Full wwPDB X-ray Structure Validation Report (i)

Mar 8, 2026 – 04:03 PM UTC

PDB ID	:	9QAS / pdb_00009qas
Title	:	Human angiotensin-1 converting enzyme N-domain in complex with trandolaprilat
Authors	:	Gregory, K.S.; Acharya, K.R.
Deposited on	:	2025-02-28
Resolution	:	2.20 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 (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:

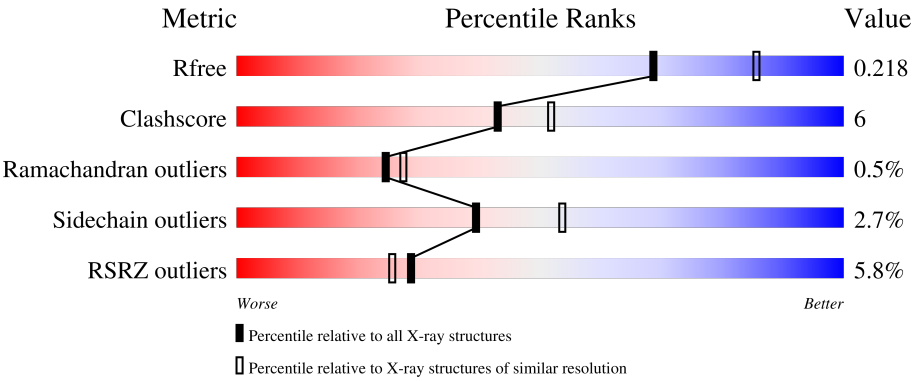
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.20 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.



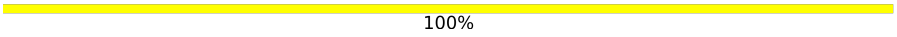
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	609	% 84% 13%
1	B	609	11% 80% 16%
2	F	4	75% 25%
3	G	3	33% 67%
3	I	3	100%

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Mol	Chain	Length	Quality of chain
4	H	2	
5	J	2	

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
7	ACT	A	702	-	-	X	-
8	PEG	A	710	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 11028 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

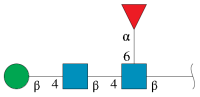
- Molecule 1 is a protein called Angiotensin-converting enzyme, soluble form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	604	Total	C	N	O	S	0	9	0
			5006	3211	858	917	20			
1	B	603	Total	C	N	O	S	0	3	0
			4948	3177	849	903	19			

There are 14 discrepancies between the modelled and reference sequences:

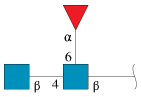
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	engineered mutation	UNP P12821
A	25	GLN	ASN	engineered mutation	UNP P12821
A	82	GLN	ASN	engineered mutation	UNP P12821
A	117	GLN	ASN	engineered mutation	UNP P12821
A	289	GLN	ASN	engineered mutation	UNP P12821
A	545	ARG	GLN	engineered mutation	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	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 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
2	F	4	Total C N O 49 28 2 19	0	0	0

- Molecule 3 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
3	G	3	Total C N O 38 22 2 14	0	0	0
3	I	3	Total C N O 38 22 2 14	0	0	0

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



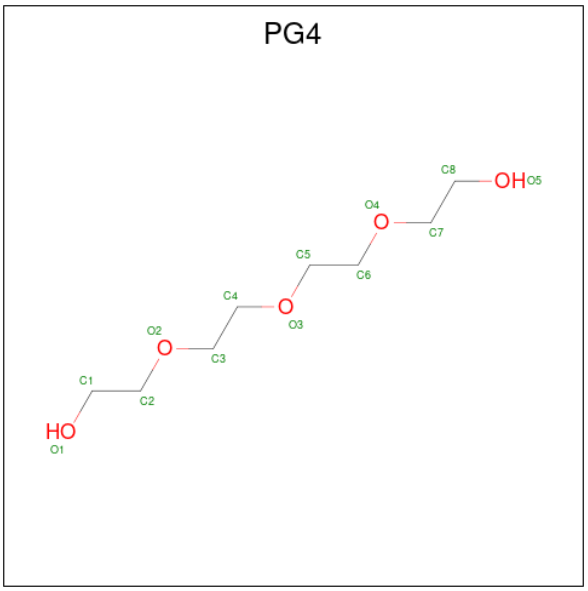
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	H	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



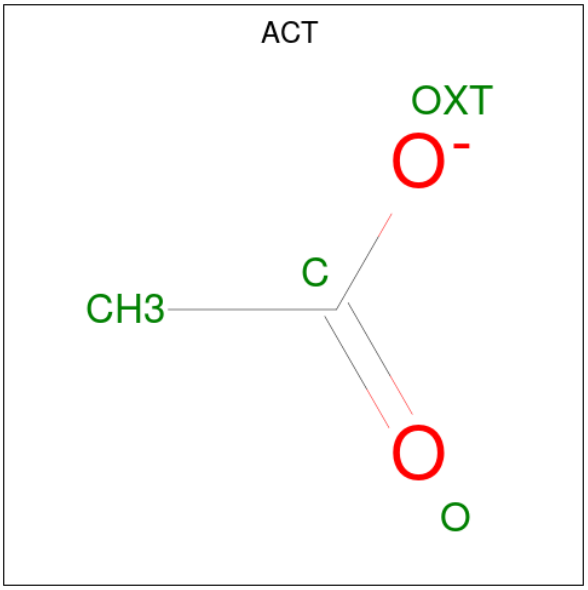
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	J	2	Total C N O 24 14 1 9	0	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



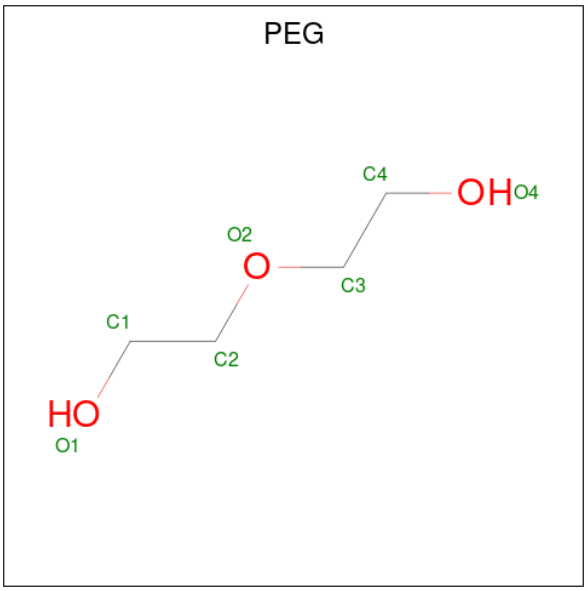
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 13 8 5	0	0
6	B	1	Total C O 13 8 5	0	0

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



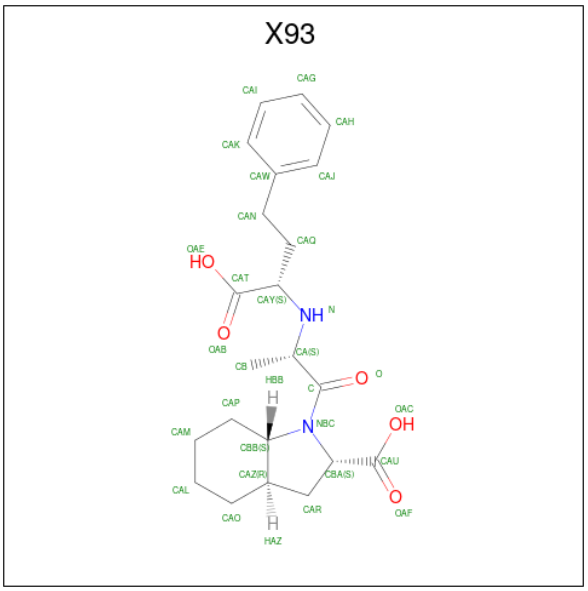
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



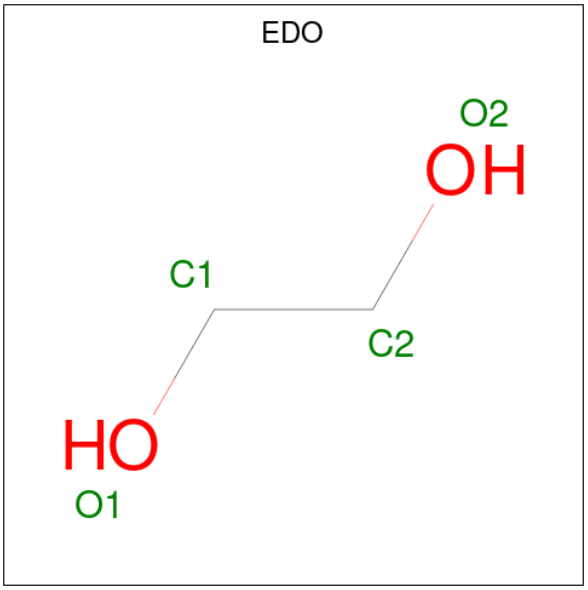
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	B	1	Total C O 7 4 3	0	0
8	B	1	Total C O 7 4 3	0	0
8	B	1	Total C O 7 4 3	0	0

- Molecule 9 is TRANDOLAPRILAT (CCD ID: X93) (formula: $C_{22}H_{30}N_2O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			29	22	2	5		
9	B	1	Total	C	N	O	0	0
			29	22	2	5		

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



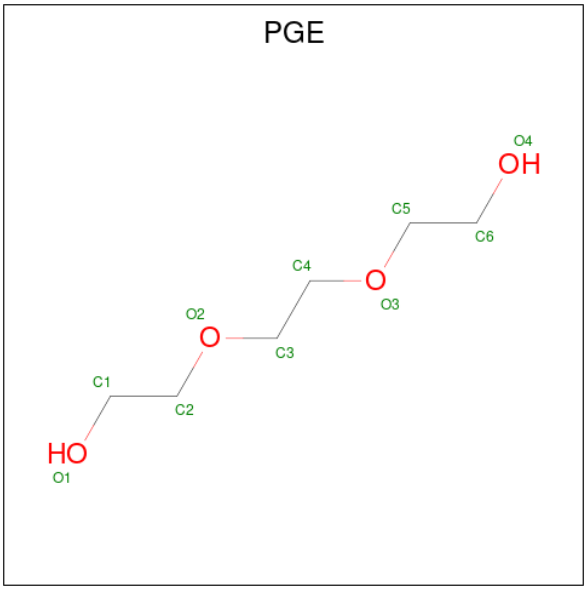
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0

- Molecule 11 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 10 6 4	0	0
11	B	1	Total C O 10 6 4	0	0

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

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

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

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

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

- Molecule 15 is water.

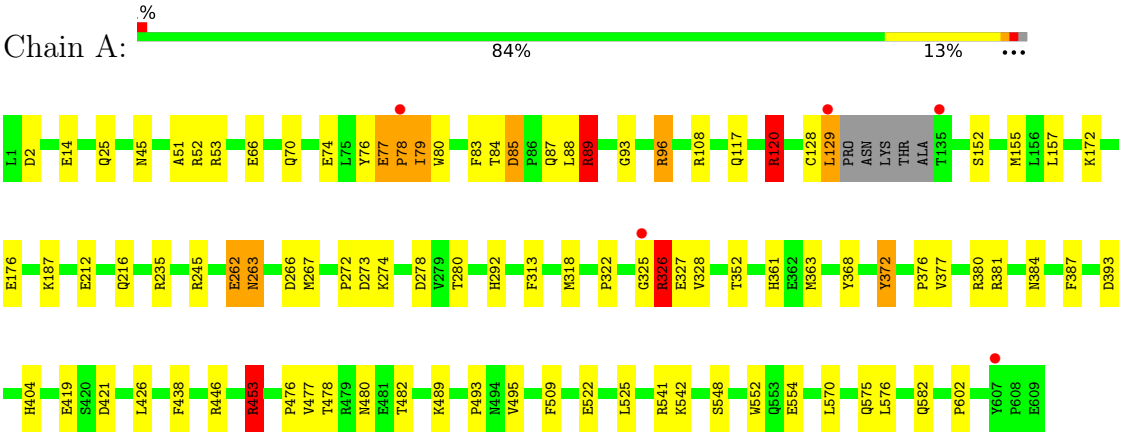
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	449	Total O 449 449	0	0
15	B	278	Total O 278 278	0	0

3 Residue-property plots (i)

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

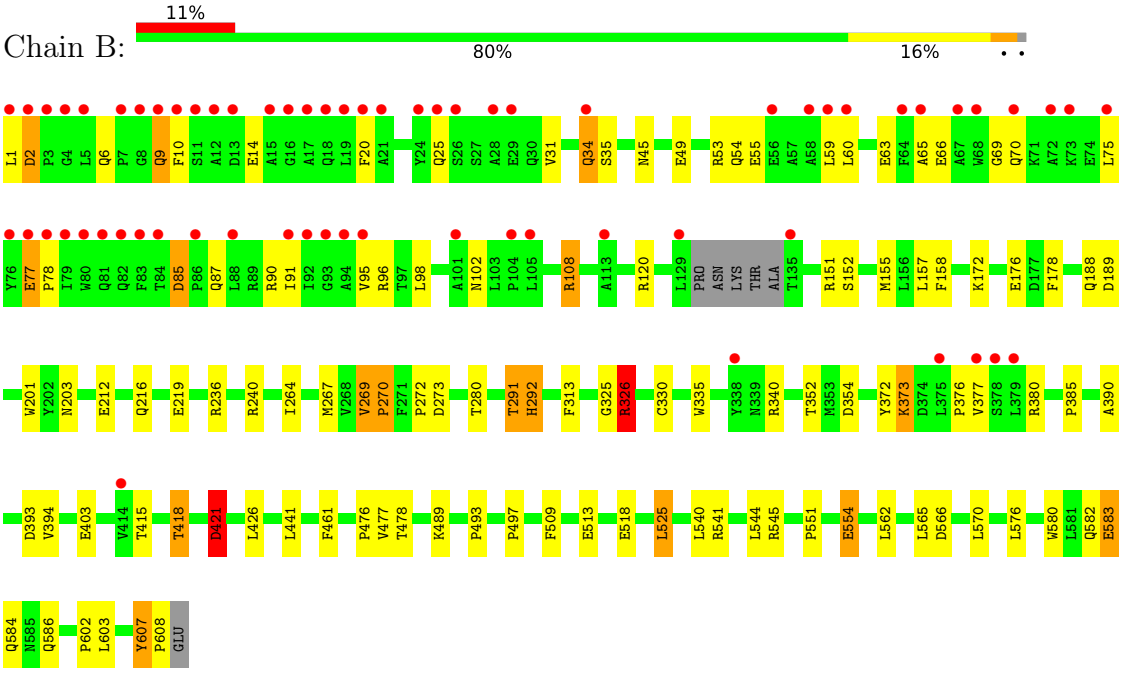
• Molecule 1: Angiotensin-converting enzyme, soluble form

Chain A:



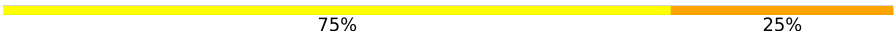
• Molecule 1: Angiotensin-converting enzyme, soluble form

Chain B:



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

Chain G:





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

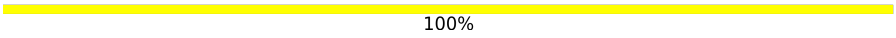
Chain I:





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

Chain H:





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

Chain J:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	73.18Å 77.60Å 82.46Å 88.47° 64.40° 74.77°	Depositor
Resolution (Å)	74.10 – 2.20 74.10 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (74.10-2.20) 92.9 (74.10-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.62 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, R_{free}	0.169 , 0.213 0.177 , 0.218	Depositor DCC
R_{free} test set	3923 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	27.2	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 48.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11028	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: X93, EDO, CA, BMA, PG4, FUC, ZN, CL, PEG, NAG, PGE, ACT

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	0.94	3/5161 (0.1%)	1.39	48/7029 (0.7%)
1	B	0.83	0/5103	1.36	35/6951 (0.5%)
All	All	0.89	3/10264 (0.0%)	1.37	83/13980 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	6
All	All	0	12

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	GLN	C-O	-5.44	1.17	1.24
1	A	262	GLU	CD-OE1	5.41	1.35	1.25
1	A	93	GLY	C-O	-5.21	1.17	1.23

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	54	GLN	CB-CA-C	12.46	132.02	110.85
1	B	54	GLN	N-CA-CB	-10.90	94.03	110.16
1	B	270	PRO	CB-CA-C	-8.96	98.60	111.68
1	B	291	THR	CA-CB-OG1	-8.51	96.83	109.60
1	B	85	ASP	CA-CB-CG	8.25	120.85	112.60
1	A	96	ARG	NE-CZ-NH2	7.94	126.35	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	602	PRO	CB-CA-C	7.92	122.47	110.75
1	A	267	MET	CG-SD-CE	-7.43	84.55	100.90
1	B	354	ASP	CA-CB-CG	7.39	119.99	112.60
1	B	415	THR	CA-CB-OG1	-7.37	98.55	109.60
1	B	418	THR	CA-CB-OG1	-7.29	98.66	109.60
1	A	419	GLU	CG-CD-OE2	-7.15	101.97	118.40
1	A	541	ARG	CD-NE-CZ	7.14	134.40	124.40
1	A	446	ARG	N-CA-CB	6.89	120.35	110.16
1	B	272	PRO	N-CA-C	6.84	122.89	113.65
1	A	582	GLN	CB-CA-C	-6.76	99.99	110.81
1	A	542	LYS	CB-CA-C	6.72	121.95	110.79
1	A	14	GLU	CB-CG-CD	6.64	123.89	112.60
1	B	2	ASP	CB-CA-C	6.57	118.14	108.87
1	A	76	TYR	N-CA-CB	-6.52	102.08	111.54
1	A	393	ASP	CA-CB-CG	6.52	119.12	112.60
1	A	327	GLU	CG-CD-OE2	-6.42	103.64	118.40
1	B	203	ASN	CB-CA-C	-6.41	102.00	112.06
1	B	403	GLU	CB-CG-CD	6.40	123.48	112.60
1	B	509	PHE	CA-CB-CG	-6.33	107.47	113.80
1	A	25	GLN	N-CA-CB	-6.33	100.82	110.12
1	B	393	ASP	CA-CB-CG	6.27	118.87	112.60
1	A	74	GLU	CB-CG-CD	6.22	123.17	112.60
1	B	272	PRO	CB-CA-C	-6.21	102.52	112.21
1	A	77	GLU	CB-CG-CD	6.07	122.92	112.60
1	A	263	ASN	CB-CA-C	-6.05	97.84	110.17
1	A	387	PHE	CB-CA-C	-6.03	100.78	110.79
1	A	87	GLN	N-CA-CB	6.01	118.96	110.12
1	A	273	ASP	N-CA-CB	5.98	119.61	110.70
1	B	583	GLU	CB-CA-C	-5.94	101.56	110.88
1	A	509	PHE	CA-CB-CG	-5.93	107.86	113.80
1	B	421	ASP	CA-CB-CG	5.93	118.53	112.60
1	B	90	ARG	CB-CA-C	-5.93	100.77	110.85
1	A	478	THR	CA-CB-OG1	-5.92	100.73	109.60
1	B	55	GLU	CB-CG-CD	5.88	122.59	112.60
1	B	77	GLU	N-CA-CB	5.87	119.05	110.30
1	A	361	HIS	CA-CB-CG	-5.83	107.97	113.80
1	B	216	GLN	CB-CA-C	-5.77	101.21	110.79
1	B	554	GLU	CB-CG-CD	-5.75	102.82	112.60
1	A	453	ARG	CG-CD-NE	5.68	124.50	112.00
1	B	373	LYS	CG-CD-CE	5.68	124.37	111.30
1	A	262	GLU	CB-CG-CD	5.63	122.17	112.60
1	A	77	GLU	N-CA-CB	5.58	118.61	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	554	GLU	CG-CD-OE2	-5.55	105.64	118.40
1	A	89	ARG	CB-CA-C	-5.53	100.41	110.63
1	A	83	PHE	CA-CB-CG	5.52	119.32	113.80
1	A	272	PRO	CA-C-N	-5.47	113.93	122.73
1	A	272	PRO	C-N-CA	-5.47	113.93	122.73
1	A	575	GLN	N-CA-CB	5.45	118.23	110.06
1	A	85	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	446	ARG	CB-CA-C	-5.35	101.75	110.85
1	B	34	GLN	CB-CA-C	5.33	120.90	110.67
1	B	566	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	372	TYR	CA-CB-CG	5.29	123.42	113.90
1	A	326	ARG	CB-CA-C	-5.27	99.93	110.42
1	B	461	PHE	CA-CB-CG	5.27	119.07	113.80
1	B	602	PRO	CB-CA-C	5.23	118.48	110.75
1	A	404	HIS	CA-CB-CG	-5.22	108.58	113.80
1	B	292	HIS	CA-CB-CG	-5.22	108.58	113.80
1	B	607	TYR	CB-CA-C	5.22	115.63	109.47
1	A	96	ARG	NE-CZ-NH1	-5.18	116.32	121.50
1	A	278	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	438	PHE	CA-C-N	5.17	125.81	120.03
1	A	438	PHE	C-N-CA	5.17	125.81	120.03
1	B	178	PHE	CA-CB-CG	-5.16	108.64	113.80
1	A	554	GLU	CB-CA-C	-5.13	102.12	110.85
1	A	120	ARG	CB-CG-CD	5.13	123.10	111.30
1	B	158	PHE	CA-CB-CG	-5.09	108.71	113.80
1	B	541	ARG	CD-NE-CZ	5.09	131.53	124.40
1	A	53	ARG	CG-CD-NE	-5.07	100.85	112.00
1	A	582	GLN	N-CA-CB	5.06	117.47	109.94
1	A	421	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	273	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	318	MET	CG-SD-CE	5.04	111.98	100.90
1	B	34	GLN	N-CA-CB	-5.04	102.47	110.28
1	B	385	PRO	CA-C-N	5.02	126.42	120.14
1	B	385	PRO	C-N-CA	5.02	126.42	120.14
1	A	327	GLU	CB-CG-CD	-5.00	104.09	112.60

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	ARG	Sidechain
1	A	245	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	326	ARG	Sidechain
1	A	380	ARG	Sidechain
1	A	453	ARG	Sidechain
1	A	89	ARG	Sidechain
1	B	108	ARG	Sidechain
1	B	120	ARG	Sidechain
1	B	326	ARG	Sidechain
1	B	380	ARG	Sidechain
1	B	53	ARG	Sidechain
1	B	545	ARG	Sidechain

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	5006	0	4772	56	0
1	B	4948	0	4725	54	0
2	F	49	0	43	1	0
3	G	38	0	34	5	0
3	I	38	0	34	4	0
4	H	28	0	25	0	0
5	J	24	0	22	1	0
6	A	13	0	16	2	0
6	B	13	0	18	2	0
7	A	4	0	3	2	0
8	A	14	0	20	6	0
8	B	21	0	30	3	0
9	A	29	0	28	2	0
9	B	29	0	28	1	0
10	A	20	0	30	5	0
11	A	10	0	14	1	0
11	B	10	0	14	2	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	2	0	0	0	0
14	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	A	449	0	0	11	0
15	B	278	0	0	7	0
All	All	11028	0	9856	124	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 6.

All (124) 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:235:ARG:HH12	10:A:707:EDO:H12	1.50	0.76
1:B:10:PHE:CE2	1:B:20:PHE:HA	2.24	0.72
1:B:91:ILE:O	1:B:95:VAL:HG23	1.91	0.71
1:A:235:ARG:HH12	10:A:707:EDO:C1	2.03	0.71
1:A:129:LEU:C	1:A:129:LEU:HD12	2.18	0.68
1:A:187:LYS:HE2	15:A:1173:HOH:O	1.95	0.67
1:B:155:MET:HE3	1:B:155:MET:HA	1.76	0.66
1:B:518:GLU:OE2	15:B:801:HOH:O	2.14	0.66
11:B:701:PGE:H32	15:B:862:HOH:O	1.96	0.66
1:A:453:ARG:NH2	1:B:212:GLU:HG2	2.14	0.63
1:A:80:TRP:O	1:A:89:ARG:HG2	1.99	0.63
1:B:66:GLU:HG2	1:B:70:GLN:OE1	1.98	0.63
10:A:708:EDO:H22	15:A:1183:HOH:O	1.97	0.63
1:B:66:GLU:CD	1:B:108:ARG:HH22	2.06	0.63
1:A:66:GLU:O	1:A:70:GLN:HG3	2.01	0.61
1:A:292:HIS:NE2	11:A:709:PGE:H12	2.16	0.60
1:B:59:LEU:O	1:B:63:GLU:HG3	2.02	0.59
1:A:155:MET:HE3	1:A:155:MET:HA	1.85	0.58
1:A:78:PRO:HA	15:A:1015:HOH:O	2.05	0.57
1:A:51:ALA:HB2	8:A:710:PEG:H42	1.87	0.56
1:A:381:ARG:HG3	1:A:548:SER:HB3	1.85	0.56
1:A:172:LYS:O	1:A:176[B]:GLU:HG3	2.05	0.56
1:B:270:PRO:HD3	1:B:426:LEU:HD22	1.88	0.56
6:A:701:PG4:H12	15:A:1187:HOH:O	2.06	0.56
1:A:482[B]:THR:CG2	3:G:1:NAG:O7	2.54	0.55
1:B:264:ILE:HB	1:B:267:MET:HE3	1.87	0.55
1:A:120:ARG:HD3	8:A:710:PEG:C2	2.37	0.55
1:A:129:LEU:CG	1:A:129:LEU:O	2.53	0.55
1:A:129:LEU:HD12	1:A:129:LEU:O	2.06	0.55
1:A:262:GLU:OE1	1:A:263:ASN:ND2	2.40	0.55
1:B:77:GLU:HA	1:B:77:GLU:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:GLU:N	1:B:78:PRO:HD2	2.21	0.55
1:A:52:ARG:HG2	1:A:52:ARG:HH11	1.73	0.54
3:I:1:NAG:H62	3:I:2:NAG:H82	1.89	0.54
1:B:270:PRO:HB3	1:B:580:TRP:CH2	2.43	0.54
1:B:330:CYS:O	15:B:802:HOH:O	2.18	0.54
1:A:117:GLN:HG2	15:A:1149:HOH:O	2.07	0.54
1:A:266:ASP:HB3	15:A:803:HOH:O	2.09	0.53
1:B:240:ARG:HG3	1:B:240:ARG:HH11	1.72	0.53
1:B:478:THR:HB	5:J:2:FUC:H2	1.91	0.53
1:A:85:ASP:HB3	1:A:88:LEU:HB3	1.91	0.52
11:B:701:PGE:C3	15:B:862:HOH:O	2.57	0.51
1:A:129:LEU:O	1:A:129:LEU:HG	2.11	0.51
1:B:201:TRP:HZ3	1:B:497:PRO:HG2	1.76	0.51
1:A:96:ARG:HH11	1:A:96:ARG:HG3	1.77	0.49
1:B:65:ALA:O	1:B:66:GLU:C	2.56	0.49
1:B:441:LEU:C	1:B:441:LEU:HD12	2.37	0.49
1:A:482[B]:THR:HG23	3:G:1:NAG:O7	2.12	0.48
1:B:376:PRO:O	1:B:377:VAL:C	2.56	0.48
1:A:120:ARG:HD3	8:A:710:PEG:H21	1.94	0.48
1:A:77:GLU:OE1	1:A:96:ARG:NE	2.47	0.48
7:A:702:ACT:H3	15:A:909:HOH:O	2.14	0.48
1:B:325:GLY:O	1:B:326:ARG:C	2.56	0.48
1:B:14:GLU:OE2	1:B:85:ASP:HB3	2.14	0.47
1:B:172:LYS:O	1:B:176:GLU:HG3	2.14	0.47
1:B:513:GLU:HA	1:B:525:LEU:HD21	1.95	0.47
1:B:551:PRO:HG2	1:B:554:GLU:OE2	2.15	0.47
1:B:335:TRP:CE2	6:B:705:PG4:H81	2.50	0.47
1:B:570:LEU:C	1:B:570:LEU:HD23	2.40	0.47
1:B:69:GLY:HA3	1:B:98:LEU:HD11	1.96	0.47
8:B:706:PEG:H22	15:B:834:HOH:O	2.15	0.47
3:G:1:NAG:O7	3:G:1:NAG:H3	2.14	0.47
1:A:235:ARG:NH1	10:A:707:EDO:H12	2.24	0.46
8:A:710:PEG:H21	8:A:710:PEG:H41	1.71	0.46
1:A:128:CYS:O	1:A:129:LEU:C	2.59	0.46
1:A:66:GLU:CD	1:A:108:ARG:HH22	2.23	0.46
1:A:482[B]:THR:HG21	3:G:1:NAG:O7	2.16	0.46
1:A:522:GLU:OE2	2:F:3:BMA:H3	2.16	0.46
1:A:157:LEU:HD13	1:A:476:PRO:HB2	1.98	0.45
1:A:381:ARG:CG	1:A:548:SER:HB3	2.47	0.45
9:A:704:X93:HAM1	10:A:706:EDO:H22	1.98	0.45
1:A:274:LYS:NZ	15:A:827:HOH:O	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:VAL:HG12	1:A:495:VAL:O	2.18	0.44
1:A:120:ARG:HB2	8:A:710:PEG:C4	2.48	0.44
1:B:1:LEU:HD23	1:B:6:GLN:HG3	1.98	0.44
1:A:96:ARG:HG3	1:A:96:ARG:NH1	2.31	0.44
1:A:120:ARG:HB2	8:A:710:PEG:O4	2.17	0.44
1:B:418:THR:HG23	3:I:3:FUC:O3	2.18	0.44
1:A:96:ARG:HH11	1:A:96:ARG:CG	2.31	0.44
1:A:480:ASN:ND2	3:G:3:FUC:H61	2.32	0.44
1:B:565:LEU:O	8:B:706:PEG:H41	2.18	0.43
1:B:102:ASN:ND2	1:B:189:ASP:OD1	2.35	0.43
1:B:292:HIS:CE1	8:B:703:PEG:H21	2.52	0.43
1:B:151:ARG:NE	1:B:267:MET:HE2	2.34	0.43
1:B:583:GLU:O	1:B:584:GLN:C	2.62	0.43
1:A:363[B]:MET:HE3	1:A:363[B]:MET:HB3	1.90	0.43
1:A:489:LYS:O	1:A:493:PRO:HD2	2.19	0.43
1:A:570:LEU:C	1:A:570:LEU:HD23	2.43	0.43
1:B:540:LEU:O	1:B:544:LEU:HG	2.18	0.43
1:A:129:LEU:O	1:A:129:LEU:CD1	2.67	0.43
1:A:77:GLU:N	1:A:78:PRO:CD	2.83	0.42
1:B:10:PHE:O	1:B:75:LEU:CD2	2.68	0.42
1:B:489:LYS:O	1:B:493:PRO:HD2	2.19	0.42
7:A:702:ACT:H1	15:A:1030:HOH:O	2.20	0.42
1:B:477:VAL:HG12	1:B:603:LEU:HD21	2.02	0.42
1:A:78:PRO:C	1:A:79:ILE:HG23	2.44	0.42
1:A:376:PRO:O	1:A:377:VAL:C	2.63	0.42
6:B:705:PG4:H22	15:B:1043:HOH:O	2.19	0.42
1:A:157:LEU:HD11	1:A:477:VAL:HG13	2.01	0.42
1:B:270:PRO:HD3	1:B:426:LEU:CD2	2.49	0.42
1:B:607:TYR:HA	1:B:608:PRO:HA	1.77	0.42
1:B:157:LEU:HD13	1:B:476:PRO:HB2	2.02	0.42
1:B:390:ALA:O	1:B:394:VAL:HG23	2.20	0.42
1:B:9:GLN:C	1:B:10:PHE:CD1	2.98	0.41
1:B:340:ARG:HG2	1:B:373:LYS:O	2.20	0.41
1:B:31:VAL:O	1:B:34:GLN:HG3	2.19	0.41
1:B:201:TRP:CZ3	1:B:497:PRO:HG2	2.53	0.41
1:A:313:PHE:CD1	1:A:313:PHE:C	2.99	0.41
1:A:322:PRO:HG2	1:A:328:VAL:HG11	2.03	0.41
1:A:266:ASP:CG	15:A:803:HOH:O	2.63	0.41
1:A:384:ASN:HD22	1:A:552:TRP:CG	2.39	0.41
1:B:219:GLU:OE2	15:B:803:HOH:O	2.22	0.41
1:B:269:VAL:HA	1:B:270:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:704:X93:HAP2	9:B:704:X93:HA	2.03	0.41
1:B:582:GLN:O	1:B:586:GLN:HG3	2.21	0.40
1:A:325:GLY:O	1:A:326:ARG:C	2.63	0.40
1:B:421:ASP:OD2	3:I:3:FUC:C6	2.70	0.40
3:I:2:NAG:H82	3:I:3:FUC:C1	2.51	0.40
1:B:273:ASP:OD1	1:B:273:ASP:N	2.53	0.40
1:A:84:THR:HA	15:A:1052:HOH:O	2.22	0.40
1:B:280:THR:HG23	1:B:352:THR:HA	2.04	0.40
1:A:280:THR:HG23	1:A:352:THR:HA	2.03	0.40
6:A:701:PG4:H51	9:A:704:X93:CAK	2.51	0.40
1:B:313:PHE:CD1	1:B:313:PHE:C	3.00	0.40

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	609/609 (100%)	593 (97%)	12 (2%)	4 (1%)	18	19
1	B	602/609 (99%)	586 (97%)	14 (2%)	2 (0%)	36	42
All	All	1211/1218 (99%)	1179 (97%)	26 (2%)	6 (0%)	24	27

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	ARG
1	B	45	ASN
1	B	326	ARG
1	A	45	ASN
1	A	79	ILE
1	A	78	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	529/524 (101%)	519 (98%)	10 (2%)	50 66
1	B	522/524 (100%)	504 (97%)	18 (3%)	32 44
All	All	1051/1048 (100%)	1023 (97%)	28 (3%)	39 53

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	129	LEU
1	A	152	SER
1	A	212	GLU
1	A	368	TYR
1	A	372	TYR
1	A	426	LEU
1	A	453	ARG
1	A	525	LEU
1	A	576	LEU
1	B	2	ASP
1	B	9	GLN
1	B	25	GLN
1	B	35	SER
1	B	49	GLU
1	B	60	LEU
1	B	87	GLN
1	B	96	ARG
1	B	152	SER
1	B	188	GLN
1	B	236	ARG
1	B	269	VAL
1	B	291	THR
1	B	372	TYR
1	B	421	ASP
1	B	525	LEU
1	B	562	LEU

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Mol	Chain	Res	Type
1	B	576	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	81	GLN
1	A	213	HIS
1	B	9	GLN
1	B	81	GLN
1	B	213	HIS
1	B	527	GLN
1	B	568	GLN
1	B	579	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

14 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	F	1	2,1	14,14,15	0.91	1 (7%)	17,19,21	2.03	3 (17%)
2	NAG	F	2	2	14,14,15	0.41	0	17,19,21	1.50	3 (17%)
2	BMA	F	3	2	11,11,12	1.65	1 (9%)	15,15,17	1.22	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FUC	F	4	2	10,10,11	1.14	1 (10%)	14,14,16	1.27	1 (7%)
3	NAG	G	1	3,1	14,14,15	0.56	0	17,19,21	1.15	1 (5%)
3	NAG	G	2	3	14,14,15	0.72	1 (7%)	17,19,21	1.47	3 (17%)
3	FUC	G	3	3	10,10,11	0.65	0	14,14,16	1.19	1 (7%)
4	NAG	H	1	4,1	14,14,15	0.48	0	17,19,21	1.50	3 (17%)
4	NAG	H	2	4	14,14,15	0.63	0	17,19,21	2.47	5 (29%)
3	NAG	I	1	3,1	14,14,15	0.74	0	17,19,21	1.64	4 (23%)
3	NAG	I	2	3	14,14,15	0.39	0	17,19,21	1.24	2 (11%)
3	FUC	I	3	3	10,10,11	0.81	0	14,14,16	1.35	2 (14%)
5	NAG	J	1	5,1	14,14,15	0.55	0	17,19,21	1.70	2 (11%)
5	FUC	J	2	5	10,10,11	1.12	1 (10%)	14,14,16	1.85	2 (14%)

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	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	FUC	F	4	2	-	-	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	5/6/23/26	0/1/1/1
3	FUC	G	3	3	-	-	0/1/1/1
4	NAG	H	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1
3	FUC	I	3	3	-	-	0/1/1/1
5	NAG	J	1	5,1	-	2/6/23/26	0/1/1/1
5	FUC	J	2	5	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3	BMA	C2-C3	4.96	1.60	1.52
2	F	4	FUC	C2-C3	-3.23	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	2	FUC	C2-C3	2.69	1.56	1.52
3	G	2	NAG	C1-C2	2.17	1.55	1.52
2	F	1	NAG	O6-C6	2.03	1.50	1.42

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	2	NAG	C1-O5-C5	7.26	121.92	112.19
2	F	1	NAG	C2-N2-C7	5.75	130.61	122.90
5	J	2	FUC	O2-C2-C3	5.60	121.76	110.15
5	J	1	NAG	C1-C2-N2	4.89	118.14	110.43
4	H	2	NAG	C1-C2-N2	4.52	117.56	110.43
2	F	2	NAG	C1-O5-C5	4.32	117.98	112.19
2	F	1	NAG	C1-C2-N2	-4.20	103.82	110.43
3	I	1	NAG	O3-C3-C2	3.91	117.51	109.40
4	H	1	NAG	C2-N2-C7	-3.83	117.77	122.90
2	F	4	FUC	O3-C3-C2	-3.68	102.54	110.05
3	I	2	NAG	C1-O5-C5	3.43	116.78	112.19
3	G	1	NAG	O3-C3-C2	3.36	116.38	109.40
2	F	1	NAG	C1-O5-C5	3.19	116.46	112.19
3	I	1	NAG	C2-N2-C7	3.16	127.13	122.90
4	H	1	NAG	C1-C2-N2	3.11	115.33	110.43
2	F	3	BMA	C1-C2-C3	3.00	114.01	109.64
4	H	2	NAG	O5-C5-C4	2.98	118.08	110.83
3	I	1	NAG	C1-C2-N2	2.82	114.87	110.43
3	G	2	NAG	C4-C3-C2	2.81	115.14	111.02
3	G	2	NAG	C1-O5-C5	-2.79	108.45	112.19
5	J	2	FUC	C1-C2-C3	-2.59	105.88	109.64
3	I	3	FUC	C1-O5-C5	2.55	118.99	112.97
3	G	2	NAG	O5-C5-C4	-2.49	104.76	110.83
4	H	2	NAG	C4-C3-C2	-2.41	107.48	111.02
4	H	2	NAG	O3-C3-C2	2.37	114.33	109.40
3	I	2	NAG	O5-C5-C6	-2.32	103.16	107.66
3	I	1	NAG	C1-O5-C5	2.27	115.23	112.19
3	I	3	FUC	C1-C2-C3	2.27	112.95	109.64
2	F	2	NAG	C1-C2-N2	2.19	113.89	110.43
4	H	1	NAG	O5-C5-C4	-2.11	105.69	110.83
3	G	3	FUC	C1-C2-C3	2.10	112.71	109.64
2	F	3	BMA	O2-C2-C3	2.09	114.47	110.15
2	F	2	NAG	C6-C5-C4	-2.02	108.05	113.02
5	J	1	NAG	C6-C5-C4	2.01	117.95	113.02

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	1	NAG	C1-C2-N2-C7
4	H	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	G	2	NAG	C4-C5-C6-O6
3	I	2	NAG	O7-C7-N2-C2
4	H	1	NAG	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	I	1	NAG	C3-C2-N2-C7
3	G	2	NAG	C1-C2-N2-C7
5	J	1	NAG	C1-C2-N2-C7
3	I	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C8-C7-N2-C2
3	G	1	NAG	C3-C2-N2-C7
3	G	2	NAG	C3-C2-N2-C7
3	G	1	NAG	C1-C2-N2-C7
5	J	1	NAG	C3-C2-N2-C7

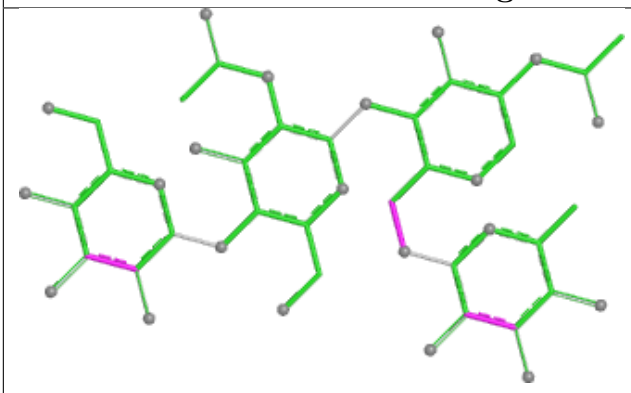
There are no ring outliers.

7 monomers are involved in 11 short contacts:

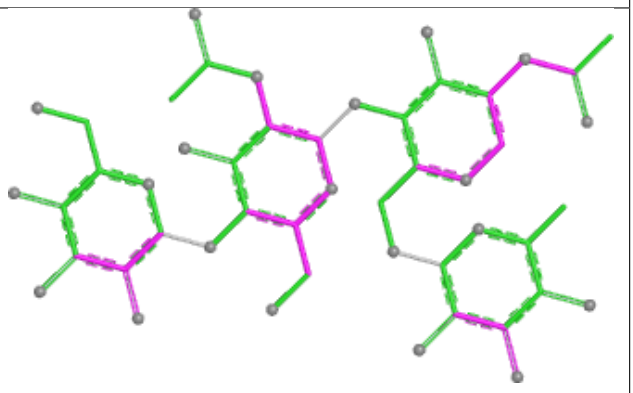
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	2	NAG	2	0
3	G	3	FUC	1	0
3	G	1	NAG	4	0
3	I	1	NAG	1	0
3	I	3	FUC	3	0
2	F	3	BMA	1	0
5	J	2	FUC	1	0

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

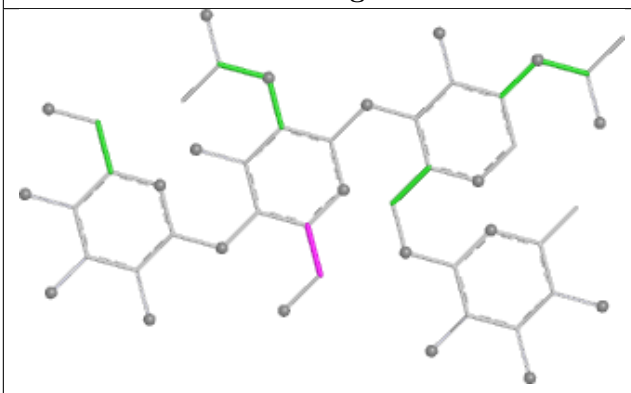
Oligosaccharide Chain F



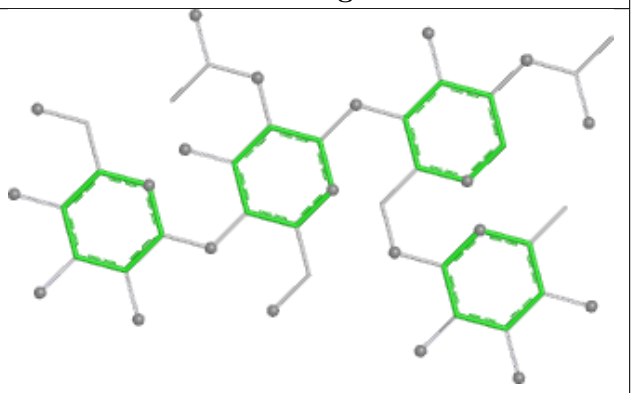
Bond lengths



Bond angles

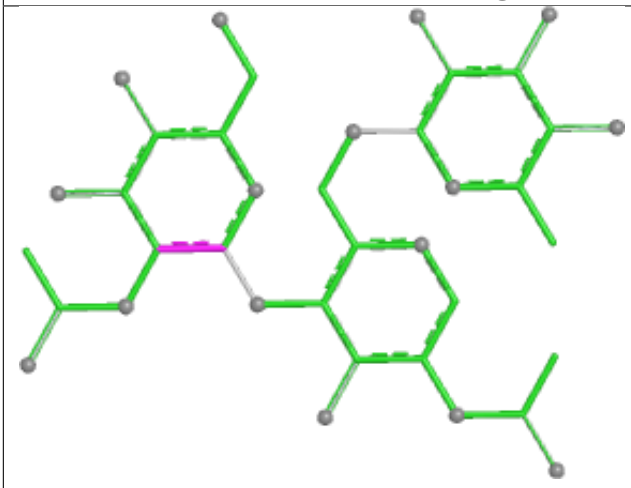


Torsions

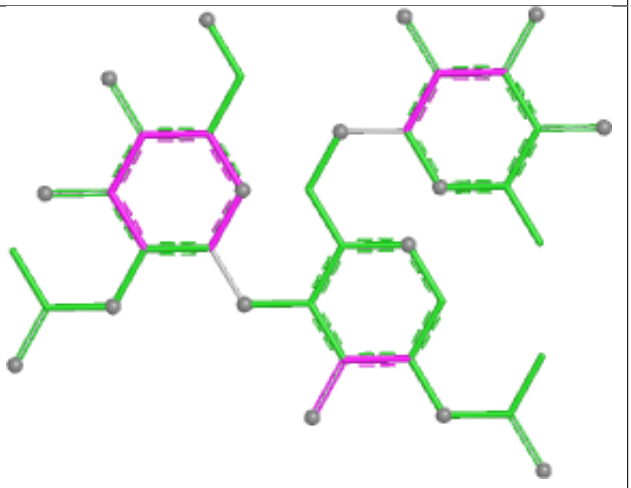


Rings

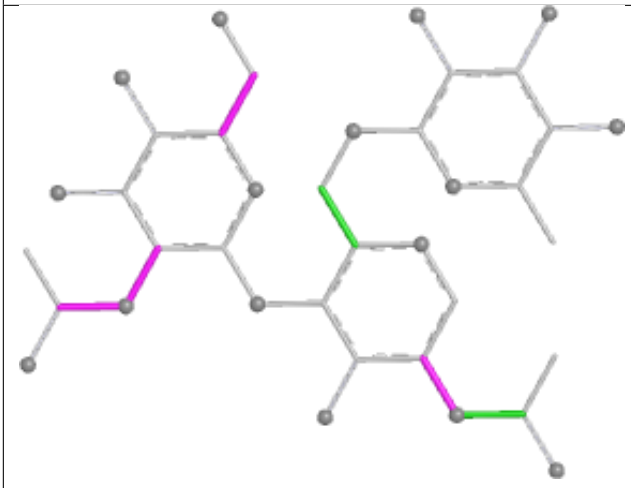
Oligosaccharide Chain G



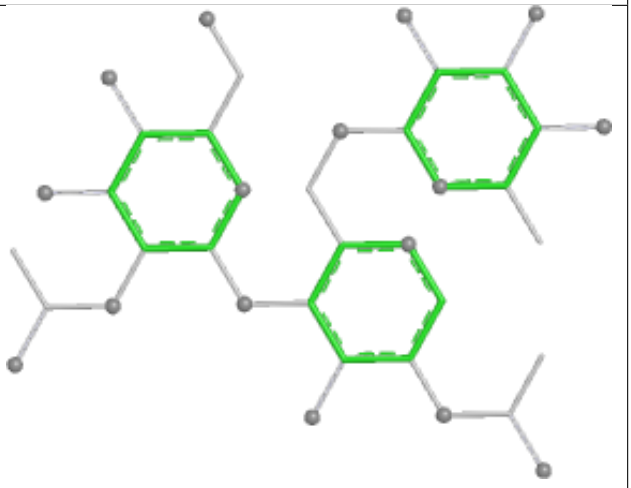
Bond lengths



Bond angles

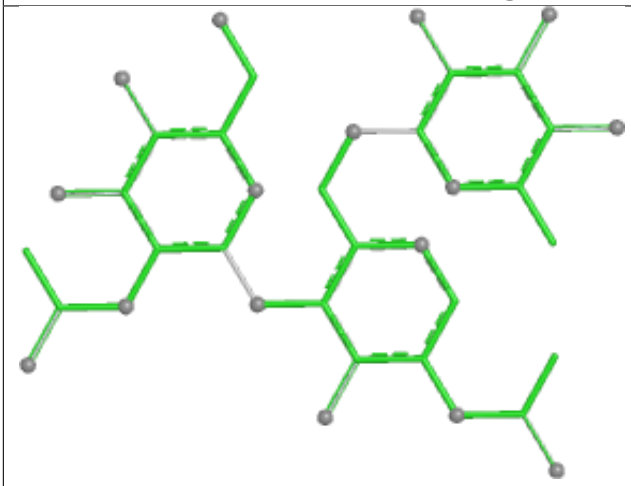


Torsions

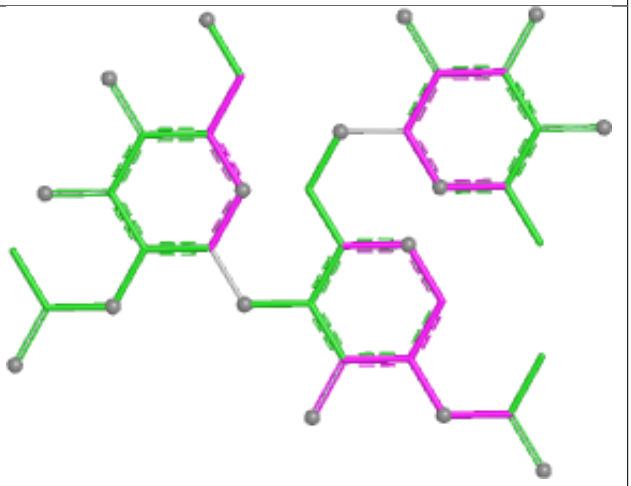


Rings

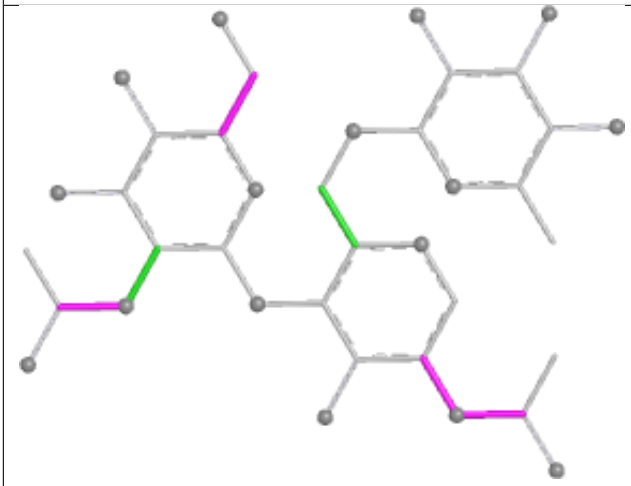
Oligosaccharide Chain I



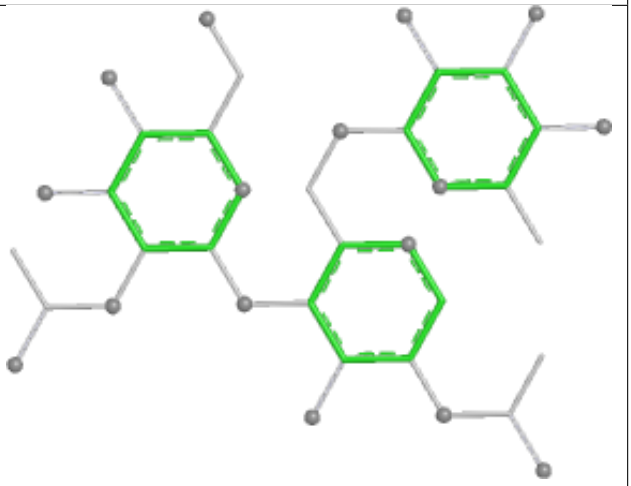
Bond lengths



Bond angles

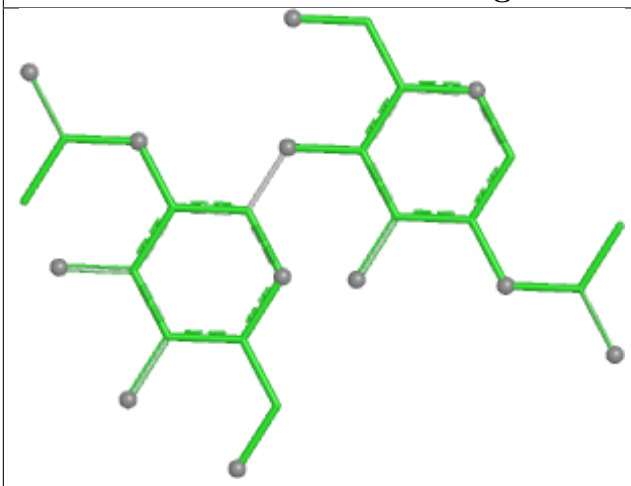


Torsions

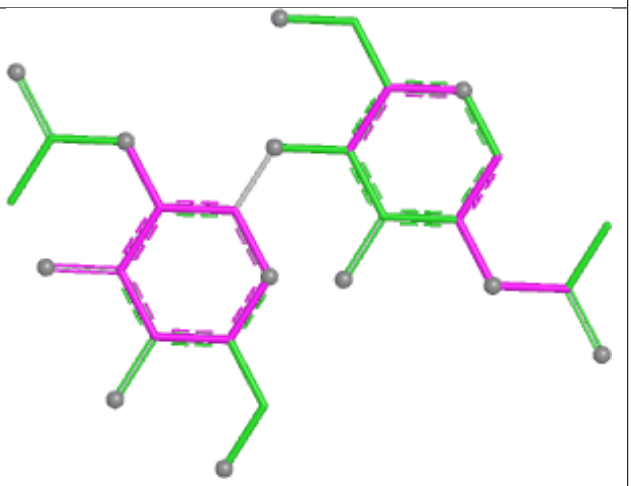


Rings

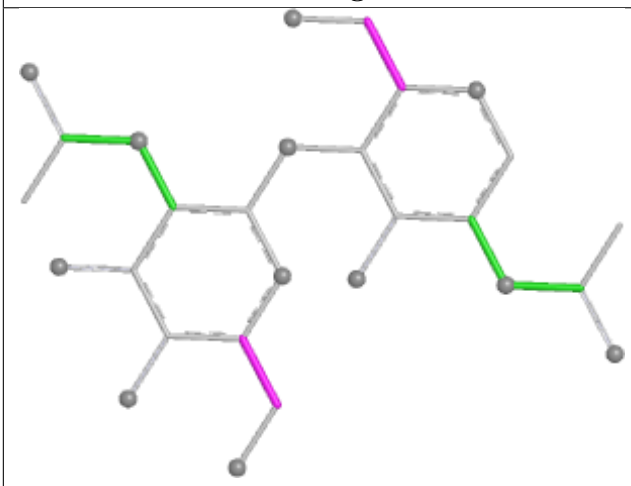
Oligosaccharide Chain H



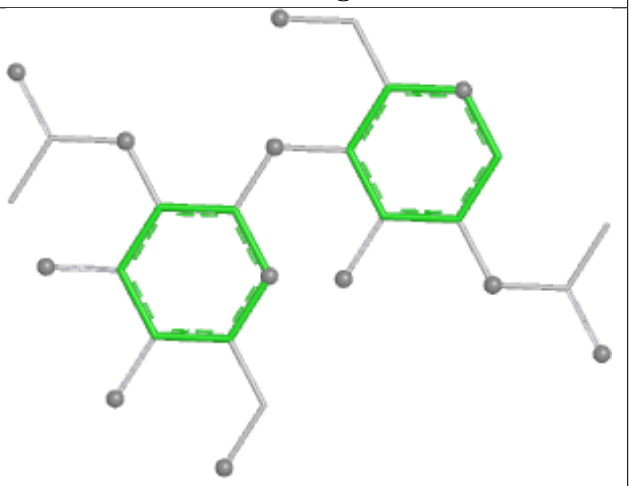
Bond lengths



Bond angles

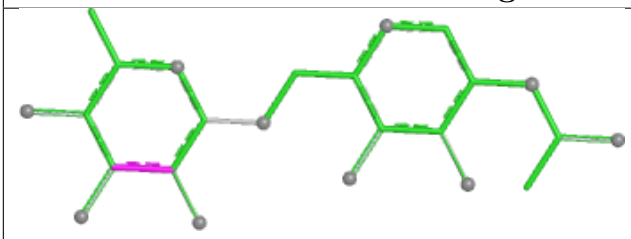


Torsions

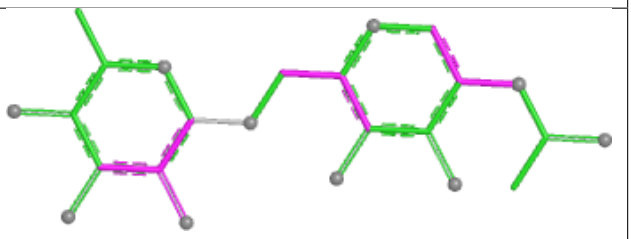


Rings

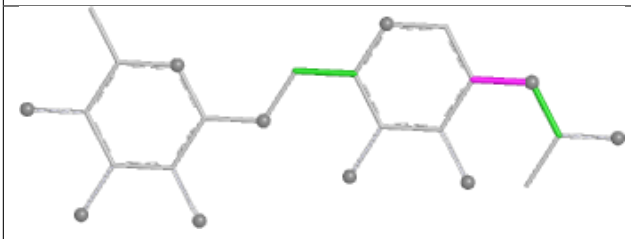
Oligosaccharide Chain J



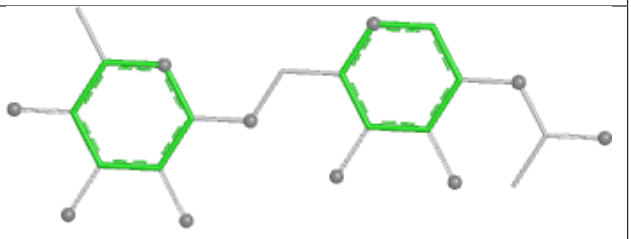
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 7 are monoatomic - leaving 17 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	$\#\|Z\| > 2$
10	EDO	A	708	-	3,3,3	0.17	0	2,2,2	0.36	0
8	PEG	B	706	-	6,6,6	0.65	0	5,5,5	0.60	0
9	X93	A	704	12	31,31,31	0.93	0	40,43,43	1.61	7 (17%)
10	EDO	A	706	-	3,3,3	0.52	0	2,2,2	0.57	0
10	EDO	A	707	-	3,3,3	0.56	0	2,2,2	0.30	0
8	PEG	A	703	-	6,6,6	0.22	0	5,5,5	0.34	0
10	EDO	A	705	-	3,3,3	0.31	0	2,2,2	0.49	0
8	PEG	B	703	-	6,6,6	0.55	0	5,5,5	0.32	0
6	PG4	B	705	-	12,12,12	0.65	0	11,11,11	0.45	0
8	PEG	B	702	-	6,6,6	0.48	0	5,5,5	0.50	0
11	PGE	A	709	-	9,9,9	0.90	0	8,8,8	0.68	0
6	PG4	A	701	-	12,12,12	0.55	0	11,11,11	0.57	0
9	X93	B	704	12	31,31,31	1.02	2 (6%)	40,43,43	1.44	4 (10%)
7	ACT	A	702	-	3,3,3	1.32	0	3,3,3	0.85	0
10	EDO	A	711	-	3,3,3	0.41	0	2,2,2	0.28	0
8	PEG	A	710	-	6,6,6	0.60	0	5,5,5	0.53	0
11	PGE	B	701	-	9,9,9	0.49	0	8,8,8	0.44	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
10	EDO	A	708	-	-	0/1/1/1	-
8	PEG	B	706	-	-	2/4/4/4	-
9	X93	A	704	12	-	2/25/48/48	0/3/3/3
10	EDO	A	706	-	-	1/1/1/1	-
10	EDO	A	707	-	-	0/1/1/1	-
8	PEG	A	703	-	-	1/4/4/4	-
10	EDO	A	705	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PEG	B	703	-	-	3/4/4/4	-
6	PG4	B	705	-	-	5/10/10/10	-
11	PGE	A	709	-	-	4/7/7/7	-
6	PG4	A	701	-	-	5/10/10/10	-
9	X93	B	704	12	-	5/25/48/48	0/3/3/3
8	PEG	B	702	-	-	2/4/4/4	-
10	EDO	A	711	-	-	1/1/1/1	-
8	PEG	A	710	-	-	3/4/4/4	-
11	PGE	B	701	-	-	4/7/7/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	704	X93	OAE-CAT	-3.08	1.20	1.30
9	B	704	X93	CBB-NBC	2.41	1.51	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	704	X93	CAP-CBB-CAZ	-5.41	106.37	113.09
9	A	704	X93	CAP-CBB-CAZ	-4.97	106.92	113.09
9	A	704	X93	CAR-CBA-CAU	3.41	114.98	111.01
9	A	704	X93	OAF-CAU-CBA	-3.05	113.09	122.44
9	B	704	X93	OAF-CAU-CBA	-2.99	113.28	122.44
9	B	704	X93	CAQ-CAN-CAW	2.49	121.42	113.22
9	B	704	X93	CAP-CBB-NBC	2.47	120.39	112.89
9	A	704	X93	CAR-CBA-NBC	2.39	106.47	103.48
9	A	704	X93	CBB-NBC-C	2.34	133.74	126.84
9	A	704	X93	CAP-CBB-NBC	2.07	119.16	112.89
9	A	704	X93	CAQ-CAN-CAW	2.06	120.01	113.22

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	710	PEG	C4-C3-O2-C2
11	A	709	PGE	O2-C3-C4-O3
6	B	705	PG4	O4-C7-C8-O5
6	A	701	PG4	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
8	B	702	PEG	O1-C1-C2-O2
8	B	703	PEG	O1-C1-C2-O2
6	A	701	PG4	O1-C1-C2-O2
8	B	706	PEG	O2-C3-C4-O4
11	A	709	PGE	O1-C1-C2-O2
11	A	709	PGE	O3-C5-C6-O4
11	B	701	PGE	O3-C5-C6-O4
10	A	705	EDO	O1-C1-C2-O2
9	B	704	X93	CAN-CAQ-CAY-N
6	B	705	PG4	O2-C3-C4-O3
8	A	703	PEG	O2-C3-C4-O4
8	A	710	PEG	O1-C1-C2-O2
8	B	703	PEG	O2-C3-C4-O4
10	A	706	EDO	O1-C1-C2-O2
10	A	711	EDO	O1-C1-C2-O2
6	B	705	PG4	O3-C5-C6-O4
11	B	701	PGE	O2-C3-C4-O3
11	A	709	PGE	C4-C3-O2-C2
8	B	706	PEG	C4-C3-O2-C2
9	B	704	X93	OAE-CAT-CAY-N
11	B	701	PGE	C4-C3-O2-C2
9	B	704	X93	CAN-CAQ-CAY-CAT
8	B	702	PEG	C4-C3-O2-C2
6	B	705	PG4	C5-C6-O4-C7
6	A	701	PG4	O2-C3-C4-O3
9	B	704	X93	CAQ-CAN-CAW-CAJ
8	A	710	PEG	C1-C2-O2-C3
6	B	705	PG4	C1-C2-O2-C3
9	B	704	X93	CAQ-CAN-CAW-CAK
6	A	701	PG4	C3-C4-O3-C5
8	B	703	PEG	C1-C2-O2-C3
9	A	704	X93	CAQ-CAN-CAW-CAJ
11	B	701	PGE	C3-C4-O3-C5
9	A	704	X93	CAQ-CAN-CAW-CAK
6	A	701	PG4	O4-C7-C8-O5

There are no ring outliers.

13 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	708	EDO	1	0
8	B	706	PEG	2	0

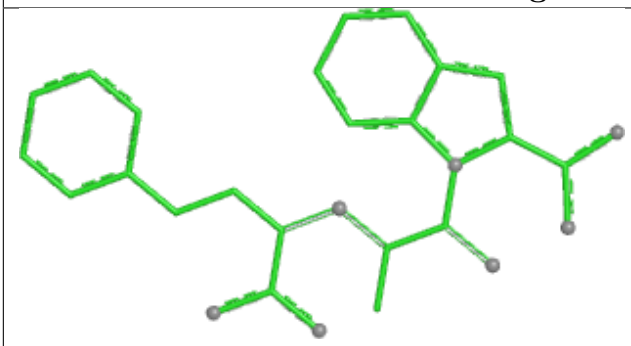
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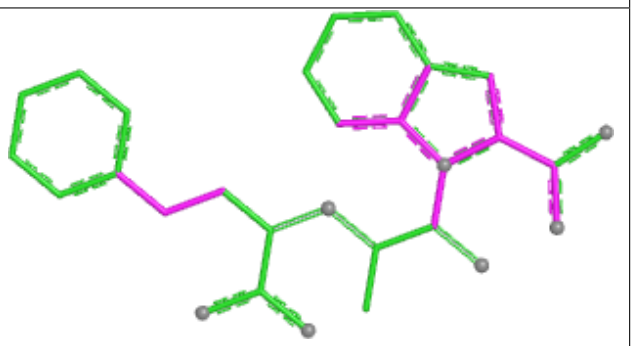
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	704	X93	2	0
10	A	706	EDO	1	0
10	A	707	EDO	3	0
8	B	703	PEG	1	0
6	B	705	PG4	2	0
11	A	709	PGE	1	0
6	A	701	PG4	2	0
9	B	704	X93	1	0
7	A	702	ACT	2	0
8	A	710	PEG	6	0
11	B	701	PGE	2	0

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.

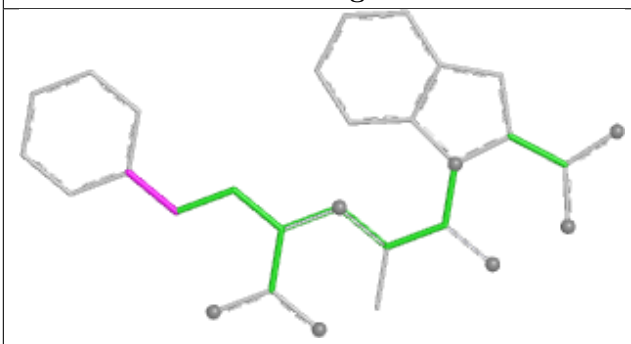
Ligand X93 A 704



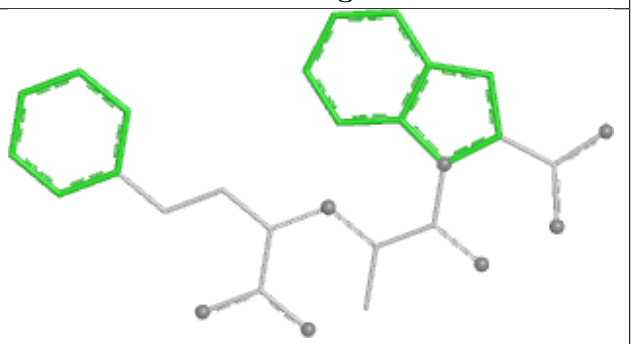
Bond lengths



Bond angles

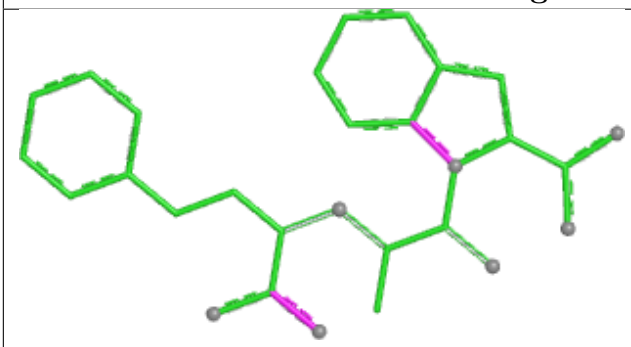


Torsions

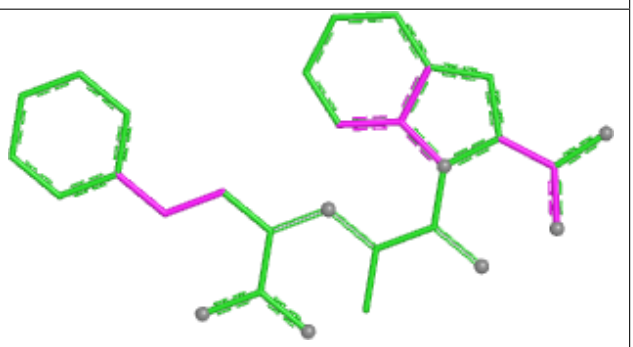


Rings

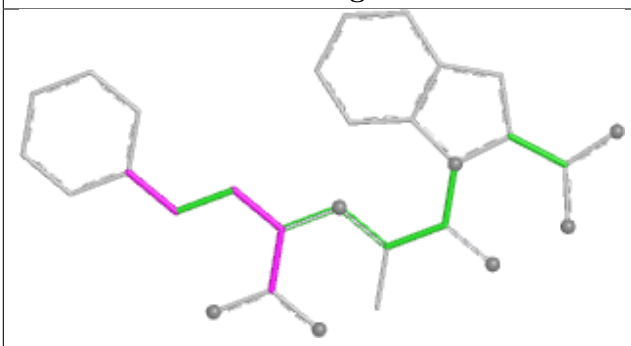
Ligand X93 B 704



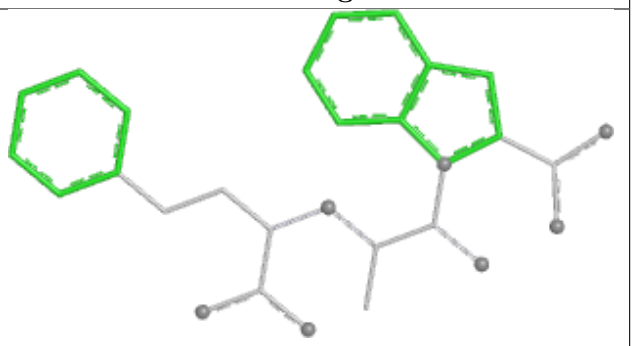
Bond lengths



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	604/609 (99%)	-0.37	5 (0%) 82 80	8, 24, 48, 75	9 (1%)
1	B	603/609 (99%)	0.28	65 (10%) 11 8	11, 34, 76, 104	3 (0%)
All	All	1207/1218 (99%)	-0.05	70 (5%) 29 25	8, 28, 66, 104	12 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	19	LEU	5.3
1	B	67	ALA	4.4
1	B	1	LEU	4.4
1	B	20	PHE	4.2
1	B	15	ALA	4.1
1	B	21	ALA	4.1
1	B	80	TRP	4.0
1	B	378	SER	3.9
1	B	79	ILE	3.9
1	B	92	ILE	3.9
1	B	8	GLY	3.9
1	B	65	ALA	3.9
1	B	78	PRO	3.8
1	A	129	LEU	3.8
1	B	10	PHE	3.8
1	B	5	LEU	3.7
1	B	11	SER	3.5
1	B	83	PHE	3.5
1	B	91	ILE	3.5
1	B	25	GLN	3.5
1	B	82	GLN	3.5
1	A	325	GLY	3.4
1	B	64	PHE	3.4
1	B	56	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	72	ALA	3.4
1	B	17	ALA	3.3
1	B	84	THR	3.3
1	B	4	GLY	3.3
1	B	24	TYR	3.3
1	B	75	LEU	3.2
1	B	135	THR	3.2
1	B	101	ALA	3.2
1	B	129	LEU	3.0
1	B	377	VAL	3.0
1	B	379	LEU	3.0
1	B	13	ASP	2.9
1	B	93	GLY	2.9
1	B	12	ALA	2.8
1	A	135	THR	2.7
1	B	77	GLU	2.6
1	B	16	GLY	2.6
1	B	34	GLN	2.5
1	B	68	TRP	2.5
1	B	88	LEU	2.5
1	B	414	VAL	2.5
1	B	94	ALA	2.5
1	B	86	PRO	2.4
1	B	26	SER	2.4
1	B	375	LEU	2.4
1	B	60	LEU	2.4
1	B	76	TYR	2.4
1	B	2	ASP	2.3
1	B	3	PRO	2.3
1	B	7	PRO	2.3
1	B	9	GLN	2.3
1	B	338	TYR	2.3
1	B	29	GLU	2.3
1	B	95	VAL	2.3
1	B	105	LEU	2.2
1	A	607	TYR	2.2
1	B	18	GLN	2.2
1	B	58	ALA	2.2
1	B	113	ALA	2.2
1	B	59	LEU	2.2
1	B	104	PRO	2.2
1	A	78	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	81	GLN	2.1
1	B	70	GLN	2.1
1	B	73	LYS	2.1
1	B	28	ALA	2.1

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

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

6.3 Carbohydrates (i)

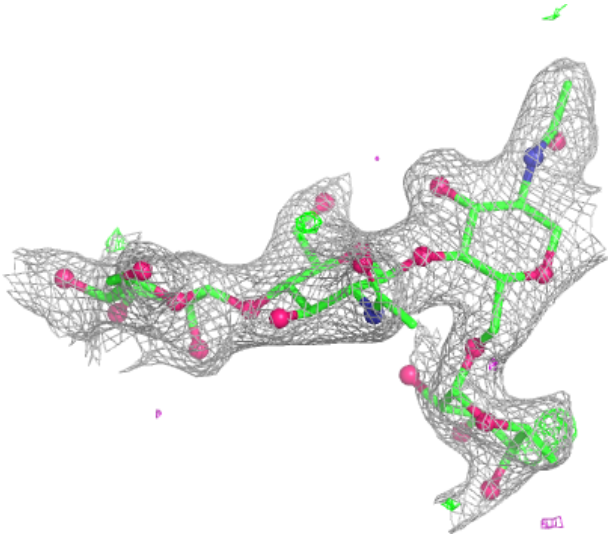
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

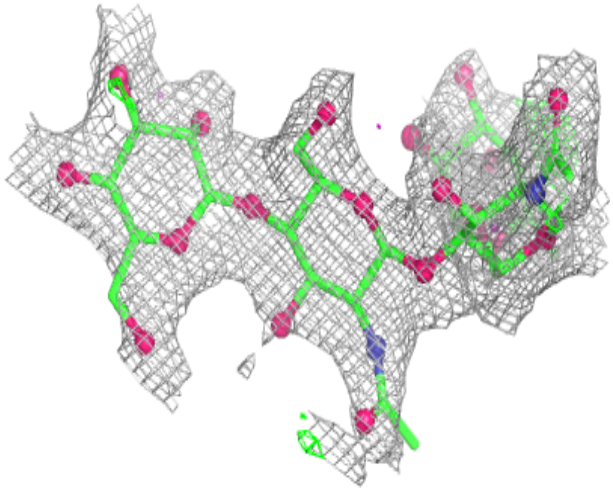
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	F	2	14/15	0.76	0.12	31,37,52,63	0
2	NAG	F	1	14/15	0.83	0.11	25,33,41,41	0
2	BMA	F	3	11/12	-	-	48,54,60,63	0
2	FUC	F	4	10/11	-	-	28,32,34,44	10
3	NAG	G	1	14/15	0.90	0.09	26,35,44,52	0
3	NAG	G	2	14/15	-	-	45,59,65,72	0
3	FUC	G	3	10/11	-	-	45,50,56,57	0
3	NAG	I	1	14/15	-	-	39,51,62,64	0
3	NAG	I	2	14/15	-	-	42,61,64,68	0
3	FUC	I	3	10/11	-	-	54,73,98,109	0
4	NAG	H	1	14/15	-	-	39,50,64,66	0
4	NAG	H	2	14/15	-	-	56,66,84,84	0
5	NAG	J	1	14/15	-	-	25,38,48,61	0
5	FUC	J	2	10/11	-	-	46,71,85,88	0

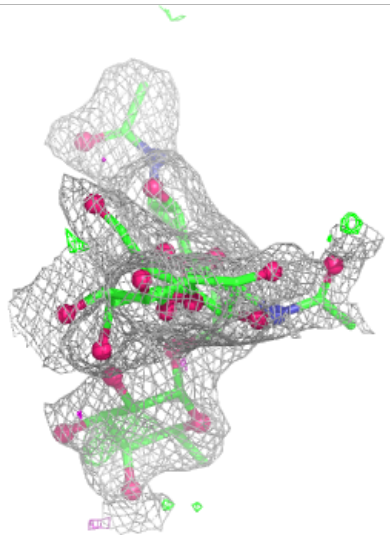
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain F:

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

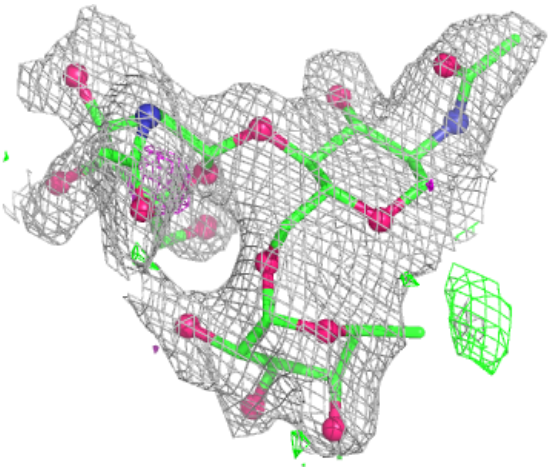


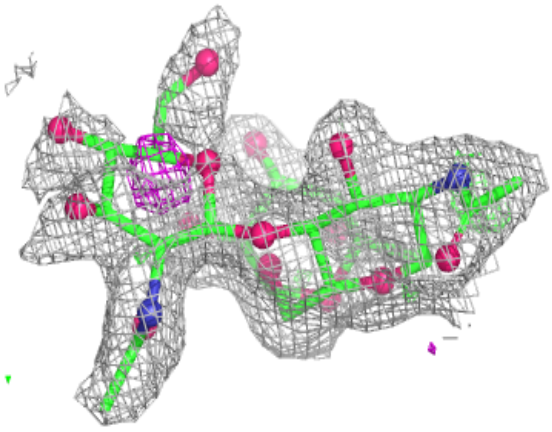


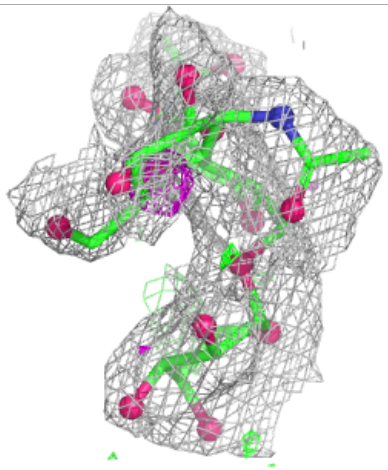


Electron density around Chain G:

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

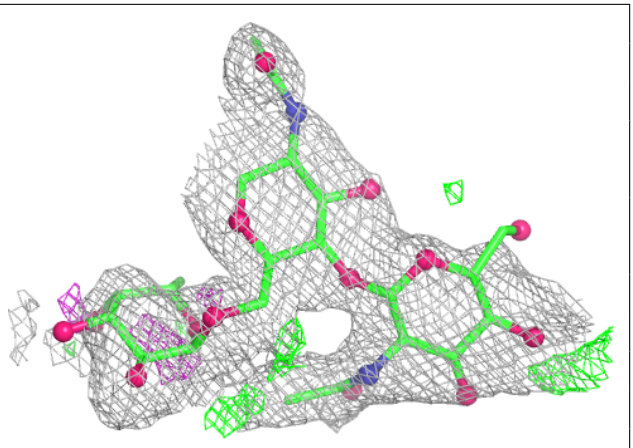


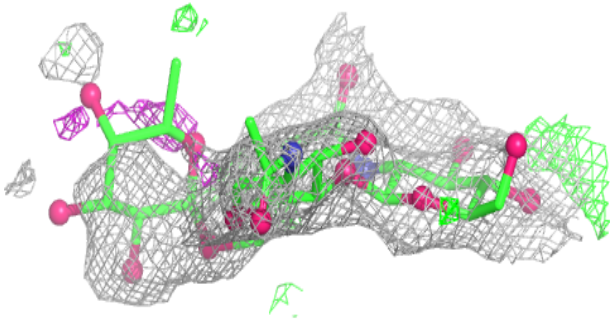


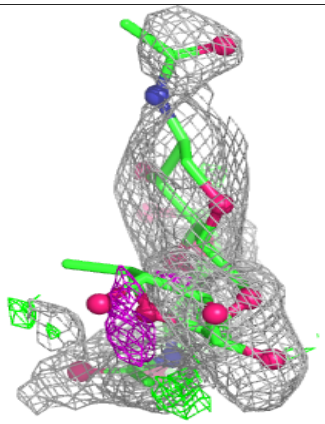


Electron density around Chain I:

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

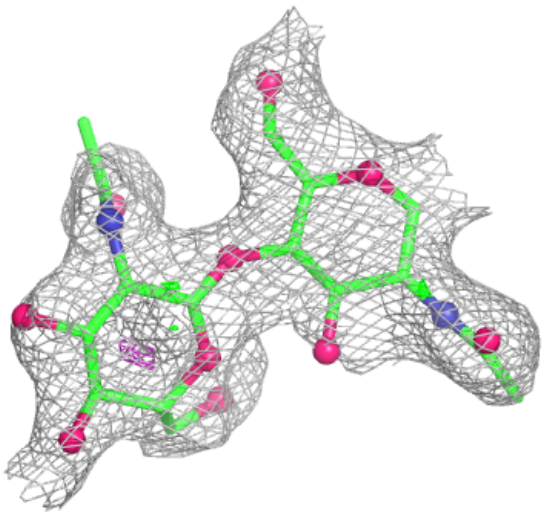


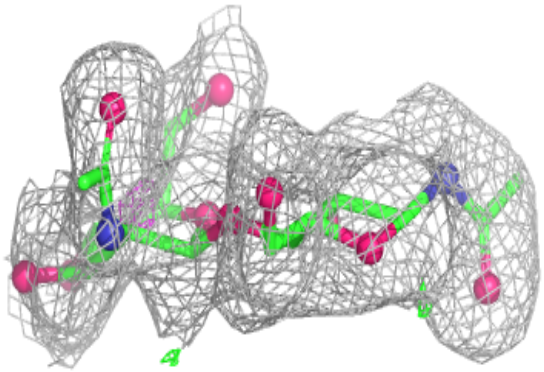


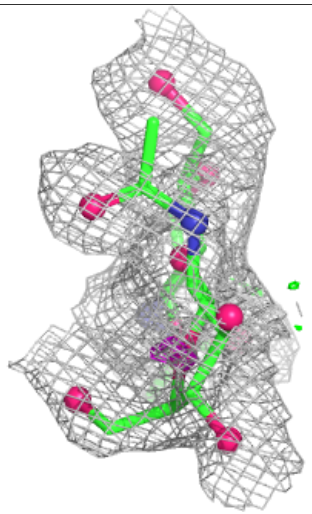


Electron density around Chain H:

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

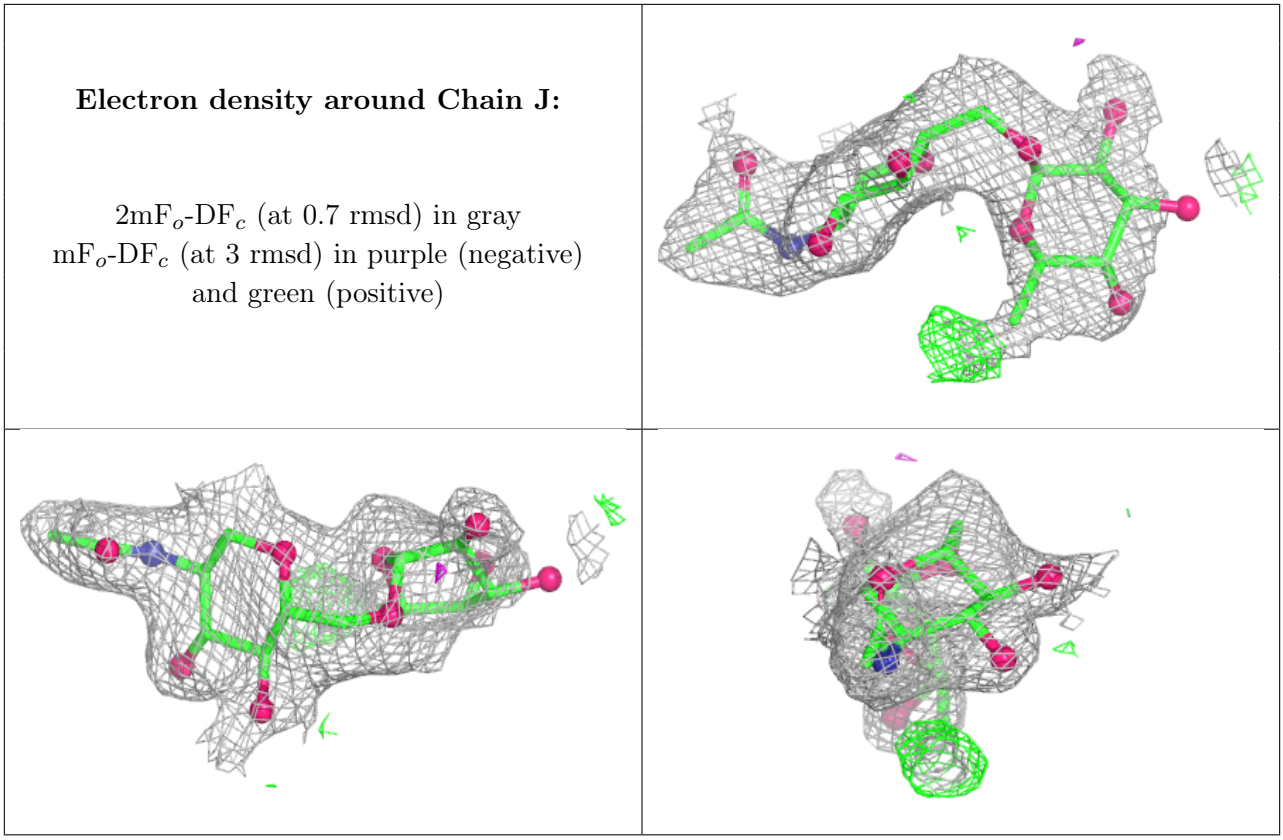






Electron density around Chain J:

$2mF_o$-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
8	PEG	B	703	7/7	0.78	0.15	49,50,56,60	0
10	EDO	A	707	4/4	0.83	0.17	39,42,43,53	0
10	EDO	A	708	4/4	0.85	0.12	48,53,57,59	0
11	PGE	A	709	10/10	0.85	0.15	41,47,58,58	0
11	PGE	B	701	10/10	0.86	0.14	40,42,49,51	0
7	ACT	A	702	4/4	0.88	0.13	29,40,40,44	0
6	PG4	B	705	13/13	0.89	0.12	31,34,50,54	0
10	EDO	A	706	4/4	0.89	0.15	42,43,43,46	0
8	PEG	A	703	7/7	0.89	0.12	39,41,47,50	0
8	PEG	A	710	7/7	0.90	0.14	42,56,71,72	0
8	PEG	B	706	7/7	0.91	0.12	48,50,54,55	0
10	EDO	A	711	4/4	0.92	0.10	46,54,55,57	0
8	PEG	B	702	7/7	0.93	0.10	37,40,44,45	0
10	EDO	A	705	4/4	0.93	0.15	41,43,46,46	0

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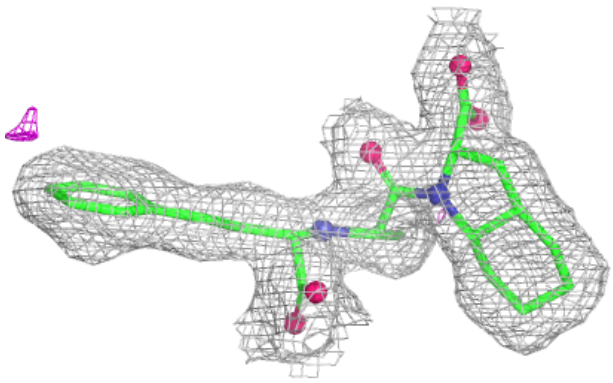
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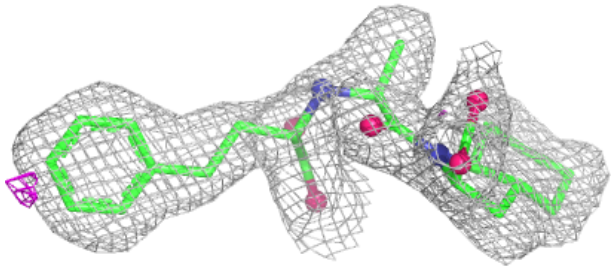
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	CA	A	714	1/1	0.95	0.15	50,50,50,50	0
6	PG4	A	701	13/13	0.96	0.06	22,23,32,35	0
9	X93	A	704	29/29	0.97	0.06	14,17,23,23	0
9	X93	B	704	29/29	0.97	0.06	13,17,29,30	0
14	CA	A	715	1/1	0.97	0.05	50,50,50,50	0
13	CL	B	708	1/1	0.98	0.05	22,22,22,22	0
14	CA	B	709	1/1	0.99	0.04	32,32,32,32	0
12	ZN	B	707	1/1	1.00	0.01	18,18,18,18	0
13	CL	A	713	1/1	1.00	0.02	16,16,16,16	0
12	ZN	A	712	1/1	1.00	0.01	15,15,15,15	0

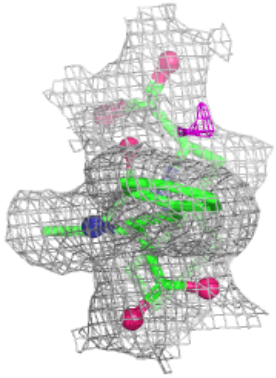
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around X93 A 704:

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

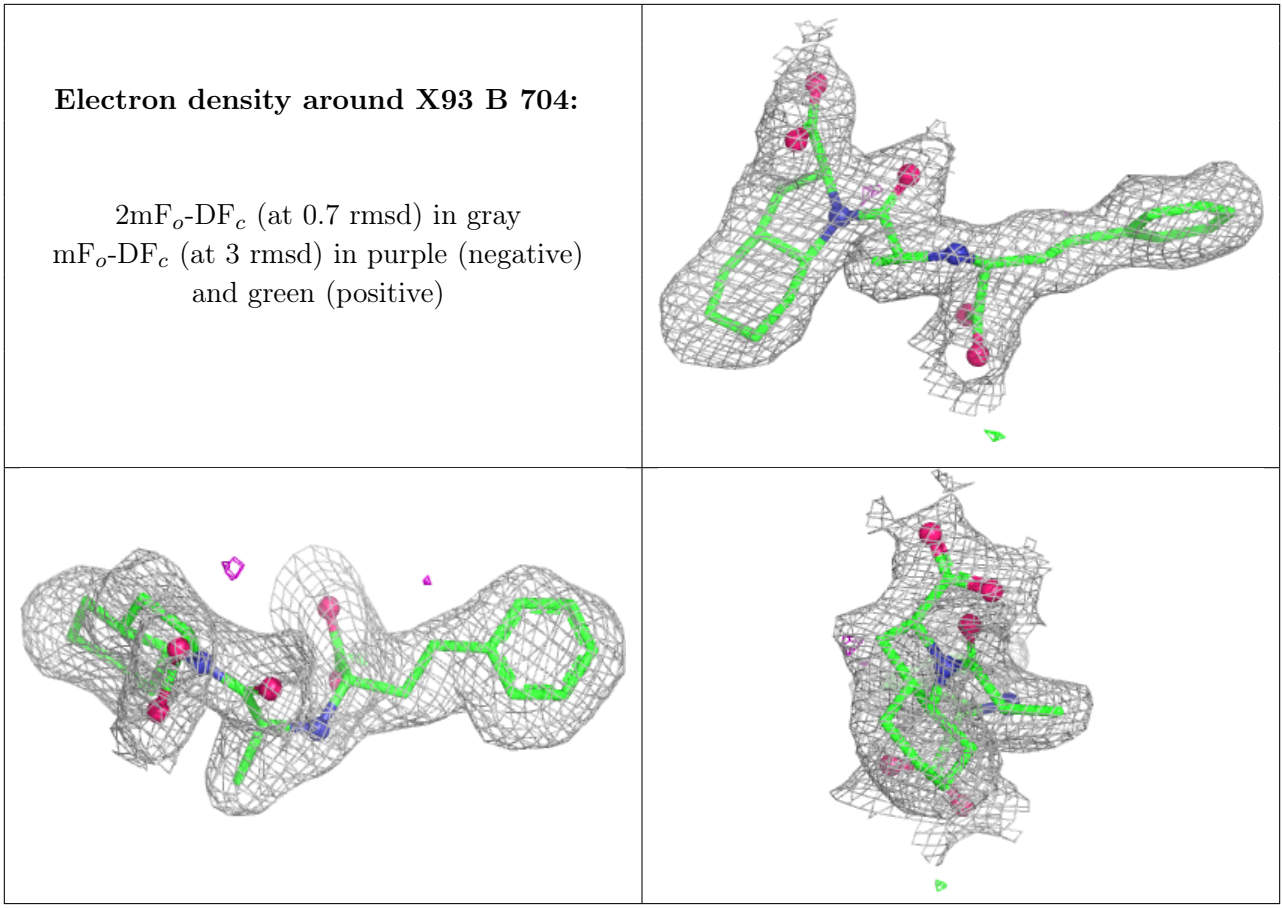






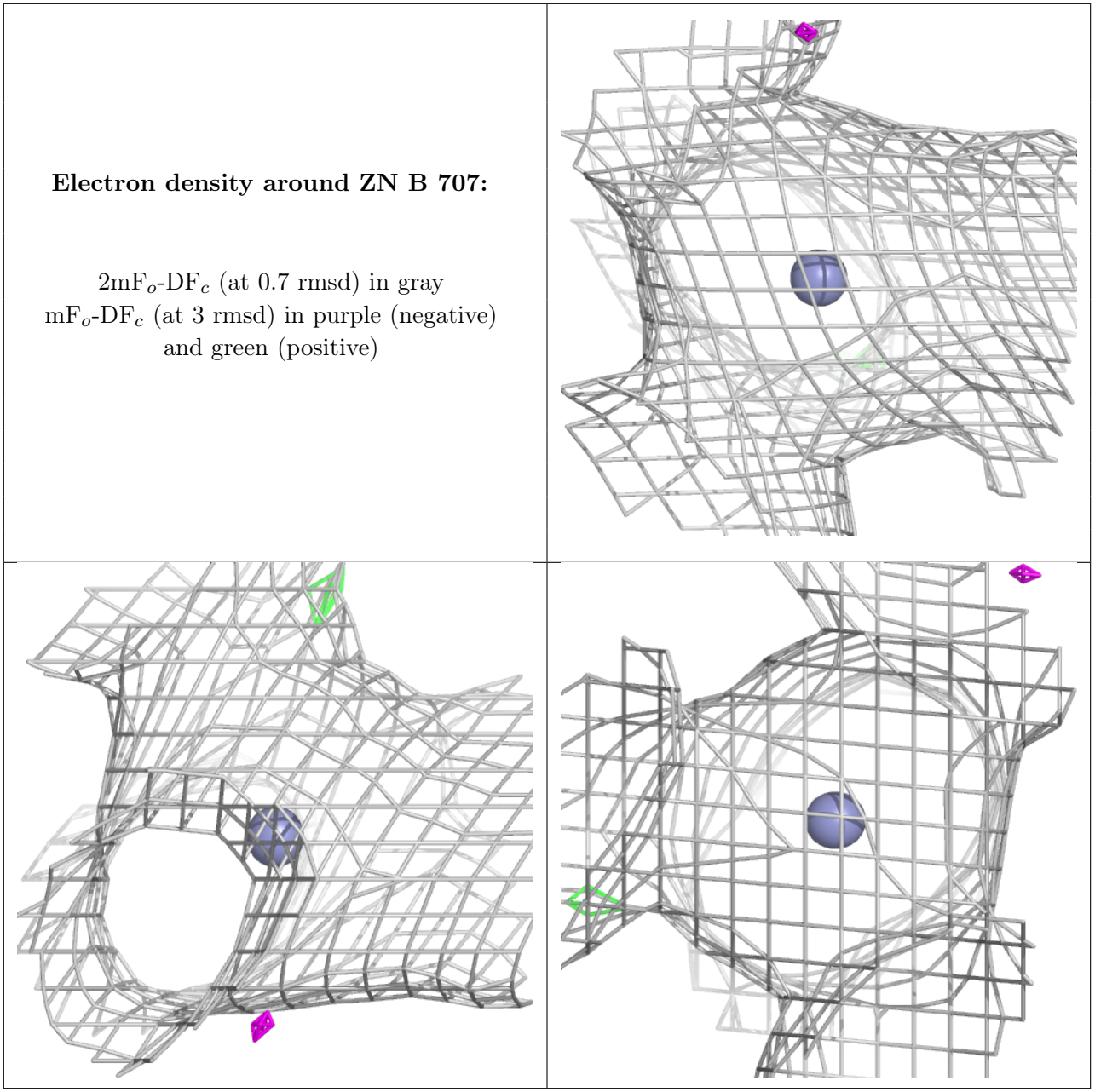
Electron density around X93 B 704:

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



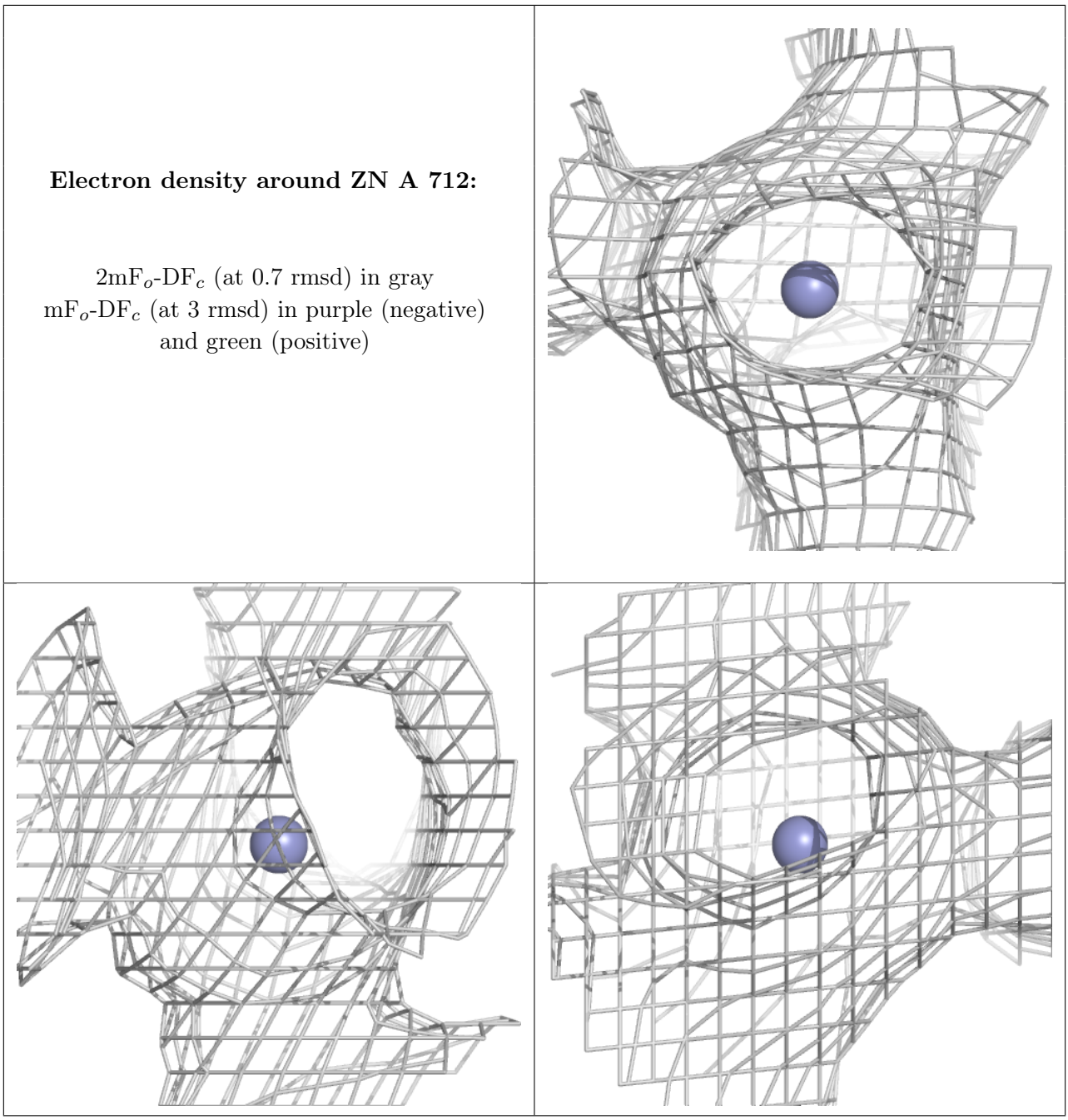
Electron density around ZN B 707:

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



Electron density around ZN A 712:

$2mF_o$-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.