Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:11 AM GMT

PDB ID	:	2FZM
Title	:	Structure of the E. coli PutA proline dehydrogenase domain reduced by dithionite and complexed with SO2
Authors	:	Tanner, J.J.
Deposited on	:	2006-02-09
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
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:

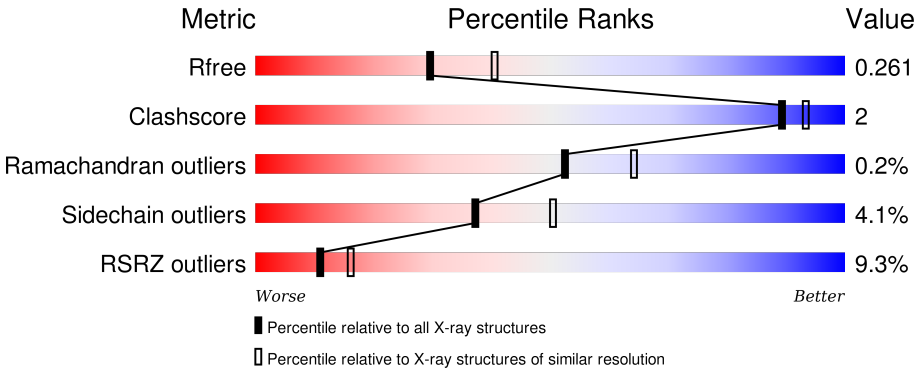
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 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	602	7%, 67%, 7%, 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FAD	A	2001	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3633 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.

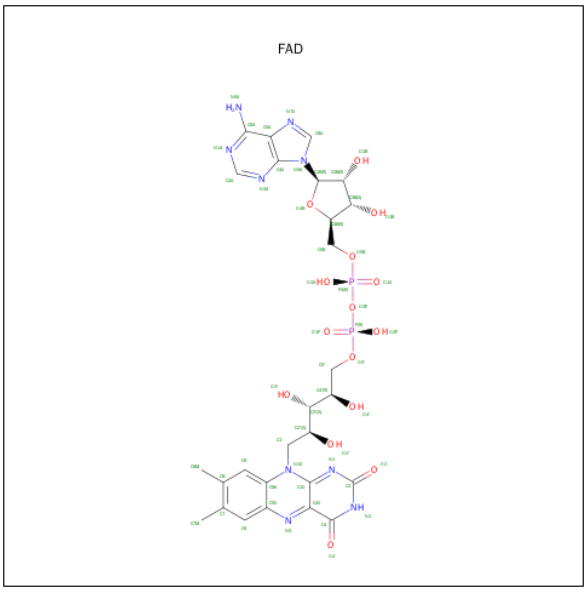
- Molecule 1 is a protein called Bifunctional protein putA, Proline dehydrogenase (EC 1.5.99.8) (Proline oxidase).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	450	3460	2197	609	637	17	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

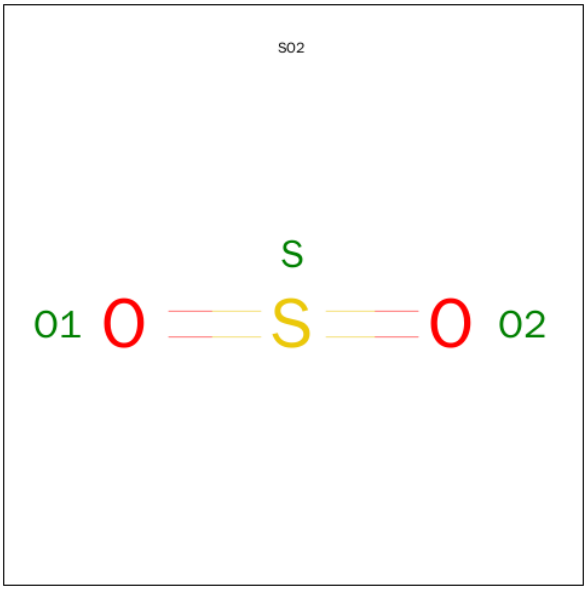
Chain	Residue	Modelled	Actual	Comment	Reference
A	670	SER	-	CLONING ARTIFACT	UNP P09546
A	671	SER	-	CLONING ARTIFACT	UNP P09546
A	672	SER	-	CLONING ARTIFACT	UNP P09546
A	673	VAL	-	CLONING ARTIFACT	UNP P09546
A	674	ASP	-	CLONING ARTIFACT	UNP P09546
A	675	LYS	-	CLONING ARTIFACT	UNP P09546
A	676	LEU	-	CLONING ARTIFACT	UNP P09546
A	677	ALA	-	CLONING ARTIFACT	UNP P09546
A	678	ALA	-	CLONING ARTIFACT	UNP P09546
A	679	ALA	-	CLONING ARTIFACT	UNP P09546
A	680	LEU	-	CLONING ARTIFACT	UNP P09546
A	681	GLU	-	CLONING ARTIFACT	UNP P09546
A	682	HIS	-	EXPRESSION TAG	UNP P09546
A	683	HIS	-	EXPRESSION TAG	UNP P09546
A	684	HIS	-	EXPRESSION TAG	UNP P09546
A	685	HIS	-	EXPRESSION TAG	UNP P09546
A	686	HIS	-	EXPRESSION TAG	UNP P09546
A	687	HIS	-	EXPRESSION TAG	UNP P09546

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is SULFUR DIOXIDE (three-letter code: SO2) (formula: O_2S).



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

- Molecule 4 is water.

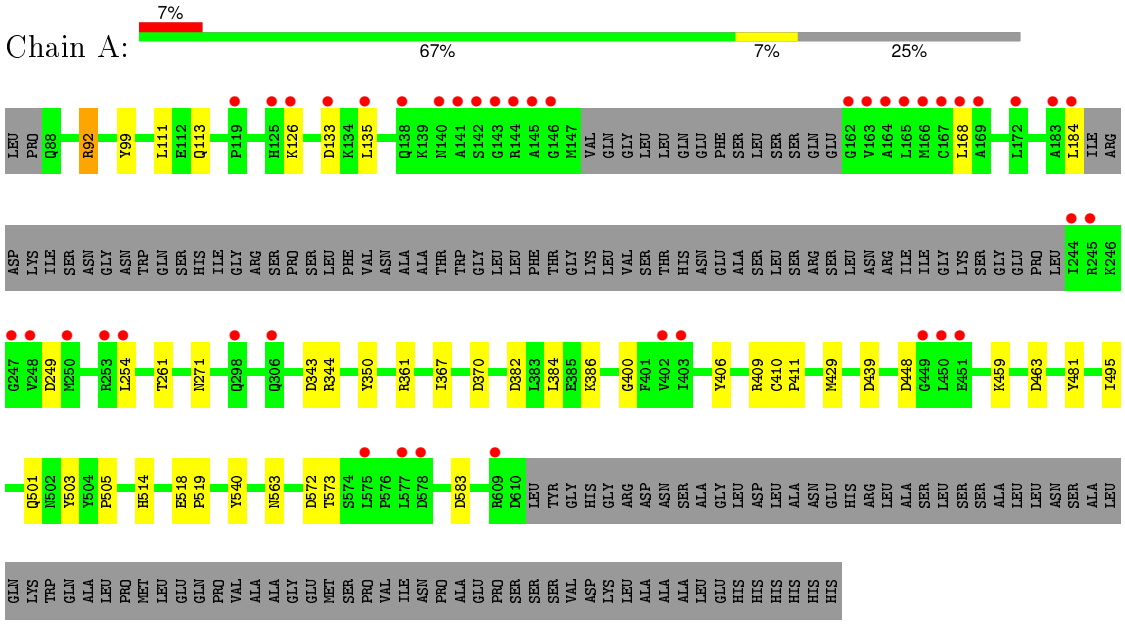
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	117	Total	O	0	0
			117	117		

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: Bifunctional protein putA, Proline dehydrogenase (EC 1.5.99.8) (Proline oxidase)

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	73.11Å 141.42Å 145.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.13 – 2.30 45.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.13-2.30) 97.9 (45.93-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.14 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.209 , 0.257 0.215 , 0.261	Depositor DCC
R_{free} test set	1635 reflections (5.20%)	DCC
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.714	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.6	EDS
Estimated twinning fraction	0.005 for -h,-l,-k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 33071 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3633	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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: SO2, FAD

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	0.70	1/3523 (0.0%)	0.81	8/4774 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	481	TYR	CD1-CE1	6.01	1.48	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	439	ASP	CB-CG-OD2	7.09	124.69	118.30
1	A	343	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	370	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	448	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	583	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	133	ASP	CB-CG-OD2	5.58	123.33	118.30
1	A	249	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	92	ARG	NE-CZ-NH2	-5.26	117.67	120.30

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	3460	0	3453	16	0
2	A	53	0	30	2	0
3	A	3	0	0	0	0
4	A	117	0	0	3	0
All	All	3633	0	3483	17	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 2.

All (17) 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:540:TYR:HB2	2:A:2001:FAD:HM72	1.76	0.67
1:A:92:ARG:NH2	1:A:382:ASP:OD2	2.27	0.67
1:A:135:LEU:HD11	1:A:519:PRO:HB2	1.82	0.62
1:A:409:ARG:HD2	4:A:2005:HOH:O	2.04	0.57
1:A:350:TYR:CE1	1:A:386:LYS:HE3	2.44	0.52
1:A:410:CYS:HB3	1:A:411:PRO:HD3	1.91	0.52
1:A:409:ARG:CD	4:A:2005:HOH:O	2.59	0.51
1:A:261:THR:HG22	1:A:514:HIS:CG	2.46	0.50
1:A:503:TYR:OH	1:A:505:PRO:HA	2.12	0.49
1:A:367:ILE:O	1:A:367:ILE:HG23	2.15	0.47
2:A:2001:FAD:H9	2:A:2001:FAD:H2'	1.96	0.47
1:A:400:GLY:HA2	1:A:429:MET:O	2.15	0.46
1:A:113:GLN:HB3	4:A:2085:HOH:O	2.15	0.45
1:A:271:ASN:N	1:A:271:ASN:HD22	2.14	0.45
1:A:518:GLU:HB2	1:A:519:PRO:HD3	2.01	0.43
1:A:518:GLU:N	1:A:519:PRO:CD	2.82	0.42
1:A:459:LYS:NZ	1:A:463:ASP:OD2	2.51	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	444/602 (74%)	433 (98%)	10 (2%)	1 (0%)	52 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	572	ASP

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	345/490 (70%)	331 (96%)	14 (4%)	37 50

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	TYR
1	A	111	LEU
1	A	126	LYS
1	A	168	LEU
1	A	184	LEU
1	A	254	LEU
1	A	344	ARG
1	A	361	ARG
1	A	384	LEU
1	A	406	TYR
1	A	495	ILE
1	A	501	GLN
1	A	563	ASN
1	A	573	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	GLN

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Mol	Chain	Res	Type
1	A	123	GLN
1	A	130	GLN
1	A	137	ASN
1	A	271	ASN
1	A	298	GLN
1	A	305	GLN
1	A	368	ASN
1	A	501	GLN
1	A	534	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	FAD	A	2001	-	48,58,58	1.57	11 (22%)	54,89,89	2.19	11 (20%)
3	SO2	A	2002	-	2,2,2	1.67	1 (50%)	1,1,1	0.70	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	FAD	A	2001	-	1/1/9/9	0/30/50/50	0/6/6/6
3	SO2	A	2002	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	FAD	O4B-C4B	-3.69	1.36	1.45
2	A	2001	FAD	P-O2P	-2.35	1.44	1.54
2	A	2001	FAD	C4A-N3A	-2.35	1.32	1.35
2	A	2001	FAD	PA-O2A	-2.27	1.45	1.54
2	A	2001	FAD	C6-C5X	-2.05	1.38	1.41
3	A	2002	SO2	O2-S	2.03	1.54	1.40
2	A	2001	FAD	C5'-C4'	2.17	1.55	1.51
2	A	2001	FAD	C5X-N5	2.22	1.38	1.35
2	A	2001	FAD	C2A-N1A	2.98	1.39	1.33
2	A	2001	FAD	C4-N3	3.54	1.39	1.33
2	A	2001	FAD	C4X-N5	3.74	1.39	1.33
2	A	2001	FAD	O4B-C1B	4.46	1.46	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2001	FAD	N3A-C2A-N1A	-9.00	122.00	128.89
2	A	2001	FAD	C4A-C5A-N7A	-3.99	105.81	109.48
2	A	2001	FAD	C4X-C4-N3	-3.50	118.80	123.59
2	A	2001	FAD	C1B-N9A-C4A	-3.26	122.03	126.94
2	A	2001	FAD	C2B-C1B-N9A	-2.80	110.01	114.29
2	A	2001	FAD	C5B-C4B-C3B	2.22	124.04	115.21
2	A	2001	FAD	O2A-PA-O3P	2.39	115.95	105.09
2	A	2001	FAD	O4B-C4B-C3B	2.52	110.22	105.15
2	A	2001	FAD	C4-C4X-N5	3.29	122.72	118.72
2	A	2001	FAD	O4B-C4B-C5B	4.59	125.72	109.32
2	A	2001	FAD	C4-N3-C2	6.60	120.95	115.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2001	FAD	C4B

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	FAD	2	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	450/602 (74%)	0.46	42 (9%)	11	16	19, 37, 79, 96	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	ILE	10.8
1	A	164	ALA	7.0
1	A	141	ALA	5.1
1	A	163	VAL	4.5
1	A	142	SER	4.4
1	A	165	LEU	4.3
1	A	168	LEU	3.8
1	A	145	ALA	3.6
1	A	172	LEU	3.5
1	A	609	ARG	3.5
1	A	577	LEU	3.4
1	A	166	MET	3.3
1	A	140	ASN	3.3
1	A	184	LEU	3.3
1	A	167	CYS	3.2
1	A	169	ALA	3.1
1	A	162	GLY	3.1
1	A	247	GLY	3.0
1	A	143	GLY	3.0
1	A	119	PRO	3.0
1	A	575	LEU	2.9
1	A	248	VAL	2.7
1	A	126	LYS	2.7
1	A	250	MET	2.6
1	A	144	ARG	2.6
1	A	403	ILE	2.5
1	A	183	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	253	ARG	2.5
1	A	133	ASP	2.5
1	A	578	ASP	2.5
1	A	138	GLN	2.5
1	A	254	LEU	2.5
1	A	245	ARG	2.5
1	A	125	HIS	2.4
1	A	402	VAL	2.3
1	A	146	GLY	2.3
1	A	135	LEU	2.2
1	A	298	GLN	2.2
1	A	451	GLU	2.2
1	A	449	GLY	2.2
1	A	450	LEU	2.1
1	A	306	GLN	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	SO2	A	2002	3/3	0.98	0.17	-0.18	48,48,49,51	0
2	FAD	A	2001	53/53	0.99	0.12	-0.72	29,34,40,42	0

6.5 Other polymers (i)

There are no such residues in this entry.