



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:39 PM UTC

PDB ID : 3UWW / pdb_00003uww
Title : Crystal structure of Staphylococcus Aureus triosephosphate isomerase complexed with 3-phosphoglyceric acid
Authors : Mukherjee, S.; Roychowdhury, A.; Dutta, D.; Das, A.K.
Deposited on : 2011-12-03
Resolution : 2.25 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

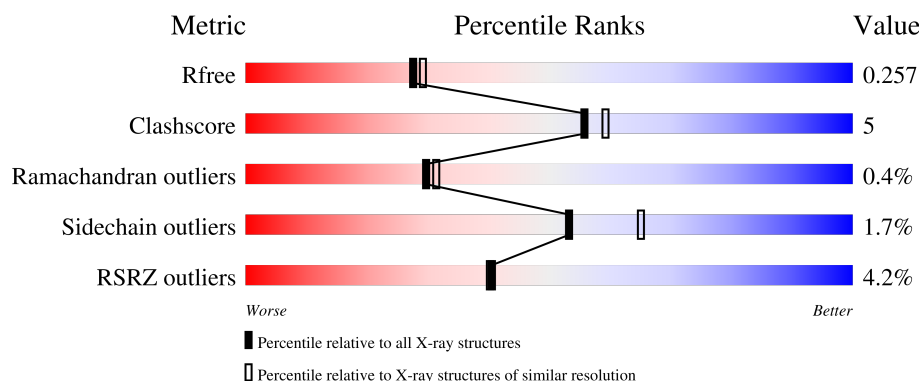
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	261	3% 90% 7% .
1	B	261	5% 86% 9% . .

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
3	3PG	A	254	-	X	-	-
3	3PG	B	255	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4051 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.

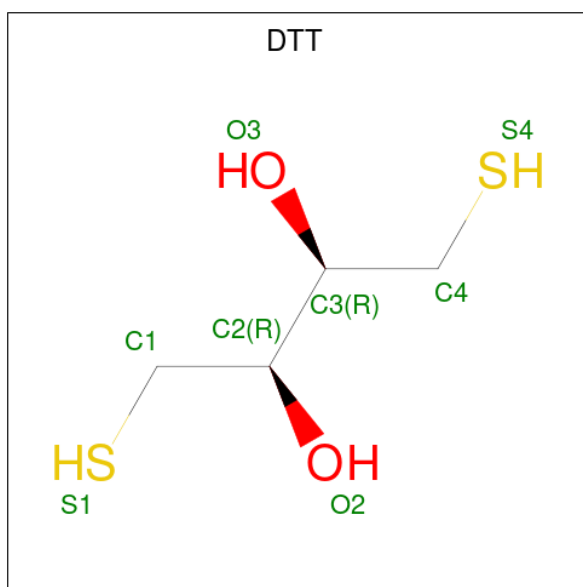
- Molecule 1 is a protein called Triosephosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1918	1197	322	391	8			
1	B	251	Total	C	N	O	S	0	0	0
			1891	1180	317	387	7			

There are 16 discrepancies between the modelled and reference sequences:

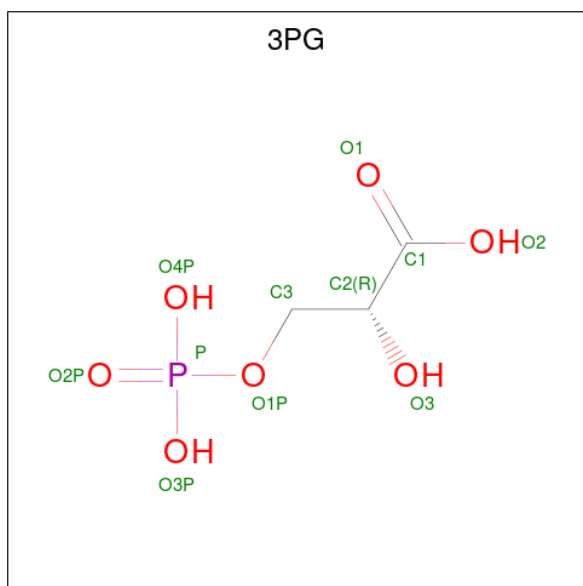
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	HIS	-	expression tag	UNP Q6GIL6
A	-6	HIS	-	expression tag	UNP Q6GIL6
A	-5	HIS	-	expression tag	UNP Q6GIL6
A	-4	HIS	-	expression tag	UNP Q6GIL6
A	-3	HIS	-	expression tag	UNP Q6GIL6
A	-2	HIS	-	expression tag	UNP Q6GIL6
A	-1	GLY	-	expression tag	UNP Q6GIL6
A	0	SER	-	expression tag	UNP Q6GIL6
B	-7	HIS	-	expression tag	UNP Q6GIL6
B	-6	HIS	-	expression tag	UNP Q6GIL6
B	-5	HIS	-	expression tag	UNP Q6GIL6
B	-4	HIS	-	expression tag	UNP Q6GIL6
B	-3	HIS	-	expression tag	UNP Q6GIL6
B	-2	HIS	-	expression tag	UNP Q6GIL6
B	-1	GLY	-	expression tag	UNP Q6GIL6
B	0	SER	-	expression tag	UNP Q6GIL6

- Molecule 2 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: C₄H₁₀O₂S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			8	4	2	2		

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



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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Na 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	126	Total 126	O 126	0	0
5	B	85	Total 85	O 85	0	0

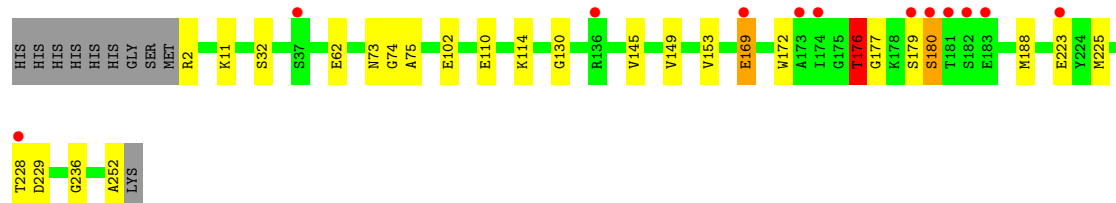
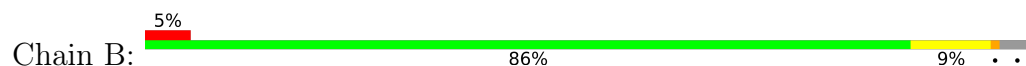
3 Residue-property plots [i](#)

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



• Molecule 1: Triosephosphate isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	80.58Å 80.58Å 174.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.56 – 2.25 29.56 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.56-2.25) 99.7 (29.56-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.206 , 0.248 0.222 , 0.257	Depositor DCC
R_{free} test set	1412 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4051	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 5.90% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.52	0/1945	0.80	0/2629
1	B	0.53	0/1918	0.82	2/2596 (0.1%)
All	All	0.53	0/3863	0.81	2/5225 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	GLY	N-CA-C	5.30	117.91	110.38
1	B	176	THR	N-CA-C	5.22	118.12	111.69

There are no chirality outliers.

There are no planarity outliers.

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	1918	0	1904	16	0
1	B	1891	0	1862	21	0
2	A	8	0	10	0	0
3	A	11	0	4	2	0
3	B	11	0	4	4	0
4	B	1	0	0	0	0
5	A	126	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	85	0	0	6	0
All	All	4051	0	3784	36	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 5.

All (36) 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:175:GLY:HA3	1:A:176:THR:HB	1.17	1.16
1:B:62:GLU:HG3	5:B:307:HOH:O	1.63	0.99
1:A:175:GLY:CA	1:A:176:THR:HB	1.99	0.92
1:B:145:VAL:HG11	1:B:188:MET:HE1	1.61	0.80
1:A:175:GLY:HA3	1:A:176:THR:CB	2.09	0.76
1:A:174:ILE:HG22	1:A:174:ILE:O	1.97	0.64
1:B:102:GLU:HB2	5:B:291:HOH:O	1.98	0.61
1:B:11:LYS:NZ	3:B:255:3PG:H31	2.16	0.61
1:A:131:GLU:OE2	1:A:172:TRP:CD1	2.54	0.60
1:A:236:GLY:HA3	3:A:254:3PG:O2P	2.02	0.60
1:A:13:ASN:HA	1:B:73:ASN:HD22	1.70	0.57
1:B:2:ARG:N	5:B:335:HOH:O	2.40	0.54
1:B:176:THR:N	1:B:177:GLY:HA2	2.23	0.53
1:B:179:SER:O	1:B:180:SER:HB3	2.09	0.53
1:A:175:GLY:CA	1:A:176:THR:CB	2.78	0.51
1:A:174:ILE:O	1:A:174:ILE:CG2	2.58	0.50
1:B:73:ASN:ND2	5:B:273:HOH:O	2.45	0.49
1:B:228:THR:HG23	1:B:229:ASP:OD2	2.13	0.49
1:A:11:LYS:HD3	1:B:75:ALA:HA	1.97	0.47
3:A:254:3PG:O3P	5:A:271:HOH:O	2.21	0.47
1:B:169:GLU:HB3	5:B:283:HOH:O	2.15	0.46
1:B:11:LYS:CE	3:B:255:3PG:H31	2.46	0.45
1:B:225:MET:HG3	1:B:252:ALA:HA	1.97	0.45
1:B:223:GLU:HG3	5:B:300:HOH:O	2.16	0.45
1:B:11:LYS:HZ1	3:B:255:3PG:H31	1.81	0.44
1:A:130:GLY:HA3	1:A:169:GLU:O	2.18	0.44
1:B:149:VAL:O	1:B:153:VAL:HG22	2.19	0.42
1:B:130:GLY:HA3	1:B:169:GLU:O	2.19	0.42
1:A:131:GLU:OE2	1:A:172:TRP:NE1	2.52	0.42
1:B:236:GLY:HA3	3:B:255:3PG:H32	2.02	0.41
1:B:110:GLU:O	1:B:114:LYS:HG3	2.20	0.41
1:A:110:GLU:O	1:A:114:LYS:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:MET:HG3	1:A:252:ALA:HA	2.03	0.41
1:A:13:ASN:O	1:A:14:LYS:HB2	2.21	0.40
1:A:133:ASP:O	1:A:137:GLU:HG2	2.21	0.40
1:B:172:TRP:CH2	1:B:180:SER:HB2	2.57	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	252/261 (97%)	243 (96%)	8 (3%)	1 (0%)	30	31
1	B	249/261 (95%)	241 (97%)	7 (3%)	1 (0%)	30	31
All	All	501/522 (96%)	484 (97%)	15 (3%)	2 (0%)	30	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	THR
1	B	180	SER

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/212 (97%)	202 (98%)	4 (2%)	50	61
1	B	202/212 (95%)	199 (98%)	3 (2%)	57	68
All	All	408/424 (96%)	401 (98%)	7 (2%)	53	65

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	SER
1	A	169	GLU
1	A	176	THR
1	A	216	VAL
1	B	32	SER
1	B	169	GLU
1	B	176	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	GLN
1	A	247	GLN
1	B	73	ASN
1	B	142	ASN
1	B	227	GLN
1	B	247	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

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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	$\# Z > 2$
3	3PG	B	255	-	9,10,10	0.95	0	11,14,14	1.33	2 (18%)
2	DTT	A	255	-	7,7,7	0.57	0	4,8,8	0.85	0
3	3PG	A	254	-	9,10,10	1.68	2 (22%)	11,14,14	1.59	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
3	3PG	B	255	-	-	1/10/10/10	-
2	DTT	A	255	-	-	2/8/8/8	-
3	3PG	A	254	-	-	8/10/10/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	254	3PG	P-O2P	2.85	1.59	1.50
3	A	254	3PG	C2-C1	2.20	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	254	3PG	O4P-P-O1P	2.76	113.86	106.67
3	B	255	3PG	O2-C1-C2	2.48	117.99	112.74
3	A	254	3PG	O1-C1-C2	-2.38	117.84	122.60
3	A	254	3PG	O2-C1-C2	2.23	117.46	112.74
3	A	254	3PG	O3P-P-O2P	-2.21	102.24	110.83
3	B	255	3PG	O1P-P-O2P	-2.03	100.96	106.44

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	255	DTT	O3-C3-C4-S4
3	A	254	3PG	C1-C2-C3-O1P
3	A	254	3PG	C2-C3-O1P-P
3	A	254	3PG	O3-C2-C3-O1P
3	B	255	3PG	C1-C2-C3-O1P
3	A	254	3PG	O1-C1-C2-C3
3	A	254	3PG	O2-C1-C2-C3
2	A	255	DTT	C2-C3-C4-S4
3	A	254	3PG	O1-C1-C2-O3
3	A	254	3PG	O2-C1-C2-O3
3	A	254	3PG	C3-O1P-P-O3P

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	255	3PG	4	0
3	A	254	3PG	2	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

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	254/261 (97%)	0.16	9 (3%) 47 47	20, 30, 51, 60	1 (0%)
1	B	251/261 (96%)	0.40	12 (4%) 35 35	20, 35, 59, 68	1 (0%)
All	All	505/522 (96%)	0.28	21 (4%) 40 40	20, 32, 56, 68	2 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	GLY	3.9
1	A	174	ILE	3.8
1	B	179	SER	3.1
1	B	136	ARG	2.9
1	A	37	SER	2.8
1	B	37	SER	2.7
1	A	33	LYS	2.6
1	A	243	GLU	2.6
1	B	183	GLU	2.5
1	B	223	GLU	2.5
1	B	174	ILE	2.4
1	A	0	SER	2.4
1	A	176	THR	2.4
1	B	173	ALA	2.3
1	B	228	THR	2.1
1	A	143	ASP	2.1
1	B	181	THR	2.0
1	B	182	SER	2.0
1	A	218	PRO	2.0
1	B	169	GLU	2.0
1	B	180	SER	2.0

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($\text{\AA}^2$)	Q<0.9
3	3PG	A	254	11/11	0.78	0.18	53,61,62,63	3
3	3PG	B	255	11/11	0.87	0.11	35,44,49,49	0
2	DTT	A	255	8/8	0.90	0.16	30,35,36,36	8
4	NA	B	254	1/1	0.90	0.15	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.