



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 01:49 pm BST

PDB ID : 6JP6
Title : The X-ray structure of yeast tRNA methyltransferase complex of Trm7 and Trm734 essential for 2'-O-methylation at the first position of anticodon in specific tRNAs
Authors : Hirata, A.; Okada, K.; Yoshii, K.; Shiraisi, H.; Saijo, S.; Yonezawa, K.; Shimizu, N.; Hori, H.
Deposited on : 2019-03-26
Resolution : 2.70 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

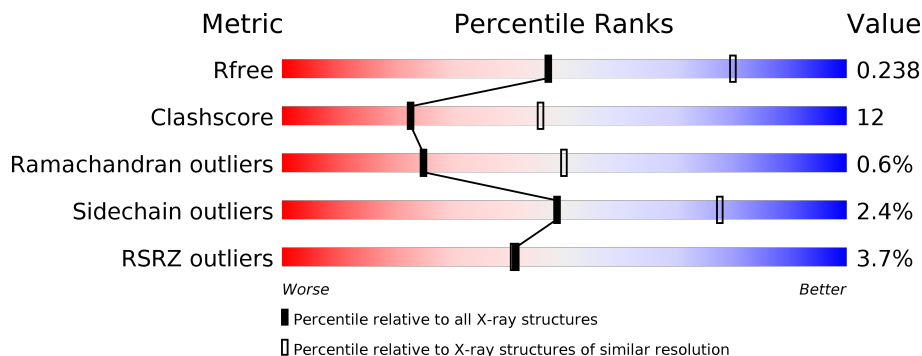
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	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 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	A	1028	
1	C	1028	
2	B	325	
2	D	325	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19867 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 tRNA (guanosine(34)-2'-O)-methyltransferase non-catalytic subunit TRM734.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	998	7951	5074	1328	1517	32	0	0	0
1	C	998	7951	5074	1328	1517	32	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1014	LEU	-	expression tag	UNP Q08924
A	1015	GLU	-	expression tag	UNP Q08924
A	1016	VAL	-	expression tag	UNP Q08924
A	1017	LEU	-	expression tag	UNP Q08924
A	1018	PHE	-	expression tag	UNP Q08924
A	1019	GLN	-	expression tag	UNP Q08924
A	1020	GLY	-	expression tag	UNP Q08924
A	1021	PRO	-	expression tag	UNP Q08924
A	1022	SER	-	expression tag	UNP Q08924
A	1023	HIS	-	expression tag	UNP Q08924
A	1024	HIS	-	expression tag	UNP Q08924
A	1025	HIS	-	expression tag	UNP Q08924
A	1026	HIS	-	expression tag	UNP Q08924
A	1027	HIS	-	expression tag	UNP Q08924
A	1028	HIS	-	expression tag	UNP Q08924
C	1014	LEU	-	expression tag	UNP Q08924
C	1015	GLU	-	expression tag	UNP Q08924
C	1016	VAL	-	expression tag	UNP Q08924
C	1017	LEU	-	expression tag	UNP Q08924
C	1018	PHE	-	expression tag	UNP Q08924
C	1019	GLN	-	expression tag	UNP Q08924
C	1020	GLY	-	expression tag	UNP Q08924
C	1021	PRO	-	expression tag	UNP Q08924
C	1022	SER	-	expression tag	UNP Q08924

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1023	HIS	-	expression tag	UNP Q08924
C	1024	HIS	-	expression tag	UNP Q08924
C	1025	HIS	-	expression tag	UNP Q08924
C	1026	HIS	-	expression tag	UNP Q08924
C	1027	HIS	-	expression tag	UNP Q08924
C	1028	HIS	-	expression tag	UNP Q08924

- Molecule 2 is a protein called tRNA (cytidine(34)/guanosine(34)-2'-O)-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	231	1829	1158	318	342	11	0	0	0
2	D	231	1829	1158	318	342	11	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

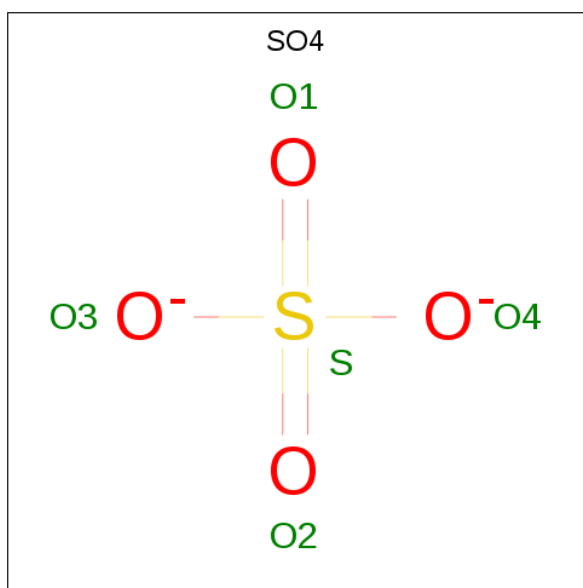
Chain	Residue	Modelled	Actual	Comment	Reference
B	311	LEU	-	expression tag	UNP P38238
B	312	GLU	-	expression tag	UNP P38238
B	313	VAL	-	expression tag	UNP P38238
B	314	LEU	-	expression tag	UNP P38238
B	315	PHE	-	expression tag	UNP P38238
B	316	GLN	-	expression tag	UNP P38238
B	317	GLY	-	expression tag	UNP P38238
B	318	PRO	-	expression tag	UNP P38238
B	319	SER	-	expression tag	UNP P38238
B	320	HIS	-	expression tag	UNP P38238
B	321	HIS	-	expression tag	UNP P38238
B	322	HIS	-	expression tag	UNP P38238
B	323	HIS	-	expression tag	UNP P38238
B	324	HIS	-	expression tag	UNP P38238
B	325	HIS	-	expression tag	UNP P38238
D	311	LEU	-	expression tag	UNP P38238
D	312	GLU	-	expression tag	UNP P38238
D	313	VAL	-	expression tag	UNP P38238
D	314	LEU	-	expression tag	UNP P38238
D	315	PHE	-	expression tag	UNP P38238
D	316	GLN	-	expression tag	UNP P38238
D	317	GLY	-	expression tag	UNP P38238
D	318	PRO	-	expression tag	UNP P38238
D	319	SER	-	expression tag	UNP P38238

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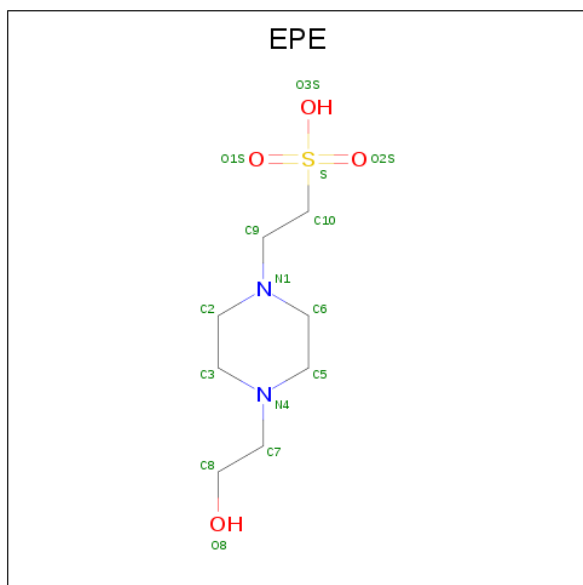
Chain	Residue	Modelled	Actual	Comment	Reference
D	320	HIS	-	expression tag	UNP P38238
D	321	HIS	-	expression tag	UNP P38238
D	322	HIS	-	expression tag	UNP P38238
D	323	HIS	-	expression tag	UNP P38238
D	324	HIS	-	expression tag	UNP P38238
D	325	HIS	-	expression tag	UNP P38238

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	15	8	2	4	1	0	0
4	C	1	15	8	2	4	1	0	0

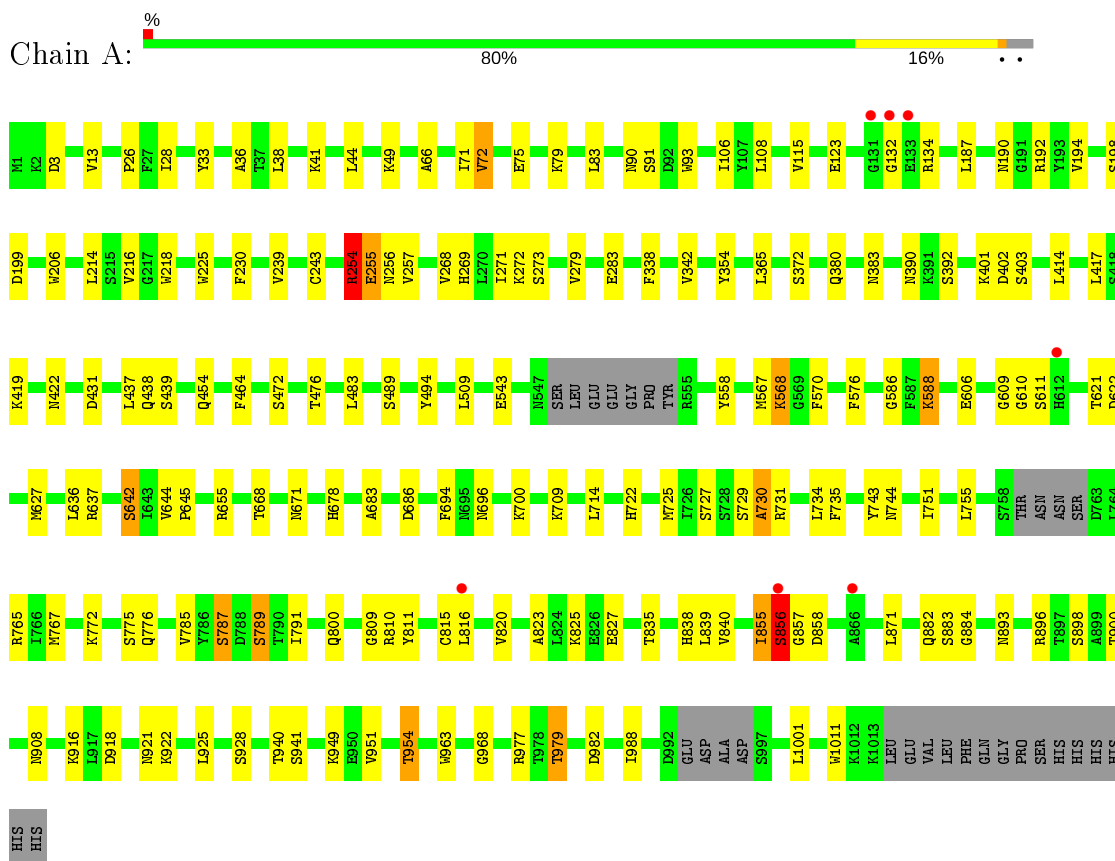
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	121	Total	O	0	0
			121	121		
5	B	10	Total	O	0	0
			10	10		
5	C	114	Total	O	0	0
			114	114		
5	D	12	Total	O	0	0
			12	12		

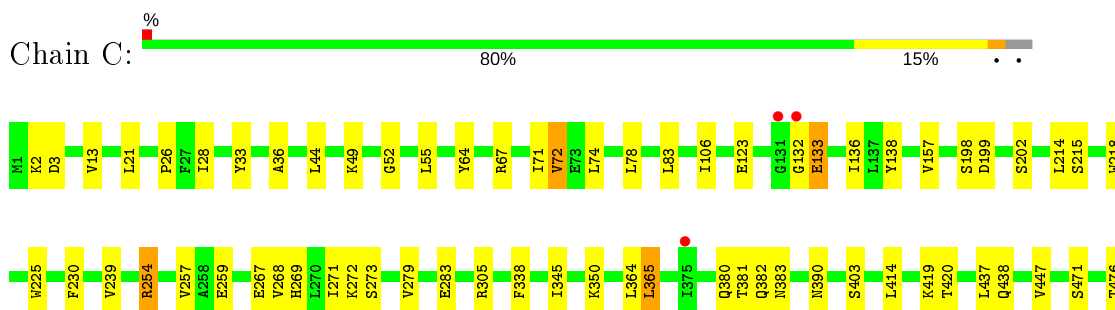
3 Residue-property plots [i](#)

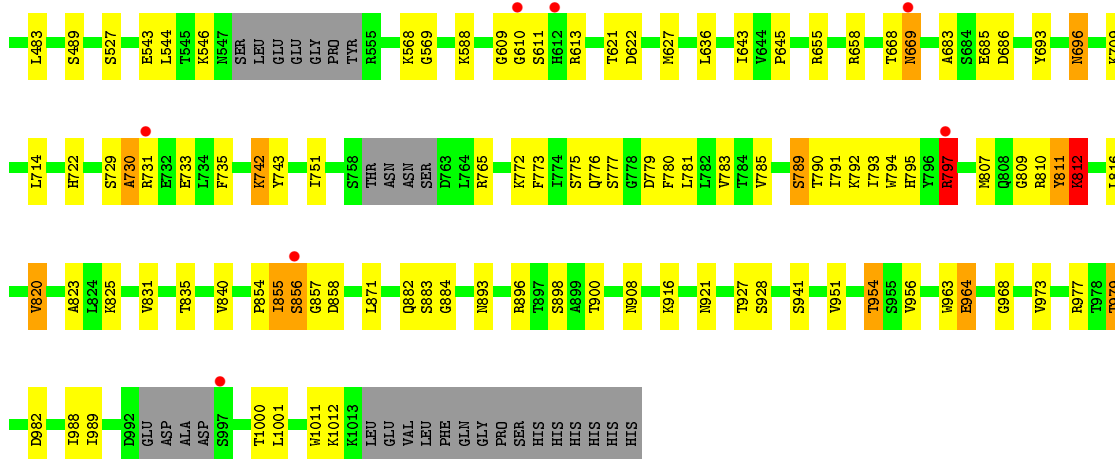
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: tRNA (guanosine(34)-2'-O)-methyltransferase non-catalytic subunit TRM734

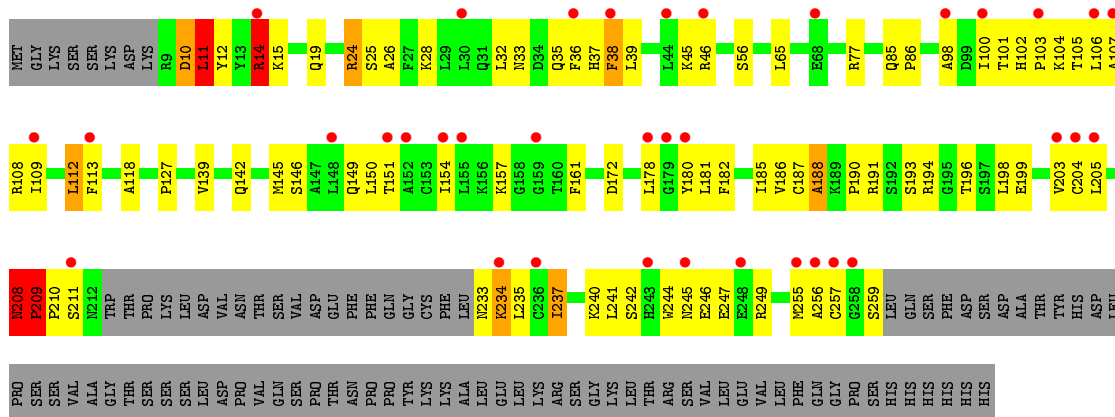


- Molecule 1: tRNA (guanosine(34)-2'-O)-methyltransferase non-catalytic subunit TRM734

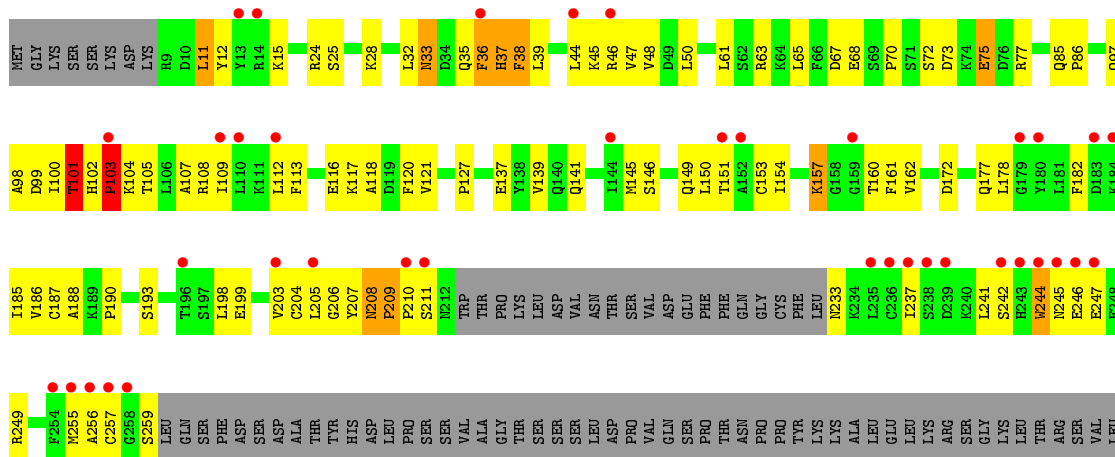




• Molecule 2: tRNA (cytidine(34)/guanosine(34)-2'-O)-methyltransferase



• Molecule 2: tRNA (cytidine(34)/guanosine(34)-2'-O)-methyltransferase



GLU
VAL
LEU
PHE
GLN
GLY
PRO
SER
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	253.64Å 110.35Å 133.50Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	36.43 – 2.70 36.43 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (36.43-2.70) 99.6 (36.43-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.68Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.194 , 0.239 0.194 , 0.238	Depositor DCC
R_{free} test set	5048 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtrriage
Anisotropy	0.048	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 22.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.477 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19867	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, SO4

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	0.60	8/8110 (0.1%)	0.71	3/10972 (0.0%)
1	C	0.53	1/8110 (0.0%)	0.71	6/10972 (0.1%)
2	B	0.58	2/1865 (0.1%)	0.87	8/2516 (0.3%)
2	D	0.60	0/1865	0.85	8/2516 (0.3%)
All	All	0.57	11/19950 (0.1%)	0.74	25/26976 (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	A	0	2
1	C	0	2
2	B	0	4
2	D	0	2
All	All	0	10

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	ARG	NE-CZ	-7.90	1.22	1.33
1	A	588	LYS	CA-CB	-7.43	1.37	1.53
1	A	254	ARG	CZ-NH2	-6.75	1.24	1.33
1	A	254	ARG	CZ-NH1	-6.46	1.24	1.33
1	A	255	GLU	CD-OE1	6.31	1.32	1.25

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	ARG	NE-CZ-NH2	-9.23	115.68	120.30
1	C	797	ARG	CD-NE-CZ	8.72	135.81	123.60
1	C	812	LYS	N-CA-C	-7.71	90.19	111.00
2	B	11	LEU	CA-CB-CG	7.60	132.77	115.30
2	D	11	LEU	CB-CG-CD2	7.13	123.12	111.00

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	855	ILE	Peptide
1	A	856	SER	Peptide
2	B	101	THR	Peptide
2	B	11	LEU	Mainchain
2	B	188	ALA	Peptide

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	7951	0	7901	119	0
1	C	7951	0	7901	130	0
2	B	1829	0	1829	103	0
2	D	1829	0	1829	117	0
3	A	10	0	0	0	0
3	C	10	0	0	0	0
4	A	15	0	17	2	0
4	C	15	0	17	1	0
5	A	121	0	0	8	0
5	B	10	0	0	0	0
5	C	114	0	0	7	0
5	D	12	0	0	0	0
All	All	19867	0	19494	451	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 12.

The worst 5 of 451 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:669:ASN:HD21	1:C:742:LYS:CE	1.15	1.59
2:D:11:LEU:HD22	2:D:15:LYS:NZ	1.22	1.40
1:C:669:ASN:ND2	1:C:742:LYS:CE	1.94	1.28
2:D:11:LEU:CD2	2:D:15:LYS:HZ2	1.51	1.23
1:C:789:SER:CB	1:C:812:LYS:O	1.89	1.21

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	990/1028 (96%)	943 (95%)	44 (4%)	3 (0%)	41 66
1	C	990/1028 (96%)	942 (95%)	45 (4%)	3 (0%)	41 66
2	B	227/325 (70%)	211 (93%)	13 (6%)	3 (1%)	12 30
2	D	227/325 (70%)	206 (91%)	16 (7%)	5 (2%)	6 17
All	All	2434/2706 (90%)	2302 (95%)	118 (5%)	14 (1%)	25 50

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	610	GLY
1	A	856	SER
2	B	211	SER
1	C	610	GLY
1	C	730	ALA

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	900/927 (97%)	883 (98%)	17 (2%)	57	82
1	C	900/927 (97%)	878 (98%)	22 (2%)	49	77
2	B	203/289 (70%)	195 (96%)	8 (4%)	32	61
2	D	203/289 (70%)	196 (97%)	7 (3%)	37	66
All	All	2206/2432 (91%)	2152 (98%)	54 (2%)	49	77

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	259	SER
1	C	365	LEU
2	D	38	PHE
1	C	13	VAL
1	C	133	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	673	ASN
1	C	696	ASN
2	D	102	HIS
1	C	678	HIS
1	C	722	HIS

5.3.3 RNA [i](#)

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](#)

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
3	SO4	C	1102	-	4,4,4	0.13	0	6,6,6	0.30	0
4	EPE	A	1103	-	15,15,15	0.84	1 (6%)	18,20,20	1.82	4 (22%)
4	EPE	C	1103	-	15,15,15	0.82	1 (6%)	18,20,20	2.08	5 (27%)
3	SO4	A	1101	-	4,4,4	0.23	0	6,6,6	0.40	0
3	SO4	C	1101	-	4,4,4	0.13	0	6,6,6	0.33	0
3	SO4	A	1102	-	4,4,4	0.30	0	6,6,6	0.37	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
4	EPE	A	1103	-	-	4/9/19/19	0/1/1/1
4	EPE	C	1103	-	-	2/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1103	EPE	C10-S	2.67	1.81	1.77
4	A	1103	EPE	C10-S	2.58	1.81	1.77

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1103	EPE	C5-N4-C3	5.17	120.46	108.83
4	A	1103	EPE	C5-N4-C3	4.63	119.25	108.83
4	C	1103	EPE	O3S-S-C10	3.63	111.64	105.77
4	A	1103	EPE	C7-N4-C5	3.50	120.19	111.23
4	C	1103	EPE	C7-N4-C3	3.28	119.62	111.23

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1103	EPE	C10-C9-N1-C2
4	A	1103	EPE	C8-C7-N4-C5
4	A	1103	EPE	S-C10-C9-N1
4	C	1103	EPE	C8-C7-N4-C5
4	C	1103	EPE	N4-C7-C8-O8

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1103	EPE	2	0
4	C	1103	EPE	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	998/1028 (97%)	0.12	7 (0%) 87 89	22, 39, 66, 96	0
1	C	998/1028 (97%)	0.14	10 (1%) 82 83	22, 39, 66, 94	0
2	B	231/325 (71%)	0.87	36 (15%) 2 1	27, 68, 96, 109	0
2	D	231/325 (71%)	0.92	38 (16%) 1 1	26, 68, 96, 106	0
All	All	2458/2706 (90%)	0.27	91 (3%) 41 41	22, 42, 83, 109	0

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	237	ILE	5.6
2	B	14	ARG	5.3
1	A	856	SER	4.9
2	D	257	CYS	4.9
2	D	235	LEU	4.8

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
4	EPE	C	1103	15/15	0.93	0.22	42,50,69,74	0
4	EPE	A	1103	15/15	0.95	0.21	41,50,63,69	0
3	SO4	A	1102	5/5	0.95	0.13	57,59,63,79	0
3	SO4	C	1102	5/5	0.96	0.15	57,59,65,71	0
3	SO4	C	1101	5/5	0.99	0.18	29,34,38,42	0
3	SO4	A	1101	5/5	0.99	0.16	31,36,39,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.