



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 06:15 AM UTC

PDB ID : 6H8K / pdb_00006h8k
Title : Crystal structure of a variant (Q133C in PSST) of Yarrowia lipolytica complex I
Authors : Wirth, C.; Galemou Yoga, E.; Zickermann, V.; Hunte, C.
Deposited on : 2018-08-02
Resolution : 3.79 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:

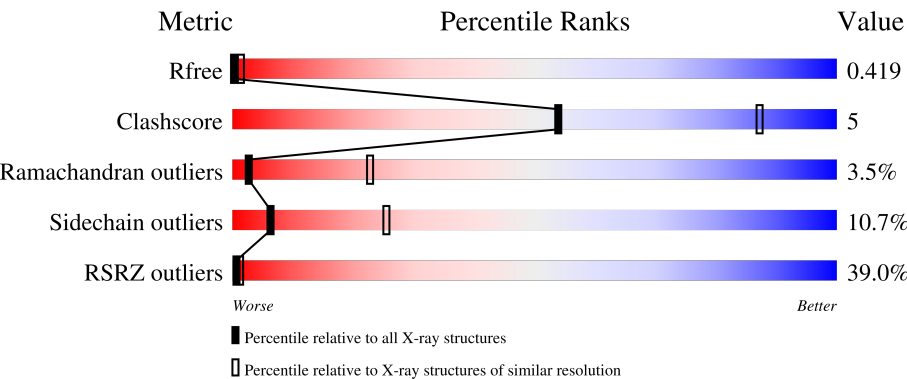
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 3.79 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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 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	1	335	52% 64%27%6% . .
2	2	434	15% 77%20% .
3	3	110	31% 56%18%5%20%
4	4	470	13% 82%15% .
5	5	616	23% 85%13% .

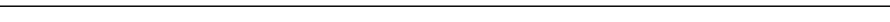
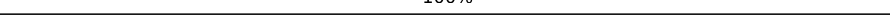
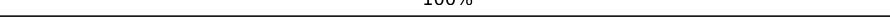
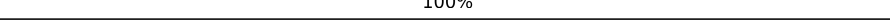
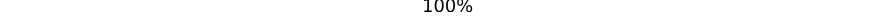
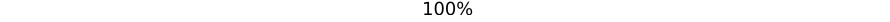
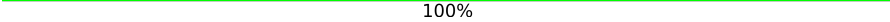
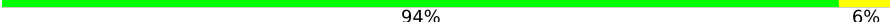
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Mol	Chain	Length	Quality of chain
6	6	184	
7	A	634	
8	B	370	
9	C	383	
10	E	195	
11	G	133	
12	H	154	
13	I	140	
14	K	147	
15	L	79	
16	Z	17	
16	r	17	
17	AF	40	
17	Y	40	
18	U	10	
19	X	57	
20	W	54	
21	V	63	
22	AI	20	
22	T	20	
22	m	20	
23	AJ	19	
23	AL	19	
23	S	19	
24	R	50	

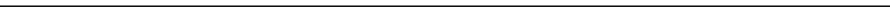
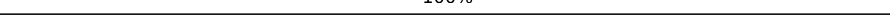
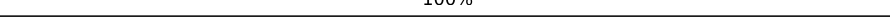
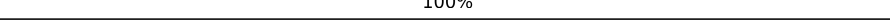
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Mol	Chain	Length	Quality of chain
25	Q	70	 100%
26	P	28	 100%
27	AC	18	 100%
27	AH	18	 100%
27	AM	18	 100%
27	F	18	 100%
27	f	18	 100%
28	O	25	 100%
28	l	25	 100%
29	M	51	 100%
30	D	30	 100%
31	J	69	 100%
32	N	15	 100%
33	a	26	 100%
33	i	26	 100%
34	b	22	 100%
35	AE	9	 100%
35	AK	9	 100%
35	AO	9	 100%
35	c	9	 100%
35	g	9	 100%
36	AB	16	 100%
36	AN	16	 94% 6%
36	d	16	 100%
36	o	16	 100%

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Mol	Chain	Length	Quality of chain
37	e	13	 100%
37	w	13	 100%
37	z	13	 100%
38	h	47	 91% 9%
39	j	48	 100%
40	k	23	 100%
40	s	23	 100%
41	n	36	 100%
41	q	36	 100%
42	p	76	 100%
43	t	45	 100%
44	u	32	 100%
45	v	11	 100%
45	y	11	 100%
46	AG	8	 100%
46	x	8	 100%
47	AA	58	 100%
48	AD	39	 100%

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 35631 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 NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	325	Total	C	N	O	S	0	0	0
			2581	1758	375	441	7			

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 2,NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	434	Total	C	N	O	S	0	0	0
			3122	2080	478	552	12			

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	88	Total	C	N	O	S	0	0	0
			685	475	94	113	3			

- Molecule 4 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	470	Total	C	N	O	S	0	0	0
			3017	1952	507	546	12			

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	5	616	Total	C	N	O	S	0	0	0
			4050	2627	674	724	25			

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	6	118	Total	C	N	O	S	0	0	0
			870	597	124	143	6			

- Molecule 7 is a protein called NUAM protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	A	628	Total	C	N	O	S	0	0	0
			3221	1929	639	639	14			

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	B	367	Total	C	N	O	S	0	0	0
			1997	1204	388	396	9			

- Molecule 9 is a protein called NUCM protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	C	369	Total	C	N	O	S	0	0	0
			2882	1845	486	530	21			

- Molecule 10 is a protein called NUEM protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	E	195	Total	C	N	O	0	0	0
			975	585	195	195			

- Molecule 11 is a protein called NUGM protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	G	133	Total	C	N	O	S	0	0	0
			880	558	154	164	4			

- Molecule 12 is a protein called Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	H	154	Total	C	N	O	S	0	0	0
			803	476	156	164	7			

- Molecule 13 is a protein called Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Com-

plex I).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	I	137	Total	C	N	O	S	0	0	0
			857	533	145	169	10			

- Molecule 14 is a protein called Subunit NUKM of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	K	143	Total	C	N	O	S	5	0	0
			1069	675	187	193	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	133	CYS	GLN	engineered mutation	UNP Q9UUT7

- Molecule 15 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	L	79	Total	C	N	O	S	6	0	0
			612	412	95	102	3			

- Molecule 16 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	Z	17	Total	C	N	O		0	0	0
			85	51	17	17				
16	r	17	Total	C	N	O		0	0	0
			85	51	17	17				

- Molecule 17 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	40	Total	C	N	O		0	0	0
			200	120	40	40				
17	AF	40	Total	C	N	O		0	0	0
			200	120	40	40				

- Molecule 18 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	U	10	Total	C	N	O	0	0	0
			50	30	10	10			

- Molecule 19 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	X	57	Total	C	N	O	0	0	0
			285	171	57	57			

- Molecule 20 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	W	54	Total	C	N	O	0	0	0
			270	162	54	54			

- Molecule 21 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	V	63	Total	C	N	O	0	0	0
			315	189	63	63			

- Molecule 22 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	T	20	Total	C	N	O	0	0	0
			100	60	20	20			
22	m	20	Total	C	N	O	0	0	0
			100	60	20	20			
22	AI	20	Total	C	N	O	0	0	0
			100	60	20	20			

- Molecule 23 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	S	19	Total	C	N	O	0	0	0
			95	57	19	19			
23	AJ	19	Total	C	N	O	0	0	0
			95	57	19	19			
23	AL	19	Total	C	N	O	0	0	0
			95	57	19	19			

- Molecule 24 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	R	50	Total	C	N	O	0	0	0
			250	150	50	50			

- Molecule 25 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	Q	70	Total	C	N	O	0	0	0
			350	210	70	70			

- Molecule 26 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	P	28	Total	C	N	O	0	0	0
			140	84	28	28			

- Molecule 27 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	F	18	Total	C	N	O	0	0	0
			90	54	18	18			
27	f	18	Total	C	N	O	0	0	0
			90	54	18	18			
27	AC	18	Total	C	N	O	0	0	0
			90	54	18	18			
27	AH	18	Total	C	N	O	0	0	0
			90	54	18	18			
27	AM	18	Total	C	N	O	0	0	0
			90	54	18	18			

- Molecule 28 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	O	25	Total	C	N	O	0	0	0
			125	75	25	25			
28	l	25	Total	C	N	O	0	0	0
			125	75	25	25			

- Molecule 29 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
29	M	51	Total	C	N	O	0	0	0
			255	153	51	51			

- Molecule 30 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
30	D	30	Total	C	N	O	0	0	0
			150	90	30	30			

- Molecule 31 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
31	J	69	Total	C	N	O	0	0	0
			345	207	69	69			

- Molecule 32 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
32	N	15	Total	C	N	O	0	0	0
			75	45	15	15			

- Molecule 33 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
33	a	26	Total	C	N	O	0	0	0
			130	78	26	26			
33	i	26	Total	C	N	O	0	0	0
			130	78	26	26			

- Molecule 34 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
34	b	22	Total	C	N	O	0	0	0
			110	66	22	22			

- Molecule 35 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	c	9	Total	C	N	O	0	0	0
			45	27	9	9			
35	g	9	Total	C	N	O	0	0	0
			45	27	9	9			
35	AE	9	Total	C	N	O	0	0	0
			45	27	9	9			
35	AK	9	Total	C	N	O	0	0	0
			45	27	9	9			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	AO	9	Total	C	N	O	0	0	0
			45	27	9	9			

- Molecule 36 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	d	16	Total	C	N	O	0	0	0
			80	48	16	16			
36	o	16	Total	C	N	O	0	0	0
			80	48	16	16			
36	AB	16	Total	C	N	O	0	0	0
			80	48	16	16			
36	AN	16	Total	C	N	O	0	0	0
			80	48	16	16			

- Molecule 37 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	e	13	Total	C	N	O	0	0	0
			65	39	13	13			
37	w	13	Total	C	N	O	0	0	0
			65	39	13	13			
37	z	13	Total	C	N	O	0	0	0
			65	39	13	13			

- Molecule 38 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	h	47	Total	C	N	O	0	0	0
			235	141	47	47			

- Molecule 39 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	j	48	Total	C	N	O	0	0	0
			240	144	48	48			

- Molecule 40 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	k	23	Total	C	N	O	0	0	0
			115	69	23	23			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	s	23	Total	C	N	O	0	0	0
			115	69	23	23			

- Molecule 41 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	n	36	Total	C	N	O	0	0	0
			180	108	36	36			
41	q	36	Total	C	N	O	0	0	0
			180	108	36	36			

- Molecule 42 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	p	76	Total	C	N	O	0	0	0
			380	228	76	76			

- Molecule 43 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	t	45	Total	C	N	O	0	0	0
			225	135	45	45			

- Molecule 44 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	u	32	Total	C	N	O	0	0	0
			160	96	32	32			

- Molecule 45 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	v	11	Total	C	N	O	0	0	0
			55	33	11	11			
45	y	11	Total	C	N	O	0	0	0
			54	32	11	11			

- Molecule 46 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	x	8	Total	C	N	O	0	0	0
			40	24	8	8			
46	AG	8	Total	C	N	O	0	0	0
			40	24	8	8			

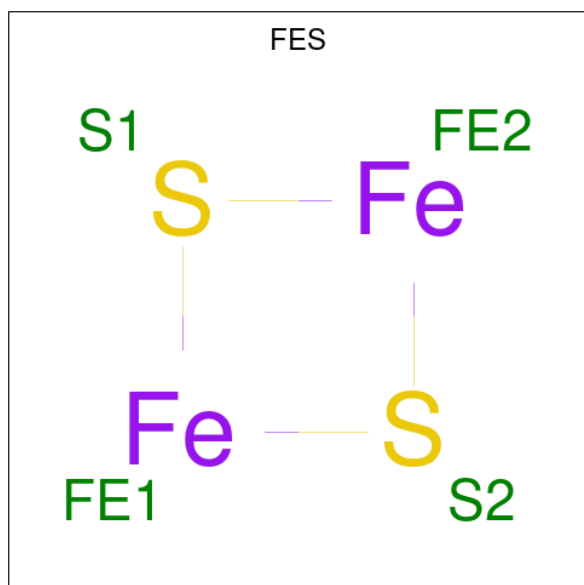
- Molecule 47 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	AA	58	Total	C	N	O	0	0	0
			290	174	58	58			

- Molecule 48 is a protein called Unknown polypeptide.

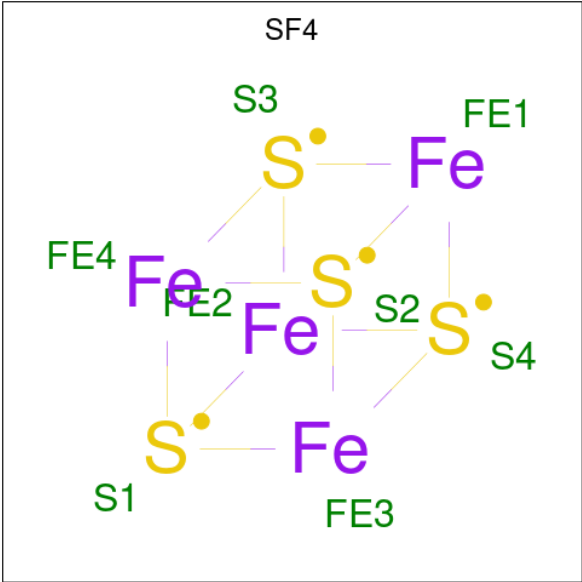
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	AD	39	Total	C	N	O	0	0	0
			195	117	39	39			

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
49	A	1	Total	Fe	S	0	0
			4	2	2		
49	H	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 50 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

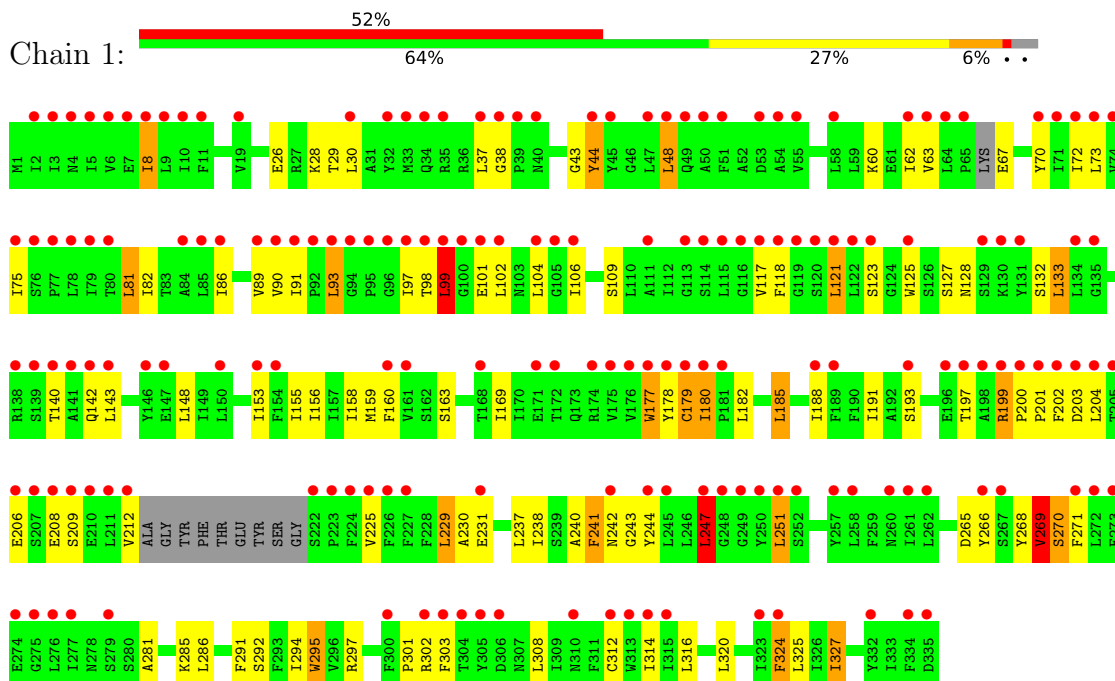


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
50	A	1	Total	Fe	S	0	0
			8	4	4		
50	A	1	Total	Fe	S	0	0
			8	4	4		
50	B	1	Total	Fe	S	0	0
			8	4	4		
50	I	1	Total	Fe	S	0	0
			8	4	4		
50	I	1	Total	Fe	S	0	0
			8	4	4		
50	K	1	Total	Fe	S	0	0
			8	4	4		

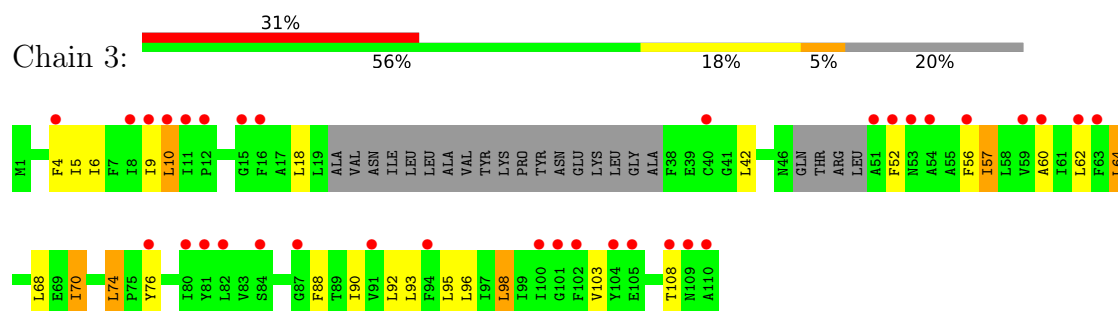
3 Residue-property plots [i](#)

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.

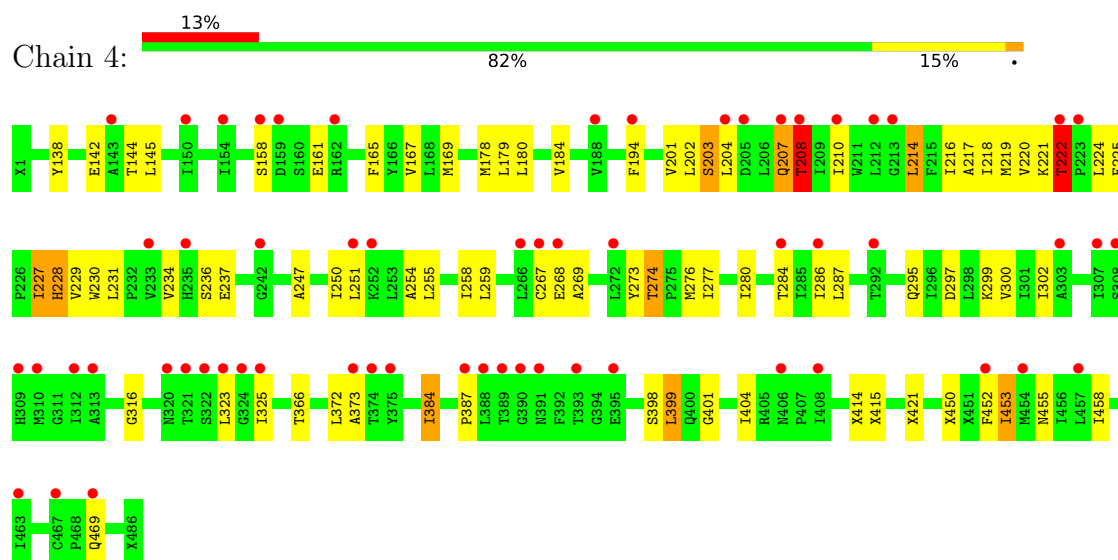
• Molecule 1: NADH-ubiquinone oxidoreductase chain 1



- Molecule 3: NADH-ubiquinone oxidoreductase chain 3



- Molecule 4: NADH-ubiquinone oxidoreductase chain 4



- Molecule 5: NADH-ubiquinone oxidoreductase chain 5



Chain 6:

Amino Acid	Percentage
T123	5%
T124	5%
T134	5%
T167	5%
T180	5%
T181	5%
T183	5%
T145	5%
T148	5%
T149	5%
T150	5%
G151	5%
N152	5%
T153	5%
T154	5%

Chain A:

9%

98%

..

Chain B:

17%

95%

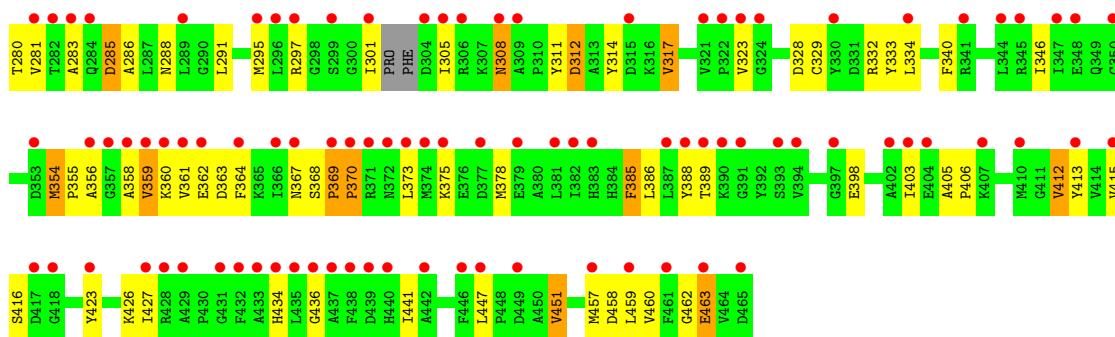
• •

T391 T392 W393 L394 L395 K396 A397 M398 D399 R400 F401 R402 T403 GLN GLY ALA K407 E408 E409 E410 T411 D412 M413 L414 Y415 E416 L417 T418 K419 D420 T421 H424 T425 L426 C427 A428 L429 C433 X434 X435 X436 X437 X438 X439 X440 X441 X442 X443 X444 X445 X446 X447 X448 X449 X450 X451 X452 X453 X454 X455 X456 X457 X458 X459 X460 X461 X462 X463 X464 X465 X466 X467 X468 X469 X470 X471 X472 X473 X474 X475 X476 X477 X478 X479 X480 X481 X482 X483 X484 X485 X486 X487 X488 X489 X490 X491 X492 X493 X494 X495 X496 X497 X498 X499 X500 X501 X502 X503 X504 X505 X506 X507 X508 X509 X510 X511 X512 X513 X514 X515 X516 X517 X518 X519 X520 X521 X522 X523 X524 X525 X526 X527 X528 X529 X530 X531 X532 X533 X534 X535 X536 X537 X538 X539 X540 X541 X542 X543 X544 X545 X546 X547 X548 X549 X550 X551 X552 X553 X554 X555 X556 X557 X558 X559 X560 X561 X562 X563 X564 X565 X566 X567 X568 X569 X570 X571 X572 X573 X574 X575 X576 X577 X578 X579 X580 X581 X582 X583 X584 X585 X586 X587 X588 X589 X590 X591 X592 X593 X594 X595 X596 X597 X598 X599 X600 X601 X602 X603 X604 X605 X606 X607 X608 X609 X610 X611 X612 X613 X614 X615 X616 X617 X618 X619 X620 X621 X622 X623 X624 X625 X626 X627 X628 X629 X630 X631 X632 X633 X634 X635 X636 X637 X638 X639 X640 X641 X642 X643 X644 X645 X646 X647 X648 X649 X650 X651 X652 X653 X654 X655 X656 X657 X658 X659 X660 X661 X662 X663 X664 X665 X666 X667 X668 X669 X670 X671 X672 X673 X674 X675 X676 X677 X678 X679 X680 X681 X682 X683 X684 X685 X686 X687 X688 X689 X690 X691 X692 X693 X694 X695 X696 X697 X698 X699 X700 X701 X702 X703 X704 X705 X706 X707 X708 X709 X710 X711 X712 X713 X714 X715 X716 X717 X718 X719 X720 X721 X722 X723 X724 X725 X726 X727 X728 X729 X730 X731 X732 X733 X734 X735 X736 X737 X738 X739 X740 X741 X742 X743 X744 X745 X746 X747 X748 X749 X750 X751 X752 X753 X754 X755 X756 X757 X758 X759 X760 X761 X762 X763 X764 X765 X766 X767 X768 X769 X770 X771 X772 X773 X774 X775 X776 X777 X778 X779 X780 X781 X782 X783 X784 X785 X786 X787 X788 X789 X790 X791 X792 X793 X794 X795 X796 X797 X798 X799 X800 X801 X802 X803 X804 X805 X806 X807 X808 X809 X810 X811 X812 X813 X814 X815 X816 X817 X818 X819 X820 X821 X822 X823 X824 X825 X826 X827 X828 X829 X830 X831 X832 X833 X834 X835 X836 X837 X838 X839 X840 X841 X842 X843 X844 X845 X846 X847 X848 X849 X850 X851 X852 X853 X854 X855 X856 X857 X858 X859 X860 X861 X862 X863 X864 X865 X866 X867 X868 X869 X870 X871 X872 X873 X874 X875 X876 X877 X878 X879 X880 X881 X882 X883 X884 X885 X886 X887 X888 X889 X890 X891 X892 X893 X894 X895 X896 X897 X898 X899 X900 X901 X902 X903 X904 X905 X906 X907 X908 X909 X910 X911 X912 X913 X914 X915 X916 X917 X918 X919 X920 X921 X922 X923 X924 X925 X926 X927 X928 X929 X930 X931 X932 X933 X934 X935 X936 X937 X938 X939 X940 X941 X942 X943 X944 X945 X946 X947 X948 X949 X950 X951 X952 X953 X954 X955 X956 X957 X958 X959 X960 X961 X962 X963 X964 X965 X966 X967 X968 X969 X970 X971 X972 X973 X974 X975 X976 X977 X978 X979 X980 X981 X982 X983 X984 X985 X986 X987 X988 X989 X990 X991 X992 X993 X994 X995 X996 X997 X998 X999

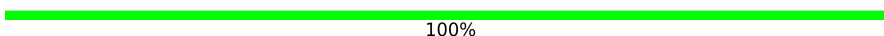
Chain C:

52% 64% 27% 5%

F83 T84 I85 M86 F87 G88 F89 G90 H91 P92 A93 A94 A95 G96 V97 L98 L99 H99 I100 I101 L104 S105 G106 F107 E108 I109 I110 I111 S112 D113 P114 H115 V116 G117 L118 L119 H119 H118 A119 G119 G120 G121 G122 G123 G124 G125 G126 G127 G128 G129 G130 G131 G132 G133 G134 A135 A136 P137 F138 F139 D140 R141 L142 D143 Y144 V145 S146 M147 L148 T149 N150 E151 Q152 L153 F154 S155 V156 E157 E158 E159 I160 V164 E165 V166 P167 L168 L169 R169 Y172 I173 F177 I180 I181 I182 V183 L184 R185 S185 S186 S187 S188 S189 S190 S191 S192 S193 S194 S195 S196 S197 S198 S199 S200 S201 S202 S203 S204 S205 S206 S207 S208 S209 S210 S211 S212 S213 S214 S215 S216 S217 S218 S219 S220 S221 S222 S223 S224 S225 S226 S227 S228 S229 S230 S231 S232 S233 S234 S235 S236 S237 S238 S239 S240 L243 L244 L245 L246 L247 L248 L249 L250 Q253 F254 G255 G256 G257 G258 G259 G260 G261 G262 G263 G264 G265 G266 G267 G268 G269 G270 G271 G272 G273 G274 G275 G276 G277 G278 G279

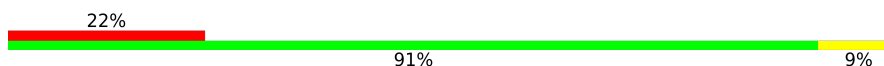


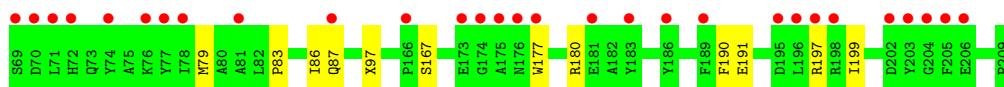
• Molecule 10: NUEM protein

Chain E:  100%

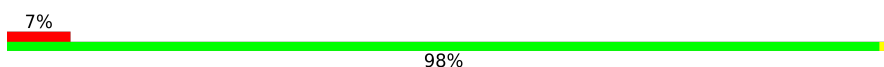
There are no outlier residues recorded for this chain.

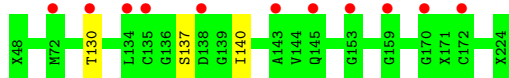
• Molecule 11: NUGM protein

Chain G:  22% 91% 9%



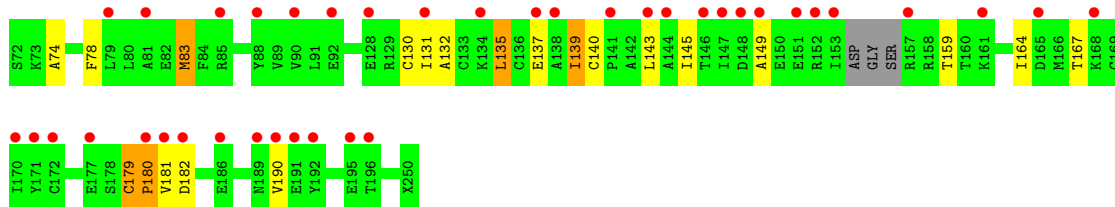
• Molecule 12: Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain H:  7% 98% .



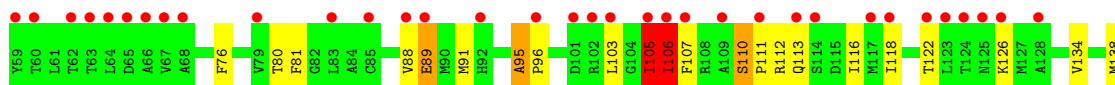
• Molecule 13: Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I)

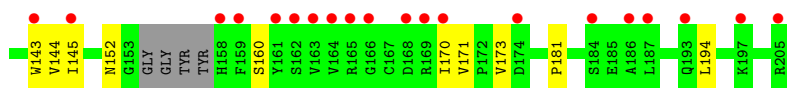
Chain I:  28% 83% 11% . .



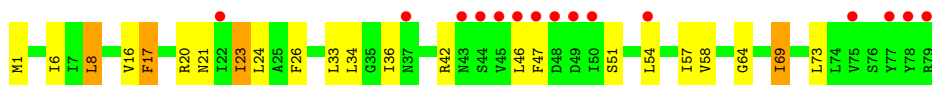
• Molecule 14: Subunit NUKM of protein NADH:Ubiquinone Oxidoreductase (Complex I)

Chain K:  37% 76% 18% . . .





- Molecule 15: NADH-ubiquinone oxidoreductase chain 4L



- Molecule 16: Unknown polypeptide



There are no outlier residues recorded for this chain.

- Molecule 16: Unknown polypeptide



There are no outlier residues recorded for this chain.

- Molecule 17: Unknown polypeptide



There are no outlier residues recorded for this chain.

- Molecule 17: Unknown polypeptide

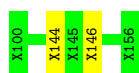


- Molecule 18: Unknown polypeptide



There are no outlier residues recorded for this chain.

- Molecule 19: Unknown polypeptide

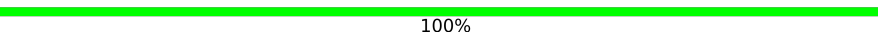


- Molecule 20: Unknown polypeptide



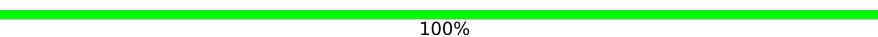
There are no outlier residues recorded for this chain.

- Molecule 21: Unknown polypeptide

Chain V:  100%

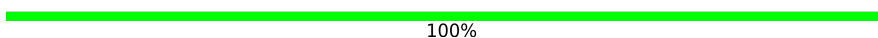
There are no outlier residues recorded for this chain.

- Molecule 22: Unknown polypeptide

Chain T:  100%

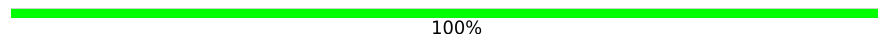
There are no outlier residues recorded for this chain.

- Molecule 22: Unknown polypeptide

Chain m:  100%

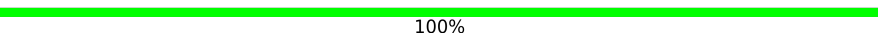
There are no outlier residues recorded for this chain.

- Molecule 22: Unknown polypeptide

Chain AI:  100%

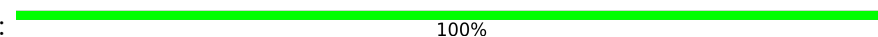
There are no outlier residues recorded for this chain.

- Molecule 23: Unknown polypeptide

Chain S:  100%

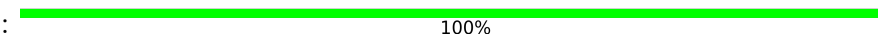
There are no outlier residues recorded for this chain.

- Molecule 23: Unknown polypeptide

Chain AJ:  100%

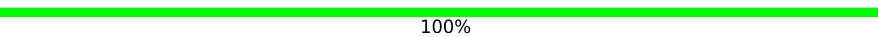
There are no outlier residues recorded for this chain.

- Molecule 23: Unknown polypeptide

Chain AL:  100%

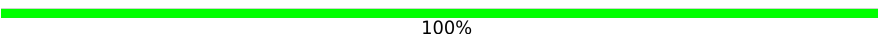
There are no outlier residues recorded for this chain.

- Molecule 24: Unknown polypeptide

Chain R:  100%

There are no outlier residues recorded for this chain.

- Molecule 25: Unknown polypeptide

Chain Q:  100%

There are no outlier residues recorded for this chain.

- Molecule 26: Unknown polypeptide

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: Unknown polypeptide

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: Unknown polypeptide

Chain f:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: Unknown polypeptide

Chain AC:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: Unknown polypeptide

Chain AH:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: Unknown polypeptide

Chain AM:  100%

There are no outlier residues recorded for this chain.

- Molecule 28: Unknown polypeptide

Chain O:  100%

There are no outlier residues recorded for this chain.

- Molecule 28: Unknown polypeptide

Chain l:  100%

There are no outlier residues recorded for this chain.

- Molecule 29: Unknown polypeptide

Chain M:  100%

There are no outlier residues recorded for this chain.

- Molecule 30: Unknown polypeptide

Chain D:  100%

There are no outlier residues recorded for this chain.

- Molecule 31: Unknown polypeptide

Chain J:  100%

There are no outlier residues recorded for this chain.

- Molecule 32: Unknown polypeptide

Chain N:  100%

There are no outlier residues recorded for this chain.

- Molecule 33: Unknown polypeptide

Chain a:  100%

There are no outlier residues recorded for this chain.

- Molecule 33: Unknown polypeptide

Chain i:  100%

There are no outlier residues recorded for this chain.

- Molecule 34: Unknown polypeptide

Chain b:  100%

There are no outlier residues recorded for this chain.

- Molecule 35: Unknown polypeptide

Chain c:  100%

There are no outlier residues recorded for this chain.

- Molecule 35: Unknown polypeptide

Chain g:  100%

There are no outlier residues recorded for this chain.

- Molecule 35: Unknown polypeptide

Chain AE:  100%

There are no outlier residues recorded for this chain.

- Molecule 35: Unknown polypeptide

Chain AK:  100%

There are no outlier residues recorded for this chain.

- Molecule 35: Unknown polypeptide

Chain AO:  100%

There are no outlier residues recorded for this chain.

- Molecule 36: Unknown polypeptide

Chain d:  100%

There are no outlier residues recorded for this chain.

- Molecule 36: Unknown polypeptide

Chain o:  100%

There are no outlier residues recorded for this chain.

- Molecule 36: Unknown polypeptide

Chain AB:  100%

There are no outlier residues recorded for this chain.

- Molecule 36: Unknown polypeptide

Chain AN:  94% 6%



- Molecule 37: Unknown polypeptide

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 37: Unknown polypeptide

Chain w:  100%

There are no outlier residues recorded for this chain.

- Molecule 37: Unknown polypeptide

Chain z:  100%

There are no outlier residues recorded for this chain.

- Molecule 38: Unknown polypeptide

Chain h:  91% 9%



- Molecule 39: Unknown polypeptide

Chain j:  100%

There are no outlier residues recorded for this chain.

- Molecule 40: Unknown polypeptide

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 40: Unknown polypeptide

Chain s:  100%

There are no outlier residues recorded for this chain.

- Molecule 41: Unknown polypeptide

Chain n:  100%

There are no outlier residues recorded for this chain.

- Molecule 41: Unknown polypeptide

Chain q:  100%

There are no outlier residues recorded for this chain.

- Molecule 42: Unknown polypeptide

Chain p:  100%

There are no outlier residues recorded for this chain.

- Molecule 43: Unknown polypeptide

Chain t:  100%

There are no outlier residues recorded for this chain.

- Molecule 44: Unknown polypeptide

Chain u:  100%

There are no outlier residues recorded for this chain.

- Molecule 45: Unknown polypeptide

Chain v:  100%

There are no outlier residues recorded for this chain.

- Molecule 45: Unknown polypeptide

Chain y:  100%

There are no outlier residues recorded for this chain.

- Molecule 46: Unknown polypeptide

Chain x:  100%

There are no outlier residues recorded for this chain.

- Molecule 46: Unknown polypeptide

Chain AG:  100%

There are no outlier residues recorded for this chain.

- Molecule 47: Unknown polypeptide

Chain AA:  100%

There are no outlier residues recorded for this chain.

- Molecule 48: Unknown polypeptide

Chain AD:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	316.31Å 316.31Å 819.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.79 40.00 – 3.79	Depositor EDS
% Data completeness (in resolution range)	77.1 (40.00-3.79) 77.2 (40.00-3.79)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.77Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.361 , 0.363 0.412 , 0.419	Depositor DCC
R_{free} test set	5835 reflections (3.61%)	wwPDB-VP
Wilson B-factor (Å ²)	142.0	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 226.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	35631	wwPDB-VP
Average B, all atoms (Å ²)	164.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, FES

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	1	0.82	1/2648 (0.0%)	1.48	14/3616 (0.4%)
2	2	0.77	1/2699 (0.0%)	1.45	8/3672 (0.2%)
3	3	0.88	0/699	1.55	5/954 (0.5%)
4	4	0.81	0/1991	1.48	14/2716 (0.5%)
5	5	0.80	1/2797 (0.0%)	1.46	14/3796 (0.4%)
6	6	0.83	0/836	1.46	1/1141 (0.1%)
7	A	0.79	0/547	1.53	5/740 (0.7%)
8	B	0.73	0/670	1.41	2/901 (0.2%)
9	C	0.79	1/2946 (0.0%)	1.42	18/3989 (0.5%)
11	G	0.72	0/581	1.22	0/787
12	H	0.72	0/172	1.40	0/210
13	I	0.83	0/614	1.40	7/836 (0.8%)
14	K	0.83	0/1092	1.35	1/1489 (0.1%)
15	L	0.79	0/620	1.65	3/839 (0.4%)
All	All	0.80	4/18912 (0.0%)	1.45	92/25686 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	5	643	ILE	CA-CB	6.40	1.57	1.54
9	C	91	HIS	CA-C	5.63	1.57	1.53
2	2	239	ILE	CA-CB	5.24	1.56	1.54
1	1	327	ILE	CA-C	5.08	1.56	1.52

The worst 5 of 92 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	241	PHE	CA-CB-CG	12.02	125.81	113.80
7	A	91	PRO	N-CA-CB	10.53	110.18	102.28
1	1	179	CYS	CA-C-N	10.36	126.77	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	179	CYS	C-N-CA	10.36	126.77	120.24
3	3	88	PHE	CA-CB-CG	8.04	121.84	113.80

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	1	2581	0	2675	56	0
2	2	3122	0	2880	49	0
3	3	685	0	719	16	0
4	4	3017	0	2290	38	0
5	5	4050	0	3162	41	0
6	6	870	0	916	25	0
7	A	3221	0	1001	2	0
8	B	1997	0	856	5	0
9	C	2882	0	2825	49	0
10	E	975	0	228	0	0
11	G	880	0	582	6	0
12	H	803	0	299	1	0
13	I	857	0	582	6	0
14	K	1069	0	1038	20	0
15	L	612	0	664	14	0
16	Z	85	0	19	0	0
16	r	85	0	20	0	0
17	AF	200	0	46	1	0
17	Y	200	0	43	0	0
18	U	50	0	13	0	0
19	X	285	0	64	1	0
20	W	270	0	59	0	0
21	V	315	0	69	0	0
22	AI	100	0	22	0	0
22	T	100	0	22	0	0
22	m	100	0	22	0	0
23	AJ	95	0	22	0	0

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Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	AL	95	0	21	0	0
23	S	95	0	21	0	0
24	R	250	0	53	0	0
25	Q	350	0	75	0	0
26	P	140	0	32	0	0
27	AC	90	0	22	0	0
27	AH	90	0	20	0	0
27	AM	90	0	21	0	0
27	F	90	0	20	0	0
27	f	90	0	20	0	0
28	O	125	0	27	0	0
28	l	125	0	27	0	0
29	M	255	0	56	0	0
30	D	150	0	32	0	0
31	J	345	0	74	0	0
32	N	75	0	17	0	0
33	a	130	0	29	0	0
33	i	130	0	31	0	0
34	b	110	0	24	0	0
35	AE	45	0	11	0	0
35	AK	45	0	11	0	0
35	AO	45	0	11	0	0
35	c	45	0	11	0	0
35	g	45	0	12	0	0
36	AB	80	0	19	0	0
36	AN	80	0	18	1	0
36	d	80	0	19	0	0
36	o	80	0	19	0	0
37	e	65	0	15	0	0
37	w	65	0	17	0	0
37	z	65	0	15	0	0
38	h	235	0	49	2	0
39	j	240	0	52	0	0
40	k	115	0	25	0	0
40	s	115	0	26	0	0
41	n	180	0	38	0	0
41	q	180	0	44	0	0
42	p	380	0	78	0	0
43	t	225	0	47	0	0
44	u	160	0	34	0	0
45	v	55	0	14	0	0
45	y	54	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	AG	40	0	10	0	0
46	x	40	0	10	0	0
47	AA	290	0	64	0	0
48	AD	195	0	43	0	0
49	A	4	0	0	0	0
49	H	4	0	0	0	0
50	A	16	0	0	0	0
50	B	8	0	0	0	0
50	I	16	0	0	0	0
50	K	8	0	0	0	0
All	All	35631	0	22486	287	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 5.

The worst 5 of 287 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)
9:C:295:MET:HE3	9:C:457:MET:HA	1.38	1.05
4:4:225:PHE:H	4:4:284:THR:HG22	1.39	0.86
1:1:142:GLN:HG3	1:1:308:LEU:HD23	1.62	0.82
2:2:125:THR:HA	6:6:161:ILE:HD11	1.70	0.73
5:5:126:TRP:CZ3	5:5:146:ILE:HG12	2.24	0.72

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	1	319/335 (95%)	274 (86%)	29 (9%)	16 (5%)	1 17
2	2	337/434 (78%)	309 (92%)	24 (7%)	4 (1%)	10 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	3	82/110 (74%)	68 (83%)	12 (15%)	2 (2%)	4	29
4	4	257/470 (55%)	228 (89%)	24 (9%)	5 (2%)	6	32
5	5	353/616 (57%)	315 (89%)	31 (9%)	7 (2%)	6	32
6	6	104/184 (56%)	89 (86%)	10 (10%)	5 (5%)	2	17
7	A	84/634 (13%)	72 (86%)	9 (11%)	3 (4%)	2	22
8	B	95/370 (26%)	90 (95%)	4 (4%)	1 (1%)	11	41
9	C	361/383 (94%)	296 (82%)	41 (11%)	24 (7%)	1	13
11	G	67/133 (50%)	58 (87%)	7 (10%)	2 (3%)	3	25
12	H	29/154 (19%)	27 (93%)	2 (7%)	0	100	100
13	I	82/140 (59%)	63 (77%)	13 (16%)	6 (7%)	1	11
14	K	139/147 (95%)	122 (88%)	11 (8%)	6 (4%)	2	19
15	L	77/79 (98%)	69 (90%)	5 (6%)	3 (4%)	2	20
All	All	2386/4189 (57%)	2080 (87%)	222 (9%)	84 (4%)	3	23

5 of 84 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	60	LYS
1	1	269	VAL
2	2	62	ASN
5	5	346	ALA
7	A	133	CYS

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	1	286/296 (97%)	246 (86%)	40 (14%)	3	18
2	2	291/308 (94%)	258 (89%)	33 (11%)	5	23
3	3	75/96 (78%)	65 (87%)	10 (13%)	4	19
4	4	215/229 (94%)	192 (89%)	23 (11%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	5	301/302 (100%)	274 (91%)	27 (9%)	9	32
6	6	90/157 (57%)	74 (82%)	16 (18%)	2	12
7	A	37/83 (45%)	37 (100%)	0	100	100
8	B	53/83 (64%)	50 (94%)	3 (6%)	18	44
9	C	305/324 (94%)	269 (88%)	36 (12%)	5	22
11	G	55/58 (95%)	54 (98%)	1 (2%)	51	67
12	H	19/19 (100%)	18 (95%)	1 (5%)	20	45
13	I	55/78 (70%)	47 (86%)	8 (14%)	3	17
14	K	114/125 (91%)	108 (95%)	6 (5%)	20	45
15	L	68/69 (99%)	61 (90%)	7 (10%)	7	27
All	All	1964/2227 (88%)	1753 (89%)	211 (11%)	6	25

5 of 211 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	5	215	ILE
6	6	154	LEU
14	K	105	ILE
5	5	329	LEU
5	5	649	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
9	C	288	ASN
14	K	195	GLN
9	C	349	GLN
13	I	176	GLN
3	3	107	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands 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	$\# Z > 2$
49	FES	A	900	7	0,4,4	-	-	-		
50	SF4	I	501	13	0,12,12	-	-	-		
50	SF4	A	901	7	0,12,12	-	-	-		
50	SF4	A	902	7	0,12,12	-	-	-		
50	SF4	K	500	14	0,12,12	-	-	-		
49	FES	H	300	12	0,4,4	-	-	-		
50	SF4	B	500	8	0,12,12	-	-	-		
50	SF4	I	500	13	0,12,12	-	-	-		

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
49	FES	A	900	7	-	-	0/1/1/1
50	SF4	I	501	13	-	-	0/6/5/5
50	SF4	A	901	7	-	-	0/6/5/5
50	SF4	A	902	7	-	-	0/6/5/5
50	SF4	K	500	14	-	-	0/6/5/5
49	FES	H	300	12	-	-	0/1/1/1
50	SF4	B	500	8	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	SF4	I	500	13	-	-	0/6/5/5

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	A	27
10	E	10
8	B	10
5	5	8
12	H	5
13	I	4
2	2	4
4	4	4
11	G	2
41	q	1
25	Q	1

The worst 5 of 76 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	422:UNK	C	499:UNK	N	48.59
1	B	270:UNK	C	279:UNK	N	26.48
1	A	148:SER	C	152:UNK	N	24.96
1	E	513:UNK	C	604:UNK	N	24.71
1	I	92:GLU	C	103:UNK	N	24.13

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	1	325/335 (97%)	2.38	175 (53%) 0 0	46, 169, 254, 284	0
2	2	339/434 (78%)	1.16	67 (19%) 3 5	46, 83, 126, 144	0
3	3	88/110 (80%)	1.97	34 (38%) 1 1	55, 126, 252, 271	0
4	4	257/470 (54%)	1.18	60 (23%) 2 3	60, 93, 130, 184	0
5	5	354/616 (57%)	1.86	140 (39%) 1 1	93, 127, 226, 291	0
6	6	109/184 (59%)	0.69	9 (8%) 17 17	47, 81, 132, 209	0
7	A	92/634 (14%)	3.08	57 (61%) 0 0	154, 245, 279, 284	0
8	B	101/370 (27%)	2.78	63 (62%) 0 0	153, 259, 286, 297	0
9	C	369/383 (96%)	2.49	199 (53%) 0 0	93, 186, 223, 240	0
10	E	0/195	-	-	-	-
11	G	69/133 (51%)	2.12	29 (42%) 0 1	134, 166, 282, 295	0
12	H	30/154 (19%)	1.85	11 (36%) 1 1	103, 258, 293, 297	0
13	I	87/140 (62%)	2.23	39 (44%) 0 1	121, 169, 255, 268	0
14	K	143/147 (97%)	1.89	54 (37%) 1 1	93, 165, 227, 243	1 (0%)
15	L	79/79 (100%)	1.60	15 (18%) 3 5	15, 93, 186, 219	1 (1%)
16	Z	0/17	-	-	-	-
16	r	0/17	-	-	-	-
17	AF	0/40	-	-	-	-
17	Y	0/40	-	-	-	-
18	U	0/10	-	-	-	-
19	X	0/57	-	-	-	-
20	W	0/54	-	-	-	-
21	V	0/63	-	-	-	-
22	AI	0/20	-	-	-	-
22	T	0/20	-	-	-	-
22	m	0/20	-	-	-	-
23	AJ	0/19	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
23	AL	0/19	-	-	-	-
23	S	0/19	-	-	-	-
24	R	0/50	-	-	-	-
25	Q	0/70	-	-	-	-
26	P	0/28	-	-	-	-
27	AC	0/18	-	-	-	-
27	AH	0/18	-	-	-	-
27	AM	0/18	-	-	-	-
27	F	0/18	-	-	-	-
27	f	0/18	-	-	-	-
28	O	0/25	-	-	-	-
28	l	0/25	-	-	-	-
29	M	0/51	-	-	-	-
30	D	0/30	-	-	-	-
31	J	0/69	-	-	-	-
32	N	0/15	-	-	-	-
33	a	0/26	-	-	-	-
33	i	0/26	-	-	-	-
34	b	0/22	-	-	-	-
35	AE	0/9	-	-	-	-
35	AK	0/9	-	-	-	-
35	AO	0/9	-	-	-	-
35	c	0/9	-	-	-	-
35	g	0/9	-	-	-	-
36	AB	0/16	-	-	-	-
36	AN	0/16	-	-	-	-
36	d	0/16	-	-	-	-
36	o	0/16	-	-	-	-
37	e	0/13	-	-	-	-
37	w	0/13	-	-	-	-
37	z	0/13	-	-	-	-
38	h	0/47	-	-	-	-
39	j	0/48	-	-	-	-
40	k	0/23	-	-	-	-
40	s	0/23	-	-	-	-
41	n	0/36	-	-	-	-
41	q	0/36	-	-	-	-
42	p	0/76	-	-	-	-
43	t	0/45	-	-	-	-
44	u	0/32	-	-	-	-
45	v	0/11	-	-	-	-
45	y	0/11	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
46	AG	0/8	-	-	-	-
46	x	0/8	-	-	-	-
47	AA	0/58	-	-	-	-
48	AD	0/39	-	-	-	-
All	All	2442/5975 (40%)	1.91	952 (38%) 1 1	15, 134, 261, 297	2 (0%)

The worst 5 of 952 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	L	48	ASP	14.8
9	C	119	LEU	12.4
9	C	208	GLU	11.1
14	K	158	HIS	10.1
1	1	139	SER	10.1

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
50	SF4	A	901	8/8	0.89	0.09	226,234,244,247	0
50	SF4	B	500	8/8	0.91	0.07	255,259,260,260	0
49	FES	H	300	4/4	0.93	0.09	172,174,182,183	0
50	SF4	A	902	8/8	0.95	0.06	195,221,242,242	0
49	FES	A	900	4/4	0.95	0.09	221,222,223,223	0
50	SF4	K	500	8/8	0.95	0.07	138,142,150,186	0
50	SF4	I	501	8/8	0.96	0.05	165,170,173,175	0
50	SF4	I	500	8/8	0.97	0.05	169,173,176,177	0

6.5 Other polymers [i](#)

There are no such residues in this entry.