



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:45 PM GMT

PDB ID : 4Z35  
Title : Crystal Structure of Human Lysophosphatidic Acid Receptor 1 in complex with ONO-9910539  
Authors : Chrencik, J.E.; Roth, C.B.; Terakado, M.; Kurata, H.; Omi, R.; Kihara, Y.; Warshaviak, D.; Nakade, S.; Asmar-Rovira, G.; Mileni, M.; Mizuno, H.; Griffith, M.T.; Rodgers, C.; Han, G.W.; Velasquez, J.; Chun, J.; Stevens, R.C.; Hanson, M.A.; GPCR Network (GPCR)  
Deposited on : 2015-03-30  
Resolution : 2.90 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.

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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 : 1.7 (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

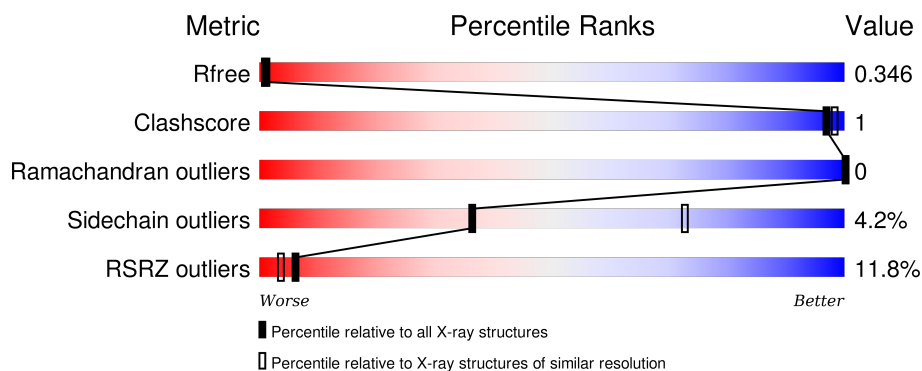
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	464	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3039 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 Lysophosphatidic acid receptor 1, Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			2977	1938	487	526	26			

There are 59 discrepancies between the modelled and reference sequences:

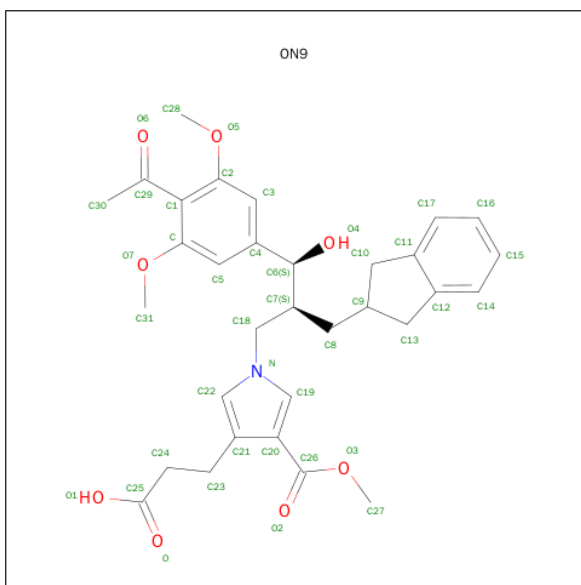
Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP Q92633
A	-16	LYS	-	expression tag	UNP Q92633
A	-15	THR	-	expression tag	UNP Q92633
A	-14	ILE	-	expression tag	UNP Q92633
A	-13	ILE	-	expression tag	UNP Q92633
A	-12	ALA	-	expression tag	UNP Q92633
A	-11	LEU	-	expression tag	UNP Q92633
A	-10	SER	-	expression tag	UNP Q92633
A	-9	TYR	-	expression tag	UNP Q92633
A	-8	ILE	-	expression tag	UNP Q92633
A	-7	PHE	-	expression tag	UNP Q92633
A	-6	CYS	-	expression tag	UNP Q92633
A	-5	LEU	-	expression tag	UNP Q92633
A	-4	VAL	-	expression tag	UNP Q92633
A	-3	PHE	-	expression tag	UNP Q92633
A	-2	ALA	-	expression tag	UNP Q92633
A	-1	GLY	-	expression tag	UNP Q92633
A	0	ALA	-	expression tag	UNP Q92633
A	1	PRO	-	expression tag	UNP Q92633
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1043	ALA	-	linker	UNP P0ABE7
A	1044	THR	-	linker	UNP P0ABE7
A	1045	PRO	-	linker	UNP P0ABE7
A	1046	PRO	-	linker	UNP P0ABE7
A	1047	LYS	-	linker	UNP P0ABE7
A	1048	LEU	-	linker	UNP P0ABE7
A	1049	GLU	-	linker	UNP P0ABE7

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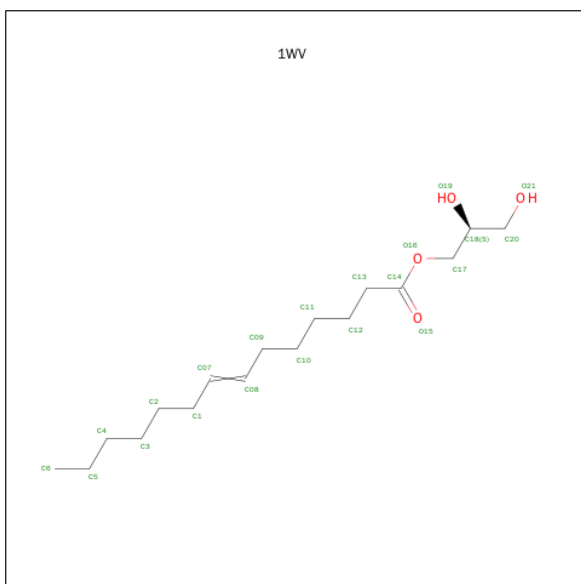
Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	ASP	-	linker	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	-	linker	UNP P0ABE7
A	327	GLY	-	expression tag	UNP Q92633
A	328	ARG	-	expression tag	UNP Q92633
A	329	PRO	-	expression tag	UNP Q92633
A	330	LEU	-	expression tag	UNP Q92633
A	331	GLU	-	expression tag	UNP Q92633
A	332	VAL	-	expression tag	UNP Q92633
A	333	LEU	-	expression tag	UNP Q92633
A	334	PHE	-	expression tag	UNP Q92633
A	335	GLN	-	expression tag	UNP Q92633
A	336	GLY	-	expression tag	UNP Q92633
A	337	PRO	-	expression tag	UNP Q92633
A	338	HIS	-	expression tag	UNP Q92633
A	339	HIS	-	expression tag	UNP Q92633
A	340	HIS	-	expression tag	UNP Q92633
A	341	HIS	-	expression tag	UNP Q92633
A	342	HIS	-	expression tag	UNP Q92633
A	343	HIS	-	expression tag	UNP Q92633
A	344	HIS	-	expression tag	UNP Q92633
A	345	HIS	-	expression tag	UNP Q92633
A	346	HIS	-	expression tag	UNP Q92633
A	347	HIS	-	expression tag	UNP Q92633
A	348	ASP	-	expression tag	UNP Q92633
A	349	TYR	-	expression tag	UNP Q92633
A	350	LYS	-	expression tag	UNP Q92633
A	351	ASP	-	expression tag	UNP Q92633
A	352	ASP	-	expression tag	UNP Q92633
A	353	ASP	-	expression tag	UNP Q92633
A	354	ASP	-	expression tag	UNP Q92633
A	355	LYS	-	expression tag	UNP Q92633

- Molecule 2 is 3-{1-[(2S,3S)-3-(4-acetyl-3,5-dimethoxyphenyl)-2-(2,3-dihydro-1H-inden-2-yl methyl)-3-hydroxypropyl]-4-(methoxycarbonyl)-1H-pyrrol-3-yl}propanoic acid (three-letter code: ON9) (formula: C<sub>32</sub>H<sub>37</sub>NO<sub>8</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			41	32	1	8		

- Molecule 3 is (2S)-2,3-dihydroxypropyl (7Z)-tetradec-7-enoate (three-letter code: 1WV) (formula: C<sub>17</sub>H<sub>32</sub>O<sub>4</sub>).



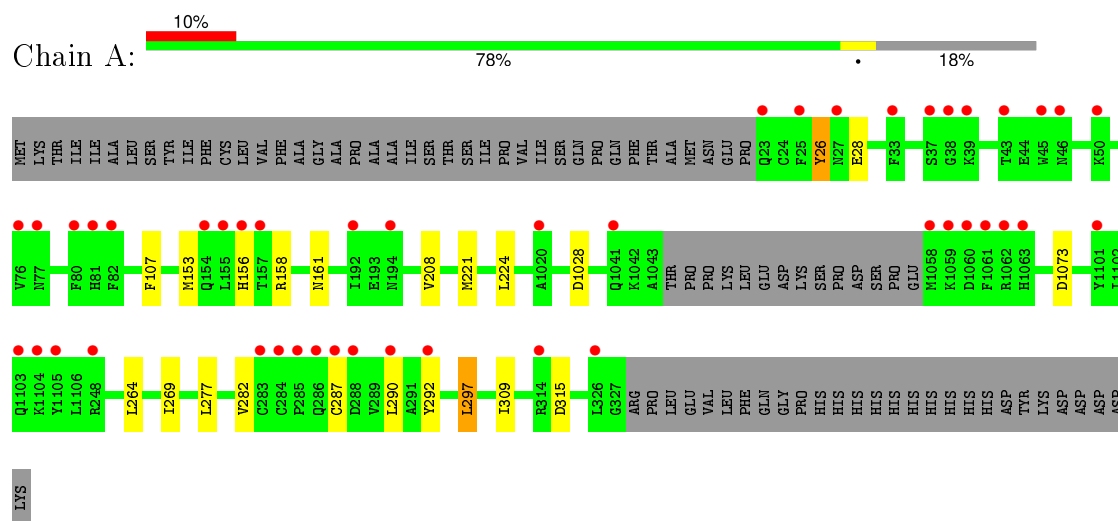
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			18	14	4		

- Molecule 4 is water.

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



- Molecule 1: Lysophosphatidic acid receptor 1, Soluble cytochrome b562



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	34.61Å 112.40Å 155.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.47 – 2.90	Depositor EDS
% Data completeness (in resolution range)	81.9 (30.00-2.90) 81.9 (29.47-2.90)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 2.90Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.265 , 0.279 0.321 , 0.346	Depositor DCC
$R_{free}$ test set	584 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.0	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 61.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 11627 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	3039	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.18% 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, 0.375 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: 1WV, ON9

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	0.45	0/3039	0.56	0/4134

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	2977	0	2967	8	0
2	A	41	0	36	2	0
3	A	18	0	23	0	0
4	A	3	0	0	0	0
All	All	3039	0	3026	8	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 1.

All (8) 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:297:LEU:HG	2:A:2001:ON9:H12	1.83	0.60
1:A:158:ARG:HA	1:A:161:ASN:HD22	1.71	0.56
1:A:208:VAL:HG23	1:A:282:VAL:HG21	1.88	0.56
1:A:297:LEU:HD23	2:A:2001:ON9:H22	1.92	0.51
1:A:26:TYR:HB3	1:A:28:GLU:HG2	1.96	0.47
1:A:208:VAL:CG2	1:A:282:VAL:HG21	2.44	0.47
1:A:221:MET:HA	1:A:224:LEU:HD12	2.02	0.42
1:A:277:LEU:HG	1:A:290:LEU:HD23	2.02	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	378/464 (82%)	366 (97%)	12 (3%)	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	312/400 (78%)	299 (96%)	13 (4%)	36	73

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	TYR
1	A	107	PHE
1	A	153	MET
1	A	156	HIS
1	A	1028	ASP
1	A	1073	ASP
1	A	264	LEU
1	A	269	ILE
1	A	287	CYS
1	A	292	TYR
1	A	297	LEU
1	A	309	ILE
1	A	315	ASP

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

Mol	Chain	Res	Type
1	A	161	ASN
1	A	1013	ASN
1	A	1080	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

2 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	ON9	A	2001	-	38,44,44	1.51	5 (13%)	47,62,62	2.05	8 (17%)
3	1WV	A	2002	-	17,17,20	1.33	1 (5%)	17,18,21	0.92	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	ON9	A	2001	-	-	0/33/43/43	0/4/4/4
3	1WV	A	2002	-	-	0/17/17/20	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	ON9	C1-C	2.01	1.44	1.40
2	A	2001	ON9	O5-C2	2.23	1.40	1.37
2	A	2001	ON9	O3-C26	2.97	1.40	1.33
2	A	2001	ON9	C20-C21	3.92	1.44	1.39
3	A	2002	1WV	C07-C08	4.02	1.54	1.31
2	A	2001	ON9	C7-C6	4.22	1.59	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	ON9	O3-C26-O2	-6.14	110.67	123.44
2	A	2001	ON9	O5-C2-C3	-2.88	119.28	124.21
2	A	2001	ON9	O7-C-C5	-2.67	119.65	124.21
2	A	2001	ON9	C8-C9-C13	-2.58	107.50	115.43
2	A	2001	ON9	C5-C4-C6	2.16	123.20	119.60
2	A	2001	ON9	O5-C2-C1	2.66	119.91	115.78
2	A	2001	ON9	C27-O3-C26	4.59	125.27	115.84
2	A	2001	ON9	O3-C26-C20	8.63	126.87	112.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	ON9	2	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	382/464 (82%)	0.65	45 (11%) 6 4	59, 97, 135, 159	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1063	HIS	8.9
1	A	287	CYS	6.2
1	A	156	HIS	6.1
1	A	286	GLN	5.6
1	A	1103	GLN	5.1
1	A	285	PRO	4.5
1	A	38	GLY	4.4
1	A	154	GLN	3.9
1	A	288	ASP	3.5
1	A	1058	MET	3.4
1	A	1061	PHE	3.3
1	A	1059	LYS	3.3
1	A	1062	ARG	3.2
1	A	326	LEU	3.2
1	A	157	THR	3.1
1	A	283	CYS	3.0
1	A	37	SER	3.0
1	A	1060	ASP	2.9
1	A	23	GLN	2.8
1	A	1101	TYR	2.8
1	A	284	CYS	2.8
1	A	155	LEU	2.7
1	A	314	ARG	2.6
1	A	39	LYS	2.6
1	A	81	HIS	2.6
1	A	76	VAL	2.6
1	A	1020	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	248	ARG	2.6
1	A	43	THR	2.5
1	A	1041	GLN	2.5
1	A	27	ASN	2.5
1	A	82	PHE	2.5
1	A	290	LEU	2.5
1	A	45	TRP	2.5
1	A	77	ASN	2.4
1	A	292	TYR	2.4
1	A	46	ASN	2.4
1	A	25	PHE	2.3
1	A	33	PHE	2.2
1	A	194	ASN	2.2
1	A	50	LYS	2.1
1	A	1105	TYR	2.1
1	A	1104	LYS	2.1
1	A	80	PHE	2.0
1	A	192	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<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(Å <sup>2</sup> )	Q<0.9
2	ON9	A	2001	41/41	0.88	0.29	0.58	56,70,84,87	0
3	1WV	A	2002	18/21	0.82	0.26	0.46	84,87,92,92	0

## 6.5 Other polymers

There are no such residues in this entry.