



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 21, 2020 – 08:54 PM BST

PDB ID : 6UYN
Title : Crystal structure of influenza A virus hemagglutinin from A/Ohio/09/2015 bound to the stalk-binding CR6261 antibody Fab
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2019-11-13
Resolution : 2.85 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

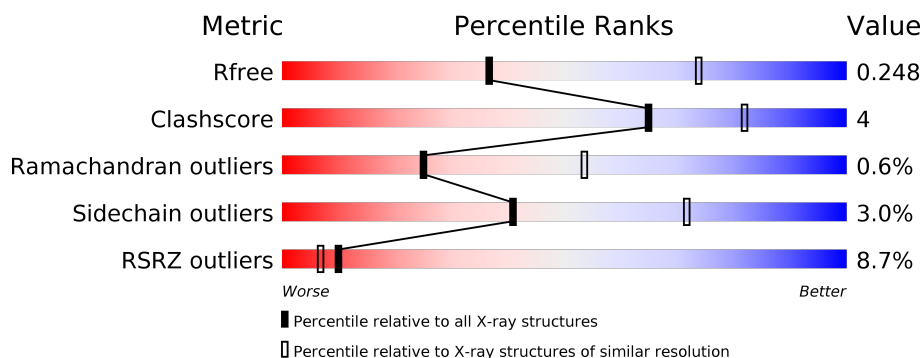
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 on 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	566	<div> <div>4%</div> <div> <div></div> <div>49%</div> <div>8%</div> <div>42%</div> </div> </div>
1	B	566	<div> <div>27%</div> <div>70%</div> </div>
2	H	232	<div> <div>3%</div> <div> <div></div> <div>55%</div> <div>8%</div> <div>36%</div> </div> </div>
3	L	221	<div> <div>17%</div> <div> <div></div> <div>57%</div> <div>10%</div> <div>33%</div> </div> </div>
4	C	2	<div> <div>100%</div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5967 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2396	1510	414	461	11			
1	B	167	Total	C	N	O	S	0	0	0
			1331	837	223	265	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	ASN	ILE	variant	UNP A0A6C0TB04
A	6	LEU	ILE	variant	UNP A0A6C0TB04
A	10	CYS	TYR	variant	UNP A0A6C0TB04
A	11	ALA	THR	variant	UNP A0A6C0TB04
A	12	LEU	PHE	variant	UNP A0A6C0TB04
A	13	ALA	THR	variant	UNP A0A6C0TB04
A	14	ALA	THR	variant	UNP A0A6C0TB04
A	16	ASP	ASN	variant	UNP A0A6C0TB04
A	544	LEU	VAL	variant	UNP A0A6C0TB04
A	564	ILE	VAL	variant	UNP A0A6C0TB04
B	4	ASN	ILE	variant	UNP A0A6C0TB04
B	6	LEU	ILE	variant	UNP A0A6C0TB04
B	10	CYS	TYR	variant	UNP A0A6C0TB04
B	11	ALA	THR	variant	UNP A0A6C0TB04
B	12	LEU	PHE	variant	UNP A0A6C0TB04
B	13	ALA	THR	variant	UNP A0A6C0TB04
B	14	ALA	THR	variant	UNP A0A6C0TB04
B	16	ASP	ASN	variant	UNP A0A6C0TB04
B	544	LEU	VAL	variant	UNP A0A6C0TB04
B	564	ILE	VAL	variant	UNP A0A6C0TB04

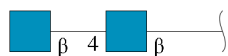
- Molecule 2 is a protein called CR6261 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	148	Total	C	N	O	S	0	1	0
			1115	707	185	216	7			

- Molecule 3 is a protein called CR6261 Fab light chain.

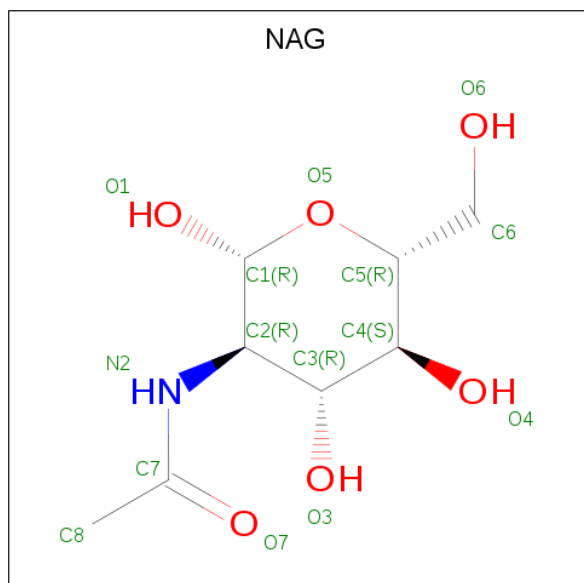
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	149	Total	C	N	O	S	0	0	0
			1030	641	172	214	3			

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

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



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

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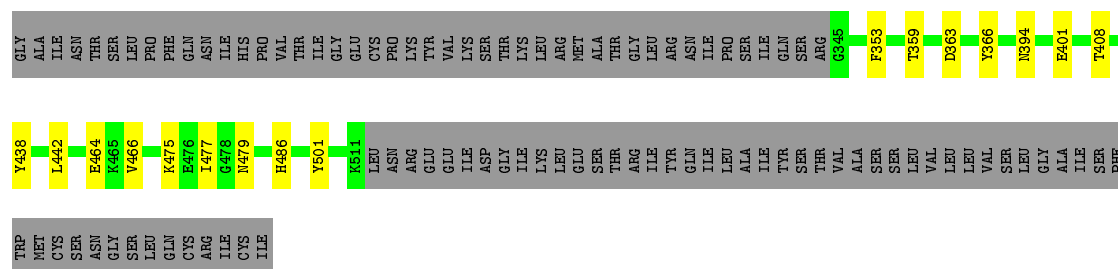
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

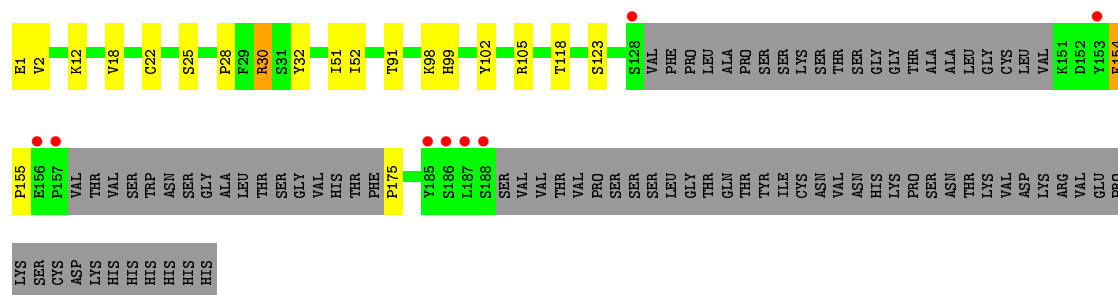
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is water.

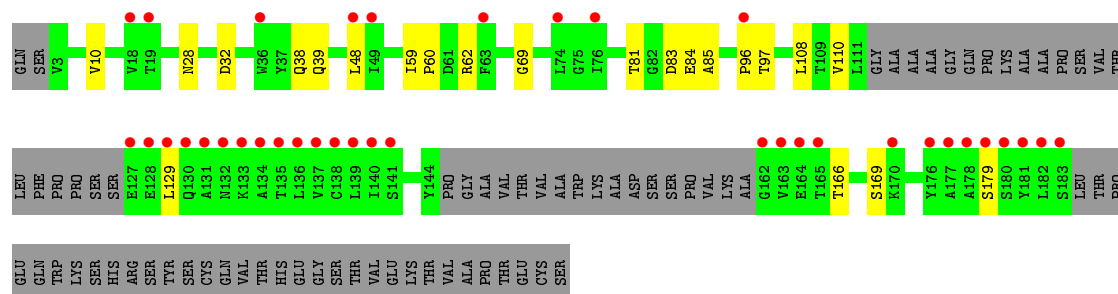
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	13	Total	O	0	0
			13	13		
7	B	17	Total	O	0	0
			17	17		
7	H	7	Total	O	0	0
			7	7		
7	L	1	Total	O	0	0
			1	1		



• Molecule 2: CR6261 Fab heavy chain



• Molecule 3: CR6261 Fab light chain



• 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	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	205.59 Å 205.59 Å 205.59 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.26 – 2.85 48.46 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.26-2.85) 99.9 (48.46-2.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.86 Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.209 , 0.247 0.209 , 0.248	Depositor DCC
R_{free} test set	1615 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	75.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5967	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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: NAG, CL

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	0.29	0/2459	0.48	0/3376
1	B	0.36	0/1359	0.52	0/1833
2	H	0.34	0/1145	0.54	0/1550
3	L	0.30	0/1049	0.51	0/1439
All	All	0.32	0/6012	0.51	0/8198

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 [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	2396	0	2175	22	0
1	B	1331	0	1243	8	0
2	H	1115	0	1076	11	0
3	L	1030	0	921	10	0
4	C	28	0	25	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	1	0	0	0	0
7	A	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	17	0	0	0	0
7	H	7	0	0	0	0
7	L	1	0	0	0	0
All	All	5967	0	5466	47	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 4.

The worst 5 of 47 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:154:PHE:HB3	2:H:155:PRO:HD3	1.77	0.67
2:H:25:SER:O	2:H:30[B]:ARG:NH1	2.29	0.66
1:A:140:TRP:HZ3	1:A:178:ILE:HG21	1.60	0.66
3:L:38:GLN:HB2	3:L:48:LEU:HD11	1.78	0.64
2:H:1:GLU:HG2	2:H:2:VAL:H	1.65	0.61

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	324/566 (57%)	297 (92%)	25 (8%)	2 (1%)	25	53
1	B	165/566 (29%)	155 (94%)	10 (6%)	0	100	100
2	H	143/232 (62%)	140 (98%)	2 (1%)	1 (1%)	22	50
3	L	143/221 (65%)	133 (93%)	8 (6%)	2 (1%)	11	31
All	All	775/1585 (49%)	725 (94%)	45 (6%)	5 (1%)	25	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	154	PHE
3	L	96	PRO
1	A	141	PRO
1	A	212	ALA
3	L	69	GLY

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	246/491 (50%)	238 (97%)	8 (3%)	38	68
1	B	140/491 (28%)	136 (97%)	4 (3%)	42	72
2	H	118/195 (60%)	114 (97%)	4 (3%)	37	67
3	L	101/182 (56%)	98 (97%)	3 (3%)	41	72
All	All	605/1359 (44%)	586 (97%)	19 (3%)	41	71

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	366	TYR
1	B	401	GLU
2	H	123	SER
1	A	335	LEU
3	L	28	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	ASN

5.3.3 RNA [i](#)

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 ⓘ

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	C	1	1,4	14,14,15	0.43	0	17,19,21	0.62	0
4	NAG	C	2	4	14,14,15	0.44	0	17,19,21	0.61	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	C	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is 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	$\# Z > 2$
5	NAG	B	601	1	14,14,15	0.50	0	17,19,21	0.67	1 (5%)
5	NAG	A	601	1	14,14,15	0.44	0	17,19,21	0.46	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
5	NAG	B	601	1	-	0/6/23/26	0/1/1/1
5	NAG	A	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	601	NAG	C1-O5-C5	2.38	115.41	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	NAG	C4-C5-C6-O6
5	A	601	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	326/566 (57%)	0.45	24 (7%) 14 10	39, 111, 185, 204	0
1	B	167/566 (29%)	0.20	0 100 100	38, 54, 103, 144	0
2	H	148/232 (63%)	0.28	8 (5%) 25 21	44, 62, 150, 187	0
3	L	149/221 (67%)	1.34	37 (24%) 0 0	57, 104, 223, 255	0
All	All	790/1585 (49%)	0.53	69 (8%) 10 7	38, 84, 191, 255	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	178	ALA	12.8
2	H	188	SER	9.8
3	L	177	ALA	7.6
3	L	183	SER	7.5
3	L	140	ILE	7.4

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
4	NAG	C	2	14/15	0.83	0.24	135,138,141,141	0
4	NAG	C	1	14/15	0.88	0.30	103,120,124,128	0

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
5	NAG	B	601	14/15	0.80	0.18	92,102,106,108	0
5	NAG	A	601	14/15	0.85	0.16	100,111,116,122	0
6	CL	A	604	1/1	0.97	0.21	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.