



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:31 AM UTC

PDB ID : 7Z0X / pdb_00007z0x
Title : THSC20.HVTR26 Fab bound to SARS-CoV-2 Receptor Binding Domain
Authors : Wibmer, C.K.
Deposited on : 2022-02-23
Resolution : 1.80 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

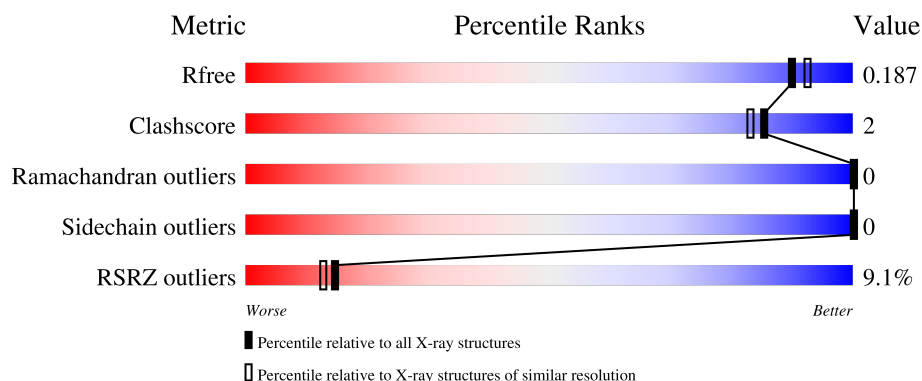
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	H	237	5% 90% • 5%
2	L	216	18% 91% 9%
3	R	205	4% 93% • 5%
4	A	3	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10126 atoms, of which 4669 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 THSC20.HVTR26 Fab heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	H	224	Total	C	H	N	O	S	0	0	0
			3278	1042	1625	278	325	8			

- Molecule 2 is a protein called THSC20.HVTR26 Fab light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	215	Total	C	H	N	O	S	0	0	0
			3140	998	1542	263	330	7			

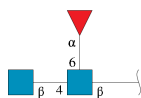
- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	R	195	Total	C	H	N	O	S	0	1	0
			3008	991	1462	257	290	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	330	GLN	-	expression tag	UNP P0DTC2
R	528	GLY	-	expression tag	UNP P0DTC2
R	529	LEU	-	expression tag	UNP P0DTC2
R	530	GLU	-	expression tag	UNP P0DTC2
R	531	VAL	-	expression tag	UNP P0DTC2
R	532	LEU	-	expression tag	UNP P0DTC2
R	533	PHE	-	expression tag	UNP P0DTC2
R	534	GLN	-	expression tag	UNP P0DTC2

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	3	Total	C	H	N	O	0	0	0
			61	22	23	2	14			

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	H	1	Total	C	H	N	O S	0	0
			32	8	17	2	4 1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	168	Total	O	0	0
			168	168		
6	L	155	Total	O	0	0
			155	155		
6	R	284	Total	O	0	0
			284	284		

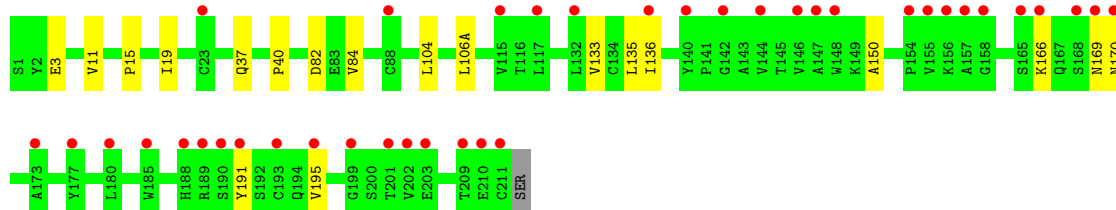
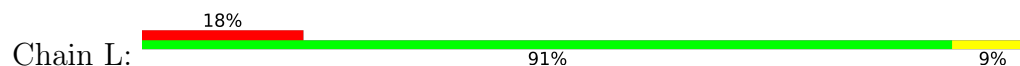
3 Residue-property plots [i](#)

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: THSC20.HVTR26 Fab heavy chain



- Molecule 2: THSC20.HVTR26 Fab light chain



- Molecule 3: Spike protein S1



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	90.29Å 104.21Å 89.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.0 (50.00-1.80) 88.3 (50.00-1.80)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.163 , 0.188 0.165 , 0.187	Depositor DCC
R_{free} test set	3530 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10126	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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: EPE, FUC, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	H	0.41	0/1690	0.56	0/2303
2	L	0.35	0/1637	0.52	0/2233
3	R	0.47	0/1593	0.60	1/2169 (0.0%)
All	All	0.41	0/4920	0.56	1/6705 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	495	TYR	N-CA-C	-5.33	102.99	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1653	1625	1625	6	0
2	L	1598	1542	1542	12	0
3	R	1546	1462	1464	3	0
4	A	38	23	34	0	0
5	H	15	17	17	0	0
6	H	168	0	0	0	1
6	L	155	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	284	0	0	1	1
All	All	5457	4669	4682	21	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 2.

All (21) 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:L:3:GLU:OE2	6:L:301:HOH:O	1.86	0.93
2:L:11:VAL:HG23	2:L:104:LEU:HD13	1.82	0.60
2:L:150:ALA:HB2	2:L:191:TYR:CE1	2.36	0.60
3:R:462:LYS:NZ	6:R:603:HOH:O	2.36	0.57
2:L:133:VAL:HG12	2:L:135:LEU:HD13	1.87	0.55
2:L:136:ILE:HG12	2:L:195:VAL:HG11	1.91	0.53
2:L:37:GLN:HG3	2:L:84:VAL:HG21	1.92	0.50
2:L:82:ASP:O	2:L:84:VAL:HG22	2.12	0.50
1:H:20:LEU:HG	1:H:82:MET:HE2	1.96	0.47
2:L:15:PRO:HD3	2:L:106(A):LEU:O	2.16	0.46
1:H:178:LEU:C	1:H:178:LEU:HD12	2.42	0.44
1:H:201:LYS:N	1:H:202:PRO:CD	2.81	0.43
2:L:37:GLN:CG	2:L:84:VAL:HG21	2.49	0.43
3:R:354:ASN:O	3:R:398:ASP:HA	2.19	0.42
3:R:334:ASN:OD1	3:R:334:ASN:N	2.52	0.41
1:H:119:PRO:CB	1:H:142:VAL:HG12	2.51	0.41
1:H:119:PRO:HB3	1:H:145:TYR:HB3	2.02	0.41
1:H:126:PRO:HG3	1:H:138:LEU:HB3	2.02	0.41
2:L:19:ILE:HD12	2:L:19:ILE:HA	1.96	0.40
2:L:169:ASN:O	2:L:170:ASN:HB2	2.21	0.40
2:L:40:PRO:HG2	2:L:166:LYS:HB3	2.04	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)
6:H:556:HOH:O	6:R:792:HOH:O[4_455]	2.10	0.10

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	H	220/237 (93%)	216 (98%)	4 (2%)	0	100	100
2	L	213/216 (99%)	204 (96%)	9 (4%)	0	100	100
3	R	194/205 (95%)	188 (97%)	6 (3%)	0	100	100
All	All	627/658 (95%)	608 (97%)	19 (3%)	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	H	185/196 (94%)	185 (100%)	0	100	100
2	L	182/183 (100%)	182 (100%)	0	100	100
3	R	169/177 (96%)	169 (100%)	0	100	100
All	All	536/556 (96%)	536 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	H	192	GLN
2	L	108	GLN
3	R	460	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	$\# Z > 2$
4	NAG	A	1	4,3	14,14,15	0.59	0	17,19,21	0.54	0
4	NAG	A	2	4	14,14,15	0.31	0	17,19,21	0.42	0
4	FUC	A	3	4	10,10,11	1.00	0	14,14,16	0.70	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	4,3	-	0/6/23/26	0/1/1/1
4	NAG	A	2	4	-	0/6/23/26	0/1/1/1
4	FUC	A	3	4	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

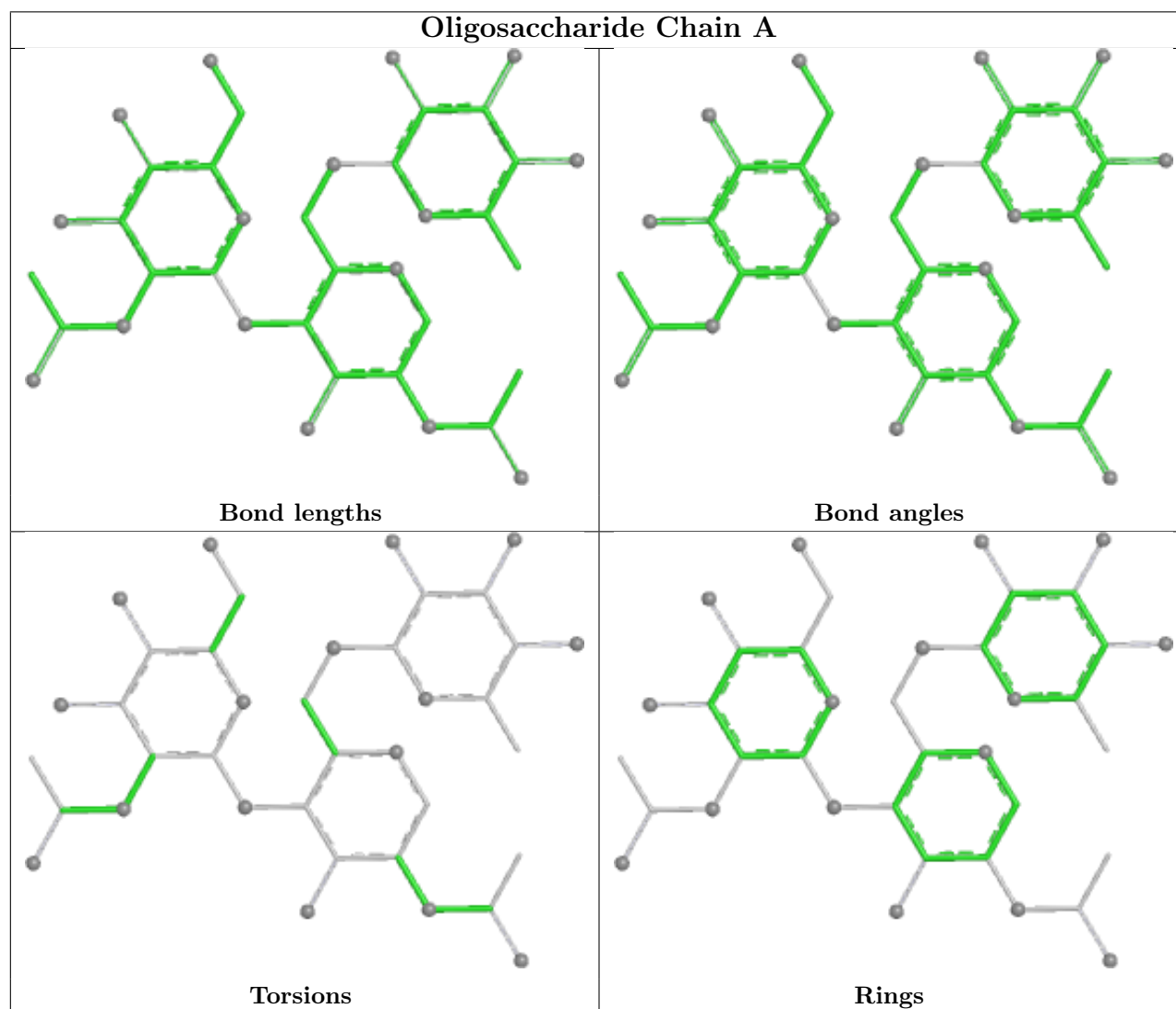
There are no chirality outliers.

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](#)

1 ligand 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
5	EPE	H	301	-	15,15,15	0.79	1 (6%)	19,20,20	1.60	4 (21%)

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	EPE	H	301	-	-	0/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	301	EPE	C10-S	2.53	1.81	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	301	EPE	C5-N4-C3	4.16	117.80	108.84
5	H	301	EPE	O2S-S-C10	3.74	112.39	106.73
5	H	301	EPE	C7-N4-C3	2.24	117.20	111.24
5	H	301	EPE	C7-N4-C5	2.16	116.99	111.24

There are no chirality outliers.

There are no torsion outliers.

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

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	H	224/237 (94%)	0.31	11 (4%) 35 33	21, 45, 97, 131	0
2	L	215/216 (99%)	0.70	39 (18%) 3 3	18, 63, 123, 137	0
3	R	195/205 (95%)	-0.20	8 (4%) 41 41	19, 31, 64, 105	1 (0%)
All	All	634/658 (96%)	0.29	58 (9%) 15 13	18, 40, 105, 137	1 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	195	VAL	4.3
1	H	134	GLY	4.1
2	L	202	VAL	4.0
3	R	333	THR	4.0
2	L	211	CYS	4.0
2	L	23	CYS	3.9
1	H	127	SER	3.7
1	H	216	CYS	3.6
2	L	168	SER	3.5
2	L	190	SER	3.3
1	H	215	SER	3.3
2	L	189	ARG	3.2
3	R	385	THR	3.2
2	L	155	VAL	3.1
2	L	165	SER	3.0
2	L	210	GLU	3.0
2	L	88	CYS	2.9
2	L	148	TRP	2.8
3	R	505	TYR	2.7
2	L	157	ALA	2.7
2	L	185	TRP	2.7
3	R	519	HIS	2.7
2	L	154	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
2	L	199	GLY	2.6
2	L	140	TYR	2.5
2	L	117	LEU	2.5
2	L	132	LEU	2.4
2	L	115	VAL	2.4
2	L	146	VAL	2.4
1	H	210	LYS	2.4
2	L	166	LYS	2.4
3	R	527	PRO	2.4
3	R	382	VAL	2.4
2	L	142	GLY	2.4
2	L	201	THR	2.4
2	L	169	ASN	2.3
2	L	158	GLY	2.3
2	L	193	CYS	2.3
1	H	151	THR	2.3
2	L	147	ALA	2.2
2	L	188	HIS	2.2
3	R	373	SER	2.2
2	L	136	ILE	2.2
1	H	199	ASN	2.2
2	L	144	VAL	2.2
1	H	150	VAL	2.1
2	L	173	ALA	2.1
2	L	156	LYS	2.1
2	L	203	GLU	2.1
2	L	177	TYR	2.0
2	L	170	ASN	2.0
3	R	367	VAL	2.0
1	H	124	LEU	2.0
1	H	141	LEU	2.0
2	L	180	LEU	2.0
2	L	209	THR	2.0
2	L	191	TYR	2.0
1	H	211	VAL	2.0

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

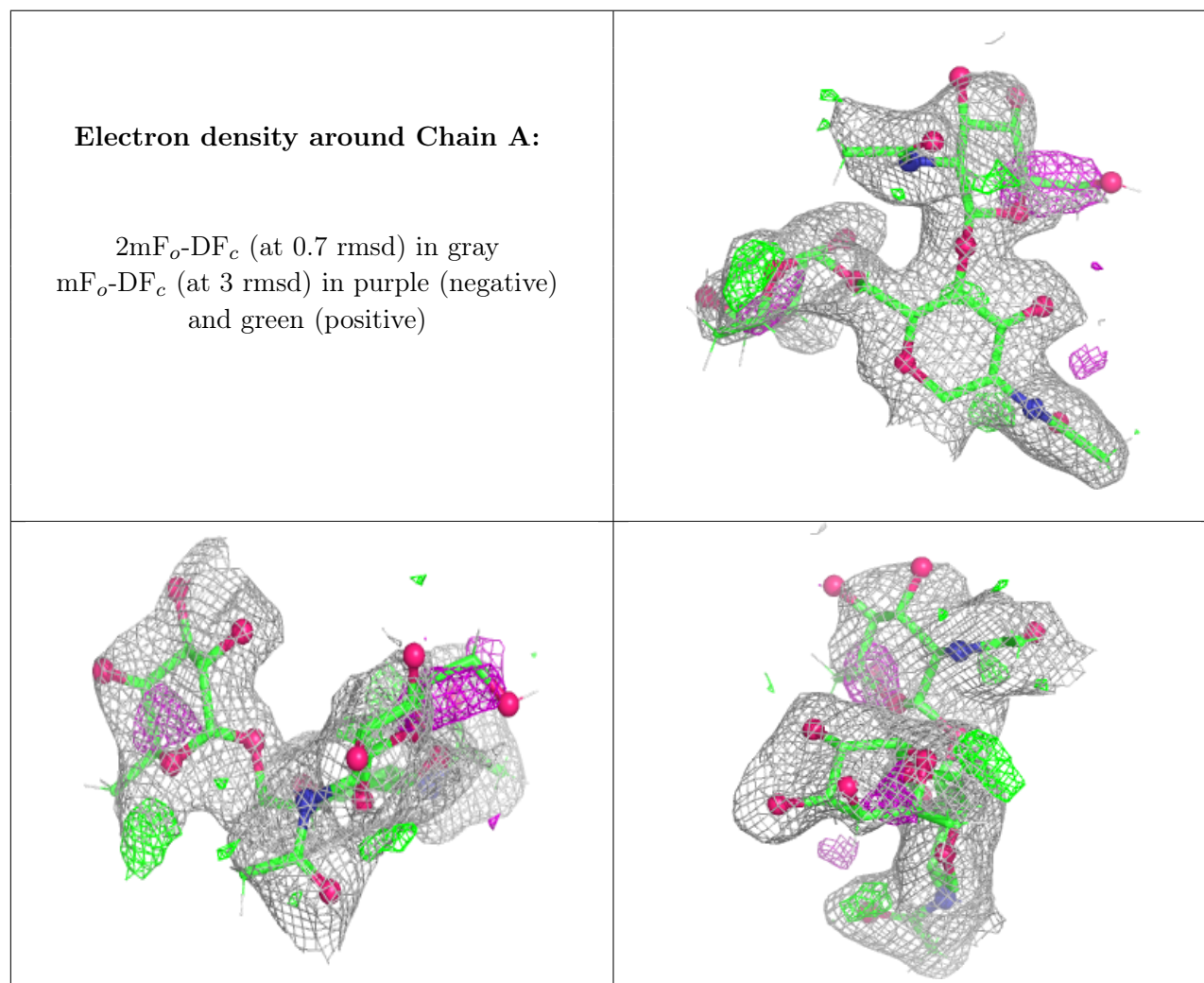
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [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
4	NAG	A	1	14/15	-	-	37,44,64,68	0
4	NAG	A	2	14/15	-	-	59,71,83,91	0
4	FUC	A	3	10/11	-	-	60,73,82,88	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

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	EPE	H	301	15/15	0.89	0.13	34,59,72,74	0

6.5 Other polymers

There are no such residues in this entry.