



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:27 AM GMT

PDB ID : 2H6R
Title : Crystal Structure of triosephosphate isomerase (TIM) from *Methanocaldococcus jannaschii*
Authors : Gayathri, P.; Banerjee, M.; Vijayalakshmi, A.; Balaram, H.; Balaram, P.; Murthy, M.R.N.
Deposited on : 2006-06-01
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

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

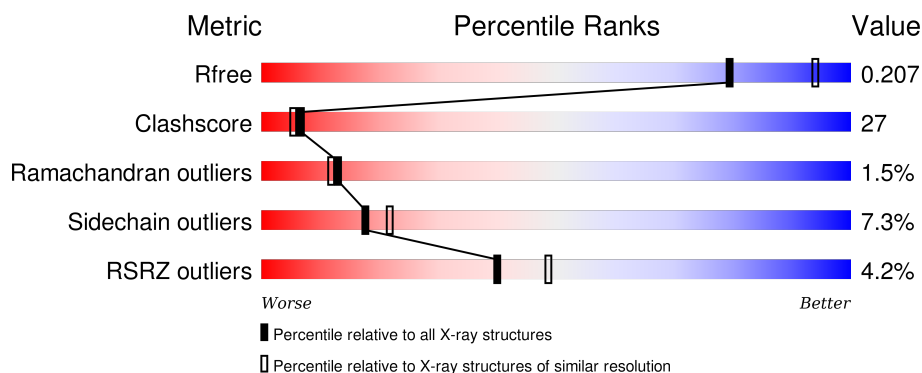
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 $\leq 5\%$. 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	219	<div> <div>2%</div> <div> <div></div> <div>50%</div> <div>37%</div> <div>• • 7%</div> </div> </div>
1	B	219	<div> <div>0%</div> <div> <div></div> <div>59%</div> <div>32%</div> <div>• 5%</div> </div> </div>
1	C	219	<div> <div>4%</div> <div> <div></div> <div>56%</div> <div>34%</div> <div>• 7%</div> </div> </div>
1	D	219	<div> <div>3%</div> <div> <div></div> <div>51%</div> <div>33%</div> <div>6% 9%</div> </div> </div>
1	E	219	<div> <div>3%</div> <div> <div></div> <div>50%</div> <div>38%</div> <div>6% • 5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	219	
1	G	219	
1	H	219	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12422 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	203	Total	C	N	O	S	0	0	0
			1504	943	258	294	9			
1	B	209	Total	C	N	O	S	0	0	0
			1548	971	265	303	9			
1	C	204	Total	C	N	O	S	0	0	0
			1508	946	260	293	9			
1	D	200	Total	C	N	O	S	0	0	0
			1480	927	255	289	9			
1	E	207	Total	C	N	O	S	0	0	0
			1538	966	264	299	9			
1	F	201	Total	C	N	O	S	0	0	0
			1490	934	257	290	9			
1	G	200	Total	C	N	O	S	0	0	0
			1477	925	254	289	9			
1	H	201	Total	C	N	O	S	0	0	0
			1493	937	257	290	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	LEU	ENGINEERED	UNP Q58923
A	134	CYS	TYR	ENGINEERED	UNP Q58923
B	2	VAL	LEU	ENGINEERED	UNP Q58923
B	134	CYS	TYR	ENGINEERED	UNP Q58923
C	2	VAL	LEU	ENGINEERED	UNP Q58923
C	134	CYS	TYR	ENGINEERED	UNP Q58923
D	2	VAL	LEU	ENGINEERED	UNP Q58923
D	134	CYS	TYR	ENGINEERED	UNP Q58923
E	2	VAL	LEU	ENGINEERED	UNP Q58923
E	134	CYS	TYR	ENGINEERED	UNP Q58923
F	2	VAL	LEU	ENGINEERED	UNP Q58923
F	134	CYS	TYR	ENGINEERED	UNP Q58923
G	2	VAL	LEU	ENGINEERED	UNP Q58923

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Chain	Residue	Modelled	Actual	Comment	Reference
G	134	CYS	TYR	ENGINEERED	UNP Q58923
H	2	VAL	LEU	ENGINEERED	UNP Q58923
H	134	CYS	TYR	ENGINEERED	UNP Q58923

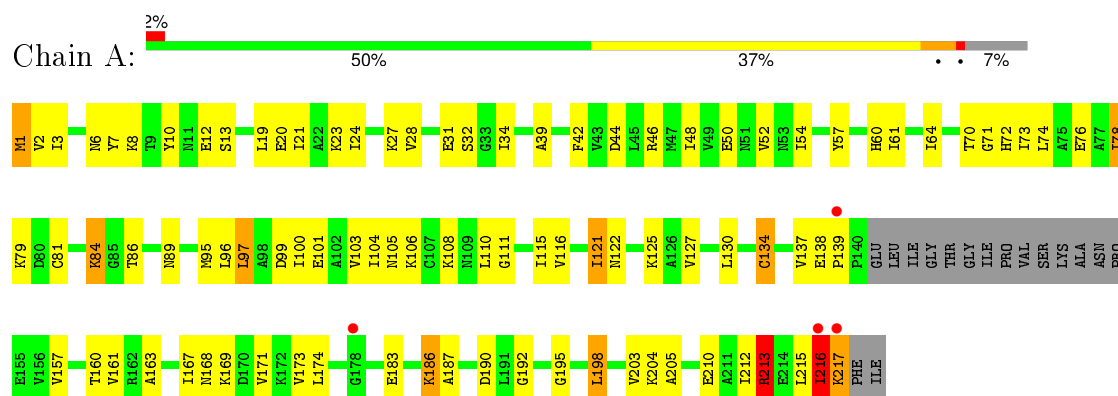
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	58	Total	O	0	0
			58	58		
2	B	55	Total	O	0	0
			55	55		
2	C	45	Total	O	0	0
			45	45		
2	D	46	Total	O	0	0
			46	46		
2	E	53	Total	O	0	0
			53	53		
2	F	34	Total	O	0	0
			34	34		
2	G	36	Total	O	0	0
			36	36		
2	H	57	Total	O	0	0
			57	57		

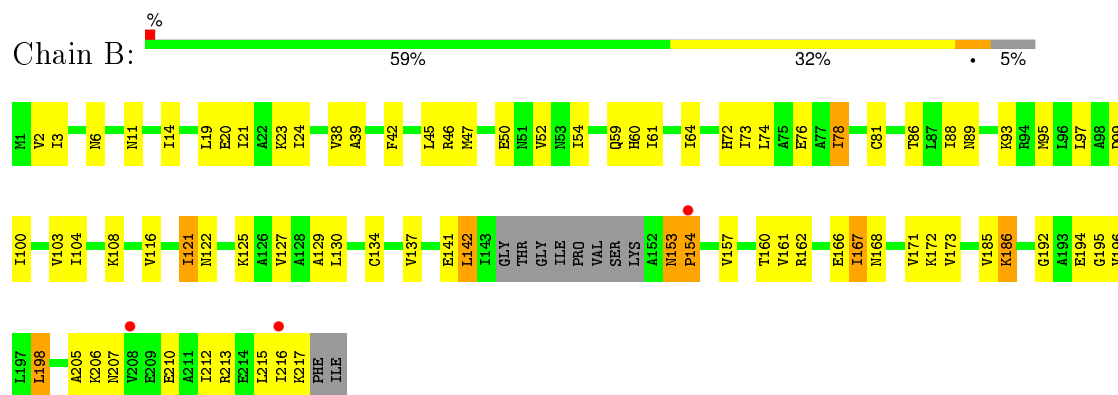
3 Residue-property plots

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.

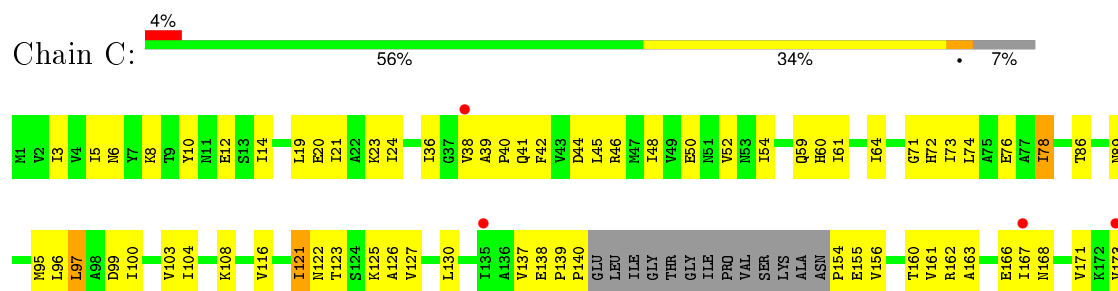
• Molecule 1: Triosephosphate isomerase

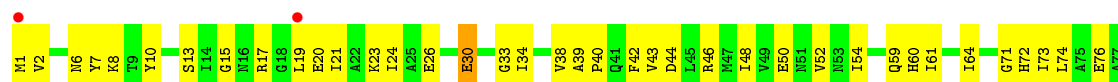


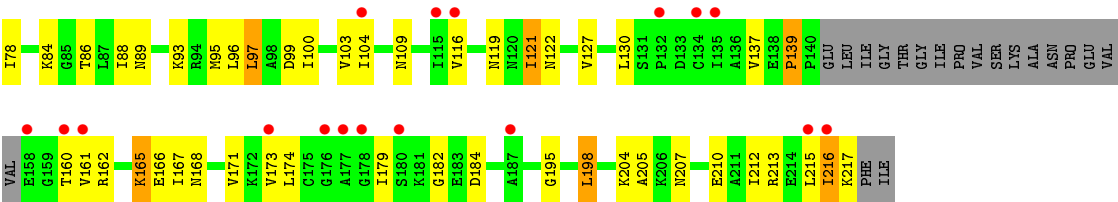
• Molecule 1: Triosephosphate isomerase



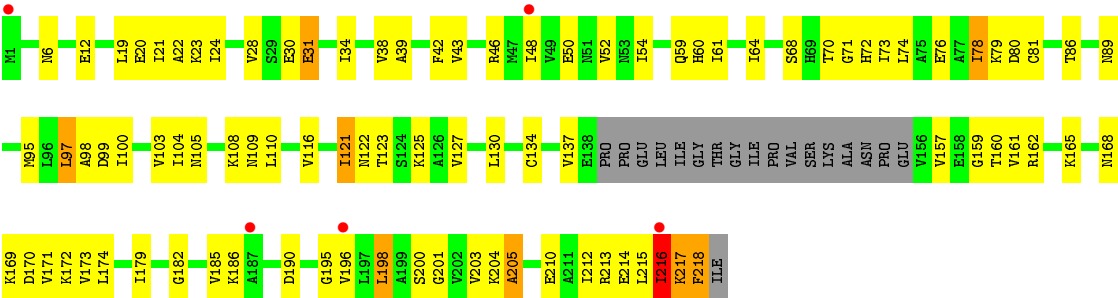
• Molecule 1: Triosephosphate isomerase







• Molecule 1: Triosephosphate isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	139.34Å 139.34Å 80.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.28 – 2.30 34.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.7 (34.28-2.30) 96.2 (34.98-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.56 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.278 0.208 , 0.207	Depositor DCC
R_{free} test set	3415 reflections (4.75%)	DCC
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 20.4	EDS
Estimated twinning fraction	0.250 for h,k,l 0.250 for k,h,-l 0.250 for -k,-h,-l 0.250 for -h,-k,l 0.467 for -h,-k,l 0.426 for h,-h-k,-l 0.420 for -k,-h,-l	Xtriage
Reported twinning fraction	0.250 for h,k,l 0.250 for k,h,-l 0.250 for -k,-h,-l 0.250 for -h,-k,l	Depositor
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 75331 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12422	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.30	0/1516	1.01	8/2051 (0.4%)
1	B	0.23	0/1561	0.58	1/2114 (0.0%)
1	C	0.28	0/1521	0.60	1/2058 (0.0%)
1	D	0.30	0/1490	0.81	5/2014 (0.2%)
1	E	0.27	0/1552	0.58	0/2100
1	F	0.29	0/1502	0.64	2/2031 (0.1%)
1	G	0.24	0/1489	0.57	0/2015
1	H	0.31	1/1504 (0.1%)	0.64	4/2032 (0.2%)
All	All	0.28	1/12135 (0.0%)	0.69	21/16415 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	216	ILE	C-O	-5.05	1.13	1.23

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	ARG	NE-CZ-NH1	-21.76	109.42	120.30
1	A	213	ARG	NE-CZ-NH2	21.27	130.94	120.30
1	D	216	ILE	CA-C-N	-16.48	80.94	117.20
1	A	216	ILE	CA-C-N	-13.72	87.02	117.20
1	D	216	ILE	C-N-CA	12.72	153.51	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	216	ILE	Mainchain

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	1504	0	1560	98	0
1	B	1548	0	1604	67	0
1	C	1508	0	1569	75	0
1	D	1480	0	1537	96	0
1	E	1538	0	1596	105	0
1	F	1490	0	1552	111	0
1	G	1477	0	1525	84	0
1	H	1493	0	1554	83	0
2	A	58	0	0	0	0
2	B	55	0	0	1	0
2	C	45	0	0	0	0
2	D	46	0	0	0	0
2	E	53	0	0	0	0
2	F	34	0	0	0	0
2	G	36	0	0	0	0
2	H	57	0	0	0	0
All	All	12422	0	12497	665	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 27.

The worst 5 of 665 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:F:215:LEU:O	1:F:217:LYS:HD3	1.46	1.13
1:D:217:LYS:HZ3	1:D:217:LYS:HB2	1.01	1.11
1:E:207:ASN:HD21	1:E:210:GLU:HB3	1.07	1.11
1:C:138:GLU:HB3	1:C:139:PRO:HD2	1.12	1.10
1:H:19:LEU:HA	1:H:48:ILE:HD11	1.23	1.09

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	199/219 (91%)	176 (88%)	20 (10%)	3 (2%)	13	12
1	B	205/219 (94%)	177 (86%)	23 (11%)	5 (2%)	7	5
1	C	200/219 (91%)	173 (86%)	26 (13%)	1 (0%)	34	41
1	D	196/219 (90%)	176 (90%)	17 (9%)	3 (2%)	13	12
1	E	203/219 (93%)	181 (89%)	20 (10%)	2 (1%)	19	21
1	F	197/219 (90%)	173 (88%)	20 (10%)	4 (2%)	9	7
1	G	196/219 (90%)	178 (91%)	16 (8%)	2 (1%)	19	21
1	H	197/219 (90%)	174 (88%)	19 (10%)	4 (2%)	9	7
All	All	1593/1752 (91%)	1408 (88%)	161 (10%)	24 (2%)	13	12

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ILE
1	B	142	LEU
1	D	216	ILE
1	G	205	ALA
1	H	205	ALA

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	165/180 (92%)	151 (92%)	14 (8%)	13	16
1	B	170/180 (94%)	160 (94%)	10 (6%)	24	32
1	C	166/180 (92%)	158 (95%)	8 (5%)	31	42
1	D	162/180 (90%)	146 (90%)	16 (10%)	10	11
1	E	169/180 (94%)	152 (90%)	17 (10%)	9	11
1	F	164/180 (91%)	152 (93%)	12 (7%)	17	22
1	G	161/180 (89%)	151 (94%)	10 (6%)	23	30
1	H	164/180 (91%)	155 (94%)	9 (6%)	27	36
All	All	1321/1440 (92%)	1225 (93%)	96 (7%)	17	22

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	198	LEU
1	E	121	ILE
1	H	78	ILE
1	D	207	ASN
1	E	21	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	11	ASN
1	E	120	ASN
1	H	89	ASN
1	E	59	GLN
1	E	105	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 ⓘ

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	203/219 (92%)	0.24	4 (1%) 68 75	13, 29, 42, 53	0
1	B	209/219 (95%)	0.35	3 (1%) 78 83	16, 33, 44, 50	0
1	C	204/219 (93%)	0.48	9 (4%) 38 47	17, 32, 50, 57	0
1	D	200/219 (91%)	0.37	7 (3%) 48 56	15, 32, 51, 60	0
1	E	207/219 (94%)	0.51	7 (3%) 49 58	17, 35, 52, 60	0
1	F	201/219 (91%)	0.66	14 (6%) 19 27	21, 37, 55, 61	0
1	G	200/219 (91%)	0.71	19 (9%) 10 15	22, 39, 60, 69	0
1	H	201/219 (91%)	0.32	5 (2%) 61 70	9, 32, 43, 57	0
All	All	1625/1752 (92%)	0.45	68 (4%) 40 49	9, 34, 51, 69	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	217	LYS	11.6
1	F	216	ILE	6.5
1	A	217	LYS	6.3
1	C	217	LYS	6.1
1	F	177	ALA	5.7

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.