Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:04 AM GMT

PDB ID	:	2FIC
Title	:	The crystal structure of the BAR domain from human Bin1/Amphiphysin II and its implications for molecular recognition
Authors	:	Casal, E.; Federici, L.; Zhang, W.; Fernandez-Recio, J.; Priego, E.M.; Miguel, R.N.; Duhadaway, J.B.; Prendergast, G.C.; Luisi, B.F.; Laue, E.D.
Deposited on	:	2005-12-29
Resolution	:	1.99 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:

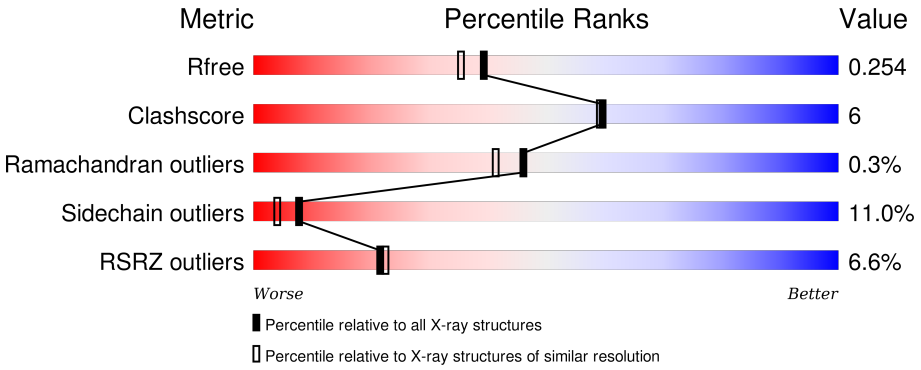
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.99 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 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	251	6% 61% 13% • 24%
1	B	251	4% 63% 13% • 20%

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	XE	B	1002	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3400 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 bridging integrator 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1566	986	271	302	7			
1	B	201	Total	C	N	O	S	0	0	0
			1640	1029	283	321	7			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	CLONING ARTIFACT	UNP O00499
A	2	SER	-	CLONING ARTIFACT	UNP O00499
A	3	GLY	-	CLONING ARTIFACT	UNP O00499
A	4	LEU	-	CLONING ARTIFACT	UNP O00499
A	5	VAL	-	CLONING ARTIFACT	UNP O00499
A	6	PRO	-	CLONING ARTIFACT	UNP O00499
A	7	ARG	-	CLONING ARTIFACT	UNP O00499
A	8	GLY	-	CLONING ARTIFACT	UNP O00499
A	9	SER	-	CLONING ARTIFACT	UNP O00499
A	10	HIS	-	CLONING ARTIFACT	UNP O00499
B	1	SER	-	CLONING ARTIFACT	UNP 30582569
B	2	SER	-	CLONING ARTIFACT	UNP 30582569
B	3	GLY	-	CLONING ARTIFACT	UNP 30582569
B	4	LEU	-	CLONING ARTIFACT	UNP 30582569
B	5	VAL	-	CLONING ARTIFACT	UNP 30582569
B	6	PRO	-	CLONING ARTIFACT	UNP 30582569
B	7	ARG	-	CLONING ARTIFACT	UNP 30582569
B	8	GLY	-	CLONING ARTIFACT	UNP 30582569
B	9	SER	-	CLONING ARTIFACT	UNP 30582569
B	10	HIS	-	CLONING ARTIFACT	UNP 30582569

- Molecule 2 is XENON (three-letter code: XE) (formula: Xe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Xe 1 1	0	0
2	A	1	Total Xe 1 1	0	0

- Molecule 3 is water.

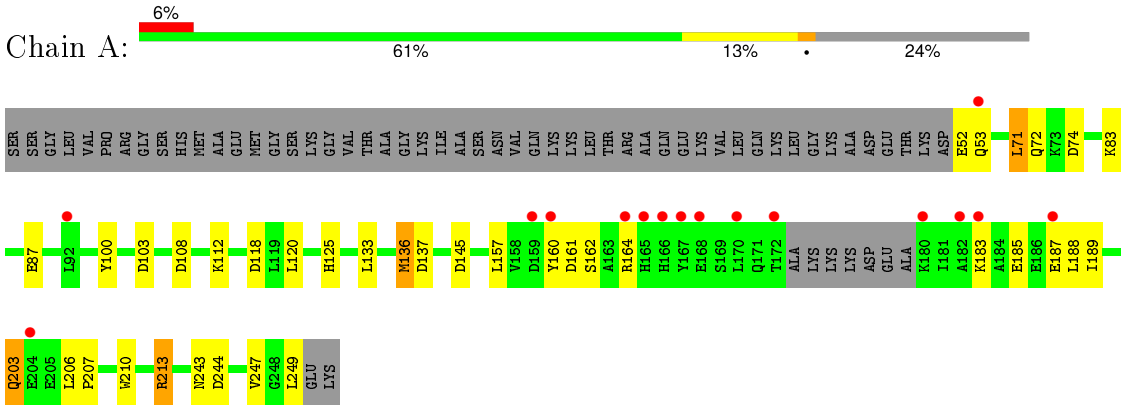
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	102	Total O 102 102	0	0
3	B	90	Total O 90 90	0	0

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.

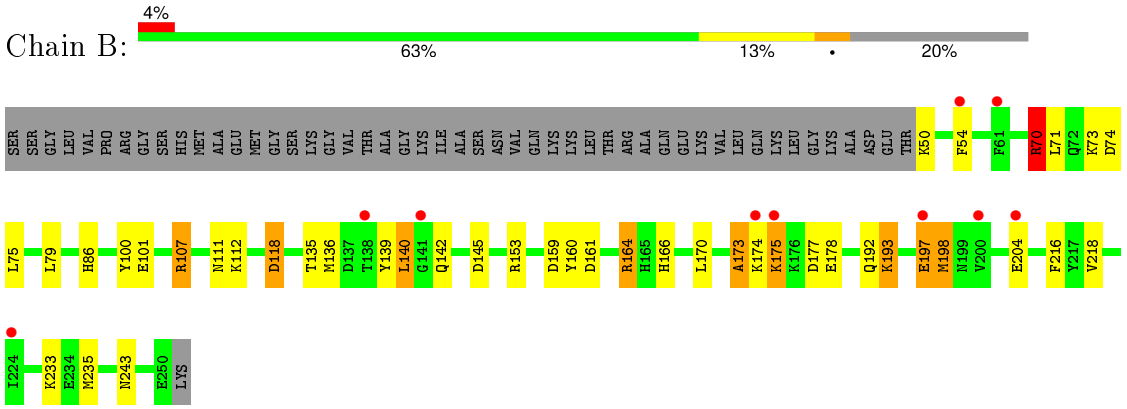
- Molecule 1: bridging integrator 1

Chain A:



- Molecule 1: bridging integrator 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.92Å 59.09Å 75.01Å 90.00° 117.53° 90.00°	Depositor
Resolution (Å)	15.00 – 1.99 27.45 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.3 (15.00-1.99) 98.2 (27.45-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.27 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.230 , 0.280 0.245 , 0.254	Depositor DCC
R_{free} test set	1820 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.4	EDS
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 36616 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3400	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.46% 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: XE

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	0.79	0/1593	0.87	7/2145 (0.3%)
1	B	0.85	1/1668 (0.1%)	0.96	10/2246 (0.4%)
All	All	0.82	1/3261 (0.0%)	0.92	17/4391 (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	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	70	ARG	CZ-NH2	-5.98	1.25	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	70	ARG	NE-CZ-NH1	11.13	125.86	120.30
1	B	70	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	A	74	ASP	CB-CG-OD2	7.13	124.72	118.30
1	B	74	ASP	CB-CG-OD2	6.45	124.11	118.30
1	A	118	ASP	CB-CG-OD2	6.38	124.04	118.30
1	B	177	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	244	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	145	ASP	CB-CG-OD2	5.86	123.57	118.30
1	B	118	ASP	CB-CG-OD2	5.72	123.45	118.30
1	B	161	ASP	CB-CG-OD2	5.62	123.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	70	ARG	CD-NE-CZ	5.44	131.21	123.60
1	B	145	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	108	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	159	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	164	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	103	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	161	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	173	ALA	Peptide
1	B	50	LYS	Peptide

5.2 Too-close contacts (i)

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	1566	0	1528	11	0
1	B	1640	0	1594	25	0
2	A	1	0	0	0	0
2	B	1	0	0	2	0
3	A	102	0	0	1	0
3	B	90	0	0	0	0
All	All	3400	0	3122	36	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 6.

All (36) 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:52:GLU:HG2	1:A:53:GLN:H	1.11	1.10
1:B:139:TYR:HD2	1:B:140:LEU:HD13	1.22	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ALA:HB1	1:B:174:LYS:O	1.61	0.99
1:A:52:GLU:HG2	1:A:53:GLN:N	1.83	0.93
1:B:139:TYR:CD2	1:B:140:LEU:HD13	2.04	0.92
1:B:54:PHE:CZ	1:B:153:ARG:CD	2.82	0.63
1:B:193:LYS:HD3	1:B:193:LYS:O	1.99	0.61
1:B:139:TYR:CD2	1:B:140:LEU:CD1	2.82	0.60
1:A:52:GLU:CG	1:A:53:GLN:H	2.00	0.59
1:A:210:TRP:CE2	1:A:213:ARG:NH2	2.71	0.59
1:B:174:LYS:O	1:B:175:LYS:O	2.21	0.58
1:B:173:ALA:CB	1:B:174:LYS:O	2.45	0.55
1:B:136:MET:HB3	1:B:140:LEU:HD22	1.89	0.54
1:B:86:HIS:HE1	1:B:118:ASP:OD2	1.91	0.54
1:B:136:MET:HG2	1:B:216:PHE:CE1	2.45	0.51
1:B:107:ARG:HD2	1:B:107:ARG:C	2.31	0.51
1:B:139:TYR:O	1:B:142:GLN:HB2	2.12	0.50
1:B:54:PHE:CZ	1:B:153:ARG:HD3	2.48	0.49
1:B:86:HIS:CE1	1:B:118:ASP:OD2	2.66	0.48
1:B:173:ALA:HB1	1:B:174:LYS:C	2.31	0.48
1:B:54:PHE:CE2	1:B:153:ARG:CZ	2.96	0.48
1:A:83:LYS:HE2	1:A:125:HIS:CD2	2.48	0.48
1:B:218:VAL:HG22	2:B:1002:XE:XE	2.92	0.47
1:A:203:GLN:NE2	3:A:1049:HOH:O	2.47	0.47
1:B:136:MET:HB3	1:B:140:LEU:CD2	2.46	0.46
1:B:166:HIS:O	1:B:170:LEU:HD13	2.17	0.45
1:A:72:GLN:NE2	1:A:137:ASP:OD1	2.49	0.44
1:A:83:LYS:O	1:A:87:GLU:HG2	2.18	0.43
1:B:54:PHE:CZ	1:B:153:ARG:NE	2.86	0.42
1:A:206:LEU:HB2	1:A:207:PRO:HD3	2.00	0.42
1:A:243:ASN:O	1:A:247:VAL:HG23	2.19	0.42
1:B:160:TYR:CZ	1:B:192:GLN:HG3	2.55	0.42
1:B:70:ARG:HG3	1:B:71:LEU:N	2.33	0.41
1:B:218:VAL:HA	2:B:1002:XE:XE	2.99	0.41
1:B:197:GLU:HG3	1:B:198:MET:N	2.35	0.40
1:A:71:LEU:HD13	1:A:136:MET:SD	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	187/251 (74%)	186 (100%)	1 (0%)	0	100 100
1	B	199/251 (79%)	196 (98%)	2 (1%)	1 (0%)	34 26
All	All	386/502 (77%)	382 (99%)	3 (1%)	1 (0%)	46 41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	175	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	170/219 (78%)	152 (89%)	18 (11%)	8 4
1	B	177/219 (81%)	157 (89%)	20 (11%)	7 4
All	All	347/438 (79%)	309 (89%)	38 (11%)	8 4

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	LEU
1	A	100	TYR
1	A	112	LYS
1	A	120	LEU
1	A	133	LEU

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Mol	Chain	Res	Type
1	A	136	MET
1	A	157	LEU
1	A	160	TYR
1	A	162	SER
1	A	164	ARG
1	A	183	LYS
1	A	185	GLU
1	A	187	GLU
1	A	188	LEU
1	A	189	ILE
1	A	203	GLN
1	A	213	ARG
1	A	249	LEU
1	B	70	ARG
1	B	73	LYS
1	B	75	LEU
1	B	79	LEU
1	B	100	TYR
1	B	101	GLU
1	B	107	ARG
1	B	111	ASN
1	B	112	LYS
1	B	135	THR
1	B	140	LEU
1	B	164	ARG
1	B	178	GLU
1	B	193	LYS
1	B	197	GLU
1	B	198	MET
1	B	204	GLU
1	B	233	LYS
1	B	235	MET
1	B	243	ASN

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

Mol	Chain	Res	Type
1	A	62	ASN
1	A	93	ASN
1	A	171	GLN
1	A	203	GLN
1	B	62	ASN

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Mol	Chain	Res	Type
1	B	86	HIS
1	B	97	GLN
1	B	116	ASN
1	B	131	GLN
1	B	211	ASN
1	B	232	HIS
1	B	239	ASN
1	B	243	ASN

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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

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	191/251 (76%)	0.55	16 (8%)	14	14	8, 18, 43, 50	0
1	B	201/251 (80%)	0.55	10 (4%)	32	34	9, 19, 37, 74	0
All	All	392/502 (78%)	0.55	26 (6%)	22	22	8, 19, 42, 74	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	LYS	4.4
1	B	174	LYS	4.1
1	B	138	THR	4.0
1	A	182	ALA	4.0
1	B	175	LYS	4.0
1	A	204	GLU	3.2
1	A	172	THR	2.9
1	A	164	ARG	2.8
1	B	141	GLY	2.8
1	A	165	HIS	2.8
1	B	204	GLU	2.8
1	A	160	TYR	2.6
1	A	166	HIS	2.5
1	A	167	TYR	2.5
1	A	187	GLU	2.5
1	B	197	GLU	2.4
1	A	168	GLU	2.3
1	A	53	GLN	2.3
1	B	54	PHE	2.3
1	A	92	LEU	2.3
1	A	170	LEU	2.2
1	A	183	LYS	2.2
1	B	61	PHE	2.2
1	A	159	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	224	ILE	2.1
1	B	200	VAL	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
2	XE	A	1001	1/1	0.97	0.13	0.61	35,35,35,35	1
2	XE	B	1002	1/1	0.98	0.05	-3.22	52,52,52,52	1

6.5 Other polymers (i)

There are no such residues in this entry.