



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:01 PM UTC

PDB ID : 1M7O / pdb_00001m7o
Title : Plasmodium Falciparum Triosephosphate isomerase (PfTIM) compled to substrate analog 3-phosphoglycerate (3PG)
Authors : Parthasarathy, S.; Balaram, H.; Balaram, P.; Murthy, M.R.N.
Deposited on : 2002-07-22
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)	:	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

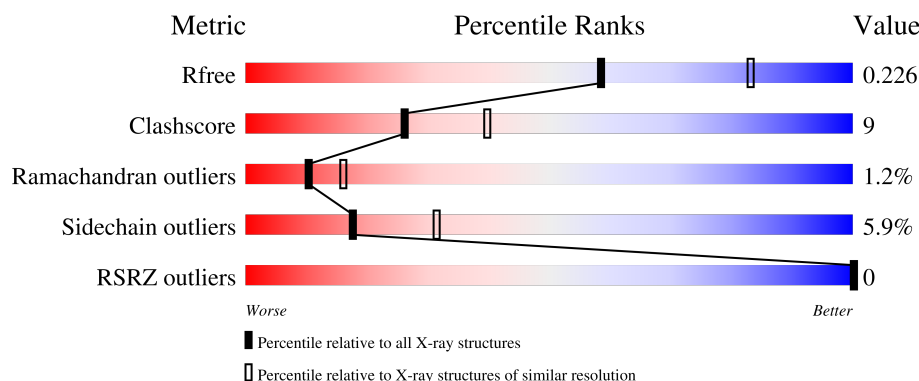
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. 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	248	 73% 21% . .
1	B	248	 75% 17% . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4066 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.

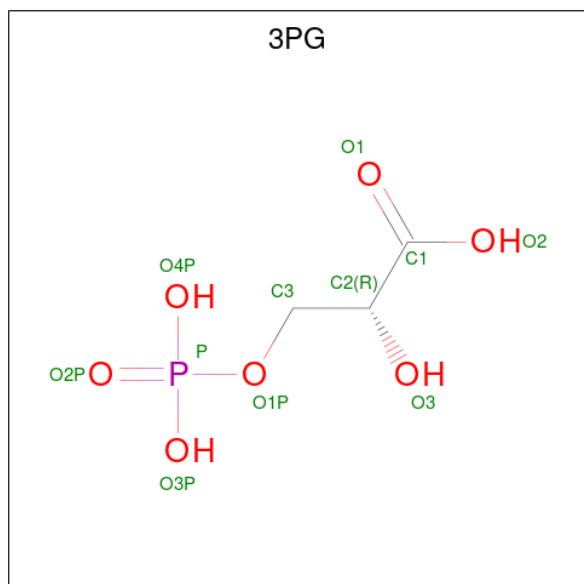
- Molecule 1 is a protein called Triosephosphate Isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1957	1239	333	380	5			
1	B	246	Total	C	N	O	S	0	0	0
			1957	1239	333	380	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	163	VAL	ALA	conflict	UNP Q07412
B	163	VAL	ALA	conflict	UNP Q07412

- Molecule 2 is 3-PHOSPHOGLYCERIC ACID (CCD ID: 3PG) (formula: $C_3H_7O_7P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			11	3	7	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			11	3	7	1		

- Molecule 3 is water.

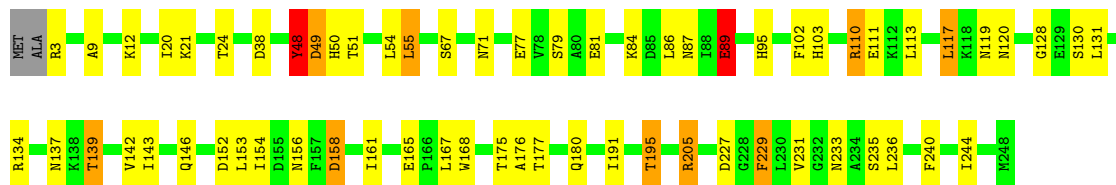
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	60	Total	O	0	0
			60	60		
3	B	70	Total	O	0	0
			70	70		

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.

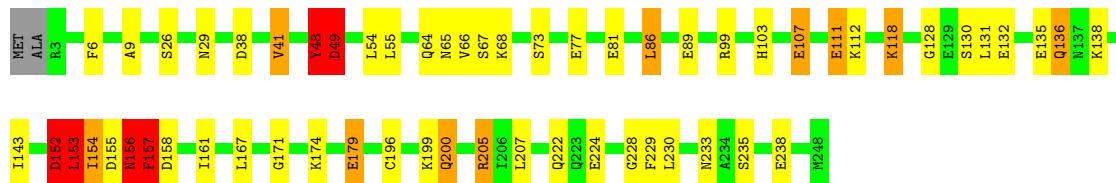
• Molecule 1: Triosephosphate Isomerase

Chain A:  73% 21% . .



• Molecule 1: Triosephosphate Isomerase

Chain B:  75% 17% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.26Å 51.34Å 90.36Å 90.00° 91.38° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.3 (20.00-2.40) 93.4 (20.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.29 (at 2.41Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.183 , 0.225 0.183 , 0.226	Depositor DCC
R_{free} test set	1813 reflections (9.83%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4066	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.39% 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

Bond lengths and bond angles in the following residue types are not validated in this section: 3PG

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	0.75	3/1989 (0.2%)	1.03	13/2682 (0.5%)
1	B	1.04	6/1989 (0.3%)	1.37	21/2682 (0.8%)
All	All	0.91	9/3978 (0.2%)	1.21	34/5364 (0.6%)

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	B	0	5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	49	ASP	C-N	-32.05	0.93	1.33
1	A	48	TYR	C-N	23.45	1.66	1.33
1	B	48	TYR	C-N	17.04	1.57	1.33
1	B	153	LEU	C-N	-16.25	1.11	1.33
1	A	95	HIS	C-N	10.56	1.49	1.33
1	A	49	ASP	C-N	-7.22	1.24	1.33
1	B	152	ASP	C-N	-6.13	1.25	1.34
1	B	152	ASP	CA-C	5.98	1.60	1.52
1	B	153	LEU	C-O	5.56	1.31	1.24

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	ASP	O-C-N	-35.10	75.91	122.59
1	B	49	ASP	CA-C-N	17.55	147.14	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	ASP	C-N-CA	17.55	147.14	120.82
1	B	153	LEU	O-C-N	-16.89	102.46	122.22
1	A	48	TYR	CA-C-N	-9.74	102.94	121.54
1	A	48	TYR	C-N-CA	-9.74	102.94	121.54
1	A	49	ASP	O-C-N	-9.46	110.01	122.59
1	B	152	ASP	CA-C-N	8.44	132.43	120.28
1	B	152	ASP	C-N-CA	8.44	132.43	120.28
1	B	48	TYR	CA-C-N	-7.24	107.72	121.54
1	B	48	TYR	C-N-CA	-7.24	107.72	121.54
1	A	103	HIS	N-CA-C	6.91	120.94	111.54
1	B	89	GLU	N-CA-C	6.66	118.33	111.14
1	A	102	PHE	N-CA-C	6.37	120.69	112.41
1	B	157	PHE	N-CA-C	6.34	124.30	110.80
1	B	152	ASP	O-C-N	-6.23	114.61	122.27
1	A	89	GLU	N-CA-C	6.16	119.27	111.69
1	A	229	PHE	N-CA-C	6.07	118.00	108.96
1	A	120	ASN	N-CA-C	5.93	119.75	111.74
1	A	95	HIS	CA-C-N	-5.76	111.06	121.14
1	A	95	HIS	C-N-CA	-5.76	111.06	121.14
1	B	158	ASP	N-CA-C	-5.72	106.65	113.97
1	B	103	HIS	N-CA-C	5.69	119.41	111.90
1	A	158	ASP	N-CA-C	-5.67	106.91	113.88
1	B	174	LYS	N-CA-C	-5.62	102.21	110.52
1	B	68	LYS	N-CA-C	-5.40	106.69	113.28
1	B	64	GLN	N-CA-C	5.27	119.46	113.19
1	A	231	VAL	N-CA-C	5.26	116.16	108.58
1	B	156	ASN	N-CA-CB	-5.21	102.77	110.37
1	A	49	ASP	N-CA-C	5.16	121.78	110.80
1	B	233	ASN	N-CA-C	5.15	117.63	111.71
1	B	230	LEU	N-CA-C	-5.04	97.70	107.62
1	B	224	GLU	CA-C-N	-5.02	114.77	122.60
1	B	224	GLU	C-N-CA	-5.02	114.77	122.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	152	ASP	Mainchain
1	B	153	LEU	Mainchain
1	B	48	TYR	Mainchain
1	B	49	ASP	Peptide,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	1957	0	1953	39	0
1	B	1957	0	1951	36	0
2	A	11	0	4	2	0
2	B	11	0	4	0	0
3	A	60	0	0	1	0
3	B	70	0	0	4	0
All	All	4066	0	3912	74	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 9.

All (74) 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:191:ILE:O	1:A:195:THR:HG22	1.78	0.82
1:B:136:GLN:HG3	1:B:138:LYS:HE2	1.63	0.80
1:B:156:ASN:C	1:B:156:ASN:HD22	1.94	0.74
1:B:196:CYS:O	1:B:200:GLN:NE2	2.31	0.64
1:B:132:GLU:O	1:B:136:GLN:HG2	1.97	0.64
1:A:49:ASP:O	1:A:50:HIS:C	2.38	0.63
1:B:153:LEU:O	1:B:155:ASP:N	2.32	0.62
1:B:131:LEU:O	1:B:135:GLU:HG3	2.01	0.60
1:B:65:ASN:HD21	1:B:112:LYS:NZ	2.02	0.57
1:B:200:GLN:N	1:B:200:GLN:OE1	2.37	0.57
1:B:26:SER:OG	1:B:238:GLU:HG2	2.05	0.57
1:B:152:ASP:OD1	1:B:152:ASP:N	2.38	0.56
1:B:118:LYS:HB2	1:B:118:LYS:NZ	2.21	0.55
1:B:6:PHE:HB3	1:B:207:LEU:HD21	1.90	0.54
1:A:205:ARG:HA	1:A:227:ASP:OD2	2.08	0.54
1:A:191:ILE:O	1:A:195:THR:CG2	2.51	0.54
1:B:138:LYS:HG2	3:B:615:HOH:O	2.07	0.53
1:B:153:LEU:O	1:B:154:ILE:C	2.48	0.53
1:A:175:THR:HG22	1:A:176:ALA:N	2.22	0.53
1:B:179:GLU:H	1:B:179:GLU:CD	2.17	0.53
1:A:161:ILE:HD12	1:A:161:ILE:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:THR:O	1:A:143:ILE:HG12	2.09	0.52
1:B:9:ALA:HB1	1:B:235:SER:HB2	1.92	0.52
1:A:113:LEU:HD13	1:A:117:LEU:HD22	1.92	0.51
1:A:20:ILE:O	1:A:24:THR:HG23	2.10	0.51
1:A:3:ARG:HD2	1:A:227:ASP:OD2	2.10	0.50
1:A:67:SER:HB2	1:A:77:GLU:HB3	1.94	0.50
1:A:113:LEU:HD12	1:A:153:LEU:HD12	1.94	0.50
1:A:12:LYS:HD3	1:B:73:SER:HA	1.94	0.49
1:A:84:LYS:HE3	1:A:119:ASN:O	2.11	0.49
1:A:110:ARG:HG3	1:A:111:GLU:N	2.28	0.48
1:A:9:ALA:HB1	1:A:235:SER:HB2	1.94	0.48
3:A:582:HOH:O	1:B:86:LEU:HD13	2.13	0.48
1:B:67:SER:HB2	1:B:77:GLU:HB3	1.95	0.48
1:B:130:SER:HA	1:B:167:LEU:HB2	1.96	0.48
1:B:65:ASN:HD21	1:B:112:LYS:HZ3	1.61	0.48
1:B:161:ILE:HD12	1:B:161:ILE:N	2.30	0.47
1:A:156:ASN:OD1	1:A:158:ASP:HB2	2.14	0.47
1:B:156:ASN:C	1:B:156:ASN:ND2	2.67	0.47
1:A:12:LYS:NZ	2:A:5401:3PG:H32	2.30	0.47
1:A:134:ARG:HD2	1:A:168:TRP:CG	2.50	0.47
1:A:134:ARG:HD2	1:A:168:TRP:CD2	2.50	0.47
1:B:6:PHE:O	1:B:228:GLY:HA3	2.15	0.46
1:A:21:LYS:HA	1:A:54:LEU:HD13	1.97	0.46
1:A:240:PHE:CE2	1:A:244:ILE:HD11	2.50	0.46
1:B:38:ASP:OD2	1:B:205:ARG:NH2	2.47	0.46
1:A:86:LEU:O	1:A:87:ASN:HB2	2.17	0.45
1:A:131:LEU:HA	1:A:168:TRP:HB3	1.99	0.45
1:B:199:LYS:HB2	1:B:200:GLN:OE1	2.17	0.45
1:A:38:ASP:OD2	1:A:205:ARG:NH2	2.49	0.45
1:A:240:PHE:O	1:A:244:ILE:HG13	2.16	0.45
1:A:51:THR:HG22	1:A:55:LEU:HD22	1.98	0.44
1:A:142:VAL:O	1:A:146:GLN:HG3	2.17	0.44
1:B:128:GLY:HA2	1:B:143:ILE:HD11	2.00	0.43
1:A:71:ASN:ND2	1:A:79:SER:OG	2.51	0.43
1:A:131:LEU:HA	1:A:168:TRP:CB	2.48	0.43
1:A:130:SER:HA	1:A:167:LEU:HB2	2.00	0.43
1:A:177:THR:OG1	1:A:180:GLN:HG3	2.19	0.43
1:B:81:GLU:H	1:B:81:GLU:HG3	1.66	0.43
1:A:3:ARG:HD2	1:A:227:ASP:CG	2.44	0.42
1:A:128:GLY:HA3	1:A:165:GLU:O	2.19	0.42
1:B:99:ARG:HD3	3:B:546:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:GLN:CG	1:B:138:LYS:HE2	2.44	0.42
1:A:12:LYS:HZ1	2:A:5401:3PG:H32	1.85	0.42
1:A:110:ARG:NH2	1:A:152:ASP:OD1	2.53	0.42
1:A:175:THR:CG2	1:A:176:ALA:N	2.83	0.42
1:B:107:GLU:O	1:B:111:GLU:HG3	2.20	0.42
1:B:136:GLN:HB2	1:B:138:LYS:HG3	2.01	0.41
1:B:41:VAL:HG11	1:B:55:LEU:CD1	2.50	0.41
1:B:171:GLY:N	3:B:631:HOH:O	2.39	0.41
1:A:89:GLU:H	1:A:89:GLU:HG2	1.64	0.40
1:B:29:ASN:ND2	3:B:613:HOH:O	2.53	0.40
1:B:157:PHE:CD1	1:B:157:PHE:N	2.88	0.40
1:A:48:TYR:O	1:A:49:ASP:C	2.65	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	244/248 (98%)	234 (96%)	8 (3%)	2 (1%)	16	25
1	B	244/248 (98%)	232 (95%)	8 (3%)	4 (2%)	7	11
All	All	488/496 (98%)	466 (96%)	16 (3%)	6 (1%)	10	16

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	49	ASP
1	A	48	TYR
1	B	48	TYR
1	B	154	ILE
1	B	157	PHE
1	A	154	ILE

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	219/220 (100%)	207 (94%)	12 (6%)	19	34
1	B	219/220 (100%)	205 (94%)	14 (6%)	16	28
All	All	438/440 (100%)	412 (94%)	26 (6%)	18	31

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	81	GLU
1	A	89	GLU
1	A	110	ARG
1	A	117	LEU
1	A	137	ASN
1	A	139	THR
1	A	195	THR
1	A	205	ARG
1	A	229	PHE
1	A	233	ASN
1	A	236	LEU
1	B	41	VAL
1	B	54	LEU
1	B	66	VAL
1	B	86	LEU
1	B	107	GLU
1	B	111	GLU
1	B	118	LYS
1	B	136	GLN
1	B	156	ASN
1	B	179	GLU
1	B	200	GLN
1	B	205	ARG
1	B	222	GLN
1	B	229	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	71	ASN
1	A	159	ASN
1	A	202	ASN
1	A	223	GLN
1	A	233	ASN
1	B	25	ASN
1	B	29	ASN
1	B	56	GLN
1	B	65	ASN
1	B	71	ASN
1	B	120	ASN
1	B	156	ASN
1	B	185	HIS
1	B	222	GLN
1	B	223	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](#)

2 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	3PG	B	6401	-	9,10,10	3.31	6 (66%)	11,14,14	1.72	3 (27%)
2	3PG	A	5401	-	9,10,10	3.45	6 (66%)	11,14,14	1.87	4 (36%)

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	3PG	B	6401	-	-	2/10/10/10	-
2	3PG	A	5401	-	-	0/10/10/10	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6401	3PG	P-O2P	6.17	1.69	1.50
2	A	5401	3PG	P-O2P	6.03	1.69	1.50
2	A	5401	3PG	O1-C1	4.53	1.35	1.22
2	A	5401	3PG	P-O4P	4.19	1.70	1.54
2	B	6401	3PG	O1-C1	4.14	1.34	1.22
2	B	6401	3PG	P-O3P	3.90	1.69	1.54
2	B	6401	3PG	P-O4P	3.88	1.69	1.54
2	A	5401	3PG	P-O3P	3.81	1.69	1.54
2	A	5401	3PG	P-O1P	3.49	1.71	1.60
2	B	6401	3PG	P-O1P	2.49	1.68	1.60
2	B	6401	3PG	C2-C1	-2.31	1.49	1.52
2	A	5401	3PG	C2-C1	-2.08	1.49	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6401	3PG	O2-C1-C2	3.91	121.00	112.74
2	A	5401	3PG	O2-C1-C2	3.51	120.17	112.74
2	A	5401	3PG	O2-C1-O1	-3.07	117.12	124.08
2	B	6401	3PG	O2-C1-O1	-2.81	117.71	124.08
2	A	5401	3PG	O4P-P-O1P	2.68	113.65	106.67
2	A	5401	3PG	O1P-C3-C2	2.36	114.59	107.96
2	B	6401	3PG	O4P-P-O1P	2.08	112.10	106.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	6401	3PG	C1-C2-C3-O1P
2	B	6401	3PG	O3-C2-C3-O1P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5401	3PG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	48:TYR	C	49:ASP	N	1.66
1	B	153:LEU	C	154:ILE	N	1.11
1	B	49:ASP	C	50:HIS	N	0.93

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	246/248 (99%)	-0.39	0 100 100	9, 22, 40, 59	0
1	B	246/248 (99%)	-0.40	0 100 100	7, 20, 39, 58	0
All	All	492/496 (99%)	-0.40	0 100 100	7, 21, 39, 59	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	3PG	B	6401	11/11	0.78	0.19	70,72,73,74	0
2	3PG	A	5401	11/11	0.81	0.18	69,71,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.