Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:20 AM GMT

PDB ID : 3LQ1

Title : Crystal structure of 2-succinyl-6-hydroxy-2,4-cyclohexadiene 1-carboxylic acid synthase/2-oxoglutarate decarboxylase FROM Listeria monocytogenes str. 4b F2365

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Deposited on : 2010-02-08

Resolution : 2.60 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.
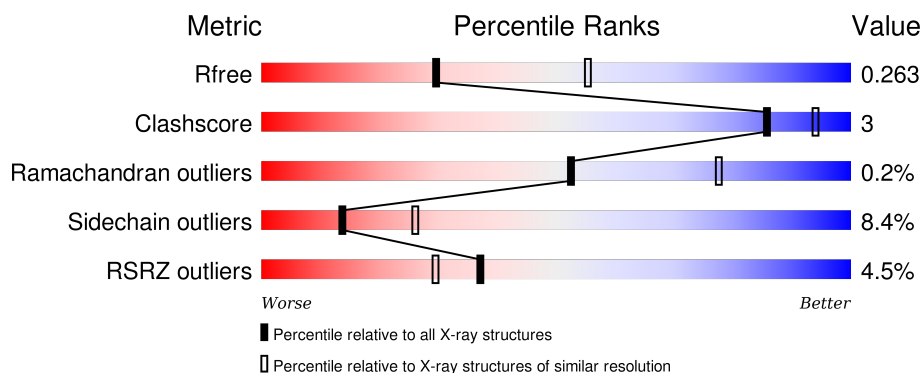
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	578	
1	B	578	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8131 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 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total 4020	C 2581	N 665	O 752	S 22	0	0	0
1	B	518	Total 4057	C 2605	N 670	O 760	S 22	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP Q71YZ2
A	0	SER	-	EXPRESSION TAG	UNP Q71YZ2
A	1	LEU	-	EXPRESSION TAG	UNP Q71YZ2
A	569	GLU	-	EXPRESSION TAG	UNP Q71YZ2
A	570	GLY	-	EXPRESSION TAG	UNP Q71YZ2
A	571	HIS	-	EXPRESSION TAG	UNP Q71YZ2
A	572	HIS	-	EXPRESSION TAG	UNP Q71YZ2
A	573	HIS	-	EXPRESSION TAG	UNP Q71YZ2
A	574	HIS	-	EXPRESSION TAG	UNP Q71YZ2
A	575	HIS	-	EXPRESSION TAG	UNP Q71YZ2
A	576	HIS	-	EXPRESSION TAG	UNP Q71YZ2
B	-1	MET	-	EXPRESSION TAG	UNP Q71YZ2
B	0	SER	-	EXPRESSION TAG	UNP Q71YZ2
B	1	LEU	-	EXPRESSION TAG	UNP Q71YZ2
B	569	GLU	-	EXPRESSION TAG	UNP Q71YZ2
B	570	GLY	-	EXPRESSION TAG	UNP Q71YZ2
B	571	HIS	-	EXPRESSION TAG	UNP Q71YZ2
B	572	HIS	-	EXPRESSION TAG	UNP Q71YZ2
B	573	HIS	-	EXPRESSION TAG	UNP Q71YZ2
B	574	HIS	-	EXPRESSION TAG	UNP Q71YZ2
B	575	HIS	-	EXPRESSION TAG	UNP Q71YZ2
B	576	HIS	-	EXPRESSION TAG	UNP Q71YZ2

- Molecule 2 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	32	Total 32	O 32	0	0
2	B	22	Total 22	O 22	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: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase
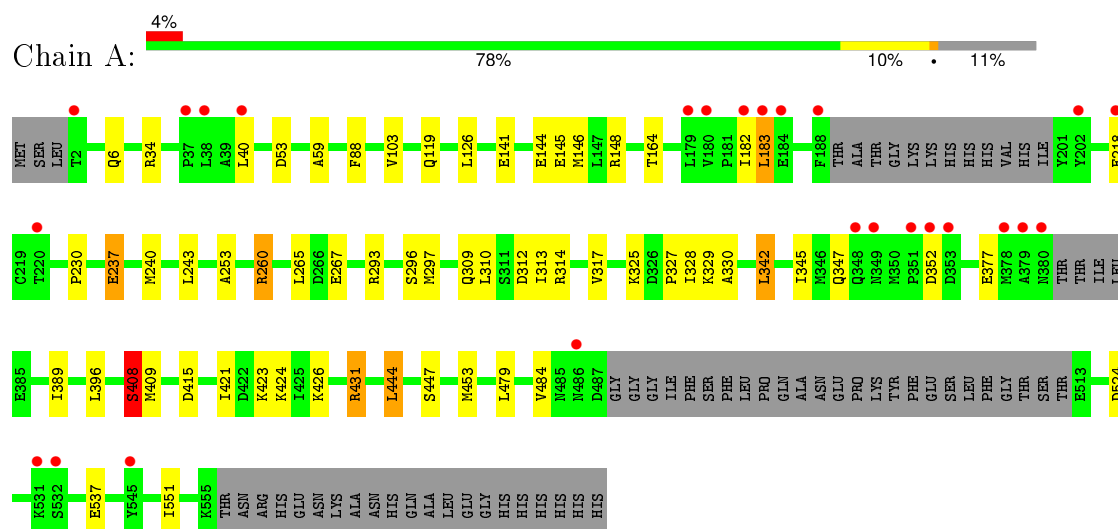
Chain A:

• Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

Chain B:
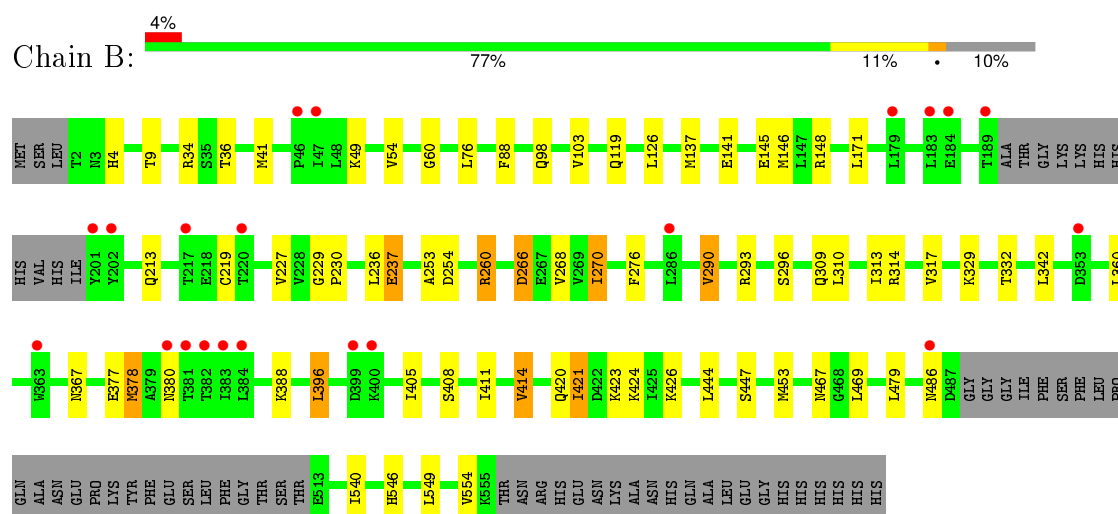
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	99.69Å 99.69Å 259.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 39.74 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-2.60) 99.5 (39.74-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.222 , 0.265 0.220 , 0.263	Depositor DCC
R_{free} test set	1280 reflections (3.23%)	DCC
Wilson B-factor (Å²)	71.4	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.30 , 45.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Outliers	1 of 41109 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8131	wwPDB-VP
Average B, all atoms (Å²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.35	0/4106	0.55	0/5566
1	B	0.34	0/4144	0.53	0/5621
All	All	0.35	0/8250	0.54	0/11187

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 (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	4020	0	4030	20	0
1	B	4057	0	4074	25	0
2	A	32	0	0	0	0
2	B	22	0	0	0	0
All	All	8131	0	8104	45	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 3.

All (45) 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:290:VAL:HG12	1:B:314:ARG:HB2	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ILE:HD11	1:B:276:PHE:HZ	1.70	0.57
1:B:230:PRO:HG2	1:B:296:SER:HB2	1.88	0.55
1:A:328:ILE:HG22	1:A:330:ALA:HB2	1.88	0.54
1:B:266:ASP:HB2	1:B:420:GLN:HE22	1.73	0.53
1:A:447:SER:HA	1:A:453:MET:HG3	1.90	0.52
1:B:141:GLU:HB2	1:B:146:MET:HG2	1.91	0.52
1:B:421:ILE:HG12	1:B:423:LYS:HE2	1.91	0.52
1:A:53:ASP:HB3	1:A:59:ALA:HB2	1.91	0.51
1:B:219:CYS:HB3	1:B:290:VAL:HG11	1.92	0.51
1:B:270:ILE:HD11	1:B:276:PHE:CZ	2.47	0.50
1:A:421:ILE:HG12	1:A:423:LYS:HE2	1.92	0.50
1:A:230:PRO:HG2	1:A:296:SER:HB2	1.94	0.49
1:A:389:ILE:HD13	1:A:484:VAL:HG22	1.94	0.49
1:B:227:VAL:HB	1:B:293:ARG:HG2	1.95	0.48
1:A:342:LEU:HD23	1:A:345:ILE:HD11	1.96	0.47
1:A:293:ARG:NH2	1:A:325:LYS:O	2.47	0.47
1:B:137:MET:CE	1:B:171:LEU:HD23	2.45	0.47
1:B:268:VAL:HG12	1:B:360:LEU:HD11	1.97	0.47
1:A:297:MET:HG3	1:A:327:PRO:HD2	1.96	0.47
1:B:378:MET:HG3	1:B:388:LYS:HG2	1.96	0.46
1:A:444:LEU:HD13	1:A:479:LEU:HD22	1.99	0.45
1:B:421:ILE:HG23	1:B:423:LYS:H	1.82	0.45
1:A:260:ARG:NH2	1:A:415:ASP:O	2.50	0.45
1:A:408:SER:HB2	1:A:409:MET:H	1.53	0.44
1:A:237:GLU:H	1:A:237:GLU:HG2	1.52	0.43
1:A:40:LEU:HB3	1:A:183:LEU:HD21	2.00	0.43
1:B:447:SER:HA	1:B:453:MET:HG3	1.99	0.43
1:B:396:LEU:HB3	1:B:540:ILE:HG21	2.00	0.43
1:A:431:ARG:CG	1:A:431:ARG:HH11	2.31	0.42
1:B:229:GLY:HA2	1:B:254:ASP:HB2	2.01	0.42
1:B:119:GLN:HB3	1:B:119:GLN:HE21	1.66	0.42
1:A:253:ALA:O	1:A:260:ARG:NH1	2.43	0.42
1:B:270:ILE:HD12	1:B:367:ASN:HB2	2.02	0.42
1:B:469:LEU:HD22	1:B:549:LEU:HD21	2.02	0.42
1:A:6:GLN:HG2	1:A:182:ILE:HD12	2.02	0.42
1:B:9:THR:HA	1:B:41:MET:HE1	2.02	0.41
1:B:237:GLU:HG2	1:B:237:GLU:H	1.60	0.41
1:A:141:GLU:HB2	1:A:146:MET:HG2	2.02	0.41
1:A:396:LEU:HD11	1:A:537:GLU:HG2	2.03	0.41
1:B:60:GLY:HA2	1:B:76:LEU:HD11	2.03	0.41
1:B:405:ILE:HD13	1:B:414:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LEU:HA	1:A:347:GLN:HE21	1.85	0.40
1:B:253:ALA:O	1:B:260:ARG:NH1	2.53	0.40
1:B:137:MET:HE2	1:B:171:LEU:HD23	2.03	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	505/578 (87%)	489 (97%)	15 (3%)	1 (0%)	52 77
1	B	512/578 (89%)	498 (97%)	13 (2%)	1 (0%)	52 77
All	All	1017/1156 (88%)	987 (97%)	28 (3%)	2 (0%)	52 77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	408	SER
1	A	408	SER

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	434/489 (89%)	401 (92%)	33 (8%)	16 32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	439/489 (90%)	399 (91%)	40 (9%)	12	22
All	All	873/978 (89%)	800 (92%)	73 (8%)	14	26

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ARG
1	A	88	PHE
1	A	103	VAL
1	A	119	GLN
1	A	126	LEU
1	A	144	GLU
1	A	145	GLU
1	A	148	ARG
1	A	164	THR
1	A	183	LEU
1	A	218	GLU
1	A	237	GLU
1	A	240	MET
1	A	260	ARG
1	A	265	LEU
1	A	267	GLU
1	A	309	GLN
1	A	310	LEU
1	A	312	ASP
1	A	313	ILE
1	A	314	ARG
1	A	317	VAL
1	A	329	LYS
1	A	342	LEU
1	A	352	ASP
1	A	377	GLU
1	A	408	SER
1	A	424	LYS
1	A	426	LYS
1	A	431	ARG
1	A	444	LEU
1	A	524	ASP
1	A	551	ILE
1	B	4	HIS
1	B	34	ARG
1	B	36	THR

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Mol	Chain	Res	Type
1	B	49	LYS
1	B	54	VAL
1	B	88	PHE
1	B	98	GLN
1	B	103	VAL
1	B	126	LEU
1	B	145	GLU
1	B	148	ARG
1	B	213	GLN
1	B	236	LEU
1	B	237	GLU
1	B	260	ARG
1	B	266	ASP
1	B	270	ILE
1	B	290	VAL
1	B	309	GLN
1	B	310	LEU
1	B	313	ILE
1	B	317	VAL
1	B	329	LYS
1	B	332	THR
1	B	342	LEU
1	B	377	GLU
1	B	378	MET
1	B	380	ASN
1	B	396	LEU
1	B	411	ILE
1	B	414	VAL
1	B	421	ILE
1	B	424	LYS
1	B	426	LYS
1	B	444	LEU
1	B	467	ASN
1	B	479	LEU
1	B	486	ASN
1	B	546	HIS
1	B	554	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS

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Mol	Chain	Res	Type
1	A	309	GLN
1	A	347	GLN
1	B	98	GLN
1	B	119	GLN
1	B	309	GLN
1	B	347	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	513/578 (88%)	0.25	25 (4%)	33	26	55, 80, 119, 151	0
1	B	518/578 (89%)	0.16	21 (4%)	41	33	48, 85, 126, 157	0
All	All	1031/1156 (89%)	0.21	46 (4%)	37	29	48, 82, 123, 157	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	353	ASP	5.0
1	A	2	THR	4.6
1	B	399	ASP	4.3
1	B	382	THR	4.3
1	A	379	ALA	4.2
1	A	352	ASP	3.9
1	B	383	ILE	3.8
1	A	183	LEU	3.8
1	B	380	ASN	3.8
1	B	184	GLU	3.7
1	A	202	TYR	3.6
1	B	363	TRP	3.3
1	B	201	TYR	3.3
1	A	40	LEU	3.3
1	A	378	MET	3.1
1	A	380	ASN	3.1
1	B	381	THR	3.1
1	B	183	LEU	3.1
1	A	37	PRO	3.0
1	A	531	LYS	3.0
1	A	486	ASN	2.8
1	A	184	GLU	2.8
1	A	349	ASN	2.8
1	A	351	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	220	THR	2.7
1	A	545	TYR	2.6
1	B	220	THR	2.6
1	B	384	LEU	2.6
1	A	182	ILE	2.6
1	B	400	LYS	2.6
1	B	179	LEU	2.5
1	A	532	SER	2.5
1	B	353	ASP	2.4
1	A	348	GLN	2.4
1	A	38	LEU	2.4
1	A	188	PHE	2.3
1	B	202	TYR	2.3
1	A	179	LEU	2.3
1	A	218	GLU	2.3
1	B	486	ASN	2.3
1	B	189	THR	2.3
1	B	217	THR	2.3
1	B	46	PRO	2.3
1	B	47	ILE	2.2
1	A	180	VAL	2.2
1	B	286	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.