



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:15 AM GMT

PDB ID : 3O98
Title : Glutathionylspermidine synthetase/amidase C59A complex with ADP and Gsp
Authors : Pai, C.H.; Lin, C.H.; Wang, A.H.-J.
Deposited on : 2010-08-04
Resolution : 2.80 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

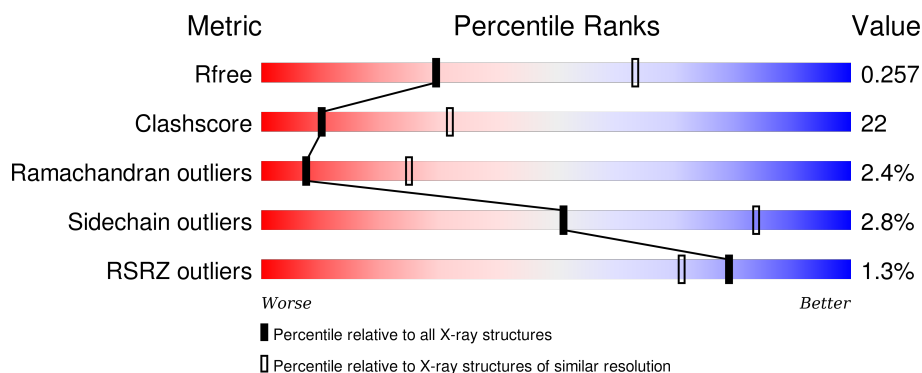
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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. 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	619	<div> <div> <div></div> <div>57%</div> <div>36%</div> <div>• •</div> </div> </div>
1	B	619	<div> <div> <div>2%</div> <div>59%</div> <div>36%</div> <div>• •</div> </div> </div>

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
2	TS5	A	620	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9968 atoms, of which 3 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.

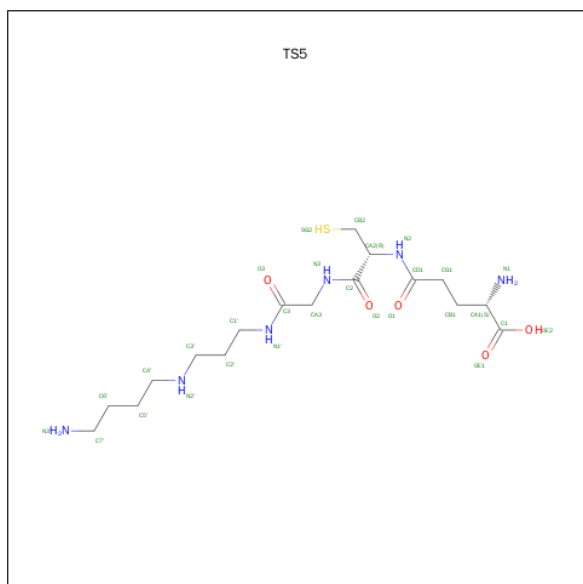
- Molecule 1 is a protein called Bifunctional glutathionylspermidine synthetase/amidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	599	Total	C	H	N	O	S	0	0	0
			4823	3087	2	826	890	18			
1	B	603	Total	C	H	N	O	S	0	0	0
			4852	3104	1	830	899	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	ALA	CYS	ENGINEERED MUTATION	UNP P0AES0
B	59	ALA	CYS	ENGINEERED MUTATION	UNP P0AES0

- Molecule 2 is GLUTATHIONYLSPERMIDINE (three-letter code: TS5) (formula: C₁₇H₃₄N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			29	17	6	5	1		

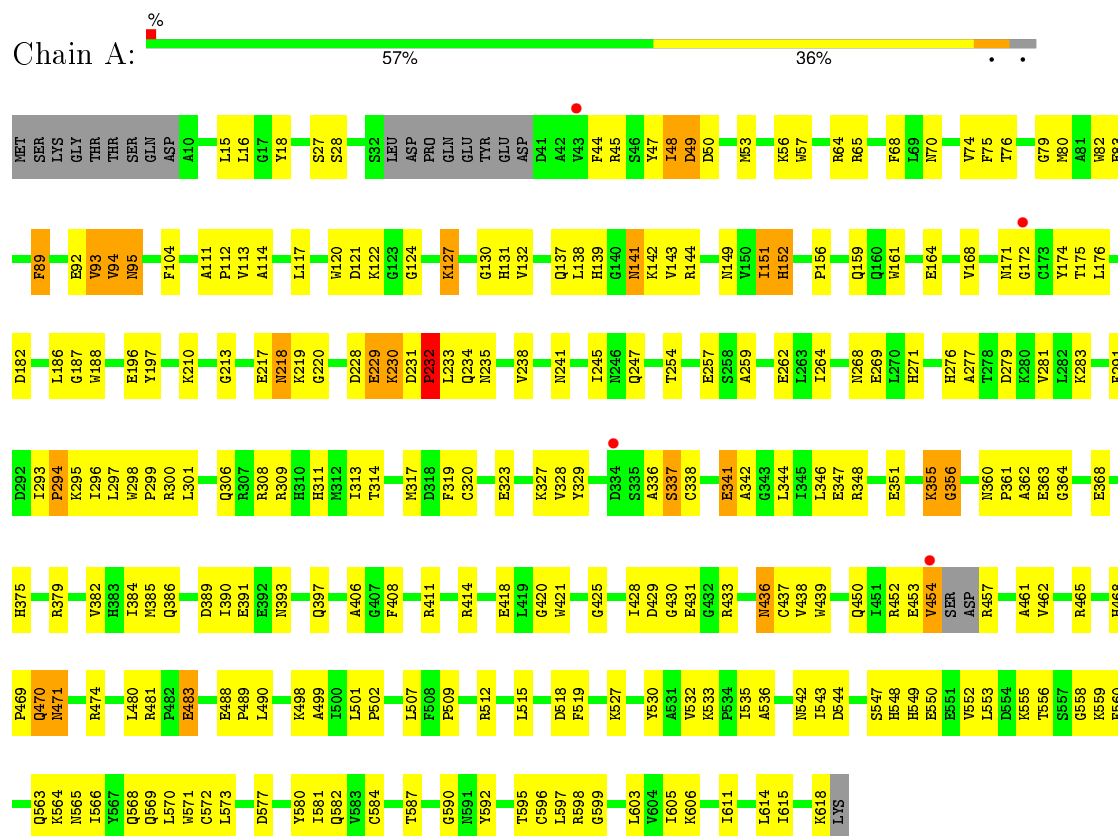
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	113	Total O 113 113	0	0
5	B	93	Total O 93 93	0	0

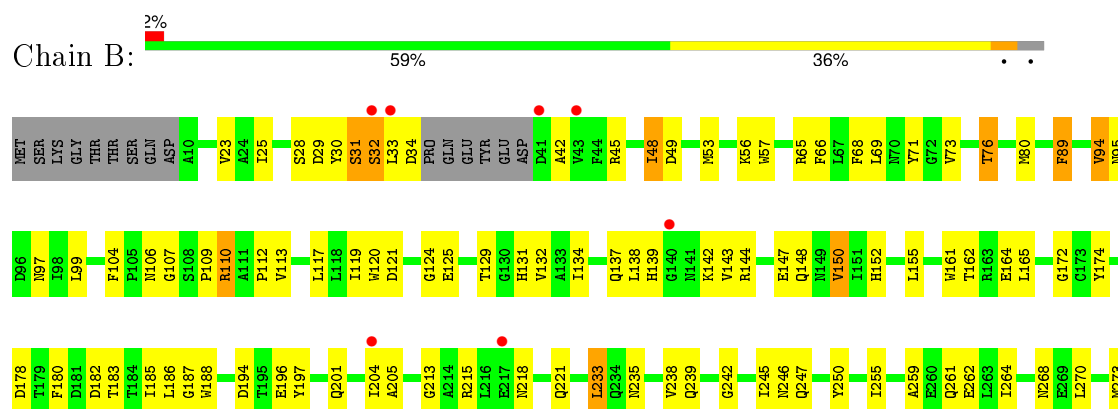
3 Residue-property plots

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.

- Molecule 1: Bifunctional glutathionylspermidine synthetase/amidase



- Molecule 1: Bifunctional glutathionylspermidine synthetase/amidase



Y274	S376	L475	G558	Y275	R377	●
L275	R377	●	R359	D279	I384	●
D279	I384	V478	A561	D285	I385	
D285	I385	L479	E562	D286	L480	
D286	I386	R481	E563	D287	R482	
L287	D387	E483	I566	L290	E484	
L290	D388	V484	Y567	L294	L485	
L294	D389	V486	Q568	L295	V487	
L295	E391	F487	W571	L296	E488	
L296	I393	F489	D577	L301	L490	
L301	I394	L491	Y580	L302	T492	
L302	R395	T492	I581	L303	Q401	
L303	Q401	Q405	Q582	L306	Q405	
L306	Q405	T410	Y583	L307	Q405	
L307	T410	L501	C584	L308	L501	
L308	R414	P502	Y587	L309	P502	
L309	E418	R511	G590	L313	R511	
L313	E418	R512	W591	L314	Y513	
L314	E418	Y513	Y592	F319	T517	
F319	W421	T517	T595	C320	D618	
C320	D422	D618	C596	W321	F519	
W321	G425	F519	L597	D322	T520	
D322	Q426	T520	R598	L326	Y521	
L326	L427	Y521	G599	K327	R522	
K327	I428	R522	D600	V328	D623	
V328	D429	D623	E601	D334	E524	
D334	Q430	E524	S602	C338	L525	
C338	Q430	L525	L603	H339	V526	
H339	R433	V526	K606	I340	V532	
I340	L434	V532	T611	E341	I535	
E341	C437	I535	L614	A342	A536	
A342	W439	A536	I615	I345	G537	
I345	K440	G537	I616	L346	R538	
L346	T441	R538	W617	E347	I542	
E347	W444	I542	K618	L348	I543	
L348	D456	I543	LYS	E358	D544	
E358	D456	D544		F359	S547	
F359	F469	S547		A362	I549	●
A362	A460	I549		E363	E550	
E363	A461	E550		G364	E551	
G364	V462	E551		L365	V552	●
L365	H468	V552		I366	I553	
I366	P469	I553		N367	D554	
N367	Q470	D554		E368	R555	
E368	W471	R555		H375	T556	
H375	W471	T556			S557	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.38Å 76.20Å 84.22Å 70.81° 74.37° 78.64°	Depositor
Resolution (Å)	30.00 – 2.80 29.57 – 2.82	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.80) 83.0 (29.57-2.82)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.262 0.211 , 0.257	Depositor DCC
R_{free} test set	1463 reflections (4.94%)	DCC
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 31316 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9968	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 6.47% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, TS5, ADP

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	0.47	1/4944 (0.0%)	0.60	2/6713 (0.0%)
1	B	0.44	0/4975	0.58	1/6757 (0.0%)
All	All	0.46	1/9919 (0.0%)	0.59	3/13470 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	454	VAL	C-O	10.34	1.43	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	453	GLU	O-C-N	-6.34	112.55	122.70
1	B	48	ILE	N-CA-C	-5.32	96.65	111.00
1	A	48	ILE	N-CA-C	-5.15	97.11	111.00

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	4821	2	4697	232	0
1	B	4851	1	4722	189	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	29	0	31	5	0
3	A	27	0	12	2	0
3	B	27	0	12	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	113	0	0	1	0
5	B	93	0	0	3	0
All	All	9965	3	9474	417	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 22.

The worst 5 of 417 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:536:ALA:H	1:A:563:GLN:NE2	1.55	1.02
1:A:355:LYS:HD2	1:A:356:GLY:N	1.75	1.02
1:B:342:ALA:HA	1:B:346:LEU:HD12	1.46	0.97
1:A:89:PHE:HE1	1:A:269:GLU:HG3	1.32	0.94
1:A:355:LYS:HD2	1:A:356:GLY:H	1.29	0.91

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	593/619 (96%)	525 (88%)	54 (9%)	14 (2%)	7	25
1	B	599/619 (97%)	540 (90%)	44 (7%)	15 (2%)	7	24
All	All	1192/1238 (96%)	1065 (89%)	98 (8%)	29 (2%)	7	25

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	LYS
1	A	341	GLU
1	B	150	VAL
1	A	94	VAL
1	A	356	GLY

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	510/529 (96%)	495 (97%)	15 (3%)	50	83
1	B	514/529 (97%)	500 (97%)	14 (3%)	52	85
All	All	1024/1058 (97%)	995 (97%)	29 (3%)	51	84

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	483	GLU
1	B	89	PHE
1	B	459	PHE
1	A	569	GLN
1	B	110	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	471	ASN
1	B	102	GLN
1	B	522	ASN
1	A	563	GLN
1	A	568	GLN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are 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	ADP	A	3001	4	22,29,29	1.03	1 (4%)	27,45,45	1.66	3 (11%)
2	TS5	A	620	-	25,28,28	4.54	14 (56%)	27,33,33	5.41	12 (44%)
3	ADP	B	3002	4	22,29,29	1.08	1 (4%)	27,45,45	1.70	3 (11%)

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	ADP	A	3001	4	-	0/12/32/32	0/3/3/3
2	TS5	A	620	-	1/1/6/10	0/30/34/34	0/0/0/0
3	ADP	B	3002	4	-	0/12/32/32	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	620	TS5	CB2-CA2	-11.09	1.40	1.53
2	A	620	TS5	CA2-C2	-5.09	1.38	1.52
2	A	620	TS5	C2'-C1'	-3.64	1.36	1.51
2	A	620	TS5	CA3-C3	-2.04	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	620	TS5	C2'-C3'	2.95	1.63	1.51

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	620	TS5	CB2-CA2-N2	-10.47	96.69	111.40
2	A	620	TS5	C1'-N1'-C3	-10.11	102.90	122.79
3	A	3001	ADP	N3-C2-N1	-6.47	123.94	128.89
3	B	3002	ADP	N3-C2-N1	-6.38	124.01	128.89
2	A	620	TS5	C2'-C3'-N2'	-4.93	99.64	111.96

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	620	TS5	CA2

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3001	ADP	2	0
2	A	620	TS5	5	0
3	B	3002	ADP	1	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 [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	599/619 (96%)	-0.37	4 (0%) 89 84	18, 43, 65, 84	0
1	B	603/619 (97%)	-0.27	12 (1%) 68 58	20, 46, 69, 86	0
All	All	1202/1238 (97%)	-0.32	16 (1%) 79 71	18, 44, 67, 86	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	SER	6.1
1	B	33	LEU	3.8
1	B	456	ASP	3.8
1	A	43	VAL	3.2
1	B	558	GLY	2.6

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	TS5	A	620	29/29	0.86	0.23	1.50	39,45,75,78	0
3	ADP	B	3002	27/27	0.98	0.15	-0.51	32,39,40,42	0
3	ADP	A	3001	27/27	0.97	0.13	-1.25	30,33,34,36	0
4	MG	A	4000	1/1	0.95	0.11	-1.54	37,37,37,37	0
4	MG	B	6000	1/1	0.95	0.11	-1.58	39,39,39,39	0
4	MG	B	7000	1/1	0.95	0.11	-	34,34,34,34	0
4	MG	A	5000	1/1	0.97	0.15	-	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.