Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2023 – 02:07 am GMT

PDB ID	:	3ZV3
Title	:	CRYSTAL STRUCTURE OF CIS-BIPHENYL-2,3-DIHYDRODIOL-2,3-DEHYDROGENASE (BPHB)FROM PANDORAEA PNOMENUSA STRAIN B-356 IN INTERMEDIATE STATE OF SUBSTRATE BINDING LOOP
Authors	:	Dhindwal, S.; Patil, D.N.; Kumar, P.
Deposited on	:	2011-07-23
Resolution	:	2.90 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:

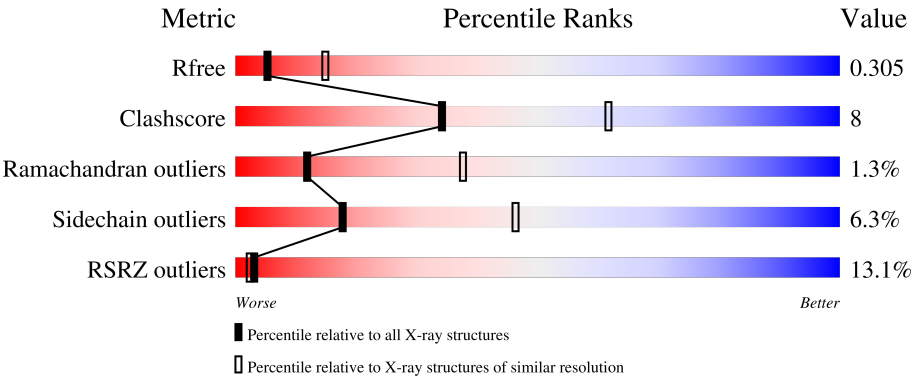
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	281	9% 72% 18% · 7%
1	B	281	16% 77% 19% · ·

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3955 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 CIS-2,3-DIHYDROBIPHENYL-2,3-DIOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	1
			1901	1205	335	353	8			
1	B	276	Total	C	N	O	S	0	0	1
			2015	1273	355	379	8			

- Molecule 2 is water.

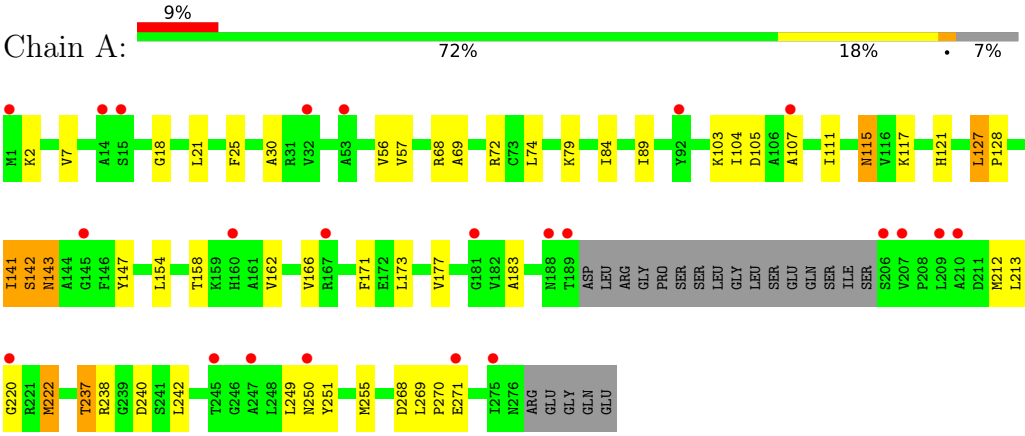
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total	O	0	0
			19	19		
2	B	20	Total	O	0	0
			20	20		

3 Residue-property plots (i)

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.

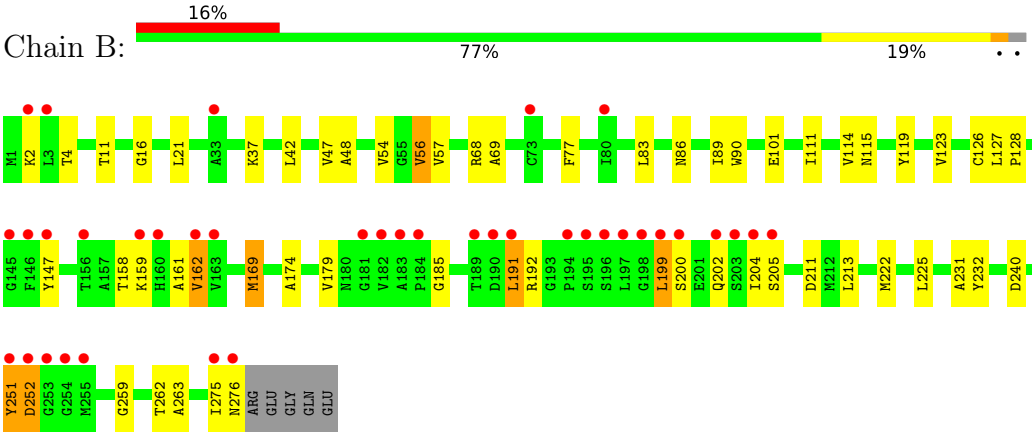
• Molecule 1: CIS-2,3-DIHYDROBIPHENYL-2,3-DIOL DEHYDROGENASE

Chain A:



• Molecule 1: CIS-2,3-DIHYDROBIPHENYL-2,3-DIOL DEHYDROGENASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	75.73Å 75.73Å 178.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.67 – 2.90 46.86 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (69.67-2.90) 98.4 (46.86-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.268 , 0.295 0.266 , 0.305	Depositor DCC
R_{free} test set	663 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	59.6	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 26.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	3955	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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, 0.333 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	0.39	0/1935	0.54	0/2625
1	B	0.40	0/2051	0.56	0/2783
All	All	0.40	0/3986	0.55	0/5408

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	1901	0	1919	32	0
1	B	2015	0	2033	38	0
2	A	19	0	0	1	0
2	B	20	0	0	4	1
All	All	3955	0	3952	66	1

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 (66) 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:204:ILE:HG22	1:B:204:ILE:O	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ILE:HD12	1:B:114:VAL:HG21	1.64	0.78
1:B:111:ILE:HG22	1:B:158:THR:HG21	1.71	0.71
1:B:90:TRP:HB2	1:B:191:LEU:HB3	1.73	0.71
1:A:89:ILE:H	1:A:115:ASN:HD21	1.41	0.68
1:A:115:ASN:HD22	1:A:115:ASN:N	1.97	0.62
1:B:204:ILE:O	1:B:204:ILE:CG2	2.49	0.60
1:B:262:THR:HB	2:B:2017:HOH:O	2.01	0.59
1:A:171:PHE:CE1	1:B:259:GLY:HA3	2.39	0.58
1:A:56:VAL:HG11	1:A:69:ALA:HA	1.84	0.58
1:A:84:ILE:HG12	1:A:138:VAL:HG13	1.87	0.56
1:B:89:ILE:CD1	1:B:114:VAL:HG21	2.35	0.56
1:A:104:ILE:HD12	1:A:105:ASP:H	1.73	0.54
1:A:7:VAL:HG23	1:A:79:LYS:HE3	1.91	0.53
1:A:141:ILE:O	1:A:142:SER:HB2	2.09	0.53
1:B:101:GLU:HG3	2:B:2008:HOH:O	2.09	0.52
1:B:83:LEU:HD22	1:B:126:CYS:HB2	1.92	0.52
1:A:143:ASN:HD22	1:A:255:MET:CE	2.22	0.51
1:B:276:ASN:N	2:B:2020:HOH:O	2.43	0.51
1:A:127:LEU:HB3	1:A:128:PRO:HD3	1.93	0.50
1:A:173:LEU:HB3	1:A:177:VAL:HB	1.92	0.50
1:A:183:ALA:HB3	1:A:250:ASN:HA	1.92	0.50
1:A:162:VAL:O	1:A:166:VAL:HG23	2.12	0.50
1:A:212:MET:HG2	1:A:222:MET:SD	2.53	0.49
1:B:119:TYR:O	1:B:123:VAL:HG23	2.12	0.49
1:B:21:LEU:HD21	1:B:232:TYR:CD1	2.47	0.49
1:B:54:VAL:HG22	1:B:77:PHE:CE2	2.47	0.49
1:B:159:LYS:HA	1:B:162:VAL:HG13	1.94	0.49
1:A:213:LEU:HD22	1:A:220:GLY:O	2.13	0.49
1:A:111:ILE:HG21	1:A:154:LEU:HB3	1.95	0.48
1:B:169:MET:HB3	1:B:179:VAL:HG21	1.95	0.48
1:A:117:LYS:HG2	1:A:121:HIS:CE1	2.50	0.47
1:B:185:GLY:HA3	1:B:252:ASP:HA	1.96	0.47
1:B:213:LEU:HD12	1:B:222:MET:HG3	1.95	0.47
1:B:158:THR:O	1:B:161:ALA:HB3	2.15	0.47
1:A:2:LYS:NZ	2:A:2001:HOH:O	2.42	0.46
1:B:54:VAL:HG22	1:B:77:PHE:HE2	1.80	0.46
1:A:158:THR:O	1:A:162:VAL:HG13	2.15	0.46
1:B:42:LEU:HD12	1:B:57:VAL:HG22	1.97	0.46
1:A:139:PHE:HD2	1:A:166:VAL:HG22	1.81	0.45
1:B:89:ILE:CG1	1:B:114:VAL:HG21	2.47	0.45
1:B:11:THR:O	1:B:86:ASN:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:SER:OG	1:A:143:ASN:OD1	2.33	0.44
1:A:251:TYR:OH	1:B:240:ASP:O	2.35	0.44
1:B:127:LEU:HB3	1:B:128:PRO:HD3	1.98	0.44
1:B:89:ILE:HD12	1:B:114:VAL:CG2	2.40	0.44
1:B:199:LEU:HA	1:B:202:GLN:OE1	2.18	0.44
1:B:263:ALA:N	2:B:2017:HOH:O	2.51	0.44
1:A:25:PHE:O	1:A:30:ALA:HB3	2.17	0.43
1:A:57:VAL:O	1:A:68:ARG:NH2	2.48	0.43
1:A:132:SER:HA	1:B:275:ILE:HG21	2.01	0.43
1:A:269:LEU:N	1:A:270:PRO:CD	2.83	0.42
1:A:237:THR:HB	1:A:240:ASP:HB2	2.01	0.42
1:A:218:PRO:O	1:B:174:ALA:HB1	2.20	0.42
1:B:114:VAL:HG23	1:B:115:ASN:N	2.35	0.42
1:A:18:GLY:HA2	1:A:21:LEU:HD12	2.01	0.42
1:B:47:VAL:HG23	1:B:48:ALA:N	2.35	0.41
1:A:104:ILE:HD12	1:A:105:ASP:N	2.32	0.41
1:B:16:GLY:C	1:B:225:LEU:HD21	2.41	0.41
1:A:115:ASN:N	1:A:115:ASN:ND2	2.65	0.41
1:A:107:ALA:O	1:A:111:ILE:HG22	2.21	0.41
1:B:57:VAL:O	1:B:68:ARG:NH2	2.54	0.41
1:B:114:VAL:HG23	1:B:115:ASN:H	1.85	0.41
1:B:231:ALA:HB2	1:B:251:TYR:CZ	2.56	0.41
1:B:89:ILE:HB	1:B:114:VAL:HG21	2.03	0.41
1:B:56:VAL:HG21	1:B:69:ALA:HA	2.04	0.40

All (1) 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:B:2003:HOH:O	2:B:2003:HOH:O[7_555]	1.98	0.22

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	256/281 (91%)	237 (93%)	15 (6%)	4 (2%)	9 32
1	B	274/281 (98%)	255 (93%)	16 (6%)	3 (1%)	14 42
All	All	530/562 (94%)	492 (93%)	31 (6%)	7 (1%)	12 37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	238	ARG
1	A	141	ILE
1	A	142	SER
1	B	191	LEU
1	B	200	SER
1	B	141	ILE
1	A	143	ASN

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	191/210 (91%)	179 (94%)	12 (6%)	18 46
1	B	205/210 (98%)	192 (94%)	13 (6%)	18 46
All	All	396/420 (94%)	371 (94%)	25 (6%)	18 46

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ARG
1	A	74	LEU
1	A	103	LYS
1	A	115	ASN
1	A	127	LEU
1	A	147	TYR
1	A	222	MET

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Mol	Chain	Res	Type
1	A	237	THR
1	A	242	LEU
1	A	249	LEU
1	A	268	ASP
1	A	271	GLU
1	B	2	LYS
1	B	4	THR
1	B	37	LYS
1	B	56	VAL
1	B	147	TYR
1	B	162	VAL
1	B	169	MET
1	B	192	ARG
1	B	199	LEU
1	B	205	SER
1	B	211	ASP
1	B	251	TYR
1	B	252	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	115	ASN
1	A	121	HIS
1	A	250	ASN

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 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, 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	260/281 (92%)	0.60	24 (9%) 9 6	60, 60, 60, 60	0
1	B	276/281 (98%)	0.72	46 (16%) 1 1	60, 60, 60, 60	0
All	All	536/562 (95%)	0.66	70 (13%) 3 2	60, 60, 60, 60	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	276	ASN	6.7
1	B	2	LYS	6.1
1	B	200	SER	5.1
1	A	188	ASN	5.0
1	B	189	THR	4.8
1	B	203	SER	4.7
1	A	275	ILE	4.6
1	B	250	ASN	4.6
1	A	206	SER	4.3
1	B	248	LEU	4.3
1	B	196	SER	3.9
1	B	275	ILE	3.9
1	B	204	ILE	3.9
1	B	142	SER	3.9
1	A	207	VAL	3.8
1	B	205	SER	3.5
1	B	252	ASP	3.5
1	A	15	SER	3.4
1	B	33	ALA	3.4
1	A	215	SER	3.3
1	B	198	GLY	3.3
1	B	247	ALA	3.3
1	B	194	PRO	3.3
1	B	147	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	209	LEU	3.1
1	A	210	ALA	3.1
1	A	271	GLU	3.0
1	A	14	ALA	2.9
1	B	191	LEU	2.9
1	B	145	GLY	2.8
1	B	195	SER	2.8
1	A	189	THR	2.8
1	A	247	ALA	2.8
1	A	167	ARG	2.7
1	A	250	ASN	2.6
1	B	143	ASN	2.6
1	B	73	CYS	2.6
1	B	160	HIS	2.6
1	A	53	ALA	2.6
1	B	202	GLN	2.6
1	B	183	ALA	2.6
1	B	80	ILE	2.5
1	B	182	VAL	2.5
1	B	249	LEU	2.5
1	B	146	PHE	2.5
1	B	162	VAL	2.4
1	B	141	ILE	2.4
1	A	107	ALA	2.4
1	B	199	LEU	2.3
1	B	197	LEU	2.3
1	B	184	PRO	2.3
1	B	255	MET	2.3
1	B	159	LYS	2.3
1	B	190	ASP	2.2
1	B	253	GLY	2.2
1	B	254	GLY	2.2
1	A	181	GLY	2.2
1	B	3	LEU	2.2
1	A	92	TYR	2.2
1	A	145	GLY	2.2
1	B	251	TYR	2.2
1	A	32	VAL	2.1
1	B	181	GLY	2.1
1	A	1	MET	2.1
1	A	245	THR	2.1
1	A	160	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	220	GLY	2.1
1	B	156	THR	2.0
1	B	144	ALA	2.0
1	B	163	VAL	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 monosaccharides 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.