Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:53 AM GMT

PDB ID	:	2J7U
Title	:	DENGUE VIRUS NS5 RNA DEPENDENT RNA POLYMERASE DOMAIN
Authors	:	Yap, T.L.; Xu, T.; Chen, Y.L.; Malet, H.; Egloff, M.P.; Canard, B.; Vasudevan, S.G.; Lescar, J.
Deposited on	:	2006-10-17
Resolution	:	1.85 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

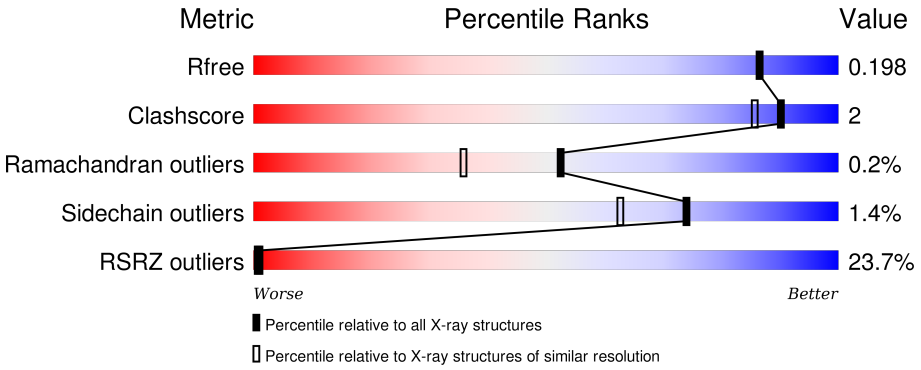
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.85 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}	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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 <=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	635	21% 83% 6% 10%

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	MG	A	1886	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	A	1887	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5220 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 RNA DEPENDENT RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	573	Total	C	N	O	S	0	11	0
			4701	2980	842	849	30			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	266	GLY	-	EXPRESSION TAG	UNP Q6DLV0
A	267	SER	-	EXPRESSION TAG	UNP Q6DLV0
A	268	HIS	-	EXPRESSION TAG	UNP Q6DLV0
A	269	MET	-	EXPRESSION TAG	UNP Q6DLV0
A	270	LEU	-	EXPRESSION TAG	UNP Q6DLV0
A	271	ASP	-	EXPRESSION TAG	UNP Q6DLV0
A	374	GLU	GLY	CONFLICT	UNP Q6DLV0
A	480	ALA	VAL	CONFLICT	UNP Q6DLV0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

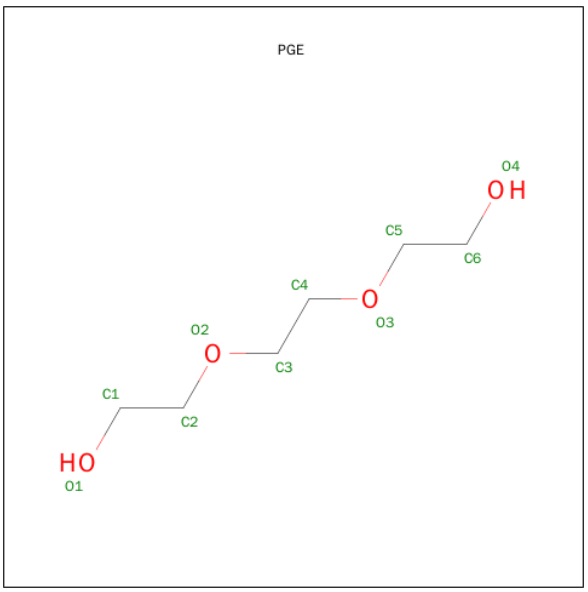
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 6 is water.

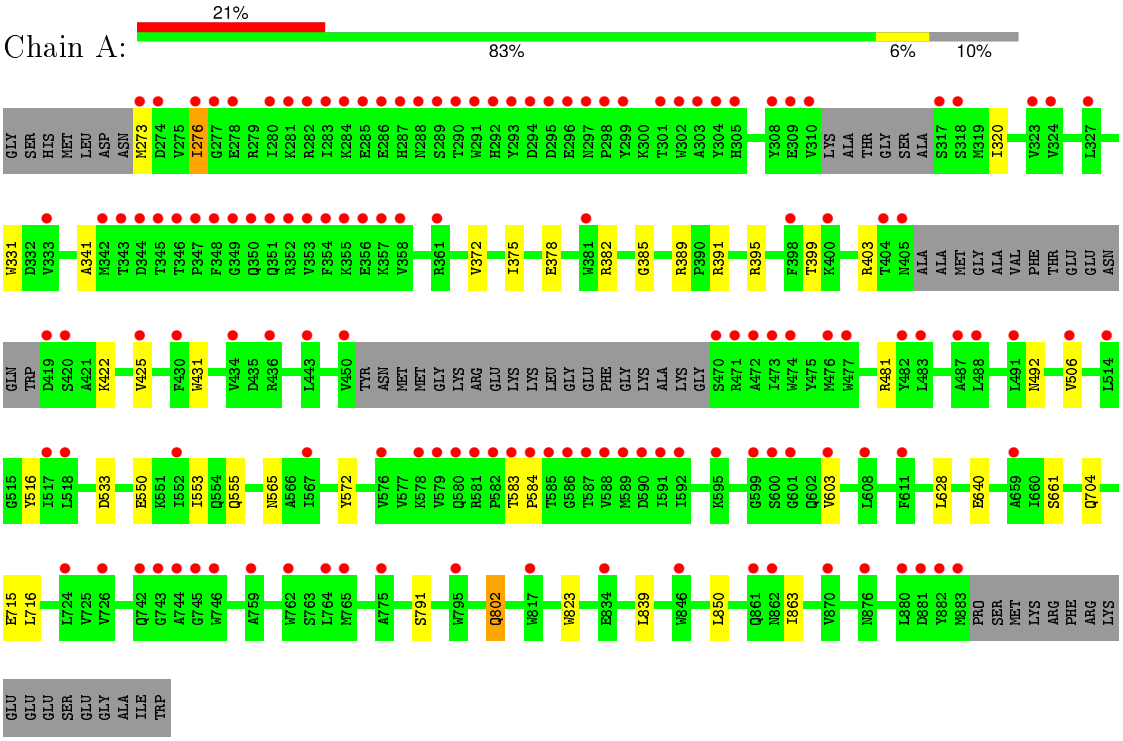
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	505	Total O 505 505	0	0

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: RNA DEPENDENT RNA POLYMERASE

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	160.15Å 180.48Å 57.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.85 19.96 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-1.85) 99.9 (19.96-1.85)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.234 0.200 , 0.198	Depositor DCC
R_{free} test set	3601 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 72006 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5220	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, PGE, MG, 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	0.35	0/4854	0.49	0/6576

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

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	4701	0	4598	21	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	1	0	0	1	0
5	A	10	0	14	0	0
6	A	505	0	0	0	0
All	All	5220	0	4612	21	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 (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)
1:A:716:LEU:HD21	1:A:839:LEU:HD23	1.60	0.83
1:A:802:GLN:HE21	1:A:802:GLN:H	1.30	0.77
1:A:385:GLY:HA3	1:A:555:GLN:HE22	1.64	0.61
1:A:704:GLN:NE2	1:A:715:GLU:H	2.05	0.55
1:A:716:LEU:CD2	1:A:839:LEU:HD23	2.36	0.53
1:A:403:ARG:HA	1:A:422:LYS:HD3	1.89	0.53
1:A:375:ILE:HD11	1:A:640:GLU:HG2	1.91	0.53
1:A:273:MET:HB3	1:A:276:ILE:HG22	1.96	0.47
1:A:572:TYR:OH	1:A:603:VAL:O	2.33	0.47
1:A:331:TRP:CE2	1:A:850:LEU:HD22	2.51	0.45
1:A:583:THR:HA	1:A:584:PRO:HD3	1.87	0.44
1:A:399:THR:HG23	1:A:425:VAL:CG1	2.47	0.44
1:A:395:ARG:HG3	1:A:431:TRP:CZ2	2.53	0.43
1:A:378:GLU:O	1:A:382:ARG:HG3	2.19	0.43
1:A:320:ILE:HD11	1:A:341:ALA:HB1	2.01	0.43
1:A:372[A]:VAL:HG11	1:A:628:LEU:HD11	2.00	0.43
1:A:492:ASN:ND2	4:A:1887:CL:CL	2.89	0.42
1:A:506:VAL:CG2	1:A:661[B]:SER:OG	2.68	0.41
1:A:550:GLU:O	1:A:553:ILE:HG12	2.21	0.41
1:A:516:TYR:HB3	1:A:823:TRP:CE2	2.57	0.40

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	576/635 (91%)	553 (96%)	22 (4%)	1 (0%)	52 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	791	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	502/551 (91%)	495 (99%)	7 (1%)	74 63

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	276	ILE
1	A	389	ARG
1	A	391	ARG
1	A	481	ARG
1	A	533	ASP
1	A	802	GLN
1	A	863	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	339	GLN
1	A	387	ASN
1	A	548	ASN
1	A	555	GLN
1	A	645	GLN
1	A	701	HIS
1	A	704	GLN
1	A	760	GLN
1	A	768	HIS
1	A	802	GLN
1	A	835	ASN
1	A	869	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	PGE	A	1888	-	9,9,9	0.43	0	8,8,8	0.62	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	PGE	A	1888	-	-	0/7/7/7	0/0/0/0

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.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	573/635 (90%)	1.57	136 (23%) 1 1	28, 36, 42, 51	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	347	PRO	19.3
1	A	345	THR	16.9
1	A	348	PHE	15.0
1	A	583	THR	14.8
1	A	587	THR	14.3
1	A	353	VAL	13.8
1	A	293	TYR	12.7
1	A	310	VAL	12.3
1	A	346	THR	12.0
1	A	355	LYS	11.1
1	A	349	GLY	11.1
1	A	343	THR	9.9
1	A	354	PHE	9.6
1	A	582	PRO	9.2
1	A	291	TRP	8.9
1	A	344	ASP	8.6
1	A	580	GLN	8.4
1	A	304	TYR	8.4
1	A	317	SER	8.2
1	A	295	ASP	8.0
1	A	280	ILE	7.9
1	A	352	ARG	7.8
1	A	579	VAL	7.8
1	A	585	THR	7.4
1	A	289	SER	7.4
1	A	584	PRO	7.3
1	A	473	ILE	7.3

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Mol	Chain	Res	Type	RSRZ
1	A	287	HIS	7.2
1	A	746	TRP	7.0
1	A	290	THR	6.8
1	A	288	ASN	6.8
1	A	305	HIS	6.7
1	A	358	VAL	6.6
1	A	292	HIS	6.5
1	A	586	GLY	6.5
1	A	273	MET	6.2
1	A	303	ALA	6.1
1	A	474	TRP	5.9
1	A	443	LEU	5.7
1	A	880	LEU	5.6
1	A	356	GLU	5.6
1	A	742	GLN	5.3
1	A	276	ILE	5.2
1	A	743	GLY	5.1
1	A	283	ILE	5.1
1	A	470	SER	5.1
1	A	581	ARG	5.0
1	A	876	ASN	5.0
1	A	285	GLU	5.0
1	A	590	ASP	4.8
1	A	342	MET	4.8
1	A	296	GLU	4.7
1	A	588	VAL	4.7
1	A	591	ILE	4.6
1	A	350	GLN	4.4
1	A	589	MET	4.4
1	A	881	ASP	4.4
1	A	351	GLN	4.4
1	A	284	LYS	4.3
1	A	333	VAL	4.3
1	A	302	TRP	4.3
1	A	795	TRP	4.3
1	A	318	SER	4.1
1	A	277	GLY	4.1
1	A	603	VAL	4.0
1	A	308	TYR	4.0
1	A	294	ASP	3.8
1	A	323	VAL	3.8
1	A	882	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	745	GLY	3.7
1	A	567	ILE	3.7
1	A	309	GLU	3.6
1	A	601	GLY	3.6
1	A	286	GLU	3.6
1	A	576	VAL	3.4
1	A	477	TRP	3.4
1	A	298	PRO	3.3
1	A	281	LYS	3.3
1	A	600	SER	3.3
1	A	472	ALA	3.2
1	A	301	THR	3.2
1	A	861	GLN	3.2
1	A	299	TYR	3.2
1	A	282	ARG	3.1
1	A	608	LEU	3.1
1	A	552	ILE	3.0
1	A	471	ARG	3.0
1	A	744	ALA	3.0
1	A	578	LYS	2.9
1	A	297	ASN	2.9
1	A	278	GLU	2.9
1	A	883	MET	2.9
1	A	361	ARG	2.9
1	A	592	ILE	2.9
1	A	450	VAL	2.9
1	A	491	LEU	2.8
1	A	357	LYS	2.8
1	A	327	LEU	2.8
1	A	324	VAL	2.8
1	A	595	LYS	2.7
1	A	483	LEU	2.7
1	A	405	ASN	2.6
1	A	599	GLY	2.6
1	A	274	ASP	2.5
1	A	476	MET	2.5
1	A	487	ALA	2.4
1	A	514	LEU	2.4
1	A	726	VAL	2.4
1	A	817	TRP	2.4
1	A	400	LYS	2.3
1	A	775	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	436	ARG	2.3
1	A	488	LEU	2.3
1	A	834	GLU	2.3
1	A	420	SER	2.3
1	A	846	TRP	2.3
1	A	425	VAL	2.3
1	A	659	ALA	2.2
1	A	870	VAL	2.2
1	A	611	PHE	2.2
1	A	764	LEU	2.2
1	A	759	ALA	2.2
1	A	765	MET	2.2
1	A	762	TRP	2.1
1	A	724	LEU	2.1
1	A	862	ASN	2.1
1	A	398	PHE	2.1
1	A	404	THR	2.1
1	A	419	ASP	2.1
1	A	482	TYR	2.0
1	A	506	VAL	2.0
1	A	430	PHE	2.0
1	A	518	LEU	2.0
1	A	381	TRP	2.0
1	A	434	VAL	2.0
1	A	517	ILE	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, 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	LLDF	B-factors(Å^2)	Q<0.9
4	CL	A	1887	1/1	0.93	0.31	3.12	51,51,51,51	0
3	MG	A	1886	1/1	0.89	0.25	2.87	47,47,47,47	0
2	ZN	A	1884	1/1	0.99	0.07	-2.26	25,25,25,25	0
2	ZN	A	1885	1/1	0.97	0.08	-2.42	31,31,31,31	1
5	PGE	A	1888	10/10	0.85	0.22	-	48,49,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.