



Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 12:34 PM GMT

PDB ID : 6TIM
Title : THE ADAPTABILITY OF THE ACTIVE SITE OF TRYPANOSOMAL
TRIOSEPHOSPHATE ISOMERASE AS OBSERVED IN THE CRYSTAL
STRUCTURES OF THREE DIFFERENT COMPLEXES
Authors : Noble, M.E.M.; Wierenga, R.K.; Hol, W.G.J.
Deposited on : 1991-04-23
Resolution : 2.20 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

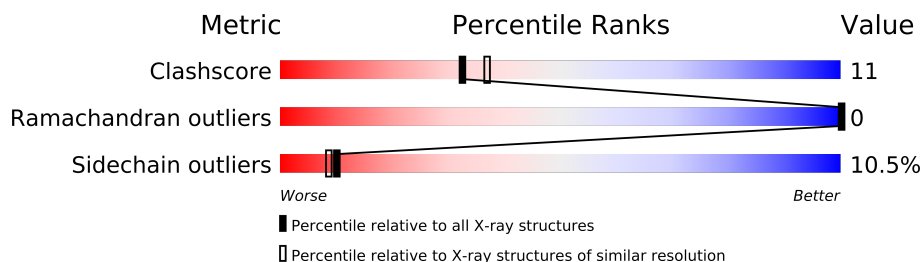
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.20 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	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

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

2 Entry composition i

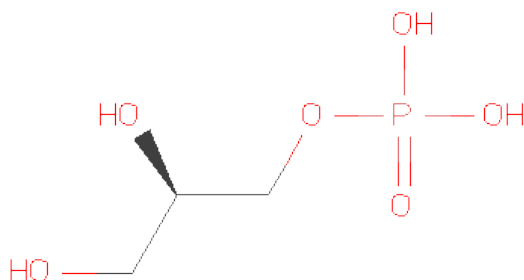
There are 3 unique types of molecules in this entry. The entry contains 3867 atoms, of which 0 are hydrogen and 0 are deuterium.

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	249	Total	C	N	O	S	0	0	0
			1883	1197	331	350	5			
1	B	249	Total	C	N	O	S	0	0	0
			1883	1197	331	350	5			

- Molecule 2 is SN-GLYCEROL-3-PHOSPHATE (three-letter code: G3P) (formula: $C_3H_9O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	53	Total	O	0	0
			53	53		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	38	Total	O	0	0
			38	38		

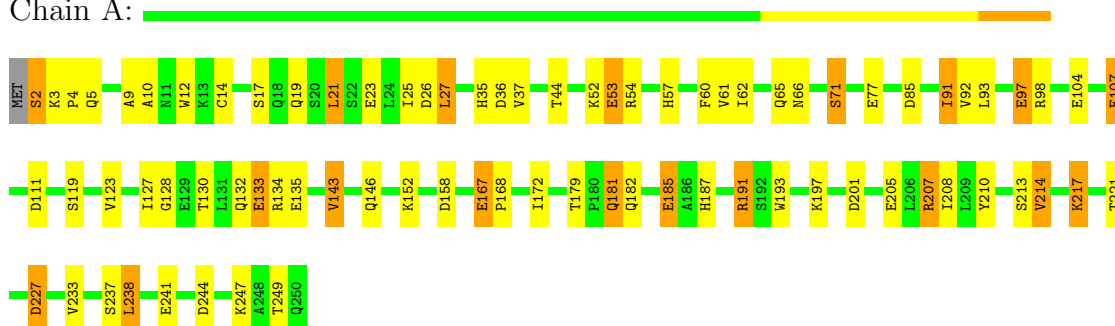
3 Residue-property plots

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.

Note EDS was not executed.

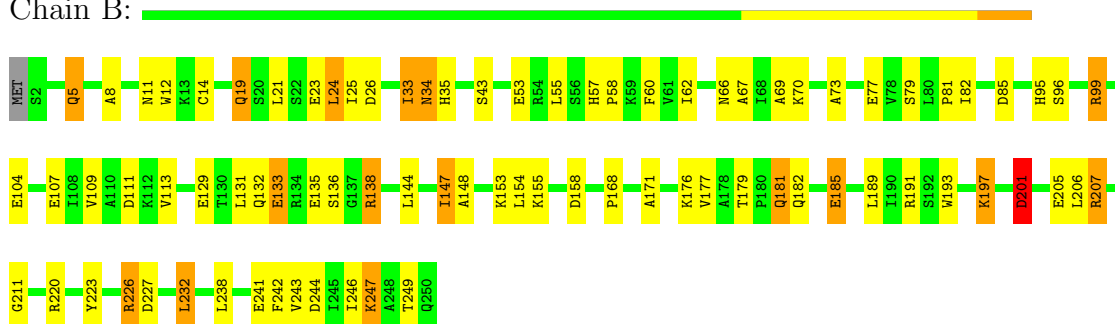
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain A:



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain B:



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.36Å 97.59Å 46.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.370 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3867	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: G3P

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	0.95	12/1917 (0.6%)	1.37	20/2599 (0.8%)
1	B	0.92	10/1917 (0.5%)	1.32	11/2599 (0.4%)
All	All	0.93	22/3834 (0.6%)	1.35	31/5198 (0.6%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	GLU	CD-OE2	9.89	1.36	1.25
1	B	107	GLU	CD-OE1	8.02	1.34	1.25
1	A	97	GLU	CD-OE2	7.48	1.33	1.25
1	B	185	GLU	CD-OE1	7.41	1.33	1.25
1	B	77	GLU	CD-OE2	7.23	1.33	1.25
1	A	167	GLU	CD-OE2	7.19	1.33	1.25
1	A	23	GLU	CD-OE2	6.98	1.33	1.25
1	B	53	GLU	CD-OE1	6.73	1.33	1.25
1	A	185	GLU	CD-OE2	6.72	1.33	1.25
1	B	133	GLU	CD-OE2	6.71	1.33	1.25
1	A	107	GLU	CD-OE2	6.60	1.32	1.25
1	B	135	GLU	CD-OE2	6.02	1.32	1.25
1	B	205	GLU	CD-OE2	5.84	1.32	1.25
1	B	241	GLU	CD-OE1	5.77	1.31	1.25
1	A	77	GLU	CD-OE2	5.53	1.31	1.25
1	A	135	GLU	CD-OE1	5.48	1.31	1.25
1	B	104	GLU	CD-OE2	5.39	1.31	1.25
1	A	241	GLU	CD-OE2	5.38	1.31	1.25
1	B	23	GLU	CD-OE2	5.32	1.31	1.25
1	A	133	GLU	CD-OE1	5.29	1.31	1.25
1	A	205	GLU	CD-OE2	5.06	1.31	1.25
1	A	53	GLU	CD-OE2	5.04	1.31	1.25

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	ARG	NE-CZ-NH2	-10.74	114.93	120.30
1	A	191	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	A	227	ASP	CB-CG-OD1	7.21	124.79	118.30
1	B	201	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	B	8	ALA	N-CA-CB	7.02	119.93	110.10
1	A	227	ASP	CB-CG-OD2	-6.87	112.11	118.30
1	B	26	ASP	CB-CG-OD1	6.69	124.32	118.30
1	A	26	ASP	CB-CG-OD1	-6.56	112.39	118.30
1	B	244	ASP	CB-CG-OD1	-6.47	112.48	118.30
1	A	2	SER	N-CA-CB	6.45	120.18	110.50
1	B	201	ASP	CB-CG-OD1	6.45	124.10	118.30
1	B	111	ASP	CB-CG-OD2	-6.03	112.88	118.30
1	A	111	ASP	CB-CG-OD1	6.00	123.70	118.30
1	B	19	GLN	CB-CA-C	5.87	122.14	110.40
1	A	36	ASP	CB-CG-OD1	-5.86	113.03	118.30
1	A	158	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	A	111	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	A	210	TYR	CB-CG-CD2	-5.71	117.57	121.00
1	A	201	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	191	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	214	VAL	CB-CA-C	5.57	121.97	111.40
1	A	37	VAL	CG1-CB-CG2	-5.48	102.13	110.90
1	A	244	ASP	CB-CG-OD1	-5.46	113.39	118.30
1	A	98	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	B	96	SER	N-CA-CB	5.39	118.59	110.50
1	A	201	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	17	SER	N-CA-CB	5.26	118.39	110.50
1	B	85	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	B	223	TYR	CB-CG-CD1	-5.09	117.94	121.00
1	A	143	VAL	N-CA-CB	5.08	122.69	111.50
1	B	99	ARG	NE-CZ-NH2	5.07	122.84	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1883	0	1917	39	0
1	B	1883	0	1917	50	0
2	B	10	0	7	4	0
3	A	53	0	0	0	0
3	B	38	0	0	0	0
All	All	3867	0	3841	86	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (86) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:132:GLN:HE22	1:B:138:ARG:NH2	1.53	1.06
1:A:179:THR:H	1:A:182:GLN:HE21	1.21	0.84
1:A:52:LYS:HG3	1:A:62:ILE:HD13	1.59	0.84
1:A:10:ALA:HB1	1:A:237:SER:HB2	1.67	0.76
1:A:179:THR:H	1:A:182:GLN:NE2	1.85	0.75
1:A:52:LYS:HG3	1:A:62:ILE:CD1	2.20	0.72
1:B:226:ARG:O	1:B:226:ARG:HD2	1.89	0.72
1:B:79:SER:HB2	1:B:81:PRO:HD2	1.72	0.71
1:B:132:GLN:HE22	1:B:138:ARG:HH21	1.38	0.69
1:B:5:GLN:HE21	1:B:207:ARG:HH12	1.41	0.69
1:B:21:LEU:O	1:B:25:ILE:HG13	1.93	0.68
1:B:168:PRO:HD2	1:B:211:GLY:O	1.93	0.67
1:A:10:ALA:CB	1:A:237:SER:HB2	2.27	0.63
1:B:11:ASN:HB2	1:B:232:LEU:HD21	1.80	0.62
1:B:133:GLU:HG2	1:B:138:ARG:NH1	2.14	0.62
1:A:191:ARG:HH21	1:A:227:ASP:HB3	1.66	0.60
1:B:133:GLU:HG2	1:B:138:ARG:HH12	1.69	0.58
1:B:181:GLN:O	1:B:185:GLU:HG2	2.03	0.58
1:B:24:LEU:HD21	1:B:238:LEU:O	2.05	0.57
1:B:226:ARG:C	1:B:226:ARG:HD2	2.26	0.55
1:A:25:ILE:HG21	1:A:54:ARG:HB3	1.88	0.54
1:A:132:GLN:N	1:A:132:GLN:OE1	2.40	0.54
1:B:55:LEU:HD11	1:B:60:PHE:CB	2.38	0.53
1:A:181:GLN:O	1:A:185:GLU:HG3	2.07	0.53
1:B:154:LEU:HD22	1:B:158:ASP:HB3	1.91	0.53
1:A:71:SER:HB3	1:B:14:CYS:O	2.08	0.53
1:B:168:PRO:HG2	1:B:171:ALA:HB3	1.91	0.53
1:B:179:THR:H	1:B:182:GLN:NE2	2.06	0.53
1:A:168:PRO:O	1:A:172:ILE:HD12	2.09	0.52
1:A:57:HIS:HB3	1:A:60:PHE:HD1	1.73	0.52
1:A:57:HIS:HB3	1:A:60:PHE:CD1	2.45	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:201:ASP:N	1:B:201:ASP:OD1	2.42	0.51
1:B:95:HIS:HE2	2:B:300:G3P:H11	1.75	0.51
1:B:193:TRP:CE2	1:B:197:LYS:HD3	2.46	0.51
1:B:11:ASN:HD22	2:B:300:G3P:H11	1.76	0.51
1:B:55:LEU:HD11	1:B:60:PHE:HB2	1.93	0.50
1:A:35:HIS:CD2	1:A:35:HIS:H	2.30	0.49
1:A:3:LYS:HB3	1:A:4:PRO:HD2	1.94	0.49
1:A:127:ILE:HB	1:A:146:GLN:OE1	2.12	0.48
1:B:155:LYS:O	1:B:158:ASP:HB2	2.13	0.47
1:A:217:LYS:HD2	1:A:217:LYS:N	2.29	0.47
1:A:65:GLN:O	1:A:66:ASN:HB2	2.14	0.47
1:A:12:TRP:CE3	1:A:21:LEU:HD22	2.49	0.47
1:B:136:SER:HB2	1:B:138:ARG:HG3	1.96	0.47
1:B:11:ASN:HD22	2:B:300:G3P:C1	2.27	0.47
1:A:91:ILE:HG23	1:A:123:VAL:HG13	1.96	0.47
1:B:147:ILE:CG2	1:B:148:ALA:N	2.78	0.47
1:B:57:HIS:ND1	1:B:58:PRO:HD2	2.30	0.47
1:B:79:SER:CB	1:B:81:PRO:HD2	2.42	0.47
1:A:193:TRP:CZ2	1:A:197:LYS:HG3	2.50	0.47
1:A:130:THR:OG1	1:A:133:GLU:HG3	2.15	0.47
1:B:11:ASN:HB2	1:B:232:LEU:CD2	2.44	0.46
1:A:187:HIS:CE1	1:A:208:ILE:HG22	2.51	0.46
1:B:191:ARG:HD2	1:B:227:ASP:OD1	2.15	0.46
1:B:12:TRP:CE3	1:B:43:SER:HB3	2.52	0.45
1:B:132:GLN:NE2	1:B:138:ARG:NH2	2.39	0.45
1:B:69:ALA:O	1:B:70:LYS:HG2	2.16	0.45
1:A:181:GLN:H	1:A:181:GLN:CD	2.21	0.45
1:A:12:TRP:CD1	1:A:238:LEU:HD13	2.52	0.45
1:B:147:ILE:HG22	1:B:148:ALA:N	2.32	0.44
1:B:191:ARG:NH2	1:B:206:LEU:O	2.51	0.44
1:B:242:PHE:O	1:B:246:ILE:HG13	2.18	0.44
1:B:34:ASN:HD22	1:B:35:HIS:N	2.16	0.43
1:A:97:GLU:OE2	1:B:73:ALA:HB1	2.18	0.43
1:A:91:ILE:HG12	1:A:93:LEU:HG	2.00	0.43
1:B:247:LYS:HB2	1:B:247:LYS:HE3	1.68	0.43
1:B:144:LEU:HD11	1:B:189:LEU:HD11	2.00	0.43
1:B:249:THR:O	1:B:249:THR:OG1	2.29	0.42
1:B:232:LEU:HD22	2:B:300:G3P:O1	2.20	0.42
1:A:5:GLN:OE1	1:A:207:ARG:NH2	2.53	0.42
1:B:243:VAL:HG12	1:B:247:LYS:HE2	2.02	0.42
1:A:14:CYS:SG	1:A:14:CYS:O	2.77	0.42
1:A:128:GLY:HA3	1:A:167:GLU:O	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:91:ILE:HG13	1:A:92:VAL:N	2.34	0.42
1:A:197:LYS:HD2	1:A:197:LYS:HA	1.93	0.42
1:A:44:THR:HG21	1:B:82:ILE:HD13	2.00	0.41
1:B:129:GLU:OE1	1:B:129:GLU:N	2.52	0.41
1:A:133:GLU:HG3	1:A:133:GLU:H	1.48	0.41
1:B:99:ARG:HH11	1:B:99:ARG:HD3	1.62	0.41
1:B:109:VAL:O	1:B:113:VAL:HG23	2.20	0.41
1:A:9:ALA:O	1:A:233:VAL:N	2.38	0.41
1:A:35:HIS:HE1	1:A:249:THR:OG1	2.04	0.40
1:A:193:TRP:CE2	1:A:197:LYS:HG3	2.55	0.40
1:B:66:ASN:CG	1:B:67:ALA:H	2.25	0.40
1:A:27:LEU:HD22	1:A:27:LEU:C	2.42	0.40
1:B:33:ILE:HG21	1:B:33:ILE:HD13	1.81	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	247/250 (99%)	232 (94%)	15 (6%)	0	100	100
1	B	247/250 (99%)	238 (96%)	9 (4%)	0	100	100
All	All	494/500 (99%)	470 (95%)	24 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	196/197 (100%)	175 (89%)	21 (11%)	10	8
1	B	196/197 (100%)	176 (90%)	20 (10%)	11	9
All	All	392/394 (100%)	351 (90%)	41 (10%)	10	9

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	19	GLN
1	A	21	LEU
1	A	27	LEU
1	A	53	GLU
1	A	61	VAL
1	A	71	SER
1	A	85	ASP
1	A	91	ILE
1	A	107	GLU
1	A	119	SER
1	A	143	VAL
1	A	152	LYS
1	A	181	GLN
1	A	207	ARG
1	A	213	SER
1	A	214	VAL
1	A	217	LYS
1	A	221	THR
1	A	238	LEU
1	A	247	LYS
1	B	5	GLN
1	B	19	GLN
1	B	24	LEU
1	B	33	ILE
1	B	34	ASN
1	B	62	ILE
1	B	131	LEU
1	B	138	ARG
1	B	147	ILE
1	B	153	LYS
1	B	176	LYS
1	B	177	VAL
1	B	181	GLN
1	B	197	LYS

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Mol	Chain	Res	Type
1	B	201	ASP
1	B	207	ARG
1	B	220	ARG
1	B	226	ARG
1	B	232	LEU
1	B	247	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	34	ASN
1	A	35	HIS
1	A	182	GLN
1	B	5	GLN
1	B	34	ASN
1	B	66	ASN
1	B	132	GLN
1	B	182	GLN
1	B	224	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	G3P	B	300	-	9,9,9	0.44	0	12,12,12	1.57	2 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G3P	B	300	-	1/1/2/2	0/8/8/8	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	300	G3P	O1P-C3-C2	3.97	121.07	108.62
2	B	300	G3P	O3P-P-O1P	-2.37	100.12	106.65

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	300	G3P	C2

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.