



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:35 PM UTC

PDB ID : 3CDZ / pdb_00003cdz
Title : Crystal structure of human factor VIII
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Deposited on : 2008-02-27
Resolution : 3.98 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
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

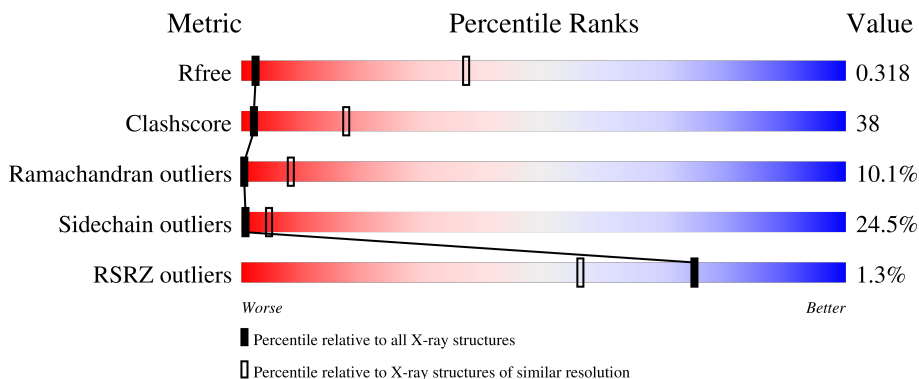
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.98 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	1016 (4.18-3.78)
Clashscore	190562	1007 (4.16-3.80)
Ramachandran outliers	187476	1000 (4.18-3.78)
Sidechain outliers	187428	1131 (4.20-3.76)
RSRZ outliers	180081	1016 (4.18-3.78)

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	754	 25% 37% 17% 5% 16%
2	B	684	 34% 39% 16% 8%
3	C	2	 50% 50%
4	D	4	 75% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MAN	D	2	X	-	-	-
4	MAN	D	4	X	-	-	-
7	NAG	B	2333	X	-	-	-
7	NAG	B	2334	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10317 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 Coagulation factor VIII heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	630	5086	3278	855	928	25	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	741	SER	-	SEE REMARK 999	UNP P00451
A	742	PHE	-	SEE REMARK 999	UNP P00451
A	743	SER	-	SEE REMARK 999	UNP P00451
A	744	GLN	-	SEE REMARK 999	UNP P00451
A	745	ASN	-	SEE REMARK 999	UNP P00451
A	746	PRO	-	SEE REMARK 999	UNP P00451
A	747	PRO	-	SEE REMARK 999	UNP P00451
A	748	VAL	-	SEE REMARK 999	UNP P00451
A	749	LEU	-	SEE REMARK 999	UNP P00451
A	750	LYS	-	SEE REMARK 999	UNP P00451
A	751	ARG	-	SEE REMARK 999	UNP P00451
A	752	HIS	-	SEE REMARK 999	UNP P00451
A	753	GLN	-	SEE REMARK 999	UNP P00451
A	754	ARG	-	SEE REMARK 999	UNP P00451

- Molecule 2 is a protein called Coagulation factor VIII light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	631	5125	3288	881	924	32	0	0	0

There is a discrepancy between the modelled and reference sequences:

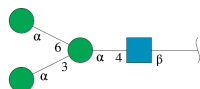
Chain	Residue	Modelled	Actual	Comment	Reference
B	1880	LEU	PHE	variant	UNP P00451

- 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
			Total	C	N	O			
3	C	2	28	16	2	10	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	4	47	26	1	20	0	0	0

- Molecule 5 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cu	0	0
			1	1		
5	B	1	Total	Cu	0	0
			1	1		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		

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

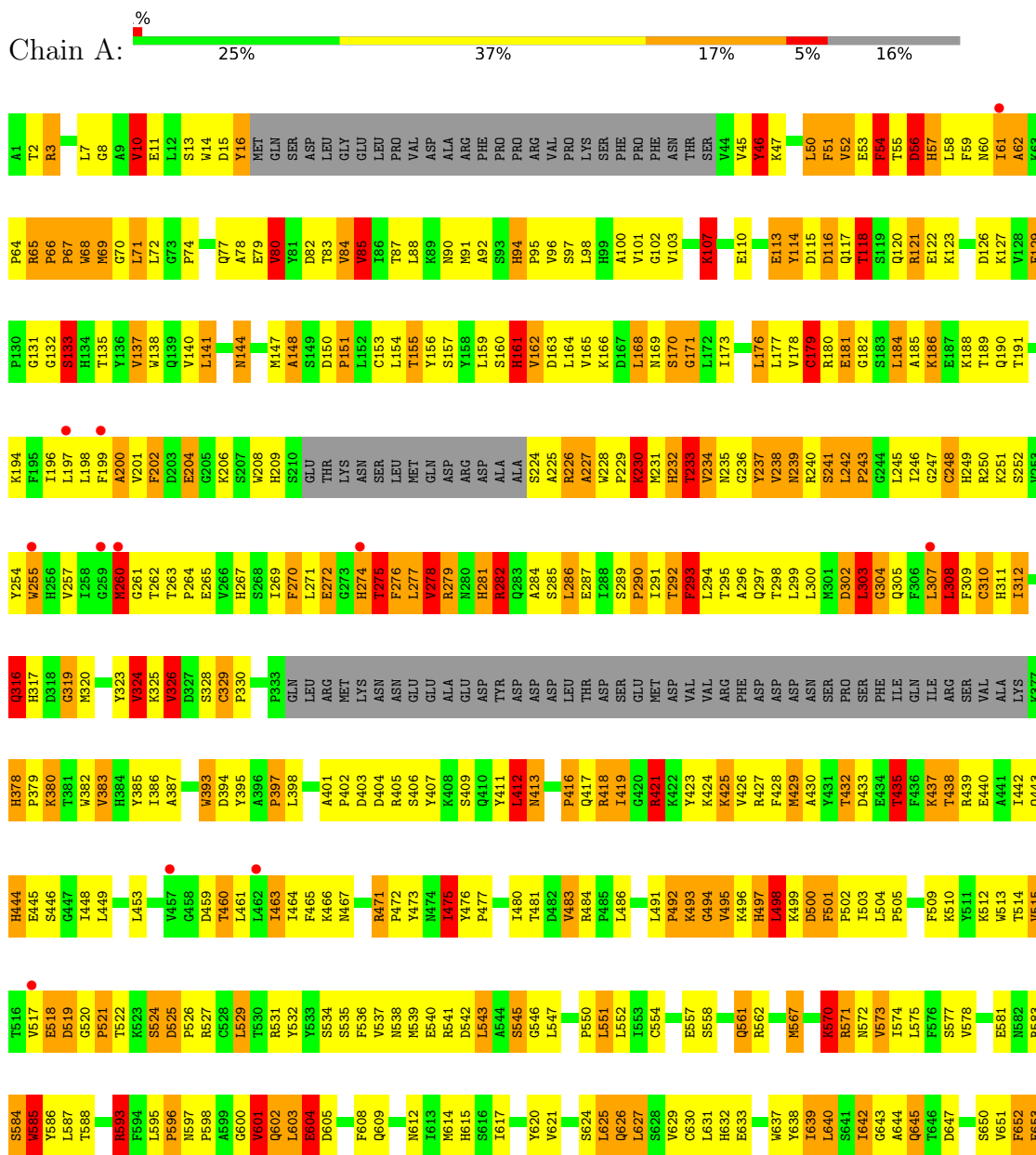


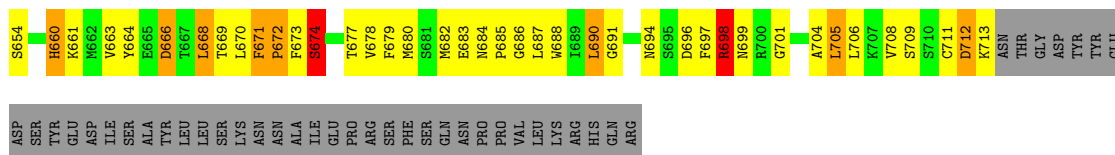
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots

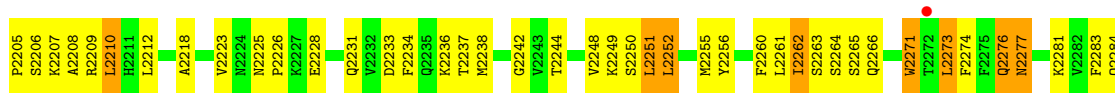
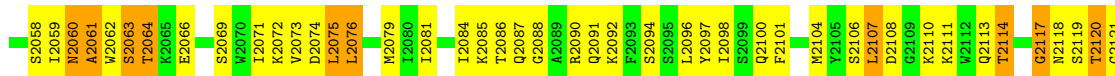
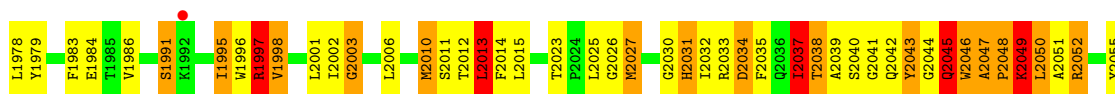
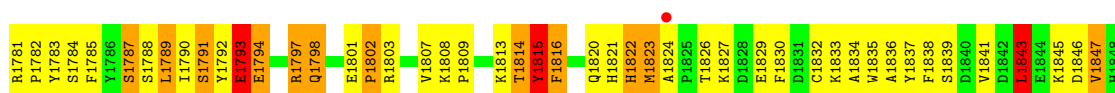
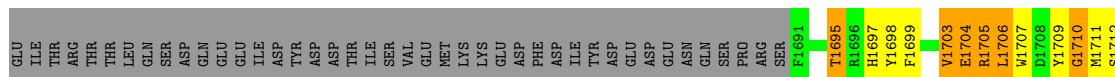
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Coagulation factor VIII heavy chain





• Molecule 2: Coagulation factor VIII light chain



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



MAG1
MAG2

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

Chain D:



MAG1
MAN2
MAN3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	134.11Å 134.11Å 349.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.98 50.00 – 3.98	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-3.98) 98.5 (50.00-3.98)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.92 (at 4.00Å)	Xtrriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.256 , 0.327 0.251 , 0.318	Depositor DCC
R_{free} test set	1399 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	151.1	Xtrriage
Anisotropy	0.480	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 221.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10317	wwPDB-VP
Average B, all atoms (Å ²)	199.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MAN, NAG, CU

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	0.91	10/5230 (0.2%)	1.19	49/7098 (0.7%)
2	B	0.78	4/5270 (0.1%)	1.08	34/7136 (0.5%)
All	All	0.85	14/10500 (0.1%)	1.14	83/14234 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
2	B	0	6
All	All	0	13

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	ARG	CZ-NH1	12.41	1.50	1.32
2	B	1904	ASN	CG-OD1	11.46	1.45	1.23
1	A	121	ARG	NE-CZ	10.23	1.44	1.33
2	B	1904	ASN	CG-ND2	9.73	1.53	1.33
1	A	107	LYS	CG-CD	7.40	1.74	1.52

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	ARG	NE-CZ-NH2	-12.12	108.29	119.20
1	A	121	ARG	NE-CZ-NH1	10.56	132.06	121.50
1	A	233	THR	N-CA-C	9.85	124.49	109.23
1	A	329	CYS	N-CA-C	8.83	123.65	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1904	ASN	OD1-CG-ND2	8.52	131.12	122.60

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	TYR	Peptide
1	A	278	VAL	Peptide
1	A	281	HIS	Peptide
1	A	282	ARG	Peptide
1	A	56	ASP	Peptide

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	5086	0	4971	420	0
2	B	5125	0	4994	370	0
3	C	28	0	25	1	0
4	D	47	0	40	2	0
5	A	1	0	0	1	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
7	B	28	0	26	0	0
All	All	10317	0	10056	770	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 38.

The worst 5 of 770 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:107:LYS:CG	1:A:107:LYS:CD	1.74	1.58
1:A:378:HIS:HB3	1:A:379:PRO:CD	1.71	1.19
2:B:1963:PHE:CD2	2:B:1986:VAL:HG21	1.77	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:LEU:CB	1:A:421:ARG:HG2	1.76	1.15
1:A:572:ASN:HB3	1:A:637:TRP:CZ3	1.82	1.15

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	622/754 (82%)	430 (69%)	130 (21%)	62 (10%)	0 8
2	B	627/684 (92%)	437 (70%)	126 (20%)	64 (10%)	0 8
All	All	1249/1438 (87%)	867 (69%)	256 (20%)	126 (10%)	0 8

5 of 126 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	THR
1	A	133	SER
1	A	181	GLU
1	A	227	ALA
1	A	232	HIS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	559/674 (83%)	401 (72%)	158 (28%)	0	3
2	B	560/612 (92%)	444 (79%)	116 (21%)	1	7
All	All	1119/1286 (87%)	845 (76%)	274 (24%)	1	4

5 of 274 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	2058	SER
2	B	2086	THR
2	B	2178	LEU
1	A	435	THR
1	A	427	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	2036	GLN
2	B	2042	GLN
2	B	2222	GLN
1	A	615	HIS
1	A	609	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

6 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	C	1	3,1	14,14,15	0.88	0	17,19,21	1.10	1 (5%)
3	NAG	C	2	3	14,14,15	2.92	3 (21%)	17,19,21	1.73	2 (11%)
4	NAG	D	1	4	14,14,15	0.97	0	17,19,21	1.59	5 (29%)
4	MAN	D	2	4	11,11,12	0.64	0	15,15,17	1.61	2 (13%)
4	MAN	D	3	4	11,11,12	0.68	0	15,15,17	1.98	2 (13%)
4	MAN	D	4	4	11,11,12	0.78	0	15,15,17	1.57	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
4	NAG	D	1	4	-	5/6/23/26	0/1/1/1
4	MAN	D	2	4	1/1/4/5	2/2/19/22	0/1/1/1
4	MAN	D	3	4	-	2/2/19/22	0/1/1/1
4	MAN	D	4	4	1/1/4/5	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	O7-C7	8.08	1.41	1.23
3	C	2	NAG	C8-C7	-6.02	1.38	1.50
3	C	2	NAG	C1-C2	2.94	1.56	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3	MAN	C1-O5-C5	6.55	120.96	112.19
3	C	2	NAG	C4-C3-C2	5.16	118.58	111.02
4	D	2	MAN	C1-O5-C5	4.56	118.30	112.19
4	D	4	MAN	C2-C3-C4	3.75	117.45	110.86
4	D	4	MAN	C1-C2-C3	3.28	114.42	109.64

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	2	MAN	C1
4	D	4	MAN	C1

5 of 18 torsion outliers are listed below:

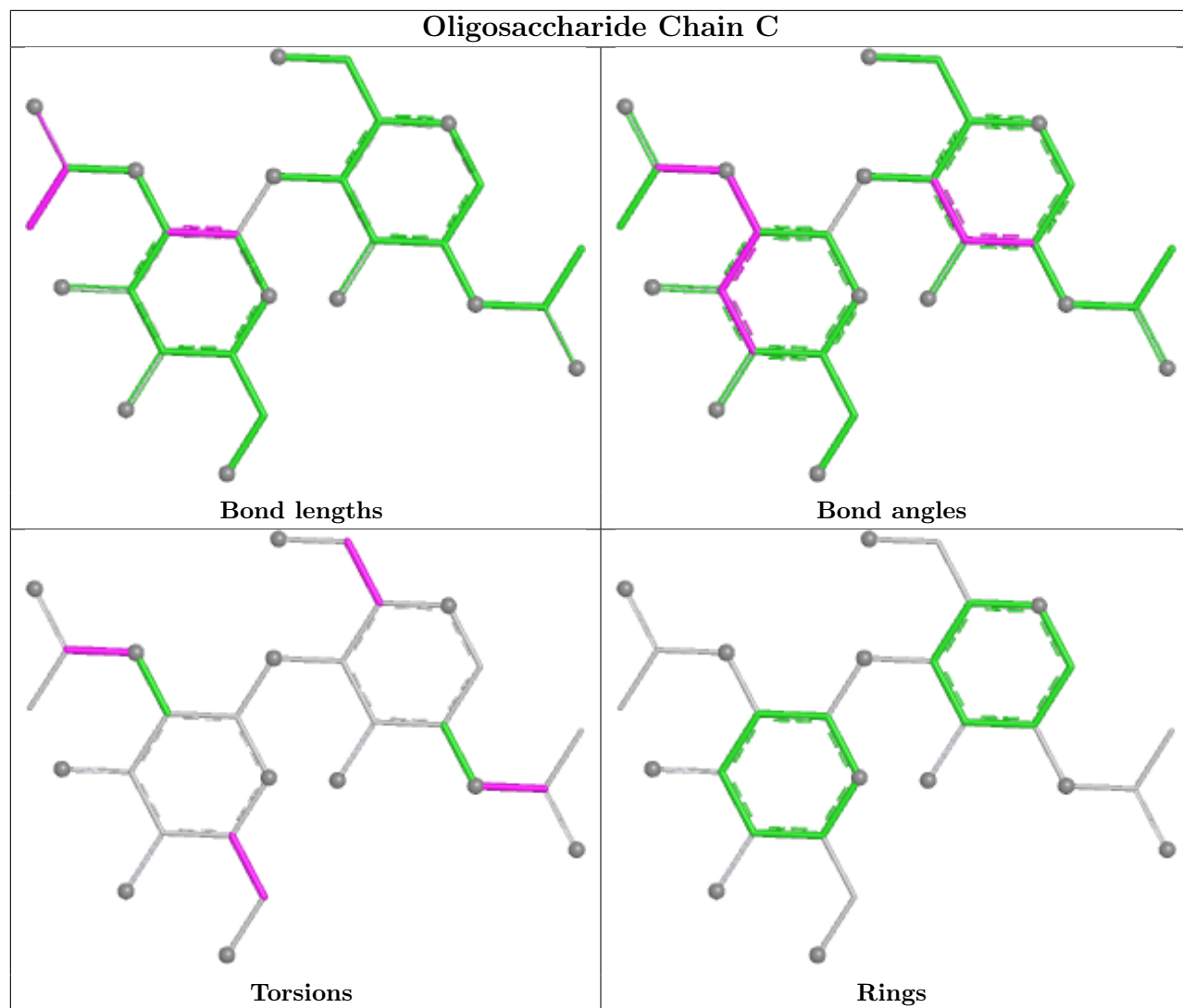
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
4	D	1	NAG	C3-C2-N2-C7
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2

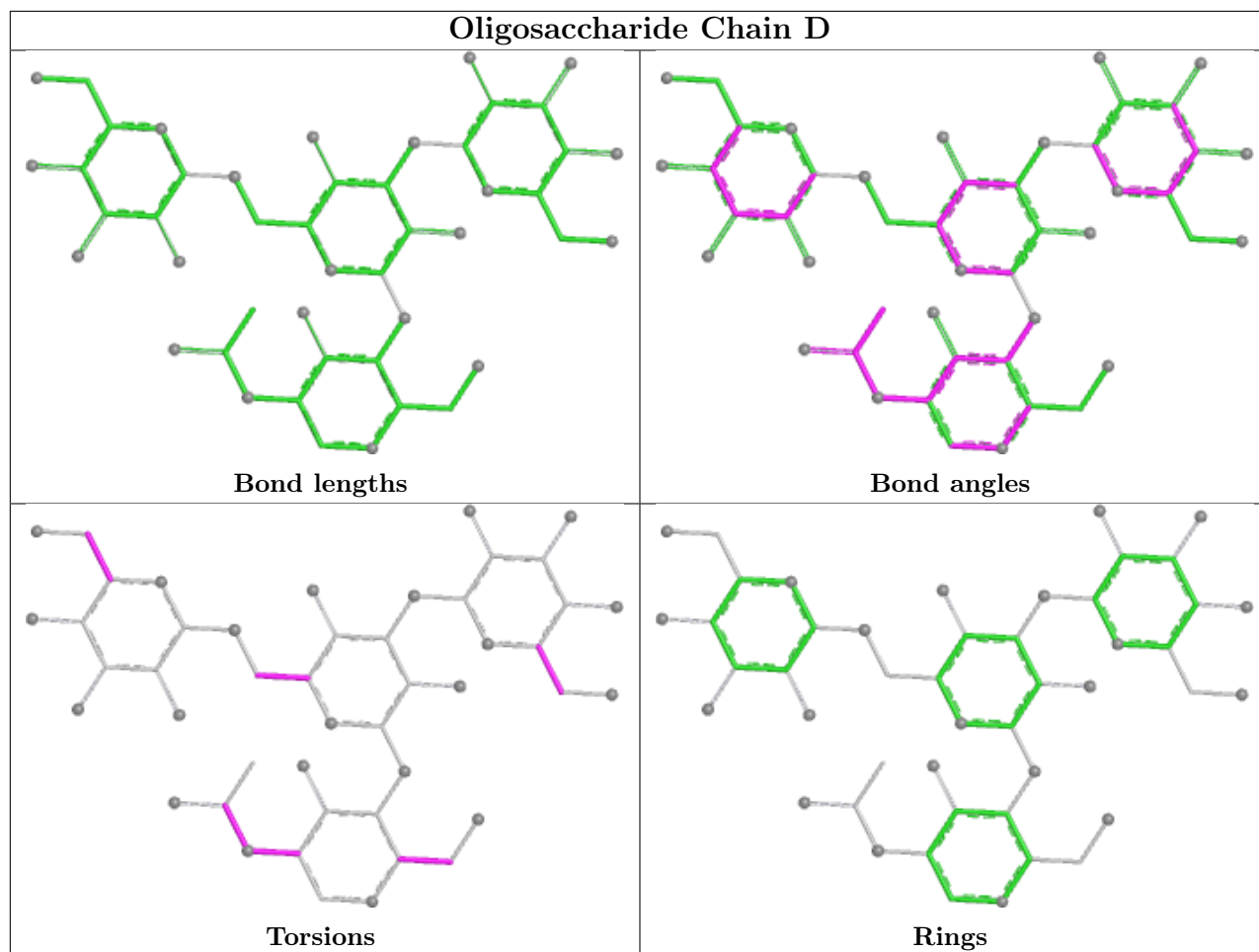
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	1	0
4	D	1	NAG	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 oligosaccharide.





5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\# Z > 2$
7	NAG	B	2333	2	14,14,15	0.76	0	17,19,21	2.05	5 (29%)
7	NAG	B	2334	2	14,14,15	0.84	0	17,19,21	1.29	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
7	NAG	B	2333	2	1/1/5/7	3/6/23/26	0/1/1/1
7	NAG	B	2334	2	1/1/5/7	4/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	B	2333	NAG	C1-O5-C5	5.12	119.05	112.19
7	B	2333	NAG	C3-C4-C5	4.36	118.14	110.23
7	B	2334	NAG	C1-O5-C5	3.03	116.25	112.19
7	B	2333	NAG	C2-N2-C7	2.70	126.52	122.90
7	B	2334	NAG	C2-N2-C7	2.63	126.42	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	2333	NAG	C1
7	B	2334	NAG	C1

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	2333	NAG	C8-C7-N2-C2
7	B	2333	NAG	O7-C7-N2-C2
7	B	2334	NAG	C8-C7-N2-C2
7	B	2334	NAG	O7-C7-N2-C2
7	B	2334	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 [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(Å ²)	Q<0.9
1	A	630/754 (83%)	-0.21	11 (1%) 69 50	182, 196, 215, 239	0
2	B	631/684 (92%)	-0.21	5 (0%) 82 65	101, 198, 214, 231	1 (0%)
All	All	1261/1438 (87%)	-0.21	16 (1%) 75 56	101, 197, 215, 239	1 (0%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1992	LYS	3.1
2	B	2272	THR	3.1
1	A	197	LEU	3.0
1	A	517	VAL	2.6
1	A	307	LEU	2.5

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.

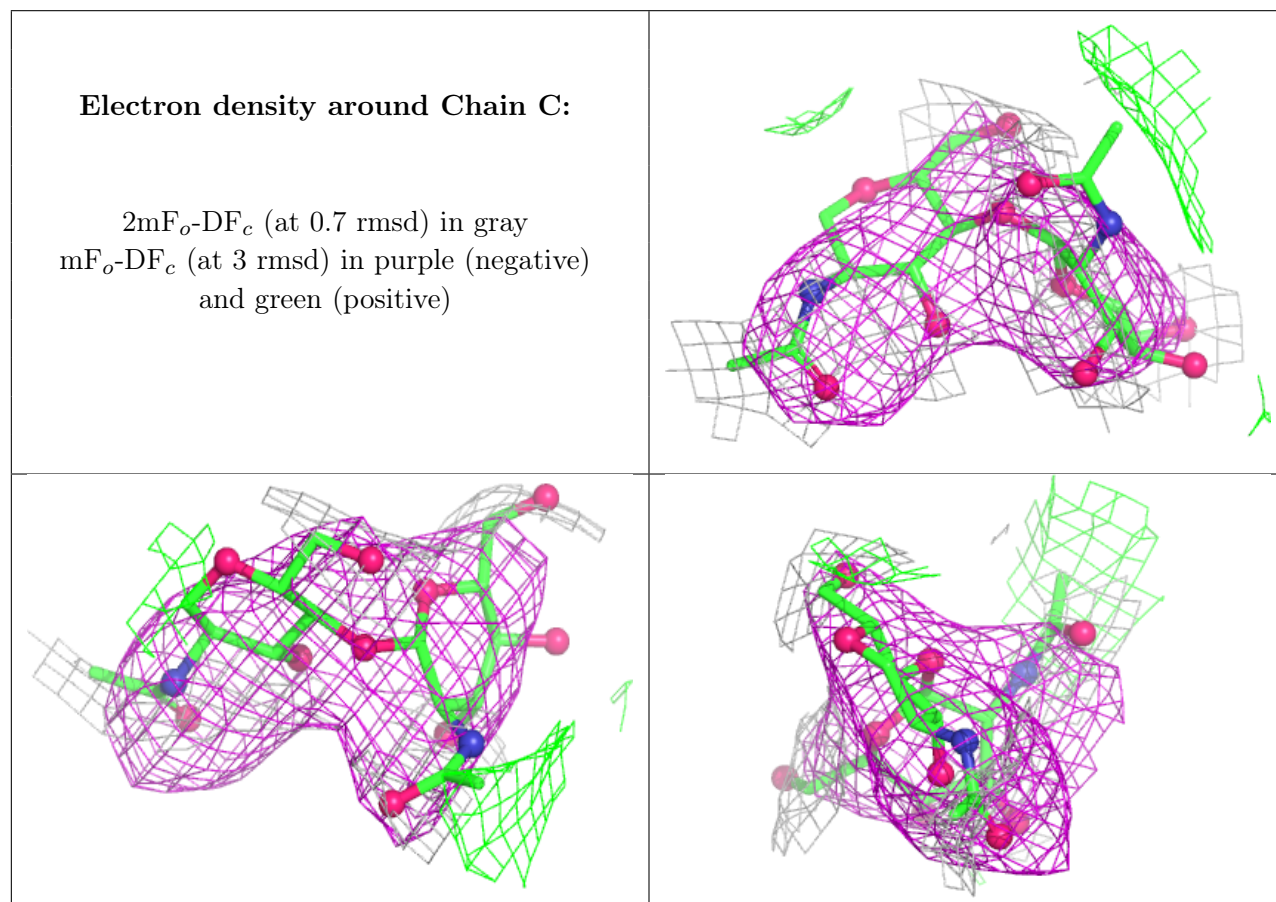
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	2	14/15	-0.20	0.20	227,229,230,231	0
4	MAN	D	2	11/12	0.17	0.14	257,259,260,261	0
3	NAG	C	1	14/15	0.32	0.14	210,216,218,222	0
4	MAN	D	3	11/12	0.34	0.12	258,261,261,261	0
4	MAN	D	4	11/12	0.45	0.15	254,255,256,256	0

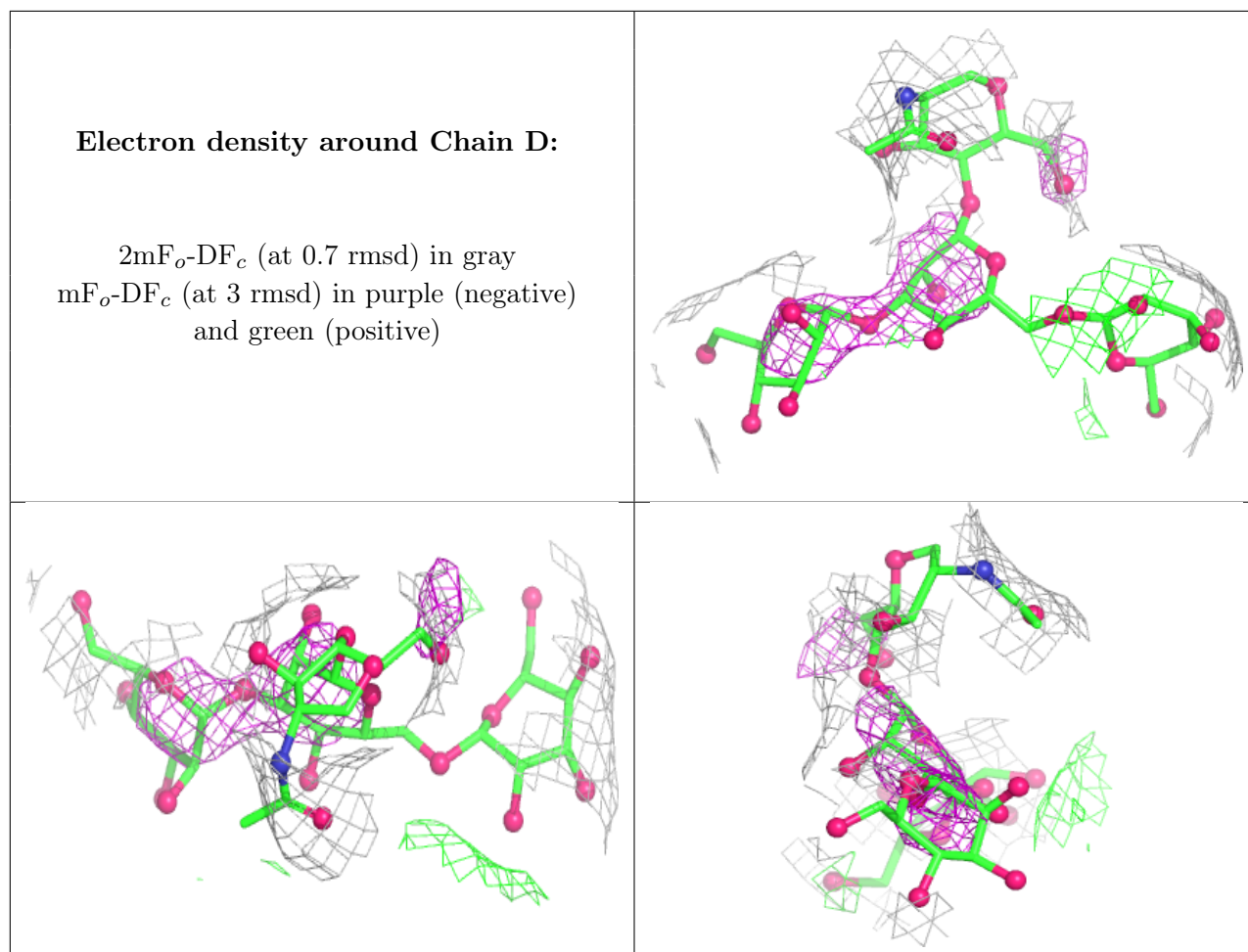
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	D	1	14/15	0.67	0.10	257,257,257,258	0

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.





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(Å ²)	Q<0.9
7	NAG	B	2333	14/15	0.16	0.14	210,213,214,214	0
7	NAG	B	2334	14/15	0.70	0.14	191,194,196,197	0
6	CA	A	758	1/1	0.98	0.06	172,172,172,172	0
5	CU	B	1	1/1	0.99	0.07	174,174,174,174	0
5	CU	A	757	1/1	1.00	0.04	171,171,171,171	0

6.5 Other polymers [i](#)

There are no such residues in this entry.