Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:46 PM GMT

PDB ID	:	4Z36
Title	:	Crystal Structure of Human Lysophosphatidic Acid Receptor 1 in complex with ONO-3080573
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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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

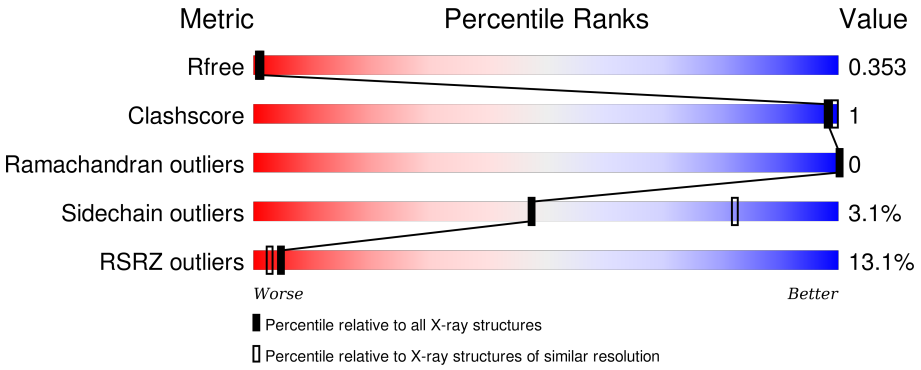
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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 >=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 <=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	459	11% 79% 17%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3073 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
			3014	1963	497	526	28			

There are 61 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	204	CYS	ASP	engineered mutation	UNP Q92633
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1043	GLY	-	linker	UNP P0ABE7
A	1049	GLY	-	linker	UNP P0ABE7
A	1050	SER	-	linker	UNP P0ABE7
A	1051	GLY	-	linker	UNP P0ABE7
A	1052	GLY	-	linker	UNP P0ABE7
A	1053	SER	-	linker	UNP P0ABE7

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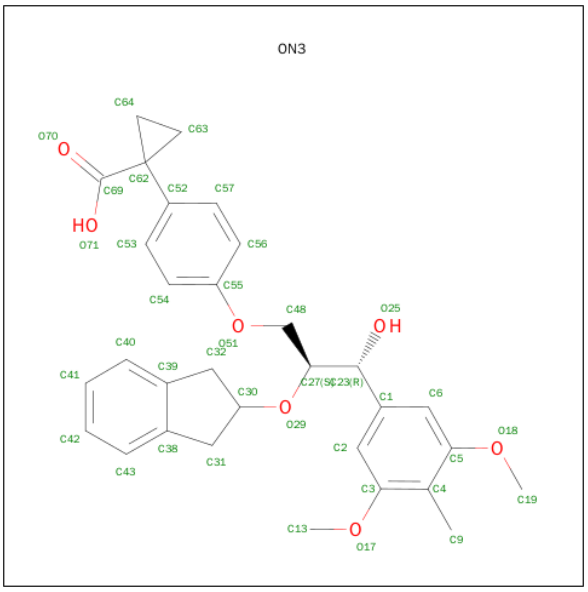
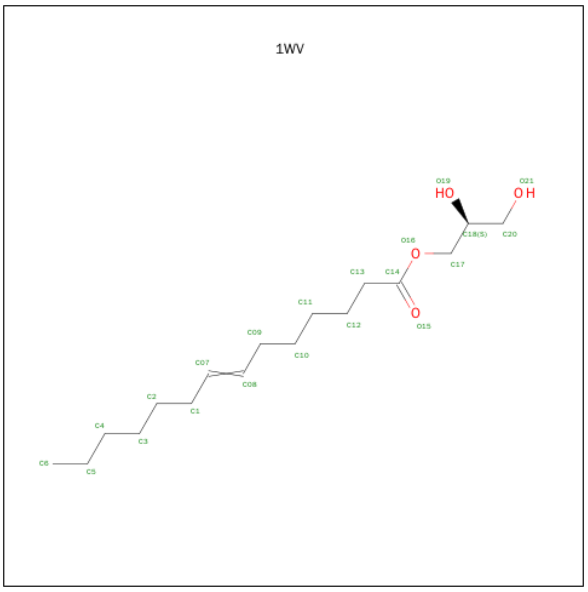
Chain	Residue	Modelled	Actual	Comment	Reference
A	1054	ASP	-	linker	UNP P0ABE7
A	1055	SER	-	linker	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	-	linker	UNP P0ABE7
A	282	CYS	VAL	conflict	UNP Q92633
A	327	GLY	-	expression tag	UNP Q92633
A	328	ARG	-	expression tag	UNP Q92633
A	329	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 1-(4-{[(2S,3R)-2-(2,3-dihydro-1H-inden-2-yloxy)-3-(3,5-dimethoxy-4-methylphenyl)-3-hydroxypropyl]oxy}phenyl)cyclopropanecarboxylic acid (three-letter code: ON3) (formula: $C_{31}H_{34}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 38 31 7	0	0

- Molecule 3 is (2S)-2,3-dihydroxypropyl (7Z)-tetradec-7-enoate (three-letter code: 1WV) (formula: $C_{17}H_{32}O_4$).



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

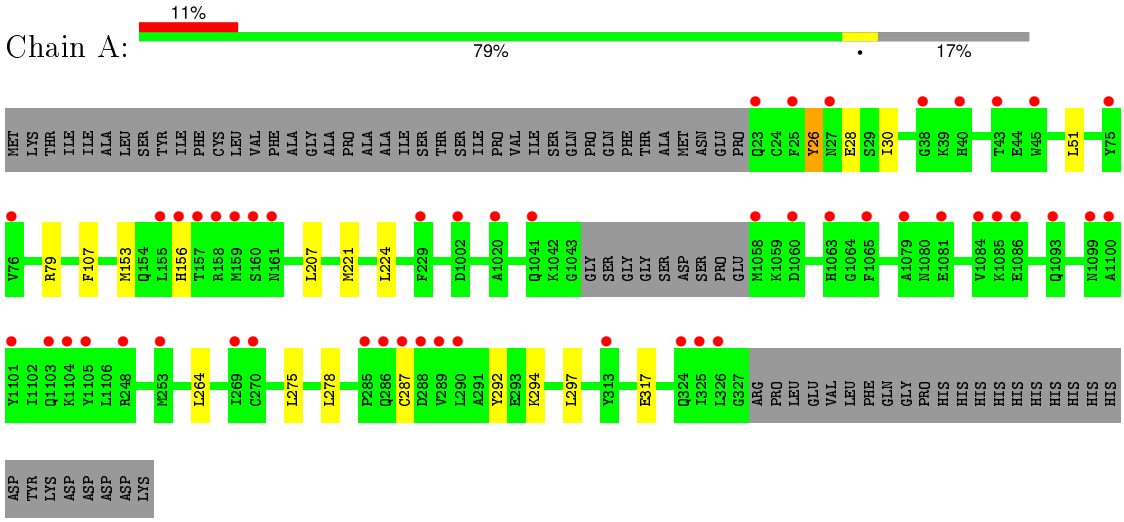
- Molecule 4 is water.

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

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 (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: Lysophosphatidic acid receptor 1,Soluble cytochrome b562



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	34.35Å 111.93Å 153.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.28 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.1 (30.00-2.90) 91.1 (29.28-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.90Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.272 , 0.292 0.324 , 0.353	Depositor DCC
R_{free} test set	625 reflections (5.19%)	DCC
Wilson B-factor (Å^2)	74.0	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 37.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 12660 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	3073	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ON3, 1WV

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	0.44	0/3077	0.53	0/4178

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	3014	0	3042	6	0
2	A	38	0	33	1	0
3	A	18	0	23	0	0
4	A	3	0	0	0	0
All	All	3073	0	3098	6	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 (6) 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:294:LYS:HA	2:A:2000:ON3:H26	1.88	0.54
1:A:26:TYR:HB3	1:A:28:GLU:HG2	1.97	0.46
1:A:221:MET:HA	1:A:224:LEU:HD12	2.00	0.43
1:A:275:LEU:HA	1:A:278:LEU:HD12	2.01	0.43
1:A:207:LEU:HD22	1:A:278:LEU:HD22	2.02	0.42
1:A:79:ARG:HE	1:A:317:GLU:HG2	1.86	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	378/459 (82%)	368 (97%)	10 (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	321/392 (82%)	311 (97%)	10 (3%)	47 82

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	TYR

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Mol	Chain	Res	Type
1	A	30	ILE
1	A	51	LEU
1	A	107	PHE
1	A	153	MET
1	A	156	HIS
1	A	264	LEU
1	A	287	CYS
1	A	292	TYR
1	A	297	LEU

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

Mol	Chain	Res	Type
1	A	1006	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	ON3	A	2000	-	38,42,42	1.86	9 (23%)	50,61,61	1.10	4 (8%)
3	1WV	A	2001	-	17,17,20	1.31	1 (5%)	17,18,21	0.98	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	ON3	A	2000	-	-	0/27/45/45	0/4/5/5
3	1WV	A	2001	-	-	0/17/17/20	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2000	ON3	C62-C52	-3.39	1.49	1.54
2	A	2000	ON3	C2-C3	2.10	1.42	1.38
2	A	2000	ON3	C56-C55	2.20	1.43	1.38
2	A	2000	ON3	C57-C52	2.31	1.42	1.39
2	A	2000	ON3	O17-C3	2.70	1.41	1.37
2	A	2000	ON3	C3-C4	2.73	1.43	1.40
2	A	2000	ON3	C62-C69	3.24	1.56	1.50
2	A	2000	ON3	C5-C4	3.35	1.44	1.40
3	A	2001	1WV	C07-C08	3.96	1.54	1.31
2	A	2000	ON3	C27-C23	5.60	1.57	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2000	ON3	O17-C3-C2	-2.06	120.69	124.21
2	A	2000	ON3	C1-C23-C27	2.17	115.64	112.57
2	A	2000	ON3	C6-C1-C23	2.20	123.26	119.60
2	A	2000	ON3	O17-C3-C4	3.20	117.67	115.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2000	ON3	1	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, 95^{th} 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	382/459 (83%)	0.81	50 (13%) 5 3	50, 92, 143, 172	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	287	CYS	8.1
1	A	1063	HIS	7.3
1	A	157	THR	6.9
1	A	1105	TYR	6.1
1	A	156	HIS	6.0
1	A	1103	GLN	5.1
1	A	288	ASP	5.0
1	A	1060	ASP	5.0
1	A	27	ASN	4.8
1	A	158	ARG	4.4
1	A	1081	GLU	4.4
1	A	23	GLN	4.4
1	A	286	GLN	4.2
1	A	1020	ALA	4.1
1	A	289	VAL	4.0
1	A	45	TRP	3.9
1	A	159	MET	3.8
1	A	155	LEU	3.5
1	A	1002	ASP	3.5
1	A	248	ARG	3.4
1	A	1065	PHE	3.4
1	A	1041	GLN	3.4
1	A	324	GLN	3.4
1	A	1104	LYS	3.3
1	A	1100	ALA	3.2
1	A	40	HIS	3.2
1	A	1101	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1058	MET	3.0
1	A	161	ASN	3.0
1	A	1084	VAL	2.7
1	A	25	PHE	2.7
1	A	253	MET	2.7
1	A	229	PHE	2.6
1	A	285	PRO	2.6
1	A	1099	ASN	2.5
1	A	1085	LYS	2.5
1	A	38	GLY	2.4
1	A	76	VAL	2.4
1	A	75	TYR	2.4
1	A	269	ILE	2.3
1	A	43	THR	2.3
1	A	270	CYS	2.2
1	A	326	LEU	2.2
1	A	1093	GLN	2.1
1	A	1079	ALA	2.1
1	A	160	SER	2.1
1	A	290	LEU	2.1
1	A	313	TYR	2.1
1	A	325	ILE	2.0
1	A	1086	GLU	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^{th} 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^2)	Q<0.9
3	1WV	A	2001	18/21	0.87	0.27	0.85	62,63,64,65	0
2	ON3	A	2000	38/38	0.86	0.28	0.80	59,63,69,69	0

6.5 Other polymers (i)

There are no such residues in this entry.