wwPDB X-ray Structure Validation Summary Report (i)

Nov 14, 2026 – 03:05 PM EST

PDB ID	:	7UG3 / pdb_00007ug3
Title	:	Crystal structure of adenosylmethionie-8-amino-7-oxononanoate aminotransferase from Klebsiella pneumoniae
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2022-03-23
Resolution	:	1.90 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 (i) 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 (1)) were used in the production of this report:

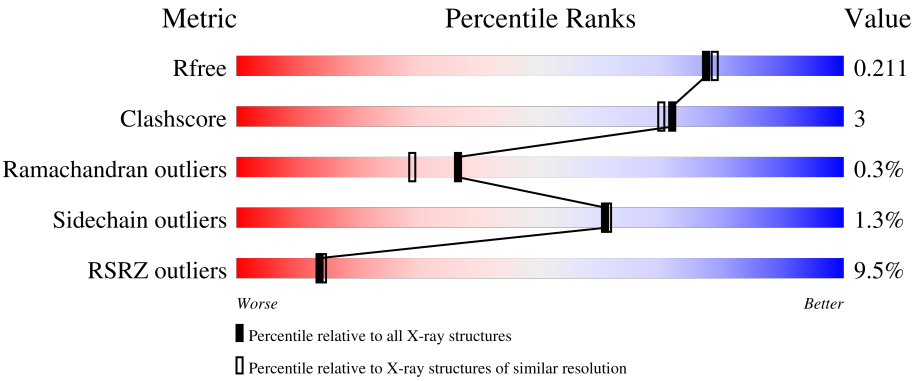
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	438	8% 82% 7% 11%
1	B	438	7% 82% 7% 11%
1	C	438	8% 79% 10% 11%
1	D	438	11% 81% 7% 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12851 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 Adenosylmethionine-8-amino-7-oxononanoate aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	4	0
			3018	1924	536	532	26			
1	B	389	Total	C	N	O	S	0	2	0
			2999	1910	529	534	26			
1	C	390	Total	C	N	O	S	0	0	0
			2975	1893	524	533	25			
1	D	387	Total	C	N	O	S	0	2	0
			2914	1862	506	522	24			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	expression tag	UNP A0A422Z2E3
A	-7	ALA	-	expression tag	UNP A0A422Z2E3
A	-6	HIS	-	expression tag	UNP A0A422Z2E3
A	-5	HIS	-	expression tag	UNP A0A422Z2E3
A	-4	HIS	-	expression tag	UNP A0A422Z2E3
A	-3	HIS	-	expression tag	UNP A0A422Z2E3
A	-2	HIS	-	expression tag	UNP A0A422Z2E3
A	-1	HIS	-	expression tag	UNP A0A422Z2E3
A	0	HIS	-	expression tag	UNP A0A422Z2E3
B	-8	MET	-	expression tag	UNP A0A422Z2E3
B	-7	ALA	-	expression tag	UNP A0A422Z2E3
B	-6	HIS	-	expression tag	UNP A0A422Z2E3
B	-5	HIS	-	expression tag	UNP A0A422Z2E3
B	-4	HIS	-	expression tag	UNP A0A422Z2E3
B	-3	HIS	-	expression tag	UNP A0A422Z2E3
B	-2	HIS	-	expression tag	UNP A0A422Z2E3
B	-1	HIS	-	expression tag	UNP A0A422Z2E3
B	0	HIS	-	expression tag	UNP A0A422Z2E3
C	-8	MET	-	expression tag	UNP A0A422Z2E3
C	-7	ALA	-	expression tag	UNP A0A422Z2E3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	HIS	-	expression tag	UNP A0A422Z2E3
C	-5	HIS	-	expression tag	UNP A0A422Z2E3
C	-4	HIS	-	expression tag	UNP A0A422Z2E3
C	-3	HIS	-	expression tag	UNP A0A422Z2E3
C	-2	HIS	-	expression tag	UNP A0A422Z2E3
C	-1	HIS	-	expression tag	UNP A0A422Z2E3
C	0	HIS	-	expression tag	UNP A0A422Z2E3
D	-8	MET	-	expression tag	UNP A0A422Z2E3
D	-7	ALA	-	expression tag	UNP A0A422Z2E3
D	-6	HIS	-	expression tag	UNP A0A422Z2E3
D	-5	HIS	-	expression tag	UNP A0A422Z2E3
D	-4	HIS	-	expression tag	UNP A0A422Z2E3
D	-3	HIS	-	expression tag	UNP A0A422Z2E3
D	-2	HIS	-	expression tag	UNP A0A422Z2E3
D	-1	HIS	-	expression tag	UNP A0A422Z2E3
D	0	HIS	-	expression tag	UNP A0A422Z2E3

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0

- Molecule 3 is water.

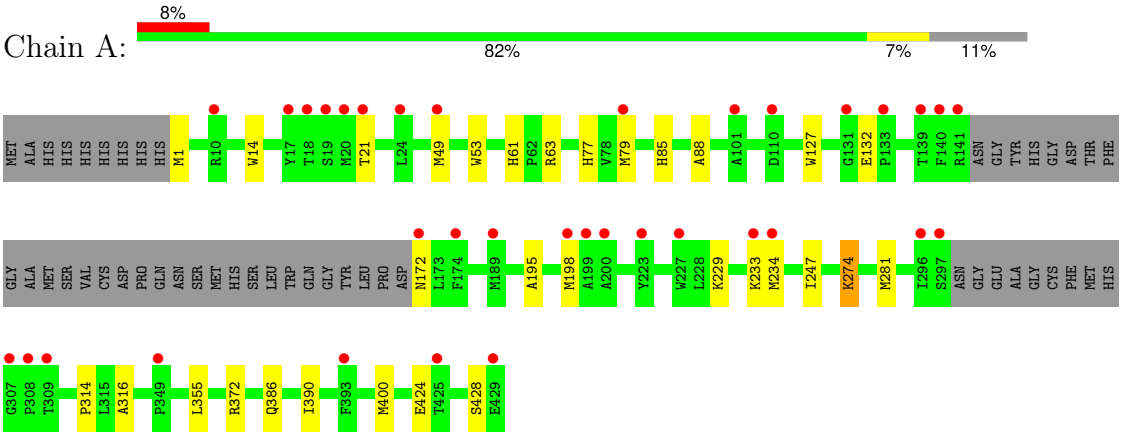
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	287	Total O 287 287	0	0
3	B	302	Total O 302 302	0	0
3	C	172	Total O 172 172	0	0
3	D	180	Total O 180 180	0	0

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.

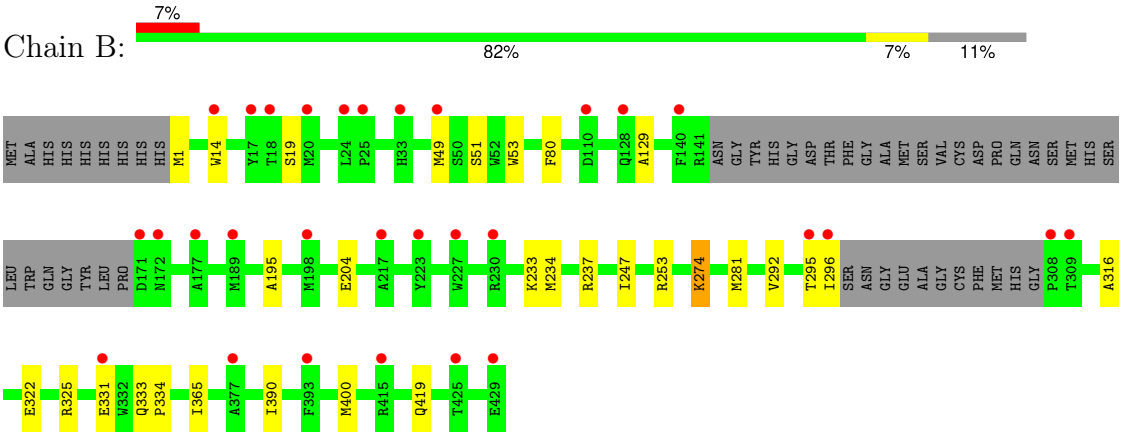
• Molecule 1: Adenosylmethionine-8-amino-7-oxononanoate aminotransferase

Chain A:



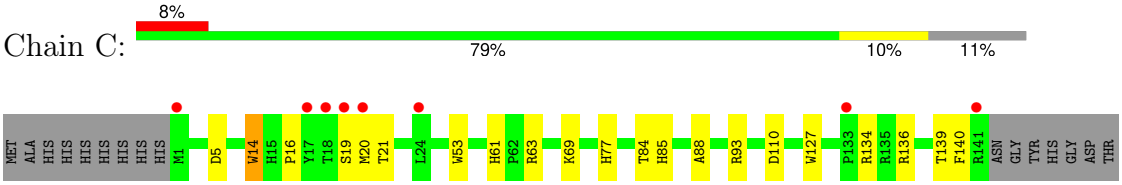
• Molecule 1: Adenosylmethionine-8-amino-7-oxononanoate aminotransferase

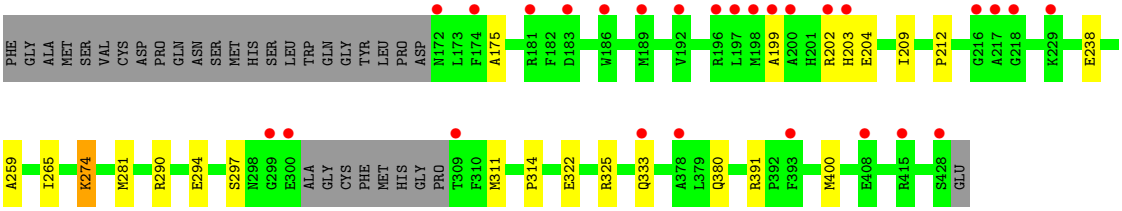
Chain B:



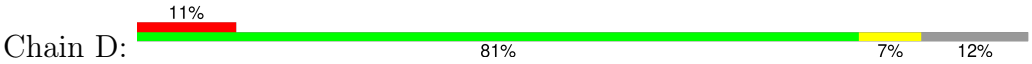
• Molecule 1: Adenosylmethionine-8-amino-7-oxononanoate aminotransferase

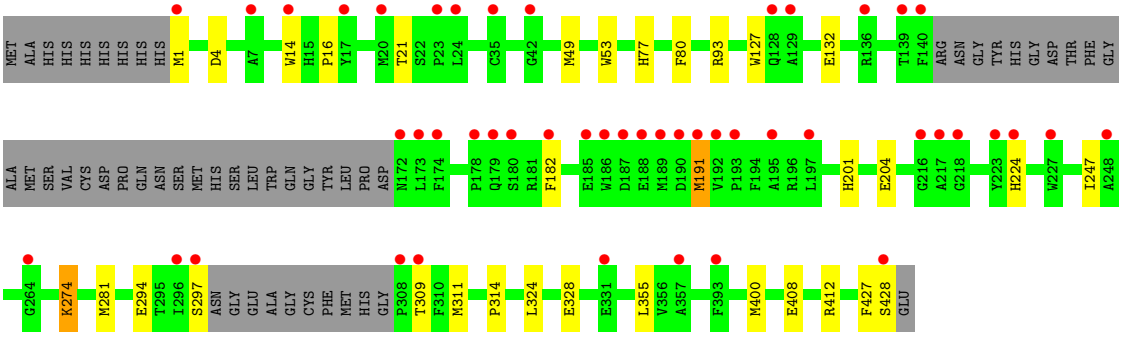
Chain C:





• Molecule 1: Adenosylmethionine-8-amino-7-oxononanoate aminotransferase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.07Å 90.83Å 103.86Å 90.00° 93.87° 90.00°	Depositor
Resolution (Å)	45.42 – 1.90 45.42 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.42-1.90) 99.8 (45.42-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
R, R_{free}	0.225 , 0.260 0.195 , 0.211	Depositor DCC
R_{free} test set	1954 reflections (1.57%)	wwPDB-VP
Wilson B-factor (Å^2)	28.5	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12851	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 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: NA

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	0/3098	0.48	0/4208
1	B	0.35	0/3075	0.51	0/4175
1	C	0.25	0/3043	0.43	0/4136
1	D	0.25	0/2988	0.43	0/4069
All	All	0.31	0/12204	0.46	0/16588

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3018	0	3022	22	0
1	B	2999	0	2997	19	0
1	C	2975	0	2954	28	0
1	D	2914	0	2881	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	287	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	302	0	0	3	0
3	C	172	0	0	1	0
3	D	180	0	0	0	0
All	All	12851	0	11854	78	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 3.

The worst 5 of 78 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:372[A]:ARG:HH22	1:A:424:GLU:HG3	1.50	0.77
1:C:136:ARG:NH2	1:C:204:GLU:OE1	2.26	0.69
1:C:281:MET:HE3	1:D:281:MET:HE3	1.74	0.68
1:D:247:ILE:HG22	1:D:274:LYS:HE2	1.74	0.67
1:C:139:THR:HG22	1:C:209:ILE:HB	1.81	0.61

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	387/438 (88%)	374 (97%)	12 (3%)	1 (0%)	36	29
1	B	384/438 (88%)	374 (97%)	9 (2%)	1 (0%)	36	29
1	C	384/438 (88%)	373 (97%)	10 (3%)	1 (0%)	36	29
1	D	383/438 (87%)	372 (97%)	10 (3%)	1 (0%)	36	29
All	All	1538/1752 (88%)	1493 (97%)	41 (3%)	4 (0%)	36	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	274	LYS
1	B	274	LYS
1	D	274	LYS
1	A	274	LYS

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	A	311/350 (89%)	308 (99%)	3 (1%)	68	70
1	B	310/350 (89%)	306 (99%)	4 (1%)	61	61
1	C	305/350 (87%)	300 (98%)	5 (2%)	55	54
1	D	296/350 (85%)	292 (99%)	4 (1%)	59	59
All	All	1222/1400 (87%)	1206 (99%)	16 (1%)	61	61

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	191	MET
1	D	80	PHE
1	C	19	SER
1	D	14	TRP
1	C	14	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	74	GLN
1	C	418	ASN
1	D	418	ASN
1	D	125	GLN
1	D	313	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	390/438 (89%)	0.62	35 (8%)	15	16	21, 38, 67, 87	4 (1%)
1	B	389/438 (88%)	0.62	30 (7%)	19	21	22, 38, 61, 101	2 (0%)
1	C	390/438 (89%)	0.85	35 (8%)	15	16	31, 46, 76, 105	0
1	D	387/438 (88%)	0.97	48 (12%)	8	8	28, 48, 75, 100	2 (0%)
All	All	1556/1752 (88%)	0.76	148 (9%)	14	14	21, 43, 72, 105	8 (0%)

The worst 5 of 148 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17	TYR	7.2
1	B	296	ILE	5.5
1	C	189	MET	4.9
1	B	308	PRO	4.7
1	D	227	TRP	4.6

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 oligosaccharides 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	NA	A	501	1/1	0.96	0.05	35,35,35,35	0
2	NA	B	501	1/1	0.96	0.12	35,35,35,35	0
2	NA	C	501	1/1	0.98	0.06	35,35,35,35	0
2	NA	D	501	1/1	0.99	0.09	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.