



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2016 – 05:49 PM EDT

PDB ID : 5AYP  
Title : Crystal structure of Bacillus stearothermophilus Farnesyl pyrophosphate synthase  
Authors : Makabe, K.; Kijima, T.  
Deposited on : 2015-08-26  
Resolution : 2.31 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
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)	:	rb-20027939

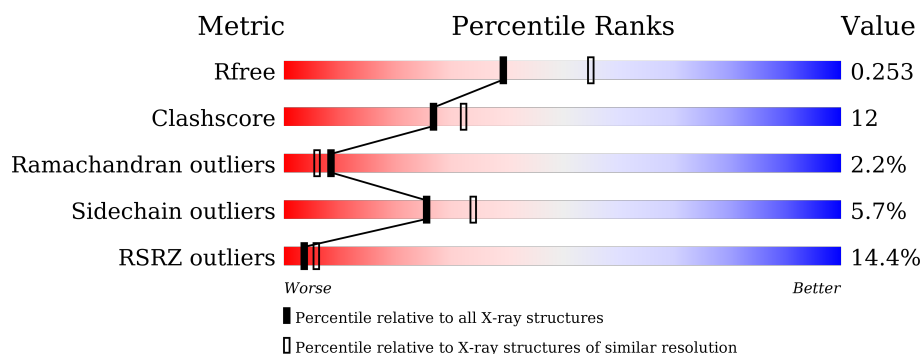
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 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	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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  $\geq 3$ , 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	297	
1	B	297	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4029 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 Farnesyl diphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1977	1244	358	366	9			
1	B	264	Total	C	N	O	S	0	0	0
			2020	1278	357	376	9			

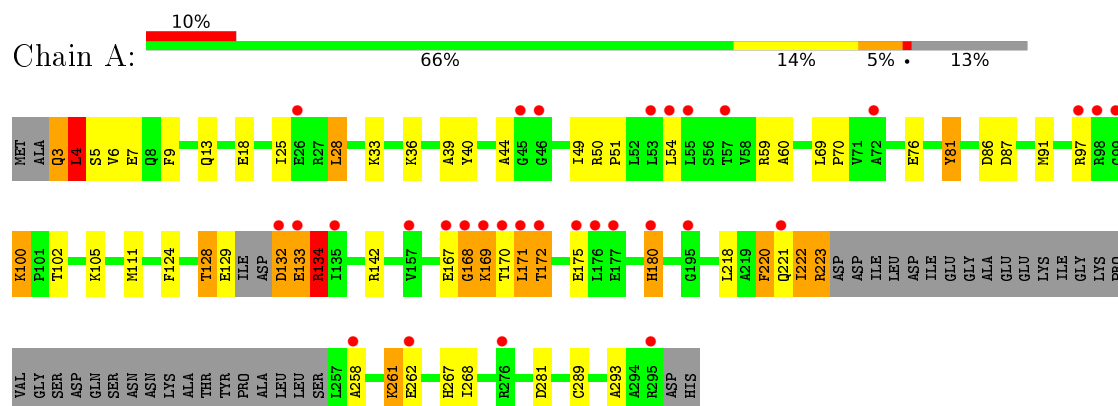
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	20	Total	O	0	0
			20	20		
2	B	12	Total	O	0	0
			12	12		

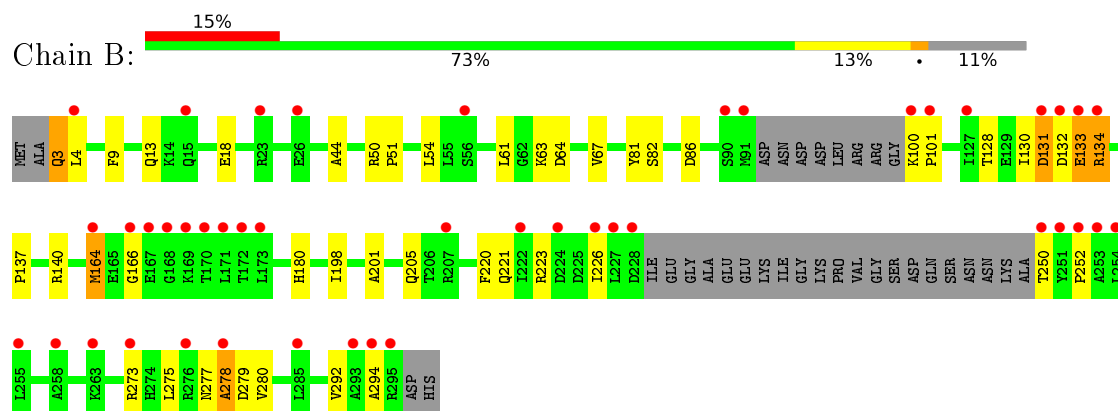
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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: Farnesyl diphosphate synthase



#### • Molecule 1: Farnesyl diphosphate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.02Å 95.16Å 103.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.31 20.08 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-2.31) 99.6 (20.08-2.31)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.48 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.211 , 0.252 0.219 , 0.253	Depositor DCC
$R_{free}$ test set	1117 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.6	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 56.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4029	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.56	0/2005	0.70	0/2699
1	B	0.56	0/2050	0.72	0/2765
All	All	0.56	0/4055	0.71	0/5464

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	THR	Peptide
1	A	134	ARG	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	1977	0	2017	60	0
1	B	2020	0	2063	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	20	0	0	0	0
2	B	12	0	0	0	0
All	All	4029	0	4080	98	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 12.

All (98) 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:278:ALA:HB3	1:B:279:ASP:HA	1.24	1.13
1:B:132:ASP:HB2	1:B:133:GLU:HB2	1.48	0.94
1:B:278:ALA:HB3	1:B:279:ASP:CA	2.00	0.92
1:A:180:HIS:ND1	1:A:221:GLN:HG3	1.86	0.91
1:A:3:GLN:OE1	1:A:3:GLN:N	2.03	0.91
1:A:171:LEU:O	1:A:172:THR:OG1	1.92	0.86
1:B:132:ASP:CB	1:B:133:GLU:HB2	2.07	0.85
1:A:49:ILE:HD13	1:A:220:PHE:HZ	1.44	0.81
1:A:3:GLN:HB3	1:A:6:VAL:H	1.54	0.72
1:B:130:ILE:HG22	1:B:131:ASP:N	2.05	0.71
1:A:87:ASP:OD2	1:A:97:ARG:HD2	1.91	0.70
1:A:49:ILE:HD13	1:A:220:PHE:CZ	2.27	0.69
1:B:275:LEU:O	1:B:278:ALA:HB2	1.93	0.69
1:A:180:HIS:CE1	1:A:221:GLN:HG3	2.29	0.67
1:B:278:ALA:CB	1:B:279:ASP:CA	2.67	0.66
1:A:3:GLN:HA	1:A:4:LEU:CB	2.25	0.66
1:B:63:LYS:NZ	1:B:198:ILE:O	2.23	0.66
1:A:169:LYS:HE2	1:A:170:THR:N	2.10	0.65
1:A:218:LEU:HD13	1:A:267:HIS:CE1	2.31	0.65
1:B:130:ILE:O	1:B:131:ASP:CB	2.45	0.63
1:A:223:ARG:HH11	1:A:223:ARG:HG3	1.64	0.63
1:A:222:ILE:O	1:A:223:ARG:HG2	2.00	0.62
1:A:169:LYS:O	1:A:171:LEU:HD12	1.99	0.61
1:A:180:HIS:C	1:A:180:HIS:ND1	2.53	0.61
1:B:134:ARG:HG2	1:B:134:ARG:HH11	1.64	0.61
1:A:220:PHE:O	1:A:223:ARG:HD3	2.00	0.61
1:A:180:HIS:CG	1:A:221:GLN:HG3	2.36	0.60
1:A:171:LEU:O	1:A:172:THR:CB	2.50	0.59
1:A:111:MET:HE2	1:B:164:MET:HG2	1.83	0.59
1:B:132:ASP:CA	1:B:133:GLU:HB2	2.32	0.59
1:B:128:THR:O	1:B:140:ARG:NH2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PHE:CE1	1:A:59:ARG:HD2	2.38	0.58
1:A:167:GLU:O	1:A:169:LYS:N	2.37	0.57
1:A:167:GLU:O	1:A:168:GLY:C	2.43	0.56
1:A:258:ALA:O	1:A:261:LYS:HG3	2.05	0.56
1:A:128:THR:O	1:A:132:ASP:N	2.37	0.56
1:B:275:LEU:O	1:B:278:ALA:CB	2.53	0.56
1:A:268:ILE:HG13	1:A:293:ALA:HB2	1.88	0.56
1:A:180:HIS:HB2	1:A:221:GLN:HE21	1.71	0.55
1:A:3:GLN:CG	1:A:5:SER:HB2	2.37	0.55
1:B:273:ARG:NH2	1:B:277:ASN:OD1	2.39	0.55
1:B:223:ARG:HD2	1:B:292:VAL:HG13	1.89	0.55
1:B:130:ILE:CG2	1:B:131:ASP:N	2.70	0.54
1:A:172:THR:HB	1:A:175:GLU:HB2	1.91	0.53
1:A:258:ALA:O	1:A:261:LYS:CG	2.57	0.53
1:B:250:THR:HB	1:B:252:PRO:HD2	1.92	0.51
1:B:131:ASP:HB2	1:B:140:ARG:NH1	2.25	0.50
1:B:223:ARG:HA	1:B:226:ILE:HG22	1.92	0.50
1:A:51:PRO:HG3	1:A:76:GLU:HB2	1.93	0.50
1:A:9:PHE:O	1:A:13:GLN:HG2	2.12	0.50
1:B:220:PHE:O	1:B:223:ARG:HG2	2.12	0.50
1:A:133:GLU:HA	1:A:134:ARG:HH21	1.77	0.49
1:A:261:LYS:HG3	1:A:262:GLU:N	2.28	0.49
1:A:132:ASP:OD1	1:A:132:ASP:C	2.51	0.49
1:A:3:GLN:HA	1:A:4:LEU:HB3	1.95	0.48
1:B:50:ARG:HB2	1:B:51:PRO:HD3	1.95	0.48
1:A:132:ASP:O	1:A:133:GLU:O	2.32	0.48
1:B:205:GLN:HG2	1:B:278:ALA:O	2.15	0.47
1:A:25:ILE:O	1:A:28:LEU:HB2	2.15	0.47
1:B:180:HIS:CE1	1:B:221:GLN:HG2	2.50	0.47
1:B:180:HIS:CD2	1:B:221:GLN:HG2	2.49	0.47
1:A:40:TYR:OH	1:A:100:LYS:HD3	2.14	0.47
1:A:223:ARG:N	1:A:223:ARG:HD3	2.29	0.46
1:A:33:LYS:HA	1:A:36:LYS:HE3	1.96	0.46
1:A:60:ALA:HA	1:A:281:ASP:O	2.16	0.46
1:A:3:GLN:HG2	1:A:5:SER:HB2	1.97	0.46
1:A:3:GLN:HB3	1:A:5:SER:N	2.31	0.46
1:A:3:GLN:HB2	1:A:6:VAL:HG13	1.98	0.45
1:B:3:GLN:HB2	1:B:4:LEU:H	1.66	0.45
1:B:180:HIS:CG	1:B:221:GLN:HG2	2.51	0.45
1:A:97:ARG:HG3	1:A:102:THR:HG22	1.99	0.45
1:B:9:PHE:O	1:B:13:GLN:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ILE:O	1:B:131:ASP:HB3	2.16	0.45
1:B:82:SER:O	1:B:86:ASP:HB2	2.17	0.44
1:A:4:LEU:HA	1:A:7:GLU:HG2	1.99	0.44
1:A:81:TYR:CD1	1:A:81:TYR:C	2.91	0.44
1:B:133:GLU:O	1:B:134:ARG:HB2	2.18	0.44
1:A:180:HIS:C	1:A:180:HIS:HD1	2.21	0.43
1:A:40:TYR:O	1:A:44:ALA:HB2	2.19	0.43
1:A:25:ILE:HG21	1:A:39:ALA:HB2	2.00	0.43
1:A:50:ARG:HB2	1:A:51:PRO:HD3	2.01	0.43
1:A:180:HIS:NE2	1:A:218:LEU:HD23	2.34	0.43
1:B:44:ALA:CB	1:B:101:PRO:HG3	2.49	0.43
1:B:223:ARG:CD	1:B:292:VAL:HG13	2.49	0.42
1:A:129:GLU:O	1:A:132:ASP:HA	2.20	0.42
1:B:134:ARG:CG	1:B:134:ARG:HH11	2.31	0.42
1:A:222:ILE:C	1:A:223:ARG:HG2	2.39	0.41
1:B:278:ALA:CB	1:B:280:VAL:HG22	2.50	0.41
1:B:61:LEU:HD11	1:B:201:ALA:HB2	2.01	0.41
1:B:54:LEU:HD23	1:B:54:LEU:C	2.41	0.41
1:B:279:ASP:OD1	1:B:279:ASP:N	2.54	0.41
1:A:220:PHE:C	1:A:222:ILE:H	2.22	0.40
1:A:124:PHE:O	1:A:128:THR:HG23	2.20	0.40
1:A:54:LEU:C	1:A:54:LEU:HD23	2.41	0.40
1:A:86:ASP:HA	1:A:91:MET:HG2	2.02	0.40
1:A:69:LEU:HB3	1:A:70:PRO:HD3	2.03	0.40
1:A:3:GLN:CB	1:A:6:VAL:HG13	2.52	0.40
1:B:64:ASP:O	1:B:67:VAL:HG12	2.21	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	252/297 (85%)	240 (95%)	7 (3%)	5 (2%)	9	7
1	B	258/297 (87%)	244 (95%)	8 (3%)	6 (2%)	8	5
All	All	510/594 (86%)	484 (95%)	15 (3%)	11 (2%)	8	6

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	133	GLU
1	A	172	THR
1	B	131	ASP
1	B	133	GLU
1	B	134	ARG
1	B	278	ALA
1	A	168	GLY
1	A	222	ILE
1	B	294	ALA
1	B	166	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	199/231 (86%)	182 (92%)	17 (8%)	13	15
1	B	205/231 (89%)	199 (97%)	6 (3%)	50	66
All	All	404/462 (87%)	381 (94%)	23 (6%)	25	34

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	4	LEU
1	A	18	GLU
1	A	28	LEU
1	A	81	TYR

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Mol	Chain	Res	Type
1	A	100	LYS
1	A	105	LYS
1	A	132	ASP
1	A	134	ARG
1	A	142	ARG
1	A	169	LYS
1	A	171	LEU
1	A	180	HIS
1	A	220	PHE
1	A	223	ARG
1	A	261	LYS
1	A	289	CYS
1	B	3	GLN
1	B	18	GLU
1	B	81	TYR
1	B	100	LYS
1	B	137	PRO
1	B	164	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	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 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	258/297 (86%)	0.57	31 (12%) 6 9	30, 42, 82, 106	0
1	B	264/297 (88%)	0.82	44 (16%) 2 4	30, 45, 82, 101	0
All	All	522/594 (87%)	0.69	75 (14%) 3 6	30, 43, 82, 106	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	132	ASP	9.6
1	B	227	LEU	8.3
1	B	133	GLU	7.6
1	A	168	GLY	7.2
1	B	170	THR	7.1
1	A	295	ARG	6.8
1	A	171	LEU	6.7
1	B	250	THR	5.5
1	A	170	THR	5.4
1	B	226	ILE	5.4
1	B	295	ARG	5.2
1	A	172	THR	4.9
1	B	294	ALA	4.8
1	B	167	GLU	4.8
1	B	169	LYS	4.8
1	B	134	ARG	4.6
1	A	98	ARG	4.5
1	B	131	ASP	4.3
1	B	168	GLY	4.2
1	B	278	ALA	4.2
1	A	167	GLU	4.1
1	B	258	ALA	4.1
1	B	255	LEU	3.8
1	A	169	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	26	GLU	3.8
1	A	133	GLU	3.6
1	A	258	ALA	3.6
1	A	54	LEU	3.5
1	B	91	MET	3.3
1	A	99	GLY	3.2
1	B	251	TYR	3.2
1	A	46	GLY	3.2
1	B	171	LEU	3.2
1	B	173	LEU	3.1
1	A	97	ARG	3.1
1	B	252	PRO	3.1
1	B	276	ARG	3.1
1	B	207	ARG	3.1
1	A	45	GLY	3.1
1	A	135	ILE	3.1
1	B	4	LEU	3.0
1	B	15	GLN	2.9
1	B	26	GLU	2.9
1	B	100	LYS	2.9
1	B	164	MET	2.9
1	A	132	ASP	2.9
1	B	224	ASP	2.8
1	A	177	GLU	2.7
1	A	276	ARG	2.6
1	B	127	ILE	2.6
1	A	57	THR	2.5
1	A	180	HIS	2.5
1	B	90	SER	2.4
1	A	195	GLY	2.4
1	B	172	THR	2.4
1	B	273	ARG	2.4
1	A	175	GLU	2.3
1	B	253	ALA	2.3
1	B	263	LYS	2.3
1	B	166	GLY	2.3
1	B	293	ALA	2.3
1	B	254	LEU	2.3
1	B	101	PRO	2.3
1	B	222	ILE	2.3
1	A	55	LEU	2.2
1	A	176	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	157	VAL	2.2
1	B	228	ASP	2.2
1	B	285	LEU	2.2
1	B	23	ARG	2.2
1	B	56	SER	2.2
1	A	262	GLU	2.1
1	A	72	ALA	2.1
1	A	221	GLN	2.0
1	A	53	LEU	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.