



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:03 PM UTC

PDB ID : 4LA5 / pdb_00004la5
Title : Crystal structure of 2-methylisoborneol synthase from *Streptomyces coelicolor* A3(2)
Authors : Koksai, M.; Christianson, D.W.
Deposited on : 2013-06-19
Resolution : 1.85 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

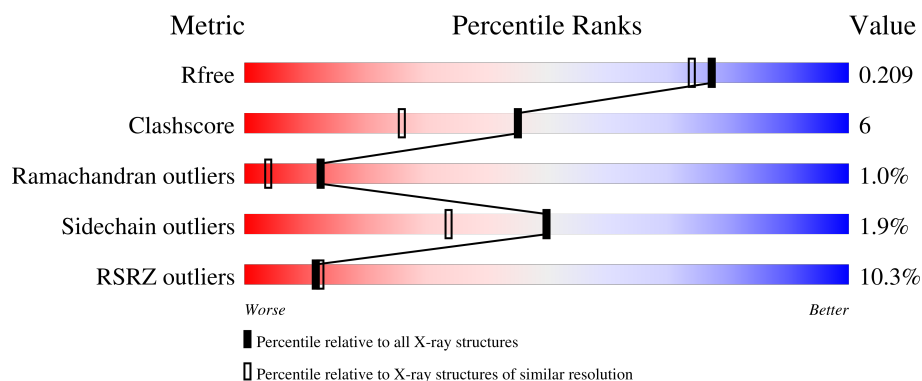
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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 $\leq 5\%$. 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	461	7% 47% 19% . 31%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2679 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-methylisoborneol synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	2	0
			2534	1600	458	463	13			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q9F1Y6
A	-19	GLY	-	expression tag	UNP Q9F1Y6
A	-18	SER	-	expression tag	UNP Q9F1Y6
A	-17	SER	-	expression tag	UNP Q9F1Y6
A	-16	HIS	-	expression tag	UNP Q9F1Y6
A	-15	HIS	-	expression tag	UNP Q9F1Y6
A	-14	HIS	-	expression tag	UNP Q9F1Y6
A	-13	HIS	-	expression tag	UNP Q9F1Y6
A	-12	HIS	-	expression tag	UNP Q9F1Y6
A	-11	HIS	-	expression tag	UNP Q9F1Y6
A	-10	SER	-	expression tag	UNP Q9F1Y6
A	-9	SER	-	expression tag	UNP Q9F1Y6
A	-8	GLY	-	expression tag	UNP Q9F1Y6
A	-7	LEU	-	expression tag	UNP Q9F1Y6
A	-6	VAL	-	expression tag	UNP Q9F1Y6
A	-5	PRO	-	expression tag	UNP Q9F1Y6
A	-4	ARG	-	expression tag	UNP Q9F1Y6
A	-3	GLY	-	expression tag	UNP Q9F1Y6
A	-2	SER	-	expression tag	UNP Q9F1Y6
A	-1	HIS	-	expression tag	UNP Q9F1Y6
A	0	MET	-	expression tag	UNP Q9F1Y6

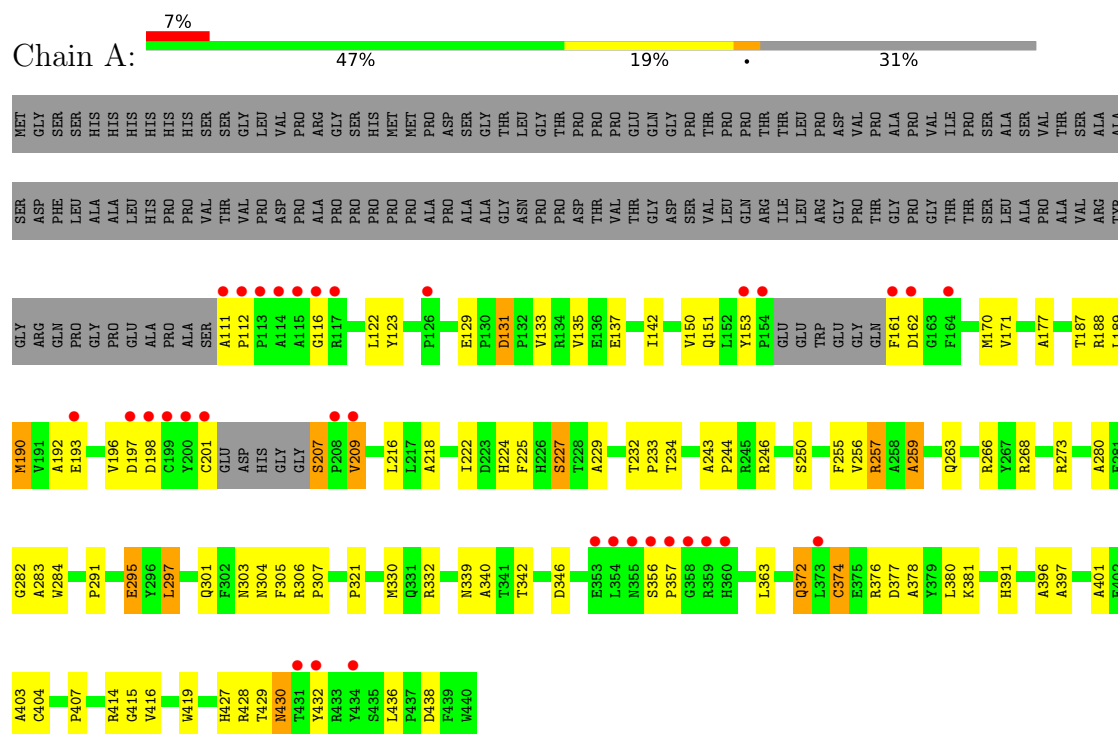
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	145	Total	O	0	0
			145	145		

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: 2-methylisoborneol synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	99.45Å 99.45Å 104.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.73 – 1.85 49.73 – 1.85	Depositor EDS
% Data completeness (in resolution range)	93.8 (49.73-1.85) 91.6 (49.73-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 1.86Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.186 , 0.214 0.182 , 0.209	Depositor DCC
R_{free} test set	1983 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2679	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	1.95	53/2623 (2.0%)	1.56	28/3584 (0.8%)

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	187	THR	CA-CB	8.36	1.66	1.53
1	A	259	ALA	CA-CB	8.31	1.67	1.53
1	A	227	SER	CA-C	7.81	1.62	1.53
1	A	342	THR	CA-CB	7.51	1.65	1.53
1	A	189	LEU	N-CA	7.45	1.55	1.46
1	A	142	ILE	N-CA	7.35	1.55	1.46
1	A	177	ALA	CA-C	7.33	1.61	1.52
1	A	268	ARG	CB-CG	7.20	1.74	1.52
1	A	415	GLY	CA-C	7.05	1.60	1.52
1	A	332	ARG	CZ-NH1	7.02	1.42	1.32
1	A	257[A]	ARG	N-CA	6.96	1.55	1.46
1	A	257[B]	ARG	N-CA	6.96	1.55	1.46
1	A	188	ARG	CA-C	6.64	1.61	1.52
1	A	372	GLN	CA-C	6.63	1.61	1.52
1	A	372	GLN	CB-CG	6.62	1.72	1.52
1	A	330	MET	CA-C	6.58	1.61	1.52
1	A	372	GLN	CG-CD	6.30	1.67	1.52
1	A	218	ALA	CA-CB	-6.30	1.42	1.53
1	A	340	ALA	CA-CB	6.27	1.63	1.53
1	A	266	ARG	CD-NE	6.15	1.54	1.46
1	A	188	ARG	CB-CG	6.02	1.70	1.52
1	A	396	ALA	CA-CB	5.93	1.62	1.53
1	A	256	VAL	CA-C	5.80	1.61	1.52
1	A	284	TRP	N-CA	5.72	1.53	1.46
1	A	305	PHE	N-CA	5.70	1.53	1.46
1	A	229	ALA	CA-CB	5.68	1.62	1.53
1	A	280	ALA	N-CA	5.67	1.53	1.46
1	A	250	SER	CA-CB	5.65	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	407	PRO	CA-C	5.64	1.57	1.52
1	A	192	ALA	CA-C	5.62	1.60	1.52
1	A	162	ASP	CA-C	5.60	1.59	1.53
1	A	381	LYS	CA-C	5.59	1.60	1.52
1	A	304	ASN	CA-C	5.53	1.59	1.52
1	A	193	GLU	CG-CD	5.52	1.65	1.52
1	A	273	ARG	N-CA	5.49	1.52	1.46
1	A	133	VAL	CA-CB	5.44	1.60	1.54
1	A	404	CYS	N-CA	-5.42	1.40	1.46
1	A	193	GLU	CD-OE2	5.38	1.35	1.25
1	A	295	GLU	CG-CD	5.32	1.65	1.52
1	A	283	ALA	CA-CB	-5.30	1.44	1.53
1	A	401	ALA	CA-CB	-5.30	1.44	1.53
1	A	401	ALA	CA-C	5.30	1.59	1.52
1	A	255	PHE	CA-CB	5.28	1.61	1.53
1	A	427	HIS	CA-CB	5.21	1.61	1.53
1	A	137	GLU	CA-C	5.17	1.59	1.52
1	A	346	ASP	N-CA	5.17	1.52	1.46
1	A	303	ASN	C-N	5.15	1.40	1.33
1	A	416	VAL	N-CA	5.14	1.52	1.46
1	A	397	ALA	C-O	-5.12	1.18	1.24
1	A	171	VAL	CA-CB	5.09	1.60	1.54
1	A	381	LYS	N-CA	5.05	1.52	1.46
1	A	363	LEU	CA-C	5.03	1.58	1.52
1	A	246	ARG	CG-CD	5.01	1.67	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	ILE	N-CA-C	-9.04	104.58	111.90
1	A	306	ARG	CA-C-N	-8.90	110.62	119.87
1	A	306	ARG	C-N-CA	-8.90	110.62	119.87
1	A	209	VAL	CA-C-N	-7.99	111.20	122.86
1	A	209	VAL	C-N-CA	-7.99	111.20	122.86
1	A	111	ALA	CA-C-N	7.26	124.96	119.66
1	A	111	ALA	C-N-CA	7.26	124.96	119.66
1	A	116	GLY	N-CA-C	-6.33	106.69	114.92
1	A	419	TRP	N-CA-C	-6.05	104.77	111.36
1	A	216	LEU	N-CA-C	-6.04	104.69	111.28
1	A	192	ALA	N-CA-C	-5.95	104.88	111.36
1	A	378	ALA	N-CA-C	-5.81	105.03	111.36
1	A	207	SER	CA-C-N	-5.81	113.67	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	SER	C-N-CA	-5.81	113.67	120.12
1	A	372	GLN	CB-CG-CD	5.77	122.40	112.60
1	A	162	ASP	N-CA-C	5.70	118.44	108.52
1	A	131	ASP	CA-C-N	5.68	125.53	119.28
1	A	131	ASP	C-N-CA	5.68	125.53	119.28
1	A	321	PRO	CB-CA-C	-5.64	104.00	111.23
1	A	403	ALA	CA-C-N	-5.60	117.16	122.37
1	A	403	ALA	C-N-CA	-5.60	117.16	122.37
1	A	224	HIS	N-CA-C	5.58	117.94	110.35
1	A	374	CYS	N-CA-C	-5.47	103.17	110.55
1	A	430	ASN	N-CA-C	5.25	119.54	113.18
1	A	297	LEU	N-CA-C	-5.22	105.67	111.36
1	A	307	PRO	CB-CA-C	-5.19	103.60	111.44
1	A	282	GLY	N-CA-C	-5.19	106.13	112.77
1	A	193	GLU	CG-CD-OE2	5.05	130.01	118.40

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	2534	0	2404	29	0
2	A	145	0	0	3	0
All	All	2679	0	2404	29	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 6.

All (29) 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:257[A]:ARG:NH2	2:A:598:HOH:O	1.57	1.29
1:A:374:CYS:SG	1:A:377:ASP:OD2	2.22	0.97
1:A:257[A]:ARG:CZ	2:A:598:HOH:O	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:MET:HA	1:A:170:MET:HE2	1.79	0.64
1:A:112:PRO:HG3	1:A:438:ASP:HB2	1.79	0.63
1:A:153:TYR:CE2	1:A:161:PHE:HB2	2.37	0.59
1:A:429:THR:O	1:A:432:TYR:HD2	1.88	0.56
1:A:428:ARG:HG2	1:A:428:ARG:HH11	1.75	0.52
1:A:259:ALA:HB1	1:A:263:GLN:HB2	1.92	0.51
1:A:414:ARG:HG3	2:A:569:HOH:O	2.12	0.48
1:A:190:MET:O	1:A:190:MET:HG3	2.11	0.47
1:A:243:ALA:N	1:A:244:PRO:CD	2.77	0.47
1:A:301:GLN:HA	1:A:339:ASN:OD1	2.16	0.46
1:A:197:ASP:O	1:A:201:CYS:HB2	2.16	0.45
1:A:122:LEU:C	1:A:122:LEU:HD23	2.41	0.45
1:A:428:ARG:HG2	1:A:428:ARG:NH1	2.32	0.45
1:A:232:THR:HB	1:A:233:PRO:HD3	2.00	0.44
1:A:150:VAL:O	1:A:151:GLN:C	2.62	0.43
1:A:291:PRO:HB2	1:A:295:GLU:HB2	2.00	0.42
1:A:376:ARG:O	1:A:380:LEU:HG	2.19	0.42
1:A:225:PHE:CZ	1:A:227:SER:HB2	2.56	0.41
1:A:131:ASP:O	1:A:135:VAL:HG23	2.21	0.41
1:A:129:GLU:HA	1:A:129:GLU:OE1	2.21	0.41
1:A:243:ALA:HB3	1:A:244:PRO:HD3	2.03	0.41
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.98	0.41
1:A:436:LEU:HD23	1:A:436:LEU:HA	1.87	0.41
1:A:190:MET:HE3	1:A:190:MET:HB2	1.84	0.40
1:A:207:SER:OG	1:A:209:VAL:HG23	2.21	0.40
1:A:123:TYR:CE2	1:A:391:HIS:CE1	3.10	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	315/461 (68%)	304 (96%)	8 (2%)	3 (1%)	12 4

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	372	GLN
1	A	357	PRO
1	A	356	SER

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	262/372 (70%)	257 (98%)	5 (2%)	50 34

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	MET
1	A	196	VAL
1	A	198	ASP
1	A	234	THR
1	A	430	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	345	ASN
1	A	360	HIS
1	A	391	HIS

5.3.3 RNA ⓘ

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 oligosaccharides 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	319/461 (69%)	0.33	33 (10%)	12 12	17, 32, 70, 108	2 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	357	PRO	4.8
1	A	112	PRO	4.6
1	A	358	GLY	4.1
1	A	201	CYS	4.1
1	A	154	PRO	4.0
1	A	434	TYR	3.9
1	A	111	ALA	3.8
1	A	164	PHE	3.8
1	A	153	TYR	3.7
1	A	432	TYR	3.7
1	A	114	ALA	3.4
1	A	355	ASN	3.4
1	A	200	TYR	3.4
1	A	373	LEU	3.1
1	A	354	LEU	3.0
1	A	199	CYS	3.0
1	A	193	GLU	2.9
1	A	356	SER	2.8
1	A	360	HIS	2.8
1	A	161	PHE	2.7
1	A	113	PRO	2.6
1	A	115	ALA	2.6
1	A	359	ARG	2.6
1	A	162	ASP	2.5
1	A	198	ASP	2.5
1	A	431	THR	2.4
1	A	116	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	209	VAL	2.3
1	A	126	PRO	2.2
1	A	197	ASP	2.2
1	A	117	ARG	2.1
1	A	353	GLU	2.1
1	A	208	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 oligosaccharides 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.