



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 07:53 am BST

PDB ID : 2C8M  
Title : Structure of protein Ta0514, putative lipoate protein ligase from *T. acidophilum* with bound lipoic acid  
Authors : McManus, E.; Perham, R.N.; Luisi, B.F.  
Deposited on : 2005-12-06  
Resolution : 1.89 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

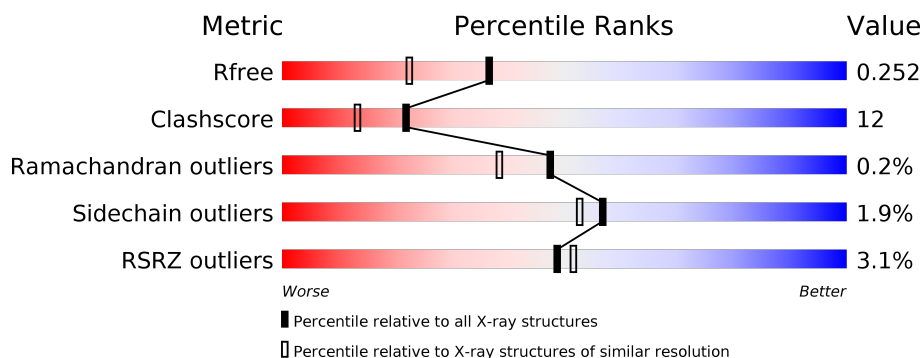
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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	262	<div> <div></div> <div>73%18%8%</div> </div>
1	B	262	<div> <div></div> <div>73%18%6%</div> </div>
1	C	262	<div> <div>5%</div> <div>67%24%6%</div> </div>
1	D	262	<div> <div>5%</div> <div>68%22%8%</div> </div>

## 2 Entry composition [i](#)

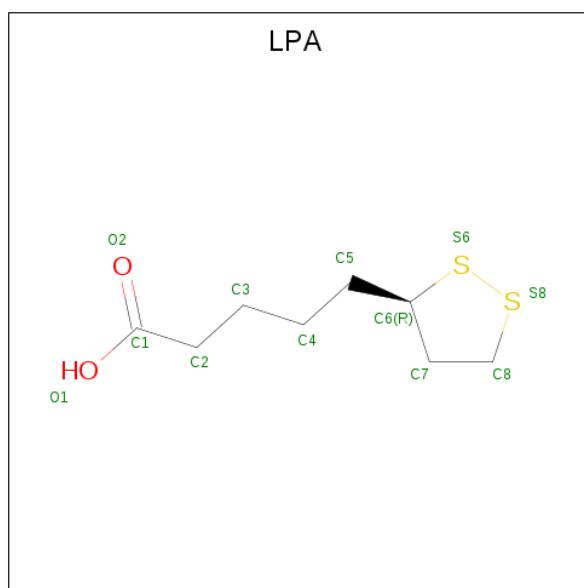
There are 3 unique types of molecules in this entry. The entry contains 8042 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LIPOATE-PROTEIN LIGASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	46	0	0
			1886	1185	322	366	13			
1	B	245	Total	C	N	O	S	54	0	0
			1920	1204	332	371	13			
1	C	245	Total	C	N	O	S	73	0	0
			1882	1182	325	363	12			
1	D	241	Total	C	N	O	S	99	0	0
			1822	1145	310	355	12			

- Molecule 2 is LIPOIC ACID (three-letter code: LPA) (formula: C<sub>8</sub>H<sub>14</sub>O<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			12	8	2	2		
2	B	1	Total	C	O	S	0	0
			12	8	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	S	0	0
			12	8	2	2		
2	D	1	Total	C	O	S	0	0
			12	8	2	2		

- Molecule 3 is water.

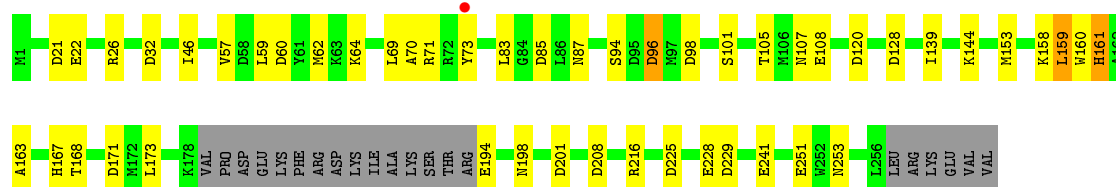
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	191	Total	O	0	0
			191	191		
3	B	162	Total	O	0	0
			162	162		
3	C	65	Total	O	0	0
			65	65		
3	D	66	Total	O	0	0
			66	66		

### 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 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.

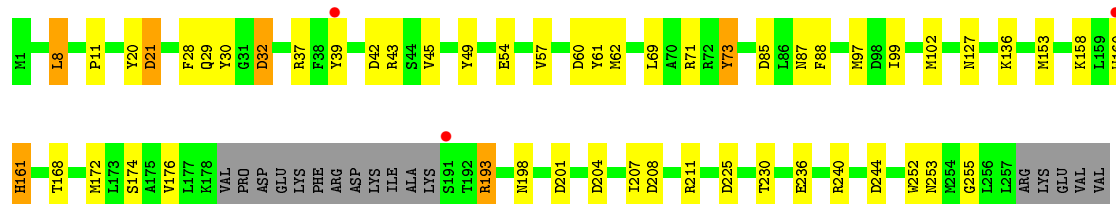
#### • Molecule 1: LIPOATE-PROTEIN LIGASE A

Chain A:



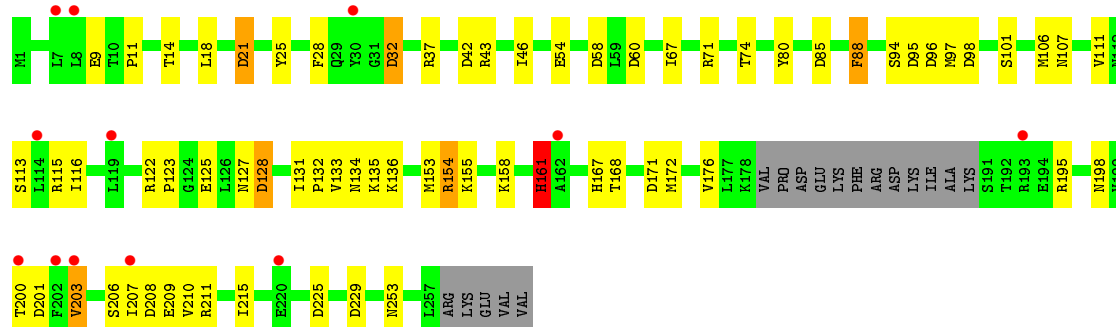
#### • Molecule 1: LIPOATE-PROTEIN LIGASE A

Chain B:



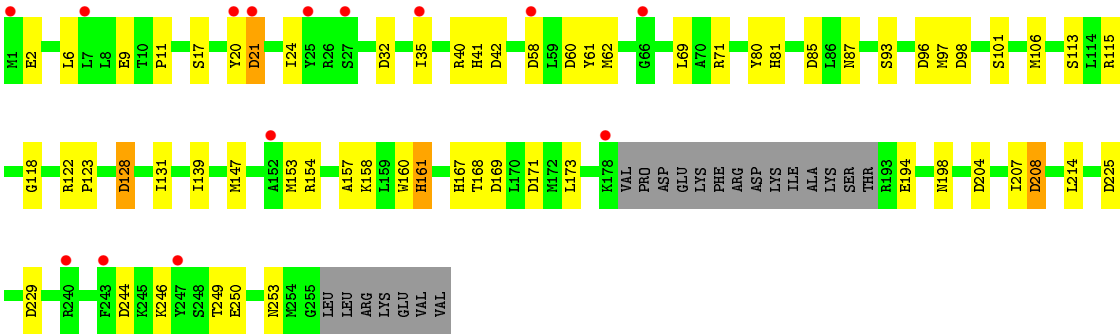
#### • Molecule 1: LIPOATE-PROTEIN LIGASE A

Chain C:



#### • Molecule 1: LIPOATE-PROTEIN LIGASE A

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.38Å 117.88Å 105.66Å 90.00° 93.51° 90.00°	Depositor
Resolution (Å)	53.30 – 1.89 53.28 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.2 (53.30-1.89) 99.2 (53.28-1.89)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.207 , 0.239 0.224 , 0.252	Depositor DCC
$R_{free}$ test set	5132 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.5	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 73.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8042	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LPA

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	0.63	3/1915 (0.2%)	0.87	16/2583 (0.6%)
1	B	0.53	3/1949 (0.2%)	0.86	11/2628 (0.4%)
1	C	0.41	2/1911 (0.1%)	0.73	14/2583 (0.5%)
1	D	0.47	4/1850 (0.2%)	0.94	22/2505 (0.9%)
All	All	0.52	12/7625 (0.2%)	0.85	63/10299 (0.6%)

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	B	1	0
1	C	1	2
1	D	0	2
All	All	2	4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	GLU	CD-OE2	-15.97	1.08	1.25
1	A	216	ARG	NE-CZ	11.85	1.48	1.33
1	D	40	ARG	CZ-NH2	-8.63	1.21	1.33
1	C	203	VAL	CB-CG1	-8.27	1.35	1.52
1	B	73	TYR	CG-CD1	8.01	1.49	1.39

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	154	ARG	NE-CZ-NH1	-23.09	108.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	ARG	NE-CZ-NH2	16.89	128.75	120.30
1	A	216	ARG	NE-CZ-NH1	-14.39	113.10	120.30
1	A	216	ARG	NE-CZ-NH2	13.98	127.29	120.30
1	D	40	ARG	NE-CZ-NH2	11.63	126.11	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	192	THR	CB
1	C	192	THR	CB

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	161	HIS	Peptide
1	C	207	ILE	Peptide
1	D	21	ASP	Peptide
1	D	61	TYR	Sidechain

## 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	1886	0	1836	41	0
1	B	1920	0	1871	52	1
1	C	1882	0	1806	43	0
1	D	1822	0	1718	32	1
2	A	12	0	13	0	0
2	B	12	0	13	0	0
2	C	12	0	13	0	0
2	D	12	0	13	0	0
3	A	191	0	0	3	1
3	B	162	0	0	6	1
3	C	65	0	0	3	0
3	D	66	0	0	3	0
All	All	8042	0	7283	166	2

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 12.

The worst 5 of 166 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:C:94:SER:OG	1:C:158:LYS:HE3	1.63	0.98
1:C:80:TYR:OH	1:C:172:MET:SD	2.27	0.91
1:B:61:TYR:CE2	1:B:176:VAL:HG22	2.08	0.88
1:A:153:MET:HG2	1:A:158:LYS:HG2	1.54	0.87
1:B:127:ASN:OD1	1:B:136:LYS:HE2	1.78	0.83

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2008:HOH:O	3:B:2029:HOH:O[2_545]	1.86	0.34
1:B:73:TYR:O	1:D:122:ARG:NH1[2_555]	2.03	0.17

## 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	237/262 (90%)	231 (98%)	6 (2%)	0	100	100
1	B	241/262 (92%)	236 (98%)	5 (2%)	0	100	100
1	C	241/262 (92%)	227 (94%)	12 (5%)	2 (1%)	19	9
1	D	237/262 (90%)	228 (96%)	9 (4%)	0	100	100
All	All	956/1048 (91%)	922 (96%)	32 (3%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	154	ARG
1	C	155	LYS

### 5.3.2 Protein sidechains ⓘ

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	199/226 (88%)	197 (99%)	2 (1%)	76	76
1	B	202/226 (89%)	198 (98%)	4 (2%)	55	51
1	C	193/226 (85%)	189 (98%)	4 (2%)	53	48
1	D	183/226 (81%)	178 (97%)	5 (3%)	44	38
All	All	777/904 (86%)	762 (98%)	15 (2%)	57	53

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	21	ASP
1	C	88	PHE
1	D	161	HIS
1	B	207	ILE
1	D	101	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	253	ASN
1	C	161	HIS
1	D	167	HIS
1	B	198	ASN
1	D	41	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 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	LPA	B	900	-	9,12,12	1.04	1 (11%)	10,14,14	1.65	2 (20%)
2	LPA	D	900	-	9,12,12	1.10	1 (11%)	10,14,14	1.79	3 (30%)
2	LPA	A	900	-	9,12,12	1.01	1 (11%)	10,14,14	2.19	3 (30%)
2	LPA	C	900	-	9,12,12	1.08	1 (11%)	10,14,14	1.78	2 (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	LPA	B	900	-	-	0/5/14/14	0/1/1/1
2	LPA	D	900	-	-	0/5/14/14	0/1/1/1
2	LPA	A	900	-	-	0/5/14/14	0/1/1/1
2	LPA	C	900	-	-	0/5/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	900	LPA	S6-S8	-2.90	1.82	2.04
2	D	900	LPA	S6-S8	-2.89	1.82	2.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	LPA	S6-S8	-2.77	1.83	2.04
2	A	900	LPA	S6-S8	-2.64	1.84	2.04

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	LPA	C8-S8-S6	4.94	112.24	95.01
2	C	900	LPA	C8-S8-S6	4.07	109.22	95.01
2	A	900	LPA	C7-C8-S8	-3.80	98.98	109.05
2	D	900	LPA	C8-S8-S6	3.69	107.88	95.01
2	B	900	LPA	C8-S8-S6	3.65	107.75	95.01

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	20:TYR	C	21:ASP	N	1.16

## 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	241/262 (91%)	0.39	1 (0%) 92 93	19, 27, 38, 46	28 (11%)
1	B	245/262 (93%)	0.38	3 (1%) 79 81	19, 26, 39, 51	29 (11%)
1	C	245/262 (93%)	0.45	12 (4%) 29 33	24, 38, 46, 55	46 (18%)
1	D	241/262 (91%)	0.64	14 (5%) 23 25	24, 39, 47, 52	58 (24%)
All	All	972/1048 (92%)	0.46	30 (3%) 49 51	19, 33, 45, 55	161 (16%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	5.6
1	B	39	TYR	5.1
1	D	7	LEU	3.9
1	D	240	ARG	3.6
1	C	202	PHE	3.3

### 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. 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	LPA	C	900	12/12	0.89	0.20	14,20,24,25	12
2	LPA	A	900	12/12	0.92	0.24	7,12,19,22	12
2	LPA	B	900	12/12	0.93	0.24	6,8,16,18	12
2	LPA	D	900	12/12	0.93	0.20	15,23,29,35	12

## 6.5 Other polymers [i](#)

There are no such residues in this entry.