



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:21 AM UTC

PDB ID : 5LFE / pdb_00005lfe
Title : Protruding domain of GII.4 human norovirus isolate 8-14 in complex with HBGA type B (triglycan)
Authors : Singh, B.K.; Hansman, G.S.
Deposited on : 2016-07-01
Resolution : 2.30 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
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

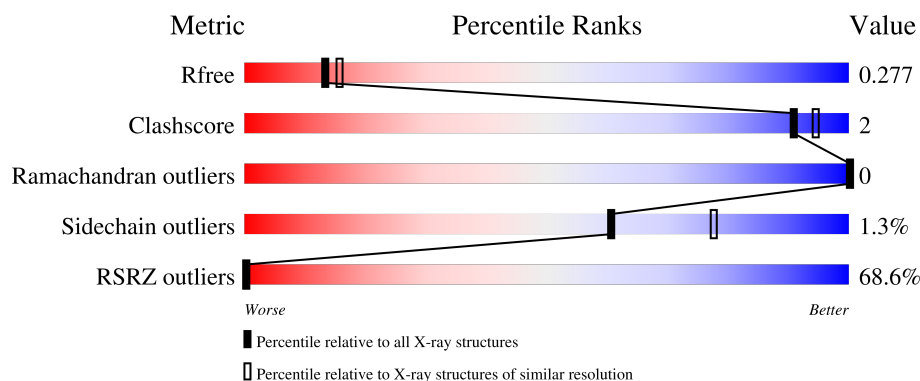
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	309	70% 95% 5%
1	B	309	67% 93% 6%
2	C	3	33% 67%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9639 atoms, of which 4508 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.

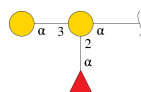
- Molecule 1 is a protein called VP1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	309	Total	C	H	N	O	S	0	0	0
			4667	1520	2273	409	454	11			
1	B	306	Total	C	H	N	O	S	0	0	0
			4606	1505	2235	404	451	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	PRO	-	expression tag	UNP M4QNL3
A	223	GLY	-	expression tag	UNP M4QNL3
A	224	SER	-	expression tag	UNP M4QNL3
B	222	PRO	-	expression tag	UNP M4QNL3
B	223	GLY	-	expression tag	UNP M4QNL3
B	224	SER	-	expression tag	UNP M4QNL3

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-2)-[alpha-D-galactopyranoside-(1-3)]alpha-D-galactopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	3	Total	C	O	0	0	0
			33	18	15			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	150	Total	O	0	0
			150	150		

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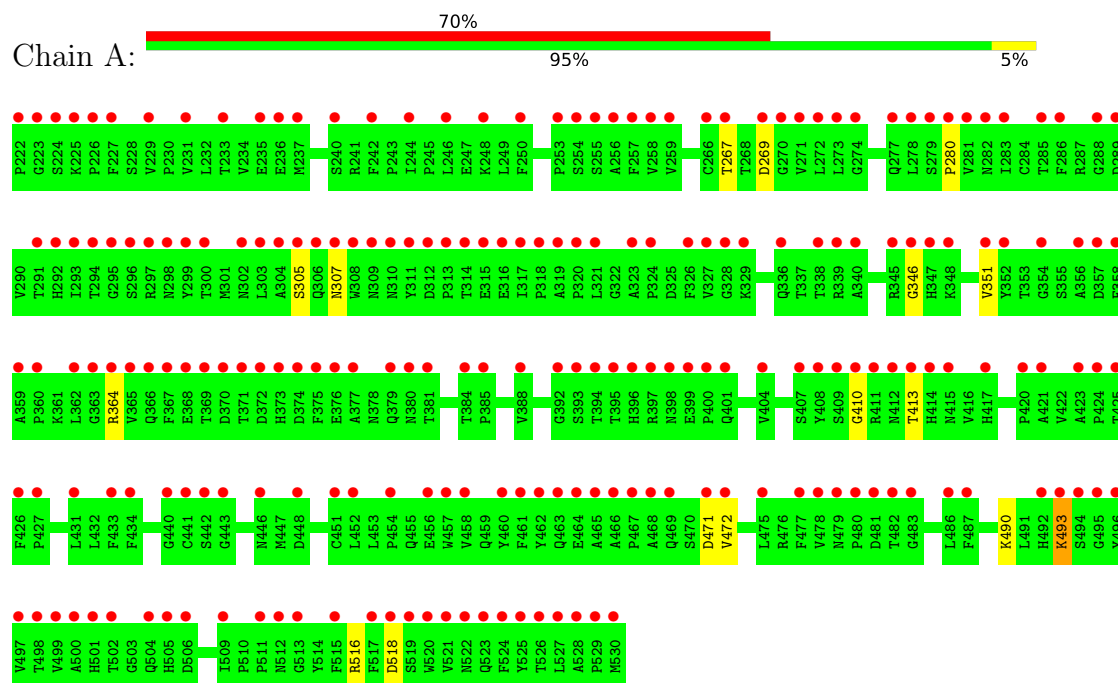
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	183	Total 183	O 183	0	0

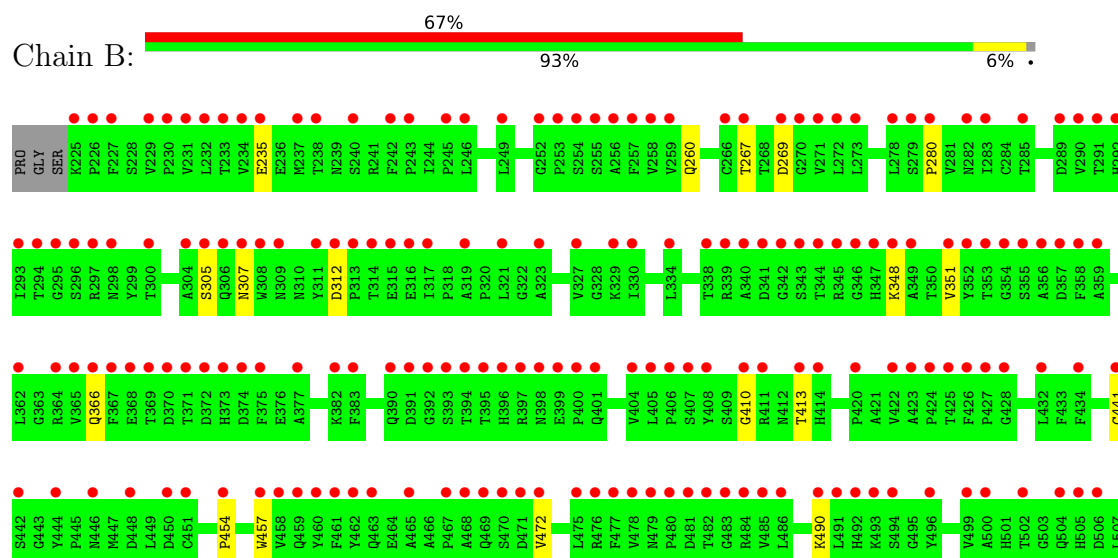
3 Residue-property plots

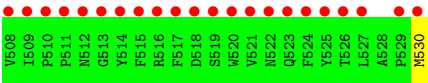
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: VP1



• Molecule 1: VP1





● Molecule 2: α -L-fucopyranose-(1-2)-[α -D-galactopyranose-(1-3)] α -D-galactopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.83Å 55.42Å 87.10Å 90.00° 99.38° 90.00°	Depositor
Resolution (Å)	46.58 – 2.30 46.58 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.4 (46.58-2.30) 94.8 (46.58-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.27Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.233 , 0.277 0.235 , 0.277	Depositor DCC
R_{free} test set	1326 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	9639	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 78.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4942e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLA, FUC

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	0.32	0/2466	0.64	0/3374
1	B	0.31	0/2442	0.62	0/3344
All	All	0.32	0/4908	0.63	0/6718

There are no bond length outliers.

There are no bond angle outliers.

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	2394	2273	2275	8	0
1	B	2371	2235	2248	10	0
2	C	33	0	30	0	0
3	A	150	0	0	0	0
3	B	183	0	0	2	0
All	All	5131	4508	4553	16	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 2.

All (16) 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:B:305:SER:OG	1:B:307:ASN:OD1	2.04	0.76
1:B:267:THR:OG1	1:B:269:ASP:OD2	2.18	0.61
1:A:267:THR:OG1	1:A:269:ASP:OD1	2.13	0.59
1:B:410:GLY:O	1:B:413:THR:OG1	2.22	0.56
1:B:260:GLN:NE2	3:B:608:HOH:O	2.39	0.51
1:A:305:SER:OG	1:A:307:ASN:OD1	2.27	0.50
1:A:280:PRO:HG2	1:B:280:PRO:HG2	1.93	0.49
1:A:472:VAL:HG11	1:A:490:LYS:HG2	1.94	0.49
1:A:516:ARG:NE	1:A:518:ASP:OD1	2.43	0.49
1:B:235:GLU:OE1	3:B:601:HOH:O	2.19	0.48
1:A:410:GLY:O	1:A:413:THR:OG1	2.29	0.45
1:A:471:ASP:HA	1:A:493:LYS:HE2	2.01	0.42
1:A:346:GLY:N	1:B:441:CYS:O	2.53	0.42
1:B:472:VAL:HG11	1:B:490:LYS:HG2	2.03	0.41
1:B:312:ASP:OD1	1:B:312:ASP:N	2.54	0.40
1:B:454:PRO:HG2	1:B:457:TRP:CG	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	307/309 (99%)	303 (99%)	4 (1%)	0	100	100
1	B	304/309 (98%)	300 (99%)	4 (1%)	0	100	100
All	All	611/618 (99%)	603 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	262/267 (98%)	259 (99%)	3 (1%)	65	81
1	B	260/267 (97%)	256 (98%)	4 (2%)	57	75
All	All	522/534 (98%)	515 (99%)	7 (1%)	61	77

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	351	VAL
1	A	364	ARG
1	A	493	LYS
1	B	348	LYS
1	B	351	VAL
1	B	366	GLN
1	B	530	MET

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

Mol	Chain	Res	Type
1	A	263	ASN
1	A	523	GLN
1	B	522	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 ⓘ

3 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	GLA	C	1	2	12,12,12	0.50	0	17,17,17	0.94	1 (5%)
2	FUC	C	2	2	10,10,11	0.66	0	14,14,16	0.77	0
2	GLA	C	3	2	11,11,12	0.77	0	15,15,17	1.11	1 (6%)

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	GLA	C	1	2	-	0/2/22/22	0/1/1/1
2	FUC	C	2	2	-	-	0/1/1/1
2	GLA	C	3	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	C	3	GLA	C1-O5-C5	-3.50	107.49	112.19
2	C	1	GLA	C1-O5-C5	-2.94	107.96	113.65

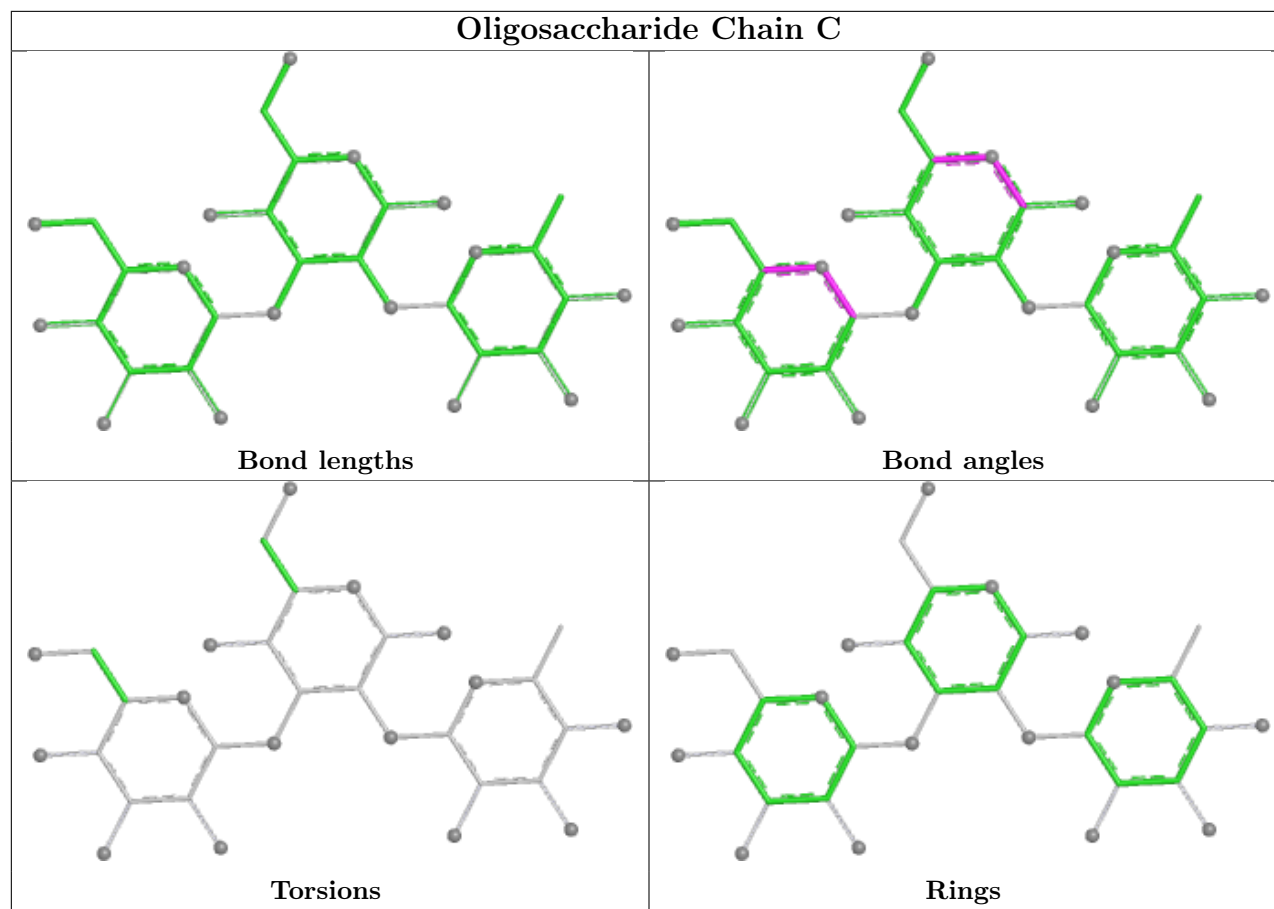
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	309/309 (100%)	2.63	216 (69%) 0 0	22, 37, 55, 86	0
1	B	306/309 (99%)	2.60	206 (67%) 0 0	24, 35, 59, 87	1 (0%)
All	All	615/618 (99%)	2.62	422 (68%) 0 0	22, 36, 57, 87	1 (0%)

All (422) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	THR	8.9
1	A	374	ASP	8.4
1	B	481	ASP	7.8
1	B	312	ASP	7.5
1	B	294	THR	7.0
1	A	359	ALA	6.8
1	A	293	ILE	6.5
1	B	483	GLY	6.4
1	B	482	THR	6.3
1	A	295	GLY	6.1
1	A	372	ASP	6.0
1	B	370	ASP	6.0
1	B	479	ASN	6.0
1	B	480	PRO	6.0
1	B	511	PRO	5.9
1	B	226	PRO	5.8
1	A	375	PHE	5.6
1	B	357	ASP	5.4
1	B	514	TYR	5.4
1	A	357	ASP	5.3
1	A	294	THR	5.3
1	A	424	PRO	5.2
1	B	346	GLY	5.2
1	B	414	HIS	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	375	PHE	5.1
1	B	425	THR	5.1
1	B	522	ASN	5.0
1	B	478	VAL	5.0
1	B	524	PHE	4.9
1	A	365	VAL	4.9
1	A	272	LEU	4.9
1	A	310	ASN	4.9
1	A	393	SER	4.8
1	B	293	ILE	4.8
1	A	307	ASN	4.8
1	A	296	SER	4.8
1	B	442	SER	4.8
1	B	295	GLY	4.7
1	A	257	PHE	4.7
1	A	223	GLY	4.7
1	B	231	VAL	4.7
1	B	485	VAL	4.7
1	A	392	GLY	4.7
1	B	523	GLN	4.6
1	A	256	ALA	4.6
1	A	528	ALA	4.6
1	A	258	VAL	4.6
1	A	302	ASN	4.6
1	A	499	VAL	4.6
1	B	314	THR	4.5
1	A	226	PRO	4.4
1	B	296	SER	4.4
1	A	278	LEU	4.4
1	B	410	GLY	4.4
1	A	279	SER	4.4
1	A	339	ARG	4.3
1	B	407	SER	4.3
1	A	469	GLN	4.2
1	A	340	ALA	4.2
1	A	466	ALA	4.2
1	A	314	THR	4.2
1	A	306	GLN	4.2
1	A	370	ASP	4.1
1	B	484	ARG	4.1
1	A	338	THR	4.1
1	A	270	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	339	ARG	4.1
1	A	345	ARG	4.0
1	A	313	PRO	4.0
1	A	346	GLY	4.0
1	A	397	ARG	4.0
1	B	469	GLN	4.0
1	A	395	THR	4.0
1	A	227	PHE	4.0
1	B	400	PRO	3.9
1	A	323	ALA	3.9
1	B	279	SER	3.9
1	B	356	ALA	3.9
1	A	366	GLN	3.9
1	A	254	SER	3.8
1	A	440	GLY	3.8
1	A	497	VAL	3.8
1	B	477	PHE	3.7
1	B	428	GLY	3.7
1	B	242	PHE	3.7
1	A	520	TRP	3.7
1	A	371	THR	3.7
1	B	238	THR	3.7
1	B	300	THR	3.7
1	B	353	THR	3.7
1	B	509	ILE	3.6
1	B	432	LEU	3.6
1	A	356	ALA	3.6
1	B	225	LYS	3.6
1	B	291	THR	3.6
1	B	413	THR	3.6
1	A	523	GLN	3.6
1	A	517	PHE	3.6
1	A	271	VAL	3.6
1	A	358	PHE	3.6
1	B	517	PHE	3.6
1	A	312	ASP	3.5
1	A	285	THR	3.5
1	B	366	GLN	3.5
1	B	512	ASN	3.5
1	A	316	GLU	3.5
1	B	313	PRO	3.5
1	B	508	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	256	ALA	3.5
1	A	364	ARG	3.5
1	B	502	THR	3.5
1	B	510	PRO	3.5
1	A	425	THR	3.4
1	B	271	VAL	3.4
1	A	483	GLY	3.4
1	A	482	THR	3.4
1	B	395	THR	3.4
1	A	319	ALA	3.4
1	A	417	HIS	3.4
1	A	521	VAL	3.4
1	A	292	HIS	3.4
1	B	513	GLY	3.4
1	B	372	ASP	3.4
1	A	426	PHE	3.4
1	B	472	VAL	3.4
1	A	421	ALA	3.4
1	A	495	GLY	3.4
1	B	457	TRP	3.3
1	A	527	LEU	3.3
1	A	511	PRO	3.3
1	B	467	PRO	3.3
1	B	526	THR	3.3
1	B	499	VAL	3.3
1	A	398	ASN	3.3
1	A	267	THR	3.3
1	A	494	SER	3.3
1	A	512	ASN	3.3
1	B	232	LEU	3.3
1	A	308	TRP	3.3
1	A	471	ASP	3.2
1	B	420	PRO	3.2
1	A	305	SER	3.2
1	B	462	TYR	3.2
1	A	522	ASN	3.2
1	B	307	ASN	3.2
1	B	486	LEU	3.2
1	A	253	PRO	3.2
1	A	315	GLU	3.2
1	A	456	GLU	3.2
1	B	368	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	373	HIS	3.2
1	B	308	TRP	3.2
1	B	330	ILE	3.2
1	A	367	PHE	3.1
1	B	355	SER	3.1
1	A	235	GLU	3.1
1	B	374	ASP	3.1
1	B	468	ALA	3.1
1	A	427	PRO	3.1
1	A	255	SER	3.1
1	A	513	GLY	3.1
1	A	529	PRO	3.1
1	B	246	LEU	3.1
1	B	519	SER	3.1
1	A	250	PHE	3.1
1	B	392	GLY	3.1
1	B	349	ALA	3.1
1	A	321	LEU	3.1
1	B	362	LEU	3.1
1	B	444	TYR	3.1
1	B	460	TYR	3.1
1	A	274	GLY	3.1
1	A	412	ASN	3.1
1	B	309	ASN	3.1
1	A	320	PRO	3.1
1	A	411	ARG	3.1
1	A	518	ASP	3.0
1	A	441	CYS	3.0
1	A	304	ALA	3.0
1	B	230	PRO	3.0
1	B	525	TYR	3.0
1	A	414	HIS	3.0
1	B	390	GLN	3.0
1	B	342	GLY	3.0
1	A	242	PHE	3.0
1	B	500	ALA	3.0
1	B	422	VAL	3.0
1	B	397	ARG	3.0
1	A	237	MET	3.0
1	B	237	MET	3.0
1	B	292	HIS	3.0
1	A	493	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	462	TYR	3.0
1	B	476	ARG	3.0
1	A	224	SER	3.0
1	B	405	LEU	2.9
1	A	231	VAL	2.9
1	B	470	SER	2.9
1	B	494	SER	2.9
1	A	269	ASP	2.9
1	B	282	ASN	2.9
1	B	520	TRP	2.9
1	B	423	ALA	2.9
1	B	297	ARG	2.9
1	A	291	THR	2.9
1	A	289	ASP	2.9
1	B	529	PRO	2.9
1	B	369	THR	2.9
1	B	347	HIS	2.9
1	A	229	VAL	2.9
1	A	280	PRO	2.8
1	A	400	PRO	2.8
1	B	424	PRO	2.8
1	B	454	PRO	2.8
1	A	423	ALA	2.8
1	A	477	PHE	2.8
1	B	461	PHE	2.8
1	A	464	GLU	2.8
1	A	248	LYS	2.8
1	A	454	PRO	2.8
1	A	408	TYR	2.8
1	B	352	TYR	2.8
1	B	496	TYR	2.8
1	B	458	VAL	2.8
1	A	266	CYS	2.8
1	A	282	ASN	2.8
1	A	318	PRO	2.8
1	B	383	PHE	2.8
1	B	426	PHE	2.8
1	B	259	VAL	2.8
1	B	521	VAL	2.8
1	A	347	HIS	2.8
1	A	222	PRO	2.8
1	A	480	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	530	MET	2.8
1	B	359	ALA	2.8
1	B	377	ALA	2.8
1	A	515	PHE	2.8
1	A	381	THR	2.7
1	B	371	THR	2.7
1	A	442	SER	2.7
1	B	393	SER	2.7
1	B	491	LEU	2.7
1	A	496	TYR	2.7
1	B	323	ALA	2.7
1	A	373	HIS	2.7
1	A	502	THR	2.7
1	A	504	GLN	2.7
1	B	298	ASN	2.7
1	B	329	LYS	2.7
1	B	493	LYS	2.7
1	A	303	LEU	2.7
1	A	396	HIS	2.7
1	A	492	HIS	2.7
1	B	227	PHE	2.7
1	B	515	PHE	2.7
1	B	258	VAL	2.7
1	B	365	VAL	2.7
1	A	233	THR	2.7
1	A	385	PRO	2.7
1	B	492	HIS	2.7
1	A	525	TYR	2.7
1	A	259	VAL	2.7
1	A	225	LYS	2.7
1	B	316	GLU	2.7
1	B	252	GLY	2.7
1	B	240	SER	2.7
1	B	305	SER	2.7
1	B	249	LEU	2.7
1	A	376	GLU	2.6
1	B	391	ASP	2.6
1	A	244	ILE	2.6
1	B	343	SER	2.6
1	B	319	ALA	2.6
1	A	309	ASN	2.6
1	B	358	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	311	TYR	2.6
1	B	448	ASP	2.6
1	A	363	GLY	2.6
1	A	413	THR	2.6
1	B	229	VAL	2.6
1	B	394	THR	2.6
1	B	283	ILE	2.6
1	B	434	PHE	2.6
1	A	327	VAL	2.6
1	B	408	TYR	2.6
1	B	396	HIS	2.6
1	B	233	THR	2.6
1	B	351	VAL	2.6
1	A	246	LEU	2.5
1	B	273	LEU	2.5
1	B	364	ARG	2.5
1	A	465	ALA	2.5
1	A	500	ALA	2.5
1	B	354	GLY	2.5
1	B	257	PHE	2.5
1	B	367	PHE	2.5
1	A	236	GLU	2.5
1	B	334	LEU	2.5
1	B	530	MET	2.5
1	A	360	PRO	2.5
1	A	467	PRO	2.5
1	A	524	PHE	2.5
1	B	404	VAL	2.5
1	A	352	TYR	2.5
1	A	368	GLU	2.5
1	A	460	TYR	2.5
1	B	321	LEU	2.5
1	A	468	ALA	2.5
1	A	505	HIS	2.5
1	B	243	PRO	2.5
1	B	280	PRO	2.5
1	B	306	GLN	2.5
1	B	315	GLU	2.5
1	B	411	ARG	2.5
1	B	518	ASP	2.5
1	B	272	LEU	2.4
1	A	446	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	506	ASP	2.4
1	B	459	GLN	2.4
1	A	328	GLY	2.4
1	A	354	GLY	2.4
1	B	253	PRO	2.4
1	B	399	GLU	2.4
1	B	327	VAL	2.4
1	A	475	LEU	2.4
1	B	341	ASP	2.4
1	B	398	ASN	2.4
1	B	304	ALA	2.4
1	A	498	THR	2.4
1	B	255	SER	2.4
1	B	348	LYS	2.4
1	B	382	LYS	2.4
1	A	388	VAL	2.4
1	A	404	VAL	2.4
1	A	362	LEU	2.4
1	B	504	GLN	2.4
1	A	399	GLU	2.4
1	A	377	ALA	2.4
1	A	336	GLN	2.4
1	B	446	ASN	2.3
1	B	471	ASP	2.3
1	A	410	GLY	2.3
1	A	283	ILE	2.3
1	B	266	CYS	2.3
1	B	267	THR	2.3
1	A	326	PHE	2.3
1	A	463	GLN	2.3
1	B	463	GLN	2.3
1	A	451	CYS	2.3
1	B	527	LEU	2.3
1	A	324	PRO	2.3
1	A	526	THR	2.3
1	B	344	THR	2.3
1	A	407	SER	2.3
1	A	401	GLN	2.3
1	B	235	GLU	2.3
1	A	434	PHE	2.3
1	A	273	LEU	2.3
1	A	448	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	269	ASP	2.3
1	A	299	TYR	2.3
1	A	240	SER	2.3
1	A	329	LYS	2.3
1	A	380	ASN	2.2
1	A	479	ASN	2.2
1	B	450	ASP	2.2
1	A	288	GLY	2.2
1	B	278	LEU	2.2
1	A	481	ASP	2.2
1	B	506	ASP	2.2
1	B	441	CYS	2.2
1	A	379	GLN	2.2
1	A	300	THR	2.2
1	B	340	ALA	2.2
1	B	465	ALA	2.2
1	B	311	TYR	2.2
1	A	478	VAL	2.2
1	A	298	ASN	2.2
1	B	490	LYS	2.2
1	B	505	HIS	2.2
1	A	519	SER	2.2
1	A	457	TRP	2.2
1	A	461	PHE	2.2
1	B	451	CYS	2.2
1	A	409	SER	2.2
1	A	415	ASN	2.1
1	A	458	VAL	2.1
1	B	290	VAL	2.1
1	A	487	PHE	2.1
1	B	285	THR	2.1
1	B	345	ARG	2.1
1	A	317	ILE	2.1
1	A	431	LEU	2.1
1	A	501	HIS	2.1
1	B	427	PRO	2.1
1	A	348	LYS	2.1
1	A	509	ILE	2.1
1	A	277	GLN	2.1
1	A	433	PHE	2.1
1	A	384	THR	2.1
1	B	401	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	475	LEU	2.1
1	A	281	VAL	2.1
1	A	351	VAL	2.1
1	B	234	VAL	2.1
1	B	516	ARG	2.1
1	A	369	THR	2.0
1	A	452	LEU	2.0
1	B	245	PRO	2.0
1	B	406	PRO	2.0
1	A	297	ARG	2.0
1	A	472	VAL	2.0
1	A	443	GLY	2.0
1	B	270	GLY	2.0
1	A	286	PHE	2.0
1	B	254	SER	2.0
1	B	338	THR	2.0
1	A	486	LEU	2.0
1	B	289	ASP	2.0
1	A	420	PRO	2.0
1	B	317	ILE	2.0

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

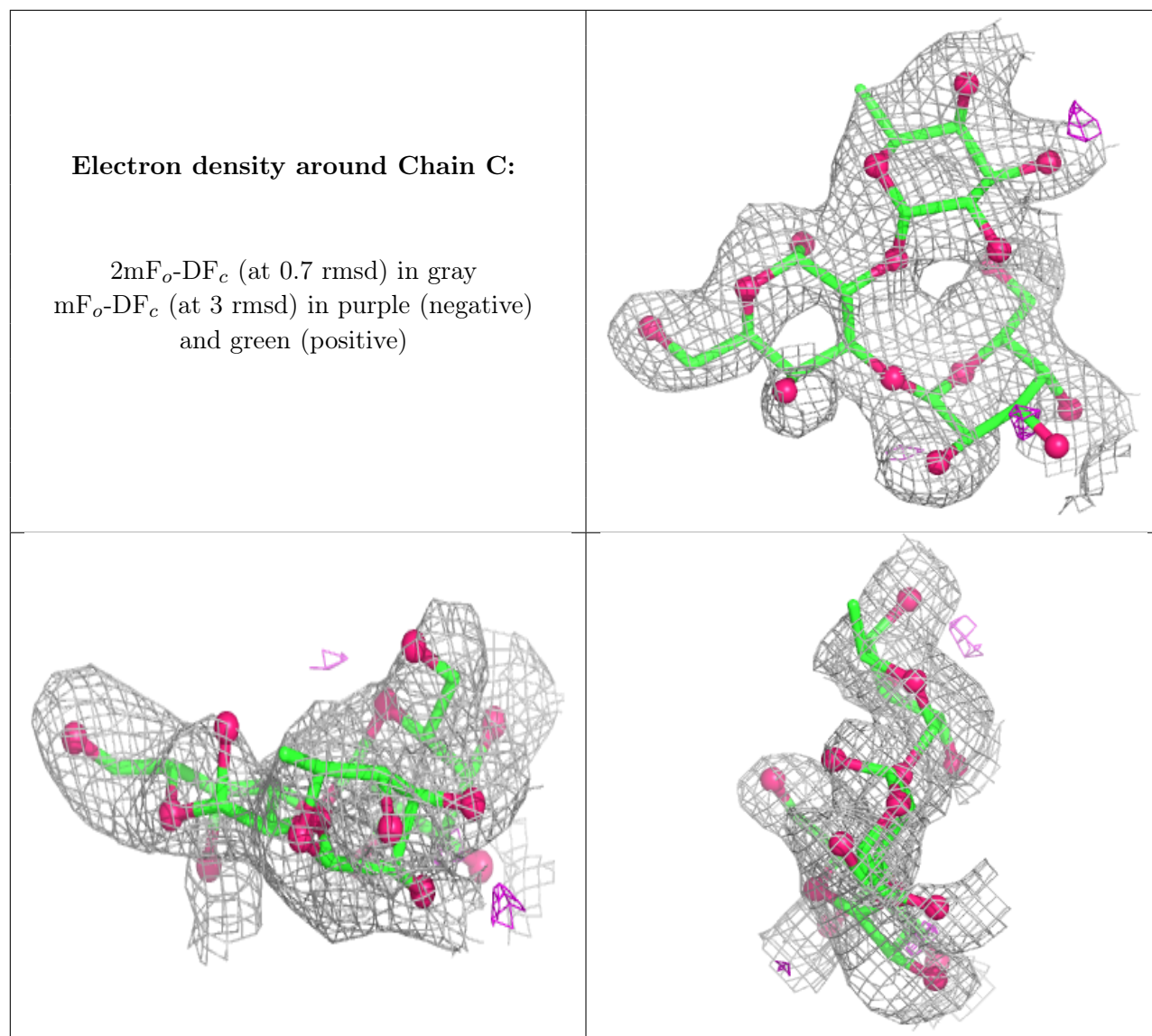
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	GLA	C	3	11/12	0.59	0.27	37,42,44,46	0
2	GLA	C	1	12/12	0.68	0.21	30,34,37,39	0
2	FUC	C	2	10/11	0.83	0.16	26,31,33,33	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.