



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:13 PM EDT

PDB ID : 4Z97 / pdb_00004z97
Title : Crystal structure of USP7 in complex with DNMT1(K1115Q)
Authors : Zhang, Z.M.; Song, J.
Deposited on : 2015-04-09
Resolution : 3.00 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

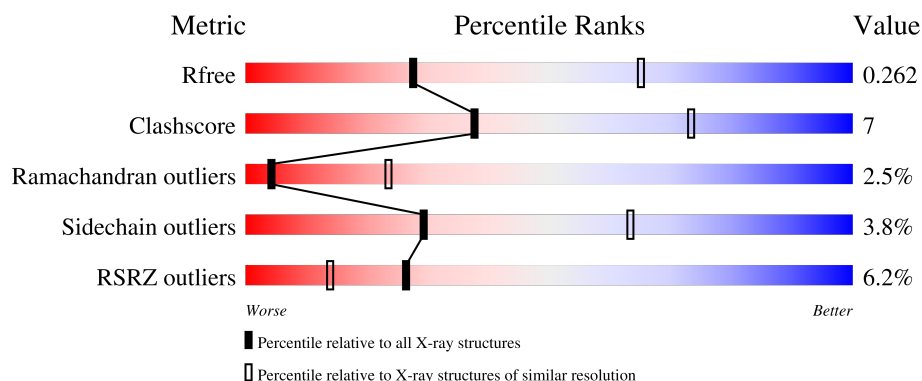
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. 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	530	
2	C	33	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4127 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 Ubiquitin carboxyl-terminal hydrolase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	1	0
			4047	2575	686	760	26			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	554	SER	-	expression tag	UNP Q93009
A	555	GLY	-	expression tag	UNP Q93009
A	556	PRO	-	expression tag	UNP Q93009
A	557	LEU	-	expression tag	UNP Q93009
A	558	GLY	-	expression tag	UNP Q93009
A	559	SER	-	expression tag	UNP Q93009

- Molecule 2 is a protein called DNA (cytosine-5)-methyltransferase 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	0	5	0
			74	44	17	13			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

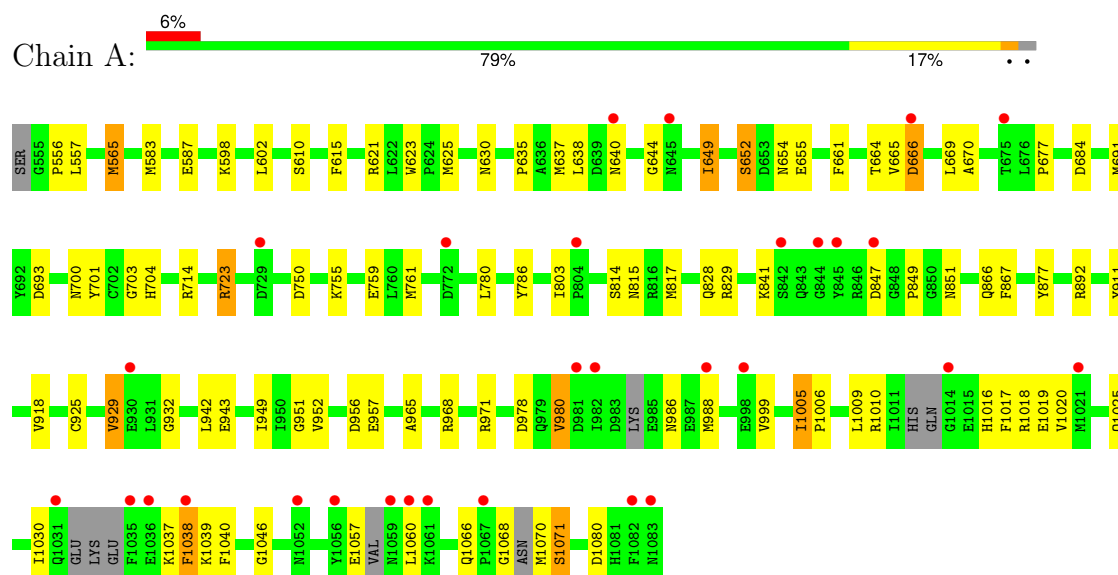


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

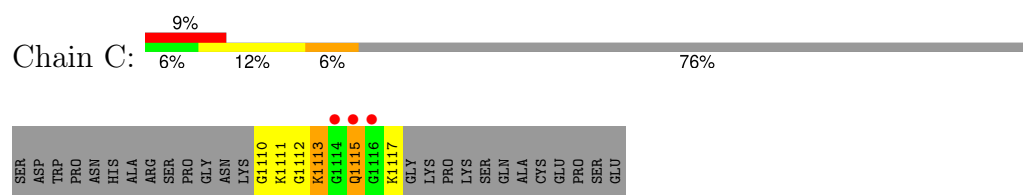
3 Residue-property plots [i](#)

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: Ubiquitin carboxyl-terminal hydrolase 7



- Molecule 2: DNA (cytosine-5)-methyltransferase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.66Å 123.66Å 152.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.86 – 3.00 43.86 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.86-3.00) 96.9 (43.86-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.209 , 0.254 0.217 , 0.262	Depositor DCC
R_{free} test set	2016 reflections (7.29%)	wwPDB-VP
Wilson B-factor (Å ²)	89.1	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 75.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4127	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: 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	0.50	0/4137	0.90	8/5614 (0.1%)
2	C	0.29	0/71	0.54	0/84
All	All	0.49	0/4208	0.89	8/5698 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1005	ILE	N-CA-C	7.47	115.59	107.60
1	A	1071	SER	N-CA-C	7.03	118.94	111.28
1	A	951	GLY	N-CA-C	6.20	119.55	110.38
1	A	693	ASP	CA-C-N	5.51	125.17	119.05
1	A	693	ASP	C-N-CA	5.51	125.17	119.05
1	A	929	VAL	N-CA-C	5.20	116.21	108.46
1	A	666	ASP	CA-C-N	5.00	125.27	119.47
1	A	666	ASP	C-N-CA	5.00	125.27	119.47

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	4047	0	3759	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	74	0	82	6	0
3	A	6	0	8	3	0
All	All	4127	0	3849	56	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 7.

All (56) 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:761:MET:HG3	3:A:1101:GOL:H32	1.58	0.84
1:A:625:MET:HE1	1:A:661:PHE:HB2	1.64	0.80
1:A:649:ILE:HD12	1:A:649:ILE:H	1.54	0.73
1:A:1016:HIS:CE1	1:A:1020:VAL:HG23	2.31	0.65
1:A:602:LEU:HB3	1:A:644:GLY:HA2	1.80	0.63
1:A:598:LYS:HB3	1:A:649:ILE:HD11	1.82	0.62
1:A:978:ASP:N	1:A:978:ASP:OD1	2.34	0.61
1:A:1009:LEU:HD12	1:A:1010:ARG:H	1.67	0.60
1:A:949:ILE:HG13	1:A:1006:PRO:HB2	1.86	0.57
1:A:814:SER:HB3	1:A:817:MET:HG3	1.88	0.56
1:A:630:ASN:HB3	2:C:1112:GLY:HA3	1.87	0.55
1:A:610:SER:OG	1:A:615:PHE:O	2.23	0.55
1:A:965:ALA:HB3	1:A:968:ARG:HG3	1.90	0.54
1:A:1017:PHE:O	1:A:1019:GLU:N	2.40	0.54
1:A:849:PRO:HB3	1:A:877:TYR:HB2	1.90	0.53
1:A:1017:PHE:O	1:A:1020:VAL:N	2.30	0.53
1:A:691:MET:HE3	1:A:700:ASN:HB2	1.91	0.52
1:A:1016:HIS:HA	1:A:1057:GLU:HB2	1.91	0.51
1:A:1039:LYS:C	1:A:1040:PHE:HD1	2.19	0.51
1:A:701:TYR:CZ	1:A:703:GLY:HA2	2.46	0.50
1:A:759:GLU:HB2	2:C:1113[B]:LYS:HD3	1.93	0.50
1:A:665:VAL:HG23	1:A:670:ALA:HB2	1.93	0.50
1:A:943:GLU:OE2	1:A:968:ARG:NH1	2.46	0.48
1:A:1070:MET:HG2	1:A:1071:SER:N	2.27	0.48
3:A:1101:GOL:H31	2:C:1115[B]:GLN:OE1	2.14	0.48
1:A:925:CYS:O	1:A:929:VAL:HG22	2.14	0.47
1:A:583:MET:HE2	1:A:635:PRO:HD2	1.97	0.46
1:A:892:ARG:O	1:A:911:TYR:HA	2.15	0.46
1:A:1066:GLN:O	1:A:1068:GLY:N	2.49	0.46
1:A:701:TYR:CE2	1:A:703:GLY:HA2	2.51	0.46
2:C:1110:GLY:HA3	2:C:1111:LYS:HA	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:MET:HE2	1:A:625:MET:HB2	1.62	0.46
1:A:1038:PHE:HA	1:A:1080:ASP:O	2.16	0.45
1:A:978:ASP:HB2	1:A:1010:ARG:HD2	1.98	0.45
1:A:565:MET:HE1	1:A:649:ILE:HA	1.98	0.45
1:A:866:GLN:HG3	1:A:867:PHE:CD1	2.51	0.45
1:A:714:ARG:HH21	1:A:750:ASP:CG	2.24	0.44
1:A:942:LEU:HD22	1:A:952:VAL:HG22	1.99	0.44
1:A:761:MET:HB2	1:A:761:MET:HE3	1.55	0.44
1:A:918:VAL:HG23	1:A:957:GLU:O	2.18	0.43
1:A:704:HIS:O	1:A:723:ARG:NH2	2.52	0.43
3:A:1101:GOL:O3	2:C:1117[B]:LYS:HE3	2.19	0.43
1:A:649:ILE:HG22	1:A:654:ASN:HA	2.00	0.42
1:A:1039:LYS:C	1:A:1040:PHE:CD1	2.97	0.42
1:A:652:SER:OG	1:A:655:GLU:N	2.52	0.42
1:A:666:ASP:O	1:A:669:LEU:N	2.53	0.42
1:A:621[A]:ARG:NH2	1:A:677:PRO:O	2.52	0.42
1:A:971:ARG:NH1	1:A:1005:ILE:HG23	2.36	0.41
1:A:828:GLN:O	1:A:829:ARG:HB2	2.21	0.41
1:A:621[B]:ARG:HD3	1:A:623:TRP:CZ2	2.56	0.41
1:A:684:ASP:O	2:C:1117[B]:LYS:NZ	2.50	0.41
1:A:780:LEU:HD13	1:A:786:TYR:HA	2.03	0.41
1:A:841:LYS:HG3	1:A:851:ASN:O	2.22	0.40
1:A:755:LYS:HB3	1:A:755:LYS:HE3	1.70	0.40
1:A:598:LYS:C	1:A:649:ILE:HD11	2.46	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	510/530 (96%)	471 (92%)	27 (5%)	12 (2%)	4 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	9/33 (27%)	5 (56%)	2 (22%)	2 (22%)	0	0
All	All	519/563 (92%)	476 (92%)	29 (6%)	14 (3%)	4	22

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1037	LYS
1	A	1060	LEU
1	A	815	ASN
1	A	1018	ARG
1	A	1046	GLY
1	A	847	ASP
1	A	932	GLY
1	A	986	ASN
2	C	1115[A]	GLN
2	C	1115[B]	GLN
1	A	1030	ILE
1	A	1038	PHE
1	A	980	VAL
1	A	556	PRO

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	417/485 (86%)	402 (96%)	15 (4%)	31	65
2	C	6/25 (24%)	4 (67%)	2 (33%)	0	1
All	All	423/510 (83%)	406 (96%)	17 (4%)	29	62

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	557	LEU
1	A	565	MET

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Mol	Chain	Res	Type
1	A	587	GLU
1	A	637	MET
1	A	638	LEU
1	A	649	ILE
1	A	652	SER
1	A	664	THR
1	A	723	ARG
1	A	803	ILE
1	A	956	ASP
1	A	980	VAL
1	A	988	MET
1	A	999	VAL
1	A	1025	GLN
2	C	1113[A]	LYS
2	C	1113[B]	LYS

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

Mol	Chain	Res	Type
1	A	986	ASN

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	GOL	A	1101	-	5,5,5	0.45	0	5,5,5	0.38	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	GOL	A	1101	-	-	4/4/4/4	-

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	1101	GOL	C1-C2-C3-O3
3	A	1101	GOL	O1-C1-C2-C3
3	A	1101	GOL	O1-C1-C2-O2
3	A	1101	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	GOL	3	0

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, 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	521/530 (98%)	0.16	30 (5%) 29 15	38, 95, 150, 194	1 (0%)
2	C	8/33 (24%)	3.22	3 (37%) 1 1	42, 93, 111, 143	3 (37%)
All	All	529/563 (93%)	0.20	33 (6%) 26 14	38, 95, 150, 194	4 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1114[A]	GLY	11.3
2	C	1115[A]	GLN	8.0
1	A	1014	GLY	6.4
1	A	645	ASN	6.0
1	A	1031	GLN	5.7
1	A	1052	ASN	3.9
1	A	1059	ASN	3.4
1	A	772	ASP	3.3
1	A	640	ASN	3.2
1	A	666	ASP	3.1
1	A	1067	PRO	3.1
1	A	729	ASP	3.0
1	A	1061	LYS	2.9
1	A	844	GLY	2.7
1	A	981	ASP	2.6
1	A	675	THR	2.6
1	A	930	GLU	2.6
1	A	998	GLU	2.6
1	A	1056	TYR	2.6
1	A	804	PRO	2.5
1	A	845	TYR	2.5
1	A	1035	PHE	2.5
1	A	988	MET	2.4
1	A	1021	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	842	SER	2.4
1	A	1082	PHE	2.4
1	A	1083	ASN	2.3
2	C	1116[B]	GLY	2.3
1	A	1036	GLU	2.3
1	A	847	ASP	2.3
1	A	982	ILE	2.1
1	A	1038	PHE	2.0
1	A	1060	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 oligosaccharides 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	1101	6/6	0.89	0.30	118,133,136,136	0

6.5 Other polymers [i](#)

There are no such residues in this entry.