



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:45 AM UTC

PDB ID : 1K21 / pdb_00001k21
Title : HUMAN THROMBIN-INHIBITOR COMPLEX
Authors : Stubbs, M.T.; Musil, D.
Deposited on : 2001-09-26
Resolution : 1.86 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

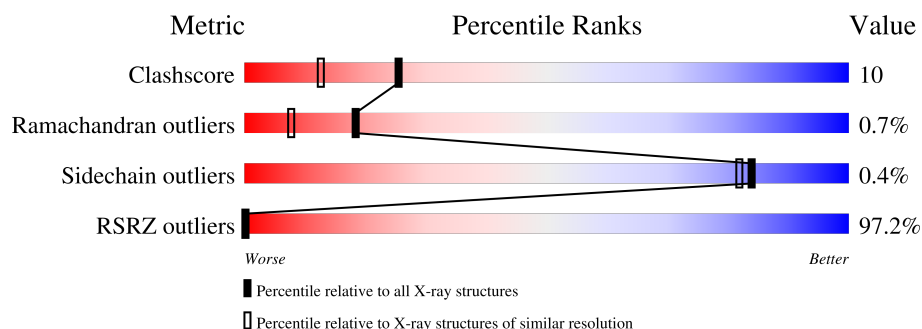
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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))
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	L	36	69% 67% 8% 25%
2	H	259	94% 76% 19% . .
3	I	12	75% 67% 17% 17%
4	A	2	50% 50%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 2634 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 Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	27	Total	C	N	O	S	0	0	0
			222	140	36	45	1			

- Molecule 2 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	249	Total	C	N	O	S	0	0	0
			2014	1283	357	360	14			

- Molecule 3 is a protein called Hirudin variant-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	10	Total	C	N	O	S	0	0	0
			90	56	10	23	1			

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

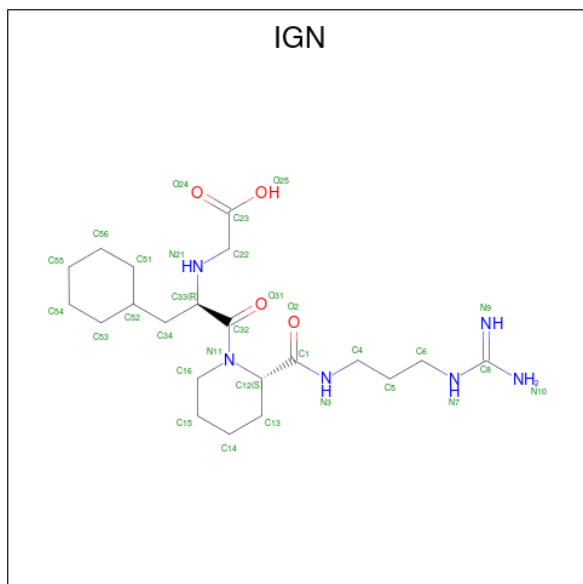


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	2	Total	C	N	O		14	0	0
			28	16	2	10				

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	2	Total	Na	0	0
			2	2		

- Molecule 6 is {[(1R)-2-((2S)-2-{[(3-{[AMINO(IMINO)METHYL]AMINO}PROPYL)AMINO]CARBONYL}PIPERIDINYL)-1-(CYCLOHEXYLMETHYL)-2-OXOETHYL]AMINO} ACETIC ACID (CCD ID: IGN) (formula: $C_{21}H_{38}N_6O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	H	1	Total	C	N	O	0	0
			31	21	6	4		

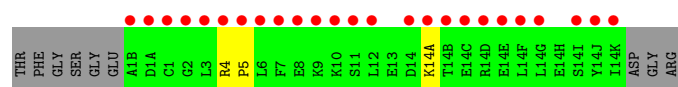
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	34	Total	O	0	0
			34	34		
7	H	207	Total	O	0	0
			207	207		
7	I	6	Total	O	0	0
			6	6		

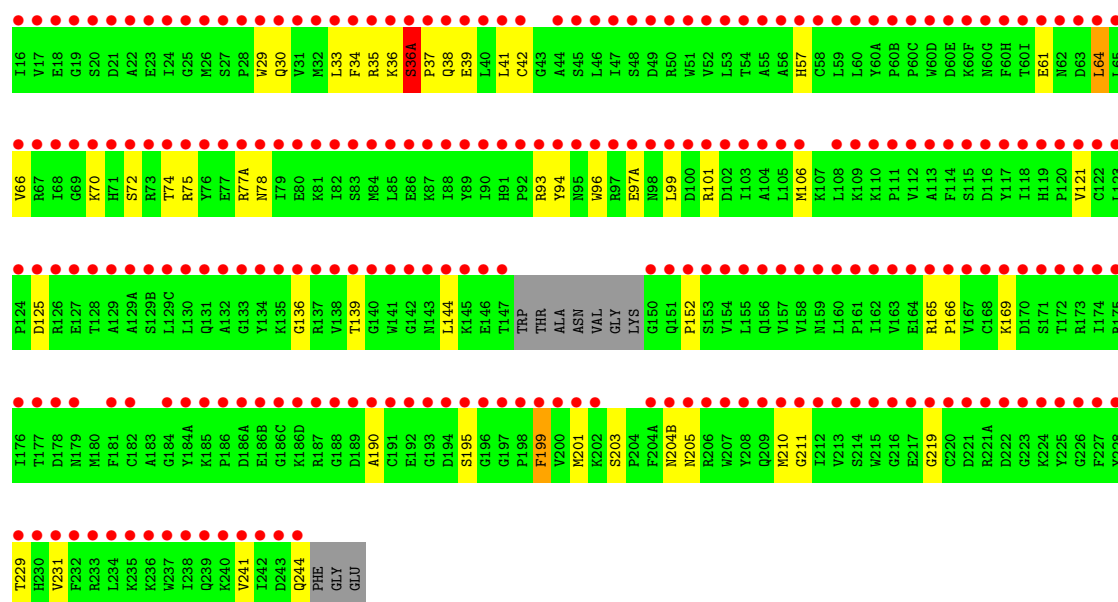
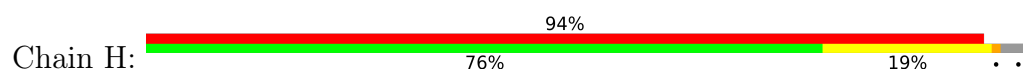
3 Residue-property plots

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.

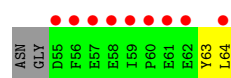
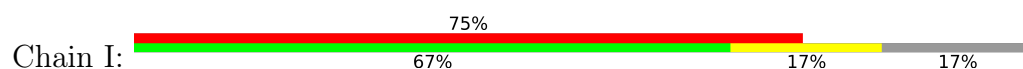
• Molecule 1: Prothrombin



• Molecule 2: Prothrombin



• Molecule 3: Hirudin variant-2



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	69.62Å 71.55Å 71.82Å 90.00° 100.12° 90.00°	Depositor
Resolution (Å)	500.00 – 1.86 70.70 – 2.26	Depositor EDS
% Data completeness (in resolution range)	96.5 (500.00-1.86) 34.8 (70.70-2.26)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.85 (at 2.27Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.216 , 0.256 0.564 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 125.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.30	EDS
Total number of atoms	2634	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, NAG, IGN, TYS

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	L	0.38	0/224	0.90	1/298 (0.3%)
2	H	0.35	0/2065	0.93	11/2790 (0.4%)
3	I	0.38	0/74	0.51	0/96
All	All	0.35	0/2363	0.91	12/3184 (0.4%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	36(A)	SER	CA-C-N	-7.34	110.67	119.84
2	H	36(A)	SER	C-N-CA	-7.34	110.67	119.84
2	H	190	ALA	N-CA-C	-6.73	101.85	110.53
1	L	14(A)	LYS	N-CA-C	6.57	120.39	112.38
2	H	97(A)	GLU	N-CA-C	6.37	120.66	112.12
2	H	64	LEU	N-CA-C	6.18	117.58	108.86
2	H	74	THR	N-CA-C	5.86	120.56	113.41
2	H	231	VAL	N-CA-C	5.51	116.14	110.36
2	H	125	ASP	N-CA-C	-5.14	102.85	110.46
2	H	219	GLY	N-CA-C	-5.13	103.02	112.62
2	H	199	PHE	N-CA-C	-5.08	98.99	107.99
2	H	70	LYS	N-CA-C	5.07	117.40	110.55

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	L	222	0	226	1	0
2	H	2014	0	1998	38	0
3	I	90	0	69	1	0
4	A	28	0	25	1	0
5	H	2	0	0	0	0
6	H	31	0	36	1	0
7	H	207	0	0	6	1
7	I	6	0	0	0	0
7	L	34	0	0	0	0
All	All	2634	0	2354	41	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (41) 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)
2:H:33:LEU:HD21	2:H:106:MET:HE1	1.57	0.84
2:H:72:SER:OG	2:H:75:ARG:HG2	1.78	0.82
7:H:609:HOH:O	4:A:1:NAG:H81	1.80	0.81
2:H:144:LEU:HD21	2:H:152:PRO:HB3	1.69	0.73
2:H:36(A):SER:CB	2:H:37:PRO:HD3	2.25	0.66
2:H:36(A):SER:OG	2:H:37:PRO:HD3	1.98	0.64
2:H:35:ARG:HD2	2:H:41:LEU:HD21	1.80	0.62
2:H:169:LYS:HB2	7:H:559:HOH:O	2.01	0.60
2:H:36(A):SER:HB2	2:H:37:PRO:HD3	1.88	0.56
2:H:57:HIS:CD2	6:H:999:IGN:H131	2.41	0.55
2:H:35:ARG:HB2	2:H:41:LEU:HD21	1.93	0.51
2:H:36(A):SER:CB	2:H:37:PRO:CD	2.89	0.50
2:H:241:VAL:O	2:H:244:GLN:HG3	2.11	0.50
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.19	0.50
2:H:77(A):ARG:O	2:H:78:ASN:HB2	2.11	0.49
2:H:203:SER:HB3	2:H:204(B):ASN:ND2	2.28	0.49
2:H:36(A):SER:OG	2:H:37:PRO:CD	2.60	0.49
2:H:30:GLN:NE2	2:H:139:THR:OG1	2.45	0.49
2:H:61:GLU:H	2:H:61:GLU:CD	2.21	0.47
2:H:41:LEU:O	2:H:42:CYS:SG	2.72	0.47
2:H:29:TRP:CG	2:H:121:VAL:HB	2.51	0.46
2:H:34:PHE:O	2:H:64:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:165:ARG:NH1	7:H:499:HOH:O	2.49	0.45
3:I:64:LEU:HD12	3:I:64:LEU:N	2.31	0.45
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.51	0.45
2:H:165:ARG:NH2	7:H:623:HOH:O	2.49	0.45
2:H:36(A):SER:O	2:H:38:GLN:N	2.50	0.44
2:H:57:HIS:NE2	2:H:195:SER:HB3	2.32	0.44
2:H:93:ARG:HB2	2:H:101:ARG:HD2	2.00	0.43
1:L:4:ARG:HA	1:L:5:PRO:HD3	1.93	0.43
2:H:33:LEU:CD2	2:H:66:VAL:HG12	2.48	0.43
2:H:203:SER:O	2:H:205:ASN:HA	2.18	0.43
2:H:37:PRO:O	2:H:39:GLU:HG2	2.19	0.43
2:H:211:GLY:HA2	2:H:229:THR:O	2.19	0.43
2:H:169:LYS:HG2	7:H:574:HOH:O	2.18	0.42
2:H:201:MET:SD	2:H:210:MET:HG3	2.59	0.42
2:H:33:LEU:HD23	2:H:66:VAL:HG12	2.01	0.42
2:H:203:SER:HB3	2:H:204(B):ASN:HD21	1.85	0.41
2:H:94:TYR:CZ	2:H:96:TRP:HB3	2.56	0.41
2:H:165:ARG:HB3	2:H:166:PRO:HD3	2.03	0.40
2:H:169:LYS:HD2	7:H:559:HOH:O	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:660:HOH:O	7:H:660:HOH:O[2_555]	1.14	1.06

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	L	25/36 (69%)	24 (96%)	1 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	245/259 (95%)	233 (95%)	10 (4%)	2 (1%)	16	6
3	I	7/12 (58%)	7 (100%)	0	0	100	100
All	All	277/307 (90%)	264 (95%)	11 (4%)	2 (1%)	18	8

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	36(A)	SER
2	H	36	LYS

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	L	25/31 (81%)	25 (100%)	0	100	100
2	H	218/225 (97%)	217 (100%)	1 (0%)	81	77
3	I	8/10 (80%)	8 (100%)	0	100	100
All	All	251/266 (94%)	250 (100%)	1 (0%)	84	82

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

Mol	Chain	Res	Type
2	H	99	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	30	GLN
2	H	62	ASN
2	H	204(B)	ASN
2	H	205	ASN
2	H	209	GLN
2	H	244	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	TYS	I	63	3	15,16,17	1.79	2 (13%)	15,22,24	0.35	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
3	TYS	I	63	3	-	1/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	63	TYS	OH-S	5.98	1.70	1.58
3	I	63	TYS	OH-CZ	-2.50	1.38	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	63	TYS	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

2 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	$\# Z > 2$
4	NAG	A	1	2,4	14,14,15	0.53	0	17,19,21	0.64	0
4	NAG	A	2	4	14,14,15	0.52	0	17,19,21	0.63	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
4	NAG	A	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	A	2	4	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

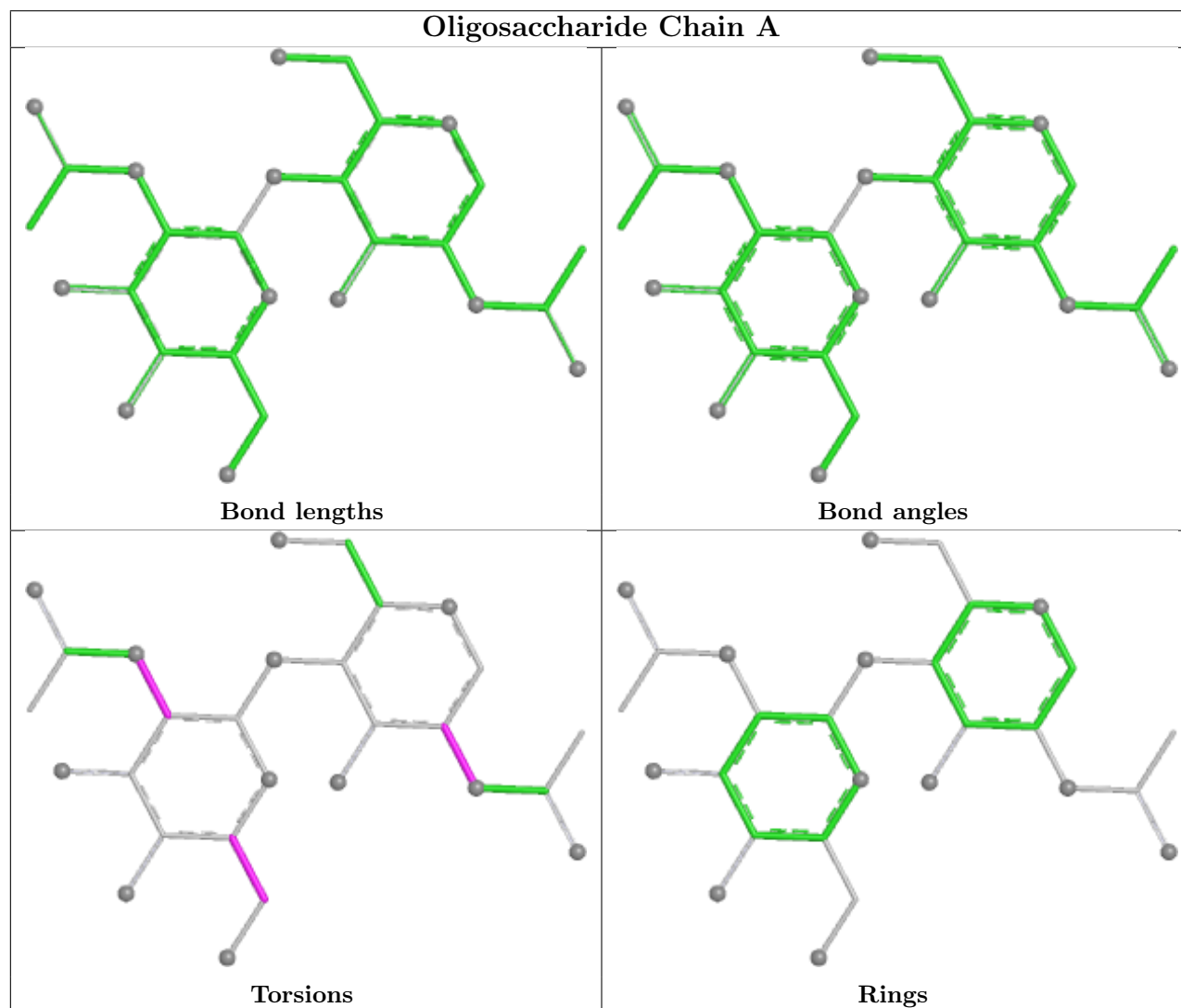
Mol	Chain	Res	Type	Atoms
4	A	2	NAG	O5-C5-C6-O6
4	A	2	NAG	C4-C5-C6-O6
4	A	1	NAG	C1-C2-N2-C7
4	A	1	NAG	C3-C2-N2-C7
4	A	2	NAG	C3-C2-N2-C7
4	A	2	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	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.



5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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
6	IGN	H	999	-	32,32,32	2.14	8 (25%)	37,41,41	1.74	7 (18%)

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
6	IGN	H	999	-	-	6/29/48/48	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	999	IGN	C8-N7	5.65	1.44	1.33
6	H	999	IGN	C12-N11	5.63	1.54	1.47
6	H	999	IGN	C34-C52	3.47	1.58	1.53
6	H	999	IGN	C16-N11	3.19	1.52	1.47
6	H	999	IGN	C22-N21	3.09	1.50	1.46
6	H	999	IGN	C33-C32	2.63	1.58	1.53
6	H	999	IGN	C51-C52	2.57	1.59	1.52
6	H	999	IGN	C32-N11	2.37	1.39	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	999	IGN	C15-C16-N11	5.18	118.66	110.65
6	H	999	IGN	C22-N21-C33	4.78	123.73	113.93
6	H	999	IGN	C33-C32-N11	3.11	124.79	118.71
6	H	999	IGN	C13-C12-C1	-2.93	106.67	112.17
6	H	999	IGN	O31-C32-C33	-2.70	114.67	119.61
6	H	999	IGN	C34-C33-C32	2.51	114.16	109.28
6	H	999	IGN	C14-C15-C16	2.31	115.47	111.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	999	IGN	C33-C34-C52-C51
6	H	999	IGN	C33-C34-C52-C53
6	H	999	IGN	C4-C5-C6-N7
6	H	999	IGN	N3-C4-C5-C6

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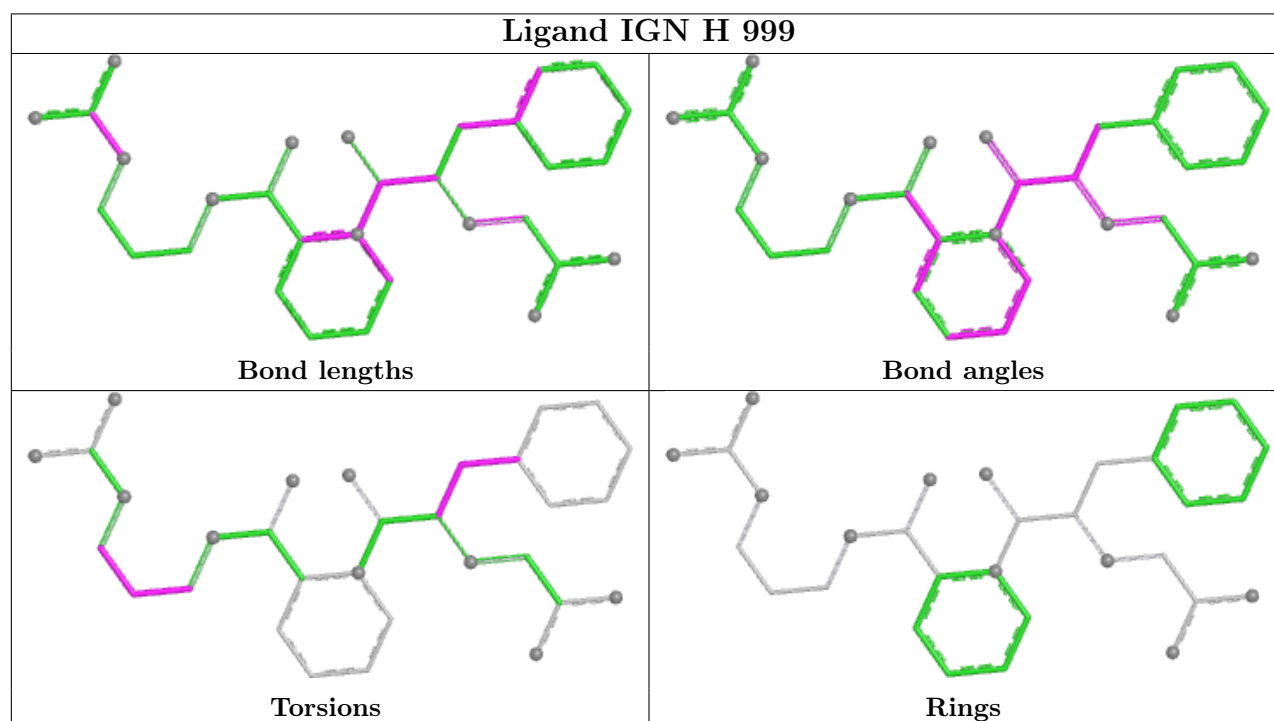
Mol	Chain	Res	Type	Atoms
6	H	999	IGN	C32-C33-C34-C52
6	H	999	IGN	N21-C33-C34-C52

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	999	IGN	1	0

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



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	L	27/36 (75%)	4.60	25 (92%) 0 0	20, 26, 38, 41	0
2	H	249/259 (96%)	4.86	243 (97%) 0 0	19, 28, 43, 52	0
3	I	9/12 (75%)	5.69	9 (100%) 0 0	43, 49, 55, 60	0
All	All	285/307 (92%)	4.86	277 (97%) 0 0	19, 28, 44, 60	0

All (277) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	128	THR	13.6
2	H	231	VAL	12.6
2	H	60(B)	PRO	11.1
1	L	3	LEU	10.4
2	H	37	PRO	9.9
1	L	1(B)	ALA	9.9
2	H	197	GLY	9.5
2	H	111	PRO	9.4
2	H	150	GLY	9.3
2	H	133	GLY	9.2
2	H	195	SER	9.1
2	H	53	LEU	9.0
2	H	176	ILE	9.0
2	H	168	CYS	8.8
2	H	117	TYR	8.6
2	H	237	TRP	8.5
2	H	118	ILE	8.5
2	H	60(D)	TRP	8.3
2	H	60(H)	PHE	8.2
3	I	59	ILE	8.2
2	H	42	CYS	8.0
3	I	64	LEU	7.8
2	H	124	PRO	7.8

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Mol	Chain	Res	Type	RSRZ
2	H	215	TRP	7.8
2	H	112	VAL	7.8
3	I	56	PHE	7.6
2	H	144	LEU	7.6
1	L	14(K)	ILE	7.5
1	L	14(A)	LYS	7.5
2	H	147	THR	7.4
2	H	89	TYR	7.3
1	L	6	LEU	7.3
2	H	232	PHE	7.3
2	H	51	TRP	7.3
2	H	68	ILE	7.2
2	H	191	CYS	7.2
2	H	52	VAL	7.2
2	H	60(C)	PRO	7.2
2	H	178	ASP	7.2
2	H	19	GLY	7.1
2	H	207	TRP	7.1
3	I	61	GLU	6.9
2	H	119	HIS	6.9
2	H	154	VAL	6.8
2	H	88	ILE	6.8
2	H	160	LEU	6.7
2	H	79	ILE	6.7
2	H	38	GLN	6.6
2	H	35	ARG	6.6
2	H	123	LEU	6.6
2	H	33	LEU	6.5
2	H	24	ILE	6.5
2	H	213	VAL	6.5
2	H	241	VAL	6.4
2	H	163	VAL	6.4
3	I	60	PRO	6.3
2	H	72	SER	6.3
2	H	186(C)	GLY	6.3
2	H	104	ALA	6.2
2	H	229	THR	6.2
2	H	64	LEU	6.2
2	H	125	ASP	6.1
2	H	239	GLN	6.1
2	H	40	LEU	6.1
2	H	211	GLY	6.1

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Mol	Chain	Res	Type	RSRZ
2	H	90	ILE	6.0
2	H	48	SER	5.9
2	H	214	SER	5.9
2	H	223	GLY	5.9
2	H	196	GLY	5.8
2	H	41	LEU	5.8
2	H	45	SER	5.8
2	H	220	CYS	5.8
2	H	161	PRO	5.8
2	H	61	GLU	5.8
2	H	22	ALA	5.8
2	H	222	ASP	5.7
2	H	217	GLU	5.7
2	H	82	ILE	5.6
2	H	93	ARG	5.6
2	H	227	PHE	5.6
2	H	184(A)	TYR	5.6
2	H	244	GLN	5.5
2	H	78	ASN	5.5
2	H	179	ASN	5.5
2	H	120	PRO	5.5
2	H	165	ARG	5.5
2	H	59	LEU	5.4
2	H	105	LEU	5.4
2	H	131	GLN	5.4
1	L	14(I)	SER	5.4
2	H	71	HIS	5.4
2	H	175	ARG	5.4
2	H	181	PHE	5.4
2	H	129(B)	SER	5.4
2	H	36(A)	SER	5.4
2	H	29	TRP	5.3
2	H	39	GLU	5.3
2	H	77	GLU	5.3
2	H	60(I)	THR	5.2
2	H	204(A)	PHE	5.2
2	H	130	LEU	5.2
2	H	243	ASP	5.2
1	L	11	SER	5.2
2	H	228	TYR	5.2
1	L	14(G)	LEU	5.2
2	H	174	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
2	H	169	LYS	5.2
2	H	151	GLN	5.1
2	H	199	PHE	5.1
2	H	212	ILE	5.1
2	H	185	LYS	5.1
2	H	164	GLU	5.1
2	H	44	ALA	5.1
2	H	134	TYR	5.1
2	H	141	TRP	5.1
2	H	129(C)	LEU	5.0
2	H	242	ILE	5.0
2	H	86	GLU	5.0
2	H	193	GLY	5.0
2	H	162	ILE	4.9
1	L	12	LEU	4.9
2	H	210	MET	4.9
1	L	8	GLU	4.9
2	H	103	ILE	4.9
2	H	198	PRO	4.8
2	H	110	LYS	4.8
2	H	28	PRO	4.8
2	H	60(A)	TYR	4.8
2	H	94	TYR	4.8
2	H	132	ALA	4.8
2	H	234	LEU	4.8
2	H	60	LEU	4.7
2	H	167	VAL	4.7
2	H	122	CYS	4.7
3	I	58	GLU	4.6
2	H	166	PRO	4.6
2	H	225	TYR	4.6
2	H	106	MET	4.6
2	H	114	PHE	4.6
2	H	200	VAL	4.6
2	H	63	ASP	4.6
2	H	186(D)	LYS	4.6
2	H	77(A)	ARG	4.6
2	H	126	ARG	4.6
2	H	140	GLY	4.6
2	H	145	LYS	4.5
1	L	14(B)	THR	4.5
2	H	66	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
2	H	102	ASP	4.5
2	H	69	GLY	4.5
2	H	142	GLY	4.5
2	H	74	THR	4.5
2	H	137	ARG	4.5
2	H	32	MET	4.5
2	H	138	VAL	4.5
2	H	25	GLY	4.5
2	H	186	PRO	4.4
2	H	230	HIS	4.4
2	H	127	GLU	4.4
2	H	26	MET	4.4
1	L	14(D)	ARG	4.3
2	H	115	SER	4.3
2	H	91	HIS	4.3
2	H	60(E)	ASP	4.3
2	H	17	VAL	4.2
3	I	62	GLU	4.2
2	H	96	TRP	4.2
2	H	58	CYS	4.2
2	H	27	SER	4.2
2	H	92	PRO	4.2
2	H	65	LEU	4.2
2	H	83	SER	4.1
2	H	67	ARG	4.1
2	H	76	TYR	4.1
2	H	36	LYS	4.1
2	H	18	GLU	4.1
2	H	116	ASP	4.1
1	L	10	LYS	4.1
1	L	14(E)	GLU	4.1
2	H	152	PRO	4.1
2	H	55	ALA	4.0
2	H	54	THR	4.0
2	H	129	ALA	4.0
2	H	60(G)	ASN	4.0
1	L	2	GLY	4.0
2	H	85	LEU	4.0
2	H	121	VAL	4.0
2	H	46	LEU	3.9
2	H	238	ILE	3.9
2	H	155	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
2	H	31	VAL	3.9
1	L	14(J)	TYR	3.9
2	H	30	GLN	3.9
2	H	240	LYS	3.9
2	H	171	SER	3.8
2	H	100	ASP	3.8
2	H	170	ASP	3.8
2	H	23	GLU	3.8
2	H	187	ARG	3.8
2	H	21	ASP	3.8
2	H	219	GLY	3.7
1	L	7	PHE	3.7
2	H	136	GLY	3.7
1	L	1(A)	ASP	3.6
2	H	98	ASN	3.6
2	H	129(A)	ALA	3.5
2	H	84	MET	3.5
2	H	49	ASP	3.5
2	H	233	ARG	3.5
2	H	34	PHE	3.5
2	H	216	GLY	3.5
1	L	1	CYS	3.5
2	H	182	CYS	3.5
2	H	189	ASP	3.5
2	H	221	ASP	3.4
2	H	73	ARG	3.4
1	L	14(F)	LEU	3.4
2	H	135	LYS	3.3
2	H	194	ASP	3.3
2	H	56	ALA	3.3
2	H	62	ASN	3.3
2	H	109	LYS	3.2
2	H	87	LYS	3.2
2	H	188	GLY	3.2
2	H	75	ARG	3.2
3	I	55	ASP	3.2
2	H	97	ARG	3.2
2	H	206	ARG	3.1
2	H	173	ARG	3.1
2	H	224	LYS	3.0
2	H	236	LYS	3.0
2	H	143	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	57	HIS	3.0
2	H	108	LEU	3.0
2	H	202	LYS	3.0
2	H	97(A)	GLU	3.0
2	H	99	LEU	2.9
2	H	157	VAL	2.9
2	H	113	ALA	2.9
2	H	177	THR	2.8
1	L	4	ARG	2.8
2	H	50	ARG	2.8
2	H	101	ARG	2.8
1	L	5	PRO	2.8
2	H	209	GLN	2.7
2	H	47	ILE	2.7
2	H	184	GLY	2.7
1	L	14	ASP	2.6
2	H	146	GLU	2.6
2	H	192	GLU	2.6
2	H	190	ALA	2.6
2	H	156	GLN	2.6
2	H	159	ASN	2.6
1	L	14(C)	GLU	2.5
2	H	153	SER	2.5
2	H	139	THR	2.5
2	H	158	VAL	2.5
2	H	20	SER	2.4
2	H	201	MET	2.4
2	H	235	LYS	2.4
2	H	186(B)	GLU	2.4
2	H	204(B)	ASN	2.4
1	L	9	LYS	2.4
2	H	205	ASN	2.4
2	H	186(A)	ASP	2.3
2	H	208	TYR	2.3
2	H	80	GLU	2.3
3	I	57	GLU	2.2
2	H	221(A)	ARG	2.2
2	H	226	GLY	2.2
2	H	60(F)	LYS	2.1
2	H	70	LYS	2.1
2	H	172	THR	2.1
2	H	95	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	81	LYS	2.0
2	H	16	ILE	2.0

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

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.

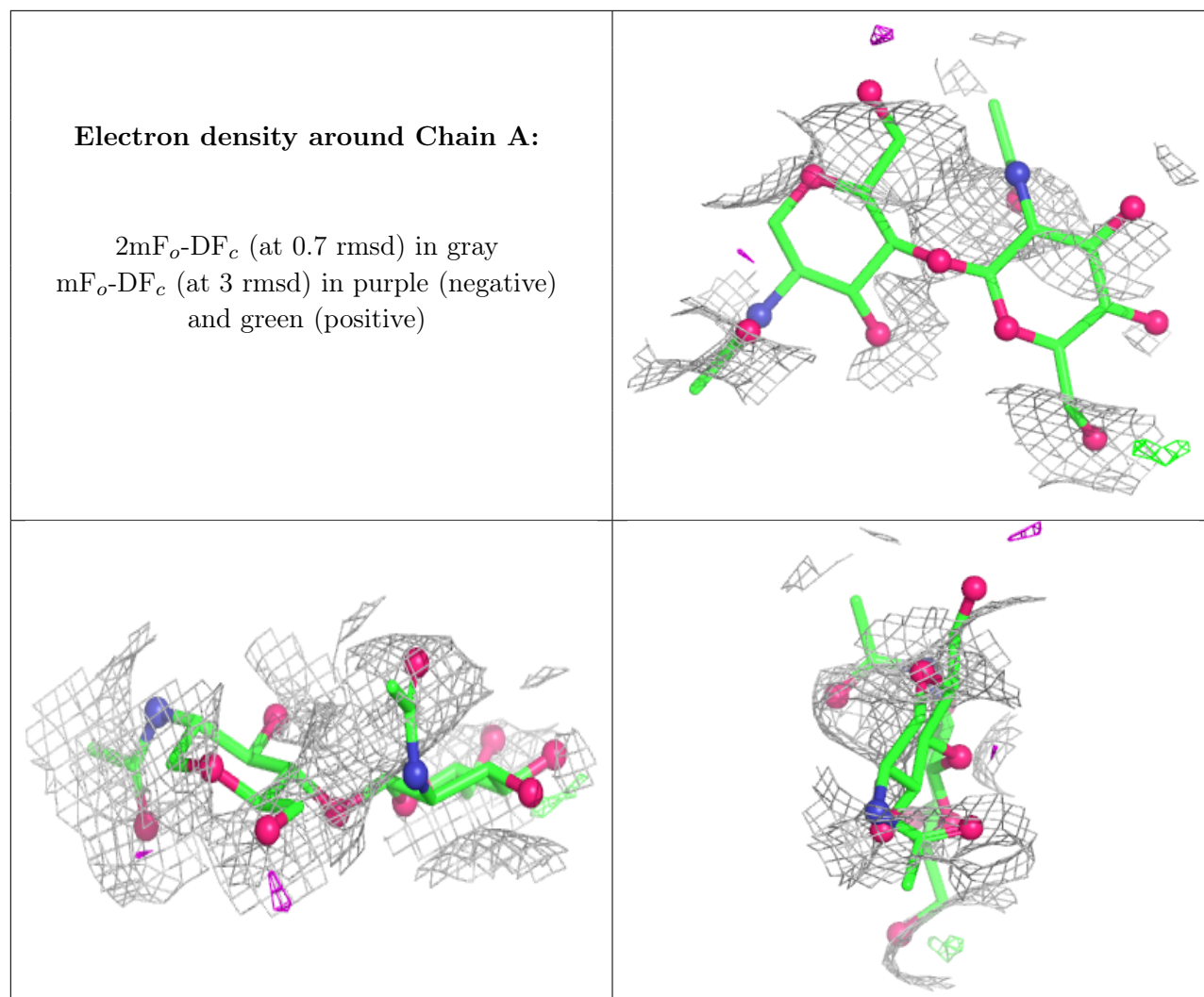
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TYS	I	63	16/17	0.57	0.24	40,45,55,56	0

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	NAG	A	1	14/15	-	-	49,52,53,53	0
4	NAG	A	2	14/15	-	-	49,50,50,50	14

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.



6.4 Ligands [i](#)

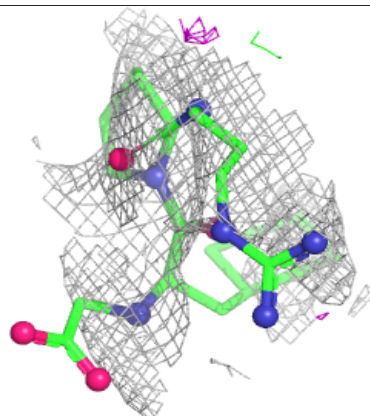
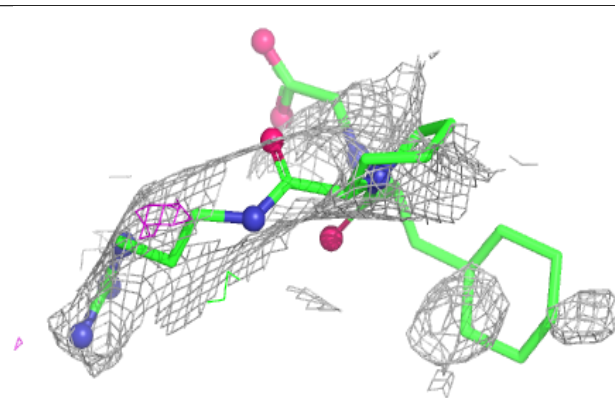
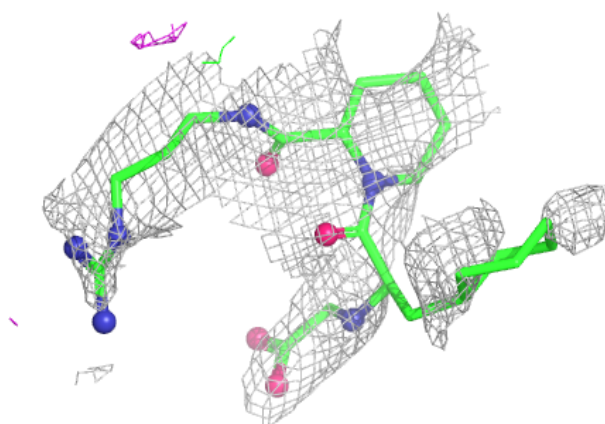
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NA	H	392	1/1	0.49	0.23	24,24,24,24	0
6	IGN	H	999	31/31	0.58	0.21	27,31,37,37	0
5	NA	H	391	1/1	0.79	0.08	27,27,27,27	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 IGN H 999:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.