



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2024 – 08:23 pm BST

PDB ID : 1W81  
Title : Crystal structure of apical membrane antigen 1 from Plasmodium vivax  
Authors : Pizarro, J.C.; Vulliez-Le Normand, B.; Chesne-Seck, M.-L.; Kocken, C.H.M.; Thomas, A.W.; Bentley, G.A.  
Deposited on : 2004-09-15  
Resolution : 2.01 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

<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>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

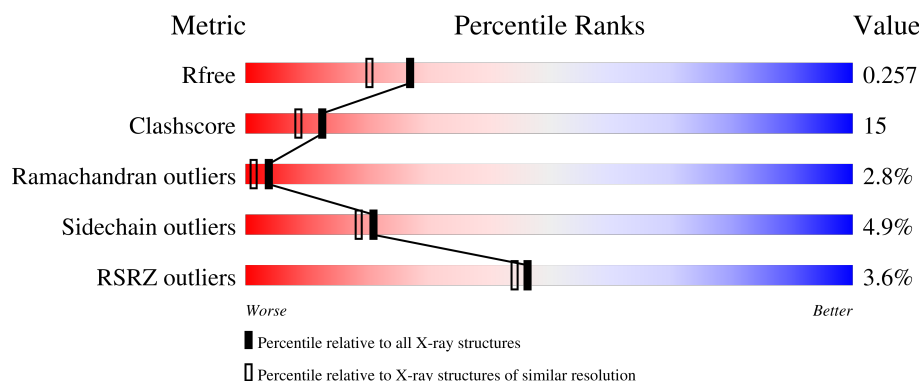
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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))
$R_{free}$	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	447	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3237 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.

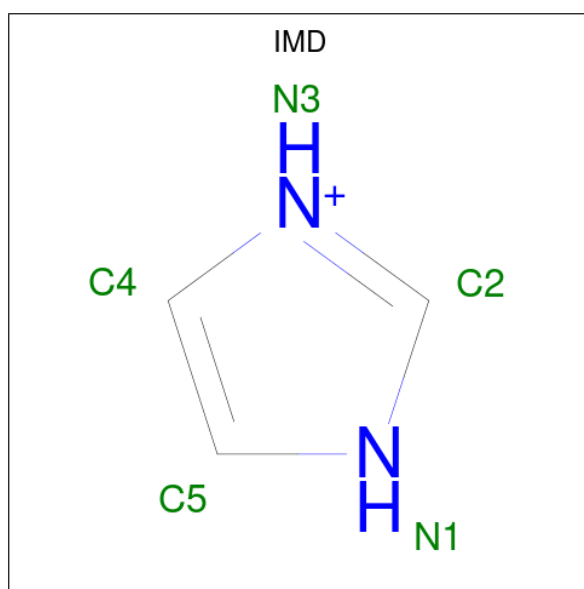
- Molecule 1 is a protein called APICAL MEMBRANE ANTIGEN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	364	2944	1845	514	563	22	0	2	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	SER	GLY	conflict	UNP Q9TY14
A	178	ASN	SER	engineered mutation	UNP Q9TY14
A	226	ASP	ASN	engineered mutation	UNP Q9TY14
A	441	GLN	ASN	engineered mutation	UNP Q9TY14
A	472	ASP	ASN	conflict	UNP Q9TY14

- Molecule 2 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
2	A	1	5	3	2	0	0

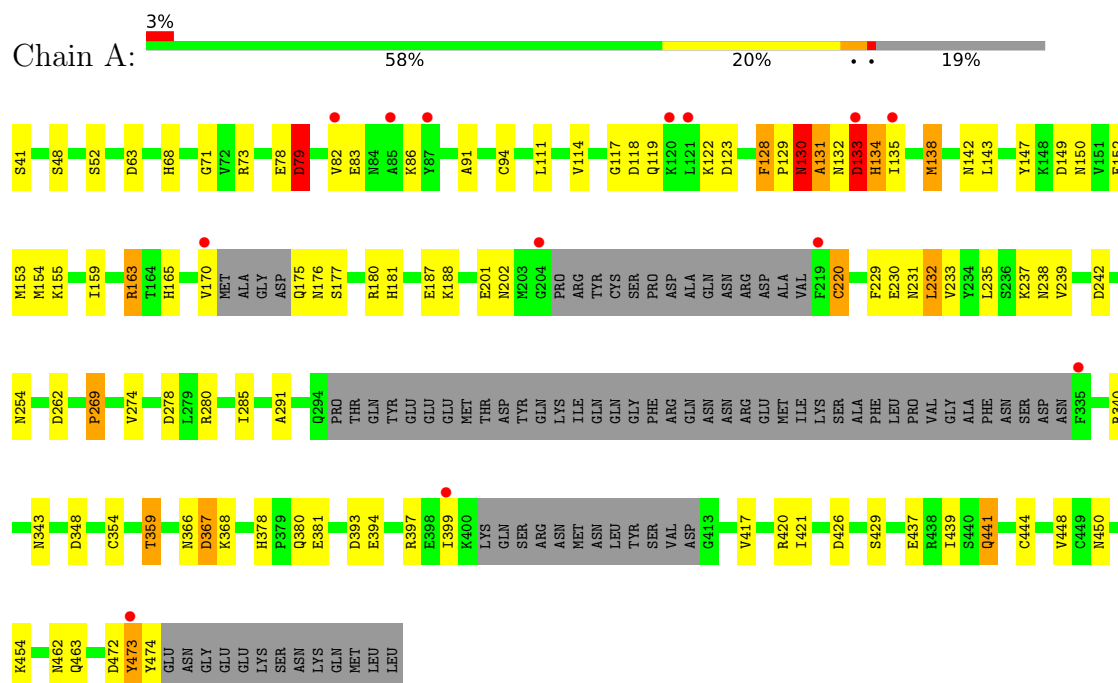
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	288	Total 288	O 288	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: APICAL MEMBRANE ANTIGEN 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.10Å 76.10Å 103.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.01 20.00 – 2.01	Depositor EDS
% Data completeness (in resolution range)	88.7 (20.00-2.01) 88.8 (20.00-2.01)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, $R_{free}$	0.194 , 0.259 0.193 , 0.257	Depositor DCC
$R_{free}$ test set	1345 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 35.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3237	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 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: IMD

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	0.83	1/3012 (0.0%)	0.95	16/4052 (0.4%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	SER	CB-OG	5.12	1.49	1.42

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79[A]	ASP	CB-CG-OD2	8.54	125.98	118.30
1	A	79[B]	ASP	CB-CG-OD2	8.54	125.98	118.30
1	A	348	ASP	CB-CG-OD2	7.43	124.99	118.30
1	A	393	ASP	CB-CG-OD2	6.87	124.49	118.30
1	A	63	ASP	CB-CG-OD2	6.45	124.10	118.30
1	A	278	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	340	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	123	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	149	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	133	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	262	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	242	ASP	CB-CG-OD2	5.27	123.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	420	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	472	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	367	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	163	ARG	NE-CZ-NH1	-5.08	117.76	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	LYS	Peptide
1	A	132	ASN	Peptide

## 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	2944	0	2849	87	0
2	A	5	0	5	0	0
3	A	288	0	0	16	0
All	All	3237	0	2854	87	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 15.

All (87) 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:187:GLU:CD	3:A:2125:HOH:O	1.92	1.04
1:A:130:ASN:HD22	1:A:131:ALA:H	0.97	0.93
1:A:359:THR:HB	3:A:2277:HOH:O	1.75	0.86
1:A:130:ASN:ND2	1:A:131:ALA:H	1.74	0.85
1:A:359:THR:HG21	1:A:462:ASN:HD22	1.40	0.85
1:A:147:TYR:OH	1:A:165:HIS:HD2	1.59	0.83
1:A:131:ALA:HB1	1:A:134:HIS:HE1	1.42	0.83
1:A:439:ILE:HD11	1:A:448:VAL:HG23	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASN:HD22	1:A:131:ALA:N	1.77	0.81
1:A:394:GLU:OE2	3:A:2236:HOH:O	1.98	0.81
1:A:152:GLU:O	1:A:155:LYS:HG2	1.83	0.78
1:A:177:SER:O	1:A:180:ARG:NH1	2.16	0.78
1:A:73:ARG:NH2	1:A:201:GLU:OE2	2.19	0.76
1:A:473:TYR:HB3	3:A:2286:HOH:O	1.85	0.75
1:A:188:LYS:HE2	3:A:2123:HOH:O	1.88	0.72
1:A:378:HIS:HD2	1:A:380:GLN:H	1.37	0.70
1:A:439:ILE:CD1	1:A:448:VAL:HG23	2.24	0.68
1:A:78:GLU:HB2	1:A:91:ALA:HB2	1.77	0.67
1:A:274:VAL:HG21	1:A:285:ILE:HG21	1.78	0.66
1:A:359:THR:CG2	1:A:462:ASN:HD22	2.08	0.66
1:A:170:VAL:HG11	1:A:175:GLN:HA	1.78	0.65
1:A:187:GLU:OE2	3:A:2125:HOH:O	2.07	0.65
1:A:473:TYR:HA	3:A:2287:HOH:O	1.97	0.65
1:A:439:ILE:HD11	1:A:448:VAL:CG2	2.27	0.64
1:A:73:ARG:HH22	1:A:201:GLU:CD	2.01	0.64
1:A:176:ASN:O	3:A:2119:HOH:O	2.15	0.64
1:A:359:THR:HG21	1:A:462:ASN:ND2	2.12	0.64
1:A:378:HIS:CD2	1:A:380:GLN:H	2.16	0.64
1:A:68:HIS:HE1	1:A:71:GLY:O	1.81	0.63
1:A:280[A]:ARG:NH2	3:A:2190:HOH:O	2.17	0.63
1:A:68:HIS:HD2	1:A:94:CYS:H	1.47	0.63
1:A:138:MET:HG2	1:A:143:LEU:HG	1.81	0.62
1:A:230:GLU:OE1	1:A:280[A]:ARG:NH1	2.25	0.61
1:A:291:ALA:H	1:A:343:ASN:HD21	1.48	0.59
1:A:133:ASP:O	1:A:134:HIS:ND1	2.34	0.58
1:A:187:GLU:OE1	3:A:2125:HOH:O	2.11	0.57
1:A:366:ASN:HD21	1:A:444:CYS:H	1.52	0.57
1:A:237:LYS:NZ	1:A:238:ASN:HD21	2.03	0.57
1:A:368:LYS:HG2	1:A:441:GLN:HG3	1.86	0.57
1:A:147:TYR:OH	1:A:165:HIS:CD2	2.51	0.56
1:A:473:TYR:O	1:A:474:TYR:HB2	2.07	0.54
1:A:437:GLU:HB2	3:A:2270:HOH:O	2.06	0.54
1:A:291:ALA:H	1:A:343:ASN:ND2	2.06	0.54
1:A:187:GLU:OE2	3:A:2126:HOH:O	2.18	0.53
1:A:231:ASN:ND2	3:A:2146:HOH:O	2.39	0.53
1:A:426:ASP:O	1:A:429:SER:OG	2.20	0.52
1:A:133:ASP:C	1:A:134:HIS:HD1	2.13	0.52
1:A:439:ILE:HD12	1:A:439:ILE:N	2.25	0.52
1:A:131:ALA:HB1	1:A:134:HIS:CE1	2.32	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ASP:O	1:A:135:ILE:N	2.38	0.51
1:A:131:ALA:CB	1:A:134:HIS:HE1	2.21	0.51
1:A:73:ARG:NH2	1:A:201:GLU:CD	2.64	0.51
1:A:68:HIS:CD2	1:A:94:CYS:H	2.29	0.50
1:A:473:TYR:O	1:A:474:TYR:CB	2.60	0.49
1:A:378:HIS:HD2	1:A:381:GLU:H	1.61	0.49
1:A:378:HIS:CD2	1:A:381:GLU:H	2.30	0.49
1:A:274:VAL:HG22	1:A:354:CYS:HB3	1.95	0.48
1:A:463:GLN:CD	3:A:2281:HOH:O	2.51	0.48
1:A:68:HIS:CD2	1:A:94:CYS:HB2	2.48	0.48
1:A:229:PHE:HA	1:A:232:LEU:HD22	1.96	0.48
1:A:367:ASP:OD2	1:A:441:GLN:HG2	2.15	0.47
1:A:114:VAL:HG12	1:A:129:PRO:HG3	1.95	0.47
1:A:150:ASN:HB3	1:A:153:MET:HB2	1.97	0.46
1:A:269:PRO:HD2	1:A:462:ASN:OD1	2.16	0.46
1:A:159:ILE:HG23	1:A:235:LEU:HD21	1.98	0.46
1:A:128:PHE:HE1	1:A:181:HIS:CD2	2.34	0.46
1:A:274:VAL:CG2	1:A:354:CYS:HB3	2.46	0.45
1:A:138:MET:HE2	1:A:138:MET:HB2	1.71	0.45
1:A:254:ASN:HD22	1:A:368:LYS:HA	1.80	0.44
1:A:274:VAL:CG2	1:A:285:ILE:HD13	2.48	0.44
1:A:450:ASN:HA	3:A:2269:HOH:O	2.16	0.44
1:A:128:PHE:CE1	1:A:181:HIS:CD2	3.06	0.44
1:A:394:GLU:HG2	1:A:421:ILE:HD11	2.00	0.44
1:A:138:MET:HG3	1:A:142:ASN:HB2	1.98	0.44
1:A:135:ILE:O	1:A:165:HIS:HE1	2.01	0.43
1:A:163:ARG:HG3	1:A:239:VAL:HB	1.99	0.43
1:A:237:LYS:HZ1	1:A:238:ASN:HD21	1.64	0.43
1:A:128:PHE:HA	1:A:129:PRO:HD3	1.83	0.43
1:A:170:VAL:HG11	1:A:175:GLN:CA	2.46	0.43
1:A:48:SER:HB2	1:A:417:VAL:HG12	2.01	0.42
1:A:68:HIS:HD2	1:A:94:CYS:HB2	1.84	0.42
1:A:274:VAL:HG21	1:A:285:ILE:HD13	2.03	0.41
1:A:202:ASN:O	1:A:220:CYS:HA	2.20	0.41
1:A:439:ILE:CD1	1:A:439:ILE:N	2.83	0.41
1:A:82:VAL:HG12	1:A:82:VAL:O	2.20	0.40
1:A:378:HIS:HE1	3:A:2146:HOH:O	2.03	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	356/447 (80%)	333 (94%)	13 (4%)	10 (3%)	<b>4</b> <b>1</b>

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	A	134	HIS
1	A	220	CYS
1	A	83	GLU
1	A	119	GLN
1	A	399	ILE
1	A	473	TYR
1	A	131	ALA
1	A	133	ASP
1	A	117	GLY

### 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	328/401 (82%)	311 (95%)	17 (5%)	<b>19</b> <b>17</b>

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

Mol	Chain	Res	Type
1	A	41	SER

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Mol	Chain	Res	Type
1	A	79[A]	ASP
1	A	79[B]	ASP
1	A	86	LYS
1	A	111	LEU
1	A	118	ASP
1	A	128	PHE
1	A	130	ASN
1	A	138	MET
1	A	154	MET
1	A	232	LEU
1	A	233	VAL
1	A	269	PRO
1	A	359	THR
1	A	397	ARG
1	A	441	GLN
1	A	454	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	130	ASN
1	A	132	ASN
1	A	165	HIS
1	A	181	HIS
1	A	238	ASN
1	A	241	ASN
1	A	251	ASN
1	A	254	ASN
1	A	264	ASN
1	A	343	ASN
1	A	366	ASN
1	A	378	HIS

### 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 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	$\# Z  > 2$
2	IMD	A	1475	-	3,5,5	0.64	0	4,5,5	0.50	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	IMD	A	1475	-	-	-	0/1/1/1

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 [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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	364/447 (81%)	-0.17	13 (3%) 46 44	17, 33, 72, 99	2 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	335	PHE	4.8
1	A	135	ILE	4.0
1	A	121	LEU	4.0
1	A	170	VAL	3.6
1	A	82	VAL	3.5
1	A	204	GLY	3.1
1	A	219	PHE	3.0
1	A	120	LYS	2.7
1	A	473	TYR	2.5
1	A	85	ALA	2.4
1	A	399	ILE	2.3
1	A	87	TYR	2.1
1	A	133	ASP	2.1

### 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

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<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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	IMD	A	1475	5/5	0.95	0.09	21,23,26,28	0

## 6.5 Other polymers

There are no such residues in this entry.