



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2016 – 11:27 AM EDT

PDB ID : 5LK3
Title : Structure of hantavirus envelope glycoprotein Gc in postfusion conformation
in presence of 500 mM KCL
Authors : Guardado-Calvo, P.; Rey, F.A.
Deposited on : 2016-07-20
Resolution : 1.50 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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028320
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

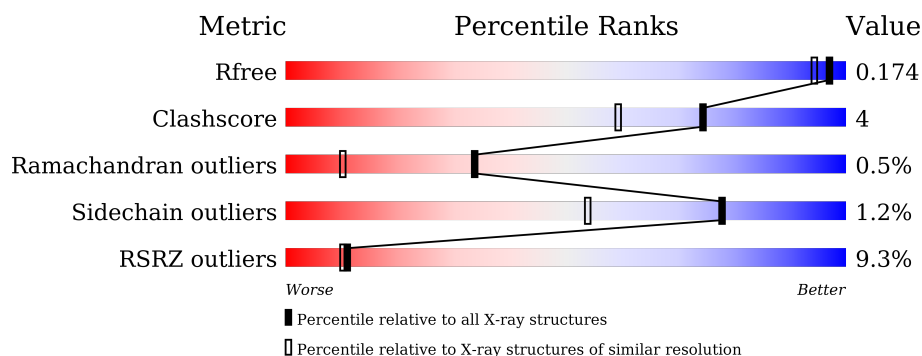
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 1.50 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}	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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. 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	495	

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
2	NAG	A	501	-	-	-	X
2	NAG	A	502	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FUL	A	503	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3397 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 Envelopment polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	9	0
			2989	1884	509	568	28			

There are 39 discrepancies between the modelled and reference sequences:

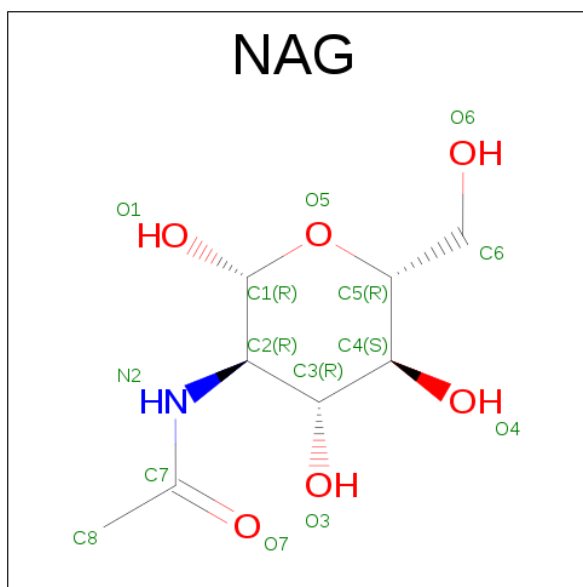
Chain	Residue	Modelled	Actual	Comment	Reference
A	115	HIS	TRP	conflict	UNP P08668
A	458	GLY	-	expression tag	UNP P08668
A	459	GLY	-	expression tag	UNP P08668
A	460	SER	-	expression tag	UNP P08668
A	461	ASP	-	expression tag	UNP P08668
A	462	ASP	-	expression tag	UNP P08668
A	463	ASP	-	expression tag	UNP P08668
A	464	ASP	-	expression tag	UNP P08668
A	465	LYS	-	expression tag	UNP P08668
A	466	ALA	-	expression tag	UNP P08668
A	467	GLY	-	expression tag	UNP P08668
A	468	TRP	-	expression tag	UNP P08668
A	469	SER	-	expression tag	UNP P08668
A	470	HIS	-	expression tag	UNP P08668
A	471	PRO	-	expression tag	UNP P08668
A	472	GLN	-	expression tag	UNP P08668
A	473	PHE	-	expression tag	UNP P08668
A	474	GLU	-	expression tag	UNP P08668
A	475	LYS	-	expression tag	UNP P08668
A	476	GLY	-	expression tag	UNP P08668
A	477	GLY	-	expression tag	UNP P08668
A	478	GLY	-	expression tag	UNP P08668
A	479	SER	-	expression tag	UNP P08668
A	480	GLY	-	expression tag	UNP P08668
A	481	GLY	-	expression tag	UNP P08668
A	482	GLY	-	expression tag	UNP P08668
A	483	SER	-	expression tag	UNP P08668

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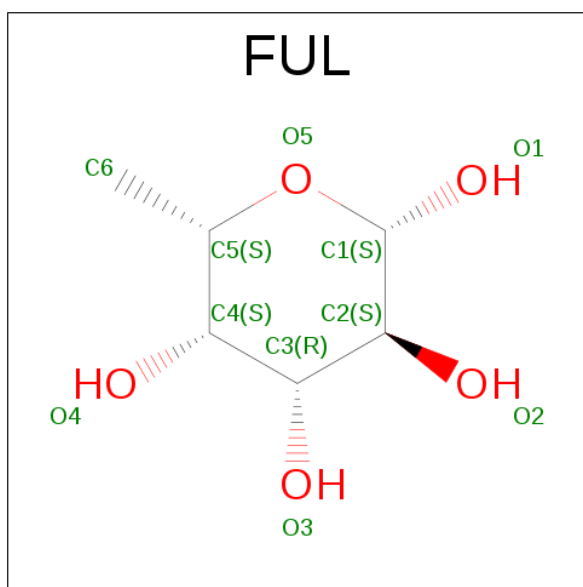
Chain	Residue	Modelled	Actual	Comment	Reference
A	484	GLY	-	expression tag	UNP P08668
A	485	GLY	-	expression tag	UNP P08668
A	486	GLY	-	expression tag	UNP P08668
A	487	SER	-	expression tag	UNP P08668
A	488	TRP	-	expression tag	UNP P08668
A	489	SER	-	expression tag	UNP P08668
A	490	HIS	-	expression tag	UNP P08668
A	491	PRO	-	expression tag	UNP P08668
A	492	GLN	-	expression tag	UNP P08668
A	493	PHE	-	expression tag	UNP P08668
A	494	GLU	-	expression tag	UNP P08668
A	495	LYS	-	expression tag	UNP P08668

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 3 is BETA-L-FUCOSE (three-letter code: FUL) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

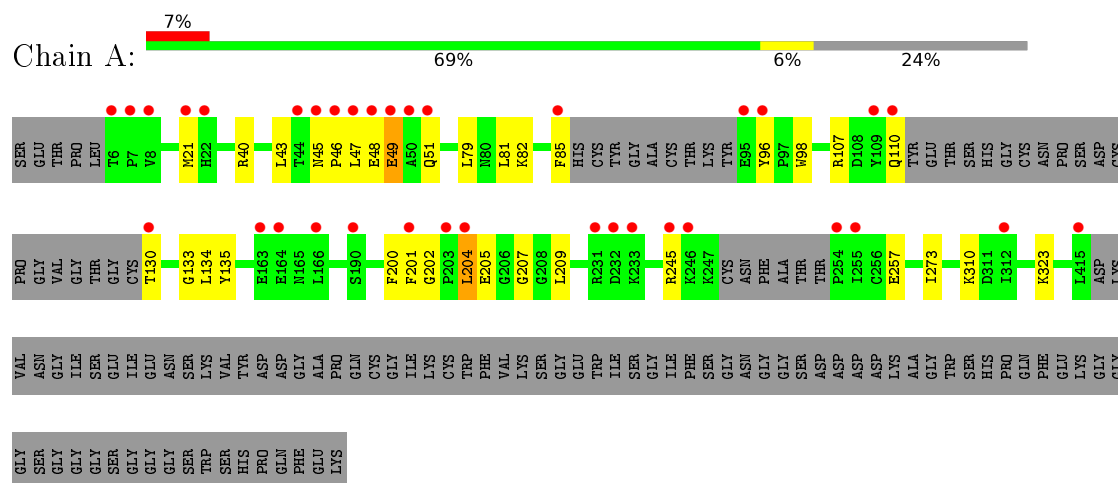
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	368	Total	O	0	0
			368	368		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Envelopment polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	107.14Å 107.14Å 127.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.52 – 1.50 37.52 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (37.52-1.50) 99.6 (37.52-1.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 1.50Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.171 , 0.201 0.152 , 0.174	Depositor DCC
R_{free} test set	4392 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	16.3	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.065 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.044 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.048 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l 0.047 for -h,2/3*h+1/3*k-2/3*l,-2/3*h-4/3*k-1/3*l 0.046 for 1/3*h+2/3*k+2/3*l,-k,4/3*h+2/3*k-1/3*l 0.066 for -1/3*h-2/3*k-2/3*l,-2/3*h-1/3*k+2/3*l,-2/3*h+2/3*k-1/3*l 0.188 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3397	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, K, FUL, 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	0.62	0/3067	0.71	0/4143

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204	LEU	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	2989	0	2873	24	0
2	A	28	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	10	0	10	0	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	368	0	0	4	0
All	All	3397	0	2907	24	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.

All (24) 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:201:PHE:H	1:A:204:LEU:HD12	1.22	0.99
1:A:201:PHE:N	1:A:204:LEU:HD12	1.94	0.83
1:A:245:ARG:NH2	6:A:601:HOH:O	2.13	0.79
1:A:202:GLY:H	1:A:204:LEU:HG	1.49	0.77
1:A:45:ASN:O	1:A:47:LEU:N	2.22	0.72
1:A:43:LEU:HB3	1:A:310:LYS:HD3	1.75	0.67
1:A:205:GLU:OE1	1:A:205:GLU:N	2.28	0.67
1:A:204:LEU:HD13	1:A:207:GLY:O	1.99	0.62
1:A:49:GLU:HB3	1:A:51:GLN:HG2	1.82	0.61
1:A:200:PHE:HB3	1:A:204:LEU:HB2	1.85	0.58
1:A:48:GLU:O	1:A:49:GLU:HB2	2.05	0.56
1:A:45:ASN:HB3	1:A:48:GLU:O	2.13	0.48
1:A:82:LYS:HG3	1:A:135:TYR:HE2	1.78	0.48
1:A:209:LEU:HD11	1:A:273:ILE:HD11	1.96	0.46
1:A:81:LEU:HD21	1:A:257:GLU:HA	1.98	0.46
1:A:40:ARG:NH2	6:A:618:HOH:O	2.49	0.45
1:A:81:LEU:HD12	1:A:133:GLY:O	2.16	0.45
1:A:98:TRP:CZ2	1:A:133:GLY:HA3	2.53	0.44
1:A:323:LYS:NZ	6:A:621:HOH:O	2.50	0.43
1:A:79:LEU:HG	1:A:134:LEU:HD22	1.99	0.43
1:A:205:GLU:HB3	6:A:729:HOH:O	2.19	0.43
1:A:204:LEU:HD23	1:A:204:LEU:HA	1.79	0.41
1:A:21:MET:HG3	1:A:21:MET:H	1.69	0.40
1:A:96:TYR:HB3	1:A:98:TRP:CE2	2.56	0.40

There are no symmetry-related clashes.

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	377/495 (76%)	363 (96%)	12 (3%)	2 (0%)	34	10

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	PRO
1	A	49	GLU

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	336/419 (80%)	332 (99%)	4 (1%)	78	54

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	PHE
1	A	107	ARG
1	A	110	GLN
1	A	130	THR

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z > 2$
2	NAG	A	501	1,3,2	14,14,15	0.53	0	15,19,21	0.73	0
2	NAG	A	502	2	14,14,15	0.27	0	15,19,21	0.40	0
3	FUL	A	503	2	10,10,11	1.26	1 (10%)	13,14,16	0.91	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
2	NAG	A	501	1,3,2	-	0/6/23/26	0/1/1/1
2	NAG	A	502	2	-	0/6/23/26	0/1/1/1
3	FUL	A	503	2	-	0/0/17/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	FUL	O5-C1	-3.20	1.38	1.43

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.

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	376/495 (75%)	0.32	35 (9%) 11 10	11, 21, 55, 75	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	85	PHE	14.3
1	A	204	LEU	10.6
1	A	47	LEU	9.1
1	A	46	PRO	8.9
1	A	232	ASP	6.7
1	A	6	THR	6.3
1	A	255	ILE	5.0
1	A	45	ASN	4.9
1	A	7	PRO	4.7
1	A	203	PRO	4.2
1	A	51	GLN	3.9
1	A	233	LYS	3.9
1	A	415	LEU	3.8
1	A	50	ALA	3.7
1	A	48	GLU	3.6
1	A	231	ARG	3.4
1	A	49	GLU	3.2
1	A	163	GLU	3.0
1	A	95	GLU	3.0
1	A	21	MET	3.0
1	A	201	PHE	2.9
1	A	8	VAL	2.9
1	A	246	LYS	2.8
1	A	96	TYR	2.7
1	A	110	GLN	2.7
1	A	44	THR	2.5
1	A	109	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	130	THR	2.4
1	A	254	PRO	2.4
1	A	22	HIS	2.3
1	A	190	SER	2.2
1	A	312	ILE	2.2
1	A	166	LEU	2.1
1	A	245	ARG	2.1
1	A	164	GLU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	502	14/15	0.49	0.32	10.86	60,62,66,68	0
3	FUL	A	503	10/11	0.54	0.48	2.87	61,62,63,64	0
2	NAG	A	501	14/15	0.78	0.17	2.86	43,49,56,57	0
4	K	A	504	1/1	1.00	0.06	-2.24	19,19,19,19	0
5	NA	A	505	1/1	1.00	0.06	-	15,15,15,15	1

6.5 Other polymers [i](#)

There are no such residues in this entry.