



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:33 AM UTC

PDB ID : 1TPF / pdb_00001tpf
Title : COMPARISON OF THE STRUCTURES AND THE CRYSTAL CONTACTS
OF TRYPANOSOMAL TRIOSEPHOSPHATE ISOMERASE IN FOUR DIF-
FERENT CRYSTAL FORMS
Authors : Radha Kishan, K.V.; Zeelen, J.Ph.; Wierenga, R.K.
Deposited on : 1994-02-28
Resolution : 1.80 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

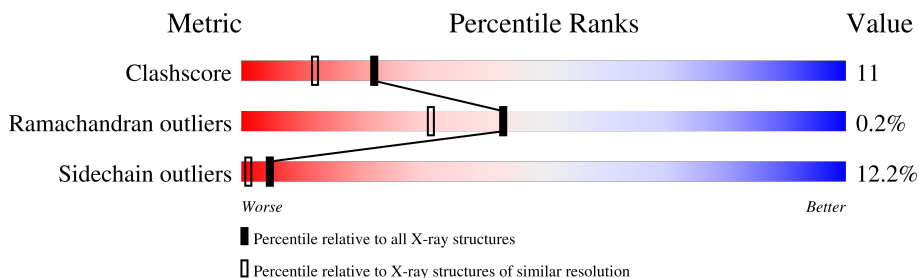
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	250	
1	B	250	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DMS	B	252	-	-	X	-

2 Entry composition [i](#)

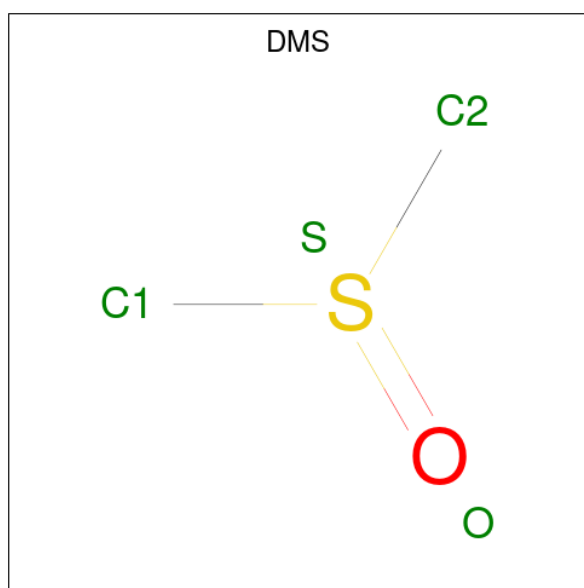
There are 3 unique types of molecules in this entry. The entry contains 3948 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	250	Total	C	N	O	S	0	0	0
			1891	1202	332	351	6			
1	B	249	Total	C	N	O	S	0	0	0
			1883	1197	331	350	5			

- Molecule 2 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	75	Total 75	O 75	0	0
3	B	83	Total 83	O 83	0	0

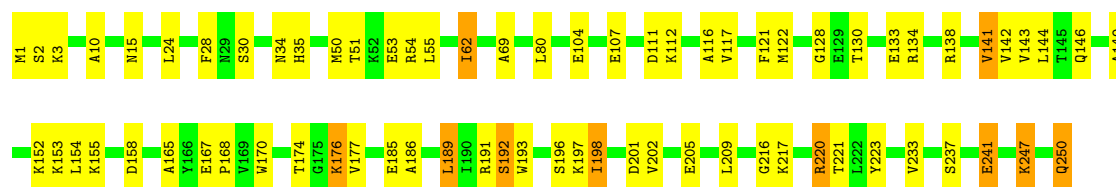
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

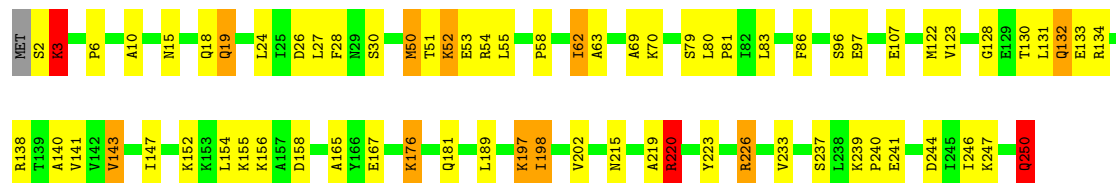
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain A: 



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain B: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.08Å 53.45Å 64.71Å 92.27° 74.63° 116.74°	Depositor
Resolution (Å)	32.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (32.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, R_{free}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3948	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DMS

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	0.85	0/1925	1.49	17/2609 (0.7%)
1	B	0.88	0/1917	1.49	18/2599 (0.7%)
All	All	0.86	0/3842	1.49	35/5208 (0.7%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	ASN	CA-CB-CG	-8.38	104.22	112.60
1	A	141	VAL	CB-CA-C	-7.99	101.74	111.97
1	A	2	SER	N-CA-C	-7.72	98.40	110.36
1	B	69	ALA	N-CA-C	7.38	119.41	111.36
1	A	69	ALA	N-CA-C	6.96	118.94	111.36
1	B	143	VAL	N-CA-CB	6.95	119.99	110.54
1	B	30	SER	CB-CA-C	-6.71	99.21	110.56
1	B	6	PRO	CB-CA-C	-6.48	101.66	110.60
1	A	34	ASN	N-CA-C	6.33	120.21	112.23
1	B	244	ASP	CA-CB-CG	-6.30	106.30	112.60
1	A	15	ASN	CA-CB-CG	6.02	118.62	112.60
1	B	220	ARG	N-CA-CB	6.00	118.95	110.12
1	B	122	MET	N-CA-C	-5.99	99.44	108.96
1	A	189	LEU	N-CA-CB	5.89	118.78	110.12
1	B	3	LYS	N-CA-CB	5.86	120.80	110.37
1	B	123	VAL	N-CA-C	5.84	116.89	108.48
1	B	58	PRO	N-CA-CB	5.65	108.72	103.41
1	B	176	LYS	CB-CA-C	-5.58	99.97	109.51
1	B	165	ALA	N-CA-CB	5.43	119.07	110.55
1	A	192	SER	N-CA-CB	5.42	118.09	110.12
1	B	15	ASN	CA-CB-CG	5.40	118.00	112.60
1	A	30	SER	CB-CA-C	-5.40	100.77	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	ALA	N-CA-CB	-5.36	103.09	111.56
1	A	191	ARG	CD-NE-CZ	-5.30	116.98	124.40
1	A	121	PHE	CB-CA-C	-5.28	100.59	109.83
1	A	165	ALA	N-CA-CB	5.26	118.86	110.65
1	A	250	GLN	N-CA-CB	5.26	119.44	110.50
1	A	233	VAL	N-CA-C	5.24	116.52	108.71
1	B	246	ILE	CB-CA-C	-5.21	105.11	112.14
1	A	122	MET	N-CA-C	-5.18	100.86	109.46
1	B	250	GLN	N-CA-CB	5.17	119.30	110.50
1	A	30	SER	N-CA-CB	-5.17	102.97	110.47
1	B	233	VAL	N-CA-C	5.16	116.40	108.71
1	A	168	PRO	CB-CA-C	-5.11	104.31	112.27
1	B	219	ALA	N-CA-C	5.04	116.78	111.28

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	1891	0	1929	36	0
1	B	1883	0	1917	46	0
2	A	8	0	12	0	0
2	B	8	0	12	7	0
3	A	75	0	0	0	0
3	B	83	0	0	0	0
All	All	3948	0	3870	82	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 11.

All (82) 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:226:ARG:HG3	1:B:226:ARG:HH11	1.34	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:GLN:HE21	1:B:19:GLN:HA	1.34	0.91
1:B:197:LYS:C	1:B:198:ILE:HD13	2.08	0.77
1:A:51:THR:HG22	1:A:62:ILE:HD11	1.65	0.76
1:B:96:SER:C	2:B:252:DMS:H22	2.11	0.75
1:B:97:GLU:HA	2:B:252:DMS:C2	2.17	0.74
1:A:24:LEU:HD21	1:A:28:PHE:CZ	2.22	0.73
1:B:226:ARG:HG3	1:B:226:ARG:NH1	2.00	0.73
1:B:10:ALA:HB1	1:B:237:SER:HB2	1.74	0.70
1:A:185:GLU:O	1:A:189:LEU:HD23	1.94	0.67
1:B:220:ARG:NH2	1:B:250:GLN:OXT	2.29	0.66
1:B:220:ARG:HH21	1:B:223:TYR:HD2	1.45	0.65
1:A:10:ALA:HB1	1:A:237:SER:HB2	1.79	0.64
1:A:3:LYS:NZ	1:A:223:TYR:O	2.33	0.61
1:A:186:ALA:HA	1:A:189:LEU:CD2	2.30	0.61
1:B:19:GLN:HE21	1:B:19:GLN:CA	2.08	0.61
1:A:51:THR:HG22	1:A:62:ILE:CD1	2.32	0.60
1:B:96:SER:O	2:B:252:DMS:H22	2.03	0.58
1:A:174:THR:O	1:A:176:LYS:NZ	2.30	0.58
1:B:97:GLU:HA	2:B:252:DMS:H22	1.84	0.58
1:B:154:LEU:HB3	1:B:158:ASP:HB2	1.85	0.58
1:A:186:ALA:HA	1:A:189:LEU:HD21	1.86	0.57
1:B:18:GLN:O	1:B:50:MET:HE1	2.04	0.57
1:A:220:ARG:NH2	1:A:250:GLN:O	2.35	0.57
1:A:247:LYS:O	1:A:250:GLN:HG2	2.04	0.57
1:B:27:LEU:CD2	1:B:240:PRO:HB3	2.34	0.56
1:B:3:LYS:NZ	1:B:223:TYR:O	2.39	0.55
1:A:104:GLU:OE2	1:A:112:LYS:NZ	2.40	0.53
1:A:197:LYS:C	1:A:198:ILE:HD13	2.33	0.53
1:A:201:ASP:N	1:A:201:ASP:OD1	2.39	0.53
1:B:220:ARG:NH2	1:B:223:TYR:HD2	2.07	0.53
1:B:198:ILE:HD13	1:B:198:ILE:N	2.23	0.52
1:B:80:LEU:HB2	1:B:81:PRO:HD3	1.92	0.52
1:B:97:GLU:HA	2:B:252:DMS:H23	1.90	0.52
1:A:198:ILE:HD13	1:A:198:ILE:N	2.25	0.52
1:B:220:ARG:O	1:B:220:ARG:HG3	2.09	0.51
1:B:27:LEU:HD21	1:B:240:PRO:HB3	1.93	0.50
1:A:193:TRP:CE2	1:A:197:LYS:HG3	2.47	0.50
1:B:52:LYS:HE2	1:B:86:PHE:CE2	2.47	0.49
1:A:220:ARG:NH1	1:A:250:GLN:O	2.45	0.49
1:B:97:GLU:N	2:B:252:DMS:H22	2.29	0.48
1:B:197:LYS:O	1:B:198:ILE:HD13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:HD21	1:A:28:PHE:CE2	2.49	0.47
1:A:117:VAL:HG11	1:A:158:ASP:HB3	1.97	0.47
1:A:186:ALA:HA	1:A:189:LEU:HD23	1.97	0.47
1:B:10:ALA:CB	1:B:237:SER:HB2	2.42	0.46
1:B:226:ARG:HH11	1:B:226:ARG:CG	2.15	0.46
1:A:80:LEU:HD13	1:A:116:ALA:HA	1.98	0.46
1:A:24:LEU:C	1:A:24:LEU:HD23	2.41	0.45
1:A:111:ASP:OD1	1:A:153:LYS:HE3	2.17	0.45
1:B:80:LEU:N	1:B:81:PRO:CD	2.80	0.45
1:A:130:THR:OG1	1:A:133:GLU:HG3	2.17	0.44
1:B:247:LYS:O	1:B:250:GLN:HG3	2.17	0.44
1:B:220:ARG:NH1	1:B:250:GLN:OXT	2.51	0.44
1:A:154:LEU:HB3	1:A:158:ASP:HB2	2.00	0.44
1:B:26:ASP:OD1	1:B:54:ARG:NH2	2.50	0.44
1:B:140:ALA:HA	1:B:189:LEU:HD21	1.99	0.43
1:B:130:THR:OG1	1:B:133:GLU:HG3	2.19	0.43
1:A:128:GLY:HA3	1:A:167:GLU:O	2.19	0.43
1:A:142:VAL:O	1:A:146:GLN:HG3	2.18	0.43
1:A:201:ASP:OD1	1:A:202:VAL:N	2.50	0.43
1:B:51:THR:HG22	1:B:62:ILE:HG21	2.00	0.43
1:A:149:ALA:O	1:A:152:LYS:HG2	2.19	0.43
1:B:83:LEU:HD23	1:B:83:LEU:HA	1.89	0.43
1:A:216:GLY:N	1:A:241:GLU:OE2	2.39	0.42
1:B:220:ARG:NH2	1:B:223:TYR:CD2	2.85	0.42
1:A:144:LEU:HD22	1:A:193:TRP:CG	2.54	0.42
1:B:28:PHE:N	1:B:28:PHE:CD1	2.87	0.42
1:A:134:ARG:HD2	1:A:170:TRP:CD2	2.54	0.42
1:A:10:ALA:CB	1:A:237:SER:HB2	2.48	0.41
1:B:226:ARG:O	1:B:226:ARG:HD2	2.20	0.41
1:A:193:TRP:CD1	1:A:197:LYS:HZ3	2.39	0.41
1:B:97:GLU:CA	2:B:252:DMS:H22	2.48	0.41
1:B:79:SER:HB2	1:B:81:PRO:HD2	2.01	0.41
1:B:215:ASN:HB2	1:B:241:GLU:OE2	2.21	0.41
1:A:35:HIS:ND1	1:A:35:HIS:N	2.66	0.41
1:B:181:GLN:CD	1:B:181:GLN:H	2.29	0.41
1:B:156:LYS:HE3	1:B:202:VAL:HG23	2.02	0.40
1:B:132:GLN:HE21	1:B:132:GLN:HB3	1.67	0.40
1:B:181:GLN:CD	1:B:181:GLN:N	2.80	0.40
1:A:107:GLU:H	1:A:107:GLU:CD	2.29	0.40
1:B:128:GLY:HA3	1:B:167:GLU:O	2.22	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	248/250 (99%)	244 (98%)	4 (2%)	0	100	100
1	B	247/250 (99%)	241 (98%)	5 (2%)	1 (0%)	30	19
All	All	495/500 (99%)	485 (98%)	9 (2%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	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	197/197 (100%)	175 (89%)	22 (11%)	6	1
1	B	196/197 (100%)	170 (87%)	26 (13%)	4	1
All	All	393/394 (100%)	345 (88%)	48 (12%)	5	1

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	50	MET
1	A	53	GLU
1	A	54	ARG
1	A	55	LEU

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Mol	Chain	Res	Type
1	A	62	ILE
1	A	138	ARG
1	A	141	VAL
1	A	143	VAL
1	A	155	LYS
1	A	176	LYS
1	A	177	VAL
1	A	192	SER
1	A	196	SER
1	A	198	ILE
1	A	205	GLU
1	A	209	LEU
1	A	217	LYS
1	A	220	ARG
1	A	221	THR
1	A	241	GLU
1	A	247	LYS
1	B	2	SER
1	B	19	GLN
1	B	24	LEU
1	B	50	MET
1	B	52	LYS
1	B	53	GLU
1	B	55	LEU
1	B	62	ILE
1	B	70	LYS
1	B	107	GLU
1	B	131	LEU
1	B	132	GLN
1	B	134	ARG
1	B	138	ARG
1	B	141	VAL
1	B	143	VAL
1	B	147	ILE
1	B	152	LYS
1	B	155	LYS
1	B	176	LYS
1	B	197	LYS
1	B	198	ILE
1	B	220	ARG
1	B	226	ARG
1	B	239	LYS

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Mol	Chain	Res	Type
1	B	250	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	19	GLN
1	B	132	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	DMS	B	252	-	3,3,3	0.39	0	3,3,3	0.57	0
2	DMS	A	252	-	3,3,3	0.43	0	3,3,3	0.53	0
2	DMS	B	251	-	3,3,3	0.57	0	3,3,3	0.28	0
2	DMS	A	251	-	3,3,3	0.42	0	3,3,3	0.73	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	252	DMS	7	0

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.