WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Aug 28, 2024 – 04:21 pm BST

PDB ID	:	8P0I
Title	:	Crystal structure of the open conformation of insulin-regulated aminopeptidase in complex with a small-MW inhibitor
Authors	:	Mpakali, A.; Giastas, P.; Stratikos, E.
Deposited on	:	2023-05-10
Resolution	:	3.50 Å(reported)

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

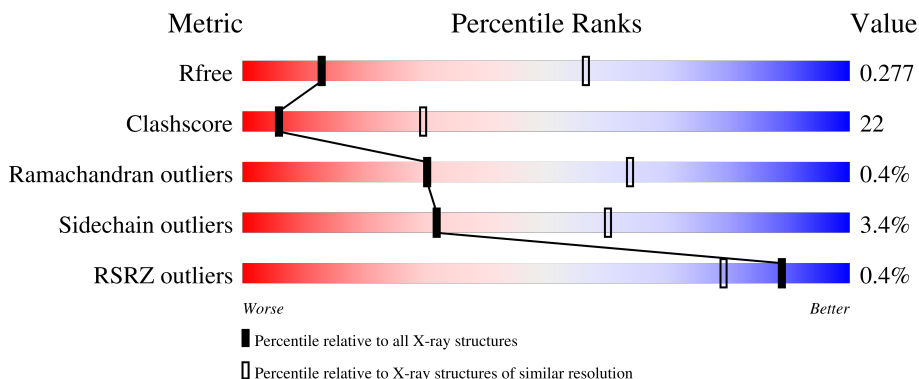|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 3.50 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	Percentile Ranks	Value
Rfree		0.277
Clashscore		22
Ramachandran outliers		0.4%
Sidechain outliers		3.4%
RSRZ outliers		0.4%

Worse ▮ *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	164625	1094 (3.56-3.44)
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)

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

Mol	Chain	Length	Quality of chain
1	A	871	55% 42% ‥
1	B	871	.% 56% 40% ‥
2	C	3	67% 33%
2	E	3	33% 67%
2	G	3	100%

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Mol	Chain	Length	Quality of chain
2	I	3	67% 33%
3	D	4	50% 50%
3	F	4	75% 25%
4	H	2	100%
4	J	2	100%
4	K	2	100%
4	L	2	100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13992 atoms, of which 56 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	857	Total 6700	C 4328	N 1091	O 1255	S 26	0	0	0
1	B	851	Total 6614	C 4290	N 1061	O 1239	S 24	0	0	0

- Molecule 2 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
2	C	3	Total 39	C 22	N 2	O 15	0	0	0
2	E	3	Total 39	C 22	N 2	O 15	0	0	0
2	G	3	Total 39	C 22	N 2	O 15	0	0	0
2	I	3	Total 39	C 22	N 2	O 15	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
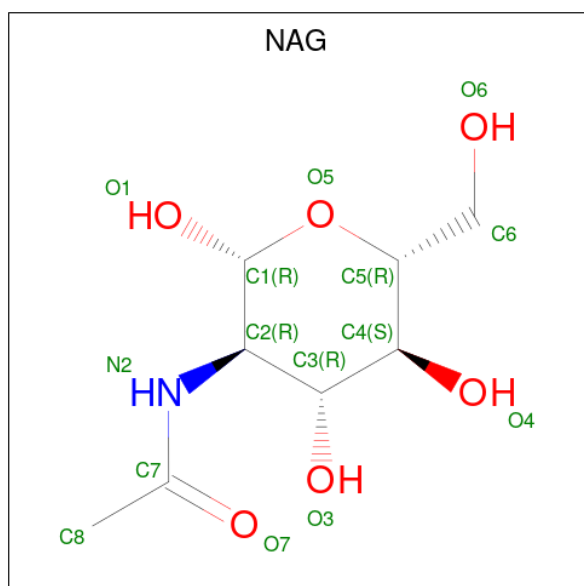
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	4	Total 50	C 28	N 2	O 20	0	0	0
3	F	4	Total 50	C 28	N 2	O 20	0	0	0

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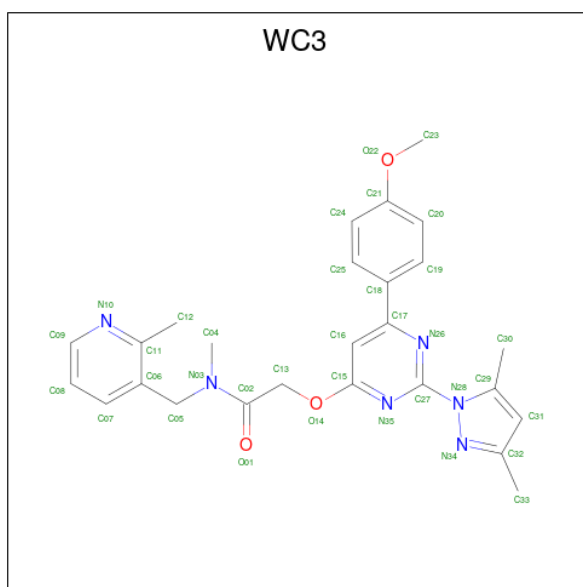

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	2	Total 28	C 16	N 2	O 10	0	0	0
4	J	2	Total 28	C 16	N 2	O 10	0	0	0
4	K	2	Total 28	C 16	N 2	O 10	0	0	0
4	L	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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

- Molecule 6 is 2-[2-(3,5-dimethylpyrazol-1-yl)-6-(4-methoxyphenyl)pyrimidin-4-yl]oxy-N-methyl-N-[(2-methylpyridin-3-yl)methyl]ethanamide (three-letter code: WC3) (formula: $C_{26}H_{28}N_6O_3$) (labeled as "Ligand of Interest" by depositor).

WC3

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	0	0
			63	26	28	6	3		
6	B	1	Total	C	H	N	O	0	0
			63	26	28	6	3		

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

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

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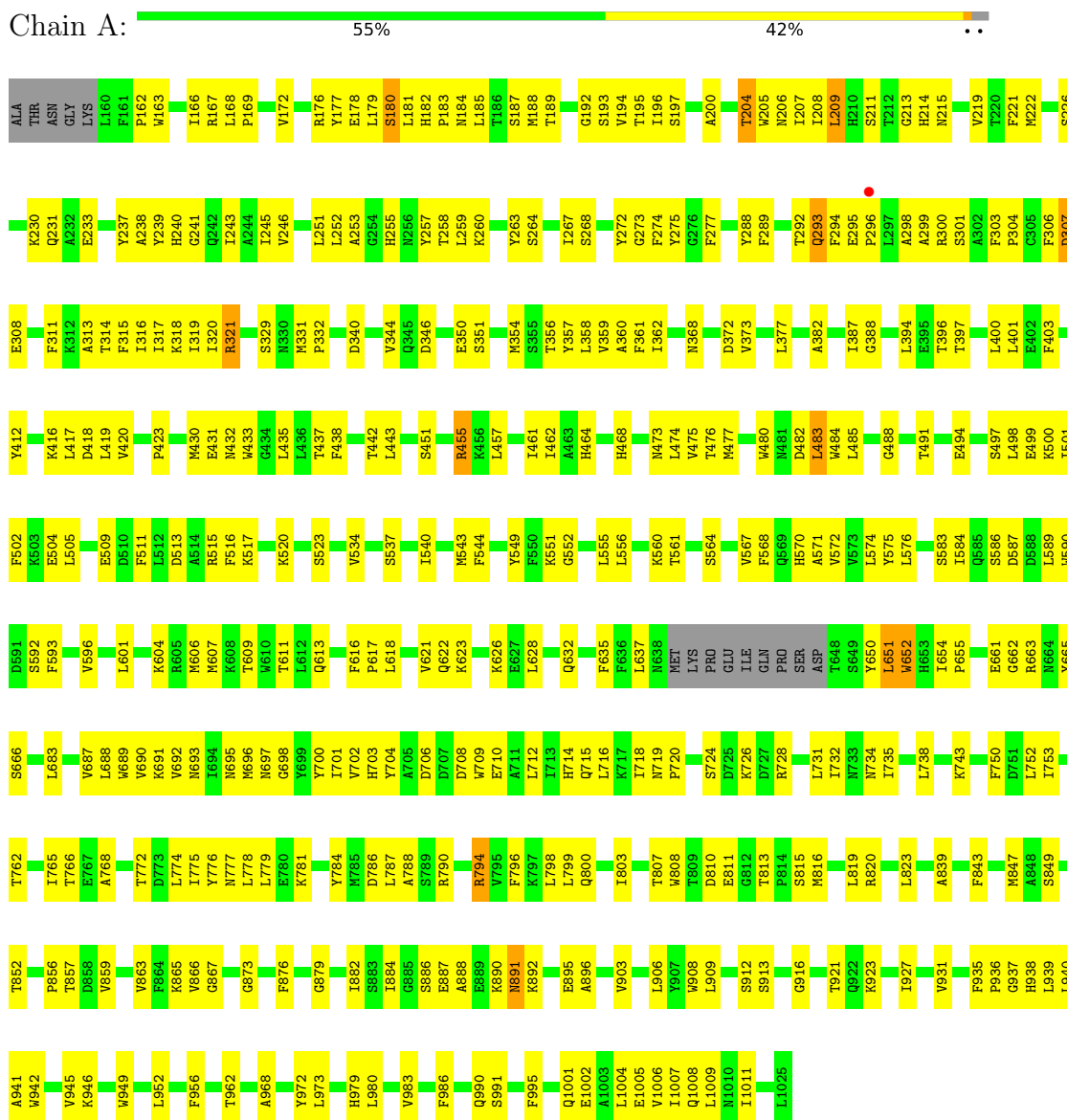
- Molecule 1: Leucyl-cystinyl aminopeptidase, pregnancy serum form
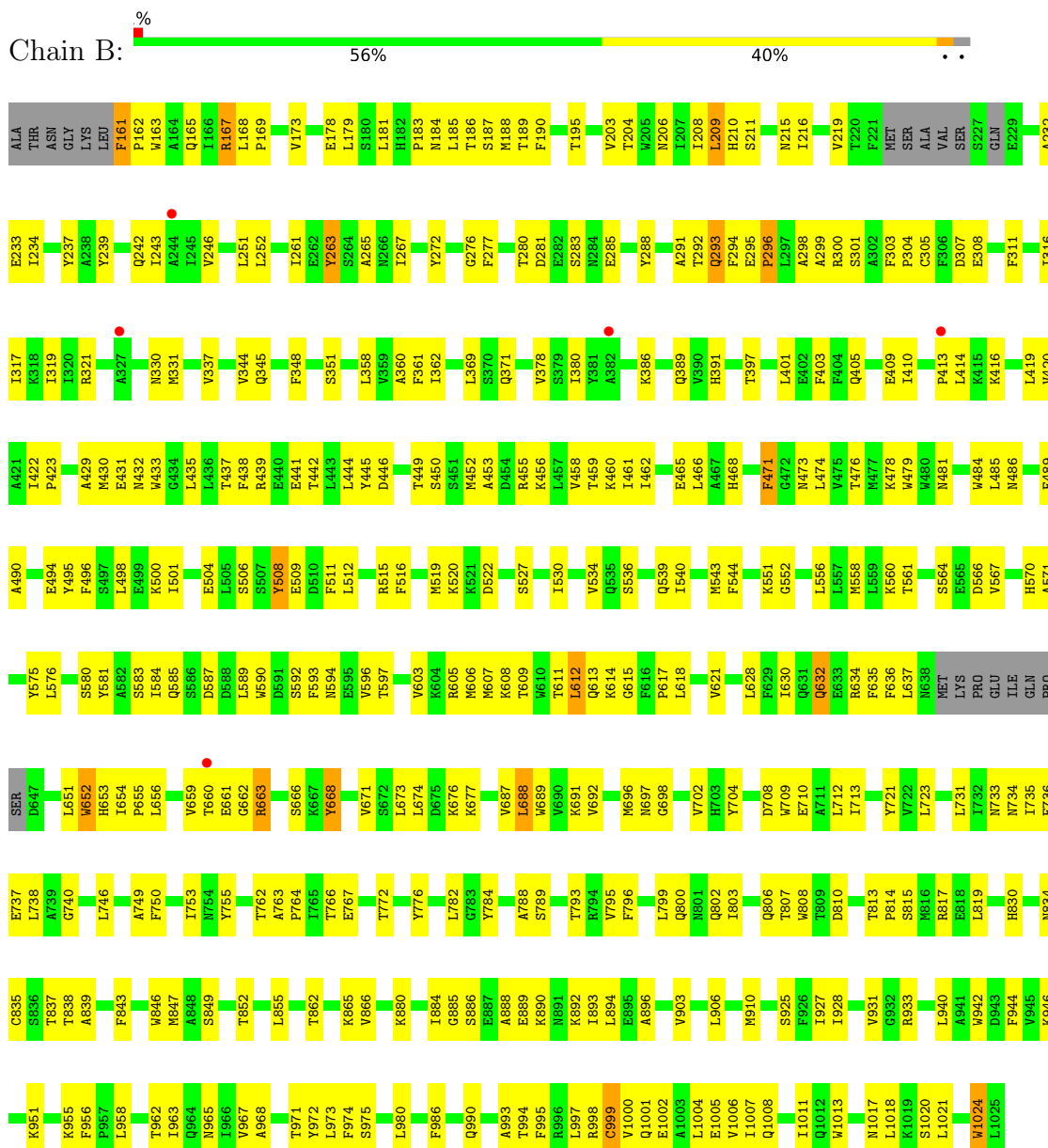
Chain B:

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

Chain C:

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

Chain E:

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

Chain G:

100%

NAG1 NAG2 BMA3

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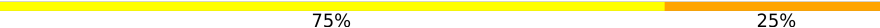etamido-2-deoxy-beta-D-glucopyranose

Chain I:

67%　　　　33%

NAG1 NAG2 BMA3

• Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b
eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
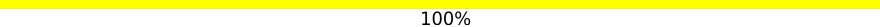
Chain D:

50%　　　　50%

NAG1 NAG2 BMA3 MAN4

• Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b
eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
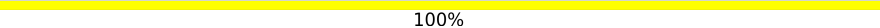
Chain F:

75%　　　　25%

NAG1 NAG2 BMA3 MAN4

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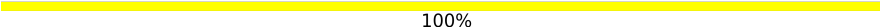opyranose

Chain H:

100%

NAG1 NAG2

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

Chain J:

100%

NAG1 NAG2

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

Chain K:

100%

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NAG1
NAG2

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

Chain L:

100%

NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.23Å 255.12Å 73.27Å 90.00° 110.00° 90.00°	Depositor
Resolution (Å)	64.11 – 3.50 64.11 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (64.11-3.50) 99.7 (64.11-3.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.240 , 0.277 0.240 , 0.277	Depositor DCC
R_{free} test set	27885 reflections (5.73%)	wwPDB-VP
Wilson B-factor (Å^2)	117.4	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 65.8	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13992	wwPDB-VP
Average B, all atoms (Å^2)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MAN, ZN, BMA, WC3

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	0.37	0/6867	0.58	3/9360 (0.0%)
1	B	0.35	0/6778	0.57	2/9245 (0.0%)
All	All	0.36	0/13645	0.57	5/18605 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	651	LEU	CD1-CG-CD2	-7.83	87.00	110.50
1	A	483	LEU	CB-CG-CD2	-7.42	98.38	111.00
1	B	173	VAL	CG1-CB-CG2	-6.51	100.48	110.90
1	B	209	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	204	THR	CA-CB-CG2	-5.08	105.29	112.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6700	0	6340	296	0
1	B	6614	0	6240	304	0
2	C	39	0	34	0	0
2	E	39	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	39	0	34	0	0
2	I	39	0	34	1	0
3	D	50	0	43	3	0
3	F	50	0	43	1	0
4	H	28	0	25	0	0
4	J	28	0	25	1	0
4	K	28	0	25	0	0
4	L	28	0	25	0	0
5	A	98	0	91	1	0
5	B	84	0	78	2	0
6	A	35	28	0	0	0
6	B	35	28	0	3	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
All	All	13936	56	13071	606	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 22.

The worst 5 of 606 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:609:THR:HG21	1:A:652:TRP:HA	1.41	1.00
1:A:571:ALA:HA	1:A:596:VAL:HG21	1.44	0.97
1:B:661:GLU:HA	1:B:666:SER:HB3	1.49	0.93
1:A:477:MET:HE1	1:A:485:LEU:HD12	1.51	0.91
1:B:762:THR:HG22	1:B:819:LEU:HB2	1.53	0.90

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	853/871 (98%)	784 (92%)	64 (8%)	5 (1%)	22	56
1	B	844/871 (97%)	775 (92%)	67 (8%)	2 (0%)	44	75
All	All	1697/1742 (97%)	1559 (92%)	131 (8%)	7 (0%)	30	64

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	601	LEU
1	A	388	GLY
1	B	183	PRO
1	A	183	PRO
1	A	213	GLY

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	701/780 (90%)	676 (96%)	25 (4%)	30	59
1	B	688/780 (88%)	666 (97%)	22 (3%)	34	62
All	All	1389/1560 (89%)	1342 (97%)	47 (3%)	32	60

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	293	GLN
1	B	632	GLN
1	B	301	SER
1	B	508	TYR
1	B	652	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	473	ASN

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Mol	Chain	Res	Type
1	B	632	GLN
1	B	730	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	2,1	14,14,15	0.66	1 (7%)	17,19,21	0.68	0
2	NAG	C	2	2	14,14,15	0.47	0	17,19,21	0.51	0
2	BMA	C	3	2	11,11,12	0.74	0	15,15,17	0.84	0
3	NAG	D	1	3,1	14,14,15	0.37	0	17,19,21	0.47	0
3	NAG	D	2	3	14,14,15	0.70	1 (7%)	17,19,21	0.81	0
3	BMA	D	3	3	11,11,12	1.29	0	15,15,17	1.27	2 (13%)
3	MAN	D	4	3	11,11,12	0.83	0	15,15,17	1.32	2 (13%)
2	NAG	E	1	2,1	14,14,15	0.26	0	17,19,21	0.78	0
2	NAG	E	2	2	14,14,15	0.38	0	17,19,21	1.47	3 (17%)
2	BMA	E	3	2	11,11,12	0.41	0	15,15,17	1.00	1 (6%)
3	NAG	F	1	3,1	14,14,15	1.41	1 (7%)	17,19,21	2.03	5 (29%)
3	NAG	F	2	3	14,14,15	0.78	1 (7%)	17,19,21	1.08	2 (11%)
3	BMA	F	3	3	11,11,12	1.15	0	15,15,17	1.00	0
3	MAN	F	4	3	11,11,12	1.82	3 (27%)	15,15,17	1.53	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	NAG	G	1	2,1	14,14,15	0.50	0	17,19,21	0.52	0
2	NAG	G	2	2	14,14,15	0.51	0	17,19,21	0.45	0
2	BMA	G	3	2	11,11,12	0.69	0	15,15,17	0.77	0
4	NAG	H	1	4,1	14,14,15	0.57	0	17,19,21	0.98	2 (11%)
4	NAG	H	2	4	14,14,15	1.04	1 (7%)	17,19,21	1.97	3 (17%)
2	NAG	I	1	2,1	14,14,15	0.94	1 (7%)	17,19,21	1.12	2 (11%)
2	NAG	I	2	2	14,14,15	0.36	0	17,19,21	0.55	0
2	BMA	I	3	2	11,11,12	0.56	0	15,15,17	0.98	1 (6%)
4	NAG	J	1	4,1	14,14,15	0.36	0	17,19,21	0.57	0
4	NAG	J	2	4	14,14,15	1.23	1 (7%)	17,19,21	0.68	0
4	NAG	K	1	4,1	14,14,15	0.44	0	17,19,21	0.96	1 (5%)
4	NAG	K	2	4	14,14,15	0.39	0	17,19,21	0.94	1 (5%)
4	NAG	L	1	4,1	14,14,15	0.83	1 (7%)	17,19,21	1.85	2 (11%)
4	NAG	L	2	4	14,14,15	0.93	1 (7%)	17,19,21	1.41	3 (17%)

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

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

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

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	O5-C1	-5.10	1.35	1.43
3	F	4	MAN	O5-C5	4.50	1.52	1.43
4	J	2	NAG	C1-C2	4.05	1.58	1.52
4	H	2	NAG	C1-C2	3.39	1.57	1.52
2	I	1	NAG	C1-C2	3.32	1.57	1.52

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	1	NAG	C2-N2-C7	6.30	131.88	122.90
4	H	2	NAG	C2-N2-C7	6.20	131.73	122.90
3	F	1	NAG	C1-O5-C5	-4.39	106.24	112.19
2	E	2	NAG	C1-O5-C5	3.98	117.59	112.19
3	F	1	NAG	C4-C3-C2	3.85	116.66	111.02

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C1-C2-N2-C7
4	L	1	NAG	C3-C2-N2-C7
4	H	1	NAG	C4-C5-C6-O6
4	H	2	NAG	C1-C2-N2-C7
3	F	1	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	4	MAN	C1-C2-C3-C4-C5-O5

10 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	3	BMA	1	0
2	E	2	NAG	1	0
2	I	2	NAG	1	0
2	E	3	BMA	1	0
3	F	4	MAN	1	0
3	D	1	NAG	2	0
3	D	2	NAG	2	0
2	I	3	BMA	1	0
3	D	3	BMA	1	0
4	J	1	NAG	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 C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain J

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain K

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain L

Bond lengths

Bond angles

Torsions

Rings

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	#$|Z| > 2$
5	NAG	B	1103	1	14,14,15	0.29	0	17,19,21	0.45	0
5	NAG	B	1101	1	14,14,15	1.92	2 (14%)	17,19,21	2.02	3 (17%)
6	WC3	A	1107	7	37,38,38	2.92	3 (8%)	43,53,53	3.17	16 (37%)
6	WC3	B	1107	7	37,38,38	2.80	7 (18%)	43,53,53	3.45	17 (39%)
5	NAG	A	1102	1	14,14,15	0.45	0	17,19,21	1.62	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	1105	1	14,14,15	0.22	0	17,19,21	0.40	0
5	NAG	A	1101	1	14,14,15	0.94	1 (7%)	17,19,21	1.32	2 (11%)
5	NAG	A	1109	1	14,14,15	1.04	1 (7%)	17,19,21	1.69	2 (11%)
5	NAG	B	1105	1	14,14,15	0.56	0	17,19,21	0.69	1 (5%)
5	NAG	A	1104	1	14,14,15	0.19	0	17,19,21	0.93	1 (5%)
5	NAG	A	1103	1	14,14,15	0.36	0	17,19,21	0.54	0
5	NAG	B	1104	1	14,14,15	0.46	0	17,19,21	0.73	0
5	NAG	B	1102	1	14,14,15	0.41	0	17,19,21	0.44	0
5	NAG	A	1106	1	14,14,15	0.59	0	17,19,21	0.57	0
5	NAG	B	1106	1	14,14,15	0.33	0	17,19,21	1.46	2 (11%)

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
5	NAG	B	1103	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1101	1	-	3/6/23/26	0/1/1/1
6	WC3	A	1107	7	-	10/21/23/23	0/4/4/4
6	WC3	B	1107	7	-	12/21/23/23	0/4/4/4
5	NAG	A	1102	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1105	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1101	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1109	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1105	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1104	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1103	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1104	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1102	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1106	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1106	1	-	5/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1107	WC3	C02-N03	15.94	1.54	1.34
6	B	1107	WC3	C02-N03	14.67	1.52	1.34
5	B	1101	NAG	O5-C1	6.39	1.53	1.43
6	A	1107	WC3	C05-C06	4.43	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1109	NAG	C1-C2	3.57	1.57	1.52

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1107	WC3	C12-C11-C06	13.04	132.06	121.83
6	A	1107	WC3	O01-C02-N03	12.58	140.37	122.12
6	A	1107	WC3	O01-C02-C13	-6.90	103.94	120.66
6	A	1107	WC3	C29-N28-N34	-6.73	105.82	111.81
6	B	1107	WC3	C06-C11-N10	-6.71	117.84	122.04

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1102	NAG	C3-C2-N2-C7
5	B	1101	NAG	C8-C7-N2-C2
6	A	1107	WC3	C16-C15-O14-C13
6	A	1107	WC3	N35-C15-O14-C13
6	A	1107	WC3	N26-C27-N28-N34

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1101	NAG	1	0
6	B	1107	WC3	3	0
5	A	1104	NAG	1	0
5	B	1106	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand WC3 A 1107

Bond lengths

Bond angles

Torsions

Rings

Ligand WC3 B 1107

Bond lengths

Bond angles

Torsions

Rings
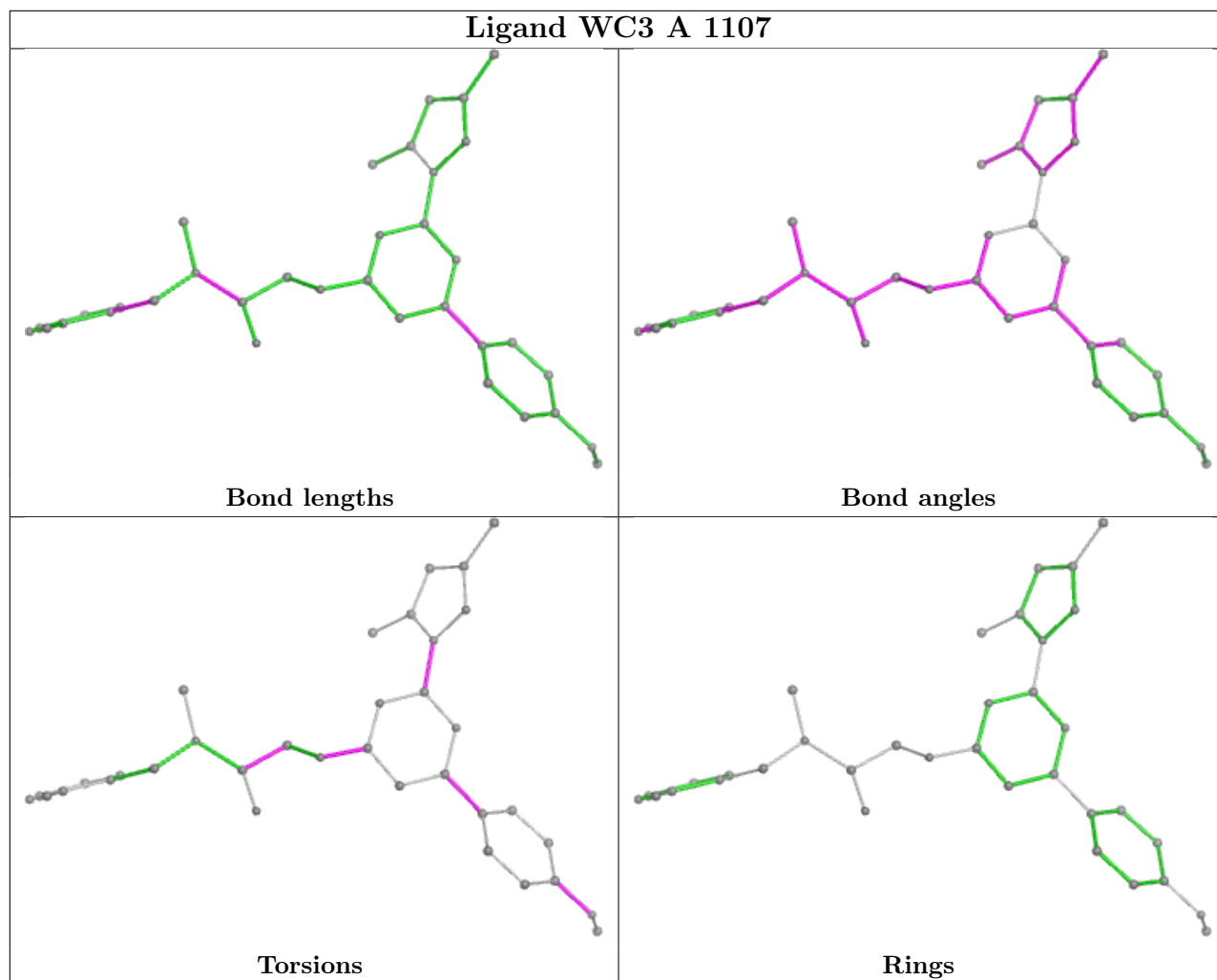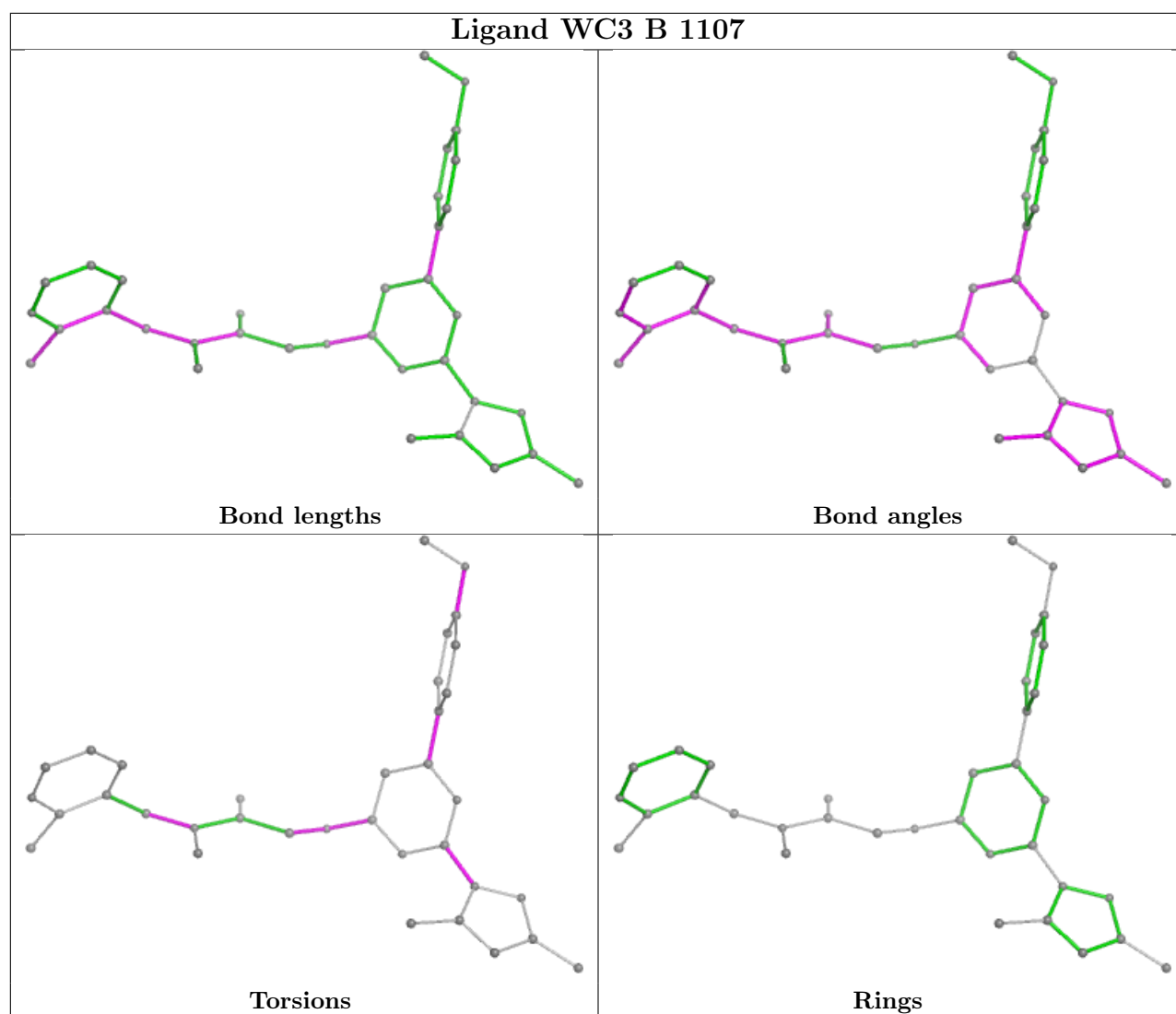
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	857/871 (98%)	-0.39	1 (0%)	92	89	83, 112, 140, 156	1 (0%)
1	B	851/871 (97%)	-0.37	5 (0%)	85	72	92, 118, 144, 165	0
All	All	1708/1742 (98%)	-0.38	6 (0%)	89	79	83, 115, 142, 165	1 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	327	ALA	3.0
1	B	382	ALA	3.0
1	B	660	THR	2.3
1	A	296	PRO	2.2
1	B	244	ALA	2.1

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å²)	Q<0.9
3	NAG	F	1	14/15	0.34	0.13	155,168,178,180	0
2	BMA	G	3	11/12	0.35	0.11	141,160,167,170	0
4	NAG	H	2	14/15	0.37	0.09	159,168,174,174	0
3	BMA	D	3	11/12	0.38	0.09	165,177,181,183	0
3	MAN	D	4	11/12	0.39	0.08	154,178,181,184	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	NAG	G	2	14/15	0.45	0.08	143,157,160,162	0
3	BMA	F	3	11/12	0.46	0.14	129,149,156,158	0
4	NAG	K	1	14/15	0.49	0.11	142,156,162,172	0
2	NAG	C	1	14/15	0.50	0.12	127,139,148,150	0
2	BMA	E	3	11/12	0.50	0.08	134,136,139,144	0
4	NAG	J	1	14/15	0.57	0.11	125,138,143,144	0
2	BMA	C	3	11/12	0.57	0.08	138,146,151,152	0
4	NAG	H	1	14/15	0.61	0.08	134,160,170,174	0
3	NAG	D	1	14/15	0.61	0.08	115,143,159,164	0
3	MAN	F	4	11/12	0.65	0.12	126,139,145,148	0
3	NAG	F	2	14/15	0.66	0.09	145,157,163,166	0
4	NAG	K	2	14/15	0.67	0.08	132,155,164,167	0
2	NAG	G	1	14/15	0.68	0.10	135,149,156,156	0
2	BMA	I	3	11/12	0.70	0.06	139,142,144,144	0
4	NAG	J	2	14/15	0.71	0.08	147,157,164,165	0
2	NAG	C	2	14/15	0.72	0.07	132,156,168,191	0
2	NAG	E	1	14/15	0.77	0.09	124,127,131,134	0
3	NAG	D	2	14/15	0.77	0.07	146,166,175,177	0
4	NAG	L	2	14/15	0.77	0.07	135,146,150,151	0
2	NAG	E	2	14/15	0.81	0.08	131,136,143,144	0
2	NAG	I	1	14/15	0.82	0.10	138,145,152,153	0
2	NAG	I	2	14/15	0.88	0.06	120,143,148,153	0
4	NAG	L	1	14/15	0.90	0.09	147,152,157,160	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.
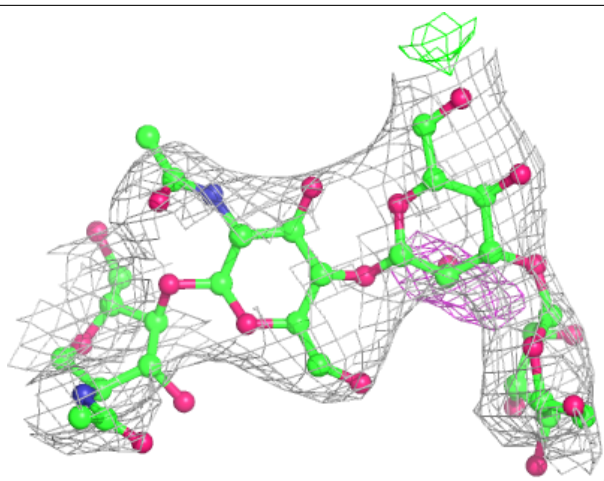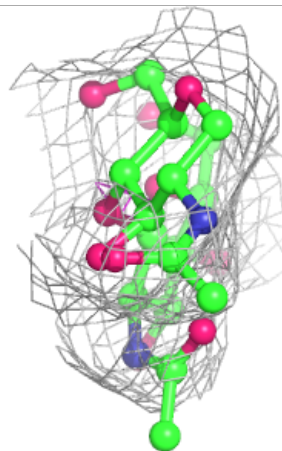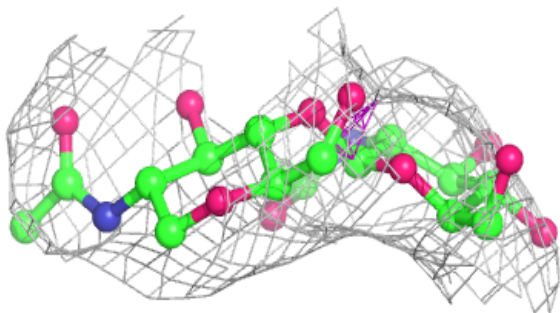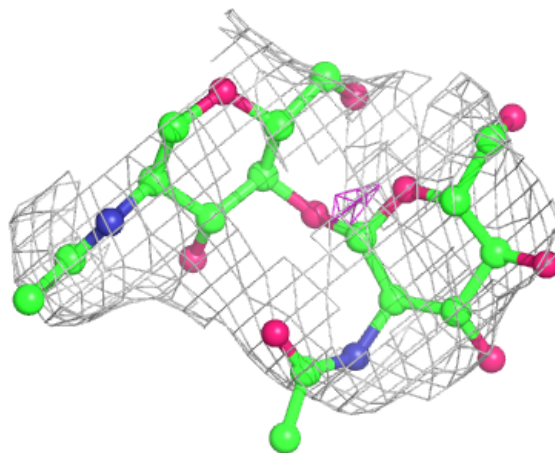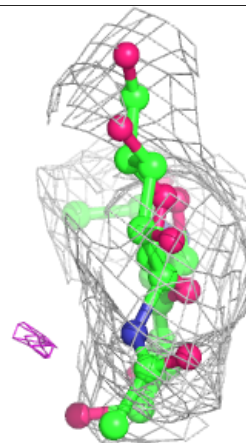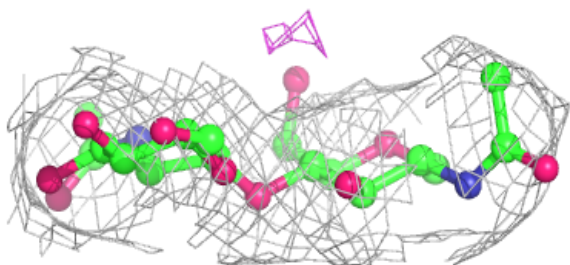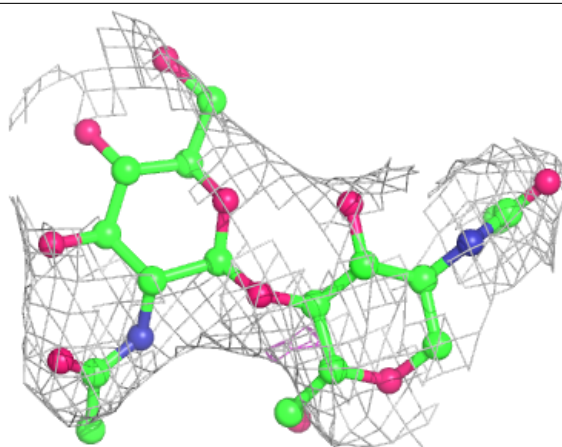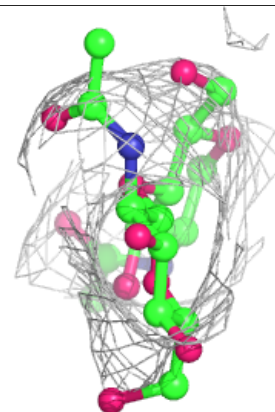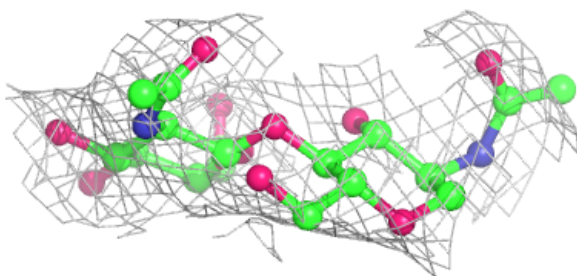
Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
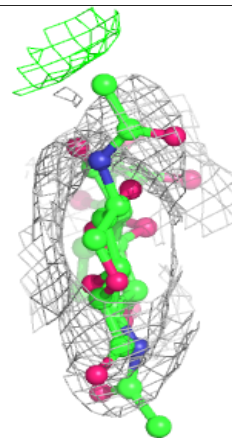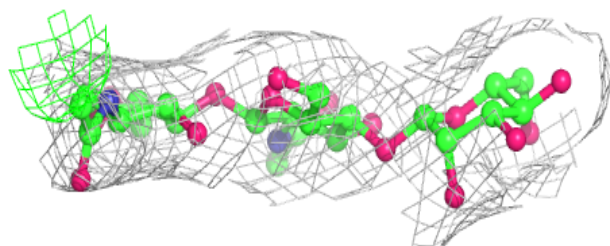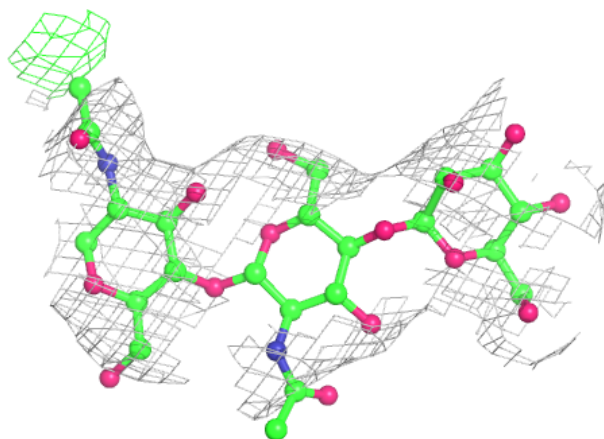
Electron density around Chain E:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
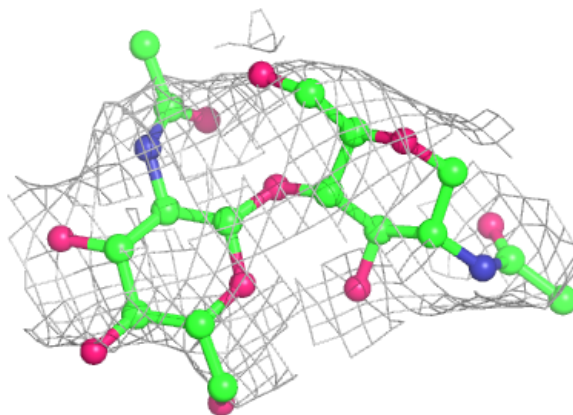mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
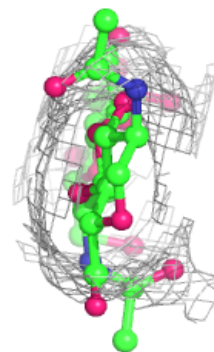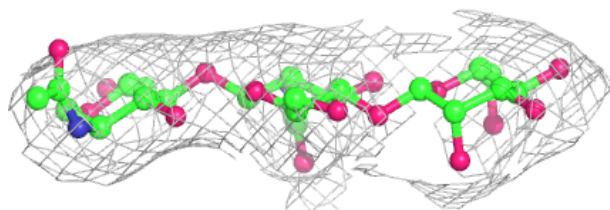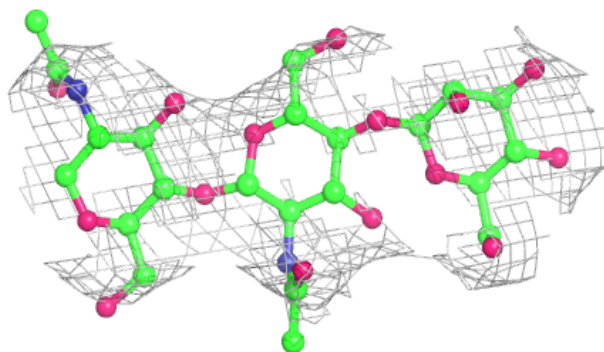
Electron density around Chain G:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
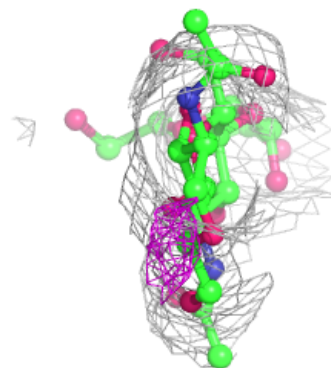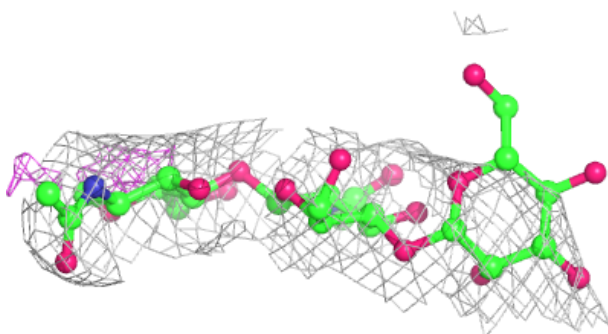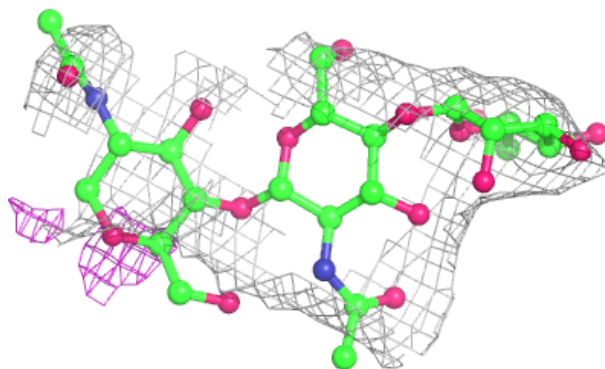
Electron density around Chain I:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
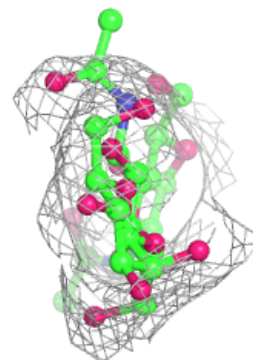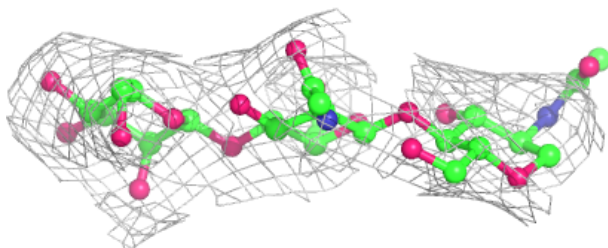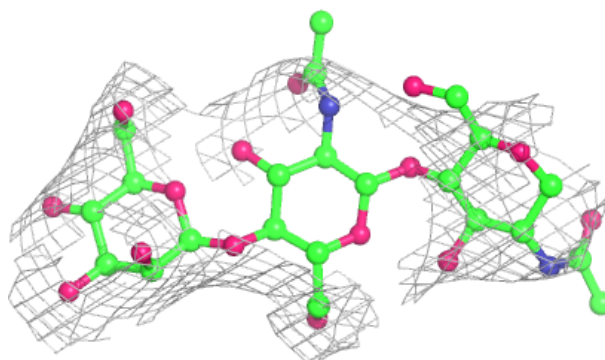
Electron density around Chain D:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
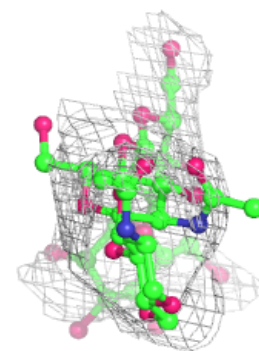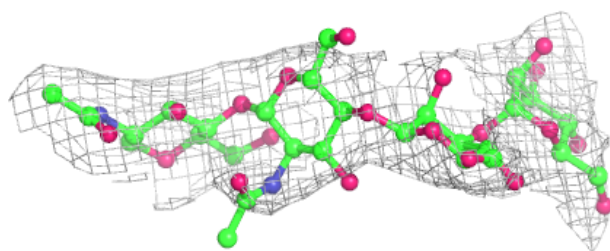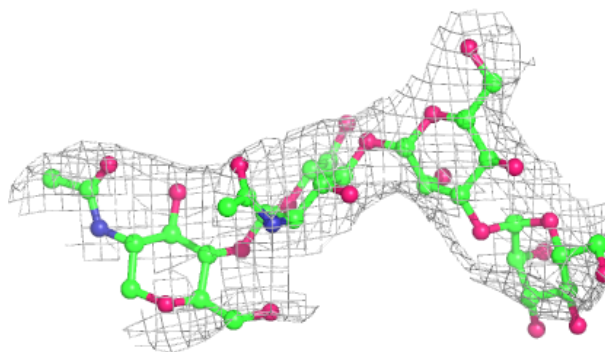
Electron density around Chain F:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
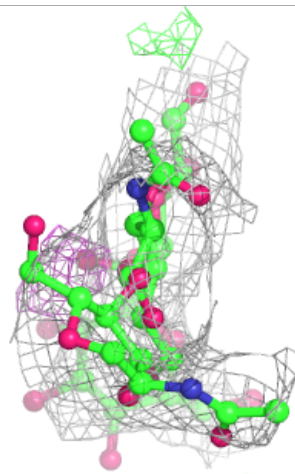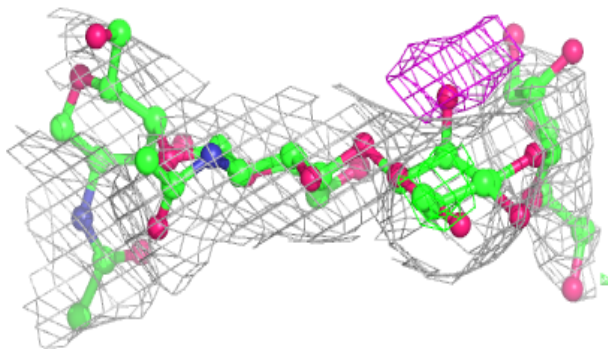
Electron density around Chain H:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
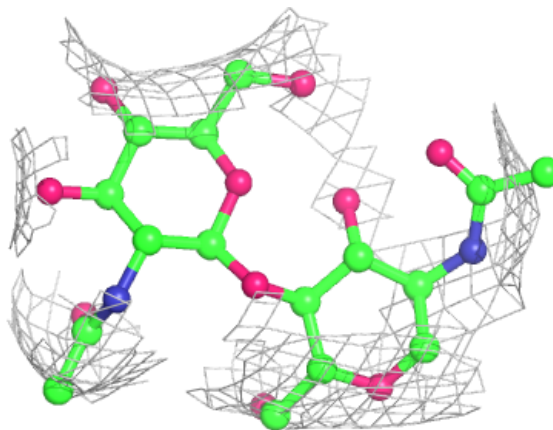and green (positive)

Electron density around Chain J:

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

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 L:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
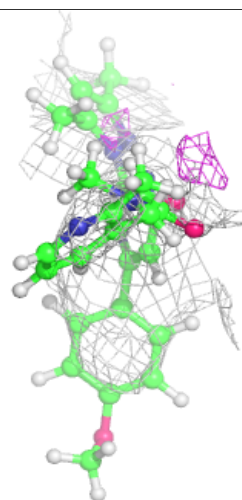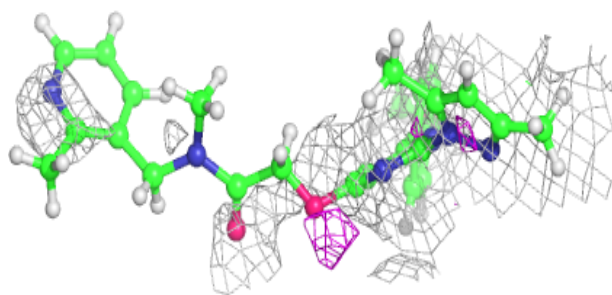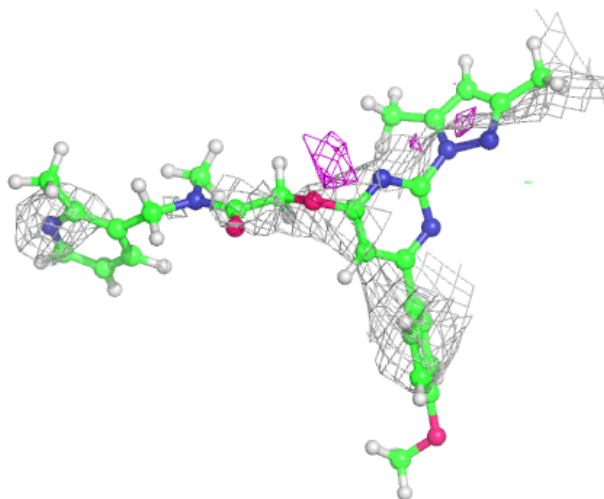and green (positive)
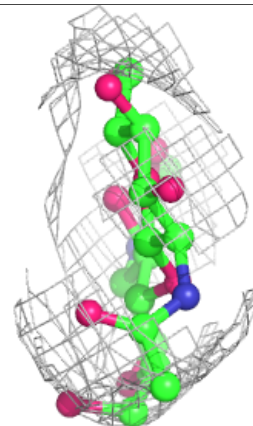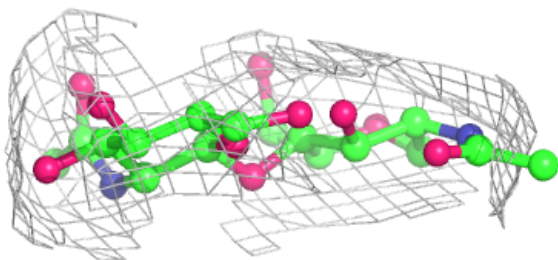
6.4 Ligands ⓘ

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.
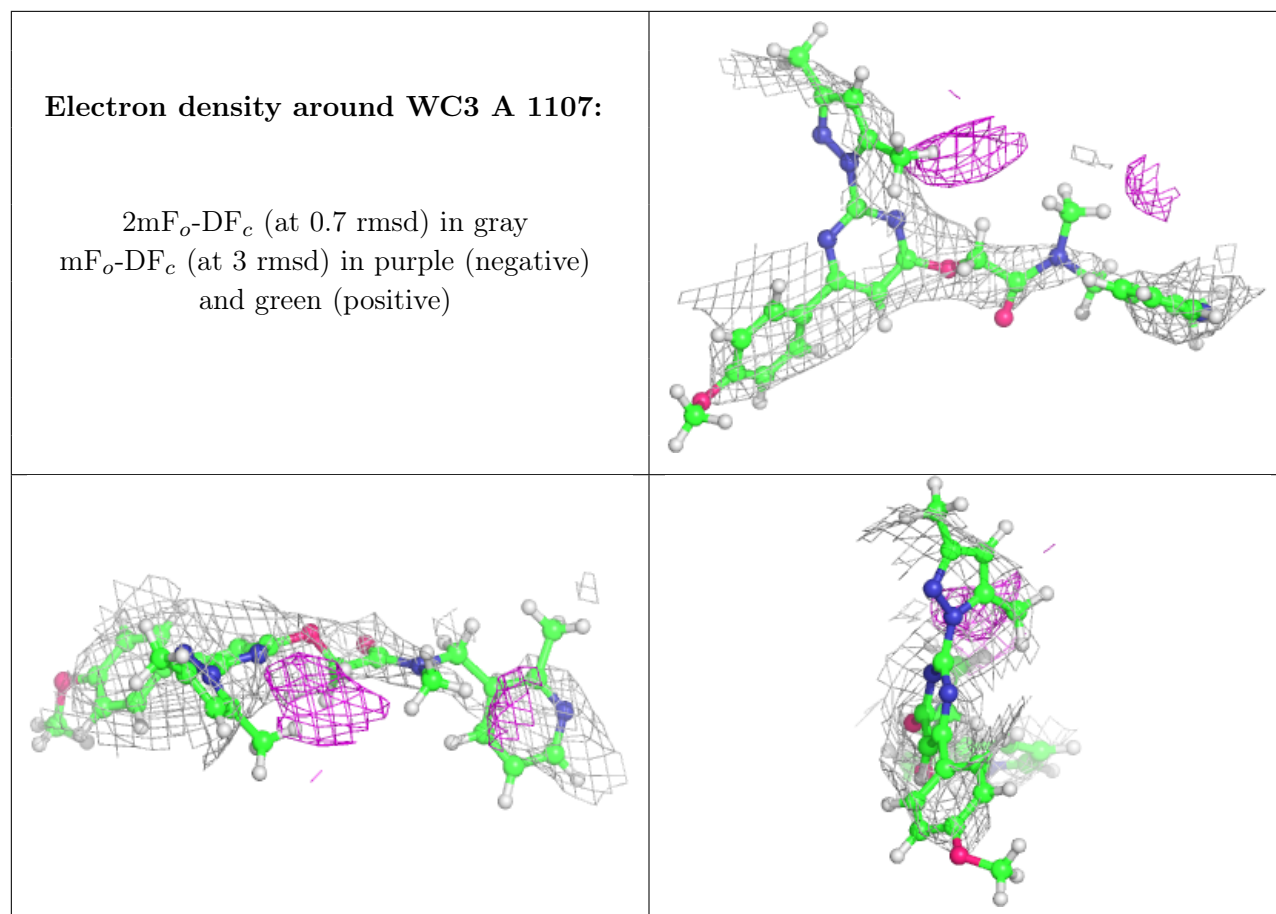
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
5	NAG	B	1106	14/15	0.42	0.09	153,162,168,172	0
5	NAG	B	1105	14/15	0.50	0.09	146,166,170,171	0
5	NAG	A	1105	14/15	0.51	0.11	137,154,169,179	0
5	NAG	A	1104	14/15	0.62	0.08	135,154,158,159	0
5	NAG	B	1101	14/15	0.63	0.09	141,159,163,167	0
5	NAG	B	1104	14/15	0.65	0.08	147,162,167,168	0
5	NAG	A	1102	14/15	0.66	0.08	141,158,169,172	0
5	NAG	A	1109	14/15	0.66	0.09	130,139,149,150	0
5	NAG	A	1106	14/15	0.72	0.07	142,150,158,160	0
5	NAG	B	1102	14/15	0.78	0.07	109,134,142,144	0
5	NAG	A	1101	14/15	0.83	0.07	139,146,149,150	0
6	WC3	B	1107	35/35	0.83	0.13	126,158,194,209	0
5	NAG	B	1103	14/15	0.84	0.07	123,132,141,147	0
6	WC3	A	1107	35/35	0.86	0.11	120,144,172,175	0
5	NAG	A	1103	14/15	0.91	0.08	107,115,124,127	0
7	ZN	B	1108	1/1	0.97	0.03	105,105,105,105	0
7	ZN	A	1108	1/1	0.98	0.04	114,114,114,114	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 WC3 B 1107:

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

Electron density around WC3 A 1107:

$2mF_o$-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.