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wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2024 – 06:21 PM EDT

PDB ID	:	4QEZ
Title	:	Crystal structure of 5'-methylthioadenosine/S-adenosylhomocysteine nucleosidase from Bacillus anthracis
Authors	:	Tarique, K.F.; Devi, S.; Abdul Rehman, S.A.; Gourinath, S.
Deposited on	:	2014-05-19
Resolution	:	2.70 Å(reported)

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

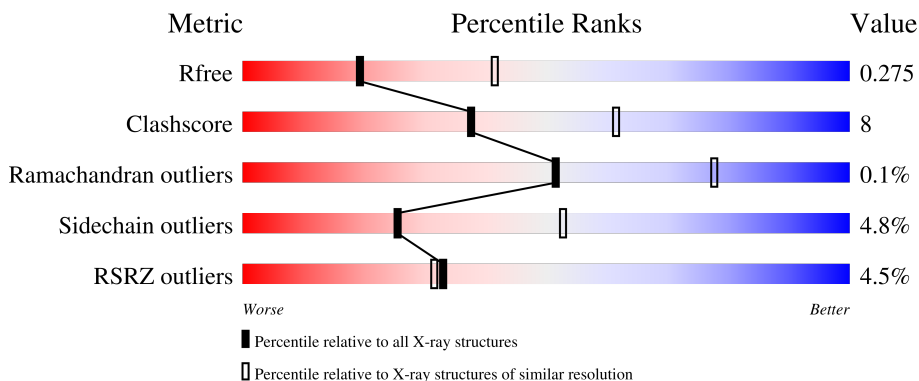|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.70 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	Percentile Ranks	Value
Rfree		0.275
Clashscore		8
Ramachandran outliers		0.1%
Sidechain outliers		4.8%
RSRZ outliers		4.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	239	3% / 81% 11% · 7%
1	B	239	4% / 80% 13% · ·
1	C	239	6% / 81% 12% · ·

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 5319 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 5'-methylthioadenosine/S-adenosylhomocysteine nucleosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	231	Total	C	N	O	S	0	0	0
			1780	1123	307	340	10			
1	A	223	Total	C	N	O	S	0	0	0
			1705	1077	289	329	10			
1	C	231	Total	C	N	O	S	0	0	0
			1780	1123	307	340	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	232	LEU	-	expression tag	UNP Q81LL4
B	233	GLU	-	expression tag	UNP Q81LL4
B	234	HIS	-	expression tag	UNP Q81LL4
B	235	HIS	-	expression tag	UNP Q81LL4
B	236	HIS	-	expression tag	UNP Q81LL4
B	237	HIS	-	expression tag	UNP Q81LL4
B	238	HIS	-	expression tag	UNP Q81LL4
B	239	HIS	-	expression tag	UNP Q81LL4
A	232	LEU	-	expression tag	UNP Q81LL4
A	233	GLU	-	expression tag	UNP Q81LL4
A	234	HIS	-	expression tag	UNP Q81LL4
A	235	HIS	-	expression tag	UNP Q81LL4
A	236	HIS	-	expression tag	UNP Q81LL4
A	237	HIS	-	expression tag	UNP Q81LL4
A	238	HIS	-	expression tag	UNP Q81LL4
A	239	HIS	-	expression tag	UNP Q81LL4
C	232	LEU	-	expression tag	UNP Q81LL4
C	233	GLU	-	expression tag	UNP Q81LL4
C	234	HIS	-	expression tag	UNP Q81LL4
C	235	HIS	-	expression tag	UNP Q81LL4
C	236	HIS	-	expression tag	UNP Q81LL4
C	237	HIS	-	expression tag	UNP Q81LL4
C	238	HIS	-	expression tag	UNP Q81LL4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	239	HIS	-	expression tag	UNP Q81LL4

- Molecule 2 is ADENINE (three-letter code: ADE) (formula: $C_5H_5N_5$).
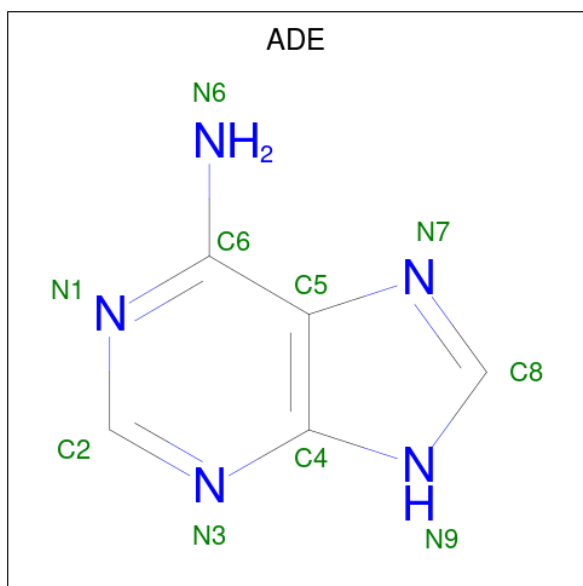
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 10	C 5	N 5	0	0
2	A	1	Total 10	C 5	N 5	0	0
2	C	1	Total 10	C 5	N 5	0	0

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).

TRS

O2
HO
C2

C1

C

NH$_3^+$ N

HO
O1

C3
OH
O3

| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			8	4	1	3		
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	C	1	Total	C	N	O	0	0
			8	4	1	3		

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3 Residue-property plots ⓘ

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.
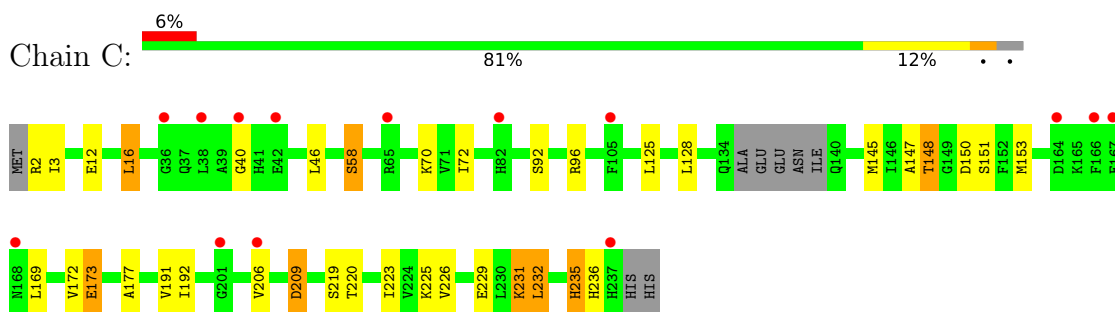
- Molecule 1: 5'-methylthioadenosine/S-adenosylhomocysteine nucleosidase
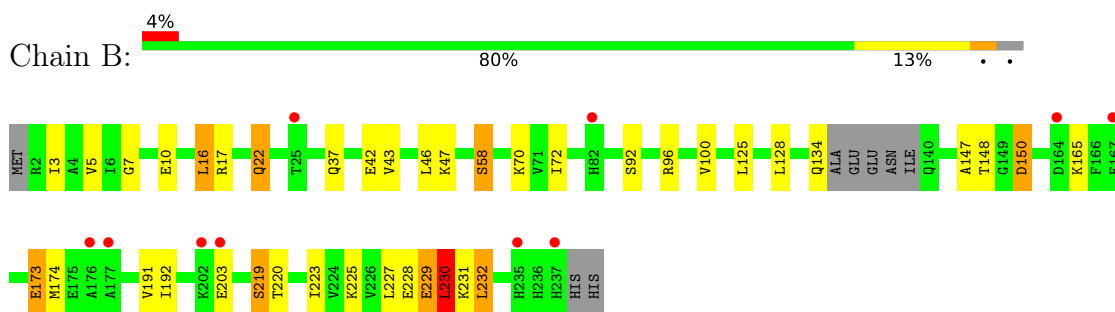
- Molecule 1: 5'-methylthioadenosine/S-adenosylhomocysteine nucleosidase
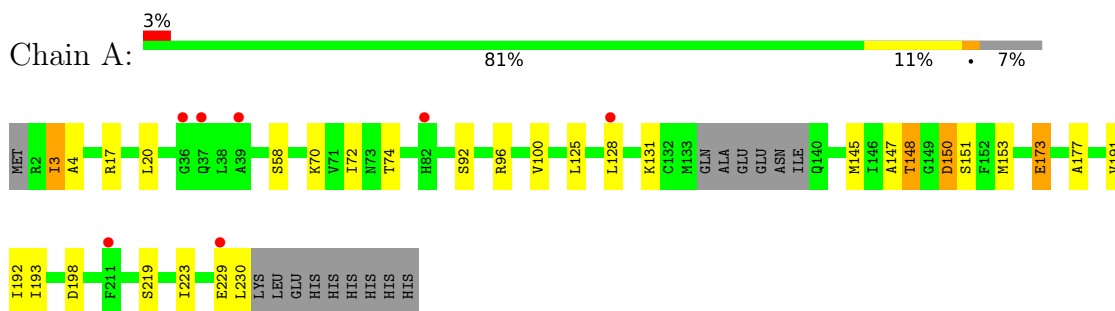
- Molecule 1: 5'-methylthioadenosine/S-adenosylhomocysteine nucleosidase

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	181.27Å 74.64Å 46.69Å 90.00° 95.26° 90.00°	Depositor
Resolution (Å)	34.49 – 2.70 34.49 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.9 (34.49-2.70) 95.0 (34.49-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.241 , 0.271 0.243 , 0.275	Depositor DCC
R_{free} test set	819 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	51.5	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 34.1	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5319	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: TRS, ADE

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	0.35	0/1731	0.62	0/2339
1	B	0.44	0/1810	0.61	0/2445
1	C	0.34	0/1810	0.59	0/2445
All	All	0.38	0/5351	0.61	0/7229

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
1	C	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	230	LEU	Peptide
1	C	232	LEU	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

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the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1705	0	1697	22	0
1	B	1780	0	1763	30	0
1	C	1780	0	1763	32	0
2	A	10	0	4	2	0
2	B	10	0	4	1	0
2	C	10	0	4	1	0
3	A	8	0	12	0	0
3	B	8	0	12	0	0
3	C	8	0	12	3	0
All	All	5319	0	5271	82	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 8.

The worst 5 of 82 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:C:148:THR:HG21	1:C:177:ALA:H	1.50	0.76
1:A:148:THR:HG21	1:A:177:ALA:H	1.50	0.74
1:A:148:THR:HG22	1:A:173:GLU:OE1	1.89	0.72
1:C:40:GLY:HA3	1:C:231:LYS:HD2	1.73	0.71
1:C:148:THR:HG22	1:C:173:GLU:OE1	1.89	0.71

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	219/239 (92%)	214 (98%)	5 (2%)	0	100	100
1	B	227/239 (95%)	216 (95%)	10 (4%)	1 (0%)	34	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	227/239 (95%)	218 (96%)	9 (4%)	0	100	100
All	All	673/717 (94%)	648 (96%)	24 (4%)	1 (0%)	51	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	229	GLU

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	182/197 (92%)	176 (97%)	6 (3%)	38	67
1	B	190/197 (96%)	179 (94%)	11 (6%)	20	43
1	C	190/197 (96%)	180 (95%)	10 (5%)	22	48
All	All	562/591 (95%)	535 (95%)	27 (5%)	25	53

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	THR
1	C	16	LEU
1	C	231	LYS
1	A	173	GLU
1	C	58	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	235	HIS
1	C	185	GLN
1	A	185	GLN
1	B	235	HIS

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Mol	Chain	Res	Type
1	C	106	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	ADE	A	301	-	9,11,11	1.35	1 (11%)	7,15,15	2.11	4 (57%)
3	TRS	C	301	-	7,7,7	0.30	0	9,9,9	0.48	0
2	ADE	C	302	-	9,11,11	1.33	1 (11%)	7,15,15	2.21	4 (57%)
2	ADE	B	301	-	9,11,11	1.30	1 (11%)	7,15,15	2.17	5 (71%)
3	TRS	A	302	-	7,7,7	0.31	0	9,9,9	0.46	0
3	TRS	B	302	-	7,7,7	0.25	0	9,9,9	0.34	0

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	TRS	C	301	-	-	3/9/9/9	-
2	ADE	A	301	-	-	-	0/2/2/2
2	ADE	C	302	-	-	-	0/2/2/2
2	ADE	B	301	-	-	-	0/2/2/2
3	TRS	A	302	-	-	2/9/9/9	-
3	TRS	B	302	-	-	0/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	ADE	C5-C4	2.51	1.47	1.40
2	C	302	ADE	C5-C4	2.49	1.47	1.40
2	B	301	ADE	C5-C4	2.46	1.47	1.40

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	302	ADE	N3-C2-N1	-3.20	123.68	128.68
2	B	301	ADE	N3-C2-N1	-2.90	124.15	128.68
2	C	302	ADE	C2-N3-C4	2.82	120.07	113.45
2	A	301	ADE	N3-C2-N1	-2.80	124.31	128.68
2	C	302	ADE	C4-C5-N7	-2.70	106.58	109.40

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	301	TRS	C3-C-C2-O2
3	C	301	TRS	N-C-C2-O2
3	A	302	TRS	C3-C-C2-O2
3	C	301	TRS	C1-C-C2-O2
3	A	302	TRS	C2-C-C3-O3

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	ADE	2	0
3	C	301	TRS	3	0
2	C	302	ADE	1	0
2	B	301	ADE	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   ⓘ

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	223/239 (93%)	0.30	7 (3%)	49	49	44, 60, 78, 87	0
1	B	231/239 (96%)	0.40	10 (4%)	35	33	40, 53, 68, 91	0
1	C	231/239 (96%)	0.46	14 (6%)	21	20	49, 62, 80, 94	0
All	All	685/717 (95%)	0.39	31 (4%)	33	31	40, 58, 77, 94	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	HIS	4.1
1	C	167	GLU	3.6
1	C	36	GLY	3.4
1	A	36	GLY	3.3
1	C	164	ASP	3.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3   Carbohydrates   ⓘ

There are no monosaccharides in this entry.

6.4   Ligands   ⓘ

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	ADE	A	301	10/10	0.78	0.35	72,72,72,72	0
2	ADE	B	301	10/10	0.81	0.31	72,72,72,72	0
2	ADE	C	302	10/10	0.87	0.24	72,72,72,72	0
3	TRS	C	301	8/8	0.90	0.35	72,72,72,72	0
3	TRS	A	302	8/8	0.92	0.31	72,72,72,72	0
3	TRS	B	302	8/8	0.94	0.38	72,72,72,72	0

6.5 Other polymers ⓘ

There are no such residues in this entry.