



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:17 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 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 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:

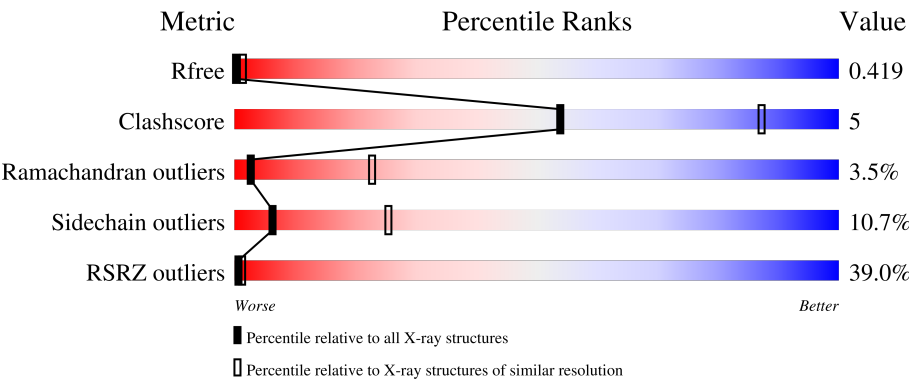
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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% .

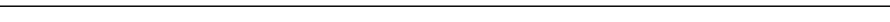
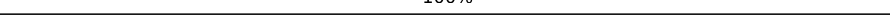
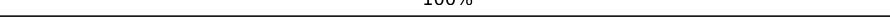
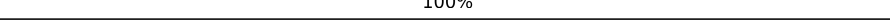
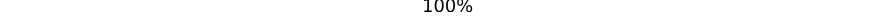
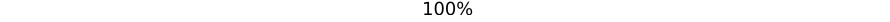
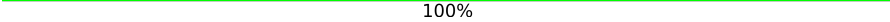
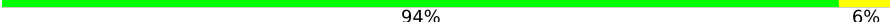
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Mol	Chain	Length	Quality of chain
6	6	184	
7	A	634	
8	B	370	
9	C	383	
10	E	195	
11	G	133	
12	H	154	
13	I	140	
14	K	147	
15	L	79	
16	Z	17	
16	r	17	
17	AF	40	
17	Y	40	
18	U	10	
19	X	57	
20	W	54	
21	V	63	
22	AI	20	
22	T	20	
22	m	20	
23	AJ	19	
23	AL	19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

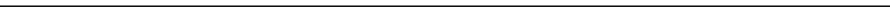
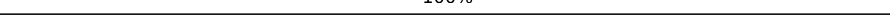
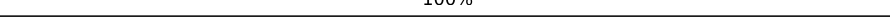
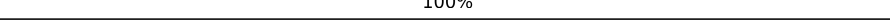
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Mol	Chain	Length	Quality of chain
25	Q	70	 100%
26	P	28	 100%
27	AC	18	 100%
27	AH	18	 100%
27	AM	18	 100%
27	F	18	 100%
27	f	18	 100%
28	O	25	 100%
28	l	25	 100%
29	M	51	 100%
30	D	30	 100%
31	J	69	 100%
32	N	15	 100%
33	a	26	 100%
33	i	26	 100%
34	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			

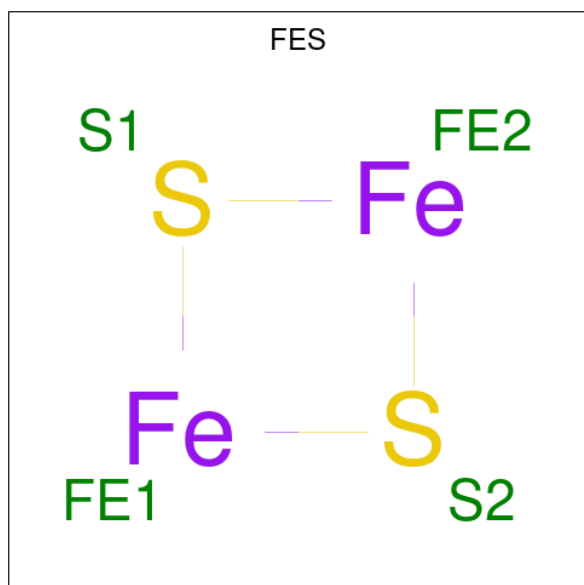
- Molecule 47 is a protein called Unknown polypeptide.

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.

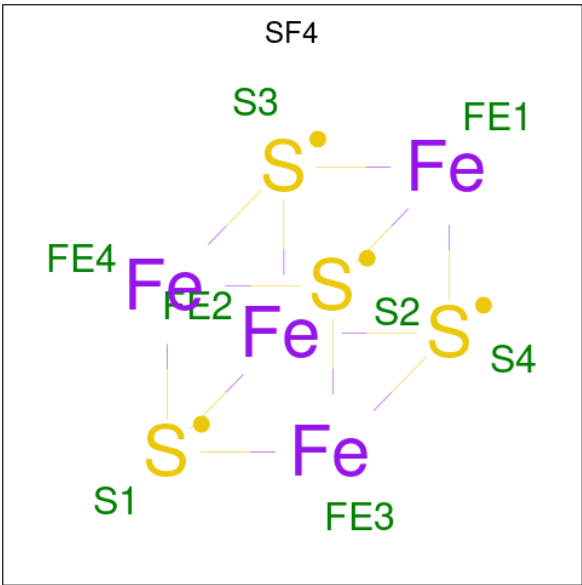
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	AD	39	Total	C	N	O	0	0	0
			195	117	39	39			

- 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).

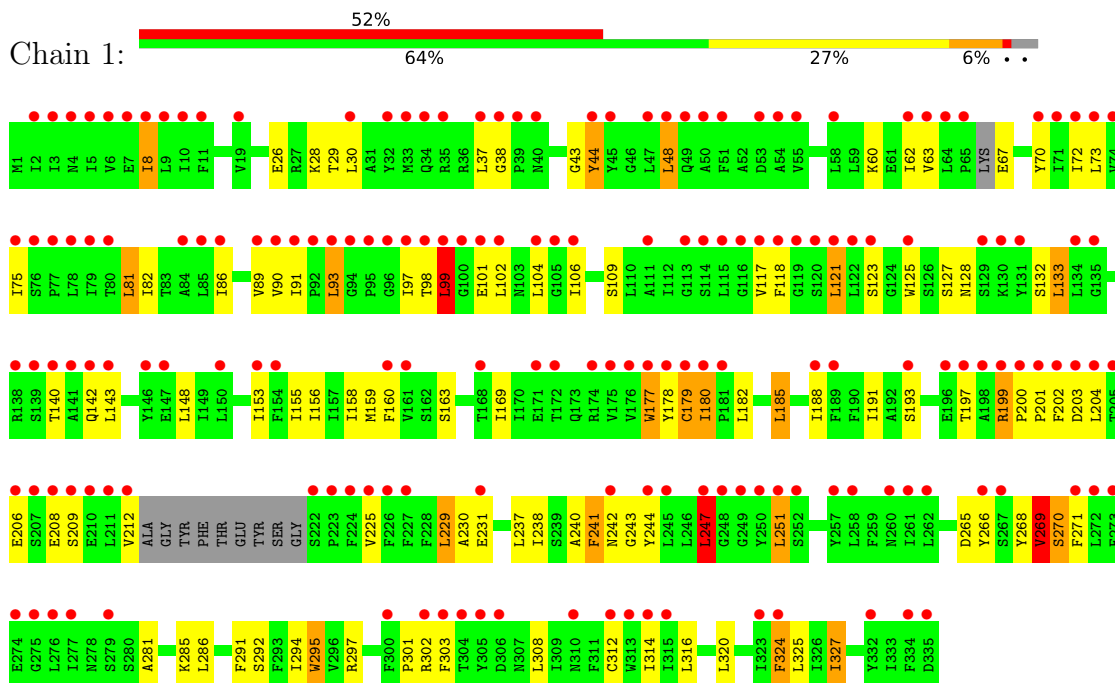


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
50	A	1	Total	Fe	S	0	0
			8	4	4		
50	A	1	Total	Fe	S	0	0
			8	4	4		
50	B	1	Total	Fe	S	0	0
			8	4	4		
50	I	1	Total	Fe	S	0	0
			8	4	4		
50	I	1	Total	Fe	S	0	0
			8	4	4		
50	K	1	Total	Fe	S	0	0
			8	4	4		

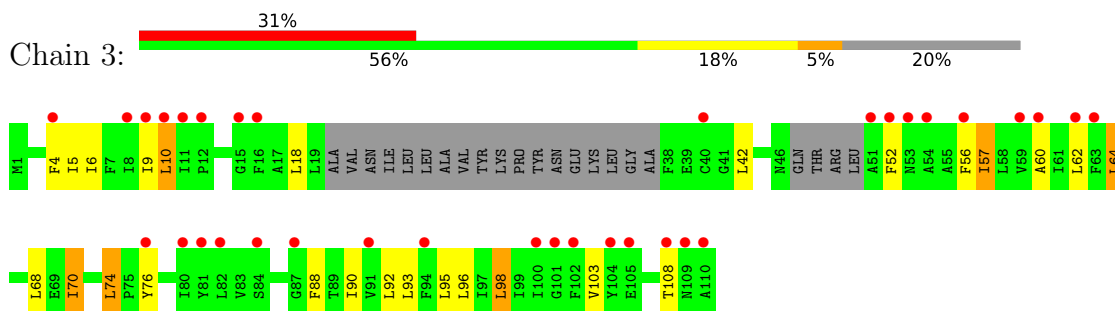
3 Residue-property plots [i](#)

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.

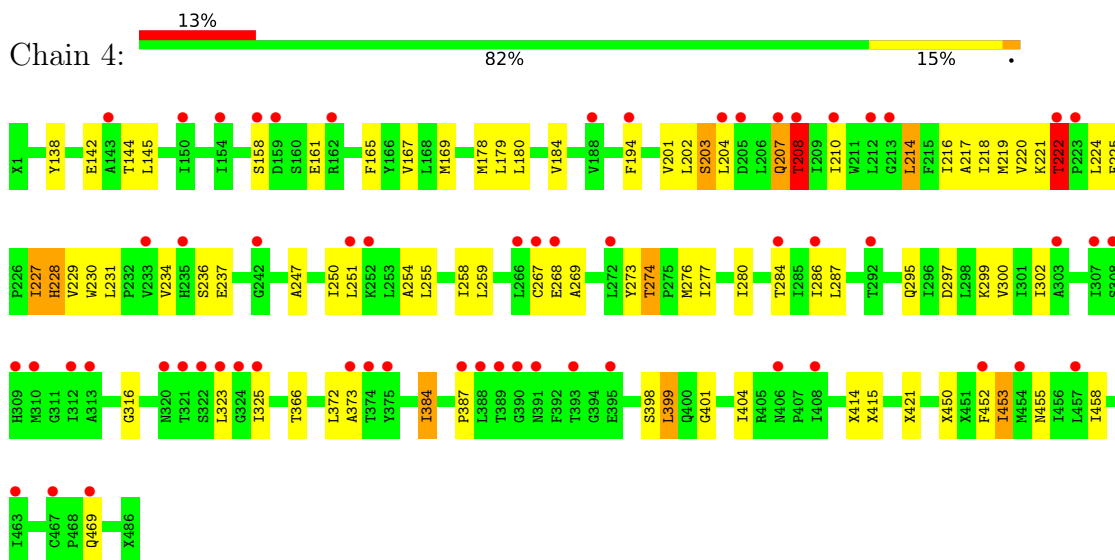
• Molecule 1: NADH-ubiquinone oxidoreductase chain 1



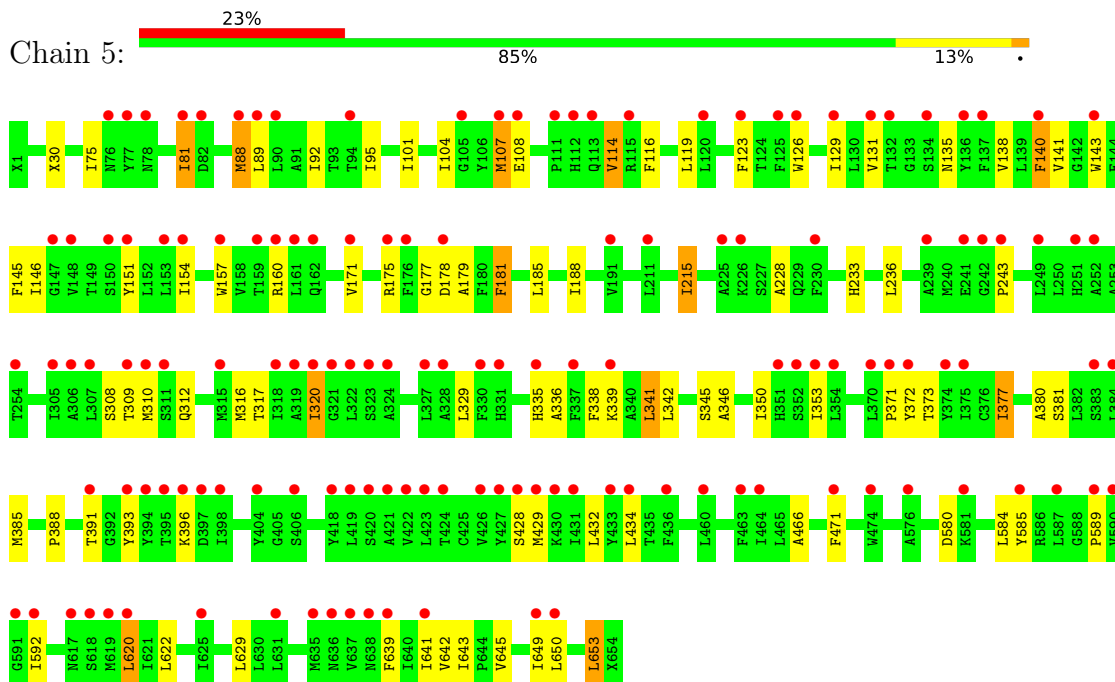
- Molecule 3: NADH-ubiquinone oxidoreductase chain 3



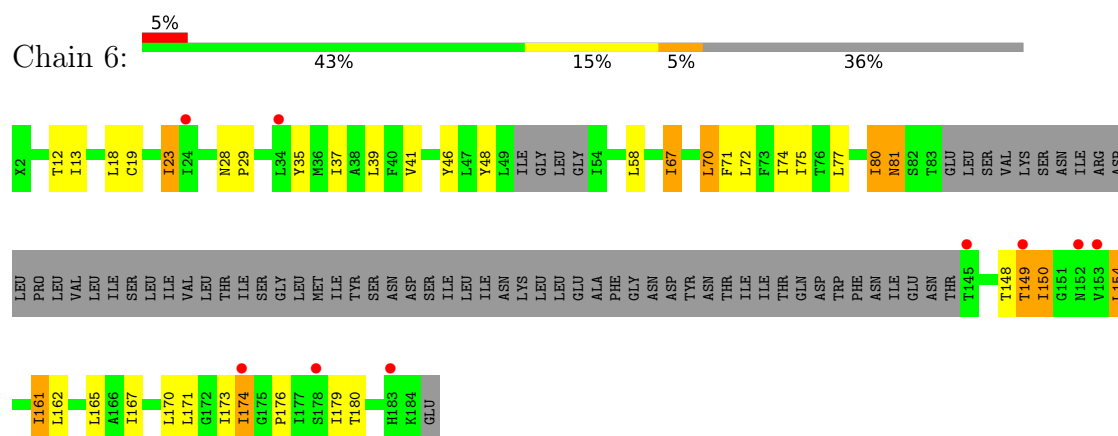
- Molecule 4: NADH-ubiquinone oxidoreductase chain 4



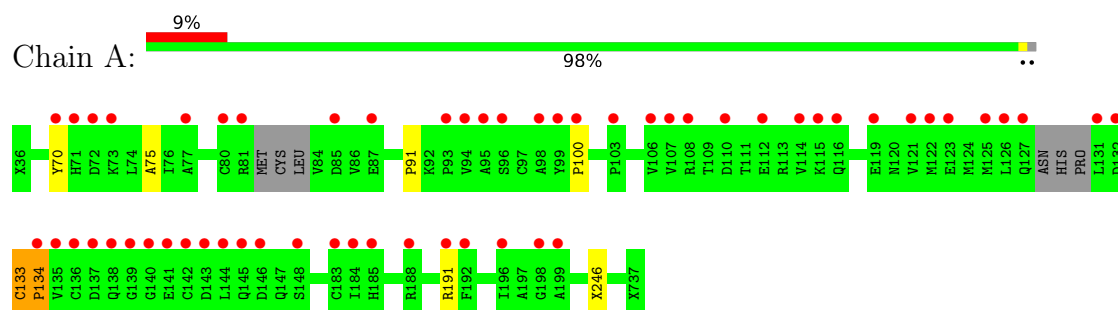
- Molecule 5: NADH-ubiquinone oxidoreductase chain 5



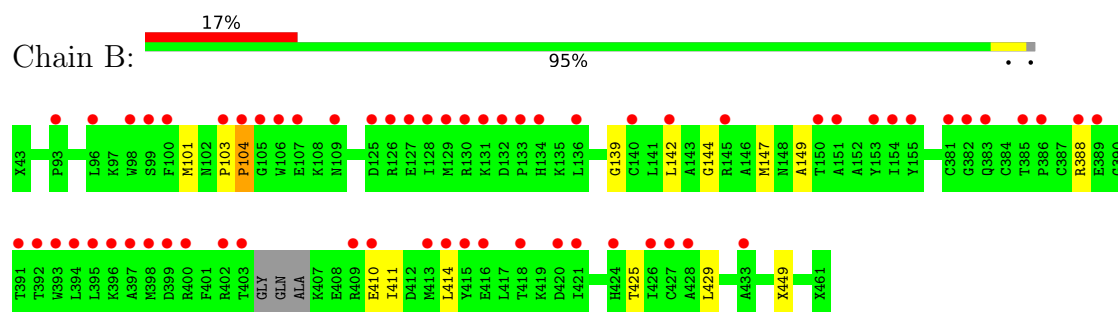
- Molecule 6: NADH-ubiquinone oxidoreductase chain 6



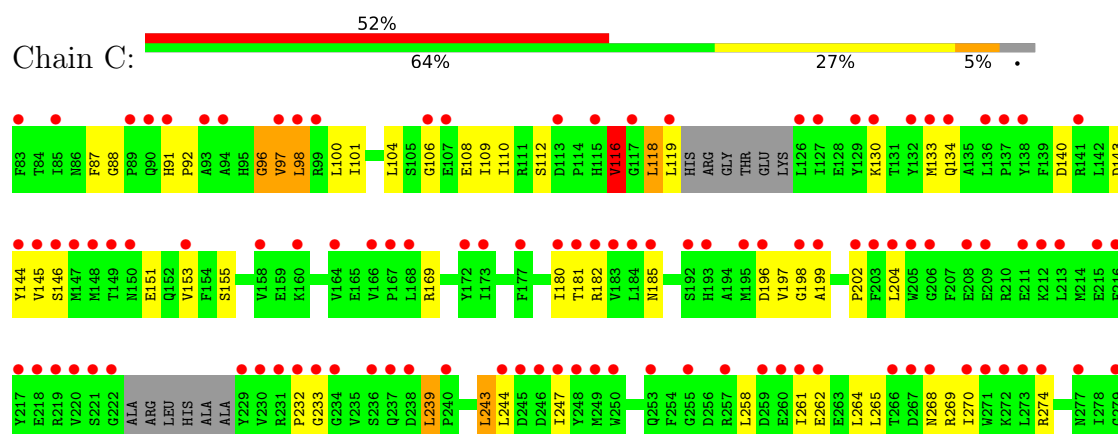
- Molecule 7: NUAM protein

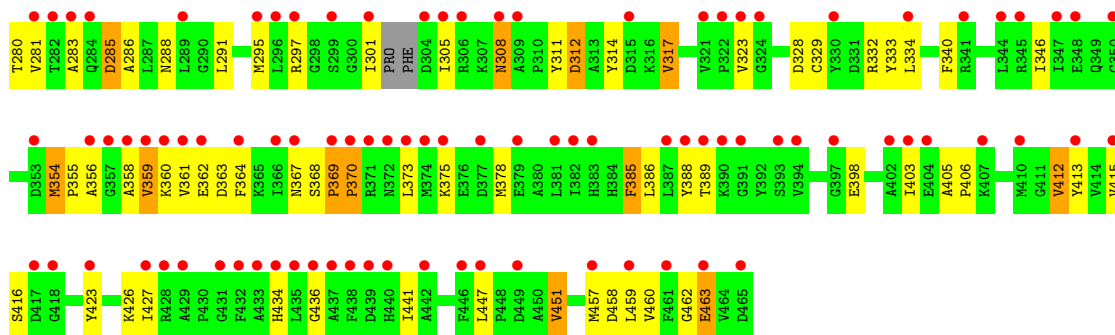


- Molecule 8: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

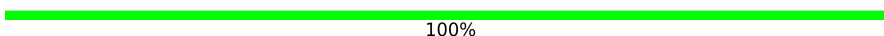


- Molecule 9: NUCM protein



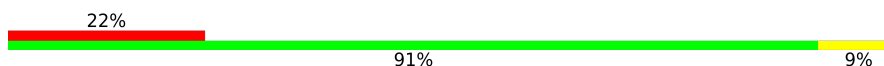


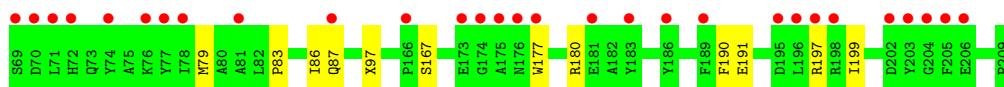
• Molecule 10: NUEM protein

Chain E:  100%

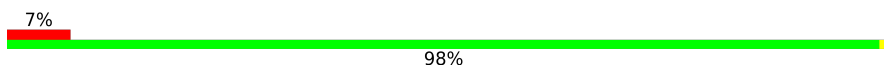
There are no outlier residues recorded for this chain.

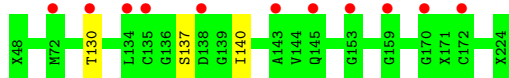
• Molecule 11: NUGM protein

Chain G:  22% 91% 9%



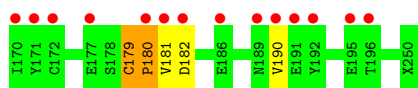
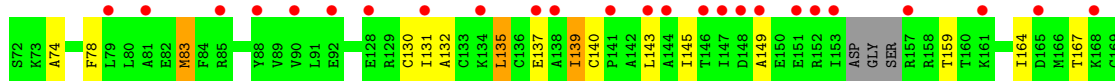
• Molecule 12: Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain H:  7% 98%



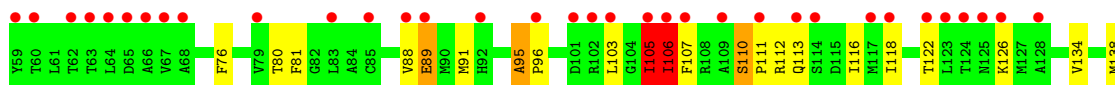
• Molecule 13: Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I)

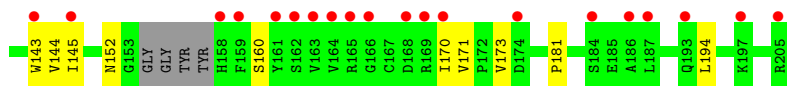
Chain I:  28% 83% 11%



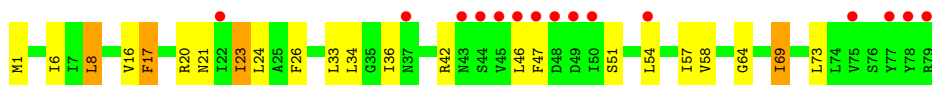
• Molecule 14: Subunit NUKM of protein NADH:Ubiquinone Oxidoreductase (Complex I)

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

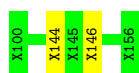


- Molecule 18: Unknown polypeptide



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.

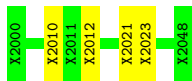
- Molecule 37: Unknown polypeptide

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

All (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
7	A	134	PRO	N-CA-CB	7.86	111.50	103.25
8	B	103	PRO	N-CA-CB	7.43	110.29	103.08
13	I	78	PHE	CA-CB-CG	7.33	121.13	113.80
13	I	180	PRO	CA-C-N	7.12	129.79	120.60
13	I	180	PRO	C-N-CA	7.12	129.79	120.60
9	C	247	ILE	N-CA-C	-7.08	106.17	112.12
4	4	228	HIS	CA-C-N	7.03	130.44	120.53
4	4	228	HIS	C-N-CA	7.03	130.44	120.53
1	1	240	ALA	CA-C-N	7.01	129.68	120.28
1	1	240	ALA	C-N-CA	7.01	129.68	120.28
7	A	133	CYS	CA-C-N	6.96	128.54	119.84
7	A	133	CYS	C-N-CA	6.96	128.54	119.84
2	2	375	PRO	N-CA-C	6.92	119.15	110.70
4	4	384	ILE	N-CA-C	-6.85	106.36	112.12
7	A	100	PRO	N-CA-CB	6.82	110.10	102.67
8	B	104	PRO	N-CA-CB	6.81	110.40	103.25
5	5	642	VAL	CA-C-N	6.79	126.94	120.43
5	5	642	VAL	C-N-CA	6.79	126.94	120.43
2	2	46	PHE	CA-CB-CG	6.70	120.50	113.80
3	3	4	PHE	CA-CB-CG	6.53	120.33	113.80
1	1	133	LEU	N-CA-C	-6.51	104.03	112.23
5	5	338	PHE	CA-CB-CG	6.50	120.30	113.80
1	1	324	PHE	CA-CB-CG	6.33	120.13	113.80
9	C	269	ARG	CA-C-N	6.25	128.66	120.60
9	C	269	ARG	C-N-CA	6.25	128.66	120.60
3	3	10	LEU	CA-C-N	6.21	125.30	120.33
3	3	10	LEU	C-N-CA	6.21	125.30	120.33
5	5	140	PHE	CA-CB-CG	6.20	120.00	113.80
4	4	207	GLN	CA-C-N	5.96	129.08	120.38
4	4	207	GLN	C-N-CA	5.96	129.08	120.38
2	2	306	GLU	CA-C-N	5.94	128.56	120.54
2	2	306	GLU	C-N-CA	5.94	128.56	120.54
1	1	303	PHE	CA-CB-CG	5.94	119.74	113.80
6	6	48	TYR	N-CA-C	-5.93	106.02	113.72
5	5	645	VAL	N-CA-C	-5.91	107.05	112.96
15	L	17	PHE	CA-CB-CG	5.91	119.71	113.80
9	C	118	LEU	CA-C-N	5.83	132.20	121.70
9	C	118	LEU	C-N-CA	5.83	132.20	121.70
2	2	184	LEU	CA-C-N	5.82	128.08	120.28
2	2	184	LEU	C-N-CA	5.82	128.08	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	180	ILE	N-CA-C	-5.79	107.21	111.90
9	C	112	SER	CA-C-N	5.68	127.28	122.28
9	C	112	SER	C-N-CA	5.68	127.28	122.28
5	5	181	PHE	CA-CB-CG	5.68	119.48	113.80
4	4	222	THR	CB-CA-C	5.67	116.87	108.87
9	C	312	ASP	CA-CB-CG	5.66	118.25	112.60
1	1	271	PHE	CA-CB-CG	5.64	119.44	113.80
9	C	314	TYR	CA-C-N	5.62	127.74	120.44
9	C	314	TYR	C-N-CA	5.62	127.74	120.44
4	4	208	THR	CA-C-N	5.56	127.77	120.60
4	4	208	THR	C-N-CA	5.56	127.77	120.60
9	C	308	ASN	CA-CB-CG	5.56	118.16	112.60
3	3	56	PHE	N-CA-C	-5.50	108.36	114.62
5	5	434	LEU	N-CA-C	-5.46	106.62	113.72
9	C	311	TYR	CA-C-N	5.38	131.81	121.54
9	C	311	TYR	C-N-CA	5.38	131.81	121.54
1	1	180	ILE	N-CA-CB	5.35	113.87	110.50
5	5	620	LEU	CA-C-N	5.35	128.07	120.53
5	5	620	LEU	C-N-CA	5.35	128.07	120.53
9	C	364	PHE	CA-CB-CG	5.33	119.13	113.80
2	2	42	LEU	CA-C-N	5.25	128.04	120.38
2	2	42	LEU	C-N-CA	5.25	128.04	120.38
15	L	20	ARG	CA-C-N	5.24	131.54	121.54
15	L	20	ARG	C-N-CA	5.24	131.54	121.54
5	5	371	PRO	CA-C-N	5.21	127.79	120.28
5	5	371	PRO	C-N-CA	5.21	127.79	120.28
4	4	453	ILE	N-CA-C	-5.20	105.47	110.72
13	I	83	MET	CA-C-N	5.15	127.43	120.38
13	I	83	MET	C-N-CA	5.15	127.43	120.38
13	I	181	VAL	CA-C-N	5.13	131.33	121.54
13	I	181	VAL	C-N-CA	5.13	131.33	121.54
4	4	167	VAL	CA-C-N	5.12	127.46	120.54
4	4	167	VAL	C-N-CA	5.12	127.46	120.54
9	C	362	GLU	CA-C-N	5.10	131.27	121.54
9	C	362	GLU	C-N-CA	5.10	131.27	121.54
5	5	391	THR	CA-C-N	5.08	125.62	119.98
5	5	391	THR	C-N-CA	5.08	125.62	119.98
4	4	228	HIS	N-CA-C	-5.07	106.51	113.30
4	4	269	ALA	CA-C-N	5.06	127.06	120.28
4	4	269	ALA	C-N-CA	5.06	127.06	120.28
5	5	81	ILE	N-CA-C	5.06	111.62	106.21
9	C	369	PRO	N-CA-C	5.05	116.86	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	63	VAL	CA-C-N	5.05	127.03	120.26
1	1	63	VAL	C-N-CA	5.05	127.03	120.26
1	1	327	ILE	N-CA-CB	5.05	113.68	110.50
1	1	101	GLU	N-CA-C	-5.04	105.86	112.72
14	K	89	GLU	N-CA-C	-5.04	105.98	111.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
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
5:5:233:HIS:HB2	5:5:310:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:98:LEU:HA	9:C:116:VAL:HG11	1.86	0.57
9:C:258:LEU:HD11	9:C:340:PHE:HB3	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
2:2:375:PRO:HG2	4:4:138:TYR:HE2	1.70	0.57
3:3:64:LEU:HD21	6:6:67:ILE:HG13	1.87	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:1:295:TRP:H	1:1:295:TRP:CD1	2.26	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
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
38:h:2021:UNK:HA	38:h:2023:UNK:CB	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:1:291:PHE:O	1:1:295:TRP:HD1	1.96	0.49
1:1:292:SER:HA	1:1:295:TRP:NE1	2.28	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
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
2:2:46:PHE:HB3	2:2:62:ASN:CB	2.44	0.47
2:2:262:ILE:O	2:2:266:LEU:HG	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:118:LEU:HD21	14:K:126:LYS:HD3	1.98	0.46
9:C:436:GLY:HA2	11:G:177:TRP:CD1	2.51	0.46
2:2:369:PHE:HD1	2:2:374:ILE:HG13	1.79	0.46
8:B:101:MET:HE2	8:B:147:MET:HB3	1.98	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
2:2:325:MET:HE3	2:2:453:UNK:HA	1.99	0.45
9:C:388:TYR:HA	13:I:139:ILE:HD13	1.99	0.45
38:h:2010:UNK:C	38:h:2012:UNK:N	2.80	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
1:1:180:ILE:C	1:1:182:LEU:H	2.25	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:1:199:ARG:HD3	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
7:A:246:UNK:HA	13:I:149:ALA:HB3	2.00	0.43
11:G:167:SER:HB3	11:G:190:PHE:HB3	2.01	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
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
2:2:10:ILE:HD11	6:6:174:ILE:HG12	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	9:C:332:ARG:HG2	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
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:96:GLY:O	9:C:97:VAL:HB	2.20	0.41
9:C:280:THR:HB	9:C:441:ILE:HA	2.02	0.41
1:1:67:GLU:HB2	1:1:70:TYR:HB3	2.03	0.41
1:1:302:ARG:HD2	9:C:274:ARG:HH22	1.86	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
5:5:335:HIS:O	5:5:339:LYS:HB2	2.21	0.41
5:5:345:SER:CB	5:5:377:ILE:HD12	2.50	0.41
5:5:381:SER:HB2	5:5:428:SER:HB3	2.03	0.41
5:5:385:MET:HE1	5:5:429:MET:HE2	2.02	0.41
1:1:99:LEU:H	1:1:99:LEU:HG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:1:43:GLY:HA3	1:1:48:LEU:HB2	2.04	0.40
1:1:153:ILE:HG12	1:1:185:LEU:HD21	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
11:G:79:MET:HE2	36:AN:1101:UNK:HA	2.04	0.40
1:1:199:ARG:O	1:1:200:PRO:C	2.62	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
9:C:368:SER:C	9:C:370:PRO:HD3	2.47	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%)	1	17
2	2	337/434 (78%)	309 (92%)	24 (7%)	4 (1%)	10	40
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	8	ILE
1	1	30	LEU
1	1	37	LEU
1	1	44	TYR
1	1	48	LEU
1	1	62	ILE
1	1	72	ILE
1	1	73	LEU
1	1	75	ILE
1	1	81	LEU
1	1	82	ILE
1	1	90	VAL
1	1	93	LEU
1	1	98	THR
1	1	99	LEU
1	1	102	LEU
1	1	104	LEU
1	1	121	LEU
1	1	123	SER
1	1	156	ILE
1	1	159	MET
1	1	160	PHE
1	1	169	ILE
1	1	185	LEU
1	1	191	ILE
1	1	199	ARG
1	1	208	GLU
1	1	212	VAL
1	1	229	LEU
1	1	231	GLU

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Mol	Chain	Res	Type
1	1	242	ASN
1	1	247	LEU
1	1	265	ASP
1	1	269	VAL
1	1	270	SER
1	1	286	LEU
1	1	295	TRP
1	1	297	ARG
1	1	325	LEU
1	1	327	ILE
2	2	59	LEU
2	2	67	TYR
2	2	68	ILE
2	2	71	LEU
2	2	72	ILE
2	2	79	ILE
2	2	130	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	204	LEU
2	2	212	ILE
2	2	217	LEU
2	2	221	LEU
2	2	230	ILE
2	2	232	ILE
2	2	233	THR
2	2	276	LEU
2	2	281	ILE
2	2	290	LEU
2	2	297	MET
2	2	300	LEU
2	2	302	LEU
2	2	313	ILE
2	2	327	ILE
2	2	328	ILE
2	2	362	LEU
2	2	367	VAL
2	2	368	VAL

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Mol	Chain	Res	Type
2	2	384	LEU
3	3	10	LEU
3	3	18	LEU
3	3	42	LEU
3	3	57	ILE
3	3	62	LEU
3	3	64	LEU
3	3	70	ILE
3	3	74	LEU
3	3	96	LEU
3	3	98	LEU
4	4	144	THR
4	4	169	MET
4	4	201	VAL
4	4	208	THR
4	4	210	ILE
4	4	214	LEU
4	4	216	ILE
4	4	222	THR
4	4	227	ILE
4	4	229	VAL
4	4	231	LEU
4	4	237	GLU
4	4	250	ILE
4	4	259	LEU
4	4	267	CYS
4	4	274	THR
4	4	276	MET
4	4	286	ILE
4	4	302	ILE
4	4	323	LEU
4	4	325	ILE
4	4	372	LEU
4	4	399	LEU
5	5	81	ILE
5	5	88	MET
5	5	107	MET
5	5	108	GLU
5	5	114	VAL
5	5	145	PHE
5	5	154	ILE
5	5	160	ARG

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Mol	Chain	Res	Type
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	373	THR
5	5	377	ILE
5	5	396	LYS
5	5	471	PHE
5	5	580	ASP
5	5	584	LEU
5	5	629	LEU
5	5	649	ILE
5	5	650	LEU
5	5	653	LEU
6	6	18	LEU
6	6	23	ILE
6	6	41	VAL
6	6	58	LEU
6	6	67	ILE
6	6	70	LEU
6	6	74	ILE
6	6	75	ILE
6	6	149	THR
6	6	150	ILE
6	6	154	LEU
6	6	161	ILE
6	6	162	LEU
6	6	171	LEU
6	6	173	ILE
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	101	ILE
9	C	104	LEU

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Mol	Chain	Res	Type
9	C	109	ILE
9	C	116	VAL
9	C	133	MET
9	C	145	VAL
9	C	196	ASP
9	C	204	LEU
9	C	239	LEU
9	C	243	LEU
9	C	262	GLU
9	C	265	LEU
9	C	268	ASN
9	C	270	ILE
9	C	281	VAL
9	C	285	ASP
9	C	297	ARG
9	C	301	ILE
9	C	305	ILE
9	C	317	VAL
9	C	333	TYR
9	C	334	LEU
9	C	361	VAL
9	C	373	LEU
9	C	375	LYS
9	C	378	MET
9	C	385	PHE
9	C	386	LEU
9	C	403	ILE
9	C	412	VAL
9	C	427	ILE
9	C	447	LEU
9	C	451	VAL
9	C	463	GLU
11	G	86	ILE
12	H	130	THR
13	I	83	MET
13	I	130	CYS
13	I	131	ILE
13	I	135	LEU
13	I	137	GLU
13	I	143	LEU
13	I	164	ILE
13	I	190	VAL

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Mol	Chain	Res	Type
14	K	80	THR
14	K	105	ILE
14	K	106	ILE
14	K	138	MET
14	K	160	SER
14	K	194	LEU
15	L	8	LEU
15	L	23	ILE
15	L	24	LEU
15	L	34	LEU
15	L	46	LEU
15	L	57	ILE
15	L	69	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	103	ASN
1	1	165	ASN
1	1	173	GLN
1	1	307	ASN
2	2	49	ASN
2	2	62	ASN
2	2	173	ASN
2	2	198	ASN
2	2	227	ASN
2	2	315	GLN
3	3	46	ASN
3	3	85	ASN
3	3	107	ASN
4	4	235	HIS
4	4	270	GLN
4	4	295	GLN
4	4	400	GLN
5	5	78	ASN
5	5	112	HIS
5	5	229	GLN
5	5	577	HIS
6	6	81	ASN
6	6	152	ASN
6	6	157	ASN
9	C	95	HIS

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Mol	Chain	Res	Type
9	C	163	ASN
9	C	185	ASN
9	C	268	ASN
9	C	288	ASN
9	C	349	GLN
9	C	352	ASN
11	G	176	ASN
13	I	176	GLN
14	K	125	ASN
14	K	152	ASN
14	K	195	GLN
15	L	37	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

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Mol	Chain	Number of breaks
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

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
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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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
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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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

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%)

All (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
7	A	145	GLN	10.0
15	L	50	ILE	9.6
7	A	185	HIS	8.8
7	A	81	ARG	8.7
8	B	389	GLU	8.6
15	L	45	VAL	8.6
11	G	197	ARG	8.4
12	H	170	GLY	8.3
15	L	47	PHE	8.2
9	C	144	TYR	8.2
1	1	249	GLY	8.2
8	B	409	ARG	8.2
13	I	172	CYS	8.0
7	A	131	LEU	8.0
9	C	222	GLY	7.9
9	C	434	HIS	7.9
1	1	76	SER	7.6
9	C	138	TYR	7.6
9	C	393	SER	7.5
5	5	353	ILE	7.5
9	C	465	ASP	7.4
9	C	216	PHE	7.4
1	1	123	SER	7.3
13	I	137	GLU	7.3
15	L	46	LEU	7.3
5	5	132	THR	7.2
9	C	359	VAL	7.1
9	C	232	PRO	7.0

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Mol	Chain	Res	Type	RSRZ
5	5	327	LEU	6.9
1	1	334	PHE	6.9
4	4	309	HIS	6.9
8	B	155	TYR	6.9
1	1	35	ARG	6.8
7	A	115	LYS	6.8
7	A	144	LEU	6.7
8	B	132	ASP	6.7
5	5	320	ILE	6.7
3	3	51	ALA	6.6
6	6	152	ASN	6.6
14	K	170	ILE	6.6
1	1	206	GLU	6.6
1	1	105	GLY	6.6
11	G	77	TYR	6.5
5	5	354	LEU	6.5
1	1	117	VAL	6.5
5	5	434	LEU	6.5
9	C	248	TYR	6.4
5	5	649	ILE	6.2
3	3	110	ALA	6.2
13	I	170	ILE	6.2
11	G	196	LEU	6.1
13	I	168	LYS	6.1
1	1	116	GLY	6.1
1	1	210	GLU	6.1
5	5	371	PRO	6.1
8	B	153	TYR	6.0
5	5	396	LYS	6.0
11	G	189	PHE	6.0
9	C	362	GLU	5.9
5	5	617	ASN	5.9
7	A	122	MET	5.9
12	H	153	GLY	5.9
8	B	134	HIS	5.9
9	C	204	LEU	5.9
7	A	123	GLU	5.9
5	5	88	MET	5.9
13	I	182	ASP	5.8
1	1	174	ARG	5.8
8	B	125	ASP	5.8
1	1	6	VAL	5.8

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Mol	Chain	Res	Type	RSRZ
2	2	211	LYS	5.8
1	1	146	TYR	5.7
3	3	76	TYR	5.7
7	A	140	GLY	5.7
8	B	127	GLU	5.7
1	1	45	TYR	5.7
9	C	217	TYR	5.6
3	3	54	ALA	5.6
9	C	205	TRP	5.6
8	B	382	GLY	5.5
13	I	181	VAL	5.5
8	B	133	PRO	5.5
2	2	160	MET	5.5
1	1	222	SER	5.5
14	K	106	ILE	5.5
2	2	315	GLN	5.5
1	1	179	CYS	5.5
7	A	183	CYS	5.5
9	C	195	MET	5.5
4	4	469	GLN	5.4
1	1	141	ALA	5.4
7	A	125	MET	5.4
7	A	139	GLY	5.4
8	B	96	LEU	5.4
9	C	407	LYS	5.4
9	C	132	TYR	5.4
1	1	118	PHE	5.3
5	5	321	GLY	5.3
15	L	22	ILE	5.3
1	1	75	ILE	5.3
9	C	260	GLU	5.3
9	C	141	ARG	5.3
9	C	372	ASN	5.3
3	3	100	ILE	5.3
1	1	303	PHE	5.2
4	4	308	SER	5.2
9	C	382	ILE	5.2
3	3	60	ALA	5.2
1	1	250	TYR	5.2
1	1	212	VAL	5.2
9	C	126	LEU	5.2
9	C	305	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
14	K	125	ASN	5.1
5	5	242	GLY	5.1
7	A	138	GLN	5.1
5	5	433	TYR	5.1
9	C	127	ILE	5.1
1	1	172	THR	5.1
3	3	81	TYR	5.1
9	C	272	LYS	5.0
8	B	130	ARG	5.0
9	C	246	ASP	5.0
9	C	233	GLY	5.0
9	C	404	GLU	5.0
5	5	618	SER	5.0
13	I	147	ILE	5.0
9	C	145	VAL	5.0
9	C	348	GLU	5.0
13	I	189	ASN	4.9
2	2	293	ALA	4.9
1	1	80	THR	4.9
3	3	12	PRO	4.9
8	B	104	PRO	4.9
9	C	249	MET	4.9
7	A	98	ALA	4.8
8	B	109	ASN	4.8
1	1	223	PRO	4.8
5	5	418	TYR	4.8
9	C	129	TYR	4.8
1	1	3	ILE	4.8
14	K	143	TRP	4.8
11	G	69	SER	4.8
13	I	134	LYS	4.8
1	1	9	LEU	4.8
3	3	8	ILE	4.7
5	5	419	LEU	4.7
14	K	107	PHE	4.7
7	A	71	HIS	4.7
5	5	230	PHE	4.7
4	4	395	GLU	4.7
7	A	127	GLN	4.7
9	C	431	GLY	4.7
9	C	267	ASP	4.7
9	C	99	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
9	C	230	VAL	4.6
11	G	70	ASP	4.6
1	1	38	GLY	4.6
5	5	397	ASP	4.6
1	1	198	ALA	4.6
14	K	64	LEU	4.6
3	3	11	ILE	4.6
7	A	184	ILE	4.6
1	1	34	GLN	4.6
1	1	140	THR	4.6
1	1	251	LEU	4.6
5	5	89	LEU	4.6
8	B	100	PHE	4.5
1	1	143	LEU	4.5
1	1	207	SER	4.5
1	1	131	TYR	4.5
1	1	147	GLU	4.5
8	B	128	ILE	4.5
11	G	76	LYS	4.5
7	A	148	SER	4.5
2	2	138	TYR	4.5
7	A	141	GLU	4.5
8	B	129	MET	4.5
12	H	172	CYS	4.5
8	B	399	ASP	4.5
14	K	65	ASP	4.5
9	C	379	GLU	4.4
4	4	162	ARG	4.4
5	5	352	SER	4.4
1	1	64	LEU	4.4
5	5	322	LEU	4.4
5	5	157	TRP	4.4
8	B	381	CYS	4.4
7	A	199	ALA	4.4
1	1	171	GLU	4.4
9	C	410	MET	4.4
9	C	304	ASP	4.4
13	I	180	PRO	4.4
9	C	373	LEU	4.4
9	C	206	GLY	4.4
8	B	154	ILE	4.4
5	5	430	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	1	74	VAL	4.3
5	5	374	TYR	4.3
9	C	433	ALA	4.3
9	C	213	LEU	4.3
1	1	63	VAL	4.3
7	A	112	GLU	4.3
9	C	334	LEU	4.3
9	C	344	LEU	4.3
11	G	87	GLN	4.3
4	4	310	MET	4.3
9	C	389	THR	4.3
1	1	95	PRO	4.3
7	A	132	ASP	4.3
9	C	238	ASP	4.3
1	1	40	ASN	4.2
7	A	135	VAL	4.2
3	3	104	TYR	4.2
14	K	66	ALA	4.2
1	1	177	TRP	4.2
15	L	78	TYR	4.2
4	4	251	LEU	4.2
4	4	390	GLY	4.2
1	1	142	GLN	4.2
5	5	585	TYR	4.1
2	2	279	ILE	4.1
9	C	133	MET	4.1
1	1	306	ASP	4.1
1	1	258	LEU	4.1
9	C	459	LEU	4.1
9	C	215	GLU	4.1
9	C	417	ASP	4.1
2	2	156	LEU	4.1
5	5	394	TYR	4.1
11	G	181	GLU	4.1
5	5	131	VAL	4.1
14	K	109	ALA	4.1
7	A	110	ASP	4.1
9	C	211	GLU	4.1
13	I	191	GLU	4.1
9	C	429	ALA	4.1
1	1	227	PHE	4.1
9	C	237	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
1	1	209	SER	4.1
14	K	162	SER	4.1
13	I	138	ALA	4.1
6	6	149	THR	4.0
9	C	308	ASN	4.0
1	1	335	ASP	4.0
1	1	55	VAL	4.0
1	1	196	GLU	4.0
8	B	402	ARG	4.0
9	C	177	PHE	4.0
2	2	309	TYR	4.0
4	4	312	ILE	4.0
1	1	260	ASN	4.0
2	2	292	ASN	4.0
8	B	131	LYS	4.0
13	I	157	ARG	4.0
14	K	169	ARG	4.0
13	I	92	GLU	4.0
1	1	100	GLY	4.0
13	I	141	PRO	4.0
1	1	201	PRO	4.0
1	1	72	ILE	3.9
14	K	105	ILE	3.9
1	1	120	SER	3.9
14	K	103	LEU	3.9
2	2	216	PRO	3.9
6	6	153	VAL	3.9
4	4	204	LEU	3.9
6	6	145	THR	3.9
3	3	56	PHE	3.9
11	G	81	ALA	3.9
7	A	146	ASP	3.9
1	1	224	PHE	3.9
1	1	39	PRO	3.9
11	G	195	ASP	3.9
1	1	58	LEU	3.9
1	1	122	LEU	3.9
9	C	402	ALA	3.9
3	3	82	LEU	3.9
3	3	91	VAL	3.9
14	K	184	SER	3.9
4	4	235	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
7	A	95	ALA	3.9
1	1	305	TYR	3.8
9	C	350	CYS	3.8
8	B	106	TRP	3.8
5	5	426	VAL	3.8
5	5	431	ILE	3.8
8	B	415	TYR	3.8
2	2	305	ASN	3.8
1	1	54	ALA	3.8
1	1	77	PRO	3.8
8	B	383	GLN	3.8
4	4	286	ILE	3.8
11	G	198	ARG	3.8
4	4	313	ALA	3.8
8	B	397	ALA	3.8
11	G	183	TYR	3.8
4	4	388	LEU	3.8
5	5	372	TYR	3.8
9	C	115	HIS	3.8
11	G	72	HIS	3.8
7	A	103	PRO	3.8
4	4	158	SER	3.8
11	G	203	TYR	3.8
5	5	211	LEU	3.7
7	A	188	ARG	3.7
7	A	99	TYR	3.7
7	A	72	ASP	3.7
9	C	236	SER	3.7
1	1	202	PHE	3.7
1	1	2	ILE	3.7
13	I	148	ASP	3.7
9	C	158	VAL	3.7
9	C	192	SER	3.7
5	5	115	ARG	3.7
9	C	322	PRO	3.7
9	C	390	LYS	3.7
9	C	245	ASP	3.7
5	5	398	ILE	3.6
12	H	135	CYS	3.6
8	B	388	ARG	3.6
9	C	203	PHE	3.6
2	2	190	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
11	G	176	ASN	3.6
2	2	360	LEU	3.6
7	A	191	ARG	3.6
8	B	418	THR	3.6
1	1	47	LEU	3.6
4	4	323	LEU	3.6
9	C	296	LEU	3.6
12	H	134	LEU	3.6
9	C	330	TYR	3.6
9	C	436	GLY	3.6
11	G	166	PRO	3.6
2	2	413	TYR	3.6
8	B	396	LYS	3.6
4	4	208	THR	3.6
5	5	591	GLY	3.6
9	C	160	LYS	3.6
1	1	111	ALA	3.6
9	C	149	THR	3.6
7	A	143	ASP	3.6
1	1	65	PRO	3.5
1	1	138	ARG	3.5
14	K	79	VAL	3.5
3	3	84	SER	3.5
11	G	71	LEU	3.5
1	1	93	LEU	3.5
9	C	219	ARG	3.5
9	C	442	ALA	3.5
9	C	261	ILE	3.5
5	5	150	SER	3.5
9	C	284	GLN	3.5
9	C	137	PRO	3.5
9	C	153	VAL	3.5
9	C	281	VAL	3.5
1	1	150	LEU	3.5
5	5	120	LEU	3.5
14	K	67	VAL	3.5
9	C	279	GLY	3.5
8	B	386	PRO	3.5
4	4	205	ASP	3.4
13	I	192	TYR	3.4
5	5	148	VAL	3.4
5	5	424	THR	3.4

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Mol	Chain	Res	Type	RSRZ
12	H	130	THR	3.4
3	3	53	ASN	3.4
9	C	93	ALA	3.4
7	A	94	VAL	3.4
7	A	121	VAL	3.4
14	K	88	VAL	3.4
1	1	252	SER	3.4
5	5	254	THR	3.4
2	2	62	ASN	3.4
5	5	339	LYS	3.4
5	5	328	ALA	3.4
9	C	184	LEU	3.4
13	I	177	GLU	3.4
5	5	395	THR	3.4
1	1	85	LEU	3.4
1	1	272	LEU	3.4
7	A	126	LEU	3.4
8	B	428	ALA	3.4
9	C	166	VAL	3.4
9	C	361	VAL	3.4
1	1	70	TYR	3.4
2	2	63	SER	3.4
9	C	117	GLY	3.4
1	1	168	THR	3.4
3	3	108	THR	3.4
13	I	165	ASP	3.4
1	1	79	ILE	3.4
5	5	153	LEU	3.4
8	B	103	PRO	3.4
7	A	107	VAL	3.4
9	C	371	ARG	3.4
2	2	278	GLN	3.4
5	5	319	ALA	3.3
5	5	420	SER	3.3
9	C	221	SER	3.3
8	B	126	ARG	3.3
14	K	161	TYR	3.3
1	1	197	THR	3.3
14	K	123	LEU	3.3
9	C	147	MET	3.3
2	2	276	LEU	3.3
9	C	229	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
4	4	143	ALA	3.3
9	C	437	ALA	3.3
9	C	403	ILE	3.3
1	1	205	THR	3.3
11	G	206	GLU	3.3
9	C	440	HIS	3.3
13	I	149	ALA	3.3
1	1	73	LEU	3.3
7	A	142	CYS	3.3
8	B	140	CYS	3.3
7	A	119	GLU	3.3
9	C	218	GLU	3.3
2	2	280	LYS	3.3
9	C	196	ASP	3.3
9	C	150	ASN	3.3
1	1	178	TYR	3.3
5	5	159	THR	3.3
11	G	173	GLU	3.3
13	I	153	ILE	3.2
3	3	109	ASN	3.2
5	5	404	TYR	3.2
2	2	60	ILE	3.2
5	5	251	HIS	3.2
14	K	126	LYS	3.2
1	1	98	THR	3.2
2	2	412	TYR	3.2
3	3	9	ILE	3.2
14	K	159	PHE	3.2
9	C	306	ARG	3.2
5	5	191	VAL	3.2
5	5	619	MET	3.2
9	C	315	ASP	3.2
9	C	202	PRO	3.2
1	1	4	ASN	3.2
8	B	392	THR	3.2
8	B	403	THR	3.2
9	C	438	PHE	3.2
4	4	159	ASP	3.2
4	4	207	GLN	3.2
13	I	186	GLU	3.2
2	2	273	VAL	3.2
8	B	136	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
3	3	102	PHE	3.2
9	C	247	ILE	3.2
11	G	202	ASP	3.2
5	5	226	LYS	3.2
9	C	358	ALA	3.2
1	1	134	LEU	3.2
12	H	72	MET	3.1
15	L	49	ASP	3.1
5	5	323	SER	3.1
5	5	324	ALA	3.1
1	1	273	PHE	3.1
3	3	4	PHE	3.1
5	5	436	PHE	3.1
1	1	257	TYR	3.1
14	K	89	GLU	3.1
1	1	119	GLY	3.1
4	4	374	THR	3.1
1	1	115	LEU	3.1
1	1	332	TYR	3.1
4	4	373	ALA	3.1
9	C	394	VAL	3.1
1	1	97	ILE	3.1
9	C	89	PRO	3.1
9	C	364	PHE	3.1
14	K	102	ARG	3.1
5	5	94	THR	3.1
9	C	435	LEU	3.1
13	I	196	THR	3.1
1	1	175	VAL	3.1
5	5	125	PHE	3.1
5	5	463	PHE	3.1
2	2	15	MET	3.1
1	1	211	LEU	3.1
8	B	150	THR	3.1
1	1	8	ILE	3.1
9	C	309	ALA	3.1
5	5	429	MET	3.1
9	C	374	MET	3.1
9	C	377	ASP	3.1
1	1	62	ILE	3.0
9	C	148	MET	3.0
4	4	213	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
4	4	267	CYS	3.0
4	4	325	ILE	3.0
5	5	331	HIS	3.0
7	A	96	SER	3.0
2	2	55	MET	3.0
5	5	160	ARG	3.0
9	C	172	TYR	3.0
2	2	164	LEU	3.0
1	1	248	GLY	3.0
9	C	180	ILE	3.0
1	1	279	SER	3.0
14	K	85	CYS	3.0
11	G	177	TRP	3.0
4	4	223	PRO	3.0
2	2	143	ILE	3.0
5	5	305	ILE	3.0
5	5	318	ILE	3.0
9	C	357	GLY	3.0
1	1	304	THR	3.0
14	K	101	ASP	3.0
2	2	411	LEU	3.0
5	5	635	MET	3.0
5	5	243	PRO	3.0
5	5	423	LEU	3.0
14	K	68	ALA	3.0
9	C	91	HIS	3.0
2	2	212	ILE	3.0
5	5	581	LYS	3.0
5	5	171	VAL	3.0
3	3	101	GLY	2.9
5	5	310	MET	2.9
14	K	145	ILE	2.9
14	K	96	PRO	2.9
4	4	194	PHE	2.9
13	I	85	ARG	2.9
5	5	307	LEU	2.9
1	1	181	PRO	2.9
1	1	19	VAL	2.9
14	K	113	GLN	2.9
13	I	143	LEU	2.9
1	1	44	TYR	2.9
5	5	636	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
9	C	231	ARG	2.9
2	2	44	LEU	2.9
3	3	10	LEU	2.9
9	C	457	MET	2.9
2	2	20	ASP	2.9
5	5	178	ASP	2.9
13	I	151	GLU	2.9
1	1	96	GLY	2.9
2	2	197	LEU	2.9
2	2	312	TYR	2.9
1	1	7	GLU	2.9
14	K	168	ASP	2.8
1	1	90	VAL	2.8
8	B	410	GLU	2.8
1	1	99	LEU	2.8
3	3	15	GLY	2.8
9	C	387	LEU	2.8
14	K	128	ALA	2.8
8	B	398	MET	2.8
9	C	432	PHE	2.8
1	1	199	ARG	2.8
14	K	165	ARG	2.8
9	C	369	PRO	2.8
5	5	384	LEU	2.8
1	1	121	LEU	2.8
7	A	198	GLY	2.8
8	B	105	GLY	2.8
13	I	195	GLU	2.8
1	1	312	CYS	2.8
3	3	52	PHE	2.8
9	C	461	PHE	2.8
14	K	92	HIS	2.8
7	A	136	CYS	2.8
7	A	137	ASP	2.8
7	A	108	ARG	2.8
2	2	263	LEU	2.8
9	C	381	LEU	2.8
4	4	324	GLY	2.8
14	K	122	THR	2.8
7	A	85	ASP	2.8
9	C	439	ASP	2.8
2	2	269	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
9	C	271	TRP	2.8
4	4	210	ILE	2.8
9	C	366	ILE	2.8
5	5	111	PRO	2.8
9	C	370	PRO	2.8
1	1	94	GLY	2.8
9	C	234	GLY	2.8
4	4	284	THR	2.8
5	5	239	ALA	2.8
9	C	282	THR	2.8
8	B	424	HIS	2.7
1	1	104	LEU	2.7
1	1	53	ASP	2.7
5	5	129	ILE	2.7
9	C	173	ILE	2.7
5	5	406	SER	2.7
5	5	590	VAL	2.7
9	C	388	TYR	2.7
9	C	324	GLY	2.7
14	K	174	ASP	2.7
4	4	233	VAL	2.7
7	A	116	GLN	2.7
5	5	638	ASN	2.7
5	5	641	ILE	2.7
3	3	63	PHE	2.7
7	A	106	VAL	2.7
7	A	192	PHE	2.7
1	1	113	GLY	2.7
9	C	244	LEU	2.7
9	C	94	ALA	2.7
11	G	204	GLY	2.7
9	C	212	LYS	2.7
5	5	140	PHE	2.7
1	1	204	LEU	2.7
8	B	395	LEU	2.7
3	3	87	GLY	2.7
15	L	79	ARG	2.7
1	1	86	ILE	2.7
4	4	389	THR	2.7
5	5	78	ASN	2.7
15	L	43	ASN	2.7
5	5	176	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
5	5	143	TRP	2.7
7	A	100	PRO	2.7
7	A	134	PRO	2.7
9	C	167	PRO	2.7
9	C	134	GLN	2.7
9	C	341	ARG	2.7
9	C	428	ARG	2.7
1	1	315	ILE	2.7
8	B	151	ALA	2.7
7	A	87	GLU	2.7
13	I	161	LYS	2.7
1	1	129	SER	2.7
5	5	134	SER	2.7
5	5	112	HIS	2.6
9	C	415	VAL	2.6
14	K	163	VAL	2.6
5	5	375	ILE	2.6
7	A	196	ILE	2.6
2	2	267	THR	2.6
9	C	209	GLU	2.6
2	2	297	MET	2.6
1	1	276	LEU	2.6
5	5	137	PHE	2.6
5	5	637	VAL	2.6
1	1	314	ILE	2.6
1	1	135	GLY	2.6
15	L	77	TYR	2.6
2	2	210	PHE	2.6
4	4	467	CYS	2.6
12	H	145	GLN	2.6
1	1	48	LEU	2.6
9	C	449	ASP	2.6
1	1	161	VAL	2.6
5	5	162	GLN	2.6
5	5	351	HIS	2.6
5	5	77	TYR	2.6
13	I	88	TYR	2.6
9	C	268	ASN	2.6
9	C	345	ARG	2.6
14	K	205	ARG	2.6
1	1	49	GLN	2.6
4	4	457	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
13	I	79	LEU	2.6
5	5	471	PHE	2.6
3	3	59	VAL	2.6
1	1	102	LEU	2.6
5	5	225	ALA	2.6
9	C	418	GLY	2.6
8	B	427	CYS	2.5
11	G	186	TYR	2.5
13	I	131	ILE	2.5
9	C	463	GLU	2.5
9	C	273	LEU	2.5
7	A	93	PRO	2.5
13	I	81	ALA	2.5
5	5	105	GLY	2.5
5	5	154	ILE	2.5
1	1	176	VAL	2.5
9	C	183	VAL	2.5
5	5	620	LEU	2.5
2	2	393	ASN	2.5
4	4	391	ASN	2.5
5	5	107	MET	2.5
9	C	353	ASP	2.5
4	4	387	PRO	2.5
2	2	84	GLY	2.5
4	4	321	THR	2.5
5	5	175	ARG	2.5
1	1	267	SER	2.5
2	2	245	LEU	2.5
4	4	452	PHE	2.5
5	5	82	ASP	2.5
4	4	307	ILE	2.5
9	C	255	GLY	2.5
9	C	297	ARG	2.5
4	4	212	LEU	2.5
5	5	90	LEU	2.5
5	5	460	LEU	2.5
8	B	394	LEU	2.5
8	B	98	TRP	2.5
15	L	37	ASN	2.5
5	5	576	ALA	2.5
7	A	73	LYS	2.5
7	A	80	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
9	C	259	ASP	2.5
14	K	166	GLY	2.5
1	1	262	LEU	2.5
5	5	650	LEU	2.5
1	1	225	VAL	2.5
9	C	295	MET	2.5
9	C	423	TYR	2.5
1	1	231	GLU	2.5
5	5	474	TRP	2.5
2	2	21	ASN	2.5
2	2	323	ILE	2.5
8	B	433	ALA	2.5
9	C	85	ILE	2.5
2	2	161	GLY	2.5
2	2	289	GLY	2.5
5	5	631	LEU	2.5
9	C	97	VAL	2.5
13	I	171	TYR	2.5
1	1	189	PHE	2.4
5	5	241	GLU	2.4
1	1	313	TRP	2.4
1	1	247	LEU	2.4
5	5	370	LEU	2.4
8	B	385	THR	2.4
8	B	391	THR	2.4
2	2	74	PHE	2.4
5	5	136	TYR	2.4
4	4	463	ILE	2.4
5	5	81	ILE	2.4
6	6	34	LEU	2.4
2	2	50	GLN	2.4
14	K	193	GLN	2.4
5	5	315	MET	2.4
9	C	106	GLY	2.4
9	C	113	ASP	2.4
9	C	146	SER	2.4
5	5	330	PHE	2.4
5	5	126	TRP	2.4
8	B	393	TRP	2.4
9	C	257	ARG	2.4
4	4	320	ASN	2.4
2	2	296	MET	2.4

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Mol	Chain	Res	Type	RSRZ
14	K	111	PRO	2.4
2	2	65	THR	2.4
9	C	299	SER	2.4
9	C	375	LYS	2.4
15	L	44	SER	2.4
3	3	62	LEU	2.4
9	C	262	GLU	2.4
1	1	50	ALA	2.4
1	1	92	PRO	2.4
5	5	383	SER	2.4
9	C	220	VAL	2.4
9	C	90	GLN	2.4
9	C	367	ASN	2.4
5	5	422	VAL	2.4
6	6	174	ILE	2.4
13	I	146	THR	2.4
14	K	60	THR	2.4
5	5	393	TYR	2.4
11	G	74	TYR	2.4
2	2	155	MET	2.4
1	1	208	GLU	2.4
1	1	300	PHE	2.3
9	C	240	PRO	2.3
9	C	446	PHE	2.3
1	1	188	ILE	2.3
5	5	464	ILE	2.3
7	A	114	VAL	2.3
15	L	75	VAL	2.3
1	1	323	ILE	2.3
2	2	166	ILE	2.3
9	C	270	ILE	2.3
9	C	427	ILE	2.3
9	C	321	VAL	2.3
9	C	274	ARG	2.3
5	5	427	TYR	2.3
7	A	77	ALA	2.3
1	1	11	PHE	2.3
1	1	261	ILE	2.3
1	1	324	PHE	2.3
2	2	200	ILE	2.3
6	6	24	ILE	2.3
8	B	421	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
9	C	136	LEU	2.3
4	4	406	ASN	2.3
8	B	142	LEU	2.3
12	H	143	ALA	2.3
1	1	71	ILE	2.3
1	1	153	ILE	2.3
14	K	118	ILE	2.3
1	1	203	ASP	2.3
9	C	198	GLY	2.3
2	2	185	HIS	2.3
2	2	180	ASN	2.3
9	C	266	THR	2.3
4	4	252	LYS	2.3
9	C	360	LYS	2.3
5	5	161	LEU	2.3
14	K	83	LEU	2.3
1	1	91	ILE	2.3
4	4	408	ILE	2.3
5	5	123	PHE	2.3
5	5	306	ALA	2.3
9	C	83	PHE	2.3
1	1	200	PRO	2.3
14	K	187	LEU	2.3
1	1	5	ILE	2.3
9	C	347	ILE	2.3
1	1	310	ASN	2.2
2	2	208	LEU	2.2
2	2	285	LEU	2.2
2	2	220	TRP	2.2
1	1	180	ILE	2.2
5	5	639	PHE	2.2
4	4	375	TYR	2.2
5	5	113	GLN	2.2
14	K	197	LYS	2.2
9	C	107	GLU	2.2
4	4	188	VAL	2.2
4	4	292	THR	2.2
4	4	393	THR	2.2
8	B	414	LEU	2.2
3	3	16	PHE	2.2
11	G	175	ALA	2.2
9	C	253	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	1	89	VAL	2.2
1	1	302	ARG	2.2
5	5	249	LEU	2.2
8	B	93	PRO	2.2
9	C	447	LEU	2.2
14	K	63	THR	2.2
1	1	277	ILE	2.2
2	2	380	PHE	2.2
8	B	420	ASP	2.2
1	1	125	TRP	2.2
1	1	114	SER	2.2
9	C	413	TYR	2.2
4	4	268	GLU	2.2
14	K	62	THR	2.2
3	3	40	CYS	2.2
11	G	205	PHE	2.2
9	C	185	ASN	2.2
6	6	183	HIS	2.2
13	I	144	ALA	2.2
4	4	266	LEU	2.2
8	B	400	ARG	2.2
9	C	289	LEU	2.2
14	K	114	SER	2.2
15	L	54	LEU	2.2
1	1	275	GLY	2.2
4	4	242	GLY	2.2
5	5	108	GLU	2.2
5	5	589	PRO	2.2
11	G	78	ILE	2.2
9	C	168	LEU	2.2
2	2	318	ILE	2.2
8	B	426	ILE	2.2
3	3	105	GLU	2.2
4	4	454	MET	2.2
5	5	587	LEU	2.2
5	5	311	SER	2.1
9	C	182	ARG	2.1
5	5	147	GLY	2.1
9	C	130	LYS	2.1
14	K	124	THR	2.1
14	K	186	ALA	2.1
9	C	193	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
2	2	262	ILE	2.1
4	4	154	ILE	2.1
1	1	32	TYR	2.1
5	5	151	TYR	2.1
14	K	59	TYR	2.1
4	4	222	THR	2.1
9	C	283	ALA	2.1
1	1	193	SER	2.1
2	2	186	SER	2.1
1	1	10	ILE	2.1
2	2	408	ILE	2.1
3	3	80	ILE	2.1
3	3	94	PHE	2.1
13	I	90	VAL	2.1
11	G	174	GLY	2.1
1	1	78	LEU	2.1
14	K	117	MET	2.1
1	1	84	ALA	2.1
5	5	252	ALA	2.1
2	2	14	SER	2.1
5	5	592	ILE	2.1
5	5	625	ILE	2.1
9	C	277	ASN	2.1
14	K	164	VAL	2.1
2	2	299	LEU	2.1
1	1	274	GLU	2.1
8	B	416	GLU	2.1
9	C	181	THR	2.1
8	B	145	ARG	2.1
2	2	72	ILE	2.1
8	B	99	SER	2.1
1	1	51	PHE	2.1
1	1	271	PHE	2.1
9	C	323	VAL	2.1
9	C	383	HIS	2.1
1	1	33	MET	2.1
1	1	266	TYR	2.1
1	1	101	GLU	2.1
5	5	391	THR	2.1
9	C	301	ILE	2.1
6	6	178	SER	2.1
5	5	76	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
4	4	272	LEU	2.1
9	C	98	LEU	2.1
2	2	157	TYR	2.0
7	A	70	TYR	2.0
9	C	397	GLY	2.0
1	1	106	ILE	2.0
4	4	150	ILE	2.0
8	B	107	GLU	2.0
9	C	199	ALA	2.0
9	C	356	ALA	2.0
1	1	154	PHE	2.0
9	C	164	VAL	2.0
1	1	242	ASN	2.0
9	C	391	GLY	2.0
12	H	159	GLY	2.0
1	1	130	LYS	2.0
2	2	230	ILE	2.0
13	I	152	ARG	2.0
9	C	250	TRP	2.0
1	1	30	LEU	2.0
1	1	37	LEU	2.0
4	4	303	ALA	2.0
4	4	322	SER	2.0
5	5	428	SER	2.0
8	B	413	MET	2.0
2	2	49	ASN	2.0
1	1	244	TYR	2.0
5	5	309	THR	2.0
5	5	335	HIS	2.0
1	1	160	PHE	2.0
1	1	226	PHE	2.0
1	1	245	LEU	2.0
5	5	337	PHE	2.0
13	I	128	GLU	2.0
5	5	421	ALA	2.0
12	H	138	ASP	2.0
13	I	190	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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($\text{\AA}^2$)	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.