Full wwPDB X-ray Structure Validation Report (i)

May 13, 2024 – 04:40 pm BST

PDB ID	:	9EQH
Title	:	WWP2 WW2-2,3-linker-HECT (WWP2-LH)
Authors	:	Dudey, A.P.; Hemmings, A.M.
Deposited on	:	2024-03-21
Resolution	:	2.05 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 (i) 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 (i)) were used in the production of this report:

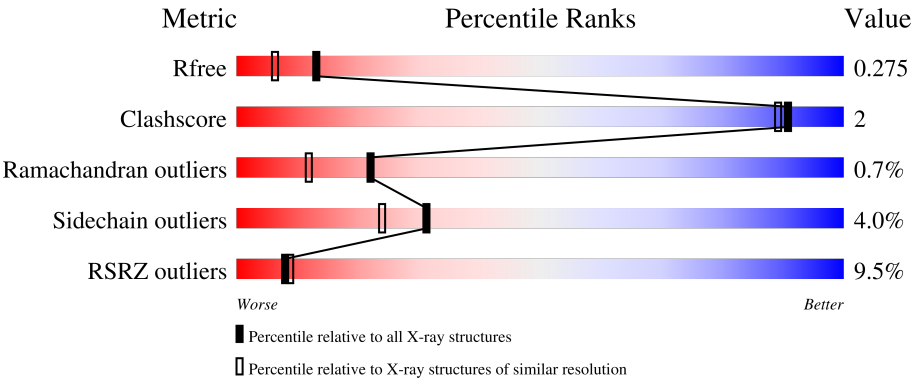
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 <=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	447	9% 84% 10% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7071 atoms, of which 3429 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 Isoform 2 of NEDD4-like E3 ubiquitin-protein ligase WWP2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	422	6937	2262	3413	597	643	22	110	2	0

There are 87 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	333	GLY	-	expression tag	UNP O00308
A	?	-	THR	deletion	UNP O00308
A	?	-	ASP	deletion	UNP O00308
A	?	-	HIS	deletion	UNP O00308
A	?	-	ASP	deletion	UNP O00308
A	?	-	PRO	deletion	UNP O00308
A	?	-	LEU	deletion	UNP O00308
A	?	-	GLY	deletion	UNP O00308
A	?	-	PRO	deletion	UNP O00308
A	?	-	LEU	deletion	UNP O00308
A	?	-	PRO	deletion	UNP O00308
A	?	-	PRO	deletion	UNP O00308
A	?	-	GLY	deletion	UNP O00308
A	?	-	TRP	deletion	UNP O00308
A	?	-	GLU	deletion	UNP O00308
A	?	-	LYS	deletion	UNP O00308
A	?	-	ARG	deletion	UNP O00308
A	?	-	GLN	deletion	UNP O00308
A	?	-	ASP	deletion	UNP O00308
A	?	-	ASN	deletion	UNP O00308
A	?	-	GLY	deletion	UNP O00308
A	?	-	ARG	deletion	UNP O00308
A	?	-	VAL	deletion	UNP O00308
A	?	-	TYR	deletion	UNP O00308
A	?	-	TYR	deletion	UNP O00308
A	?	-	VAL	deletion	UNP O00308
A	?	-	ASN	deletion	UNP O00308

Continued on next page...

Continued from previous page...

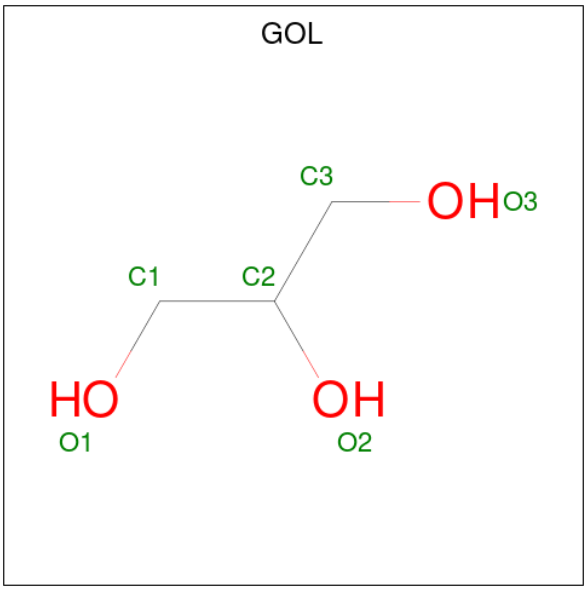
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	HIS	deletion	UNP O00308
A	?	-	ASN	deletion	UNP O00308
A	?	-	THR	deletion	UNP O00308
A	?	-	ARG	deletion	UNP O00308
A	?	-	THR	deletion	UNP O00308
A	?	-	THR	deletion	UNP O00308
A	?	-	GLN	deletion	UNP O00308
A	?	-	TRP	deletion	UNP O00308
A	?	-	GLU	deletion	UNP O00308
A	?	-	ASP	deletion	UNP O00308
A	?	-	PRO	deletion	UNP O00308
A	?	-	ARG	deletion	UNP O00308
A	?	-	THR	deletion	UNP O00308
A	?	-	GLN	deletion	UNP O00308
A	?	-	GLY	deletion	UNP O00308
A	?	-	MET	deletion	UNP O00308
A	?	-	ILE	deletion	UNP O00308
A	?	-	GLN	deletion	UNP O00308
A	?	-	GLU	deletion	UNP O00308
A	?	-	PRO	deletion	UNP O00308
A	?	-	ALA	deletion	UNP O00308
A	?	-	LEU	deletion	UNP O00308
A	?	-	PRO	deletion	UNP O00308
A	?	-	PRO	deletion	UNP O00308
A	?	-	GLY	deletion	UNP O00308
A	?	-	TRP	deletion	UNP O00308
A	?	-	GLU	deletion	UNP O00308
A	?	-	MET	deletion	UNP O00308
A	?	-	LYS	deletion	UNP O00308
A	?	-	TYR	deletion	UNP O00308
A	?	-	THR	deletion	UNP O00308
A	?	-	SER	deletion	UNP O00308
A	?	-	GLU	deletion	UNP O00308
A	?	-	GLY	deletion	UNP O00308
A	?	-	VAL	deletion	UNP O00308
A	?	-	ARG	deletion	UNP O00308
A	?	-	TYR	deletion	UNP O00308
A	?	-	PHE	deletion	UNP O00308
A	?	-	VAL	deletion	UNP O00308
A	?	-	ASP	deletion	UNP O00308
A	?	-	HIS	deletion	UNP O00308
A	?	-	ASN	deletion	UNP O00308

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP O00308
A	?	-	ARG	deletion	UNP O00308
A	?	-	THR	deletion	UNP O00308
A	?	-	THR	deletion	UNP O00308
A	?	-	THR	deletion	UNP O00308
A	?	-	PHE	deletion	UNP O00308
A	?	-	LYS	deletion	UNP O00308
A	?	-	ASP	deletion	UNP O00308
A	?	-	PRO	deletion	UNP O00308
A	?	-	ARG	deletion	UNP O00308
A	?	-	PRO	deletion	UNP O00308
A	?	-	GLY	deletion	UNP O00308
A	?	-	PHE	deletion	UNP O00308
A	?	-	GLU	deletion	UNP O00308
A	?	-	SER	deletion	UNP O00308
A	?	-	GLY	deletion	UNP O00308
A	?	-	THR	deletion	UNP O00308
A	?	-	LYS	deletion	UNP O00308

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	3	0
			14	3	8	3		
2	A	1	Total	C	H	O	3	0
			14	3	8	3		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

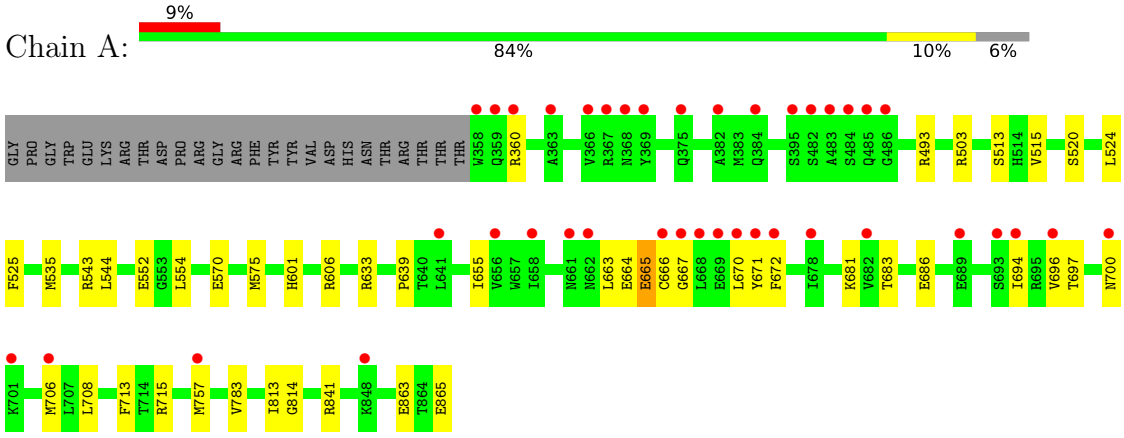
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	105	Total O 105 105	0	0

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: Isoform 2 of NEDD4-like E3 ubiquitin-protein ligase WWP2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	44.01Å 90.27Å 111.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.08 – 2.05 70.08 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.3 (70.08-2.05) 99.2 (70.08-2.05)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.213 , 0.275 0.220 , 0.275	Depositor DCC
R_{free} test set	1367 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 49.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7071	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NA, GOL

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	0.60	0/3631	1.12	6/4902 (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	4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	706	MET	CG-SD-CE	7.77	112.64	100.20
1	A	575	MET	CG-SD-CE	7.08	111.53	100.20
1	A	863	GLU	CB-CA-C	-6.36	97.67	110.40
1	A	552	GLU	CB-CA-C	5.43	121.25	110.40
1	A	686	GLU	CB-CA-C	5.13	120.67	110.40
1	A	606	ARG	NE-CZ-NH2	5.05	122.83	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	ARG	Sidechain
1	A	503	ARG	Sidechain
1	A	543	ARG	Sidechain
1	A	841	ARG	Sidechain

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	3524	3413	3378	12	0
2	A	12	16	16	0	0
3	A	1	0	0	0	0
4	A	105	0	0	0	0
All	All	3642	3429	3394	12	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 (12) 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:813:ILE:HG22	1:A:814:GLY:O	2.07	0.54
1:A:515:VAL:HG21	1:A:535:MET:CE	2.40	0.52
1:A:655:ILE:HD13	1:A:708:LEU:HD23	1.92	0.52
1:A:664:GLU:O	1:A:667:GLY:N	2.44	0.50
1:A:672:PHE:CE1	1:A:696:VAL:HG22	2.48	0.49
1:A:639:PRO:HB2	1:A:713:PHE:CE2	2.49	0.47
1:A:757:MET:HE1	1:A:783:VAL:HG12	1.97	0.47
1:A:672:PHE:CD1	1:A:696:VAL:HG22	2.51	0.46
1:A:671:TYR:C	1:A:696:VAL:HG23	2.36	0.45
1:A:515:VAL:HG21	1:A:535:MET:HE1	1.98	0.44
1:A:665:GLU:O	1:A:666:CYS:SG	2.79	0.41
1:A:525:PHE:HB2	1:A:570:GLU:HG3	2.03	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	422/447 (94%)	388 (92%)	31 (7%)	3 (1%)	22 12

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	681	LYS
1	A	513	SER
1	A	694	ILE

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	379/406 (93%)	364 (96%)	15 (4%)	31 24

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	493	ARG
1	A	520	SER
1	A	524	LEU
1	A	544	LEU
1	A	554	LEU
1	A	601	HIS
1	A	633	ARG
1	A	663	LEU
1	A	665	GLU
1	A	670	LEU
1	A	683	THR
1	A	697	THR
1	A	700	ASN
1	A	715	ARG
1	A	865	GLU

Sometimes 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

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	$\#\|Z\| > 2$
2	GOL	A	902	-	5,5,5	0.21	0	5,5,5	0.46	0
2	GOL	A	901	-	5,5,5	0.20	0	5,5,5	0.58	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	GOL	A	902	-	-	0/4/4/4	-
2	GOL	A	901	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	GOL	O1-C1-C2-O2
2	A	901	GOL	O1-C1-C2-C3
2	A	901	GOL	O2-C2-C3-O3

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, 95^{th} 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	422/447 (94%)	0.46	40 (9%) 8 9	24, 46, 100, 122	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	666	CYS	5.8
1	A	678	ILE	5.1
1	A	367	ARG	4.0
1	A	662	ASN	3.7
1	A	375	GLN	3.7
1	A	670	LEU	3.6
1	A	486	GLY	3.6
1	A	358	TRP	3.6
1	A	366	VAL	3.4
1	A	482	SER	3.3
1	A	694	ILE	3.3
1	A	360	ARG	3.3
1	A	484	SER	3.2
1	A	669	GLU	3.1
1	A	706	MET	3.0
1	A	641	LEU	2.9
1	A	700	ASN	2.9
1	A	369	TYR	2.7
1	A	848	LYS	2.7
1	A	693	SER	2.7
1	A	363	ALA	2.6
1	A	661	ASN	2.6
1	A	382	ALA	2.5
1	A	368	ASN	2.5
1	A	689	GLU	2.5
1	A	671	TYR	2.5
1	A	682	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	395	SER	2.5
1	A	696	VAL	2.4
1	A	672	PHE	2.3
1	A	359	GLN	2.3
1	A	384	GLN	2.3
1	A	658	ILE	2.3
1	A	656	VAL	2.2
1	A	485	GLN	2.2
1	A	701	LYS	2.2
1	A	667	GLY	2.2
1	A	483	ALA	2.1
1	A	757	MET	2.0
1	A	668	LEU	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, 95^{th} 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
2	GOL	A	901	6/6	0.73	0.27	58,73,84,87	3
3	NA	A	903	1/1	0.89	0.14	39,39,39,39	0
2	GOL	A	902	6/6	0.93	0.13	46,60,63,67	3

6.5 Other polymers (i)

There are no such residues in this entry.