



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:01 AM GMT

PDB ID : 3M0G  
Title : CRYSTAL STRUCTURE OF putative farnesyl diphosphate synthase from Rhodobacter capsulatus  
Authors : Malashkevich, V.N.; Toro, R.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2010-03-03  
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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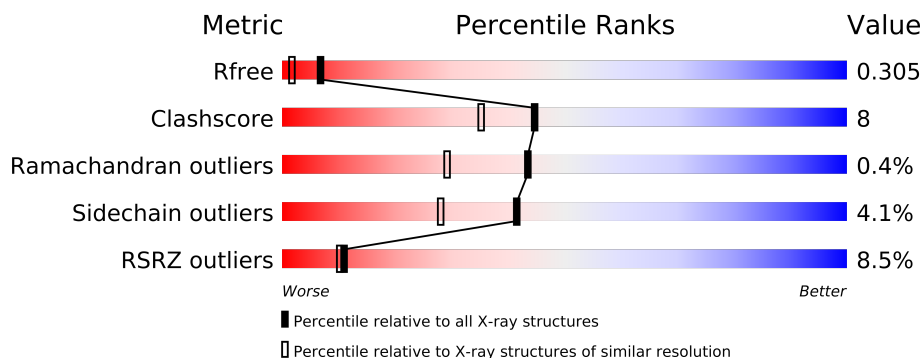
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.90 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))
$R_{free}$	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 4142 atoms, of which 0 are hydrogen and 0 are deuterium.

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	264	Total	C	N	O	S	Se	0	0	0
			1896	1189	329	368	3	7			
1	B	268	Total	C	N	O	S	Se	0	0	0
			1931	1210	337	374	3	7			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP Q9KWR7
A	2	SER	-	expression tag	UNP Q9KWR7
A	3	LEU	-	expression tag	UNP Q9KWR7
A	13	ALA	GLY	see remark 999	UNP Q9KWR7
A	16	THR	ALA	see remark 999	UNP Q9KWR7
A	61	ALA	GLU	see remark 999	UNP Q9KWR7
A	100	LYS	ARG	see remark 999	UNP Q9KWR7
A	104	ASP	GLU	see remark 999	UNP Q9KWR7
A	193	LEU	ILE	see remark 999	UNP Q9KWR7
A	199	GLY	ALA	see remark 999	UNP Q9KWR7
A	200	PRO	LEU	see remark 999	UNP Q9KWR7
A	202	THR	ALA	see remark 999	UNP Q9KWR7
A	224	ASN	ASP	see remark 999	UNP Q9KWR7
A	250	ALA	PRO	see remark 999	UNP Q9KWR7
A	254	SER	ALA	see remark 999	UNP Q9KWR7
A	275	SER	ALA	see remark 999	UNP Q9KWR7
A	290	GLU	-	expression tag	UNP Q9KWR7
A	291	GLY	-	expression tag	UNP Q9KWR7
A	292	HIS	-	expression tag	UNP Q9KWR7
A	293	HIS	-	expression tag	UNP Q9KWR7
A	294	HIS	-	expression tag	UNP Q9KWR7
A	295	HIS	-	expression tag	UNP Q9KWR7
A	296	HIS	-	expression tag	UNP Q9KWR7
A	297	HIS	-	expression tag	UNP Q9KWR7
B	1	MSE	-	expression tag	UNP Q9KWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	SER	-	expression tag	UNP Q9KWR7
B	3	LEU	-	expression tag	UNP Q9KWR7
B	13	ALA	GLY	see remark 999	UNP Q9KWR7
B	16	THR	ALA	see remark 999	UNP Q9KWR7
B	61	ALA	GLU	see remark 999	UNP Q9KWR7
B	100	LYS	ARG	see remark 999	UNP Q9KWR7
B	104	ASP	GLU	see remark 999	UNP Q9KWR7
B	193	LEU	ILE	see remark 999	UNP Q9KWR7
B	199	GLY	ALA	see remark 999	UNP Q9KWR7
B	200	PRO	LEU	see remark 999	UNP Q9KWR7
B	202	THR	ALA	see remark 999	UNP Q9KWR7
B	224	ASN	ASP	see remark 999	UNP Q9KWR7
B	250	ALA	PRO	see remark 999	UNP Q9KWR7
B	254	SER	ALA	see remark 999	UNP Q9KWR7
B	275	SER	ALA	see remark 999	UNP Q9KWR7
B	290	GLU	-	expression tag	UNP Q9KWR7
B	291	GLY	-	expression tag	UNP Q9KWR7
B	292	HIS	-	expression tag	UNP Q9KWR7
B	293	HIS	-	expression tag	UNP Q9KWR7
B	294	HIS	-	expression tag	UNP Q9KWR7
B	295	HIS	-	expression tag	UNP Q9KWR7
B	296	HIS	-	expression tag	UNP Q9KWR7
B	297	HIS	-	expression tag	UNP Q9KWR7

- Molecule 2 is water.

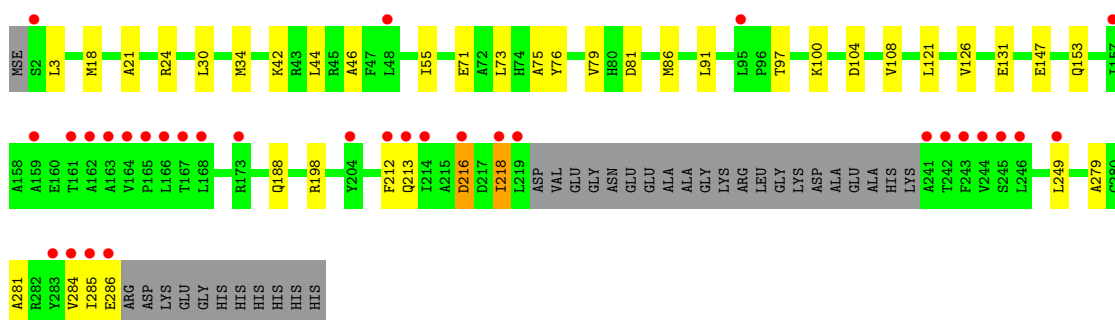
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	135	Total O 135 135	0	0
2	B	180	Total O 180 180	0	0

### 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.

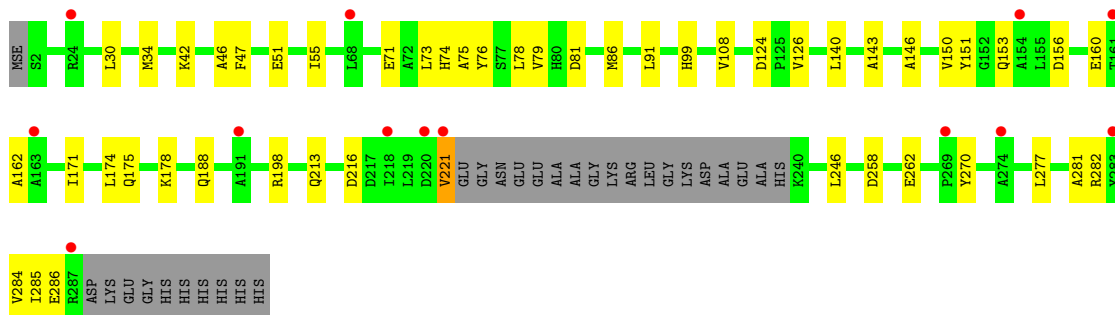
- Molecule 1: Farnesyl diphosphate synthase

Chain A: 



- Molecule 1: Farnesyl diphosphate synthase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.23Å 90.68Å 133.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.97 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-1.90) 99.5 (19.97-1.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.83 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.261 , 0.294 0.267 , 0.305	Depositor DCC
$R_{free}$ test set	2396 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.7	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 23.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	1 of 47500 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	4142	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.50	0/1912	0.61	0/2587
1	B	0.52	0/1947	0.64	0/2633
All	All	0.51	0/3859	0.62	0/5220

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1896	0	1912	19	0
1	B	1931	0	1951	46	0
2	A	135	0	0	3	0
2	B	180	0	0	18	0
All	All	4142	0	3863	65	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (65) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:42:LYS:HE2	1:A:44:LEU:HB2	1.38	1.05

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:281:ALA:O	1:B:284:VAL:HG12	1.75	0.85
1:B:143:ALA:HB3	2:B:410:HOH:O	1.83	0.78
1:B:282:ARG:HB3	1:B:286:GLU:OE1	1.86	0.74
1:B:188:GLN:OE1	1:B:198:ARG:HD2	1.89	0.73
1:B:153:GLN:CA	2:B:363:HOH:O	2.40	0.68
1:A:18:MSE:HG2	2:A:300:HOH:O	1.97	0.63
1:A:188:GLN:OE1	1:A:198:ARG:HD2	1.98	0.63
1:B:171:ILE:CD1	1:B:246:LEU:HD12	2.28	0.63
1:B:178:LYS:HG3	2:B:363:HOH:O	1.98	0.63
1:B:284:VAL:HG13	1:B:285:ILE:HG23	1.82	0.61
1:B:42:LYS:NZ	2:B:370:HOH:O	2.36	0.58
1:B:47:PHE:O	1:B:51:GLU:HG2	2.05	0.56
1:A:281:ALA:O	1:A:284:VAL:HG22	2.06	0.56
1:B:258:ASP:O	1:B:262:GLU:HG2	2.06	0.56
1:B:30:LEU:O	1:B:34:MSE:HG3	2.06	0.55
1:B:221:VAL:HG12	2:B:464:HOH:O	2.05	0.55
1:B:153:GLN:HA	2:B:363:HOH:O	2.05	0.55
2:A:407:HOH:O	1:B:108:VAL:HG13	2.07	0.54
1:B:153:GLN:N	2:B:363:HOH:O	2.40	0.54
1:B:156:ASP:HA	1:B:174:LEU:HD11	1.89	0.53
1:A:285:ILE:O	1:A:286:GLU:HB2	2.09	0.52
1:A:46:ALA:HB2	1:A:71:GLU:CG	2.39	0.52
1:B:46:ALA:HB2	1:B:71:GLU:HG2	1.92	0.52
1:B:175:GLN:HG3	1:B:213:GLN:HG2	1.92	0.52
1:B:156:ASP:OD2	1:B:178:LYS:HE3	2.11	0.51
1:B:175:GLN:CD	1:B:213:GLN:HG2	2.31	0.50
1:B:150:VAL:HA	2:B:401:HOH:O	2.11	0.50
1:B:46:ALA:HB2	1:B:71:GLU:CG	2.42	0.50
1:A:42:LYS:CE	1:A:44:LEU:HB2	2.28	0.49
1:A:147:GLU:HB2	2:A:381:HOH:O	2.13	0.49
1:B:171:ILE:HD13	1:B:246:LEU:HD12	1.95	0.48
1:B:81:ASP:OD1	1:B:86:MSE:CE	2.62	0.48
1:B:140:LEU:HD12	2:B:410:HOH:O	2.15	0.47
1:B:124:ASP:N	2:B:341:HOH:O	2.48	0.47
1:B:198:ARG:NH2	2:B:323:HOH:O	2.48	0.47
1:A:86:MSE:HE1	1:A:153:GLN:CG	2.44	0.47
1:A:30:LEU:O	1:A:34:MSE:HG3	2.15	0.47
1:B:74:HIS:CE1	1:B:78:LEU:HD11	2.50	0.46
1:B:171:ILE:HD11	1:B:246:LEU:HD12	1.97	0.46
1:A:81:ASP:HA	1:A:86:MSE:HE2	1.96	0.46
1:B:270:TYR:OH	2:B:305:HOH:O	2.19	0.45
1:A:212:PHE:O	1:A:216:ASP:HB2	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:153:GLN:NE2	1:B:178:LYS:HE2	2.32	0.45
1:A:3:LEU:HD13	1:A:279:ALA:HB3	1.99	0.45
1:A:218:ILE:O	1:A:218:ILE:HG22	2.17	0.45
1:A:81:ASP:OD1	1:A:86:MSE:HE2	2.17	0.45
1:B:42:LYS:HG2	2:B:398:HOH:O	2.17	0.44
1:B:178:LYS:HD3	2:B:414:HOH:O	2.17	0.44
1:A:75:ALA:O	1:A:79:VAL:HG23	2.17	0.44
1:A:21:ALA:O	1:A:24:ARG:HG2	2.18	0.43
1:B:175:GLN:CG	1:B:213:GLN:HG2	2.47	0.43
1:B:146:ALA:O	1:B:151:TYR:HB2	2.18	0.43
1:B:153:GLN:HB2	2:B:363:HOH:O	2.18	0.43
1:B:47:PHE:CE2	1:B:51:GLU:HG3	2.54	0.42
1:B:124:ASP:OD1	1:B:126:VAL:HB	2.20	0.42
1:A:104:ASP:O	1:A:108:VAL:HG23	2.19	0.42
1:B:156:ASP:O	1:B:160:GLU:HG2	2.19	0.42
1:B:55:ILE:HD11	1:B:277:LEU:HD12	2.02	0.42
1:B:153:GLN:CB	2:B:363:HOH:O	2.67	0.41
1:B:153:GLN:HE22	1:B:178:LYS:HE2	1.85	0.41
1:A:97:THR:OG1	1:A:100:LYS:HG2	2.21	0.41
1:B:75:ALA:O	1:B:79:VAL:HG23	2.22	0.40
1:B:99:HIS:HD2	2:B:405:HOH:O	2.03	0.40
1:B:124:ASP:HB2	2:B:341:HOH:O	2.20	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	260/297 (88%)	253 (97%)	6 (2%)	1 (0%)	43	29
1	B	264/297 (89%)	256 (97%)	7 (3%)	1 (0%)	43	29
All	All	524/594 (88%)	509 (97%)	13 (2%)	2 (0%)	43	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	162	ALA
1	A	218	ILE

### 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	179/196 (91%)	169 (94%)	10 (6%)	30	16
1	B	183/196 (93%)	178 (97%)	5 (3%)	57	47
All	All	362/392 (92%)	347 (96%)	15 (4%)	41	28

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ILE
1	A	73	LEU
1	A	76	TYR
1	A	91	LEU
1	A	121	LEU
1	A	126	VAL
1	A	131	GLU
1	A	213	GLN
1	A	216	ASP
1	A	249	LEU
1	B	73	LEU
1	B	76	TYR
1	B	91	LEU
1	B	216	ASP
1	B	221	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	88	ASN
1	A	153	GLN
1	B	88	ASN

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Mol	Chain	Res	Type
1	B	99	HIS
1	B	153	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

### 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<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	264/297 (88%)	0.91	32 (12%) 5 4	3, 11, 36, 41	0
1	B	268/297 (90%)	0.68	13 (4%) 28 28	2, 11, 23, 37	0
All	All	532/594 (89%)	0.79	45 (8%) 11 10	2, 11, 31, 41	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164	VAL	6.7
1	A	245	SER	6.1
1	B	287	ARG	4.9
1	A	163	ALA	4.9
1	A	241	ALA	3.9
1	A	161	THR	3.8
1	A	167	THR	3.6
1	A	242	THR	3.6
1	A	283	TYR	3.5
1	A	243	PHE	3.5
1	A	244	VAL	3.4
1	A	95	LEU	3.3
1	A	284	VAL	3.3
1	A	173	ARG	3.2
1	A	249	LEU	3.1
1	A	219	LEU	2.9
1	A	168	LEU	2.8
1	B	269	PRO	2.8
1	A	285	ILE	2.8
1	A	162	ALA	2.6
1	A	246	LEU	2.6
1	A	157	ILE	2.6
1	B	191	ALA	2.6
1	B	161	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	221	VAL	2.6
1	A	2	SER	2.5
1	A	166	LEU	2.5
1	B	220	ASP	2.4
1	B	283	TYR	2.4
1	A	159	ALA	2.3
1	A	214	ILE	2.3
1	B	218	ILE	2.3
1	A	48	LEU	2.3
1	A	213	GLN	2.2
1	A	218	ILE	2.2
1	B	68	LEU	2.2
1	A	165	PRO	2.2
1	B	163	ALA	2.2
1	A	212	PHE	2.2
1	B	274	ALA	2.1
1	B	24	ARG	2.1
1	A	216	ASP	2.1
1	A	204	TYR	2.1
1	A	286	GLU	2.1
1	B	154	ALA	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 ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.