



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:04 PM UTC

PDB ID : 7RGC / pdb_00007rgc
Title : Crystal structure of triosephosphate isomerase from Candidatus Absconditabacteria (Sr1) bacterium
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Deposited on : 2021-07-15
Resolution : 2.09 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

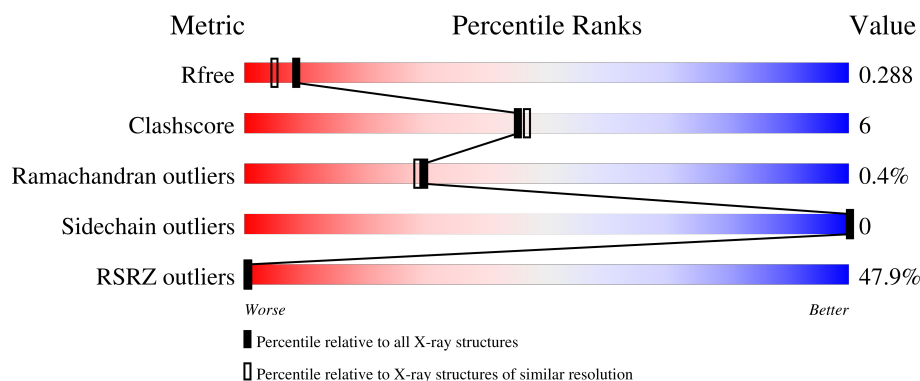
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	247	53% 82%14%.
1	B	247	40% 86%12%.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3694 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 Triosephosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	0	0
			1778	1128	300	340	10			
1	B	242	Total	C	N	O	S	0	0	0
			1804	1144	301	348	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP A0A288DKP7
A	0	HIS	-	expression tag	UNP A0A288DKP7
B	-1	SER	-	expression tag	UNP A0A288DKP7
B	0	HIS	-	expression tag	UNP A0A288DKP7

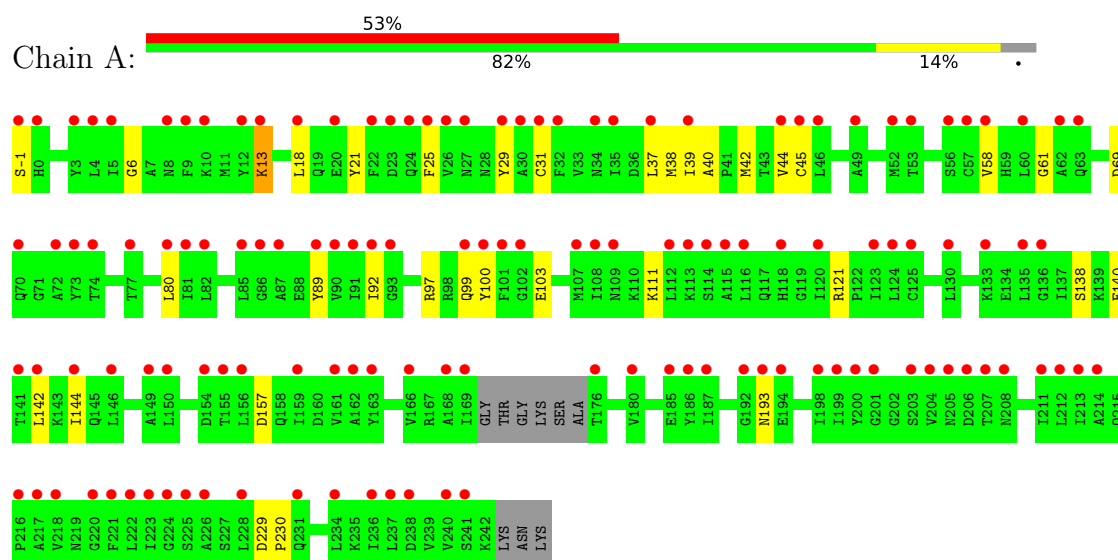
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	49	Total	O	0	0
			49	49		
2	B	63	Total	O	0	0
			63	63		

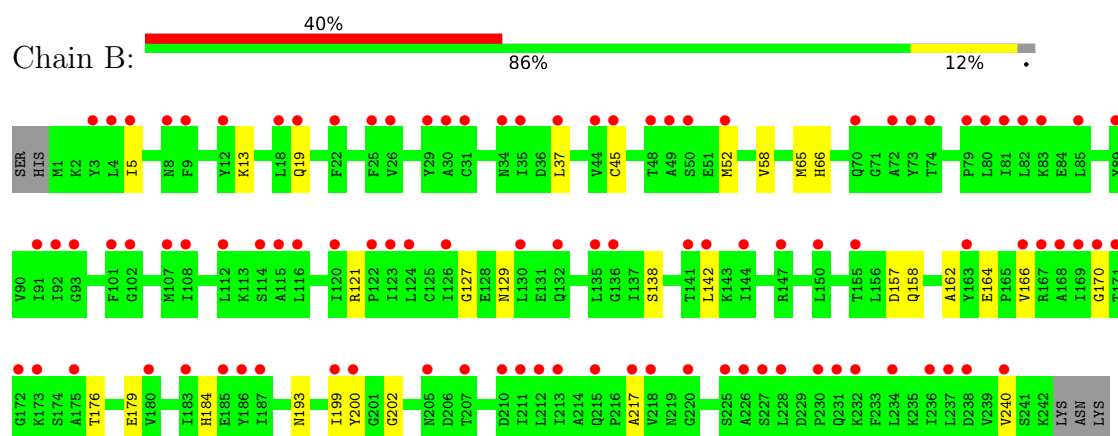
3 Residue-property plots [i](#)

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: Triosephosphate isomerase



• Molecule 1: Triosephosphate isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	151.80Å 151.80Å 118.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.00 – 2.09 44.00 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.00-2.09) 99.3 (44.00-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.236 , 0.289 0.236 , 0.288	Depositor DCC
R_{free} test set	2000 reflections (6.47%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.887	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3694	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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	0.32	0/1808	0.57	0/2456
1	B	0.30	0/1834	0.50	0/2491
All	All	0.31	0/3642	0.53	0/4947

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	1778	0	1689	23	0
1	B	1804	0	1726	19	0
2	A	49	0	0	1	0
2	B	63	0	0	1	0
All	All	3694	0	3415	41	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 (41) 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:5:ILE:HD11	1:B:240:VAL:HG11	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASP:HA	1:A:193:ASN:HD21	1.55	0.71
1:B:157:ASP:HB3	1:B:193:ASN:HD21	1.57	0.67
1:B:176:THR:HG23	1:B:179:GLU:H	1.62	0.64
1:B:45:CYS:SG	2:B:327:HOH:O	2.55	0.63
1:B:157:ASP:HB3	1:B:193:ASN:ND2	2.15	0.62
1:A:18:LEU:HD22	1:A:45:CYS:HB3	1.87	0.57
1:B:37:LEU:HD22	1:B:58:VAL:HG22	1.87	0.57
1:A:229:ASP:HB2	1:B:170:GLY:HA3	1.89	0.55
1:A:140:GLU:O	1:A:144:ILE:HG12	2.07	0.54
1:B:127:GLY:HA3	1:B:164:GLU:O	2.10	0.51
1:A:69:ASP:HB3	1:A:80:LEU:HD12	1.91	0.51
1:A:-1:SER:N	2:A:303:HOH:O	2.37	0.50
1:A:157:ASP:HA	1:A:193:ASN:ND2	2.24	0.49
1:A:29:TYR:CE1	1:A:31:CYS:HA	2.48	0.49
1:A:157:ASP:HB3	1:A:193:ASN:HD22	1.77	0.49
1:B:200:TYR:CZ	1:B:202:GLY:HA3	2.48	0.48
1:B:65:MET:HG2	1:B:66:HIS:O	2.13	0.48
1:B:138:SER:O	1:B:142:LEU:HG	2.14	0.48
1:A:97:ARG:HB2	1:A:103:GLU:HG3	1.95	0.47
1:B:37:LEU:C	1:B:37:LEU:HD23	2.40	0.47
1:B:121:ARG:HH12	1:B:158:GLN:HA	1.80	0.47
1:A:138:SER:O	1:A:142:LEU:HG	2.14	0.46
1:A:39:ILE:HD12	1:A:58:VAL:HG11	1.97	0.46
1:A:40:ALA:HA	1:A:61:GLY:O	2.16	0.45
1:A:92:ILE:HD12	1:A:111:LYS:HB3	1.99	0.44
1:A:6:GLY:CA	1:A:38:MET:HE3	2.48	0.43
1:A:157:ASP:HB3	1:A:193:ASN:ND2	2.33	0.43
1:A:89:TYR:HA	1:A:121:ARG:O	2.18	0.43
1:B:129:ASN:HA	1:B:166:VAL:O	2.19	0.42
1:A:42:MET:HE2	1:A:44:VAL:HG12	2.01	0.42
1:A:99:GLN:HG3	1:A:100:TYR:N	2.34	0.42
1:B:157:ASP:N	1:B:157:ASP:OD1	2.52	0.42
1:A:25:PHE:HZ	1:A:37:LEU:HD11	1.84	0.42
1:B:184:HIS:HB3	1:B:217:ALA:HB1	2.02	0.42
1:B:121:ARG:NH1	1:B:158:GLN:HA	2.35	0.41
1:A:13:LYS:HE3	1:A:21:TYR:CD1	2.56	0.41
1:A:21:TYR:CD1	1:A:230:PRO:HG3	2.56	0.41
1:A:6:GLY:HA3	1:A:38:MET:HE3	2.03	0.40
1:B:162:ALA:HA	1:B:199:ILE:O	2.22	0.40
1:B:19:GLN:HA	1:B:52:MET:HE1	2.03	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	234/247 (95%)	224 (96%)	9 (4%)	1 (0%)	30	28
1	B	240/247 (97%)	231 (96%)	8 (3%)	1 (0%)	30	28
All	All	474/494 (96%)	455 (96%)	17 (4%)	2 (0%)	30	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	13	LYS
1	A	13	LYS

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	180/212 (85%)	180 (100%)	0	100	100
1	B	184/212 (87%)	184 (100%)	0	100	100
All	All	364/424 (86%)	364 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	28	ASN
1	A	106	GLN

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Mol	Chain	Res	Type
1	A	193	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 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

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	238/247 (96%)	2.12	131 (55%) 0 0	37, 47, 64, 70	0
1	B	242/247 (97%)	1.91	99 (40%) 0 1	38, 46, 59, 67	0
All	All	480/494 (97%)	2.02	230 (47%) 0 0	37, 46, 63, 70	0

All (230) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	92	ILE	5.7
1	B	169	ILE	4.9
1	B	172	GLY	4.6
1	B	92	ILE	4.4
1	A	204	VAL	4.4
1	A	149	ALA	4.2
1	A	22	PHE	4.1
1	A	35	ILE	3.9
1	B	30	ALA	3.9
1	B	171	THR	3.8
1	B	163	TYR	3.8
1	A	5	ILE	3.7
1	B	175	ALA	3.7
1	A	163	TYR	3.6
1	A	180	VAL	3.6
1	B	26	VAL	3.6
1	A	221	PHE	3.6
1	B	89	TYR	3.6
1	B	130	LEU	3.5
1	A	89	TYR	3.5
1	A	112	LEU	3.5
1	B	144	ILE	3.4
1	A	87	ALA	3.4
1	A	4	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	46	LEU	3.4
1	A	222	LEU	3.4
1	B	217	ALA	3.3
1	A	82	LEU	3.3
1	A	45	CYS	3.3
1	A	74	THR	3.3
1	A	3	TYR	3.3
1	A	37	LEU	3.3
1	B	25	PHE	3.3
1	A	29	TYR	3.3
1	A	18	LEU	3.2
1	B	52	MET	3.2
1	B	74	THR	3.2
1	B	49	ALA	3.2
1	A	58	VAL	3.1
1	B	5	ILE	3.1
1	B	120	ILE	3.1
1	B	150	LEU	3.1
1	A	100	TYR	3.1
1	B	101	PHE	3.1
1	B	173	LYS	3.1
1	B	45	CYS	3.1
1	A	168	ALA	3.1
1	A	206	ASP	3.1
1	A	169	ILE	3.1
1	A	8	ASN	3.1
1	A	231	GLN	3.1
1	B	37	LEU	3.1
1	B	34	ASN	3.0
1	A	91	ILE	3.0
1	B	35	ILE	3.0
1	A	115	ALA	3.0
1	A	241	SER	3.0
1	B	135	LEU	3.0
1	A	9	PHE	3.0
1	A	26	VAL	3.0
1	B	48	THR	2.9
1	B	231	GLN	2.9
1	B	115	ALA	2.9
1	B	18	LEU	2.9
1	B	93	GLY	2.9
1	B	212	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	81	ILE	2.9
1	B	91	ILE	2.9
1	B	225	SER	2.9
1	A	72	ALA	2.9
1	A	70	GLN	2.8
1	A	142	LEU	2.8
1	A	44	VAL	2.8
1	A	203	SER	2.8
1	A	214	ALA	2.8
1	A	146	LEU	2.8
1	B	237	LEU	2.8
1	A	205	ASN	2.8
1	A	114	SER	2.8
1	A	93	GLY	2.8
1	A	135	LEU	2.8
1	B	124	LEU	2.8
1	A	187	ILE	2.8
1	A	116	LEU	2.7
1	A	207	THR	2.7
1	A	118	HIS	2.7
1	B	226	ALA	2.7
1	A	130	LEU	2.7
1	A	156	LEU	2.7
1	A	234	LEU	2.7
1	B	73	TYR	2.7
1	A	90	VAL	2.7
1	B	108	ILE	2.7
1	B	232	LYS	2.7
1	A	99	GLN	2.6
1	A	20	GLU	2.6
1	B	50	SER	2.6
1	B	236	ILE	2.6
1	A	57	CYS	2.6
1	A	226	ALA	2.6
1	A	212	LEU	2.6
1	A	0	HIS	2.6
1	A	217	ALA	2.6
1	A	124	LEU	2.6
1	B	4	LEU	2.6
1	B	80	LEU	2.6
1	B	22	PHE	2.6
1	A	166	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	240	VAL	2.6
1	A	27	ASN	2.6
1	A	80	LEU	2.6
1	B	44	VAL	2.5
1	A	136	GLY	2.5
1	A	238	ASP	2.5
1	B	234	LEU	2.5
1	A	218	VAL	2.5
1	A	236	ILE	2.5
1	B	166	VAL	2.5
1	A	176	THR	2.5
1	B	79	PRO	2.5
1	B	122	PRO	2.5
1	B	82	LEU	2.5
1	A	199	ILE	2.5
1	A	200	TYR	2.5
1	A	32	PHE	2.5
1	A	220	GLY	2.5
1	A	144	ILE	2.5
1	A	223	ILE	2.5
1	B	211	ILE	2.5
1	B	240	VAL	2.4
1	B	19	GLN	2.4
1	B	210	ASP	2.4
1	A	73	TYR	2.4
1	A	162	ALA	2.4
1	B	107	MET	2.4
1	B	168	ALA	2.4
1	A	86	GLY	2.4
1	A	201	GLY	2.4
1	A	109	ASN	2.4
1	A	123	ILE	2.4
1	A	154	ASP	2.4
1	A	159	ILE	2.4
1	B	132	GLN	2.4
1	B	29	TYR	2.4
1	A	155	THR	2.4
1	A	85	LEU	2.4
1	B	116	LEU	2.4
1	B	187	ILE	2.4
1	B	218	VAL	2.4
1	A	141	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	155	THR	2.4
1	A	216	PRO	2.4
1	B	170	GLY	2.4
1	A	198	ILE	2.4
1	B	207	THR	2.4
1	A	186	TYR	2.3
1	B	3	TYR	2.3
1	B	238	ASP	2.3
1	A	133	LYS	2.3
1	A	108	ILE	2.3
1	A	30	ALA	2.3
1	B	72	ALA	2.3
1	B	186	TYR	2.3
1	A	237	LEU	2.3
1	B	112	LEU	2.3
1	A	101	PHE	2.3
1	A	213	ILE	2.3
1	B	185	GLU	2.3
1	A	228	LEU	2.3
1	B	102	GLY	2.3
1	A	24	GLN	2.3
1	B	70	GLN	2.3
1	B	183	ILE	2.3
1	A	53	THR	2.3
1	B	136	GLY	2.3
1	A	-1	SER	2.2
1	B	9	PHE	2.2
1	A	224	GLY	2.2
1	B	228	LEU	2.2
1	B	12	TYR	2.2
1	A	25	PHE	2.2
1	A	77	THR	2.2
1	A	81	ILE	2.2
1	A	113	LYS	2.2
1	B	205	ASN	2.2
1	A	60	LEU	2.2
1	B	114	SER	2.2
1	B	167	ARG	2.2
1	B	123	ILE	2.2
1	A	62	ALA	2.2
1	B	215	GLN	2.2
1	A	31	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	150	LEU	2.2
1	B	31	CYS	2.2
1	B	227	SER	2.2
1	A	12	TYR	2.2
1	A	34	ASN	2.2
1	A	120	ILE	2.1
1	A	194	GLU	2.1
1	A	63	GLN	2.1
1	A	10	LYS	2.1
1	A	107	MET	2.1
1	B	8	ASN	2.1
1	A	23	ASP	2.1
1	B	230	PRO	2.1
1	B	199	ILE	2.1
1	A	161	VAL	2.1
1	A	225	SER	2.1
1	A	185	GLU	2.1
1	B	220	GLY	2.1
1	A	208	ASN	2.1
1	A	39	ILE	2.1
1	B	83	LYS	2.1
1	B	180	VAL	2.1
1	A	56	SER	2.1
1	A	52	MET	2.0
1	B	142	LEU	2.0
1	A	125	CYS	2.0
1	B	147	ARG	2.0
1	A	211	ILE	2.0
1	B	126	ILE	2.0
1	B	213	ILE	2.0
1	A	49	ALA	2.0
1	A	193	ASN	2.0
1	B	85	LEU	2.0
1	A	13	LYS	2.0
1	B	141	THR	2.0
1	A	102	GLY	2.0
1	A	192	GLY	2.0
1	B	200	TYR	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 [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.