



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 02:59 PM GMT

PDB ID : 2CV2
Title : Glutamyl-tRNA synthetase from *Thermus thermophilus* in complex with tRNA(Glu) and an enzyme inhibitor, Glu-AMS
Authors : Sekine, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-05-31
Resolution : 2.69 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

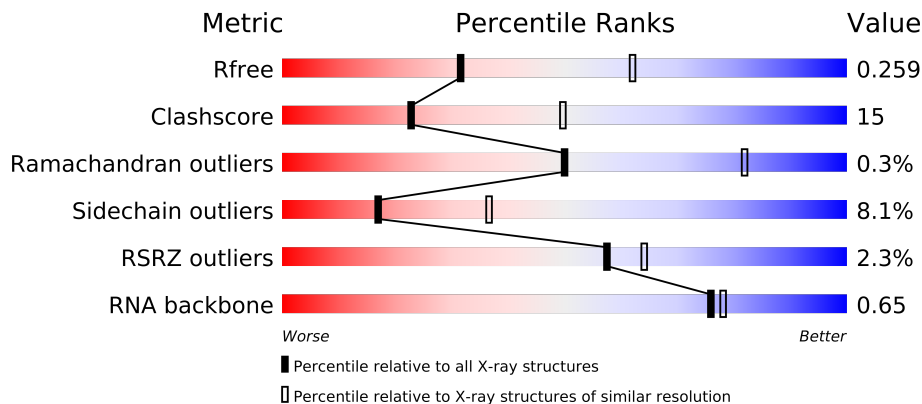
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.69 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)
RNA backbone	1838	1042 (3.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	C	75	
1	D	75	
2	A	468	
2	B	468	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	C	902	-	X
3	MG	D	901	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	CL	A	904	-	X
4	CL	B	903	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11215 atoms, of which 0 are hydrogen and 0 are deuterium.

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 RNA chain called tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	75	Total	C	N	O	P	0	0	0
			1597	711	284	527	75			
1	D	75	Total	C	N	O	P	0	0	0
			1597	711	284	527	75			

- Molecule 2 is a protein called glutamyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	468	Total	C	N	O	S	0	0	0
			3814	2443	676	687	8			
2	B	468	Total	C	N	O	S	0	0	0
			3814	2443	676	687	8			

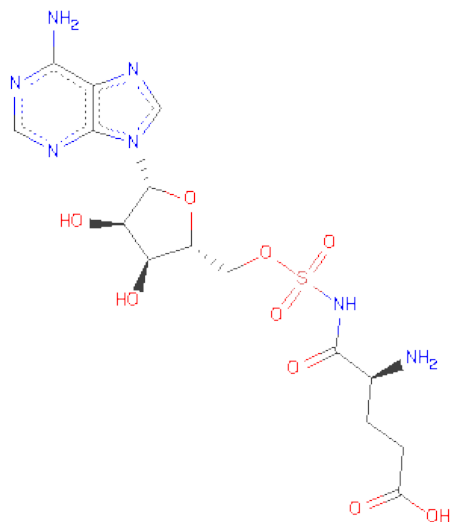
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is O5'-(L-GLUTAMYL-SULFAMOYL)-ADENOSINE (three-letter code: GSU) (formula: C₁₅H₂₁N₇O₉S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			32	15	7	9	1		
5	B	1	Total	C	N	O	S	0	0
			32	15	7	9	1		

- Molecule 6 is water.

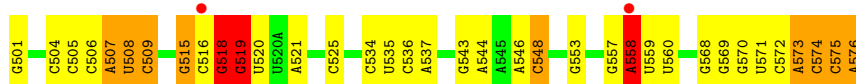
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	125	Total	O	0	0
			125	125		
6	B	116	Total	O	0	0
			116	116		
6	C	48	Total	O	0	0
			48	48		
6	D	36	Total	O	0	0
			36	36		

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: tRNA

Chain C: 



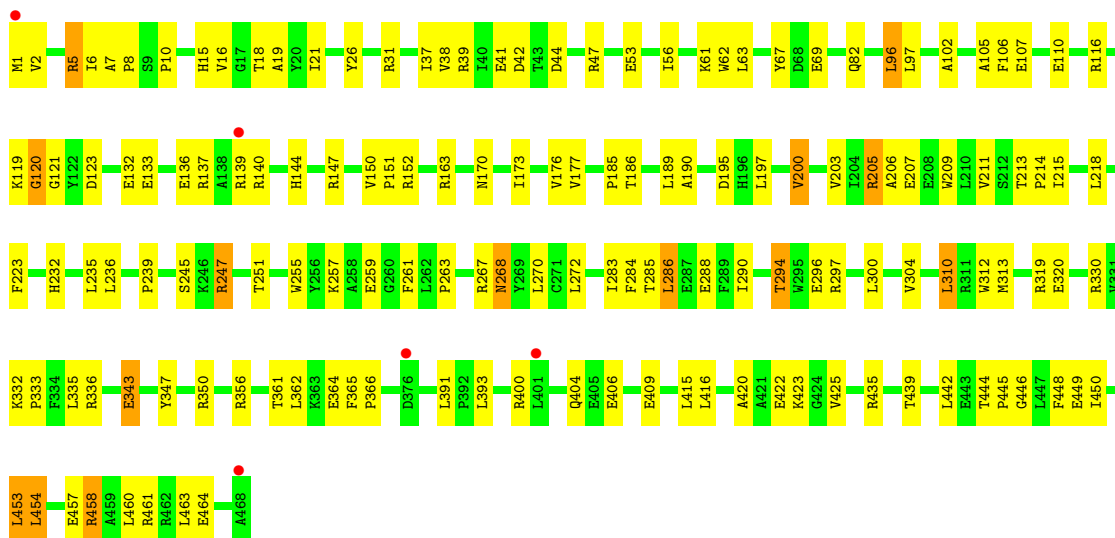
- Molecule 1: tRNA

Chain D: 



- Molecule 2: glutamyl-tRNA synthetase

Chain A: 



- Molecule 2: glutamyl-tRNA synthetase

Chain B: 



E405	E406	E409	L412	L416	R417	K423	G424	Y425	Q429	V430	A431	Q432	R435	L438	L442	E443	T444	F445	G446	L447	F448	E449	T450	L451	A452	L453	L454	A459	L463	E464	R465	A466	L467	A468																	
A292	F293	T294	W295	E296	R297	V298	G302	P303	V304	L310	Y317	I318	R319	E320	V321	L324	E325	E326	R330	F334	R350	L354	K355	R356	P357	R358	F365	P366	E367	K368	A369	L372	K382	A383	K386	L391	P392	L393	L394	K395	Y398	P399	R402								
Y187	H188	L189	D194	D195	H196	L197	R205	A206	V211	S212	T213	P214	I215	L218	H232	N233	P234	L235	L236	R237	N238	P239	D240	K241	T242	K248	L253	D254	W255	E259	G260	F261	L262	L266	R267	N268	Y269	L270	G271	L272	R273	G274	T285	L286	F287	E288	F289	T290	Q291		
R104	A105	F106	E107	E110	E111	L112	E113	Q114	I115	R116	K117	E118	K119	G120	G121	Y122	D123	G124	R127	N128	I129	P130	P131	E132	E133	A134	I135	E136	R137	A138	R139	R140	E141	G142	P143	H144	P151	R152	E157	V167	V168	P174	D175	V176	V177	L178	L179	G183	Y184	P185	L186

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	110.32Å 219.82Å 135.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.34 – 2.69 46.34 – 2.63	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.34-2.69) 96.4 (46.34-2.63)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.260 0.200 , 0.259	Depositor DCC
R_{free} test set	2378 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 26.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 47476 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11215	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GSU, CL

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	C	0.55	1/1782 (0.1%)	0.86	9/2774 (0.3%)
1	D	0.54	1/1782 (0.1%)	0.87	9/2774 (0.3%)
2	A	0.52	0/3910	0.70	0/5293
2	B	0.52	0/3910	0.68	0/5293
All	All	0.53	2/11384 (0.0%)	0.75	18/16134 (0.1%)

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	C	1	3
1	D	1	3
All	All	2	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	501	G	OP3-P	-7.12	1.52	1.61
1	D	501	G	OP3-P	-5.85	1.54	1.61

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	558	A	C2'-C3'-O3'	8.16	127.46	109.50
1	C	558	A	C2'-C3'-O3'	7.83	126.72	109.50
1	D	507	A	C2'-C3'-O3'	7.76	126.56	109.50
1	C	573	A	C2'-C3'-O3'	7.31	125.58	109.50
1	D	573	A	C2'-C3'-O3'	7.30	125.57	109.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	558	A	C3'
1	D	558	A	C3'

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	515	G	Sidechain
1	C	535	U	Sidechain
1	C	568	G	Sidechain
1	D	515	G	Sidechain
1	D	522	G	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1597	0	813	19	0
1	D	1597	0	813	19	0
2	A	3814	0	3818	115	1
2	B	3814	0	3818	157	1
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	32	0	20	2	0
5	B	32	0	20	2	0
6	A	125	0	0	6	0
6	B	116	0	0	6	0
6	C	48	0	0	0	0
6	D	36	0	0	0	0
All	All	11215	0	9302	297	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

The worst 5 of 297 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:247:ARG:HD3	2:A:247:ARG:H	1.29	0.96
2:A:177:VAL:HG23	2:A:186:THR:HG21	1.49	0.95
2:A:163:ARG:HH12	2:A:300:LEU:HD22	1.31	0.92
2:B:454:LEU:H	2:B:454:LEU:HD22	1.38	0.86
2:B:435:ARG:HH11	2:B:444:THR:CG2	1.89	0.85

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:343:GLU:O	2:B:50:PRO:O[6_654]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	
2	A	466/468 (100%)	453 (97%)	12 (3%)	1 (0%)	56	86
2	B	466/468 (100%)	448 (96%)	16 (3%)	2 (0%)	43	76
All	All	932/936 (100%)	901 (97%)	28 (3%)	3 (0%)	50	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	120	GLY
2	B	120	GLY
2	B	151	PRO

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	
2	A	393/393 (100%)	366 (93%)	27 (7%)	22	48
2	B	393/393 (100%)	356 (91%)	37 (9%)	13	28
All	All	786/786 (100%)	722 (92%)	64 (8%)	17	36

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	5	ARG
2	B	123	ASP
2	B	442	LEU
2	B	21	ILE
2	B	115	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	25	ASN
2	B	432	GLN
2	B	191	ASN
2	A	404	GLN
2	B	90	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	74/75 (98%)	14 (18%)	6 (8%)
1	D	74/75 (98%)	13 (17%)	6 (8%)
All	All	148/150 (98%)	27 (18%)	12 (8%)

5 of 27 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	507	A
1	C	508	U
1	C	509	C
1	C	516	C
1	C	518	G

5 of 12 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	573	A
1	D	507	A
1	D	558	A
1	C	558	A
1	D	519	G

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 ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
5	GSU	A	601	-	34,34,34	1.82	7 (20%)	50,50,50	2.01	8 (16%)
5	GSU	B	602	-	34,34,34	1.55	6 (17%)	50,50,50	2.00	10 (20%)

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
5	GSU	A	601	-	-	0/24/40/40	0/1/3/3
5	GSU	B	602	-	-	0/24/40/40	0/1/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	GSU	O2S-S	5.45	1.47	1.42
5	A	601	GSU	S-N10	5.08	1.65	1.60
5	A	601	GSU	O1S-S	4.38	1.46	1.42
5	B	602	GSU	O1S-S	4.37	1.46	1.42
5	B	602	GSU	S-N10	4.18	1.64	1.60

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	GSU	O2S-S-O1S	-9.88	111.16	121.45
5	B	602	GSU	O2S-S-O1S	-9.27	111.80	121.45
5	B	602	GSU	O4'-C1'-N9	5.58	113.63	108.44
5	A	601	GSU	O5'-C5'-C4'	4.65	116.65	107.81
5	B	602	GSU	O5'-C5'-C4'	4.31	116.01	107.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	C	75/75 (100%)	0.07	2 (2%) 52 57	25, 43, 76, 83	0
1	D	75/75 (100%)	0.13	6 (8%) 12 13	21, 41, 75, 96	0
2	A	468/468 (100%)	-0.32	5 (1%) 77 82	13, 29, 61, 75	0
2	B	468/468 (100%)	-0.19	12 (2%) 53 59	13, 32, 76, 95	0
All	All	1086/1086 (100%)	-0.20	25 (2%) 57 64	13, 32, 70, 96	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	516	C	5.4
2	B	128	ASN	4.9
2	B	140	ARG	4.1
2	B	141	GLY	3.6
2	A	468	ALA	3.6

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 carbohydrates 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. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	D	901	1/1	0.24	8.37	33,33,33,33	0
4	CL	B	903	1/1	0.25	4.55	27,27,27,27	0
4	CL	A	904	1/1	0.27	3.79	33,33,33,33	0
3	MG	C	902	1/1	0.17	2.76	36,36,36,36	0
5	GSU	A	601	32/32	0.13	-0.88	16,22,28,31	0
5	GSU	B	602	32/32	0.13	-1.14	16,25,31,32	0

6.5 Other polymers ⓘ

There are no such residues in this entry.