wwPDB X-ray Structure Validation Summary Report (i)

Oct 7, 2023 – 10:30 PM EDT

PDB ID	:	6DV2
Title	:	Crystal Structure of Human Mitochondrial Trifunctional Protein
Authors	:	Fu, Z.; Xia, C.; Battaile, K.P.; Kim, J.P.
Deposited on	:	2018-06-22
Resolution	:	3.60 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:

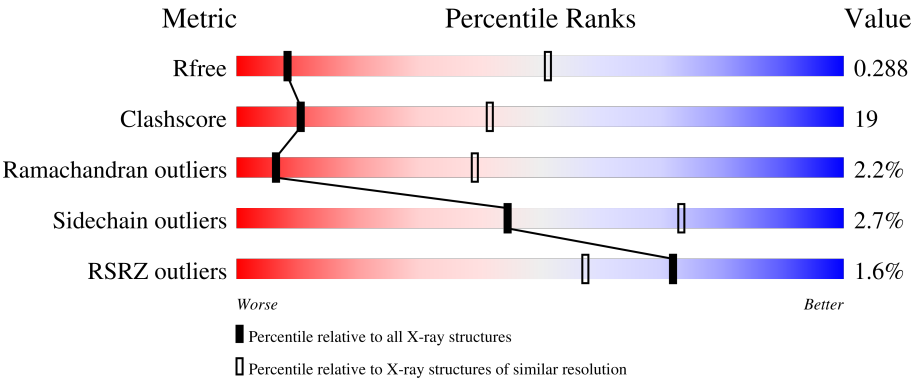
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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% 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	457	5% 56% 34% 5% 5%
1	B	457	2% 55% 31% 5% 8%
1	C	457	2% 60% 29% • 8%
1	D	457	4% 58% 32% • 7%
1	E	457	2% 60% 29% • 7%

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Mol	Chain	Length	Quality of chain
1	F	457	2% 61% 29% 7%
2	G	727	64% 34%
2	H	727	% 65% 33%
2	I	727	2% 65% 32%
2	J	727	% 68% 29%
2	K	727	% 67% 31%
2	L	727	% 65% 32%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 51375 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 Trifunctional enzyme subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3267	2071	566	608	22			
1	B	419	Total	C	N	O	S	0	0	0
			3170	2012	548	589	21			
1	C	421	Total	C	N	O	S	0	0	0
			3073	1938	530	586	19			
1	D	424	Total	C	N	O	S	0	0	0
			3087	1946	533	589	19			
1	E	423	Total	C	N	O	S	0	0	0
			3082	1943	532	588	19			
1	F	425	Total	C	N	O	S	0	0	0
			3092	1949	534	590	19			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	HIS	-	expression tag	UNP P55084
A	19	HIS	-	expression tag	UNP P55084
A	20	HIS	-	expression tag	UNP P55084
A	21	HIS	-	expression tag	UNP P55084
A	22	HIS	-	expression tag	UNP P55084
A	23	HIS	-	expression tag	UNP P55084
A	24	SER	-	expression tag	UNP P55084
A	25	SER	-	expression tag	UNP P55084
A	26	GLY	-	expression tag	UNP P55084
A	27	LEU	-	expression tag	UNP P55084
A	28	VAL	-	expression tag	UNP P55084
A	29	PRO	-	expression tag	UNP P55084
A	30	ARG	-	expression tag	UNP P55084
A	31	GLY	-	expression tag	UNP P55084
A	32	SER	-	expression tag	UNP P55084
A	33	HIS	-	expression tag	UNP P55084
B	18	HIS	-	expression tag	UNP P55084

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Chain	Residue	Modelled	Actual	Comment	Reference
B	19	HIS	-	expression tag	UNP P55084
B	20	HIS	-	expression tag	UNP P55084
B	21	HIS	-	expression tag	UNP P55084
B	22	HIS	-	expression tag	UNP P55084
B	23	HIS	-	expression tag	UNP P55084
B	24	SER	-	expression tag	UNP P55084
B	25	SER	-	expression tag	UNP P55084
B	26	GLY	-	expression tag	UNP P55084
B	27	LEU	-	expression tag	UNP P55084
B	28	VAL	-	expression tag	UNP P55084
B	29	PRO	-	expression tag	UNP P55084
B	30	ARG	-	expression tag	UNP P55084
B	31	GLY	-	expression tag	UNP P55084
B	32	SER	-	expression tag	UNP P55084
B	33	HIS	-	expression tag	UNP P55084
C	18	HIS	-	expression tag	UNP P55084
C	19	HIS	-	expression tag	UNP P55084
C	20	HIS	-	expression tag	UNP P55084
C	21	HIS	-	expression tag	UNP P55084
C	22	HIS	-	expression tag	UNP P55084
C	23	HIS	-	expression tag	UNP P55084
C	24	SER	-	expression tag	UNP P55084
C	25	SER	-	expression tag	UNP P55084
C	26	GLY	-	expression tag	UNP P55084
C	27	LEU	-	expression tag	UNP P55084
C	28	VAL	-	expression tag	UNP P55084
C	29	PRO	-	expression tag	UNP P55084
C	30	ARG	-	expression tag	UNP P55084
C	31	GLY	-	expression tag	UNP P55084
C	32	SER	-	expression tag	UNP P55084
C	33	HIS	-	expression tag	UNP P55084
D	18	HIS	-	expression tag	UNP P55084
D	19	HIS	-	expression tag	UNP P55084
D	20	HIS	-	expression tag	UNP P55084
D	21	HIS	-	expression tag	UNP P55084
D	22	HIS	-	expression tag	UNP P55084
D	23	HIS	-	expression tag	UNP P55084
D	24	SER	-	expression tag	UNP P55084
D	25	SER	-	expression tag	UNP P55084
D	26	GLY	-	expression tag	UNP P55084
D	27	LEU	-	expression tag	UNP P55084
D	28	VAL	-	expression tag	UNP P55084

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Chain	Residue	Modelled	Actual	Comment	Reference
D	29	PRO	-	expression tag	UNP P55084
D	30	ARG	-	expression tag	UNP P55084
D	31	GLY	-	expression tag	UNP P55084
D	32	SER	-	expression tag	UNP P55084
D	33	HIS	-	expression tag	UNP P55084
E	18	HIS	-	expression tag	UNP P55084
E	19	HIS	-	expression tag	UNP P55084
E	20	HIS	-	expression tag	UNP P55084
E	21	HIS	-	expression tag	UNP P55084
E	22	HIS	-	expression tag	UNP P55084
E	23	HIS	-	expression tag	UNP P55084
E	24	SER	-	expression tag	UNP P55084
E	25	SER	-	expression tag	UNP P55084
E	26	GLY	-	expression tag	UNP P55084
E	27	LEU	-	expression tag	UNP P55084
E	28	VAL	-	expression tag	UNP P55084
E	29	PRO	-	expression tag	UNP P55084
E	30	ARG	-	expression tag	UNP P55084
E	31	GLY	-	expression tag	UNP P55084
E	32	SER	-	expression tag	UNP P55084
E	33	HIS	-	expression tag	UNP P55084
F	18	HIS	-	expression tag	UNP P55084
F	19	HIS	-	expression tag	UNP P55084
F	20	HIS	-	expression tag	UNP P55084
F	21	HIS	-	expression tag	UNP P55084
F	22	HIS	-	expression tag	UNP P55084
F	23	HIS	-	expression tag	UNP P55084
F	24	SER	-	expression tag	UNP P55084
F	25	SER	-	expression tag	UNP P55084
F	26	GLY	-	expression tag	UNP P55084
F	27	LEU	-	expression tag	UNP P55084
F	28	VAL	-	expression tag	UNP P55084
F	29	PRO	-	expression tag	UNP P55084
F	30	ARG	-	expression tag	UNP P55084
F	31	GLY	-	expression tag	UNP P55084
F	32	SER	-	expression tag	UNP P55084
F	33	HIS	-	expression tag	UNP P55084

- Molecule 2 is a protein called Trifunctional enzyme subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	725	Total	C	N	O	S	0	0	0
			5440	3455	929	1027	29			

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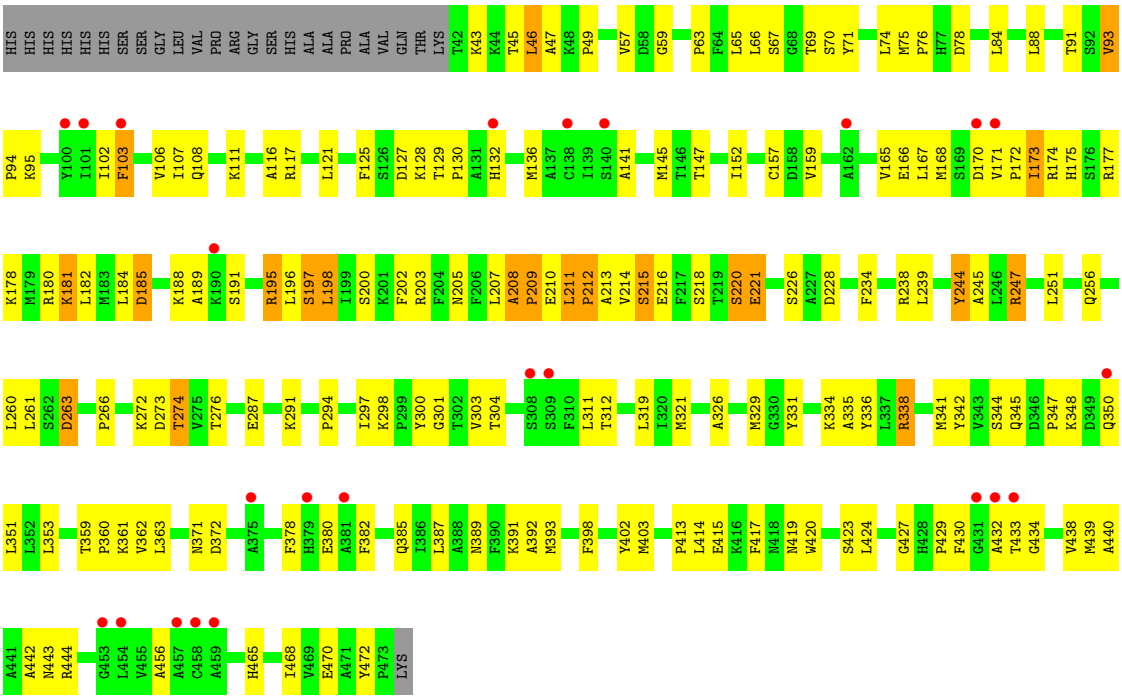
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	725	Total	C	N	O	S	0	0	0
			5440	3455	929	1027	29			
2	I	714	Total	C	N	O	S	0	0	0
			5431	3454	928	1020	29			
2	J	714	Total	C	N	O	S	0	0	0
			5431	3454	928	1020	29			
2	K	714	Total	C	N	O	S	0	0	0
			5431	3454	928	1020	29			
2	L	714	Total	C	N	O	S	0	0	0
			5431	3454	928	1020	29			

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 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.

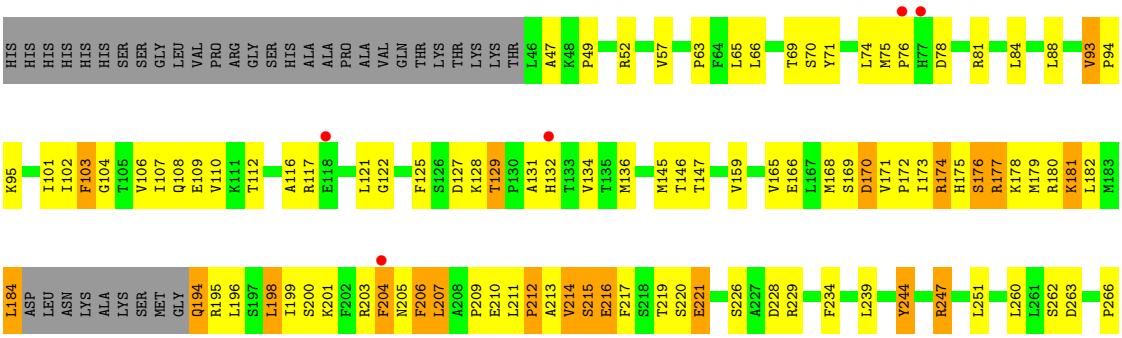
• Molecule 1: Trifunctional enzyme subunit beta, mitochondrial

Chain A:



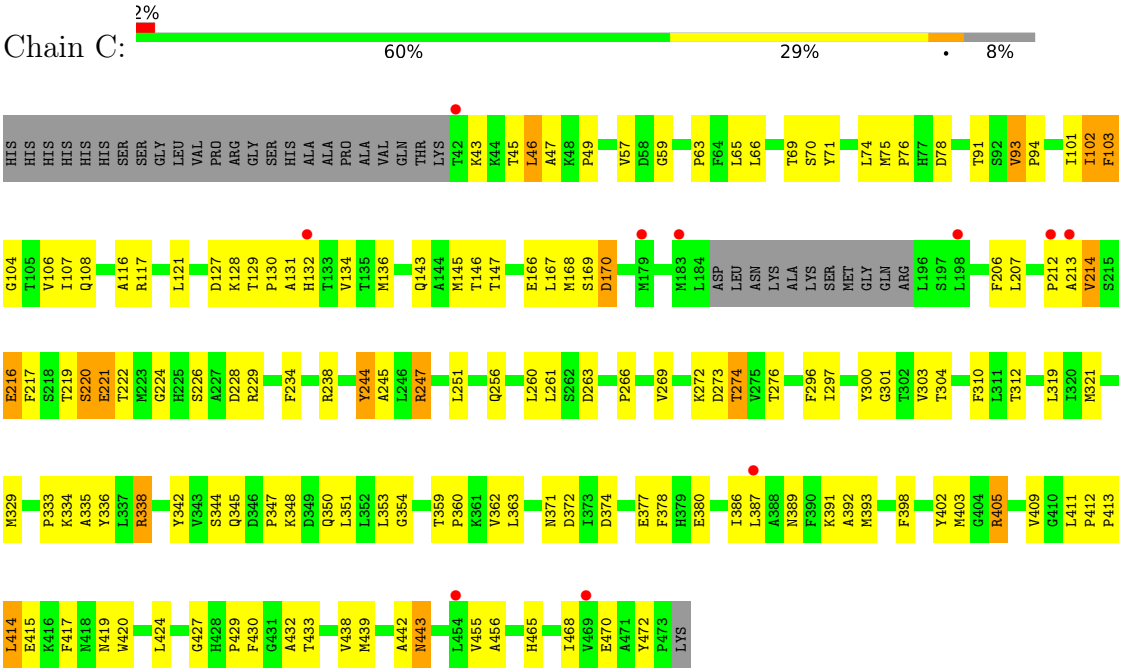
• Molecule 1: Trifunctional enzyme subunit beta, mitochondrial

Chain B:



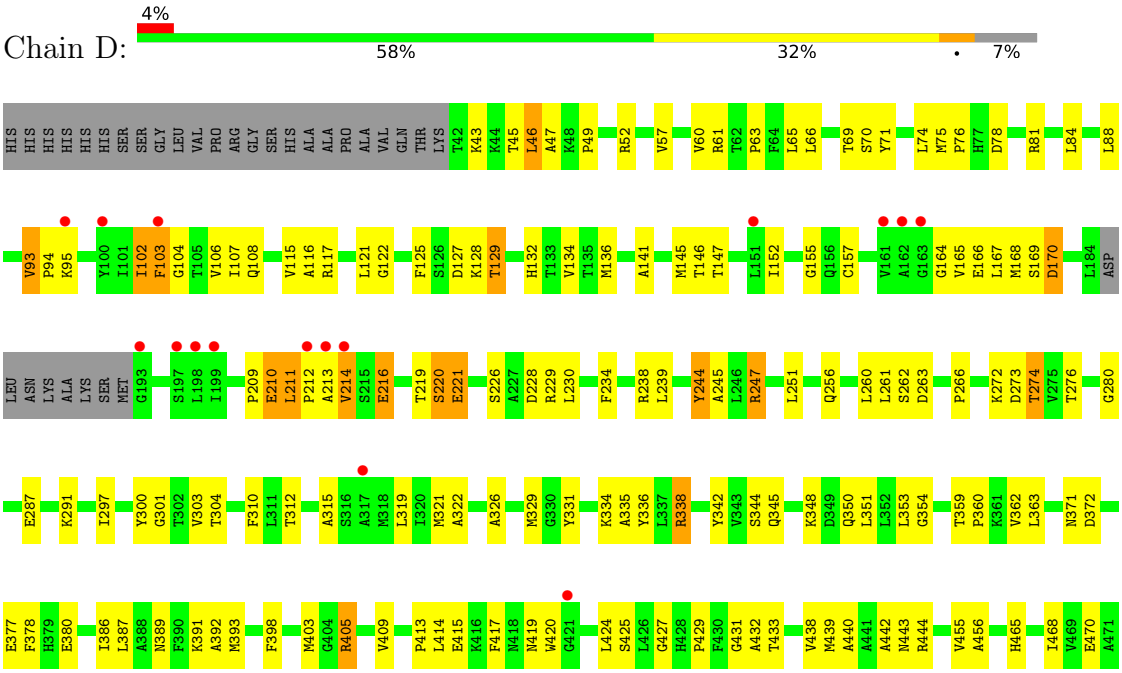
• Molecule 1: Trifunctional enzyme subunit beta, mitochondrial

Chain C:



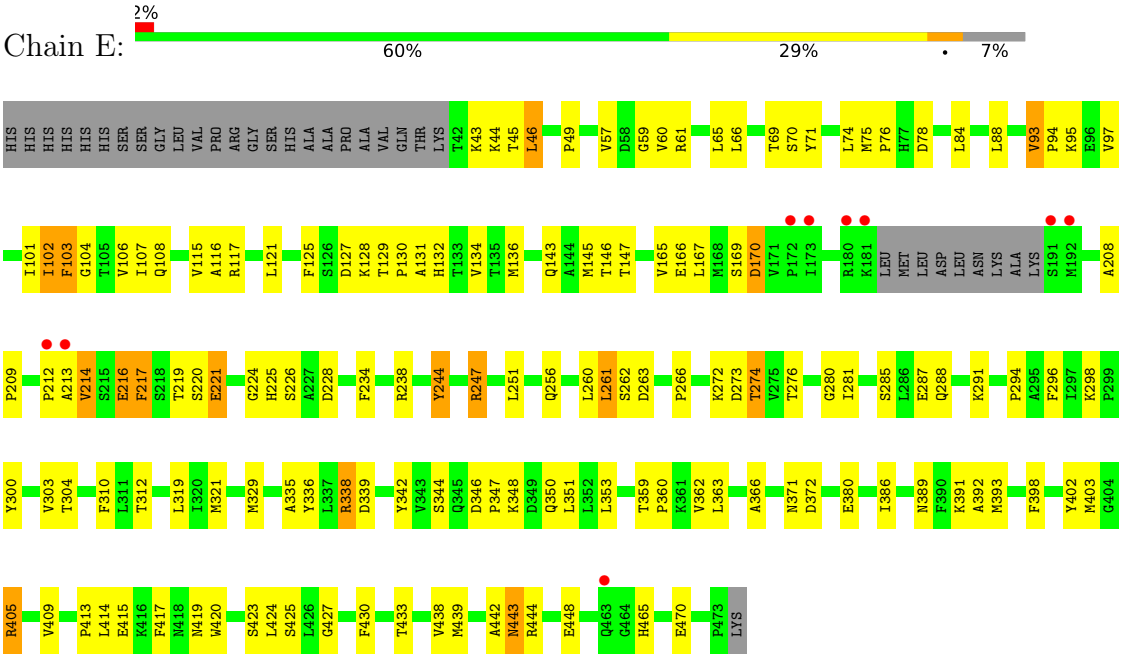
• Molecule 1: Trifunctional enzyme subunit beta, mitochondrial

Chain D:



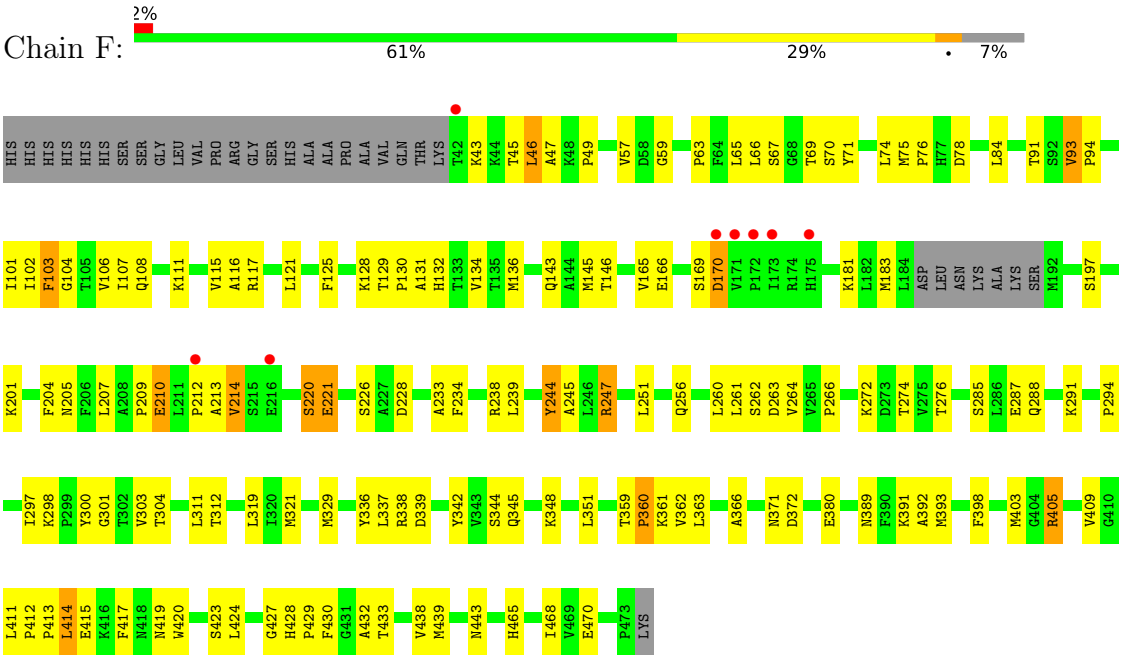
• Molecule 1: Trifunctional enzyme subunit beta, mitochondrial

Chain E:



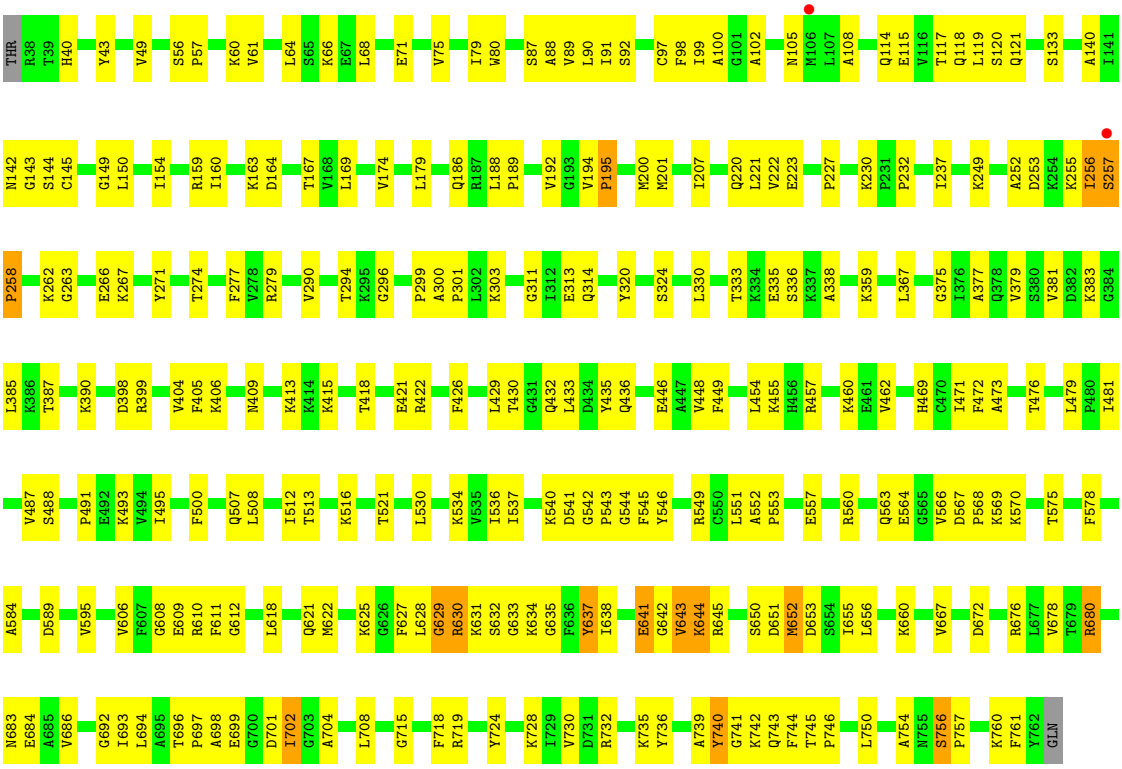
• Molecule 1: Trifunctional enzyme subunit beta, mitochondrial

Chain F:



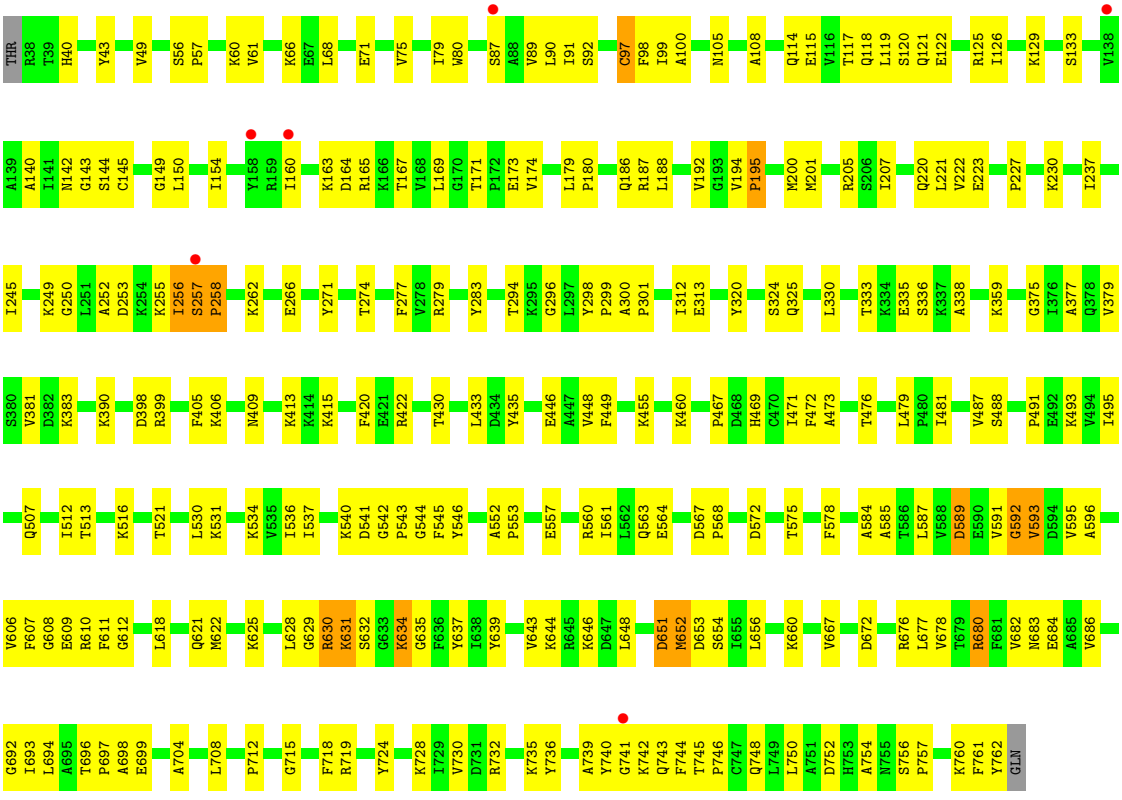
• Molecule 2: Trifunctional enzyme subunit alpha, mitochondrial

Chain G:



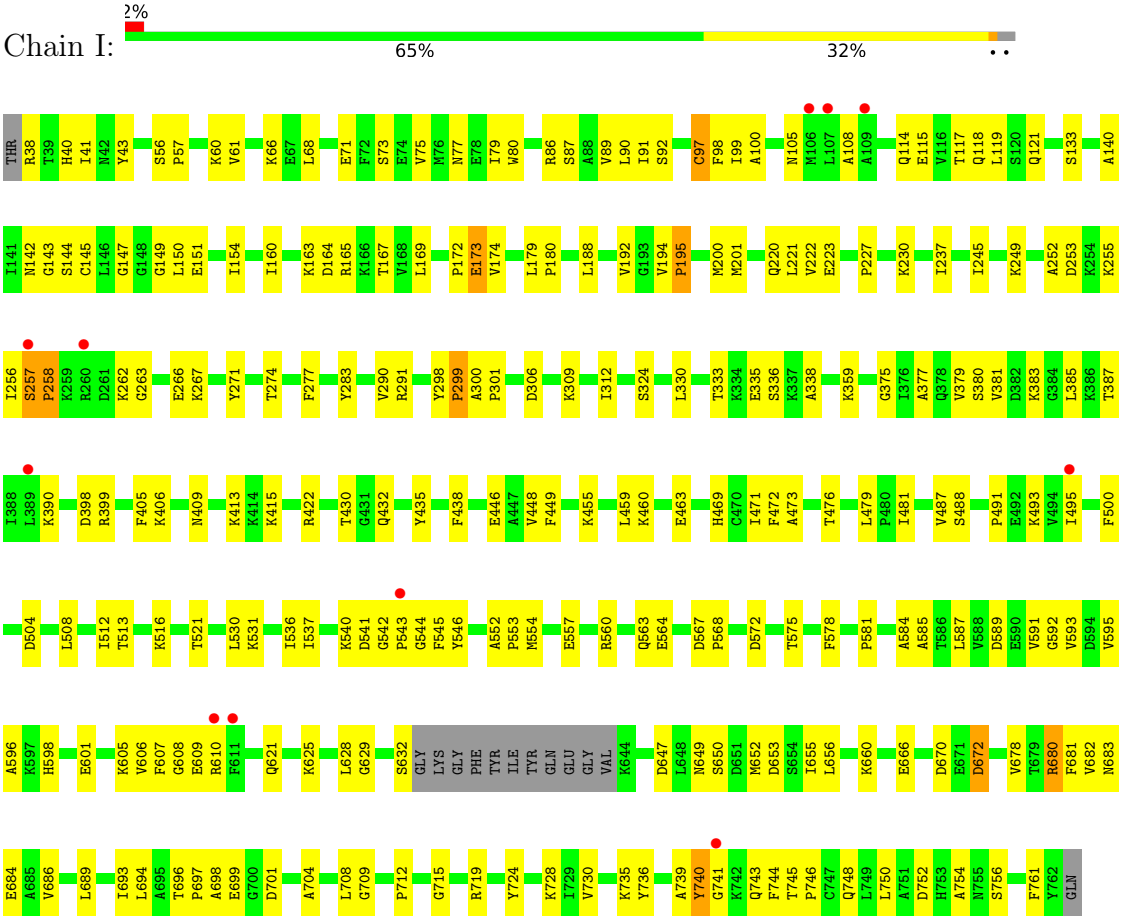
• Molecule 2: Trifunctional enzyme subunit alpha, mitochondrial

Chain H:



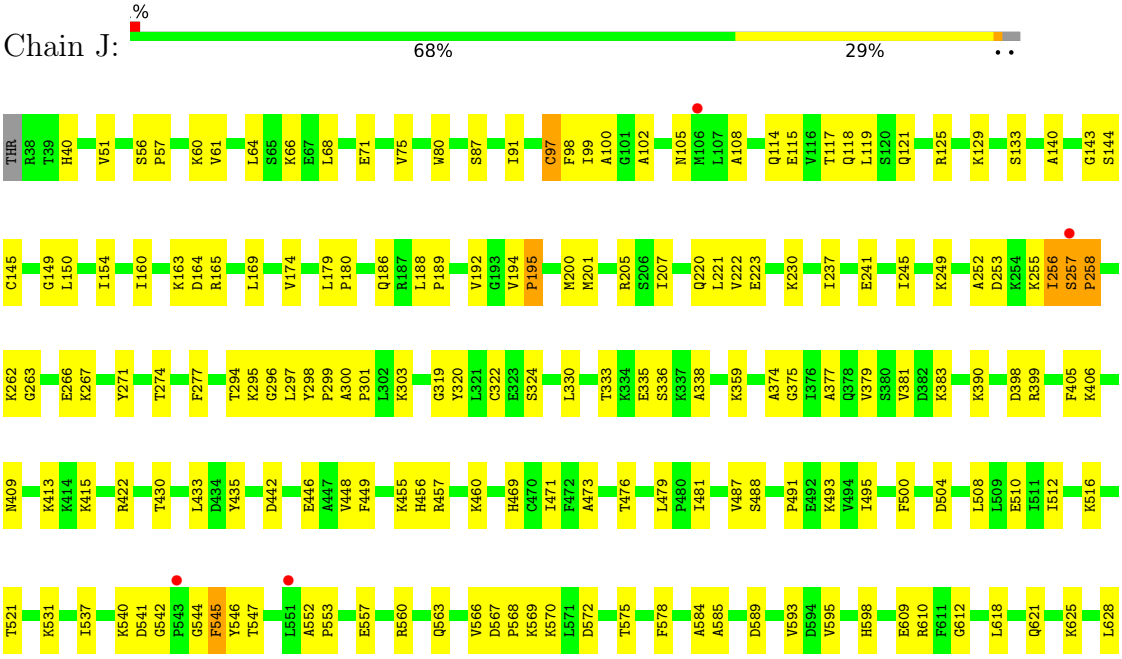
• Molecule 2: Trifunctional enzyme subunit alpha, mitochondrial

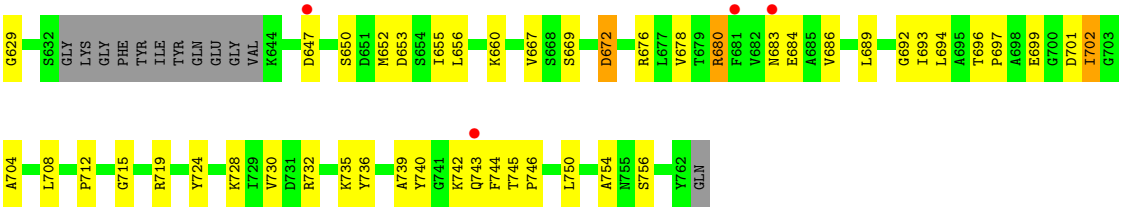
Chain I:



• Molecule 2: Trifunctional enzyme subunit alpha, mitochondrial

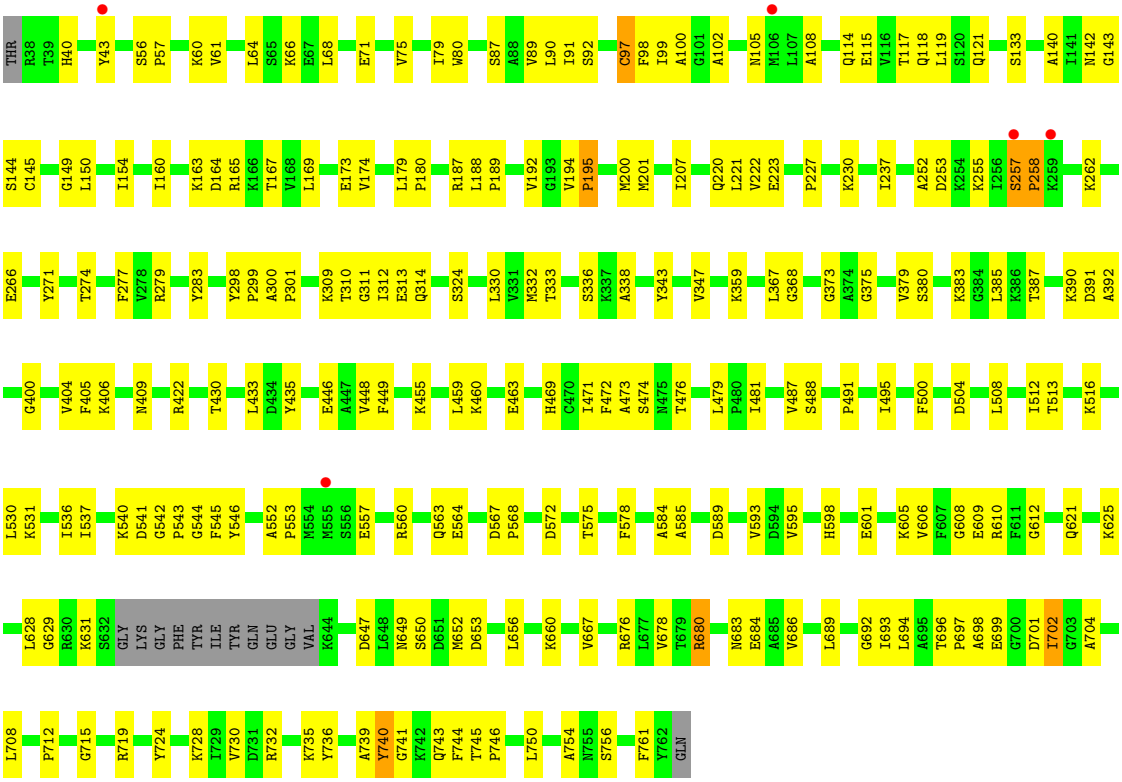
Chain J:

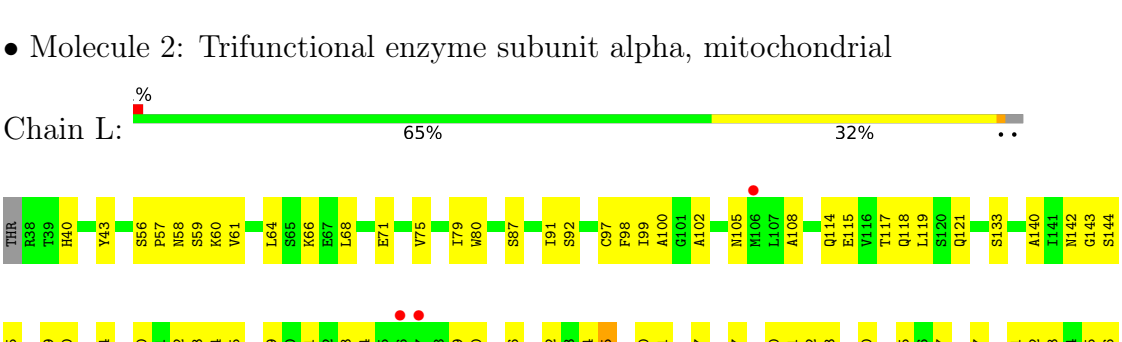


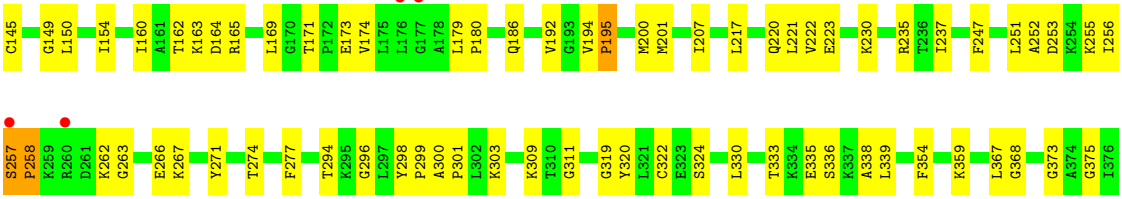


• Molecule 2: Trifunctional enzyme subunit alpha, mitochondrial

Chain K:

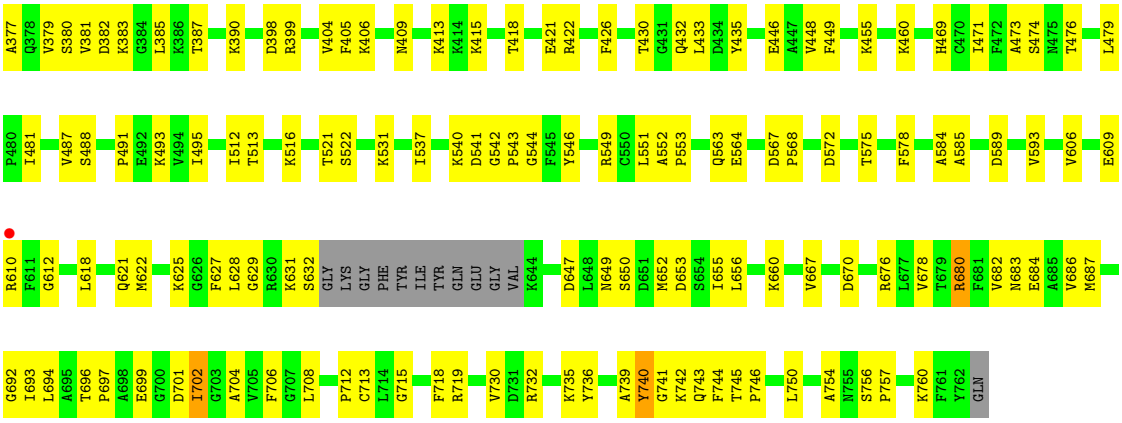






• Molecule 2: Trifunctional enzyme subunit alpha, mitochondrial

Chain L:


A377 Q378 V379 S380 V381 D382 K383 G384 L385 K386 T387 K390 D398 R399 V404 F405 K406 N409 K413 K414 K415 T418 E421 R422 F426 T430 G431 Q432 L433 D434 Y435 E446 A447 V448 F449 K455 K460 H469 C470 I471 F472 A473 S474 N475 T476 L479
P480 I481 V487 S488 P491 E492 K493 V494 I495 I512 T513 K516 T521 S522 K531 I537 K540 D541 G542 P543 G544 F545 Y546 R549 C550 L551 A552 P553 Q563 E564 D567 P568 D572 T575 F578 A584 A585 D589 V593 V606 E609
R610 F611 G612 L618 Q621 M622 K625 G626 F627 L628 G629 R630 K631 S632 GLY LYS GLY PHE TYR ILE TYR GLN GLU GLY VAL K644 D647 L648 N649 S650 D651 M652 D653 S654 I655 L656 K660 V667 D670 R676 L677 V678 T679 R680 F681 V682 N683 E684 A685 V686 M687
G692 I693 L694 A695 T696 P697 A698 E699 G700 D701 I702 G703 A704 V705 F706 G707 L708 P712 C713 L714 G715 F718 R719 V730 D731 R732 K735 Y736 A739 Y740 G741 K742 Q743 F744 T745 P746 L750 A754 N755 S756 P757 K760 F761 Y762 GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	136.54Å 237.94Å 141.32Å 90.00° 105.61° 90.00°	Depositor
Resolution (Å)	89.56 – 3.60 89.57 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (89.56-3.60) 98.7 (89.57-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 3.58Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.244 , 0.289 0.243 , 0.288	Depositor DCC
R_{free} test set	4957 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	110.8	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 66.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	51375	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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

5.1 Standard geometry

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	0/3330	0.49	0/4498
1	B	0.29	0/3232	0.49	0/4368
1	C	0.24	0/3128	0.44	0/4238
1	D	0.24	0/3142	0.44	0/4257
1	E	0.25	0/3137	0.46	0/4250
1	F	0.26	0/3147	0.46	0/4264
2	G	0.25	0/5524	0.45	0/7453
2	H	0.24	0/5524	0.44	0/7453
2	I	0.23	0/5515	0.43	0/7431
2	J	0.23	0/5515	0.43	0/7431
2	K	0.23	0/5515	0.42	0/7431
2	L	0.23	0/5515	0.43	0/7431
All	All	0.25	0/52224	0.45	0/70505

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

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	3267	0	3317	194	0
1	B	3170	0	3207	205	0
1	C	3073	0	2988	117	0
1	D	3087	0	2995	119	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3082	0	2993	117	0
1	F	3092	0	2997	115	0
2	G	5440	0	5569	213	0
2	H	5440	0	5569	198	0
2	I	5431	0	5632	175	0
2	J	5431	0	5632	178	0
2	K	5431	0	5632	172	0
2	L	5431	0	5632	180	0
All	All	51375	0	52163	1919	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 1919 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:A:174:ARG:HB2	1:A:178:LYS:HG2	1.29	1.15
1:A:173:ILE:HG23	1:B:173:ILE:HG22	1.23	1.11
1:B:178:LYS:HD3	1:B:181:LYS:HD3	1.31	1.11
1:B:174:ARG:HB3	1:B:177:ARG:HB3	1.40	1.02
1:E:45:THR:O	1:E:46:LEU:HG	1.63	0.98

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	430/457 (94%)	353 (82%)	61 (14%)	16 (4%)	3 28
1	B	415/457 (91%)	347 (84%)	54 (13%)	14 (3%)	3 31
1	C	417/457 (91%)	355 (85%)	48 (12%)	14 (3%)	3 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	420/457 (92%)	347 (83%)	59 (14%)	14 (3%)	4	31
1	E	419/457 (92%)	357 (85%)	48 (12%)	14 (3%)	4	31
1	F	421/457 (92%)	357 (85%)	53 (13%)	11 (3%)	5	35
2	G	723/727 (99%)	613 (85%)	91 (13%)	19 (3%)	5	35
2	H	723/727 (99%)	619 (86%)	87 (12%)	17 (2%)	6	37
2	I	710/727 (98%)	621 (88%)	82 (12%)	7 (1%)	15	55
2	J	710/727 (98%)	608 (86%)	95 (13%)	7 (1%)	15	55
2	K	710/727 (98%)	614 (86%)	87 (12%)	9 (1%)	12	50
2	L	710/727 (98%)	617 (87%)	86 (12%)	7 (1%)	15	55
All	All	6808/7104 (96%)	5808 (85%)	851 (12%)	149 (2%)	6	39

5 of 149 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	PRO
1	A	208	ALA
1	A	216	GLU
1	A	221	GLU
1	B	49	PRO

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	345/365 (94%)	330 (96%)	15 (4%)	29	63
1	B	334/365 (92%)	316 (95%)	18 (5%)	22	57
1	C	305/365 (84%)	294 (96%)	11 (4%)	35	67
1	D	305/365 (84%)	295 (97%)	10 (3%)	38	69
1	E	305/365 (84%)	291 (95%)	14 (5%)	27	61
1	F	305/365 (84%)	292 (96%)	13 (4%)	29	63
2	G	580/603 (96%)	571 (98%)	9 (2%)	62	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	580/603 (96%)	566 (98%)	14 (2%)	49 75
2	I	591/603 (98%)	579 (98%)	12 (2%)	55 79
2	J	591/603 (98%)	580 (98%)	11 (2%)	57 80
2	K	591/603 (98%)	580 (98%)	11 (2%)	57 80
2	L	591/603 (98%)	582 (98%)	9 (2%)	65 84
All	All	5423/5808 (93%)	5276 (97%)	147 (3%)	44 73

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	756	SER
2	L	680	ARG
2	J	430	THR
2	K	430	THR
1	D	244	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	358	GLN
2	L	469	HIS
2	J	105	ASN
2	K	358	GLN
1	C	379	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

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, 95^{th} 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	432/457 (94%)	0.34	24 (5%)	24	14	78, 115, 154, 202	0
1	B	419/457 (91%)	0.13	7 (1%)	70	55	77, 114, 150, 211	0
1	C	421/457 (92%)	0.14	10 (2%)	59	42	74, 116, 181, 239	0
1	D	424/457 (92%)	0.19	16 (3%)	40	26	78, 122, 186, 224	0
1	E	423/457 (92%)	0.04	9 (2%)	63	48	57, 91, 191, 228	0
1	F	425/457 (92%)	-0.05	8 (1%)	66	51	59, 93, 186, 231	0
2	G	725/727 (99%)	-0.14	2 (0%)	94	88	68, 123, 180, 234	0
2	H	725/727 (99%)	-0.15	6 (0%)	86	75	76, 130, 186, 241	0
2	I	714/727 (98%)	-0.04	11 (1%)	73	60	86, 128, 184, 234	0
2	J	714/727 (98%)	-0.14	8 (1%)	80	68	78, 123, 183, 237	0
2	K	714/727 (98%)	-0.18	5 (0%)	87	78	66, 121, 178, 226	0
2	L	714/727 (98%)	-0.22	6 (0%)	86	75	67, 119, 179, 214	0
All	All	6850/7104 (96%)	-0.04	112 (1%)	72	57	57, 119, 181, 241	0

The worst 5 of 112 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	212	PRO	6.9
1	E	213	ALA	4.4
1	A	453	GLY	4.2
2	J	257	SER	4.1
1	D	214	VAL	4.0

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.