



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:09 PM GMT

PDB ID : 1EAM  
Title : VACCINIA METHYLTRANSFERASE VP39 MUTANT (EC: 2.7.7.19)  
Authors : Hu, G.; Hodel, A.E.; Gershon, P.D.; Quirocho, F.A.  
Deposited on : 1999-01-26  
Resolution : 2.00 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](mailto: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 (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

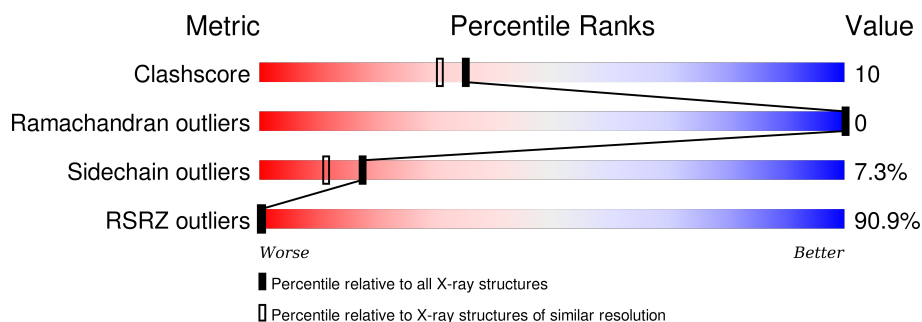
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	307	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3183 atoms, of which 709 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.

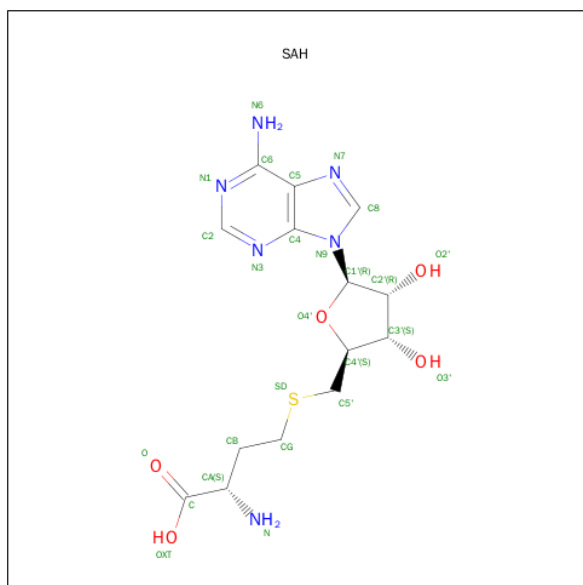
- Molecule 1 is a protein called PROTEIN (VP39).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	285	2871	1540	517	391	411	12	517	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	233	ALA	GLU	ENGINEERED	UNP P07617

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
2	A	1	30	14	4	6	5	1	4	0

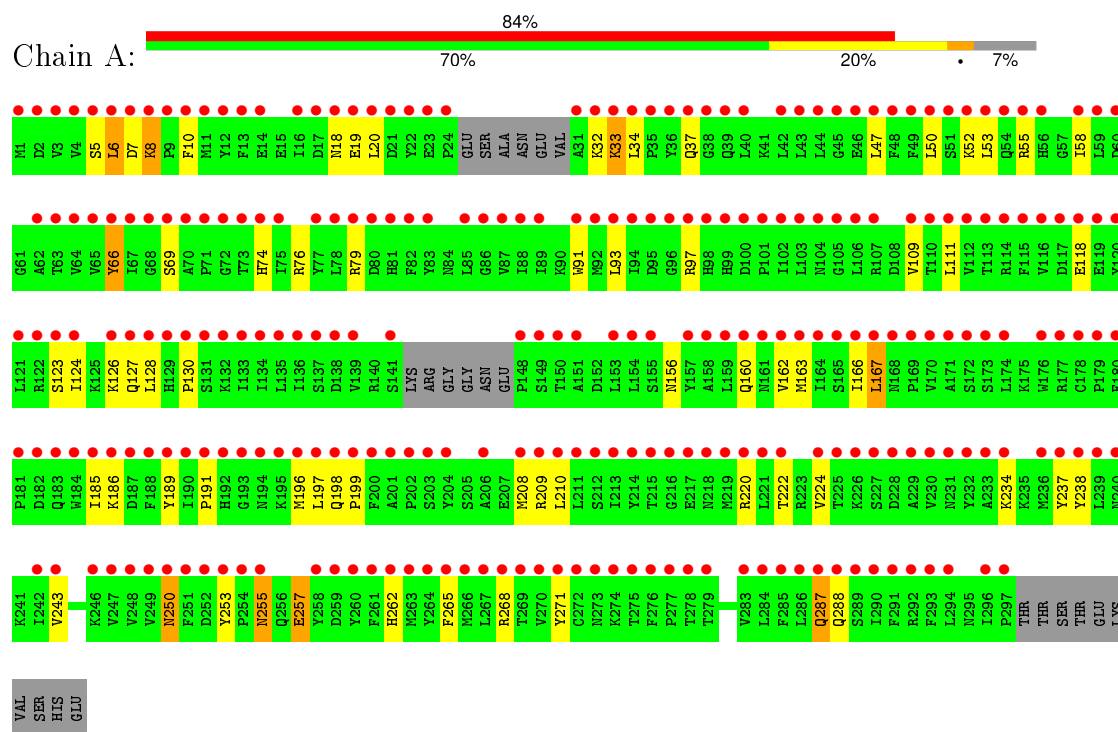
- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	94	Total	H	O	188	0
			282	188	94		

### 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 ( $\text{RSRZ} > 2$ ). 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: PROTEIN (VP39)



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.00Å 67.51Å 79.92Å 90.00° 117.42° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00 14.17 – 1.31	Depositor EDS
% Data completeness (in resolution range)	79.3 (8.00-2.00) 8.7 (14.17-1.31)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.83 (at 1.31Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.222 , 0.268 0.466 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	1.5	Xtriage
Anisotropy	2.523	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	1.52 , 155.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 9717 reflections	Xtriage
$F_o, F_c$ correlation	0.30	EDS
Total number of atoms	3183	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 100.00 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 0.0000e+00. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: SAH

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	0.52	0/2416	0.73	0/3271

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	2354	517	2375	47	0
2	A	26	4	19	3	0
3	A	94	188	0	1	0
All	All	2474	709	2394	47	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 10.

All (47) 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:124:ILE:HA	1:A:127:GLN:HG2	1.42	1.02

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:SER:HA	1:A:126:LYS:HE2	1.49	0.91
1:A:19:GLU:HB2	1:A:234:LYS:HB3	1.71	0.72
1:A:163:MET:O	1:A:167:LEU:HB2	1.91	0.70
1:A:32:LYS:HA	3:A:466:HOH:O	1.90	0.70
1:A:6:LEU:H	1:A:250:ASN:HD21	1.40	0.69
1:A:34:LEU:H	1:A:37:GLN:HE21	1.43	0.67
1:A:185:ILE:HG22	1:A:186:LYS:HG2	1.77	0.66
1:A:118:GLU:HG3	1:A:166:ILE:HD11	1.77	0.66
1:A:20:LEU:HB3	1:A:237:TYR:HD2	1.63	0.63
1:A:34:LEU:H	1:A:37:GLN:NE2	1.97	0.62
1:A:124:ILE:HA	1:A:127:GLN:CG	2.27	0.60
1:A:156:ASN:O	1:A:160:GLN:HG3	2.04	0.57
1:A:33:LYS:H	1:A:37:GLN:HE22	1.51	0.57
1:A:124:ILE:CA	1:A:127:GLN:HG2	2.25	0.57
1:A:53:LEU:HD22	1:A:58:ILE:HD11	1.86	0.56
1:A:18:ASN:HB3	1:A:238:TYR:CE2	2.41	0.55
1:A:55:ARG:HB2	1:A:271:TYR:OH	2.08	0.54
1:A:250:ASN:H	1:A:250:ASN:HD22	1.57	0.52
1:A:5:SER:HA	1:A:250:ASN:ND2	2.25	0.52
1:A:74:HIS:HE1	2:A:400:SAH:O	1.93	0.52
1:A:93:LEU:HD12	1:A:111:LEU:CD2	2.40	0.51
1:A:118:GLU:CG	1:A:166:ILE:HD11	2.40	0.51
1:A:255:ASN:ND2	1:A:257:GLU:H	2.08	0.50
1:A:198:GLN:OE1	1:A:209:ARG:HD3	2.11	0.50
1:A:255:ASN:HD21	1:A:257:GLU:CD	2.15	0.49
1:A:97:ARG:HD3	2:A:400:SAH:O3'	2.12	0.49
1:A:191:PRO:O	1:A:210:LEU:HD21	2.13	0.49
1:A:8:LYS:O	1:A:8:LYS:HD2	2.13	0.48
1:A:91:TRP:HB2	1:A:109:VAL:HB	1.95	0.48
1:A:74:HIS:CE1	2:A:400:SAH:O	2.67	0.48
1:A:33:LYS:HD2	1:A:34:LEU:HG	1.96	0.47
1:A:79:ARG:C	1:A:79:ARG:HD3	2.34	0.47
1:A:253:TYR:OH	1:A:287:GLN:NE2	2.45	0.47
1:A:189:TYR:HA	1:A:222:THR:O	2.15	0.46
1:A:265:PHE:O	1:A:268:ARG:HG2	2.17	0.45
1:A:18:ASN:HB3	1:A:238:TYR:CZ	2.51	0.45
1:A:19:GLU:HB2	1:A:234:LYS:CB	2.44	0.44
1:A:10:PHE:HE2	1:A:243:VAL:HG21	1.84	0.43
1:A:93:LEU:HD12	1:A:111:LEU:HD23	2.01	0.42
1:A:66:TYR:CD1	1:A:69:SER:HB3	2.53	0.42
1:A:52:LYS:HA	1:A:55:ARG:NH2	2.34	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:MET:O	1:A:208:MET:HB2	2.19	0.42
1:A:76:ARG:HD2	1:A:76:ARG:HA	1.92	0.42
1:A:208:MET:O	1:A:209:ARG:HD2	2.21	0.41
1:A:126:LYS:HE3	1:A:126:LYS:HB2	1.83	0.41
1:A:199:PRO:HD3	1:A:262:HIS:CE1	2.56	0.41

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	279/307 (91%)	274 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	261/282 (93%)	242 (93%)	19 (7%)	17	11

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	7	ASP
1	A	8	LYS
1	A	33	LYS
1	A	47	LEU
1	A	50	LEU
1	A	66	TYR
1	A	128	LEU
1	A	130	PRO
1	A	162	VAL
1	A	167	LEU
1	A	197	LEU
1	A	220	ARG
1	A	224	VAL
1	A	250	ASN
1	A	255	ASN
1	A	257	GLU
1	A	287	GLN
1	A	288	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	84	ASN
1	A	104	ASN
1	A	127	GLN
1	A	156	ASN
1	A	168	ASN
1	A	183	GLN
1	A	250	ASN
1	A	255	ASN
1	A	287	GLN
1	A	295	ASN

### 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](#)

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$
2	SAH	A	400	-	20,28,28	1.31	3 (15%)	19,40,40	1.86	3 (15%)

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	SAH	A	400	-	-	0/7/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	SAH	C8-N7	-2.83	1.29	1.34
2	A	400	SAH	C5-C4	-2.42	1.35	1.40
2	A	400	SAH	O3'-C3'	3.10	1.50	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	SAH	C4'-O4'-C1'	-5.21	104.00	109.72

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	400	SAH	N3-C2-N1	-4.10	125.75	128.89
2	A	400	SAH	C1'-N9-C4	-2.07	123.82	126.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	SAH	3	0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	285/307 (92%)	3.46	259 (90%) 0 0	9, 21, 50, 77	0

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	LEU	10.8
1	A	22	TYR	10.0
1	A	216	GLY	9.8
1	A	1	MET	8.8
1	A	24	PRO	8.3
1	A	31	ALA	8.0
1	A	18	ASN	7.5
1	A	3	VAL	7.0
1	A	215	THR	6.5
1	A	130	PRO	6.5
1	A	23	GLU	6.4
1	A	19	GLU	6.3
1	A	184	TRP	6.1
1	A	180	PHE	6.0
1	A	21	ASP	5.9
1	A	129	HIS	5.7
1	A	56	HIS	5.4
1	A	297	PRO	5.2
1	A	36	TYR	5.2
1	A	5	SER	5.1
1	A	34	LEU	5.1
1	A	128	LEU	5.0
1	A	32	LYS	4.9
1	A	6	LEU	4.9
1	A	75	ILE	4.9
1	A	47	LEU	4.8
1	A	218	ASN	4.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	296	ILE	4.8
1	A	127	GLN	4.8
1	A	48	PHE	4.7
1	A	181	PRO	4.7
1	A	141	SER	4.7
1	A	217	GLU	4.7
1	A	2	ASP	4.6
1	A	271	TYR	4.6
1	A	35	PRO	4.6
1	A	176	TRP	4.5
1	A	16	ILE	4.5
1	A	285	PHE	4.5
1	A	7	ASP	4.5
1	A	214	TYR	4.4
1	A	139	VAL	4.4
1	A	232	TYR	4.4
1	A	225	THR	4.3
1	A	103	LEU	4.3
1	A	78	LEU	4.3
1	A	66	TYR	4.3
1	A	131	SER	4.2
1	A	197	LEU	4.2
1	A	4	VAL	4.2
1	A	12	TYR	4.2
1	A	82	PHE	4.1
1	A	83	TYR	4.1
1	A	258	TYR	4.1
1	A	185	ILE	4.1
1	A	237	TYR	4.1
1	A	178	CYS	4.0
1	A	93	LEU	4.0
1	A	249	VAL	4.0
1	A	164	ILE	4.0
1	A	290	ILE	4.0
1	A	201	ALA	4.0
1	A	279	THR	4.0
1	A	67	ILE	4.0
1	A	9	PRO	3.9
1	A	44	LEU	3.9
1	A	115	PHE	3.9
1	A	247	VAL	3.9
1	A	120	TYR	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	220	ARG	3.9
1	A	55	ARG	3.9
1	A	118	GLU	3.9
1	A	111	LEU	3.8
1	A	148	PRO	3.8
1	A	284	LEU	3.8
1	A	219	MET	3.8
1	A	260	TYR	3.8
1	A	210	LEU	3.8
1	A	14	GLU	3.8
1	A	277	PRO	3.8
1	A	53	LEU	3.8
1	A	179	PRO	3.8
1	A	151	ALA	3.8
1	A	109	VAL	3.7
1	A	59	LEU	3.7
1	A	135	LEU	3.7
1	A	270	VAL	3.7
1	A	45	GLY	3.7
1	A	33	LYS	3.7
1	A	51	SER	3.7
1	A	190	ILE	3.7
1	A	49	PHE	3.7
1	A	291	PHE	3.7
1	A	77	TYR	3.7
1	A	102	ILE	3.7
1	A	123	SER	3.7
1	A	275	THR	3.7
1	A	293	PHE	3.6
1	A	42	LEU	3.6
1	A	43	LEU	3.6
1	A	276	PHE	3.6
1	A	89	ILE	3.6
1	A	136	ILE	3.6
1	A	238	TYR	3.6
1	A	253	TYR	3.6
1	A	13	PHE	3.6
1	A	121	LEU	3.6
1	A	124	ILE	3.6
1	A	98	HIS	3.6
1	A	70	ALA	3.6
1	A	159	LEU	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	91	TRP	3.6
1	A	200	PHE	3.6
1	A	199	PRO	3.6
1	A	264	TYR	3.5
1	A	174	LEU	3.5
1	A	157	TYR	3.5
1	A	10	PHE	3.5
1	A	183	GLN	3.5
1	A	206	ALA	3.5
1	A	211	LEU	3.5
1	A	213	ILE	3.5
1	A	68	GLY	3.5
1	A	194	ASN	3.5
1	A	191	PRO	3.5
1	A	166	ILE	3.5
1	A	243	VAL	3.5
1	A	272	CYS	3.5
1	A	170	VAL	3.4
1	A	188	PHE	3.4
1	A	64	VAL	3.4
1	A	153	LEU	3.4
1	A	69	SER	3.4
1	A	65	VAL	3.4
1	A	40	LEU	3.4
1	A	177	ARG	3.4
1	A	224	VAL	3.4
1	A	236	MET	3.4
1	A	114	ARG	3.4
1	A	86	GLY	3.4
1	A	150	THR	3.3
1	A	38	GLY	3.3
1	A	133	ILE	3.3
1	A	229	ALA	3.3
1	A	50	LEU	3.3
1	A	167	LEU	3.3
1	A	163	MET	3.3
1	A	196	MET	3.3
1	A	265	PHE	3.3
1	A	54	GLN	3.3
1	A	182	ASP	3.3
1	A	251	PHE	3.3
1	A	106	LEU	3.3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	208	MET	3.2
1	A	286	LEU	3.2
1	A	169	PRO	3.2
1	A	222	THR	3.2
1	A	239	LEU	3.2
1	A	263	MET	3.2
1	A	72	GLY	3.2
1	A	269	THR	3.2
1	A	117	ASP	3.2
1	A	242	ILE	3.2
1	A	74	HIS	3.2
1	A	189	TYR	3.2
1	A	112	VAL	3.2
1	A	161	ASN	3.1
1	A	116	VAL	3.1
1	A	221	LEU	3.1
1	A	254	PRO	3.1
1	A	134	ILE	3.1
1	A	294	LEU	3.1
1	A	193	GLY	3.1
1	A	17	ASP	3.1
1	A	252	ASP	3.1
1	A	287	GLN	3.0
1	A	274	LYS	3.0
1	A	104	ASN	3.0
1	A	231	ASN	3.0
1	A	92	MET	3.0
1	A	73	THR	3.0
1	A	110	THR	3.0
1	A	278	THR	3.0
1	A	283	VAL	3.0
1	A	266	MET	2.9
1	A	71	PRO	2.9
1	A	94	ILE	2.9
1	A	212	SER	2.9
1	A	204	TYR	2.9
1	A	261	PHE	2.9
1	A	234	LYS	2.9
1	A	273	ASN	2.9
1	A	173	SER	2.9
1	A	87	VAL	2.9
1	A	88	ILE	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	85	LEU	2.9
1	A	202	PRO	2.8
1	A	155	SER	2.8
1	A	268	ARG	2.8
1	A	81	HIS	2.8
1	A	246	LYS	2.8
1	A	113	THR	2.8
1	A	209	ARG	2.8
1	A	171	ALA	2.8
1	A	248	VAL	2.8
1	A	96	GLY	2.8
1	A	52	LYS	2.8
1	A	226	LYS	2.8
1	A	267	LEU	2.8
1	A	262	HIS	2.7
1	A	8	LYS	2.7
1	A	63	THR	2.7
1	A	99	HIS	2.7
1	A	58	ILE	2.7
1	A	138	ASP	2.7
1	A	255	ASN	2.7
1	A	119	GLU	2.7
1	A	80	ASP	2.6
1	A	192	HIS	2.6
1	A	240	ASN	2.6
1	A	137	SER	2.6
1	A	39	GLN	2.6
1	A	172	SER	2.6
1	A	230	VAL	2.6
1	A	158	ALA	2.6
1	A	97	ARG	2.6
1	A	160	GLN	2.6
1	A	288	GLN	2.5
1	A	122	ARG	2.5
1	A	162	VAL	2.5
1	A	233	ALA	2.5
1	A	292	ARG	2.5
1	A	101	PRO	2.5
1	A	107	ARG	2.5
1	A	149	SER	2.4
1	A	154	LEU	2.4
1	A	95	ASP	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	165	SER	2.3
1	A	259	ASP	2.3
1	A	289	SER	2.3
1	A	79	ARG	2.3
1	A	60	ASP	2.3
1	A	11	MET	2.3
1	A	126	LYS	2.3
1	A	105	GLY	2.2
1	A	203	SER	2.2
1	A	132	LYS	2.2
1	A	195	LYS	2.2
1	A	198	GLN	2.2
1	A	250	ASN	2.2
1	A	100	ASP	2.2
1	A	37	GLN	2.1
1	A	228	ASP	2.1
1	A	187	ASP	2.1
1	A	227	SER	2.1
1	A	62	ALA	2.1
1	A	168	ASN	2.1
1	A	46	GLU	2.1
1	A	186	LYS	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	SAH	A	400	26/26	0.84	0.29	-0.27	0,17,22,22	4

## 6.5 Other polymers [i](#)

There are no such residues in this entry.