



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:58 PM UTC

PDB ID : 7ZYF / pdb_00007zyf
Title : Insulin regulated aminopeptidase (IRAP) in complex with a nanomolar alpha hydroxy beta amino acid based inhibitor.
Authors : Mpakali, A.; Stratikos, E.; Giastas, P.; Papakyriakou, A.
Deposited on : 2022-05-24
Resolution : 2.81 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

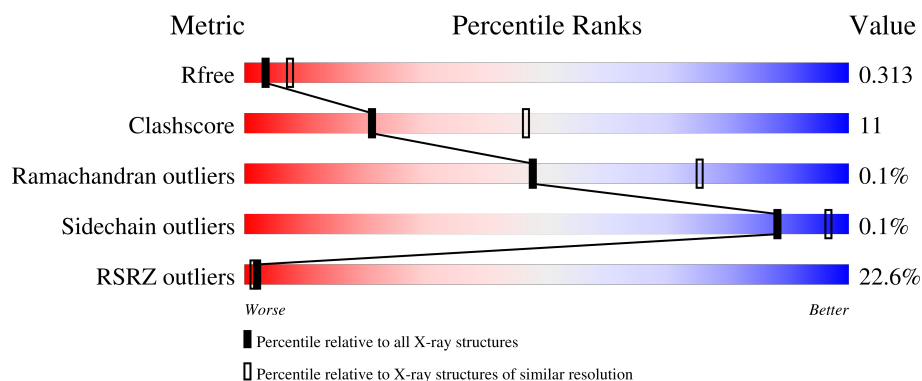
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	871	18% 77% 21%
1	B	871	26% 69% 29%
2	C	4	50% 50%
3	D	2	100%
3	F	2	100%

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Mol	Chain	Length	Quality of chain
3	G	2	 100%
3	K	2	 50% 50%
4	E	3	 33% 67%
4	J	3	 100%
5	H	5	 20% 80%
5	I	5	 40% 60%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 14588 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 Leucyl-cystinyl aminopeptidase, pregnancy serum form.

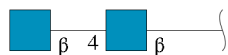
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	852	Total	C	N	O	S	0	4	0
			6910	4481	1123	1279	27			
1	B	854	Total	C	N	O	S	0	2	0
			6882	4457	1122	1277	26			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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
2	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



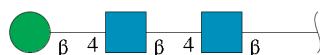
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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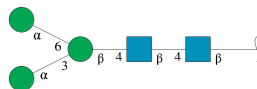
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	J	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	5	Total	C	N	O	0	0	0
			61	34	2	25			
5	I	5	Total	C	N	O	0	0	0
			61	34	2	25			

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

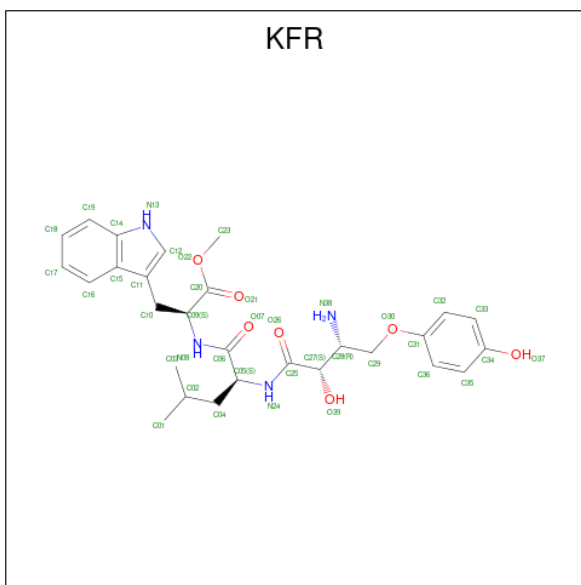
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		
6	B	1	Total	Zn	0	0
			1	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



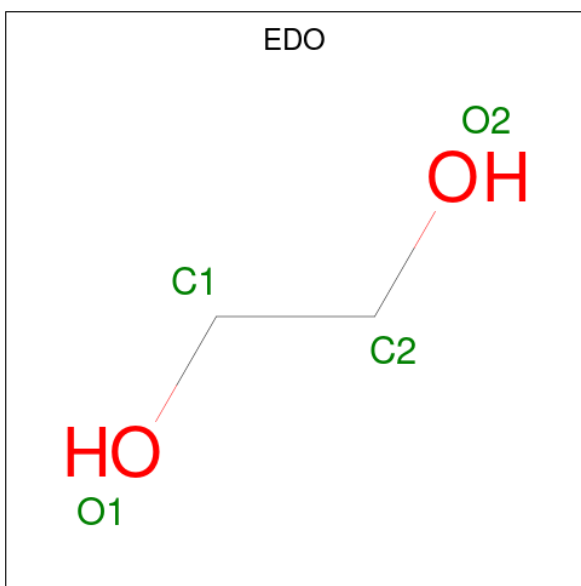
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1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

- Molecule 8 is methyl (2S)-2-[[[(2S)-2-[[[(2S,3R)-3-azanyl-2-oxidanyl-4-(4-oxidanylphenoxy)butanoyl]amino]-4-methyl-pentanoyl]amino]-3-(1H-indol-3-yl)propanoate (CCD ID: KFR) (formula: C₂₈H₃₆N₄O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total 39	C 28	N 4	O 7	0	0
8	B	1	Total 78	C 56	N 8	O 14	0	1

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



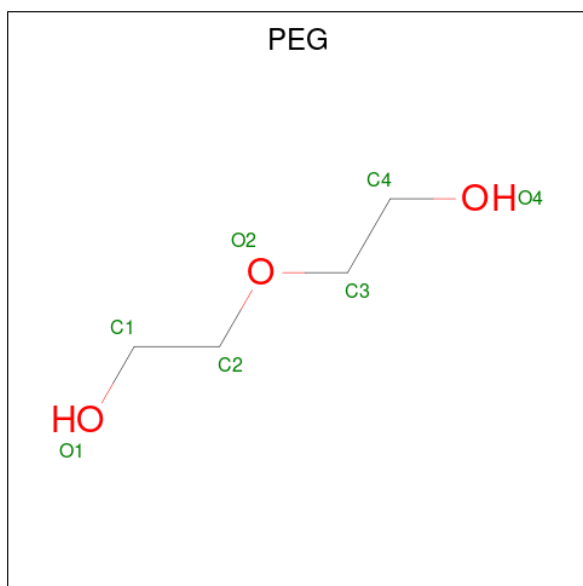
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0

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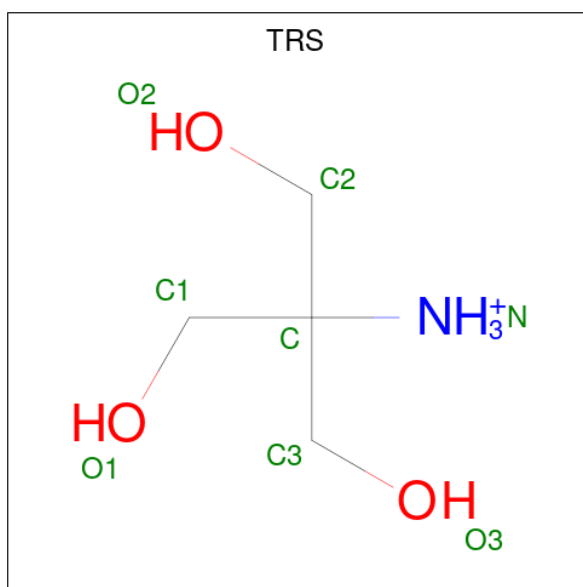
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		

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



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

- Molecule 11 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			8	4	1	3		

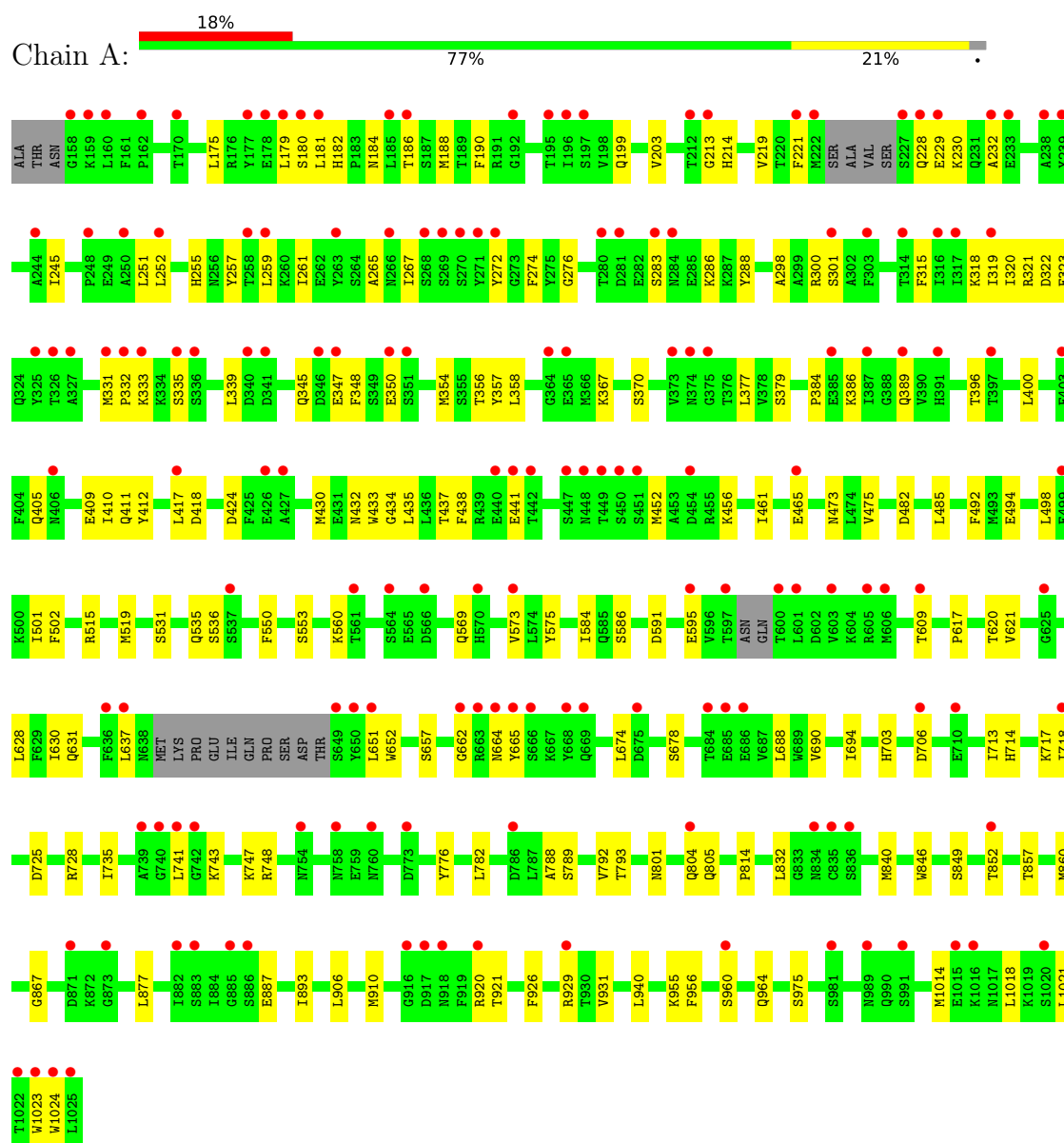
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	51	Total	O	0	0
			51	51		
12	B	53	Total	O	0	0
			53	53		

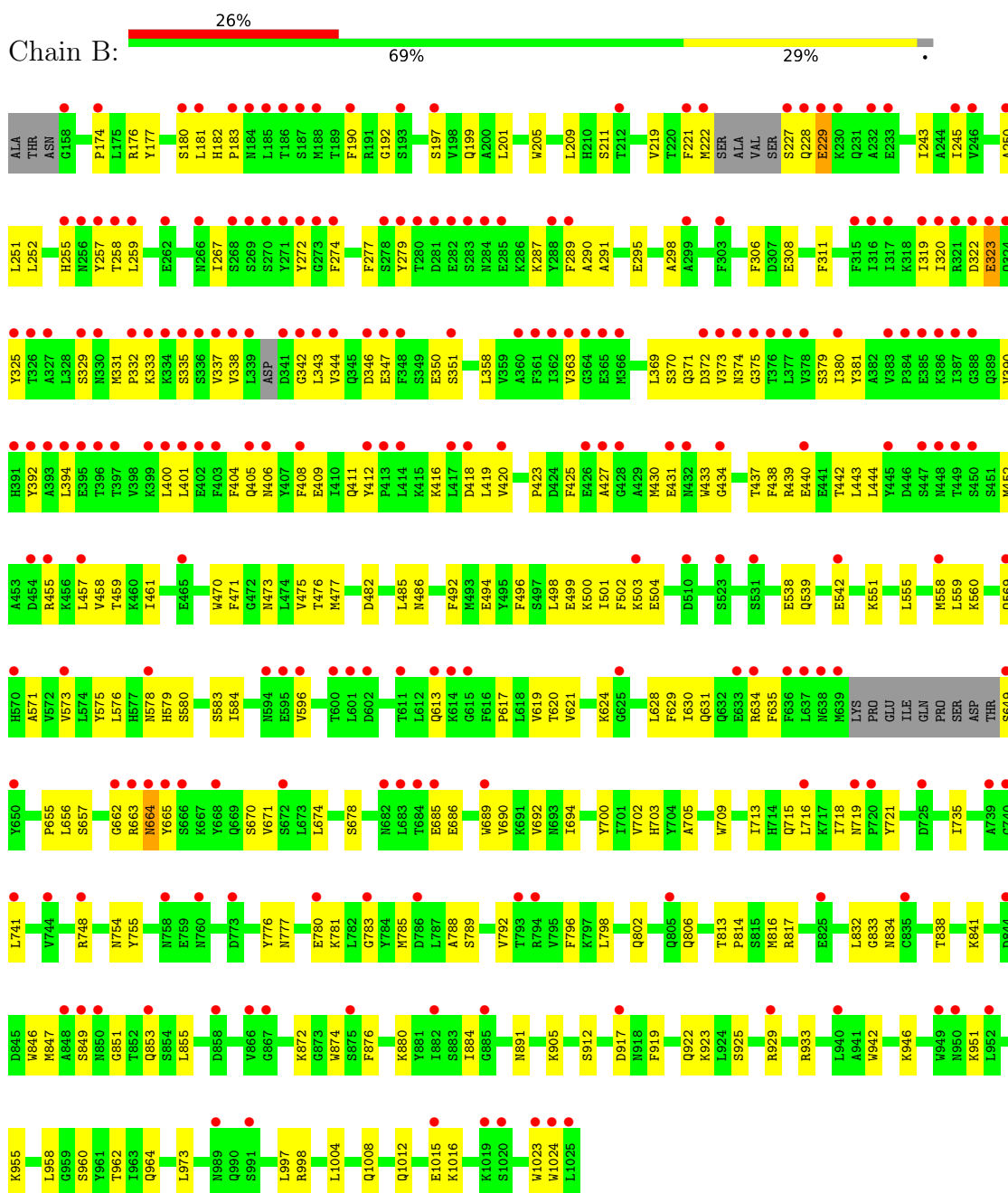
3 Residue-property plots

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

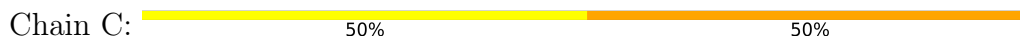
- Molecule 1: Leucyl-cystinyl aminopeptidase, pregnancy serum form



- Molecule 1: Leucyl-cystinyl aminopeptidase, pregnancy serum form



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



MAG1
MAG2
EMA3
MAV4

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





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

Chain F: 100%



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

Chain G: 100%



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

Chain K: 50% 50%



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

Chain E: 33% 67%



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

Chain J: 100%



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 20% 80%



- Molecule 5: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain I:



MAG1	MAG2	MAG3	MAG4	MAG5
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.48Å 120.05Å 141.25Å 90.00° 103.28° 90.00°	Depositor
Resolution (Å)	137.47 – 2.81 137.47 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.5 (137.47-2.81) 99.6 (137.47-2.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.271 , 0.314 0.271 , 0.313	Depositor DCC
R_{free} test set	2883 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	14588	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8538e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, EDO, ZN, PEG, KFR, TRS, BMA, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.21	0/7091	0.50	0/9615
1	B	0.24	0/7057	0.56	4/9576 (0.0%)
All	All	0.23	0/14148	0.53	4/19191 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	227	SER	CA-C-N	7.36	135.59	121.54
1	B	227	SER	C-N-CA	7.36	135.59	121.54
1	B	664	ASN	N-CA-C	-5.38	104.83	113.28
1	B	374	ASN	CB-CA-C	-5.25	102.51	111.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6910	0	6805	130	0
1	B	6882	0	6717	180	0
2	C	50	0	43	4	0
3	D	28	0	25	0	0
3	F	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	28	0	25	0	0
3	K	28	0	25	2	0
4	E	39	0	34	0	0
4	J	39	0	34	0	0
5	H	61	0	52	1	0
5	I	61	0	52	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	56	0	52	4	0
7	B	98	0	89	8	0
8	A	39	0	0	0	0
8	B	78	0	0	4	0
9	A	12	0	18	0	0
9	B	16	0	24	0	0
10	A	14	0	20	0	0
10	B	7	0	10	0	0
11	B	8	0	12	0	0
12	A	51	0	0	0	0
12	B	53	0	0	1	0
All	All	14588	0	14062	315	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 11.

All (315) 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:441:GLU:HG2	1:A:887:GLU:HB3	1.46	0.97
1:B:735:ILE:HD11	1:B:748:ARG:HG3	1.51	0.92
1:B:833:GLY:HA3	3:K:1:NAG:H82	1.55	0.88
1:B:847:MET:HE1	1:B:872:LYS:HG2	1.62	0.82
1:A:245:ILE:HD13	1:A:259:LEU:HD21	1.62	0.81
1:B:219:VAL:HG21	1:B:245:ILE:HD12	1.60	0.81
1:B:335:SER:HB3	1:B:347:GLU:HB3	1.63	0.81
1:B:392:TYR:HH	1:B:459:THR:HG1	1.28	0.80
1:A:628:LEU:HD11	1:A:690:VAL:HG21	1.63	0.79
1:A:412:TYR:CZ	1:A:417:LEU:HD13	2.21	0.76
1:B:199:GLN:CD	7:B:1802:NAG:H82	2.10	0.75
1:B:405:GLN:HG2	1:B:411:GLN:HA	1.69	0.74
1:A:405:GLN:HG2	1:A:411:GLN:HA	1.68	0.74
1:A:179:LEU:HD21	1:A:181:LEU:HD11	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:849:SER:HB2	1:B:853:GLN:H	1.52	0.73
1:A:662:GLY:O	1:A:688:LEU:HD13	1.88	0.73
1:B:181:LEU:HD12	1:B:183:PRO:HD3	1.70	0.73
1:A:179:LEU:CD2	1:A:181:LEU:HD11	2.19	0.72
1:B:813:THR:HG23	1:B:816:MET:HE2	1.73	0.70
7:B:1814:NAG:H3	7:B:1814:NAG:H83	1.72	0.70
1:B:846:TRP:HB2	1:B:855:LEU:HD11	1.72	0.69
1:B:176:ARG:HB2	1:B:197:SER:HB3	1.74	0.69
1:A:186:THR:HG21	2:C:2:NAG:HN2	1.59	0.68
1:A:857:THR:HA	1:A:860:MET:HE2	1.76	0.68
1:B:442:THR:HG22	1:B:461:ILE:HG21	1.76	0.68
1:B:630:ILE:HD12	1:B:674:LEU:HD22	1.76	0.67
1:A:318:LYS:HG3	1:A:347:GLU:HG3	1.76	0.67
1:B:337:VAL:O	1:B:344:VAL:HA	1.94	0.67
1:B:408:PHE:CZ	1:B:471:PHE:HE2	2.13	0.67
1:B:323:GLU:O	1:B:325:TYR:N	2.27	0.67
1:B:624:LYS:HD2	1:B:629:PHE:HB2	1.76	0.67
1:A:339:LEU:HD11	1:A:345:GLN:HB2	1.77	0.66
1:B:442:THR:HG21	1:B:461:ILE:HD13	1.77	0.66
7:B:1814:NAG:H3	7:B:1814:NAG:C8	2.25	0.66
1:A:370:SER:HB3	1:A:377:LEU:HD11	1.77	0.66
1:B:381:TYR:HB2	1:B:420:VAL:HG22	1.77	0.66
1:A:320:ILE:HG12	1:A:345:GLN:HG3	1.78	0.66
1:A:569:GLN:O	1:A:573:VAL:HG23	1.96	0.65
1:B:709:TRP:O	1:B:713:ILE:HG13	1.96	0.65
1:B:575:TYR:OH	1:B:584:ILE:HD12	1.98	0.64
1:A:485:LEU:HD11	1:A:586:SER:HA	1.80	0.64
1:A:181:LEU:HD23	1:A:190:PHE:CE2	2.33	0.64
1:B:783:GLY:HA2	1:B:785:MET:HE3	1.80	0.63
1:A:630:ILE:HD12	1:A:674:LEU:HD22	1.81	0.63
1:B:430:MET:HB3	1:B:437:THR:OG1	1.99	0.63
1:B:333:LYS:HD2	1:B:346:ASP:HB2	1.80	0.62
1:A:801:ASN:O	1:A:805:GLN:HG3	2.00	0.62
1:B:181:LEU:HD11	1:B:319:ILE:HG23	1.82	0.62
1:A:188:MET:HE1	1:A:276:GLY:HA3	1.82	0.62
1:B:780:GLU:OE1	1:B:781:LYS:NZ	2.32	0.62
1:A:591:ASP:O	1:A:595:GLU:HG3	2.00	0.61
1:B:477:MET:SD	1:B:486:ASN:ND2	2.74	0.61
1:B:664:ASN:HB3	7:B:1810:NAG:HN2	1.65	0.61
1:B:190:PHE:HB2	1:B:267:ILE:HD11	1.83	0.61
1:B:409:GLU:H	1:B:573:VAL:HG11	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:TYR:OH	1:B:434:GLY:HA2	2.00	0.61
1:B:558:MET:HE2	1:B:655:PRO:HD2	1.83	0.61
1:B:951:LYS:O	1:B:955:LYS:HE2	2.01	0.61
1:A:714:HIS:O	1:A:718:ILE:HG12	1.99	0.61
1:B:209:LEU:HD22	1:B:243:ILE:HD11	1.83	0.60
1:A:662:GLY:C	1:A:688:LEU:HD13	2.26	0.60
1:A:400:LEU:HD23	1:A:501:ILE:HD11	1.82	0.59
1:B:656:LEU:HD11	1:B:674:LEU:HB2	1.83	0.59
1:B:222:MET:HG3	1:B:258:THR:HB	1.85	0.59
1:B:776:TYR:CD2	1:B:788:ALA:HB1	2.38	0.59
1:B:685:GLU:HG3	1:B:686:GLU:H	1.68	0.59
1:A:482:ASP:HB3	1:A:485:LEU:HD12	1.85	0.58
1:B:891:ASN:HD21	1:B:923:LYS:HZ2	1.51	0.58
1:B:408:PHE:CZ	1:B:471:PHE:CE2	2.92	0.58
1:B:408:PHE:CE1	1:B:471:PHE:HE2	2.22	0.58
1:A:354:MET:HE2	1:A:433:TRP:HE3	1.69	0.57
1:B:663:ARG:HA	1:B:665:TYR:CD2	2.40	0.56
1:A:637:LEU:HB2	1:A:741:LEU:HD12	1.87	0.56
1:B:569:GLN:O	1:B:573:VAL:HG22	2.05	0.56
1:B:578:ASN:OD1	1:B:579:HIS:N	2.37	0.56
1:B:718:ILE:HG13	1:B:719:ASN:H	1.69	0.56
1:A:621:VAL:HG22	1:A:630:ILE:HG22	1.89	0.55
1:B:628:LEU:HD11	1:B:690:VAL:HG21	1.86	0.55
1:A:713:ILE:O	1:A:717:LYS:HG3	2.07	0.55
1:A:438:PHE:HE2	1:A:461:ILE:HG23	1.71	0.55
1:B:409:GLU:H	1:B:573:VAL:CG1	2.20	0.55
1:A:175:LEU:HD11	1:A:199:GLN:HB2	1.88	0.55
1:A:412:TYR:OH	1:A:434:GLY:HA2	2.07	0.54
1:A:1023:TRP:HE3	1:A:1024:TRP:CD1	2.26	0.54
1:B:613:GLN:NE2	1:B:649:SER:OG	2.41	0.54
1:A:214:HIS:NE2	1:A:301:SER:O	2.40	0.54
1:B:718:ILE:HG13	1:B:719:ASN:N	2.23	0.54
1:A:432:ASN:HB2	1:A:435:LEU:O	2.07	0.54
1:B:617:PRO:HG2	1:B:700:TYR:HB3	1.90	0.54
1:A:846:TRP:O	1:A:849:SER:OG	2.24	0.54
1:A:186:THR:CG2	2:C:2:NAG:HN2	2.20	0.54
1:B:372:ASP:OD1	1:B:375:GLY:N	2.39	0.54
1:B:358:LEU:HD21	1:B:431:GLU:HG2	1.90	0.53
1:A:657:SER:HB2	1:A:694:ILE:HD12	1.91	0.53
1:B:631:GLN:HG2	1:B:678:SER:HB3	1.90	0.52
1:B:279:TYR:CZ	1:B:287:LYS:HB2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:PRO:HB2	1:B:177:TYR:HE1	1.74	0.52
1:A:665:TYR:CG	1:A:665:TYR:O	2.62	0.52
1:A:747:LYS:HB2	1:A:1024:TRP:CE2	2.45	0.52
1:B:656:LEU:HD11	1:B:674:LEU:CB	2.39	0.52
1:A:492:PHE:HZ	1:A:560:LYS:HD3	1.74	0.51
1:B:439:ARG:HH21	1:B:922:GLN:HB2	1.75	0.51
1:B:662:GLY:O	1:B:665:TYR:HA	2.11	0.51
1:A:214:HIS:HE1	1:A:300:ARG:O	1.94	0.51
1:A:793:THR:HG22	1:A:832:LEU:HD21	1.92	0.51
1:B:199:GLN:NE2	1:B:201:LEU:HG	2.25	0.51
1:B:322:ASP:HB2	1:B:325:TYR:CD2	2.45	0.51
1:A:367:LYS:HG2	1:A:384:PRO:HG3	1.92	0.51
1:A:535:GLN:HG3	1:A:536:SER:N	2.24	0.51
1:A:219:VAL:HG12	1:A:259:LEU:HD11	1.92	0.51
1:B:440:GLU:HG2	1:B:444:LEU:HD11	1.93	0.50
1:B:912:SER:HB3	1:B:917:ASP:O	2.12	0.50
1:A:180:SER:HA	1:A:318:LYS:O	2.12	0.50
1:B:408:PHE:CE1	1:B:471:PHE:CE2	2.99	0.50
1:B:333:LYS:NZ	1:B:346:ASP:HB3	2.27	0.50
1:B:620:THR:HA	1:B:703:HIS:O	2.12	0.50
1:A:789:SER:HA	1:A:792:VAL:HG22	1.93	0.50
1:A:354:MET:HE2	1:A:433:TRP:CE3	2.46	0.50
1:A:789:SER:O	1:A:793:THR:HG23	2.12	0.50
1:B:425:PHE:CE2	1:B:427:ALA:HB3	2.47	0.50
1:B:874:TRP:CD2	1:B:905:LYS:HD3	2.46	0.50
1:B:181:LEU:HB2	1:B:190:PHE:CE1	2.47	0.49
1:B:338:VAL:HG12	1:B:342:GLY:HA2	1.94	0.49
1:B:504:GLU:H	1:B:504:GLU:CD	2.19	0.49
1:B:634:ARG:NH1	1:B:635:PHE:O	2.44	0.49
1:A:877:LEU:HD22	1:A:893:ILE:HG12	1.94	0.49
1:B:452:MET:HG2	1:B:814:PRO:HB3	1.93	0.49
1:B:499:GLU:O	1:B:503:LYS:HD2	2.10	0.49
1:B:777:ASN:O	1:B:781:LYS:HG2	2.12	0.49
1:A:357:TYR:CE1	1:A:358:LEU:HG	2.47	0.49
1:A:617:PRO:HB3	1:A:652:TRP:CE3	2.48	0.49
1:B:847:MET:HE3	1:B:876:PHE:HB2	1.93	0.49
1:B:333:LYS:HD2	1:B:346:ASP:CB	2.42	0.49
1:B:380:ILE:HG13	1:B:419:LEU:HB2	1.93	0.49
1:A:213:GLY:C	7:A:1104:NAG:H83	2.38	0.49
1:A:386:LYS:O	1:A:389:GLN:HB2	2.13	0.49
1:A:849:SER:HB2	1:A:852:THR:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:789:SER:HA	1:B:792:VAL:HG22	1.95	0.48
1:B:571:ALA:HB2	1:B:596:VAL:HG21	1.96	0.48
1:A:221:PHE:HE1	1:A:232:ALA:HB2	1.78	0.48
1:A:631:GLN:HG3	1:A:678:SER:HB3	1.95	0.48
1:A:741:LEU:HD23	1:A:743:LYS:HG2	1.94	0.48
1:A:804:GLN:HB3	7:A:1103:NAG:H61	1.96	0.48
1:B:925:SER:HB3	1:B:962:THR:HG23	1.95	0.48
1:A:203:VAL:HA	1:A:251:LEU:O	2.14	0.48
1:B:501:ILE:HG13	1:B:502:PHE:CD2	2.48	0.48
1:B:369:LEU:HA	7:B:1813:NAG:H83	1.96	0.48
1:B:322:ASP:HB2	1:B:325:TYR:CE2	2.48	0.47
1:B:754:ASN:HA	1:B:798:LEU:HD21	1.95	0.47
1:A:921:THR:HG22	1:A:956:PHE:HZ	1.79	0.47
1:B:1004:LEU:O	1:B:1008:GLN:HG3	2.14	0.47
1:B:370:SER:OG	7:B:1813:NAG:H2	2.15	0.47
1:B:834:ASN:ND2	3:K:1:NAG:O7	2.47	0.47
1:B:329:SER:O	1:B:416:LYS:NZ	2.38	0.47
1:B:891:ASN:HD21	1:B:923:LYS:NZ	2.12	0.47
1:A:461:ILE:O	1:A:465:GLU:HG2	2.14	0.47
1:B:251:LEU:HD23	1:B:257:TYR:CD2	2.48	0.47
1:B:802:GLN:O	1:B:806:GLN:HG2	2.15	0.47
2:C:2:NAG:O7	2:C:2:NAG:H3	2.14	0.47
1:A:412:TYR:CE1	1:A:417:LEU:HD13	2.48	0.47
1:B:917:ASP:C	1:B:919:PHE:H	2.22	0.47
1:A:181:LEU:HD23	1:A:190:PHE:CD2	2.49	0.47
1:B:331:MET:HE3	1:B:332:PRO:HD2	1.97	0.47
1:B:492:PHE:HZ	1:B:560:LYS:HD3	1.78	0.47
1:A:181:LEU:CD2	1:A:190:PHE:CE2	2.97	0.47
1:A:203:VAL:HG22	1:A:252:LEU:HD13	1.96	0.47
1:B:277:PHE:HZ	1:B:423:PRO:HD2	1.80	0.47
1:B:308:GLU:HB2	1:B:311:PHE:HD2	1.79	0.47
1:B:470:TRP:O	1:B:475:VAL:HG22	2.15	0.47
1:A:190:PHE:CE1	1:A:265:ALA:HB3	2.50	0.46
1:A:321:ARG:NH1	1:A:323:GLU:HA	2.30	0.46
1:A:515:ARG:O	1:A:519:MET:HG3	2.15	0.46
1:A:706:ASP:OD2	1:A:748:ARG:NE	2.47	0.46
1:B:182:HIS:ND1	1:B:320:ILE:HG21	2.30	0.46
1:B:657:SER:HB2	1:B:694:ILE:HD12	1.98	0.46
1:A:628:LEU:HD21	1:A:690:VAL:HG11	1.97	0.46
1:B:621:VAL:HG21	1:B:692:VAL:HG21	1.98	0.46
1:A:430:MET:HB3	1:A:437:THR:OG1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:GLU:O	1:A:498:LEU:HG	2.15	0.46
2:C:2:NAG:O3	2:C:3:BMA:O5	2.30	0.46
1:A:213:GLY:O	7:A:1104:NAG:H83	2.15	0.46
1:A:221:PHE:CE1	1:A:232:ALA:HB2	2.50	0.46
1:B:477:MET:HA	1:B:584:ILE:HG12	1.97	0.46
1:B:849:SER:CB	1:B:853:GLN:H	2.24	0.46
1:A:219:VAL:HG13	1:A:261:ILE:HG12	1.97	0.46
1:A:286:LYS:HD3	1:A:288:TYR:CE1	2.51	0.46
1:B:838:THR:O	1:B:841:LYS:HG2	2.16	0.46
1:B:1023:TRP:HE3	1:B:1024:TRP:CD1	2.35	0.45
1:A:456:LYS:HE2	1:A:456:LYS:HB3	1.79	0.45
1:A:741:LEU:HD23	1:A:743:LYS:CG	2.46	0.45
1:A:906:LEU:HD22	1:A:931:VAL:HG22	1.99	0.45
1:A:321:ARG:HD2	1:A:322:ASP:O	2.16	0.45
1:B:419:LEU:HD23	1:B:438:PHE:CE1	2.51	0.45
1:B:849:SER:OG	1:B:851:GLY:N	2.50	0.45
1:B:958:LEU:HG	1:B:997:LEU:HD11	1.99	0.45
1:A:286:LYS:HD3	1:A:288:TYR:CZ	2.51	0.45
1:B:211:SER:HB3	1:B:243:ILE:CG2	2.46	0.45
1:B:496:PHE:O	1:B:500:LYS:HG2	2.17	0.45
1:B:631:GLN:CG	1:B:678:SER:HB3	2.46	0.45
1:B:656:LEU:HD12	1:B:656:LEU:H	1.81	0.45
1:B:846:TRP:O	1:B:849:SER:OG	2.26	0.45
1:B:267:ILE:HD12	1:B:274:PHE:CD2	2.52	0.45
1:B:331:MET:HE2	1:B:350:GLU:O	2.17	0.45
1:B:295:GLU:OE1	8:B:1815[A]:KFR:N38	2.51	0.44
1:B:960:SER:O	1:B:964:GLN:HG3	2.17	0.44
1:B:1016:LYS:HA	1:B:1016:LYS:HD3	1.74	0.44
1:A:184:ASN:C	1:A:186:THR:H	2.25	0.44
1:A:396:THR:HG23	1:A:502:PHE:CZ	2.52	0.44
1:B:228:GLN:O	1:B:229:GLU:CB	2.66	0.44
1:B:290:ALA:HB3	1:B:363:VAL:HG13	1.98	0.44
1:B:576:LEU:O	1:B:580:SER:OG	2.35	0.44
1:B:664:ASN:HB3	7:B:1810:NAG:N2	2.31	0.44
1:A:190:PHE:HB3	1:A:267:ILE:HD11	1.99	0.44
1:A:255:HIS:HA	7:A:1102:NAG:H82	1.98	0.44
1:B:670:SER:OG	1:B:671:VAL:N	2.49	0.44
1:B:1012:GLN:HA	1:B:1015:GLU:HG2	1.99	0.44
1:A:320:ILE:HA	1:A:345:GLN:HA	1.98	0.44
1:A:776:TYR:CD2	1:A:788:ALA:HB1	2.52	0.44
1:B:689:TRP:CD1	1:B:715:GLN:HE21	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:960:SER:O	1:A:964:GLN:HG3	2.17	0.44
1:A:662:GLY:C	1:A:664:ASN:H	2.26	0.44
1:B:942:TRP:CE2	1:B:946:LYS:HD3	2.53	0.44
1:B:180:SER:O	1:B:192:GLY:HA2	2.18	0.44
1:A:331:MET:HE3	1:A:332:PRO:HD2	2.00	0.44
1:A:182:HIS:HD2	1:A:320:ILE:CG2	2.30	0.43
1:A:424:ASP:CG	1:A:920:ARG:HD3	2.42	0.43
1:B:433:TRP:CD1	1:B:473:ASN:HD22	2.35	0.43
1:A:221:PHE:O	1:A:229:GLU:HA	2.18	0.43
1:A:251:LEU:HD23	1:A:257:TYR:CD2	2.53	0.43
1:A:926:PHE:HD1	1:A:929:ARG:HH21	1.66	0.43
1:B:182:HIS:HA	1:B:320:ILE:HB	1.99	0.43
1:B:431:GLU:OE1	8:B:1815[A]:KFR:N38	2.52	0.43
1:B:542:GLU:HG3	1:B:542:GLU:O	2.18	0.43
1:A:331:MET:HE2	1:A:350:GLU:O	2.18	0.43
1:A:396:THR:HG22	1:A:400:LEU:HD12	2.00	0.43
1:B:289:PHE:HE1	1:B:291:ALA:HB2	1.84	0.43
1:B:331:MET:HG3	1:B:351:SER:HA	2.00	0.43
1:B:880:LYS:O	1:B:884:ILE:HG12	2.18	0.43
1:A:725:ASP:OD1	1:A:728:ARG:NH2	2.52	0.43
1:A:1021:LEU:HA	1:A:1024:TRP:CE3	2.54	0.43
1:B:295:GLU:OE1	8:B:1815[B]:KFR:N38	2.52	0.43
1:B:443:LEU:HA	1:B:458:VAL:HG13	2.00	0.43
1:B:663:ARG:HA	1:B:665:TYR:CE2	2.54	0.43
1:B:267:ILE:HD12	1:B:274:PHE:HD2	1.84	0.43
1:A:482:ASP:OD1	1:A:531:SER:OG	2.35	0.43
1:B:390:VAL:HG12	1:B:390:VAL:O	2.18	0.43
1:B:455:ARG:C	1:B:457:LEU:H	2.27	0.43
1:B:619:VAL:O	1:B:702:VAL:HA	2.19	0.43
1:A:417:LEU:HD12	1:A:417:LEU:HA	1.84	0.42
1:A:441:GLU:H	1:A:441:GLU:HG3	1.61	0.42
1:A:1014:MET:O	1:A:1018:LEU:HB2	2.19	0.42
1:B:205:TRP:CE2	1:B:250:ALA:HB2	2.54	0.42
1:B:476:THR:O	1:B:583:SER:HA	2.19	0.42
1:B:777:ASN:HB3	1:B:973:LEU:HD13	2.00	0.42
1:A:184:ASN:OD1	1:A:186:THR:HB	2.19	0.42
1:B:635:PHE:CE1	1:B:741:LEU:HD13	2.54	0.42
1:A:475:VAL:HG12	1:A:584:ILE:HG12	2.01	0.42
1:A:333:LYS:CD	1:A:335:SER:HA	2.49	0.42
1:B:221:PHE:CZ	1:B:259:LEU:HD13	2.54	0.42
1:B:482:ASP:HB3	1:B:485:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ILE:HD13	1:A:259:LEU:CD2	2.41	0.42
1:A:452:MET:HG2	1:A:814:PRO:HB3	2.01	0.42
1:A:840:MET:HE1	1:A:867:GLY:HA2	2.01	0.42
1:A:272[A]:TYR:CZ	1:A:298:ALA:HB2	2.54	0.42
1:A:319:ILE:HG13	1:A:348:PHE:HE1	1.84	0.42
1:A:433:TRP:CD2	1:A:473:ASN:HB3	2.55	0.42
1:A:379:SER:HB2	1:A:418:ASP:OD1	2.20	0.42
1:A:550:PHE:HA	1:A:553:SER:OG	2.19	0.42
1:B:400:LEU:HD23	1:B:501:ILE:HD11	2.01	0.42
1:B:538:GLU:HG2	1:B:539:GLN:N	2.35	0.42
1:B:846:TRP:CZ3	1:B:876:PHE:HE2	2.38	0.42
1:B:190:PHE:CB	1:B:267:ILE:HD11	2.50	0.42
1:B:373:VAL:HG21	1:B:401:LEU:HD12	2.01	0.42
1:B:416:LYS:HE3	1:B:418:ASP:OD2	2.20	0.42
1:B:252:LEU:HB2	1:B:255:HIS:CD2	2.55	0.42
1:B:475:VAL:HG12	1:B:579:HIS:O	2.20	0.42
1:B:663:ARG:C	1:B:665:TYR:H	2.27	0.42
1:B:705:ALA:O	1:B:709:TRP:N	2.46	0.42
1:B:813:THR:O	1:B:817:ARG:HG3	2.19	0.42
1:B:929:ARG:HG2	1:B:933:ARG:HH21	1.85	0.42
1:B:431:GLU:OE1	8:B:1815[B]:KFR:N38	2.53	0.41
1:B:998:ARG:HG2	12:B:1937:HOH:O	2.20	0.41
1:B:343:LEU:HD21	5:I:1:NAG:O6	2.20	0.41
1:A:409:GLU:O	1:A:410:ILE:HG13	2.20	0.41
1:B:181:LEU:CD1	1:B:319:ILE:HG23	2.49	0.41
1:B:796:PHE:HB2	1:B:832:LEU:HD13	2.02	0.41
1:A:315:PHE:HZ	1:A:356:THR:HG22	1.85	0.41
1:A:620:THR:HA	1:A:703:HIS:O	2.20	0.41
1:A:910:MET:HE1	1:A:940:LEU:HG	2.02	0.41
1:B:494:GLU:O	1:B:498:LEU:HG	2.20	0.41
1:B:551:LYS:O	1:B:555:LEU:HG	2.21	0.41
1:A:735:ILE:HD12	1:A:735:ILE:HA	1.95	0.41
1:A:575:TYR:OH	1:A:584:ILE:HD13	2.21	0.41
1:A:228:GLN:HG3	1:A:230:LYS:HG3	2.03	0.41
1:A:320:ILE:HG12	1:A:345:GLN:CG	2.49	0.41
1:B:333:LYS:HZ2	1:B:346:ASP:HB3	1.85	0.41
1:A:272[B]:TYR:HE1	1:A:955:LYS:O	2.04	0.41
1:A:782:LEU:HD11	1:A:975:SER:HB2	2.03	0.41
1:B:272:TYR:CZ	1:B:298:ALA:HB2	2.56	0.41
1:B:390:VAL:HG22	1:B:444:LEU:HD22	2.02	0.41
1:A:320:ILE:CG1	1:A:345:GLN:HG3	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:721:TYR:HE2	5:H:1:NAG:H81	1.86	0.40
1:B:371:GLN:HB2	1:B:394:LEU:HD21	2.03	0.40
1:B:559:LEU:HD12	1:B:559:LEU:HA	1.82	0.40
1:B:245:ILE:HG21	1:B:259:LEU:HD11	2.03	0.40
1:B:245:ILE:HG13	1:B:259:LEU:HD21	2.02	0.40
1:B:379:SER:O	1:B:418:ASP:HA	2.20	0.40
1:A:609:THR:HG21	1:A:651:LEU:O	2.21	0.40
1:A:747:LYS:HB2	1:A:1024:TRP:CZ2	2.57	0.40
1:B:209:LEU:HD12	1:B:306:PHE:CE1	2.57	0.40
1:B:404:PHE:C	1:B:406:ASN:H	2.30	0.40
1:B:716:LEU:HB3	1:B:755:TYR:CG	2.56	0.40
1:A:267:ILE:HD12	1:A:274:PHE:CD2	2.57	0.40
1:B:476:THR:O	1:B:584:ILE:HG12	2.22	0.40
7:B:1814:NAG:C8	7:B:1814:NAG:C3	2.97	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	848/871 (97%)	821 (97%)	27 (3%)	0	100	100
1	B	848/871 (97%)	812 (96%)	34 (4%)	2 (0%)	43	71
All	All	1696/1742 (97%)	1633 (96%)	61 (4%)	2 (0%)	48	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	229	GLU
1	B	323	GLU

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	756/780 (97%)	755 (100%)	1 (0%)	88	96
1	B	745/780 (96%)	745 (100%)	0	100	100
All	All	1501/1560 (96%)	1500 (100%)	1 (0%)	88	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	283	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	324	GLN
1	A	800	GLN
1	A	804	GLN
1	A	805	GLN
1	A	830	HIS
1	A	915	ASN
1	A	1001	GLN
1	B	324	GLN
1	B	389	GLN
1	B	486	ASN
1	B	715	GLN
1	B	719	ASN
1	B	733	ASN
1	B	965	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

28 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1	1,2	14,14,15	0.59	0	17,19,21	1.45	2 (11%)
2	NAG	C	2	2	14,14,15	1.02	1 (7%)	17,19,21	0.92	1 (5%)
2	BMA	C	3	2	11,11,12	0.81	0	15,15,17	1.73	5 (33%)
2	MAN	C	4	2	11,11,12	0.54	0	15,15,17	0.96	2 (13%)
3	NAG	D	1	3,1	14,14,15	0.48	0	17,19,21	0.54	0
3	NAG	D	2	3	14,14,15	0.33	0	17,19,21	0.43	0
4	NAG	E	1	4,1	14,14,15	0.48	0	17,19,21	0.77	1 (5%)
4	NAG	E	2	4	14,14,15	0.31	0	17,19,21	0.58	0
4	BMA	E	3	4	11,11,12	1.12	1 (9%)	15,15,17	1.15	2 (13%)
3	NAG	F	1	3,1	14,14,15	0.57	0	17,19,21	0.71	0
3	NAG	F	2	3	14,14,15	0.54	0	17,19,21	0.53	0
3	NAG	G	1	3,1	14,14,15	0.55	0	17,19,21	0.83	0
3	NAG	G	2	3	14,14,15	0.44	0	17,19,21	0.57	0
5	NAG	H	1	5,1	14,14,15	0.29	0	17,19,21	0.81	0
5	NAG	H	2	5	14,14,15	0.20	0	17,19,21	0.53	0
5	BMA	H	3	5	11,11,12	1.46	2 (18%)	15,15,17	1.18	1 (6%)
5	MAN	H	4	5	11,11,12	0.79	1 (9%)	15,15,17	1.50	3 (20%)
5	MAN	H	5	5	11,11,12	0.90	1 (9%)	15,15,17	1.17	2 (13%)
5	NAG	I	1	5,1	14,14,15	0.37	0	17,19,21	0.55	0
5	NAG	I	2	5	14,14,15	0.39	0	17,19,21	0.54	0
5	BMA	I	3	5	11,11,12	0.62	0	15,15,17	0.77	0
5	MAN	I	4	5	11,11,12	0.72	0	15,15,17	1.01	2 (13%)
5	MAN	I	5	5	11,11,12	0.84	0	15,15,17	1.01	2 (13%)
4	NAG	J	1	4,1	14,14,15	0.33	0	17,19,21	0.77	0
4	NAG	J	2	4	14,14,15	0.46	0	17,19,21	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	J	3	4	11,11,12	0.60	0	15,15,17	0.77	0
3	NAG	K	1	3,1	14,14,15	0.36	0	17,19,21	0.70	0
3	NAG	K	2	3	14,14,15	0.63	0	17,19,21	0.45	0

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	3	BMA	C2-C3	3.73	1.58	1.52
2	C	2	NAG	O5-C1	-3.51	1.37	1.43
5	H	4	MAN	C1-C2	2.21	1.57	1.52
5	H	3	BMA	O3-C3	2.16	1.48	1.43
4	E	3	BMA	C4-C3	2.05	1.57	1.52
5	H	5	MAN	C1-C2	2.04	1.57	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O4-C4-C5	-4.29	98.75	109.32
5	H	4	MAN	C1-O5-C5	4.15	117.75	112.19
2	C	3	BMA	C1-O5-C5	3.79	117.27	112.19
5	H	3	BMA	O3-C3-C2	3.46	117.12	110.05
5	H	5	MAN	C1-O5-C5	3.30	116.61	112.19
2	C	1	NAG	O4-C4-C3	-2.95	103.42	110.38
5	I	4	MAN	C1-O5-C5	2.75	115.87	112.19
2	C	3	BMA	C1-C2-C3	2.71	113.58	109.64
4	E	3	BMA	C2-C3-C4	2.69	115.59	110.86
2	C	3	BMA	C3-C4-C5	-2.57	105.57	110.23
2	C	4	MAN	C1-O5-C5	2.53	115.57	112.19
4	E	3	BMA	C3-C4-C5	2.45	114.67	110.23
2	C	2	NAG	C2-N2-C7	2.36	126.07	122.90
2	C	3	BMA	O5-C1-C2	2.36	116.41	110.79
4	E	1	NAG	C1-O5-C5	2.34	115.33	112.19
5	H	4	MAN	C1-C2-C3	2.32	113.03	109.64
2	C	3	BMA	O2-C2-C3	-2.31	105.37	110.15
5	I	5	MAN	C1-O5-C5	2.26	115.21	112.19
2	C	4	MAN	O2-C2-C3	-2.18	105.63	110.15
5	H	5	MAN	O2-C2-C3	-2.14	105.72	110.15
5	H	4	MAN	O2-C2-C3	-2.13	105.74	110.15
5	I	4	MAN	O2-C2-C3	-2.09	105.82	110.15
5	I	5	MAN	O2-C2-C3	-2.07	105.87	110.15

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C3-C2-N2-C7
5	H	2	NAG	C1-C2-N2-C7
5	I	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6

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

There are no ring outliers.

5 monomers are involved in 8 short contacts:

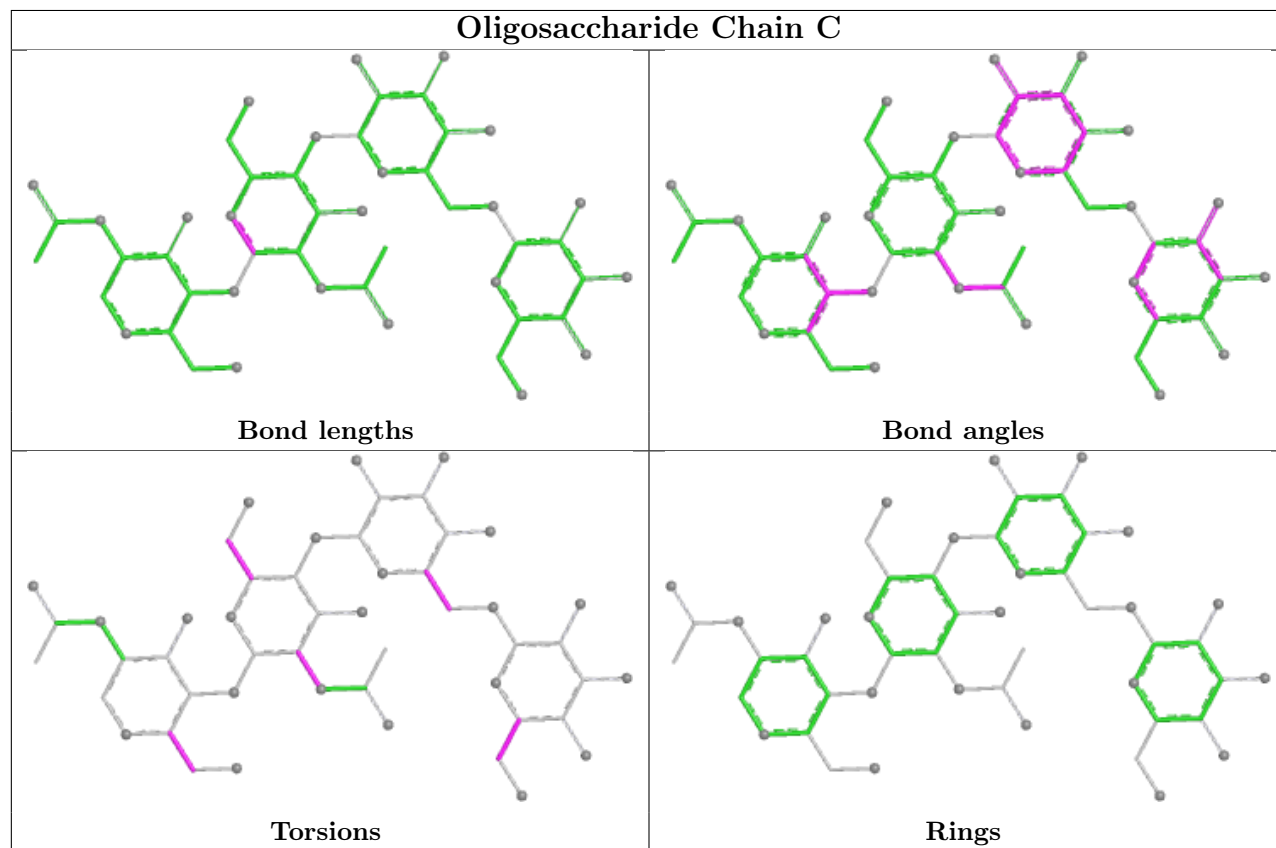
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	1	NAG	2	0
5	H	1	NAG	1	0
5	I	1	NAG	1	0
2	C	2	NAG	4	0

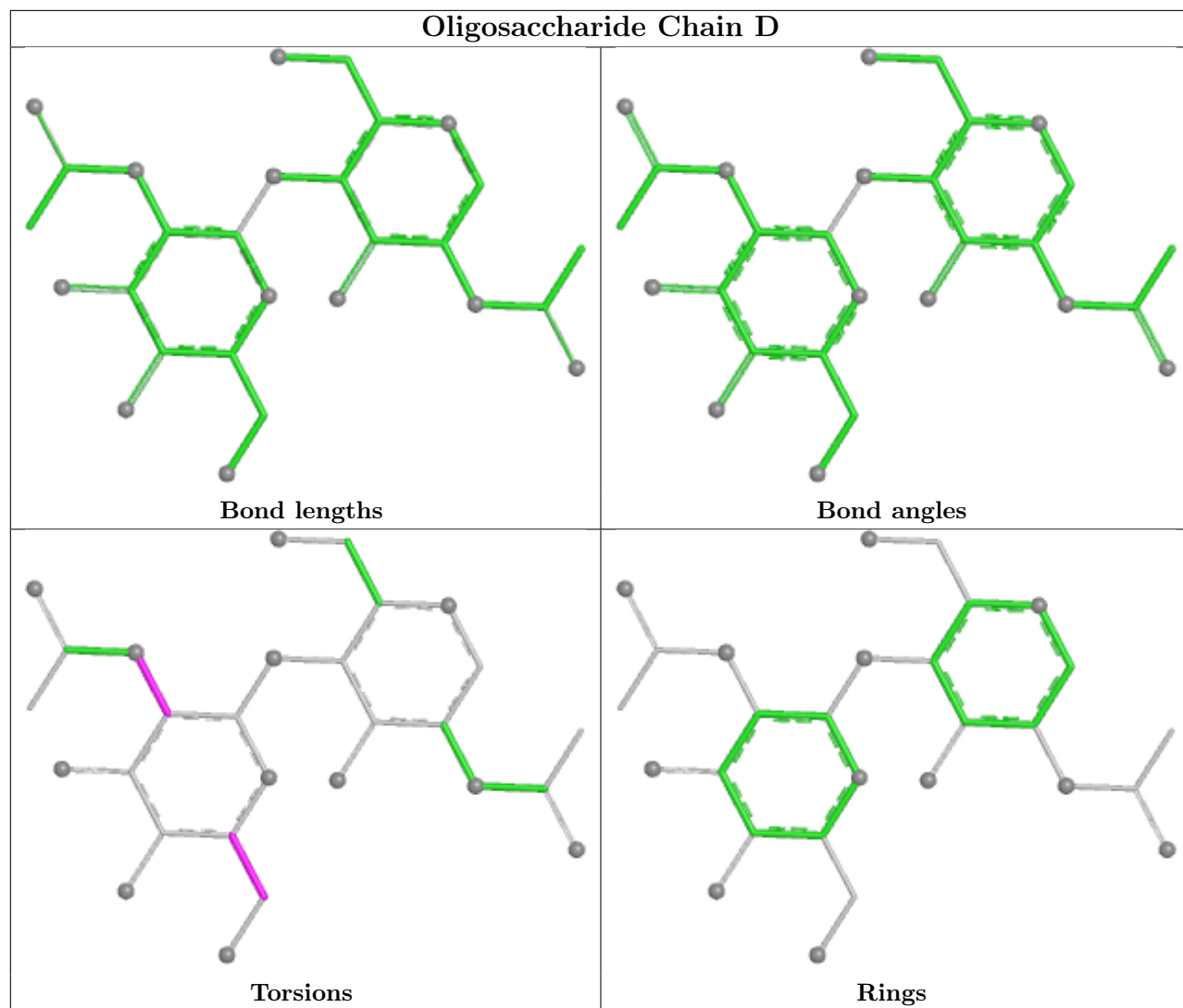
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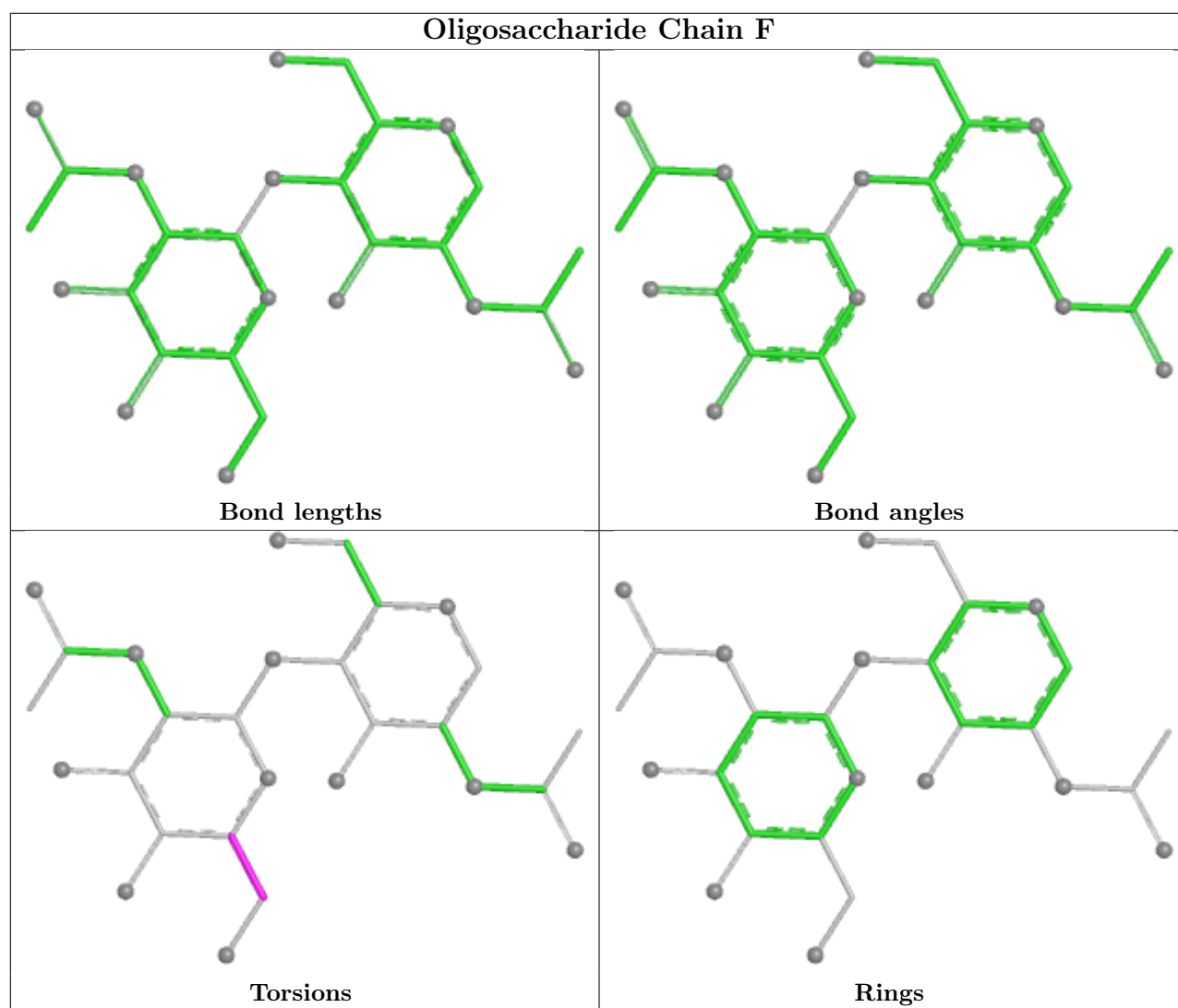
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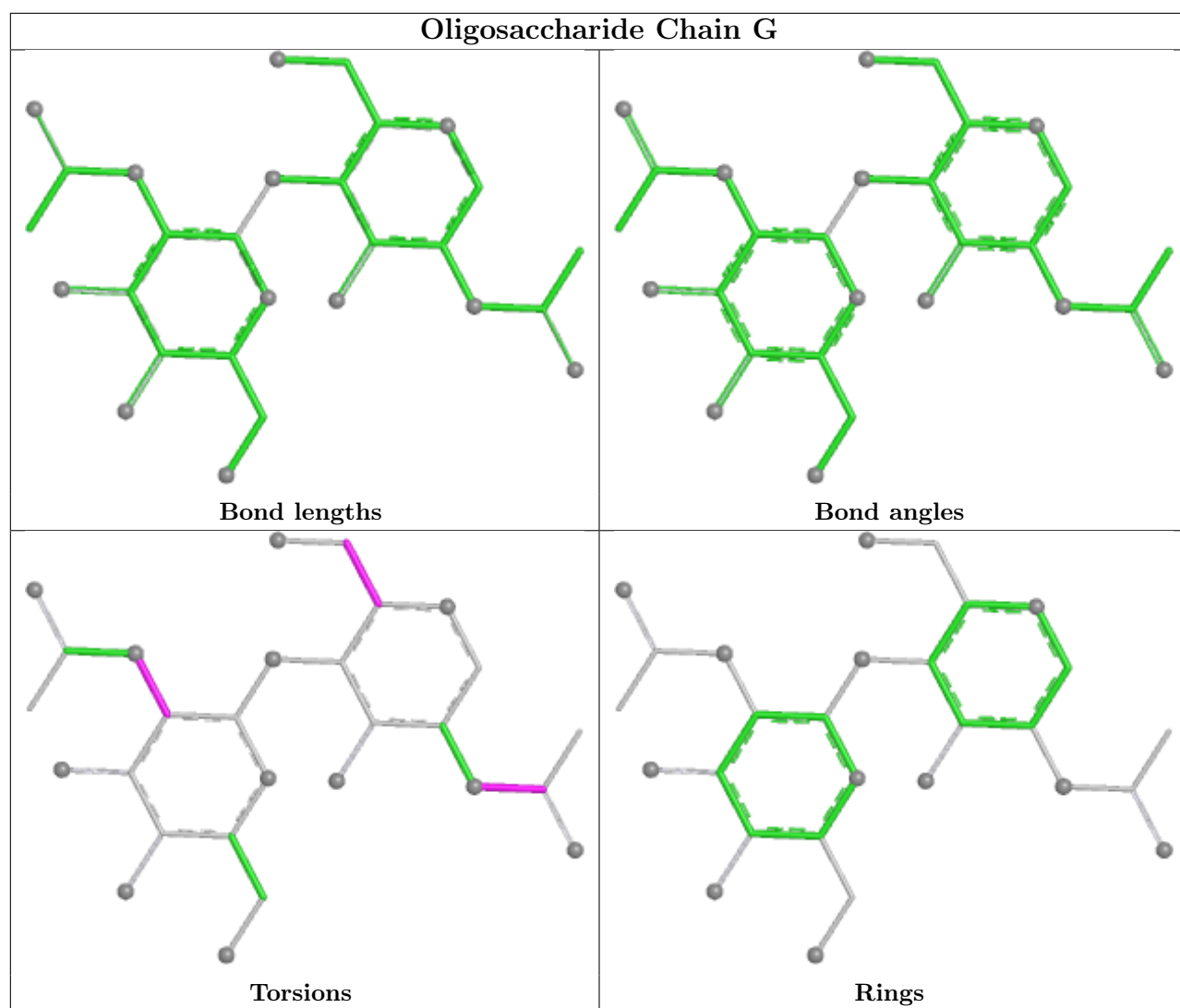
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	BMA	1	0

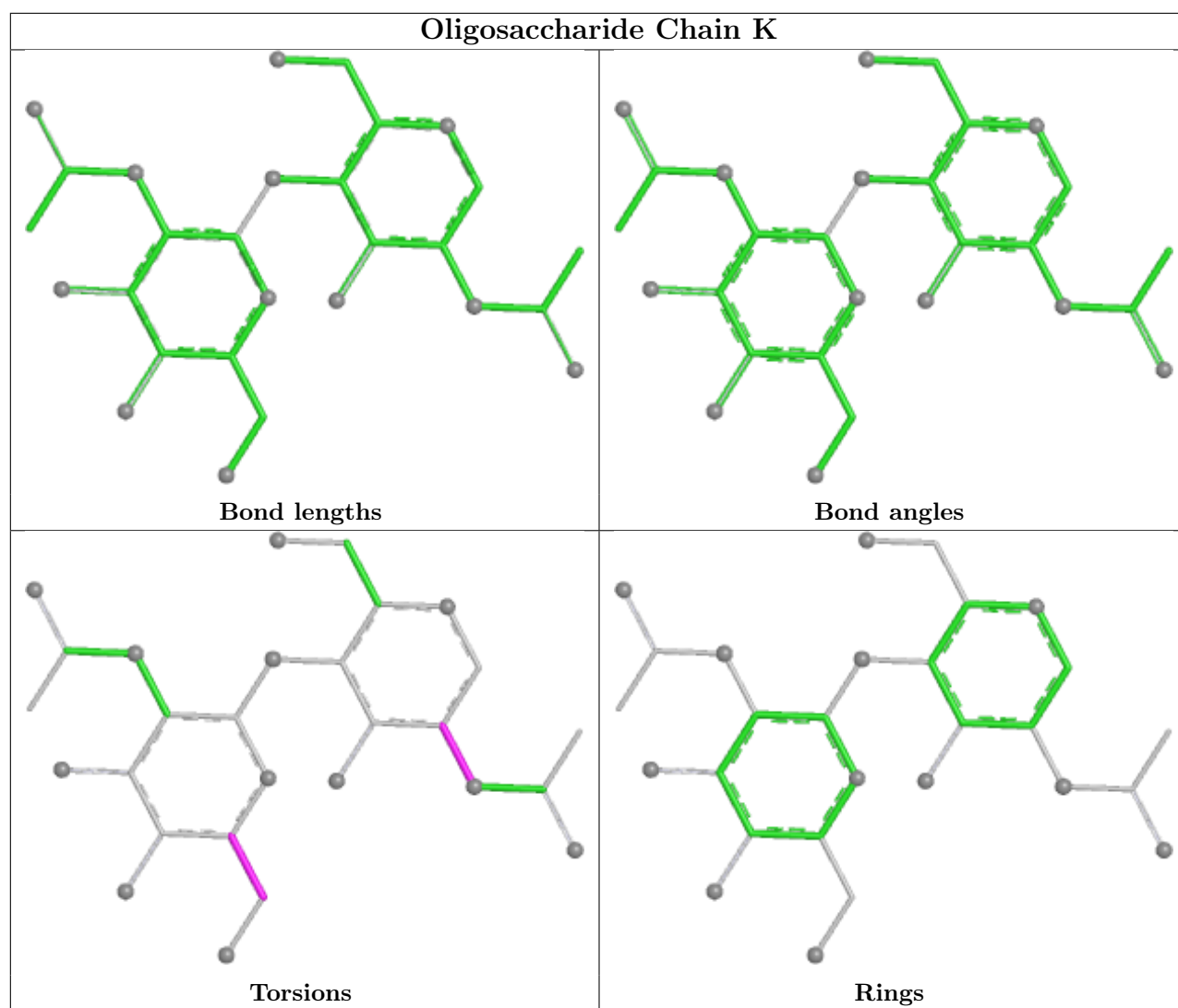
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

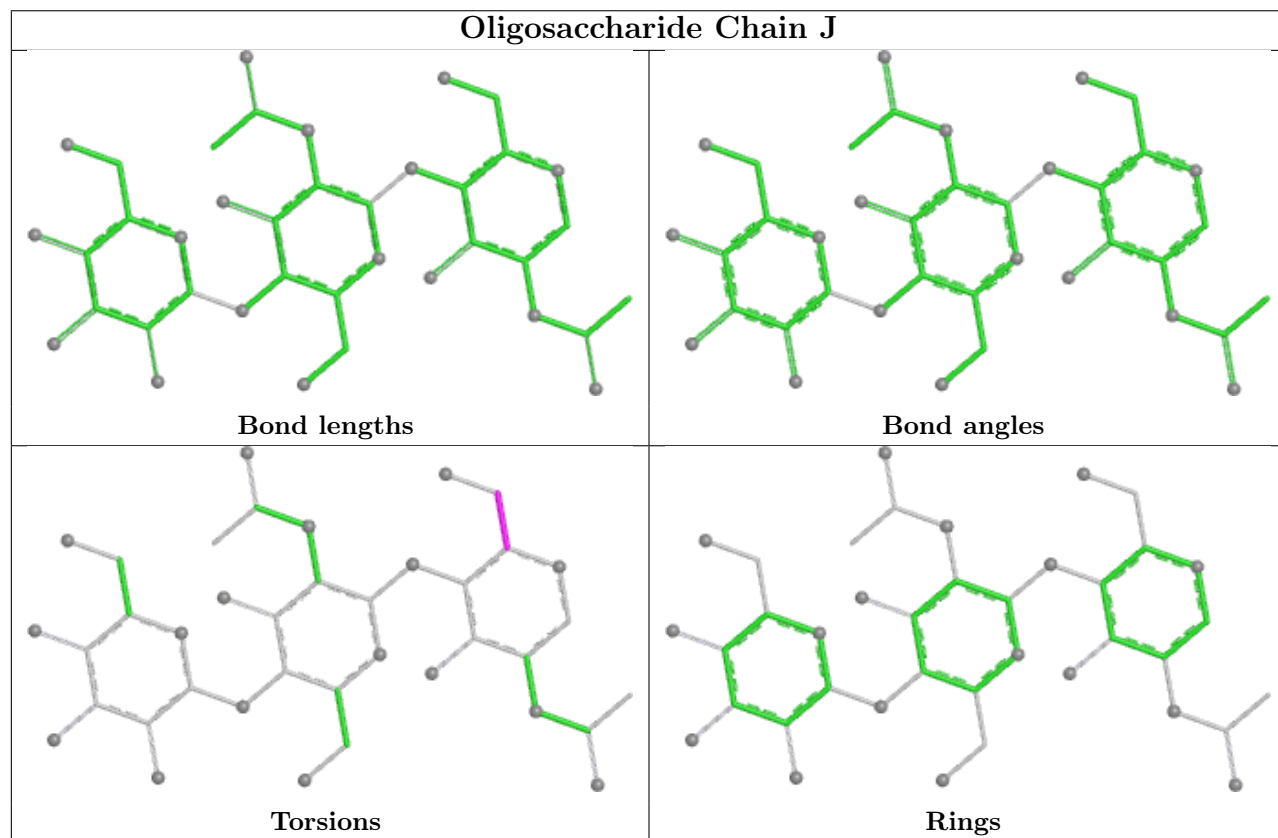
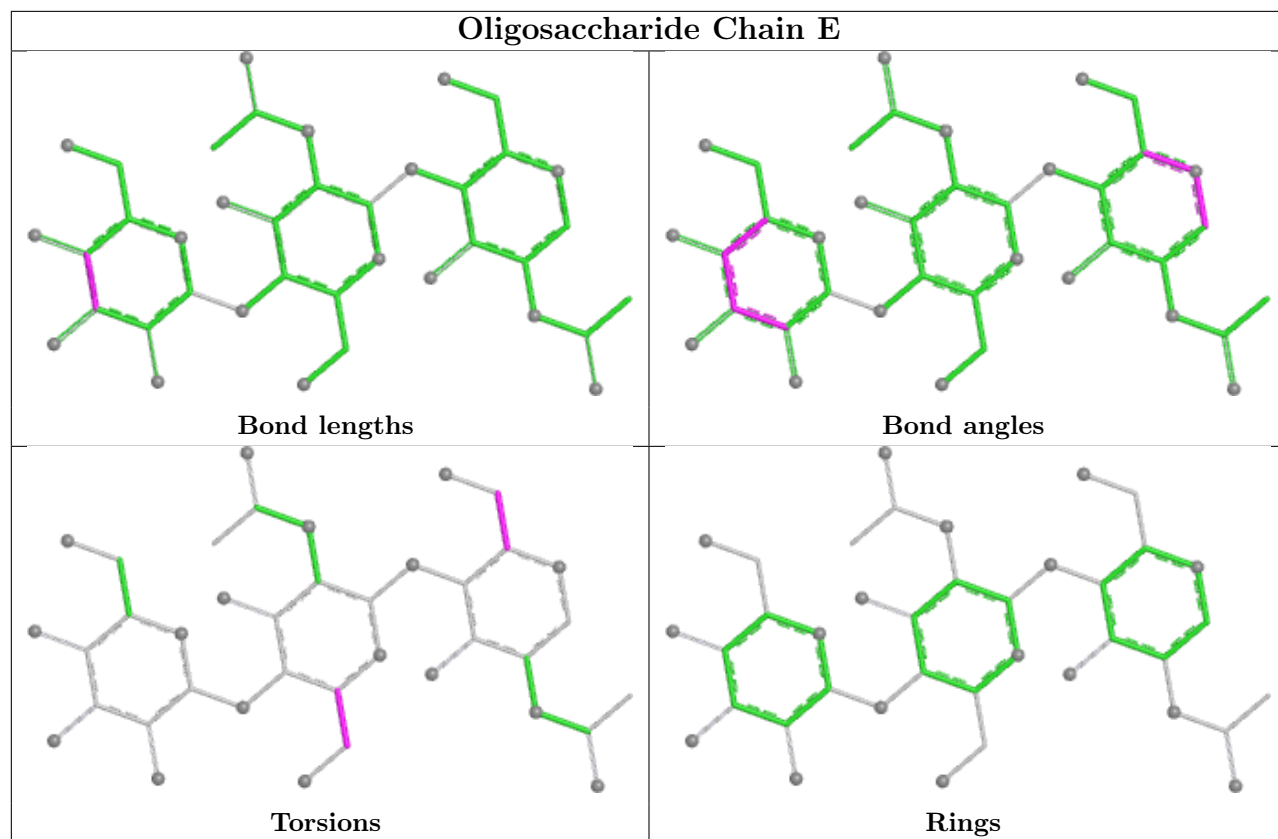


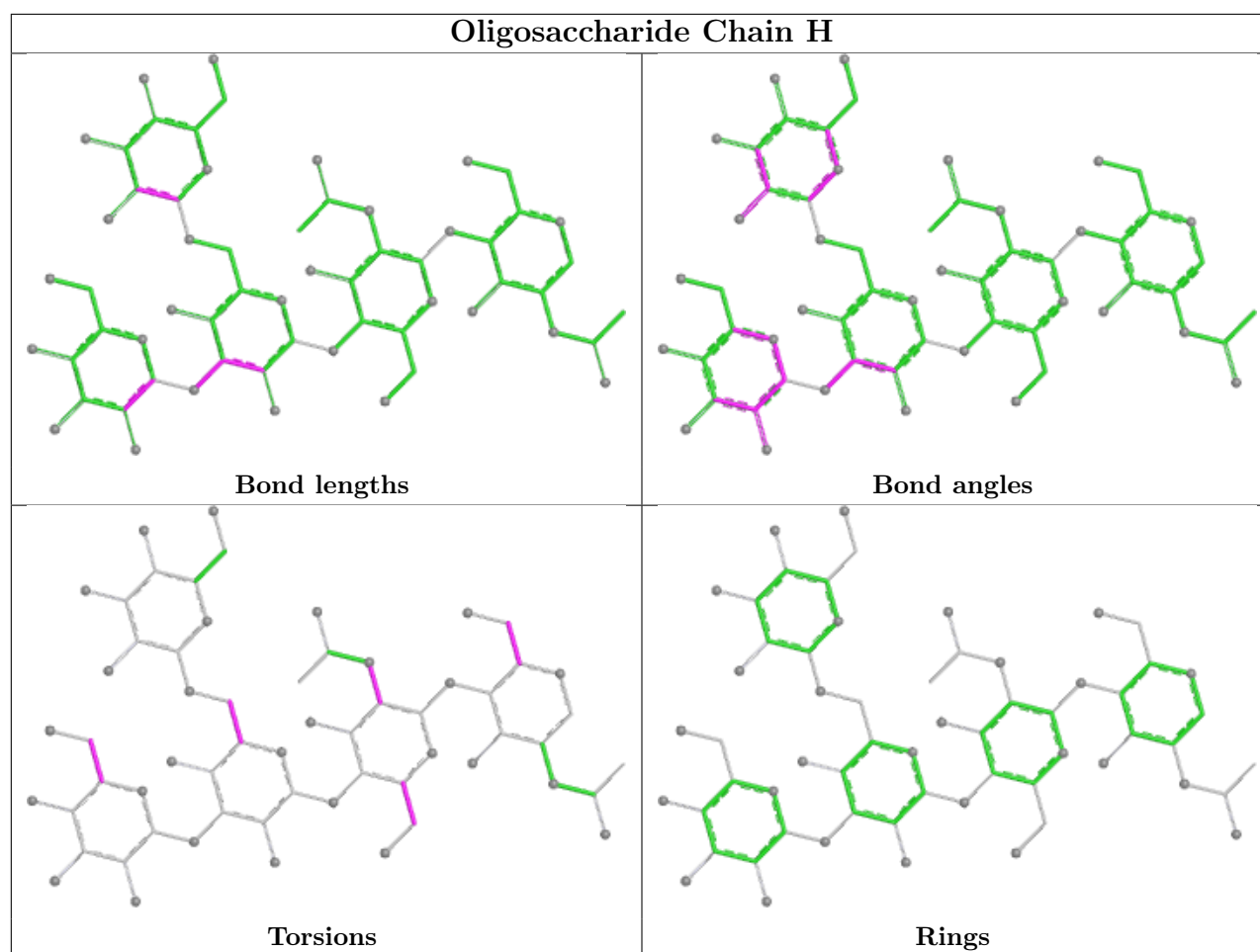


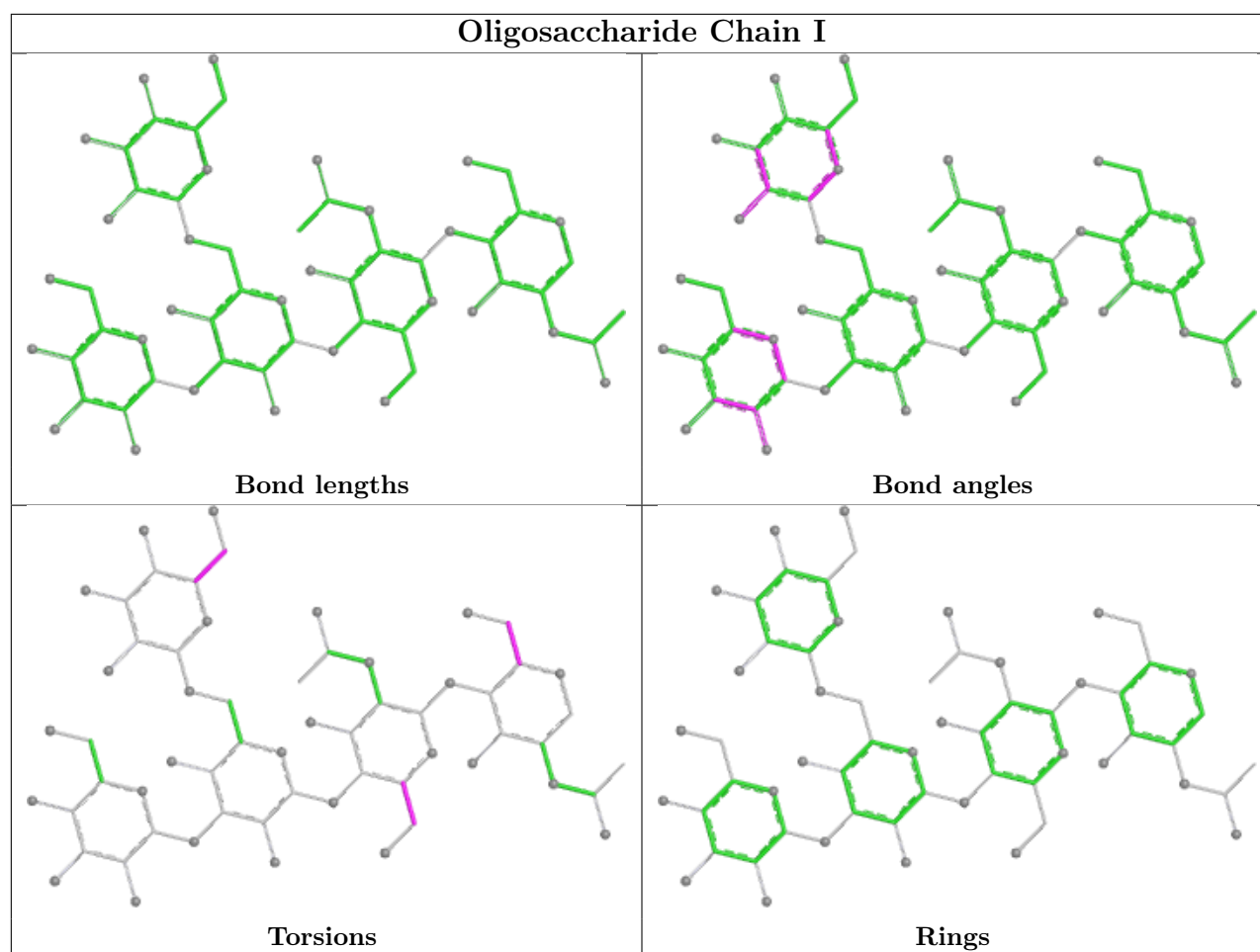












5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 2 are monoatomic - leaving 25 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	EDO	A	1108	-	3,3,3	0.42	0	2,2,2	0.39	0
7	NAG	B	1803	1	14,14,15	1.10	2 (14%)	17,19,21	0.84	1 (5%)
9	EDO	B	1808	-	3,3,3	0.42	0	2,2,2	0.43	0
9	EDO	A	1109	-	3,3,3	0.43	0	2,2,2	0.39	0
7	NAG	B	1813	1,7	14,14,15	0.48	0	17,19,21	0.86	1 (5%)
9	EDO	B	1805	-	3,3,3	0.43	0	2,2,2	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	B	1811	7	14,14,15	0.63	1 (7%)	17,19,21	0.94	0
9	EDO	A	1107	-	3,3,3	0.45	0	2,2,2	0.34	0
9	EDO	B	1806	-	3,3,3	0.44	0	2,2,2	0.40	0
10	PEG	A	1111	-	6,6,6	0.50	0	5,5,5	0.28	0
9	EDO	B	1804	-	3,3,3	0.43	0	2,2,2	0.41	0
8	KFR	A	1106	6	41,41,41	1.73	8 (19%)	53,56,56	1.07	3 (5%)
7	NAG	B	1814	1	14,14,15	0.72	1 (7%)	17,19,21	1.74	1 (5%)
11	TRS	B	1807	-	7,7,7	0.33	0	9,9,9	0.35	0
7	NAG	B	1810	1,7	14,14,15	0.79	0	17,19,21	1.41	1 (5%)
7	NAG	A	1105	1	14,14,15	0.31	0	17,19,21	0.62	0
7	NAG	A	1103	1	14,14,15	0.36	0	17,19,21	0.48	0
7	NAG	A	1102	1	14,14,15	0.19	0	17,19,21	0.57	0
8	KFR	B	1815[A]	6	41,41,41	1.76	8 (19%)	53,56,56	1.03	4 (7%)
7	NAG	B	1802	1	14,14,15	1.01	1 (7%)	17,19,21	0.80	1 (5%)
10	PEG	B	1809	-	6,6,6	0.51	0	5,5,5	0.28	0
7	NAG	B	1812	7	14,14,15	0.66	1 (7%)	17,19,21	0.70	0
7	NAG	A	1104	1	14,14,15	0.87	1 (7%)	17,19,21	0.89	0
8	KFR	B	1815[B]	6	41,41,41	1.77	8 (19%)	53,56,56	1.05	4 (7%)
10	PEG	A	1110	-	6,6,6	0.51	0	5,5,5	0.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	A	1108	-	-	0/1/1/1	-
7	NAG	B	1803	1	-	2/6/23/26	0/1/1/1
9	EDO	B	1808	-	-	0/1/1/1	-
9	EDO	A	1109	-	-	0/1/1/1	-
7	NAG	B	1813	1,7	-	1/6/23/26	0/1/1/1
9	EDO	B	1805	-	-	0/1/1/1	-
7	NAG	B	1811	7	-	1/6/23/26	0/1/1/1
9	EDO	A	1107	-	-	1/1/1/1	-
9	EDO	B	1806	-	-	1/1/1/1	-
10	PEG	A	1111	-	-	3/4/4/4	-
9	EDO	B	1804	-	-	1/1/1/1	-
8	KFR	A	1106	6	-	15/39/48/48	0/3/3/3
7	NAG	B	1814	1	-	3/6/23/26	0/1/1/1
11	TRS	B	1807	-	-	0/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	1810	1,7	-	4/6/23/26	0/1/1/1
7	NAG	A	1105	1	-	3/6/23/26	0/1/1/1
7	NAG	A	1103	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1102	1	-	0/6/23/26	0/1/1/1
8	KFR	B	1815[A]	6	-	13/39/48/48	0/3/3/3
7	NAG	B	1802	1	-	2/6/23/26	0/1/1/1
10	PEG	B	1809	-	-	0/4/4/4	-
7	NAG	B	1812	7	-	1/6/23/26	0/1/1/1
7	NAG	A	1104	1	-	3/6/23/26	0/1/1/1
8	KFR	B	1815[B]	6	-	9/39/48/48	0/3/3/3
10	PEG	A	1110	-	-	0/4/4/4	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1815[B]	KFR	C06-N08	5.66	1.46	1.34
8	B	1815[A]	KFR	C06-N08	5.60	1.46	1.34
8	B	1815[B]	KFR	C25-N24	5.50	1.45	1.34
8	A	1106	KFR	C06-N08	5.49	1.45	1.34
8	B	1815[A]	KFR	C25-N24	5.40	1.45	1.34
8	A	1106	KFR	C25-N24	5.37	1.45	1.34
8	B	1815[A]	KFR	C15-C14	-3.46	1.37	1.41
8	B	1815[B]	KFR	C15-C14	-3.40	1.37	1.41
7	B	1803	NAG	C1-C2	3.26	1.56	1.52
7	B	1802	NAG	C1-C2	3.25	1.56	1.52
8	A	1106	KFR	C15-C14	-3.22	1.37	1.41
7	A	1104	NAG	C1-C2	3.07	1.56	1.52
8	A	1106	KFR	O22-C20	2.91	1.40	1.33
8	B	1815[B]	KFR	O22-C20	2.91	1.40	1.33
8	B	1815[A]	KFR	O22-C20	2.87	1.40	1.33
8	B	1815[A]	KFR	C12-N13	-2.71	1.32	1.37
8	A	1106	KFR	C12-N13	-2.66	1.32	1.37
8	B	1815[B]	KFR	C12-N13	-2.63	1.32	1.37
8	A	1106	KFR	O07-C06	-2.39	1.18	1.23
8	B	1815[A]	KFR	O26-C25	-2.36	1.18	1.23
8	A	1106	KFR	O26-C25	-2.36	1.18	1.23
8	B	1815[B]	KFR	O26-C25	-2.35	1.18	1.23
8	B	1815[B]	KFR	O07-C06	-2.28	1.19	1.23
8	B	1815[A]	KFR	O07-C06	-2.28	1.19	1.23
7	B	1803	NAG	O5-C1	2.24	1.47	1.43
8	A	1106	KFR	O22-C23	-2.21	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1815[A]	KFR	O22-C23	-2.19	1.40	1.45
7	B	1812	NAG	O5-C1	2.18	1.47	1.43
8	B	1815[B]	KFR	O22-C23	-2.18	1.40	1.45
7	B	1811	NAG	O5-C1	2.16	1.47	1.43
7	B	1814	NAG	C1-C2	2.05	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1814	NAG	C2-N2-C7	6.52	131.64	122.90
7	B	1810	NAG	C1-O5-C5	4.56	118.30	112.19
8	B	1815[A]	KFR	O22-C20-C09	3.49	120.36	111.49
8	B	1815[B]	KFR	O22-C20-C09	3.48	120.34	111.49
8	A	1106	KFR	O22-C20-C09	3.30	119.89	111.49
8	B	1815[B]	KFR	C27-C25-N24	2.83	120.06	116.22
8	B	1815[A]	KFR	C19-C14-C15	-2.71	119.56	122.19
8	A	1106	KFR	C19-C14-C15	-2.57	119.70	122.19
8	A	1106	KFR	C27-C25-N24	2.46	119.56	116.22
8	B	1815[B]	KFR	C19-C14-C15	-2.42	119.84	122.19
8	B	1815[A]	KFR	C27-C25-N24	2.37	119.43	116.22
7	B	1803	NAG	C2-N2-C7	2.29	125.97	122.90
8	B	1815[A]	KFR	O22-C20-O21	-2.19	119.59	123.85
7	B	1802	NAG	C4-C3-C2	2.10	114.10	111.02
7	B	1813	NAG	C2-N2-C7	2.04	125.63	122.90
8	B	1815[B]	KFR	O22-C20-O21	-2.02	119.91	123.85

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1104	NAG	C1-C2-N2-C7
7	A	1105	NAG	C1-C2-N2-C7
7	B	1813	NAG	C1-C2-N2-C7
7	B	1814	NAG	C3-C2-N2-C7
8	A	1106	KFR	C25-C27-C28-C29
8	A	1106	KFR	C25-C27-C28-N38
8	A	1106	KFR	O39-C27-C28-N38
8	B	1815[A]	KFR	N08-C09-C10-C11
8	B	1815[A]	KFR	C09-C20-O22-C23
7	A	1103	NAG	C4-C5-C6-O6
8	B	1815[B]	KFR	C09-C20-O22-C23
8	B	1815[A]	KFR	O21-C20-O22-C23

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Mol	Chain	Res	Type	Atoms
7	A	1103	NAG	O5-C5-C6-O6
8	A	1106	KFR	C09-C20-O22-C23
7	B	1803	NAG	O5-C5-C6-O6
7	B	1802	NAG	C4-C5-C6-O6
8	B	1815[B]	KFR	O21-C20-O22-C23
7	A	1104	NAG	O5-C5-C6-O6
7	B	1810	NAG	O5-C5-C6-O6
7	A	1104	NAG	C4-C5-C6-O6
10	A	1111	PEG	C1-C2-O2-C3
7	B	1810	NAG	C8-C7-N2-C2
7	B	1810	NAG	O7-C7-N2-C2
7	B	1814	NAG	C8-C7-N2-C2
7	B	1814	NAG	O7-C7-N2-C2
8	B	1815[A]	KFR	C02-C04-C05-C06
10	A	1111	PEG	O2-C3-C4-O4
8	B	1815[B]	KFR	C02-C04-C05-C06
7	B	1803	NAG	C4-C5-C6-O6
10	A	1111	PEG	O1-C1-C2-O2
7	A	1105	NAG	O5-C5-C6-O6
8	A	1106	KFR	O21-C20-O22-C23
7	B	1810	NAG	C4-C5-C6-O6
7	B	1802	NAG	O5-C5-C6-O6
8	B	1815[A]	KFR	C20-C09-C10-C11
8	B	1815[A]	KFR	C02-C04-C05-N24
8	B	1815[B]	KFR	C02-C04-C05-N24
7	B	1811	NAG	O5-C5-C6-O6
9	A	1107	EDO	O1-C1-C2-O2
7	B	1812	NAG	O5-C5-C6-O6
8	A	1106	KFR	N24-C25-C27-O39
8	B	1815[A]	KFR	N24-C25-C27-O39
8	A	1106	KFR	C02-C04-C05-C06
8	B	1815[A]	KFR	C03-C02-C04-C05
8	B	1815[B]	KFR	N24-C05-C06-O07
8	A	1106	KFR	O39-C27-C28-C29
9	B	1806	EDO	O1-C1-C2-O2
8	B	1815[B]	KFR	N24-C05-C06-N08
8	B	1815[A]	KFR	N24-C05-C06-O07
8	B	1815[B]	KFR	C03-C02-C04-C05
8	A	1106	KFR	O26-C25-C27-O39
8	B	1815[A]	KFR	O26-C25-C27-O39
7	A	1105	NAG	C4-C5-C6-O6
8	A	1106	KFR	C02-C04-C05-N24

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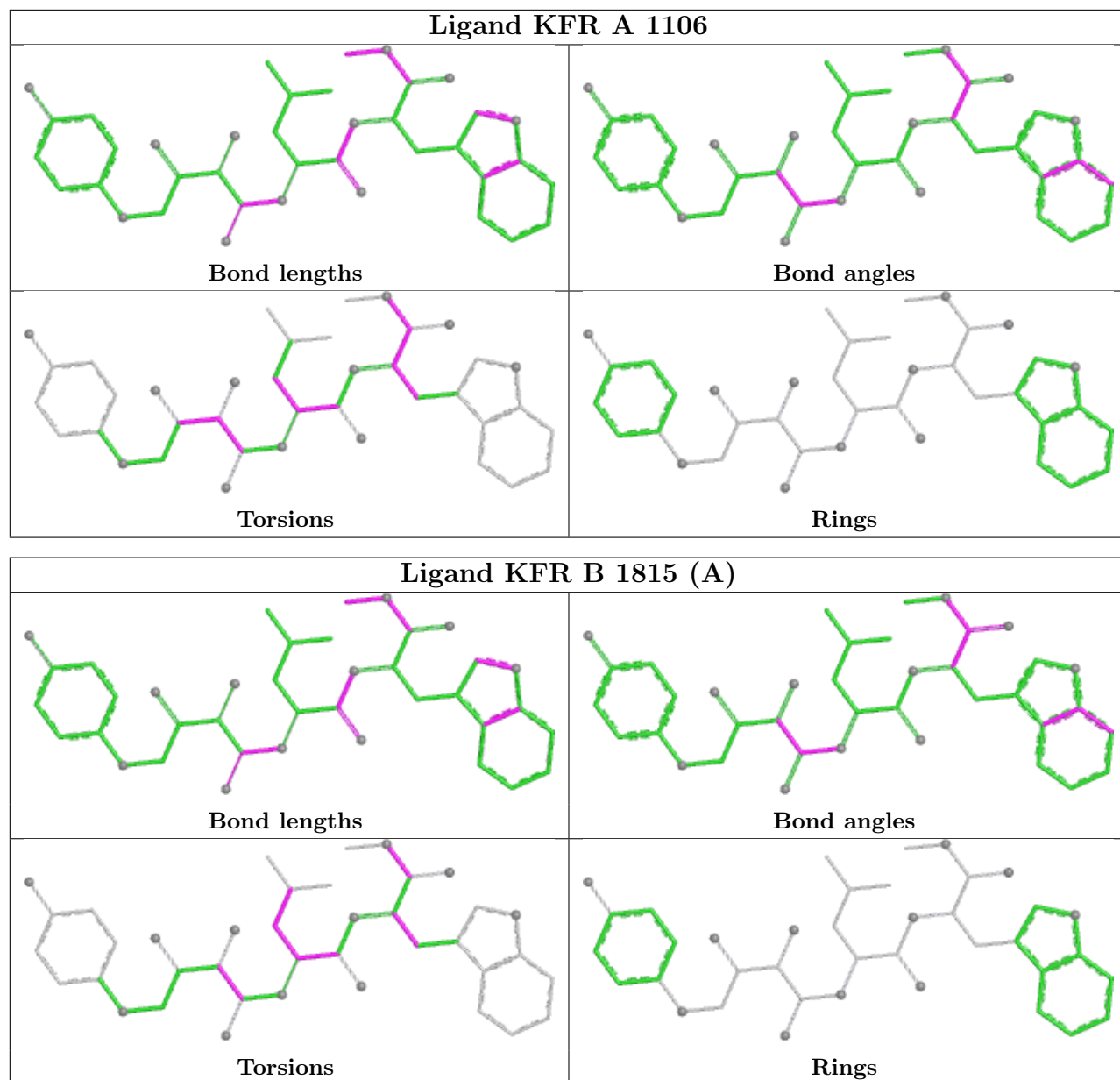
Mol	Chain	Res	Type	Atoms
8	B	1815[A]	KFR	C04-C05-C06-O07
8	B	1815[A]	KFR	N24-C05-C06-N08
9	B	1804	EDO	O1-C1-C2-O2
8	A	1106	KFR	N08-C09-C10-C11
8	B	1815[A]	KFR	C04-C05-C06-N08
8	A	1106	KFR	C20-C09-C10-C11
8	A	1106	KFR	N08-C09-C20-O22
8	A	1106	KFR	N08-C09-C20-O21
8	B	1815[B]	KFR	O26-C25-C27-O39
8	A	1106	KFR	N24-C05-C06-O07
8	B	1815[B]	KFR	N24-C25-C27-O39

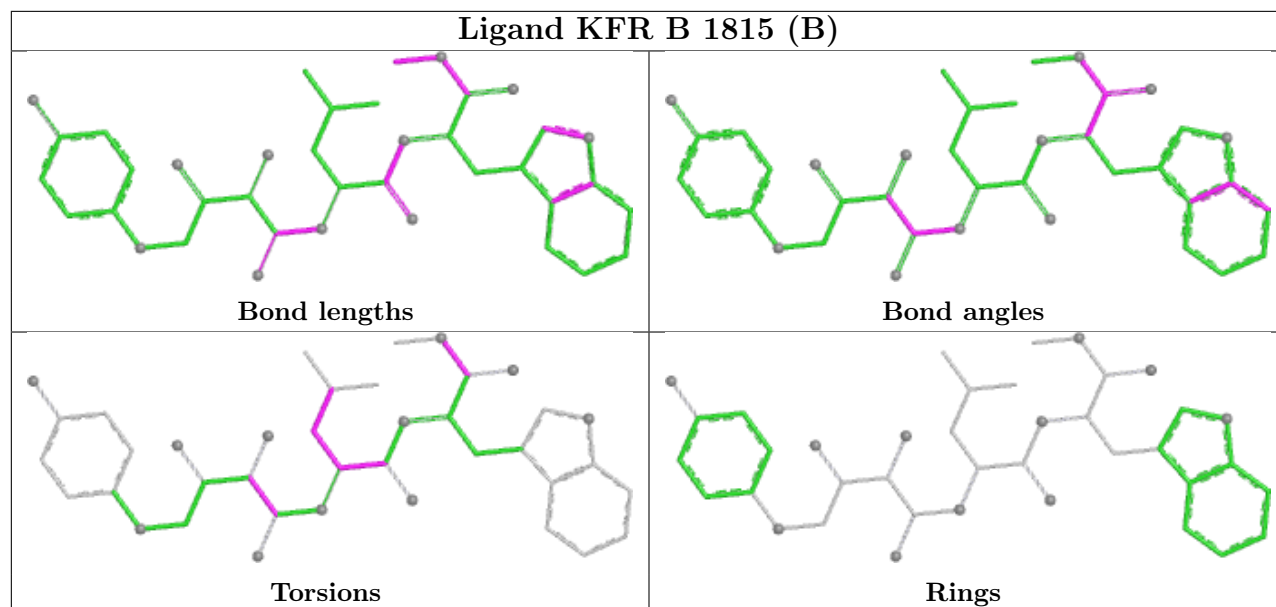
There are no ring outliers.

9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1813	NAG	2	0
7	B	1814	NAG	3	0
7	B	1810	NAG	2	0
7	A	1103	NAG	1	0
7	A	1102	NAG	1	0
8	B	1815[A]	KFR	2	0
7	B	1802	NAG	1	0
7	A	1104	NAG	2	0
8	B	1815[B]	KFR	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	852/871 (97%)	1.17	160 (18%) 3 2	8, 33, 62, 96	4 (0%)
1	B	854/871 (98%)	1.44	225 (26%) 1 1	7, 39, 68, 115	2 (0%)
All	All	1706/1742 (97%)	1.31	385 (22%) 2 1	7, 36, 66, 115	6 (0%)

All (385) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	639	MET	8.0
1	B	222	MET	7.3
1	A	665	TYR	6.8
1	B	638	ASN	6.7
1	A	917	ASP	6.2
1	A	662	GLY	6.2
1	A	347	GLU	6.1
1	B	346	ASP	5.6
1	B	326	THR	5.5
1	B	337	VAL	5.3
1	B	347	GLU	5.3
1	B	637	LEU	5.2
1	A	885	GLY	5.1
1	B	758	ASN	5.1
1	B	339	LEU	5.0
1	A	281	ASP	4.8
1	B	665	TYR	4.8
1	A	375	GLY	4.7
1	A	160	LEU	4.6
1	B	401	LEU	4.6
1	A	448	ASN	4.5
1	B	338	VAL	4.5
1	B	794[A]	ARG	4.5
1	A	186	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	184	ASN	4.3
1	A	340	ASP	4.3
1	B	664	ASN	4.3
1	A	447	SER	4.3
1	B	601	LEU	4.2
1	B	336	SER	4.2
1	B	319	ILE	4.2
1	A	666	SER	4.1
1	B	858	ASP	4.1
1	A	179	LEU	4.1
1	B	383	VAL	4.1
1	B	180	SER	4.1
1	B	343	LEU	4.1
1	A	916	GLY	4.1
1	B	375	GLY	4.1
1	B	426	GLU	4.1
1	B	281	ASP	4.1
1	B	384	PRO	4.1
1	B	662	GLY	4.0
1	A	178	GLU	4.0
1	B	434	GLY	4.0
1	B	181	LEU	4.0
1	B	268	SER	4.0
1	B	447	SER	3.9
1	B	408	PHE	3.9
1	B	666	SER	3.9
1	B	341	ASP	3.9
1	A	1024	TRP	3.9
1	A	664	ASN	3.8
1	B	197	SER	3.8
1	B	569	GLN	3.8
1	A	280	THR	3.8
1	B	335	SER	3.8
1	B	668	TYR	3.8
1	B	684	THR	3.8
1	B	454	ASP	3.7
1	A	740	GLY	3.7
1	B	324	GLN	3.7
1	A	336	SER	3.7
1	A	668	TYR	3.7
1	B	402	GLU	3.7
1	A	1023	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	229	GLU	3.7
1	B	600	THR	3.7
1	A	595	GLU	3.6
1	B	1024	TRP	3.6
1	B	284	ASN	3.6
1	B	332	PRO	3.6
1	B	317	ILE	3.5
1	B	414	LEU	3.5
1	A	886	SER	3.5
1	B	385	GLU	3.5
1	B	741	LEU	3.5
1	B	364	GLY	3.5
1	A	326	THR	3.5
1	B	374	ASN	3.5
1	B	274	PHE	3.4
1	A	499[A]	GLU	3.4
1	B	322	ASP	3.4
1	A	269	SER	3.4
1	B	227	SER	3.4
1	B	636	PHE	3.4
1	B	413	PRO	3.4
1	B	344	VAL	3.3
1	B	316	ILE	3.3
1	B	391[A]	HIS	3.3
1	B	190	PHE	3.3
1	B	342	GLY	3.3
1	A	227	SER	3.3
1	B	465	GLU	3.3
1	B	320	ILE	3.3
1	B	594	ASN	3.2
1	A	741	LEU	3.2
1	B	663	ARG	3.2
1	A	158	GLY	3.2
1	A	325	TYR	3.2
1	B	327	ALA	3.2
1	B	272	TYR	3.2
1	B	278	SER	3.2
1	B	578	ASN	3.2
1	A	365	GLU	3.2
1	B	188	MET	3.2
1	B	786	ASP	3.2
1	B	917	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	406	ASN	3.2
1	A	637	LEU	3.2
1	B	570	HIS	3.2
1	B	158	GLY	3.2
1	A	440	GLU	3.2
1	B	400	LEU	3.1
1	B	716	LEU	3.1
1	B	805	GLN	3.1
1	B	221	PHE	3.1
1	A	684	THR	3.1
1	A	185	LEU	3.1
1	A	197	SER	3.1
1	A	162	PRO	3.1
1	B	427	ALA	3.1
1	A	272[A]	TYR	3.1
1	B	1020	SER	3.1
1	B	825	GLU	3.1
1	A	373	VAL	3.0
1	A	180	SER	3.0
1	A	228	GLN	3.0
1	B	233	GLU	3.0
1	A	597	THR	3.0
1	A	222	MET	3.0
1	A	270	SER	3.0
1	A	341[A]	ASP	3.0
1	B	835	CYS	3.0
1	B	650	TYR	3.0
1	B	399	LYS	3.0
1	B	228	GLN	3.0
1	B	351	SER	3.0
1	B	395	GLU	3.0
1	A	601	LEU	2.9
1	A	758	ASN	2.9
1	B	844	ASP	2.9
1	B	380	ILE	2.9
1	B	174	PRO	2.9
1	A	374	ASN	2.9
1	A	706	ASP	2.9
1	B	682	ASN	2.9
1	A	991	SER	2.9
1	A	739	ALA	2.9
1	B	387	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	248	PRO	2.9
1	A	350	GLU	2.9
1	A	570	HIS	2.9
1	A	754	ASN	2.9
1	A	1020	SER	2.9
1	A	442	THR	2.9
1	B	229	GLU	2.8
1	B	542	GLU	2.8
1	A	636	PHE	2.8
1	B	321	ARG	2.8
1	B	719	ASN	2.8
1	B	361	PHE	2.8
1	B	1025	LEU	2.8
1	A	600	THR	2.8
1	B	366	MET	2.8
1	B	373	VAL	2.8
1	B	392	TYR	2.8
1	A	403	PHE	2.8
1	A	252	LEU	2.8
1	A	1016	LYS	2.8
1	B	885	GLY	2.8
1	A	233	GLU	2.7
1	B	289	PHE	2.7
1	A	335	SER	2.7
1	A	364	GLY	2.7
1	B	262	GLU	2.7
1	A	333	LYS	2.7
1	B	850	ASN	2.7
1	B	280	THR	2.7
1	B	595	GLU	2.7
1	B	348	PHE	2.7
1	B	683	LEU	2.7
1	B	186	THR	2.7
1	B	431	GLU	2.7
1	A	316	ILE	2.7
1	B	1023	TRP	2.7
1	A	213	GLY	2.7
1	A	385	GLU	2.7
1	B	285	GLU	2.7
1	B	323	GLU	2.7
1	A	537	SER	2.7
1	A	1025	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	760	ASN	2.6
1	B	360	ALA	2.6
1	B	991	SER	2.6
1	B	783	GLY	2.6
1	A	159	LYS	2.6
1	A	212	THR	2.6
1	B	396	THR	2.6
1	B	449	THR	2.6
1	B	503	LYS	2.6
1	B	1015	GLU	2.6
1	B	848	ALA	2.6
1	B	269	SER	2.6
1	A	742	GLY	2.6
1	B	615	GLY	2.6
1	B	334	LYS	2.6
1	A	170	THR	2.6
1	B	457	LEU	2.6
1	B	405	GLN	2.6
1	A	238	ALA	2.6
1	B	510	ASP	2.6
1	A	836	SER	2.6
1	B	428	GLY	2.6
1	B	363	VAL	2.6
1	A	426	GLU	2.6
1	A	710	GLU	2.6
1	A	266	ASN	2.6
1	B	739	ALA	2.6
1	A	773	ASP	2.6
1	A	351	SER	2.5
1	A	873	GLY	2.5
1	A	718	ILE	2.5
1	A	685	GLU	2.5
1	B	440	GLU	2.5
1	B	448	ASN	2.5
1	B	418	ASP	2.5
1	B	649	SER	2.5
1	A	603	VAL	2.5
1	B	315	PHE	2.5
1	B	330	ASN	2.5
1	B	386	LYS	2.5
1	A	268	SER	2.5
1	B	187	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	183	PRO	2.5
1	B	325	TYR	2.5
1	B	403	PHE	2.5
1	B	333	LYS	2.5
1	A	786	ASP	2.5
1	A	259	LEU	2.5
1	B	259	LEU	2.5
1	B	450	SER	2.5
1	A	271	TYR	2.5
1	B	303	PHE	2.5
1	A	663	ARG	2.5
1	B	773	ASP	2.4
1	A	450	SER	2.4
1	B	283	SER	2.4
1	B	258	THR	2.4
1	B	406	ASN	2.4
1	A	181	LEU	2.4
1	B	867	GLY	2.4
1	A	564	SER	2.4
1	A	686	GLU	2.4
1	B	271	TYR	2.4
1	A	314	THR	2.4
1	B	185	LEU	2.4
1	B	362	ILE	2.4
1	A	301	SER	2.4
1	A	649	SER	2.4
1	B	849	SER	2.4
1	B	445	TYR	2.4
1	B	376	THR	2.4
1	A	332	PRO	2.4
1	B	256	ASN	2.4
1	B	232	ALA	2.4
1	B	613	GLN	2.4
1	B	853	GLN	2.4
1	A	239	TYR	2.4
1	A	449	THR	2.4
1	A	417	LEU	2.4
1	B	573	VAL	2.3
1	B	950	ASN	2.3
1	B	625	GLY	2.3
1	A	327	ALA	2.3
1	B	780	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	949	TRP	2.3
1	B	288	TYR	2.3
1	B	793	THR	2.3
1	B	952	LEU	2.3
1	B	273	GLY	2.3
1	A	835[A]	CYS	2.3
1	A	283	SER	2.3
1	B	523	SER	2.3
1	B	255	HIS	2.3
1	A	196	ILE	2.3
1	A	319	ILE	2.3
1	A	387	ILE	2.3
1	B	397	THR	2.3
1	A	303	PHE	2.3
1	B	250	ALA	2.3
1	B	365	GLU	2.3
1	B	685	GLU	2.3
1	A	346	ASP	2.3
1	B	672	SER	2.3
1	B	212	THR	2.3
1	A	177	TYR	2.3
1	B	279	TYR	2.3
1	B	558	MET	2.3
1	A	651	LEU	2.3
1	A	609	THR	2.3
1	B	875	SER	2.3
1	B	412	TYR	2.3
1	A	918	ASN	2.2
1	A	389	GLN	2.2
1	A	920	ARG	2.2
1	A	929	ARG	2.2
1	B	634	ARG	2.2
1	A	258	THR	2.2
1	B	193	SER	2.2
1	A	232	ALA	2.2
1	B	230	LYS	2.2
1	B	760	ASN	2.2
1	B	940	LEU	2.2
1	A	573	VAL	2.2
1	A	263	TYR	2.2
1	B	270	SER	2.2
1	A	244	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	427	ALA	2.2
1	B	432	ASN	2.2
1	B	245	ILE	2.2
1	B	929	ARG	2.2
1	A	391	HIS	2.2
1	A	561	THR	2.2
1	B	329	SER	2.2
1	B	531	SER	2.2
1	B	393	ALA	2.2
1	A	605	ARG	2.2
1	A	804	GLN	2.2
1	B	420	VAL	2.2
1	B	596	VAL	2.2
1	B	602	ASP	2.2
1	B	614	LYS	2.2
1	A	221	PHE	2.2
1	B	257	TYR	2.2
1	A	960	SER	2.2
1	A	669	GLN	2.1
1	A	871	ASP	2.1
1	A	192	GLY	2.1
1	A	195	THR	2.1
1	B	611	THR	2.1
1	A	650	TYR	2.1
1	B	282	GLU	2.1
1	B	633	GLU	2.1
1	A	317	ILE	2.1
1	B	989	ASN	2.1
1	B	720	PRO	2.1
1	B	744	VAL	2.1
1	A	625	GLY	2.1
1	A	250	ALA	2.1
1	B	299	ALA	2.1
1	A	981	SER	2.1
1	A	834	ASN	2.1
1	B	266	ASN	2.1
1	B	388	GLY	2.1
1	B	725	ASP	2.1
1	B	740	GLY	2.1
1	A	331	MET	2.1
1	A	284	ASN	2.1
1	B	394	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	882	ILE	2.1
1	A	465	GLU	2.1
1	A	451	SER	2.0
1	A	989	ASN	2.0
1	B	748	ARG	2.0
1	A	454	ASP	2.0
1	A	566	ASP	2.0
1	A	675	ASP	2.0
1	A	1015	GLU	2.0
1	B	689	TRP	2.0
1	B	1019	LYS	2.0
1	A	606	MET	2.0
1	A	883	SER	2.0
1	B	378	VAL	2.0
1	B	377	LEU	2.0
1	B	417	LEU	2.0
1	B	455	ARG	2.0
1	B	882	ILE	2.0
1	A	397	THR	2.0
1	A	852	THR	2.0
1	A	1022	THR	2.0
1	A	441	GLU	2.0
1	B	372	ASP	2.0
1	B	246	VAL	2.0
1	B	866	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	J	3	11/12	0.19	0.26	92,94,97,98	0
5	BMA	H	3	11/12	0.36	0.24	90,97,100,100	0
5	MAN	H	5	11/12	0.39	0.24	83,87,89,89	0

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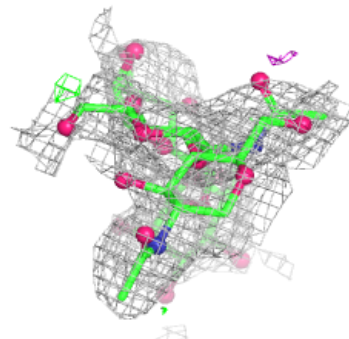
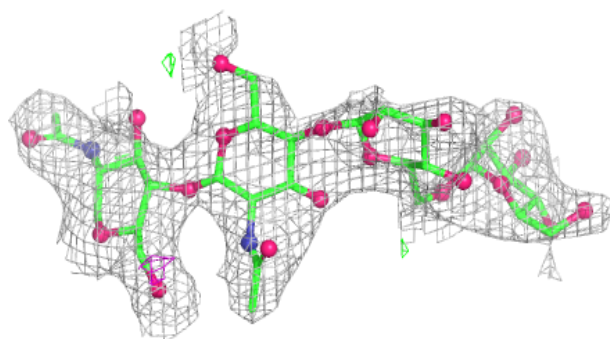
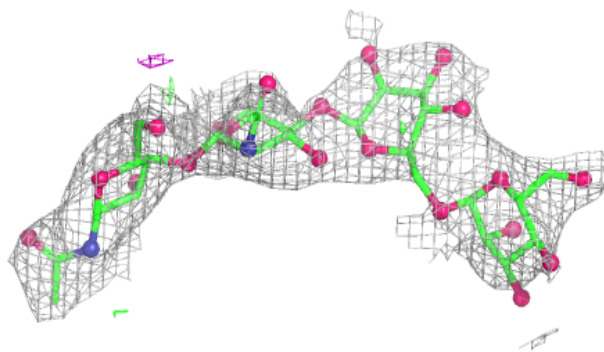
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	H	2	14/15	0.46	0.26	105,113,117,118	0
4	NAG	J	2	14/15	0.49	0.26	85,90,91,91	0
5	MAN	H	4	11/12	0.50	0.26	80,82,84,86	0
3	NAG	F	2	14/15	0.51	0.25	60,68,69,72	0
3	NAG	G	2	14/15	0.51	0.26	82,87,89,93	0
3	NAG	G	1	14/15	0.52	0.35	104,109,116,117	0
3	NAG	F	1	14/15	0.52	0.23	79,87,89,94	0
4	BMA	E	3	11/12	0.52	0.20	73,75,76,77	0
3	NAG	K	1	14/15	0.53	0.28	121,128,131,131	0
5	NAG	I	2	14/15	0.55	0.23	47,60,62,65	0
5	NAG	H	1	14/15	0.57	0.27	91,103,108,114	0
2	BMA	C	3	11/12	0.57	0.22	76,79,81,82	0
5	MAN	I	4	11/12	0.57	0.18	83,86,88,88	0
5	MAN	I	5	11/12	0.57	0.25	68,71,73,75	0
3	NAG	K	2	14/15	0.65	0.24	76,89,94,101	0
5	NAG	I	1	14/15	0.67	0.26	63,67,75,76	0
5	BMA	I	3	11/12	0.68	0.19	68,69,73,78	0
4	NAG	J	1	14/15	0.68	0.21	76,83,89,92	0
2	NAG	C	2	14/15	0.68	0.22	67,71,74,79	0
3	NAG	D	2	14/15	0.70	0.16	59,65,70,71	0
4	NAG	E	2	14/15	0.73	0.20	68,73,76,78	0
2	MAN	C	4	11/12	0.77	0.18	64,68,71,71	0
4	NAG	E	1	14/15	0.78	0.19	39,48,52,60	0
2	NAG	C	1	14/15	0.82	0.16	42,47,54,61	0
3	NAG	D	1	14/15	0.84	0.12	37,43,49,53	0

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

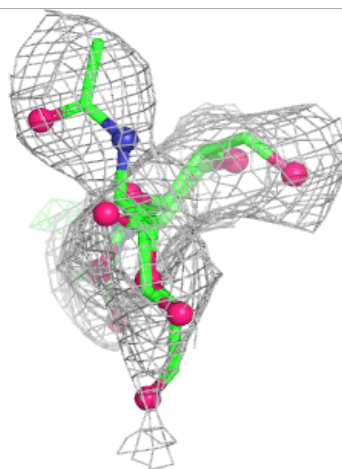
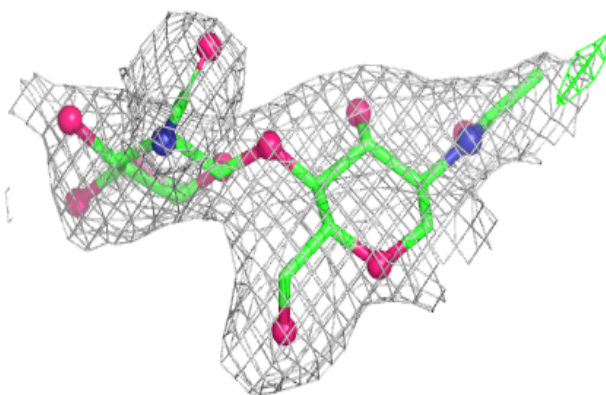
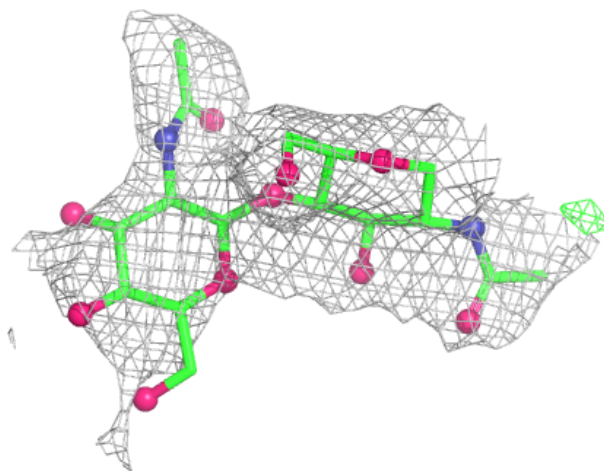
Electron density around Chain C:

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



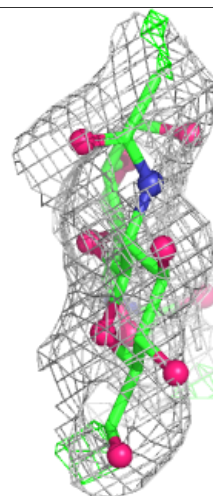
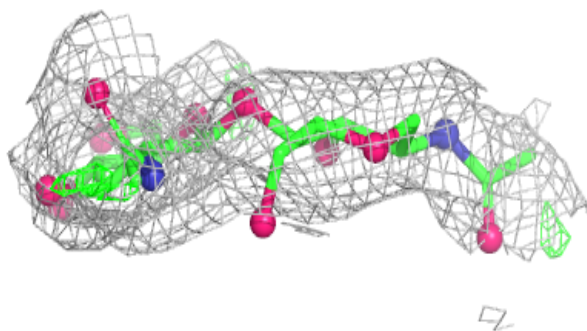
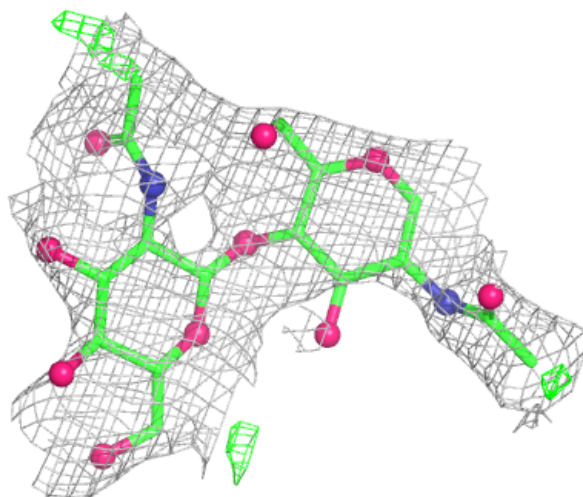
Electron density around Chain D:

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



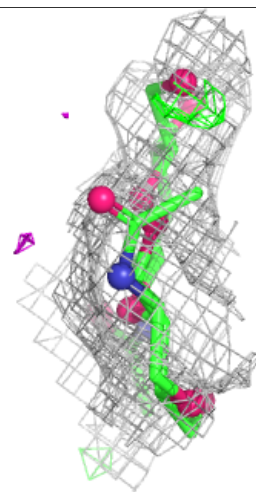
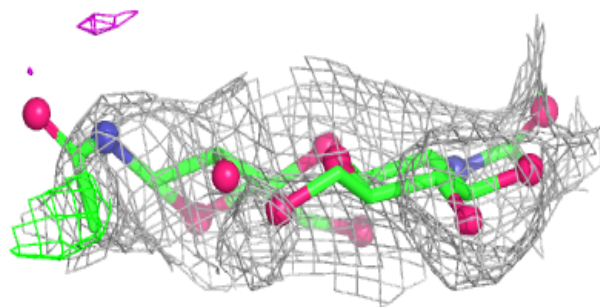
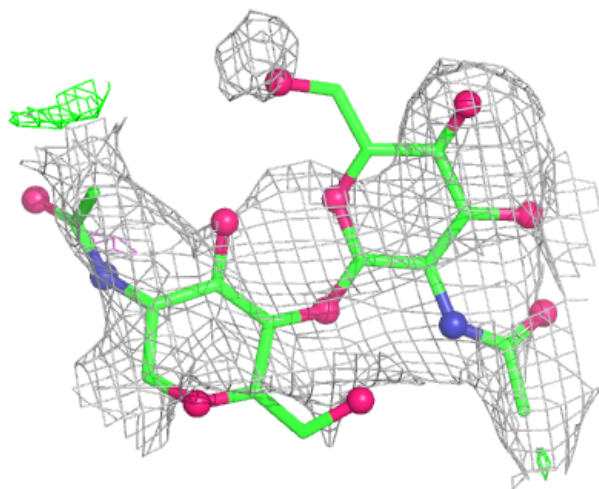
Electron density around Chain F:

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



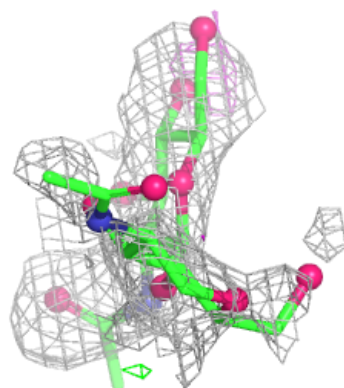
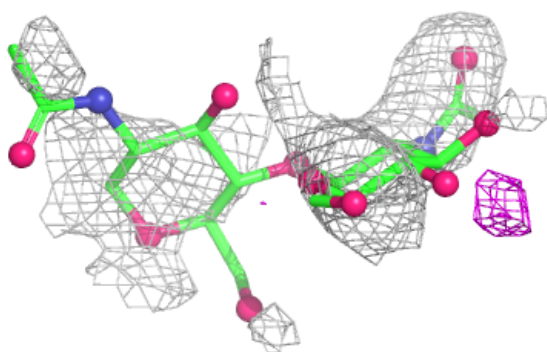
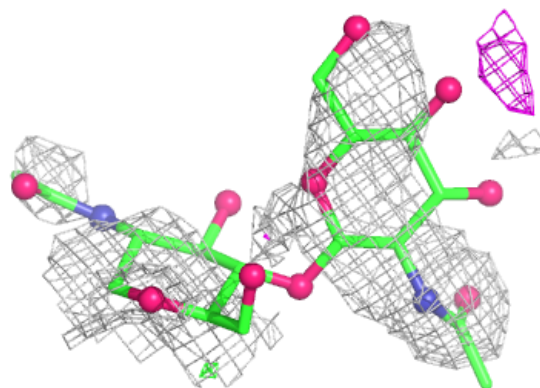
Electron density around Chain G:

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

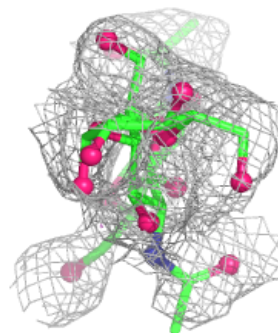
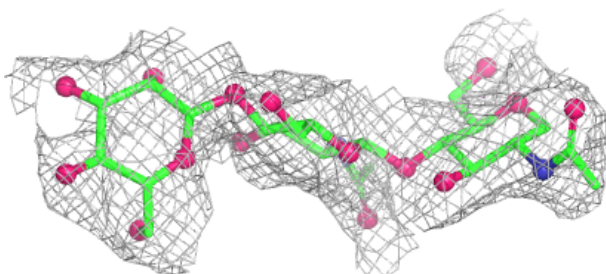
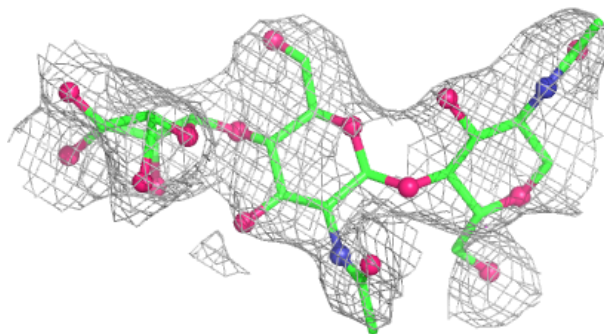


Electron density around Chain K:

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

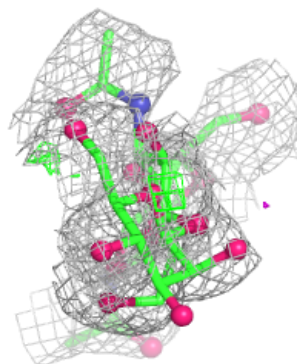
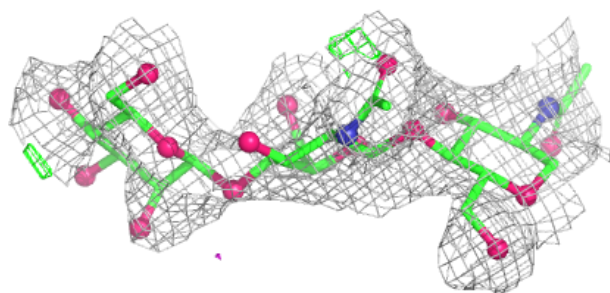
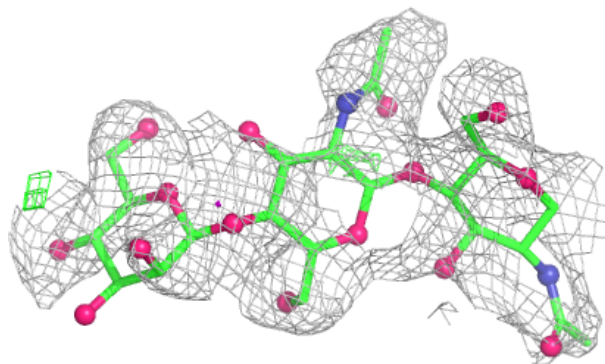
**Electron density around Chain E:**

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



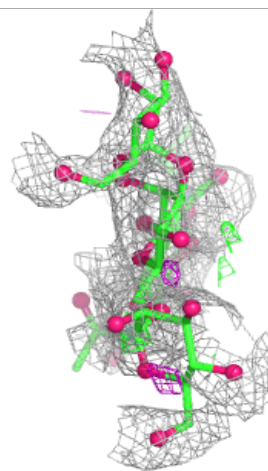
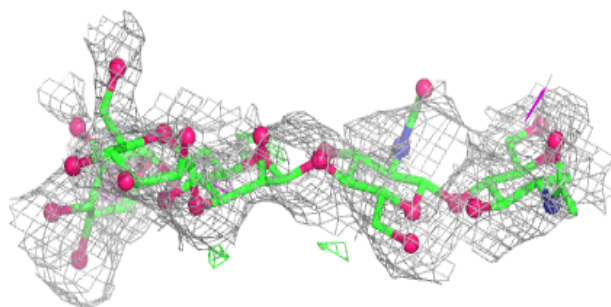
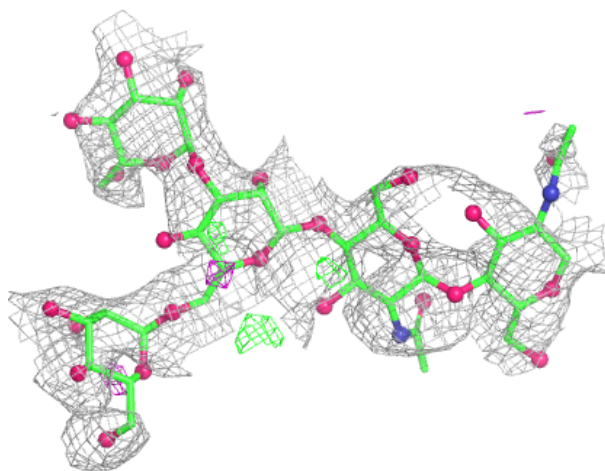
Electron density around Chain J:

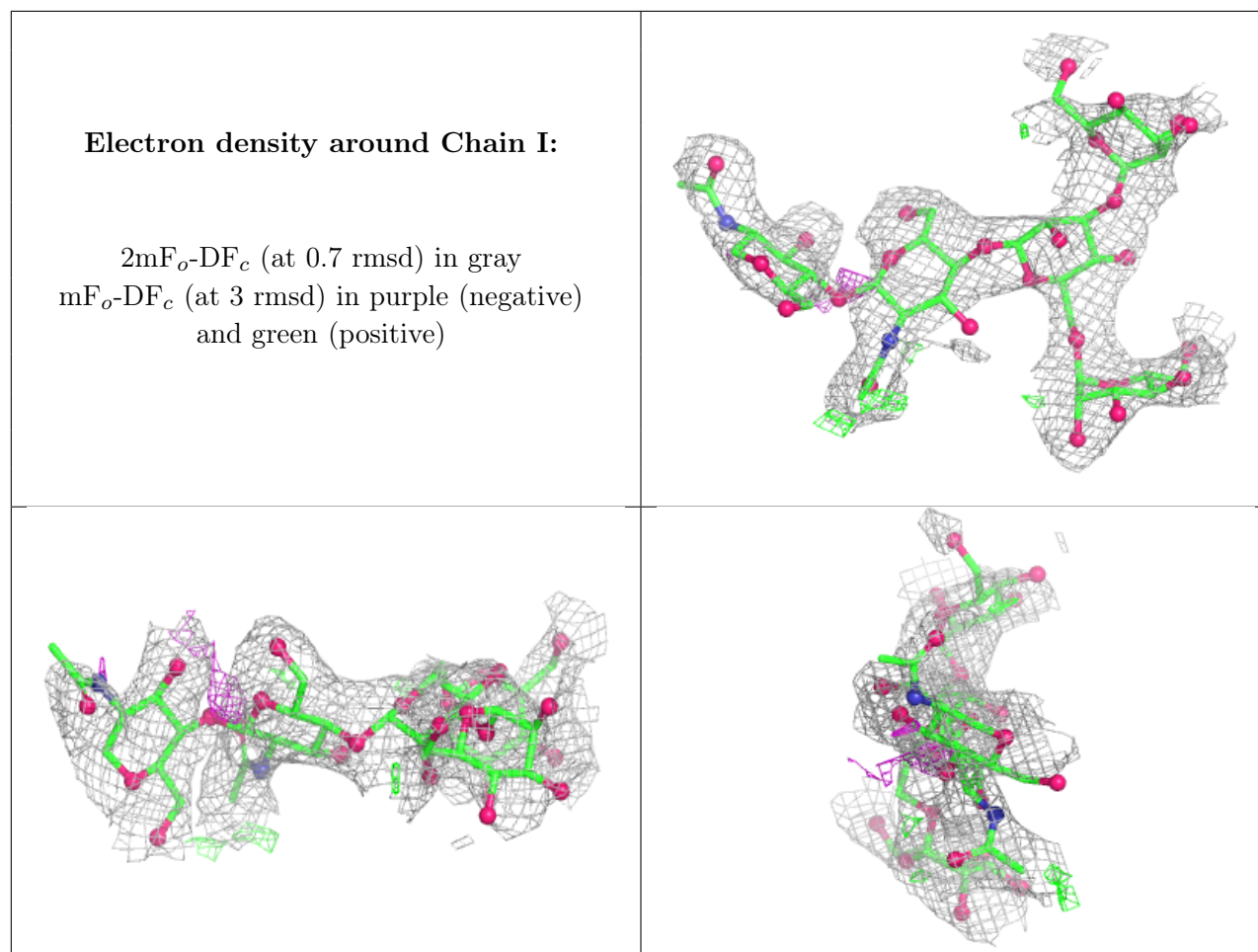
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	PEG	B	1809	7/7	0.47	0.27	55,58,62,63	0
10	PEG	A	1111	7/7	0.54	0.25	50,53,56,58	0
7	NAG	B	1812	14/15	0.57	0.22	82,85,88,88	0
7	NAG	B	1811	14/15	0.59	0.25	62,67,74,77	0
7	NAG	B	1803	14/15	0.60	0.26	70,74,75,76	0
7	NAG	B	1810	14/15	0.60	0.32	77,84,88,88	0
7	NAG	B	1802	14/15	0.60	0.27	78,84,86,86	0
7	NAG	A	1105	14/15	0.62	0.19	78,89,91,91	0
7	NAG	B	1814	14/15	0.62	0.23	74,77,82,89	0
7	NAG	A	1103	14/15	0.63	0.20	64,65,66,68	0
7	NAG	B	1813	14/15	0.67	0.19	63,66,72,78	0

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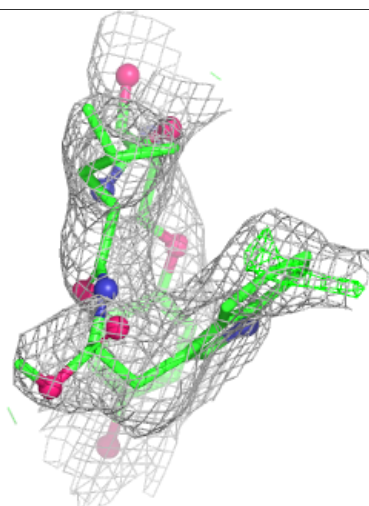
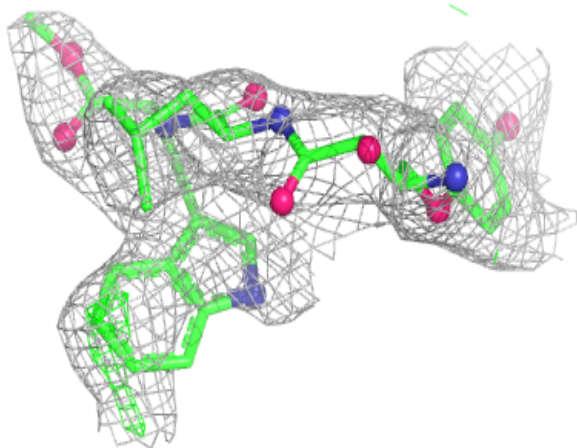
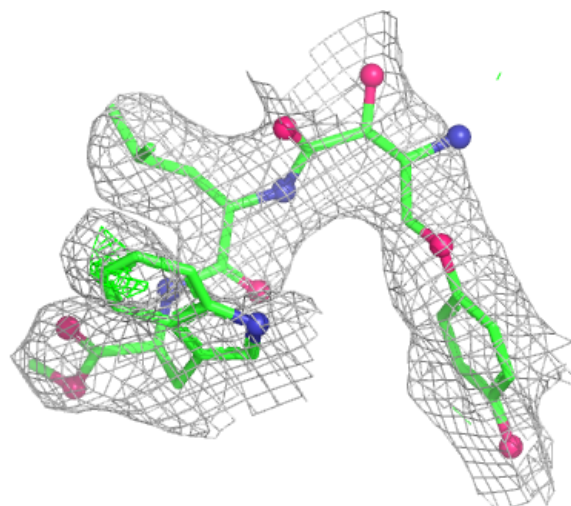
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	A	1104	14/15	0.68	0.20	65,68,73,73	0
7	NAG	A	1102	14/15	0.70	0.17	68,73,76,76	0
11	TRS	B	1807	8/8	0.71	0.17	34,36,37,37	0
9	EDO	B	1806	4/4	0.72	0.17	42,43,43,43	0
8	KFR	B	1815[A]	39/39	0.75	0.23	36,42,49,52	39
8	KFR	B	1815[B]	39/39	0.75	0.23	37,42,48,50	39
10	PEG	A	1110	7/7	0.79	0.20	34,37,40,41	0
9	EDO	A	1107	4/4	0.79	0.21	44,45,45,45	0
9	EDO	B	1805	4/4	0.81	0.14	36,37,37,38	0
9	EDO	B	1804	4/4	0.81	0.14	31,32,33,33	0
9	EDO	B	1808	4/4	0.84	0.16	40,41,41,41	0
9	EDO	A	1109	4/4	0.85	0.12	31,32,32,33	0
8	KFR	A	1106	39/39	0.86	0.16	34,43,55,58	0
9	EDO	A	1108	4/4	0.87	0.17	40,40,41,41	0
6	ZN	B	1801	1/1	1.00	0.02	29,29,29,29	0
6	ZN	A	1101	1/1	1.00	0.02	25,25,25,25	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.

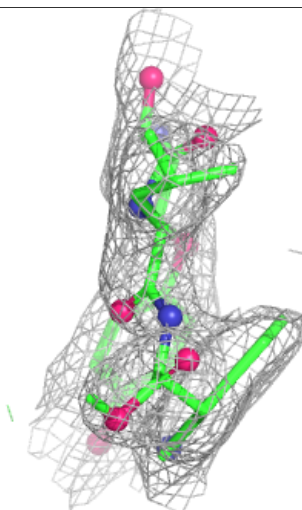
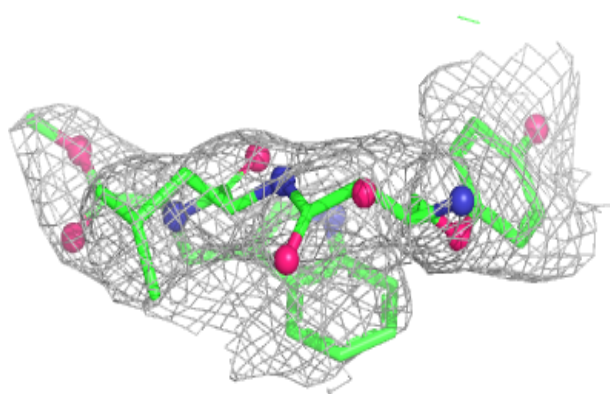
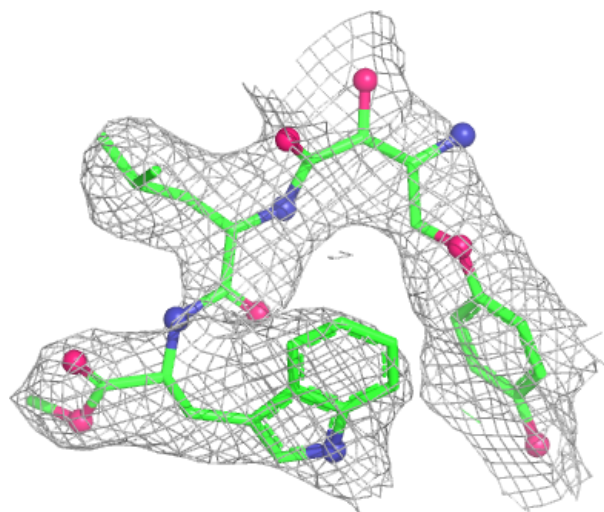
Electron density around KFR B 1815 (A):

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



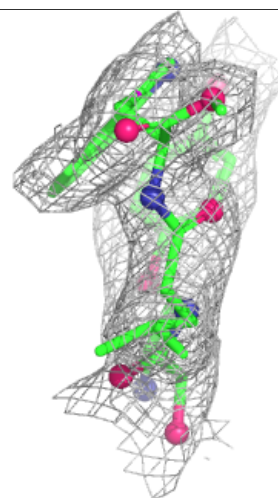
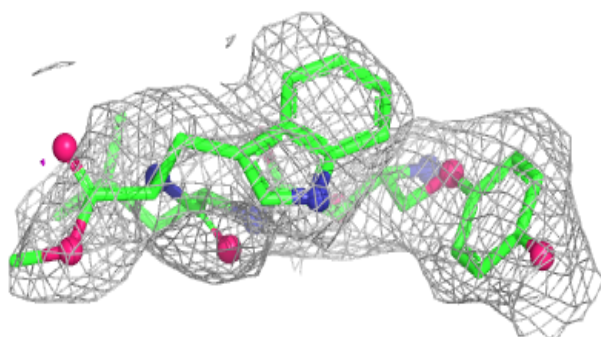
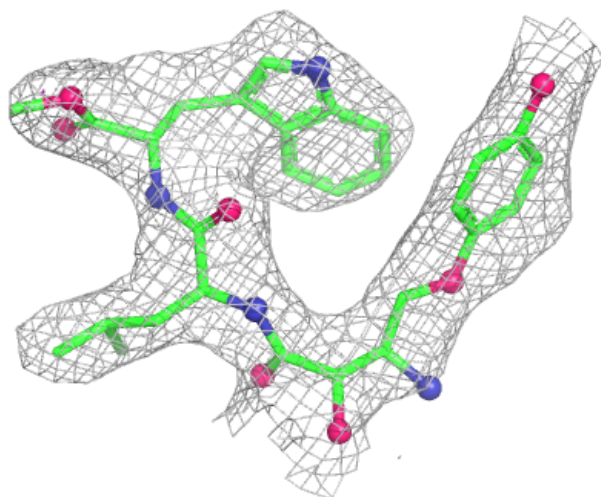
Electron density around KFR B 1815 (B):

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



Electron density around KFR A 1106:

$2mF_o-DF_c$ (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.