Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:24 PM GMT

PDB ID	:	1FHU
Title	:	CRYSTAL STRUCTURE ANALYSIS OF O-SUCCINYLBENZOATE SYNTHASE FROM E. COLI
Authors	:	Rayment, I.; Thompson, T.B.; Gerlt, J.A.
Deposited on	:	2000-08-02
Resolution	:	1.65 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

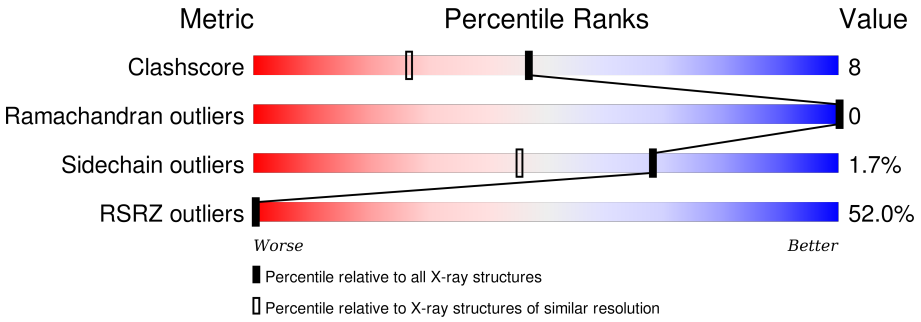
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.65 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))
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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 >=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 <=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	320	48% 69% 20% • 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2632 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 O-SUCCINYLBENZOATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2281	1447	394	430	10			

- Molecule 2 is water.

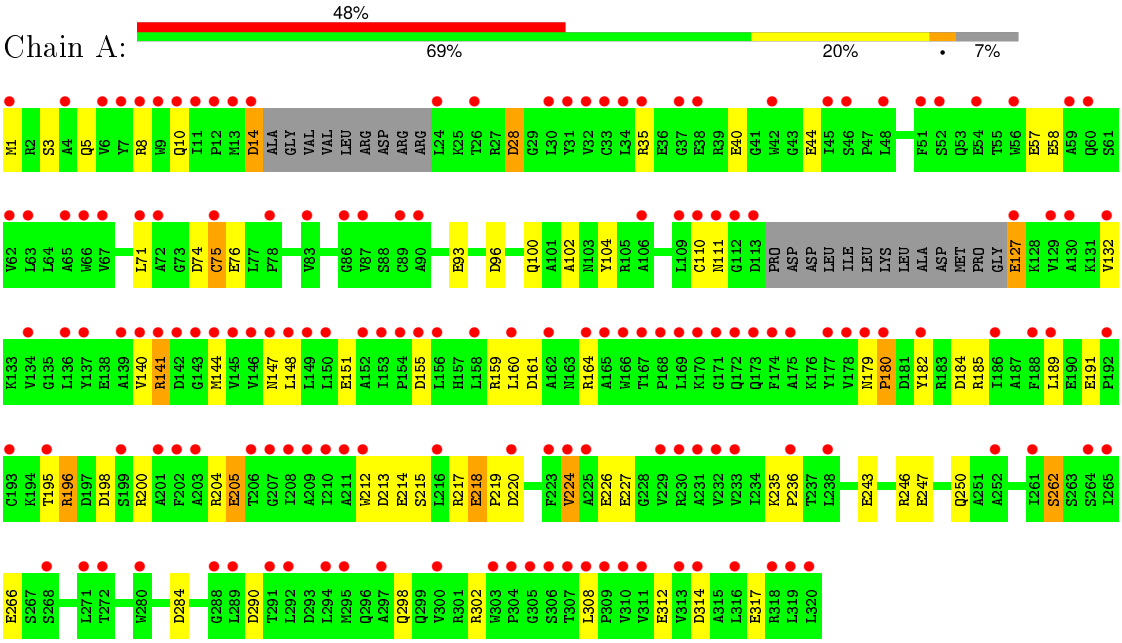
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	351	Total	O	0	0
			351	351		

3 Residue-property plots (i)

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: O-SUCCINYLBENZOATE SYNTHASE

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.10Å 70.00Å 80.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.65 20.10 – 1.52	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-1.65) 97.8 (20.10-1.52)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.03 (at 1.52Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.195 , 0.265 0.362 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	12.8	Xtriage
Anisotropy	0.654	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 150.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 48272 reflections	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	2632	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	1.47	20/2328 (0.9%)	1.64	39/3175 (1.2%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	GLU	CD-OE2	8.27	1.34	1.25
1	A	151	GLU	CD-OE2	8.16	1.34	1.25
1	A	205	GLU	CD-OE2	7.74	1.34	1.25
1	A	44	GLU	CD-OE2	7.50	1.33	1.25
1	A	227	GLU	CD-OE2	7.46	1.33	1.25
1	A	266	GLU	CD-OE2	7.19	1.33	1.25
1	A	76	GLU	CD-OE2	6.97	1.33	1.25
1	A	218	GLU	CD-OE2	6.79	1.33	1.25
1	A	214	GLU	CD-OE2	6.37	1.32	1.25
1	A	247	GLU	CD-OE2	6.33	1.32	1.25
1	A	312	GLU	CD-OE2	6.25	1.32	1.25
1	A	127	GLU	CD-OE2	6.19	1.32	1.25
1	A	243	GLU	CD-OE2	5.82	1.32	1.25
1	A	58	GLU	CD-OE1	-5.59	1.19	1.25
1	A	40	GLU	CD-OE1	-5.43	1.19	1.25
1	A	57	GLU	CD-OE2	5.41	1.31	1.25
1	A	317	GLU	CD-OE2	5.26	1.31	1.25
1	A	236	PRO	N-CD	5.17	1.55	1.47
1	A	218	GLU	CD-OE1	-5.13	1.20	1.25
1	A	191	GLU	CD-OE2	5.04	1.31	1.25

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	196	ARG	NE-CZ-NH1	19.83	130.22	120.30
1	A	8	ARG	NE-CZ-NH1	11.86	126.23	120.30
1	A	196	ARG	NE-CZ-NH2	-10.97	114.81	120.30
1	A	196	ARG	CD-NE-CZ	10.55	138.37	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	161	ASP	CB-CG-OD2	-9.91	109.38	118.30
1	A	164	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	A	185	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	A	161	ASP	CB-CG-OD1	8.58	126.02	118.30
1	A	184	ASP	CB-CG-OD1	8.32	125.79	118.30
1	A	155	ASP	CB-CG-OD2	-8.21	110.91	118.30
1	A	290	ASP	CB-CG-OD1	7.67	125.21	118.30
1	A	262	SER	N-CA-CB	-7.63	99.06	110.50
1	A	200	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	28	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	74	ASP	CB-CG-OD1	7.11	124.70	118.30
1	A	141	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	28	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	284	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	A	75	CYS	CA-CB-SG	-6.21	102.83	114.00
1	A	184	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	213	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	A	3	SER	N-CA-CB	5.93	119.40	110.50
1	A	198	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	A	204	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	284	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	182	TYR	CB-CG-CD1	-5.77	117.54	121.00
1	A	159	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	217	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	213	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	96	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	290	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	A	155	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	217	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	314	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	14	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	314	ASP	CB-CA-C	5.34	121.09	110.40
1	A	14	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	243	GLU	CG-CD-OE1	5.14	128.58	118.30
1	A	180	PRO	N-CA-CB	5.12	109.45	103.30

There are no chirality outliers.

There are no planarity outliers.

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	2281	0	2234	34	0
2	A	351	0	0	11	5
All	All	2632	0	2234	34	5

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 (34) 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:224:VAL:O	2:A:850:HOH:O	1.98	0.80
1:A:196:ARG:HD2	1:A:212:TRP:CH2	2.17	0.79
1:A:1:MET:HE2	2:A:743:HOH:O	1.86	0.75
1:A:5:GLN:HE22	1:A:35:ARG:HE	1.35	0.73
1:A:180:PRO:HB3	2:A:654:HOH:O	1.87	0.73
1:A:302:ARG:NH2	2:A:848:HOH:O	2.24	0.69
1:A:147:ASN:ND2	1:A:179:ASN:H	1.89	0.68
1:A:219:PRO:O	1:A:220:ASP:HB2	1.99	0.62
1:A:35:ARG:HD2	2:A:502:HOH:O	2.00	0.62
1:A:144:MET:HE1	2:A:705:HOH:O	2.00	0.60
1:A:196:ARG:HD2	1:A:212:TRP:CZ3	2.37	0.60
1:A:110:CYS:SG	1:A:111:ASN:N	2.75	0.60
1:A:218:GLU:OE1	2:A:622:HOH:O	2.17	0.59
1:A:10:GLN:HG2	1:A:28:ASP:OD1	2.04	0.58
1:A:140:VAL:HG12	1:A:144:MET:CE	2.35	0.57
1:A:140:VAL:HG12	1:A:144:MET:HE2	1.89	0.54
1:A:196:ARG:HD3	1:A:215:SER:OG	2.08	0.53
1:A:205:GLU:HG2	2:A:727:HOH:O	2.08	0.53
1:A:102:ALA:HB3	1:A:104:TYR:CE1	2.45	0.51
1:A:196:ARG:CD	1:A:212:TRP:CZ3	2.93	0.51
1:A:224:VAL:HG13	1:A:226:GLU:HG3	1.94	0.49
1:A:205:GLU:CG	2:A:727:HOH:O	2.60	0.49
1:A:246:ARG:HE	1:A:250:GLN:NE2	2.12	0.48
1:A:195:THR:HB	2:A:665:HOH:O	2.14	0.47
1:A:298:GLN:HG3	1:A:308:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:CYS:SG	2:A:557:HOH:O	2.39	0.45
1:A:235:LYS:HE2	1:A:262:SER:OG	2.17	0.44
1:A:110:CYS:HB3	1:A:132:VAL:HG22	1.99	0.44
1:A:224:VAL:CG1	1:A:226:GLU:HG3	2.48	0.43
1:A:160:LEU:HB2	1:A:189:LEU:HG	2.00	0.43
1:A:219:PRO:O	1:A:220:ASP:CB	2.62	0.42
1:A:141:ARG:HA	1:A:144:MET:HE2	2.01	0.42
1:A:71:LEU:HD23	1:A:71:LEU:HA	1.89	0.41
1:A:100:GLN:HB2	1:A:100:GLN:HE21	1.71	0.40

All (5) 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:767:HOH:O	2:A:843:HOH:O[2_564]	1.69	0.51
2:A:663:HOH:O	2:A:724:HOH:O[2_464]	1.77	0.43
2:A:620:HOH:O	2:A:665:HOH:O[2_564]	1.89	0.31
2:A:639:HOH:O	2:A:681:HOH:O[4_455]	1.97	0.23
2:A:575:HOH:O	2:A:598:HOH:O[2_464]	2.14	0.06

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	292/320 (91%)	286 (98%)	6 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	234/264 (89%)	230 (98%)	4 (2%)	68 45

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	127	GLU
1	A	148	LEU
1	A	224	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	5	GLN
1	A	10	GLN
1	A	100	GLN
1	A	147	ASN
1	A	250	GLN
1	A	273	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

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^{th} 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	298/320 (93%)	2.22	155 (52%)	0	0	7, 14, 44, 87	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	24	LEU	7.1
1	A	11	ILE	5.8
1	A	166	TRP	5.7
1	A	294	LEU	5.7
1	A	109	LEU	5.6
1	A	26	THR	5.5
1	A	174	PHE	5.5
1	A	320	LEU	5.1
1	A	189	LEU	5.0
1	A	1	MET	4.9
1	A	137	TYR	4.9
1	A	110	CYS	4.8
1	A	182	TYR	4.6
1	A	134	VAL	4.5
1	A	150	LEU	4.5
1	A	140	VAL	4.5
1	A	14	ASP	4.4
1	A	173	GLN	4.4
1	A	71	LEU	4.2
1	A	149	LEU	4.2
1	A	175	ALA	4.2
1	A	316	LEU	4.1
1	A	202	PHE	4.1
1	A	152	ALA	4.0
1	A	160	LEU	4.0
1	A	295	MET	4.0
1	A	193	CYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	177	TYR	3.9
1	A	56	TRP	3.9
1	A	303	TRP	3.9
1	A	158	LEU	3.9
1	A	48	LEU	3.7
1	A	308	LEU	3.7
1	A	139	ALA	3.7
1	A	75	CYS	3.7
1	A	9	TRP	3.7
1	A	292	LEU	3.7
1	A	186	ILE	3.6
1	A	10	GLN	3.6
1	A	206	THR	3.5
1	A	319	LEU	3.5
1	A	178	VAL	3.5
1	A	153	ILE	3.5
1	A	208	ILE	3.5
1	A	112	GLY	3.5
1	A	220	ASP	3.4
1	A	30	LEU	3.4
1	A	148	LEU	3.3
1	A	210	ILE	3.3
1	A	90	ALA	3.2
1	A	209	ALA	3.2
1	A	106	ALA	3.2
1	A	180	PRO	3.2
1	A	167	THR	3.2
1	A	195	THR	3.2
1	A	297	ALA	3.2
1	A	169	LEU	3.2
1	A	291	THR	3.2
1	A	141	ARG	3.2
1	A	313	VAL	3.2
1	A	7	TYR	3.2
1	A	51	PHE	3.1
1	A	192	PRO	3.1
1	A	38	GLU	3.1
1	A	223	PHE	3.1
1	A	111	ASN	3.1
1	A	146	VAL	3.1
1	A	136	LEU	3.1
1	A	113	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	304	PRO	3.0
1	A	62	VAL	2.9
1	A	130	ALA	2.9
1	A	37	GLY	2.9
1	A	31	TYR	2.9
1	A	132	VAL	2.9
1	A	203	ALA	2.9
1	A	45	ILE	2.9
1	A	65	ALA	2.9
1	A	201	ALA	2.9
1	A	156	LEU	2.9
1	A	224	VAL	2.9
1	A	311	VAL	2.9
1	A	144	MET	2.8
1	A	229	VAL	2.8
1	A	310	VAL	2.8
1	A	179	ASN	2.8
1	A	13	MET	2.8
1	A	87	VAL	2.8
1	A	231	ALA	2.7
1	A	12	PRO	2.7
1	A	145	VAL	2.7
1	A	212	TRP	2.7
1	A	154	PRO	2.7
1	A	171	GLY	2.7
1	A	271	LEU	2.7
1	A	168	PRO	2.7
1	A	265	ILE	2.7
1	A	162	ALA	2.6
1	A	66	TRP	2.6
1	A	172	GLN	2.5
1	A	165	ALA	2.5
1	A	289	LEU	2.5
1	A	143	GLY	2.5
1	A	60	GLN	2.5
1	A	216	LEU	2.5
1	A	46	SER	2.5
1	A	314	ASP	2.4
1	A	8	ARG	2.4
1	A	34	LEU	2.4
1	A	207	GLY	2.4
1	A	280	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	318	ARG	2.4
1	A	170	LYS	2.3
1	A	142	ASP	2.3
1	A	225	ALA	2.3
1	A	230	ARG	2.3
1	A	42	TRP	2.3
1	A	272	THR	2.3
1	A	33	CYS	2.3
1	A	306	SER	2.3
1	A	72	ALA	2.3
1	A	6	VAL	2.3
1	A	32	VAL	2.3
1	A	83	VAL	2.3
1	A	155	ASP	2.2
1	A	127	GLU	2.2
1	A	67	VAL	2.2
1	A	252	ALA	2.2
1	A	236	PRO	2.2
1	A	59	ALA	2.2
1	A	305	GLY	2.2
1	A	188	PHE	2.2
1	A	268	SER	2.2
1	A	54	GLU	2.2
1	A	164	ARG	2.2
1	A	4	ALA	2.2
1	A	147	ASN	2.2
1	A	52	SER	2.1
1	A	238	LEU	2.1
1	A	89	CYS	2.1
1	A	307	THR	2.1
1	A	300	VAL	2.1
1	A	35	ARG	2.1
1	A	232	VAL	2.1
1	A	233	VAL	2.1
1	A	264	SER	2.1
1	A	129	VAL	2.1
1	A	78	PRO	2.1
1	A	211	ALA	2.1
1	A	199	SER	2.0
1	A	86	GLY	2.0
1	A	63	LEU	2.0
1	A	261	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	288	GLY	2.0
1	A	309	PRO	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.