Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2021 – 07:02 PM EST

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)

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

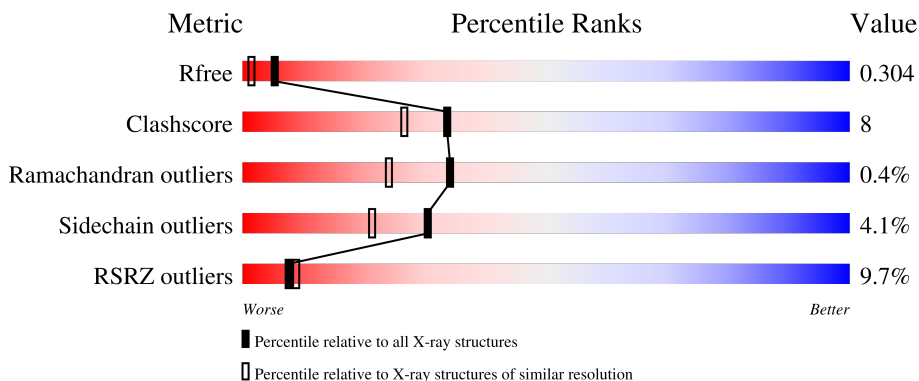|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 1.90 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	Percentile Ranks	Value
Rfree		0.304
Clashscore		8
Ramachandran outliers		0.4%
Sidechain outliers		4.1%
RSRZ outliers		9.7%

Worse *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 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	297	11% / 76% 12% · 11%
1	B	297	6% / 74% 16% 10%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 4142 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	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 135	O 135	0	0
2	B	180	Total 180	O 180	0	0

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: Farnesyl diphosphate synthase
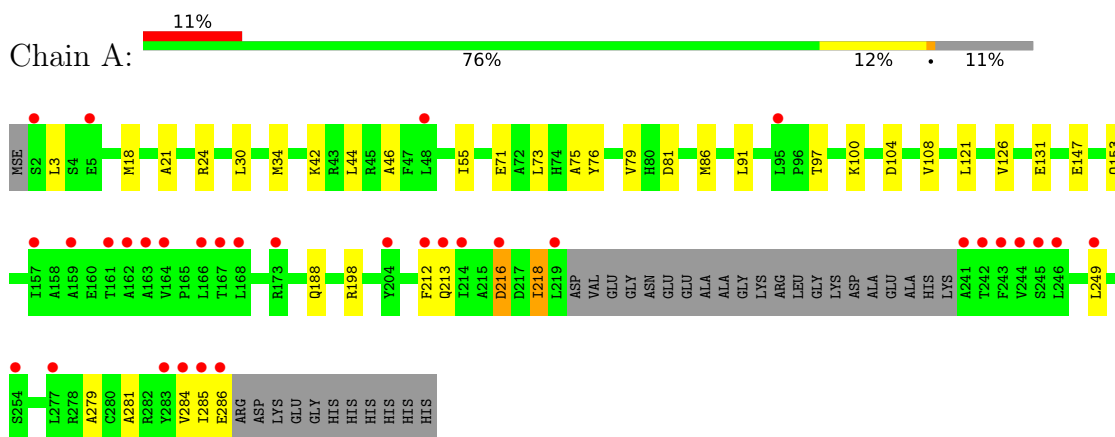
• Molecule 1: Farnesyl diphosphate synthase
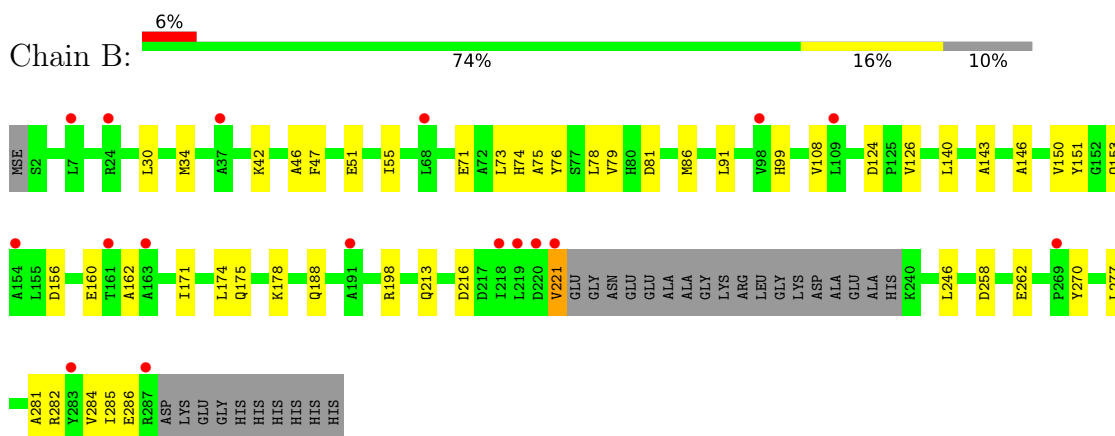
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	3.83 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.261 , 0.294 0.266 , 0.304	Depositor DCC
R_{free} test set	2396 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	19.7	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.0	EDS
L-test for twinning[2]	$< |L| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	4142	wwPDB-VP
Average B, all atoms (Å^2)	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.*

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[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	0.50	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　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	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

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 8.

All (65) 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:42:LYS:HE2	1:A:44:LEU:HB2	1.38	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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:188:GLN:OE1	1:A:198:ARG:HD2	1.98	0.63
1:A:18:MSE:HG2	2:A:300:HOH:O	1.97	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:150:VAL:HA	2:B:401:HOH:O	2.11	0.50
1:B:175:GLN:CD	1:B:213:GLN:HG2	2.31	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:A:86:MSE:HE1	1:A:153:GLN:CG	2.44	0.47
1:B:198:ARG:NH2	2:B:323:HOH:O	2.48	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:A:81:ASP:HA	1:A:86:MSE:HE2	1.96	0.46
1:B:171:ILE:HD11	1:B:246:LEU:HD12	1.97	0.46
1:B:270:TYR:OH	2:B:305:HOH:O	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:PHE:O	1:A:216:ASP:HB2	2.17	0.45
1:A:3:LEU:HD13	1:A:279:ALA:HB3	1.99	0.45
1:B:153:GLN:NE2	1:B:178:LYS:HE2	2.32	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%)	34	24
1	B	264/297 (89%)	256 (97%)	7 (3%)	1 (0%)	34	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	524/594 (88%)	509 (97%)	13 (2%)	2 (0%)	34	24

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%)	21	11
1	B	183/196 (93%)	178 (97%)	5 (3%)	44	38
All	All	362/392 (92%)	347 (96%)	15 (4%)	30	21

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

Sometimes 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
1	B	99	HIS
1	B	153	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides 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, 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	257/297 (86%)	0.97	33 (12%)	3	4	3, 11, 36, 41	0
1	B	261/297 (87%)	0.73	17 (6%)	18	21	2, 11, 23, 37	0
All	All	518/594 (87%)	0.85	50 (9%)	7	9	2, 11, 31, 41	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164	VAL	7.7
1	A	245	SER	6.4
1	A	163	ALA	5.2
1	B	287	ARG	5.1
1	A	161	THR	4.5
1	A	244	VAL	4.0
1	A	283	TYR	3.9
1	A	167	THR	3.7
1	A	95	LEU	3.7
1	A	242	THR	3.6
1	A	241	ALA	3.5
1	A	284	VAL	3.5
1	A	173	ARG	3.4
1	A	219	LEU	3.4
1	A	2	SER	3.0
1	A	243	PHE	3.0
1	A	168	LEU	2.9
1	B	221	VAL	2.8
1	B	269	PRO	2.8
1	A	162	ALA	2.8
1	A	157	ILE	2.8
1	B	163	ALA	2.7
1	B	220	ASP	2.7
1	A	285	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	191	ALA	2.7
1	A	166	LEU	2.7
1	A	249	LEU	2.7
1	A	254	SER	2.5
1	B	161	THR	2.5
1	A	159	ALA	2.5
1	B	283	TYR	2.5
1	A	286	GLU	2.5
1	A	48	LEU	2.4
1	A	216	ASP	2.4
1	B	7	LEU	2.3
1	A	204	TYR	2.3
1	B	218	ILE	2.3
1	B	68	LEU	2.3
1	A	212	PHE	2.3
1	A	246	LEU	2.3
1	A	214	ILE	2.2
1	B	24	ARG	2.2
1	B	154	ALA	2.1
1	A	277	LEU	2.1
1	B	219	LEU	2.1
1	B	109	LEU	2.1
1	A	213	GLN	2.0
1	B	37	ALA	2.0
1	B	98	VAL	2.0
1	A	5	GLU	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 monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.