



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:17 AM UTC

PDB ID : 3W1I / pdb_00003w1i
Title : Crystal structure of the N-terminal truncated selenocysteine synthase Sela
Authors : Itoh, Y.; Sekine, S.; Yokoyama, S.
Deposited on : 2012-11-15
Resolution : 3.19 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 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

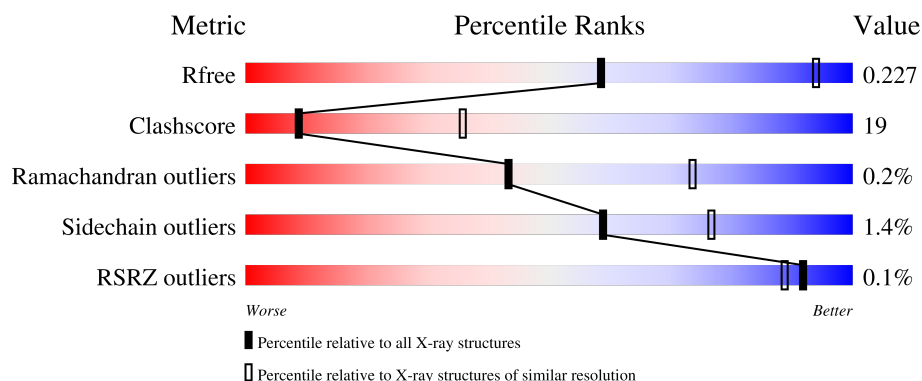
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 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	392	67% 31% .
1	B	392	62% 35% ..
1	C	392	66% 32% .
1	D	392	65% 33% ..
1	E	392	59% 40% .

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Mol	Chain	Length	Quality of chain
1	F	392	 58%39%. .
1	G	392	 57%41%.. ..
1	H	392	 63%36%.. ..
1	I	392	 66%31%.. ..
1	J	392	 61%37%.. ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30719 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 L-seryl-tRNA(Sec) selenium transferase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	P	S	Se	0	0	0
			3086	1962	535	577	1	3	8			
1	B	388	Total	C	N	O	P	S	Se	0	0	0
			3055	1942	530	572	1	3	7			
1	C	392	Total	C	N	O	P	S	Se	0	0	0
			3086	1962	535	577	1	3	8			
1	D	389	Total	C	N	O	P	S	Se	0	0	0
			3063	1948	531	573	1	3	7			
1	E	391	Total	C	N	O	P	S	Se	0	0	0
			3078	1957	534	576	1	3	7			
1	F	392	Total	C	N	O	P	S	Se	0	0	0
			3086	1962	535	577	1	3	8			
1	G	389	Total	C	N	O	P	S	Se	0	0	0
			3063	1948	531	573	1	3	7			
1	H	390	Total	C	N	O	P	S	Se	0	0	0
			3069	1951	532	575	1	3	7			
1	I	389	Total	C	N	O	P	S	Se	0	0	0
			3063	1948	531	573	1	3	7			
1	J	389	Total	C	N	O	P	S	Se	0	0	0
			3063	1948	531	573	1	3	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	MSE	-	expression tag	UNP O67140
B	61	MSE	-	expression tag	UNP O67140
C	61	MSE	-	expression tag	UNP O67140
D	61	MSE	-	expression tag	UNP O67140
E	61	MSE	-	expression tag	UNP O67140
F	61	MSE	-	expression tag	UNP O67140
G	61	MSE	-	expression tag	UNP O67140
H	61	MSE	-	expression tag	UNP O67140
I	61	MSE	-	expression tag	UNP O67140

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Chain	Residue	Modelled	Actual	Comment	Reference
J	61	MSE	-	expression tag	UNP O67140

- Molecule 2 is PLATINUM (II) ION (CCD ID: PT) (formula: Pt).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Pt 2 2	0	0

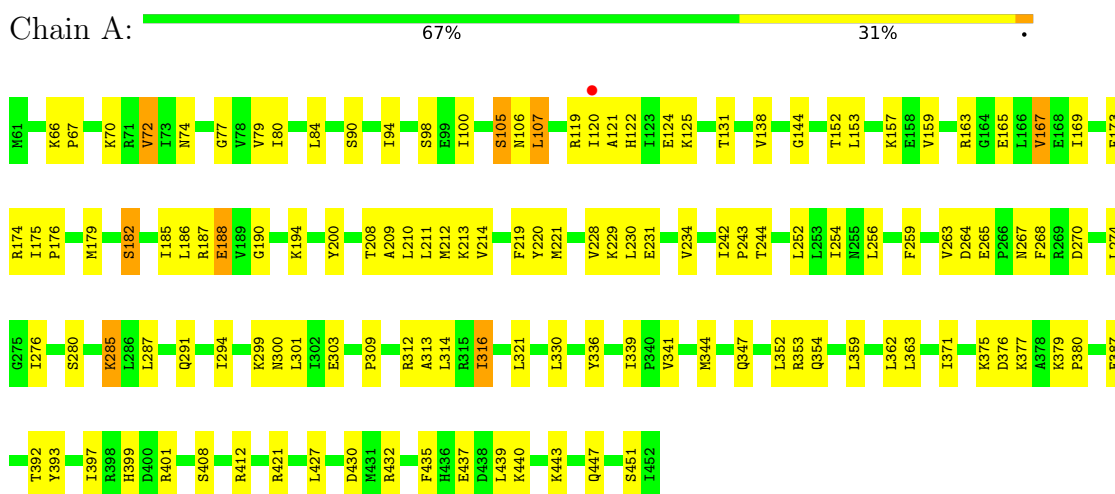
- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total K 1 1	0	0
3	C	1	Total K 1 1	0	0
3	E	1	Total K 1 1	0	0
3	H	1	Total K 1 1	0	0
3	I	1	Total K 1 1	0	0

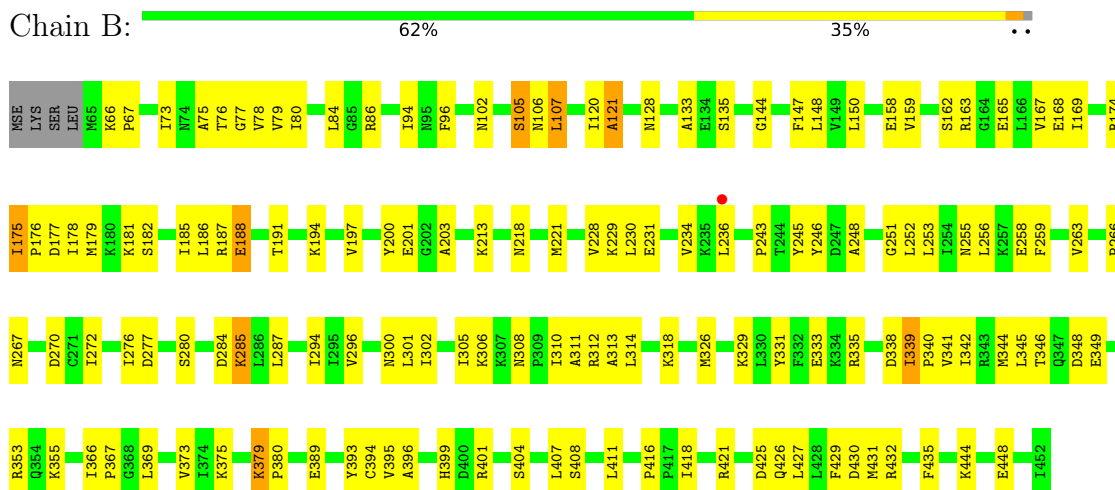
3 Residue-property plots

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: L-seryl-tRNA(Sec) selenium transferase

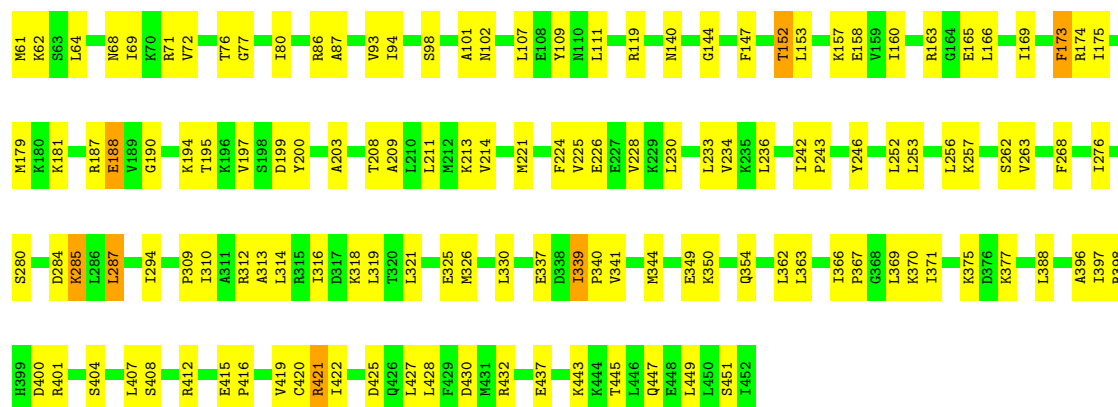


- Molecule 1: L-seryl-tRNA(Sec) selenium transferase



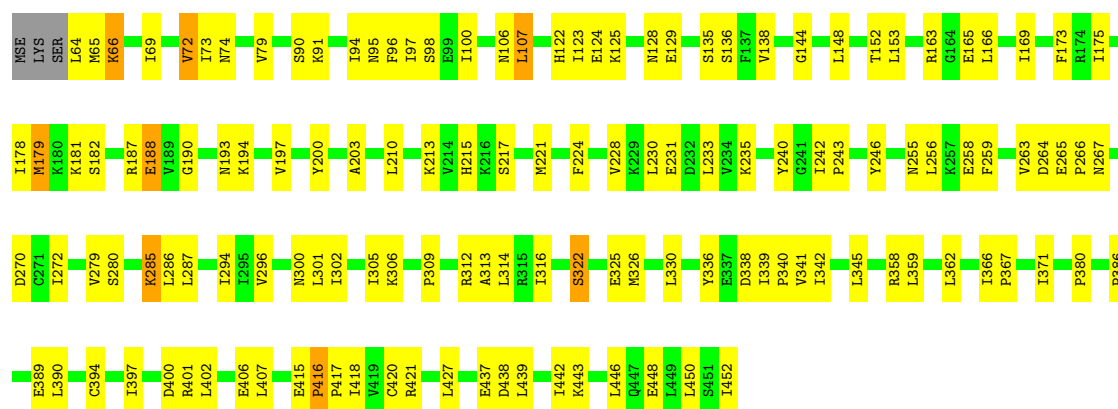
- Molecule 1: L-seryl-tRNA(Sec) selenium transferase





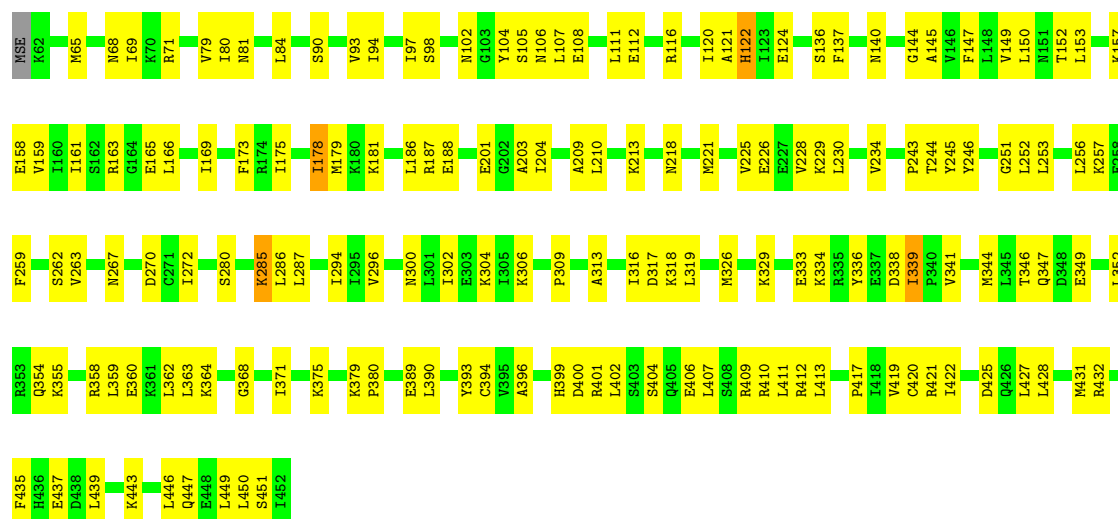
- Molecule 1: L-seryl-tRNA(Sec) selenium transferase

Chain D: 65% 33% ..



- Molecule 1: L-seryl-tRNA(Sec) selenium transferase

Chain E: 59% 40% .



- Molecule 1: L-seryl-tRNA(Sec) selenium transferase

R432	M345	T254	F147	M61
F435	L345	N255	L148	K62
H436	L256	L256	V149	
E437	E349	F259	L150	M65
D438	R353	G260	N151	K66
L439		L261	T152	P67
			L153	N68
T442	L359	E265	E158	R71
K443		P266	V159	
K444	L363			A75
Q447	I366	L278	S162	V79
E448	P367	V279	R163	
L449	G368	S280	G164	I80
			E165	
L450	K369	K285	L166	L84
S451	K370	L286	V167	
I452	I371		E168	V93
	S372	P290	I169	I94
	V373			N95
	I374	I294	R174	F96
	K375	I295	I175	I97
		V296	P176	
	K379	G297	D177	I100
	P380	K298	I178	A101
		K299	M179	N102
	L385	N300	K180	S105
	P386	I301	K181	N106
	E387	L302		L107
	L388	E303	L186	L108
	E389		E187	E108
	L390	K307	I188	I109
	P391	N308		N110
	K392	P309	L204	L111
	K393	I310		E112
	G394	A311	L210	F113
	V395	R312		G114
	A396	A313	K213	K115
	I397	L314	V214	R116
		R315		G117
	L407	I316	M218	S118
	S408	D317	F219	R119
	R409		V220	I120
	R410	T320	M221	A121
	L411		H122	H122
	R412		V225	I123
	L413	G323	E226	
	A414			
	E415	M326	L230	Y126
	P416	K329	E231	L127
	P417	L330		L130
	I418	Y331	Y240	T131
	V419	G241		
	C420	K334	T242	S135
		R335	P243	S136
		Y336		
	L427		Y246	N141
	L428	I339		
	F429	P340	L252	G144
	D430	Y241	L252	
	M431			

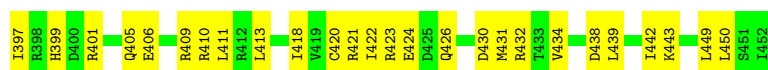
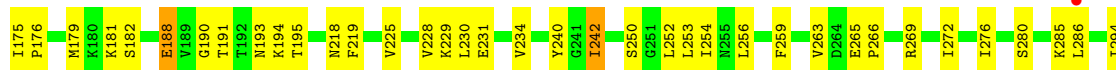
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|------|------|------|------|------|
| M431 | L345 | S273 | E168 | MSE |
| R432 | T346 | L274 | I169 | LVS |
| T433 | Q347 | | | SER |
| V434 | D348 | D277 | F173 | |
| F435 | E349 | L278 | R174 | M65 |
| H436 | K350 | V279 | I175 | K66 |
| | | S280 | | P67 |
| D437 | | G281 | K181 | N68 |
| D438 | R353 | S282 | | |
| L439 | K354 | G283 | I185 | G77 |
| | K355 | D284 | L186 | V78 |
| I442 | K356 | K285 | R187 | V79 |
| | K357 | L286 | E188 | |
| L446 | R358 | L287 | | |
| Q447 | L359 | G288 | N193 | N81 |
| E448 | E360 | G289 | | T82 |
| L449 | K361 | | | N83 |
| | L362 | | V197 | L84 |
| L450 | L363 | I294 | | G85 |
| S451 | K364 | T295 | Y200 | |
| I452 | R365 | V296 | | L89 |
| | L366 | G297 | T208 | S90 |
| | P367 | K298 | A209 | |
| | G368 | | L210 | V93 |
| | L369 | L301 | | I94 |
| | | I302 | K213 | |
| | V373 | K303 | | N102 |
| | L374 | G304 | N218 | |
| | K375 | I305 | | S105 |
| | D376 | K306 | M221 | N106 |
| | | K307 | | L107 |
| | K379 | N308 | V225 | |
| | P380 | P309 | | I120 |
| | | | V228 | A121 |
| | E389 | R312 | K229 | H122 |
| | | A313 | L230 | |
| | V395 | L314 | E231 | L130 |
| | | R315 | D232 | |
| | H399 | I316 | L233 | E134 |
| | D400 | D317 | K135 | S135 |
| | R401 | K318 | I242 | S136 |
| | | L319 | | |
| | S404 | T320 | Y246 | N141 |
| | Q405 | L321 | | N142 |
| | E406 | | G251 | A143 |
| | L407 | R324 | L252 | G144 |
| | S408 | E325 | L253 | |
| | R409 | M326 | I254 | L148 |
| | R410 | | V255 | |
| | L411 | Y331 | L256 | N151 |
| | R412 | | K257 | |
| | I418 | R335 | E258 | G156 |
| | | Y336 | F259 | K157 |
| | | E337 | | E158 |
| | I422 | D338 | S262 | V159 |
| | R423 | I339 | V263 | |
| | | P340 | D264 | R163 |
| | L427 | V341 | E265 | G164 |
| | L428 | I342 | | E165 |
| | E429 | | | L166 |
| | R420 | R343 | C271 | N167 |
| | | K344 | | |

- | |
|------|
| MSE | LVS | S63 | K66 | P67 | N68 | R71 | N74 | G77 | V78 | V79 | I80 | L84 | G85 | R86 | L89 | S90 | K91 | N95 | S98 | N106 | L107 | R116 | L119 | I120 | A121 | H122 | I123 | E124 | L130 | S135 | V139 | N140 | N141 | I142 | A145 | V146 | F147 | L148 | V149 | E158 | R163 | | | | | |
| |
| F268 | R269 | D270 | C271 | I272 | S280 | G281 | S282 | G283 | D284 | K285 | L286 | L287 | A292 | G293 | I294 | L295 | V296 | L301 | I302 | I305 | P309 | A313 | L314 | R315 | L316 | D317 | T320 | E325 | M326 | K329 | L330 | E333 | K334 | R335 | Y336 | E337 | D338 | V341 | I342 | L345 | T346 | I366 | P367 | G368 | L369 | T370 |
| V167 | I169 | F173 | R174 | I175 | P176 | D177 | N178 | K180 | K181 | R187 | E188 | V189 | G190 | T191 | I204 | N205 | L211 | M212 | K213 | V214 | H215 | K216 | F219 | G220 | M221 | F224 | E227 | V228 | K229 | L230 | V234 | Y246 | D247 | G251 | L252 | L253 | I254 | N255 | L256 | F259 | G260 | I261 | V263 | N267 | | |



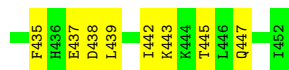
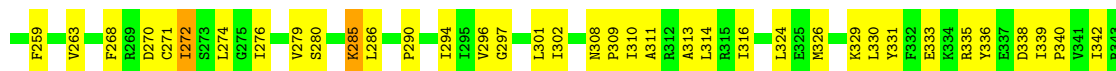
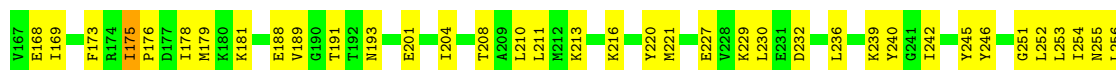
• Molecule 1: L-seryl-tRNA(Sec) selenium transferase

Chain I: 66% 31% ..



• Molecule 1: L-seryl-tRNA(Sec) selenium transferase

Chain J: 61% 37% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.83Å 280.94Å 97.64Å 90.00° 113.45° 90.00°	Depositor
Resolution (Å)	48.94 – 3.19 48.94 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.94-3.19) 99.0 (48.94-3.19)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.174 , 0.235 0.166 , 0.227	Depositor DCC
R_{free} test set	3753 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	104.4	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 102.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	30719	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: LLP, PT, K

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	0.61	0/3094	0.93	2/4144 (0.0%)
1	B	0.59	0/3064	0.96	8/4107 (0.2%)
1	C	0.61	0/3094	0.96	6/4144 (0.1%)
1	D	0.59	0/3071	0.97	11/4115 (0.3%)
1	E	0.60	1/3086 (0.0%)	0.96	7/4134 (0.2%)
1	F	0.55	0/3094	0.94	10/4144 (0.2%)
1	G	0.57	0/3071	0.97	12/4115 (0.3%)
1	H	0.55	0/3077	0.91	3/4123 (0.1%)
1	I	0.52	0/3071	0.92	8/4115 (0.2%)
1	J	0.55	0/3071	0.96	9/4115 (0.2%)
All	All	0.57	1/30793 (0.0%)	0.95	76/41256 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	175	ILE	CA-CB	6.63	1.57	1.54

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	175	ILE	CB-CA-C	-8.59	105.54	113.70
1	A	379	LYS	CA-C-N	8.54	128.53	119.05
1	A	379	LYS	C-N-CA	8.54	128.53	119.05
1	E	339	ILE	CA-C-N	7.86	129.66	119.84
1	E	339	ILE	C-N-CA	7.86	129.66	119.84

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	3086	0	3237	112	0
1	B	3055	0	3199	124	0
1	C	3086	0	3237	124	0
1	D	3063	0	3210	115	0
1	E	3078	0	3228	134	0
1	F	3086	0	3237	145	0
1	G	3063	0	3210	158	0
1	H	3069	0	3215	130	0
1	I	3063	0	3210	115	0
1	J	3063	0	3210	132	0
2	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
All	All	30719	0	32193	1177	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 19.

The worst 5 of 1177 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:G:316:ILE:HD11	1:G:321:LEU:HD13	1.40	1.03
1:A:254:ILE:HD11	1:A:259:PHE:HZ	1.27	0.97
1:F:175:ILE:HG22	1:F:179:MSE:CE	1.96	0.95
1:B:230:LEU:HD11	1:B:246:TYR:CE2	2.02	0.93
1:A:254:ILE:HD11	1:A:259:PHE:CZ	2.04	0.92

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	389/392 (99%)	374 (96%)	14 (4%)	1 (0%)	36	68
1	B	385/392 (98%)	371 (96%)	12 (3%)	2 (0%)	24	59
1	C	389/392 (99%)	371 (95%)	18 (5%)	0	100	100
1	D	386/392 (98%)	372 (96%)	13 (3%)	1 (0%)	36	68
1	E	388/392 (99%)	368 (95%)	19 (5%)	1 (0%)	36	68
1	F	389/392 (99%)	371 (95%)	17 (4%)	1 (0%)	36	68
1	G	386/392 (98%)	363 (94%)	23 (6%)	0	100	100
1	H	387/392 (99%)	370 (96%)	17 (4%)	0	100	100
1	I	386/392 (98%)	367 (95%)	18 (5%)	1 (0%)	36	68
1	J	386/392 (98%)	367 (95%)	19 (5%)	0	100	100
All	All	3871/3920 (99%)	3694 (95%)	170 (4%)	7 (0%)	43	73

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	334	LYS
1	F	107	LEU
1	I	107	LEU
1	A	107	LEU
1	B	107	LEU

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	339/331 (102%)	330 (97%)	9 (3%)	39	68
1	B	335/331 (101%)	331 (99%)	4 (1%)	63	79
1	C	339/331 (102%)	336 (99%)	3 (1%)	70	81
1	D	336/331 (102%)	330 (98%)	6 (2%)	51	74
1	E	338/331 (102%)	333 (98%)	5 (2%)	57	76
1	F	339/331 (102%)	333 (98%)	6 (2%)	51	74
1	G	336/331 (102%)	332 (99%)	4 (1%)	63	79
1	H	337/331 (102%)	335 (99%)	2 (1%)	78	84
1	I	336/331 (102%)	332 (99%)	4 (1%)	63	79
1	J	336/331 (102%)	333 (99%)	3 (1%)	70	81
All	All	3371/3310 (102%)	3325 (99%)	46 (1%)	59	77

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	106	ASN
1	G	273	SER
1	F	162	SER
1	F	369	LEU
1	H	188	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	102	ASN
1	J	399	HIS
1	I	142	ASN
1	J	83	ASN
1	D	140	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

10 non-standard protein/DNA/RNA residues 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
1	LLP	A	285	1	23,24,25	1.52	4 (17%)	25,32,34	1.41	4 (16%)
1	LLP	I	285	1	23,24,25	1.69	4 (17%)	25,32,34	1.23	1 (4%)
1	LLP	D	285	1	23,24,25	1.60	5 (21%)	25,32,34	1.27	2 (8%)
1	LLP	G	285	1	23,24,25	1.62	4 (17%)	25,32,34	1.46	1 (4%)
1	LLP	H	285	1	23,24,25	1.65	4 (17%)	25,32,34	1.18	2 (8%)
1	LLP	B	285	1	23,24,25	1.59	3 (13%)	25,32,34	1.15	2 (8%)
1	LLP	E	285	1	23,24,25	1.67	3 (13%)	25,32,34	1.17	2 (8%)
1	LLP	C	285	1	23,24,25	1.67	5 (21%)	25,32,34	1.10	2 (8%)
1	LLP	J	285	1	23,24,25	1.61	7 (30%)	25,32,34	1.04	1 (4%)
1	LLP	F	285	1	23,24,25	1.61	4 (17%)	25,32,34	1.01	1 (4%)

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
1	LLP	A	285	1	-	2/16/17/19	0/1/1/1
1	LLP	I	285	1	-	2/16/17/19	0/1/1/1
1	LLP	D	285	1	-	6/16/17/19	0/1/1/1
1	LLP	G	285	1	-	8/16/17/19	0/1/1/1
1	LLP	H	285	1	-	4/16/17/19	0/1/1/1
1	LLP	B	285	1	-	7/16/17/19	0/1/1/1
1	LLP	E	285	1	-	8/16/17/19	0/1/1/1
1	LLP	C	285	1	-	7/16/17/19	0/1/1/1
1	LLP	J	285	1	-	3/16/17/19	0/1/1/1
1	LLP	F	285	1	-	4/16/17/19	0/1/1/1

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	285	LLP	C2'-C2	3.95	1.56	1.50
1	I	285	LLP	C4-C4'	3.78	1.54	1.46
1	F	285	LLP	C2'-C2	3.61	1.56	1.50
1	E	285	LLP	C4-C4'	3.59	1.54	1.46
1	I	285	LLP	C2'-C2	3.57	1.56	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	285	LLP	OP4-C5'-C5	5.77	120.18	109.36
1	D	285	LLP	OP4-C5'-C5	4.44	117.68	109.36
1	I	285	LLP	OP4-C5'-C5	3.85	116.57	109.36
1	A	285	LLP	C4-C3-C2	-3.38	118.24	120.14
1	J	285	LLP	OP4-C5'-C5	3.37	115.67	109.36

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	285	LLP	C4-C5-C5'-OP4
1	A	285	LLP	O-C-CA-CB
1	B	285	LLP	C4-C5-C5'-OP4
1	B	285	LLP	C6-C5-C5'-OP4
1	B	285	LLP	C5'-OP4-P-OP1

There are no ring outliers.

9 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	285	LLP	4	0
1	D	285	LLP	2	0
1	G	285	LLP	5	0
1	H	285	LLP	5	0
1	B	285	LLP	2	0
1	E	285	LLP	3	0
1	C	285	LLP	4	0
1	J	285	LLP	1	0
1	F	285	LLP	3	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	383/392 (97%)	-0.77	1 (0%) 90 81	77, 108, 158, 199	0
1	B	380/392 (96%)	-0.68	1 (0%) 90 81	77, 114, 197, 238	0
1	C	383/392 (97%)	-0.82	0 100 100	65, 109, 178, 207	0
1	D	381/392 (97%)	-0.82	0 100 100	75, 114, 166, 204	0
1	E	383/392 (97%)	-0.64	0 100 100	67, 119, 203, 262	0
1	F	383/392 (97%)	-0.79	0 100 100	73, 123, 184, 234	0
1	G	381/392 (97%)	-0.84	0 100 100	82, 141, 211, 255	0
1	H	382/392 (97%)	-0.83	0 100 100	75, 129, 200, 240	0
1	I	381/392 (97%)	-0.75	1 (0%) 90 81	79, 130, 187, 224	0
1	J	381/392 (97%)	-0.70	1 (0%) 90 81	81, 131, 200, 240	0
All	All	3818/3920 (97%)	-0.76	4 (0%) 92 89	65, 122, 195, 262	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	107	LEU	2.8
1	A	120	ILE	2.7
1	I	286	LEU	2.1
1	B	236	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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($\text{\AA}^2$)	Q<0.9
1	LLP	I	285	24/25	0.95	0.07	88,110,126,127	0
1	LLP	J	285	24/25	0.96	0.09	74,112,125,126	0
1	LLP	C	285	24/25	0.97	0.06	66,99,115,121	0
1	LLP	E	285	24/25	0.97	0.08	63,98,112,168	0
1	LLP	A	285	24/25	0.97	0.07	70,106,124,128	0
1	LLP	B	285	24/25	0.97	0.08	73,98,113,114	0
1	LLP	G	285	24/25	0.98	0.07	79,125,137,145	0
1	LLP	H	285	24/25	0.98	0.07	73,109,129,140	0
1	LLP	D	285	24/25	0.98	0.06	70,98,124,149	0
1	LLP	F	285	24/25	0.98	0.06	56,103,132,144	0

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($\text{\AA}^2$)	Q<0.9
3	K	I	501	1/1	0.62	0.33	141,141,141,141	0
2	PT	A	4002	1/1	0.71	0.21	145,145,145,145	1
3	K	H	501	1/1	0.82	0.29	124,124,124,124	0
3	K	E	501	1/1	0.86	0.24	137,137,137,137	0
3	K	B	2001	1/1	0.90	0.19	124,124,124,124	0
3	K	C	501	1/1	0.91	0.11	132,132,132,132	0
2	PT	A	4001	1/1	0.96	0.14	123,123,123,123	1

6.5 Other polymers [i](#)

There are no such residues in this entry.