



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:53 PM UTC

PDB ID : 3LME / pdb_00003lme
Title : Structure of probable translation initiation inhibitor from (RPA2473) from Rhodopseudomonas palustris
Authors : Ramagopal, U.A.; Toro, R.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2010-01-29
Resolution : 2.74 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

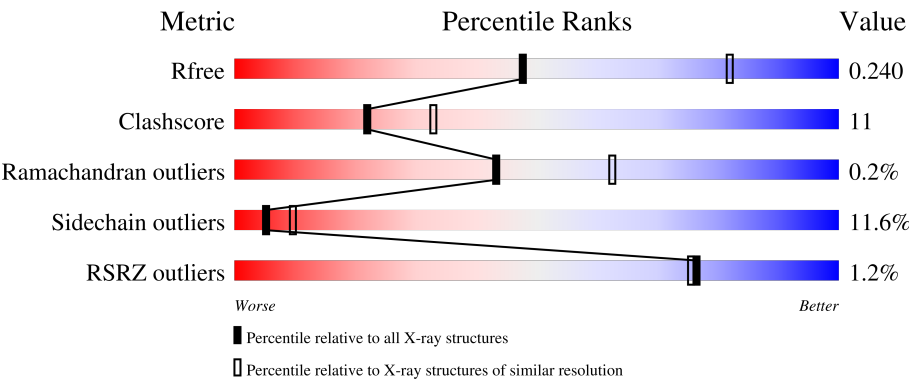
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.74 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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 $\leq 5\%$. 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	138	73%19%• 7%
1	B	138	% 70%17%6%• 7%
1	C	138	2% 62%27%• 8%
1	D	138	% 71%17%5%7%
1	E	138	% 74%14%5%7%

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Mol	Chain	Length	Quality of chain
1	F	138	
1	G	138	
1	H	138	
1	I	138	
1	J	138	
1	K	138	
1	L	138	

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	SO4	G	8	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11701 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 Possible translation initiation inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			970	614	169	183	4			
1	B	129	Total	C	N	O	S	0	0	0
			970	614	169	183	4			
1	C	127	Total	C	N	O	S	0	0	0
			958	606	167	181	4			
1	D	129	Total	C	N	O	S	0	0	0
			970	614	169	183	4			
1	E	129	Total	C	N	O	S	0	0	0
			970	614	169	183	4			
1	F	127	Total	C	N	O	S	0	0	0
			958	606	167	181	4			
1	G	129	Total	C	N	O	S	0	0	0
			970	614	169	183	4			
1	H	129	Total	C	N	O	S	0	0	0
			970	614	169	183	4			
1	I	128	Total	C	N	O	S	0	0	0
			965	611	168	182	4			
1	J	129	Total	C	N	O	S	0	0	0
			970	614	169	183	4			
1	K	129	Total	C	N	O	S	0	0	0
			970	614	169	183	4			
1	L	128	Total	C	N	O	S	0	0	0
			965	611	168	182	4			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	expression tag	UNP Q6N6Z0
A	28	SER	-	expression tag	UNP Q6N6Z0
A	29	LEU	-	expression tag	UNP Q6N6Z0
A	61	HIS	ARG	engineered mutation	UNP Q6N6Z0
A	157	GLU	-	expression tag	UNP Q6N6Z0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	158	GLY	-	expression tag	UNP Q6N6Z0
A	159	HIS	-	expression tag	UNP Q6N6Z0
A	160	HIS	-	expression tag	UNP Q6N6Z0
A	161	HIS	-	expression tag	UNP Q6N6Z0
A	162	HIS	-	expression tag	UNP Q6N6Z0
A	163	HIS	-	expression tag	UNP Q6N6Z0
A	164	HIS	-	expression tag	UNP Q6N6Z0
B	27	MET	-	expression tag	UNP Q6N6Z0
B	28	SER	-	expression tag	UNP Q6N6Z0
B	29	LEU	-	expression tag	UNP Q6N6Z0
B	61	HIS	ARG	engineered mutation	UNP Q6N6Z0
B	157	GLU	-	expression tag	UNP Q6N6Z0
B	158	GLY	-	expression tag	UNP Q6N6Z0
B	159	HIS	-	expression tag	UNP Q6N6Z0
B	160	HIS	-	expression tag	UNP Q6N6Z0
B	161	HIS	-	expression tag	UNP Q6N6Z0
B	162	HIS	-	expression tag	UNP Q6N6Z0
B	163	HIS	-	expression tag	UNP Q6N6Z0
B	164	HIS	-	expression tag	UNP Q6N6Z0
C	27	MET	-	expression tag	UNP Q6N6Z0
C	28	SER	-	expression tag	UNP Q6N6Z0
C	29	LEU	-	expression tag	UNP Q6N6Z0
C	61	HIS	ARG	engineered mutation	UNP Q6N6Z0
C	157	GLU	-	expression tag	UNP Q6N6Z0
C	158	GLY	-	expression tag	UNP Q6N6Z0
C	159	HIS	-	expression tag	UNP Q6N6Z0
C	160	HIS	-	expression tag	UNP Q6N6Z0
C	161	HIS	-	expression tag	UNP Q6N6Z0
C	162	HIS	-	expression tag	UNP Q6N6Z0
C	163	HIS	-	expression tag	UNP Q6N6Z0
C	164	HIS	-	expression tag	UNP Q6N6Z0
D	27	MET	-	expression tag	UNP Q6N6Z0
D	28	SER	-	expression tag	UNP Q6N6Z0
D	29	LEU	-	expression tag	UNP Q6N6Z0
D	61	HIS	ARG	engineered mutation	UNP Q6N6Z0
D	157	GLU	-	expression tag	UNP Q6N6Z0
D	158	GLY	-	expression tag	UNP Q6N6Z0
D	159	HIS	-	expression tag	UNP Q6N6Z0
D	160	HIS	-	expression tag	UNP Q6N6Z0
D	161	HIS	-	expression tag	UNP Q6N6Z0
D	162	HIS	-	expression tag	UNP Q6N6Z0
D	163	HIS	-	expression tag	UNP Q6N6Z0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	164	HIS	-	expression tag	UNP Q6N6Z0
E	27	MET	-	expression tag	UNP Q6N6Z0
E	28	SER	-	expression tag	UNP Q6N6Z0
E	29	LEU	-	expression tag	UNP Q6N6Z0
E	61	HIS	ARG	engineered mutation	UNP Q6N6Z0
E	157	GLU	-	expression tag	UNP Q6N6Z0
E	158	GLY	-	expression tag	UNP Q6N6Z0
E	159	HIS	-	expression tag	UNP Q6N6Z0
E	160	HIS	-	expression tag	UNP Q6N6Z0
E	161	HIS	-	expression tag	UNP Q6N6Z0
E	162	HIS	-	expression tag	UNP Q6N6Z0
E	163	HIS	-	expression tag	UNP Q6N6Z0
E	164	HIS	-	expression tag	UNP Q6N6Z0
F	27	MET	-	expression tag	UNP Q6N6Z0
F	28	SER	-	expression tag	UNP Q6N6Z0
F	29	LEU	-	expression tag	UNP Q6N6Z0
F	61	HIS	ARG	engineered mutation	UNP Q6N6Z0
F	157	GLU	-	expression tag	UNP Q6N6Z0
F	158	GLY	-	expression tag	UNP Q6N6Z0
F	159	HIS	-	expression tag	UNP Q6N6Z0
F	160	HIS	-	expression tag	UNP Q6N6Z0
F	161	HIS	-	expression tag	UNP Q6N6Z0
F	162	HIS	-	expression tag	UNP Q6N6Z0
F	163	HIS	-	expression tag	UNP Q6N6Z0
F	164	HIS	-	expression tag	UNP Q6N6Z0
G	27	MET	-	expression tag	UNP Q6N6Z0
G	28	SER	-	expression tag	UNP Q6N6Z0
G	29	LEU	-	expression tag	UNP Q6N6Z0
G	61	HIS	ARG	engineered mutation	UNP Q6N6Z0
G	157	GLU	-	expression tag	UNP Q6N6Z0
G	158	GLY	-	expression tag	UNP Q6N6Z0
G	159	HIS	-	expression tag	UNP Q6N6Z0
G	160	HIS	-	expression tag	UNP Q6N6Z0
G	161	HIS	-	expression tag	UNP Q6N6Z0
G	162	HIS	-	expression tag	UNP Q6N6Z0
G	163	HIS	-	expression tag	UNP Q6N6Z0
G	164	HIS	-	expression tag	UNP Q6N6Z0
H	27	MET	-	expression tag	UNP Q6N6Z0
H	28	SER	-	expression tag	UNP Q6N6Z0
H	29	LEU	-	expression tag	UNP Q6N6Z0
H	61	HIS	ARG	engineered mutation	UNP Q6N6Z0
H	157	GLU	-	expression tag	UNP Q6N6Z0

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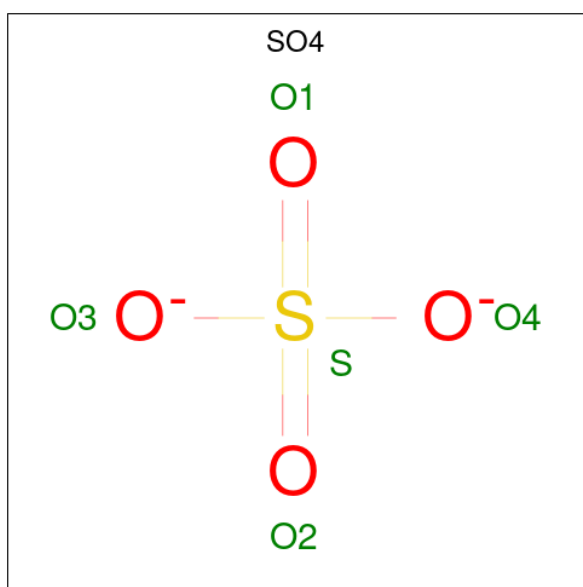
Chain	Residue	Modelled	Actual	Comment	Reference
H	158	GLY	-	expression tag	UNP Q6N6Z0
H	159	HIS	-	expression tag	UNP Q6N6Z0
H	160	HIS	-	expression tag	UNP Q6N6Z0
H	161	HIS	-	expression tag	UNP Q6N6Z0
H	162	HIS	-	expression tag	UNP Q6N6Z0
H	163	HIS	-	expression tag	UNP Q6N6Z0
H	164	HIS	-	expression tag	UNP Q6N6Z0
I	27	MET	-	expression tag	UNP Q6N6Z0
I	28	SER	-	expression tag	UNP Q6N6Z0
I	29	LEU	-	expression tag	UNP Q6N6Z0
I	61	HIS	ARG	engineered mutation	UNP Q6N6Z0
I	157	GLU	-	expression tag	UNP Q6N6Z0
I	158	GLY	-	expression tag	UNP Q6N6Z0
I	159	HIS	-	expression tag	UNP Q6N6Z0
I	160	HIS	-	expression tag	UNP Q6N6Z0
I	161	HIS	-	expression tag	UNP Q6N6Z0
I	162	HIS	-	expression tag	UNP Q6N6Z0
I	163	HIS	-	expression tag	UNP Q6N6Z0
I	164	HIS	-	expression tag	UNP Q6N6Z0
J	27	MET	-	expression tag	UNP Q6N6Z0
J	28	SER	-	expression tag	UNP Q6N6Z0
J	29	LEU	-	expression tag	UNP Q6N6Z0
J	61	HIS	ARG	engineered mutation	UNP Q6N6Z0
J	157	GLU	-	expression tag	UNP Q6N6Z0
J	158	GLY	-	expression tag	UNP Q6N6Z0
J	159	HIS	-	expression tag	UNP Q6N6Z0
J	160	HIS	-	expression tag	UNP Q6N6Z0
J	161	HIS	-	expression tag	UNP Q6N6Z0
J	162	HIS	-	expression tag	UNP Q6N6Z0
J	163	HIS	-	expression tag	UNP Q6N6Z0
J	164	HIS	-	expression tag	UNP Q6N6Z0
K	27	MET	-	expression tag	UNP Q6N6Z0
K	28	SER	-	expression tag	UNP Q6N6Z0
K	29	LEU	-	expression tag	UNP Q6N6Z0
K	61	HIS	ARG	engineered mutation	UNP Q6N6Z0
K	157	GLU	-	expression tag	UNP Q6N6Z0
K	158	GLY	-	expression tag	UNP Q6N6Z0
K	159	HIS	-	expression tag	UNP Q6N6Z0
K	160	HIS	-	expression tag	UNP Q6N6Z0
K	161	HIS	-	expression tag	UNP Q6N6Z0
K	162	HIS	-	expression tag	UNP Q6N6Z0
K	163	HIS	-	expression tag	UNP Q6N6Z0

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Chain	Residue	Modelled	Actual	Comment	Reference
K	164	HIS	-	expression tag	UNP Q6N6Z0
L	27	MET	-	expression tag	UNP Q6N6Z0
L	28	SER	-	expression tag	UNP Q6N6Z0
L	29	LEU	-	expression tag	UNP Q6N6Z0
L	61	HIS	ARG	engineered mutation	UNP Q6N6Z0
L	157	GLU	-	expression tag	UNP Q6N6Z0
L	158	GLY	-	expression tag	UNP Q6N6Z0
L	159	HIS	-	expression tag	UNP Q6N6Z0
L	160	HIS	-	expression tag	UNP Q6N6Z0
L	161	HIS	-	expression tag	UNP Q6N6Z0
L	162	HIS	-	expression tag	UNP Q6N6Z0
L	163	HIS	-	expression tag	UNP Q6N6Z0
L	164	HIS	-	expression tag	UNP Q6N6Z0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	C	2	Total	O	0	0
			2	2		
3	D	2	Total	O	0	0
			2	2		
3	E	1	Total	O	0	0
			1	1		
3	F	2	Total	O	0	0
			2	2		
3	G	2	Total	O	0	0
			2	2		
3	H	3	Total	O	0	0
			3	3		
3	I	3	Total	O	0	0
			3	3		
3	J	1	Total	O	0	0
			1	1		
3	K	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	1	Total	O	0	0
			1	1		

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.

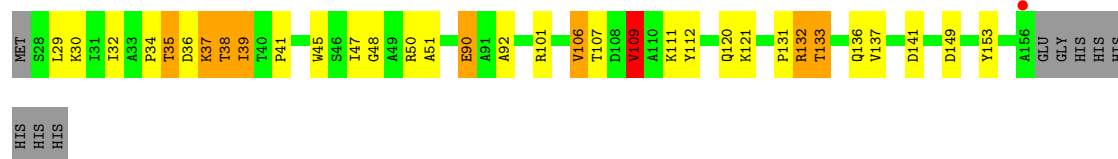
- Molecule 1: Possible translation initiation inhibitor

Chain A: 



- Molecule 1: Possible translation initiation inhibitor

Chain B: 



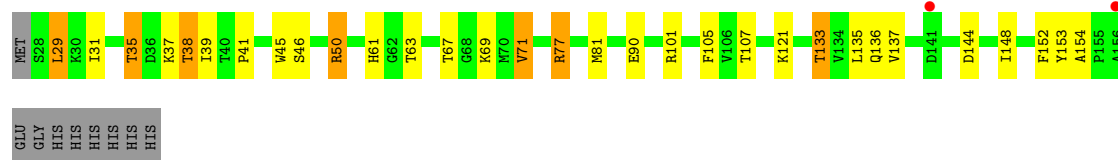
- Molecule 1: Possible translation initiation inhibitor

Chain C: 

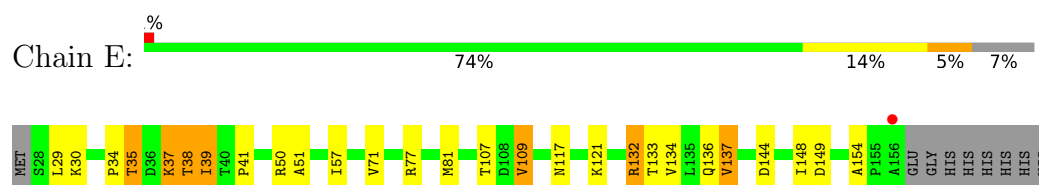


- Molecule 1: Possible translation initiation inhibitor

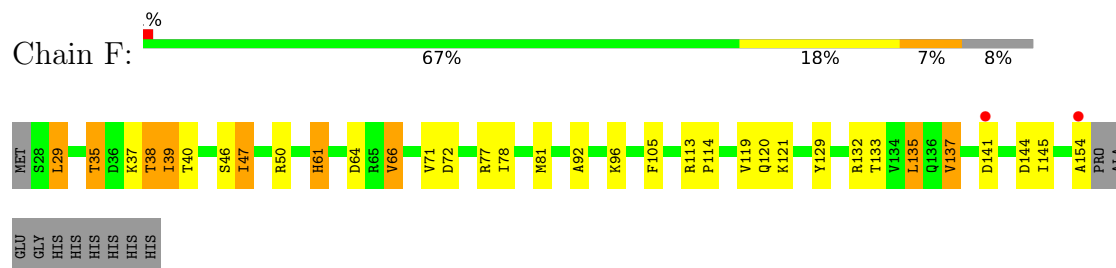
Chain D: 



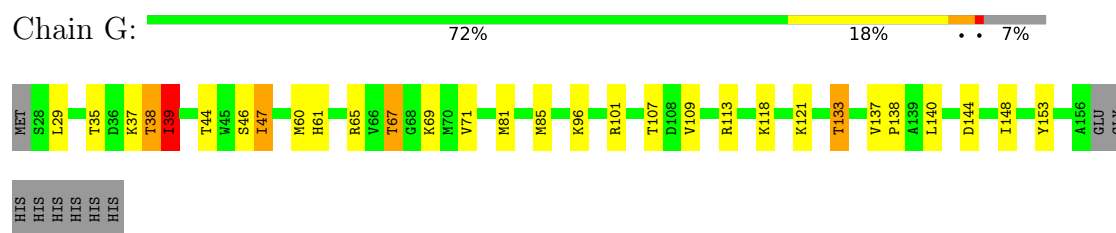
- Molecule 1: Possible translation initiation inhibitor



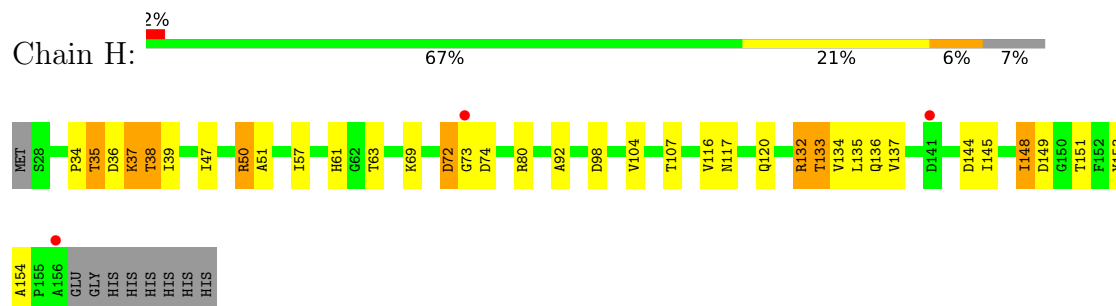
- Molecule 1: Possible translation initiation inhibitor



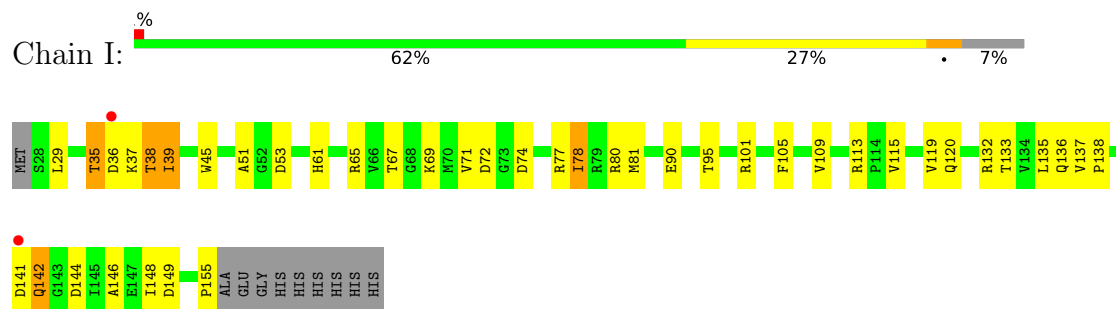
- Molecule 1: Possible translation initiation inhibitor



- Molecule 1: Possible translation initiation inhibitor



- Molecule 1: Possible translation initiation inhibitor

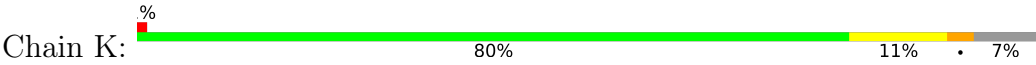


- Molecule 1: Possible translation initiation inhibitor

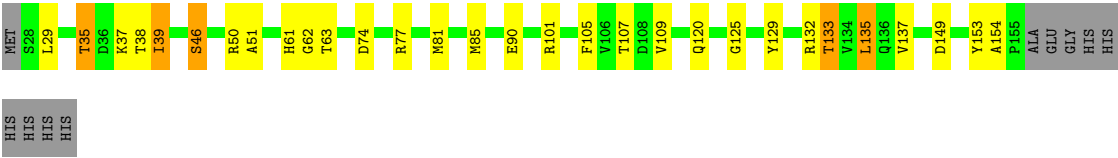




● Molecule 1: Possible translation initiation inhibitor



● Molecule 1: Possible translation initiation inhibitor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.19Å 142.24Å 147.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.19 – 2.74 49.19 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.19-2.74) 99.1 (49.19-2.74)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.37 (at 2.73Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.204 , 0.246 0.200 , 0.240	Depositor DCC
R_{free} test set	3111 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	61.1	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 15.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11701	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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, 0.333 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: 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	0.93	0/990	0.99	0/1346
1	B	0.87	0/990	1.01	2/1346 (0.1%)
1	C	0.81	0/977	1.06	3/1327 (0.2%)
1	D	0.88	0/990	1.03	0/1346
1	E	0.88	0/990	1.01	1/1346 (0.1%)
1	F	0.82	0/977	1.05	1/1327 (0.1%)
1	G	0.90	1/990 (0.1%)	1.02	1/1346 (0.1%)
1	H	0.86	0/990	1.02	1/1346 (0.1%)
1	I	0.77	0/985	0.99	0/1339
1	J	0.83	0/990	1.02	1/1346 (0.1%)
1	K	0.85	0/990	0.99	0/1346
1	L	0.87	0/985	1.09	2/1339 (0.1%)
All	All	0.86	1/11844 (0.0%)	1.02	12/16100 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	39	ILE	CA-CB	5.08	1.59	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	109	VAL	CB-CA-C	-5.87	104.22	112.14
1	C	112	TYR	N-CA-C	5.72	120.53	113.50
1	H	148	ILE	N-CA-C	5.63	115.99	108.27
1	B	112	TYR	N-CA-C	5.45	120.94	113.97
1	L	74	ASP	N-CA-C	5.31	116.75	111.07
1	J	72	ASP	N-CA-C	5.28	119.63	111.56
1	L	46	SER	CB-CA-C	-5.26	100.24	109.71
1	G	47	ILE	N-CA-CB	5.10	117.47	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	33	ALA	CA-C-N	5.07	126.18	119.84
1	C	33	ALA	C-N-CA	5.07	126.18	119.84
1	F	61	HIS	N-CA-C	5.06	116.36	109.18
1	E	109	VAL	N-CA-C	5.00	115.77	110.72

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	970	0	969	17	0
1	B	970	0	969	25	0
1	C	958	0	957	34	0
1	D	970	0	969	24	0
1	E	970	0	969	18	0
1	F	958	0	957	31	0
1	G	970	0	969	21	0
1	H	970	0	969	28	0
1	I	965	0	964	31	0
1	J	970	0	969	21	0
1	K	970	0	969	12	0
1	L	965	0	964	21	0
2	A	10	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	10	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	2	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	K	10	0	0	0	0
2	L	5	0	0	0	0
3	A	3	0	0	0	0
3	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	3	0	0	0	0
3	I	3	0	0	0	0
3	J	1	0	0	0	0
3	K	5	0	0	0	0
3	L	1	0	0	0	0
All	All	11701	0	11594	250	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 11.

All (250) 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:50:ARG:HH22	1:C:154:ALA:HB3	1.26	0.96
1:K:35:THR:HG22	1:K:37:LYS:H	1.27	0.95
1:F:35:THR:HG22	1:F:37:LYS:H	1.35	0.91
1:C:35:THR:HG22	1:C:37:LYS:H	1.34	0.90
1:H:38:THR:HG22	1:H:39:ILE:O	1.72	0.90
1:G:67:THR:HG22	1:G:69:LYS:H	1.39	0.88
1:L:120:GLN:NE2	1:L:132:ARG:HH21	1.74	0.86
1:I:35:THR:HG22	1:I:37:LYS:H	1.38	0.86
1:C:50:ARG:NH2	1:C:154:ALA:HB3	1.92	0.85
1:C:113:ARG:HG3	1:C:114:PRO:HD3	1.59	0.83
1:G:133:THR:HG21	1:H:149:ASP:OD1	1.79	0.82
1:D:35:THR:HG22	1:D:37:LYS:H	1.42	0.81
1:H:35:THR:HG22	1:H:37:LYS:H	1.44	0.80
1:F:50:ARG:HH22	1:F:154:ALA:HB3	1.47	0.79
1:B:109:VAL:HG22	1:B:136:GLN:HB2	1.66	0.77
1:A:35:THR:HG22	1:A:37:LYS:H	1.46	0.77
1:B:35:THR:HG22	1:B:37:LYS:H	1.48	0.76
1:C:50:ARG:HH22	1:C:154:ALA:CB	1.99	0.76
1:F:38:THR:HG22	1:F:39:ILE:O	1.87	0.75
1:G:35:THR:HG22	1:G:37:LYS:H	1.50	0.75
1:E:35:THR:HG22	1:E:37:LYS:H	1.49	0.75
1:A:103:THR:HG23	1:A:133:THR:HG23	1.72	0.72
1:D:136:GLN:O	1:E:137:VAL:HG22	1.91	0.71
1:L:50:ARG:NH2	1:L:154:ALA:O	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:HIS:HB2	1:D:144:ASP:OD2	1.90	0.70
1:G:67:THR:HG22	1:G:69:LYS:N	2.06	0.70
1:H:98:ASP:HB3	1:H:153:TYR:O	1.92	0.70
1:I:78:ILE:HG22	1:I:119:VAL:HG21	1.74	0.69
1:L:35:THR:HG22	1:L:37:LYS:H	1.56	0.69
1:C:65:ARG:HG3	1:C:65:ARG:HH11	1.58	0.69
1:A:113:ARG:HD3	1:B:141:ASP:OD1	1.93	0.68
1:I:35:THR:CG2	1:I:37:LYS:H	2.05	0.68
1:C:35:THR:HB	1:C:38:THR:HB	1.75	0.68
1:I:120:GLN:NE2	1:I:132:ARG:HH21	1.91	0.68
1:B:109:VAL:CG2	1:B:136:GLN:HB2	2.23	0.67
1:D:46:SER:HB2	1:F:129:TYR:O	1.96	0.66
1:F:39:ILE:HG22	1:F:40:THR:N	2.10	0.66
1:I:38:THR:CG2	1:I:39:ILE:N	2.58	0.66
1:I:38:THR:HG23	1:I:39:ILE:N	2.11	0.66
1:J:65:ARG:HH12	1:J:66:VAL:HG22	1.60	0.66
1:L:35:THR:CG2	1:L:37:LYS:H	2.08	0.66
1:J:149:ASP:OD2	1:L:133:THR:HG21	1.95	0.66
1:A:138:PRO:HD2	1:C:136:GLN:O	1.95	0.65
1:D:67:THR:HG21	1:D:69:LYS:HB2	1.79	0.65
1:C:113:ARG:HG3	1:C:114:PRO:CD	2.27	0.65
1:C:32:ILE:HG22	1:C:47:ILE:HD11	1.78	0.65
1:F:39:ILE:HG22	1:F:40:THR:H	1.62	0.64
1:A:50:ARG:NH2	1:A:154:ALA:O	2.29	0.63
1:I:120:GLN:HE22	1:I:132:ARG:HH21	1.47	0.63
1:D:38:THR:HG23	1:D:39:ILE:O	1.97	0.63
1:F:38:THR:CG2	1:F:39:ILE:N	2.62	0.63
1:D:61:HIS:HA	1:D:81:MET:HG3	1.80	0.62
1:I:71:VAL:HG21	1:I:80:ARG:HG2	1.81	0.62
1:E:117:ASN:OD1	1:E:132:ARG:NH2	2.32	0.62
1:G:101:ARG:NH2	1:H:57:ILE:O	2.33	0.61
1:F:61:HIS:HA	1:F:81:MET:HG3	1.81	0.61
1:F:120:GLN:NE2	1:F:132:ARG:HH21	1.99	0.61
1:A:153:TYR:CG	1:B:51:ALA:HB1	2.36	0.61
1:G:38:THR:HG22	1:G:39:ILE:O	2.01	0.60
1:L:62:GLY:HA3	1:L:77:ARG:HG3	1.82	0.60
1:D:31:ILE:HG23	1:D:46:SER:OG	2.00	0.60
1:J:38:THR:HG22	1:J:39:ILE:O	2.02	0.60
1:H:38:THR:HG21	1:H:47:ILE:HD13	1.84	0.60
1:L:120:GLN:NE2	1:L:132:ARG:NH2	2.47	0.60
1:B:35:THR:CG2	1:B:37:LYS:H	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:133:THR:HG21	1:H:149:ASP:CG	2.26	0.59
1:G:138:PRO:HD2	1:I:136:GLN:O	2.03	0.59
1:D:67:THR:HG22	1:D:69:LYS:HG3	1.84	0.59
1:C:36:ASP:O	1:C:65:ARG:NE	2.35	0.59
1:C:32:ILE:CG2	1:C:47:ILE:HD11	2.32	0.59
1:I:38:THR:HG22	1:I:39:ILE:O	2.02	0.59
1:G:113:ARG:NH1	2:G:8:SO4:O3	2.36	0.58
1:F:35:THR:CG2	1:F:37:LYS:H	2.14	0.58
1:I:141:ASP:O	1:I:142:GLN:HG2	2.03	0.58
1:G:38:THR:HG21	1:G:47:ILE:HD13	1.85	0.57
1:F:120:GLN:HE22	1:F:132:ARG:HD3	1.70	0.57
1:L:120:GLN:HE21	1:L:132:ARG:HH21	1.51	0.57
1:F:38:THR:HG21	1:F:47:ILE:HD12	1.86	0.57
1:D:38:THR:CG2	1:D:39:ILE:O	2.53	0.56
1:H:117:ASN:OD1	1:H:132:ARG:NH2	2.32	0.56
1:H:38:THR:CG2	1:H:47:ILE:HD13	2.35	0.56
1:F:39:ILE:CG2	1:F:40:THR:H	2.19	0.56
1:I:67:THR:CB	1:I:69:LYS:HG2	2.35	0.56
1:I:67:THR:OG1	1:I:69:LYS:HG2	2.04	0.56
1:G:67:THR:CG2	1:G:69:LYS:HG2	2.35	0.56
1:I:38:THR:HG23	1:I:39:ILE:H	1.69	0.56
1:K:129:TYR:O	1:L:46:SER:OG	2.23	0.55
1:F:35:THR:HG22	1:F:37:LYS:N	2.15	0.55
1:H:38:THR:CG2	1:H:39:ILE:O	2.51	0.55
1:F:50:ARG:NH2	1:F:154:ALA:HB3	2.17	0.55
1:I:67:THR:HB	1:I:69:LYS:HG2	1.89	0.55
1:J:144:ASP:OD1	1:J:145:ILE:N	2.32	0.54
1:C:78:ILE:HG22	1:C:119:VAL:HG21	1.88	0.54
1:J:118:LYS:HE2	1:J:122:ASP:OD2	2.07	0.54
1:L:120:GLN:HE21	1:L:132:ARG:NH2	2.05	0.54
1:C:35:THR:HG22	1:C:37:LYS:N	2.12	0.54
1:D:29:LEU:HD12	1:D:29:LEU:C	2.33	0.54
1:I:35:THR:HG22	1:I:37:LYS:N	2.17	0.54
1:D:31:ILE:CG2	1:D:46:SER:OG	2.56	0.54
1:F:113:ARG:N	1:F:114:PRO:HD2	2.23	0.54
1:G:113:ARG:NH2	2:G:8:SO4:O1	2.26	0.54
1:D:61:HIS:CD2	1:D:63:THR:HG23	2.43	0.53
1:A:50:ARG:NH1	1:A:92:ALA:O	2.41	0.53
1:J:153:TYR:CG	1:K:51:ALA:HB1	2.44	0.53
1:K:141:ASP:O	1:K:142:GLN:HB3	2.09	0.53
1:A:48:GLY:HA2	1:C:131:PRO:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:29:LEU:C	1:G:29:LEU:HD12	2.35	0.52
1:G:61:HIS:HB2	1:G:144:ASP:OD2	2.10	0.52
1:J:65:ARG:NH1	1:J:66:VAL:HG22	2.23	0.52
1:D:67:THR:CG2	1:D:69:LYS:HB2	2.39	0.52
1:L:120:GLN:HE22	1:L:132:ARG:HH21	1.51	0.52
1:F:50:ARG:NH1	1:F:92:ALA:O	2.43	0.52
1:J:35:THR:HG22	1:J:37:LYS:H	1.75	0.51
1:K:35:THR:HG22	1:K:37:LYS:N	2.11	0.51
1:A:60:MET:HG3	1:A:85:MET:HA	1.92	0.51
1:I:109:VAL:HG22	1:I:113:ARG:HH11	1.75	0.51
1:G:153:TYR:CG	1:H:51:ALA:HB1	2.45	0.51
1:C:38:THR:CG2	1:C:39:ILE:O	2.59	0.51
1:K:141:ASP:O	1:K:142:GLN:CB	2.58	0.51
1:L:39:ILE:HD11	1:L:63:THR:OG1	2.11	0.51
1:H:50:ARG:NH2	1:H:154:ALA:O	2.40	0.51
1:K:29:LEU:HD12	1:K:29:LEU:C	2.35	0.51
1:E:38:THR:CG2	1:E:39:ILE:O	2.59	0.50
1:B:120:GLN:HE22	1:B:132:ARG:HE	1.60	0.50
1:K:132:ARG:HG2	1:K:133:THR:N	2.25	0.50
1:E:34:PRO:HA	1:E:38:THR:HG21	1.93	0.50
1:F:29:LEU:HD12	1:F:29:LEU:C	2.36	0.50
1:F:144:ASP:OD1	1:F:145:ILE:N	2.43	0.50
1:F:120:GLN:HE22	1:F:132:ARG:HH21	1.58	0.50
1:D:101:ARG:NH1	1:E:57:ILE:O	2.45	0.50
1:E:35:THR:CG2	1:E:37:LYS:H	2.22	0.49
1:A:38:THR:CG2	1:A:39:ILE:O	2.61	0.49
1:E:38:THR:HG22	1:E:39:ILE:O	2.12	0.49
1:K:133:THR:HG21	1:L:149:ASP:OD2	2.12	0.49
1:C:36:ASP:HA	1:C:65:ARG:HH21	1.78	0.48
1:C:71:VAL:HG21	1:C:80:ARG:HH11	1.77	0.48
1:E:132:ARG:HD3	1:E:134:VAL:HG23	1.94	0.48
1:I:29:LEU:HD12	1:I:29:LEU:C	2.37	0.48
1:J:38:THR:CG2	1:J:39:ILE:O	2.61	0.48
1:D:152:PHE:N	1:D:152:PHE:CD1	2.82	0.48
1:J:38:THR:HG23	1:J:39:ILE:N	2.28	0.48
1:D:35:THR:CG2	1:D:37:LYS:H	2.21	0.48
1:I:35:THR:HB	1:I:38:THR:HB	1.95	0.48
1:I:105:PHE:O	1:I:146:ALA:HA	2.14	0.48
1:D:105:PHE:CE1	1:D:135:LEU:HD12	2.48	0.48
1:E:50:ARG:NH2	1:E:154:ALA:O	2.46	0.48
1:I:77:ARG:HD3	1:I:144:ASP:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:ILE:CG2	1:F:40:THR:N	2.72	0.48
1:H:34:PRO:HA	1:H:38:THR:HG21	1.96	0.48
1:F:38:THR:HG23	1:F:39:ILE:N	2.29	0.47
1:B:101:ARG:HG3	1:B:101:ARG:HH11	1.79	0.47
1:A:140:LEU:O	1:A:141:ASP:C	2.57	0.47
1:D:133:THR:HG21	1:E:149:ASP:OD1	2.15	0.47
1:J:35:THR:CG2	1:J:37:LYS:H	2.28	0.47
1:C:120:GLN:NE2	1:C:132:ARG:HH21	2.13	0.47
1:J:141:ASP:O	1:J:142:GLN:HB2	2.14	0.47
1:G:65:ARG:CZ	1:G:65:ARG:HB3	2.45	0.47
1:J:65:ARG:HH11	1:J:65:ARG:HB3	1.80	0.46
1:B:90:GLU:C	1:B:92:ALA:H	2.22	0.46
1:F:71:VAL:HG12	1:F:72:ASP:O	2.15	0.46
1:H:104:VAL:HG22	1:H:148:ILE:HG13	1.97	0.46
1:C:55:VAL:HB	1:C:152:PHE:HB2	1.96	0.46
1:D:41:PRO:HA	1:D:45:TRP:CH2	2.50	0.46
1:J:41:PRO:HA	1:J:45:TRP:CH2	2.51	0.46
1:H:35:THR:H	1:H:38:THR:HB	1.81	0.46
1:D:71:VAL:O	1:D:77:ARG:HD3	2.16	0.46
1:E:35:THR:HG22	1:E:37:LYS:N	2.26	0.46
1:H:133:THR:HG21	1:I:149:ASP:OD1	2.15	0.46
1:B:109:VAL:HG23	1:B:136:GLN:OE1	2.15	0.46
1:E:29:LEU:C	1:E:29:LEU:HD12	2.41	0.46
1:J:36:ASP:O	1:J:65:ARG:NE	2.49	0.46
1:F:77:ARG:HH11	1:F:145:ILE:HG12	1.80	0.46
1:B:38:THR:HG23	1:B:39:ILE:N	2.31	0.45
1:C:74:ASP:O	1:C:75:GLU:C	2.57	0.45
1:B:133:THR:HG21	1:C:149:ASP:CG	2.41	0.45
1:F:105:PHE:CE1	1:F:135:LEU:HD12	2.50	0.45
1:A:133:THR:HG21	1:B:149:ASP:OD2	2.17	0.45
1:C:38:THR:HG23	1:C:39:ILE:N	2.31	0.45
1:E:77:ARG:HD3	1:E:144:ASP:OD1	2.16	0.45
1:H:153:TYR:CG	1:I:51:ALA:HB1	2.52	0.45
1:I:61:HIS:HB3	1:I:144:ASP:OD2	2.17	0.45
1:D:81:MET:HG2	1:D:148:ILE:HG22	1.99	0.45
1:L:125:GLY:O	1:L:129:TYR:OH	2.33	0.45
1:C:40:THR:HA	1:C:41:PRO:HD2	1.89	0.44
1:L:29:LEU:C	1:L:29:LEU:HD12	2.42	0.44
1:C:85:MET:HE3	1:C:152:PHE:HZ	1.82	0.44
1:I:81:MET:HG2	1:I:148:ILE:HG22	1.99	0.44
1:D:50:ARG:NH2	1:D:154:ALA:O	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:TYR:CG	1:E:51:ALA:HB1	2.53	0.44
1:G:38:THR:CG2	1:G:47:ILE:HD13	2.47	0.44
1:L:105:PHE:CE1	1:L:135:LEU:HD12	2.52	0.44
1:J:104:VAL:HG22	1:J:148:ILE:HG13	1.99	0.44
1:B:90:GLU:C	1:B:92:ALA:N	2.71	0.44
1:C:29:LEU:C	1:C:29:LEU:HD12	2.43	0.44
1:G:101:ARG:NH1	1:H:151:THR:OG1	2.51	0.44
1:H:132:ARG:HD3	1:H:134:VAL:HG23	1.99	0.44
1:B:32:ILE:HG22	1:B:47:ILE:HD11	1.98	0.44
1:E:136:GLN:O	1:F:137:VAL:HG22	2.18	0.44
1:A:113:ARG:N	1:A:114:PRO:HD2	2.33	0.43
1:E:81:MET:HG2	1:E:148:ILE:HG22	2.00	0.43
1:F:38:THR:HG21	1:F:47:ILE:CD1	2.48	0.43
1:H:35:THR:CG2	1:H:37:LYS:H	2.23	0.43
1:L:61:HIS:HA	1:L:81:MET:HG3	2.00	0.43
1:C:80:ARG:HD2	1:C:80:ARG:HA	1.72	0.43
1:B:133:THR:HG21	1:C:149:ASP:OD1	2.19	0.43
1:B:34:PRO:HA	1:B:38:THR:HG21	2.01	0.43
1:B:41:PRO:HA	1:B:45:TRP:CH2	2.53	0.43
1:G:60:MET:HG3	1:G:85:MET:HA	2.00	0.43
1:C:34:PRO:HA	1:C:38:THR:HG21	2.01	0.43
1:E:34:PRO:HG3	1:E:41:PRO:HD2	2.01	0.43
1:F:38:THR:CG2	1:F:47:ILE:HD12	2.47	0.43
1:K:113:ARG:HB3	1:K:114:PRO:HD3	2.01	0.43
1:B:120:GLN:HE21	1:B:132:ARG:HH21	1.67	0.43
1:G:38:THR:CG2	1:G:39:ILE:O	2.66	0.43
1:F:38:THR:HG22	1:F:39:ILE:N	2.34	0.42
1:J:71:VAL:CG1	1:J:72:ASP:N	2.82	0.42
1:K:153:TYR:CG	1:L:51:ALA:HB1	2.54	0.42
1:A:38:THR:HG22	1:A:39:ILE:O	2.19	0.42
1:C:38:THR:HG23	1:C:39:ILE:O	2.19	0.42
1:F:78:ILE:HG22	1:F:119:VAL:HG21	2.01	0.42
1:J:65:ARG:NH1	1:J:66:VAL:CG2	2.81	0.42
1:H:50:ARG:NH1	1:H:92:ALA:O	2.53	0.42
1:L:85:MET:HE2	1:L:85:MET:HB3	1.93	0.42
1:H:136:GLN:HG2	1:I:138:PRO:HG2	2.01	0.42
1:I:78:ILE:CG2	1:I:119:VAL:HG21	2.48	0.42
1:I:115:VAL:O	1:I:119:VAL:HG23	2.20	0.42
1:B:106:VAL:O	1:B:136:GLN:HA	2.20	0.41
1:I:39:ILE:HD13	1:I:65:ARG:HA	2.01	0.41
1:B:38:THR:CG2	1:B:39:ILE:N	2.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ALA:HB2	1:C:100:VAL:HG11	2.01	0.41
1:B:131:PRO:HG3	1:C:48:GLY:HA2	2.01	0.41
1:B:153:TYR:CG	1:C:51:ALA:HB1	2.55	0.41
1:J:51:ALA:HB1	1:L:153:TYR:CG	2.55	0.41
1:J:35:THR:HG22	1:J:37:LYS:N	2.35	0.41
1:A:35:THR:CG2	1:A:36:ASP:N	2.84	0.41
1:G:81:MET:HG2	1:G:148:ILE:HG22	2.03	0.41
1:H:38:THR:CG2	1:H:39:ILE:N	2.83	0.41
1:H:72:ASP:HA	1:H:73:GLY:HA2	1.87	0.41
1:L:101:ARG:HG3	1:L:101:ARG:HH21	1.86	0.41
1:H:61:HIS:HD2	1:H:63:THR:HG23	1.85	0.41
1:H:116:VAL:O	1:H:120:GLN:HG3	2.21	0.41
1:H:132:ARG:HG2	1:I:45:TRP:HB3	2.03	0.41
1:C:57:ILE:HG22	1:C:58:GLY:O	2.21	0.40
1:K:34:PRO:HA	1:K:38:THR:HG21	2.04	0.40
1:F:64:ASP:OD1	1:F:66:VAL:HG12	2.20	0.40
1:A:131:PRO:HG3	1:B:48:GLY:HA2	2.04	0.40
1:H:144:ASP:OD1	1:H:145:ILE:N	2.50	0.40
1:B:35:THR:HB	1:B:38:THR:HB	2.02	0.40
1:I:53:ASP:OD1	1:I:155:PRO:HB3	2.22	0.40
1:J:127:GLY:HA2	1:J:128:PRO:C	2.46	0.40

There are no symmetry-related clashes.

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	
1	A	127/138 (92%)	123 (97%)	4 (3%)	0	100	100
1	B	127/138 (92%)	124 (98%)	3 (2%)	0	100	100
1	C	125/138 (91%)	119 (95%)	6 (5%)	0	100	100
1	D	127/138 (92%)	121 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	127/138 (92%)	120 (94%)	7 (6%)	0	100	100
1	F	125/138 (91%)	117 (94%)	7 (6%)	1 (1%)	16	29
1	G	127/138 (92%)	124 (98%)	3 (2%)	0	100	100
1	H	127/138 (92%)	123 (97%)	3 (2%)	1 (1%)	16	29
1	I	126/138 (91%)	119 (94%)	6 (5%)	1 (1%)	16	29
1	J	127/138 (92%)	119 (94%)	8 (6%)	0	100	100
1	K	127/138 (92%)	124 (98%)	3 (2%)	0	100	100
1	L	126/138 (91%)	120 (95%)	6 (5%)	0	100	100
All	All	1518/1656 (92%)	1453 (96%)	62 (4%)	3 (0%)	43	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	141	ASP
1	H	74	ASP
1	I	74	ASP

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	99/107 (92%)	90 (91%)	9 (9%)	9	16
1	B	99/107 (92%)	82 (83%)	17 (17%)	2	2
1	C	98/107 (92%)	88 (90%)	10 (10%)	7	13
1	D	99/107 (92%)	88 (89%)	11 (11%)	6	11
1	E	99/107 (92%)	87 (88%)	12 (12%)	5	8
1	F	98/107 (92%)	86 (88%)	12 (12%)	5	8
1	G	99/107 (92%)	85 (86%)	14 (14%)	3	5
1	H	99/107 (92%)	86 (87%)	13 (13%)	4	6
1	I	99/107 (92%)	86 (87%)	13 (13%)	4	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	99/107 (92%)	91 (92%)	8 (8%)	11	20
1	K	99/107 (92%)	90 (91%)	9 (9%)	9	16
1	L	99/107 (92%)	90 (91%)	9 (9%)	9	16
All	All	1186/1284 (92%)	1049 (88%)	137 (12%)	5	10

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	THR
1	A	38	THR
1	A	46	SER
1	A	71	VAL
1	A	77	ARG
1	A	107	THR
1	A	118	LYS
1	A	135	LEU
1	A	137	VAL
1	B	29	LEU
1	B	30	LYS
1	B	35	THR
1	B	36	ASP
1	B	37	LYS
1	B	38	THR
1	B	39	ILE
1	B	50	ARG
1	B	90	GLU
1	B	106	VAL
1	B	107	THR
1	B	109	VAL
1	B	111	LYS
1	B	121	LYS
1	B	132	ARG
1	B	133	THR
1	B	137	VAL
1	C	37	LYS
1	C	38	THR
1	C	39	ILE
1	C	65	ARG
1	C	67	THR
1	C	71	VAL
1	C	96	LYS

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Mol	Chain	Res	Type
1	C	107	THR
1	C	133	THR
1	C	137	VAL
1	D	29	LEU
1	D	35	THR
1	D	38	THR
1	D	50	ARG
1	D	71	VAL
1	D	77	ARG
1	D	90	GLU
1	D	107	THR
1	D	121	LYS
1	D	133	THR
1	D	137	VAL
1	E	30	LYS
1	E	35	THR
1	E	37	LYS
1	E	38	THR
1	E	39	ILE
1	E	71	VAL
1	E	107	THR
1	E	109	VAL
1	E	121	LYS
1	E	132	ARG
1	E	133	THR
1	E	137	VAL
1	F	29	LEU
1	F	35	THR
1	F	38	THR
1	F	39	ILE
1	F	46	SER
1	F	47	ILE
1	F	66	VAL
1	F	96	LYS
1	F	121	LYS
1	F	133	THR
1	F	135	LEU
1	F	137	VAL
1	G	38	THR
1	G	39	ILE
1	G	44	THR
1	G	46	SER

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Mol	Chain	Res	Type
1	G	67	THR
1	G	71	VAL
1	G	96	LYS
1	G	107	THR
1	G	109	VAL
1	G	118	LYS
1	G	121	LYS
1	G	133	THR
1	G	137	VAL
1	G	140	LEU
1	H	35	THR
1	H	36	ASP
1	H	37	LYS
1	H	38	THR
1	H	50	ARG
1	H	69	LYS
1	H	72	ASP
1	H	80	ARG
1	H	107	THR
1	H	132	ARG
1	H	133	THR
1	H	135	LEU
1	H	137	VAL
1	I	35	THR
1	I	36	ASP
1	I	38	THR
1	I	39	ILE
1	I	72	ASP
1	I	78	ILE
1	I	90	GLU
1	I	95	THR
1	I	101	ARG
1	I	133	THR
1	I	135	LEU
1	I	137	VAL
1	I	142	GLN
1	J	35	THR
1	J	38	THR
1	J	47	ILE
1	J	65	ARG
1	J	75	GLU
1	J	118	LYS

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Mol	Chain	Res	Type
1	J	133	THR
1	J	137	VAL
1	K	35	THR
1	K	37	LYS
1	K	38	THR
1	K	39	ILE
1	K	101	ARG
1	K	107	THR
1	K	133	THR
1	K	135	LEU
1	K	137	VAL
1	L	35	THR
1	L	38	THR
1	L	39	ILE
1	L	90	GLU
1	L	107	THR
1	L	109	VAL
1	L	133	THR
1	L	135	LEU
1	L	137	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	B	84	ASN
1	B	120	GLN
1	C	61	HIS
1	C	84	ASN
1	C	120	GLN
1	C	142	GLN
1	D	61	HIS
1	D	84	ASN
1	E	84	ASN
1	E	120	GLN
1	F	84	ASN
1	F	120	GLN
1	G	61	HIS
1	G	84	ASN
1	H	61	HIS
1	H	84	ASN
1	H	120	GLN

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Mol	Chain	Res	Type
1	I	84	ASN
1	I	120	GLN
1	I	142	GLN
1	J	84	ASN
1	K	61	HIS
1	K	84	ASN
1	L	84	ASN
1	L	120	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	SO4	I	10	-	4,4,4	0.33	0	6,6,6	0.33	0
2	SO4	K	14	-	4,4,4	0.31	0	6,6,6	0.27	0
2	SO4	A	1	-	4,4,4	0.38	0	6,6,6	0.56	0
2	SO4	J	11	-	4,4,4	0.24	0	6,6,6	0.49	0
2	SO4	D	5	-	4,4,4	0.38	0	6,6,6	0.41	0
2	SO4	K	12	-	4,4,4	0.30	0	6,6,6	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	E	6	-	4,4,4	0.23	0	6,6,6	0.21	0
2	SO4	F	7	-	4,4,4	0.24	0	6,6,6	0.25	0
2	SO4	A	15	-	4,4,4	0.37	0	6,6,6	0.17	0
2	SO4	H	9	-	4,4,4	0.39	0	6,6,6	0.61	0
2	SO4	C	3	-	4,4,4	0.30	0	6,6,6	0.15	0
2	SO4	G	8	-	4,4,4	0.28	0	6,6,6	0.43	0
2	SO4	L	13	-	4,4,4	0.29	0	6,6,6	0.51	0
2	SO4	E	4	-	4,4,4	0.24	0	6,6,6	0.42	0

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	8	SO4	2	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

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	129/138 (93%)	-0.30	0 100 100	37, 50, 61, 69	0
1	B	129/138 (93%)	-0.17	1 (0%) 82 82	38, 53, 71, 78	0
1	C	127/138 (92%)	0.07	3 (2%) 59 56	46, 61, 76, 80	0
1	D	129/138 (93%)	-0.12	2 (1%) 70 68	39, 53, 67, 78	0
1	E	129/138 (93%)	-0.11	1 (0%) 82 82	42, 56, 71, 76	0
1	F	127/138 (92%)	0.14	2 (1%) 70 68	48, 64, 78, 81	0
1	G	129/138 (93%)	-0.27	0 100 100	38, 51, 64, 71	0
1	H	129/138 (93%)	-0.11	3 (2%) 61 58	41, 56, 70, 73	0
1	I	128/138 (92%)	0.08	2 (1%) 70 68	43, 61, 73, 79	0
1	J	129/138 (93%)	-0.01	2 (1%) 70 68	46, 58, 80, 84	0
1	K	129/138 (93%)	-0.14	2 (1%) 70 68	41, 53, 66, 77	0
1	L	128/138 (92%)	-0.19	0 100 100	39, 50, 66, 69	0
All	All	1542/1656 (93%)	-0.09	18 (1%) 76 75	37, 56, 73, 84	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	154	ALA	3.9
1	B	156	ALA	3.4
1	F	154	ALA	3.0
1	K	156	ALA	2.9
1	F	141	ASP	2.8
1	J	156	ALA	2.7
1	K	141	ASP	2.6
1	D	156	ALA	2.6
1	C	141	ASP	2.6
1	H	141	ASP	2.6
1	J	141	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	156	ALA	2.5
1	I	141	ASP	2.5
1	H	73	GLY	2.4
1	I	36	ASP	2.3
1	D	141	ASP	2.2
1	E	156	ALA	2.1
1	C	61	HIS	2.0

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 oligosaccharides 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(Å ²)	Q<0.9
2	SO4	A	15	5/5	0.59	0.32	52,53,54,55	5
2	SO4	H	9	5/5	0.70	0.19	88,89,90,91	0
2	SO4	A	1	5/5	0.86	0.10	76,79,79,80	0
2	SO4	F	7	5/5	0.87	0.10	83,83,84,85	0
2	SO4	K	14	5/5	0.88	0.13	80,81,81,82	0
2	SO4	J	11	5/5	0.89	0.10	80,81,82,82	0
2	SO4	G	8	5/5	0.91	0.10	80,80,81,81	0
2	SO4	I	10	5/5	0.91	0.12	72,74,75,77	0
2	SO4	L	13	5/5	0.91	0.08	75,76,76,76	0
2	SO4	E	6	5/5	0.94	0.08	72,73,74,76	0
2	SO4	D	5	5/5	0.94	0.08	68,68,69,70	0
2	SO4	C	3	5/5	0.95	0.06	74,75,75,76	0
2	SO4	E	4	5/5	0.97	0.08	54,56,56,57	0
2	SO4	K	12	5/5	0.97	0.06	55,55,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.