



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:09 am BST

PDB ID : 6H8K
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 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

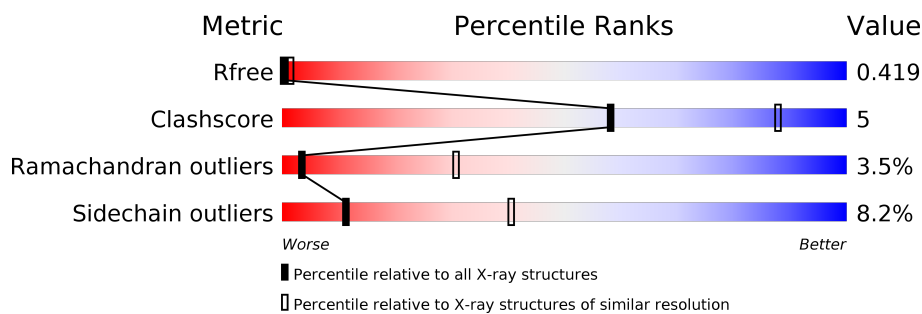
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



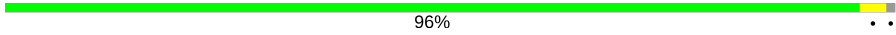

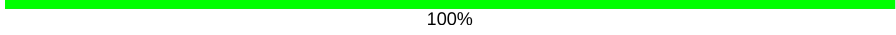

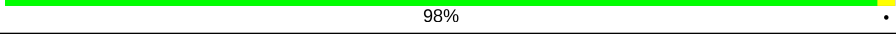


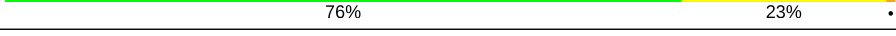
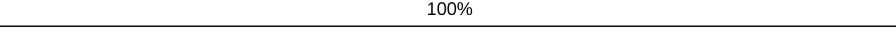
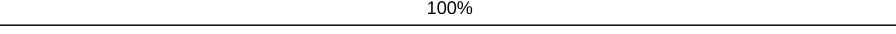
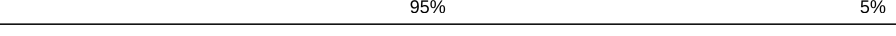
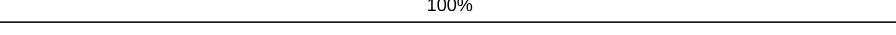
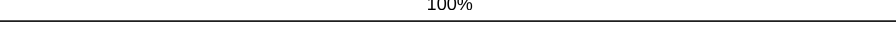
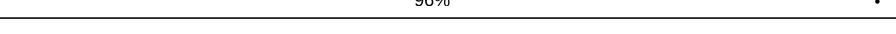
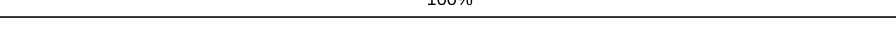
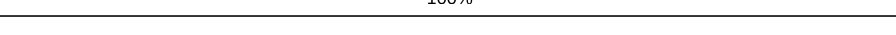
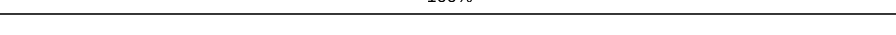
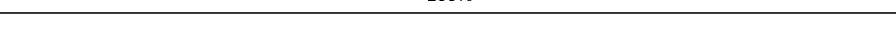


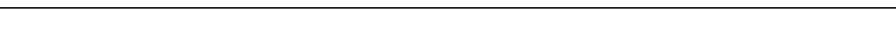
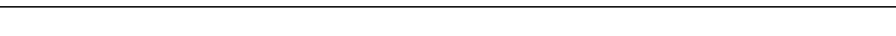



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1	335	66% 27% . .
2	2	434	79% 19% .
3	3	110	60% 17% . 20%
4	4	470	83% 16% .
5	5	616	86% 13% .
6	6	184	46% 14% . 36%
7	A	634	98% ..
















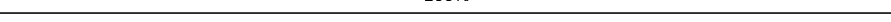
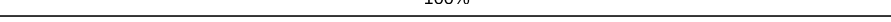
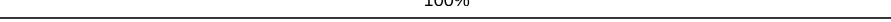
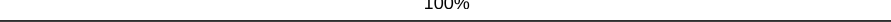
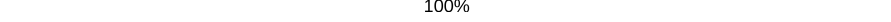
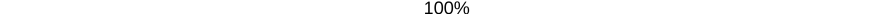
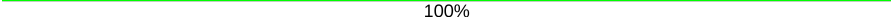
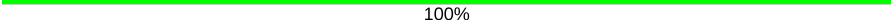

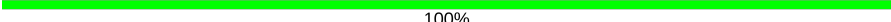
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Mol	Chain	Length	Quality of chain
8	B	370	 96%
9	C	383	 68% 26%
10	E	195	 100%
11	G	133	 92% 8%
12	H	154	 98%
13	I	140	 86% 10%
14	K	147	 75% 20%
15	L	79	 76% 23%
16	Z	17	 100%
16	r	17	 100%
17	AF	40	 95% 5%
17	Y	40	 100%
18	U	10	 100%
19	X	57	 96%
20	W	54	 100%
21	V	63	 100%
22	AI	20	 100%
22	T	20	 100%
22	m	20	 100%
23	AJ	19	 100%
23	AL	19	 100%
23	S	19	 100%
24	R	50	 100%
25	Q	70	 100%
26	P	28	 100%

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Mol	Chain	Length	Quality of chain
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	 100%
36	d	16	 100%
36	o	16	 100%
37	e	13	 100%
37	w	13	 100%

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Mol	Chain	Length	Quality of chain
37	z	13	 100%
38	h	47	 100%
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			

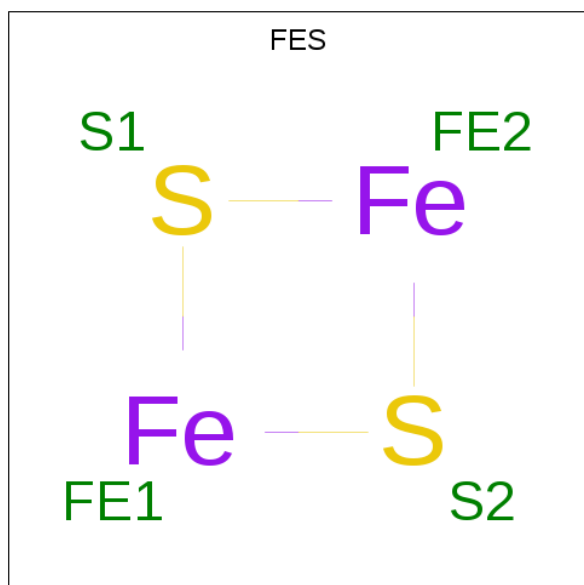
- Molecule 47 is a protein called Unknown polypeptide.

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.

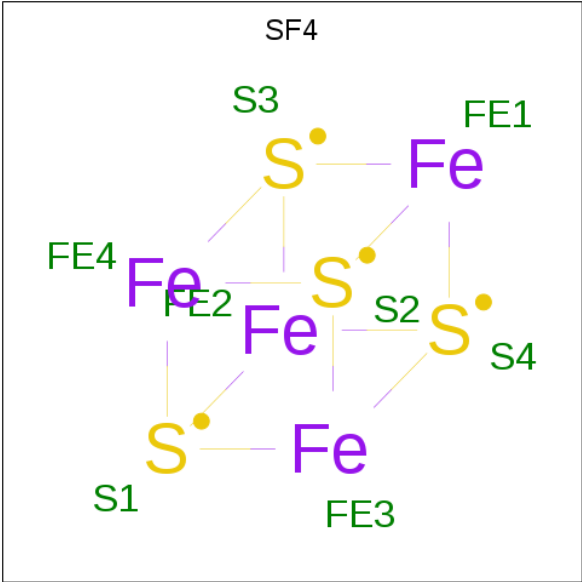
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	AD	39	Total	C	N	O	0	0	0
			195	117	39	39			

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



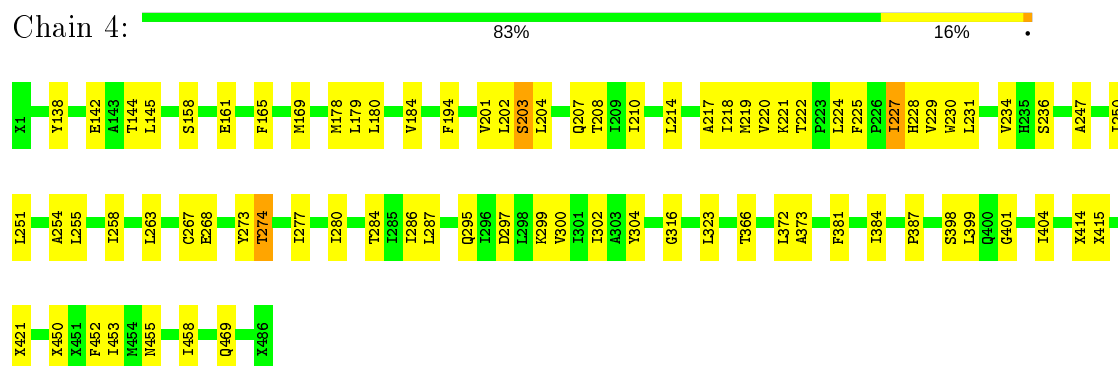
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
49	A	1	Total	Fe	S	0	0
			4	2	2		
49	H	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 50 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

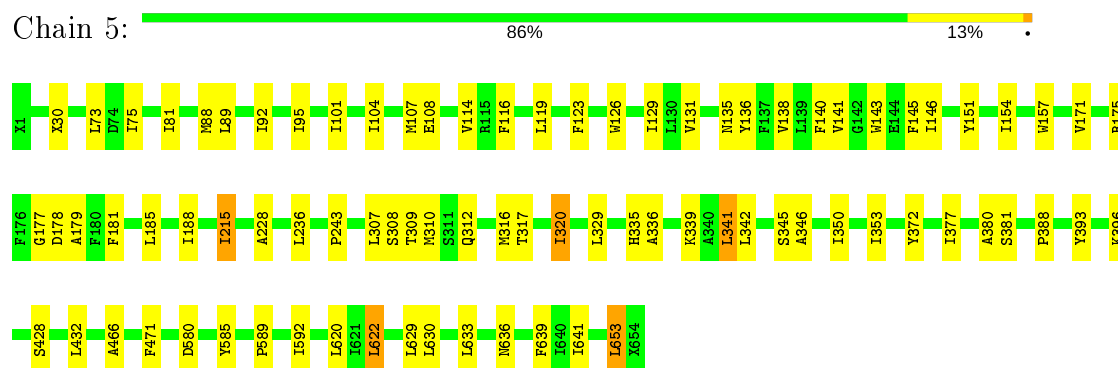


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
50	A	1	Total	Fe	S	0	0
			8	4	4		
50	A	1	Total	Fe	S	0	0
			8	4	4		
50	B	1	Total	Fe	S	0	0
			8	4	4		
50	I	1	Total	Fe	S	0	0
			8	4	4		
50	I	1	Total	Fe	S	0	0
			8	4	4		
50	K	1	Total	Fe	S	0	0
			8	4	4		

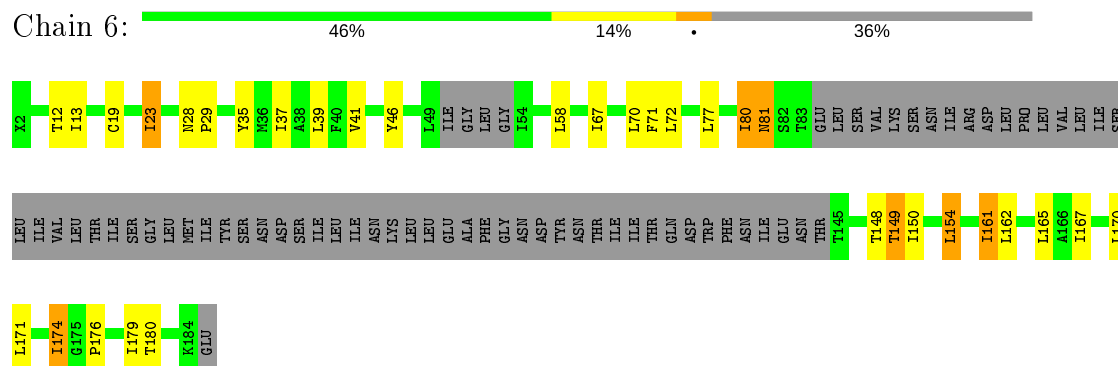
- Molecule 4: NADH-ubiquinone oxidoreductase chain 4



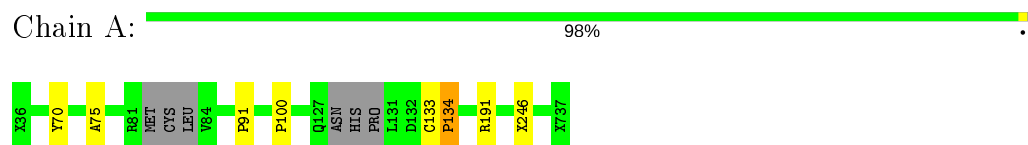
- Molecule 5: NADH-ubiquinone oxidoreductase chain 5



- Molecule 6: NADH-ubiquinone oxidoreductase chain 6

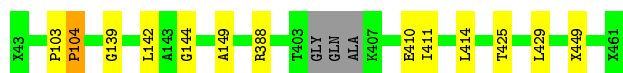


- Molecule 7: NUAM protein



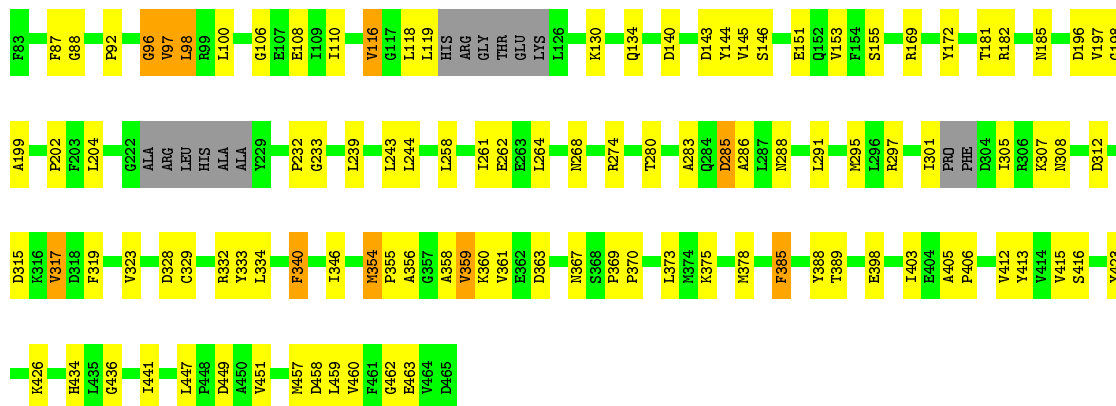
- Molecule 8: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial





- Molecule 9: NUCM protein

Chain C: 68% 26%



- Molecule 10: NUEM protein

Chain E: 100%

There are no outlier residues recorded for this chain.

- Molecule 11: NUGM protein

Chain G: 92% 8%



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

Chain H: 98%



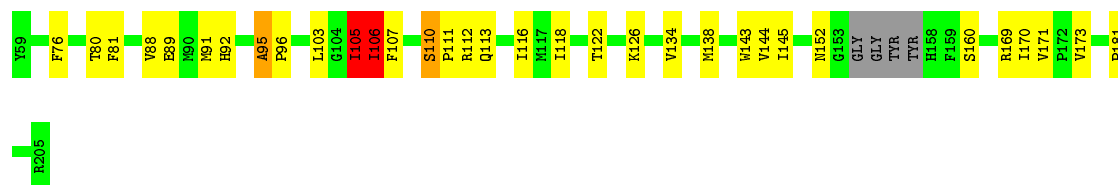
- Molecule 13: Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain I: 86% 10%



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

Chain K: 75% 20%



- 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

Chain W:  100%

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:  100%

There are no outlier residues recorded for this chain.

- 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:  100%

There are no outlier residues recorded for this chain.

- 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 49.18 – 3.79	Depositor EDS
% Data completeness (in resolution range)	77.1 (40.00-3.79) 77.4 (49.18-3.79)	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 (4.86%)	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 , 238.0	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	0.46	0/2648	0.70	0/3616
2	2	0.42	0/2699	0.64	0/3672
3	3	0.48	0/699	0.74	0/954
4	4	0.45	0/1991	0.66	0/2716
5	5	0.43	0/2797	0.62	0/3796
6	6	0.45	0/836	0.70	0/1141
7	A	0.43	0/547	0.71	3/740 (0.4%)
8	B	0.41	0/670	0.62	2/901 (0.2%)
9	C	0.42	0/2946	0.66	0/3989
11	G	0.39	0/581	0.55	0/787
12	H	0.39	0/172	0.63	0/210
13	I	0.45	0/614	0.69	0/836
14	K	0.44	0/1092	0.66	0/1489
15	L	0.44	0/620	0.71	0/839
All	All	0.44	0/18912	0.66	5/25686 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	134	PRO	N-CA-CB	6.84	111.50	103.30
8	B	104	PRO	N-CA-CB	5.92	110.40	103.30
8	B	103	PRO	N-CA-CB	5.83	110.29	103.30
7	A	91	PRO	N-CA-CB	5.73	110.18	103.30
7	A	100	PRO	N-CA-CB	5.67	110.10	103.30

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	53	0
2	2	3122	0	2880	48	0
3	3	685	0	719	16	0
4	4	3017	0	2290	38	0
5	5	4050	0	3162	40	0
6	6	870	0	916	25	0
7	A	3221	0	1001	2	0
8	B	1997	0	856	4	0
9	C	2882	0	2825	50	0
10	E	975	0	228	0	0
11	G	880	0	582	5	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	O	125	0	27	0	0
28	I	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	0	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	0	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	35631	0	22486	279	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.

All (279) 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)
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
6:6:167:ILE:HA	6:6:170:LEU:HG	1.70	0.71
9:C:144:TYR:CE1	14:K:88:VAL:HG21	2.25	0.71
5:5:175:ARG:HA	5:5:178:ASP:HB2	1.71	0.71
2:2:208:LEU:HB3	2:2:244:ILE:HD11	1.73	0.70
3:3:57:ILE:HG12	6:6:77:LEU:HD21	1.72	0.70
6:6:176:PRO:HA	6:6:179:ILE:HG22	1.74	0.69
1:1:302:ARG:HH22	9:C:451:VAL:HB	1.56	0.69
2:2:123:PHE:HB2	2:2:182:TYR:HB3	1.74	0.68
3:3:98:LEU:HD21	6:6:170:LEU:HA	1.76	0.67
1:1:121:LEU:HB3	1:1:140:THR:HG21	1.76	0.66
2:2:166:ILE:HD11	15:L:33:LEU:HG	1.78	0.66
6:6:12:THR:HG21	6:6:46:TYR:HB2	1.78	0.66
1:1:302:ARG:HG2	9:C:197:VAL:HA	1.78	0.64
5:5:95:ILE:HD11	5:5:336:ALA:HB1	1.78	0.64
5:5:345:SER:HB2	5:5:377:ILE:HD12	1.79	0.64
2:2:59:LEU:HB2	2:2:121:ASN:HB2	1.79	0.63
6:6:80:ILE:HG23	6:6:81:ASN:H	1.62	0.63
2:2:414:LEU:HB3	4:4:165:PHE:HE2	1.63	0.63
3:3:6:ILE:O	3:3:9:ILE:HG12	1.99	0.62
15:L:1:MET:HB2	15:L:42:ARG:HG2	1.81	0.62
5:5:341:LEU:HD11	5:5:466:ALA:HA	1.81	0.62
14:K:110:SER:HB2	14:K:111:PRO:HA	1.80	0.62
1:1:109:SER:HB3	1:1:241:PHE:HE1	1.65	0.62
5:5:151:TYR:HB2	5:5:171:VAL:HG21	1.80	0.62
9:C:295:MET:CE	9:C:457:MET:HA	2.30	0.62
9:C:140:ASP:HB3	9:C:151:GLU:HG3	1.82	0.62
5:5:140:PHE:HD1	5:5:181:PHE:CZ	2.18	0.61
14:K:116:ILE:HG13	14:K:143:TRP:HB2	1.83	0.61
4:4:228:HIS:HE1	4:4:287:LEU:HD23	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:46:PHE:HB3	2:2:62:ASN:HB3	1.84	0.60
14:K:95:ALA:HB1	14:K:96:PRO:CD	2.32	0.60
4:4:452:PHE:HA	4:4:455:ASN:HB2	1.82	0.60
4:4:280:ILE:O	4:4:284:THR:HG23	2.02	0.59
9:C:119:LEU:HD13	9:C:462:GLY:HA2	1.83	0.59
9:C:413:TYR:HB3	9:C:426:LYS:HB2	1.85	0.59
4:4:221:LYS:HG3	4:4:254:ALA:HB2	1.85	0.58
2:2:276:LEU:HG	2:2:287:PHE:HB3	1.84	0.58
2:2:49:ASN:ND2	2:2:63:SER:HB3	2.19	0.58
14:K:89:GLU:HG3	14:K:181:PRO:HB2	1.86	0.58
4:4:450:UNK:HA	4:4:453:ILE:HD12	1.85	0.57
2:2:214:ILE:HG23	2:2:268:LEU:HD22	1.85	0.57
4:4:202:LEU:HB3	4:4:207:GLN:HG2	1.85	0.57
6:6:179:ILE:HG23	6:6:180:THR:HG23	1.86	0.57
5:5:585:TYR:O	5:5:589:PRO:HD2	2.03	0.57
9:C:258:LEU:HD11	9:C:340:PHE:HB3	1.86	0.57
9:C:98:LEU:HA	9:C:116:VAL:HG11	1.86	0.57
2:2:299:LEU:HD11	2:2:386:ILE:HG12	1.87	0.57
1:1:302:ARG:HE	9:C:197:VAL:HA	1.68	0.57
3:3:64:LEU:HD21	6:6:67:ILE:HG13	1.87	0.57
2:2:375:PRO:HG2	4:4:138:TYR:HE2	1.70	0.57
1:1:81:LEU:HD22	1:1:230:ALA:HB2	1.87	0.56
8:B:410:GLU:O	8:B:414:LEU:HG	2.06	0.56
9:C:295:MET:HE2	9:C:457:MET:HA	1.87	0.56
1:1:295:TRP:HD1	1:1:295:TRP:H	1.55	0.55
4:4:142:GLU:HA	4:4:145:LEU:HD13	1.89	0.55
9:C:130:LYS:HB3	9:C:134:GLN:HB3	1.89	0.55
1:1:117:VAL:HG22	1:1:143:LEU:HG	1.89	0.55
14:K:95:ALA:CB	14:K:96:PRO:CD	2.86	0.54
1:1:269:VAL:HG12	1:1:270:SER:H	1.72	0.54
4:4:203:SER:HB2	4:4:207:GLN:HB2	1.91	0.53
1:1:177:TRP:HA	1:1:251:LEU:HD23	1.91	0.53
5:5:377:ILE:HG23	5:5:432:LEU:HD13	1.91	0.53
12:H:137:SER:HA	12:H:140:ILE:HD12	1.90	0.53
4:4:220:VAL:HG22	4:4:227:ILE:HG21	1.90	0.53
5:5:101:ILE:HA	5:5:104:ILE:HD12	1.90	0.53
5:5:177:GLY:O	5:5:181:PHE:HB2	2.09	0.53
5:5:188:ILE:HD13	5:5:215:ILE:HG12	1.91	0.53
19:X:144:UNK:C	19:X:146:UNK:H	2.22	0.53
1:1:121:LEU:HD11	6:6:72:LEU:HB3	1.90	0.53
1:1:237:LEU:O	1:1:241:PHE:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:341:LEU:HB3	5:5:380:ALA:HB2	1.91	0.52
5:5:317:THR:HA	5:5:320:ILE:HG22	1.92	0.52
2:2:273:VAL:HG21	2:2:405:ALA:HB1	1.91	0.52
4:4:178:MET:HB2	4:4:217:ALA:HB2	1.91	0.52
4:4:455:ASN:HA	4:4:458:ILE:HD12	1.92	0.52
6:6:71:PHE:CE1	15:L:26:PHE:HB3	2.45	0.52
6:6:13:ILE:HD11	15:L:6:ILE:HD12	1.92	0.52
4:4:138:TYR:CZ	4:4:179:LEU:HB2	2.45	0.52
4:4:415:UNK:HA	5:5:179:ALA:HB1	1.91	0.52
6:6:29:PRO:HB3	15:L:23:ILE:HD13	1.92	0.52
3:3:68:LEU:HD11	15:L:64:GLY:HA3	1.92	0.51
14:K:76:PHE:HB2	14:K:116:ILE:HD13	1.91	0.51
9:C:146:SER:HB3	9:C:185:ASN:HB2	1.92	0.51
2:2:187:LEU:HD11	2:2:197:LEU:HD21	1.92	0.51
3:3:76:TYR:HE1	6:6:154:LEU:HB3	1.74	0.51
9:C:405:ALA:HB1	9:C:406:PRO:CD	2.40	0.51
1:1:26:GLU:HG3	1:1:294:ILE:HG12	1.91	0.51
1:1:204:LEU:HD22	1:1:302:ARG:HD3	1.93	0.51
4:4:384:ILE:HG12	4:4:421:UNK:HA	1.92	0.51
5:5:622:LEU:HB2	15:L:16:VAL:HG21	1.93	0.51
2:2:295:TYR:HA	2:2:298:LEU:HD12	1.92	0.51
1:1:109:SER:HB3	1:1:241:PHE:CE1	2.45	0.50
1:1:314:ILE:HD11	3:3:108:THR:HB	1.93	0.50
9:C:202:PRO:HG3	9:C:264:LEU:HD23	1.92	0.50
11:G:180:ARG:HB3	11:G:199:ILE:HD11	1.94	0.50
2:2:139:LEU:HD11	15:L:69:ILE:HD11	1.93	0.50
3:3:60:ALA:O	6:6:70:LEU:HD21	2.11	0.50
9:C:434:HIS:CE1	9:C:459:LEU:HB2	2.47	0.50
1:1:155:ILE:HG22	3:3:74:LEU:HD23	1.94	0.50
2:2:140:ILE:HA	2:2:143:ILE:HD12	1.94	0.50
5:5:126:TRP:HA	5:5:129:ILE:HD12	1.94	0.49
1:1:125:TRP:HA	1:1:133:LEU:HD13	1.93	0.49
9:C:146:SER:HA	9:C:181:THR:HG22	1.95	0.49
2:2:54:VAL:HG21	2:2:60:ILE:HG12	1.95	0.49
4:4:219:MET:HA	4:4:224:LEU:HD12	1.95	0.49
4:4:399:LEU:HD21	4:4:414:UNK:HA	1.92	0.49
5:5:308:SER:O	5:5:312:GLN:HG2	2.13	0.49
9:C:119:LEU:HD12	14:K:122:THR:HG21	1.94	0.49
14:K:110:SER:HB3	14:K:113:GLN:H	1.77	0.49
6:6:71:PHE:HE1	15:L:26:PHE:HB3	1.77	0.49
1:1:292:SER:HA	1:1:295:TRP:NE1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:291:PHE:O	1:1:295:TRP:HD1	1.96	0.49
5:5:89:LEU:HG	5:5:131:VAL:HG11	1.93	0.49
1:1:193:SER:O	1:1:197:THR:HG22	2.12	0.49
9:C:169:ARG:H	9:C:358:ALA:HB3	1.78	0.49
1:1:238:ILE:HA	1:1:241:PHE:HB3	1.95	0.49
9:C:359:VAL:HG13	9:C:360:LYS:H	1.78	0.49
2:2:375:PRO:HG2	4:4:138:TYR:CE2	2.48	0.49
1:1:8:ILE:HG23	1:1:99:LEU:HD21	1.95	0.48
2:2:138:TYR:HE2	15:L:73:LEU:HD13	1.77	0.48
3:3:98:LEU:HD11	6:6:170:LEU:HB3	1.95	0.48
14:K:118:ILE:HG12	14:K:145:ILE:HB	1.96	0.48
1:1:324:PHE:HE1	3:3:92:LEU:HD22	1.78	0.48
5:5:589:PRO:HA	5:5:592:ILE:HB	1.94	0.48
9:C:295:MET:HE3	9:C:457:MET:HA	1.96	0.48
1:1:106:ILE:HG21	1:1:158:ILE:HD11	1.95	0.47
6:6:165:LEU:HD11	15:L:58:VAL:HG22	1.95	0.47
7:A:75:ALA:HB3	7:A:191:ARG:HD2	1.96	0.47
2:2:78:VAL:HG21	2:2:321:LEU:HD21	1.96	0.47
2:2:262:ILE:O	2:2:266:LEU:HG	2.14	0.47
2:2:46:PHE:HB3	2:2:62:ASN:CB	2.44	0.47
4:4:274:THR:HA	4:4:277:ILE:HD12	1.96	0.47
5:5:388:PRO:HA	5:5:393:TYR:HB2	1.96	0.47
8:B:411:ILE:HD13	8:B:449:UNK:HA	1.96	0.47
4:4:236:SER:HB2	4:4:299:LYS:HG3	1.97	0.47
9:C:317:VAL:HG11	9:C:346:ILE:HG13	1.96	0.47
8:B:139:GLY:HA2	8:B:142:LEU:HD12	1.96	0.47
1:1:178:TYR:CE1	1:1:180:ILE:HA	2.49	0.47
4:4:401:GLY:HA2	4:4:404:ILE:HD12	1.95	0.47
6:6:23:ILE:HG22	6:6:35:TYR:HB3	1.97	0.47
6:6:150:ILE:HG23	15:L:54:LEU:HD12	1.97	0.47
2:2:215:ALA:H	2:2:268:LEU:HD13	1.79	0.47
4:4:366:THR:HG22	4:4:373:ALA:HB1	1.97	0.47
2:2:277:LEU:HB2	2:2:412:TYR:CE1	2.49	0.46
5:5:350:ILE:HA	5:5:353:ILE:HD12	1.97	0.46
9:C:244:LEU:HD13	9:C:354:MET:HG3	1.97	0.46
13:I:132:ALA:HA	13:I:159:THR:HG23	1.98	0.46
2:2:242:ILE:HG23	2:2:313:ILE:HG21	1.97	0.46
14:K:95:ALA:CB	14:K:96:PRO:HD2	2.45	0.46
1:1:179:CYS:HB3	1:1:182:LEU:HD13	1.98	0.46
1:1:243:GLY:HA2	1:1:247:LEU:HB2	1.96	0.46
1:1:312:CYS:HA	1:1:316:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:314:ILE:HG23	3:3:103:VAL:HG21	1.98	0.46
3:3:57:ILE:HG12	6:6:77:LEU:CD2	2.41	0.46
9:C:436:GLY:HA2	11:G:177:TRP:CD1	2.51	0.46
9:C:118:LEU:HD21	14:K:126:LYS:HD3	1.98	0.46
2:2:369:PHE:HD1	2:2:374:ILE:HG13	1.79	0.46
9:C:182:ARG:HG3	9:C:406:PRO:HB3	1.98	0.46
11:G:180:ARG:HH11	11:G:197:ARG:HB3	1.80	0.46
4:4:178:MET:HG3	4:4:214:LEU:HA	1.97	0.46
4:4:219:MET:HG2	4:4:224:LEU:HD12	1.98	0.46
17:AF:320:UNK:CB	17:AF:321:UNK:HA	2.46	0.46
14:K:170:ILE:HG22	14:K:171:VAL:HG23	1.97	0.45
5:5:88:MET:O	5:5:92:ILE:HG12	2.15	0.45
1:1:86:ILE:O	1:1:89:VAL:HG22	2.17	0.45
14:K:144:VAL:HB	14:K:173:VAL:HA	1.99	0.45
1:1:91:ILE:HD11	1:1:237:LEU:HD12	1.99	0.45
2:2:262:ILE:O	2:2:265:ILE:HG12	2.16	0.45
9:C:388:TYR:HA	13:I:139:ILE:HD13	1.99	0.45
5:5:307:LEU:HD23	5:5:310:MET:HE1	1.98	0.45
1:1:8:ILE:CG2	1:1:99:LEU:HD21	2.47	0.45
9:C:460:VAL:HG12	9:C:463:GLU:H	1.82	0.45
5:5:30:UNK:HA	5:5:114:VAL:HG22	2.00	0.44
6:6:176:PRO:HA	6:6:179:ILE:CG2	2.45	0.44
5:5:107:MET:SD	5:5:116:PHE:HB3	2.58	0.44
2:2:386:ILE:O	2:2:390:ILE:HG12	2.18	0.44
4:4:247:ALA:HA	4:4:251:LEU:HD13	1.99	0.44
4:4:387:PRO:HB2	5:5:141:VAL:HG13	1.99	0.44
1:1:204:LEU:CD2	1:1:302:ARG:HD3	2.47	0.44
11:G:87:GLN:HA	11:G:97:UNK:HA	2.00	0.44
2:2:54:VAL:CG2	2:2:60:ILE:HG12	2.47	0.44
3:3:90:ILE:HA	3:3:93:LEU:HD12	1.99	0.44
1:1:225:VAL:O	1:1:229:LEU:HB2	2.18	0.44
9:C:98:LEU:HD22	9:C:459:LEU:HD23	2.00	0.44
2:2:354:UNK:HA	2:2:361:VAL:HG21	2.00	0.43
1:1:199:ARG:HD3	1:1:199:ARG:HA	1.62	0.43
9:C:143:ASP:HA	9:C:460:VAL:HG11	1.99	0.43
2:2:103:UNK:HA	2:2:143:ILE:HD13	2.00	0.43
5:5:140:PHE:HA	5:5:181:PHE:CZ	2.53	0.43
11:G:167:SER:HB3	11:G:190:PHE:HB3	2.01	0.43
7:A:246:UNK:HA	13:I:149:ALA:HB3	2.00	0.43
2:2:156:LEU:HB3	2:2:224:ILE:HD11	2.00	0.43
4:4:218:ILE:O	4:4:222:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:167:THR:HG22	14:K:152:ASN:HB3	2.01	0.43
13:I:179:CYS:HB3	13:I:180:PRO:HA	2.00	0.43
14:K:88:VAL:HA	14:K:91:MET:HB2	2.01	0.43
2:2:212:ILE:HG23	2:2:241:LYS:HE2	2.00	0.43
9:C:233:GLY:O	9:C:360:LYS:HG2	2.18	0.43
9:C:280:THR:H	9:C:441:ILE:HG23	1.84	0.43
4:4:255:LEU:HA	4:4:258:ILE:HD12	2.01	0.43
9:C:285:ASP:HA	9:C:288:ASN:HD22	1.84	0.42
1:1:241:PHE:HA	1:1:244:TYR:CE2	2.54	0.42
2:2:209:LEU:HB3	2:2:214:ILE:HG12	2.01	0.42
4:4:204:LEU:O	4:4:268:GLU:HB3	2.19	0.42
5:5:135:ASN:HB2	5:5:138:VAL:HG22	2.00	0.42
2:2:10:ILE:HD11	6:6:174:ILE:HG12	2.01	0.42
9:C:398:GLU:HA	9:C:415:VAL:HG22	2.01	0.42
14:K:81:PHE:HE2	14:K:134:VAL:HG21	1.84	0.42
2:2:277:LEU:HD12	2:2:412:TYR:HE1	1.85	0.42
3:3:95:LEU:HA	3:3:98:LEU:HD22	2.01	0.42
9:C:434:HIS:CE1	9:C:457:MET:HB3	2.55	0.42
1:1:118:PHE:CE1	6:6:37:ILE:HD13	2.54	0.42
2:2:66:PHE:O	2:2:70:MET:HG2	2.19	0.42
4:4:316:GLY:HA3	4:4:398:SER:HB2	2.02	0.42
9:C:286:ALA:HB1	9:C:291:LEU:HD22	2.01	0.42
1:1:29:THR:OG1	1:1:294:ILE:HG21	2.19	0.42
1:1:148:LEU:HD11	3:3:70:ILE:HD13	2.01	0.42
4:4:180:LEU:O	4:4:184:VAL:HG23	2.19	0.42
4:4:230:TRP:CE3	4:4:234:VAL:HG21	2.55	0.42
5:5:143:TRP:HZ3	5:5:178:ASP:HA	1.84	0.42
1:1:28:LYS:HG3	1:1:38:GLY:HA3	2.02	0.42
2:2:138:TYR:HB2	2:2:157:TYR:HB3	2.02	0.42
2:2:248:LEU:HB3	2:2:300:LEU:HD21	2.01	0.42
5:5:236:LEU:HD12	5:5:310:MET:HG3	2.01	0.42
6:6:19:CYS:HB3	6:6:39:LEU:HD13	2.02	0.42
9:C:153:VAL:HG22	9:C:412:VAL:HG23	2.01	0.42
9:C:329:CYS:HA	9:C:332:ARG:HD2	2.00	0.42
2:2:230:ILE:O	2:2:234:ILE:HG13	2.20	0.42
2:2:265:ILE:HD12	2:2:298:LEU:HD23	2.01	0.42
2:2:235:TYR:CZ	2:2:239:ILE:HG13	2.55	0.42
9:C:328:ASP:O	9:C:332:ARG:HG3	2.19	0.42
9:C:332:ARG:HG2	9:C:332:ARG:HH11	1.85	0.42
14:K:105:ILE:HG23	14:K:106:ILE:N	2.35	0.41
4:4:208:THR:HG23	4:4:273:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:385:PHE:HB2	13:I:135:LEU:HD21	2.02	0.41
1:1:93:LEU:H	1:1:97:ILE:HB	1.85	0.41
1:1:281:ALA:O	1:1:285:LYS:HG2	2.20	0.41
4:4:297:ASP:HB3	4:4:300:VAL:HB	2.01	0.41
9:C:280:THR:HB	9:C:441:ILE:HA	2.02	0.41
9:C:96:GLY:O	9:C:97:VAL:HB	2.20	0.41
1:1:302:ARG:HD2	9:C:274:ARG:HH22	1.86	0.41
1:1:67:GLU:HB2	1:1:70:TYR:HB3	2.03	0.41
4:4:161:GLU:O	4:4:165:PHE:HD1	2.04	0.41
9:C:416:SER:HA	9:C:423:TYR:H	1.86	0.41
14:K:95:ALA:HB1	14:K:96:PRO:HD3	2.01	0.41
1:1:188:ILE:HG21	1:1:320:LEU:HD11	2.02	0.41
2:2:180:ASN:HA	15:L:47:PHE:HE1	1.85	0.41
5:5:126:TRP:CH2	5:5:146:ILE:HG12	2.56	0.41
9:C:202:PRO:HB3	9:C:261:ILE:HG23	2.01	0.41
5:5:119:LEU:O	5:5:123:PHE:HB2	2.21	0.41
2:2:231:LEU:HD23	2:2:234:ILE:HD12	2.02	0.41
5:5:345:SER:CB	5:5:377:ILE:HD12	2.50	0.41
5:5:335:HIS:O	5:5:339:LYS:HB2	2.21	0.41
5:5:381:SER:HB2	5:5:428:SER:HB3	2.03	0.41
1:1:99:LEU:HG	1:1:99:LEU:H	1.64	0.41
5:5:140:PHE:HA	5:5:181:PHE:HZ	1.86	0.41
9:C:155:SER:HB2	9:C:232:PRO:HA	2.02	0.41
9:C:354:MET:CB	9:C:355:PRO:HD3	2.51	0.41
14:K:110:SER:HB3	14:K:112:ARG:N	2.35	0.41
1:1:203:ASP:HA	1:1:206:GLU:HG2	2.03	0.40
1:1:237:LEU:O	1:1:241:PHE:CB	2.69	0.40
8:B:144:GLY:HA2	8:B:149:ALA:HB3	2.03	0.40
9:C:239:LEU:HD13	9:C:243:LEU:HD12	2.03	0.40
1:1:200:PRO:HB2	1:1:201:PRO:HD3	2.03	0.40
2:2:368:VAL:O	2:2:372:ILE:HG23	2.21	0.40
4:4:208:THR:HG23	4:4:273:TYR:HE2	1.87	0.40
5:5:157:TRP:HE1	5:5:243:PRO:HD3	1.86	0.40
9:C:354:MET:HB2	9:C:355:PRO:HD3	2.03	0.40
15:L:8:LEU:HD11	15:L:36:ILE:HG13	2.02	0.40
1:1:153:ILE:HG12	1:1:185:LEU:HD21	2.04	0.40
1:1:43:GLY:HA3	1:1:48:LEU:HB2	2.04	0.40
5:5:123:PHE:HA	5:5:126:TRP:NE1	2.36	0.40
5:5:151:TYR:HB2	5:5:171:VAL:CG2	2.48	0.40
2:2:127:PHE:HA	2:2:130:ILE:HG22	2.03	0.40
2:2:262:ILE:HG23	2:2:301:LEU:HD22	2.04	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	1	319/335 (95%)	274 (86%)	29 (9%)	16 (5%)	2	23
2	2	337/434 (78%)	309 (92%)	24 (7%)	4 (1%)	13	50
3	3	82/110 (74%)	68 (83%)	12 (15%)	2 (2%)	6	37
4	4	257/470 (55%)	228 (89%)	24 (9%)	5 (2%)	8	42
5	5	353/616 (57%)	315 (89%)	31 (9%)	7 (2%)	7	41
6	6	104/184 (56%)	89 (86%)	10 (10%)	5 (5%)	2	24
7	A	84/634 (13%)	72 (86%)	9 (11%)	3 (4%)	3	30
8	B	95/370 (26%)	90 (95%)	4 (4%)	1 (1%)	14	51
9	C	361/383 (94%)	296 (82%)	41 (11%)	24 (7%)	1	19
11	G	67/133 (50%)	58 (87%)	7 (10%)	2 (3%)	4	33
12	H	29/154 (19%)	27 (93%)	2 (7%)	0	100	100
13	I	82/140 (59%)	63 (77%)	13 (16%)	6 (7%)	1	16
14	K	139/147 (95%)	122 (88%)	11 (8%)	6 (4%)	2	26
15	L	77/79 (98%)	69 (90%)	5 (6%)	3 (4%)	3	28
All	All	2386/4189 (57%)	2080 (87%)	222 (9%)	84 (4%)	3	31

All (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
7	A	134	PRO

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Mol	Chain	Res	Type
9	C	96	GLY
9	C	97	VAL
9	C	116	VAL
9	C	199	ALA
9	C	312	ASP
9	C	323	VAL
9	C	354	MET
13	I	74	ALA
13	I	139	ILE
13	I	179	CYS
13	I	182	ASP
14	K	95	ALA
14	K	105	ILE
14	K	110	SER
15	L	21	ASN
1	1	99	LEU
1	1	202	PHE
1	1	247	LEU
1	1	251	LEU
2	2	51	THR
2	2	218	HIS
4	4	158	SER
4	4	203	SER
4	4	295	GLN
5	5	620	LEU
6	6	80	ILE
6	6	149	THR
8	B	104	PRO
9	C	87	PHE
9	C	88	GLY
9	C	106	GLY
9	C	110	ILE
9	C	198	GLY
9	C	308	ASN
9	C	363	ASP
11	G	191	GLU
14	K	106	ILE
15	L	17	PHE
1	1	127	SER
1	1	177	TRP
1	1	209	SER
1	1	268	TYR

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Mol	Chain	Res	Type
1	1	301	PRO
3	3	52	PHE
5	5	639	PHE
5	5	653	LEU
6	6	81	ASN
7	A	70	TYR
9	C	108	GLU
9	C	283	ALA
9	C	369	PRO
9	C	458	ASP
11	G	83	PRO
13	I	140	CYS
14	K	103	LEU
15	L	51	SER
1	1	44	TYR
1	1	132	SER
1	1	163	SER
1	1	266	TYR
3	3	5	ILE
4	4	469	GLN
6	6	148	THR
9	C	356	ALA
9	C	359	VAL
9	C	367	ASN
9	C	389	THR
13	I	145	ILE
14	K	107	PHE
2	2	193	ASN
4	4	194	PHE
5	5	228	ALA
1	1	128	ASN
5	5	641	ILE
6	6	28	ASN
5	5	75	ILE
9	C	370	PRO
9	C	92	PRO

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%)	252 (88%)	34 (12%)	5	26
2	2	291/308 (94%)	266 (91%)	25 (9%)	10	40
3	3	75/96 (78%)	68 (91%)	7 (9%)	9	35
4	4	215/229 (94%)	198 (92%)	17 (8%)	12	42
5	5	301/302 (100%)	277 (92%)	24 (8%)	12	42
6	6	90/157 (57%)	81 (90%)	9 (10%)	7	32
7	A	37/83 (45%)	37 (100%)	0	100	100
8	B	53/83 (64%)	50 (94%)	3 (6%)	20	52
9	C	305/324 (94%)	278 (91%)	27 (9%)	9	38
11	G	55/58 (95%)	55 (100%)	0	100	100
12	H	19/19 (100%)	18 (95%)	1 (5%)	22	54
13	I	55/78 (70%)	49 (89%)	6 (11%)	6	29
14	K	114/125 (91%)	107 (94%)	7 (6%)	18	50
15	L	68/69 (99%)	66 (97%)	2 (3%)	42	67
All	All	1964/2227 (88%)	1802 (92%)	162 (8%)	11	40

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	37	LEU
1	1	44	TYR
1	1	48	LEU
1	1	72	ILE
1	1	75	ILE
1	1	81	LEU
1	1	93	LEU
1	1	98	THR
1	1	99	LEU
1	1	104	LEU
1	1	108	PHE
1	1	121	LEU
1	1	123	SER
1	1	156	ILE
1	1	159	MET
1	1	160	PHE

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Mol	Chain	Res	Type
1	1	174	ARG
1	1	185	LEU
1	1	191	ILE
1	1	199	ARG
1	1	227	PHE
1	1	229	LEU
1	1	242	ASN
1	1	246	LEU
1	1	250	TYR
1	1	263	PHE
1	1	265	ASP
1	1	270	SER
1	1	276	LEU
1	1	295	TRP
1	1	297	ARG
1	1	321	PHE
1	1	325	LEU
1	1	327	ILE
2	2	52	TYR
2	2	59	LEU
2	2	64	PHE
2	2	67	TYR
2	2	68	ILE
2	2	72	ILE
2	2	79	ILE
2	2	137	ILE
2	2	138	TYR
2	2	152	LYS
2	2	156	LEU
2	2	164	LEU
2	2	166	ILE
2	2	217	LEU
2	2	221	LEU
2	2	230	ILE
2	2	232	ILE
2	2	276	LEU
2	2	281	ILE
2	2	300	LEU
2	2	302	LEU
2	2	312	TYR
2	2	328	ILE
2	2	362	LEU

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Mol	Chain	Res	Type
2	2	384	LEU
3	3	18	LEU
3	3	42	LEU
3	3	57	ILE
3	3	62	LEU
3	3	64	LEU
3	3	96	LEU
3	3	98	LEU
4	4	144	THR
4	4	169	MET
4	4	201	VAL
4	4	210	ILE
4	4	227	ILE
4	4	229	VAL
4	4	231	LEU
4	4	250	ILE
4	4	263	LEU
4	4	267	CYS
4	4	274	THR
4	4	286	ILE
4	4	302	ILE
4	4	304	TYR
4	4	323	LEU
4	4	372	LEU
4	4	381	PHE
5	5	73	LEU
5	5	81	ILE
5	5	108	GLU
5	5	136	TYR
5	5	145	PHE
5	5	154	ILE
5	5	185	LEU
5	5	215	ILE
5	5	309	THR
5	5	316	MET
5	5	320	ILE
5	5	329	LEU
5	5	341	LEU
5	5	342	LEU
5	5	372	TYR
5	5	396	LYS
5	5	471	PHE

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Mol	Chain	Res	Type
5	5	580	ASP
5	5	622	LEU
5	5	629	LEU
5	5	630	LEU
5	5	633	LEU
5	5	636	ASN
5	5	653	LEU
6	6	23	ILE
6	6	41	VAL
6	6	58	LEU
6	6	149	THR
6	6	154	LEU
6	6	161	ILE
6	6	162	LEU
6	6	171	LEU
6	6	174	ILE
8	B	388	ARG
8	B	425	THR
8	B	429	LEU
9	C	98	LEU
9	C	100	LEU
9	C	145	VAL
9	C	172	TYR
9	C	196	ASP
9	C	204	LEU
9	C	262	GLU
9	C	268	ASN
9	C	285	ASP
9	C	297	ARG
9	C	301	ILE
9	C	305	ILE
9	C	307	LYS
9	C	315	ASP
9	C	317	VAL
9	C	319	PHE
9	C	333	TYR
9	C	334	LEU
9	C	340	PHE
9	C	361	VAL
9	C	373	LEU
9	C	375	LYS
9	C	378	MET

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Mol	Chain	Res	Type
9	C	385	PHE
9	C	403	ILE
9	C	447	LEU
9	C	449	ASP
12	H	130	THR
13	I	78	PHE
13	I	83	MET
13	I	130	CYS
13	I	135	LEU
13	I	164	ILE
13	I	190	VAL
14	K	80	THR
14	K	92	HIS
14	K	105	ILE
14	K	106	ILE
14	K	138	MET
14	K	160	SER
14	K	169	ARG
15	L	46	LEU
15	L	69	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	165	ASN
1	1	173	GLN
1	1	307	ASN
2	2	49	ASN
2	2	173	ASN
5	5	78	ASN
6	6	81	ASN
9	C	95	HIS
9	C	150	ASN
9	C	185	ASN
9	C	288	ASN
9	C	434	HIS
14	K	195	GLN

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 carbohydrates 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	$\# Z > 2$
50	SF4	I	500	13	0,12,12	0.00	-	-		
49	FES	H	300	12	0,4,4	0.00	-	-		
50	SF4	I	501	13	0,12,12	0.00	-	-		
50	SF4	A	902	7	0,12,12	0.00	-	-		
49	FES	A	900	7	0,4,4	0.00	-	-		
50	SF4	B	500	8	0,12,12	0.00	-	-		
50	SF4	A	901	7	0,12,12	0.00	-	-		
50	SF4	K	500	14	0,12,12	0.00	-	-		

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	SF4	K	500	14	-	-	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
4	4	4
2	2	4
11	G	2
41	q	1
25	Q	1

All 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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	325:UNK	C	404:UNK	N	23.14
1	2	422:UNK	C	446:UNK	N	21.82
1	A	358:UNK	C	360:UNK	N	17.39
1	E	637:UNK	C	785:UNK	N	17.09
1	H	121:UNK	C	127:CYS	N	16.81
1	E	65:UNK	C	83:UNK	N	16.44
1	A	560:UNK	C	565:UNK	N	16.27
1	E	109:UNK	C	161:UNK	N	16.16
1	B	109:ASN	C	115:UNK	N	16.06
1	E	180:UNK	C	235:UNK	N	16.00
1	E	795:UNK	C	887:UNK	N	14.89
1	B	195:UNK	C	201:UNK	N	14.77
1	I	212:UNK	C	233:UNK	N	14.61
1	H	174:UNK	C	181:UNK	N	14.40
1	A	510:UNK	C	515:UNK	N	12.66
1	A	363:UNK	C	367:UNK	N	12.00
1	B	343:UNK	C	356:UNK	N	11.69
1	A	642:UNK	C	647:UNK	N	11.45
1	H	109:UNK	C	117:UNK	N	11.07
1	4	52:UNK	C	57:UNK	N	10.74
1	A	708:UNK	C	712:UNK	N	10.68
1	H	90:UNK	C	94:UNK	N	10.66
1	G	138:UNK	C	145:UNK	N	10.61
1	2	84:GLY	C	97:UNK	N	10.37
1	G	125:UNK	C	128:UNK	N	10.20
1	B	120:UNK	C	125:ASP	N	9.94
1	5	297:UNK	C	301:UNK	N	9.85
1	B	155:TYR	C	159:UNK	N	9.77
1	A	530:UNK	C	534:UNK	N	9.64
1	B	245:UNK	C	251:UNK	N	9.60
1	4	67:UNK	C	76:UNK	N	9.53
1	A	414:UNK	C	416:UNK	N	9.45
1	H	162:UNK	C	165:UNK	N	9.45
1	A	427:UNK	C	432:UNK	N	9.42
1	A	457:UNK	C	464:UNK	N	9.33
1	A	541:UNK	C	543:UNK	N	9.21
1	I	120:UNK	C	128:GLU	N	9.10
1	B	87:UNK	C	92:PHE	N	8.89
1	4	18:UNK	C	22:UNK	N	8.65
1	A	435:UNK	C	438:UNK	N	8.48
1	E	242:UNK	C	316:UNK	N	8.01
1	A	704:UNK	C	707:UNK	N	7.65

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	24:UNK	C	27:UNK	N	7.56
1	A	87:GLU	C	89:ARG	N	7.29
1	4	435:UNK	C	437:UNK	N	7.16
1	5	604:UNK	C	616:MET	N	7.14
1	A	273:UNK	C	276:UNK	N	7.03
1	I	235:UNK	C	238:UNK	N	7.01
1	A	492:UNK	C	496:UNK	N	6.98
1	A	293:UNK	C	297:UNK	N	6.82
1	A	257:UNK	C	260:UNK	N	6.51
1	A	580:UNK	C	586:UNK	N	6.32
1	2	251:UNK	C	256:UNK	N	6.18
1	B	303:UNK	C	306:UNK	N	5.99
1	A	236:UNK	C	240:UNK	N	5.69
1	5	447:UNK	C	455:UNK	N	5.59
1	A	246:UNK	C	248:UNK	N	5.53
1	A	309:UNK	C	313:UNK	N	5.36
1	A	181:UNK	C	183:CYS	N	5.26
1	5	437:UNK	C	439:UNK	N	5.19
1	E	57:UNK	C	59:UNK	N	4.80
1	5	205:UNK	C	208:UNK	N	4.68
1	B	238:UNK	C	240:UNK	N	4.54
1	5	412:UNK	C	416:UNK	N	4.43
1	2	332:UNK	C	339:UNK	N	4.40
1	q	1916:UNK	C	1917:UNK	N	4.23
1	5	550:UNK	C	560:UNK	N	3.78
1	A	443:UNK	C	445:UNK	N	3.78
1	Q	639:UNK	C	641:UNK	N	3.74
1	A	397:UNK	C	400:UNK	N	3.57
1	A	334:UNK	C	336:UNK	N	3.29

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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