15-C14-O13-C12
10	B	1204	P6G	C18-C17-O16-C15
8	B	1102	NAG	O5-C5-C6-O6
9	B	1201	PEG	C4-C3-O2-C2
10	B	1204	P6G	C14-C15-O16-C17
10	A	1202	P6G	C5-C6-O7-C8
11	B	1301	SAC	CB-CA-N-C1A
10	B	1203	P6G	C8-C9-O10-C11
9	B	1202	PEG	C1-C2-O2-C3
10	B	1204	P6G	C12-C11-O10-C9
10	B	1203	P6G	C9-C8-O7-C6
12	B	1302	ASP	C-CA-CB-CG
10	A	1202	P6G	C15-C14-O13-C12
10	B	1204	P6G	C6-C5-O4-C3
11	A	1301	SAC	C-CA-N-C1A
10	A	1202	P6G	C11-C12-O13-C14
9	B	1201	PEG	O1-C1-C2-O2
10	B	1203	P6G	C2-C3-O4-C5
9	A	1201	PEG	C4-C3-O2-C2
9	A	1201	PEG	O2-C3-C4-O4
10	A	1202	P6G	C6-C5-O4-C3
10	B	1204	P6G	C15-C14-O13-C12
10	B	1203	P6G	C6-C5-O4-C3
10	B	1204	P6G	C9-C8-O7-C6
10	A	1202	P6G	C14-C15-O16-C17
11	B	1301	SAC	N-CA-CB-OG
12	A	1302	ASP	O-C-CA-N

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	1301	SAC	4	0
10	B	1204	P6G	1	0

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	607/629 (96%)	-0.07	25 (4%) 41 41	10, 23, 43, 69	2 (0%)
1	B	607/629 (96%)	0.33	50 (8%) 17 15	14, 28, 51, 73	0
All	All	1214/1258 (96%)	0.13	75 (6%) 26 25	10, 25, 48, 73	2 (0%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	607	TYR	4.9
1	B	92	ILE	4.3
1	A	133	THR	4.2
1	B	270	PRO	4.2
1	A	129	LEU	4.2
1	A	80	TRP	4.0
1	A	414	VAL	4.0
1	B	105	LEU	3.9
1	A	325	GLY	3.7
1	B	325	GLY	3.7
1	A	78	PRO	3.7
1	B	133	THR	3.6
1	B	271	PHE	3.5
1	B	83	PHE	3.4
1	B	25	GLN	3.4
1	A	134	ALA	3.4
1	B	84	THR	3.4
1	B	134	ALA	3.3
1	A	135	THR	3.2
1	A	84	THR	3.0
1	B	414	VAL	2.9
1	B	206		

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1	LEU	2.8
1	B	64	PHE	2.8
1	B	610	GLY	2.8
1	B	56	GLU	2.8
1	A	606	ASN	2.7
1	B	269	VAL	2.6
1	B	101	ALA	2.6
1	B	135	THR	2.6
1	A	79	ILE	2.6
1	A	323	ALA	2.6
1	B	129	LEU	2.6
1	A	18	GLN	2.5
1	B	81	GLN	2.5
1	B	80	TRP	2.5
1	B	5	LEU	2.5
1	B	68	TRP	2.5
1	B	95	VAL	2.5
1	B	379	LEU	2.4
1	B	9	GLN	2.4
1	B	10	PHE	2.4
1	B	78	PRO	2.4
1	B	24	TYR	2.4
1	B	375	LEU	2.3
1	A	16	GLY	2.3
1	A	20	PHE	2.3
1	B	26	SER	2.2
1	B	415	THR	2.2
1	B	418	THR	2.2
1	A	88	LEU	2.2
1	A	24	TYR	2.2
1	A	94	ALA	2.2
1	B	21	ALA	2.2
1	B	103	LEU	2.2
1	B	86	PRO	2.2
1	A	14	GLU	2.1
1	A	83	PHE	2.1
1	B	607	TYR	2.1
1	B	377	VAL	2.1
1	A	21	ALA	2.1
1	B	15	ALA	2.1
1	B	186	TYR	2.1
1	A	19	LEU	2.1

<

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	2	ASP	2.1
1	B	79	ILE	2.1
1	B	272	PRO	2.1
1	B	90	ARG	2.1
1	B	608	PRO	2.0
1	B	60	LEU	2.0
1	B	556	LEU	2.0
1	B	412	ASP	2.0
1	A	64	PHE	2.0

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

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

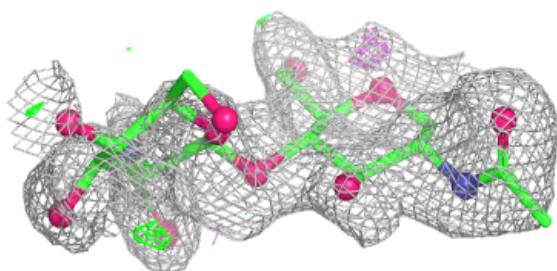
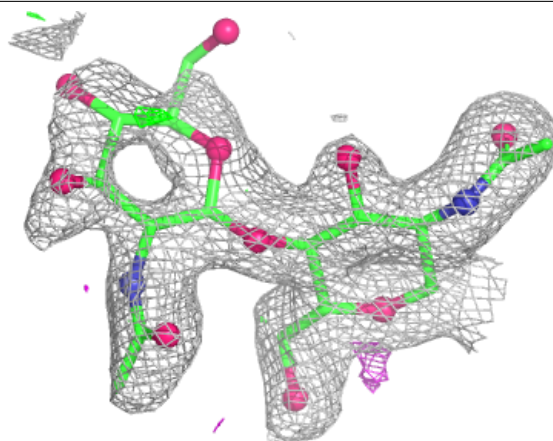
6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	F	3	11/12	0.61	0.15	82,85,85,87	0
4	FUC	E	2	10/11	0.63	0.21	61,66,70,72	0
2	NAG	C	2	14/15	0.72	0.15	57,66,73,74	0
3	BMA	D	3	11/12	0.77	0.12	63,65,67,68	0
5	NAG	F	2	14/15	0.81	0.12	71,73,75,79	0
5	NAG	F	1	14/15	0.82	0.11	58,63,68,68	0
4	NAG	E	1	14/15	0.83	0.12	39,45,52,53	0
3	FUC	D	4	10/11	0.84	0.14	44,46,48,50	0
3	NAG	D	2	14/15	0.84	0.12	45,51,58,58	0
2	NAG	C	1	14/15	0.85	0.12	38,45,51,57	0

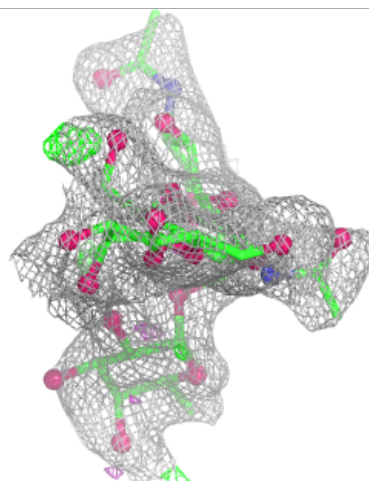
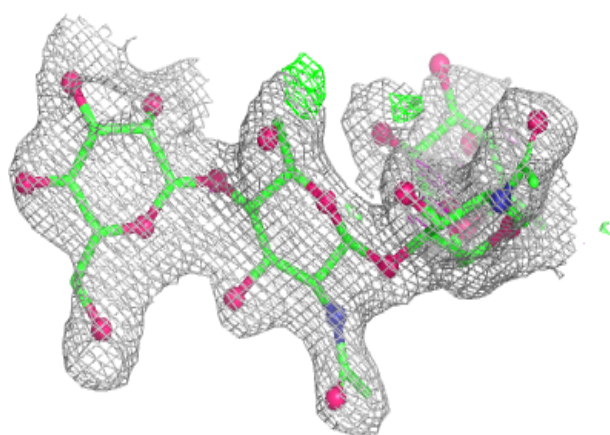
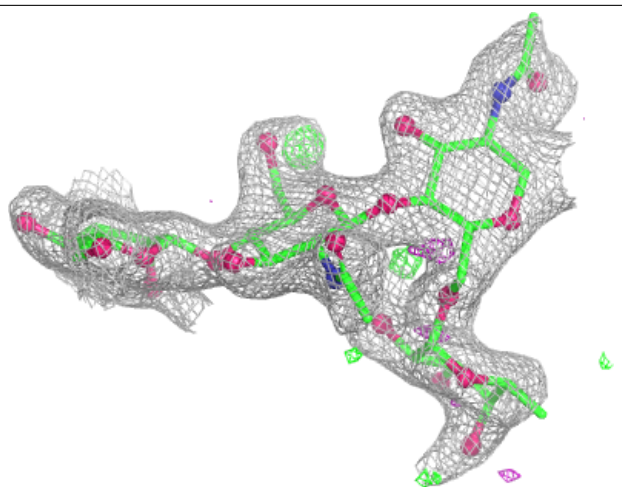
Electron density around Chain C:

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



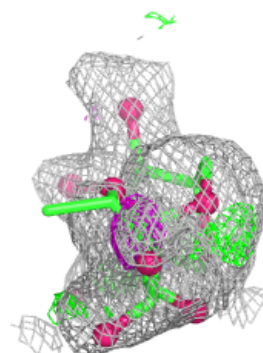
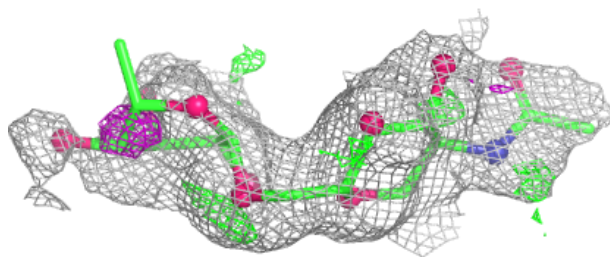
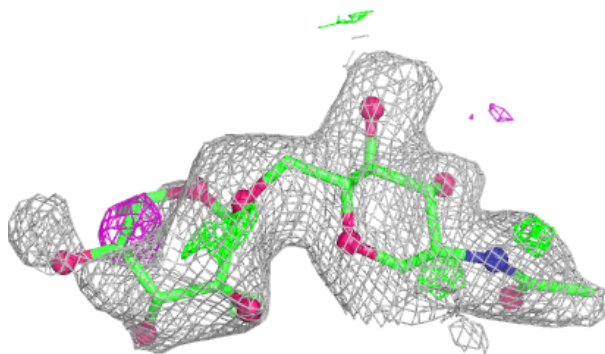
Electron density around Chain D:

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

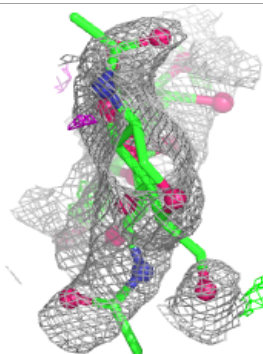
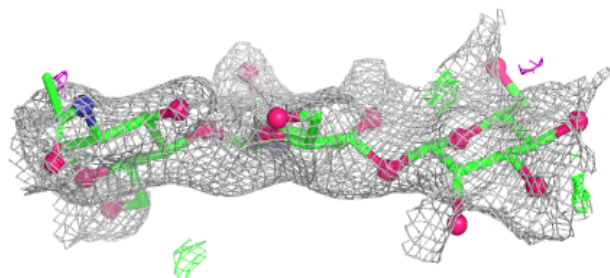
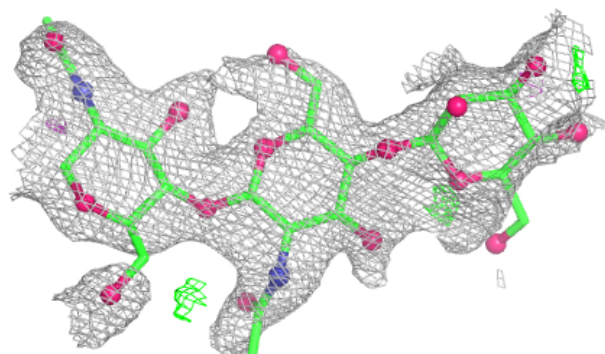


Electron density around Chain E:

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

**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)



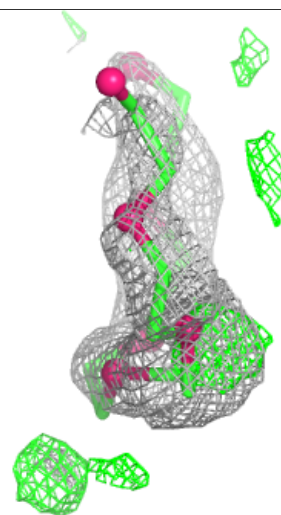
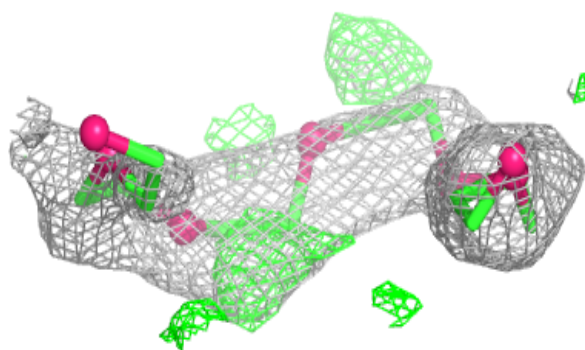
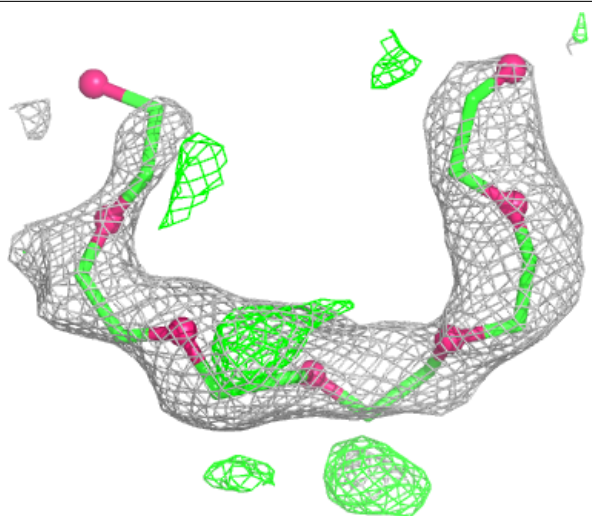
6.4 Ligands ⓘ

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
11	SAC	B	1301	9/10	0.76	0.17	41,45,49,50	0
12	ASP	A	1302	9/9	0.76	0.19	23,35,41,42	0
12	ASP	B	1302	9/9	0.79	0.15	25,31,38,41	0
10	P6G	B	1204	19/19	0.81	0.20	60,64,74,76	0
9	PEG	A	1201	7/7	0.81	0.14	53,56,61,62	0
11	SAC	A	1301	9/10	0.82	0.15	47,49,50,51	0
10	P6G	A	1202	19/19	0.82	0.20	50,65,72,73	0
8	NAG	B	1102	14/15	0.83	0.12	43,47,48,51	0
10	P6G	B	1203	19/19	0.85	0.15	41,43,52,53	0
8	NAG	A	1100	14/15	0.85	0.13	30,35,40,44	0
9	PEG	B	1201	7/7	0.87	0.12	39,41,43,46	0
9	PEG	A	1200	7/7	0.87	0.12	43,45,48,50	0
9	PEG	B	1202	7/7	0.92	0.08	35,36,41,41	0
7	CL	B	1002	1/1	0.99	0.03	21,21,21,21	0
7	CL	A	1002	1/1	1.00	0.01	17,17,17,17	0
6	ZN	A	1001	1/1	1.00	0.01	17,17,17,17	0
6	ZN	B	1001	1/1	1.00	0.01	17,17,17,17	

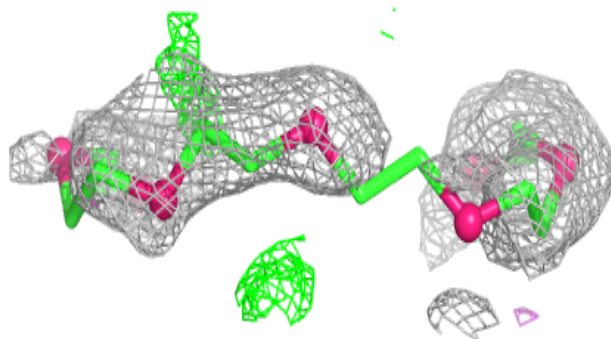
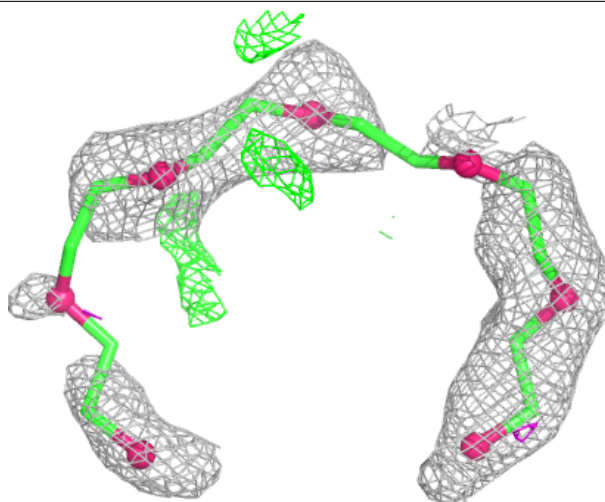
Electron density around P6G B 1204:

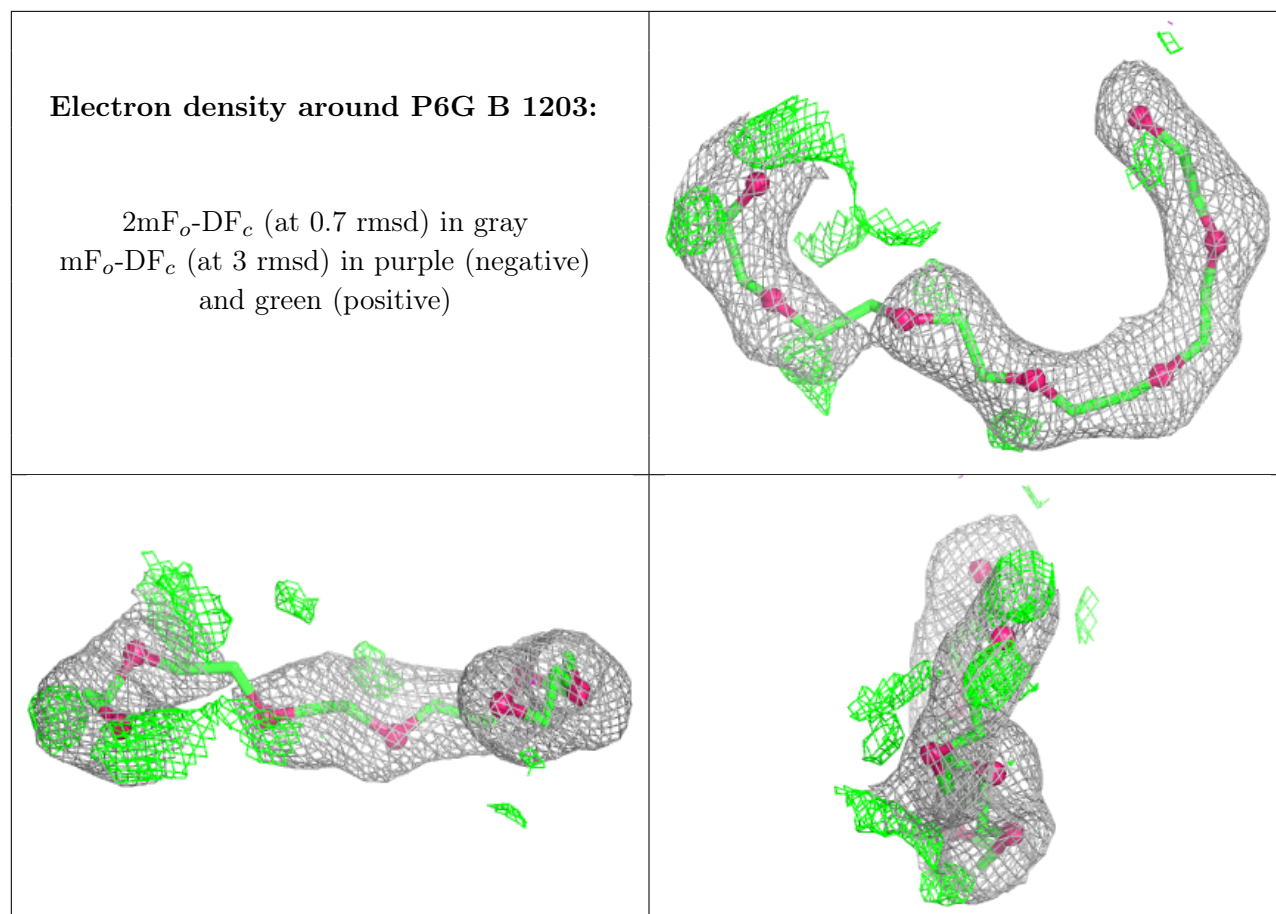
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around P6G A 1202:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.