



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:33 PM GMT

PDB ID : 1KOG
Title : Crystal structure of E. coli threonyl-tRNA synthetase interacting with the essential domain of its mRNA operator
Authors : Torres-Larrios, A.; Dock-Bregeon, A.C.; Romby, P.; Rees, B.; Sankaranarayanan, R.; Caillet, J.; Springer, M.; Ehresmann, C.; Ehresmann, B.; Moras, D.
Deposited on : 2001-12-20
Resolution : 3.50 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

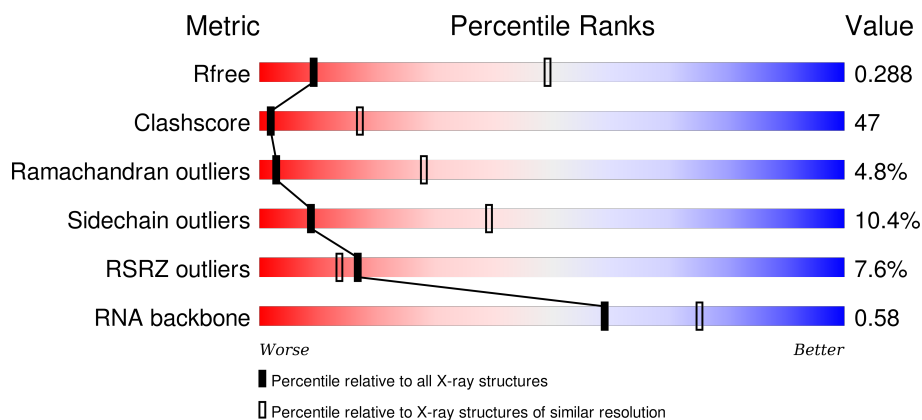
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)
RNA backbone	2183	1050 (4.20-2.80)

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. 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	I	37	<div> <div>32%</div> <div> <div>30%</div> <div>41%</div> <div>22%</div> <div>8%</div> </div> </div>
1	J	37	<div> <div>16%</div> <div>14%</div> <div>57%</div> <div>16%</div> <div>14%</div> </div>
1	K	37	<div> <div>65%</div> <div>11%</div> <div>51%</div> <div>32%</div> <div>5%</div> </div>
1	L	37	<div> <div>35%</div> <div>24%</div> <div>46%</div> <div>22%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	M	37	
1	N	37	
1	O	37	
1	P	37	
2	A	401	
2	B	401	
2	C	401	
2	D	401	
2	E	401	
2	F	401	
2	G	401	
2	H	401	

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
4	TSB	D	5002	-	-	-	X
4	TSB	E	6002	-	-	-	X
4	TSB	F	7002	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 32922 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 RNA chain called Threonyl-tRNA synthetase mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			
1	J	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			
1	K	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			
1	L	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			
1	M	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			
1	N	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			
1	O	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			
1	P	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	401	Total	C	N	O	S	0	0	0
			3278	2069	576	610	23			
2	B	401	Total	C	N	O	S	0	0	0
			3278	2069	576	610	23			
2	C	401	Total	C	N	O	S	0	0	0
			3278	2069	576	610	23			
2	D	401	Total	C	N	O	S	0	0	0
			3278	2069	576	610	23			
2	E	401	Total	C	N	O	S	0	0	0
			3278	2069	576	610	23			
2	F	401	Total	C	N	O	S	0	0	0
			3278	2069	576	610	23			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	401	Total 3278	C 2069	N 576	O 610	S 23	0	0	0
2	H	401	Total 3278	C 2069	N 576	O 610	S 23	0	0	0

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3 | G | 1 | Total Zn
1 1 | 0 | 0 |
| 3 | D | 1 | Total Zn
1 1 | 0 | 0 |
| 3 | E | 1 | Total Zn
1 1 | 0 | 0 |
| 3 | H | 1 | Total Zn
1 1 | 0 | 0 |
| 3 | B | 1 | Total Zn
1 1 | 0 | 0 |
| 3 | C | 1 | Total Zn
1 1 | 0 | 0 |
| 3 | A | 1 | Total Zn
1 1 | 0 | 0 |
| 3 | F | 1 | Total Zn
1 1 | 0 | 0 |

- [illegible]

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 30	C 14	N 7	O 8	S 1	0	0
4	B	1	Total 30	C 14	N 7	O 8	S 1	0	0
4	C	1	Total 30	C 14	N 7	O 8	S 1	0	0
4	D	1	Total 30	C 14	N 7	O 8	S 1	0	0
4	E	1	Total 30	C 14	N 7	O 8	S 1	0	0
4	F	1	Total 30	C 14	N 7	O 8	S 1	0	0
4	G	1	Total 30	C 14	N 7	O 8	S 1	0	0
4	H	1	Total 30	C 14	N 7	O 8	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total 10	O 10	0	0
5	B	15	Total 15	O 15	0	0
5	C	11	Total 11	O 11	0	0
5	D	14	Total 14	O 14	0	0
5	E	11	Total 11	O 11	0	0
5	F	13	Total 13	O 13	0	0
5	G	13	Total 13	O 13	0	0
5	H	16	Total 16	O 16	0	0
5	I	11	Total 11	O 11	0	0
5	J	12	Total 12	O 12	0	0
5	K	1	Total 1	O 1	0	0
5	L	8	Total 8	O 8	0	0

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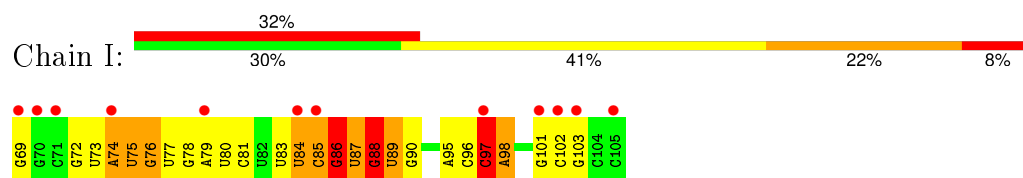
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	6	Total 6	O 6	0	0
5	N	9	Total 9	O 9	0	0
5	O	11	Total 11	O 11	0	0
5	P	9	Total 9	O 9	0	0

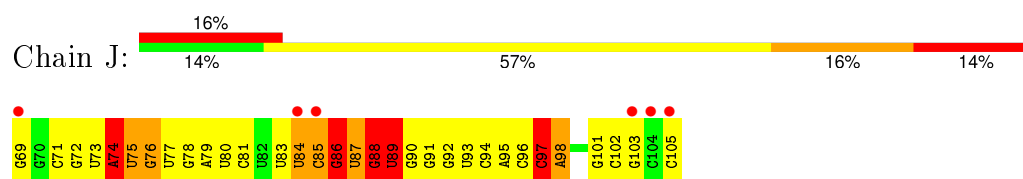
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

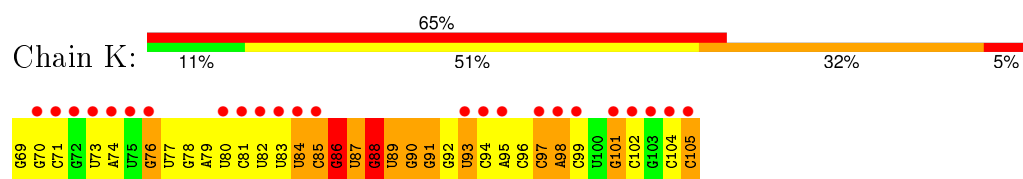
- Molecule 1: Threonyl-tRNA synthetase mRNA



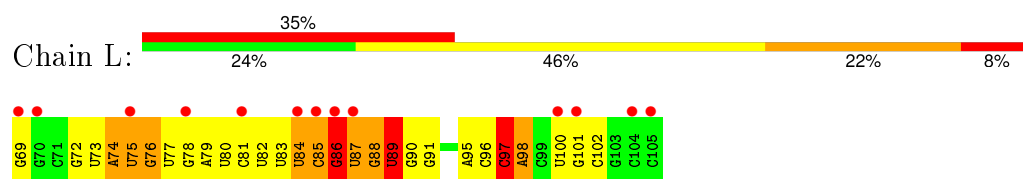
- Molecule 1: Threonyl-tRNA synthetase mRNA



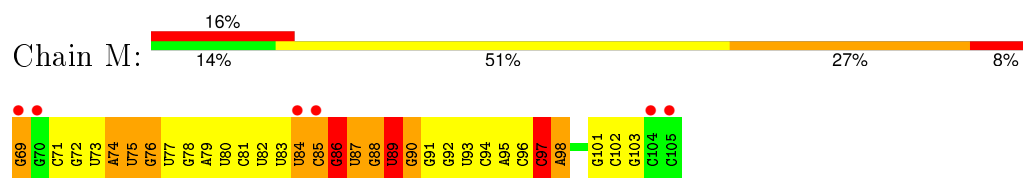
- Molecule 1: Threonyl-tRNA synthetase mRNA



- Molecule 1: Threonyl-tRNA synthetase mRNA

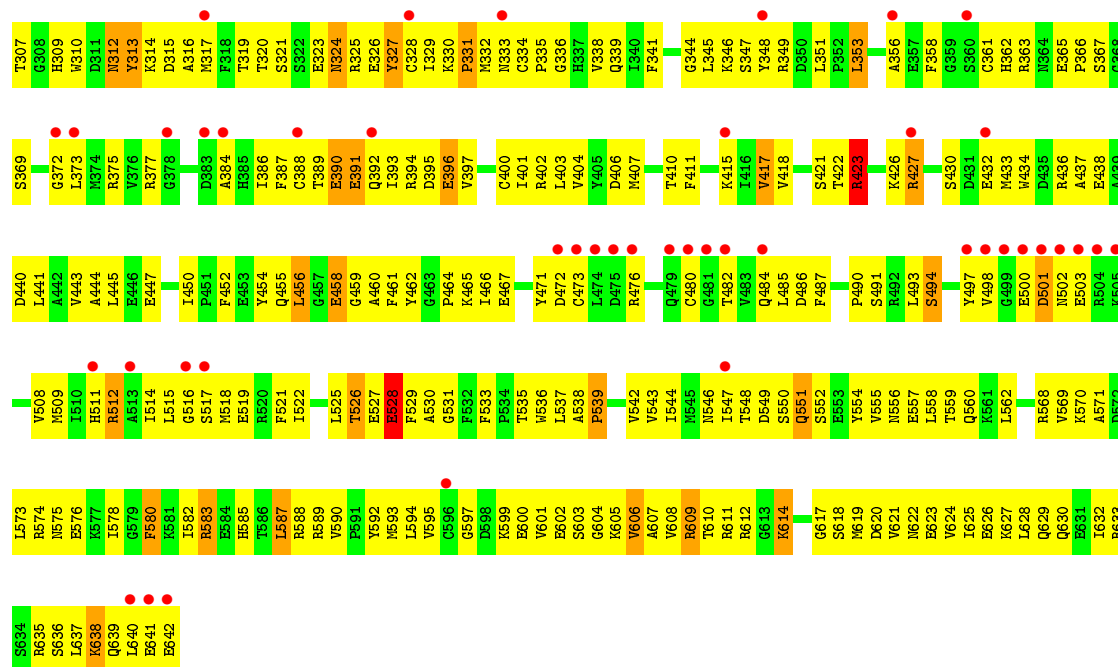


- Molecule 1: Threonyl-tRNA synthetase mRNA

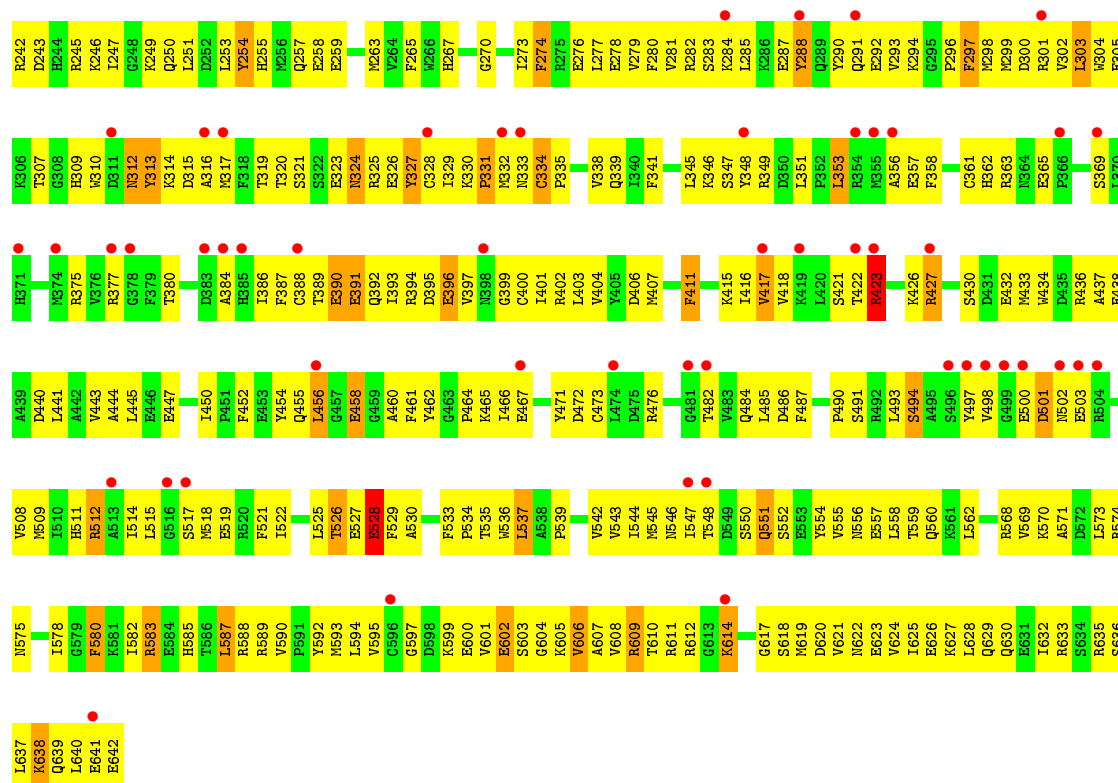


- Molecule 1: Threonyl-tRNA synthetase mRNA



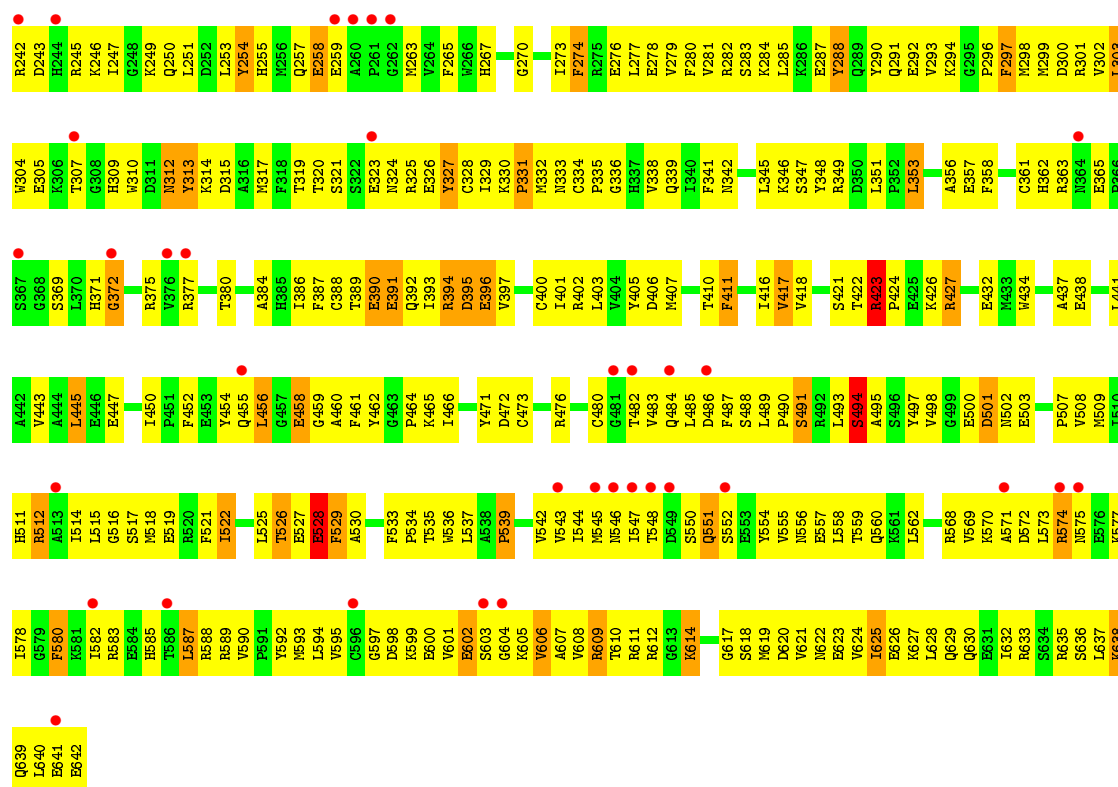


• Molecule 2: Threonyl-tRNA synthetase

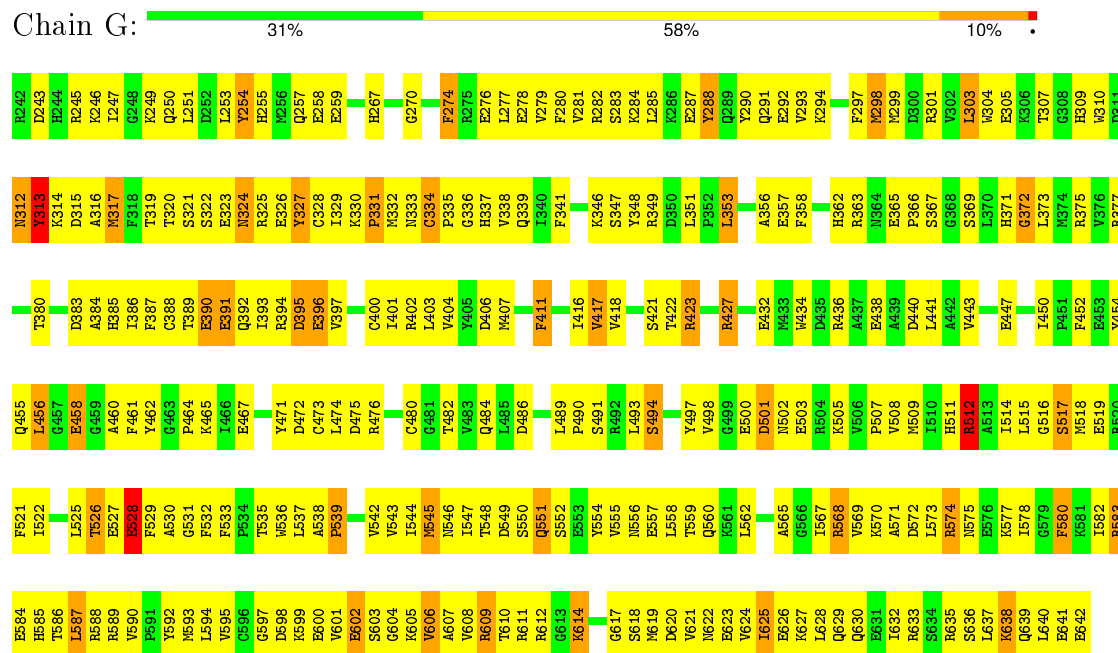


• Molecule 2: Threonyl-tRNA synthetase





• Molecule 2: Threonyl-tRNA synthetase



• Molecule 2: Threonyl-tRNA synthetase



H585	T586	L587	R588	R589	V590	P591	Y592	M593	L594	V595	G596	G597	D598	R599	E600	V601	E602	S603	G604	R605	V606	A607	V608	R609	T610	R611	R612	G613	K614	G617	S618	M619	D620	V621	M622	E623	V624	T625	E626	K627	L628	Q629	Q630	E631	T632	R633	G634	R635	S636	L637	R638	Q639	L640	E641	E642				
M518	I450	P451	F452	E453	Y454	Q455	L456	G457	E458	F459	A460	A461	Y462	G463	P464	K465	I466	E467	Y471	D472	C473	R476	Q479	C480	Q484	L485	D486	F487	S488	L489	P490	S491	E492	L493	S494	A495	S496	Y497	V498	G499	E500	D501	N502	N503	V508	M509	I510	H511	R512	A513	I514	L515	R582	R583	E584				
R375	V376	R377		T380	D383	A384	H385		R386	F387	C388	T389	E390	E391	Q392	I393	C394	I329	K330	P331	M332	N333	C334	R402	L403	Y404	Y405	D406	M407	F411	I416	V417	Y418	V419	S421	T422	R423	K426	R427	A356	E357	F358		C361	R362	R363	N364	E365	P366	S367	G368	A442	S369	I370	H371	G372	L445	E446	E447
D242	R243	R244	K245	K246	L247	G248	K249	Q250	L251	D252	L253	Y254	H255	M256	Q257	E258	E259		N266	H267		G270		I273	F274	R275	E276	L277	E278	V279	F280	V281	R282	S283	K284	L285	V286	E287	Y288	Q289	D290	Q291	E292	V293	K294			F297	M298	D300	R301	V302	L303	N304	E305	K306	T307	G308	H309

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	188.45Å 101.74Å 199.34Å 90.00° 114.40° 90.00°	Depositor
Resolution (Å)	29.80 – 3.50 29.80 – 3.46	Depositor EDS
% Data completeness (in resolution range)	90.0 (29.80-3.50) 92.6 (29.80-3.46)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.63 (at 3.47Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.251 , 0.287 0.256 , 0.288	Depositor DCC
R_{free} test set	8182 reflections (9.96%)	DCC
Wilson B-factor (Å ²)	96.2	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 93.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 88408 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	32922	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, TSB

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	I	0.71	1/874 (0.1%)	0.99	7/1358 (0.5%)
1	J	0.81	1/874 (0.1%)	1.01	7/1358 (0.5%)
1	K	0.94	1/874 (0.1%)	1.08	7/1358 (0.5%)
1	L	0.64	1/874 (0.1%)	0.96	5/1358 (0.4%)
1	M	0.79	1/874 (0.1%)	1.00	5/1358 (0.4%)
1	N	0.66	1/874 (0.1%)	0.94	4/1358 (0.3%)
1	O	0.99	3/874 (0.3%)	1.07	6/1358 (0.4%)
1	P	0.73	1/874 (0.1%)	0.99	6/1358 (0.4%)
2	A	0.64	0/3349	0.76	0/4508
2	B	0.70	1/3349 (0.0%)	0.78	0/4508
2	C	0.53	0/3349	0.71	0/4508
2	D	0.49	0/3349	0.68	0/4508
2	E	0.49	0/3349	0.69	0/4508
2	F	0.54	0/3349	0.73	0/4508
2	G	0.78	0/3349	0.85	2/4508 (0.0%)
2	H	0.66	0/3349	0.78	0/4508
All	All	0.65	11/33784 (0.0%)	0.81	49/46928 (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	I	0	2
1	J	0	4
1	K	0	1
1	L	0	3
1	M	0	2
1	N	0	2
1	O	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	3
All	All	0	20

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	69	G	OP3-P	-7.74	1.51	1.61
1	I	69	G	OP3-P	-7.56	1.52	1.61
1	K	69	G	OP3-P	-7.33	1.52	1.61
1	L	69	G	OP3-P	-7.26	1.52	1.61
1	P	69	G	OP3-P	-7.09	1.52	1.61

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	74	A	N9-C1'-C2'	11.86	129.42	114.00
1	M	74	A	N9-C1'-C2'	10.30	127.39	114.00
1	P	74	A	N9-C1'-C2'	9.87	126.84	114.00
1	K	86	G	N9-C1'-C2'	9.58	126.46	114.00
1	L	74	A	N9-C1'-C2'	9.26	126.04	114.00

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	74	A	Sidechain
1	I	86	G	Sidechain
1	J	74	A	Sidechain
1	J	86	G	Sidechain
1	J	89	U	Sidechain

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	I	785	0	397	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	785	0	397	53	0
1	K	785	0	397	76	0
1	L	785	0	397	42	0
1	M	785	0	397	72	0
1	N	785	0	397	44	0
1	O	785	0	397	56	0
1	P	785	0	397	65	0
2	A	3278	0	3208	336	0
2	B	3278	0	3208	316	0
2	C	3278	0	3208	340	0
2	D	3278	0	3208	331	0
2	E	3278	0	3208	333	0
2	F	3278	0	3208	346	0
2	G	3278	0	3208	314	0
2	H	3278	0	3208	313	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	30	0	21	3	0
4	B	30	0	20	4	0
4	C	30	0	21	3	0
4	D	30	0	21	4	0
4	E	30	0	21	4	0
4	F	30	0	21	5	0
4	G	30	0	21	4	0
4	H	30	0	21	4	0
5	A	10	0	0	0	0
5	B	15	0	0	8	0
5	C	11	0	0	3	0
5	D	14	0	0	4	0
5	E	11	0	0	5	0
5	F	13	0	0	2	0
5	G	13	0	0	4	0
5	H	16	0	0	3	0
5	I	11	0	0	10	0
5	J	12	0	0	8	0
5	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	8	0	0	3	0
5	M	6	0	0	10	0
5	N	9	0	0	2	0
5	O	11	0	0	9	0
5	P	9	0	0	14	0
All	All	32922	0	29007	2890	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 47.

The worst 5 of 2890 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)
2:G:407:MET:CE	2:G:407:MET:SD	2.05	1.44
2:D:559:THR:HG21	2:D:571:ALA:HB2	1.29	1.15
2:G:559:THR:HG21	2:G:571:ALA:HB2	1.27	1.12
2:E:559:THR:HG21	2:E:571:ALA:HB2	1.30	1.12
2:A:559:THR:HG21	2:A:571:ALA:HB2	1.27	1.11

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	
2	A	399/401 (100%)	327 (82%)	53 (13%)	19 (5%)	3	28
2	B	399/401 (100%)	325 (82%)	57 (14%)	17 (4%)	3	31
2	C	399/401 (100%)	327 (82%)	52 (13%)	20 (5%)	3	27
2	D	399/401 (100%)	327 (82%)	54 (14%)	18 (4%)	3	30
2	E	399/401 (100%)	327 (82%)	55 (14%)	17 (4%)	3	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	399/401 (100%)	327 (82%)	52 (13%)	20 (5%)	3	27
2	G	399/401 (100%)	323 (81%)	55 (14%)	21 (5%)	2	25
2	H	399/401 (100%)	323 (81%)	55 (14%)	21 (5%)	2	25
All	All	3192/3208 (100%)	2606 (82%)	433 (14%)	153 (5%)	3	28

5 of 153 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	313	TYR
2	A	324	ASN
2	A	456	LEU
2	A	528	GLU
2	A	574	ARG

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	356/356 (100%)	317 (89%)	39 (11%)	8	36
2	B	356/356 (100%)	318 (89%)	38 (11%)	8	37
2	C	356/356 (100%)	321 (90%)	35 (10%)	10	42
2	D	356/356 (100%)	321 (90%)	35 (10%)	10	42
2	E	356/356 (100%)	319 (90%)	37 (10%)	9	39
2	F	356/356 (100%)	320 (90%)	36 (10%)	9	40
2	G	356/356 (100%)	315 (88%)	41 (12%)	7	33
2	H	356/356 (100%)	320 (90%)	36 (10%)	9	40
All	All	2848/2848 (100%)	2551 (90%)	297 (10%)	9	39

5 of 297 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	512	ARG

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Mol	Chain	Res	Type
2	E	427	ARG
2	H	396	GLU
2	D	539	PRO
2	E	297	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 129 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	560	GLN
2	E	381	GLN
2	H	371	HIS
2	D	575	ASN
2	E	257	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	36/37 (97%)	6 (16%)	4 (11%)
1	J	36/37 (97%)	9 (25%)	5 (13%)
1	K	36/37 (97%)	11 (30%)	4 (11%)
1	L	36/37 (97%)	7 (19%)	4 (11%)
1	M	36/37 (97%)	8 (22%)	5 (13%)
1	N	36/37 (97%)	8 (22%)	4 (11%)
1	O	36/37 (97%)	9 (25%)	5 (13%)
1	P	36/37 (97%)	8 (22%)	5 (13%)
All	All	288/296 (97%)	66 (22%)	36 (12%)

5 of 66 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	76	G
1	I	85	C
1	I	86	G
1	I	89	U
1	I	90	G

5 of 36 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L	97	C

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Mol	Chain	Res	Type
1	M	88	G
1	P	84	U
1	M	75	U
1	M	97	C

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](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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$
4	TSB	A	2002	3	24,32,32	2.05	3 (12%)	31,48,48	1.14	1 (3%)
4	TSB	B	3002	3	24,32,32	3.06	2 (8%)	31,48,48	0.64	0
4	TSB	C	4002	3	24,32,32	2.28	2 (8%)	31,48,48	0.83	0
4	TSB	D	5002	3	24,32,32	2.57	2 (8%)	31,48,48	0.67	0
4	TSB	E	6002	3	24,32,32	2.83	2 (8%)	31,48,48	0.70	0
4	TSB	F	7002	3	24,32,32	2.06	2 (8%)	31,48,48	0.96	1 (3%)
4	TSB	G	8002	3	24,32,32	2.62	3 (12%)	31,48,48	1.20	2 (6%)
4	TSB	H	9002	3	24,32,32	2.33	2 (8%)	31,48,48	1.06	2 (6%)

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	TSB	A	2002	3	-	0/17/39/39	0/3/3/3
4	TSB	B	3002	3	-	0/17/39/39	0/3/3/3
4	TSB	C	4002	3	-	0/17/39/39	0/3/3/3
4	TSB	D	5002	3	-	0/17/39/39	0/3/3/3
4	TSB	E	6002	3	-	0/17/39/39	0/3/3/3
4	TSB	F	7002	3	-	0/17/39/39	0/3/3/3
4	TSB	G	8002	3	-	0/17/39/39	0/3/3/3
4	TSB	H	9002	3	-	0/17/39/39	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2002	TSB	C-N8	-2.56	1.33	1.37
4	G	8002	TSB	C2-N3	2.65	1.36	1.32
4	A	2002	TSB	O1S-S1	5.68	1.47	1.42
4	F	7002	TSB	O1S-S1	6.26	1.47	1.42
4	G	8002	TSB	O1S-S1	6.78	1.48	1.42

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	8002	TSB	O2S-S1-N8	-4.12	103.00	108.50
4	H	9002	TSB	O2S-S1-N8	-2.84	104.70	108.50
4	F	7002	TSB	O2S-S1-O1S	-2.19	118.15	120.77
4	H	9002	TSB	C2'-C1'-N9	-2.03	111.19	114.29
4	G	8002	TSB	CA-C-N8	2.06	120.68	116.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2002	TSB	3	0
4	B	3002	TSB	4	0
4	C	4002	TSB	3	0
4	D	5002	TSB	4	0
4	E	6002	TSB	4	0
4	F	7002	TSB	5	0
4	G	8002	TSB	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	9002	TSB	4	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	I	37/37 (100%)	1.51	12 (32%) 1 0	82, 115, 150, 153	0
1	J	37/37 (100%)	0.93	6 (16%) 3 3	55, 88, 135, 152	0
1	K	37/37 (100%)	2.67	24 (64%) 0 0	119, 148, 168, 184	0
1	L	37/37 (100%)	1.62	13 (35%) 0 0	110, 134, 170, 180	0
1	M	37/37 (100%)	1.08	6 (16%) 3 3	60, 86, 153, 166	0
1	N	37/37 (100%)	3.65	34 (91%) 0 0	140, 163, 181, 184	0
1	O	37/37 (100%)	0.47	1 (2%) 58 47	45, 67, 115, 124	0
1	P	37/37 (100%)	1.22	9 (24%) 1 1	46, 104, 155, 159	0
2	A	401/401 (100%)	-0.20	4 (0%) 84 76	15, 68, 109, 136	0
2	B	401/401 (100%)	-0.11	4 (0%) 84 76	17, 62, 105, 137	0
2	C	401/401 (100%)	0.30	19 (4%) 35 28	55, 101, 146, 160	0
2	D	401/401 (100%)	0.56	45 (11%) 7 7	80, 123, 147, 158	0
2	E	401/401 (100%)	0.69	51 (12%) 5 5	75, 126, 150, 168	0
2	F	401/401 (100%)	0.46	35 (8%) 13 12	47, 105, 148, 168	0
2	G	401/401 (100%)	-0.26	0 100 100	7, 48, 98, 132	0
2	H	401/401 (100%)	-0.17	3 (0%) 89 82	14, 68, 105, 135	0
All	All	3504/3504 (100%)	0.28	266 (7%) 17 14	7, 91, 147, 184	0

The worst 5 of 266 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	546	ASN	8.3
2	F	546	ASN	8.1
2	C	596	CYS	7.5
1	N	97	C	7.2
2	F	571	ALA	6.8

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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	TSB	G	8002	30/30	0.94	0.31	0.55	0,18,49,50	0
4	TSB	D	5002	30/30	0.75	0.57	0.49	94,112,119,120	0
4	TSB	H	9002	30/30	0.91	0.39	0.48	30,48,71,72	0
4	TSB	B	3002	30/30	0.95	0.38	0.48	32,50,57,58	0
4	TSB	E	6002	30/30	0.65	0.51	0.12	86,122,126,127	0
4	TSB	A	2002	30/30	0.96	0.29	0.11	31,44,58,65	0
4	TSB	F	7002	30/30	0.81	0.42	0.10	89,103,111,112	0
3	ZN	B	1	1/1	0.99	0.32	-0.10	52,52,52,52	0
4	TSB	C	4002	30/30	0.87	0.36	-0.29	73,88,100,102	0
3	ZN	G	1	1/1	0.95	0.24	-0.61	27,27,27,27	0
3	ZN	F	1	1/1	0.81	0.26	-0.80	101,101,101,101	0
3	ZN	A	1	1/1	0.99	0.23	-0.93	42,42,42,42	0
3	ZN	H	1	1/1	0.98	0.27	-0.98	54,54,54,54	0
3	ZN	D	1	1/1	0.77	0.30	-1.76	135,135,135,135	0
3	ZN	E	1	1/1	0.73	0.26	-1.94	185,185,185,185	0
3	ZN	C	1	1/1	0.95	0.27	-2.07	95,95,95,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.