



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:39 am BST

PDB ID : 4YRA
Title : mouse TDH in the apo form
Authors : He, C.; Li, F.
Deposited on : 2015-03-14
Resolution : 2.65 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

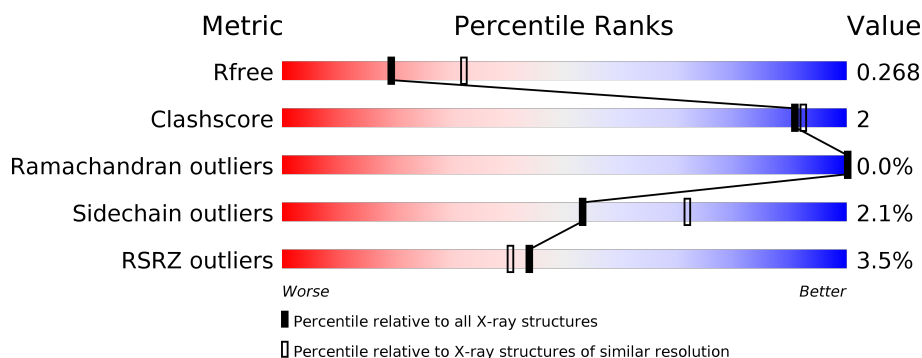
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>6%</div> <div>11%</div> </div> </div>
1	B	329	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>6%</div> <div>11%</div> </div> </div>
1	C	329	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>6%</div> <div>11%</div> </div> </div>
1	D	329	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>•</div> <div>11%</div> </div> </div>
1	E	329	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>•</div> <div>12%</div> </div> </div>
1	F	329	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>•</div> <div>13%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	329	<div><div><div></div><div></div><div></div></div><div>2%81%8%11%</div></div>
1	H	329	<div><div><div></div><div></div><div></div></div><div>3%84%5%10%</div></div>
1	I	329	<div><div><div></div><div></div><div></div></div><div>2%84%12%</div></div>
1	J	329	<div><div><div></div><div></div><div></div></div><div>3%81%8%11%</div></div>
1	K	329	<div><div><div></div><div></div><div></div></div><div>5%83%13%</div></div>
1	L	329	<div><div><div></div><div></div><div></div></div><div>2%86%9%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27791 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-threonine 3-dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2295	1465	396	421	13			
1	B	294	Total	C	N	O	S	0	0	0
			2324	1483	404	424	13			
1	C	293	Total	C	N	O	S	0	0	0
			2321	1485	403	420	13			
1	D	292	Total	C	N	O	S	0	0	0
			2307	1484	398	412	13			
1	E	291	Total	C	N	O	S	0	0	0
			2313	1483	401	416	13			
1	F	287	Total	C	N	O	S	0	0	0
			2296	1475	399	409	13			
1	G	294	Total	C	N	O	S	0	0	0
			2310	1482	399	416	13			
1	H	295	Total	C	N	O	S	0	0	0
			2334	1494	406	421	13			
1	I	291	Total	C	N	O	S	0	0	0
			2308	1480	398	417	13			
1	J	292	Total	C	N	O	S	0	0	0
			2294	1466	398	417	13			
1	K	286	Total	C	N	O	S	0	0	0
			2269	1451	393	412	13			
1	L	299	Total	C	N	O	S	0	0	0
			2350	1503	407	427	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	HIS	-	expression tag	UNP Q8K3F7
A	46	MET	-	expression tag	UNP Q8K3F7
B	45	HIS	-	expression tag	UNP Q8K3F7
B	46	MET	-	expression tag	UNP Q8K3F7
C	45	HIS	-	expression tag	UNP Q8K3F7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	46	MET	-	expression tag	UNP Q8K3F7
D	45	HIS	-	expression tag	UNP Q8K3F7
D	46	MET	-	expression tag	UNP Q8K3F7
E	45	HIS	-	expression tag	UNP Q8K3F7
E	46	MET	-	expression tag	UNP Q8K3F7
F	45	HIS	-	expression tag	UNP Q8K3F7
F	46	MET	-	expression tag	UNP Q8K3F7
G	45	HIS	-	expression tag	UNP Q8K3F7
G	46	MET	-	expression tag	UNP Q8K3F7
H	45	HIS	-	expression tag	UNP Q8K3F7
H	46	MET	-	expression tag	UNP Q8K3F7
I	45	HIS	-	expression tag	UNP Q8K3F7
I	46	MET	-	expression tag	UNP Q8K3F7
J	45	HIS	-	expression tag	UNP Q8K3F7
J	46	MET	-	expression tag	UNP Q8K3F7
K	45	HIS	-	expression tag	UNP Q8K3F7
K	46	MET	-	expression tag	UNP Q8K3F7
L	45	HIS	-	expression tag	UNP Q8K3F7
L	46	MET	-	expression tag	UNP Q8K3F7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total O 6 6	0	0
2	B	11	Total O 11 11	0	0
2	C	6	Total O 6 6	0	0
2	D	6	Total O 6 6	0	0
2	E	6	Total O 6 6	0	0
2	F	9	Total O 9 9	0	0
2	G	8	Total O 8 8	0	0
2	H	2	Total O 2 2	0	0
2	I	3	Total O 3 3	0	0
2	J	4	Total O 4 4	0	0

Continued on next page...

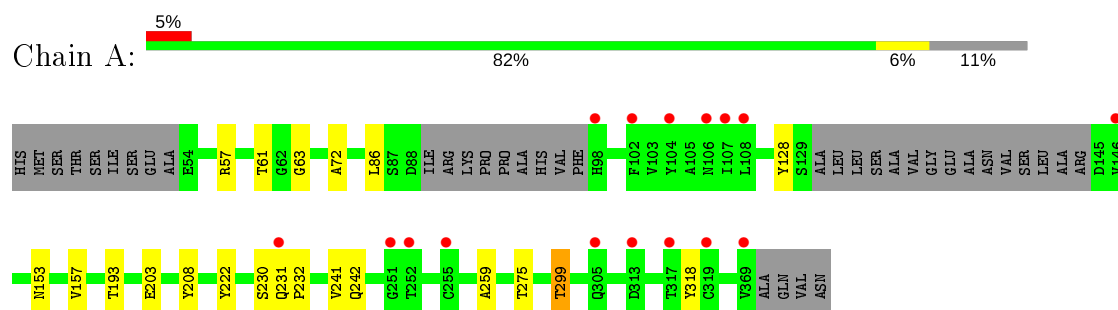
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	K	2	Total	O	0	0
			2	2		
2	L	7	Total	O	0	0
			7	7		

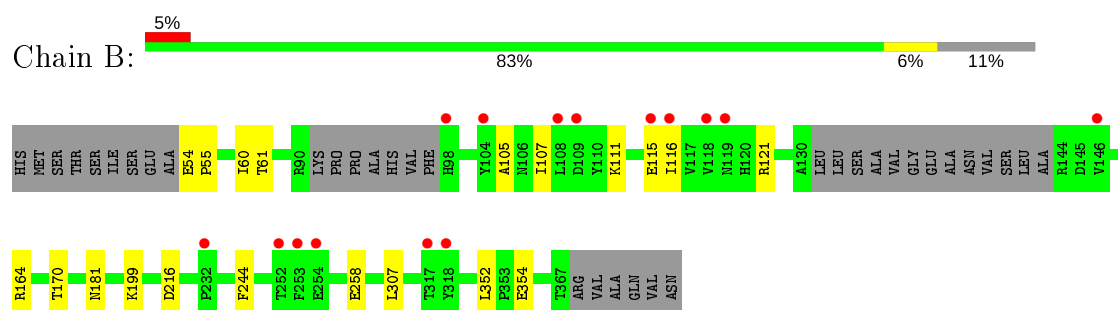
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

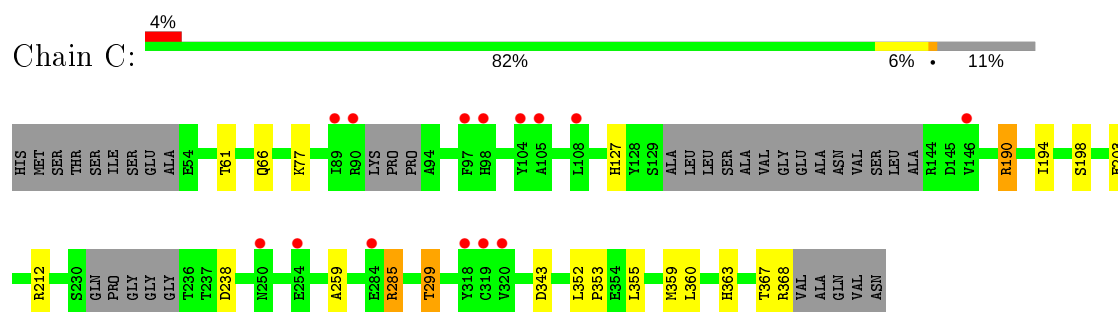
- Molecule 1: L-threonine 3-dehydrogenase, mitochondrial



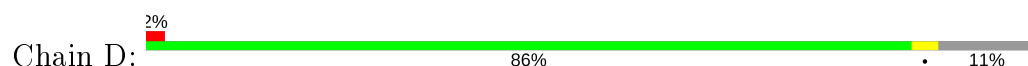
- Molecule 1: L-threonine 3-dehydrogenase, mitochondrial

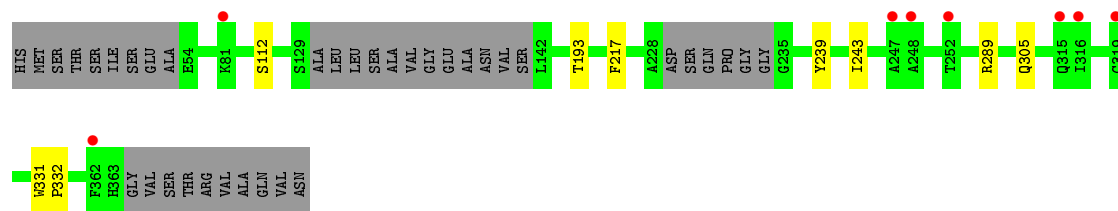


- Molecule 1: L-threonine 3-dehydrogenase, mitochondrial

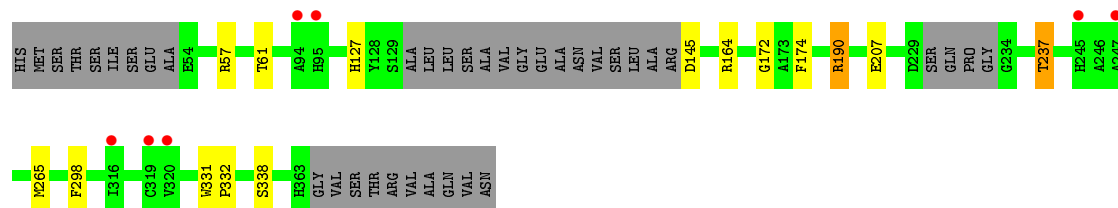
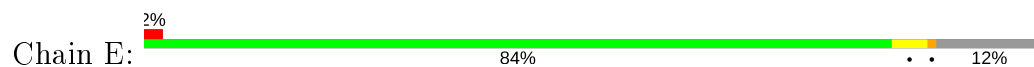


- Molecule 1: L-threonine 3-dehydrogenase, mitochondrial

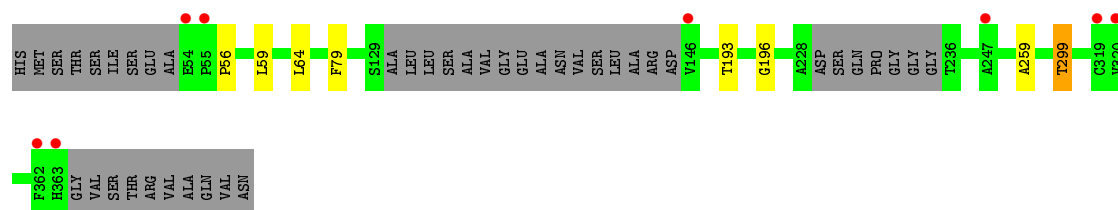
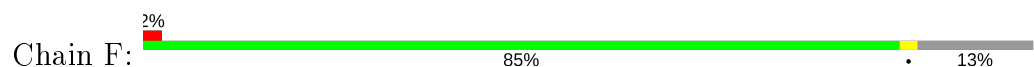




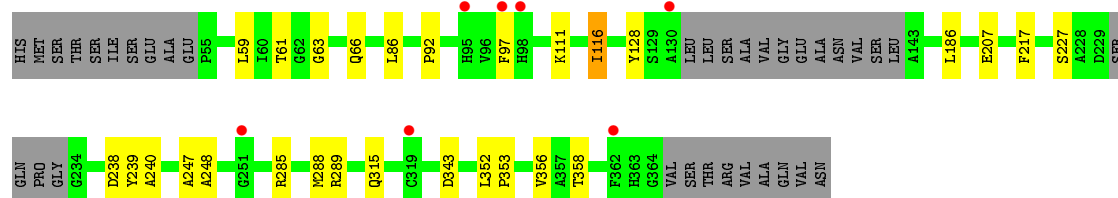
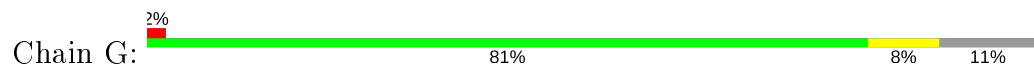
- Molecule 1: L-threonine 3-dehydrogenase, mitochondrial



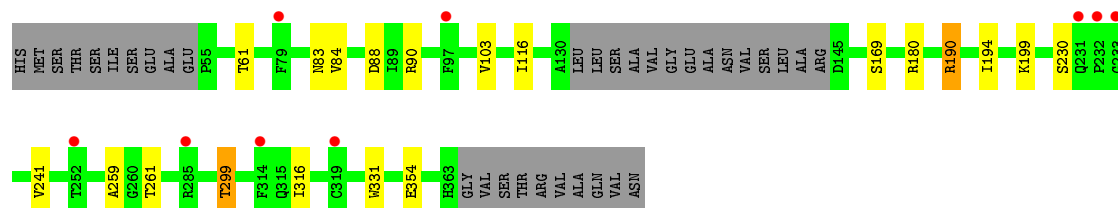
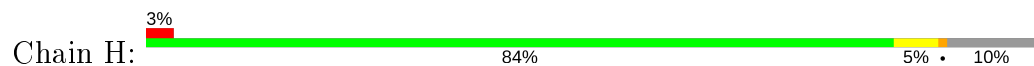
- Molecule 1: L-threonine 3-dehydrogenase, mitochondrial



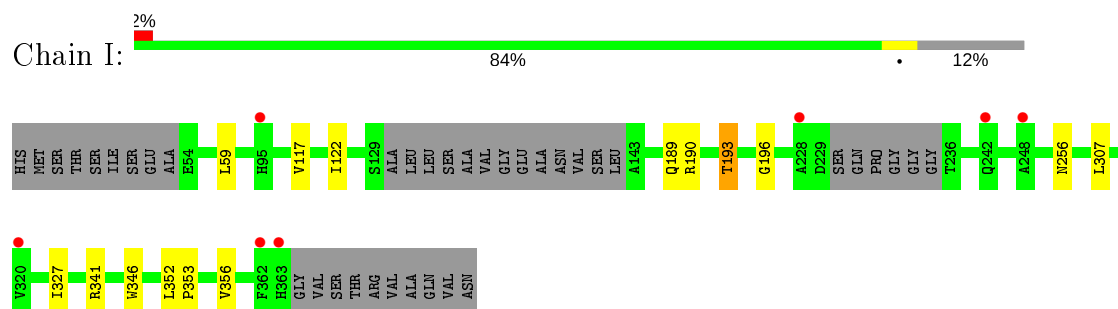
- Molecule 1: L-threonine 3-dehydrogenase, mitochondrial



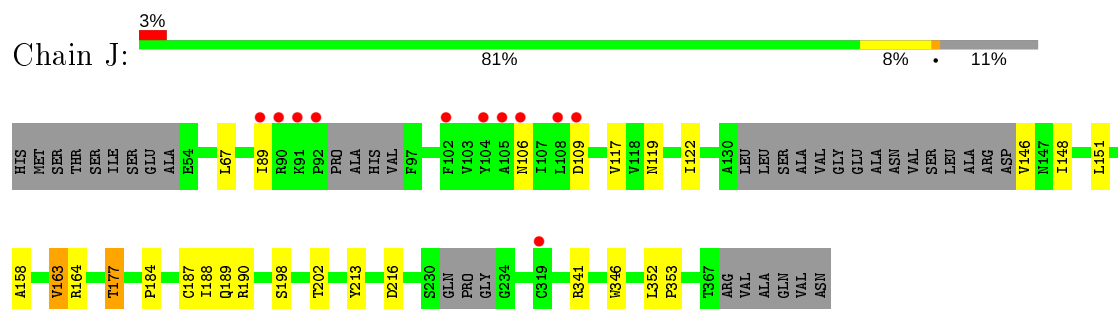
- Molecule 1: L-threonine 3-dehydrogenase, mitochondrial



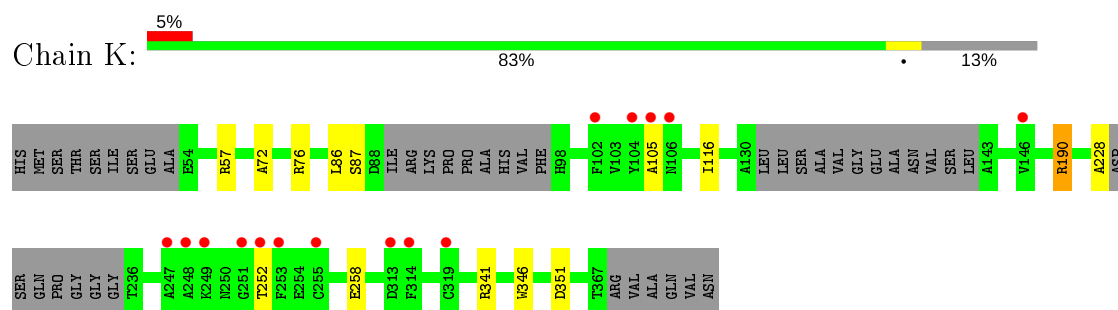
- Molecule 1: L-threonine 3-dehydrogenase, mitochondrial



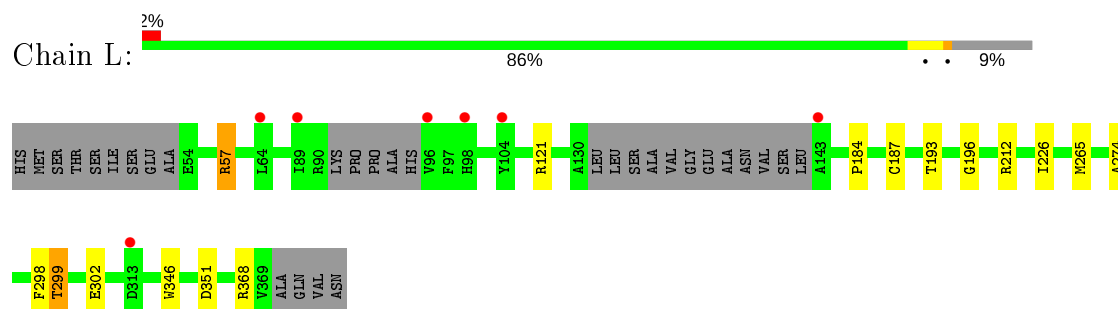
- Molecule 1: L-threonine 3-dehydrogenase, mitochondrial



- Molecule 1: L-threonine 3-dehydrogenase, mitochondrial



- Molecule 1: L-threonine 3-dehydrogenase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.44Å 157.31Å 162.34Å 90.00° 97.00° 90.00°	Depositor
Resolution (Å)	44.35 – 2.65 44.35 – 2.65	Depositor EDS
% Data completeness (in resolution range)	91.5 (44.35-2.65) 91.5 (44.35-2.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.217 , 0.271 0.217 , 0.268	Depositor DCC
R_{free} test set	6300 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	58.5	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27791	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.29	0/2353	0.52	0/3200
1	B	0.30	0/2383	0.53	0/3239
1	C	0.29	0/2380	0.50	0/3236
1	D	0.28	0/2369	0.49	0/3224
1	E	0.28	0/2375	0.48	0/3230
1	F	0.29	0/2358	0.50	0/3206
1	G	0.29	0/2372	0.52	0/3228
1	H	0.29	0/2398	0.49	0/3264
1	I	0.30	0/2370	0.53	0/3227
1	J	0.31	0/2351	0.53	0/3196
1	K	0.29	0/2325	0.50	0/3159
1	L	0.31	0/2410	0.54	0/3279
All	All	0.29	0/28444	0.51	0/38688

There are no bond length outliers.

There are no bond angle outliers.

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	2295	0	2237	11	0
1	B	2324	0	2277	8	0
1	C	2321	0	2264	11	0
1	D	2307	0	2263	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2313	0	2265	8	0
1	F	2296	0	2266	3	0
1	G	2310	0	2253	14	0
1	H	2334	0	2282	8	0
1	I	2308	0	2248	8	0
1	J	2294	0	2242	16	0
1	K	2269	0	2230	8	0
1	L	2350	0	2291	9	0
2	A	6	0	0	0	0
2	B	11	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
2	E	6	0	0	0	0
2	F	9	0	0	0	0
2	G	8	0	0	0	0
2	H	2	0	0	0	0
2	I	3	0	0	0	0
2	J	4	0	0	1	0
2	K	2	0	0	0	0
2	L	7	0	0	0	0
All	All	27791	0	27118	95	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 2.

All (95) 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:K:87:SER:OG	1:K:105:ALA:HB3	1.92	0.69
1:L:226:ILE:HD11	1:L:265:MET:CE	2.24	0.68
1:I:190:ARG:NH2	1:J:189:GLN:OE1	2.29	0.65
1:J:341:ARG:HG2	1:J:346:TRP:O	1.98	0.64
1:A:61:THR:O	1:A:128:TYR:N	2.32	0.63
1:H:230:SER:HB2	1:H:241:VAL:HG21	1.82	0.62
1:H:88:ASP:OD1	1:H:90:ARG:NH1	2.33	0.61
1:G:61:THR:O	1:G:128:TYR:N	2.30	0.60
1:J:177:THR:HG23	1:J:188:ILE:HG21	1.83	0.59
1:C:203:GLU:OE1	1:E:190:ARG:NH2	2.36	0.59
1:J:164:ARG:HG3	1:J:164:ARG:HH11	1.67	0.58
1:I:117:VAL:HA	1:I:122:ILE:HD12	1.85	0.58
1:A:259:ALA:O	1:A:299:THR:HG23	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:259:ALA:O	1:F:299:THR:HG23	2.05	0.56
1:B:111:LYS:O	1:B:115:GLU:OE1	2.23	0.55
1:I:59:LEU:HB2	1:I:122:ILE:HD13	1.87	0.55
1:A:230:SER:HB3	1:A:241:VAL:HG11	1.90	0.53
1:J:146:VAL:HG12	1:J:146:VAL:O	2.09	0.52
1:L:265:MET:HG3	1:L:298:PHE:CZ	2.44	0.52
1:I:189:GLN:OE1	1:J:190:ARG:NH2	2.42	0.52
1:J:164:ARG:NH1	1:J:216:ASP:OD2	2.43	0.52
1:A:231:GLN:N	1:A:232:PRO:HD2	2.25	0.51
1:L:299:THR:HG22	1:L:302:GLU:H	1.76	0.50
1:G:111:LYS:HD2	1:J:213:TYR:CZ	2.47	0.50
1:B:61:THR:HB	1:B:107:ILE:HD11	1.95	0.48
1:E:265:MET:HG3	1:E:298:PHE:CZ	2.48	0.48
1:E:237:THR:O	1:E:237:THR:CG2	2.61	0.48
1:K:341:ARG:HG2	1:K:346:TRP:O	2.14	0.48
1:C:259:ALA:O	1:C:299:THR:HG23	2.14	0.47
1:H:180:ARG:NH2	1:H:331:TRP:O	2.47	0.47
1:G:59:LEU:HG	1:G:116:ILE:HD11	1.97	0.47
1:H:103:VAL:HG11	1:H:116:ILE:HD12	1.94	0.47
1:C:360:LEU:O	1:C:363:HIS:O	2.33	0.47
1:D:217:PHE:O	1:D:289:ARG:HD2	2.15	0.47
1:G:92:PRO:HG2	1:G:97:PHE:CE1	2.50	0.47
1:J:198:SER:O	1:J:202:THR:HG23	2.15	0.47
1:J:117:VAL:HA	1:J:122:ILE:HD12	1.97	0.47
1:B:105:ALA:HB2	1:B:116:ILE:CD1	2.46	0.46
1:A:63:GLY:HA3	1:A:86:LEU:HD22	1.98	0.46
1:C:285:ARG:HG2	1:C:343:ASP:O	2.15	0.46
1:I:193:THR:HG22	1:I:196:GLY:H	1.80	0.46
1:G:217:PHE:O	1:G:289:ARG:HD2	2.16	0.46
1:G:285:ARG:HG3	1:G:343:ASP:O	2.16	0.46
1:H:259:ALA:O	1:H:299:THR:OG1	2.33	0.45
1:E:61:THR:OG1	1:E:127:HIS:HA	2.17	0.45
1:F:193:THR:HG23	1:F:196:GLY:H	1.82	0.45
1:G:352:LEU:HB3	1:G:353:PRO:HD3	1.98	0.45
1:E:174:PHE:HB2	1:E:332:PRO:HD3	1.98	0.45
1:E:237:THR:O	1:E:237:THR:HG23	2.16	0.45
1:B:164:ARG:NH1	1:B:216:ASP:OD2	2.50	0.44
1:C:355:LEU:O	1:C:359:MET:HB2	2.17	0.44
1:C:190:ARG:NH1	1:E:207:GLU:OE2	2.50	0.44
1:B:170:THR:HG22	1:B:199:LYS:HG3	1.99	0.44
1:L:184:PRO:HG2	1:L:187:CYS:HB3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ASN:O	1:A:157:VAL:HG23	2.18	0.44
1:G:66:GLN:NE2	1:G:227:SER:OG	2.51	0.44
1:L:193:THR:HG23	1:L:196:GLY:H	1.83	0.43
1:B:244:PHE:CE1	1:B:307:LEU:HD21	2.53	0.43
1:I:307:LEU:HD23	1:I:356:VAL:HG13	2.00	0.43
1:I:352:LEU:HB3	1:I:353:PRO:HD3	1.99	0.43
1:J:352:LEU:HB3	1:J:353:PRO:HD3	1.99	0.43
1:C:61:THR:OG1	1:C:127:HIS:HA	2.18	0.43
1:E:172:GLY:HA2	1:E:331:TRP:NE1	2.34	0.43
1:A:203:GLU:OE1	1:H:190:ARG:NH2	2.52	0.43
1:L:274:ALA:HB2	1:L:346:TRP:CZ3	2.53	0.43
1:G:247:ALA:O	1:G:248:ALA:HB3	2.19	0.43
1:J:184:PRO:HG2	1:J:187:CYS:HB3	2.00	0.43
1:A:259:ALA:HA	1:A:318:TYR:CE1	2.53	0.43
1:K:105:ALA:HB2	1:K:116:ILE:HD13	1.99	0.43
1:L:226:ILE:HD11	1:L:265:MET:HE1	2.00	0.43
1:L:57:ARG:HD2	1:L:121:ARG:O	2.18	0.43
1:G:207:GLU:OE2	1:K:190:ARG:NH1	2.52	0.42
1:G:239:TYR:CG	1:G:240:ALA:N	2.87	0.42
1:D:331:TRP:HB3	1:D:332:PRO:HD2	2.01	0.42
1:G:63:GLY:HA3	1:G:86:LEU:CD2	2.49	0.42
1:C:368:ARG:NH2	1:K:351:ASP:OD2	2.52	0.42
1:B:354:GLU:HG2	1:L:368:ARG:HD3	2.02	0.41
1:F:56:PRO:HD2	1:F:79:PHE:CD1	2.55	0.41
1:G:186:LEU:HG	1:G:288:MET:HE1	2.02	0.41
1:B:54:GLU:HB3	1:B:55:PRO:HD3	2.02	0.41
1:J:158:ALA:HA	1:J:163:VAL:HG22	2.01	0.41
1:I:341:ARG:HG2	1:I:346:TRP:O	2.20	0.41
1:J:151:LEU:HD13	1:J:202:THR:HG22	2.03	0.41
1:J:177:THR:HG22	2:J:402:HOH:O	2.20	0.41
1:K:76:ARG:NH2	1:K:86:LEU:HD13	2.35	0.41
1:A:222:TYR:OH	1:A:275:THR:OG1	2.26	0.41
1:C:360:LEU:HB2	1:C:367:THR:HG21	2.03	0.41
1:J:146:VAL:HA	1:J:148:ILE:HG22	2.03	0.41
1:C:352:LEU:HB3	1:C:353:PRO:HD3	2.03	0.41
1:G:285:ARG:CG	1:G:343:ASP:O	2.69	0.41
1:H:169:SER:HA	1:H:199:LYS:HD2	2.03	0.41
1:A:208:TYR:CZ	1:H:194:ILE:HB	2.56	0.40
1:K:72:ALA:HB2	1:K:86:LEU:HD11	2.03	0.40
1:A:72:ALA:HB2	1:A:86:LEU:HD21	2.02	0.40
1:C:77:LYS:HE2	1:K:228:ALA:HB1	2.02	0.40

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	286/329 (87%)	275 (96%)	11 (4%)	0	100	100
1	B	288/329 (88%)	279 (97%)	9 (3%)	0	100	100
1	C	285/329 (87%)	276 (97%)	9 (3%)	0	100	100
1	D	286/329 (87%)	275 (96%)	11 (4%)	0	100	100
1	E	285/329 (87%)	280 (98%)	5 (2%)	0	100	100
1	F	281/329 (85%)	271 (96%)	10 (4%)	0	100	100
1	G	288/329 (88%)	275 (96%)	13 (4%)	0	100	100
1	H	291/329 (88%)	282 (97%)	9 (3%)	0	100	100
1	I	285/329 (87%)	275 (96%)	10 (4%)	0	100	100
1	J	284/329 (86%)	278 (98%)	5 (2%)	1 (0%)	34	48
1	K	278/329 (84%)	268 (96%)	10 (4%)	0	100	100
1	L	293/329 (89%)	283 (97%)	10 (3%)	0	100	100
All	All	3430/3948 (87%)	3317 (97%)	112 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	89	ILE

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	244/277 (88%)	240 (98%)	4 (2%)	62	78
1	B	248/277 (90%)	243 (98%)	5 (2%)	55	73
1	C	247/277 (89%)	239 (97%)	8 (3%)	39	56
1	D	244/277 (88%)	239 (98%)	5 (2%)	55	73
1	E	246/277 (89%)	240 (98%)	6 (2%)	49	67
1	F	246/277 (89%)	243 (99%)	3 (1%)	71	84
1	G	243/277 (88%)	238 (98%)	5 (2%)	53	72
1	H	248/277 (90%)	240 (97%)	8 (3%)	39	56
1	I	245/277 (88%)	242 (99%)	3 (1%)	71	84
1	J	243/277 (88%)	237 (98%)	6 (2%)	47	66
1	K	242/277 (87%)	238 (98%)	4 (2%)	60	77
1	L	248/277 (90%)	244 (98%)	4 (2%)	62	78
All	All	2944/3324 (89%)	2883 (98%)	61 (2%)	53	72

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	193	THR
1	A	242	GLN
1	A	299	THR
1	B	60	ILE
1	B	121	ARG
1	B	181	ASN
1	B	258	GLU
1	B	352	LEU
1	C	66	GLN
1	C	190	ARG
1	C	194	ILE
1	C	198	SER
1	C	212	ARG
1	C	238	ASP
1	C	285	ARG
1	C	299	THR
1	D	112	SER
1	D	193	THR
1	D	239	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	243	ILE
1	D	305	GLN
1	E	57	ARG
1	E	145	ASP
1	E	164	ARG
1	E	190	ARG
1	E	237	THR
1	E	338	SER
1	F	59	LEU
1	F	64	LEU
1	F	299	THR
1	G	116	ILE
1	G	238	ASP
1	G	315	GLN
1	G	356	VAL
1	G	358	THR
1	H	61	THR
1	H	83	ASN
1	H	84	VAL
1	H	190	ARG
1	H	261	THR
1	H	299	THR
1	H	316	ILE
1	H	354	GLU
1	I	193	THR
1	I	256	ASN
1	I	327	ILE
1	J	67	LEU
1	J	106	ASN
1	J	109	ASP
1	J	119	ASN
1	J	163	VAL
1	J	177	THR
1	K	57	ARG
1	K	190	ARG
1	K	252	THR
1	K	258	GLU
1	L	57	ARG
1	L	212	ARG
1	L	299	THR
1	L	351	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	153	ASN
1	B	83	ASN
1	B	119	ASN
1	B	153	ASN
1	B	325	GLN
1	C	83	ASN
1	G	66	GLN
1	H	66	GLN
1	I	153	ASN
1	J	83	ASN
1	J	152	HIS
1	L	152	HIS
1	L	361	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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 ⓘ

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	292/329 (88%)	0.36	16 (5%) 25 21	48, 62, 94, 128	0
1	B	294/329 (89%)	0.23	15 (5%) 28 25	41, 58, 91, 122	0
1	C	293/329 (89%)	0.37	14 (4%) 30 27	52, 68, 103, 140	0
1	D	292/329 (88%)	0.18	8 (2%) 54 50	48, 67, 100, 118	0
1	E	291/329 (88%)	0.15	7 (2%) 59 54	53, 69, 101, 118	0
1	F	287/329 (87%)	0.11	8 (2%) 53 49	42, 63, 97, 116	0
1	G	294/329 (89%)	-0.01	7 (2%) 59 54	42, 61, 95, 113	0
1	H	295/329 (89%)	0.20	9 (3%) 49 45	52, 73, 101, 131	0
1	I	291/329 (88%)	0.01	7 (2%) 59 54	41, 60, 92, 107	0
1	J	292/329 (88%)	0.20	11 (3%) 40 36	37, 57, 94, 126	0
1	K	286/329 (86%)	0.17	15 (5%) 27 24	41, 62, 96, 114	0
1	L	299/329 (90%)	-0.00	7 (2%) 60 56	35, 50, 98, 128	0
All	All	3506/3948 (88%)	0.16	124 (3%) 44 40	35, 64, 98, 140	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	319	CYS	5.6
1	L	98	HIS	4.9
1	K	252	THR	4.7
1	K	248	ALA	4.6
1	C	146	VAL	4.5
1	J	106	ASN	4.3
1	H	233	GLY	4.3
1	J	89	ILE	4.3
1	K	319	CYS	4.2
1	K	105	ALA	4.1
1	E	319	CYS	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	319	CYS	4.0
1	G	97	PHE	3.9
1	C	104	TYR	3.8
1	J	91	LYS	3.8
1	H	232	PRO	3.8
1	H	97	PHE	3.7
1	D	315	GLN	3.7
1	J	104	TYR	3.7
1	A	102	PHE	3.6
1	K	146	VAL	3.6
1	A	146	VAL	3.6
1	C	319	CYS	3.6
1	C	97	PHE	3.6
1	A	369	VAL	3.5
1	E	94	ALA	3.5
1	A	319	CYS	3.5
1	L	104	TYR	3.4
1	C	108	LEU	3.4
1	E	95	HIS	3.4
1	K	253	PHE	3.4
1	J	92	PRO	3.4
1	B	232	PRO	3.4
1	F	54	GLU	3.4
1	C	98	HIS	3.3
1	E	320	VAL	3.3
1	K	102	PHE	3.2
1	B	252	THR	3.2
1	D	247	ALA	3.2
1	I	363	HIS	3.2
1	B	104	TYR	3.2
1	A	104	TYR	3.1
1	F	363	HIS	3.1
1	I	95	HIS	3.1
1	A	255	CYS	3.1
1	A	252	THR	3.1
1	E	247	ALA	3.0
1	J	109	ASP	3.0
1	J	108	LEU	3.0
1	B	98	HIS	3.0
1	C	284	GLU	3.0
1	K	314	PHE	3.0
1	D	316	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	362	PHE	2.9
1	K	247	ALA	2.9
1	K	251	GLY	2.9
1	D	319	CYS	2.9
1	J	90	ARG	2.9
1	A	313	ASP	2.9
1	K	255	CYS	2.8
1	A	231	GLN	2.8
1	H	319	CYS	2.8
1	C	89	ILE	2.8
1	B	108	LEU	2.7
1	G	130	ALA	2.7
1	K	313	ASP	2.7
1	H	314	PHE	2.7
1	B	254	GLU	2.6
1	H	79	PHE	2.6
1	B	109	ASP	2.5
1	J	102	PHE	2.5
1	I	248	ALA	2.5
1	B	317	THR	2.5
1	G	98	HIS	2.5
1	E	316	ILE	2.5
1	F	247	ALA	2.5
1	K	104	TYR	2.5
1	B	146	VAL	2.5
1	C	105	ALA	2.4
1	A	251	GLY	2.4
1	F	55	PRO	2.4
1	H	231	GLN	2.3
1	I	228	ALA	2.3
1	J	105	ALA	2.3
1	C	90	ARG	2.3
1	F	146	VAL	2.3
1	G	251	GLY	2.3
1	C	318	TYR	2.3
1	A	107	ILE	2.3
1	B	118	VAL	2.3
1	J	319	CYS	2.2
1	F	362	PHE	2.2
1	A	106	ASN	2.2
1	K	106	ASN	2.2
1	K	249	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	313	ASP	2.2
1	C	254	GLU	2.2
1	G	362	PHE	2.2
1	L	143	ALA	2.2
1	H	285	ARG	2.2
1	A	98	HIS	2.2
1	E	245	HIS	2.2
1	A	317	THR	2.2
1	I	242	GLN	2.2
1	D	248	ALA	2.2
1	B	318	TYR	2.1
1	B	116	ILE	2.1
1	A	108	LEU	2.1
1	C	250	ASN	2.1
1	C	320	VAL	2.1
1	I	320	VAL	2.1
1	B	253	PHE	2.1
1	A	305	GLN	2.0
1	D	81	LYS	2.0
1	H	252	THR	2.0
1	I	362	PHE	2.0
1	F	320	VAL	2.0
1	G	95	HIS	2.0
1	L	89	ILE	2.0
1	B	119	ASN	2.0
1	L	64	LEU	2.0
1	D	252	THR	2.0
1	B	115	GLU	2.0
1	L	96	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.