



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 6, 2022 – 12:17 PM JST

PDB ID : 7F28
Title : Crystal structure of a bacterial ketosynthase
Authors : Lee, W.C.; Kim, Y.
Deposited on : 2021-06-10
Resolution : 1.88 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 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 : 2.28.1
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) : 2.28.1

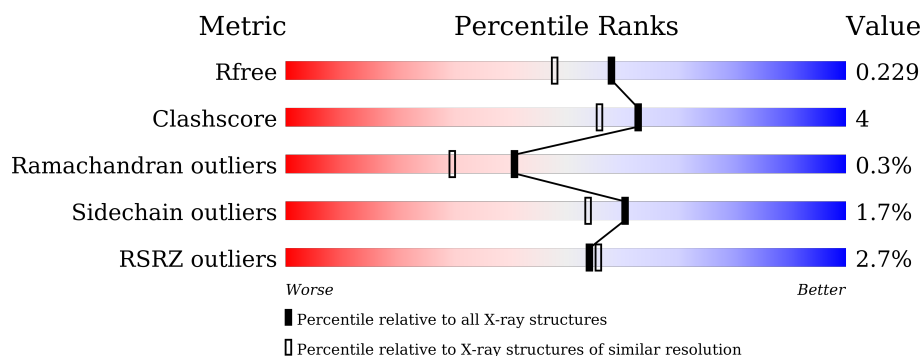
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 $\leq 5\%$. 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	204	<div> <div>4%</div> <div>86% 12% .</div> </div>
1	C	204	<div> <div>%</div> <div>88% 8% .</div> </div>
2	B	400	<div> <div>4%</div> <div>85% 12% ..</div> </div>
2	D	400	<div> <div>2%</div> <div>91% 6% .</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9395 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 Ketoacyl_synth_N domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1571	1001	259	304	7			
1	C	198	Total	C	N	O	S	0	0	0
			1519	972	250	291	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	GLU	ASP	conflict	UNP A0A0E1PUF7
C	181	GLU	ASP	conflict	UNP A0A0E1PUF7

- Molecule 2 is a protein called Putative 3-oxoacyl-[ACP] synthase FabV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	390	Total	C	N	O	S	0	0	0
			2939	1849	504	567	19			
2	D	390	Total	C	N	O	S	0	0	0
			2939	1849	504	567	19			

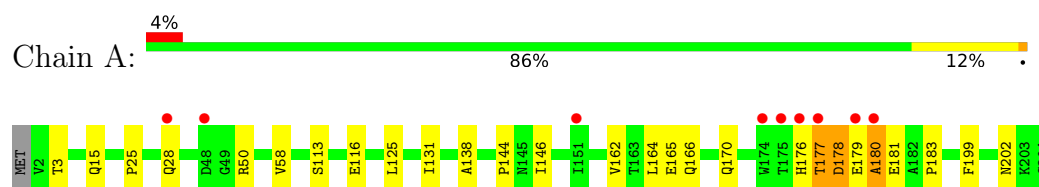
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total	O	0	0
			55	55		
3	B	134	Total	O	0	0
			134	134		
3	C	84	Total	O	0	0
			84	84		
3	D	154	Total	O	0	0
			154	154		

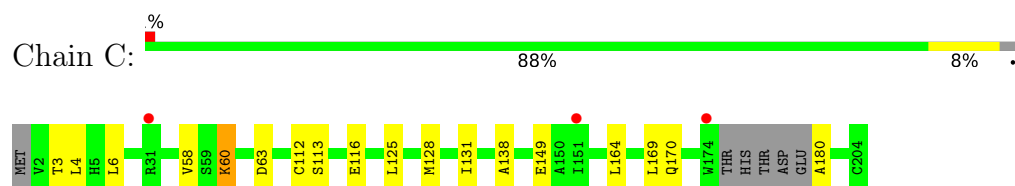
3 Residue-property plots

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.

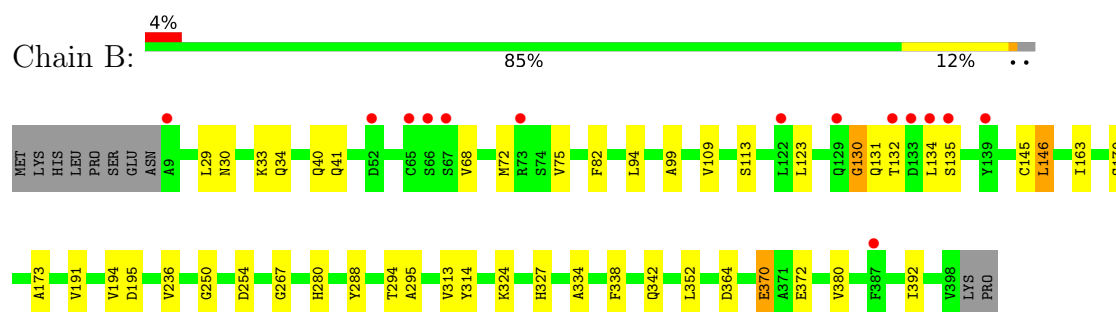
- Molecule 1: Ketoacyl_synth_N domain-containing protein



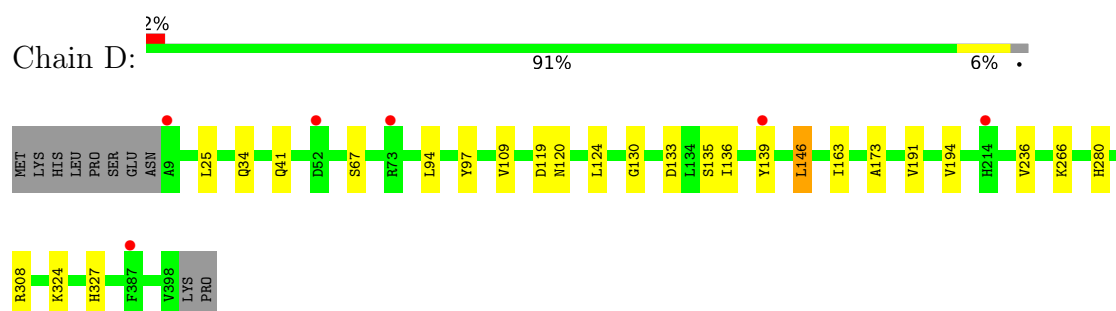
- Molecule 1: Ketoacyl_synth_N domain-containing protein



- Molecule 2: Putative 3-oxoacyl-[ACP] synthase FabV



- Molecule 2: Putative 3-oxoacyl-[ACP] synthase FabV



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.71Å 104.24Å 98.18Å 90.00° 98.24° 90.00°	Depositor
Resolution (Å)	39.05 – 1.88 48.58 – 1.88	Depositor EDS
% Data completeness (in resolution range)	97.6 (39.05-1.88) 91.3 (48.58-1.88)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.79 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.190 , 0.230 0.192 , 0.229	Depositor DCC
R_{free} test set	1984 reflections (2.28%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9395	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0076e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.38	0/1611	0.56	0/2209
1	C	0.38	0/1557	0.53	0/2135
2	B	0.41	1/2993 (0.0%)	0.56	0/4064
2	D	0.41	0/2993	0.58	0/4064
All	All	0.40	1/9154 (0.0%)	0.56	0/12472

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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	370	GLU	CD-OE1	-6.34	1.18	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	THR	Peptide

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	1571	0	1529	25	0
1	C	1519	0	1478	17	0
2	B	2939	0	2910	24	0
2	D	2939	0	2910	13	0
3	A	55	0	0	6	0
3	B	134	0	0	3	0
3	C	84	0	0	4	0
3	D	154	0	0	2	0
All	All	9395	0	8827	77	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 4.

All (77) 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:166:GLN:NE2	3:A:301:HOH:O	2.08	0.86
1:C:180:ALA:N	3:C:301:HOH:O	2.13	0.79
2:D:124:LEU:HD22	2:D:136:ILE:HD13	1.76	0.68
1:A:165:GLU:OE1	3:A:302:HOH:O	2.13	0.66
1:A:176:HIS:CD2	1:A:177:THR:H	2.14	0.65
1:C:3:THR:HG22	1:C:170:GLN:HG2	1.80	0.62
1:A:178:ASP:HB3	1:A:180:ALA:H	1.65	0.61
1:A:165:GLU:N	3:A:302:HOH:O	2.28	0.60
2:B:313:VAL:HG12	2:B:314:TYR:CD2	2.37	0.60
1:A:176:HIS:CG	1:A:177:THR:H	2.19	0.59
2:D:146:LEU:HD11	2:D:194:VAL:HG12	1.85	0.59
1:A:170:GLN:HB3	1:A:202:ASN:OD1	2.02	0.59
2:B:146:LEU:HD11	2:B:194:VAL:HG12	1.85	0.59
1:C:4:LEU:HD13	1:C:6:LEU:CD1	2.34	0.57
1:C:131:ILE:O	3:C:302:HOH:O	2.18	0.56
2:D:97:TYR:OH	3:D:501:HOH:O	1.96	0.56
1:A:179:GLU:O	1:A:181:GLU:N	2.35	0.56
1:C:4:LEU:HD11	1:C:169:LEU:HD23	1.88	0.55
1:A:28:GLN:OE1	1:A:28:GLN:N	2.28	0.54
1:A:113:SER:OG	1:A:116:GLU:OE2	2.10	0.54
2:B:99:ALA:O	3:B:502:HOH:O	2.18	0.54
1:A:125:LEU:HD11	1:A:162:VAL:HG12	1.90	0.53
3:A:301:HOH:O	2:D:133:ASP:OD2	2.18	0.53
1:A:116:GLU:OE1	1:A:177:THR:HG21	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:LYS:NZ	1:C:112:CYS:O	2.28	0.53
2:D:308:ARG:NH2	3:D:506:HOH:O	2.33	0.52
1:A:181:GLU:HG3	1:A:183:PRO:HD2	1.92	0.51
2:D:120:ASN:O	2:D:124:LEU:HD23	2.11	0.51
2:B:113:SER:OG	2:B:195:ASP:OD2	2.27	0.49
1:C:60:LYS:N	1:C:60:LYS:HD3	2.27	0.49
2:B:372:GLU:HB2	3:B:503:HOH:O	2.13	0.48
2:B:352:LEU:HD21	3:B:528:HOH:O	2.13	0.48
2:D:94:LEU:HD13	2:D:236:VAL:HG21	1.95	0.48
2:B:29:LEU:HG	2:B:33:LYS:HE3	1.96	0.48
2:B:109:VAL:O	2:B:191:VAL:HA	2.14	0.48
1:C:63:ASP:OD2	3:C:304:HOH:O	2.20	0.47
2:D:109:VAL:O	2:D:191:VAL:HA	2.14	0.47
2:B:130:GLY:O	2:B:132:THR:N	2.47	0.47
1:C:60:LYS:HD2	1:C:112:CYS:O	2.13	0.47
1:A:176:HIS:NE2	1:A:199:PHE:O	2.34	0.46
2:B:30:ASN:O	2:B:34:GLN:HG2	2.14	0.46
1:A:176:HIS:CG	1:A:177:THR:N	2.84	0.46
2:B:134:LEU:HD12	2:B:135:SER:H	1.79	0.46
1:C:125:LEU:HB3	1:C:164:LEU:HG	1.98	0.46
2:B:40:GLN:O	2:B:324:LYS:HE2	2.17	0.45
1:A:50:ARG:CZ	2:D:130:GLY:HA2	2.47	0.45
2:B:163:ILE:HD12	2:B:173:ALA:HA	1.99	0.44
1:C:149:GLU:HG2	2:D:139:TYR:CZ	2.52	0.44
2:B:313:VAL:HG13	2:B:364:ASP:HB2	1.98	0.44
1:A:144:PRO:HB2	1:A:146:ILE:HG22	1.98	0.44
2:B:94:LEU:HD13	2:B:236:VAL:HG21	2.01	0.43
1:C:4:LEU:CD1	1:C:6:LEU:HD13	2.48	0.43
2:D:25:LEU:HD21	2:D:324:LYS:HB3	2.00	0.43
2:D:163:ILE:HD12	2:D:173:ALA:HA	2.00	0.43
2:B:288:TYR:HB3	2:B:380:VAL:HG22	1.99	0.43
1:A:3:THR:HG22	1:A:170:GLN:HG3	2.01	0.42
2:B:68:VAL:CG1	2:B:72:MET:HB2	2.49	0.42
2:B:338:PHE:O	2:B:342:GLN:HG2	2.19	0.42
1:A:25:PRO:HB2	1:A:28:GLN:OE1	2.19	0.42
1:A:131:ILE:O	3:A:303:HOH:O	2.21	0.42
1:C:60:LYS:NZ	1:C:113:SER:HA	2.35	0.42
1:C:128:MET:HG3	1:C:131:ILE:HD12	2.02	0.42
2:B:250:GLY:O	2:B:392:ILE:HA	2.19	0.42
1:C:112:CYS:HB2	1:C:116:GLU:OE2	2.20	0.42
2:B:294:THR:O	2:B:295:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:HB3	1:A:164:LEU:HG	2.01	0.41
1:C:180:ALA:N	3:C:311:HOH:O	2.53	0.41
1:A:58:VAL:O	1:A:138:ALA:HA	2.20	0.41
1:A:15:GLN:NE2	3:A:305:HOH:O	2.34	0.41
2:B:75:VAL:HB	2:B:145:CYS:SG	2.61	0.41
2:B:170:SER:HB2	2:B:334:ALA:HB2	2.02	0.41
1:A:179:GLU:O	1:A:181:GLU:HG2	2.21	0.41
2:B:123:LEU:H	2:B:123:LEU:HD22	1.84	0.41
2:D:266:LYS:HE3	2:D:266:LYS:HB3	1.90	0.41
1:A:170:GLN:OE1	1:A:202:ASN:ND2	2.51	0.41
1:C:58:VAL:O	1:C:138:ALA:HA	2.21	0.40
2:B:254:ASP:OD1	2:B:267:GLY:HA3	2.22	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	201/204 (98%)	195 (97%)	5 (2%)	1 (0%)	29	17
1	C	194/204 (95%)	194 (100%)	0	0	100	100
2	B	388/400 (97%)	372 (96%)	14 (4%)	2 (0%)	29	17
2	D	388/400 (97%)	378 (97%)	10 (3%)	0	100	100
All	All	1171/1208 (97%)	1139 (97%)	29 (2%)	3 (0%)	41	30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	ALA
2	B	131	GLN
2	B	130	GLY

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	170/172 (99%)	169 (99%)	1 (1%)	86	86
1	C	162/172 (94%)	161 (99%)	1 (1%)	86	86
2	B	314/324 (97%)	308 (98%)	6 (2%)	57	49
2	D	314/324 (97%)	306 (98%)	8 (2%)	47	37
All	All	960/992 (97%)	944 (98%)	16 (2%)	60	54

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	ASP
2	B	41	GLN
2	B	82	PHE
2	B	146	LEU
2	B	280	HIS
2	B	327	HIS
2	B	370	GLU
1	C	60	LYS
2	D	34	GLN
2	D	41	GLN
2	D	67	SER
2	D	119	ASP
2	D	135	SER
2	D	146	LEU
2	D	280	HIS
2	D	327	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	GLN
1	C	76	ASN
2	D	131	GLN

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, 95th 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	203/204 (99%)	0.28	9 (4%) 34 35	16, 27, 43, 58	0
1	C	198/204 (97%)	0.05	3 (1%) 73 75	12, 23, 38, 47	0
2	B	390/400 (97%)	0.04	14 (3%) 42 44	14, 22, 39, 77	0
2	D	390/400 (97%)	-0.09	6 (1%) 73 75	12, 20, 34, 49	0
All	All	1181/1208 (97%)	0.04	32 (2%) 54 56	12, 22, 39, 77	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	176	HIS	6.9
1	A	174	TRP	6.6
1	A	175	THR	6.2
1	C	174	TRP	5.5
1	A	177	THR	5.5
2	B	133	ASP	4.9
2	B	135	SER	4.5
2	B	132	THR	4.2
2	B	129	GLN	4.0
2	B	9	ALA	3.8
2	B	122	LEU	3.7
1	A	179	GLU	3.5
1	A	180	ALA	3.5
2	B	139	TYR	3.4
2	B	52	ASP	3.4
2	B	134	LEU	3.3
2	D	52	ASP	3.3
2	D	387	PHE	3.1
2	D	73	ARG	3.1
2	D	9	ALA	2.9
2	B	66	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	387	PHE	2.8
1	A	28	GLN	2.5
1	C	151	ILE	2.3
1	C	31	ARG	2.3
1	A	151	ILE	2.2
2	B	67	SER	2.2
2	D	139	TYR	2.1
1	A	48	ASP	2.1
2	D	214	HIS	2.0
2	B	65	CYS	2.0
2	B	73	ARG	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.