



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2025 – 06:47 pm BST

PDB ID : 8QHL / pdb\_00008qhl  
Title : Human Angiotensin-1 converting enzyme N-domain in complex with the lactotripeptide VPP  
Authors : Gregory, K.S.; Cozier, G.E.; Acharya, K.R.  
Deposited on : 2023-09-08  
Resolution : 1.90 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

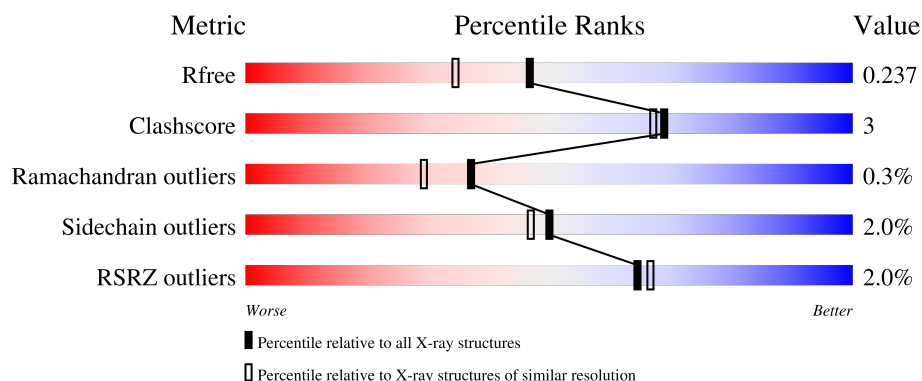
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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  $\geq 3$ , 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	
1	B	628	
2	C	3	
2	D	3	
3	E	2	

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Mol	Chain	Length	Quality of chain
3	F	2	 100%
4	G	4	 50% 50%
5	H	3	 67% 33%
6	I	2	 50% 50%
6	J	2	 50% 50%

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 10738 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	603	Total	C	N	O	S	0	4	0
			4960	3184	850	907	19			
1	A	605	Total	C	N	O	S	0	4	0
			4964	3187	850	908	19			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

- Molecule 2 is a protein called VAL-PRO-PRO.

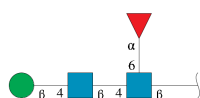
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	0	0	0
			22	15	3	4			
2	C	3	Total	C	N	O	0	0	0
			22	15	3	4			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



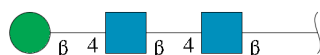
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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
4	G	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



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

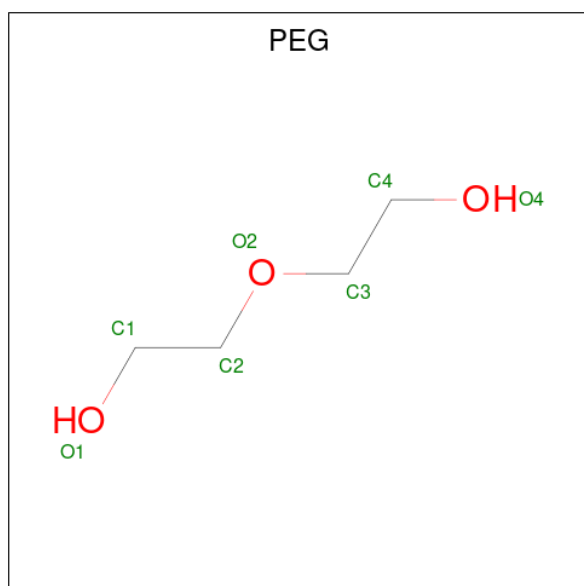
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

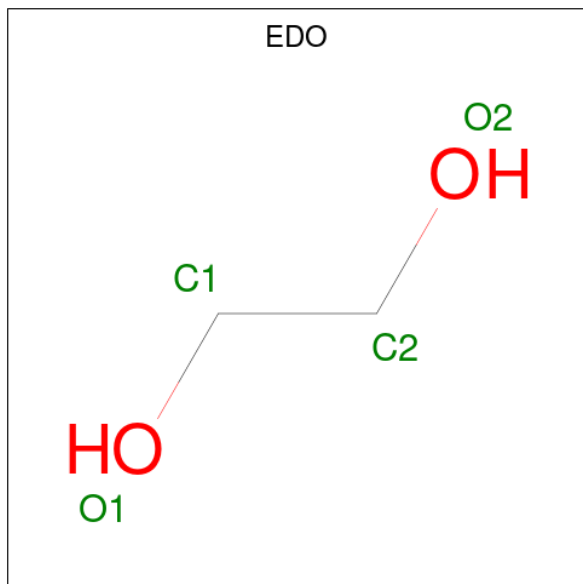
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cl	0	0
			1	1		
8	A	1	Total	Cl	0	0
			1	1		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



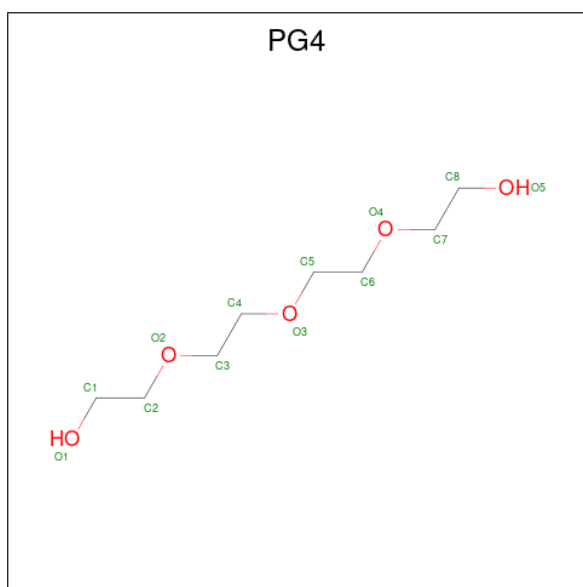
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 7 4 3	0	0
9	B	1	Total C O 7 4 3	0	0
9	B	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0

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



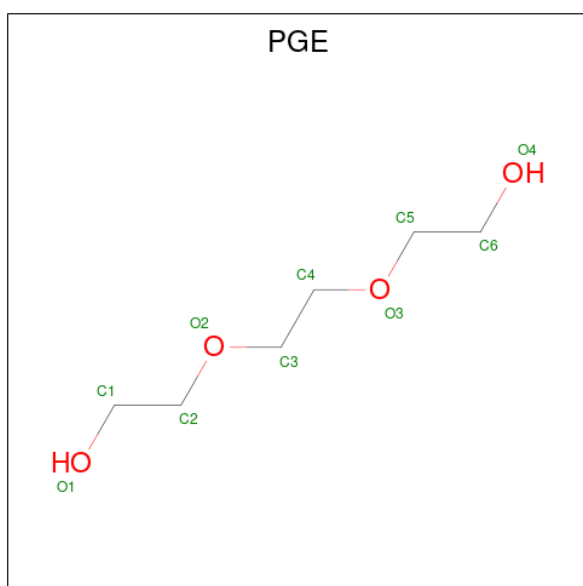
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O 4 2 2	0	0
10	B	1	Total C O 4 2 2	0	0

- Molecule 11 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula:  $C_8H_{18}O_5$ ).



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

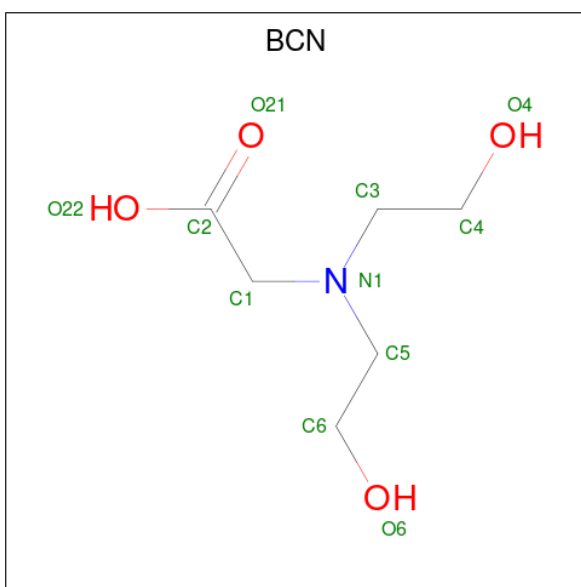
- Molecule 12 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula:  $C_6H_{14}O_4$ ).



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

- Molecule 13 is BICINE (CCD ID: BCN) (formula:  $C_6H_{13}NO_4$ ).



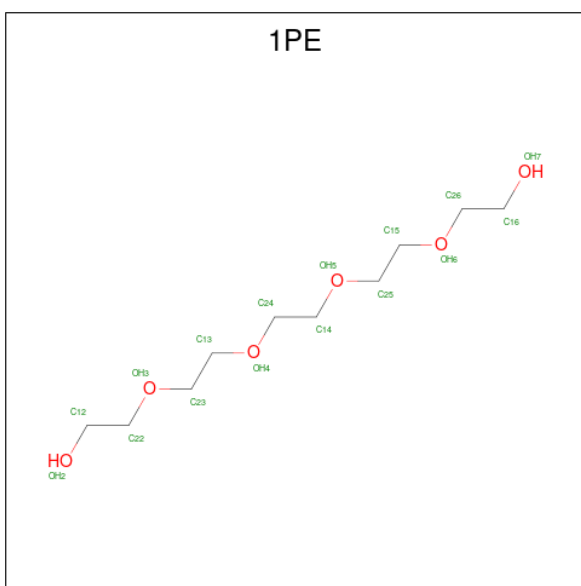


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total	Mg	0	0
			1	1		

- Molecule 15 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	A	1	Total	C	O	0	0
			16	10	6		
15	A	1	Total	C	O	0	0
			16	10	6		

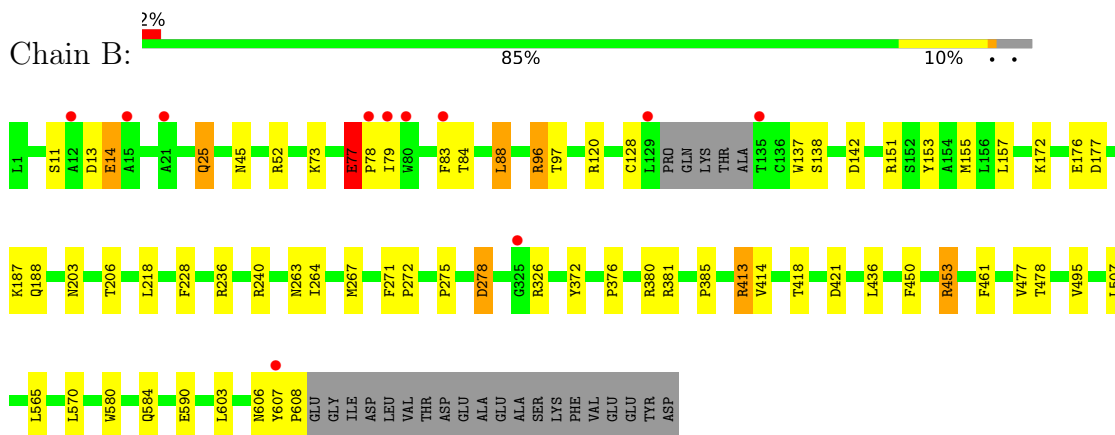
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	B	252	Total	O	0	0
			252	252		
16	D	3	Total	O	0	0
			3	3		
16	A	187	Total	O	0	0
			187	187		
16	C	2	Total	O	0	0
			2	2		

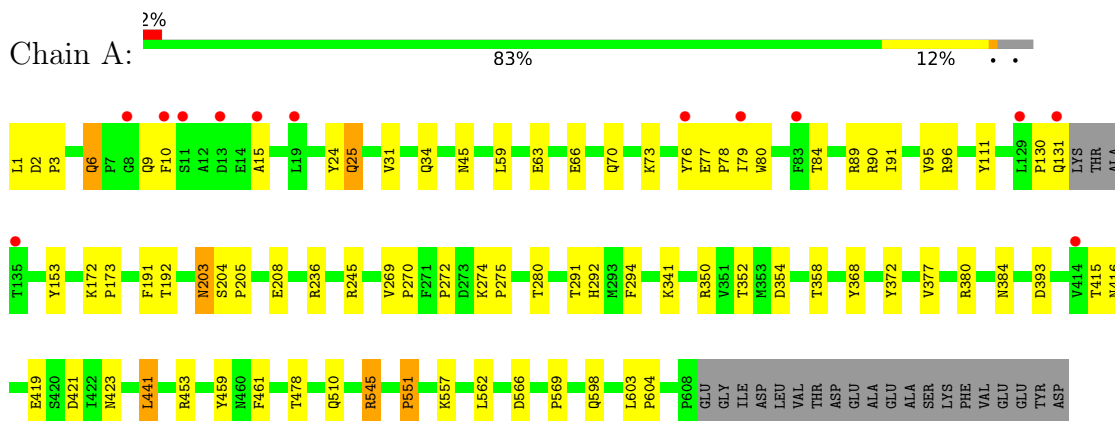
### 3 Residue-property plots [i](#)

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

- Molecule 1: Angiotensin-converting enzyme



- Molecule 1: Angiotensin-converting enzyme



- Molecule 2: VAL-PRO-PRO



There are no outlier residues recorded for this chain.

- Molecule 2: VAL-PRO-PRO



There are no outlier residues recorded for this chain.

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

NAG1  
NAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

NAG1  
NAG2

- Molecule 4: 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 G:  50% 50%

NAG1  
NAG2  
BMA3  
FUC4

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

Chain H:  67% 33%

NAG1  
NAG2  
BMA3

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

Chain I:  50% 50%

NAG1  
FUC2

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

Chain J:  50% 50%

NAG1  
FUC2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.34Å 78.22Å 83.01Å 88.75° 64.70° 75.25°	Depositor
Resolution (Å)	75.27 – 1.90 75.27 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (75.27-1.90) 95.9 (75.27-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, $R_{free}$	0.188 , 0.233 0.190 , 0.237	Depositor DCC
$R_{free}$ test set	6246 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.4	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10738	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, PEG, EDO, ZN, MG, PG4, NAG, 1PE, FUC, BMA, CL, BCN

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	0.84	1/5120 (0.0%)	1.32	25/6975 (0.4%)
1	B	0.93	0/5115	1.36	28/6966 (0.4%)
2	C	1.39	0/23	1.36	0/31
2	D	1.81	0/23	1.80	0/31
All	All	0.89	1/10281 (0.0%)	1.34	53/14003 (0.4%)

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	5
1	B	0	5
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	ALA	C-O	10.45	1.36	1.24

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ASN	CB-CA-C	-10.63	95.38	112.06
1	B	453	ARG	CB-CG-CD	7.86	129.37	111.30
1	B	418	THR	CA-CB-OG1	-7.46	98.42	109.60
1	B	97	THR	CA-CB-OG1	-7.24	98.74	109.60
1	B	84	THR	CA-CB-OG1	-7.13	98.90	109.60
1	B	326	ARG	CB-CG-CD	-6.95	95.31	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	461	PHE	CA-CB-CG	6.88	120.68	113.80
1	B	263	ASN	CA-C-N	-6.79	113.83	122.26
1	B	263	ASN	C-N-CA	-6.79	113.83	122.26
1	A	358	THR	CA-CB-OG1	-6.64	99.63	109.60
1	B	385	PRO	CA-C-N	6.42	127.22	120.03
1	B	385	PRO	C-N-CA	6.42	127.22	120.03
1	B	77	GLU	CB-CG-CD	6.20	123.14	112.60
1	B	203	ASN	CA-CB-CG	-6.17	106.43	112.60
1	A	461	PHE	CA-CB-CG	6.12	119.92	113.80
1	A	545	ARG	CG-CD-NE	-6.11	98.56	112.00
1	B	128	CYS	CA-C-N	5.87	132.26	121.70
1	B	128	CYS	C-N-CA	5.87	132.26	121.70
1	B	153	TYR	CB-CA-C	5.85	120.63	110.68
1	B	478	THR	CA-CB-OG1	-5.76	100.96	109.60
1	A	73	LYS	CA-C-N	5.63	127.83	120.28
1	A	73	LYS	C-N-CA	5.63	127.83	120.28
1	B	236	ARG	CG-CD-NE	-5.62	99.64	112.00
1	B	240	ARG	CB-CA-C	5.56	120.31	110.85
1	B	272	PRO	N-CA-C	5.54	121.12	113.98
1	B	206	THR	CA-CB-OG1	-5.46	101.41	109.60
1	A	423	ASN	CA-CB-CG	5.43	118.03	112.60
1	A	604	PRO	CB-CA-C	-5.42	104.29	111.23
1	A	25	GLN	CB-CA-C	5.42	120.56	109.67
1	B	78	PRO	N-CA-C	5.36	120.62	114.03
1	A	384	ASN	CA-CB-CG	5.35	117.95	112.60
1	A	203	ASN	CA-CB-CG	-5.35	107.25	112.60
1	A	153	TYR	CB-CA-C	5.34	119.35	110.81
1	A	6	GLN	CB-CG-CD	-5.33	103.53	112.60
1	B	590	GLU	CB-CG-CD	5.31	121.63	112.60
1	A	291	THR	CA-CB-OG1	-5.30	101.65	109.60
1	A	421	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	566	ASP	CA-CB-CG	5.24	117.84	112.60
1	B	450	PHE	CA-CB-CG	5.21	119.02	113.80
1	A	393	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	192	THR	CA-CB-OG1	-5.14	101.89	109.60
1	A	111	TYR	N-CA-CB	-5.14	102.56	110.16
1	B	188	GLN	CB-CG-CD	-5.13	103.88	112.60
1	B	271	PHE	CB-CA-C	5.08	118.90	110.87
1	A	84	THR	CB-CA-C	5.05	119.27	110.79
1	B	278	ASP	CB-CA-C	5.04	119.13	110.81
1	A	459	TYR	CA-CB-CG	5.04	122.97	113.90
1	B	421	ASP	CA-CB-CG	5.04	117.64	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	551	PRO	CB-CA-C	-5.03	105.18	111.56
1	A	294	PHE	CB-CA-C	5.02	118.77	110.88
1	B	385	PRO	N-CA-C	5.01	120.50	113.53
1	A	208	GLU	CA-C-N	5.00	127.30	120.54
1	A	208	GLU	C-N-CA	5.00	127.30	120.54

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	350	ARG	Sidechain
1	A	380	ARG	Sidechain
1	A	453	ARG	Sidechain
1	A	545	ARG	Sidechain
1	A	89	ARG	Sidechain
1	B	120	ARG	Sidechain
1	B	151	ARG	Sidechain
1	B	380	ARG	Sidechain
1	B	453	ARG	Sidechain
1	B	96	ARG	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4964	0	4732	29	0
1	B	4960	0	4730	30	0
2	C	22	0	22	0	0
2	D	22	0	22	0	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
4	G	49	0	44	1	0
5	H	39	0	34	1	0
6	I	24	0	22	1	0
6	J	24	0	22	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	21	0	30	1	0
9	B	21	0	30	2	0
10	B	8	0	12	2	0
11	A	13	0	18	2	0
11	B	13	0	18	1	0
12	B	10	0	14	0	0
13	A	11	0	12	1	0
14	A	1	0	0	0	0
15	A	32	0	44	5	0
16	A	187	0	0	4	0
16	B	252	0	0	1	0
16	C	2	0	0	0	0
16	D	3	0	0	0	0
All	All	10738	0	9856	68	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (68) 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)
5:H:1:NAG:H62	5:H:2:NAG:H82	1.52	0.90
1:A:292:HIS:NE2	15:A:708:1PE:H121	1.90	0.86
1:A:66:GLU:O	1:A:70:GLN:HG3	1.90	0.72
1:B:381:ARG:HH11	10:B:705:EDO:H12	1.57	0.70
1:B:88:LEU:O	1:B:88:LEU:HD23	1.93	0.68
1:A:1:LEU:HD23	1:A:6:GLN:HG3	1.76	0.67
1:B:275:PRO:HD3	1:B:413:ARG:CZ	2.25	0.66
1:A:270:PRO:O	1:A:272:PRO:HD3	1.95	0.65
1:A:292:HIS:CD2	15:A:708:1PE:H121	2.33	0.64
1:B:73:LYS:HG3	1:B:96:ARG:HG3	1.81	0.63
1:B:83:PHE:CD2	1:B:88:LEU:HD22	2.33	0.63
1:A:91:ILE:O	1:A:95:VAL:HG23	1.99	0.62
11:A:707:PG4:H22	16:A:833:HOH:O	1.99	0.62
15:A:708:1PE:H252	16:A:977:HOH:O	2.00	0.61
1:A:191:PHE:CZ	9:A:703:PEG:H31	2.37	0.60
1:B:52:ARG:HH11	1:B:52:ARG:HG2	1.68	0.59
15:A:708:1PE:H162	16:A:979:HOH:O	2.04	0.58
1:B:228:PHE:CZ	9:B:706:PEG:H32	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.85	0.57
1:B:137:TRP:CH2	1:B:155:MET:HE1	2.43	0.54
1:B:570:LEU:C	1:B:570:LEU:HD23	2.32	0.54
1:A:130:PRO:O	1:A:131:GLN:HB2	2.08	0.54
1:A:59:LEU:O	1:A:63:GLU:HG3	2.07	0.53
1:B:77:GLU:OE2	1:B:96:ARG:HD2	2.07	0.53
1:B:13:ASP:OD1	1:B:13:ASP:C	2.52	0.53
1:A:236:ARG:HH21	1:A:236:ARG:HG3	1.74	0.53
1:B:25:GLN:OE1	1:B:376:PRO:HA	2.10	0.52
1:B:79:ILE:O	1:B:79:ILE:HG22	2.11	0.50
1:A:24:TYR:HD2	1:A:25:GLN:HG3	1.76	0.50
1:A:77:GLU:OE2	1:A:96:ARG:HD2	2.11	0.50
1:A:31:VAL:O	1:A:34:GLN:HG3	2.12	0.49
1:A:510:GLN:HG2	1:A:569:PRO:HG2	1.94	0.49
11:B:707:PG4:H42	11:B:707:PG4:H21	1.48	0.48
1:A:478:THR:CG2	6:J:2:FUC:H63	2.43	0.48
1:B:83:PHE:HD2	1:B:88:LEU:HD22	1.76	0.48
13:A:704:BCN:O21	13:A:704:BCN:H61	2.13	0.47
1:B:477:VAL:HG12	1:B:603:LEU:HD21	1.97	0.47
1:B:187:LYS:HE3	1:B:187:LYS:HB2	1.65	0.47
10:B:704:EDO:O2	9:B:708:PEG:H12	2.15	0.46
1:A:274:LYS:HB3	1:A:275:PRO:CD	2.46	0.46
1:A:441:LEU:HD12	1:A:441:LEU:C	2.40	0.46
1:A:2:ASP:OD1	1:A:3:PRO:HD2	2.17	0.45
1:A:341:LYS:HE3	1:A:341:LYS:HB2	1.66	0.45
1:B:580:TRP:O	1:B:584:GLN:HG2	2.17	0.44
1:B:88:LEU:HD23	1:B:88:LEU:C	2.43	0.44
1:B:177:ASP:OD1	16:B:801:HOH:O	2.21	0.43
1:A:557:LYS:HA	1:A:562:LEU:O	2.19	0.43
4:G:1:NAG:C6	4:G:4:FUC:C1	2.90	0.43
1:B:138:SER:O	1:B:142:ASP:HB2	2.19	0.42
1:B:14:GLU:HB2	1:B:83:PHE:CD1	2.55	0.42
11:A:707:PG4:C2	16:A:833:HOH:O	2.65	0.42
1:B:507:LEU:HD13	1:B:565:LEU:CD2	2.49	0.42
1:B:77:GLU:OE2	1:B:77:GLU:HA	2.20	0.42
1:B:495:VAL:HG12	1:B:495:VAL:O	2.20	0.42
1:A:172:LYS:HB3	1:A:173:PRO:HD3	2.02	0.42
1:A:9:GLN:C	1:A:10:PHE:CD1	2.98	0.41
1:B:137:TRP:CZ3	1:B:155:MET:HE1	2.55	0.41
1:A:90:ARG:NH1	1:A:551:PRO:HA	2.35	0.41
1:B:172:LYS:O	1:B:176[A]:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:THR:HG23	1:A:352:THR:HA	2.02	0.41
1:A:76:TYR:O	1:A:80:TRP:HD1	2.02	0.41
1:A:204:SER:HA	1:A:205:PRO:HD2	1.88	0.41
1:B:607:TYR:HA	1:B:608:PRO:HA	1.85	0.40
1:A:292:HIS:NE2	15:A:708:1PE:C12	2.74	0.40
1:B:264:ILE:HB	1:B:267:MET:HE3	2.04	0.40
1:B:218:LEU:HD13	1:B:436:LEU:HD13	2.03	0.40
1:A:245:ARG:NH1	6:I:1:NAG:H82	2.36	0.40
1:A:603:LEU:HD22	1:A:603:LEU:H	1.87	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	605/628 (96%)	588 (97%)	14 (2%)	3 (0%)	25	17
1	B	603/628 (96%)	589 (98%)	13 (2%)	1 (0%)	44	36
2	C	1/3 (33%)	1 (100%)	0	0	100	100
2	D	1/3 (33%)	1 (100%)	0	0	100	100
All	All	1210/1262 (96%)	1179 (97%)	27 (2%)	4 (0%)	37	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	416	ASN
1	B	45	ASN
1	A	78	PRO

### 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	524/540 (97%)	513 (98%)	11 (2%)	48	45
1	B	523/540 (97%)	513 (98%)	10 (2%)	52	49
2	C	3/3 (100%)	3 (100%)	0	100	100
2	D	3/3 (100%)	3 (100%)	0	100	100
All	All	1053/1086 (97%)	1032 (98%)	21 (2%)	50	47

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	11	SER
1	B	14	GLU
1	B	25	GLN
1	B	77	GLU
1	B	88	LEU
1	B	278	ASP
1	B	372	TYR
1	B	413	ARG
1	B	414	VAL
1	B	606	ASN
1	A	79	ILE
1	A	203	ASN
1	A	269	VAL
1	A	354	ASP
1	A	368	TYR
1	A	372	TYR
1	A	377	VAL
1	A	415	THR
1	A	419	GLU
1	A	441	LEU
1	A	598	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	87	GLN
1	A	25	GLN
1	A	87	GLN
1	A	600	HIS

### 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 ⓘ

15 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	$\# Z  > 2$
3	NAG	E	1	1,3	14,14,15	0.51	0	17,19,21	1.41	2 (11%)
3	NAG	E	2	3	14,14,15	0.59	0	17,19,21	1.56	3 (17%)
3	NAG	F	1	1,3	14,14,15	0.49	0	17,19,21	1.27	3 (17%)
3	NAG	F	2	3	14,14,15	0.57	0	17,19,21	1.52	2 (11%)
4	NAG	G	1	1,4	14,14,15	0.51	0	17,19,21	1.32	2 (11%)
4	NAG	G	2	4	14,14,15	0.43	0	17,19,21	1.69	3 (17%)
4	BMA	G	3	4	11,11,12	0.98	1 (9%)	15,15,17	1.18	1 (6%)
4	FUC	G	4	4	10,10,11	0.61	0	14,14,16	1.66	3 (21%)
5	NAG	H	1	1,5	14,14,15	0.46	0	17,19,21	1.79	2 (11%)
5	NAG	H	2	5	14,14,15	0.53	0	17,19,21	0.74	0
5	BMA	H	3	5	11,11,12	0.86	0	15,15,17	0.88	1 (6%)
6	NAG	I	1	1,6	14,14,15	0.61	0	17,19,21	1.34	2 (11%)
6	FUC	I	2	6	10,10,11	0.98	1 (10%)	14,14,16	1.88	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	J	1	1,6	14,14,15	0.41	0	17,19,21	1.20	2 (11%)
6	FUC	J	2	6	10,10,11	0.82	1 (10%)	14,14,16	1.76	3 (21%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3	BMA	C2-C3	2.29	1.55	1.52
6	J	2	FUC	C2-C3	2.16	1.55	1.52
6	I	2	FUC	C4-C3	2.15	1.57	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1	NAG	C1-C2-N2	5.68	120.19	110.49
4	G	2	NAG	C1-C2-N2	4.66	118.45	110.49
3	F	2	NAG	O5-C1-C2	4.53	118.44	111.29
3	E	2	NAG	C2-N2-C7	4.43	129.21	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	2	FUC	C3-C4-C5	-4.30	103.08	109.77
3	E	1	NAG	C1-O5-C5	3.98	117.58	112.19
4	G	2	NAG	C1-O5-C5	3.91	117.49	112.19
6	I	2	FUC	O3-C3-C2	-3.73	102.86	109.99
5	H	1	NAG	C1-O5-C5	3.56	117.01	112.19
3	E	1	NAG	C2-N2-C7	3.46	127.83	122.90
6	I	2	FUC	O3-C3-C4	3.38	118.17	110.35
4	G	4	FUC	O5-C1-C2	3.36	115.95	110.77
4	G	1	NAG	C1-O5-C5	3.35	116.73	112.19
6	I	2	FUC	O4-C4-C3	3.25	117.87	110.35
4	G	3	BMA	C1-C2-C3	3.15	113.54	109.67
3	F	1	NAG	C1-O5-C5	2.93	116.16	112.19
4	G	4	FUC	C1-O5-C5	2.87	119.29	112.78
6	J	2	FUC	O3-C3-C2	2.75	115.26	109.99
3	E	2	NAG	O5-C1-C2	-2.71	107.02	111.29
3	E	2	NAG	C1-O5-C5	2.60	115.71	112.19
6	J	1	NAG	C1-C2-N2	2.51	114.77	110.49
6	I	1	NAG	O5-C1-C2	-2.50	107.35	111.29
3	F	1	NAG	C4-C3-C2	2.48	114.65	111.02
4	G	2	NAG	O3-C3-C2	-2.45	104.39	109.47
6	J	1	NAG	C2-N2-C7	2.44	126.37	122.90
4	G	1	NAG	C1-C2-N2	-2.35	106.48	110.49
3	F	1	NAG	O5-C1-C2	-2.33	107.61	111.29
6	I	1	NAG	C3-C4-C5	-2.26	106.21	110.24
6	J	2	FUC	O2-C2-C3	-2.22	105.69	110.14
6	I	2	FUC	O2-C2-C1	2.14	113.52	109.15
5	H	3	BMA	C1-C2-C3	2.13	112.28	109.67
3	F	2	NAG	C2-N2-C7	2.09	125.88	122.90
4	G	4	FUC	O2-C2-C3	2.05	114.24	110.14

There are no chirality outliers.

All (29) torsion outliers are listed below:

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

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

There are no ring outliers.

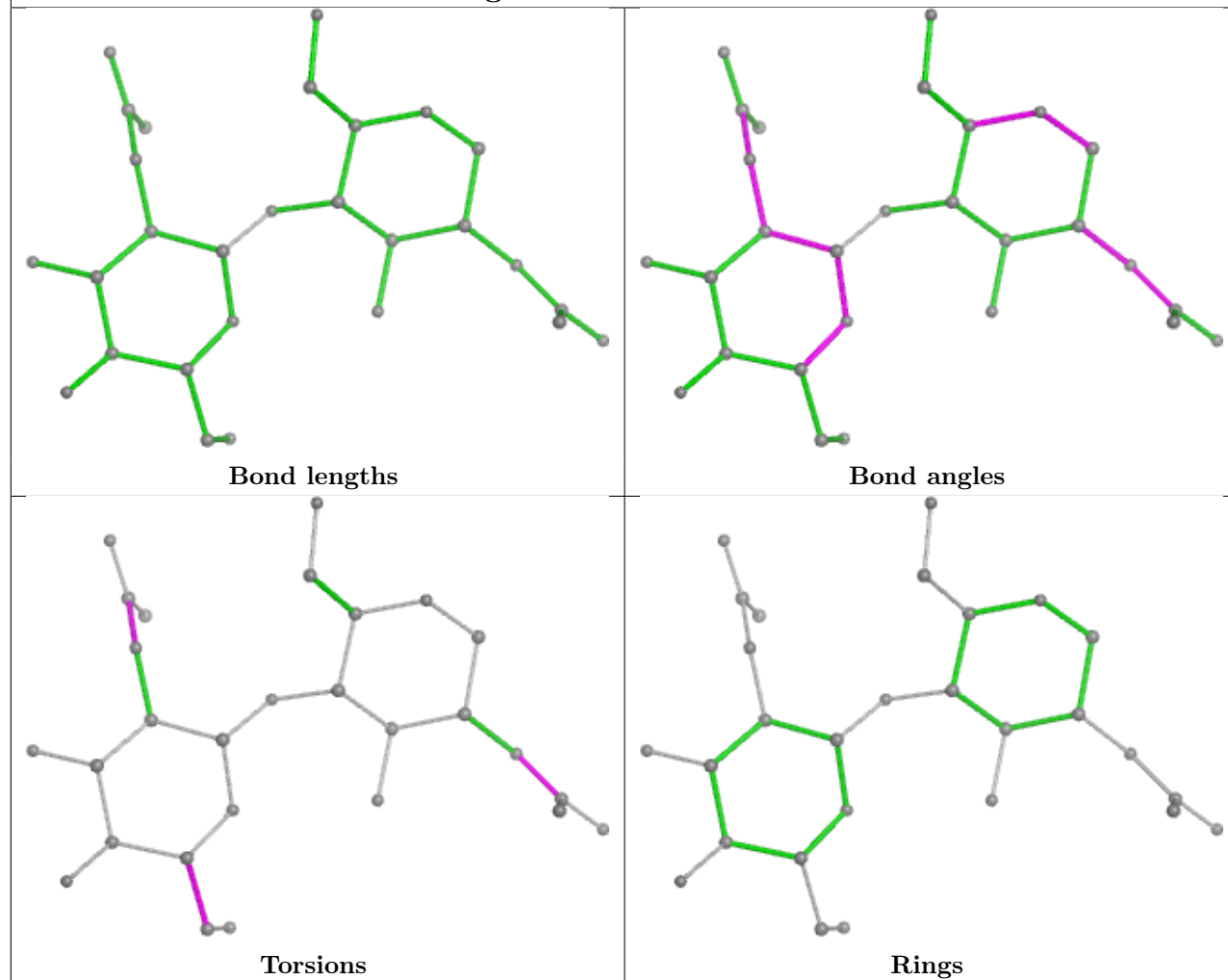
6 monomers are involved in 4 short contacts:

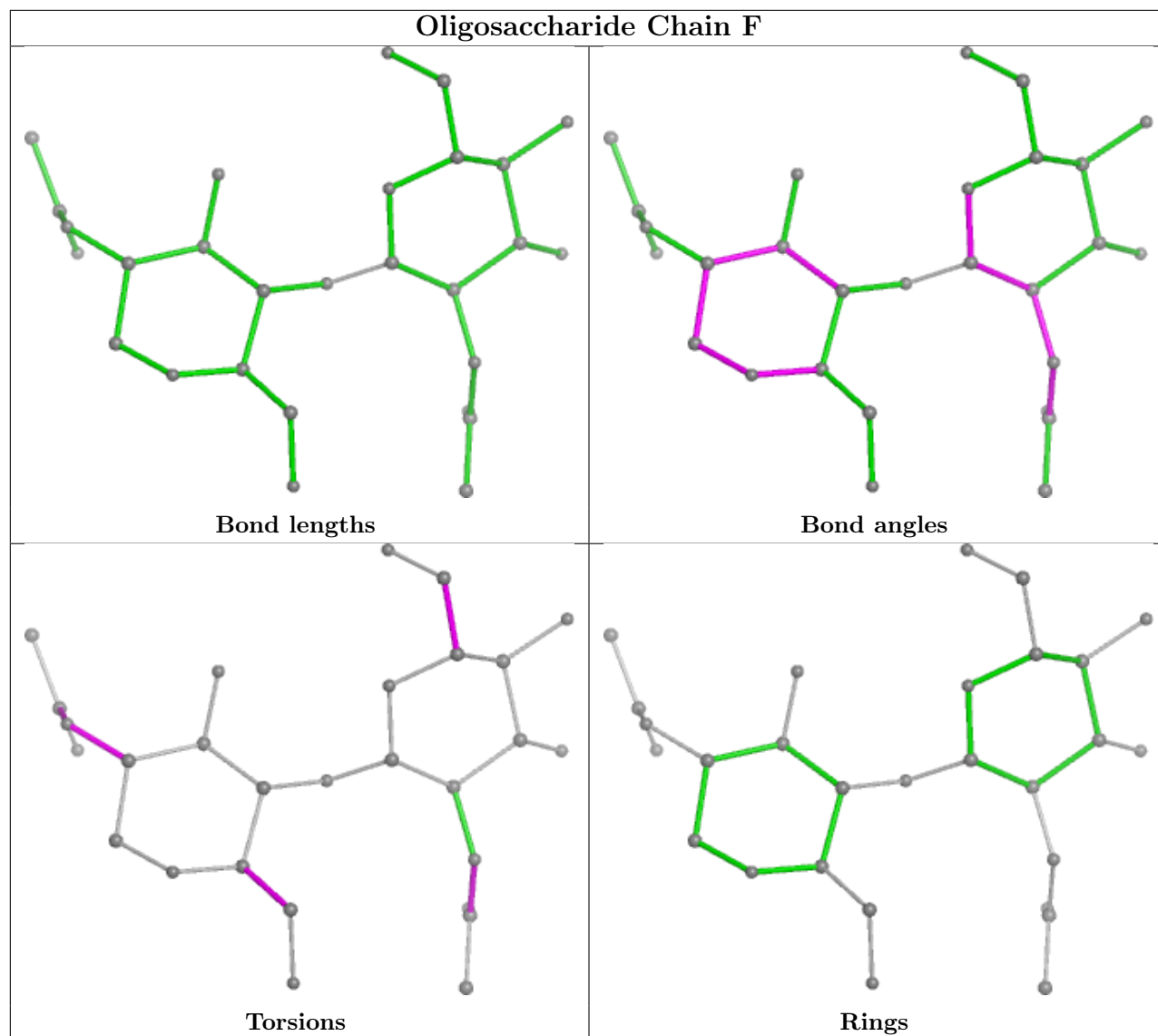
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	2	NAG	1	0
4	G	1	NAG	1	0
4	G	4	FUC	1	0
5	H	1	NAG	1	0
6	I	1	NAG	1	0
6	J	2	FUC	1	0

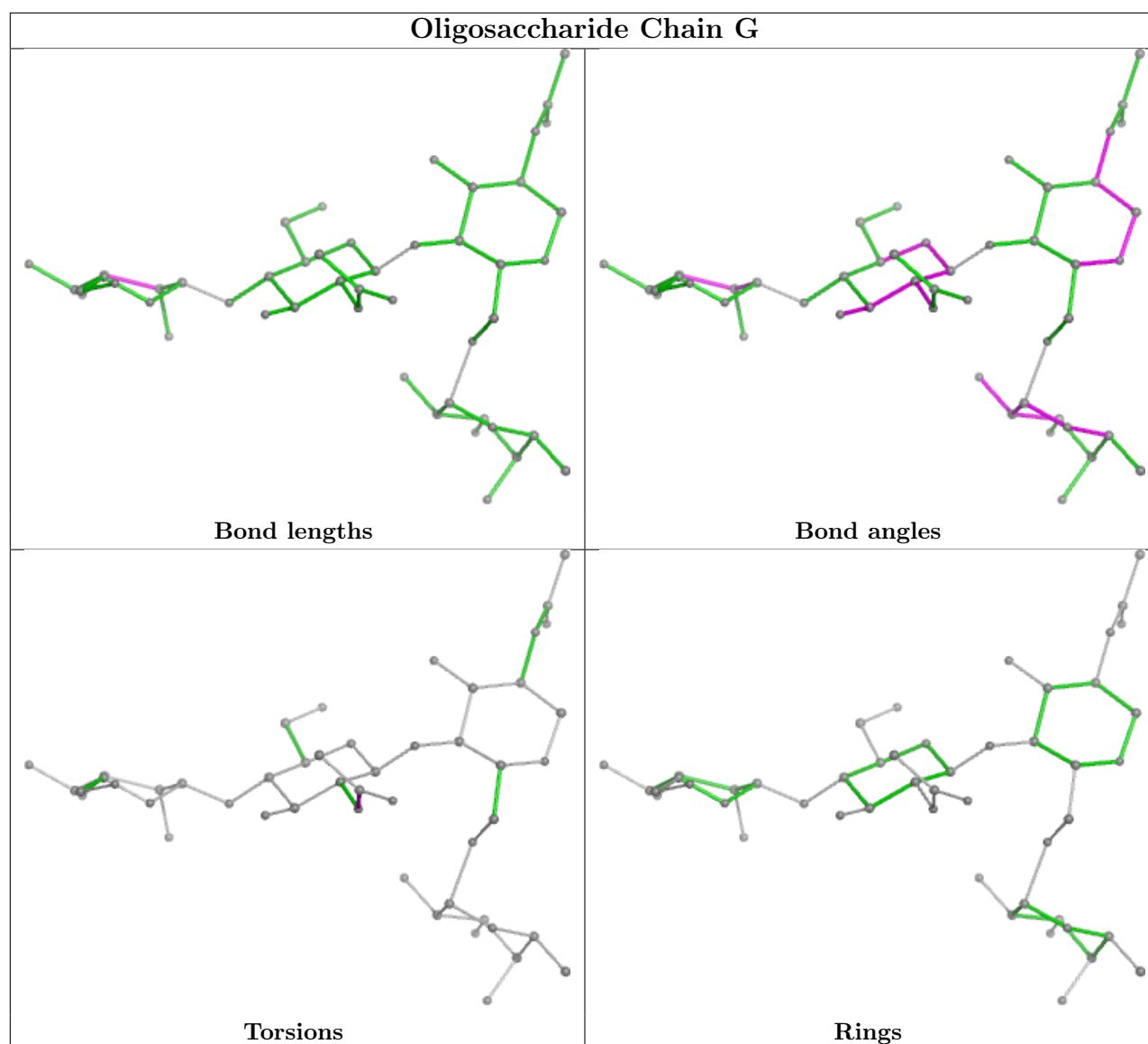
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

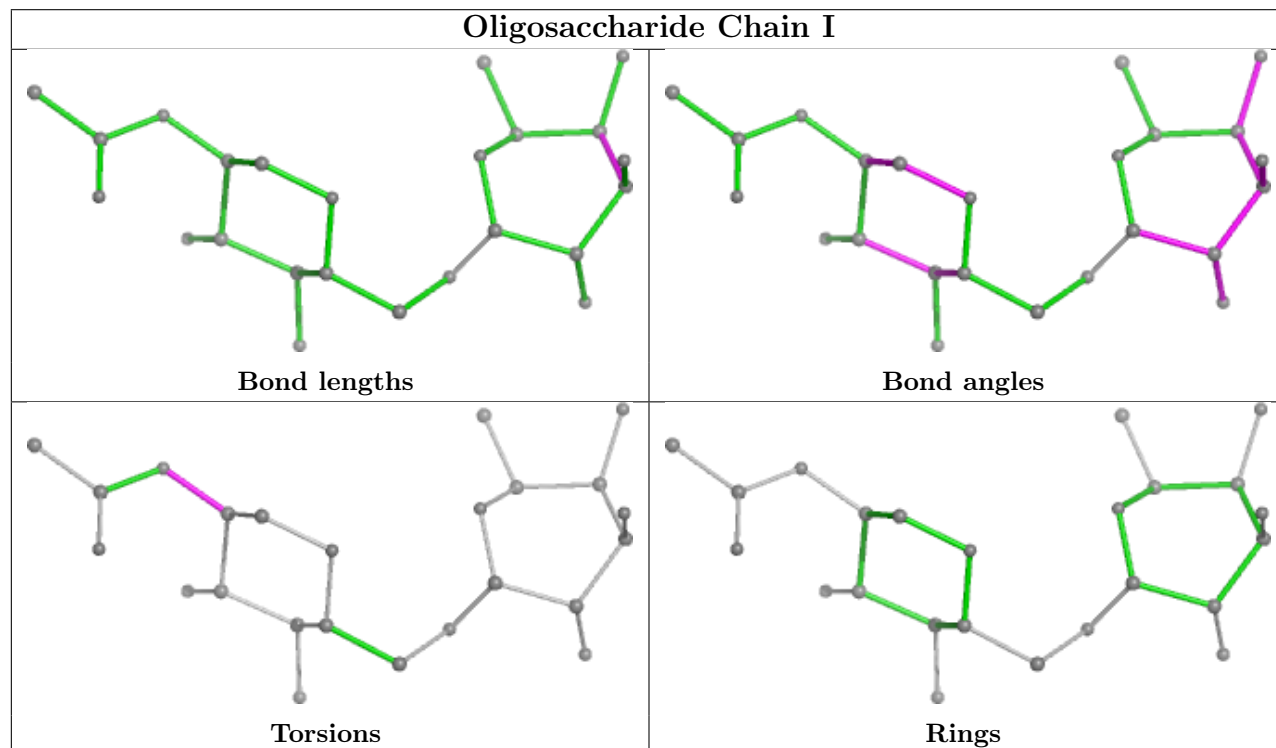
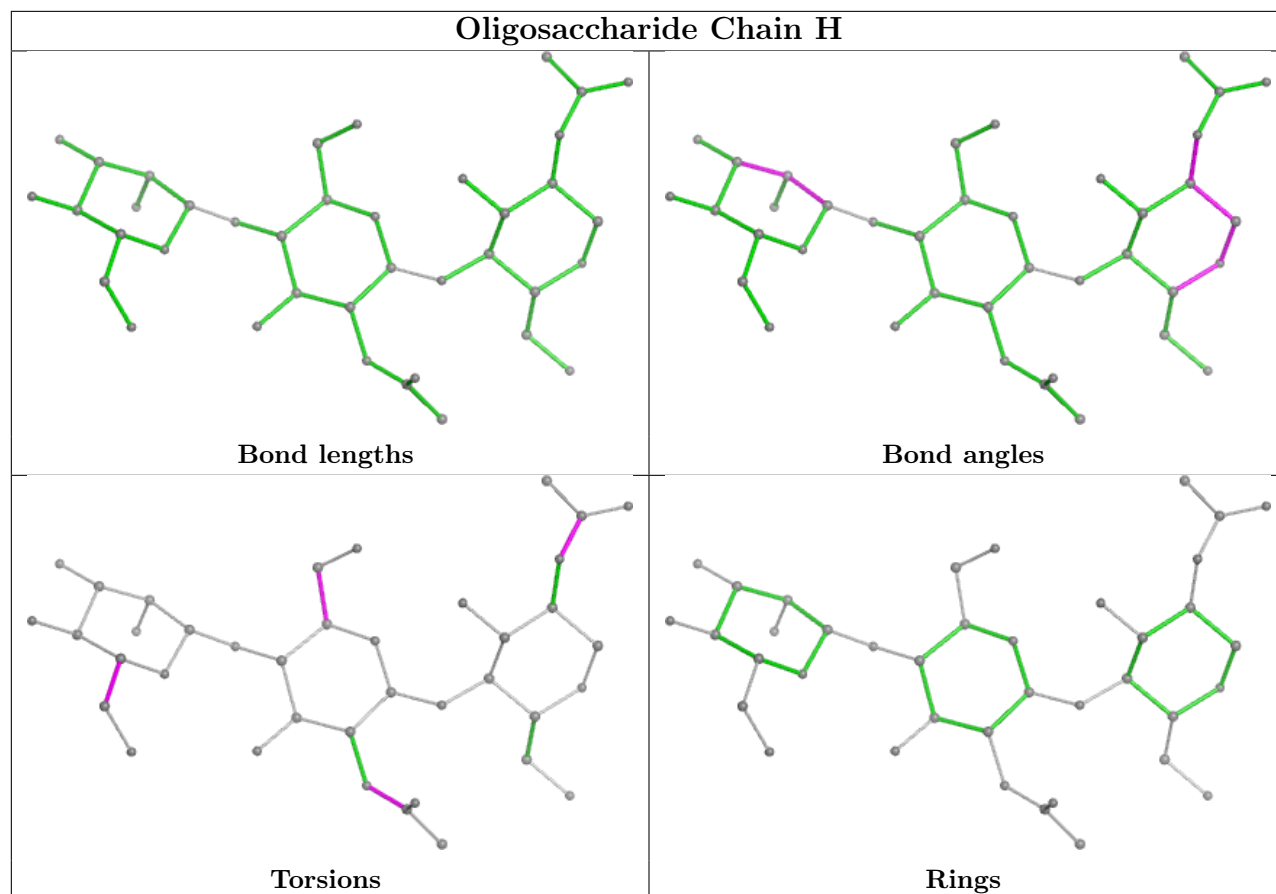


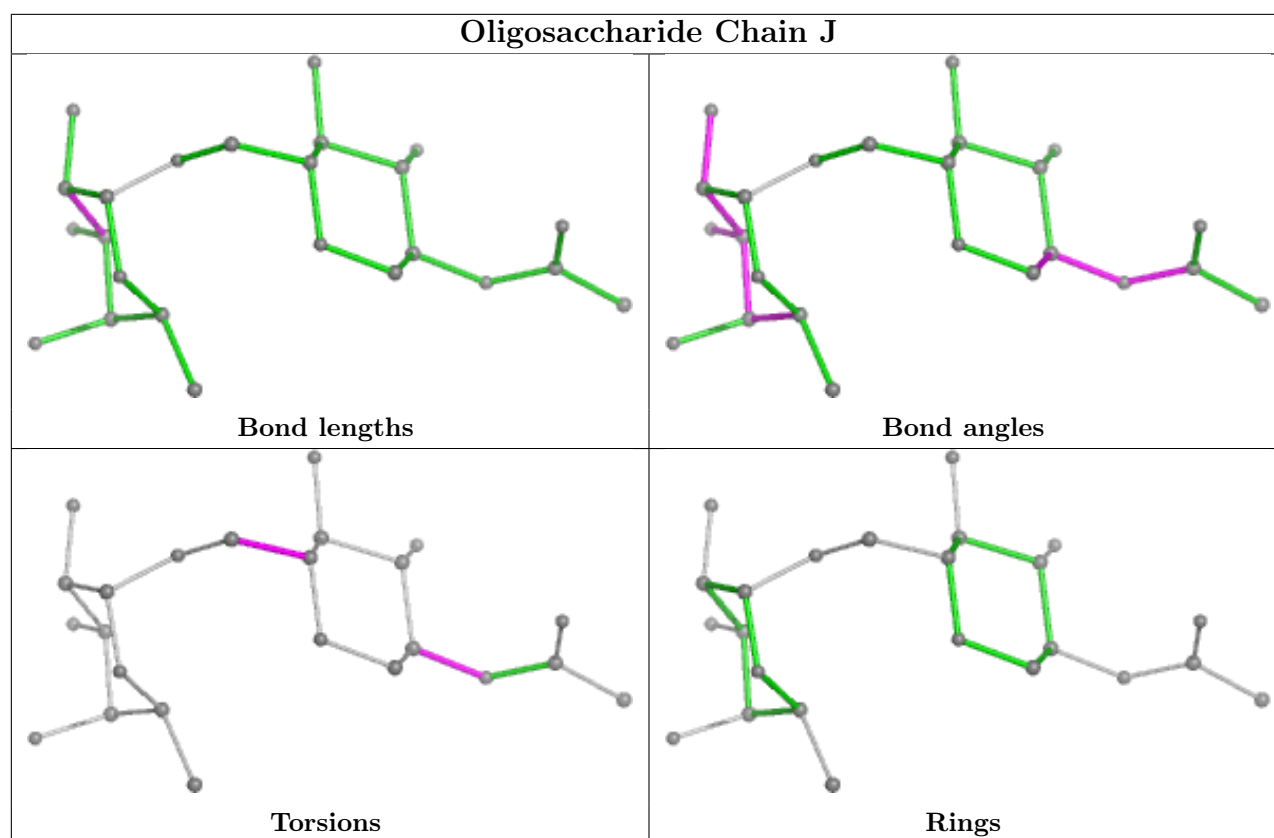
## Oligosaccharide Chain E











## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 5 are monoatomic - leaving 14 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	$\# Z  > 2$
9	PEG	B	708	-	6,6,6	0.41	0	5,5,5	0.38	0
11	PG4	B	707	-	12,12,12	0.30	0	11,11,11	0.27	0
15	1PE	A	709	-	15,15,15	0.58	0	14,14,14	0.41	0
10	EDO	B	704	-	3,3,3	0.18	0	2,2,2	0.21	0
9	PEG	A	705	-	6,6,6	0.20	0	5,5,5	0.28	0
9	PEG	B	703	-	6,6,6	0.34	0	5,5,5	0.42	0
15	1PE	A	708	-	15,15,15	0.51	0	14,14,14	0.39	0
9	PEG	A	710	-	6,6,6	0.16	0	5,5,5	0.16	0
11	PG4	A	707	-	12,12,12	0.61	0	11,11,11	0.47	0
12	PGE	B	709	-	9,9,9	0.32	0	8,8,8	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	PEG	B	706	-	6,6,6	0.60	0	5,5,5	0.77	0
9	PEG	A	703	-	6,6,6	0.26	0	5,5,5	0.16	0
10	EDO	B	705	-	3,3,3	0.26	0	2,2,2	0.53	0
13	BCN	A	704	-	10,10,10	1.11	1 (10%)	11,11,11	1.10	1 (9%)

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
9	PEG	B	708	-	-	2/4/4/4	-
11	PG4	B	707	-	-	6/10/10/10	-
15	1PE	A	709	-	-	6/13/13/13	-
10	EDO	B	704	-	-	0/1/1/1	-
9	PEG	A	705	-	-	4/4/4/4	-
9	PEG	B	703	-	-	2/4/4/4	-
15	1PE	A	708	-	-	6/13/13/13	-
9	PEG	A	710	-	-	3/4/4/4	-
11	PG4	A	707	-	-	7/10/10/10	-
12	PGE	B	709	-	-	3/7/7/7	-
9	PEG	B	706	-	-	1/4/4/4	-
9	PEG	A	703	-	-	4/4/4/4	-
10	EDO	B	705	-	-	1/1/1/1	-
13	BCN	A	704	-	-	5/10/10/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	704	BCN	C1-N1	2.32	1.52	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	704	BCN	C2-C1-N1	2.53	121.90	113.63

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	704	BCN	C6-C5-N1-C1
13	A	704	BCN	N1-C1-C2-O21
9	A	705	PEG	C1-C2-O2-C3
11	B	707	PG4	C4-C3-O2-C2
13	A	704	BCN	N1-C1-C2-O22
11	A	707	PG4	O3-C5-C6-O4
9	A	705	PEG	O1-C1-C2-O2
11	B	707	PG4	O3-C5-C6-O4
9	A	705	PEG	O2-C3-C4-O4
12	B	709	PGE	O3-C5-C6-O4
15	A	708	1PE	OH7-C16-C26-OH6
15	A	709	1PE	OH2-C12-C22-OH3
15	A	709	1PE	OH7-C16-C26-OH6
11	A	707	PG4	O4-C7-C8-O5
13	A	704	BCN	N1-C3-C4-O4
9	B	703	PEG	O1-C1-C2-O2
9	B	706	PEG	O2-C3-C4-O4
9	B	708	PEG	O1-C1-C2-O2
11	A	707	PG4	O1-C1-C2-O2
13	A	704	BCN	N1-C5-C6-O6
9	A	710	PEG	O2-C3-C4-O4
15	A	708	1PE	OH6-C15-C25-OH5
9	B	703	PEG	O2-C3-C4-O4
15	A	709	1PE	OH4-C13-C23-OH3
9	A	703	PEG	O1-C1-C2-O2
11	B	707	PG4	C8-C7-O4-C6
11	A	707	PG4	C5-C6-O4-C7
11	B	707	PG4	C1-C2-O2-C3
11	A	707	PG4	C6-C5-O3-C4
9	A	710	PEG	C1-C2-O2-C3
15	A	709	1PE	C14-C24-OH4-C13
12	B	709	PGE	C6-C5-O3-C4
15	A	708	1PE	C14-C24-OH4-C13
11	A	707	PG4	C4-C3-O2-C2
11	B	707	PG4	C5-C6-O4-C7
9	B	708	PEG	O2-C3-C4-O4
9	A	703	PEG	C4-C3-O2-C2
15	A	708	1PE	OH4-C13-C23-OH3
15	A	709	1PE	C25-C15-OH6-C26
15	A	708	1PE	C15-C25-OH5-C14
11	B	707	PG4	C3-C4-O3-C5
10	B	705	EDO	O1-C1-C2-O2
15	A	708	1PE	C12-C22-OH3-C23

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Mol	Chain	Res	Type	Atoms
12	B	709	PGE	O1-C1-C2-O2
9	A	703	PEG	C1-C2-O2-C3
9	A	705	PEG	C4-C3-O2-C2
9	A	703	PEG	O2-C3-C4-O4
15	A	709	1PE	C24-C14-OH5-C25
9	A	710	PEG	C4-C3-O2-C2
11	A	707	PG4	O2-C3-C4-O3

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	708	PEG	1	0
11	B	707	PG4	1	0
10	B	704	EDO	1	0
15	A	708	1PE	5	0
11	A	707	PG4	2	0
9	B	706	PEG	1	0
9	A	703	PEG	1	0
10	B	705	EDO	1	0
13	A	704	BCN	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	605/628 (96%)	-0.17	13 (2%) 63 65	14, 41, 72, 107	4 (0%)
1	B	603/628 (96%)	-0.44	11 (1%) 67 70	12, 34, 59, 83	4 (0%)
2	C	3/3 (100%)	-0.82	0 100 100	26, 26, 28, 28	0
2	D	3/3 (100%)	-0.57	0 100 100	26, 26, 27, 28	0
All	All	1214/1262 (96%)	-0.30	24 (1%) 64 67	12, 37, 68, 107	8 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	129	LEU	4.5
1	B	79	ILE	3.6
1	A	15	ALA	3.5
1	B	135	THR	3.4
1	A	135	THR	3.4
1	B	607	TYR	3.3
1	B	15	ALA	3.2
1	B	78	PRO	2.8
1	A	11	SER	2.7
1	A	79	ILE	2.7
1	B	80	TRP	2.6
1	A	83	PHE	2.5
1	B	83	PHE	2.4
1	B	12	ALA	2.4
1	A	129	LEU	2.3
1	A	131	GLN	2.2
1	A	8	GLY	2.2
1	A	19	LEU	2.2
1	B	21	ALA	2.2
1	B	325	GLY	2.1
1	A	414	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	13	ASP	2.0
1	A	76	TYR	2.0
1	A	10	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

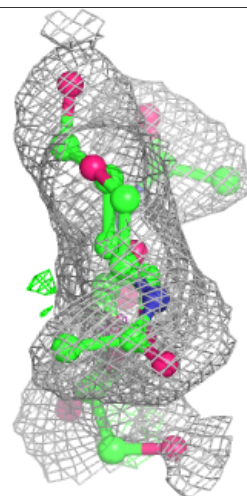
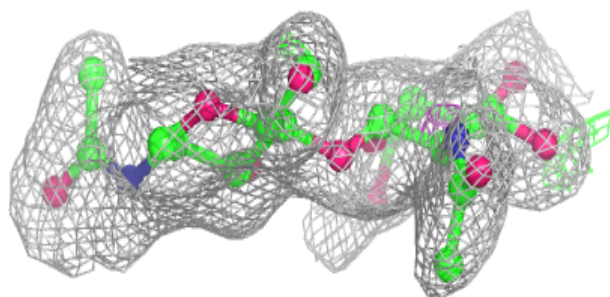
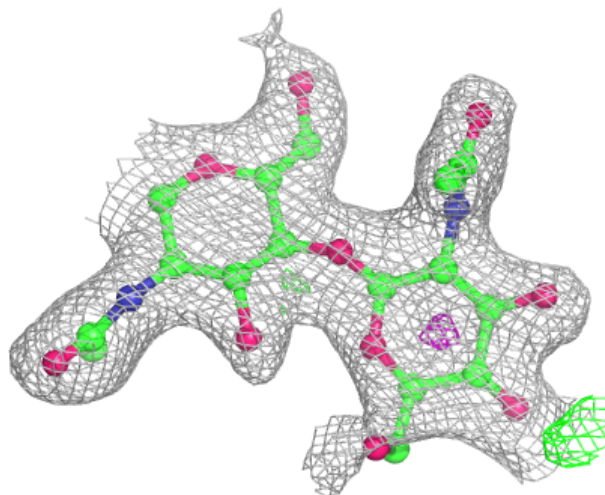
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	NAG	F	2	14/15	0.68	0.14	71,98,108,119	0
5	BMA	H	3	11/12	0.70	0.12	76,94,103,103	0
6	FUC	I	2	10/11	0.71	0.18	66,76,95,99	0
4	BMA	G	3	11/12	0.77	0.13	72,78,83,85	0
6	FUC	J	2	10/11	0.78	0.14	64,75,82,91	0
3	NAG	F	1	14/15	0.82	0.12	56,70,84,99	0
5	NAG	H	1	14/15	0.86	0.10	52,63,72,77	0
3	NAG	E	2	14/15	0.87	0.10	48,62,78,83	0
5	NAG	H	2	14/15	0.88	0.10	54,72,82,87	0
6	NAG	J	1	14/15	0.89	0.10	36,51,69,73	0
4	FUC	G	4	10/11	0.89	0.11	56,61,65,73	0
3	NAG	E	1	14/15	0.90	0.09	40,53,60,60	0
6	NAG	I	1	14/15	0.91	0.09	34,47,61,66	0
4	NAG	G	2	14/15	0.93	0.08	46,57,71,77	0
4	NAG	G	1	14/15	0.94	0.07	33,44,63,73	0

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

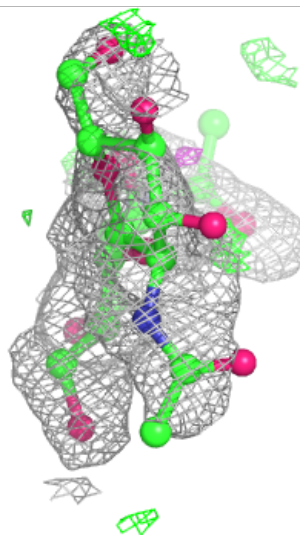
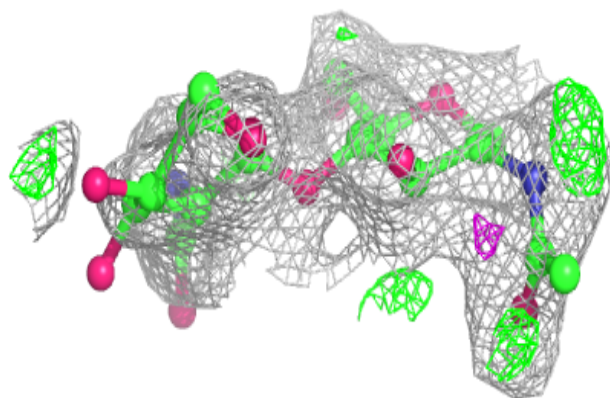
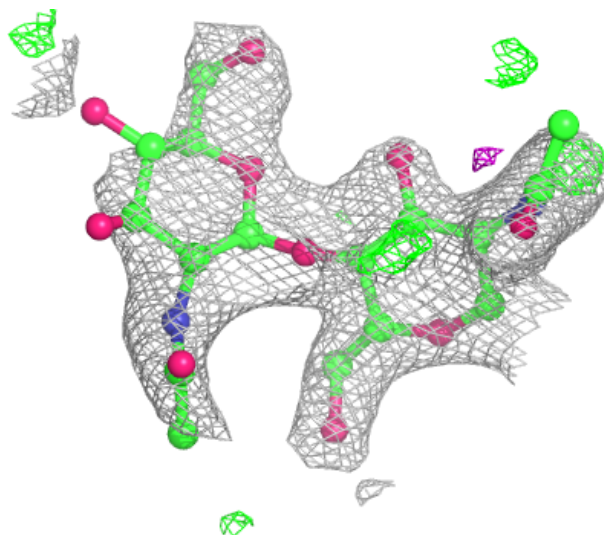
**Electron density around Chain E:**

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



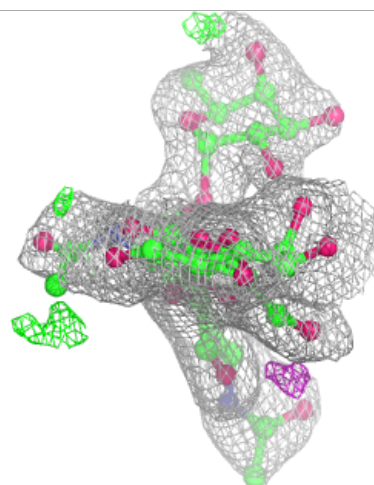
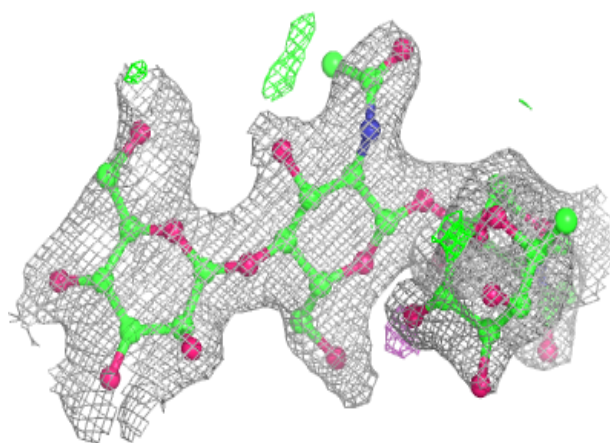
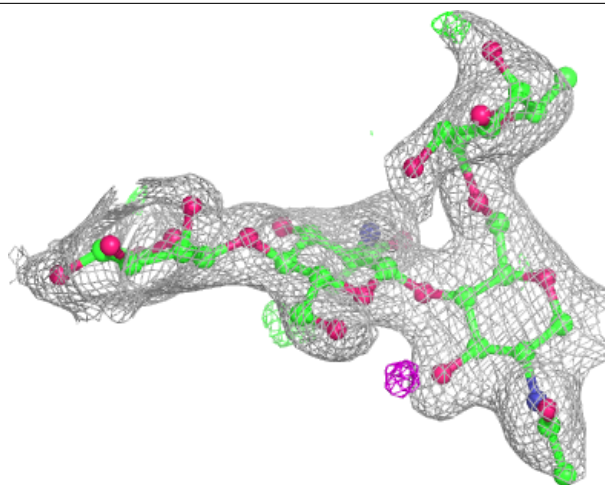
**Electron density around Chain F:**

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



**Electron density around Chain G:**

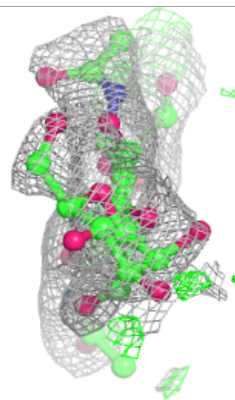
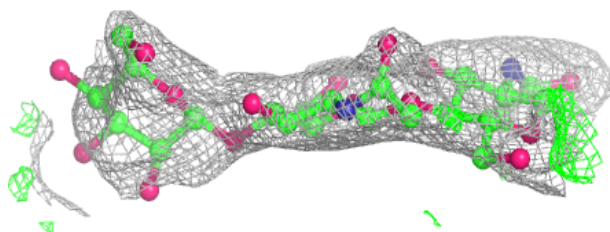
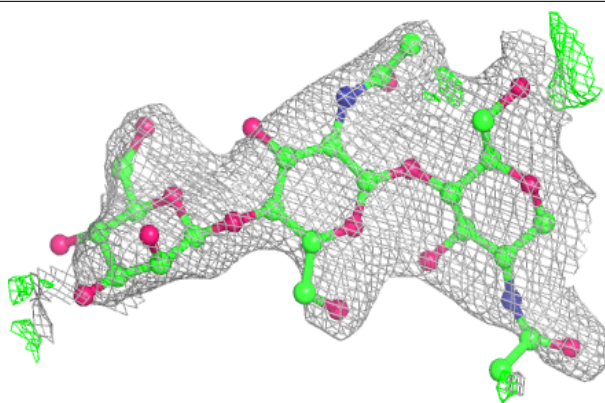
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



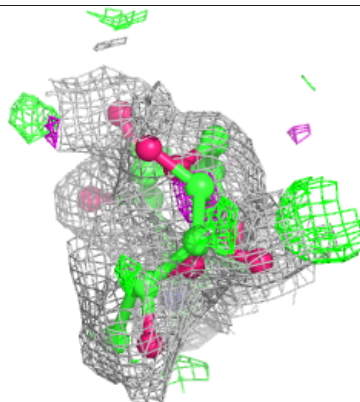
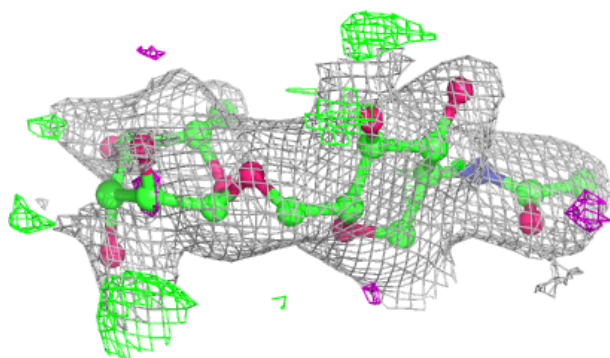
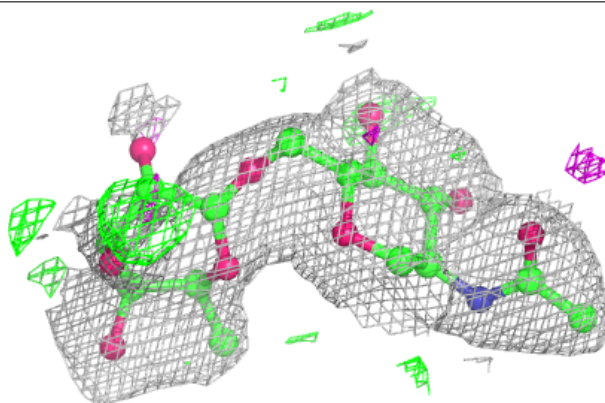


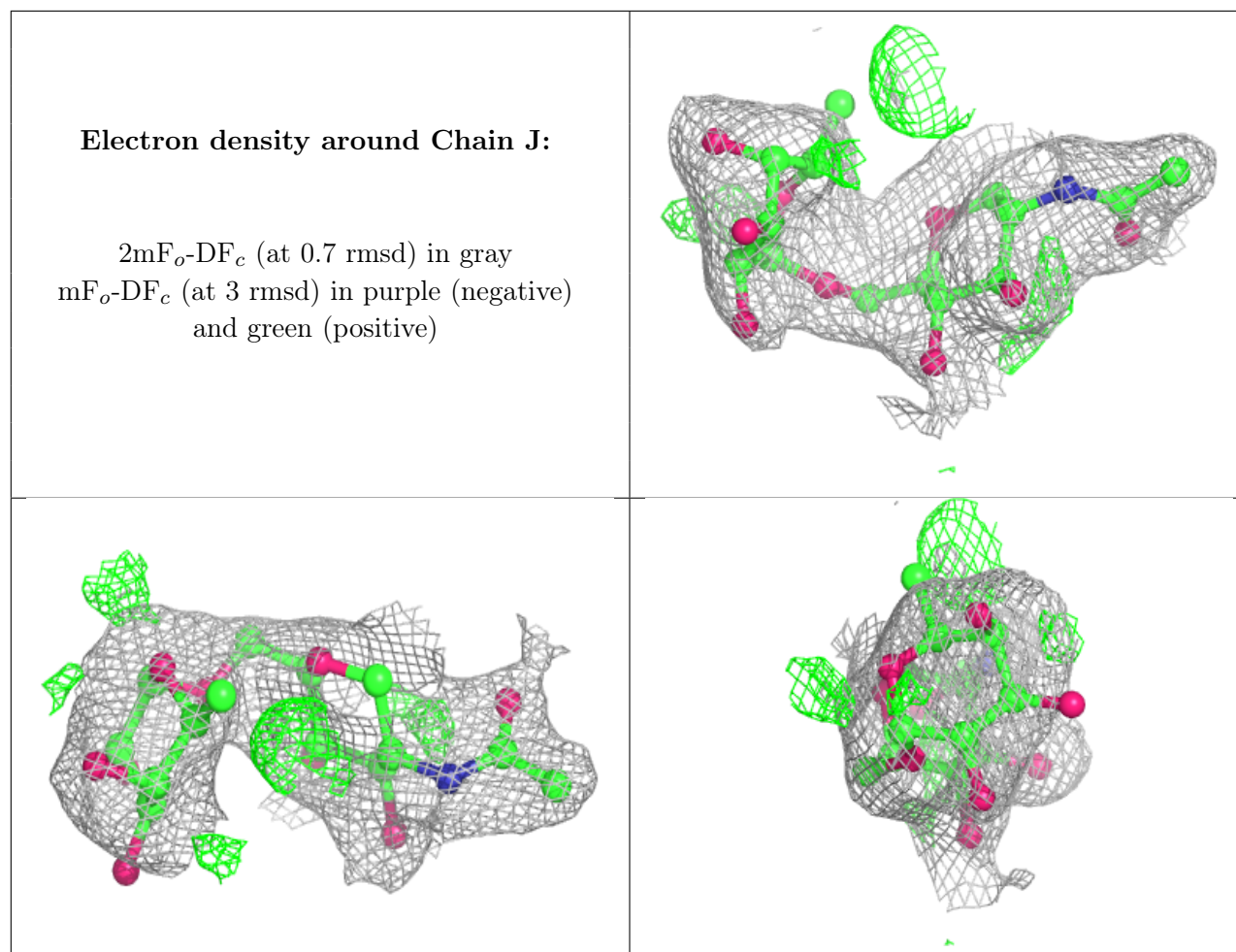
**Electron density around Chain H:**

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

**Electron density around Chain I:**

$2mF_o-DF_c$  (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, 95<sup>th</sup> 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
9	PEG	B	708	7/7	0.82	0.14	56,61,68,70	0
9	PEG	B	706	7/7	0.83	0.14	46,50,62,62	0
13	BCN	A	704	11/11	0.84	0.13	67,75,89,93	0
11	PG4	B	707	13/13	0.87	0.13	62,68,78,79	0
9	PEG	B	703	7/7	0.89	0.10	50,55,63,63	0
9	PEG	A	710	7/7	0.89	0.11	60,65,72,75	0
11	PG4	A	707	13/13	0.90	0.11	43,53,56,58	0
10	EDO	B	704	4/4	0.91	0.12	68,70,74,75	0
12	PGE	B	709	10/10	0.91	0.11	45,57,66,67	0
9	PEG	A	705	7/7	0.91	0.10	47,63,71,72	0
15	1PE	A	708	16/16	0.91	0.11	41,51,68,78	0

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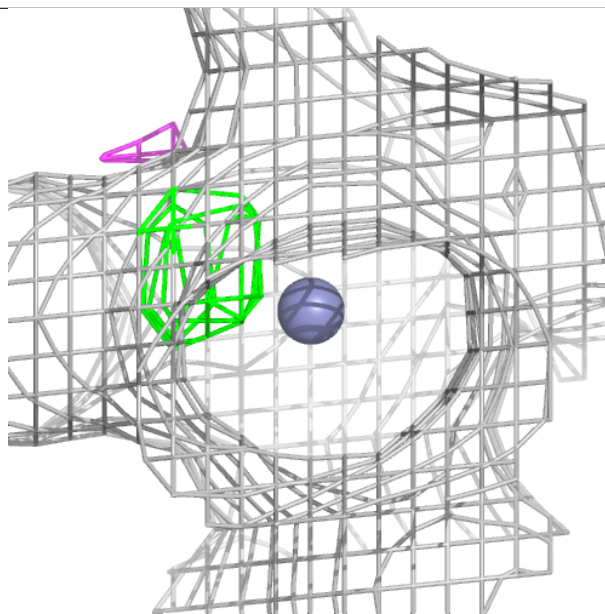
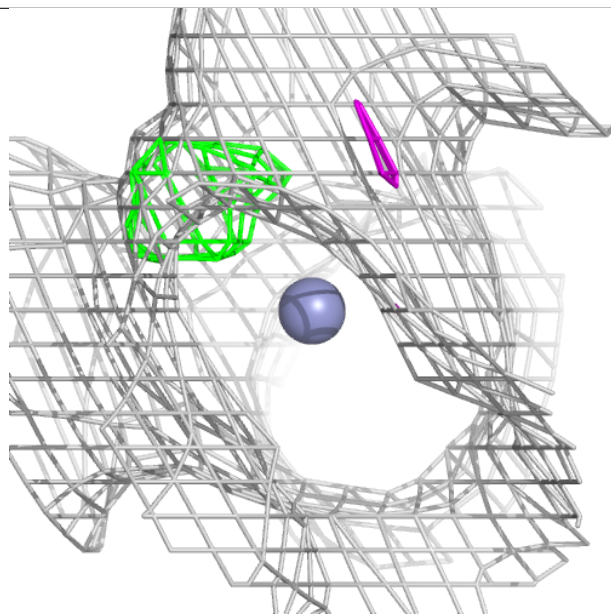
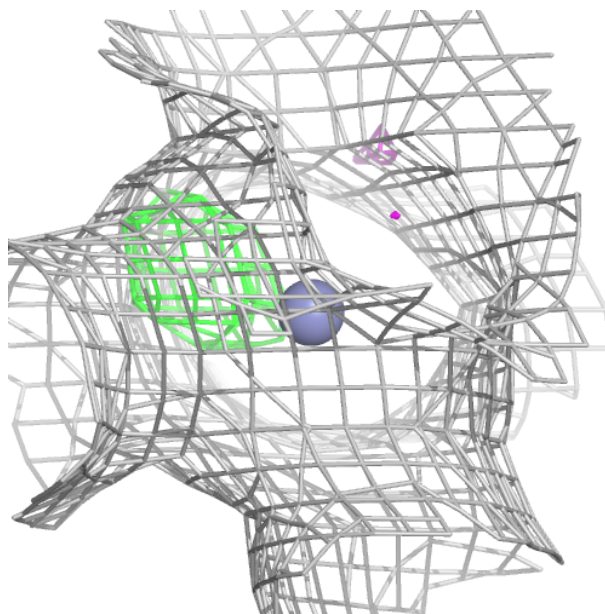
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	1PE	A	709	16/16	0.91	0.11	41,54,71,71	0
10	EDO	B	705	4/4	0.92	0.16	51,58,59,65	0
9	PEG	A	703	7/7	0.94	0.09	57,59,63,66	0
14	MG	A	706	1/1	0.97	0.08	49,49,49,49	0
7	ZN	B	701	1/1	0.99	0.02	25,25,25,25	0
7	ZN	A	701	1/1	0.99	0.03	27,27,27,27	0
8	CL	A	702	1/1	0.99	0.04	31,31,31,31	0
8	CL	B	702	1/1	1.00	0.05	24,24,24,24	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.



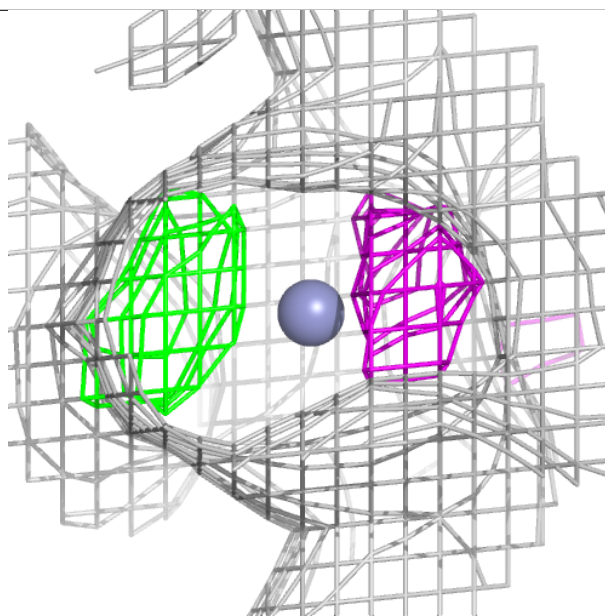
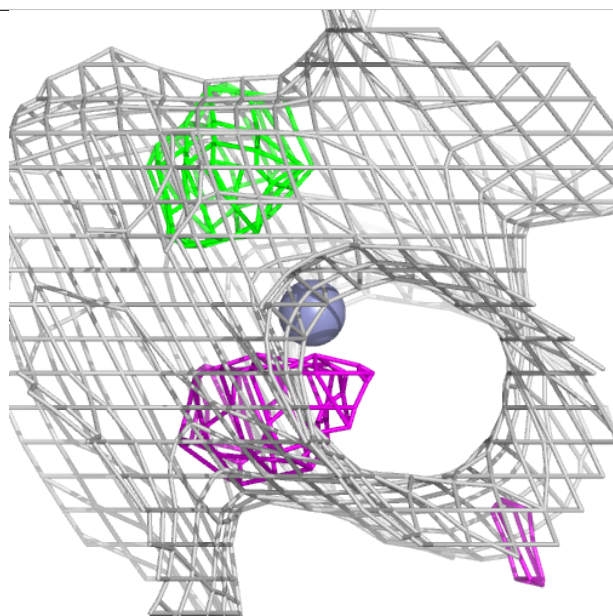
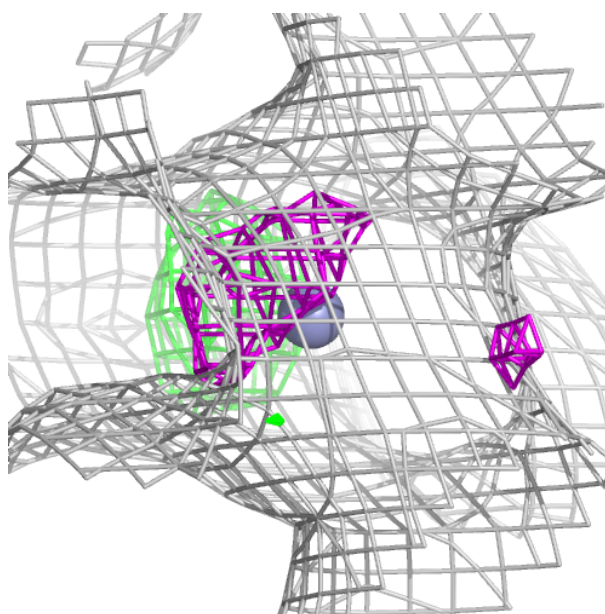
**Electron density around ZN B 701:**

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



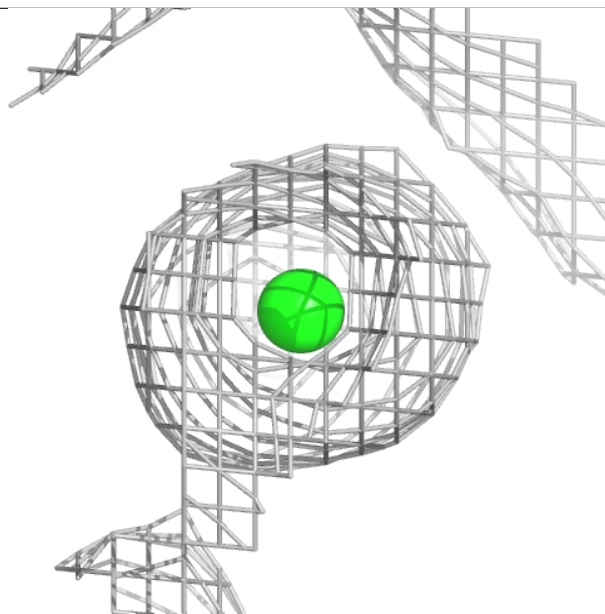
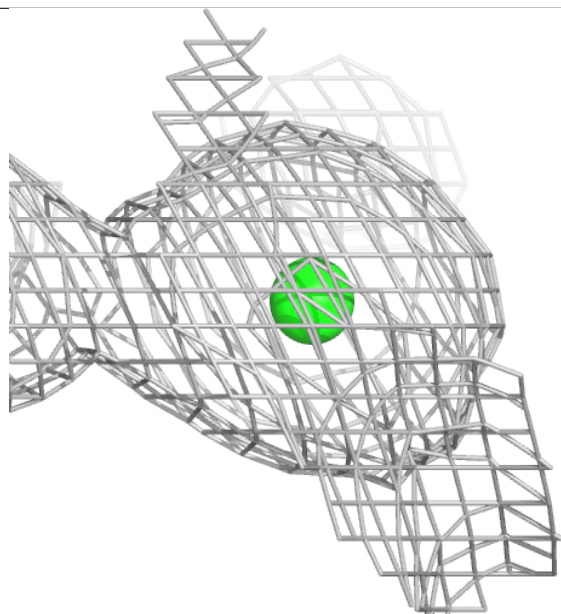
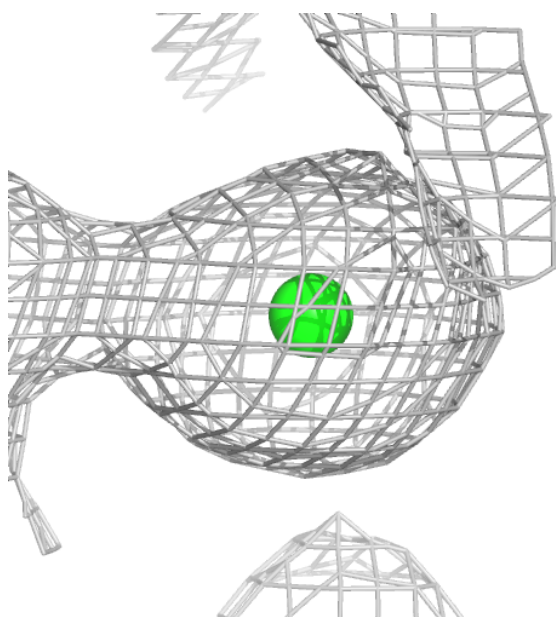
**Electron density around ZN A 701:**

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



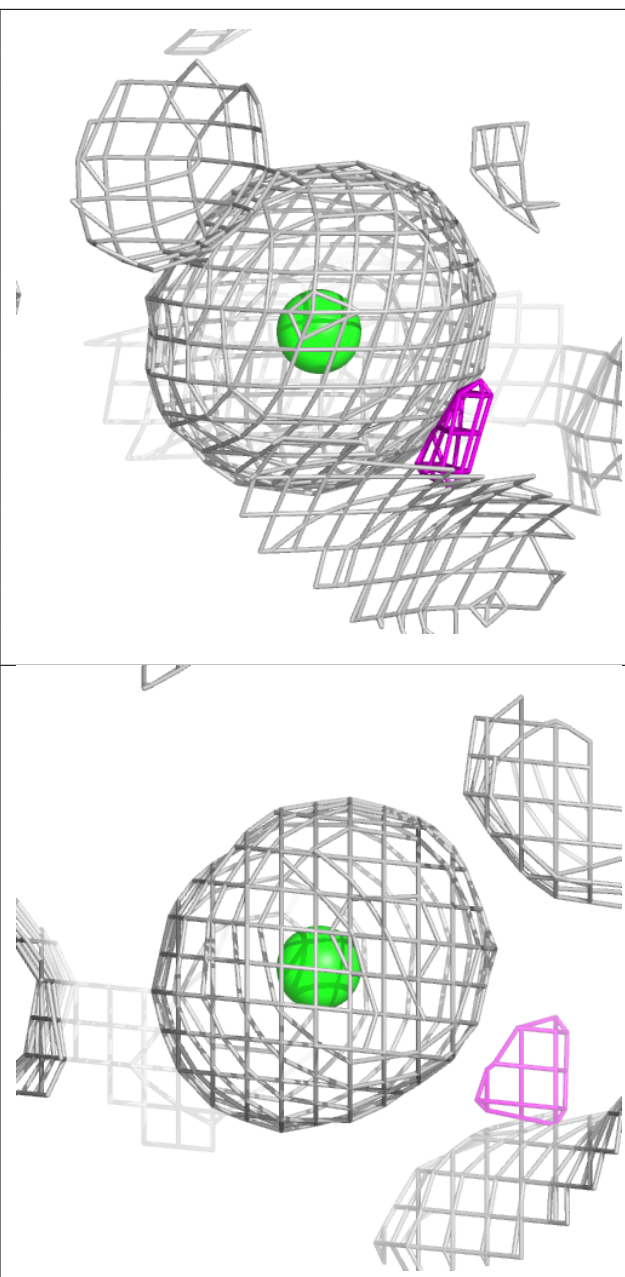
**Electron density around CL A 702:**

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



**Electron density around CL B 702:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.