



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 09:06 AM BST

PDB ID : 6ICW
Title : Crystal structure of H7 hemagglutinin mutant AH-SGTQ (A138S, V186G, P221T and L226Q) from the influenza virus A/Anhui/1/2013 (H7N9)
Authors : Gao, G.F.; Xu, Y.
Deposited on : 2018-09-07
Resolution : 2.60 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 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 : 2.13.1
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) : 2.13.1

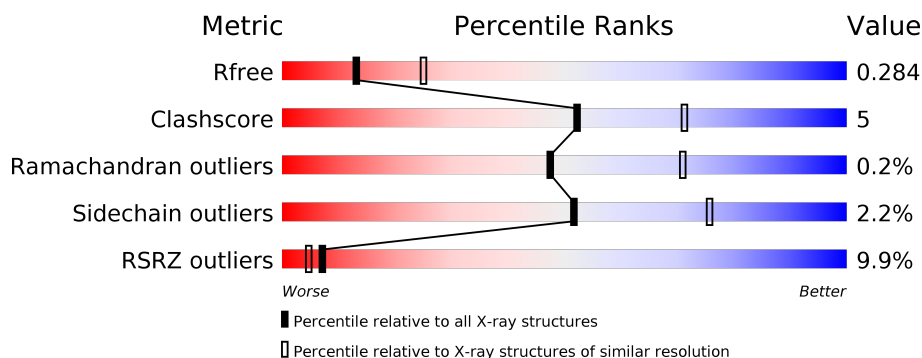
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	321	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>.</div> </div> </div>
2	B	177	<div> <div>16%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>8%</div> <div>..</div> </div> </div>

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
3	NAG	A	601	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3825 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	314	Total	C	N	O	S	0	0	0
			2386	1478	433	460	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	SER	ALA	engineered mutation	UNP R4NN21
A	177	GLY	VAL	engineered mutation	UNP R4NN21
A	212	THR	PRO	engineered mutation	UNP R4NN21
A	217	GLN	LEU	engineered mutation	UNP R4NN21

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	163	Total	C	N	O	S	0	0	0
			1328	817	231	273	7			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

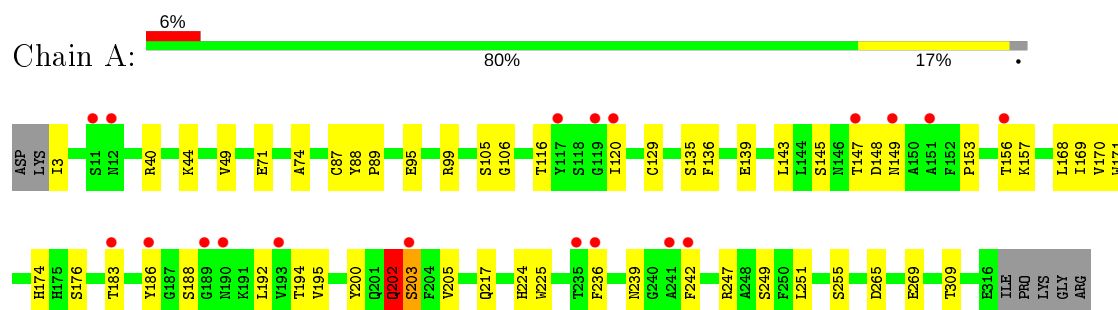
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total	O	0	0
			54	54		
4	B	15	Total	O	0	0
			15	15		

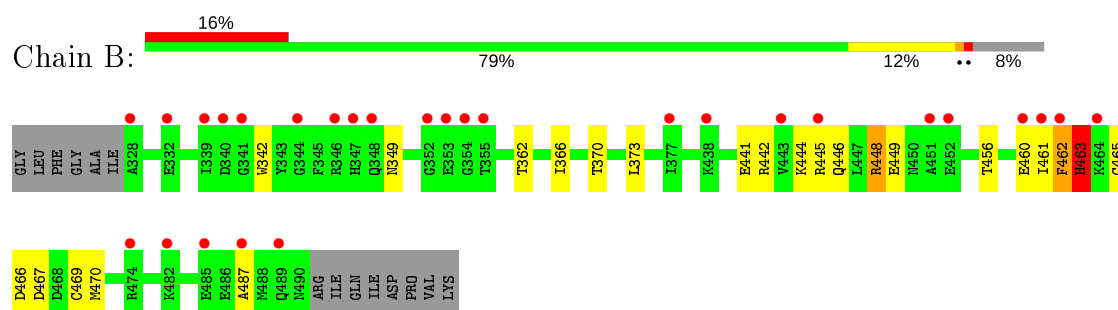
3 Residue-property plots [i](#)

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: Hemagglutinin HA1 chain



- Molecule 2: Hemagglutinin HA2 chain



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	115.61Å 115.61Å 293.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.53 – 2.60 47.38 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.53-2.60) 99.8 (47.38-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.258 , 0.283 0.258 , 0.284	Depositor DCC
R_{free} test set	1219 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for $-1/3^*h+1/3^*k+1/3^*l,-k,8/3^*h+4/3^*k+1/3^*l$ 0.021 for $-2/3^*h-1/3^*k-1/3^*l,-1/3^*h-2/3^*k+1/3^*l,-4/3^*h+4/3^*k+1/3^*l$ 0.011 for $-h,1/3^*h-1/3^*k-1/3^*l,-4/3^*h-8/3^*k+1/3^*l$	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3825	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: 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	A	0.25	0/2431	0.46	1/3286 (0.0%)
2	B	0.27	0/1351	0.67	5/1821 (0.3%)
All	All	0.26	0/3782	0.55	6/5107 (0.1%)

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	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	462	PHE	C-N-CA	11.86	151.35	121.70
2	B	462	PHE	N-CA-C	11.48	141.99	111.00
2	B	463	HIS	N-CA-C	9.25	135.97	111.00
2	B	463	HIS	N-CA-CB	-8.95	94.48	110.60
1	A	202	GLN	CB-CA-C	5.61	121.61	110.40
2	B	448	ARG	CB-CA-C	-5.05	100.31	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	GLN	Peptide
2	B	462	PHE	Peptide

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	2386	0	2328	30	0
2	B	1328	0	1221	11	1
3	A	28	0	26	0	0
3	B	14	0	13	0	0
4	A	54	0	0	1	0
4	B	15	0	0	1	0
All	All	3825	0	3588	40	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 5.

All (40) 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:169:ILE:O	1:A:225:TRP:HA	1.92	0.69
1:A:156:THR:HA	1:A:236:PHE:O	1.92	0.69
2:B:444:LYS:NZ	4:B:601:HOH:O	2.31	0.63
1:A:168:LEU:HB3	1:A:249:SER:HB2	1.81	0.63
2:B:461:ILE:HG23	2:B:461:ILE:O	2.02	0.60
1:A:309:THR:HG22	2:B:373:LEU:HD11	1.84	0.58
1:A:170:VAL:HG22	1:A:225:TRP:HB3	1.87	0.57
1:A:49:VAL:HG23	1:A:74:ALA:HB2	1.87	0.56
1:A:71:GLU:OE2	1:A:247:ARG:NH2	2.39	0.55
1:A:203:SER:O	1:A:203:SER:OG	2.21	0.54
1:A:194:THR:O	1:A:236:PHE:HA	2.07	0.54
1:A:106:GLY:HA2	1:A:255:SER:HB3	1.91	0.53
2:B:466:ASP:OD1	2:B:467:ASP:N	2.43	0.52
1:A:170:VAL:HA	1:A:224:HIS:O	2.10	0.52
2:B:463:HIS:HB3	2:B:487:ALA:HB2	1.93	0.51
1:A:202:GLN:HA	1:A:203:SER:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:441:GLU:HB3	2:B:445:ARG:NH1	2.26	0.51
1:A:87:CYS:SG	1:A:88:TYR:N	2.83	0.51
1:A:143:LEU:HD12	1:A:242:PHE:HD2	1.77	0.50
1:A:44:LYS:HE3	1:A:269:GLU:HB2	1.94	0.49
1:A:171:TRP:CE2	1:A:195:VAL:HG21	2.48	0.48
1:A:120:ILE:HD11	1:A:153:PRO:HD2	1.96	0.47
2:B:349:ASN:ND2	2:B:467:ASP:OD1	2.47	0.46
1:A:135:SER:OG	1:A:136:PHE:N	2.48	0.46
1:A:148:ASP:O	1:A:149:ASN:C	2.54	0.46
1:A:95:GLU:HB3	1:A:99:ARG:NH1	2.31	0.45
1:A:192:LEU:N	1:A:239:ASN:OD1	2.42	0.45
1:A:40:ARG:HD2	1:A:265:ASP:HB2	1.99	0.44
2:B:442:ARG:NH1	2:B:446:GLN:OE1	2.51	0.44
1:A:116:THR:O	1:A:157:LYS:NZ	2.41	0.43
1:A:174:HIS:ND1	1:A:186:TYR:OH	2.38	0.43
1:A:139:GLU:OE1	1:A:247:ARG:HD3	2.20	0.42
2:B:342:TRP:HB2	2:B:362:THR:HG22	2.01	0.42
2:B:366:ILE:O	2:B:370:THR:OG1	2.32	0.42
1:A:3:ILE:N	4:A:714:HOH:O	2.52	0.41
1:A:183:THR:HG22	1:A:188:SER:HA	2.02	0.41
1:A:200:TYR:CE2	1:A:202:GLN:HB2	2.56	0.40
1:A:89:PRO:HG3	1:A:217:GLN:HB3	2.04	0.40
1:A:105:SER:HB2	1:A:251:LEU:HD22	2.03	0.40
2:B:465:CYS:SG	2:B:470:MET:HG3	2.61	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)
2:B:448:ARG:NH1	2:B:460:GLU:OE1[2_545]	1.94	0.26

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	312/321 (97%)	286 (92%)	25 (8%)	1 (0%)	41	64
2	B	161/177 (91%)	155 (96%)	6 (4%)	0	100	100
All	All	473/498 (95%)	441 (93%)	31 (7%)	1 (0%)	47	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	SER

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	A	261/269 (97%)	256 (98%)	5 (2%)	57	79
2	B	141/152 (93%)	137 (97%)	4 (3%)	43	69
All	All	402/421 (96%)	393 (98%)	9 (2%)	52	76

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	CYS
1	A	145	SER
1	A	147	THR
1	A	176	SER
1	A	205	VAL
2	B	449	GLU
2	B	456	THR
2	B	463	HIS
2	B	469	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 ligands 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	A	602	1	14,14,15	0.20	0	17,19,21	0.44	0
3	NAG	B	501	2	14,14,15	0.27	0	17,19,21	0.46	0
3	NAG	A	601	1	14,14,15	0.25	0	17,19,21	0.41	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	NAG	A	602	1	-	2/6/23/26	0/1/1/1
3	NAG	B	501	2	-	0/6/23/26	0/1/1/1
3	NAG	A	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	NAG	O5-C5-C6-O6
3	A	601	NAG	O5-C5-C6-O6
3	A	602	NAG	C4-C5-C6-O6
3	A	601	NAG	C4-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 ⓘ

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	314/321 (97%)	0.33	19 (6%) 21 16	29, 61, 109, 142	0
2	B	163/177 (92%)	0.94	28 (17%) 1 0	30, 85, 131, 157	0
All	All	477/498 (95%)	0.54	47 (9%) 7 5	29, 67, 126, 157	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	346	ARG	4.4
2	B	464	LYS	4.2
2	B	489	GLN	4.2
1	A	190	ASN	3.9
2	B	354	GLY	3.8
1	A	147	THR	3.6
2	B	355	THR	3.6
1	A	117	TYR	3.5
1	A	12	ASN	3.5
2	B	482	LYS	3.4
2	B	341	GLY	3.4
2	B	353	GLU	3.3
2	B	348	GLN	3.3
2	B	460	GLU	3.2
1	A	120	ILE	3.2
1	A	203	SER	3.2
2	B	452	GLU	3.0
1	A	189	GLY	3.0
2	B	347	HIS	3.0
1	A	156	THR	3.0
2	B	328	ALA	2.9
2	B	487	ALA	2.8
1	A	241	ALA	2.8
1	A	186	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	377	ILE	2.7
1	A	242	PHE	2.7
1	A	236	PHE	2.6
1	A	183	THR	2.6
1	A	149	ASN	2.6
2	B	340	ASP	2.6
1	A	151	ALA	2.5
2	B	445	ARG	2.5
2	B	485	GLU	2.4
2	B	352	GLY	2.3
2	B	451	ALA	2.3
1	A	11	SER	2.3
2	B	443	VAL	2.3
2	B	474	ARG	2.2
2	B	344	GLY	2.2
2	B	462	PHE	2.2
2	B	339	ILE	2.1
2	B	461	ILE	2.1
2	B	438	LYS	2.1
1	A	193	VAL	2.1
1	A	119	GLY	2.1
2	B	332	GLU	2.0
1	A	235	THR	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](#)

There are no monosaccharides in this entry.

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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	A	601	14/15	0.71	0.40	95,112,129,130	0
3	NAG	A	602	14/15	0.82	0.33	93,108,113,115	0
3	NAG	B	501	14/15	0.93	0.15	47,72,78,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.