



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:28 PM GMT

PDB ID : 1P5H  
Title : Crystal structure of Formyl-CoA Transferase (apoenzyme) from *Oxalobacter formigenes*  
Authors : Ricagno, S.; Jonsson, S.; Richards, N.; Lindqvist, Y.  
Deposited on : 2003-04-27  
Resolution : 2.20 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : 1.7 (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

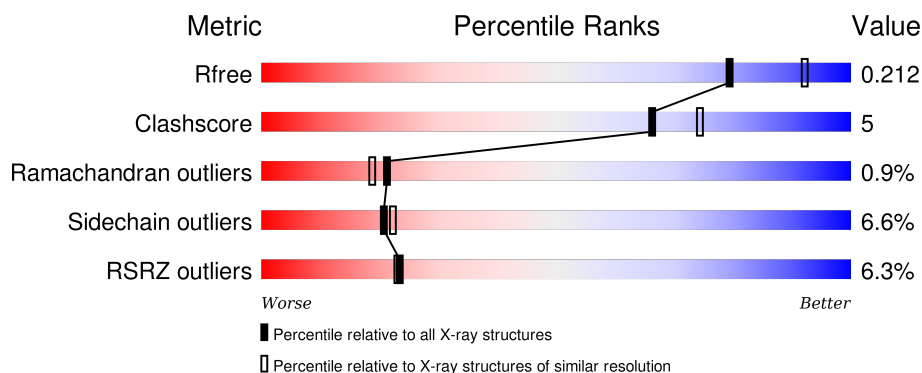
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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. 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	428	<div> <div>4%</div> <div>85%</div> <div>13%</div> </div>
1	B	428	<div> <div>8%</div> <div>81%</div> <div>17%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7154 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 Formyl-coenzyme A transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3312	2095	568	625	24			
1	B	427	Total	C	N	O	S	4	0	0
			3312	2095	568	625	24			

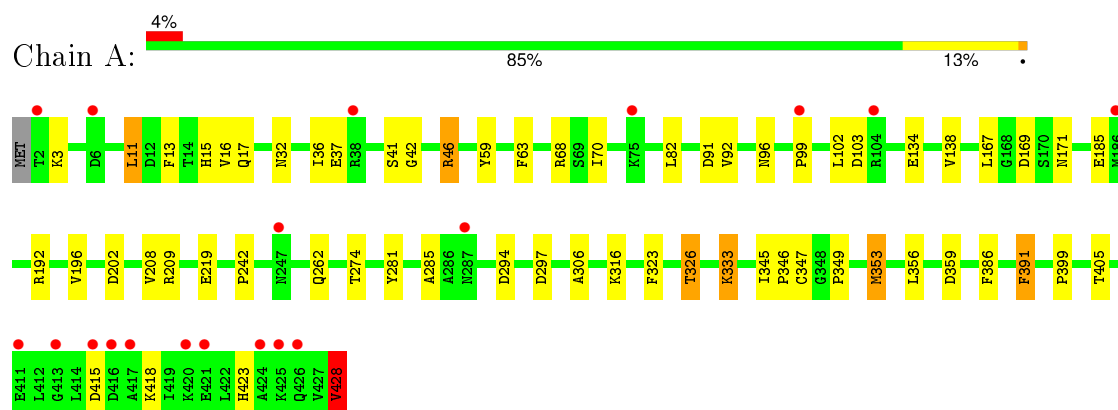
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	278	Total	O	0	0
			278	278		
2	B	252	Total	O	0	0
			252	252		

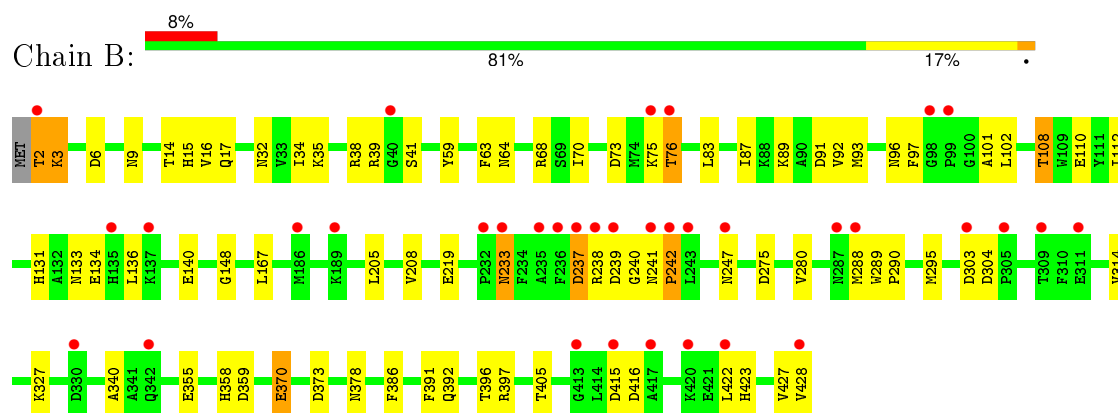
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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: Formyl-coenzyme A transferase



- Molecule 1: Formyl-coenzyme A transferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.44Å 151.44Å 99.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.62 – 2.20 24.61 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.62-2.20) 99.5 (24.61-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.97 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.171 , 0.209 0.177 , 0.212	Depositor DCC
$R_{free}$ test set	2870 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.5	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.1	EDS
Estimated twinning fraction	0.034 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 56693 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7154	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.59	2/3386 (0.1%)	0.84	9/4579 (0.2%)
1	B	0.53	0/3386	0.81	9/4579 (0.2%)
All	All	0.56	2/6772 (0.0%)	0.82	18/9158 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	428	VAL	C-O	-8.44	1.07	1.23
1	A	353	MET	SD-CE	-5.86	1.45	1.77

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	VAL	CA-C-O	14.99	151.57	120.10
1	B	275	ASP	CB-CG-OD2	7.10	124.69	118.30
1	A	202	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	297	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	169	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	359	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	6	ASP	CB-CG-OD2	5.82	123.53	118.30
1	A	91	ASP	CB-CG-OD2	5.72	123.45	118.30
1	B	73	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	46	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	A	103	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	91	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	294	ASP	CB-CG-OD2	5.43	123.18	118.30
1	B	416	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	359	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	303	ASP	CB-CG-OD2	5.26	123.04	118.30
1	B	304	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	242	PRO	CA-N-CD	-5.06	104.42	111.50

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	3312	0	3250	29	0
1	B	3312	0	3250	40	0
2	A	278	0	0	2	1
2	B	252	0	0	4	1
All	All	7154	0	6500	64	1

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 5.

All (64) 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:B:405:THR:HG21	1:B:428:VAL:HG11	1.52	0.91
1:A:405:THR:HG21	1:A:428:VAL:HG13	1.64	0.80
1:B:405:THR:HG21	1:B:428:VAL:CG1	2.17	0.74
1:B:237:ASP:OD1	1:B:239:ASP:O	2.06	0.72
1:A:167:LEU:HD21	1:B:167:LEU:CD2	2.22	0.69
1:B:93:MET:HE1	1:B:112:ILE:HD13	1.75	0.69
1:A:15:HIS:H	1:A:96:ASN:HD21	1.41	0.66
1:A:46:ARG:NH2	1:A:399:PRO:O	2.27	0.66
1:A:167:LEU:HD21	1:B:167:LEU:HD21	1.78	0.64
1:B:295:MET:CE	1:B:340:ALA:HA	2.28	0.64
1:B:9:ASN:OD1	2:B:1099:HOH:O	2.16	0.63
1:B:392:GLN:NE2	2:B:1237:HOH:O	2.13	0.62
1:B:405:THR:CG2	1:B:428:VAL:HG11	2.27	0.60
1:B:422:LEU:HD22	1:B:427:VAL:HG21	1.84	0.59
1:A:306:ALA:HB1	1:A:316:LYS:NZ	2.17	0.59
1:B:208:VAL:O	1:B:208:VAL:HG12	2.02	0.59
1:A:219:GLU:OE2	1:B:358:HIS:HE1	1.87	0.57
1:B:83:LEU:O	1:B:87:ILE:HG13	2.04	0.57
1:A:17:GLN:HG3	1:A:63:PHE:CE2	2.40	0.56
1:A:353:MET:HE3	1:B:148:GLY:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:MET:HE2	1:B:112:ILE:HG21	1.89	0.54
1:A:208:VAL:HG12	1:A:208:VAL:O	2.08	0.53
1:A:262:GLN:HE21	1:A:285:ALA:HA	1.73	0.53
1:B:131:HIS:O	1:B:134:GLU:HB2	2.08	0.53
1:B:14:THR:HB	1:B:96:ASN:ND2	2.24	0.53
1:B:423:HIS:CE1	1:B:428:VAL:HG12	2.44	0.52
1:B:239:ASP:O	1:B:241:ASN:N	2.43	0.51
1:B:14:THR:HB	1:B:96:ASN:HD21	1.75	0.51
1:A:70:ILE:HG22	1:A:405:THR:HA	1.92	0.51
1:A:32:ASN:HD21	1:A:68:ARG:HH21	1.57	0.51
1:B:34:ILE:CG2	1:B:70:ILE:HD11	2.41	0.51
1:B:70:ILE:HG23	1:B:405:THR:HA	1.93	0.50
1:A:423:HIS:CE1	1:A:428:VAL:HG12	2.47	0.50
1:B:108:THR:HG22	1:B:110:GLU:OE1	2.12	0.50
1:B:2:THR:O	1:B:3:LYS:HB2	2.12	0.49
1:A:333:LYS:HG2	1:A:349:PRO:CB	2.42	0.49
1:B:32:ASN:HD21	1:B:68:ARG:HH21	1.59	0.49
1:B:76:THR:HG21	1:B:427:VAL:HG12	1.95	0.49
1:A:242:PRO:HD3	2:A:1057:HOH:O	2.13	0.49
1:A:333:LYS:HG2	1:A:349:PRO:HB3	1.96	0.48
1:B:93:MET:CE	1:B:112:ILE:HG21	2.44	0.47
1:B:97:PHE:HB3	1:B:101:ALA:HB3	1.95	0.47
1:A:281:TYR:O	1:A:347:CYS:HA	2.15	0.47
1:B:370:GLU:HG3	2:B:1146:HOH:O	2.15	0.47
1:A:323:PHE:O	1:A:326:THR:HB	2.14	0.47
1:A:11:LEU:HD12	1:A:13:PHE:CE1	2.50	0.46
1:B:289:TRP:N	1:B:290:PRO:CD	2.79	0.46
1:B:355:GLU:OE2	2:B:1149:HOH:O	2.21	0.45
1:A:37:GLU:HB3	1:A:42:GLY:HA2	1.99	0.45
1:B:38:ARG:HB2	1:B:38:ARG:HE	1.66	0.45
1:A:405:THR:HG21	1:A:428:VAL:CG1	2.40	0.44
1:A:209:ARG:HD2	1:B:63:PHE:CZ	2.52	0.44
1:B:208:VAL:CG1	1:B:208:VAL:O	2.66	0.44
1:B:133:ASN:HB3	1:B:136:LEU:HD12	1.99	0.44
1:B:373:ASP:H	1:B:378:ASN:ND2	2.17	0.43
1:A:167:LEU:O	1:A:171:ASN:HB3	2.19	0.42
1:B:17:GLN:HG3	1:B:63:PHE:CE2	2.53	0.42
1:A:345:ILE:HA	1:A:346:PRO:HD3	1.82	0.42
1:A:3:LYS:HG2	1:A:391:PHE:CD1	2.56	0.41
1:A:306:ALA:HB1	1:A:316:LYS:HZ2	1.83	0.41
1:B:35:LYS:CE	1:B:64:ASN:OD1	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HD11	1:A:36:ILE:HD11	2.04	0.40
1:A:316:LYS:NZ	2:A:1239:HOH:O	2.45	0.40
1:B:15:HIS:H	1:B:96:ASN:HD21	1.68	0.40

All (1) 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)
2:A:1329:HOH:O	2:B:1087:HOH:O[4_555]	2.19	0.01

## 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	425/428 (99%)	408 (96%)	15 (4%)	2 (0%)	34	35
1	B	425/428 (99%)	405 (95%)	14 (3%)	6 (1%)	14	10
All	All	850/856 (99%)	813 (96%)	29 (3%)	8 (1%)	21	19

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	LYS
1	A	16	VAL
1	B	16	VAL
1	B	140	GLU
1	B	237	ASP
1	B	240	GLY
1	A	99	PRO
1	B	233	ASN

### 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	350/351 (100%)	330 (94%)	20 (6%)	25	29
1	B	350/351 (100%)	324 (93%)	26 (7%)	17	17
All	All	700/702 (100%)	654 (93%)	46 (7%)	21	22

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	41	SER
1	A	59	TYR
1	A	82	LEU
1	A	92	VAL
1	A	102	LEU
1	A	134	GLU
1	A	138	VAL
1	A	185	GLU
1	A	192	ARG
1	A	196	VAL
1	A	274	THR
1	A	326	THR
1	A	333	LYS
1	A	356	LEU
1	A	386	PHE
1	A	391	PHE
1	A	415	ASP
1	A	418	LYS
1	A	428	VAL
1	B	2	THR
1	B	39	ARG
1	B	41	SER
1	B	59	TYR
1	B	75	LYS
1	B	76	THR
1	B	89	LYS

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Mol	Chain	Res	Type
1	B	92	VAL
1	B	102	LEU
1	B	108	THR
1	B	205	LEU
1	B	219	GLU
1	B	233	ASN
1	B	238	ARG
1	B	242	PRO
1	B	247	ASN
1	B	280	VAL
1	B	288	MET
1	B	314	VAL
1	B	327	LYS
1	B	370	GLU
1	B	386	PHE
1	B	391	PHE
1	B	396	THR
1	B	397	ARG
1	B	415	ASP

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	32	ASN
1	A	54	ASN
1	A	96	ASN
1	A	262	GLN
1	B	17	GLN
1	B	32	ASN
1	B	96	ASN
1	B	188	HIS
1	B	194	GLN
1	B	206	ASN
1	B	358	HIS
1	B	378	ASN
1	B	423	HIS

### 5.3.3 RNA ⓘ

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](#)

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<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	427/428 (99%)	-0.06	19 (4%) 38 37	18, 29, 68, 95	0
1	B	426/428 (99%)	0.17	35 (8%) 14 14	21, 32, 76, 89	0
All	All	853/856 (99%)	0.06	54 (6%) 23 23	18, 30, 74, 95	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	THR	6.1
1	B	239	ASP	6.0
1	B	233	ASN	5.3
1	B	242	PRO	5.2
1	B	241	ASN	5.2
1	A	413	GLY	4.9
1	A	2	THR	4.8
1	B	303	ASP	4.6
1	B	305	PRO	4.0
1	A	415	ASP	4.0
1	B	232	PRO	3.9
1	A	417	ALA	3.9
1	A	420	LYS	3.9
1	B	236	PHE	3.6
1	A	416	ASP	3.5
1	A	99	PRO	3.5
1	B	237	ASP	3.4
1	A	38	ARG	3.4
1	A	424	ALA	3.4
1	B	417	ALA	3.2
1	B	135	HIS	3.2
1	B	330	ASP	3.1
1	A	421	GLU	3.1
1	B	428	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	247	ASN	3.0
1	B	311	GLU	3.0
1	B	137	LYS	2.9
1	B	415	ASP	2.9
1	A	75	LYS	2.8
1	B	287	ASN	2.8
1	A	186	MET	2.7
1	B	75	LYS	2.7
1	B	243	LEU	2.7
1	B	99	PRO	2.6
1	B	309	THR	2.6
1	B	288	MET	2.5
1	B	238	ARG	2.5
1	A	411	GLU	2.5
1	B	76	THR	2.5
1	A	104	ARG	2.4
1	A	425	LYS	2.4
1	A	247	ASN	2.4
1	B	342	GLN	2.4
1	B	422	LEU	2.3
1	B	420	LYS	2.3
1	B	40	GLY	2.3
1	A	426	GLN	2.3
1	B	186	MET	2.3
1	B	235	ALA	2.2
1	A	6	ASP	2.1
1	B	98	GLY	2.1
1	B	189	LYS	2.1
1	B	413	GLY	2.1
1	A	287	ASN	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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.