



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 7PHY / pdb_00007phy
Title : Vaccinia virus E2
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Deposited on : 2021-08-19
Resolution : 2.30 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)
Xtrriage (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

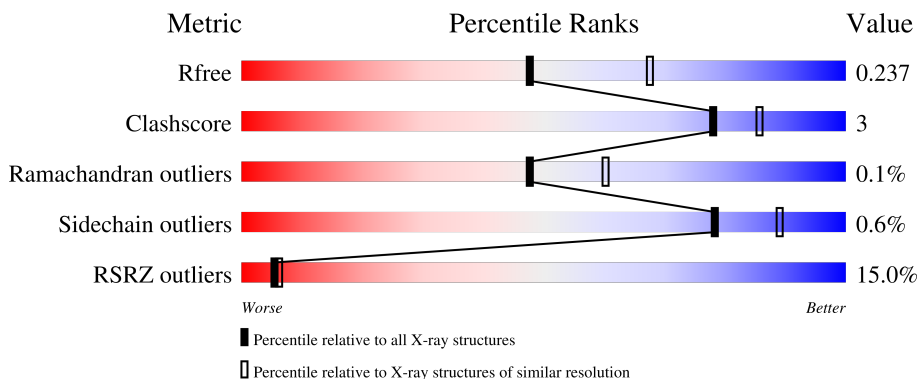
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	750	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6295 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 Protein E2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	732	6016	3893	961	1124	38	0	3	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	738	ALA	-	expression tag	UNP P21604
A	739	ALA	-	expression tag	UNP P21604
A	740	ALA	-	expression tag	UNP P21604
A	741	HIS	-	expression tag	UNP P21604
A	742	HIS	-	expression tag	UNP P21604
A	743	HIS	-	expression tag	UNP P21604
A	744	HIS	-	expression tag	UNP P21604
A	745	HIS	-	expression tag	UNP P21604
A	746	HIS	-	expression tag	UNP P21604
A	747	HIS	-	expression tag	UNP P21604
A	748	HIS	-	expression tag	UNP P21604
A	749	HIS	-	expression tag	UNP P21604
A	750	HIS	-	expression tag	UNP P21604

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

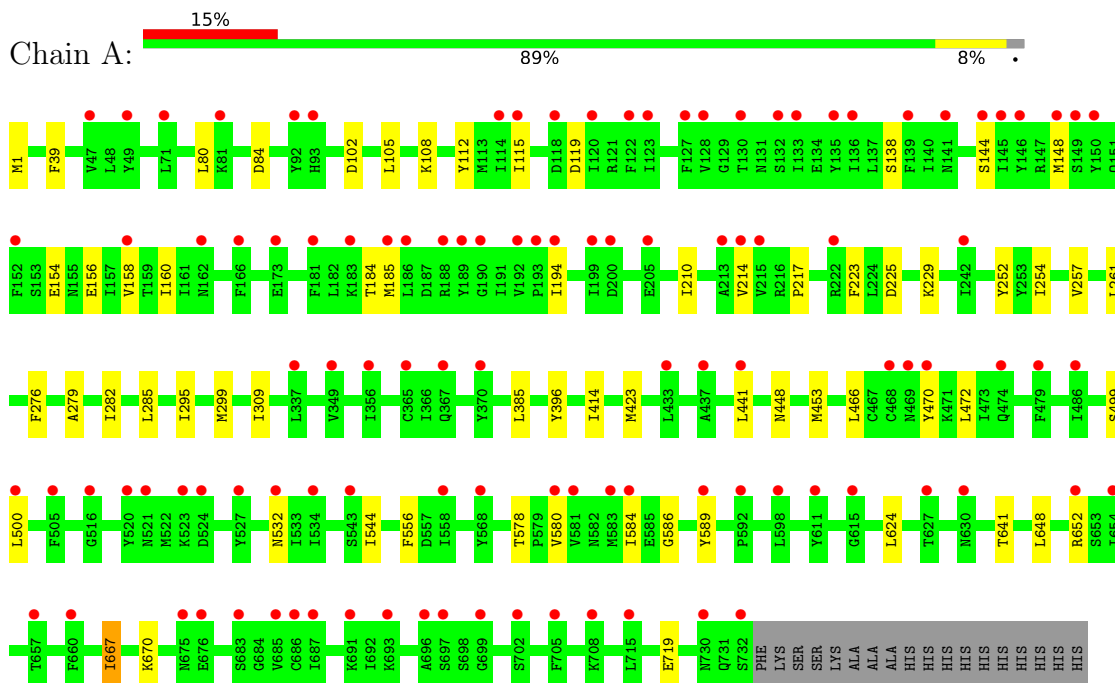
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	249	Total O 249 249	0	0

3 Residue-property plots

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: Protein E2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.17Å 90.92Å 147.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.52 – 2.30 35.52 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (35.52-2.30) 99.9 (35.52-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.192 , 0.237 0.193 , 0.237	Depositor DCC
R_{free} test set	2404 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	66.7	Xtrriage
Anisotropy	0.129	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6295	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: AME, 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	0.35	1/6135 (0.0%)	0.50	0/8313

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	ILE	CA-CB	5.56	1.57	1.54

There are no bond angle outliers.

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	6016	0	6104	34	0
2	A	30	0	40	1	0
3	A	249	0	0	2	0
All	All	6295	0	6144	34	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 3.

All (34) 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:194:ILE:HD12	1:A:223:PHE:HB2	1.72	0.70
1:A:138:SER:HA	1:A:160:ILE:HG12	1.75	0.66
1:A:225:ASP:OD1	1:A:229:LYS:NZ	2.38	0.57
1:A:556:PHE:HB2	1:A:667:ILE:HG23	1.86	0.57
1:A:282:ILE:HA	1:A:285:LEU:HD12	1.87	0.56
1:A:670:LYS:NZ	3:A:907:HOH:O	2.40	0.54
1:A:500:LEU:H	1:A:500:LEU:HD23	1.73	0.54
1:A:80:LEU:O	1:A:108:LYS:NZ	2.36	0.54
1:A:466:LEU:HB3	1:A:584:ILE:HG22	1.90	0.52
1:A:414:ILE:HD11	1:A:441:LEU:HD12	1.92	0.51
1:A:39:PHE:CE1	2:A:803:GOL:H12	2.46	0.50
1:A:144:SER:O	1:A:148:MET:HB2	2.12	0.49
1:A:257:VAL:HG22	1:A:261:LEU:HD12	1.95	0.49
1:A:448:ASN:HB3	1:A:453:MET:HG3	1.95	0.48
1:A:276:PHE:HB2	1:A:279:ALA:HB2	1.95	0.48
1:A:299:MET:HE1	1:A:309:ILE:HD13	1.95	0.48
1:A:210:ILE:O	1:A:214:VAL:HG13	2.14	0.47
1:A:589:TYR:OH	1:A:719:GLU:OE2	2.31	0.47
1:A:84:ASP:OD1	1:A:112:TYR:OH	2.28	0.45
1:A:295:ILE:HG13	1:A:299:MET:HE2	1.99	0.44
1:A:472:LEU:HD23	1:A:472:LEU:HA	1.83	0.44
1:A:115:ILE:HG23	1:A:119:ASP:HB2	2.00	0.44
1:A:102:ASP:HB3	1:A:105:LEU:HB3	1.99	0.43
1:A:156:GLU:O	1:A:160:ILE:HG13	2.18	0.43
1:A:154:GLU:O	1:A:158:VAL:HG23	2.18	0.43
1:A:544:ILE:HG23	3:A:1098:HOH:O	2.17	0.43
1:A:652:ARG:HD3	1:A:652:ARG:HA	1.72	0.43
1:A:423:MET:HE3	1:A:586:GLY:O	2.19	0.43
1:A:184:THR:HG22	1:A:185:MET:HE2	2.01	0.42
1:A:499:SER:HA	1:A:532:ASN:O	2.21	0.41
1:A:648:LEU:HD23	1:A:648:LEU:HA	1.82	0.41
1:A:217:PRO:HA	1:A:252:TYR:CD2	2.56	0.41
1:A:578:THR:HG21	1:A:624:LEU:HD21	2.02	0.40
1:A:396:TYR:CD1	1:A:396:TYR:C	2.99	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	733/750 (98%)	718 (98%)	14 (2%)	1 (0%)	48 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	470	TYR

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	693/705 (98%)	689 (99%)	4 (1%)	78 89

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

Mol	Chain	Res	Type
1	A	385	LEU
1	A	580	VAL
1	A	641	THR
1	A	667	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	492	ASN

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Mol	Chain	Res	Type
1	A	521	ASN
1	A	659	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](#)

1 non-standard protein/DNA/RNA residue 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
1	AME	A	1	1	9,10,11	1.54	1 (11%)	9,11,13	1.24	1 (11%)

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
1	AME	A	1	1	-	4/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	AME	CA-N	-3.75	1.41	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	AME	CT2-CT1-N	2.14	119.67	116.12

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	AME	CA-CB-CG-SD
1	A	1	AME	C-CA-N-CT1
1	A	1	AME	CB-CA-N-CT1
1	A	1	AME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are 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	GOL	A	805	-	5,5,5	1.06	0	5,5,5	1.29	1 (20%)
2	GOL	A	803	-	5,5,5	1.57	2 (40%)	5,5,5	0.81	0
2	GOL	A	802	-	5,5,5	0.94	0	5,5,5	1.22	0
2	GOL	A	804	-	5,5,5	0.95	0	5,5,5	0.95	0
2	GOL	A	801	-	5,5,5	1.08	0	5,5,5	1.08	1 (20%)

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	805	-	-	0/4/4/4	-
2	GOL	A	803	-	-	0/4/4/4	-
2	GOL	A	802	-	-	0/4/4/4	-
2	GOL	A	804	-	-	2/4/4/4	-
2	GOL	A	801	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	803	GOL	C1-C2	2.12	1.59	1.51
2	A	803	GOL	C3-C2	2.02	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	GOL	C3-C2-C1	-2.04	104.31	111.80
2	A	805	GOL	C3-C2-C1	-2.04	104.33	111.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	804	GOL	O1-C1-C2-C3
2	A	804	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	803	GOL	1	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, 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	731/750 (97%)	0.95	110 (15%) 5 6	41, 73, 108, 175	3 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	145	ILE	7.9
1	A	611	TYR	6.7
1	A	558	ILE	5.5
1	A	148	MET	5.5
1	A	687	ILE	5.4
1	A	589	TYR	5.4
1	A	470	TYR	5.2
1	A	615	GLY	5.1
1	A	500	LEU	4.9
1	A	158	VAL	4.8
1	A	194	ILE	4.8
1	A	468	CYS	4.5
1	A	676	GLU	4.4
1	A	71	LEU	4.2
1	A	186	LEU	4.2
1	A	122	PHE	4.1
1	A	215	VAL	4.0
1	A	193	PRO	3.9
1	A	144	SER	3.8
1	A	630	ASN	3.6
1	A	127	PHE	3.6
1	A	120	ILE	3.5
1	A	214	VAL	3.5
1	A	135	TYR	3.5
1	A	581	VAL	3.5
1	A	370	TYR	3.4
1	A	190	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	469	ASN	3.3
1	A	183	LYS	3.3
1	A	437	ALA	3.2
1	A	523	LYS	3.2
1	A	349	VAL	3.2
1	A	584	ILE	3.1
1	A	181	PHE	3.1
1	A	520	TYR	3.1
1	A	474	GLN	3.1
1	A	192	VAL	3.1
1	A	199	ILE	3.1
1	A	657	THR	3.1
1	A	693	LYS	3.0
1	A	486	ILE	3.0
1	A	654	ILE	3.0
1	A	222	ARG	3.0
1	A	705	PHE	2.9
1	A	185	MET	2.9
1	A	93	HIS	2.9
1	A	627	THR	2.9
1	A	141	ASN	2.9
1	A	516	GLY	2.8
1	A	188	ARG	2.8
1	A	441	LEU	2.8
1	A	47[A]	VAL	2.8
1	A	130	THR	2.8
1	A	685	VAL	2.8
1	A	532	ASN	2.8
1	A	133	ILE	2.7
1	A	189	TYR	2.7
1	A	132	SER	2.7
1	A	149	SER	2.7
1	A	49	TYR	2.7
1	A	123	ILE	2.7
1	A	433	LEU	2.7
1	A	527	TYR	2.7
1	A	652	ARG	2.7
1	A	479	PHE	2.6
1	A	580	VAL	2.6
1	A	115	ILE	2.6
1	A	337	LEU	2.6
1	A	715	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	114	ILE	2.5
1	A	150	TYR	2.5
1	A	128	VAL	2.4
1	A	173	GLU	2.4
1	A	683	SER	2.4
1	A	697	SER	2.4
1	A	732	SER	2.4
1	A	152	PHE	2.4
1	A	118	ASP	2.4
1	A	365	CYS	2.4
1	A	583	MET	2.4
1	A	598	LEU	2.4
1	A	696	ALA	2.4
1	A	702	SER	2.4
1	A	534	ILE	2.3
1	A	521	ASN	2.3
1	A	146	TYR	2.3
1	A	568	TYR	2.3
1	A	691	LYS	2.3
1	A	660	PHE	2.3
1	A	166	PHE	2.2
1	A	213	ALA	2.2
1	A	242	ILE	2.2
1	A	592	PRO	2.2
1	A	543	SER	2.2
1	A	730	ASN	2.2
1	A	699	GLY	2.2
1	A	205	GLU	2.2
1	A	162	ASN	2.2
1	A	524	ASP	2.2
1	A	81	LYS	2.2
1	A	367	GLN	2.2
1	A	686	CYS	2.2
1	A	200	ASP	2.1
1	A	505	PHE	2.1
1	A	92	TYR	2.1
1	A	356	ILE	2.1
1	A	139	PHE	2.1
1	A	675	ASN	2.0
1	A	136	ILE	2.0
1	A	708	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	AME	A	1	11/12	0.97	0.09	53,59,64,64	0

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(Å ²)	Q<0.9
2	GOL	A	804	6/6	0.58	0.21	87,93,108,108	0
2	GOL	A	805	6/6	0.82	0.18	91,94,96,105	0
2	GOL	A	803	6/6	0.87	0.14	75,76,80,83	0
2	GOL	A	801	6/6	0.91	0.23	116,116,117,117	0
2	GOL	A	802	6/6	0.92	0.15	89,91,93,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.