wwPDB X-ray Structure Validation Summary Report (i)

Jan 8, 2024 – 09:50 am GMT

PDB ID	:	6EN5
Title	:	Crystal structure A of the Angiotensin-1 converting enzyme N-domain in complex with a diprolyl inhibitor.
Authors	:	Cozier, G.E.; Acharya, K.R.; Fienberg, S.; Chibale, K.; Sturrock, E.D.
Deposited on	:	2017-10-04
Resolution	:	1.75 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

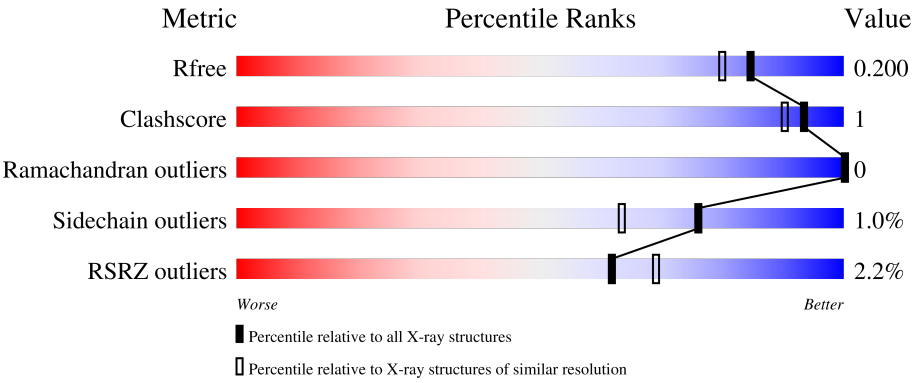
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	629	2% 92%
1	B	629	4% 93%
1	C	629	2% 93%
1	D	629	94%
2	E	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	2	50% 50%
2	K	2	100%
3	F	4	75% 25%
3	I	4	100%
4	G	3	100%
4	J	3	67% 33%
4	M	3	67% 33%
4	P	3	33% 33% 33%
5	L	3	67% 33%
5	N	3	100%
6	O	6	67% 33%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 43786 atoms, of which 20257 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	605	Total	C	H	N	O	S	0	11	0
			9849	3228	4811	870	920	20			
1	B	608	Total	C	H	N	O	S	0	9	0
			9851	3231	4810	867	923	20			
1	C	606	Total	C	H	N	O	S	0	9	0
			9789	3213	4779	862	916	19			
1	D	614	Total	C	H	N	O	S	0	14	0
			9957	3264	4865	874	934	20			

There are 36 discrepancies between the modelled and reference sequences:

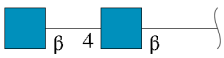
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	conflict	UNP P12821
A	25	GLN	ASN	conflict	UNP P12821
A	82	GLN	ASN	conflict	UNP P12821
A	117	GLN	ASN	conflict	UNP P12821
A	131	GLN	ASN	conflict	UNP P12821
A	289	GLN	ASN	conflict	UNP P12821
A	545	ARG	GLN	conflict	UNP P12821
A	576	LEU	PRO	conflict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

Continued on next page...

Continued from previous page...

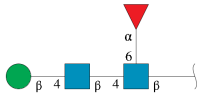
Chain	Residue	Modelled	Actual	Comment	Reference
C	117	GLN	ASN	conflict	UNP P12821
C	131	GLN	ASN	conflict	UNP P12821
C	289	GLN	ASN	conflict	UNP P12821
C	545	ARG	GLN	conflict	UNP P12821
C	576	LEU	PRO	conflict	UNP P12821
C	629	LEU	-	expression tag	UNP P12821
D	9	GLN	ASN	conflict	UNP P12821
D	25	GLN	ASN	conflict	UNP P12821
D	82	GLN	ASN	conflict	UNP P12821
D	117	GLN	ASN	conflict	UNP P12821
D	131	GLN	ASN	conflict	UNP P12821
D	289	GLN	ASN	conflict	UNP P12821
D	545	ARG	GLN	conflict	UNP P12821
D	576	LEU	PRO	conflict	UNP P12821
D	629	LEU	-	expression tag	UNP P12821

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	H	2	Total	C	H	N	O	0	0	0
			54	16	26	2	10			
2	K	2	Total	C	H	N	O	0	0	0
			54	16	26	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.



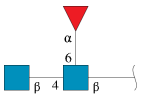
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	4	Total	C	H	N	O	0	0	0
			95	28	46	2	19			

Continued on next page...

Continued from previous page...

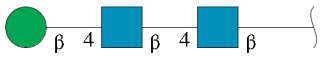
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	4	Total	C	H	N	O	0	0	0
			95	28	46	2	19			

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



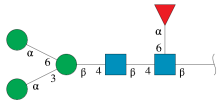
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	3	Total	C	H	N	O	0	0	0
			74	22	36	2	14			
4	J	3	Total	C	H	N	O	0	0	0
			73	22	35	2	14			
4	M	3	Total	C	H	N	O	0	0	0
			74	22	36	2	14			
4	P	3	Total	C	H	N	O	0	0	0
			72	22	34	2	14			

- Molecule 5 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
5	L	3	Total	C	H	N	O	0	0	0
			75	22	36	2	15			
5	N	3	Total	C	H	N	O	0	0	0
			75	22	36	2	15			

- Molecule 6 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

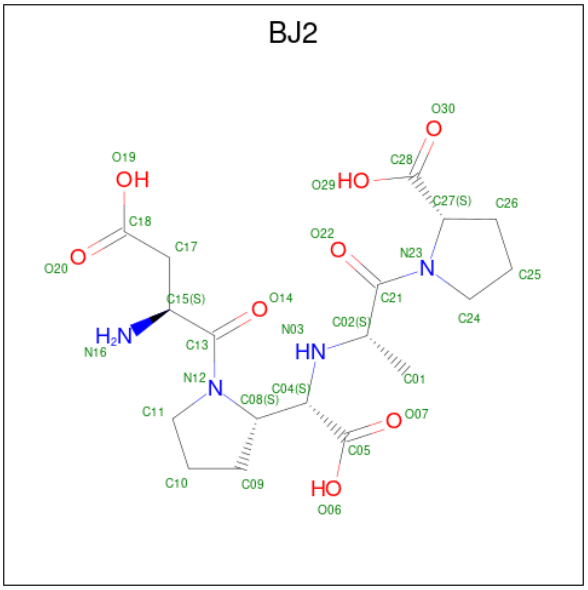


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	O	6	Total	C	H	N	O	0	0	0
			135	40	64	2	29			

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		
7	B	1	Total	Zn	0	0
			1	1		
7	C	1	Total	Zn	0	0
			1	1		
7	D	1	Total	Zn	0	0
			1	1		

- Molecule 8 is (2 {S})-1-[(2 {S})-2-[[(1 {S})-1-[(2 {S})-1-[(2 {S})-2-azanyl-4-oxidanyl-4-oxidanylidene-butanoyl]pyrrolidin-2-yl]-2-oxidanyl-2-oxidanylidene-ethyl]amino]propanoyl]pyrrolidine-2-carboxylic acid (three-letter code: BJ2) (formula: $C_{18}H_{28}N_4O_8$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	H	N	O	0	0
			55	18	25	4	8		
8	B	1	Total	C	H	N	O	0	0
			55	18	25	4	8		
8	C	1	Total	C	H	N	O	0	0
			55	18	25	4	8		
8	D	1	Total	C	H	N	O	0	0
			55	18	25	4	8		

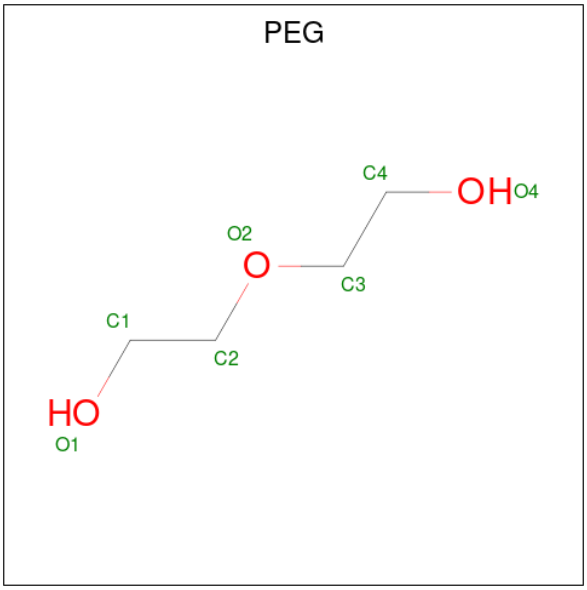
- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Cl 1 1	0	0
9	B	1	Total Cl 1 1	0	0
9	C	1	Total Cl 1 1	0	0
9	D	1	Total Cl 1 1	0	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

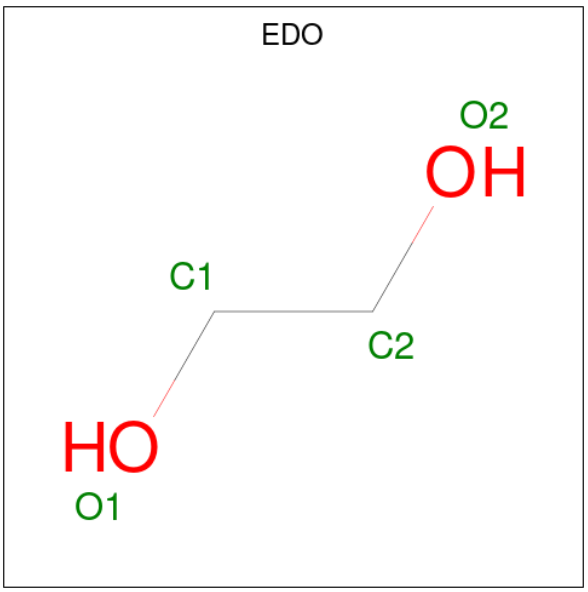
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Mg 1 1	0	0
10	B	1	Total Mg 1 1	0	0
10	C	1	Total Mg 1 1	0	0
10	D	1	Total Mg 1 1	0	0

- Molecule 11 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	H	O	0	0
			17	4	10	3		
11	A	1	Total	C	H	O	0	0
			17	4	10	3		
11	A	1	Total	C	H	O	0	0
			17	4	10	3		
11	B	1	Total	C	H	O	0	0
			17	4	10	3		
11	B	1	Total	C	H	O	0	0
			17	4	10	3		
11	B	1	Total	C	H	O	0	0
			17	4	10	3		
11	B	1	Total	C	H	O	0	0
			17	4	10	3		
11	B	1	Total	C	H	O	0	0
			17	4	10	3		
11	C	1	Total	C	H	O	0	0
			17	4	10	3		
11	C	1	Total	C	H	O	0	0
			17	4	10	3		
11	D	1	Total	C	H	O	0	0
			17	4	10	3		
11	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 12 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



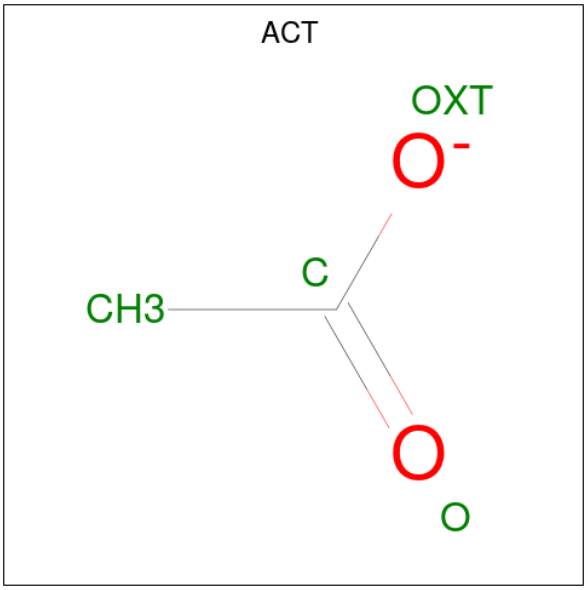
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C H O 10 2 6 2	0	0
12	A	1	Total C H O 10 2 6 2	0	0
12	A	1	Total C H O 10 2 6 2	0	0
12	A	1	Total C H O 10 2 6 2	0	0
12	A	1	Total C H O 10 2 6 2	0	0
12	A	1	Total C H O 10 2 6 2	0	0
12	A	1	Total C H O 10 2 6 2	0	0
12	B	1	Total C H O 10 2 6 2	0	0
12	B	1	Total C H O 10 2 6 2	0	0
12	B	1	Total C H O 10 2 6 2	0	0
12	B	1	Total C H O 10 2 6 2	0	0
12	B	1	Total C H O 10 2 6 2	0	0
12	C	1	Total C H O 10 2 6 2	0	0
12	C	1	Total C H O 10 2 6 2	0	0
12	C	1	Total C H O 10 2 6 2	0	0
12	C	1	Total C H O 10 2 6 2	0	0
12	C	1	Total C H O 10 2 6 2	0	0
12	C	1	Total C H O 10 2 6 2	0	0
12	C	1	Total C H O 10 2 6 2	0	0
12	C	1	Total C H O 10 2 6 2	0	0
12	D	1	Total C H O 10 2 6 2	0	0
12	D	1	Total C H O 10 2 6 2	0	0

Continued on next page...

Continued from previous page...

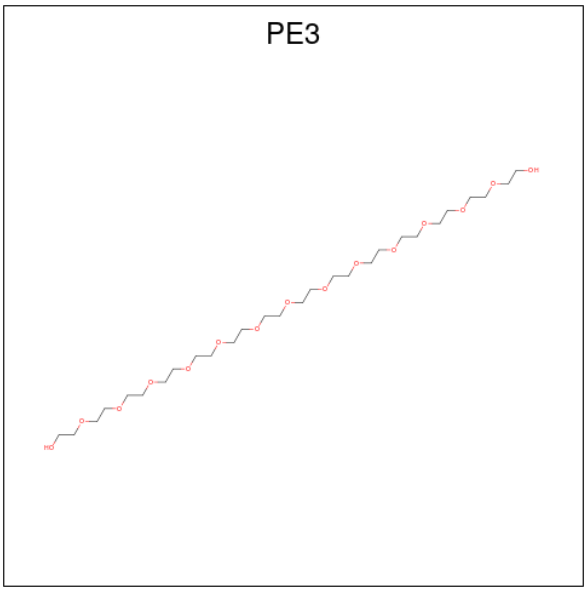
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 13 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



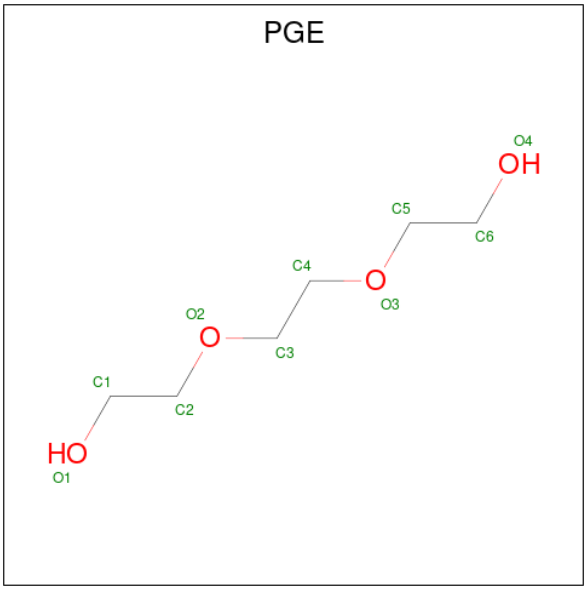
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	H	O	0	0
			7	2	3	2		
13	A	1	Total	C	H	O	0	0
			7	2	3	2		
13	B	1	Total	C	H	O	0	0
			7	2	3	2		
13	C	1	Total	C	H	O	0	0
			7	2	3	2		
13	D	1	Total	C	H	O	0	0
			7	2	3	2		
13	D	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 14 is 3,6,9,12,15,18,21,24,27,30,33,36,39-TRIDECAOXAHENTETRACONTANE-1,41-DIOL (three-letter code: PE3) (formula: $C_{28}H_{58}O_{15}$).



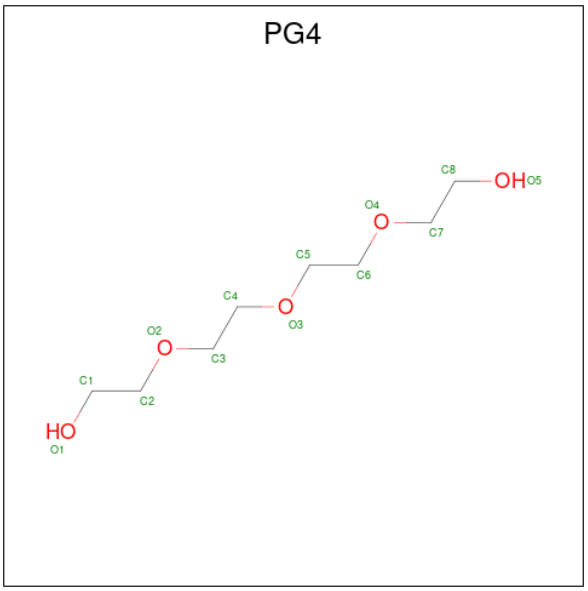
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
14	A	1	101	28	58	15	0	0

- Molecule 15 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



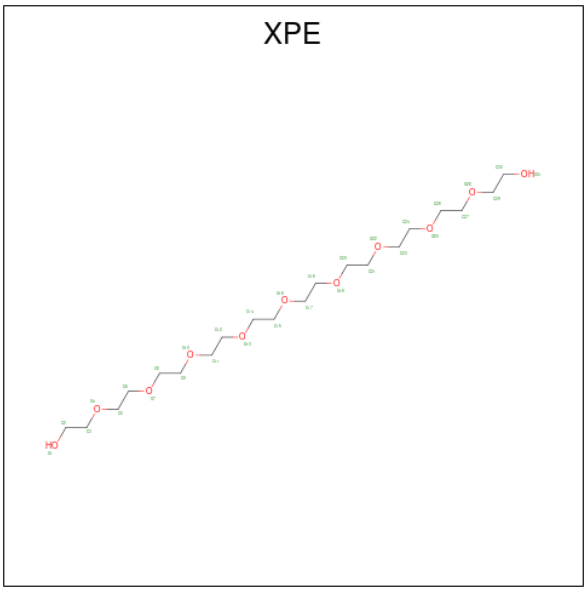
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
15	B	1	24	6	14	4	0	0

- Molecule 16 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	B	1	Total	C	H	O	0	0
			31	8	18	5		
16	C	1	Total	C	H	O	0	1
			62	16	36	10		

- Molecule 17 is 3,6,9,12,15,18,21,24,27-NONAOXANONACOSANE-1,29-DIOL (three-letter code: XPE) (formula: $C_{20}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	D	1	Total	C	H	O	0	0
			73	20	42	11		

- Molecule 18 is water.

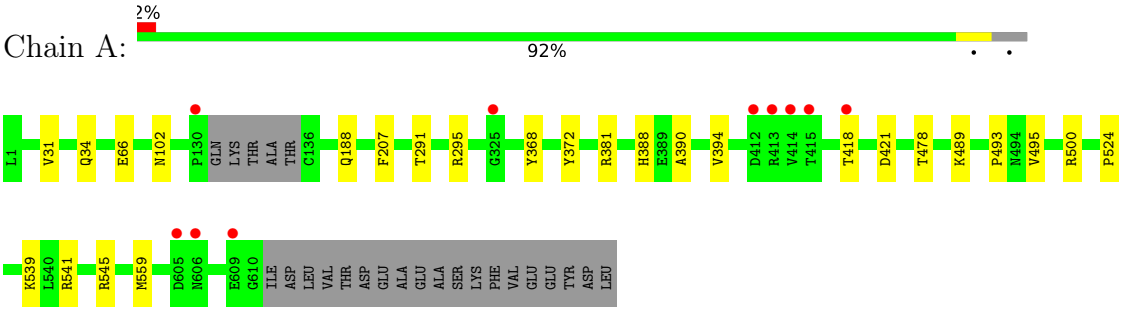
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	584	Total O 588 588	0	4
18	B	580	Total O 581 581	0	2
18	C	547	Total O 551 551	0	4
18	D	682	Total O 690 690	0	8

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.

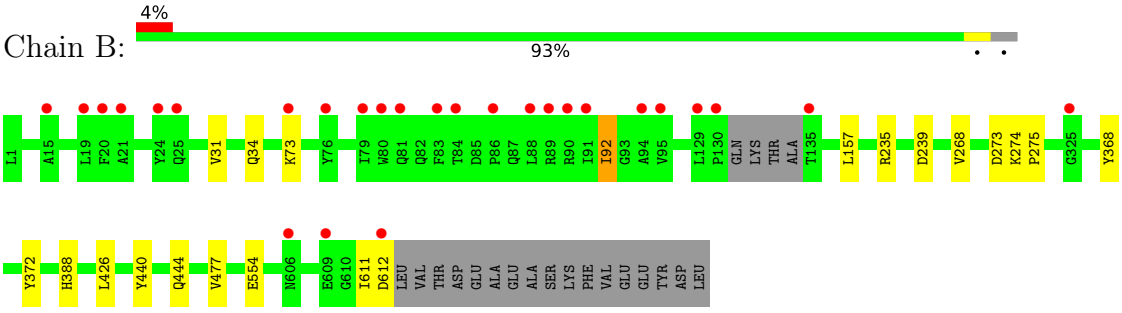
• Molecule 1: Angiotensin-converting enzyme

Chain A:



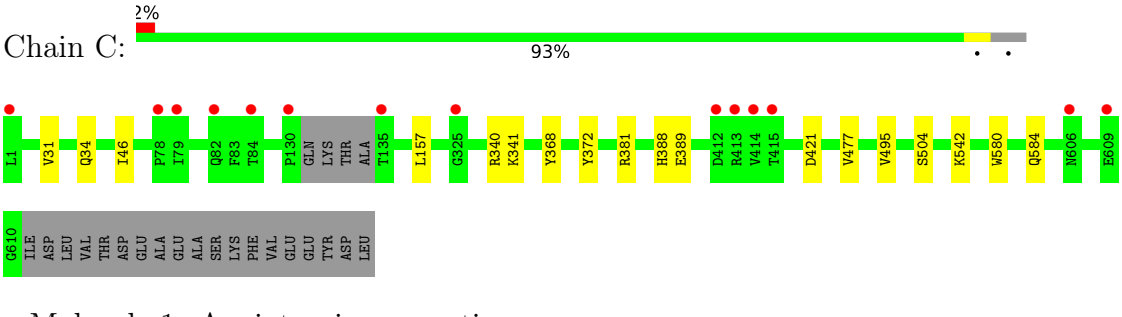
• Molecule 1: Angiotensin-converting enzyme

Chain B:



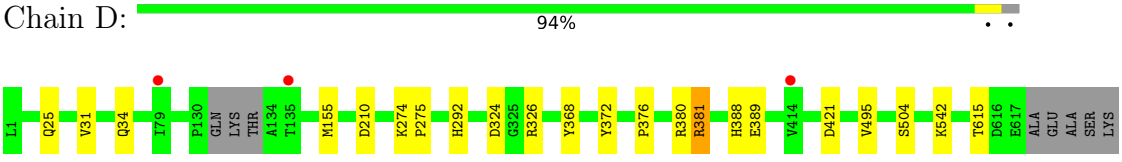
• Molecule 1: Angiotensin-converting enzyme

Chain C:



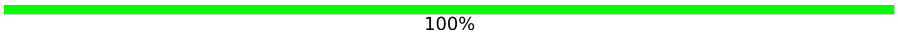
• Molecule 1: Angiotensin-converting enzyme

Chain D:



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

Chain E:

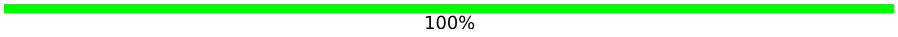


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

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

Chain K:

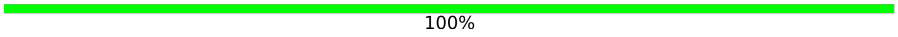


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 3: 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

Chain I:



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

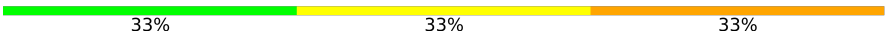
Chain J:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

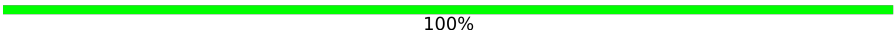


• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

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

Chain N:



• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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

Chain O:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	74.17Å 103.45Å 115.45Å 84.86° 85.49° 81.99°	Depositor
Resolution (Å)	79.48 – 1.75 102.11 – 1.75	Depositor EDS
% Data completeness (in resolution range)	97.0 (79.48-1.75) 97.1 (102.11-1.75)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 1.75Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.173 , 0.198 0.175 , 0.200	Depositor DCC
R_{free} test set	3195 reflections (0.97%)	wwPDB-VP
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	43786	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3807e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: BJ2, XPE, BMA, ZN, CL, FUC, PGE, EDO, PG4, MAN, PE3, PEG, ACT, MG, NAG

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	0.45	0/5194	0.56	0/7070
1	B	0.44	0/5197	0.57	0/7076
1	C	0.41	0/5181	0.56	0/7055
1	D	0.49	0/5280	0.60	0/7190
All	All	0.45	0/20852	0.57	0/28391

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	5038	4811	4799	15	0
1	B	5041	4810	4802	13	0
1	C	5010	4779	4758	9	0
1	D	5092	4865	4820	11	0
2	E	28	27	25	0	0
2	H	28	26	25	0	0
2	K	28	26	25	0	0
3	F	49	46	43	1	0
3	I	49	46	43	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	38	36	34	3	0
4	J	38	35	34	0	0
4	M	38	36	34	0	0
4	P	38	34	34	2	0
5	L	39	36	34	0	0
5	N	39	36	34	0	0
6	O	71	64	61	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	30	25	0	0	0
8	B	30	25	0	0	0
8	C	30	25	0	1	0
8	D	30	25	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
11	A	21	30	30	2	0
11	B	35	50	50	0	0
11	C	14	20	20	3	0
11	D	14	20	20	0	0
12	A	28	42	42	3	0
12	B	20	30	30	0	0
12	C	32	48	48	0	0
12	D	12	18	18	0	0
13	A	8	6	6	0	0
13	B	4	3	3	0	0
13	C	4	3	3	0	0
13	D	8	6	6	1	0
14	A	43	58	58	4	0
15	B	10	14	14	0	0
16	B	13	18	18	2	0
16	C	26	36	36	0	0
17	D	31	42	42	0	0
18	A	588	0	0	3	0
18	B	581	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	C	551	0	0	2	0
18	D	690	0	0	4	0
All	All	23529	20257	20049	59	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 1.

The worst 5 of 59 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)
13:D:723:ACT:H1	18:D:1087:HOH:O	1.89	0.71
1:D:542:LYS:NZ	18:D:804:HOH:O	2.25	0.69
1:C:542:LYS:NZ	18:C:804:HOH:O	2.27	0.67
1:C:340[A]:ARG:O	1:C:341:LYS:HE2	1.99	0.62
1:C:340[B]:ARG:O	1:C:341:LYS:HE2	1.99	0.62

There are no symmetry-related clashes.

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	A	612/629 (97%)	603 (98%)	9 (2%)	0	100	100
1	B	613/629 (98%)	605 (99%)	8 (1%)	0	100	100
1	C	611/629 (97%)	603 (99%)	8 (1%)	0	100	100
1	D	624/629 (99%)	615 (99%)	9 (1%)	0	100	100
All	All	2460/2516 (98%)	2426 (99%)	34 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	531/541 (98%)	526 (99%)	5 (1%)	78	67
1	B	532/541 (98%)	526 (99%)	6 (1%)	73	60
1	C	530/541 (98%)	525 (99%)	5 (1%)	78	67
1	D	542/541 (100%)	536 (99%)	6 (1%)	73	60
All	All	2135/2164 (99%)	2113 (99%)	22 (1%)	76	63

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

Mol	Chain	Res	Type
1	C	388	HIS
1	D	372	TYR
1	D	368	TYR
1	D	381[A]	ARG
1	B	239	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

38 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	E	1	1,2	14,14,15	0.43	0	17,19,21	0.59	0
2	NAG	E	2	2	14,14,15	0.27	0	17,19,21	0.51	0
3	NAG	F	1	1,3	14,14,15	0.22	0	17,19,21	0.52	0
3	NAG	F	2	3	14,14,15	0.30	0	17,19,21	0.39	0
3	BMA	F	3	3	11,11,12	0.54	0	15,15,17	0.77	0
3	FUC	F	4	3	10,10,11	0.80	0	14,14,16	0.81	0
4	NAG	G	1	1,4	14,14,15	0.51	0	17,19,21	0.90	1 (5%)
4	NAG	G	2	4	14,14,15	0.37	0	17,19,21	1.03	1 (5%)
4	FUC	G	3	4	10,10,11	0.97	0	14,14,16	1.58	3 (21%)
2	NAG	H	1	1,2	14,14,15	0.24	0	17,19,21	0.65	1 (5%)
2	NAG	H	2	2	14,14,15	0.31	0	17,19,21	0.51	0
3	NAG	I	1	1,3	14,14,15	0.55	0	17,19,21	0.67	0
3	NAG	I	2	3	14,14,15	0.26	0	17,19,21	0.35	0
3	BMA	I	3	3	11,11,12	0.73	0	15,15,17	0.71	0
3	FUC	I	4	3	10,10,11	0.67	0	14,14,16	0.79	0
4	NAG	J	1	1,4	14,14,15	0.48	0	17,19,21	0.57	0
4	NAG	J	2	4	14,14,15	0.33	0	17,19,21	0.39	0
4	FUC	J	3	4	10,10,11	0.93	0	14,14,16	0.95	1 (7%)
2	NAG	K	1	1,2	14,14,15	0.31	0	17,19,21	0.55	0
2	NAG	K	2	2	14,14,15	0.29	0	17,19,21	0.50	0
5	NAG	L	1	1,5	14,14,15	0.16	0	17,19,21	0.49	0
5	NAG	L	2	5	14,14,15	0.40	0	17,19,21	0.56	0
5	BMA	L	3	5	11,11,12	0.71	0	15,15,17	0.94	1 (6%)
4	NAG	M	1	1,4	14,14,15	0.26	0	17,19,21	0.69	0
4	NAG	M	2	4	14,14,15	0.32	0	17,19,21	0.39	0
4	FUC	M	3	4	10,10,11	1.11	1 (10%)	14,14,16	1.31	2 (14%)
5	NAG	N	1	1,5	14,14,15	0.37	0	17,19,21	0.68	0
5	NAG	N	2	5	14,14,15	0.30	0	17,19,21	0.47	0
5	BMA	N	3	5	11,11,12	0.64	0	15,15,17	0.70	0
6	NAG	O	1	6,1	14,14,15	0.64	0	17,19,21	0.80	0
6	NAG	O	2	6	14,14,15	0.47	0	17,19,21	0.56	0
6	BMA	O	3	6	11,11,12	0.79	0	15,15,17	0.89	0
6	MAN	O	4	6	11,11,12	1.06	1 (9%)	15,15,17	1.21	2 (13%)
6	MAN	O	5	6	11,11,12	0.91	1 (9%)	15,15,17	0.92	1 (6%)
6	FUC	O	6	6	10,10,11	0.93	0	14,14,16	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	P	1	1,4	14,14,15	0.37	0	17,19,21	0.77	0
4	NAG	P	2	4	14,14,15	0.50	0	17,19,21	0.41	0
4	FUC	P	3	4	10,10,11	1.49	1 (10%)	14,14,16	1.07	1 (7%)

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

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

Continued on next page...

Continued from previous page...

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	3	FUC	C1-C2	4.22	1.61	1.52
6	O	4	MAN	C1-C2	2.75	1.58	1.52
6	O	5	MAN	O5-C1	-2.20	1.40	1.43
4	M	3	FUC	O5-C1	-2.13	1.40	1.43

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	2	NAG	C2-N2-C7	3.30	127.60	122.90
4	G	3	FUC	O5-C5-C4	3.26	115.36	109.52
6	O	4	MAN	C1-O5-C5	2.76	115.93	112.19
4	P	3	FUC	O2-C2-C1	2.71	114.70	109.15
4	G	3	FUC	O2-C2-C1	2.69	114.66	109.15

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	O	4	MAN	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6

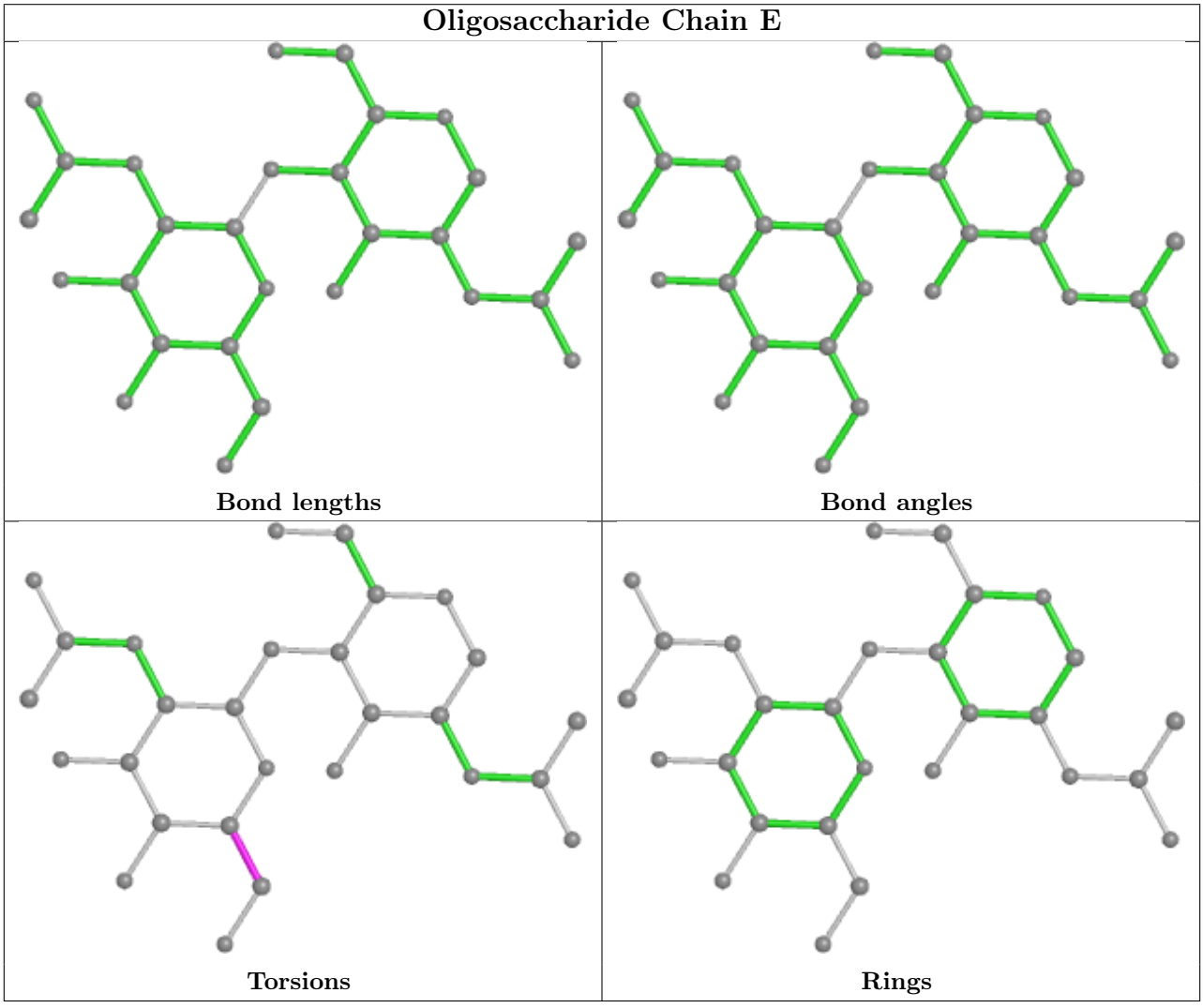
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	O	4	MAN	C1-C2-C3-C4-C5-O5

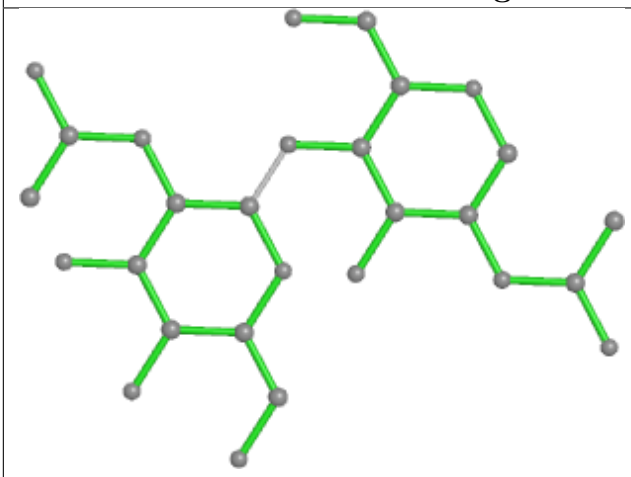
6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NAG	1	0
4	G	2	NAG	1	0
4	P	1	NAG	1	0
4	P	3	FUC	2	0
4	G	3	FUC	2	0
3	F	4	FUC	1	0

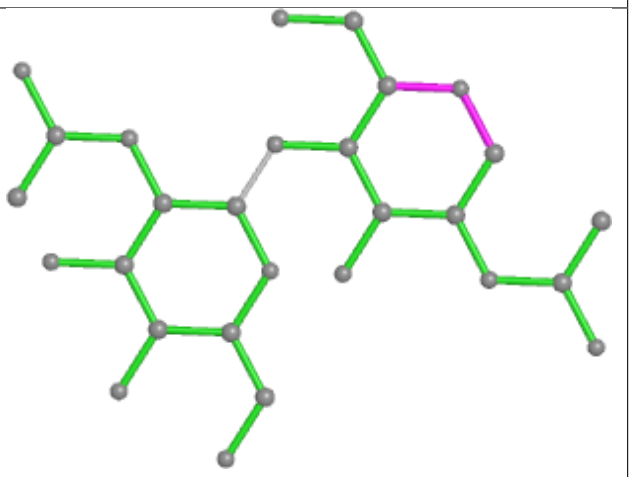
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



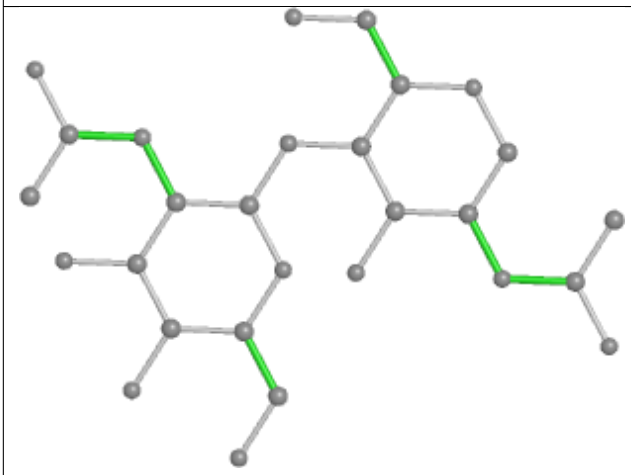
Oligosaccharide Chain H



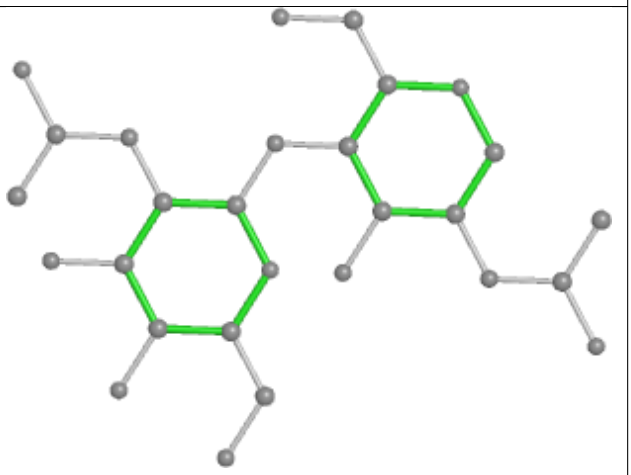
Bond lengths



Bond angles

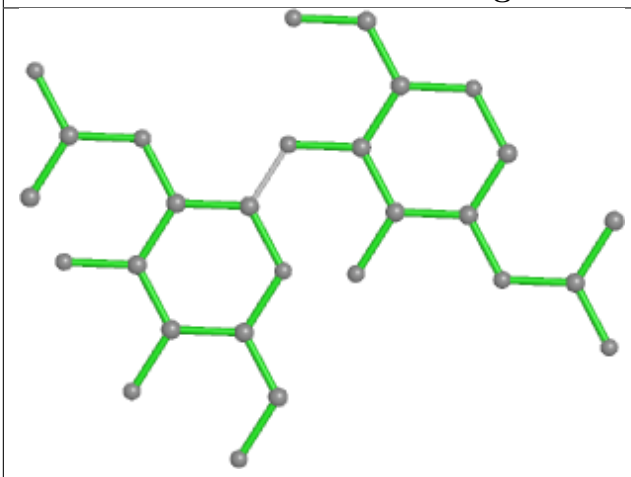


Torsions

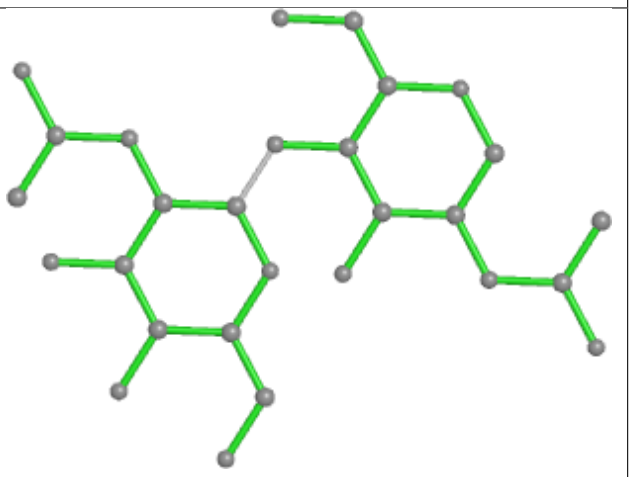


Rings

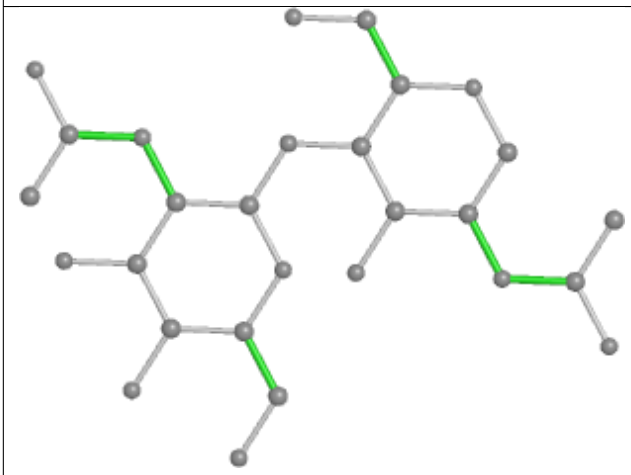
Oligosaccharide Chain K



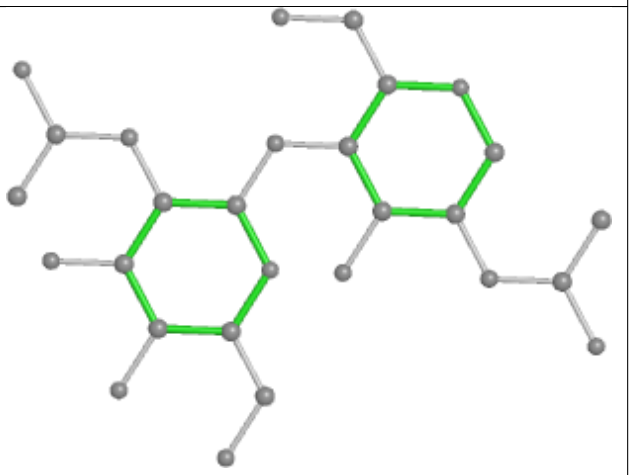
Bond lengths



Bond angles

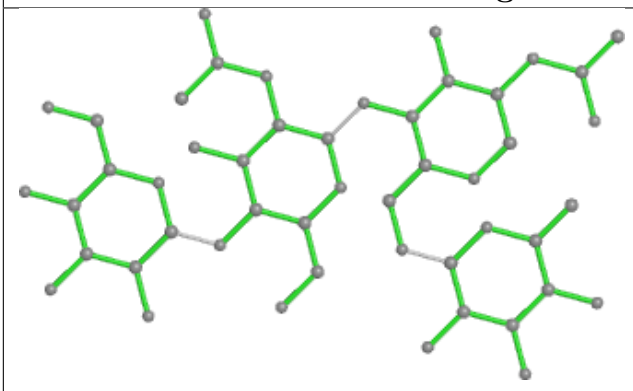


Torsions

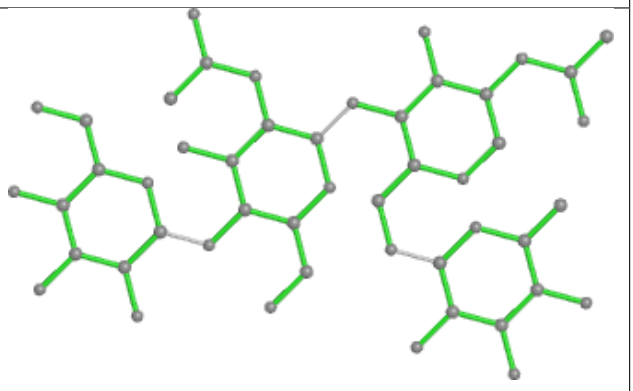


Rings

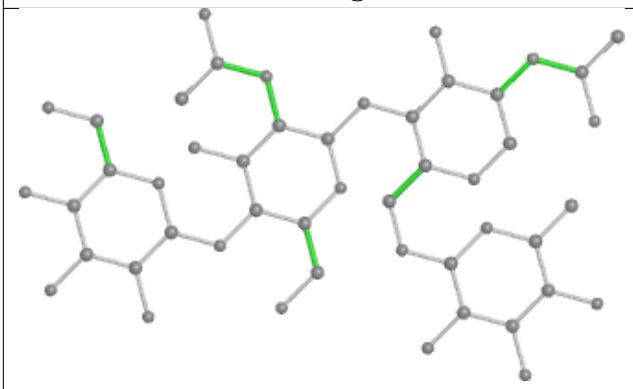
Oligosaccharide Chain F



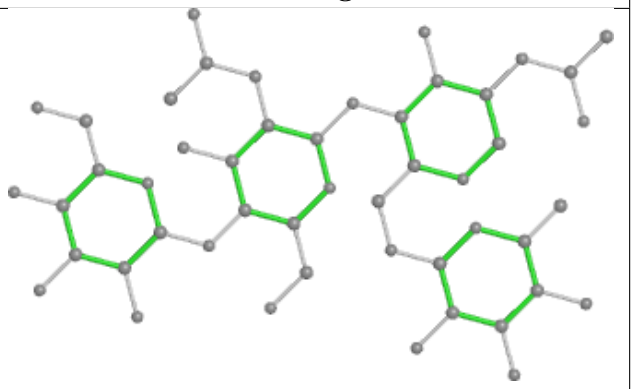
Bond lengths



Bond angles

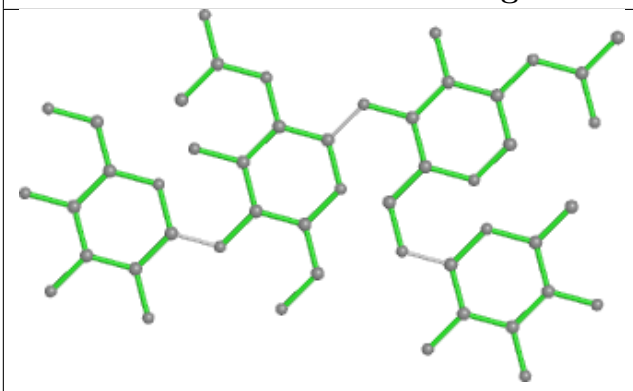


Torsions

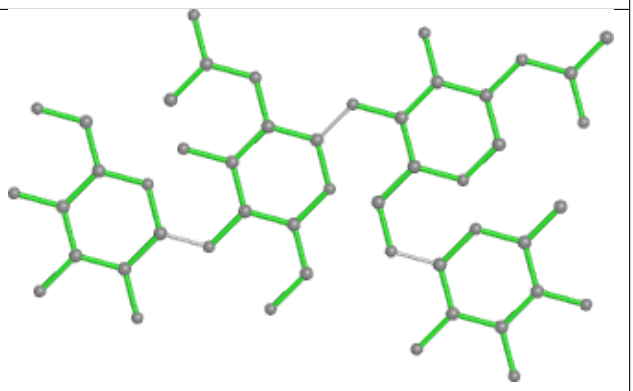


Rings

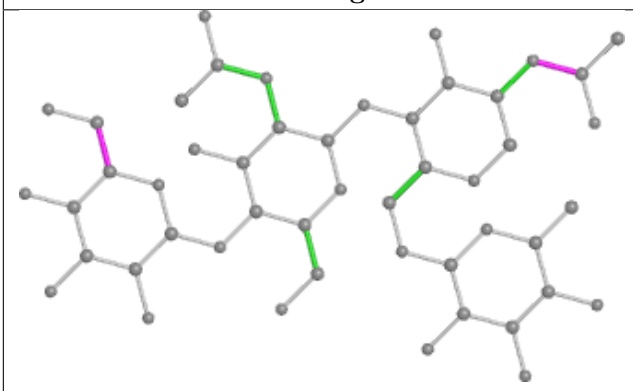
Oligosaccharide Chain I



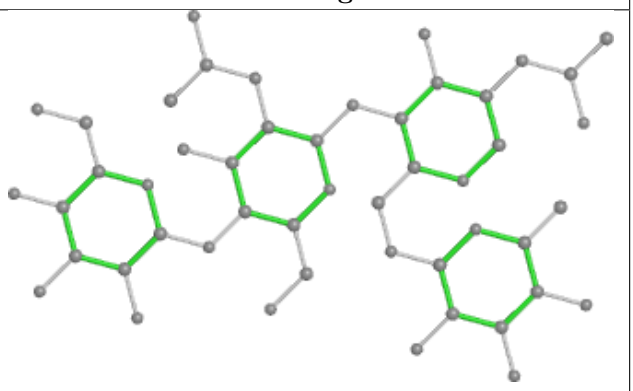
Bond lengths



Bond angles

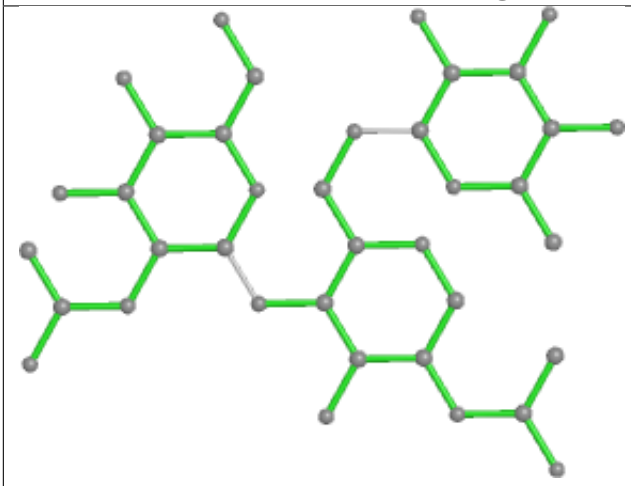


Torsions

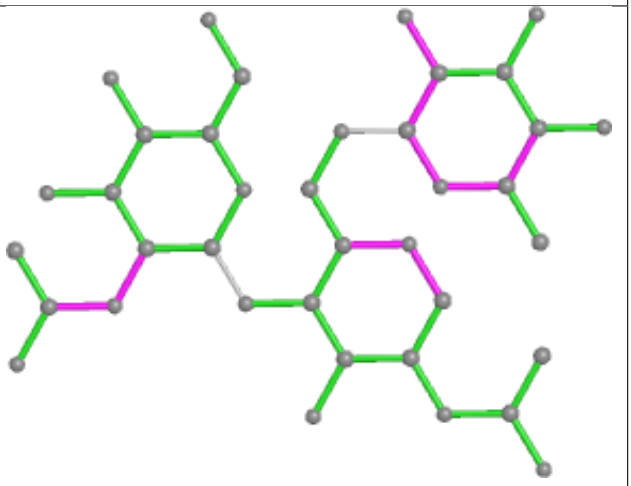


Rings

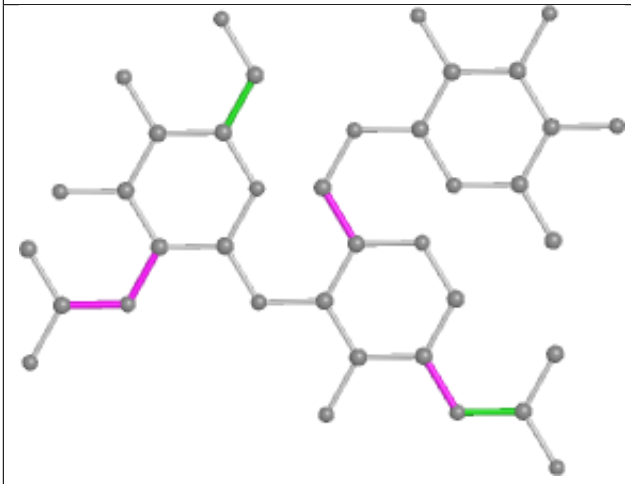
Oligosaccharide Chain G



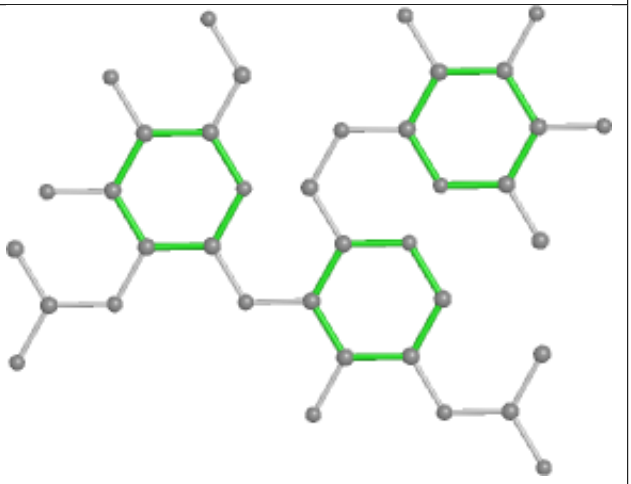
Bond lengths



Bond angles

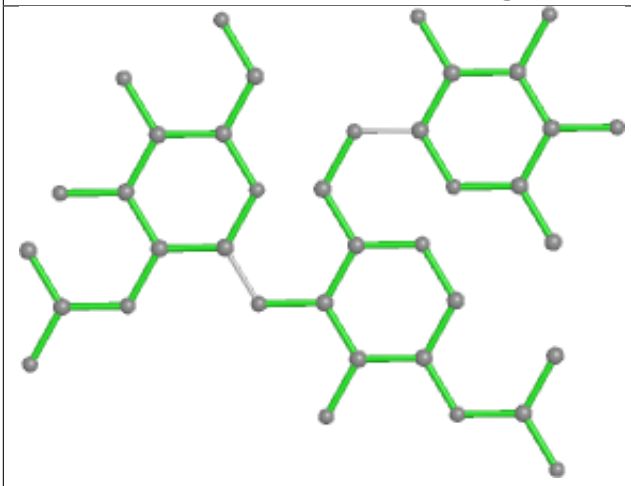


Torsions

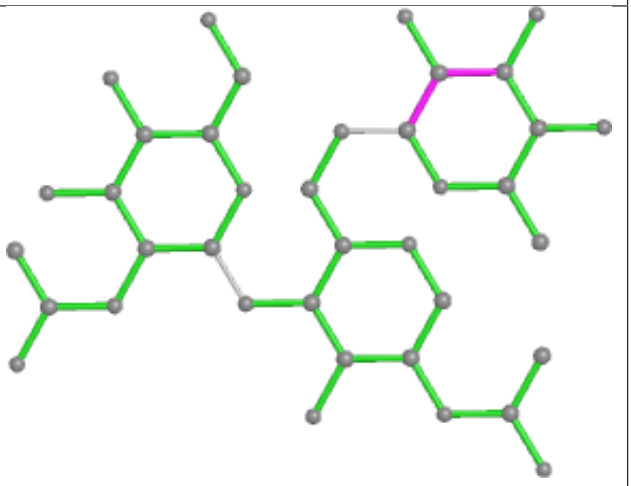


Rings

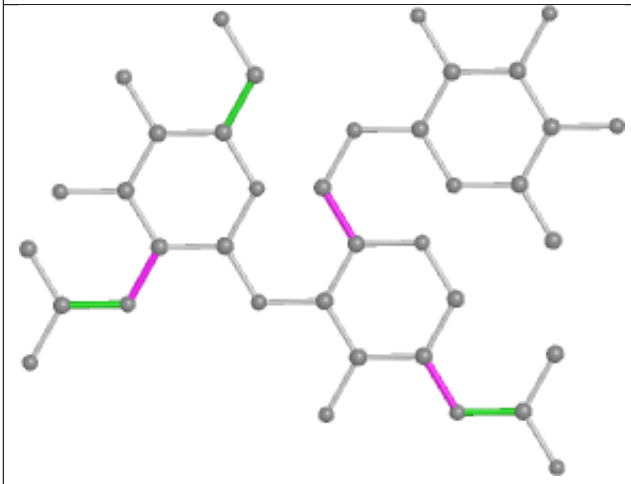
Oligosaccharide Chain J



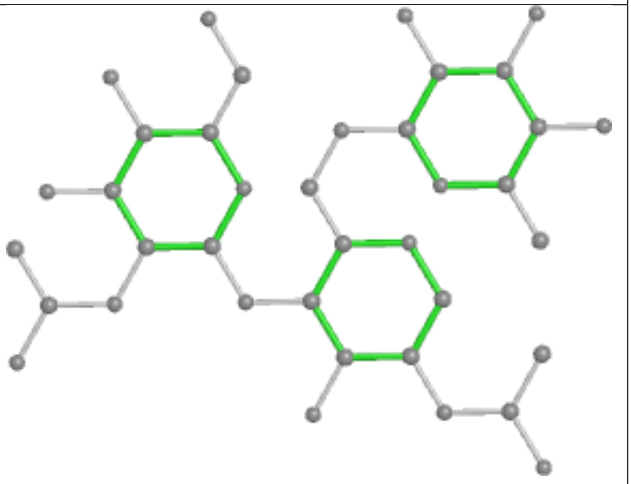
Bond lengths



Bond angles

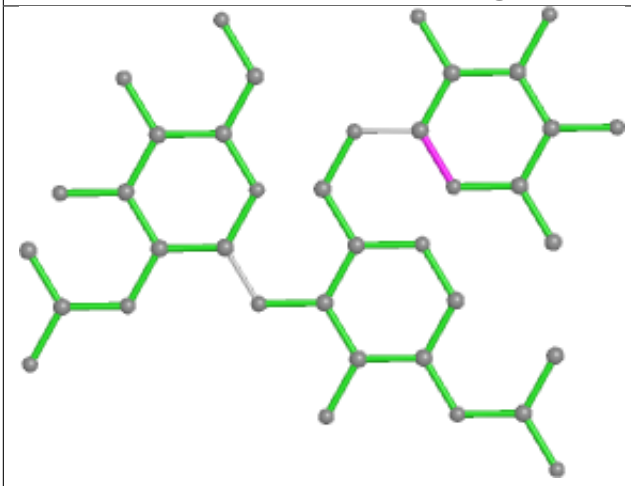


Torsions

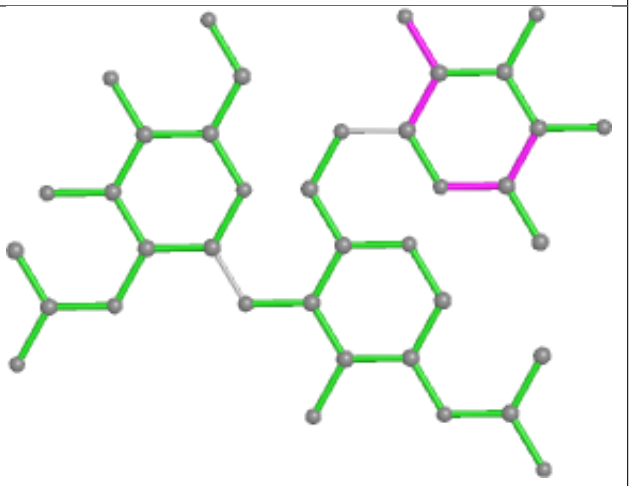


Rings

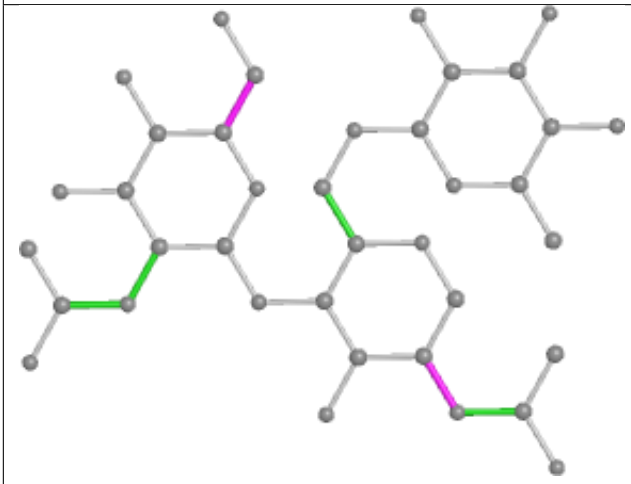
Oligosaccharide Chain M



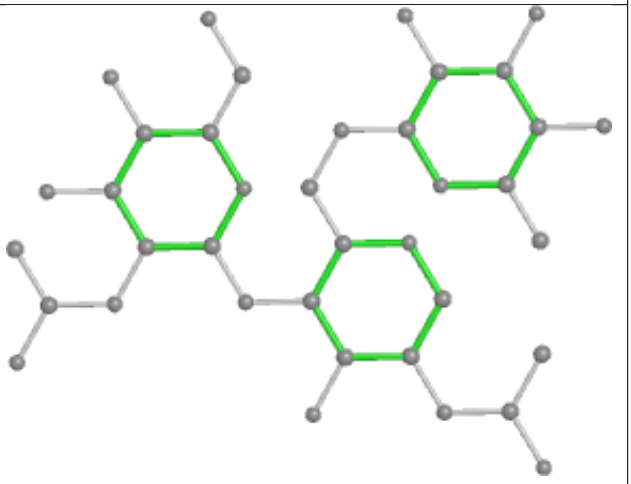
Bond lengths



Bond angles

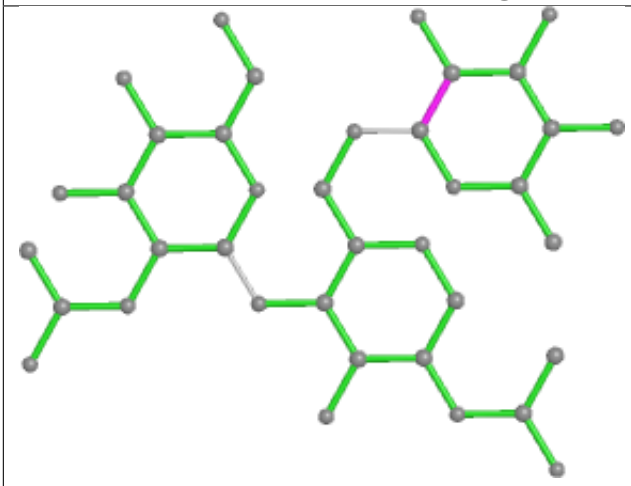


Torsions

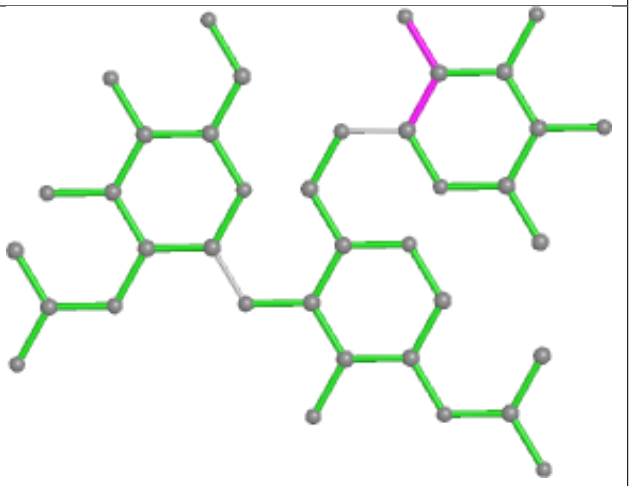


Rings

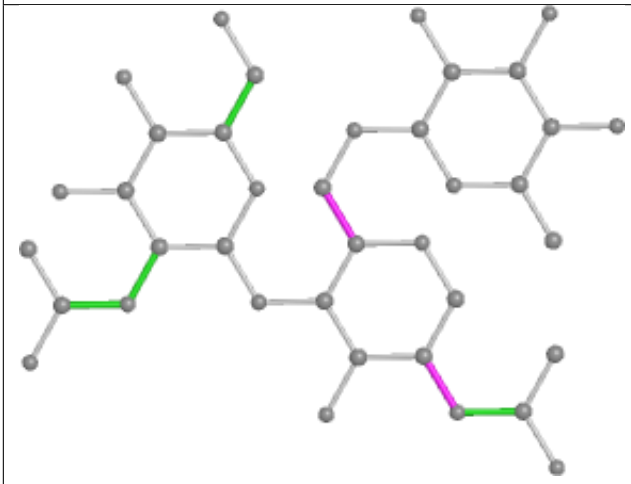
Oligosaccharide Chain P



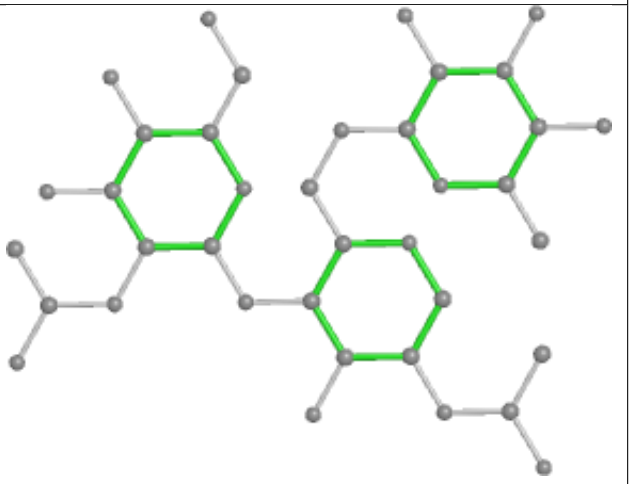
Bond lengths



Bond angles

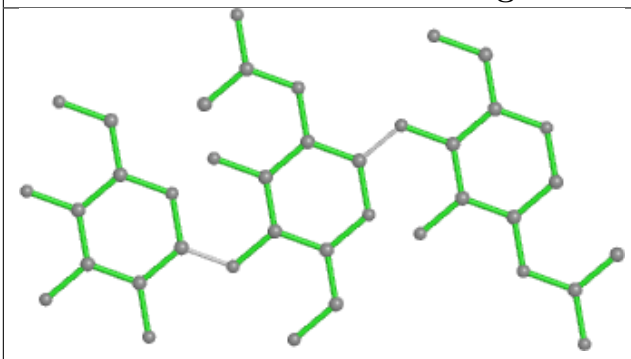


Torsions

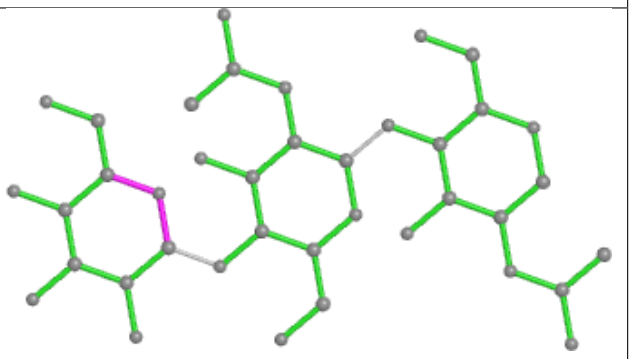


Rings

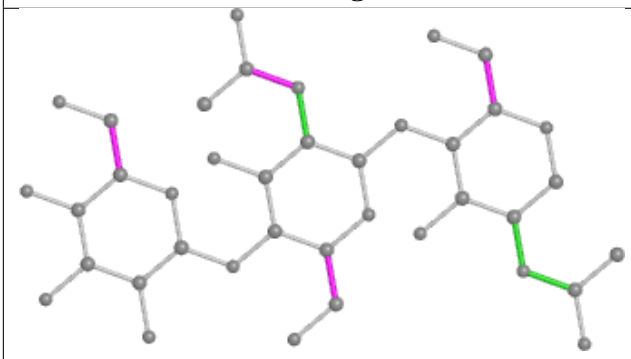
Oligosaccharide Chain L



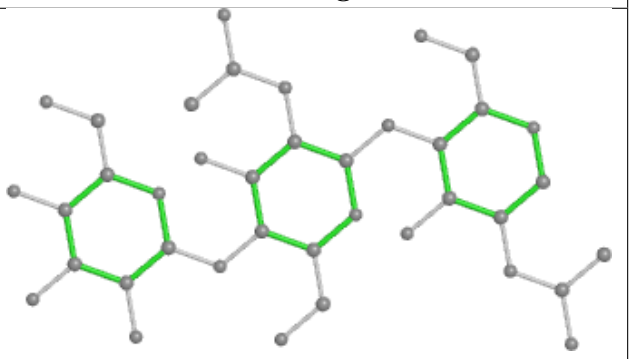
Bond lengths



Bond angles

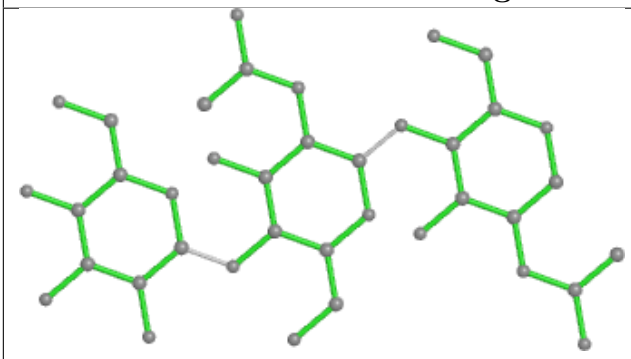


Torsions

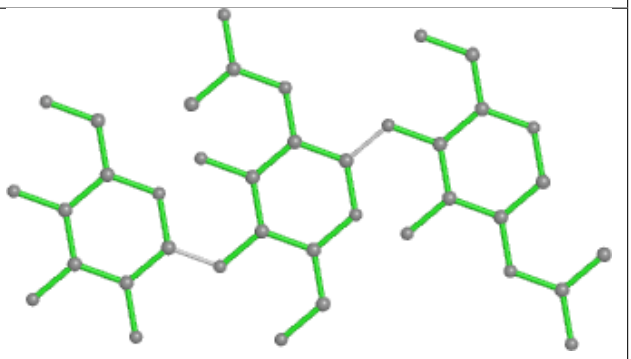


Rings

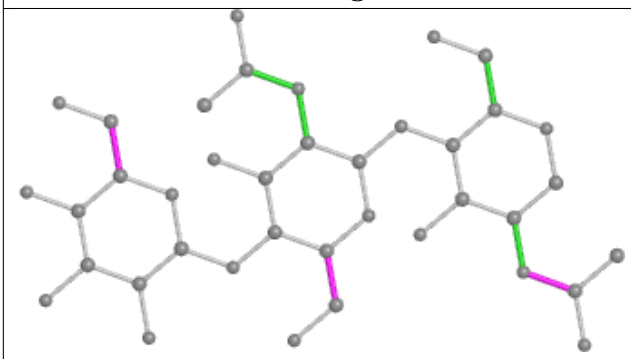
Oligosaccharide Chain N



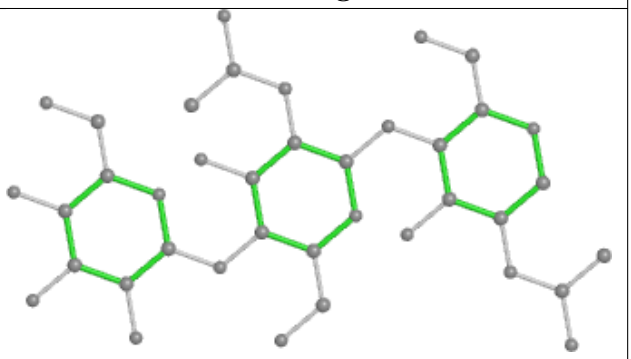
Bond lengths



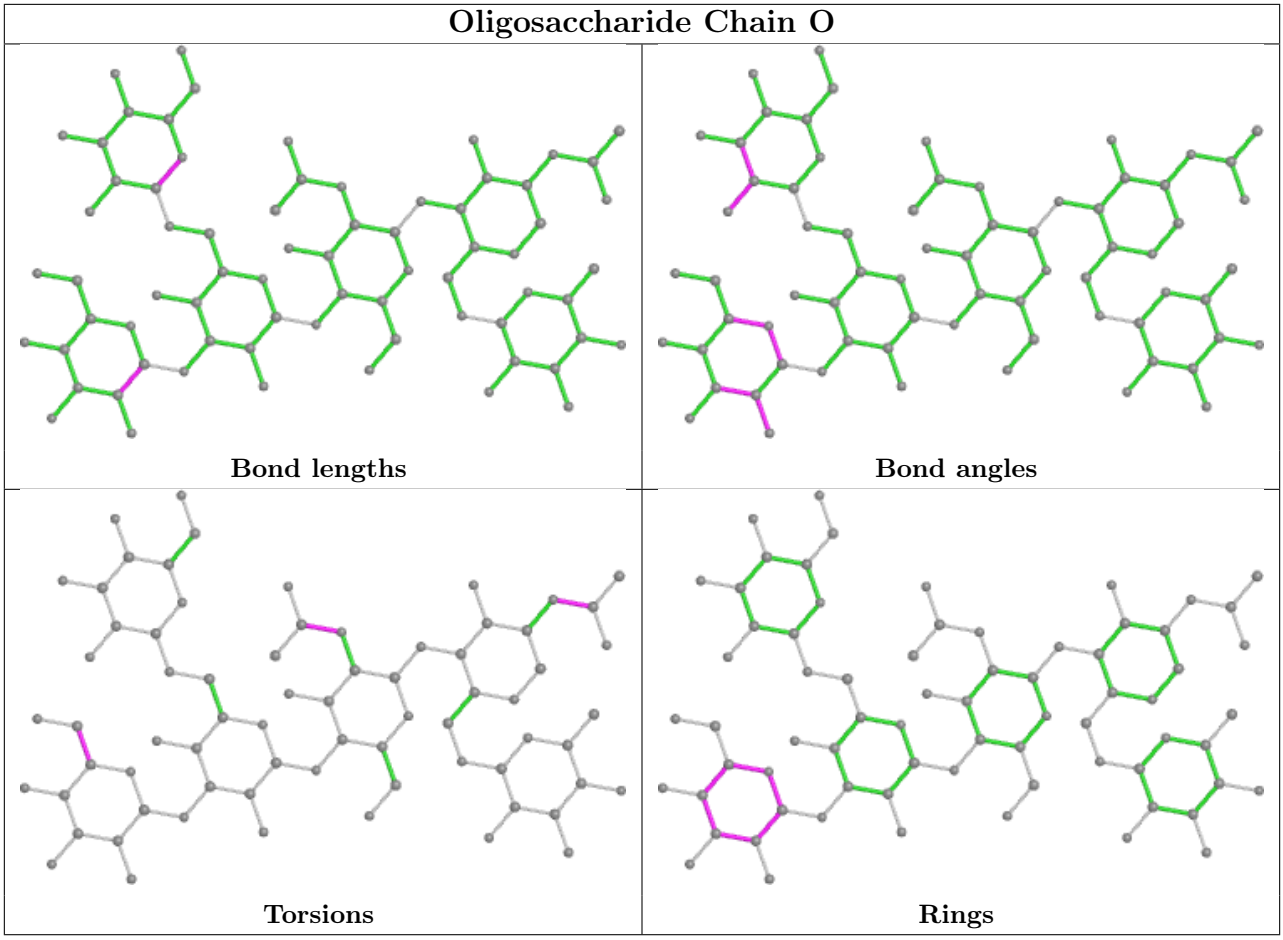
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 63 ligands modelled in this entry, 12 are monoatomic - leaving 51 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	$\#\|Z\| > 2$
12	EDO	B	721	-	3,3,3	0.46	0	2,2,2	0.29	0
11	PEG	A	716	-	6,6,6	0.39	0	5,5,5	0.45	0
12	EDO	D	721	-	3,3,3	0.41	0	2,2,2	0.37	0
8	BJ2	C	702	7	30,31,31	3.73	12 (40%)	36,44,44	1.41	7 (19%)
13	ACT	A	724	-	3,3,3	1.53	1 (33%)	3,3,3	1.39	0
13	ACT	A	725	-	3,3,3	1.35	0	3,3,3	1.44	0
17	XPE	D	724	-	30,30,30	0.54	0	29,29,29	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	PG4	C	724[B]	-	12,12,12	0.52	0	11,11,11	0.32	0
12	EDO	A	722	-	3,3,3	0.46	0	2,2,2	0.28	0
12	EDO	B	720	-	3,3,3	0.53	0	2,2,2	0.26	0
13	ACT	D	723	-	3,3,3	1.22	0	3,3,3	1.41	0
16	PG4	B	726	-	12,12,12	0.59	0	11,11,11	0.56	0
12	EDO	A	721	-	3,3,3	0.49	0	2,2,2	0.43	0
11	PEG	D	717	-	6,6,6	0.46	0	5,5,5	0.25	0
13	ACT	D	722	-	3,3,3	0.86	0	3,3,3	1.79	2 (66%)
11	PEG	B	717	-	6,6,6	0.47	0	5,5,5	0.49	0
8	BJ2	D	702	7	30,31,31	3.51	14 (46%)	36,44,44	1.45	7 (19%)
11	PEG	C	713	-	6,6,6	0.48	0	5,5,5	0.55	0
12	EDO	C	717	-	3,3,3	0.50	0	2,2,2	0.24	0
11	PEG	C	714	-	6,6,6	0.47	0	5,5,5	0.32	0
11	PEG	A	714	-	6,6,6	0.49	0	5,5,5	0.27	0
12	EDO	C	719	-	3,3,3	0.49	0	2,2,2	0.26	0
13	ACT	B	724	-	3,3,3	1.40	1 (33%)	3,3,3	1.44	0
12	EDO	A	723	-	3,3,3	0.43	0	2,2,2	0.19	0
12	EDO	B	722	-	3,3,3	0.45	0	2,2,2	0.32	0
11	PEG	B	715	-	6,6,6	0.49	0	5,5,5	0.31	0
16	PG4	C	724[A]	-	12,12,12	0.52	0	11,11,11	0.39	0
11	PEG	B	718	-	6,6,6	0.46	0	5,5,5	0.40	0
12	EDO	A	717	-	3,3,3	0.58	0	2,2,2	0.33	0
12	EDO	C	715	-	3,3,3	0.48	0	2,2,2	0.26	0
12	EDO	C	718	-	3,3,3	0.53	0	2,2,2	0.24	0
12	EDO	C	720	-	3,3,3	0.44	0	2,2,2	0.41	0
12	EDO	C	721	-	3,3,3	0.50	0	2,2,2	0.25	0
8	BJ2	B	702	7	30,31,31	3.55	10 (33%)	36,44,44	1.38	5 (13%)
8	BJ2	A	702	7	30,31,31	3.60	12 (40%)	36,44,44	1.49	4 (11%)
11	PEG	B	714	-	6,6,6	0.46	0	5,5,5	0.35	0
12	EDO	C	722	-	3,3,3	0.51	0	2,2,2	0.02	0
11	PEG	A	715	-	6,6,6	0.46	0	5,5,5	0.35	0
12	EDO	A	719	-	3,3,3	0.55	0	2,2,2	0.25	0
11	PEG	D	718	-	6,6,6	0.43	0	5,5,5	0.29	0
13	ACT	C	723	-	3,3,3	1.25	0	3,3,3	1.49	0
11	PEG	B	716	-	6,6,6	0.48	0	5,5,5	0.31	0
12	EDO	C	716	-	3,3,3	0.51	0	2,2,2	0.15	0
12	EDO	D	719	-	3,3,3	0.52	0	2,2,2	0.20	0
12	EDO	A	718	-	3,3,3	0.48	0	2,2,2	0.34	0
12	EDO	B	723	-	3,3,3	0.48	0	2,2,2	0.31	0
14	PE3	A	726	-	42,42,42	0.55	0	41,41,41	0.48	0
15	PGE	B	725	-	9,9,9	0.31	0	8,8,8	0.31	0
12	EDO	A	720	-	3,3,3	0.48	0	2,2,2	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	EDO	B	719	-	3,3,3	0.51	0	2,2,2	0.22	0
12	EDO	D	720	-	3,3,3	0.50	0	2,2,2	0.30	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
12	EDO	B	721	-	-	0/1/1/1	-
11	PEG	A	716	-	-	0/4/4/4	-
12	EDO	D	721	-	-	0/1/1/1	-
8	BJ2	C	702	7	-	7/36/56/56	0/2/2/2
17	XPE	D	724	-	-	15/28/28/28	-
16	PG4	C	724[B]	-	-	6/10/10/10	-
12	EDO	A	722	-	-	0/1/1/1	-
12	EDO	B	720	-	-	1/1/1/1	-
16	PG4	B	726	-	-	4/10/10/10	-
12	EDO	A	721	-	-	0/1/1/1	-
11	PEG	D	717	-	-	2/4/4/4	-
11	PEG	B	717	-	-	3/4/4/4	-
8	BJ2	D	702	7	-	7/36/56/56	0/2/2/2
11	PEG	C	713	-	-	2/4/4/4	-
12	EDO	C	717	-	-	0/1/1/1	-
11	PEG	C	714	-	-	1/4/4/4	-
11	PEG	A	714	-	-	1/4/4/4	-
12	EDO	C	719	-	-	0/1/1/1	-
12	EDO	A	723	-	-	0/1/1/1	-
12	EDO	B	722	-	-	1/1/1/1	-
11	PEG	B	715	-	-	2/4/4/4	-
16	PG4	C	724[A]	-	-	2/10/10/10	-
11	PEG	B	718	-	-	1/4/4/4	-
12	EDO	A	717	-	-	0/1/1/1	-
12	EDO	C	715	-	-	1/1/1/1	-
12	EDO	C	718	-	-	1/1/1/1	-
12	EDO	C	720	-	-	0/1/1/1	-
12	EDO	C	721	-	-	0/1/1/1	-
8	BJ2	B	702	7	-	7/36/56/56	0/2/2/2
8	BJ2	A	702	7	-	7/36/56/56	0/2/2/2
11	PEG	B	714	-	-	1/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	EDO	C	722	-	-	0/1/1/1	-
11	PEG	A	715	-	-	0/4/4/4	-
12	EDO	A	719	-	-	1/1/1/1	-
11	PEG	D	718	-	-	3/4/4/4	-
11	PEG	B	716	-	-	0/4/4/4	-
12	EDO	C	716	-	-	1/1/1/1	-
12	EDO	D	719	-	-	1/1/1/1	-
12	EDO	A	718	-	-	0/1/1/1	-
12	EDO	B	723	-	-	1/1/1/1	-
14	PE3	A	726	-	-	23/40/40/40	-
15	PGE	B	725	-	-	4/7/7/7	-
12	EDO	A	720	-	-	1/1/1/1	-
12	EDO	B	719	-	-	1/1/1/1	-
12	EDO	D	720	-	-	1/1/1/1	-

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	702	BJ2	C08-N12	9.30	1.58	1.47
8	A	702	BJ2	C08-N12	8.74	1.58	1.47
8	D	702	BJ2	C08-N12	8.59	1.58	1.47
8	B	702	BJ2	C08-N12	8.33	1.57	1.47
8	B	702	BJ2	C09-C08	-7.60	1.40	1.53

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	702	BJ2	C28-C27-N23	-3.99	104.17	112.26
8	A	702	BJ2	C08-C04-N03	-3.93	101.90	109.99
8	D	702	BJ2	C28-C27-N23	-3.82	104.51	112.26
8	C	702	BJ2	C08-C04-N03	-3.48	102.81	109.99
8	A	702	BJ2	C28-C27-N23	-3.20	105.77	112.26

There are no chirality outliers.

5 of 109 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	702	BJ2	N03-C04-C08-C09
8	B	702	BJ2	N03-C04-C08-C09
8	C	702	BJ2	N03-C04-C08-C09
14	A	726	PE3	C42-C41-O40-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	D	717	PEG	O2-C3-C4-O4

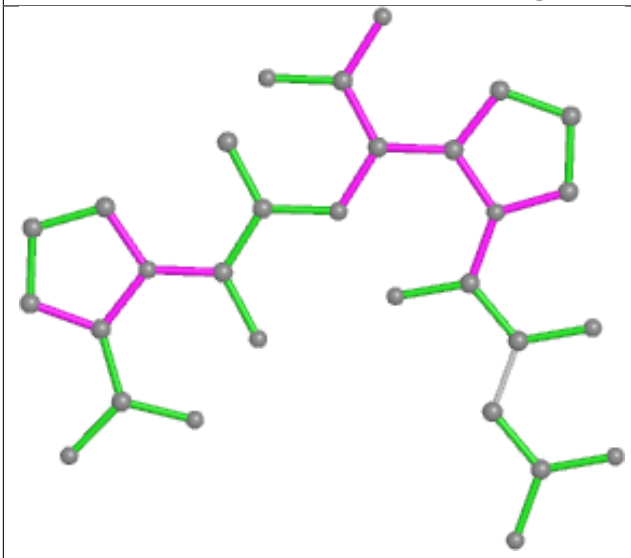
There are no ring outliers.

9 monomers are involved in 15 short contacts:

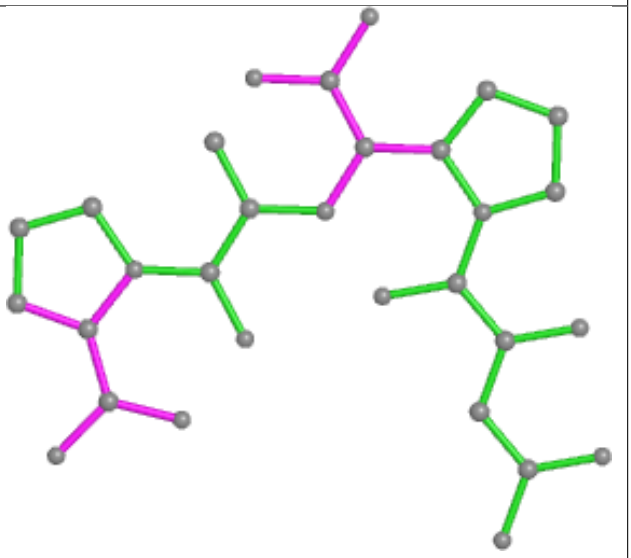
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	716	PEG	2	0
8	C	702	BJ2	1	0
13	D	723	ACT	1	0
16	B	726	PG4	2	0
11	C	713	PEG	2	0
11	C	714	PEG	1	0
12	A	723	EDO	2	0
12	A	719	EDO	1	0
14	A	726	PE3	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is 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.

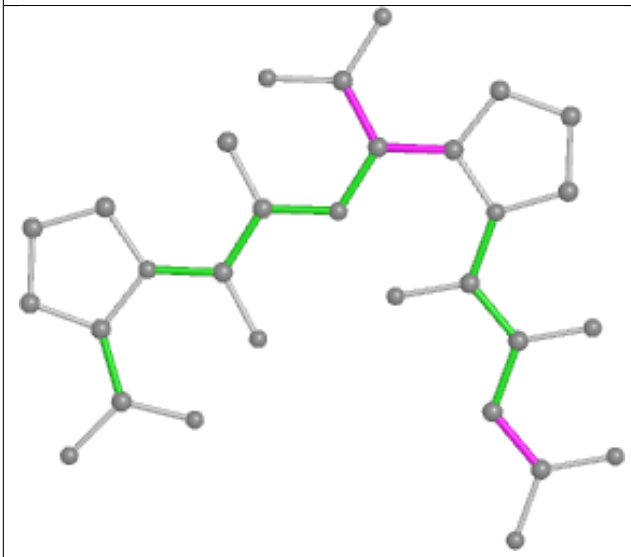
Ligand BJ2 C 702



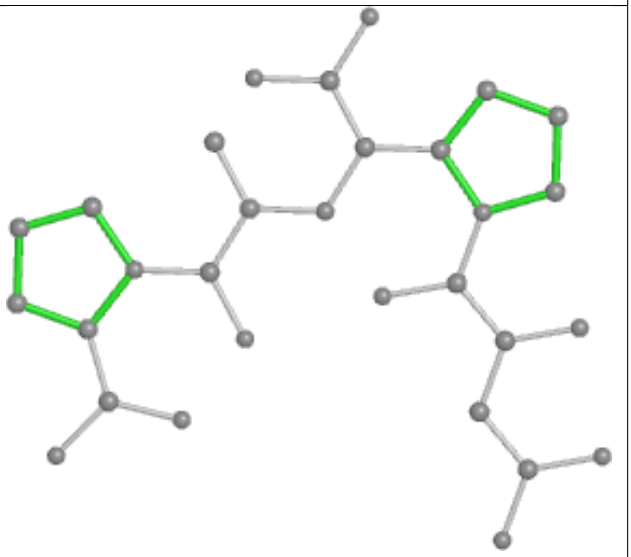
Bond lengths



Bond angles



Torsions

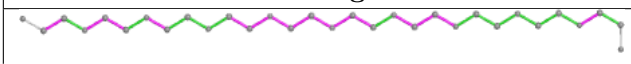


Rings

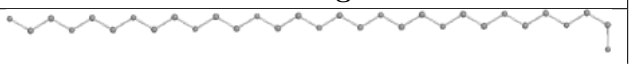
Ligand XPE D 724

Bond lengths

Bond angles

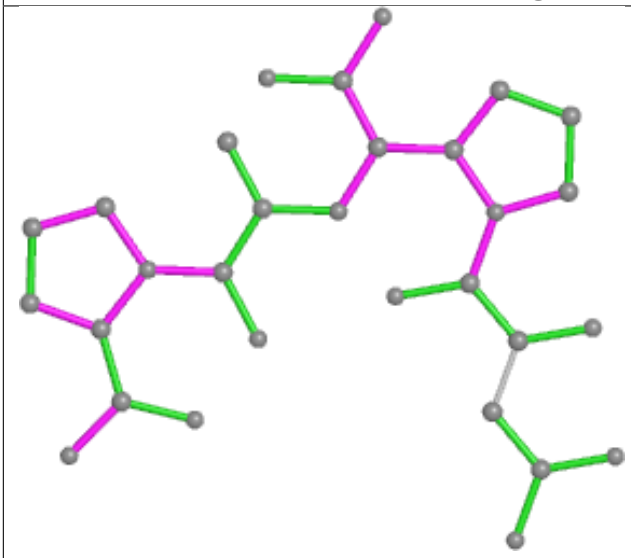


Torsions

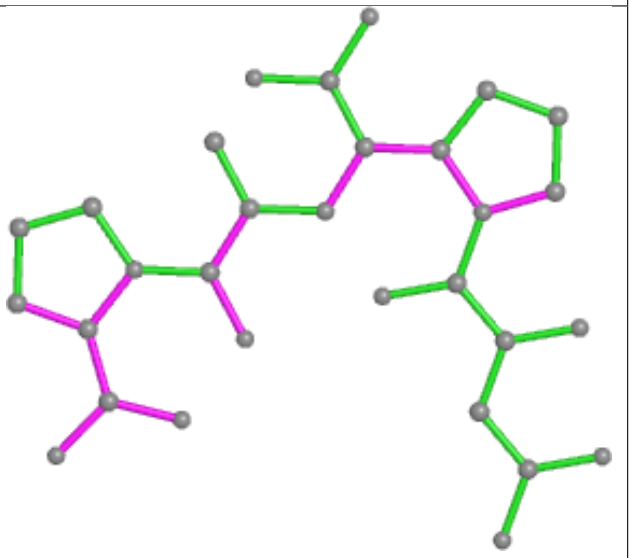


Rings

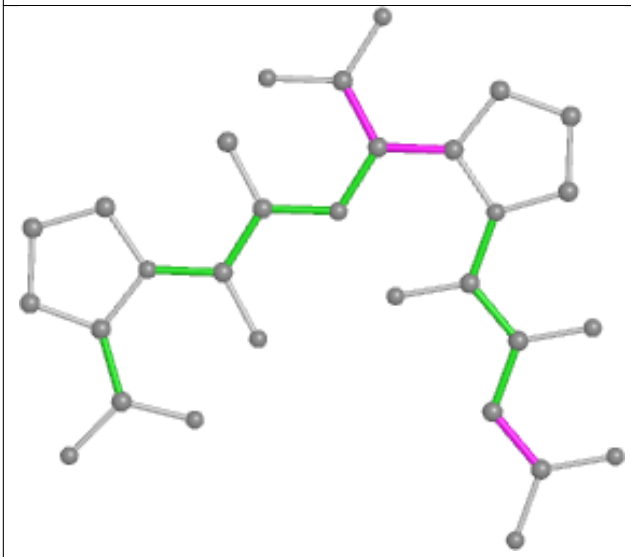
Ligand BJ2 D 702



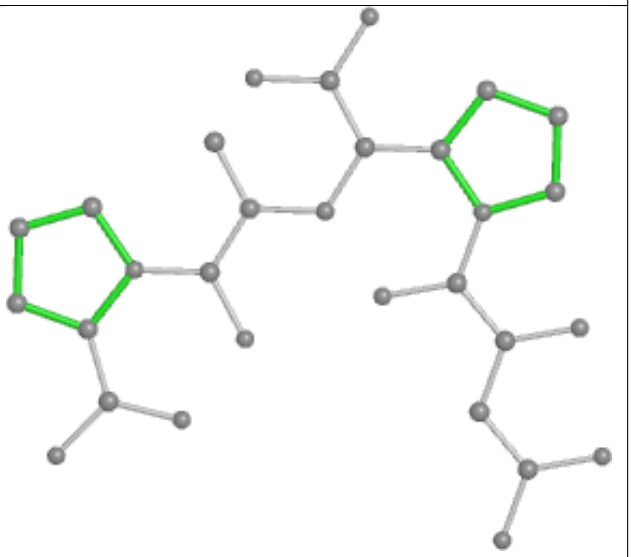
Bond lengths



Bond angles

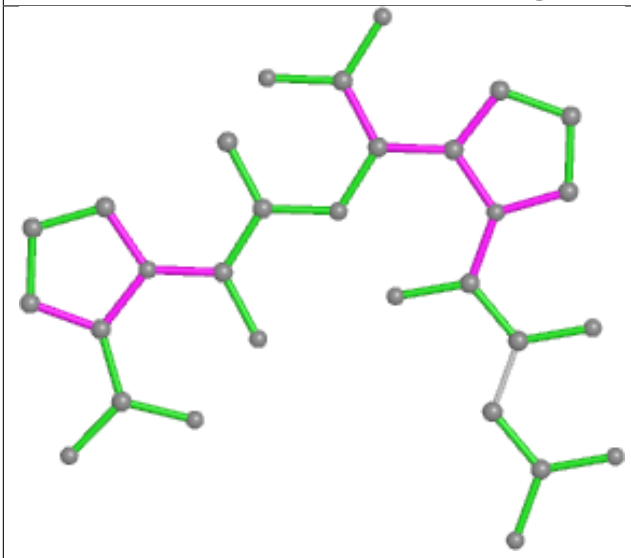


Torsions

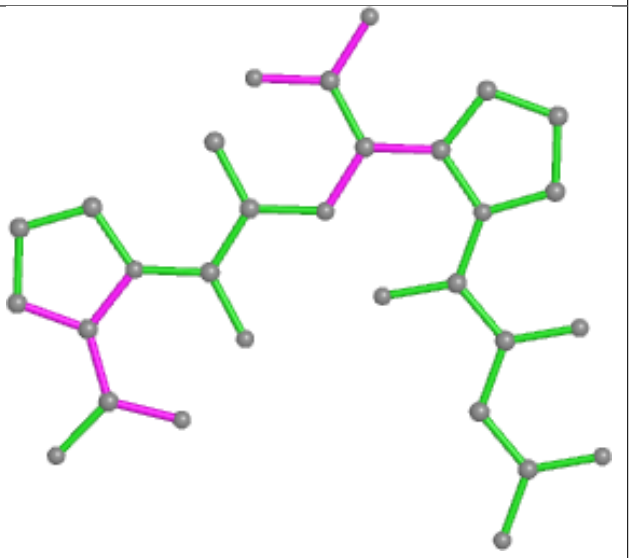


Rings

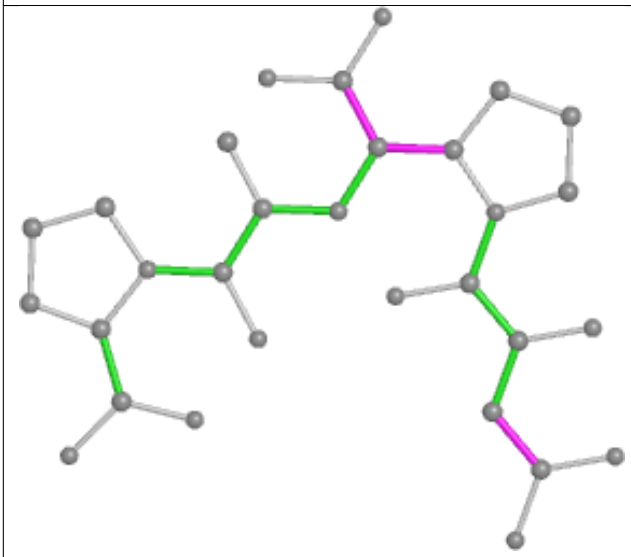
Ligand BJ2 B 702



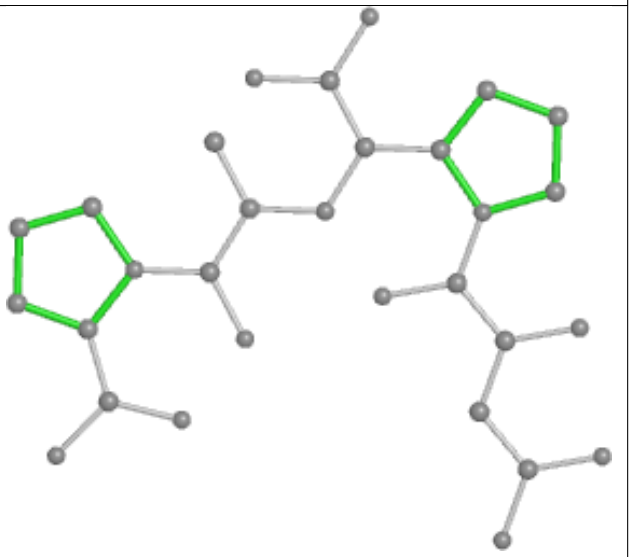
Bond lengths



Bond angles

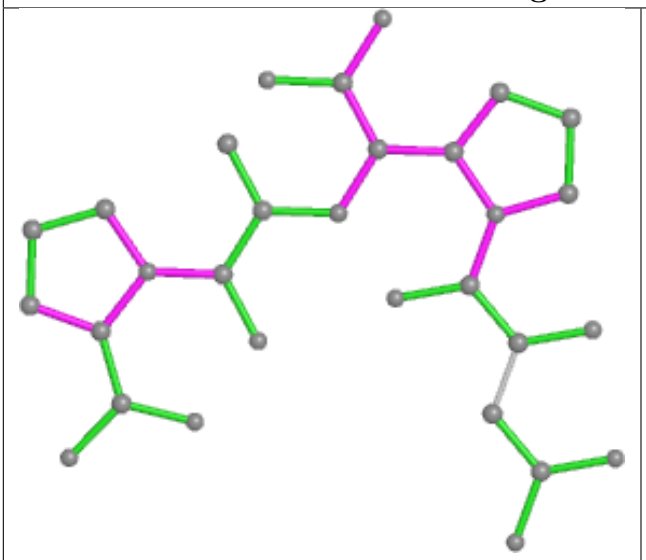


Torsions

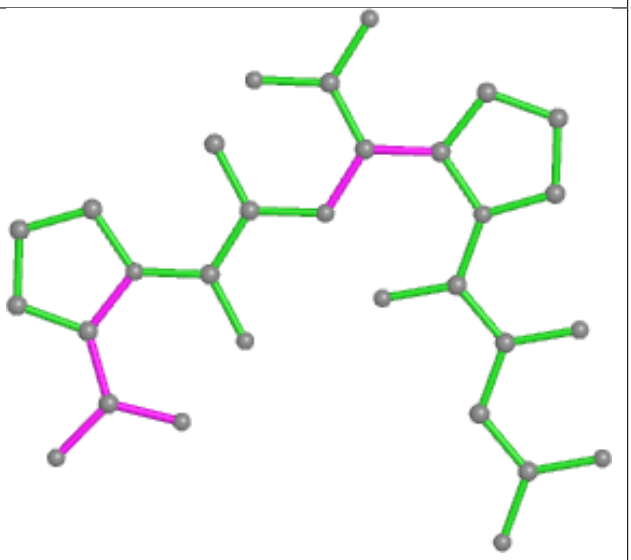


Rings

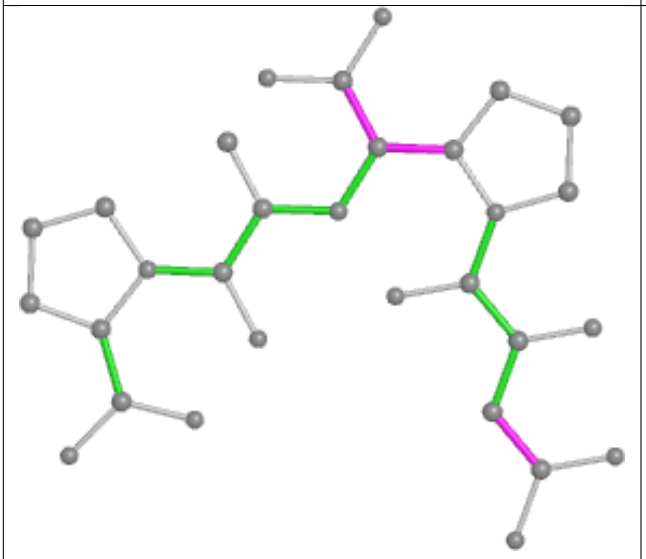
Ligand BJ2 A 702



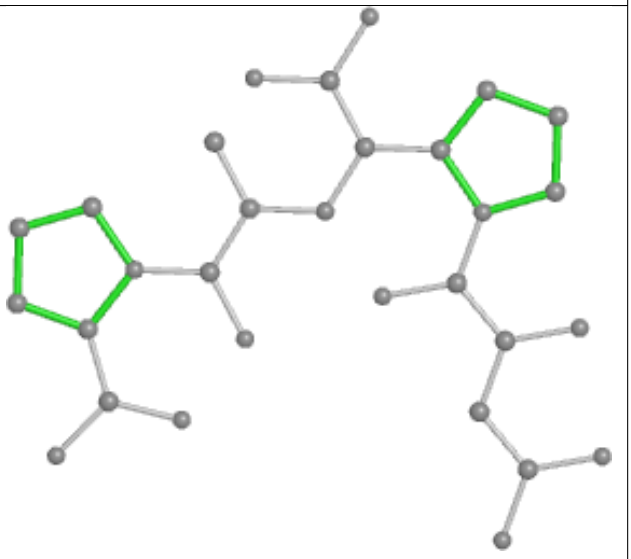
Bond lengths



Bond angles

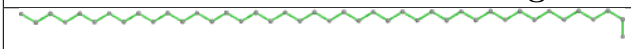


Torsions

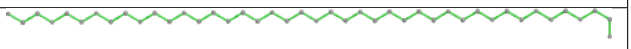


Rings

Ligand PE3 A 726



Bond lengths



Bond angles

Torsions

Rings

5.7 Other polymers

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, 95^{th} 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	605/629 (96%)	-0.18	10 (1%)	70	77	17, 26, 46, 98	0
1	B	608/629 (96%)	-0.05	27 (4%)	34	40	17, 26, 47, 75	50 (8%)
1	C	606/629 (96%)	-0.11	14 (2%)	60	67	18, 30, 53, 83	0
1	D	614/629 (97%)	-0.19	3 (0%)	91	93	16, 24, 41, 69	0
All	All	2433/2516 (96%)	-0.13	54 (2%)	62	69	16, 26, 48, 98	50 (2%)

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	414	VAL	6.9
1	D	135	THR	5.4
1	C	130	PRO	5.4
1	C	135	THR	4.9
1	A	413	ARG	4.7

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

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, 95^{th} 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
6	MAN	O	5	11/12	0.31	0.37	71,86,101,106	21
6	MAN	O	4	11/12	0.46	0.31	75,92,108,116	0

Continued on next page...

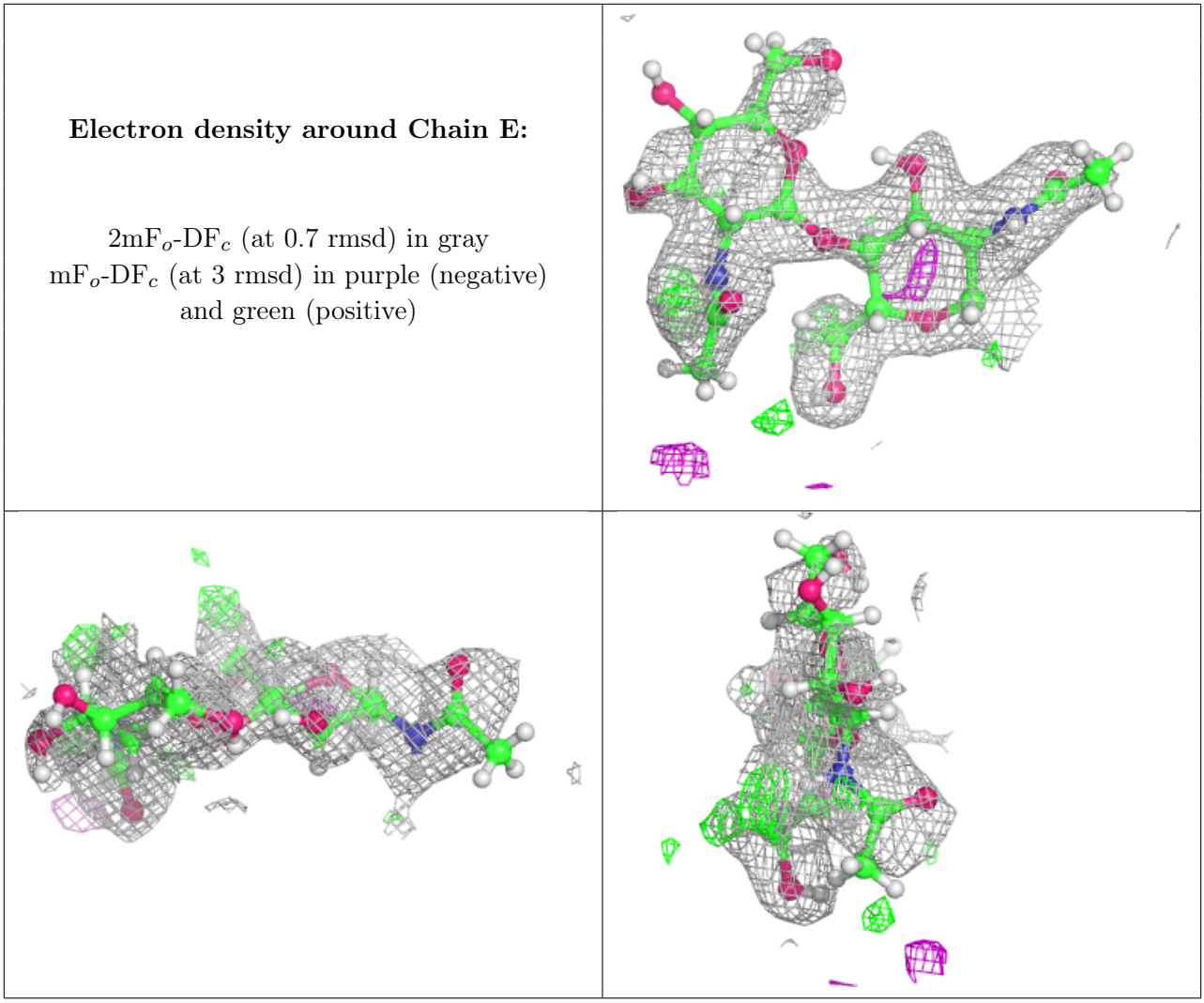
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	J	2	14/15	0.48	0.35	52,70,88,93	27
4	NAG	P	2	14/15	0.55	0.39	59,79,102,109	27
4	NAG	G	2	14/15	0.57	0.21	53,80,99,111	28
2	NAG	K	2	14/15	0.62	0.28	56,71,86,94	27
5	BMA	N	3	11/12	0.64	0.23	84,102,122,126	0
5	BMA	L	3	11/12	0.67	0.25	76,95,114,115	0
4	NAG	M	2	14/15	0.68	0.23	52,79,101,112	27
2	NAG	E	2	14/15	0.68	0.26	66,86,105,126	28
4	FUC	P	3	10/11	0.69	0.30	52,65,78,82	19
2	NAG	H	2	14/15	0.70	0.17	57,68,87,95	27
5	NAG	N	2	14/15	0.71	0.20	44,64,87,96	27
3	BMA	F	3	11/12	0.71	0.24	57,70,85,88	22
3	BMA	I	3	11/12	0.72	0.21	64,74,89,90	0
4	FUC	M	3	10/11	0.74	0.14	51,62,71,79	21
4	FUC	J	3	10/11	0.74	0.25	53,65,78,81	20
2	NAG	E	1	14/15	0.76	0.18	44,61,76,80	0
3	FUC	F	4	10/11	0.78	0.22	42,51,63,72	20
2	NAG	H	1	14/15	0.78	0.12	33,50,60,68	0
6	BMA	O	3	11/12	0.80	0.20	63,70,84,84	0
4	FUC	G	3	10/11	0.81	0.23	48,66,76,80	20
2	NAG	K	1	14/15	0.82	0.15	36,53,63,67	0
5	NAG	L	1	14/15	0.83	0.18	56,70,88,88	0
4	NAG	P	1	14/15	0.84	0.11	37,50,65,74	0
4	NAG	J	1	14/15	0.84	0.12	35,46,60,66	0
6	FUC	O	6	10/11	0.84	0.15	42,53,64,67	0
4	NAG	G	1	14/15	0.85	0.10	30,43,57,61	0
4	NAG	M	1	14/15	0.88	0.10	37,50,65,69	0
5	NAG	N	1	14/15	0.88	0.09	30,45,54,59	0
5	NAG	L	2	14/15	0.89	0.19	67,82,93,95	27
6	NAG	O	2	14/15	0.90	0.15	39,49,70,71	0
3	NAG	F	1	14/15	0.90	0.13	40,48,60,60	26
3	FUC	I	4	10/11	0.90	0.10	45,55,65,67	0
3	NAG	F	2	14/15	0.90	0.15	44,55,64,64	27
3	NAG	I	2	14/15	0.90	0.10	41,55,68,68	0
6	NAG	O	1	14/15	0.92	0.09	29,40,46,52	0
3	NAG	I	1	14/15	0.95	0.09	32,41,49,50	0

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

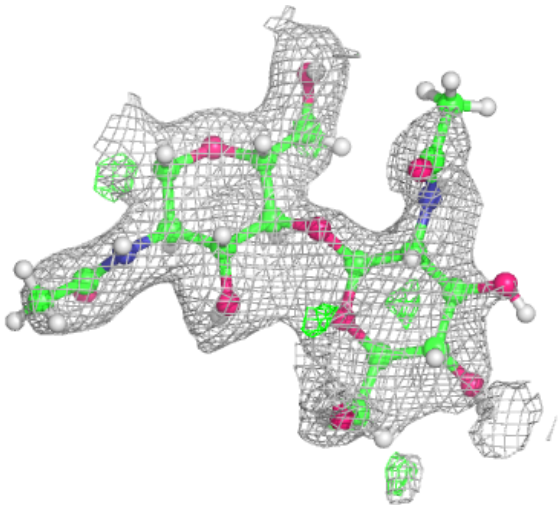
Electron density around Chain E:

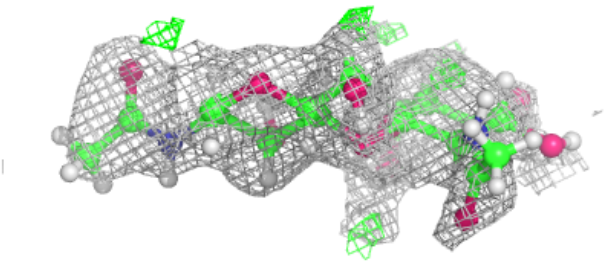
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

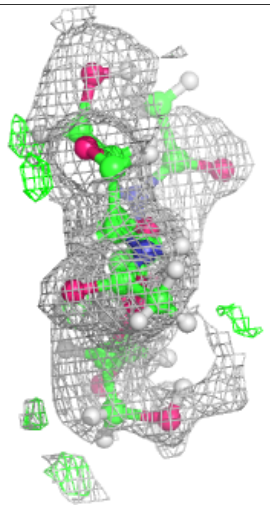


Electron density around Chain H:

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

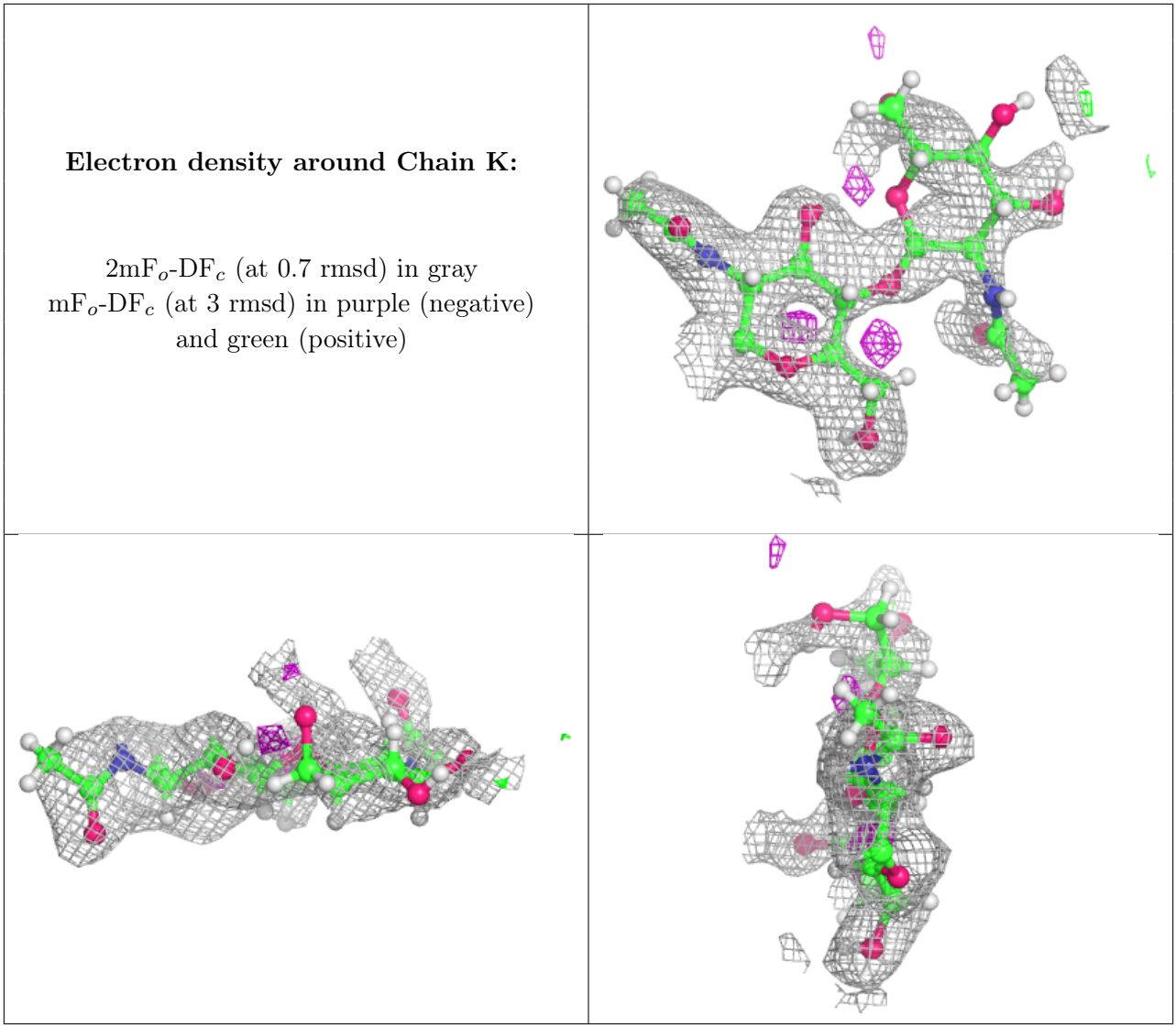






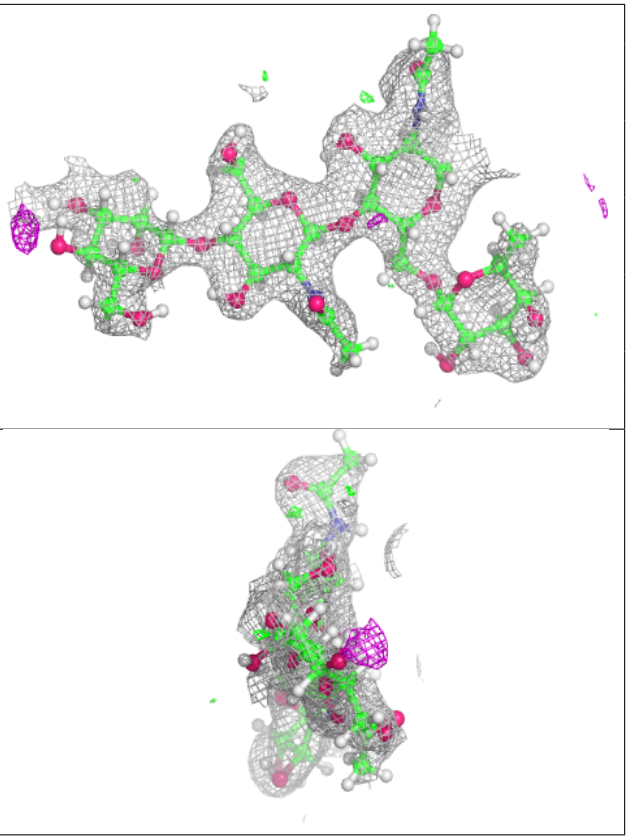
Electron density around Chain K:

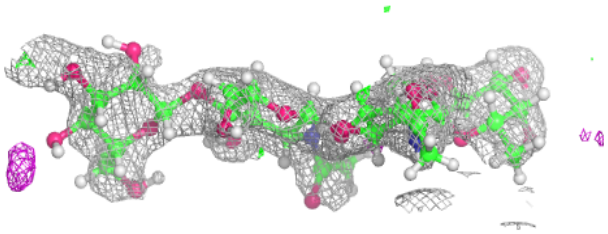
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain F:

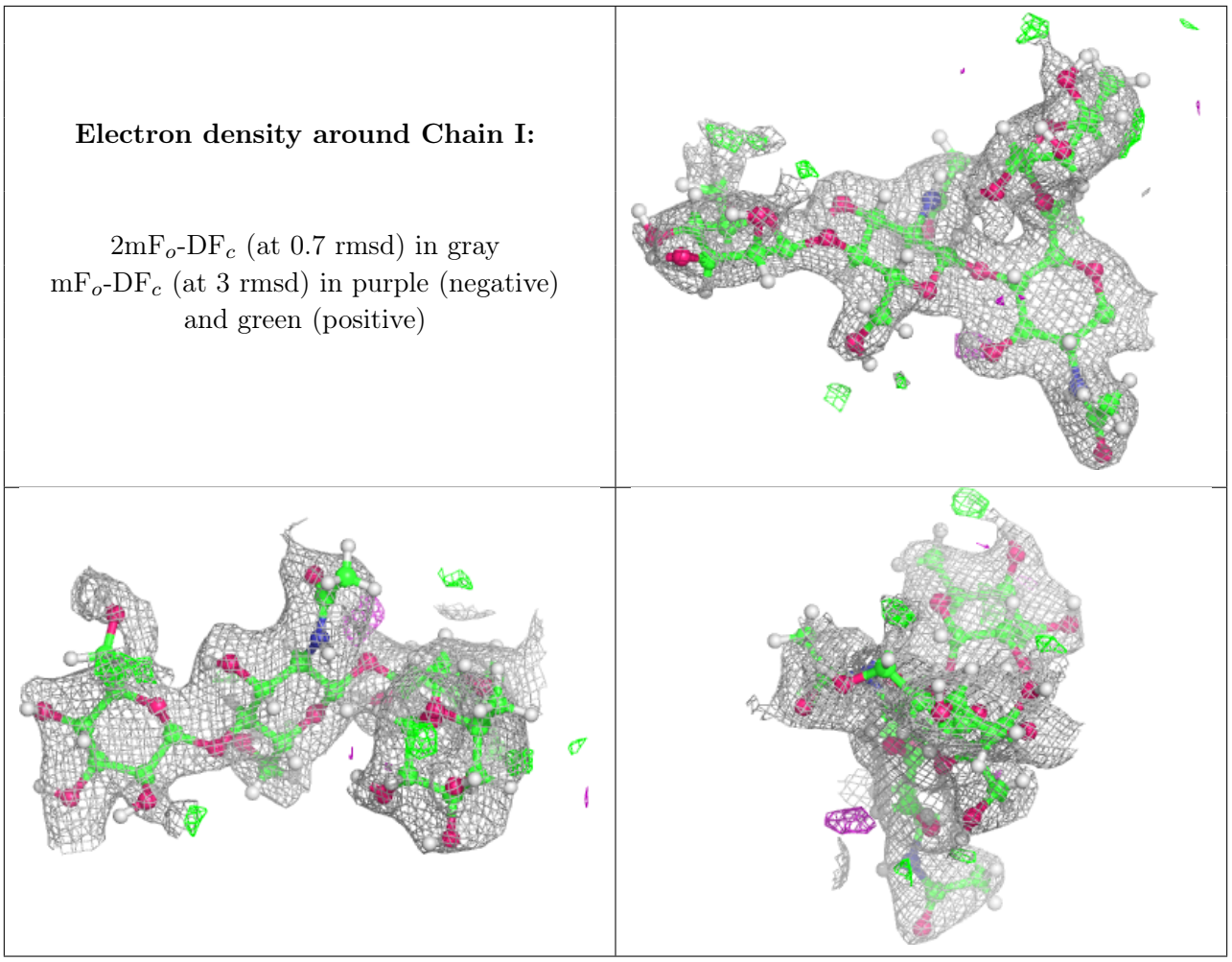
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





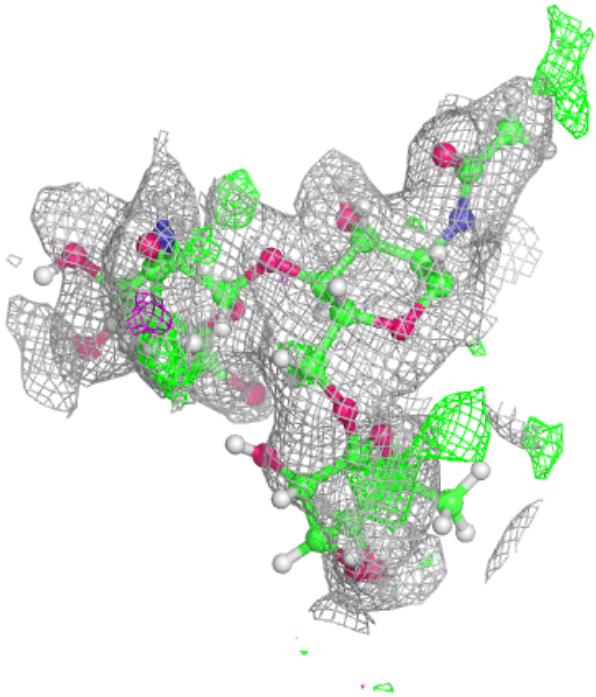
Electron density around Chain I:

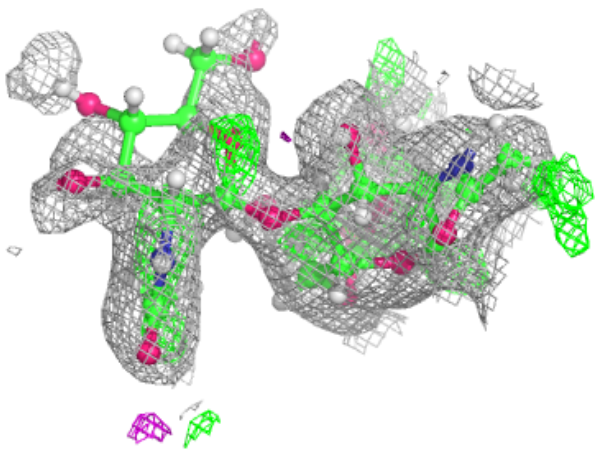
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

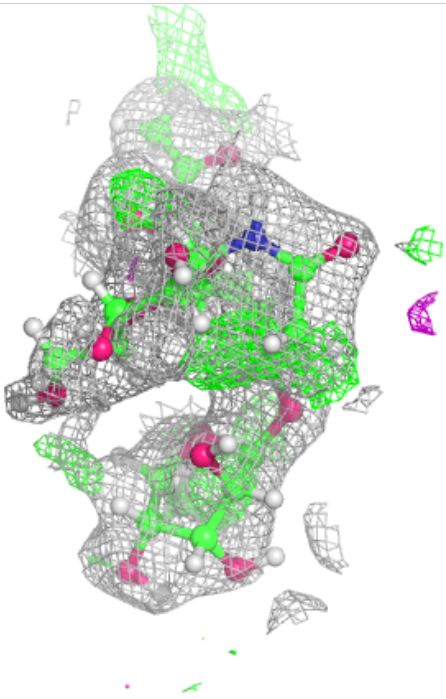


Electron density around Chain G:

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

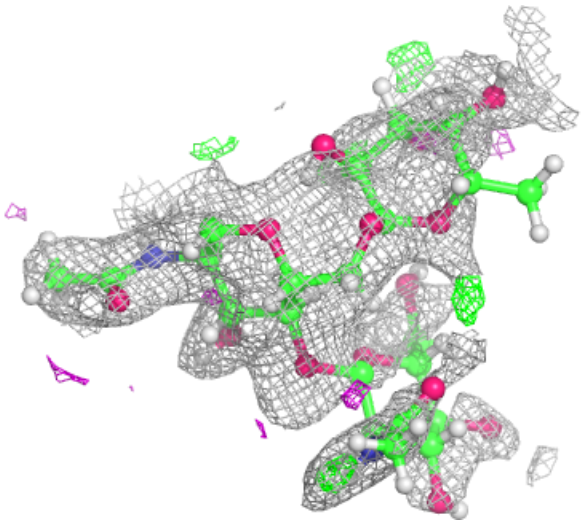


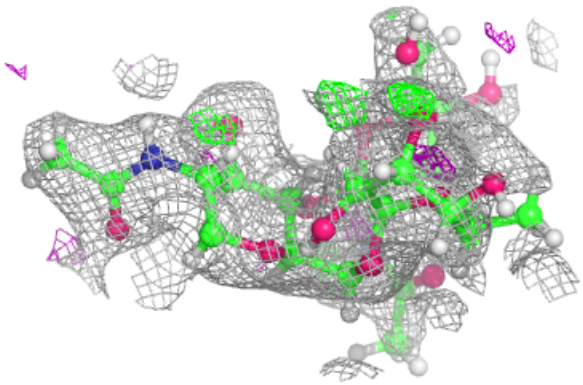


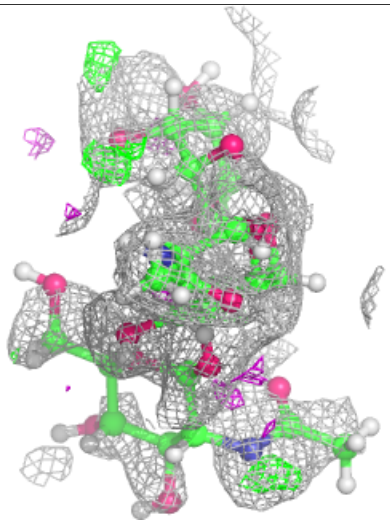


Electron density around Chain J:

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

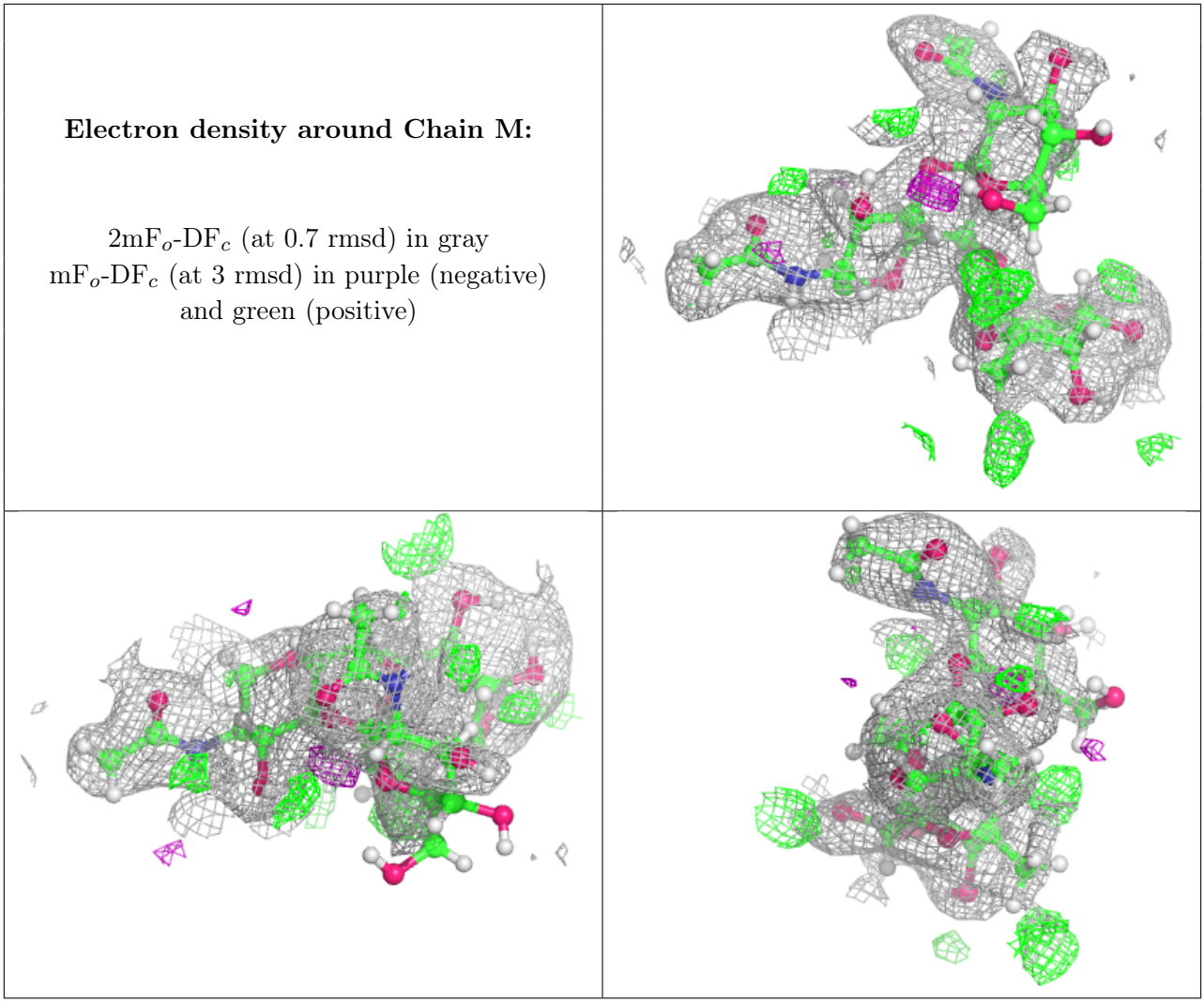






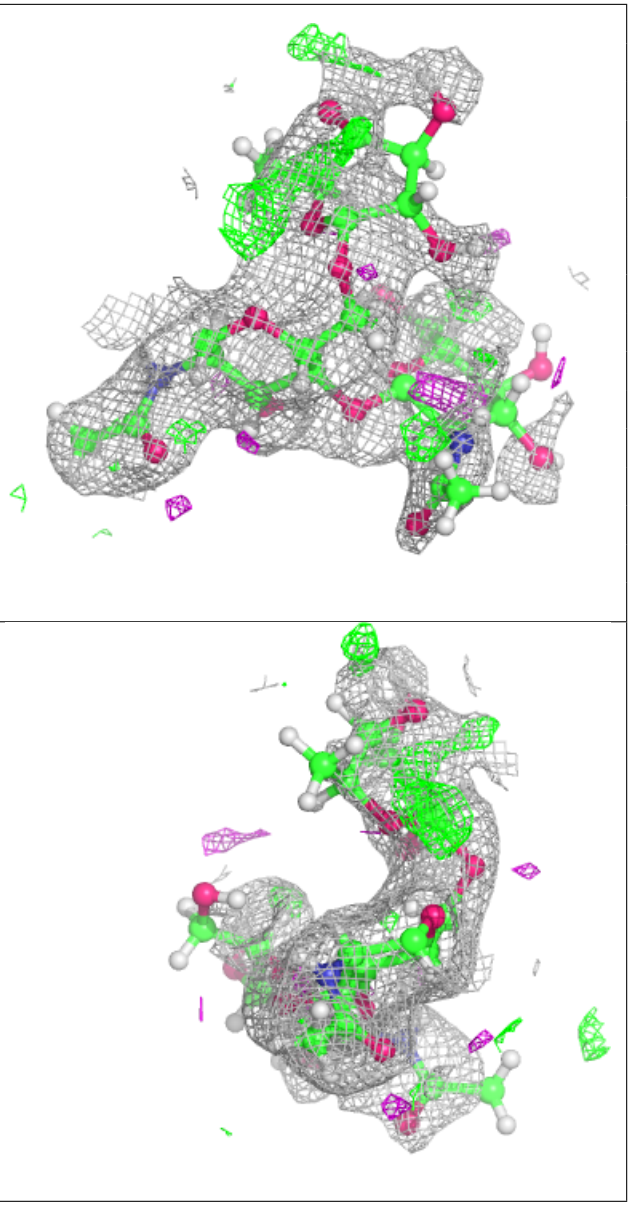
Electron density around Chain M:

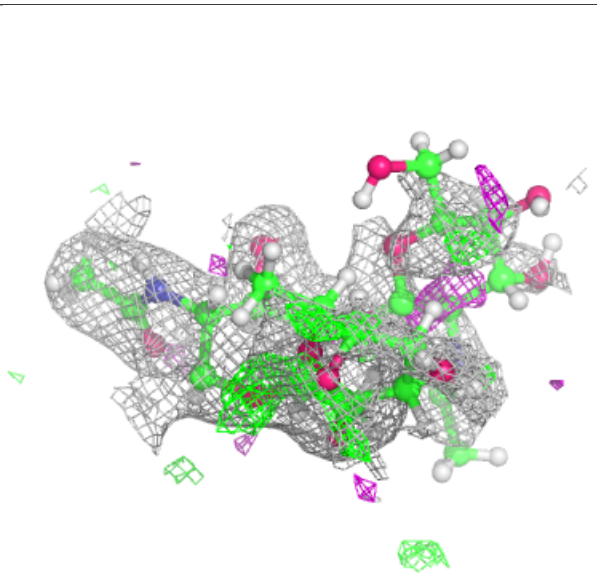
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain P:

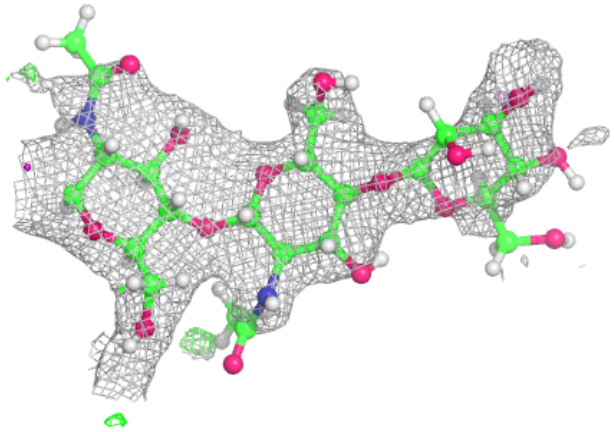
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

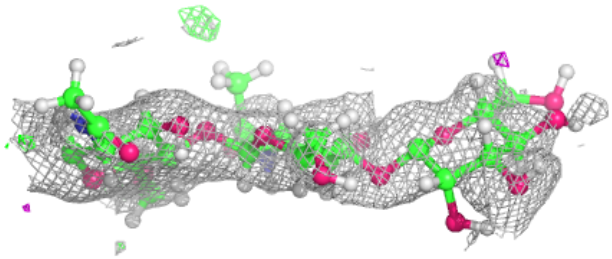


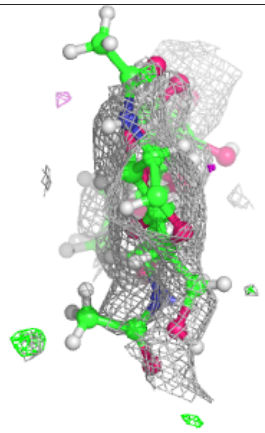


Electron density around Chain L:

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

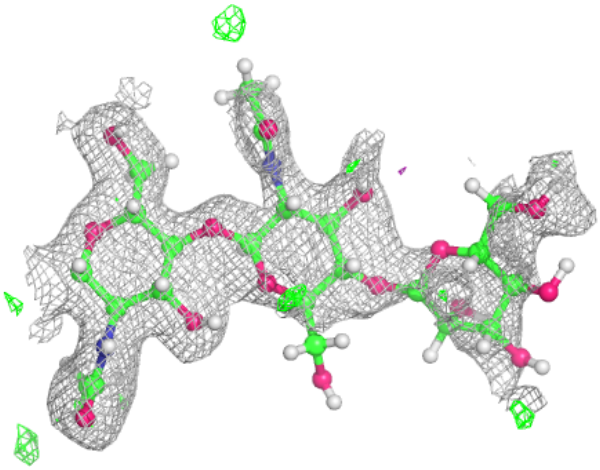


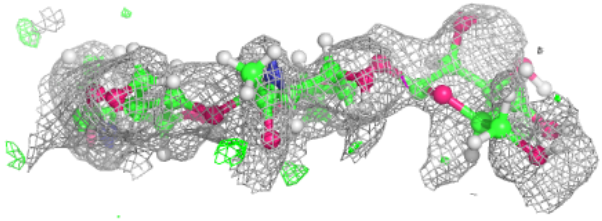


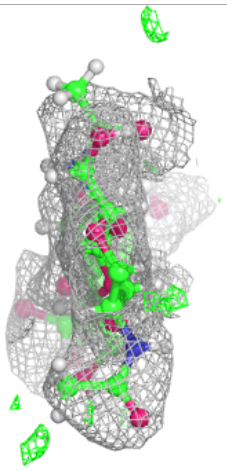


Electron density around Chain N:

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

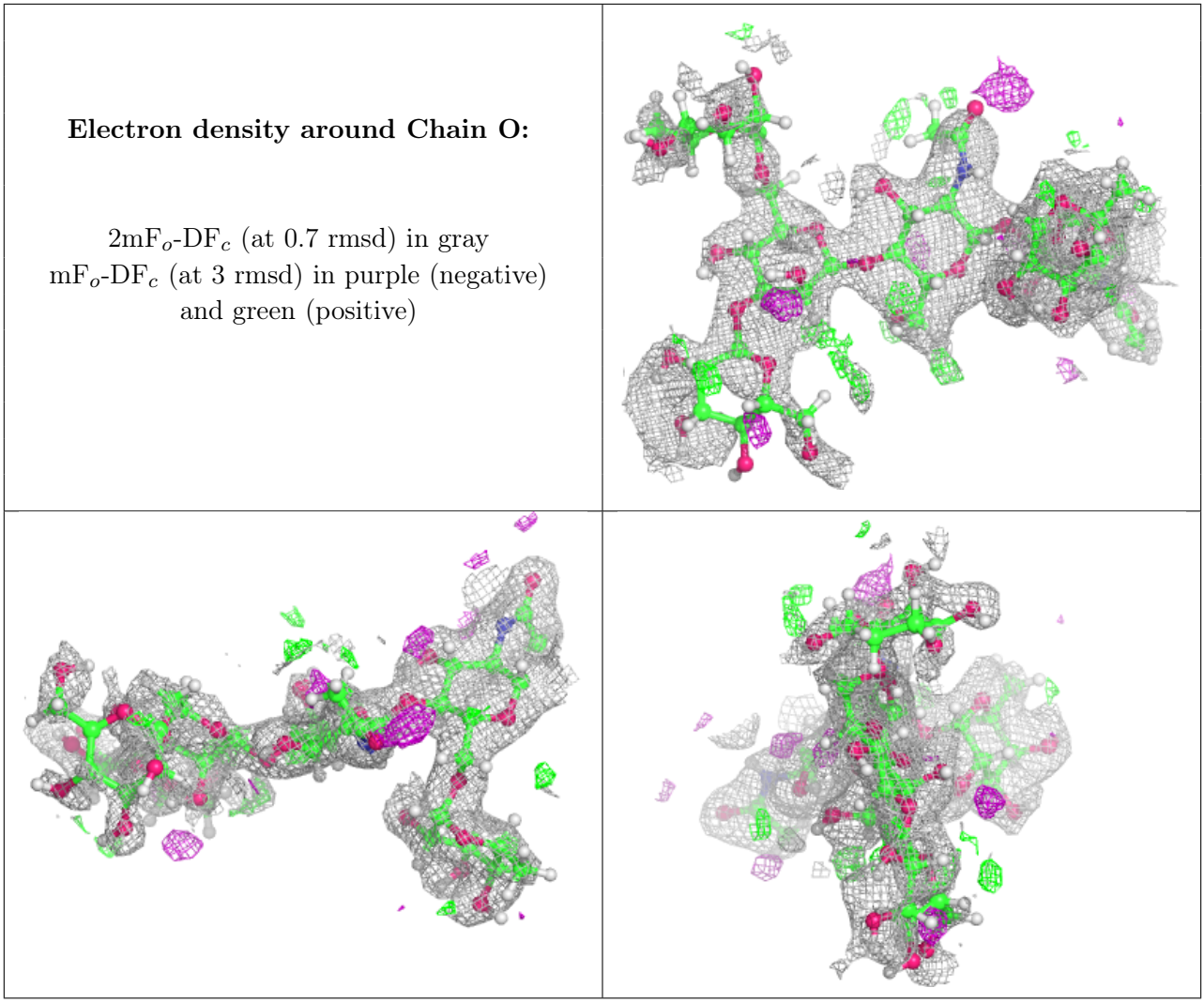






Electron density around Chain O:

$2mF_o$-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, 95^{th} 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
13	ACT	C	723	4/4	0.63	0.17	34,41,51,52	0
12	EDO	C	718	4/4	0.68	0.20	46,56,58,58	10
12	EDO	A	719	4/4	0.68	0.31	36,44,46,48	10
11	PEG	B	716	7/7	0.73	0.18	39,47,63,63	17
12	EDO	D	720	4/4	0.75	0.15	49,63,65,78	0
12	EDO	C	719	4/4	0.76	0.13	46,57,69,69	10
13	ACT	D	722	4/4	0.76	0.13	24,29,37,46	0
12	EDO	C	717	4/4	0.77	0.10	64,76,83,92	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	EDO	B	723	4/4	0.77	0.19	48,61,63,75	0
12	EDO	C	716	4/4	0.77	0.12	56,67,80,80	0
11	PEG	C	714	7/7	0.78	0.20	31,42,51,51	17
12	EDO	A	721	4/4	0.79	0.12	40,49,55,59	10
12	EDO	C	715	4/4	0.79	0.10	42,50,55,59	0
12	EDO	C	722	4/4	0.79	0.23	36,44,60,60	10
11	PEG	B	715	7/7	0.80	0.21	33,43,52,55	17
12	EDO	A	720	4/4	0.81	0.15	33,43,51,59	10
12	EDO	B	720	4/4	0.81	0.18	31,38,43,48	10
11	PEG	A	716	7/7	0.83	0.18	30,36,42,48	17
12	EDO	C	720	4/4	0.83	0.14	38,48,58,63	10
12	EDO	A	718	4/4	0.84	0.10	49,59,60,63	0
12	EDO	C	721	4/4	0.84	0.18	49,59,65,67	0
14	PE3	A	726	43/43	0.84	0.15	28,42,56,63	101
15	PGE	B	725	10/10	0.84	0.13	30,43,49,51	24
16	PG4	C	724[A]	13/13	0.84	0.14	30,37,42,53	31
16	PG4	C	724[B]	13/13	0.84	0.14	27,34,41,42	31
11	PEG	B	717	7/7	0.85	0.15	46,55,62,62	17
13	ACT	A	724	4/4	0.85	0.19	30,36,44,46	0
17	XPE	D	724	31/31	0.85	0.11	31,47,60,71	0
11	PEG	B	714	7/7	0.86	0.10	45,55,66,76	0
12	EDO	B	722	4/4	0.86	0.14	29,38,46,48	10
12	EDO	A	717	4/4	0.86	0.18	17,30,36,38	10
11	PEG	B	718	7/7	0.86	0.14	41,50,68,68	0
12	EDO	A	723	4/4	0.86	0.15	31,37,49,58	10
16	PG4	B	726	13/13	0.87	0.14	26,42,54,55	0
11	PEG	D	717	7/7	0.87	0.10	32,42,51,51	17
11	PEG	C	713	7/7	0.87	0.10	39,47,54,55	17
11	PEG	A	714	7/7	0.87	0.10	35,46,55,55	17
12	EDO	B	721	4/4	0.88	0.11	48,58,70,71	0
12	EDO	A	722	4/4	0.89	0.06	43,52,57,61	0
12	EDO	D	719	4/4	0.89	0.16	29,38,43,49	10
12	EDO	D	721	4/4	0.90	0.14	38,46,52,53	10
12	EDO	B	719	4/4	0.90	0.08	40,48,55,60	0
11	PEG	A	715	7/7	0.91	0.12	26,41,49,52	17
13	ACT	A	725	4/4	0.91	0.20	46,49,59,59	0
11	PEG	D	718	7/7	0.92	0.08	44,53,63,73	0
13	ACT	B	724	4/4	0.92	0.07	32,41,42,47	0
13	ACT	D	723	4/4	0.93	0.15	27,33,35,39	0
10	MG	C	704	1/1	0.95	0.06	31,31,31,31	0
8	BJ2	B	702	30/30	0.96	0.08	16,23,28,31	0
8	BJ2	C	702	30/30	0.96	0.08	17,24,31,31	0

Continued on next page...

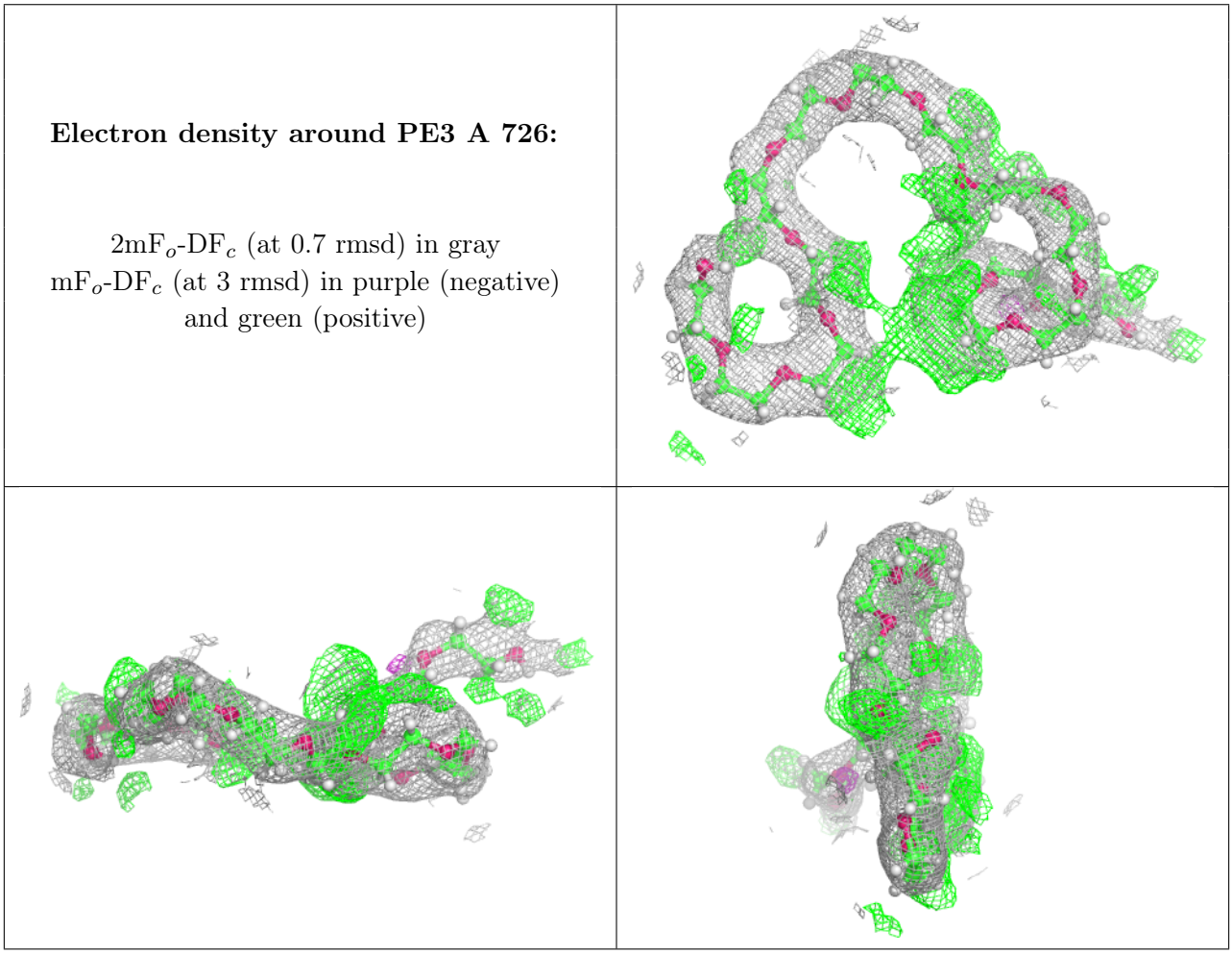
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	BJ2	A	702	30/30	0.97	0.08	14,21,28,29	0
8	BJ2	D	702	30/30	0.97	0.09	13,20,24,28	0
10	MG	A	704	1/1	0.97	0.12	23,23,23,23	0
10	MG	D	704	1/1	0.99	0.16	17,17,17,17	0
10	MG	B	704	1/1	0.99	0.07	29,29,29,29	0
9	CL	B	703	1/1	0.99	0.11	20,20,20,20	0
7	ZN	D	701	1/1	1.00	0.12	16,16,16,16	0
9	CL	A	703	1/1	1.00	0.11	19,19,19,19	0
7	ZN	A	701	1/1	1.00	0.13	17,17,17,17	0
9	CL	C	703	1/1	1.00	0.13	22,22,22,22	0
9	CL	D	703	1/1	1.00	0.12	18,18,18,18	0
7	ZN	B	701	1/1	1.00	0.12	18,18,18,18	0
7	ZN	C	701	1/1	1.00	0.11	20,20,20,20	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

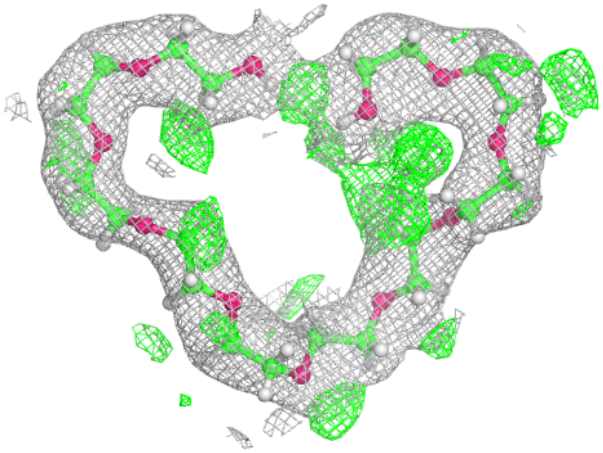
Electron density around PE3 A 726:

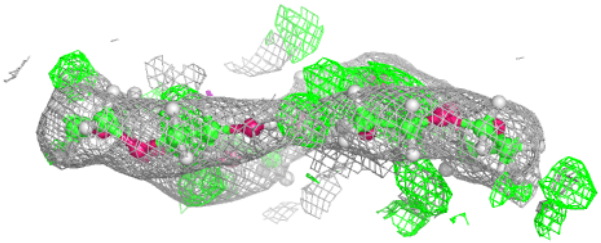
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

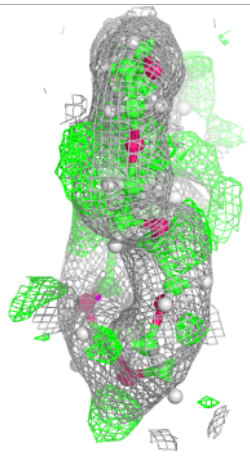


Electron density around XPE D 724:

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

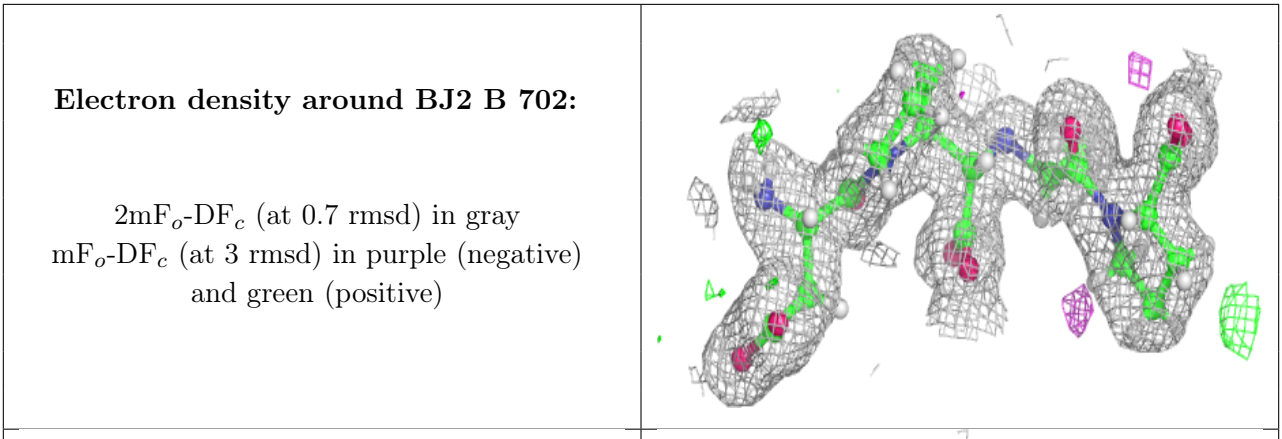


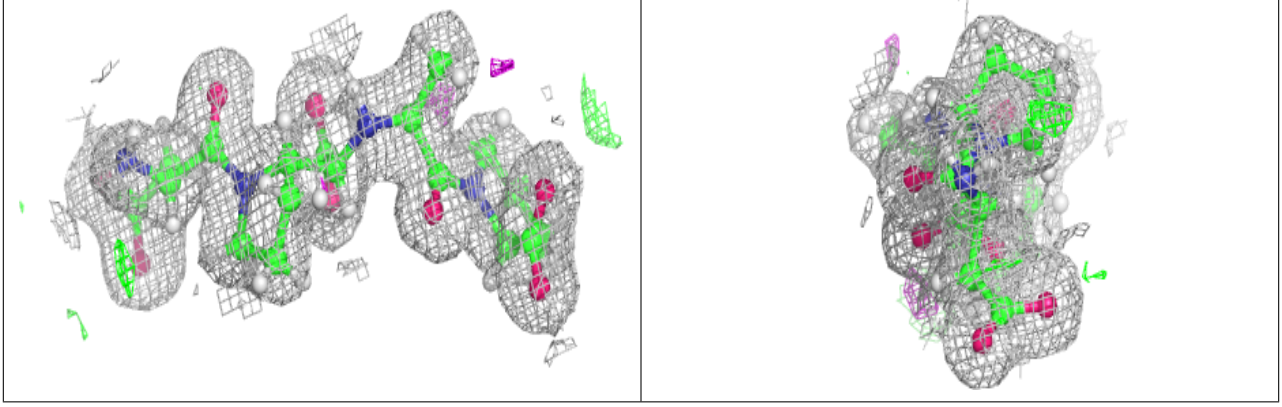




Electron density around BJ2 B 702:

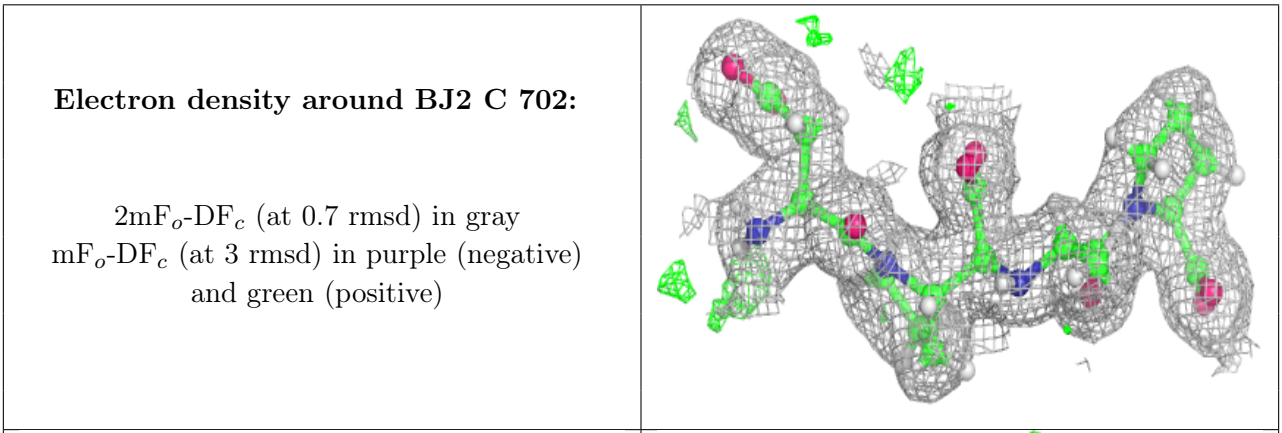
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

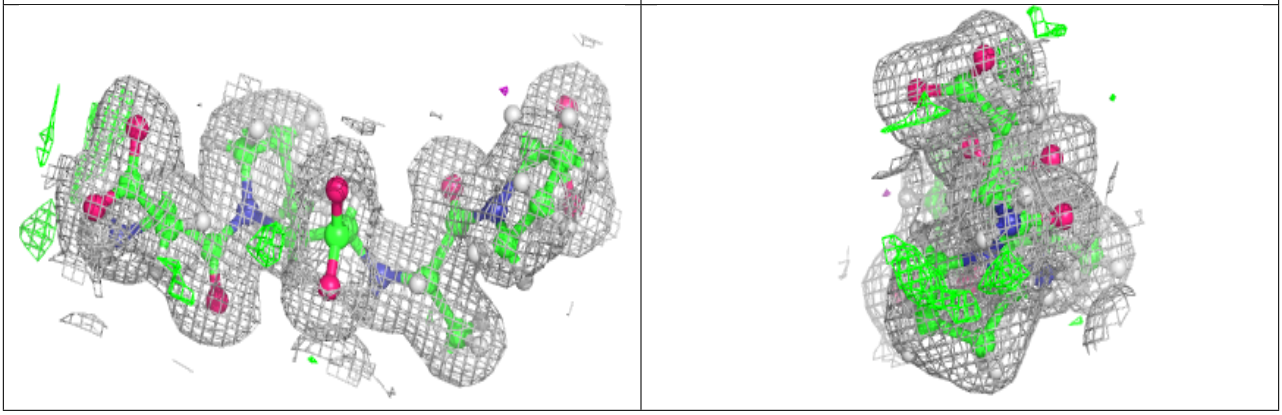




Electron density around BJ2 C 702:

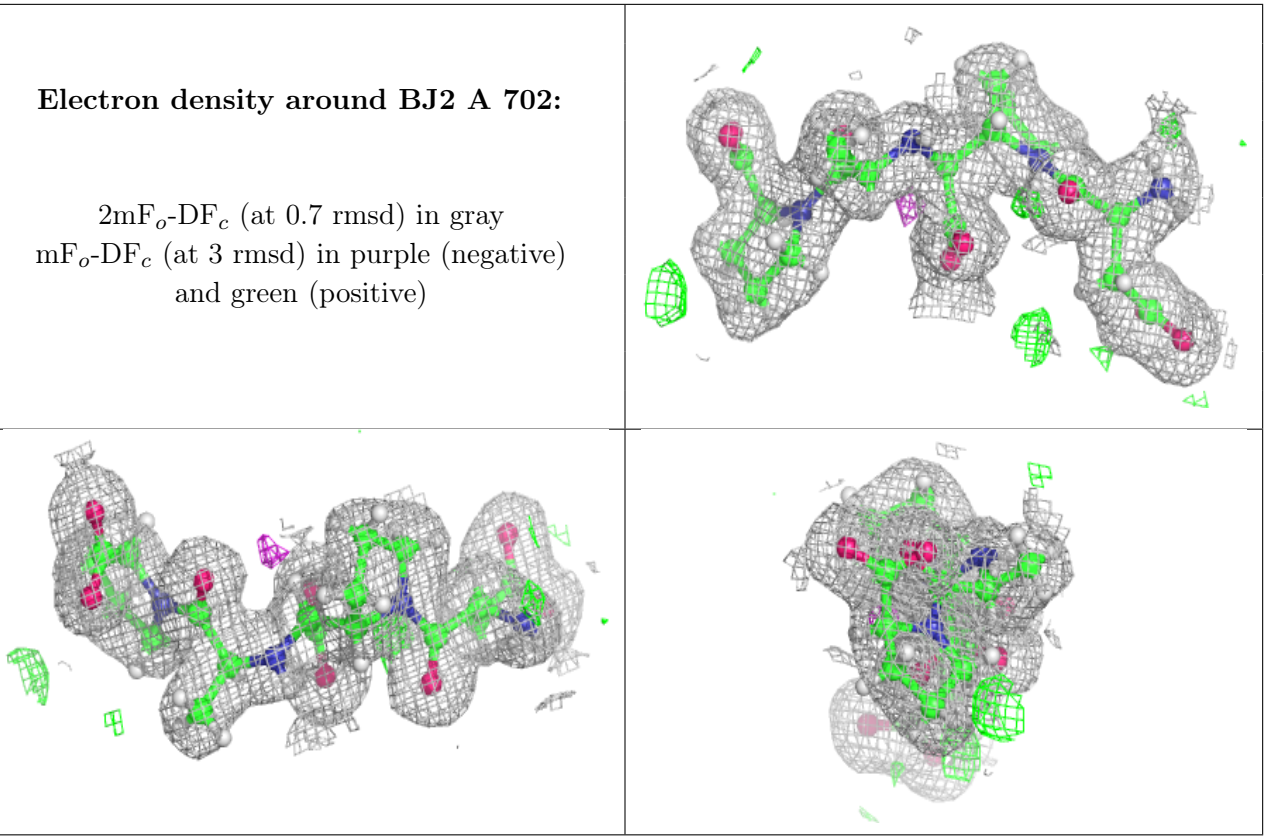
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





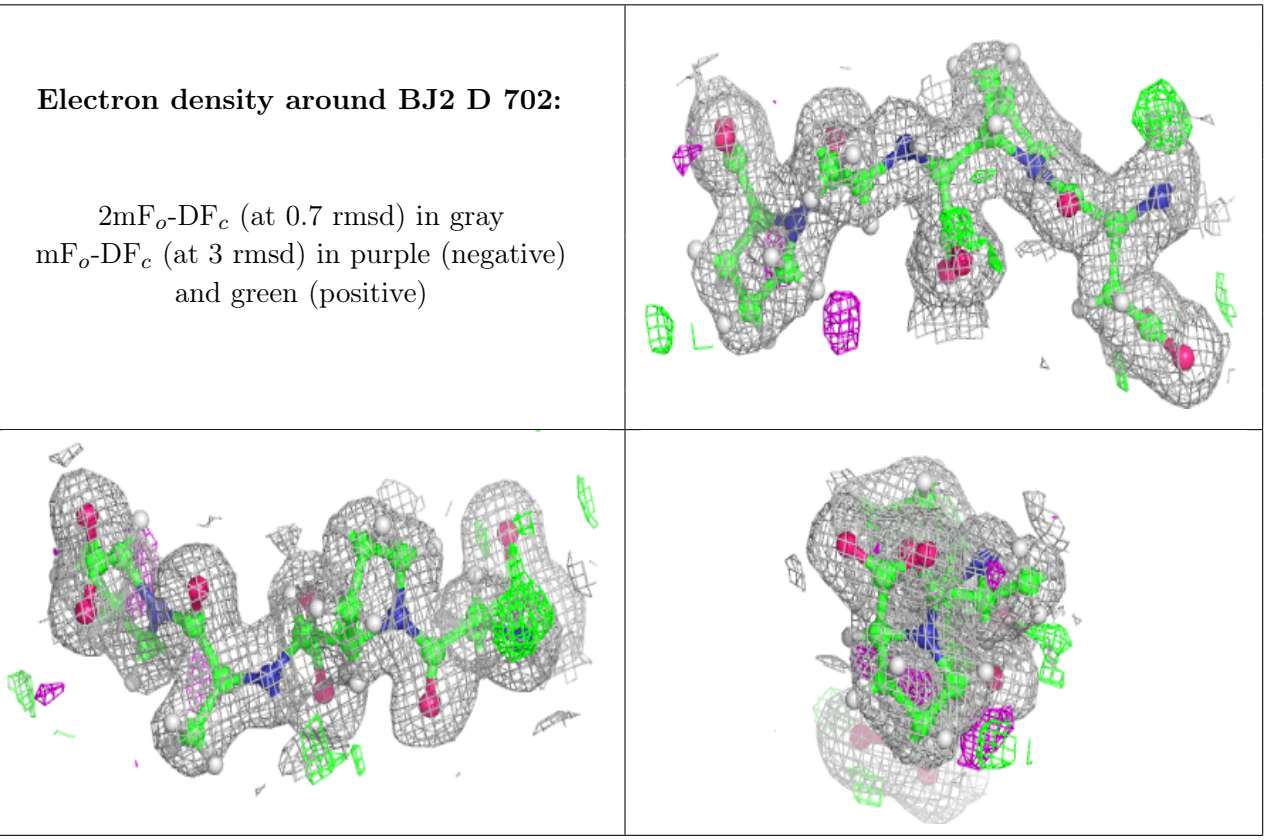
Electron density around BJ2 A 702:

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



Electron density around BJ2 D 702:

$2mF_o$-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 (i)

There are no such residues in this entry.