



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:19 AM UTC

PDB ID : 1TRI / pdb_00001tri
Title : THE CRYSTAL STRUCTURE OF AN ENGINEERED MONOMERIC
TRIOSEPHOSPHATE ISOMERASE, MONOTIM: THE CORRECT MOD-
ELLING OF AN EIGHT-RESIDUE LOOP
Authors : Wierenga, R.K.
Deposited on : 1993-10-08
Resolution : 2.40 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

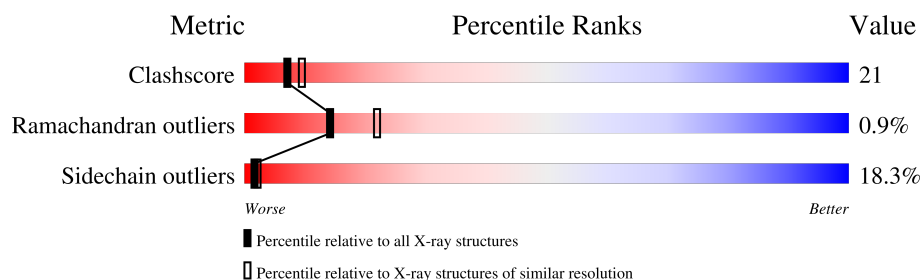
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	243	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1831 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	239	Total	C	N	O	S	0	0	0
			1805	1144	319	338	4			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	GLY	ILE	engineered mutation	UNP P04789
A	69	ASN	ALA	engineered mutation	UNP P04789
A	70	ALA	LYS	engineered mutation	UNP P04789
A	71	ASP	SER	engineered mutation	UNP P04789
A	72	ALA	GLY	engineered mutation	UNP P04789
A	?	-	ALA	deletion	UNP P04789
A	?	-	PHE	deletion	UNP P04789
A	?	-	THR	deletion	UNP P04789
A	?	-	GLU	deletion	UNP P04789
A	?	-	VAL	deletion	UNP P04789
A	?	-	SER	deletion	UNP P04789
A	81	ALA	PRO	engineered mutation	UNP P04789
A	82	SER	ILE	engineered mutation	UNP P04789

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

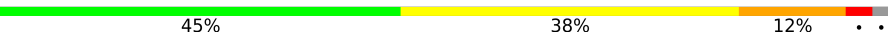
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		

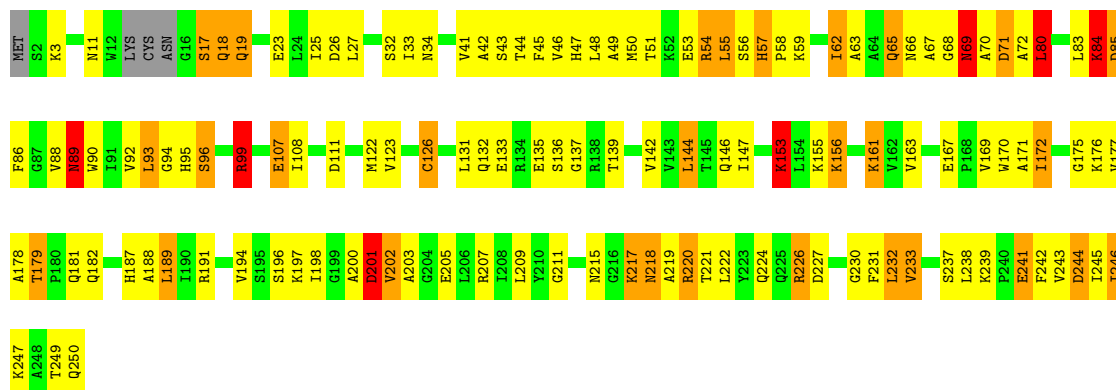
3 Residue-property plots

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: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	83.78Å 42.80Å 68.84Å 90.00° 108.22° 90.00°	Depositor
Resolution (Å)	32.60 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (32.60-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, R_{free}	0.165 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1831	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: SO4

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	1.81	26/1836 (1.4%)	1.89	40/2489 (1.6%)

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 (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	LYS	N-CA	-6.65	1.38	1.46
1	A	245	ILE	C-O	-6.29	1.16	1.24
1	A	44	THR	C-N	-6.17	1.26	1.33
1	A	207	ARG	CA-C	-6.14	1.45	1.52
1	A	211	GLY	N-CA	-6.14	1.39	1.45
1	A	49	ALA	C-N	-5.99	1.26	1.33
1	A	26	ASP	CG-OD1	5.94	1.36	1.25
1	A	239	LYS	C-N	-5.86	1.27	1.34
1	A	107	GLU	CD-OE1	5.85	1.36	1.25
1	A	178	ALA	C-O	-5.84	1.16	1.24
1	A	67	ALA	C-N	5.75	1.38	1.33
1	A	241	GLU	C-O	-5.66	1.16	1.24
1	A	191	ARG	CA-C	5.66	1.60	1.52
1	A	80	LEU	N-CA	-5.63	1.39	1.46
1	A	231	PHE	CA-C	-5.60	1.45	1.52
1	A	144	LEU	CA-C	-5.59	1.45	1.52
1	A	86	PHE	C-N	-5.50	1.26	1.33
1	A	96	SER	N-CA	-5.44	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	GLN	CA-C	-5.38	1.46	1.52
1	A	85	ASP	CG-OD2	5.33	1.35	1.25
1	A	196	SER	C-O	-5.27	1.18	1.24
1	A	222	LEU	C-O	-5.21	1.18	1.24
1	A	202	VAL	N-CA	-5.19	1.40	1.46
1	A	230	GLY	C-O	5.08	1.28	1.23
1	A	92	VAL	CA-CB	-5.08	1.47	1.54
1	A	126	CYS	CA-C	-5.02	1.46	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	GLY	N-CA-C	11.55	120.72	110.21
1	A	219	ALA	N-CA-C	8.11	121.14	111.33
1	A	89	ASN	CA-CB-CG	-7.40	105.20	112.60
1	A	153	LYS	N-CA-C	7.38	122.40	112.88
1	A	233	VAL	N-CA-C	6.77	117.62	107.80
1	A	139	THR	N-CA-C	6.67	118.24	110.97
1	A	49	ALA	CA-C-O	6.59	127.74	120.82
1	A	86	PHE	CA-C-O	6.55	126.11	118.90
1	A	88	VAL	N-CA-CB	6.41	118.68	110.99
1	A	179	THR	N-CA-C	-6.27	102.92	110.13
1	A	201	ASP	CA-C-N	6.20	128.59	120.60
1	A	201	ASP	C-N-CA	6.20	128.59	120.60
1	A	123	VAL	N-CA-C	6.02	116.54	108.11
1	A	163	VAL	CA-C-N	-6.00	115.36	123.10
1	A	163	VAL	C-N-CA	-6.00	115.36	123.10
1	A	218	ASN	N-CA-C	5.99	120.66	113.23
1	A	175	GLY	N-CA-C	-5.85	107.02	115.27
1	A	147	ILE	CA-C-N	5.77	128.49	120.29
1	A	147	ILE	C-N-CA	5.77	128.49	120.29
1	A	226	ARG	N-CA-C	5.77	118.31	111.33
1	A	244	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	84	LYS	O-C-N	5.67	128.21	122.09
1	A	221	THR	CB-CA-C	5.58	120.34	110.85
1	A	41	VAL	N-CA-CB	5.54	118.86	112.15
1	A	172	ILE	N-CA-C	5.52	115.20	107.37
1	A	92	VAL	N-CA-CB	-5.50	104.34	111.82
1	A	189	LEU	N-CA-CB	-5.45	101.82	109.94
1	A	71	ASP	CB-CA-C	5.36	119.37	110.90
1	A	99	ARG	CA-C-N	5.34	127.44	120.28
1	A	99	ARG	C-N-CA	5.34	127.44	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	ASN	N-CA-CB	-5.31	101.62	110.39
1	A	34	ASN	N-CA-C	5.30	118.59	112.97
1	A	187	HIS	CA-C-N	5.28	127.30	120.44
1	A	187	HIS	C-N-CA	5.28	127.30	120.44
1	A	71	ASP	CA-CB-CG	-5.25	107.35	112.60
1	A	57	HIS	CB-CA-C	5.25	117.52	109.60
1	A	200	ALA	CA-C-O	5.23	125.81	119.11
1	A	71	ASP	N-CA-C	5.22	116.78	111.14
1	A	232	LEU	CB-CA-C	5.16	119.20	110.79
1	A	108	ILE	N-CA-C	5.11	115.88	110.72

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	ASN	Sidechain

5.2 Too-close contacts [i](#)

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	1805	0	1826	76	0
2	A	5	0	0	0	0
3	A	21	0	0	4	0
All	All	1831	0	1826	76	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 21.

All (76) 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:45:PHE:HA	1:A:48:LEU:HD12	1.57	0.86
1:A:242:PHE:CE2	1:A:246:ILE:HD11	2.13	0.84
1:A:42:ALA:HB1	1:A:65:GLN:HE21	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:PHE:O	1:A:246:ILE:HD12	1.83	0.78
1:A:156:LYS:HD3	1:A:202:VAL:HG21	1.68	0.75
1:A:33:ILE:HG21	1:A:59:LYS:HD2	1.69	0.71
1:A:25:ILE:HG21	1:A:54:ARG:HB3	1.72	0.71
1:A:111:ASP:OD1	1:A:153:LYS:HE2	1.90	0.71
1:A:45:PHE:HA	1:A:48:LEU:CD1	2.21	0.71
1:A:33:ILE:CG2	1:A:59:LYS:HD2	2.23	0.69
1:A:57:HIS:ND1	1:A:58:PRO:HD2	2.11	0.66
1:A:18:GLN:OE1	1:A:50:MET:HE2	1.96	0.66
1:A:156:LYS:HD3	1:A:202:VAL:CG2	2.25	0.65
1:A:63:ALA:HB2	1:A:90:TRP:HB2	1.78	0.65
1:A:198:ILE:HG21	1:A:202:VAL:HG11	1.80	0.63
1:A:66:ASN:HA	1:A:93:LEU:HD12	1.81	0.63
1:A:170:TRP:CZ3	1:A:176:LYS:HE2	2.35	0.61
1:A:201:ASP:OD1	1:A:201:ASP:N	2.32	0.60
1:A:170:TRP:HZ3	1:A:176:LYS:HE2	1.67	0.59
1:A:19:GLN:O	1:A:23:GLU:HG3	2.04	0.58
1:A:142:VAL:O	1:A:146:GLN:HG3	2.04	0.57
1:A:242:PHE:CD2	1:A:246:ILE:HD11	2.40	0.57
1:A:69:ASN:OD1	1:A:71:ASP:HB2	2.06	0.56
1:A:69:ASN:CG	1:A:71:ASP:H	2.13	0.56
1:A:237:SER:HA	1:A:242:PHE:HB2	1.88	0.56
1:A:170:TRP:HZ3	1:A:176:LYS:CE	2.19	0.55
1:A:99:ARG:HH11	1:A:99:ARG:HG2	1.71	0.55
1:A:220:ARG:O	1:A:224:GLN:HG3	2.07	0.54
1:A:95:HIS:HB3	1:A:126:CYS:O	2.07	0.54
1:A:33:ILE:HG22	1:A:59:LYS:HZ2	1.72	0.54
1:A:33:ILE:HG22	1:A:59:LYS:NZ	2.22	0.54
1:A:220:ARG:HD2	1:A:224:GLN:OE1	2.08	0.54
1:A:132:GLN:H	1:A:132:GLN:CD	2.16	0.54
1:A:215:ASN:OD1	1:A:217:LYS:N	2.40	0.54
1:A:51:THR:O	1:A:55:LEU:HB2	2.07	0.53
1:A:63:ALA:HB2	1:A:90:TRP:CB	2.39	0.53
1:A:131:LEU:HG	1:A:135:GLU:OE2	2.08	0.53
1:A:233:VAL:HG12	1:A:237:SER:HB3	1.91	0.52
1:A:179:THR:N	1:A:182:GLN:OE1	2.41	0.51
1:A:33:ILE:HG22	1:A:33:ILE:O	2.09	0.51
1:A:167:GLU:OE1	1:A:232:LEU:HD23	2.12	0.50
1:A:51:THR:CG2	1:A:62:ILE:HG21	2.42	0.50
1:A:99:ARG:HG2	3:A:559:HOH:O	2.12	0.50
1:A:188:ALA:HB3	3:A:575:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ASN:ND2	1:A:70:ALA:N	2.60	0.49
1:A:135:GLU:C	1:A:137:GLY:H	2.21	0.49
1:A:51:THR:HG22	1:A:62:ILE:HG21	1.95	0.49
1:A:84:LYS:NZ	1:A:89:ASN:HA	2.28	0.49
1:A:18:GLN:HE22	1:A:47:HIS:CD2	2.31	0.49
1:A:176:LYS:HD2	1:A:176:LYS:C	2.38	0.48
1:A:171:ALA:HA	1:A:176:LYS:O	2.14	0.47
1:A:80:LEU:HD12	1:A:80:LEU:HA	1.55	0.47
1:A:246:ILE:O	1:A:249:THR:OG1	2.31	0.47
1:A:167:GLU:HG2	1:A:172:ILE:HD11	1.97	0.47
1:A:85:ASP:O	1:A:85:ASP:OD1	2.31	0.47
1:A:226:ARG:HD2	1:A:227:ASP:OD2	2.14	0.47
1:A:176:LYS:HE3	1:A:177:VAL:O	2.15	0.46
1:A:33:ILE:HG21	1:A:59:LYS:CD	2.41	0.46
1:A:198:ILE:CG2	1:A:202:VAL:HG11	2.46	0.45
1:A:94:GLY:HA2	1:A:126:CYS:HB2	1.97	0.45
1:A:84:LYS:NZ	1:A:89:ASN:OD1	2.48	0.45
1:A:72:ALA:O	1:A:83:LEU:HG	2.17	0.44
1:A:133:GLU:CD	1:A:142:VAL:HG21	2.43	0.44
1:A:17:SER:OG	1:A:19:GLN:HG3	2.18	0.44
1:A:215:ASN:OD1	1:A:218:ASN:N	2.37	0.44
1:A:217:LYS:HD2	1:A:217:LYS:HA	1.90	0.42
1:A:122:MET:SD	1:A:161:LYS:HA	2.59	0.42
1:A:194:VAL:HG12	1:A:203:ALA:HB2	2.01	0.42
1:A:144:LEU:HD23	1:A:144:LEU:HA	1.86	0.42
1:A:205:GLU:HG3	3:A:563:HOH:O	2.18	0.42
1:A:241:GLU:O	1:A:244:ASP:HB2	2.19	0.42
1:A:243:VAL:O	1:A:247:LYS:HG3	2.20	0.42
1:A:17:SER:OG	1:A:19:GLN:N	2.54	0.41
1:A:3:LYS:HB3	3:A:557:HOH:O	2.20	0.41
1:A:57:HIS:CG	1:A:58:PRO:HD2	2.54	0.41
1:A:172:ILE:O	1:A:172:ILE:HG22	2.20	0.40

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	235/243 (97%)	225 (96%)	8 (3%)	2 (1%)	14	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	SER
1	A	69	ASN

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	186/190 (98%)	152 (82%)	34 (18%)	2	2

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	SER
1	A	18	GLN
1	A	19	GLN
1	A	27	LEU
1	A	32	SER
1	A	43	SER
1	A	46	VAL
1	A	53	GLU
1	A	54	ARG
1	A	55	LEU
1	A	56	SER
1	A	62	ILE
1	A	65	GLN
1	A	69	ASN
1	A	80	LEU

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Mol	Chain	Res	Type
1	A	84	LYS
1	A	93	LEU
1	A	96	SER
1	A	99	ARG
1	A	107	GLU
1	A	153	LYS
1	A	155	LYS
1	A	156	LYS
1	A	161	LYS
1	A	169	VAL
1	A	189	LEU
1	A	197	LYS
1	A	201	ASP
1	A	209	LEU
1	A	217	LYS
1	A	220	ARG
1	A	238	LEU
1	A	246	ILE
1	A	250	GLN

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	47	HIS
1	A	65	GLN
1	A	146	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	SO4	A	555	-	4,4,4	0.78	0	6,6,6	0.66	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.

No monomer is involved in short contacts.

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.