wwPDB X-ray Structure Validation Summary Report (i)

Jun 19, 2024 – 03:49 AM EDT

PDB ID	:	3W1K
Title	:	Crystal structure of the selenocysteine synthase SelA and tRNASec complex
Authors	:	Itoh, Y.; Sekine, S.; Yokoyama, S.
Deposited on	:	2012-11-15
Resolution	:	7.50 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

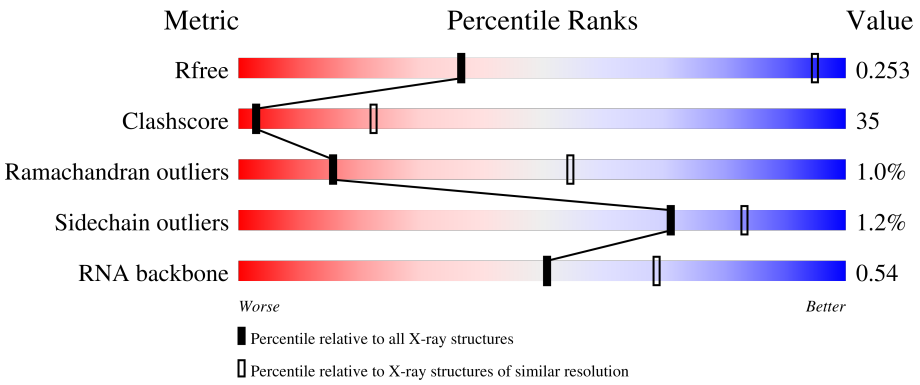
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 7.50 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}	130704	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)
RNA backbone	3102	1079 (11.50-3.00)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	452	44% 54% •
1	B	452	46% 54%
1	C	452	48% 51% •
1	D	452	47% 52% •
1	E	452	46% 53% •
2	F	95	16% 78% • •

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Mol	Chain	Length	Quality of chain
2	G	95	14% 79%
2	H	95	17% 77%
2	I	95	14% 76% 7%
2	J	95	14% 78% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 27660 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
			Total	C	N	O	P	S			
1	A	452	3575	2278	620	665	1	11	0	0	0
1	B	452	3575	2278	620	665	1	11	0	0	0
1	C	452	3575	2278	620	665	1	11	0	0	0
1	D	452	3575	2278	620	665	1	11	0	0	0
1	E	452	3575	2278	620	665	1	11	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ALA	LYS	engineered mutation	UNP O67140
A	21	ALA	LYS	engineered mutation	UNP O67140
A	46	ALA	LYS	engineered mutation	UNP O67140
A	48	ALA	LYS	engineered mutation	UNP O67140
B	19	ALA	LYS	engineered mutation	UNP O67140
B	21	ALA	LYS	engineered mutation	UNP O67140
B	46	ALA	LYS	engineered mutation	UNP O67140
B	48	ALA	LYS	engineered mutation	UNP O67140
C	19	ALA	LYS	engineered mutation	UNP O67140
C	21	ALA	LYS	engineered mutation	UNP O67140
C	46	ALA	LYS	engineered mutation	UNP O67140
C	48	ALA	LYS	engineered mutation	UNP O67140
D	19	ALA	LYS	engineered mutation	UNP O67140
D	21	ALA	LYS	engineered mutation	UNP O67140
D	46	ALA	LYS	engineered mutation	UNP O67140
D	48	ALA	LYS	engineered mutation	UNP O67140
E	19	ALA	LYS	engineered mutation	UNP O67140
E	21	ALA	LYS	engineered mutation	UNP O67140
E	46	ALA	LYS	engineered mutation	UNP O67140

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Chain	Residue	Modelled	Actual	Comment	Reference
E	48	ALA	LYS	engineered mutation	UNP O67140

- Molecule 2 is a RNA chain called selenocysteine tRNA.

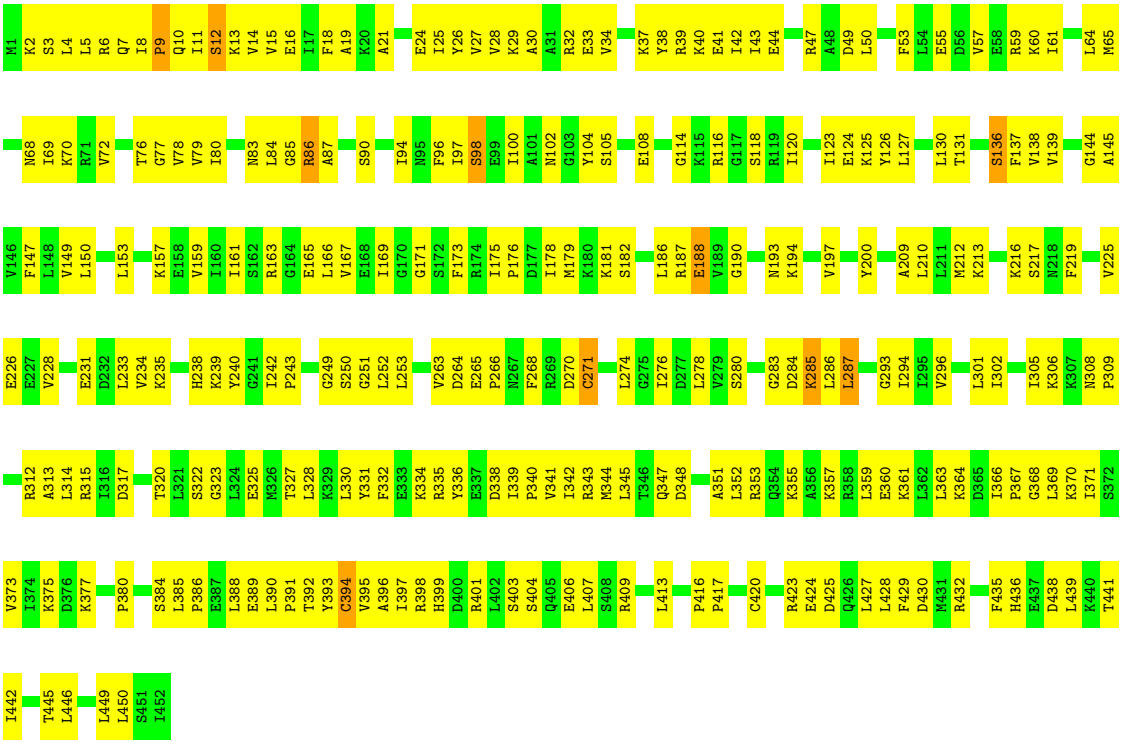
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	F	92	1957	873	342	650	92	0	0	0
2	G	92	1957	873	342	650	92	0	0	0
2	H	92	1957	873	342	650	92	0	0	0
2	I	92	1957	873	342	650	92	0	0	0
2	J	92	1957	873	342	650	92	0	0	0

3 Residue-property plots (i)

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. 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. 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.

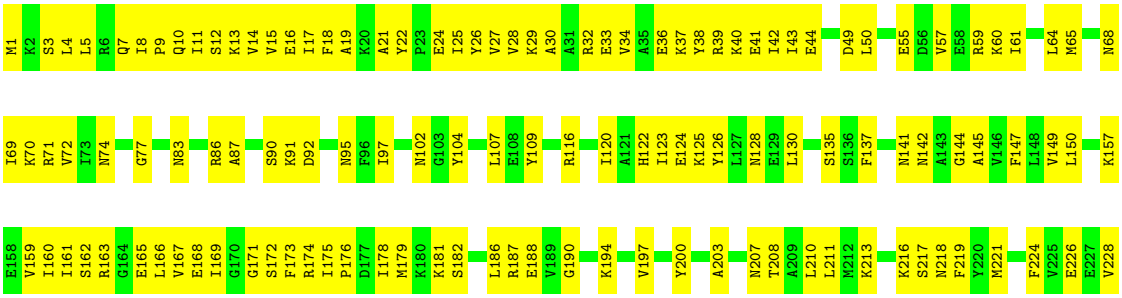
• Molecule 1: L-seryl-tRNA(Sec) selenium transferase

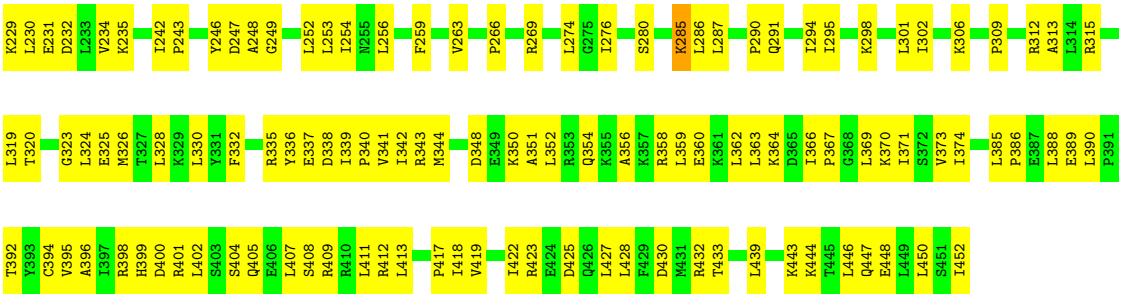
Chain A: 44% 54% •



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

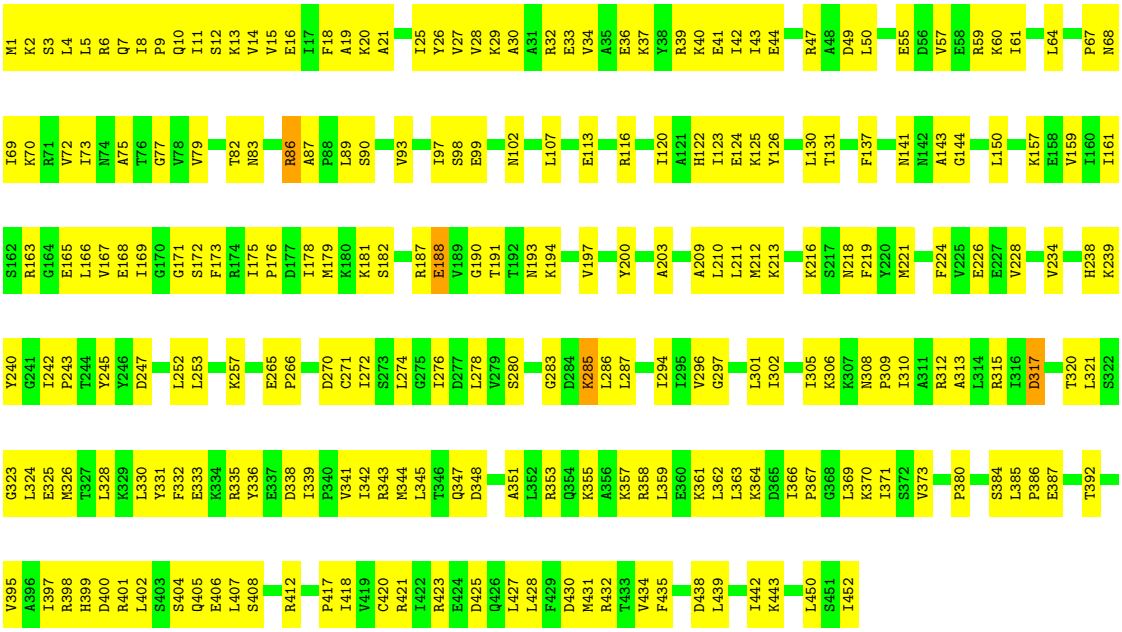
Chain B: 46% 54%





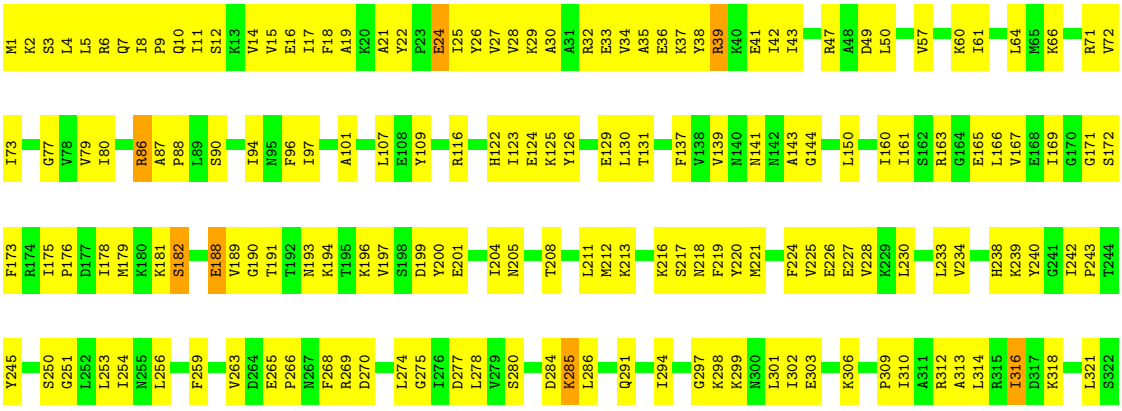
- Molecule 1: L-seryl-tRNA(Sec) selenium transferase

Chain C:



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

Chain D:



G323 L324 E325 M326 K329 L330 Y331 F332 E333 K334 R335 Y336 E337 D338 I339 P340 V341 I342 R343 M344 L345 T346 Q347 D348 A351 L352 R353 Q354 K355 R358 L359 E360 K361 L362 L363 I366 P367 G368 L369 K370 I371 S372 V373 S384 L385 P386 E387 T392 Y393 C394 V395 A396 I397 R398

H399 D400 R401 L402 Q405 E406 L407 S408 R409 R412 L413 A414 E415 P416 P417 I418 V419 C420 R421 I422 R423 Q426 L427 L428 F429 D430 M431 R432 D438 L439 K440 T441 I442 K443 L450 S451 I452

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

Chain E:

M1 K2 S3 L4 L5 R6 Q7 I8 P9 Q10 I11 S12 K13 V14 V15 E16 I17 F18 A19 K20 A21 E24 I25 Y26 V27 V28 K29 A30 A31 R32 E33 V34 A35 E36 K37 Y38 R39 K40 E41 I42 I43 E44 L50 F53 V57 K60 I61 L64 V72 I73 N74 G77

V78 V79 I80 L84 G85 R86 A87 P88 L89 S90 I94 N95 F96 I97 I100 L107 E108 Y109 N110 E113 G114 I120 A121 H122 I123 E124 K125 Y126 L130 S136 F137 V138 V139 N140 N141 N142 A143 V146 F147 L148 T152 E158 V159 I160 I161 S162 R163 G164 E165

L166 V167 E168 I169 F173 R174 I175 P176 D177 I178 M179 L186 R187 E188 V189 G190 T191 T192 N193 K194 V197 Y200 A203 I204 N205 T208 A209 L210 L211 M212 K213 K216 S217 N218 F219 Y220 M221 F224 V225 E226 E227 V228 K229 L230 E231 D232 L233 V234 H238 I242

P243 T244 Y245 Y246 S250 G251 L252 L253 I254 N255 L256 K257 E258 F259 G260 I261 S262 V263 R269 D270 C271 I272 S273 L274 G275 I276 D277 L278 V279 S280 G283 D284 K285 L286 L287 P290 I294 I295 V296 G297 K298 K299 N300 L301 I302 E303 K304 I305 L314 R315 I316 T320 L321

S322 G323 L324 E325 L330 Y331 R335 Y336 E337 D338 I339 P340 V341 I342 R343 M344 Q347 D348 A351 L352 R353 R358 L359 E360 L363 K364 D365 I366 P367 G368 L369 K370 I371 S384 L385 P386 T392 Y393 A396 I397 R398 H399 D400 R401 Q405 E406 L407 S408 R409

R412 P417 I418 V419 C420 R421 I422 R423 E424 D425 Q426 L427 L428 F429 D430 M431 R432 F435 H436 E437 D438 L439 I442 K443 K444 T445 L446 Q447 E448 L449 L450 S451 I452

- Molecule 2: selenocysteine tRNA

Chain F:

G1 G2 G3 A4 G5 U5A A6 G7 A8 U9 G14 C15 U16 G18 G19 U20 G20A C24 U25 C26 C27 U28 A29 G30 A31 C32 U33 U34 C35 A36 A37 A38 U39 C40 U41 A42 C42A G43 G44 U45 C46 U47 C47A G47B A47E U47F U47G U47H A47I A47J G47K C47L G47M A47N G47O A47P G48

G53 U54 U55 C56 G57 A58 U59 U60 C61 C62 C63 A64 C65 A66 U67 A67A C68 U69 C70 C71 C72 G73 C C A

- Molecule 2: selenocysteine tRNA

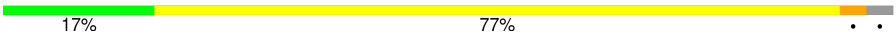
Chain G:

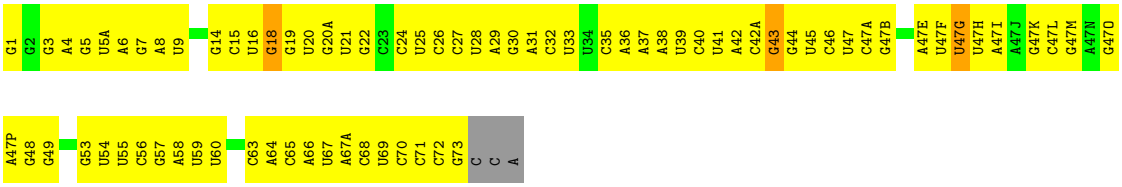
G1 G2 G3 A4 G5 U5A A6 G7 A8 U9 A10 G14 C15 U16 G18 G19 U20 G20A C24 U25 C26 C27 U28 A29 G30 A31 C32 U33 U34 C35 A36 A37 A38 U39 C40 U41 A42 C42A G43 G44 U45 C46 U47 C47A G47B C47C U47D A47E U47F U47G U47H A47I A47J G47K C47L G47M A47N G47O

A47P G48 G49 G53 U54 U55 C56 G57 A58 U59 U60 C63 A64 C65 A66 U67 A67A C68 U69 C70 C71 C72 G73 C C A

- Molecule 2: selenocysteine tRNA

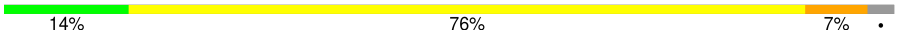
Chain H:

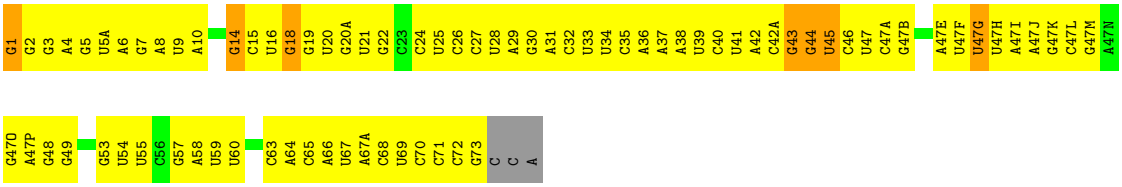




• Molecule 2: selenocysteine tRNA

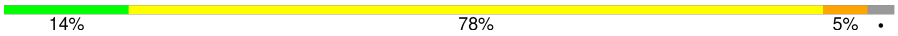
Chain I:

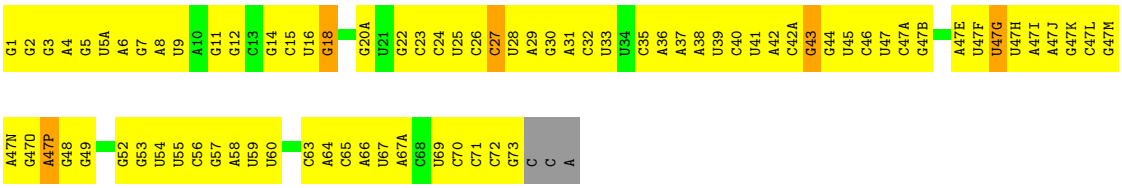




• Molecule 2: selenocysteine tRNA

Chain J:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	148.55Å 355.97Å 165.50Å 90.00° 115.41° 90.00°	Depositor
Resolution (Å)	49.94 – 7.50 49.94 – 7.49	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.94-7.50) 98.0 (49.94-7.49)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 7.37Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.194 , 0.240 0.198 , 0.253	Depositor DCC
R_{free} test set	475 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	391.5	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 562.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.085 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.70	EDS
Total number of atoms	27660	wwPDB-VP
Average B, all atoms (Å^2)	525.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.41	0/3597	0.65	0/4831
1	B	0.39	0/3597	0.65	0/4831
1	C	0.39	0/3597	0.64	0/4831
1	D	0.41	0/3597	0.65	0/4831
1	E	0.40	0/3597	0.64	0/4831
2	F	0.49	1/2185 (0.0%)	0.75	0/3401
2	G	0.44	1/2185 (0.0%)	0.73	0/3401
2	H	0.42	1/2185 (0.0%)	0.73	0/3401
2	I	0.43	1/2185 (0.0%)	0.72	0/3401
2	J	0.43	1/2185 (0.0%)	0.72	2/3401 (0.1%)
All	All	0.42	5/28910 (0.0%)	0.68	2/41160 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	G	OP3-P	-7.24	1.52	1.61
2	I	1	G	OP3-P	-7.05	1.52	1.61
2	J	1	G	OP3-P	-7.05	1.52	1.61
2	H	1	G	OP3-P	-6.86	1.52	1.61
2	G	1	G	OP3-P	-6.77	1.53	1.61

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	47(P)	A	OP2-P-O3'	6.24	118.93	105.20
2	J	27	C	OP2-P-O3'	5.73	117.81	105.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3575	0	3758	296	0
1	B	3575	0	3758	290	0
1	C	3575	0	3758	284	0
1	D	3575	0	3758	300	0
1	E	3575	0	3758	256	0
2	F	1957	0	989	102	0
2	G	1957	0	989	124	0
2	H	1957	0	989	105	0
2	I	1957	0	989	112	0
2	J	1957	0	989	91	0
All	All	27660	0	23735	1788	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 35.

The worst 5 of 1788 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:157:LYS:HE2	1:C:209:ALA:HB2	1.27	1.14
1:B:1:MET:HG3	1:B:4:LEU:HD12	1.31	1.12
1:C:102:ASN:HB3	1:D:71:ARG:HH22	1.15	1.08
1:A:10:GLN:H	1:A:13:LYS:HD2	1.13	1.08
2:J:32:C:H2'	2:J:33:U:C6	1.93	1.02

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	449/452 (99%)	423 (94%)	22 (5%)	4 (1%)	17	57
1	B	449/452 (99%)	419 (93%)	25 (6%)	5 (1%)	14	52
1	C	449/452 (99%)	421 (94%)	24 (5%)	4 (1%)	17	57
1	D	449/452 (99%)	421 (94%)	24 (5%)	4 (1%)	17	57
1	E	449/452 (99%)	420 (94%)	23 (5%)	6 (1%)	12	48
All	All	2245/2260 (99%)	2104 (94%)	118 (5%)	23 (1%)	15	54

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	9	PRO
1	E	9	PRO
1	B	124	GLU
1	C	124	GLU
1	D	124	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	390/390 (100%)	380 (97%)	10 (3%)	46	66
1	B	390/390 (100%)	389 (100%)	1 (0%)	92	95
1	C	390/390 (100%)	385 (99%)	5 (1%)	69	81
1	D	390/390 (100%)	384 (98%)	6 (2%)	65	80
1	E	390/390 (100%)	389 (100%)	1 (0%)	92	95
All	All	1950/1950 (100%)	1927 (99%)	23 (1%)	71	83

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	384	SER

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Mol	Chain	Res	Type
1	D	39	ARG
1	D	24	GLU
1	D	172	SER
1	A	271	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	122	HIS
1	E	405	GLN
1	C	405	GLN
1	E	238	HIS
1	C	347	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	F	91/95 (95%)	6 (6%)	0
2	G	91/95 (95%)	6 (6%)	0
2	H	91/95 (95%)	6 (6%)	0
2	I	91/95 (95%)	9 (9%)	1 (1%)
2	J	91/95 (95%)	6 (6%)	0
All	All	455/475 (95%)	33 (7%)	1 (0%)

5 of 33 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	F	18	G
2	F	20(A)	G
2	F	33	U
2	F	42(A)	C
2	F	43	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	I	44	G

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

5 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	1.17	2 (8%)	25,32,34	0.97	1 (4%)
1	LLP	C	285	1	23,24,25	1.14	2 (8%)	25,32,34	0.92	1 (4%)
1	LLP	E	285	1	23,24,25	1.14	1 (4%)	25,32,34	1.04	1 (4%)
1	LLP	D	285	1	23,24,25	1.14	1 (4%)	25,32,34	0.91	1 (4%)
1	LLP	B	285	1	23,24,25	1.23	2 (8%)	25,32,34	1.04	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	C	285	1	-	4/16/17/19	0/1/1/1
1	LLP	E	285	1	-	2/16/17/19	0/1/1/1
1	LLP	D	285	1	-	3/16/17/19	0/1/1/1
1	LLP	B	285	1	-	6/16/17/19	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	LLP	C4-C4'	-2.80	1.40	1.46
1	E	285	LLP	C4-C4'	-2.58	1.41	1.46
1	A	285	LLP	C4-C4'	-2.47	1.41	1.46
1	C	285	LLP	C4-C4'	-2.24	1.41	1.46
1	A	285	LLP	C2'-C2	2.24	1.53	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	285	LLP	OP4-P-OP1	2.80	114.00	106.44
1	B	285	LLP	OP4-P-OP1	2.65	113.59	106.44
1	A	285	LLP	OP4-P-OP1	2.43	113.00	106.44
1	D	285	LLP	OP4-P-OP1	2.33	112.73	106.44
1	C	285	LLP	OP4-P-OP1	2.31	112.69	106.44

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	C-CA-CB-CG
1	B	285	LLP	O-C-CA-CB

There are no ring outliers.

5 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	285	LLP	4	0
1	C	285	LLP	7	0
1	E	285	LLP	3	0
1	D	285	LLP	3	0
1	B	285	LLP	6	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.