



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 09:14 pm BST

PDB ID : 1TYG
Title : Structure of the thiazole synthase/ThiS complex
Authors : Settembre, E.C.; Dorrestein, P.C.; Zhai, H.; Chatterjee, A.; McLafferty, F.W.;
Begley, T.P.; Ealick, S.E.
Deposited on : 2004-07-07
Resolution : 3.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

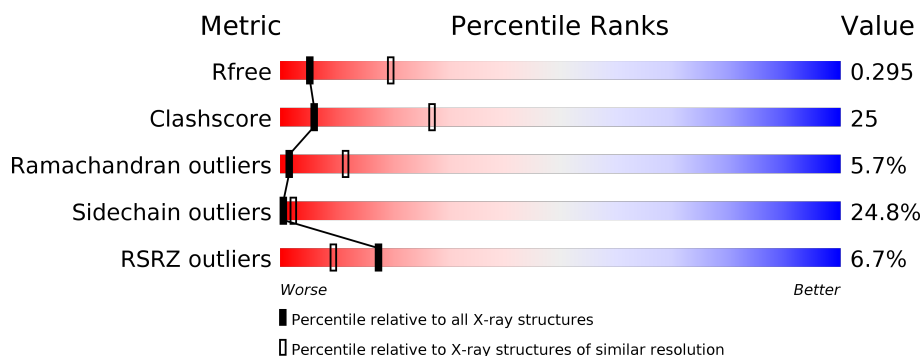
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 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	B	87	<div> <div>33%</div> <div>25%</div> <div>14%</div> <div>•</div> <div>25%</div> </div>
1	G	87	<div> <div>37%</div> <div>25%</div> <div>37%</div> <div>11%</div> <div>26%</div> </div>
2	A	253	<div> <div>58%</div> <div>28%</div> <div>7%</div> <div>• •</div> </div>
2	C	253	<div> <div>3%</div> <div>40%</div> <div>37%</div> <div>14%</div> <div>•</div> <div>6%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4555 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 yjbS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	65	Total	C	N	O	S	0	0	0
			527	334	91	100	2			
1	G	64	Total	C	N	O	S	0	0	0
			511	323	87	99	2			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	CLONING ARTIFACT	UNP O31617
B	-19	GLY	-	CLONING ARTIFACT	UNP O31617
B	-18	HIS	-	CLONING ARTIFACT	UNP O31617
B	-17	HIS	-	CLONING ARTIFACT	UNP O31617
B	-16	HIS	-	CLONING ARTIFACT	UNP O31617
B	-15	HIS	-	CLONING ARTIFACT	UNP O31617
B	-14	HIS	-	CLONING ARTIFACT	UNP O31617
B	-13	HIS	-	CLONING ARTIFACT	UNP O31617
B	-12	HIS	-	CLONING ARTIFACT	UNP O31617
B	-11	HIS	-	CLONING ARTIFACT	UNP O31617
B	-10	HIS	-	CLONING ARTIFACT	UNP O31617
B	-9	HIS	-	CLONING ARTIFACT	UNP O31617
B	-8	SER	-	CLONING ARTIFACT	UNP O31617
B	-7	SER	-	CLONING ARTIFACT	UNP O31617
B	-6	GLY	-	CLONING ARTIFACT	UNP O31617
B	-5	HIS	-	CLONING ARTIFACT	UNP O31617
B	-4	ILE	-	CLONING ARTIFACT	UNP O31617
B	-3	GLY	-	CLONING ARTIFACT	UNP O31617
B	-2	GLY	-	CLONING ARTIFACT	UNP O31617
B	-1	ARG	-	CLONING ARTIFACT	UNP O31617
B	0	HIS	-	CLONING ARTIFACT	UNP O31617
G	-20	MET	-	CLONING ARTIFACT	UNP O31617
G	-19	GLY	-	CLONING ARTIFACT	UNP O31617
G	-18	HIS	-	CLONING ARTIFACT	UNP O31617
G	-17	HIS	-	CLONING ARTIFACT	UNP O31617

Continued on next page...

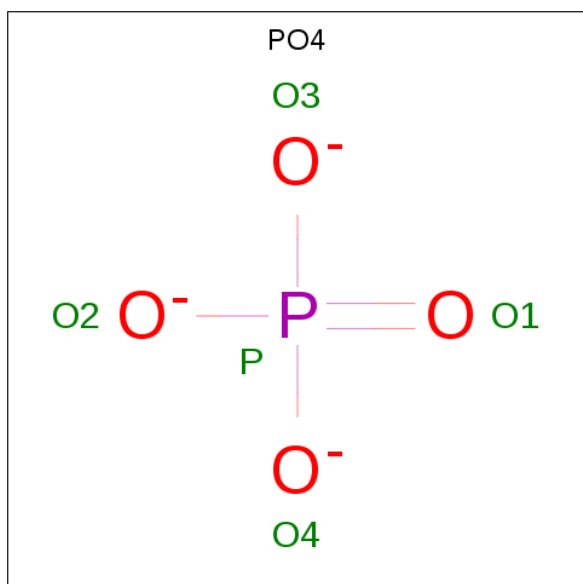
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	-16	HIS	-	CLONING ARTIFACT	UNP O31617
G	-15	HIS	-	CLONING ARTIFACT	UNP O31617
G	-14	HIS	-	CLONING ARTIFACT	UNP O31617
G	-13	HIS	-	CLONING ARTIFACT	UNP O31617
G	-12	HIS	-	CLONING ARTIFACT	UNP O31617
G	-11	HIS	-	CLONING ARTIFACT	UNP O31617
G	-10	HIS	-	CLONING ARTIFACT	UNP O31617
G	-9	HIS	-	CLONING ARTIFACT	UNP O31617
G	-8	SER	-	CLONING ARTIFACT	UNP O31617
G	-7	SER	-	CLONING ARTIFACT	UNP O31617
G	-6	GLY	-	CLONING ARTIFACT	UNP O31617
G	-5	HIS	-	CLONING ARTIFACT	UNP O31617
G	-4	ILE	-	CLONING ARTIFACT	UNP O31617
G	-3	GLY	-	CLONING ARTIFACT	UNP O31617
G	-2	GLY	-	CLONING ARTIFACT	UNP O31617
G	-1	ARG	-	CLONING ARTIFACT	UNP O31617
G	0	HIS	-	CLONING ARTIFACT	UNP O31617

- Molecule 2 is a protein called Thiazole biosynthesis protein thiG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	242	Total	C	N	O	S	0	0	0
			1784	1135	297	343	9			
2	C	237	Total	C	N	O	S	0	0	0
			1718	1090	283	338	7			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		

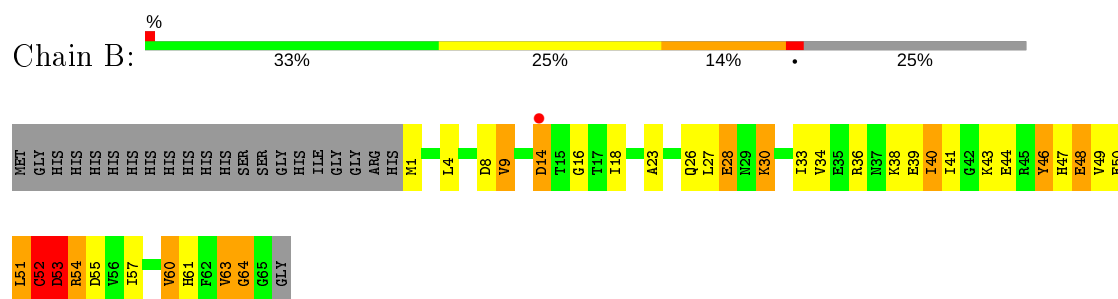
- Molecule 4 is water.

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

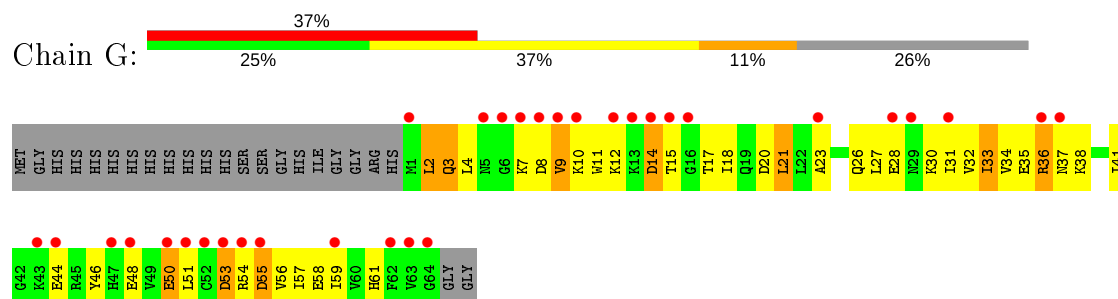
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

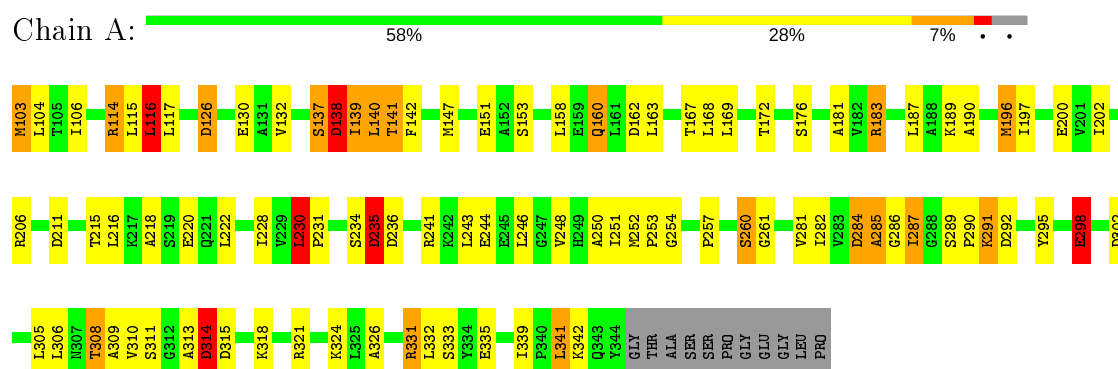
- Molecule 1: yjbS



- Molecule 1: yjbS



- Molecule 2: Thiazole biosynthesis protein thiG



- Molecule 2: Thiazole biosynthesis protein thiG





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	91.65Å 91.65Å 401.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 3.15 14.99 – 3.15	Depositor EDS
% Data completeness (in resolution range)	95.2 (15.00-3.15) 95.2 (14.99-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.242 , 0.305 0.229 , 0.295	Depositor DCC
R_{free} test set	1261 reflections (7.32%)	wwPDB-VP
Wilson B-factor (Å ²)	89.4	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4555	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: PO4

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	B	0.92	0/533	1.14	3/716 (0.4%)
1	G	0.92	0/517	1.03	3/699 (0.4%)
2	A	1.00	3/1810 (0.2%)	1.15	8/2455 (0.3%)
2	C	1.35	24/1741 (1.4%)	1.12	11/2364 (0.5%)
All	All	1.13	27/4601 (0.6%)	1.12	25/6234 (0.4%)

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	1
2	A	0	3
All	All	0	4

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	186	ARG	CZ-NH1	24.68	1.65	1.33
2	C	225	GLU	CG-CD	15.40	1.75	1.51
2	C	164	SER	CB-OG	14.96	1.61	1.42
2	C	225	GLU	CB-CG	13.71	1.78	1.52
2	C	159	GLU	CD-OE1	8.38	1.34	1.25

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	186	ARG	NE-CZ-NH2	-22.77	108.92	120.30
2	C	186	ARG	NE-CZ-NH1	11.74	126.17	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	236	ASP	CB-CG-OD2	8.21	125.69	118.30
2	C	138	ASP	CB-CG-OD2	7.76	125.28	118.30
1	G	55	ASP	CB-CG-OD2	7.07	124.67	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	235	ASP	Peptide
2	A	260	SER	Peptide
2	A	314	ASP	Peptide
1	B	53	ASP	Peptide

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	B	527	0	535	35	0
1	G	511	0	499	24	0
2	A	1784	0	1821	83	0
2	C	1718	0	1736	103	0
3	A	5	0	0	1	0
3	C	5	0	0	0	0
4	A	4	0	0	0	0
4	C	1	0	0	0	0
All	All	4555	0	4591	226	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 25.

The worst 5 of 226 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)
2:C:225:GLU:CB	2:C:225:GLU:CG	1.78	1.61
2:C:225:GLU:CG	2:C:225:GLU:CD	1.75	1.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ARG:NH2	1:B:52:CYS:HB2	1.73	1.03
1:B:18:ILE:HG13	1:B:49:VAL:HG13	1.47	0.94
1:B:36:ARG:HH22	1:B:52:CYS:HB2	1.25	0.94

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	B	63/87 (72%)	47 (75%)	9 (14%)	7 (11%)	0	2
1	G	62/87 (71%)	51 (82%)	7 (11%)	4 (6%)	1	8
2	A	240/253 (95%)	209 (87%)	22 (9%)	9 (4%)	3	19
2	C	233/253 (92%)	188 (81%)	31 (13%)	14 (6%)	1	10
All	All	598/680 (88%)	495 (83%)	69 (12%)	34 (6%)	1	12

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	47	HIS
1	B	51	LEU
1	B	53	ASP
2	A	138	ASP
2	A	314	ASP

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	58/76 (76%)	40 (69%)	18 (31%)	0	1
1	G	55/76 (72%)	34 (62%)	21 (38%)	0	0
2	A	188/201 (94%)	158 (84%)	30 (16%)	2	10
2	C	179/201 (89%)	129 (72%)	50 (28%)	0	1
All	All	480/554 (87%)	361 (75%)	119 (25%)	0	2

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	121	LYS
2	C	182	VAL
1	G	32	VAL
2	C	135	SER
2	C	161	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	249	HIS
1	G	61	HIS
1	G	5	ASN
1	B	47	HIS
1	G	26	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 carbohydrates in this entry.

5.6 Ligand geometry

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
3	PO4	C	2400	-	4,4,4	1.49	1 (25%)	6,6,6	1.21	1 (16%)
3	PO4	A	1400	-	4,4,4	0.89	0	6,6,6	1.50	1 (16%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2400	PO4	P-O1	2.65	1.57	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1400	PO4	O3-P-O2	3.06	117.79	107.97
3	C	2400	PO4	O4-P-O2	2.12	114.77	107.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1400	PO4	1	0

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 [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	B	65/87 (74%)	-0.49	1 (1%) 73 61	24, 34, 38, 40	0
1	G	64/87 (73%)	2.08	32 (50%) 0 0	137, 140, 146, 149	0
2	A	242/253 (95%)	-0.67	0 100 100	27, 33, 38, 44	0
2	C	237/253 (93%)	-0.16	8 (3%) 45 28	28, 33, 37, 54	0
All	All	608/680 (89%)	-0.16	41 (6%) 17 9	24, 34, 141, 149	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	8	ASP	8.4
1	G	63	VAL	6.9
1	G	14	ASP	6.5
1	G	15	THR	5.4
1	G	47	HIS	5.3

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 carbohydrates 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(\AA^2)	Q<0.9
3	PO4	C	2400	5/5	0.96	0.11	24,24,25,25	0
3	PO4	A	1400	5/5	0.98	0.11	25,26,29,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.