



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:23 PM UTC

PDB ID : 7Z6Z / pdb_00007z6z
Title : Crystal structure of Angiotensin-1 converting enzyme N-domain in complex with fosinoprilat
Authors : Cozier, G.E.; Acharya, K.R.
Deposited on : 2022-03-14
Resolution : 1.75 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:

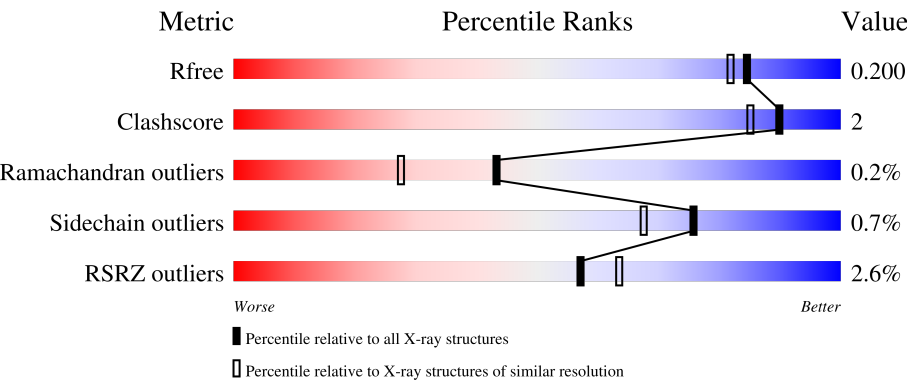
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 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}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (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 $\leq 5\%$. 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	628	% 92% . .
1	B	628	4% 92% . .
2	C	2	100%
3	D	4	100%
4	E	2	100%

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Mol	Chain	Length	Quality of chain
4	G	2	 100%
5	F	3	 100%

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
10	ACT	B	712	-	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 21256 atoms, of which 10062 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, soluble form.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	604	Total	C	H	N	O	S	0	8	0
			9785	3210	4782	861	912	20			
1	B	604	Total	C	H	N	O	S	0	13	0
			9836	3224	4807	864	922	19			

There are 16 discrepancies between the modelled and reference sequences:

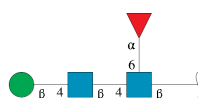
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	engineered mutation	UNP P12821
A	25	GLN	ASN	engineered mutation	UNP P12821
A	82	GLN	ASN	engineered mutation	UNP P12821
A	117	GLN	ASN	engineered mutation	UNP P12821
A	131	GLN	ASN	engineered mutation	UNP P12821
A	289	GLN	ASN	engineered mutation	UNP P12821
A	545	ARG	GLN	engineered mutation	UNP P12821
A	576	LEU	PRO	engineered mutation	UNP P12821
B	9	GLN	ASN	engineered mutation	UNP P12821
B	25	GLN	ASN	engineered mutation	UNP P12821
B	82	GLN	ASN	engineered mutation	UNP P12821
B	117	GLN	ASN	engineered mutation	UNP P12821
B	131	GLN	ASN	engineered mutation	UNP P12821
B	289	GLN	ASN	engineered mutation	UNP P12821
B	545	ARG	GLN	engineered mutation	UNP P12821
B	576	LEU	PRO	engineered mutation	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	C	2	Total	C	H	N	O	0	0	0
			53	16	25	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.



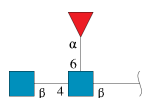
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	4	Total	C	H	N	O	0	0	0
			92	28	43	2	19			

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



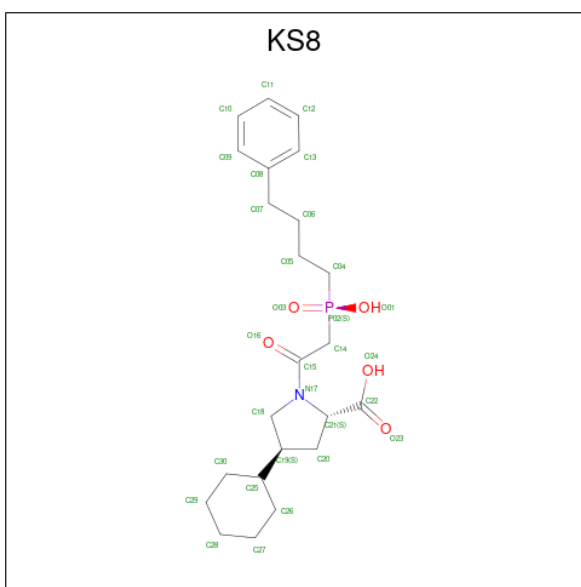
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	2	Total	C	H	N	O	0	0	0
			46	14	22	1	9			
4	G	2	Total	C	H	N	O	0	0	0
			36	14	12	1	9			

- Molecule 5 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.



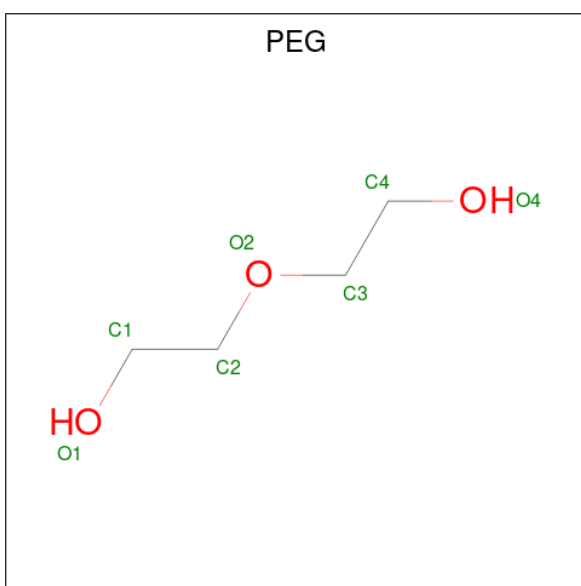
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	3	Total	C	H	N	O	0	0	0
			72	22	34	2	14			

- Molecule 6 is fosinoprilat (CCD ID: KS8) (formula: C₂₃H₃₄NO₅P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	A	1	Total 62	C 23	H 32	N 1	O 5	P 1	0	0
6	B	1	Total 62	C 23	H 32	N 1	O 5	P 1	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



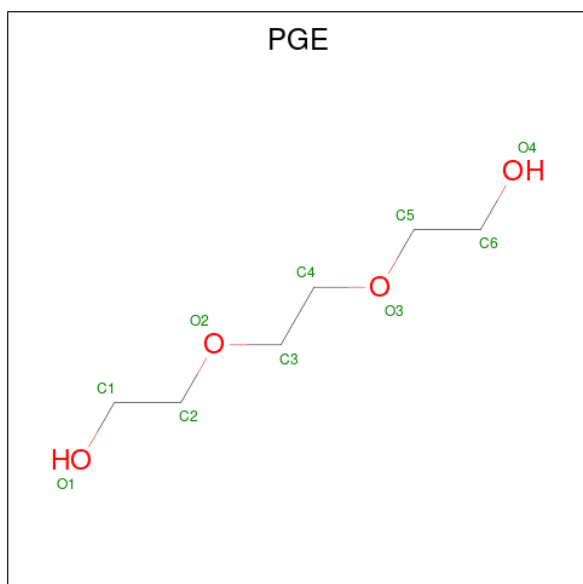
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			17	4	10	3		
7	A	1	Total	C	H	O	0	0
			17	4	10	3		

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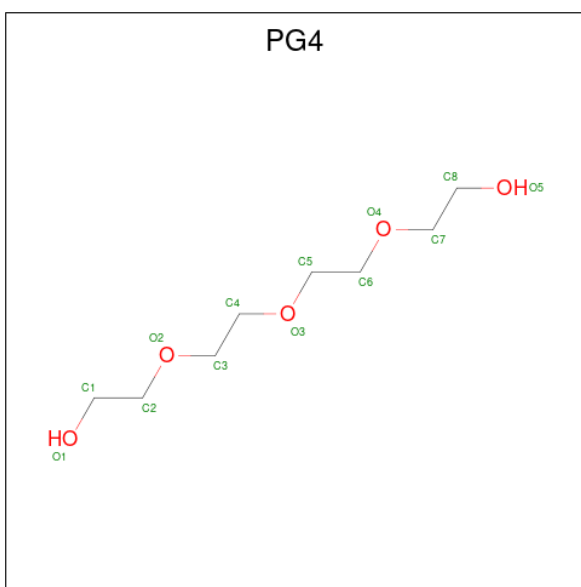
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			17	4	10	3		
7	A	1	Total	C	H	O	0	0
			17	4	10	3		
7	A	1	Total	C	H	O	0	0
			17	4	10	3		
7	B	1	Total	C	H	O	0	0
			17	4	10	3		
7	B	1	Total	C	H	O	0	0
			17	4	10	3		
7	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



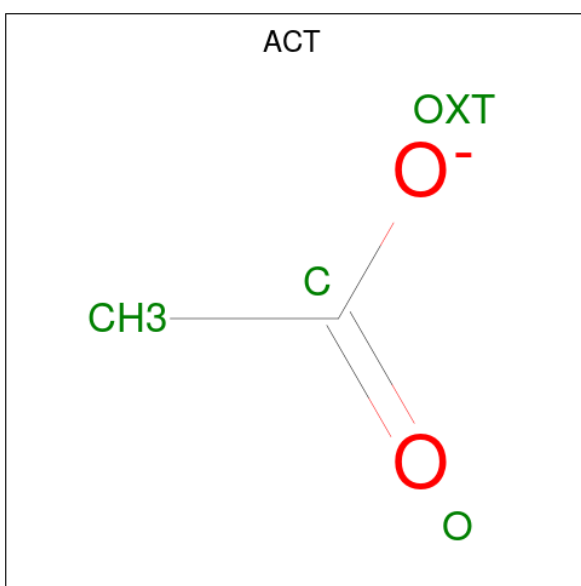
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			24	6	14	4		
8	A	1	Total	C	H	O	0	0
			24	6	14	4		
8	A	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 9 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			31	8	18	5		
9	A	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 10 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



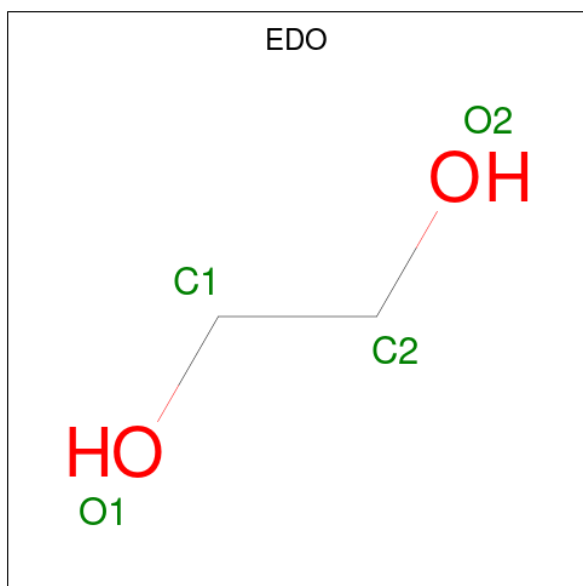
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	H	O	0	0
			7	2	3	2		
10	A	1	Total	C	H	O	0	0
			7	2	3	2		

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

- Molecule 11 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 13 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

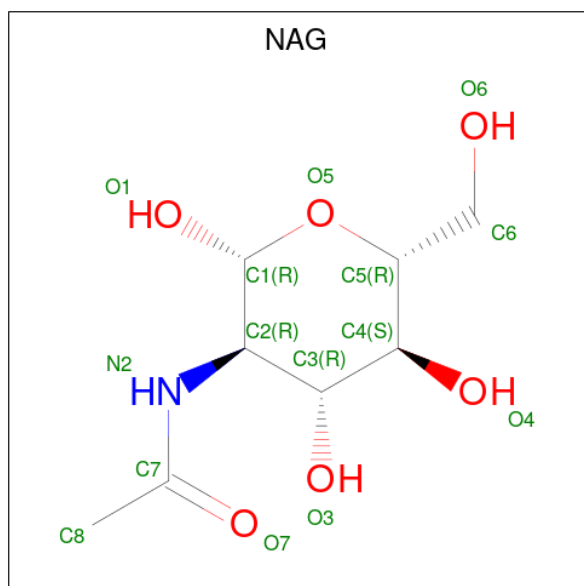
- Molecule 14 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total	Ca	0	0
			1	1		
14	B	2	Total	Ca	0	0
			2	2		

- Molecule 15 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Na	0	0
			1	1		

- Molecule 16 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

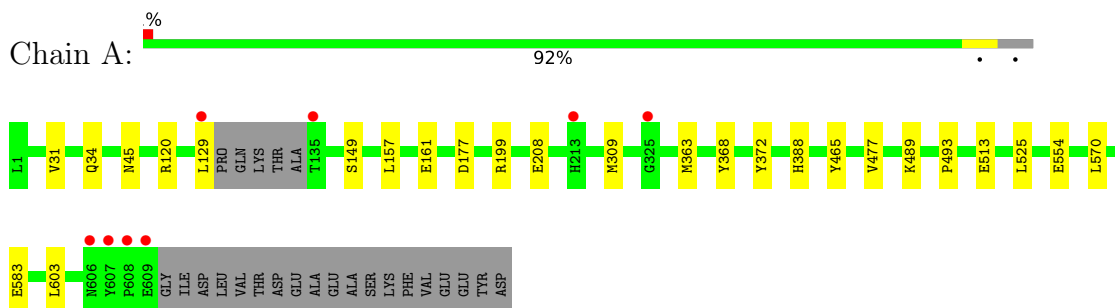
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	407	Total	O	0	4
			411	411		
17	B	306	Total	O	0	0
			306	306		

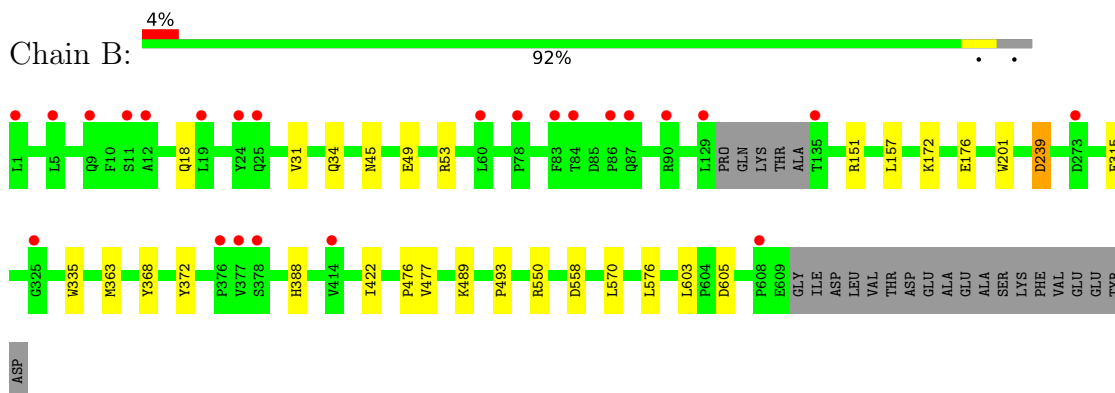
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

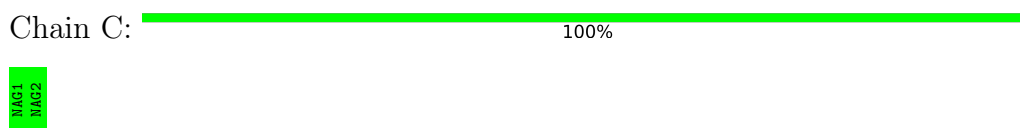
- Molecule 1: Angiotensin-converting enzyme, soluble form



- Molecule 1: Angiotensin-converting enzyme, soluble form



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



- 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



MAG1
MAG2
BMA3
FUC4

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

Chain E:  100%

MAG1
FUC2

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

Chain G:  100%

MAG1
FUC2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

MAG1
MAG2
FUC3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.58Å 77.80Å 81.59Å 88.92° 64.62° 74.81°	Depositor
Resolution (Å)	63.46 – 1.75 63.46 – 1.75	Depositor EDS
% Data completeness (in resolution range)	97.3 (63.46-1.75) 97.4 (63.46-1.75)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.172 , 0.200 0.170 , 0.200	Depositor DCC
R_{free} test set	2102 reflections (1.35%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21256	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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: PG4, BMA, NAG, CL, PEG, EDO, NA, ZN, FUC, ACT, PGE, KS8, CA

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	0.43	0/5159	0.51	0/7025
1	B	0.36	0/5196	0.47	0/7076
All	All	0.40	0/10355	0.49	0/14101

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 [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	5003	4782	4774	16	1
1	B	5029	4807	4786	19	1
2	C	28	25	25	0	0
3	D	49	43	43	0	0
4	E	24	22	22	0	0
4	G	24	12	22	0	0
5	F	38	34	34	0	0
6	A	30	32	0	0	0
6	B	30	32	0	0	0
7	A	35	50	50	0	0
7	B	21	30	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	30	42	42	0	0
9	A	26	36	36	1	0
10	A	16	12	12	2	0
10	B	24	18	18	3	0
11	A	16	24	24	0	0
11	B	32	48	47	4	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
13	A	1	0	0	0	0
13	B	1	0	0	0	0
14	A	1	0	0	0	0
14	B	2	0	0	0	0
15	A	1	0	0	0	0
16	B	14	13	13	0	0
17	A	411	0	0	5	0
17	B	306	0	0	2	0
All	All	11194	10062	9978	36	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (36) 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:A:583:GLU:OE1	17:A:801:HOH:O	2.01	0.78
1:A:199:ARG:HB3	10:A:717:ACT:H3	1.74	0.69
10:B:712:ACT:H3	11:B:716:EDO:O1	1.92	0.69
1:A:161:GLU:OE2	17:A:802:HOH:O	2.09	0.68
1:A:554:GLU:OE1	17:A:803:HOH:O	2.14	0.64
1:A:477:VAL:HG12	1:A:603:LEU:HD21	1.80	0.62
1:B:315:GLU:OE2	17:B:801:HOH:O	2.17	0.59
1:A:31:VAL:O	1:A:34:GLN:HG3	2.02	0.58
1:B:31:VAL:O	1:B:34:GLN:HG3	2.03	0.58
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.87	0.57
1:B:239:ASP:N	10:B:712:ACT:H1	2.20	0.56
1:B:201:TRP:CG	11:B:717:EDO:HO2	2.22	0.56
1:A:177:ASP:OD1	17:A:805[A]:HOH:O	2.19	0.52
1:B:201:TRP:CD1	11:B:717:EDO:HO2	2.29	0.51
1:B:605:ASP:H	11:B:719:EDO:C1	2.23	0.51
1:B:477:VAL:HG12	1:B:603:LEU:HD21	1.93	0.50
1:B:335:TRP:HA	7:B:703:PEG:H42	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.95	0.49
1:A:129:LEU:HD23	1:A:129:LEU:C	2.39	0.48
1:B:550:ARG:NH2	1:B:558:ASP:OD2	2.49	0.46
1:A:570:LEU:C	1:A:570:LEU:HD23	2.40	0.46
1:B:239:ASP:H	10:B:712:ACT:H1	1.80	0.45
1:A:120[B]:ARG:NH2	17:A:804:HOH:O	2.18	0.45
1:A:489:LYS:O	1:A:493:PRO:HD2	2.17	0.44
1:B:489:LYS:O	1:B:493:PRO:HD2	2.18	0.44
1:A:309:MET:CG	1:A:363[B]:MET:HE1	2.48	0.43
1:B:49:GLU:HG3	1:B:53:ARG:CZ	2.49	0.42
1:B:422:ILE:CD1	1:B:576[B]:LEU:HD23	2.49	0.42
1:B:570:LEU:C	1:B:570:LEU:HD23	2.45	0.42
1:A:208:GLU:OE1	10:A:707:ACT:H1	2.19	0.42
1:B:363:MET:HE3	1:B:363:MET:HB3	1.92	0.42
1:A:465:TYR:CE2	9:A:714:PG4:H42	2.54	0.42
1:B:151[B]:ARG:NH1	17:B:816:HOH:O	2.52	0.41
1:A:513:GLU:HA	1:A:525:LEU:HD21	2.03	0.41
1:B:157:LEU:HD13	1:B:476:PRO:HB2	2.03	0.41
1:B:172:LYS:O	1:B:176:GLU:HG3	2.21	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:SER:O	1:B:18:GLN:NE2[1_654]	2.15	0.05

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	608/628 (97%)	598 (98%)	9 (2%)	1 (0%)	43 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	613/628 (98%)	604 (98%)	8 (1%)	1 (0%)	43 27
All	All	1221/1256 (97%)	1202 (98%)	17 (1%)	2 (0%)	43 27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	45	ASN
1	A	45	ASN

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	528/540 (98%)	525 (99%)	3 (1%)	78 71
1	B	533/540 (99%)	529 (99%)	4 (1%)	73 64
All	All	1061/1080 (98%)	1054 (99%)	7 (1%)	76 67

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	TYR
1	A	372	TYR
1	A	388	HIS
1	B	239	ASP
1	B	368	TYR
1	B	372	TYR
1	B	388	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	371	GLN

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Mol	Chain	Res	Type
1	A	606	ASN
1	B	82	GLN
1	B	188	GLN
1	B	263	ASN
1	B	371	GLN
1	B	494	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

13 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	2,1	14,14,15	0.29	0	17,19,21	0.60	0
2	NAG	C	2	2	14,14,15	0.41	0	17,19,21	0.53	0
3	NAG	D	1	3,1	14,14,15	0.36	0	17,19,21	0.44	0
3	NAG	D	2	3	14,14,15	0.21	0	17,19,21	0.55	0
3	BMA	D	3	3	11,11,12	0.72	0	15,15,17	0.72	0
3	FUC	D	4	3	10,10,11	0.57	0	14,14,16	0.62	0
4	NAG	E	1	4,1	14,14,15	0.34	0	17,19,21	0.80	1 (5%)
4	FUC	E	2	4	10,10,11	1.20	1 (10%)	14,14,16	0.82	0
5	NAG	F	1	5,1	14,14,15	0.40	0	17,19,21	0.43	0
5	NAG	F	2	5	14,14,15	0.37	0	17,19,21	0.47	0
5	FUC	F	3	5	10,10,11	0.60	0	14,14,16	0.77	0
4	NAG	G	1	4,1	14,14,15	0.33	0	17,19,21	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FUC	G	2	4	10,10,11	1.00	0	14,14,16	0.84	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
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
3	FUC	D	4	3	-	-	0/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	FUC	E	2	4	-	-	0/1/1/1
5	NAG	F	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	F	2	5	-	1/6/23/26	0/1/1/1
5	FUC	F	3	5	-	-	0/1/1/1
4	NAG	G	1	4,1	-	1/6/23/26	0/1/1/1
4	FUC	G	2	4	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2	FUC	C1-C2	2.03	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	NAG	C1-O5-C5	2.13	115.04	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C1-C2-N2-C7
3	D	3	BMA	O5-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6

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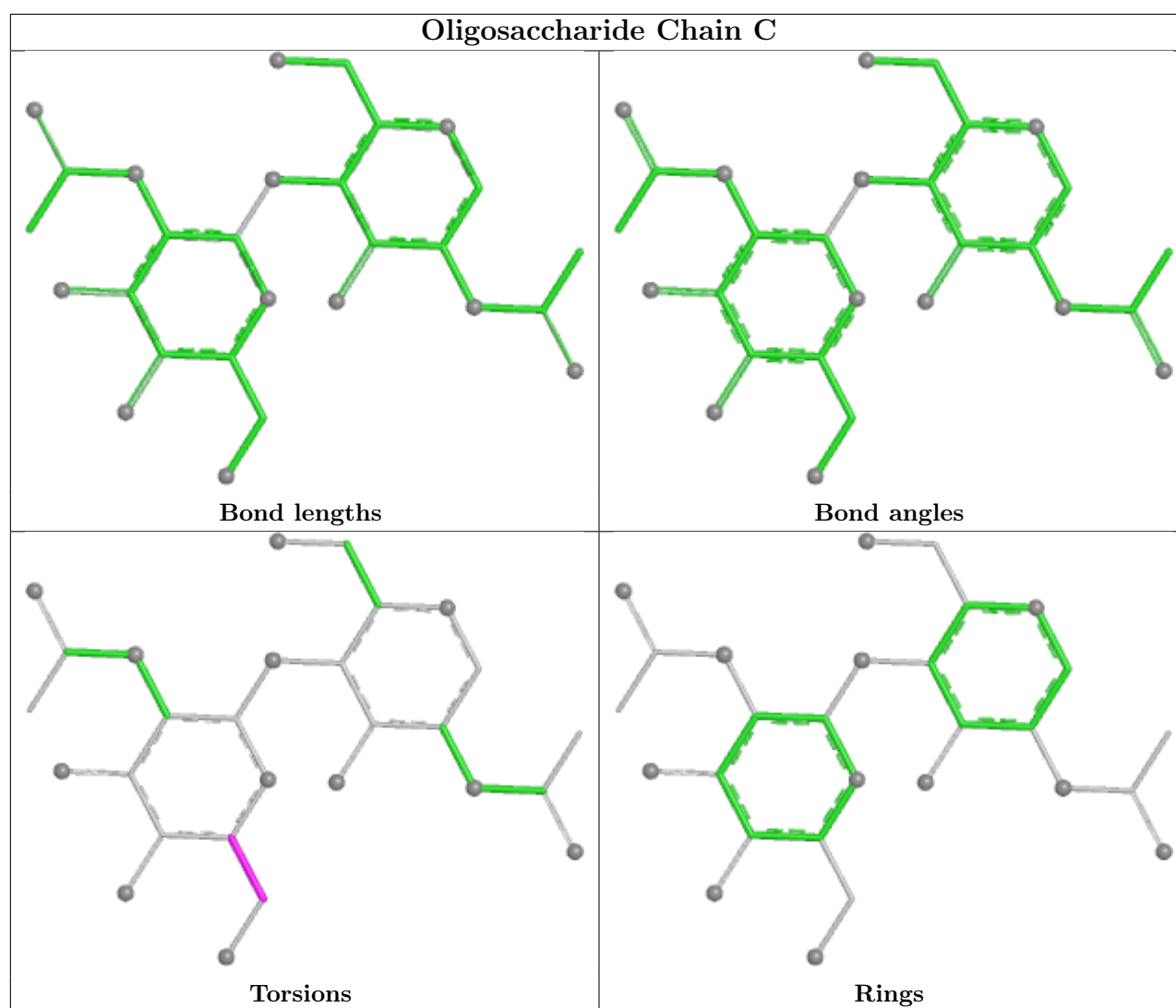
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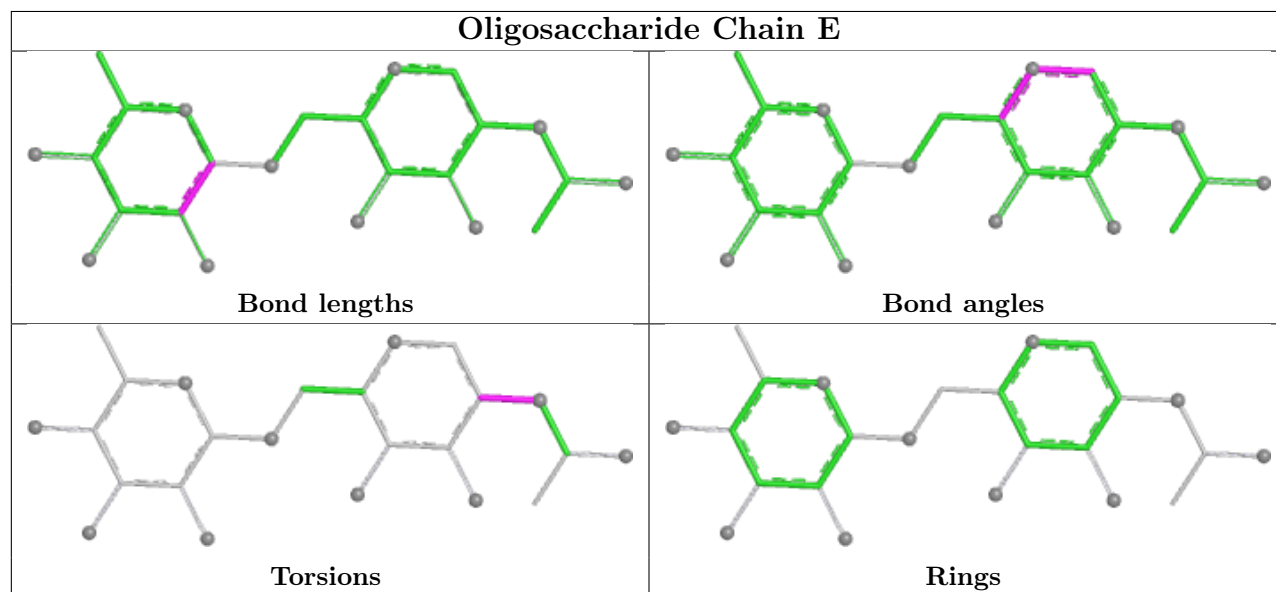
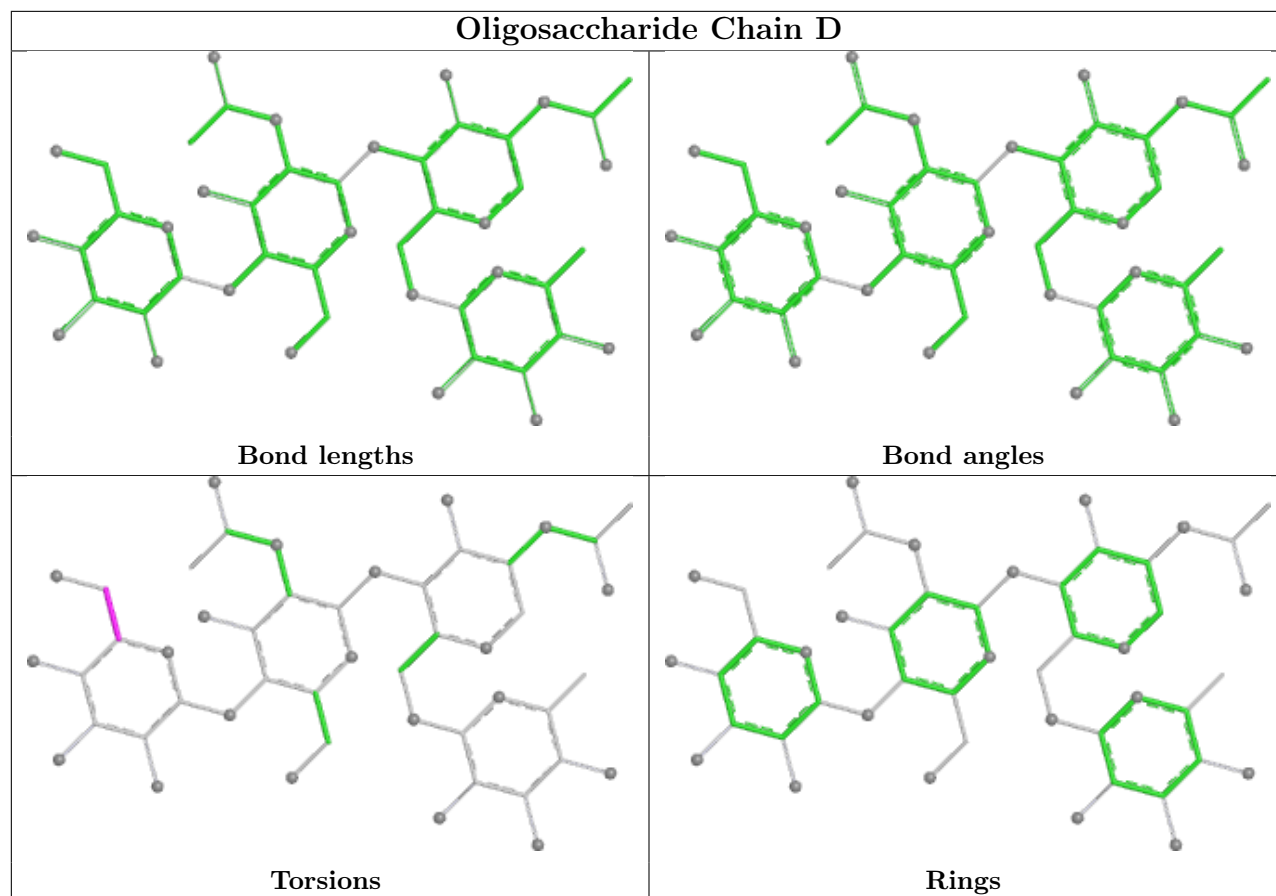
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C4-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C1-C2-N2-C7
5	F	2	NAG	C1-C2-N2-C7
4	E	1	NAG	C3-C2-N2-C7

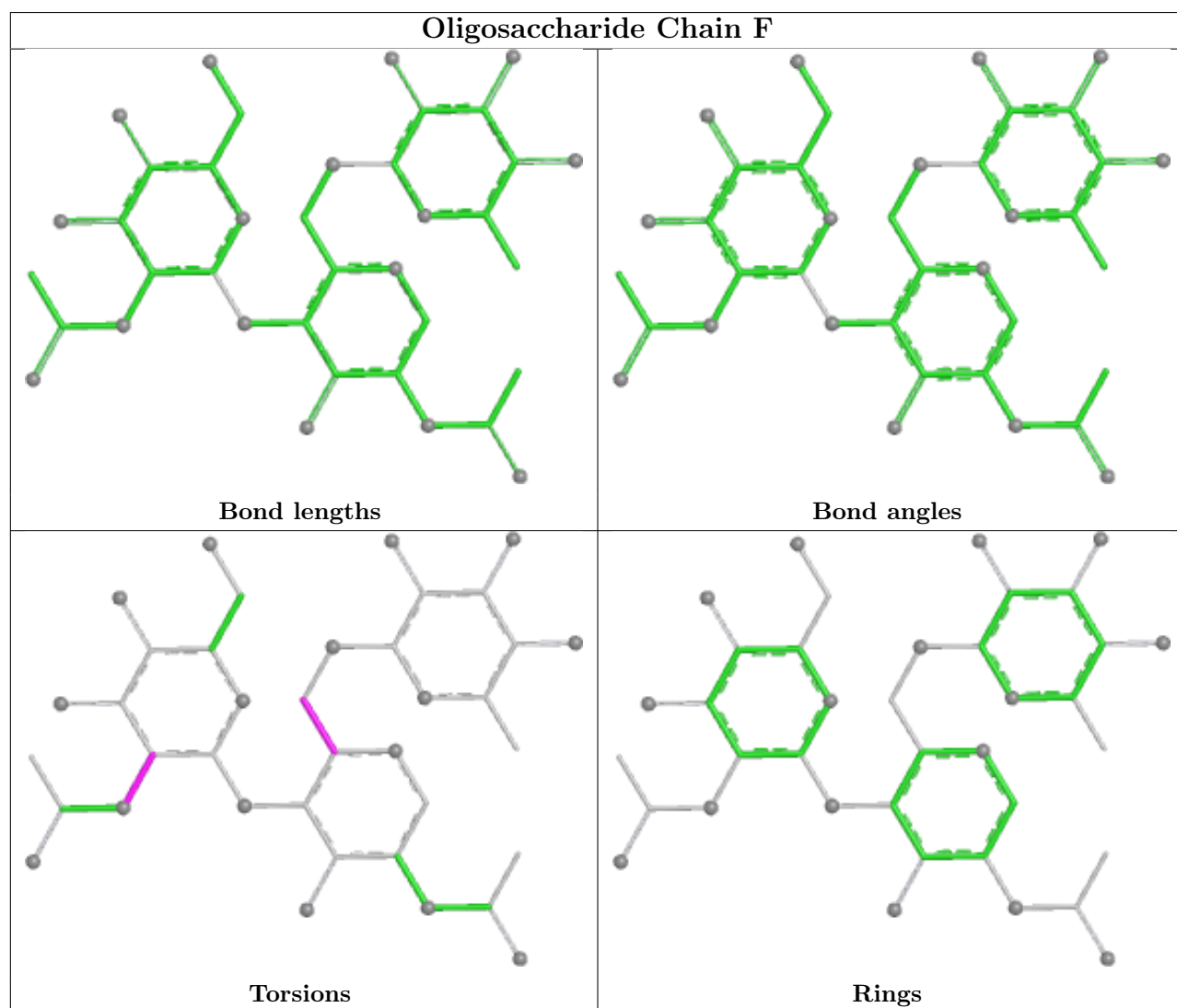
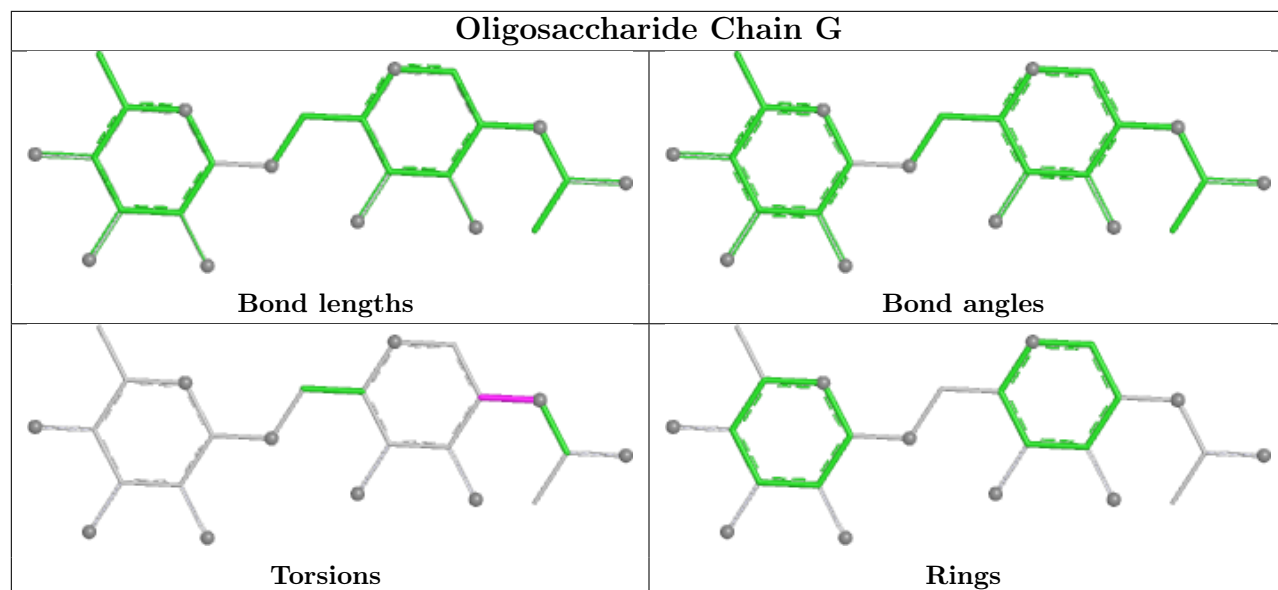
There are no ring outliers.

No monomer is involved in short contacts.

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

Of 46 ligands modelled in this entry, 8 are monoatomic - leaving 38 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	EDO	B	716	14	3,3,3	0.39	0	2,2,2	0.41	0
16	NAG	B	702	1	14,14,15	0.35	0	17,19,21	0.53	0
11	EDO	B	705	-	3,3,3	0.38	0	2,2,2	0.42	0
9	PG4	A	706	-	12,12,12	0.16	0	11,11,11	0.33	0
8	PGE	A	709	-	9,9,9	0.36	0	8,8,8	0.49	0
11	EDO	B	720	-	3,3,3	0.44	0	2,2,2	0.45	0
11	EDO	A	721	-	3,3,3	0.40	0	2,2,2	0.53	0
11	EDO	B	717	-	3,3,3	0.43	0	2,2,2	0.56	0
11	EDO	B	721	-	3,3,3	0.43	0	2,2,2	0.48	0
7	PEG	A	705	-	6,6,6	0.18	0	5,5,5	0.06	0
10	ACT	B	709	-	3,3,3	1.41	0	3,3,3	1.56	0
7	PEG	A	713	-	6,6,6	0.14	0	5,5,5	0.06	0
7	PEG	A	702	-	6,6,6	0.26	0	5,5,5	0.13	0
10	ACT	A	716	-	3,3,3	1.46	1 (33%)	3,3,3	1.26	0
7	PEG	A	712	-	6,6,6	0.15	0	5,5,5	0.12	0
11	EDO	B	718	-	3,3,3	0.40	0	2,2,2	0.56	0
10	ACT	B	708	-	3,3,3	1.18	0	3,3,3	1.64	2 (66%)
7	PEG	B	703	-	6,6,6	0.23	0	5,5,5	0.12	0
11	EDO	B	719	-	3,3,3	0.37	0	2,2,2	0.61	0
10	ACT	A	711	-	3,3,3	1.22	0	3,3,3	1.46	0
6	KS8	B	701	12	29,32,32	2.67	11 (37%)	34,44,44	1.71	10 (29%)
8	PGE	A	708	-	9,9,9	0.33	0	8,8,8	0.31	0
11	EDO	B	715	14	3,3,3	0.39	0	2,2,2	0.62	0
7	PEG	B	711	-	6,6,6	0.16	0	5,5,5	0.07	0
9	PG4	A	714	-	12,12,12	0.10	0	11,11,11	0.66	0
10	ACT	B	707	-	3,3,3	1.39	0	3,3,3	1.46	0
10	ACT	B	710	-	3,3,3	1.39	0	3,3,3	1.28	0
11	EDO	A	715	-	3,3,3	0.45	0	2,2,2	0.50	0
10	ACT	A	707	-	3,3,3	1.21	0	3,3,3	1.45	0
10	ACT	B	712	14	3,3,3	1.25	0	3,3,3	1.36	0
10	ACT	B	706	-	3,3,3	1.44	1 (33%)	3,3,3	1.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PGE	A	703	-	9,9,9	0.37	0	8,8,8	0.30	0
10	ACT	A	717	-	3,3,3	1.17	0	3,3,3	1.55	1 (33%)
11	EDO	A	710	-	3,3,3	0.41	0	2,2,2	0.44	0
7	PEG	B	704	-	6,6,6	0.14	0	5,5,5	0.13	0
7	PEG	A	704	-	6,6,6	0.12	0	5,5,5	0.03	0
6	KS8	A	701	12	29,32,32	2.40	10 (34%)	34,44,44	1.51	6 (17%)
11	EDO	A	720	-	3,3,3	0.46	0	2,2,2	0.36	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
11	EDO	B	716	14	-	1/1/1/1	-
16	NAG	B	702	1	-	0/6/23/26	0/1/1/1
11	EDO	B	705	-	-	1/1/1/1	-
9	PG4	A	706	-	-	6/10/10/10	-
8	PGE	A	709	-	-	0/7/7/7	-
11	EDO	B	720	-	-	0/1/1/1	-
11	EDO	A	721	-	-	0/1/1/1	-
11	EDO	B	717	-	-	1/1/1/1	-
11	EDO	B	721	-	-	0/1/1/1	-
7	PEG	A	705	-	-	1/4/4/4	-
7	PEG	A	713	-	-	3/4/4/4	-
7	PEG	A	702	-	-	1/4/4/4	-
7	PEG	A	712	-	-	2/4/4/4	-
11	EDO	B	718	-	-	0/1/1/1	-
7	PEG	B	703	-	-	2/4/4/4	-
11	EDO	B	719	-	-	0/1/1/1	-
6	KS8	B	701	12	-	0/25/45/45	0/3/3/3
8	PGE	A	708	-	-	0/7/7/7	-
11	EDO	B	715	14	-	0/1/1/1	-
7	PEG	B	711	-	-	0/4/4/4	-
9	PG4	A	714	-	-	4/10/10/10	-
11	EDO	A	715	-	-	0/1/1/1	-
8	PGE	A	703	-	-	2/7/7/7	-
11	EDO	A	710	-	-	1/1/1/1	-
7	PEG	B	704	-	-	2/4/4/4	-
7	PEG	A	704	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	KS8	A	701	12	-	0/25/45/45	0/3/3/3
11	EDO	A	720	-	-	1/1/1/1	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	701	KS8	C20-C21	-8.27	1.39	1.53
6	A	701	KS8	C20-C21	-8.10	1.39	1.53
6	B	701	KS8	C21-N17	5.81	1.58	1.47
6	B	701	KS8	C18-N17	-5.30	1.39	1.47
6	A	701	KS8	C21-N17	4.97	1.56	1.47
6	B	701	KS8	C14-C15	4.52	1.57	1.51
6	A	701	KS8	C15-N17	3.83	1.46	1.35
6	B	701	KS8	C15-N17	3.81	1.46	1.35
6	A	701	KS8	C18-N17	-3.17	1.42	1.47
6	A	701	KS8	O24-C22	-2.74	1.21	1.30
6	A	701	KS8	C07-C08	2.68	1.59	1.51
6	B	701	KS8	C18-C19	2.62	1.56	1.53
6	A	701	KS8	C14-C15	2.61	1.54	1.51
6	A	701	KS8	O23-C22	2.59	1.29	1.22
6	B	701	KS8	O23-C22	2.32	1.29	1.22
6	B	701	KS8	C07-C08	2.25	1.58	1.51
6	B	701	KS8	O24-C22	-2.21	1.23	1.30
6	A	701	KS8	C25-C19	-2.19	1.46	1.53
6	A	701	KS8	C18-C19	2.18	1.56	1.53
6	B	701	KS8	C25-C19	-2.17	1.46	1.53
6	B	701	KS8	P02-C14	2.11	1.85	1.81
10	A	716	ACT	CH3-C	2.09	1.57	1.49
10	B	706	ACT	CH3-C	2.09	1.57	1.49

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	701	KS8	C20-C21-C22	4.93	116.75	111.01
6	A	701	KS8	C20-C21-C22	4.73	116.51	111.01
6	A	701	KS8	C06-C05-C04	-3.42	105.45	112.61
6	B	701	KS8	C22-C21-N17	-3.19	106.14	112.54
6	B	701	KS8	C18-N17-C21	-2.92	107.97	111.83
6	B	701	KS8	C20-C21-N17	2.76	106.46	103.17
6	A	701	KS8	O16-C15-C14	2.61	122.54	119.81
6	A	701	KS8	C22-C21-N17	-2.40	107.72	112.54
6	B	701	KS8	C18-N17-C15	-2.37	124.69	129.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	701	KS8	O24-C22-O23	-2.32	118.81	124.08
6	B	701	KS8	O24-C22-C21	2.28	120.79	113.34
6	B	701	KS8	C06-C05-C04	-2.22	107.97	112.61
6	B	701	KS8	P02-C04-C05	-2.21	110.44	114.56
6	A	701	KS8	O24-C22-C21	2.18	120.44	113.34
6	A	701	KS8	O24-C22-O23	-2.17	119.16	124.08
6	B	701	KS8	C21-N17-C15	2.15	127.20	120.83
10	A	717	ACT	OXT-C-O	2.01	129.50	122.03
10	B	708	ACT	OXT-C-O	2.00	129.46	122.03
10	B	708	ACT	O-C-CH3	-2.00	114.32	122.53

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	714	PG4	O3-C5-C6-O4
8	A	703	PGE	O3-C5-C6-O4
9	A	714	PG4	O4-C7-C8-O5
7	B	703	PEG	O1-C1-C2-O2
9	A	714	PG4	O2-C3-C4-O3
9	A	706	PG4	O1-C1-C2-O2
7	A	713	PEG	O2-C3-C4-O4
9	A	714	PG4	O1-C1-C2-O2
7	A	702	PEG	O1-C1-C2-O2
7	A	712	PEG	O1-C1-C2-O2
7	A	712	PEG	O2-C3-C4-O4
7	A	705	PEG	C1-C2-O2-C3
7	A	704	PEG	O1-C1-C2-O2
9	A	706	PG4	C6-C5-O3-C4
11	B	705	EDO	O1-C1-C2-O2
11	A	710	EDO	O1-C1-C2-O2
9	A	706	PG4	C8-C7-O4-C6
11	B	716	EDO	O1-C1-C2-O2
11	B	717	EDO	O1-C1-C2-O2
9	A	706	PG4	C5-C6-O4-C7
7	B	704	PEG	C4-C3-O2-C2
9	A	706	PG4	C3-C4-O3-C5
7	A	704	PEG	C1-C2-O2-C3
9	A	706	PG4	O3-C5-C6-O4
7	A	713	PEG	O1-C1-C2-O2
7	B	703	PEG	O2-C3-C4-O4
7	A	713	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
8	A	703	PGE	C4-C3-O2-C2
11	A	720	EDO	O1-C1-C2-O2
7	B	704	PEG	O1-C1-C2-O2

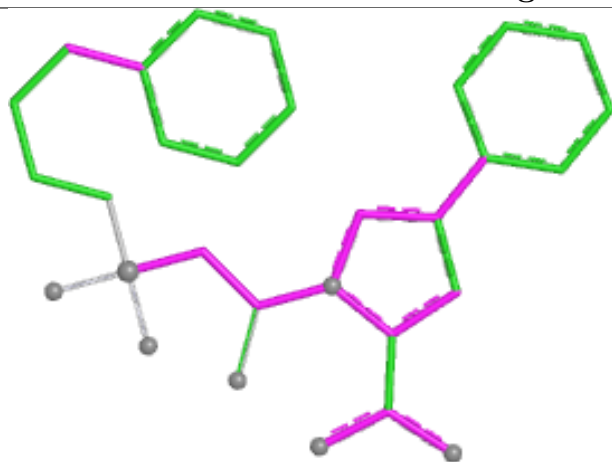
There are no ring outliers.

8 monomers are involved in 10 short contacts:

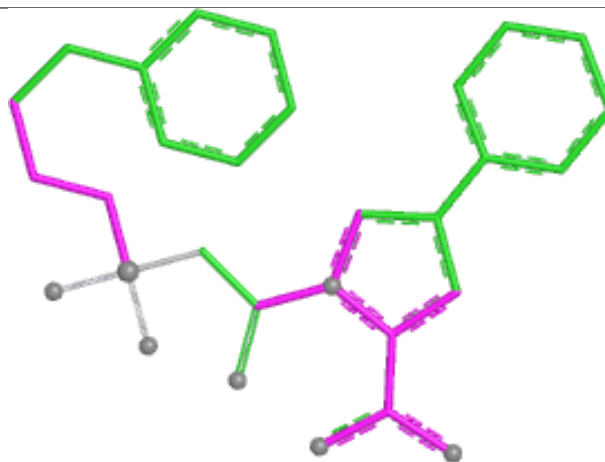
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	716	EDO	1	0
11	B	717	EDO	2	0
7	B	703	PEG	1	0
11	B	719	EDO	1	0
9	A	714	PG4	1	0
10	A	707	ACT	1	0
10	B	712	ACT	3	0
10	A	717	ACT	1	0

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

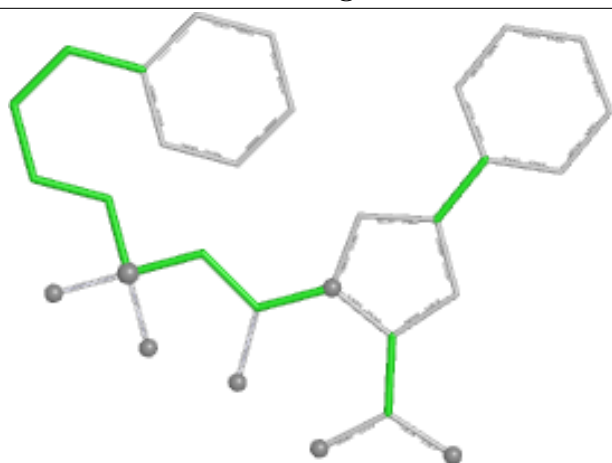
Ligand KS8 B 701



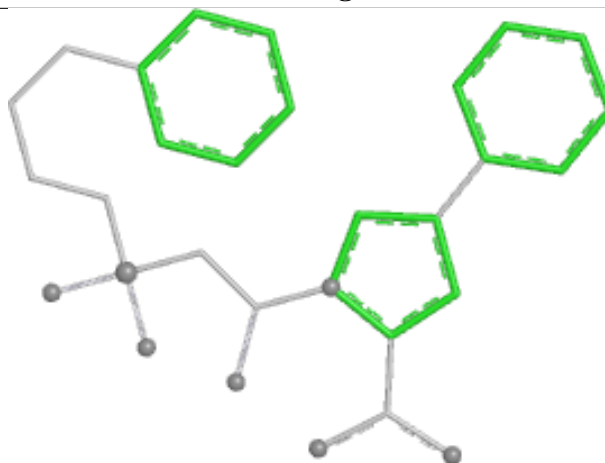
Bond lengths



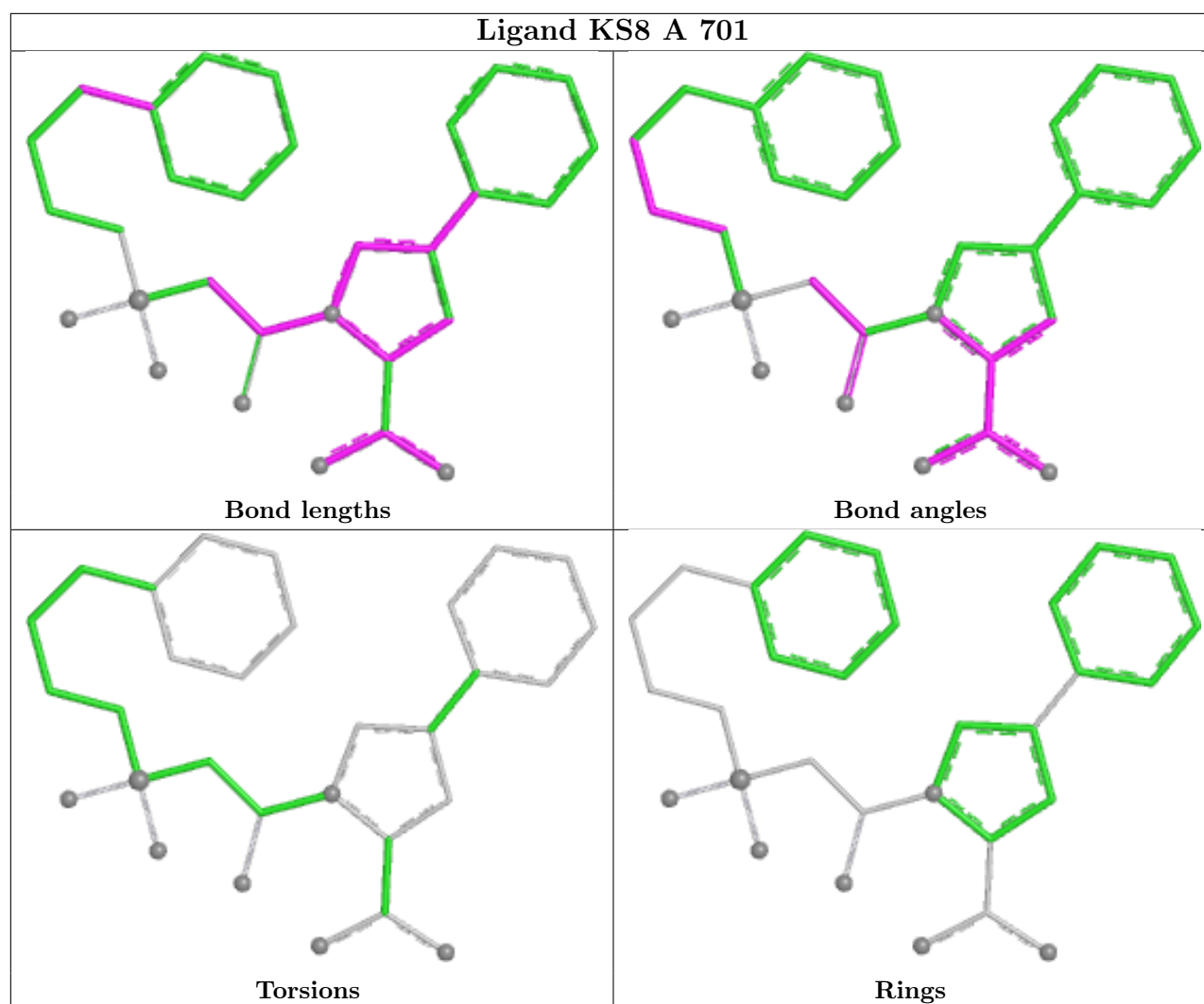
Bond angles



Torsions



Rings



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	604/628 (96%)	-0.22	8 (1%) 75 81	12, 31, 51, 97	8 (1%)
1	B	604/628 (96%)	0.15	24 (3%) 42 48	14, 39, 67, 91	12 (1%)
All	All	1208/1256 (96%)	-0.03	32 (2%) 57 63	12, 34, 62, 97	20 (1%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	LEU	6.8
1	B	129	LEU	5.6
1	A	607	TYR	3.8
1	B	325	GLY	3.6
1	B	414	VAL	3.5
1	B	376	PRO	3.4
1	B	78	PRO	3.4
1	B	19	LEU	3.2
1	B	378	SER	3.1
1	A	609	GLU	3.1
1	B	86	PRO	2.9
1	B	273	ASP	2.9
1	A	135	THR	2.8
1	B	83	PHE	2.8
1	B	377	VAL	2.8
1	A	606	ASN	2.7
1	B	84	THR	2.7
1	B	25	GLN	2.6
1	A	325	GLY	2.6
1	B	608	PRO	2.5
1	B	60	LEU	2.5
1	B	135	THR	2.3
1	B	87[A]	GLN	2.3
1	B	24	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	213[A]	HIS	2.2
1	B	90	ARG	2.2
1	B	1	LEU	2.2
1	B	5	LEU	2.2
1	A	608	PRO	2.2
1	B	9	GLN	2.1
1	B	11	SER	2.1
1	B	12	ALA	2.1

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 ⓘ

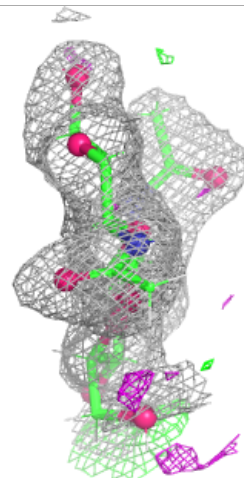
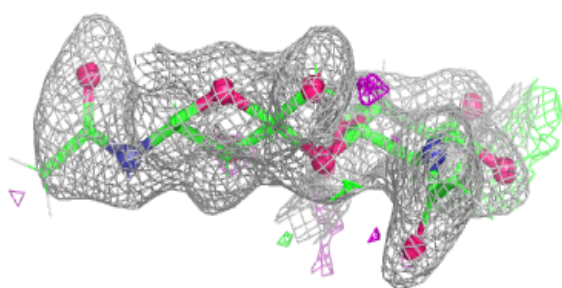
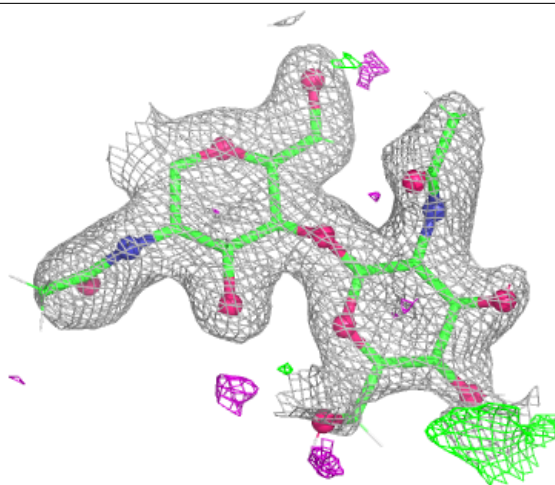
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FUC	F	3	10/11	0.66	0.17	65,78,92,108	0
3	BMA	D	3	11/12	0.67	0.14	76,84,101,102	0
4	FUC	G	2	10/11	0.75	0.18	53,61,65,67	0
4	FUC	E	2	10/11	0.79	0.17	56,70,80,85	0
4	NAG	G	1	14/15	0.79	0.16	39,53,65,72	0
5	NAG	F	1	14/15	0.81	0.12	57,65,78,83	0
2	NAG	C	2	14/15	0.81	0.13	48,60,79,84	0
5	NAG	F	2	14/15	0.86	0.12	61,72,84,89	0
3	NAG	D	2	14/15	0.87	0.12	54,65,76,80	0
4	NAG	E	1	14/15	0.88	0.13	37,49,62,62	0
3	FUC	D	4	10/11	0.89	0.13	51,61,70,82	0
3	NAG	D	1	14/15	0.91	0.10	42,52,63,63	0
2	NAG	C	1	14/15	0.93	0.09	36,43,52,52	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.

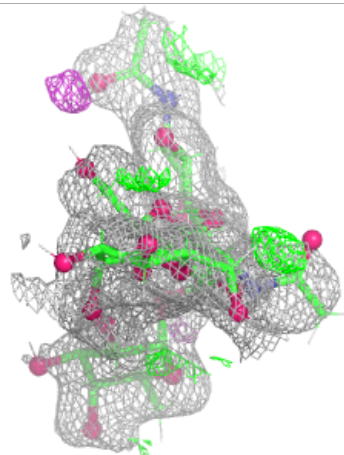
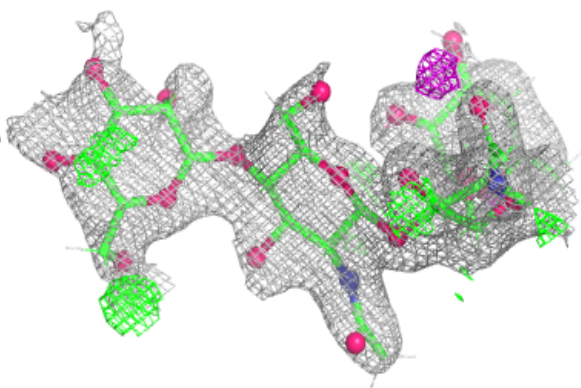
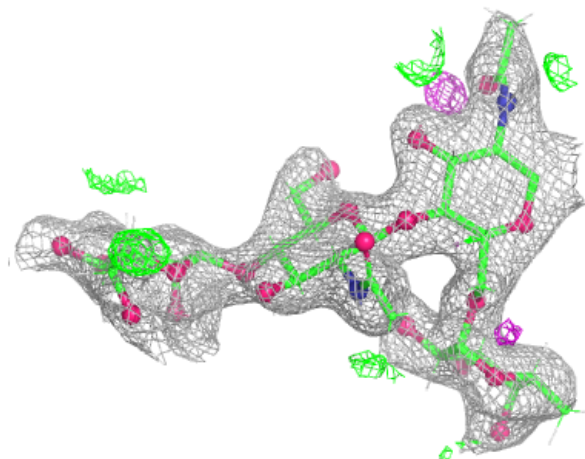
Electron density around Chain C:

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



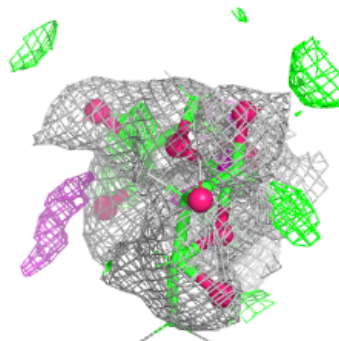
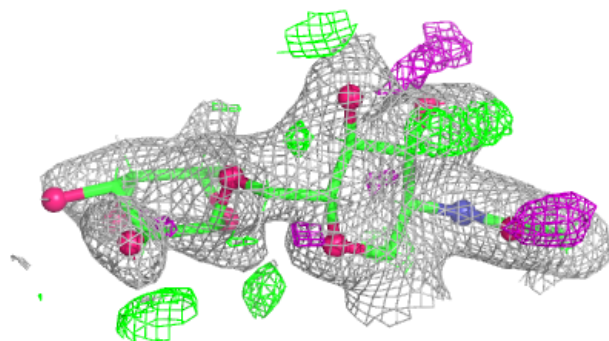
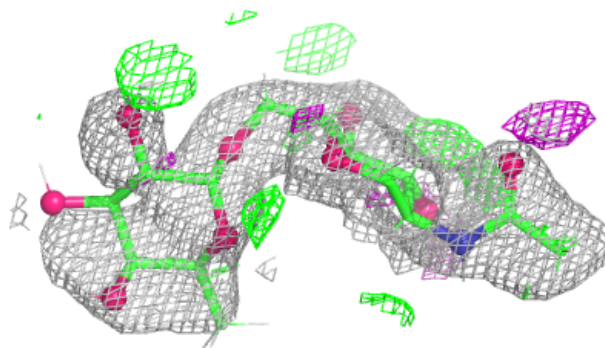
Electron density around Chain D:

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

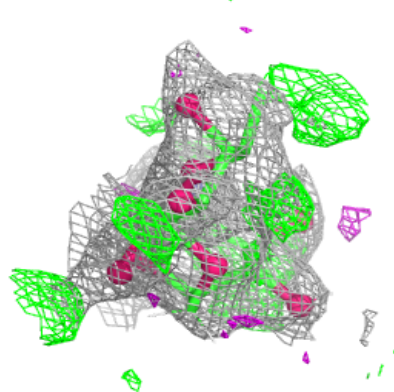
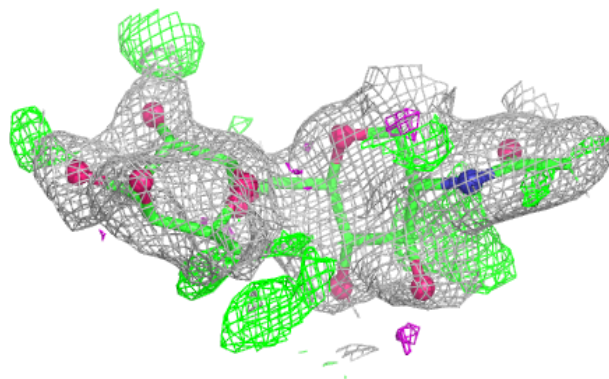
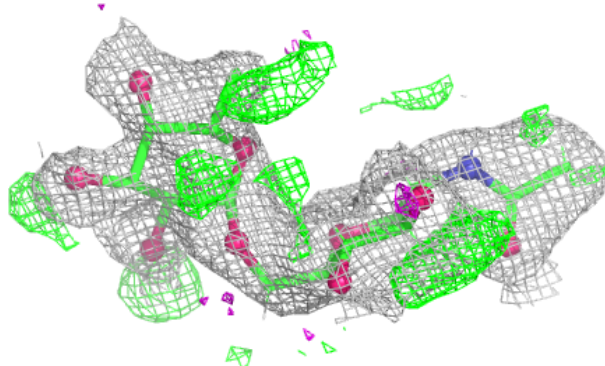


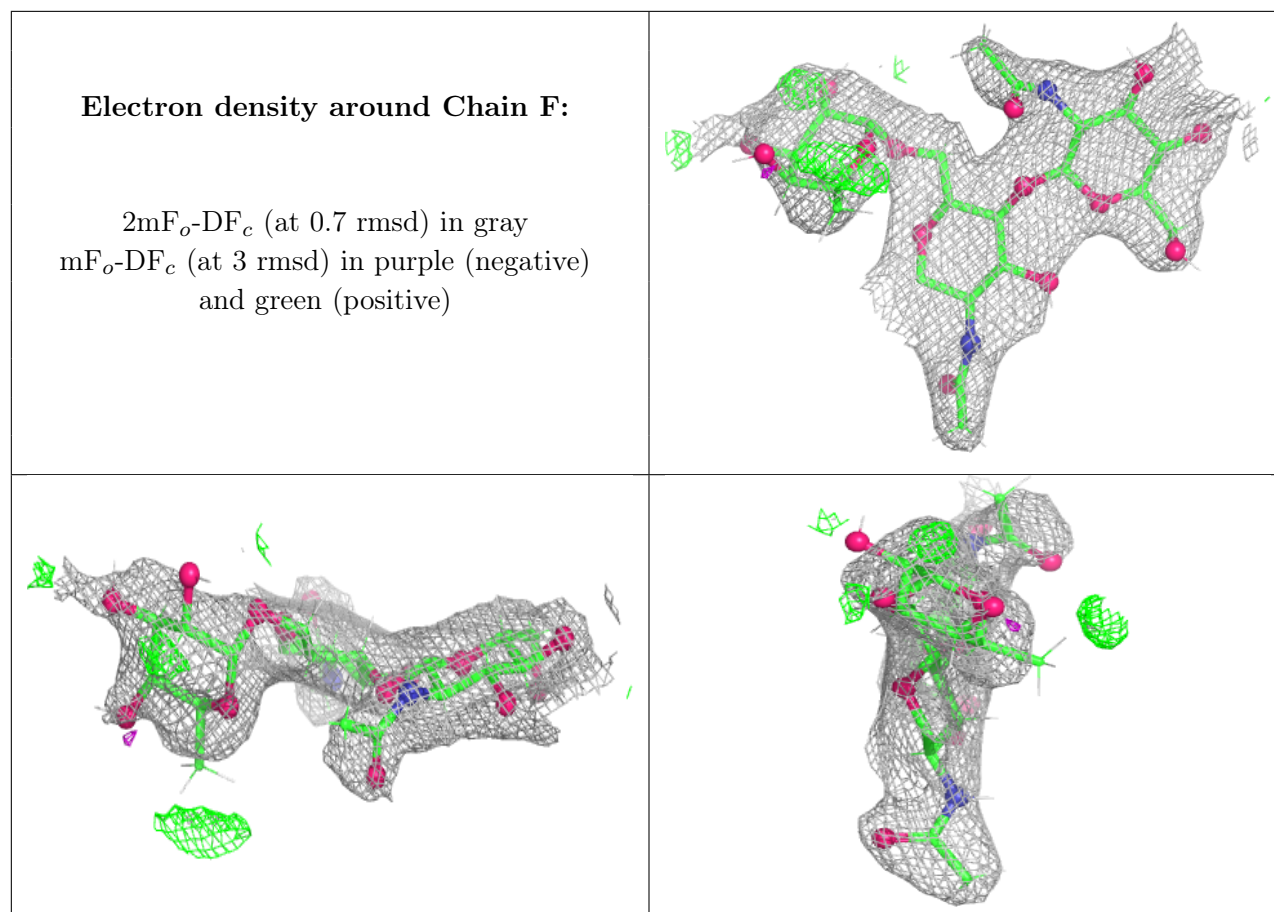
Electron density around Chain E:

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

**Electron density around Chain G:**

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	ACT	B	706	4/4	0.58	0.20	56,62,74,74	0
10	ACT	B	709	4/4	0.69	0.23	55,56,66,66	0
11	EDO	A	715	4/4	0.74	0.22	42,51,65,65	0
11	EDO	B	718	4/4	0.74	0.23	62,75,90,90	0
11	EDO	B	719	4/4	0.74	0.18	65,78,88,88	0
11	EDO	B	717	4/4	0.75	0.15	55,67,69,75	0
11	EDO	A	720	4/4	0.76	0.16	55,66,67,78	0
10	ACT	A	717	4/4	0.76	0.22	44,49,59,59	0
11	EDO	B	720	4/4	0.76	0.18	48,68,76,82	0
11	EDO	A	721	4/4	0.77	0.19	50,63,76,76	0
10	ACT	B	708	4/4	0.79	0.17	42,50,52,54	0
9	PG4	A	706	13/13	0.82	0.14	41,49,66,69	0

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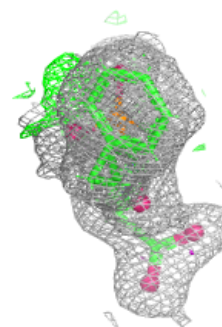
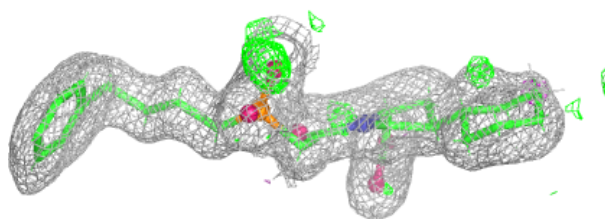
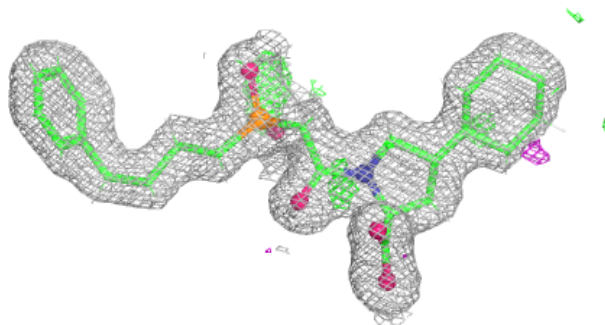
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	ACT	B	710	4/4	0.83	0.18	44,51,61,61	0
10	ACT	A	716	4/4	0.83	0.17	42,51,59,61	0
11	EDO	A	710	4/4	0.84	0.12	42,50,53,56	0
7	PEG	B	711	7/7	0.85	0.14	50,62,74,78	0
10	ACT	B	712	4/4	0.85	0.20	48,53,62,62	0
9	PG4	A	714	13/13	0.86	0.12	40,48,59,59	0
7	PEG	A	713	7/7	0.86	0.14	51,62,65,69	0
10	ACT	B	707	4/4	0.86	0.12	51,53,67,67	0
7	PEG	B	703	7/7	0.87	0.14	37,46,55,62	0
8	PGE	A	708	10/10	0.87	0.13	37,53,68,68	0
11	EDO	B	705	4/4	0.87	0.14	46,56,62,64	0
11	EDO	B	715	4/4	0.87	0.16	39,50,52,61	0
11	EDO	B	721	4/4	0.87	0.14	45,64,74,77	0
16	NAG	B	702	14/15	0.87	0.11	52,63,76,79	0
10	ACT	A	707	4/4	0.89	0.18	41,45,49,50	0
7	PEG	A	712	7/7	0.89	0.14	38,55,68,70	0
8	PGE	A	709	10/10	0.89	0.12	36,46,61,75	0
15	NA	A	723	1/1	0.90	0.12	46,46,46,46	0
7	PEG	A	704	7/7	0.90	0.10	41,50,62,74	0
8	PGE	A	703	10/10	0.91	0.11	28,45,55,60	0
7	PEG	B	704	7/7	0.91	0.11	43,52,60,60	0
7	PEG	A	705	7/7	0.91	0.12	37,47,74,74	0
11	EDO	B	716	4/4	0.92	0.09	40,48,51,54	0
7	PEG	A	702	7/7	0.93	0.09	32,39,42,50	0
14	CA	A	722	1/1	0.93	0.15	65,65,65,65	0
14	CA	B	723	1/1	0.96	0.12	55,55,55,55	0
10	ACT	A	711	4/4	0.96	0.08	39,44,53,53	0
6	KS8	B	701	30/30	0.96	0.07	22,29,39,41	0
14	CA	B	722	1/1	0.97	0.13	50,50,50,50	0
6	KS8	A	701	30/30	0.97	0.06	19,25,33,38	0
13	CL	B	714	1/1	0.98	0.06	24,24,24,24	0
12	ZN	B	713	1/1	0.99	0.02	24,24,24,24	0
12	ZN	A	718	1/1	1.00	0.01	19,19,19,19	0
13	CL	A	719	1/1	1.00	0.01	19,19,19,19	0

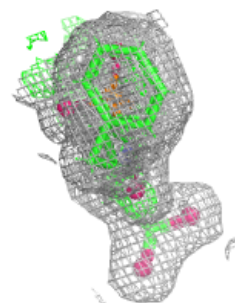
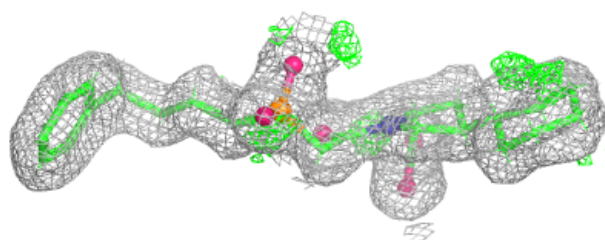
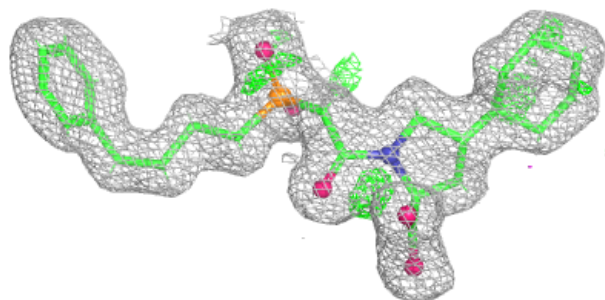
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KS8 B 701:

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

**Electron density around KS8 A 701:**

$2mF_o-DF_c$ (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.