Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2023 – 02:44 PM EDT

PDB ID	:	6DHV
Title	:	Structure of Arabidopsis Fatty Acid Amide Hydrolase
Authors	:	Aziz, M.; Wang, X.; Tripathi, A.; Bankaitis, V.; Chapman, K.D.
Deposited on	:	2018-05-21
Resolution	:	2.10 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

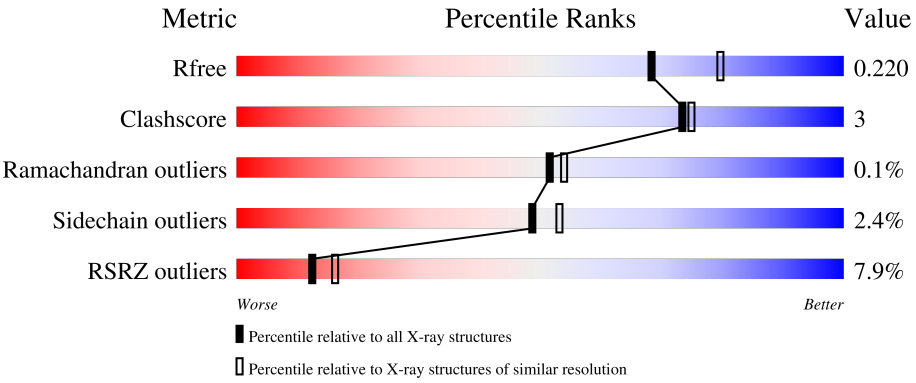
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	636	6% 86% 7% 7%
1	B	636	9% 84% 9% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9537 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 Fatty acid amide hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	594	Total	C	N	O	S	0	0	0
			4549	2887	768	871	23			
1	B	597	Total	C	N	O	S	0	0	0
			4570	2900	772	874	24			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	608	LYS	-	expression tag	UNP Q7XJJ7
A	609	GLY	-	expression tag	UNP Q7XJJ7
A	610	GLU	-	expression tag	UNP Q7XJJ7
A	611	PHE	-	expression tag	UNP Q7XJJ7
A	612	GLU	-	expression tag	UNP Q7XJJ7
A	613	ALA	-	expression tag	UNP Q7XJJ7
A	614	TYR	-	expression tag	UNP Q7XJJ7
A	615	VAL	-	expression tag	UNP Q7XJJ7
A	616	GLU	-	expression tag	UNP Q7XJJ7
A	617	GLN	-	expression tag	UNP Q7XJJ7
A	618	LYS	-	expression tag	UNP Q7XJJ7
A	619	LEU	-	expression tag	UNP Q7XJJ7
A	620	ILE	-	expression tag	UNP Q7XJJ7
A	621	SER	-	expression tag	UNP Q7XJJ7
A	622	GLU	-	expression tag	UNP Q7XJJ7
A	623	GLU	-	expression tag	UNP Q7XJJ7
A	624	ASP	-	expression tag	UNP Q7XJJ7
A	625	LEU	-	expression tag	UNP Q7XJJ7
A	626	ASN	-	expression tag	UNP Q7XJJ7
A	627	SER	-	expression tag	UNP Q7XJJ7
A	628	ALA	-	expression tag	UNP Q7XJJ7
A	629	VAL	-	expression tag	UNP Q7XJJ7
A	630	ASP	-	expression tag	UNP Q7XJJ7
A	631	HIS	-	expression tag	UNP Q7XJJ7
A	632	HIS	-	expression tag	UNP Q7XJJ7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	633	HIS	-	expression tag	UNP Q7XJJ7
A	634	HIS	-	expression tag	UNP Q7XJJ7
A	635	HIS	-	expression tag	UNP Q7XJJ7
A	636	HIS	-	expression tag	UNP Q7XJJ7
B	608	LYS	-	expression tag	UNP Q7XJJ7
B	609	GLY	-	expression tag	UNP Q7XJJ7
B	610	GLU	-	expression tag	UNP Q7XJJ7
B	611	PHE	-	expression tag	UNP Q7XJJ7
B	612	GLU	-	expression tag	UNP Q7XJJ7
B	613	ALA	-	expression tag	UNP Q7XJJ7
B	614	TYR	-	expression tag	UNP Q7XJJ7
B	615	VAL	-	expression tag	UNP Q7XJJ7
B	616	GLU	-	expression tag	UNP Q7XJJ7
B	617	GLN	-	expression tag	UNP Q7XJJ7
B	618	LYS	-	expression tag	UNP Q7XJJ7
B	619	LEU	-	expression tag	UNP Q7XJJ7
B	620	ILE	-	expression tag	UNP Q7XJJ7
B	621	SER	-	expression tag	UNP Q7XJJ7
B	622	GLU	-	expression tag	UNP Q7XJJ7
B	623	GLU	-	expression tag	UNP Q7XJJ7
B	624	ASP	-	expression tag	UNP Q7XJJ7
B	625	LEU	-	expression tag	UNP Q7XJJ7
B	626	ASN	-	expression tag	UNP Q7XJJ7
B	627	SER	-	expression tag	UNP Q7XJJ7
B	628	ALA	-	expression tag	UNP Q7XJJ7
B	629	VAL	-	expression tag	UNP Q7XJJ7
B	630	ASP	-	expression tag	UNP Q7XJJ7
B	631	HIS	-	expression tag	UNP Q7XJJ7
B	632	HIS	-	expression tag	UNP Q7XJJ7
B	633	HIS	-	expression tag	UNP Q7XJJ7
B	634	HIS	-	expression tag	UNP Q7XJJ7
B	635	HIS	-	expression tag	UNP Q7XJJ7
B	636	HIS	-	expression tag	UNP Q7XJJ7

- Molecule 2 is water.

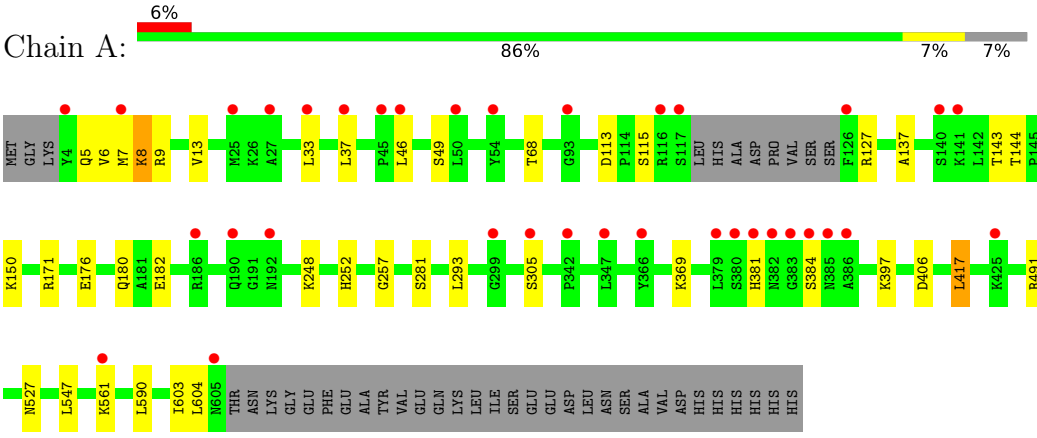
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	207	Total O 207 207	0	0
2	B	211	Total O 211 211	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

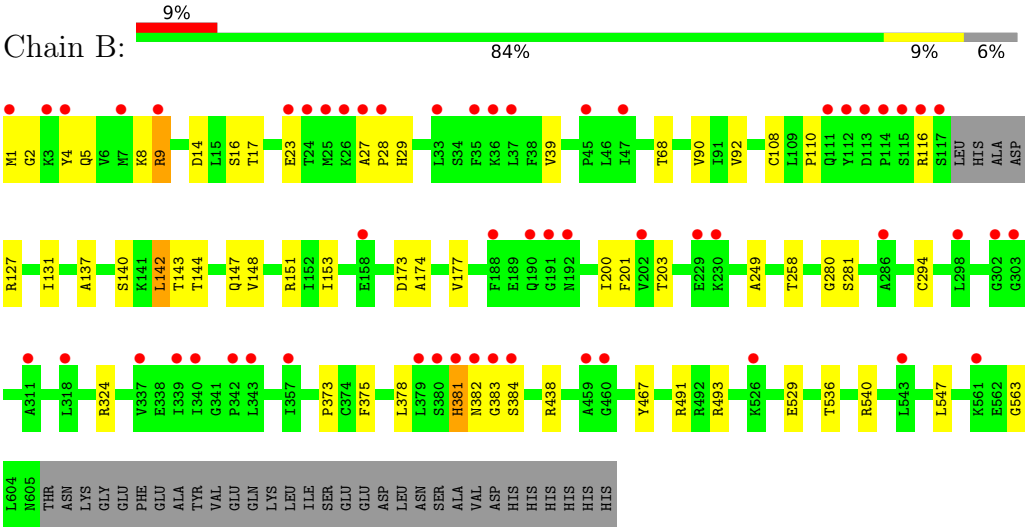
• Molecule 1: Fatty acid amide hydrolase

Chain A:



• Molecule 1: Fatty acid amide hydrolase

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	72.08Å 79.66Å 132.59Å 90.00° 104.44° 90.00°	Depositor
Resolution (Å)	33.00 – 2.10 33.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (33.00-2.10) 98.5 (33.00-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.192 , 0.220 0.193 , 0.220	Depositor DCC
R_{free} test set	4315 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 55.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9537	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.36	0/4645	0.48	0/6307
1	B	0.42	0/4666	0.49	0/6333
All	All	0.40	0/9311	0.49	0/12640

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	4549	0	4573	26	0
1	B	4570	0	4601	34	0
2	A	207	0	0	0	0
2	B	211	0	0	2	0
All	All	9537	0	9174	60	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 3.

All (60) 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:9:ARG:O	1:A:13:VAL:HG23	1.87	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:ARG:NH1	2:B:701:HOH:O	2.23	0.68
1:B:144:THR:HG23	1:B:147:GLN:H	1.59	0.68
1:A:603:ILE:HG22	1:A:604:LEU:N	2.10	0.67
1:B:23:GLU:OE2	1:B:23:GLU:HA	1.96	0.66
1:A:603:ILE:O	1:A:604:LEU:HB2	1.96	0.66
1:A:144:THR:HG23	1:A:147:GLN:H	1.63	0.64
1:A:406:ASP:OD2	1:A:561:LYS:HD2	2.00	0.61
1:B:29:HIS:NE2	1:B:529:GLU:OE1	2.32	0.60
1:A:417:LEU:HB3	1:A:590:LEU:HD13	1.85	0.58
1:B:324:ARG:HD3	2:B:846:HOH:O	2.03	0.58
1:A:171:ARG:HB2	1:A:248:LYS:HB2	1.86	0.57
1:B:140:SER:HB2	1:B:142:LEU:HD12	1.86	0.57
1:A:6:VAL:HG23	1:A:68:THR:HG23	1.86	0.56
1:B:92:VAL:HG22	1:B:373:PRO:HG2	1.86	0.56
1:A:603:ILE:CG2	1:A:604:LEU:N	2.73	0.51
1:B:563:GLY:O	1:B:595:LYS:NZ	2.41	0.51
1:A:148:VAL:HG13	1:A:603:ILE:HG21	1.92	0.51
1:A:144:THR:HG22	1:A:147:GLN:HB2	1.93	0.50
1:A:603:ILE:HG22	1:A:604:LEU:H	1.74	0.50
1:A:603:ILE:N	1:A:603:ILE:HD12	2.26	0.50
1:A:495:MET:HE3	1:A:499:LEU:HD21	1.96	0.48
1:B:9:ARG:O	1:B:493:ARG:NH2	2.45	0.48
1:B:14:ASP:OD2	1:B:16:SER:OG	2.23	0.48
1:B:23:GLU:HG3	1:B:540:ARG:HH21	1.78	0.48
1:B:90:VAL:HG11	1:B:108:CYS:SG	2.54	0.47
1:B:110:PRO:HD3	1:B:378:LEU:O	2.15	0.46
1:A:603:ILE:CG2	1:A:604:LEU:H	2.28	0.46
1:A:252:HIS:CE1	1:A:257:GLY:HA3	2.50	0.46
1:B:9:ARG:CA	1:B:493:ARG:HH12	2.29	0.46
1:B:23:GLU:OE1	1:B:536:THR:HG23	2.15	0.45
1:B:131:ILE:HG23	1:B:200:ILE:HG12	1.97	0.45
1:A:113:ASP:O	1:A:115:SER:N	2.44	0.45
1:B:14:ASP:O	1:B:17:THR:HG22	2.15	0.45
1:A:146:LEU:HG	1:A:150:LYS:HE2	1.98	0.45
1:B:381:HIS:HA	1:B:382:ASN:HA	1.68	0.45
1:A:281:SER:H	1:A:305:SER:HB3	1.80	0.45
1:B:23:GLU:CG	1:B:540:ARG:HH21	2.30	0.44
1:B:90:VAL:HG13	1:B:375:PHE:HB2	2.00	0.44
1:B:137:ALA:HB1	1:B:143:THR:HG22	2.00	0.44
1:B:203:THR:CG2	1:B:249:ALA:HB2	2.48	0.44
1:B:201:PHE:O	1:B:294:CYS:HB2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ALA:HB1	1:A:143:THR:HG22	2.00	0.43
1:A:369:LYS:HE2	1:A:369:LYS:HB2	1.67	0.43
1:A:491:ARG:HG3	1:A:547:LEU:HG	2.01	0.43
1:B:281:SER:H	1:B:305:SER:HB3	1.83	0.43
1:B:148:VAL:HG13	1:B:603:ILE:HG21	2.00	0.42
1:B:382:ASN:HA	1:B:383:GLY:HA3	1.74	0.42
1:A:8:LYS:HD2	1:A:68:THR:CG2	2.50	0.42
1:B:27:ALA:HA	1:B:28:PRO:HD3	1.84	0.42
1:B:153:ILE:HD13	1:B:174:ALA:HB1	2.02	0.42
1:B:491:ARG:HG3	1:B:547:LEU:HG	2.01	0.42
1:A:417:LEU:HD12	1:A:417:LEU:HA	1.92	0.41
1:B:258:THR:O	1:B:280:GLY:N	2.52	0.41
1:A:176:GLU:O	1:A:180:GLN:HG3	2.19	0.41
1:B:39:VAL:HG21	1:B:467:TYR:HB3	2.02	0.41
1:B:173:ASP:O	1:B:177:VAL:HG23	2.21	0.41
1:A:293:LEU:HD23	1:A:293:LEU:HA	1.92	0.40
1:B:23:GLU:OE1	1:B:536:THR:CG2	2.69	0.40
1:B:8:LYS:HD2	1:B:68:THR:HG21	2.02	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	590/636 (93%)	575 (98%)	15 (2%)	0	100	100
1	B	593/636 (93%)	571 (96%)	21 (4%)	1 (0%)	47	49
All	All	1183/1272 (93%)	1146 (97%)	36 (3%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	GLY

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	503/540 (93%)	489 (97%)	14 (3%)	43 47
1	B	505/540 (94%)	495 (98%)	10 (2%)	55 60
All	All	1008/1080 (93%)	984 (98%)	24 (2%)	49 53

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	7	MET
1	A	8	LYS
1	A	33	LEU
1	A	37	LEU
1	A	46	LEU
1	A	49	SER
1	A	127	ARG
1	A	182	GLU
1	A	381	HIS
1	A	384	SER
1	A	397	LYS
1	A	417	LEU
1	A	527	ASN
1	B	1	MET
1	B	4	TYR
1	B	5	GLN
1	B	9	ARG
1	B	116	ARG
1	B	127	ARG
1	B	142	LEU
1	B	151	ARG
1	B	381	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	384	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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^{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	594/636 (93%)	0.30	35 (5%) 22 27	32, 54, 87, 116	0
1	B	597/636 (93%)	0.45	59 (9%) 7 9	33, 57, 94, 128	0
All	All	1191/1272 (93%)	0.38	94 (7%) 12 16	32, 56, 91, 128	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	383	GLY	11.0
1	A	384	SER	8.1
1	B	384	SER	7.7
1	A	116	ARG	7.4
1	A	4	TYR	7.2
1	B	381	HIS	6.5
1	B	33	LEU	6.4
1	B	382	ASN	5.7
1	A	381	HIS	5.6
1	B	24	THR	5.1
1	B	117	SER	5.1
1	A	383	GLY	5.0
1	B	115	SER	4.9
1	B	379	LEU	4.7
1	B	26	LYS	4.6
1	B	343	LEU	4.4
1	B	116	ARG	4.4
1	B	305	SER	4.3
1	B	27	ALA	4.3
1	B	37	LEU	4.2
1	B	306	VAL	4.2
1	B	594	THR	4.1
1	B	113	ASP	4.0
1	A	141	LYS	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	192	ASN	3.7
1	A	382	ASN	3.6
1	B	526	LYS	3.6
1	A	7	MET	3.5
1	B	4	TYR	3.5
1	A	190	GLN	3.5
1	B	339	ILE	3.4
1	B	191	GLY	3.4
1	B	188	PHE	3.3
1	A	45	PRO	3.3
1	A	186	ARG	3.3
1	B	47	ILE	3.2
1	A	46	LEU	3.2
1	B	23	GLU	3.1
1	B	190	GLN	3.1
1	A	425	LYS	3.1
1	A	37	LEU	3.0
1	B	342	PRO	3.0
1	A	25	MET	3.0
1	B	192	ASN	3.0
1	B	111	GLN	3.0
1	A	347	LEU	2.9
1	B	1	MET	2.9
1	B	114	PRO	2.9
1	A	379	LEU	2.8
1	B	337	VAL	2.8
1	B	340	ILE	2.8
1	B	45	PRO	2.7
1	B	7	MET	2.7
1	A	299	GLY	2.7
1	B	229	GLU	2.7
1	A	33	LEU	2.7
1	A	54	TYR	2.6
1	A	117	SER	2.6
1	A	366	TYR	2.6
1	B	25	MET	2.6
1	A	380	SER	2.6
1	B	112	TYR	2.6
1	B	459	ALA	2.6
1	A	386	ALA	2.6
1	B	28	PRO	2.5
1	B	298	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	385	ASN	2.5
1	B	460	GLY	2.5
1	A	605	ASN	2.5
1	A	93	GLY	2.5
1	B	561	LYS	2.5
1	B	318	LEU	2.4
1	A	342	PRO	2.4
1	A	140	SER	2.4
1	B	158	GLU	2.4
1	B	36	LYS	2.4
1	B	230	LYS	2.4
1	B	380	SER	2.4
1	B	9	ARG	2.3
1	A	126	PHE	2.3
1	B	311	ALA	2.3
1	B	357	ILE	2.3
1	B	302	GLY	2.3
1	A	561	LYS	2.2
1	B	3	LYS	2.2
1	B	286	ALA	2.2
1	B	303	GLY	2.2
1	A	27	ALA	2.2
1	A	305	SER	2.2
1	A	50	LEU	2.2
1	B	308	ILE	2.2
1	B	543	LEU	2.1
1	B	202	VAL	2.0
1	B	35	PHE	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.