Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 04:03 PM EDT

PDB ID	:	4WZ7
Title	:	Crystal structure of mitochondrial NADH:ubiquinone oxidoreductase from Yarrowia lipolytica.
Authors	:	Wirth, C.; Zickermann, V.; Brandt, U.; Hunte, C.
Deposited on	:	2014-11-18
Resolution	:	3.60 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:

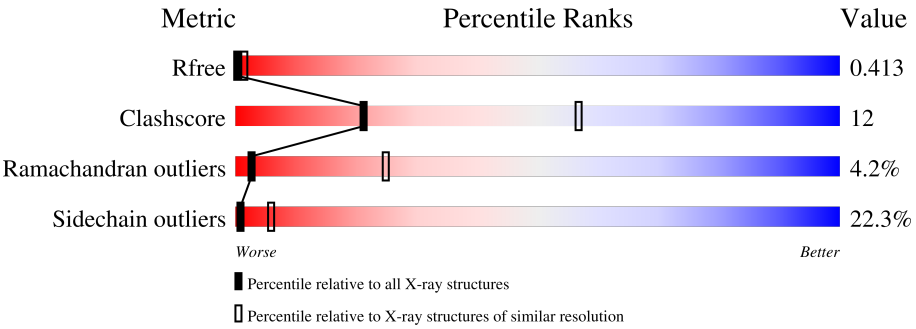
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	1	327	61% 27% 8%
2	2	438	58% 34% 8%
3	3	89	43% 45% 11%
4	4	470	64% 29% 6%
5	5	619	69% 26%
6	6	185	42% 29% 9% 19%
7	A	628	97%

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Mol	Chain	Length	Quality of chain
8	B	370	91% 9%
9	C	444	54% 24% 18%
10	E	195	99%
11	G	133	80% 20%
12	H	154	93% 6%
13	I	137	72% 23%
14	K	183	52% 26% 20%
15	L	89	44% 45% 10%
16	D	57	84% 16%
16	Z	57	89% 11%
17	F	54	100%
18	J	63	97%
19	M	29	86% 14%
20	N	50	92% 8%
21	O	70	94% 6%
22	P	46	93% 7%
23	Q	51	98%
24	R	30	100%
25	S	69	94% 6%
26	AH	15	100%
26	T	15	100%
27	U	26	100%
28	V	22	82% 18%
29	AB	9	100%
29	AY	9	100%

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Mol	Chain	Length	Quality of chain
29	BE	9	100%
29	W	9	78% 22%
30	AJ	16	100%
30	AV	16	100%
30	BH	16	88% 12%
30	X	16	100%
31	AR	13	100%
31	AT	13	100%
31	Y	13	100%
32	AA	18	100%
32	AW	18	100%
32	BB	18	100%
32	BG	18	100%
33	AC	47	85% 15%
33	AD	47	100%
34	AE	48	92% 8%
35	AF	35	100%
36	AG	25	100%
37	AI	36	100%
37	AL	36	100%
38	AK	76	100%
38	AN	76	97%
39	AM	17	100%
40	AO	32	100%
41	AP	11	100%

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Mol	Chain	Length	Quality of chain
41	AS	11	100%
42	AQ	8	100%
42	BA	8	100%
43	AU	58	100%
44	AX	39	100%
45	AZ	40	95% 5%
46	BC	20	90% 10%
47	BD	19	100%
47	BF	19	100%
48	BI	905	99%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
50	SF4	K	500	-	-	X	-

2 Entry composition (i)

There are 50 unique types of molecules in this entry. The entry contains 35169 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	318	Total	C	N	O	S	0	0	0
			2177	1431	352	389	5			

- Molecule 2 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	438	Total	C	N	O	S	0	0	0
			3142	2092	482	556	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	89	Total	C	N	O	S	0	0	0
			641	444	91	104	2			

- 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	619	Total	C	N	O	S	0	0	0
			4065	2636	677	727	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	6	149	Total	C	N	O	S	0	0	0
			1078	735	156	180	7			

- 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
			3226	1933	639	639	15			

- Molecule 8 is a protein called NUBM protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	B	370	Total	C	N	O	S	0	0	0
			2013	1214	391	399	9			

- Molecule 9 is a protein called NUCM protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	C	366	Total	C	N	O	S	0	0	0
			2647	1675	455	496	21			

- Molecule 10 is a protein called 39-kDa subunit.

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 protein 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 protein NADH:Ubiquinone Oxidoreductase (Complex 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	147	Total	C	N	O	S	0	0	0
			1023	642	182	187	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	L	89	Total	C	N	O	S	0	0	0
			660	437	108	112	3			

- Molecule 16 is a protein called unknown subunits 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	Z	57	Total	C	N	O	0	0	0
			285	171	57	57			
16	D	57	Total	C	N	O	0	0	0
			285	171	57	57			

- Molecule 17 is a protein called unknown subunits 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	F	54	Total	C	N	O	0	0	0
			270	162	54	54			

- Molecule 18 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	J	63	Total	C	N	O	0	0	0
			315	189	63	63			

- Molecule 19 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	M	29	Total	C	N	O	0	0	0
			145	87	29	29			

- Molecule 20 is a protein called unknown subunits.

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

- Molecule 21 is a protein called unknown subunits.

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

- Molecule 22 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	P	46	Total	C	N	O	0	0	0
			230	138	46	46			

- Molecule 23 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	Q	51	Total	C	N	O	0	0	0
			255	153	51	51			

- Molecule 24 is a protein called unknown subunits.

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

- Molecule 25 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	S	69	Total	C	N	O	0	0	0
			345	207	69	69			

- Molecule 26 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	T	15	Total	C	N	O	0	0	0
			75	45	15	15			
26	AH	15	Total	C	N	O	0	0	0
			75	45	15	15			

- Molecule 27 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	U	26	Total	C	N	O	0	0	0
			130	78	26	26			

- Molecule 28 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	V	22	Total	C	N	O	0	0	0
			110	66	22	22			

- Molecule 29 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
29	W	9	Total	C	N	O	0	0	0
			45	27	9	9			
29	AB	9	Total	C	N	O	0	0	0
			45	27	9	9			
29	AY	9	Total	C	N	O	0	0	0
			45	27	9	9			
29	BE	9	Total	C	N	O	0	0	0
			45	27	9	9			

- Molecule 30 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
30	X	16	Total	C	N	O	0	0	0
			80	48	16	16			
30	AJ	16	Total	C	N	O	0	0	0
			80	48	16	16			
30	AV	16	Total	C	N	O	0	0	0
			80	48	16	16			
30	BH	16	Total	C	N	O	0	0	0
			80	48	16	16			

- Molecule 31 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
31	Y	13	Total	C	N	O	0	0	0
			65	39	13	13			
31	AR	13	Total	C	N	O	0	0	0
			65	39	13	13			
31	AT	13	Total	C	N	O	0	0	0
			65	39	13	13			

- Molecule 32 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
32	AA	18	Total	C	N	O	0	0	0
			90	54	18	18			
32	AW	18	Total	C	N	O	0	0	0
			90	54	18	18			
32	BB	18	Total	C	N	O	0	0	0
			90	54	18	18			
32	BG	18	Total	C	N	O	0	0	0
			90	54	18	18			

- Molecule 33 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
33	AC	47	Total	C	N	O	0	0	0
			235	141	47	47			
33	AD	47	Total	C	N	O	0	0	0
			235	141	47	47			

- Molecule 34 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
34	AE	48	Total	C	N	O	0	0	0
			240	144	48	48			

- Molecule 35 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	AF	35	Total	C	N	O	0	0	0
			175	105	35	35			

- Molecule 36 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	AG	25	Total	C	N	O	0	0	0
			125	75	25	25			

- Molecule 37 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	AI	36	Total	C	N	O	0	0	0
			180	108	36	36			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	AL	36	Total	C	N	O	0	0	0
			180	108	36	36			

- Molecule 38 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	AK	76	Total	C	N	O	0	0	0
			380	228	76	76			
38	AN	76	Total	C	N	O	0	0	0
			380	228	76	76			

- Molecule 39 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	AM	17	Total	C	N	O	0	0	0
			85	51	17	17			

- Molecule 40 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	AO	32	Total	C	N	O	0	0	0
			160	96	32	32			

- Molecule 41 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	AP	11	Total	C	N	O	0	0	0
			55	33	11	11			
41	AS	11	Total	C	N	O	0	0	0
			54	32	11	11			

- Molecule 42 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	AQ	8	Total	C	N	O	0	0	0
			40	24	8	8			
42	BA	8	Total	C	N	O	0	0	0
			40	24	8	8			

- Molecule 43 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	AU	58	Total	C	N	O	0	0	0
			290	174	58	58			

- Molecule 44 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	AX	39	Total	C	N	O	0	0	0
			195	117	39	39			

- Molecule 45 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	AZ	40	Total	C	N	O	0	0	0
			200	120	40	40			

- Molecule 46 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	BC	20	Total	C	N	O	0	0	0
			100	60	20	20			

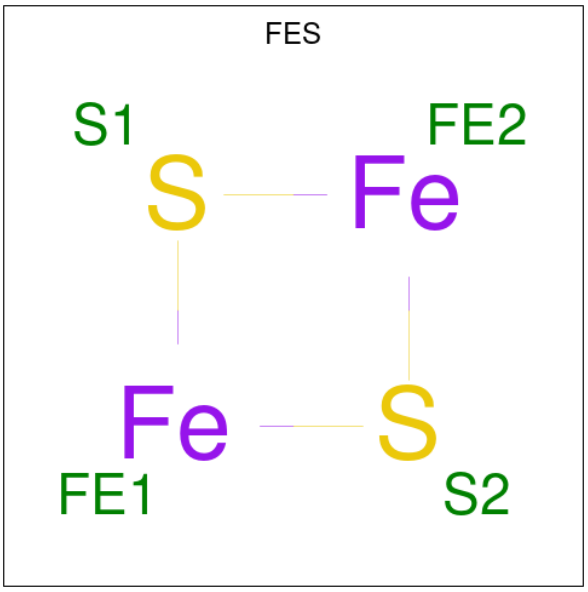
- Molecule 47 is a protein called unknown subunits.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	BD	19	Total	C	N	O	0	0	0
			95	57	19	19			
47	BF	19	Total	C	N	O	0	0	0
			95	57	19	19			

- Molecule 48 is a protein called unknown subunits.

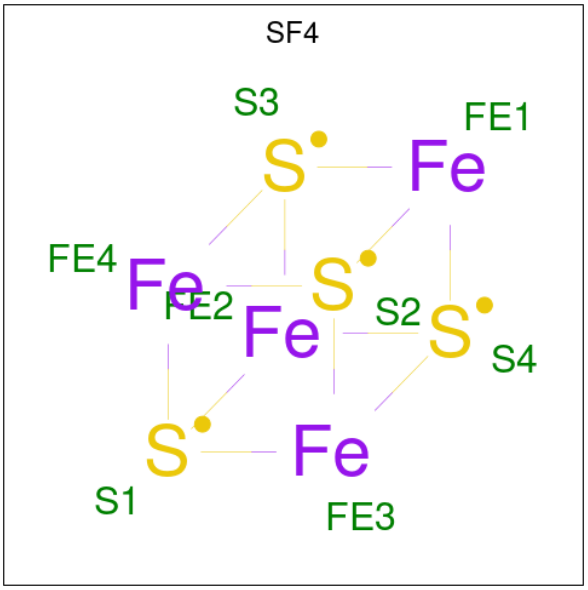
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	BI	9	Total	C	N	O	0	0	0
			45	27	9	9			

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 50 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

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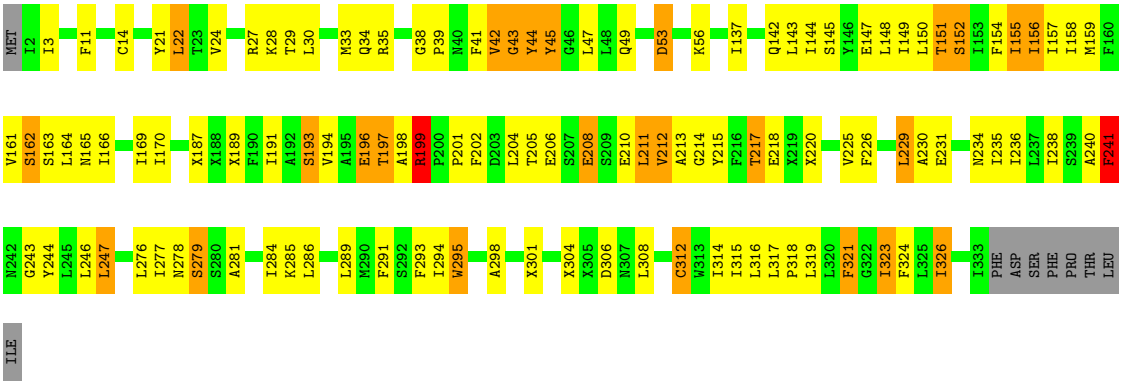
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
50	B	1	Total	Fe	S	0	0
			8	4	4		
50	I	1	Total	Fe	S	0	0
			8	4	4		
50	I	1	Total	Fe	S	0	0
			8	4	4		
50	K	1	Total	Fe	S	0	0
			8	4	4		

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. 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. 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.

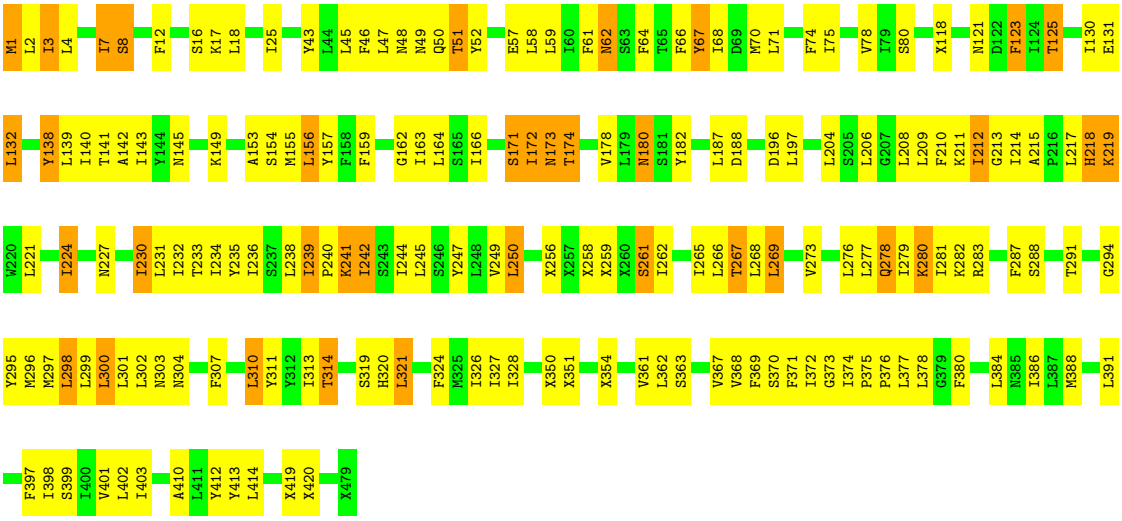
• Molecule 1: NADH-ubiquinone oxidoreductase chain 1

Chain 1:



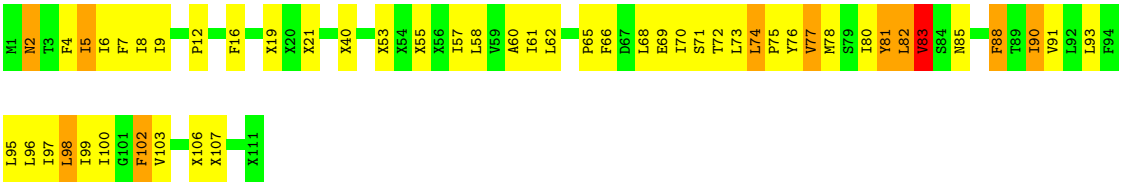
• Molecule 2: NADH dehydrogenase subunit 2

Chain 2:



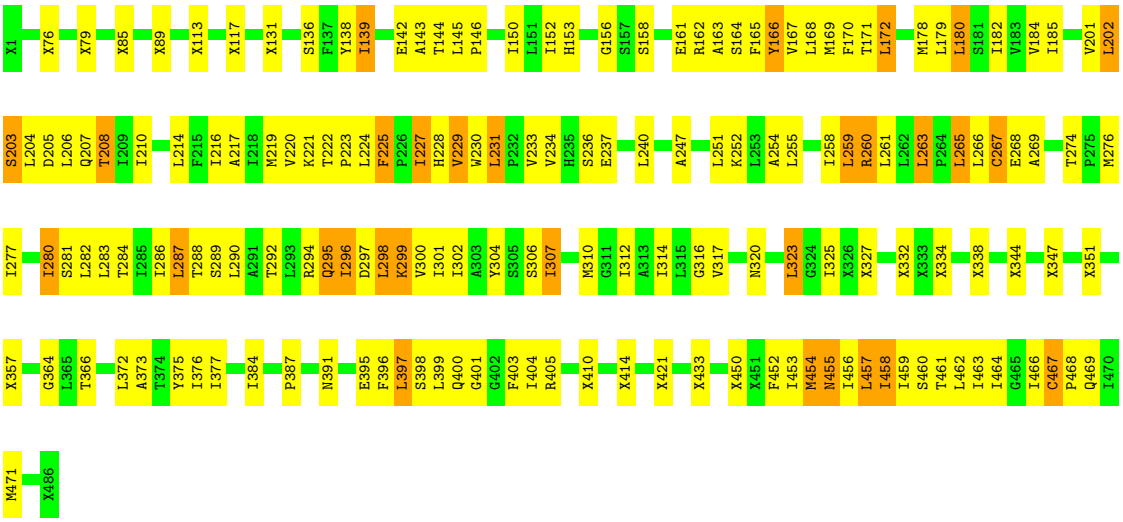
• Molecule 3: NADH-ubiquinone oxidoreductase chain 3

Chain 3:



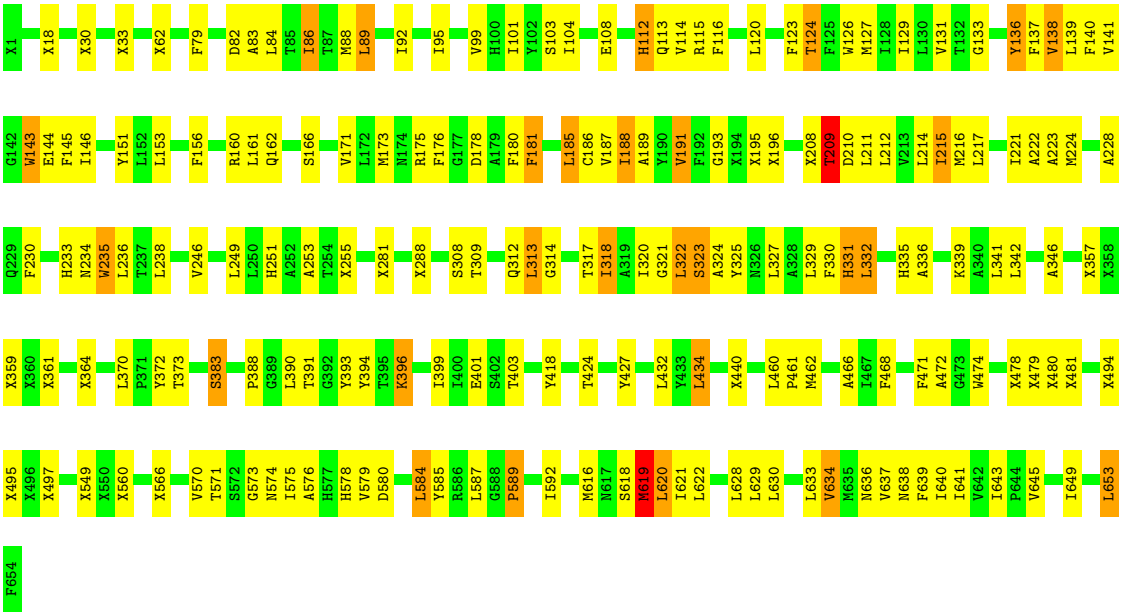
• Molecule 4: NADH-ubiquinone oxidoreductase chain 4

Chain 4:



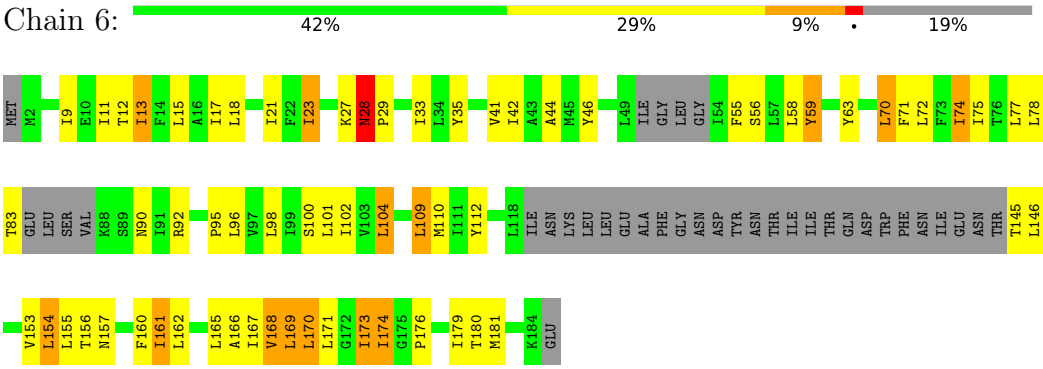
• Molecule 5: NADH-ubiquinone oxidoreductase chain 5

Chain 5:



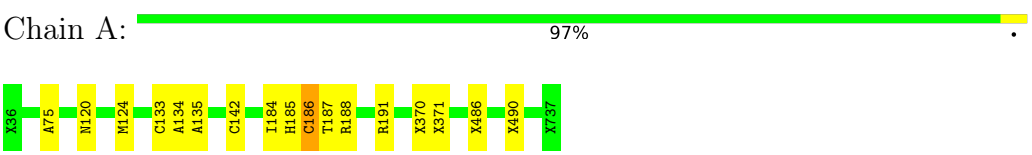
• Molecule 6: NADH-ubiquinone oxidoreductase chain 6

Chain 6:



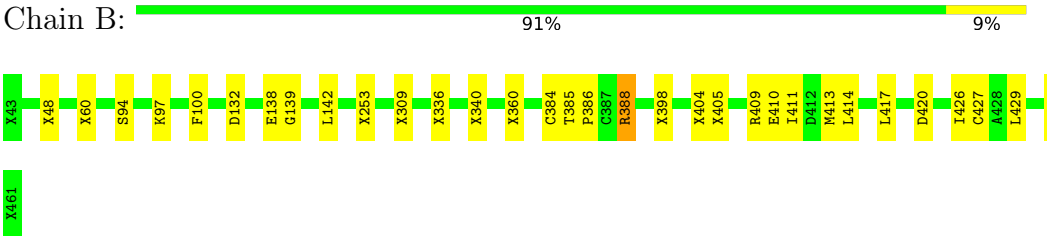
• Molecule 7: NUAM protein

Chain A:



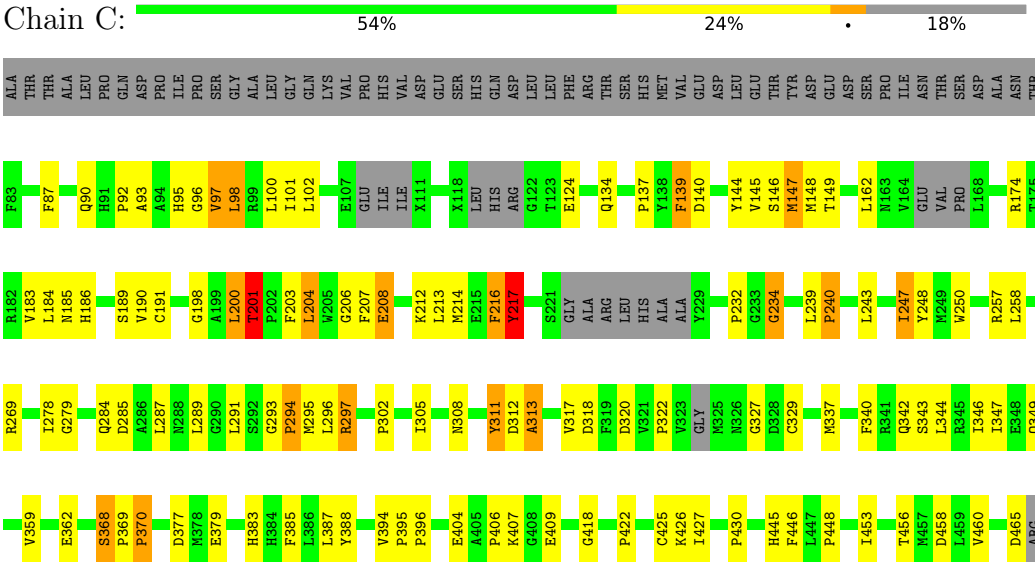
• Molecule 8: NUBM protein

Chain B:



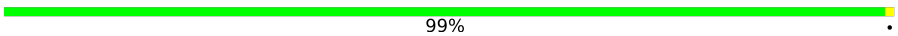
• Molecule 9: NUCM protein

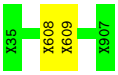
Chain C:



• Molecule 10: 39-kDa subunit

Chain E:



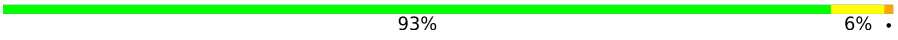


• Molecule 11: NUGM protein

Chain G:

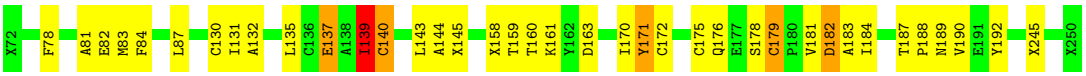
• Molecule 12: Subunit NUHM of protein NADH:Ubiquinone Oxidoreductase (Complex I)

Chain H:



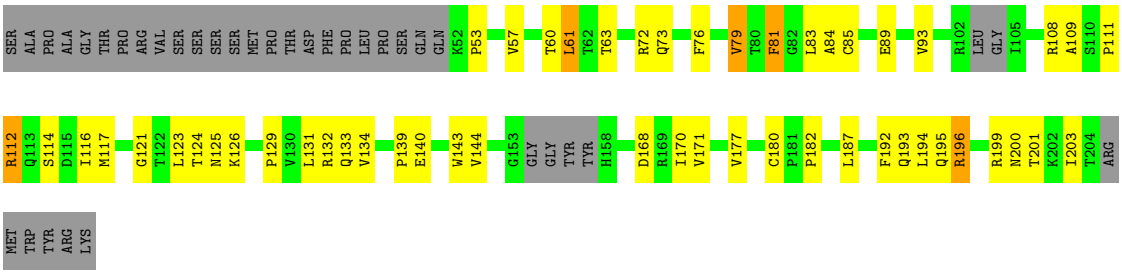
• Molecule 13: Subunit NUIM of protein NADH:Ubiquinone Oxidoreductase (Complex I)

Chain I:



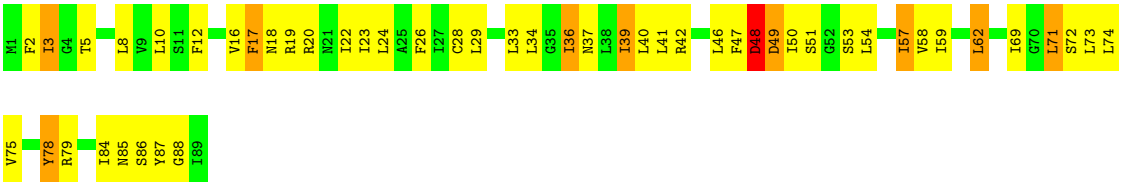
• Molecule 14: Subunit NUKM of protein NADH:Ubiquinone Oxidoreductase (Complex I)

Chain K:



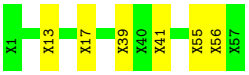
• Molecule 15: NADH-ubiquinone oxidoreductase chain 4L

Chain L:



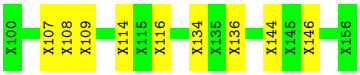
• Molecule 16: unknown subunits 1

Chain Z:



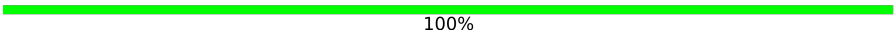
• Molecule 16: unknown subunits 1

Chain D:



• Molecule 17: unknown subunits 2

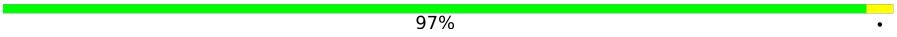
Chain F:

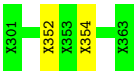


There are no outlier residues recorded for this chain.

• Molecule 18: unknown subunits

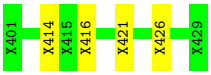
Chain J:





• Molecule 19: unknown subunits

Chain M:

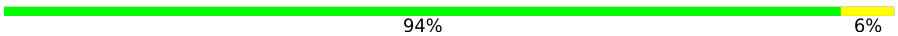


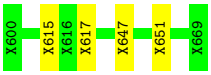
• Molecule 20: unknown subunits

Chain N:

• Molecule 21: unknown subunits

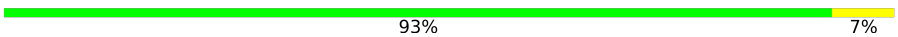
Chain O:



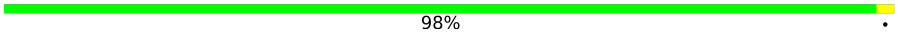


• Molecule 22: unknown subunits

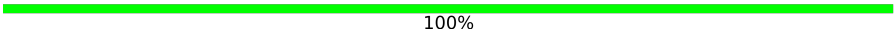
Chain P:



• Molecule 23: unknown subunits

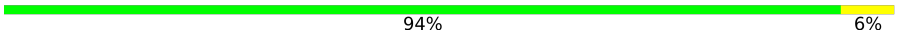
Chain Q: 

• Molecule 24: unknown subunits

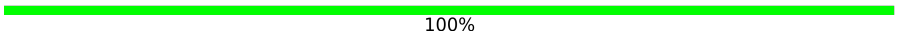
Chain R: 

There are no outlier residues recorded for this chain.

• Molecule 25: unknown subunits

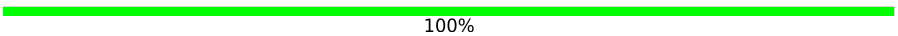
Chain S: 

• Molecule 26: unknown subunits

Chain T: 

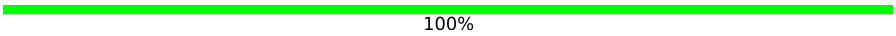
There are no outlier residues recorded for this chain.

• Molecule 26: unknown subunits

Chain AH: 

There are no outlier residues recorded for this chain.

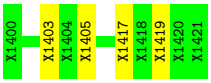
• Molecule 27: unknown subunits

Chain U: 

There are no outlier residues recorded for this chain.

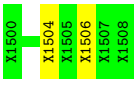
• Molecule 28: unknown subunits

Chain V: 



• Molecule 29: unknown subunits

Chain W: 



• Molecule 29: unknown subunits

Chain AB: 100%

There are no outlier residues recorded for this chain.

• Molecule 29: unknown subunits

Chain AY: 100%

There are no outlier residues recorded for this chain.

• Molecule 29: unknown subunits

Chain BE: 100%

There are no outlier residues recorded for this chain.

• Molecule 30: unknown subunits

Chain X: 100%

There are no outlier residues recorded for this chain.

• Molecule 30: unknown subunits

Chain AJ: 100%

There are no outlier residues recorded for this chain.

• Molecule 30: unknown subunits

Chain AV: 100%

There are no outlier residues recorded for this chain.

• Molecule 30: unknown subunits

Chain BH: 88% 12%

• Molecule 31: unknown subunits

Chain Y: 100%

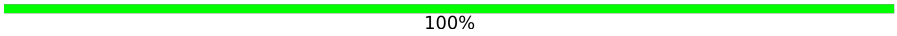
There are no outlier residues recorded for this chain.

• Molecule 31: unknown subunits

Chain AR: 100%

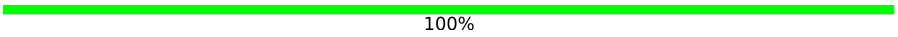
There are no outlier residues recorded for this chain.

• Molecule 31: unknown subunits

Chain AT: 

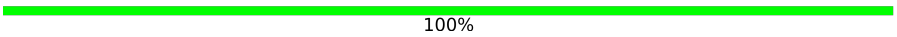
There are no outlier residues recorded for this chain.

• Molecule 32: unknown subunits

Chain AA: 

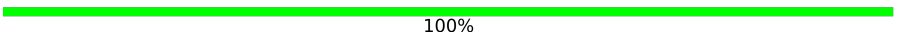
There are no outlier residues recorded for this chain.

• Molecule 32: unknown subunits

Chain AW: 

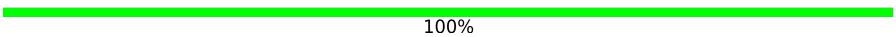
There are no outlier residues recorded for this chain.

• Molecule 32: unknown subunits

Chain BB: 

There are no outlier residues recorded for this chain.

• Molecule 32: unknown subunits

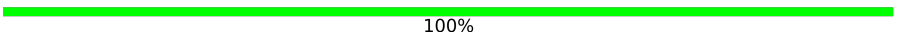
Chain BG: 

There are no outlier residues recorded for this chain.

• Molecule 33: unknown subunits

Chain AC: 

• Molecule 33: unknown subunits

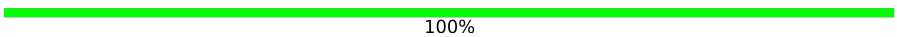
Chain AD: 

There are no outlier residues recorded for this chain.

• Molecule 34: unknown subunits

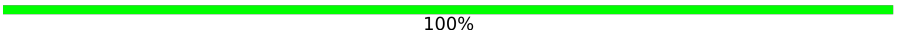
Chain AE: 

• Molecule 35: unknown subunits

Chain AF: 

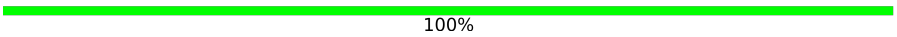
There are no outlier residues recorded for this chain.

• Molecule 36: unknown subunits

Chain AG: 

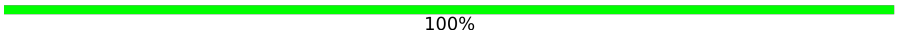
There are no outlier residues recorded for this chain.

• Molecule 37: unknown subunits

Chain AI: 

There are no outlier residues recorded for this chain.

• Molecule 37: unknown subunits

Chain AL: 

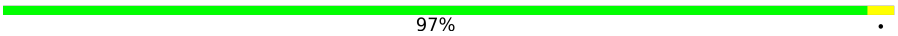
There are no outlier residues recorded for this chain.

• Molecule 38: unknown subunits

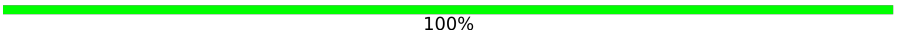
Chain AK: 

There are no outlier residues recorded for this chain.

• Molecule 38: unknown subunits

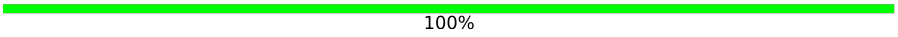
Chain AN: 

• Molecule 39: unknown subunits

Chain AM: 

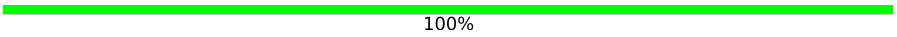
There are no outlier residues recorded for this chain.

• Molecule 40: unknown subunits

Chain AO: 

There are no outlier residues recorded for this chain.

• Molecule 41: unknown subunits

Chain AP: 

There are no outlier residues recorded for this chain.

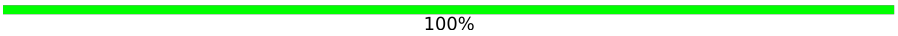
• Molecule 41: unknown subunits

Chain AS: 

There are no outlier residues recorded for this chain.

• Molecule 42: unknown subunits

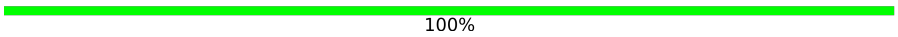
Chain AQ:



There are no outlier residues recorded for this chain.

• Molecule 42: unknown subunits

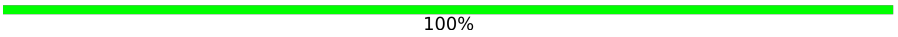
Chain BA:



There are no outlier residues recorded for this chain.

• Molecule 43: unknown subunits

Chain AU:



There are no outlier residues recorded for this chain.

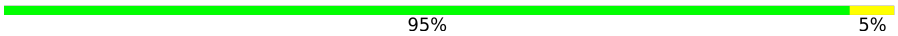
• Molecule 44: unknown subunits

Chain AX:

There are no outlier residues recorded for this chain.

• Molecule 45: unknown subunits

Chain AZ:

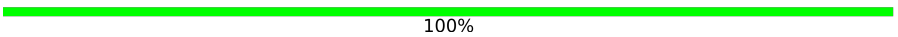


• Molecule 46: unknown subunits

Chain BC:

• Molecule 47: unknown subunits

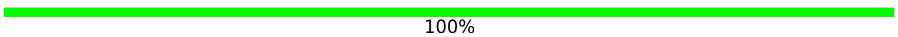
Chain BD:



There are no outlier residues recorded for this chain.

• Molecule 47: unknown subunits

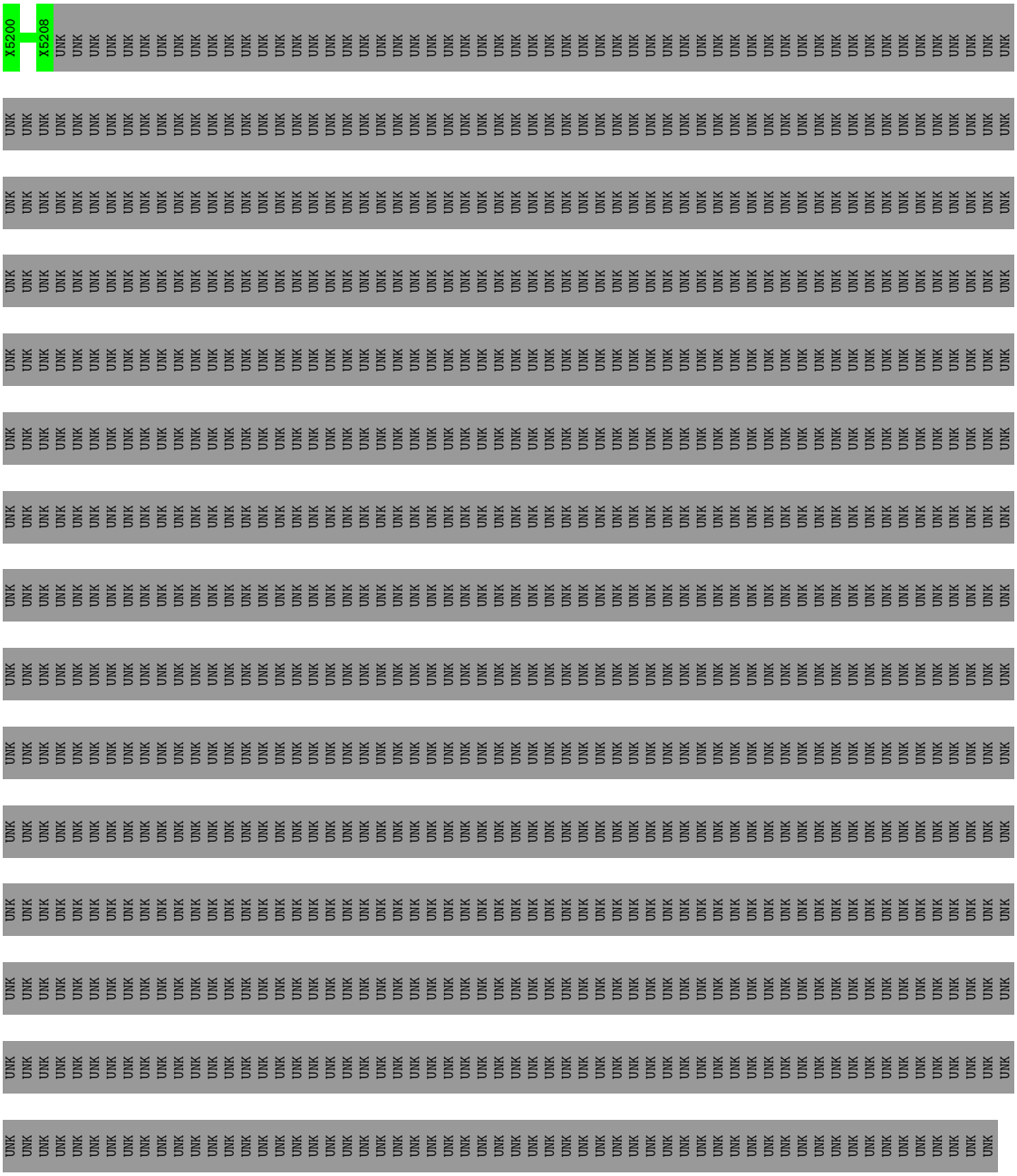
Chain BF:



There are no outlier residues recorded for this chain.

• Molecule 48: unknown subunits

Chain BI: 99%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	317.74Å 317.74Å 818.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 3.60 50.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	84.8 (25.00-3.60) 85.0 (50.00-3.60)	Depositor EDS
R_{merge}	0.52	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 3.57Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.316 , 0.341 0.379 , 0.413	Depositor DCC
R_{free} test set	2191 reflections (1.41%)	wwPDB-VP
Wilson B-factor (Å^2)	106.8	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 999.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.039 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.097 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.067 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l	Xtriage
F_o,F_c correlation	0.77	EDS
Total number of atoms	35169	wwPDB-VP
Average B, all atoms (Å^2)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.49	0/1638	0.88	3/2224 (0.1%)
2	2	0.56	0/2613	0.89	1/3550 (0.0%)
3	3	0.52	0/533	0.94	1/728 (0.1%)
4	4	0.54	0/1920	0.86	0/2615
5	5	0.51	0/2813	0.82	0/3820
6	6	0.54	0/1090	0.87	0/1491
7	A	0.48	0/412	0.79	0/531
8	B	0.46	0/527	0.73	0/701
9	C	0.46	0/2653	0.82	7/3592 (0.2%)
11	G	0.39	0/566	0.67	0/766
12	H	0.44	0/178	0.77	0/220
13	I	0.41	0/499	0.79	0/675
14	K	0.47	0/1042	0.80	2/1424 (0.1%)
15	L	0.58	0/666	0.91	0/902
All	All	0.50	0/17150	0.84	14/23239 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	82	LEU	C-N-CA	7.67	140.88	121.70
9	C	240	PRO	N-CA-CB	6.37	110.94	103.30
9	C	395	PRO	N-CA-CB	5.93	110.42	103.30
9	C	396	PRO	N-CA-CB	5.80	110.26	103.30
1	1	43	GLY	C-N-CA	5.68	135.90	121.70
9	C	232	PRO	N-CA-CB	5.60	110.02	103.30
2	2	267	THR	N-CA-CB	5.57	120.89	110.30
9	C	422	PRO	N-CA-CB	5.52	109.93	103.30
14	K	53	PRO	N-CA-CB	5.48	109.87	103.30
1	1	241	PHE	CA-CB-CG	5.36	126.77	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	K	61	LEU	C-N-CA	5.21	134.73	121.70
9	C	430	PRO	N-CA-CB	5.21	109.55	103.30
9	C	217	TYR	CA-CB-CG	5.13	123.15	113.40
1	1	326	ILE	N-CA-CB	5.02	122.34	110.80

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	2177	0	1809	76	0
2	2	3142	0	2868	136	0
3	3	641	0	608	45	0
4	4	3017	0	2276	107	0
5	5	4065	0	3176	91	0
6	6	1078	0	1125	55	0
7	A	3226	0	1029	10	0
8	B	2013	0	839	22	0
9	C	2647	0	2375	71	0
10	E	975	0	229	1	0
11	G	880	0	581	21	0
12	H	803	0	302	7	0
13	I	857	0	563	31	0
14	K	1023	0	899	24	0
15	L	660	0	701	34	0
16	D	285	0	64	5	0
16	Z	285	0	63	3	0
17	F	270	0	60	0	0
18	J	315	0	71	1	0
19	M	145	0	36	2	0
20	N	250	0	53	2	0
21	O	350	0	75	2	0
22	P	230	0	52	2	0
23	Q	255	0	55	2	0
24	R	150	0	32	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	S	345	0	77	2	0
26	AH	75	0	17	0	0
26	T	75	0	17	0	0
27	U	130	0	29	0	0
28	V	110	0	24	2	0
29	AB	45	0	14	0	0
29	AY	45	0	11	0	0
29	BE	45	0	12	0	0
29	W	45	0	11	1	0
30	AJ	80	0	19	0	0
30	AV	80	0	19	0	0
30	BH	80	0	18	1	0
30	X	80	0	19	0	0
31	AR	65	0	16	0	0
31	AT	65	0	15	0	0
31	Y	65	0	16	0	0
32	AA	90	0	20	0	0
32	AW	90	0	24	0	0
32	BB	90	0	21	0	0
32	BG	90	0	22	0	0
33	AC	235	0	49	4	0
33	AD	235	0	52	0	0
34	AE	240	0	54	2	0
35	AF	175	0	37	0	0
36	AG	125	0	29	0	0
37	AI	180	0	39	0	0
37	AL	180	0	44	0	0
38	AK	380	0	79	0	0
38	AN	380	0	84	1	0
39	AM	85	0	20	0	0
40	AO	160	0	34	0	0
41	AP	55	0	13	0	0
41	AS	54	0	13	0	0
42	AQ	40	0	10	0	0
42	BA	40	0	10	0	0
43	AU	290	0	64	0	0
44	AX	195	0	44	0	0
45	AZ	200	0	48	1	0
46	BC	100	0	22	1	0
47	BD	95	0	22	0	0
47	BF	95	0	21	0	0
48	BI	45	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	A	4	0	0	0	0
49	H	4	0	0	1	0
50	A	16	0	0	1	0
50	B	8	0	0	0	0
50	I	16	0	0	2	0
50	K	8	0	0	2	0
All	All	35169	0	21161	682	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 12.

All (682) 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)
5:5:585:TYR:O	5:5:589:PRO:HD2	1.36	1.25
3:3:98:LEU:HD11	6:6:170:LEU:HA	1.27	1.15
13:I:175:CYS:HB2	13:I:184:ILE:HD13	1.17	1.09
12:H:217:UNK:CB	12:H:220:UNK:O	2.01	1.08
6:6:28:ASN:HB3	6:6:29:PRO:HD3	1.34	1.06
5:5:95:ILE:HD11	5:5:336:ALA:HB1	1.41	1.02
4:4:225:PHE:H	4:4:284:THR:HG22	1.27	0.99
2:2:247:TYR:HA	2:2:250:LEU:HD23	1.44	0.96
1:1:208:GLU:HA	1:1:212:VAL:O	1.68	0.94
8:B:139:GLY:HA2	8:B:142:LEU:HD12	1.48	0.92
1:1:159:MET:HG2	3:3:77:VAL:HG21	1.49	0.92
5:5:585:TYR:O	5:5:589:PRO:CD	2.16	0.92
4:4:223:PRO:HG3	4:4:231:LEU:HG	1.52	0.91
9:C:385:PHE:HA	13:I:135:LEU:HD21	1.55	0.88
2:2:209:LEU:HD23	2:2:212:ILE:HD12	1.57	0.87
4:4:280:ILE:O	4:4:284:THR:HG23	1.75	0.87
8:B:410:GLU:O	8:B:414:LEU:HG	1.75	0.86
5:5:173:MET:HB3	5:5:235:TRP:HD1	1.40	0.85
9:C:293:GLY:HA2	9:C:295:MET:N	1.92	0.85
6:6:23:ILE:HG22	6:6:35:TYR:HB3	1.59	0.85
9:C:146:SER:HA	9:C:181:THR:HG22	1.58	0.85
2:2:1:MET:HA	2:2:4:LEU:HD13	1.57	0.85
5:5:151:TYR:HB2	5:5:171:VAL:HG21	1.57	0.85
13:I:175:CYS:CB	13:I:184:ILE:HD13	2.03	0.85
11:G:168:ILE:O	11:G:168:ILE:HG22	1.77	0.85
6:6:176:PRO:HA	6:6:179:ILE:HG22	1.59	0.84
9:C:388:TYR:O	13:I:139:ILE:HB	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:98:LEU:CD1	6:6:170:LEU:HA	2.06	0.83
2:2:78:VAL:HG11	2:2:321:LEU:HD21	1.60	0.83
3:3:61:ILE:O	3:3:65:PRO:HD3	1.78	0.83
13:I:139:ILE:HG23	13:I:140:CYS:H	1.42	0.82
2:2:230:ILE:O	2:2:234:ILE:HG13	1.80	0.82
5:5:576:ALA:HA	5:5:579:VAL:HB	1.61	0.82
34:AE:2212:UNK:CB	34:AE:2227:UNK:HA	2.10	0.80
1:1:194:VAL:HG12	1:1:293:PHE:HZ	1.47	0.78
12:H:217:UNK:CB	12:H:221:UNK:HA	2.13	0.78
5:5:126:TRP:CZ3	5:5:146:ILE:HG12	2.18	0.78
1:1:213:ALA:HB1	1:1:218:GLU:H	1.46	0.77
9:C:293:GLY:HA2	9:C:296:LEU:H	1.49	0.77
3:3:98:LEU:HD13	6:6:170:LEU:HD13	1.65	0.77
2:2:67:TYR:CE1	2:2:314:THR:HG21	2.21	0.76
7:A:135:ALA:HB2	13:I:131:ILE:HG22	1.66	0.76
1:1:45:TYR:HB3	1:1:47:LEU:HG	1.66	0.75
4:4:265:LEU:HG	4:4:266:LEU:N	2.01	0.75
2:2:138:TYR:OH	15:L:73:LEU:HB2	1.86	0.75
4:4:288:THR:HG21	4:4:307:ILE:HG12	1.67	0.75
13:I:176:GLN:HA	13:I:184:ILE:HG23	1.69	0.75
2:2:71:LEU:HD21	2:2:314:THR:HA	1.68	0.74
6:6:12:THR:HG21	6:6:46:TYR:HB2	1.69	0.74
2:2:125:THR:HA	6:6:161:ILE:HD11	1.68	0.74
9:C:337:MET:HA	9:C:340:PHE:HD2	1.52	0.74
13:I:181:VAL:O	13:I:182:ASP:HB2	1.87	0.73
9:C:329:CYS:HB3	9:C:456:THR:HG21	1.70	0.73
2:2:262:ILE:O	2:2:266:LEU:HG	1.88	0.73
2:2:155:MET:HA	15:L:73:LEU:HD21	1.68	0.73
1:1:240:ALA:HA	1:1:286:LEU:HD21	1.70	0.73
1:1:235:ILE:HA	1:1:238:ILE:HG22	1.71	0.73
4:4:327:UNK:CB	4:4:397:LEU:HB3	2.18	0.72
6:6:28:ASN:HB3	6:6:29:PRO:CD	2.17	0.72
34:AE:2208:UNK:CB	34:AE:2231:UNK:HA	2.19	0.72
6:6:74:ILE:HG13	6:6:78:LEU:HD13	1.71	0.72
8:B:60:UNK:HA	8:B:138:GLU:OE2	1.89	0.72
9:C:289:LEU:HD23	11:G:173:GLU:HB2	1.71	0.72
4:4:85:UNK:O	4:4:89:UNK:CB	2.37	0.72
5:5:173:MET:HB3	5:5:235:TRP:CD1	2.24	0.72
13:I:175:CYS:HB2	13:I:184:ILE:CD1	2.10	0.71
3:3:91:VAL:O	3:3:95:LEU:HG	1.90	0.71
2:2:180:ASN:HA	15:L:47:PHE:HE2	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:247:TYR:HA	2:2:250:LEU:CD2	2.18	0.71
6:6:28:ASN:CB	6:6:29:PRO:HD3	2.18	0.71
15:L:54:LEU:O	15:L:57:ILE:HG22	1.90	0.71
1:1:240:ALA:HA	1:1:286:LEU:CD2	2.21	0.71
5:5:401:GLU:HG2	5:5:495:UNK:O	1.90	0.71
4:4:163:ALA:O	4:4:167:VAL:HG23	1.91	0.71
5:5:313:LEU:O	5:5:317:THR:HG23	1.91	0.70
2:2:208:LEU:HB3	2:2:244:ILE:HD11	1.74	0.70
2:2:173:ASN:HD21	15:L:40:LEU:HD13	1.56	0.70
4:4:450:UNK:HA	4:4:453:ILE:HD12	1.71	0.70
4:4:138:TYR:CZ	4:4:179:LEU:HB2	2.25	0.70
1:1:154:PHE:CZ	1:1:241:PHE:HE1	2.10	0.69
9:C:134:GLN:O	9:C:137:PRO:HD2	1.93	0.69
3:3:61:ILE:O	3:3:65:PRO:CD	2.41	0.69
1:1:194:VAL:HG12	1:1:293:PHE:CZ	2.26	0.69
14:K:61:LEU:HA	14:K:63:THR:H	1.56	0.69
4:4:178:MET:HB2	4:4:217:ALA:HB2	1.73	0.69
4:4:254:ALA:O	4:4:258:ILE:HG13	1.93	0.69
9:C:289:LEU:CD2	11:G:173:GLU:HB2	2.24	0.68
14:K:81:PHE:HE2	14:K:134:VAL:HG11	1.59	0.68
1:1:241:PHE:HA	1:1:244:TYR:CE2	2.28	0.68
5:5:143:TRP:HA	5:5:146:ILE:HG13	1.75	0.67
5:5:126:TRP:CH2	5:5:146:ILE:HG12	2.29	0.67
5:5:619:MET:O	5:5:620:LEU:HB2	1.94	0.67
3:3:98:LEU:HD12	6:6:173:ILE:HG12	1.74	0.67
2:2:214:ILE:HG23	2:2:268:LEU:HD22	1.77	0.67
2:2:269:LEU:O	2:2:273:VAL:HB	1.94	0.67
2:2:354:UNK:HA	2:2:361:VAL:HG21	1.75	0.67
2:2:212:ILE:HG12	2:2:244:ILE:CG2	2.25	0.66
2:2:376:PRO:HD3	4:4:142:GLU:HB2	1.77	0.66
2:2:75:ILE:HG12	2:2:238:LEU:HD23	1.76	0.66
4:4:387:PRO:HB2	5:5:141:VAL:HG13	1.78	0.66
13:I:184:ILE:HG23	13:I:184:ILE:O	1.94	0.66
8:B:413:MET:O	8:B:417:LEU:HG	1.95	0.66
4:4:400:GLN:HA	5:5:186:CYS:SG	2.36	0.65
4:4:458:ILE:O	4:4:462:LEU:HG	1.97	0.65
9:C:293:GLY:CA	9:C:296:LEU:H	2.08	0.65
5:5:341:LEU:HD11	5:5:466:ALA:HA	1.78	0.65
2:2:265:ILE:HD12	2:2:298:LEU:HG	1.79	0.65
4:4:459:ILE:O	4:4:463:ILE:HG13	1.96	0.65
13:I:181:VAL:O	13:I:182:ASP:CB	2.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:89:LEU:HB2	5:5:131:VAL:HG11	1.77	0.65
9:C:95:HIS:CG	9:C:96:GLY:H	2.15	0.65
9:C:293:GLY:HA2	9:C:295:MET:H	1.60	0.65
4:4:288:THR:HG21	4:4:307:ILE:CG1	2.26	0.64
11:G:168:ILE:O	11:G:168:ILE:CG2	2.45	0.64
1:1:149:ILE:HG12	1:1:316:LEU:HD23	1.80	0.64
2:2:213:GLY:HA3	2:2:221:LEU:HD12	1.78	0.64
6:6:70:LEU:HB3	15:L:71:LEU:HD23	1.80	0.64
5:5:364:UNK:HA	5:5:440:UNK:HA	1.80	0.64
11:G:168:ILE:HG23	11:G:171:LEU:HB3	1.79	0.64
4:4:247:ALA:HA	4:4:251:LEU:HD13	1.79	0.63
14:K:196:ARG:O	14:K:201:THR:CB	2.46	0.63
2:2:3:ILE:O	2:2:7:ILE:HG13	1.98	0.63
9:C:279:GLY:H	9:C:445:HIS:CE1	2.17	0.63
2:2:212:ILE:HG12	2:2:244:ILE:HG23	1.81	0.62
3:3:9:ILE:C	3:3:12:PRO:HD2	2.19	0.62
5:5:126:TRP:HA	5:5:129:ILE:HD12	1.81	0.62
2:2:414:LEU:HB3	4:4:165:PHE:HE2	1.64	0.62
5:5:288:UNK:CB	5:5:314:GLY:HA3	2.29	0.62
2:2:123:PHE:HB2	2:2:182:TYR:HB3	1.81	0.62
2:2:212:ILE:HG23	2:2:241:LYS:HG3	1.81	0.62
7:A:120:ASN:HD21	8:B:420:ASP:HB3	1.64	0.62
2:2:164:LEU:HB3	2:2:210:PHE:HB2	1.82	0.62
2:2:262:ILE:HG23	2:2:301:LEU:HD22	1.82	0.62
4:4:240:LEU:HD11	4:4:344:UNK:HA	1.81	0.62
6:6:101:LEU:HA	6:6:104:LEU:HD23	1.81	0.62
2:2:209:LEU:HD23	2:2:212:ILE:CD1	2.30	0.61
5:5:312:GLN:HB3	5:5:335:HIS:NE2	2.15	0.61
6:6:176:PRO:HA	6:6:179:ILE:CG2	2.29	0.61
33:AC:2012:UNK:HA	33:AC:2013:UNK:C	2.30	0.61
1:1:279:SER:HB2	22:P:711:UNK:HA	1.82	0.61
9:C:320:ASP:O	9:C:322:PRO:HD3	2.01	0.61
5:5:322:LEU:HD13	5:5:403:THR:HG22	1.83	0.61
5:5:123:PHE:HA	5:5:126:TRP:CD1	2.36	0.61
9:C:180:ILE:HD11	9:C:247:ILE:HD11	1.82	0.61
2:2:132:LEU:HG	6:6:168:VAL:HG23	1.83	0.61
2:2:139:LEU:HD11	15:L:69:ILE:HD11	1.82	0.61
4:4:152:ILE:O	4:4:156:GLY:HA3	2.01	0.61
5:5:30:UNK:HA	5:5:114:VAL:HG22	1.83	0.61
2:2:391:LEU:HD13	4:4:184:VAL:HG22	1.82	0.60
6:6:33:ILE:CD1	6:6:75:ILE:HG12	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:64:PHE:CZ	2:2:250:LEU:HD22	2.37	0.60
7:A:185:HIS:CD2	8:B:388:ARG:HD3	2.36	0.60
1:1:170:ILE:HG12	1:1:244:TYR:HB2	1.84	0.60
5:5:566:UNK:O	5:5:570:VAL:HG23	2.02	0.60
1:1:225:VAL:O	1:1:229:LEU:HB2	2.02	0.60
1:1:202:PHE:HA	1:1:205:THR:HB	1.83	0.60
2:2:262:ILE:O	2:2:265:ILE:HG12	2.01	0.60
4:4:204:LEU:HD22	4:4:268:GLU:HG2	1.84	0.60
5:5:92:ILE:HG22	5:5:124:THR:HG22	1.84	0.60
1:1:22:LEU:HG	1:1:236:ILE:HD11	1.83	0.59
33:AC:2020:UNK:HA	33:AC:2021:UNK:CB	2.32	0.59
5:5:618:SER:HB2	15:L:18:ASN:CB	2.33	0.59
14:K:117:MET:HB3	14:K:144:VAL:HG22	1.84	0.59
2:2:376:PRO:HA	4:4:139:ILE:HG22	1.85	0.59
8:B:411:ILE:HD13	8:B:449:UNK:HA	1.85	0.59
2:2:59:LEU:HB2	2:2:121:ASN:HB2	1.84	0.59
5:5:143:TRP:HH2	5:5:222:ALA:O	1.86	0.59
4:4:161:GLU:O	4:4:165:PHE:HD1	1.85	0.58
4:4:316:GLY:HA3	4:4:398:SER:HB2	1.85	0.58
5:5:370:LEU:O	5:5:373:THR:HB	2.04	0.58
14:K:111:PRO:HG3	14:K:134:VAL:HG13	1.86	0.58
2:2:138:TYR:CE2	15:L:69:ILE:HG23	2.39	0.58
5:5:633:LEU:HD11	6:6:109:LEU:HD22	1.85	0.58
2:2:164:LEU:HB3	2:2:210:PHE:CB	2.34	0.58
6:6:17:ILE:HG13	15:L:10:LEU:HD11	1.86	0.58
9:C:217:TYR:C	9:C:217:TYR:HD1	2.07	0.58
9:C:191:CYS:HB3	9:C:203:PHE:HA	1.86	0.58
4:4:143:ALA:O	4:4:146:PRO:HD2	2.04	0.58
4:4:228:HIS:HE1	4:4:287:LEU:HD13	1.69	0.58
1:1:152:SER:HB3	1:1:324:PHE:HZ	1.69	0.57
1:1:213:ALA:HB1	1:1:218:GLU:N	2.18	0.57
4:4:219:MET:HG2	4:4:224:LEU:HD12	1.85	0.57
6:6:176:PRO:HB3	15:L:72:SER:HB2	1.86	0.57
2:2:171:SER:HA	2:2:174:THR:OG1	2.04	0.57
2:2:259:UNK:O	2:2:262:ILE:HG12	2.04	0.57
14:K:199:ARG:O	14:K:200:ASN:HB2	2.03	0.57
5:5:191:VAL:HG23	5:5:211:LEU:HD23	1.85	0.57
8:B:309:UNK:HA	8:B:360:UNK:HA	1.85	0.57
1:1:314:ILE:HG12	3:3:103:VAL:HG12	1.86	0.57
2:2:231:LEU:HA	2:2:234:ILE:HD12	1.86	0.57
3:3:98:LEU:HD11	6:6:170:LEU:CA	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:187:THR:HB	13:I:188:PRO:CD	2.34	0.57
3:3:66:PHE:CE1	3:3:99:ILE:HG13	2.40	0.57
1:1:24:VAL:HG13	1:1:39:PRO:HG2	1.85	0.56
2:2:369:PHE:HD1	2:2:374:ILE:HG13	1.69	0.56
13:I:132:ALA:HB2	13:I:158:UNK:C	2.35	0.56
2:2:261:SER:O	2:2:265:ILE:HG23	2.05	0.56
4:4:364:GLY:N	4:4:433:UNK:O	2.33	0.56
5:5:308:SER:O	5:5:312:GLN:HG2	2.06	0.56
5:5:312:GLN:HB3	5:5:335:HIS:CE1	2.40	0.56
10:E:608:UNK:N	10:E:609:UNK:HA	2.19	0.56
4:4:455:ASN:O	4:4:459:ILE:HD12	2.05	0.56
1:1:201:PRO:O	1:1:205:THR:N	2.29	0.56
2:2:166:ILE:HD11	15:L:33:LEU:HG	1.87	0.56
4:4:399:LEU:HD21	4:4:414:UNK:HA	1.87	0.56
13:I:137:GLU:HG3	13:I:145:UNK:O	2.06	0.56
2:2:142:ALA:HB2	2:2:154:SER:HB2	1.88	0.56
14:K:79:VAL:HB	14:K:114:SER:OG	2.06	0.56
1:1:158:ILE:O	1:1:162:SER:N	2.39	0.56
2:2:51:THR:HB	2:2:61:PHE:HA	1.88	0.56
6:6:165:LEU:HD11	15:L:58:VAL:HG22	1.87	0.56
4:4:202:LEU:HD22	4:4:207:GLN:HG2	1.86	0.56
4:4:347:UNK:O	4:4:351:UNK:N	2.38	0.56
1:1:154:PHE:CZ	1:1:241:PHE:CE1	2.94	0.56
4:4:387:PRO:HD3	5:5:144:GLU:HB3	1.88	0.56
5:5:208:UNK:HA	5:5:209:THR:HG23	1.88	0.56
5:5:388:PRO:HA	5:5:393:TYR:HB2	1.88	0.56
2:2:299:LEU:HD11	2:2:386:ILE:HG12	1.88	0.55
1:1:28:LYS:HD3	1:1:38:GLY:H	1.70	0.55
2:2:256:UNK:O	2:2:258:UNK:N	2.39	0.55
2:2:375:PRO:HG2	4:4:138:TYR:HE2	1.71	0.55
5:5:143:TRP:CZ2	5:5:223:ALA:HA	2.40	0.55
4:4:220:VAL:HG22	4:4:227:ILE:HG21	1.87	0.55
4:4:295:GLN:HE21	4:4:300:VAL:HG11	1.72	0.55
5:5:92:ILE:HD12	5:5:127:MET:HG2	1.88	0.55
1:1:161:VAL:HG12	1:1:163:SER:H	1.71	0.55
13:I:145:UNK:HA	13:I:163:ASP:O	2.07	0.55
2:2:66:PHE:O	2:2:70:MET:HG2	2.06	0.55
2:2:149:LYS:O	2:2:227:ASN:HB3	2.07	0.55
2:2:269:LEU:HD21	2:2:298:LEU:HD11	1.89	0.55
4:4:384:ILE:HG12	4:4:421:UNK:HA	1.89	0.55
14:K:79:VAL:HG23	14:K:108:ARG:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:192:PHE:HA	14:K:195:GLN:HB2	1.88	0.55
1:1:214:GLY:HA2	14:K:109:ALA:HB3	1.88	0.55
9:C:407:LYS:HE2	9:C:460:VAL:HG23	1.89	0.55
33:AC:2013:UNK:O	33:AC:2015:UNK:N	2.39	0.55
1:1:241:PHE:HA	1:1:244:TYR:CD2	2.42	0.54
2:2:211:LYS:HE3	2:2:244:ILE:HD13	1.89	0.54
2:2:295:TYR:HE1	2:2:402:LEU:HG	1.73	0.54
22:P:716:UNK:O	22:P:720:UNK:N	2.40	0.54
1:1:34:GLN:HE22	9:C:200:LEU:HD12	1.71	0.54
2:2:173:ASN:ND2	15:L:40:LEU:HD13	2.22	0.54
2:2:372:ILE:HB	2:2:410:ALA:CB	2.38	0.54
3:3:71:SER:O	3:3:74:LEU:HB3	2.06	0.54
4:4:366:THR:HG22	4:4:373:ALA:HB1	1.90	0.54
13:I:140:CYS:SG	13:I:144:ALA:HB2	2.47	0.54
9:C:140:ASP:HB2	9:C:147:MET:HB2	1.90	0.54
2:2:234:ILE:HG12	2:2:324:PHE:CG	2.43	0.54
6:6:153:VAL:HG13	6:6:157:ASN:HB3	1.89	0.54
14:K:121:GLY:HA2	50:K:500:SF4:S4	2.47	0.54
4:4:184:VAL:HB	4:4:210:ILE:HG21	1.90	0.54
8:B:142:LEU:HD11	8:B:253:UNK:CB	2.38	0.54
2:2:131:GLU:CB	15:L:62:LEU:HD21	2.38	0.54
4:4:219:MET:O	4:4:223:PRO:HA	2.07	0.54
5:5:549:UNK:O	5:5:560:UNK:N	2.41	0.54
12:H:137:SER:HA	12:H:140:ILE:HD12	1.89	0.54
3:3:65:PRO:CB	6:6:173:ILE:HG22	2.38	0.54
4:4:467:CYS:HB3	4:4:469:GLN:HG3	1.89	0.54
5:5:136:TYR:HB2	5:5:195:UNK:O	2.07	0.54
5:5:251:HIS:ND1	5:5:309:THR:HG21	2.23	0.54
5:5:424:THR:HA	5:5:427:TYR:CE2	2.43	0.53
4:4:255:LEU:HA	4:4:258:ILE:HD12	1.90	0.53
14:K:170:ILE:HG22	14:K:171:VAL:HG23	1.90	0.53
6:6:33:ILE:HD11	6:6:75:ILE:HG12	1.90	0.53
6:6:71:PHE:HE1	15:L:26:PHE:HB2	1.71	0.53
9:C:217:TYR:C	9:C:217:TYR:CD1	2.82	0.53
4:4:274:THR:HA	4:4:277:ILE:HD12	1.90	0.53
6:6:150:ILE:HD11	15:L:53:SER:HB2	1.90	0.53
13:I:189:ASN:HD21	13:I:245:UNK:CB	2.22	0.53
11:G:176:ASN:HA	11:G:193:HIS:HE1	1.73	0.53
4:4:292:THR:HA	4:4:295:GLN:HG2	1.90	0.53
9:C:149:THR:HG21	9:C:406:PRO:HD3	1.90	0.53
1:1:49:GLN:O	1:1:53:ASP:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:297:ASP:HB3	4:4:300:VAL:HB	1.90	0.53
9:C:147:MET:HG2	9:C:148:MET:N	2.24	0.53
3:3:62:LEU:O	3:3:65:PRO:HD2	2.09	0.53
5:5:331:HIS:CE1	5:5:396:LYS:HG2	2.44	0.53
6:6:173:ILE:HG12	6:6:174:ILE:HD12	1.91	0.53
9:C:87:PHE:HB3	9:C:100:LEU:HB3	1.91	0.53
6:6:55:PHE:O	6:6:59:TYR:HB2	2.09	0.52
1:1:187:UNK:HA	1:1:246:LEU:HD13	1.90	0.52
2:2:142:ALA:HB2	2:2:154:SER:CB	2.38	0.52
7:A:75:ALA:HB3	7:A:191:ARG:HD2	1.91	0.52
8:B:411:ILE:HD11	8:B:452:UNK:CB	2.39	0.52
2:2:397:PHE:O	2:2:401:VAL:HG23	2.08	0.52
4:4:251:LEU:HD23	4:4:310:MET:HG3	1.91	0.52
9:C:262:GLU:HG3	9:C:337:MET:HG2	1.92	0.52
9:C:313:ALA:O	9:C:317:VAL:HG23	2.09	0.52
16:D:144:UNK:C	16:D:146:UNK:H	2.22	0.52
3:3:69:GLU:HB3	3:3:95:LEU:HD13	1.92	0.52
4:4:375:TYR:CZ	4:4:454:MET:HG2	2.45	0.52
8:B:384:CYS:SG	8:B:426:ILE:HB	2.49	0.52
14:K:89:GLU:HG2	14:K:182:PRO:O	2.09	0.52
3:3:2:ASN:HB2	3:3:5:ILE:HG12	1.91	0.52
5:5:18:UNK:CB	5:5:115:ARG:HA	2.40	0.52
8:B:404:UNK:O	8:B:405:UNK:CB	2.57	0.52
1:1:159:MET:HG2	3:3:77:VAL:CG2	2.32	0.52
16:Z:39:UNK:C	16:Z:41:UNK:H	2.22	0.52
1:1:326:ILE:HG23	23:Q:933:UNK:CB	2.40	0.52
1:1:315:ILE:O	1:1:318:PRO:HD2	2.10	0.52
6:6:176:PRO:HB3	15:L:72:SER:CB	2.39	0.51
2:2:215:ALA:H	2:2:268:LEU:HD13	1.74	0.51
4:4:168:LEU:O	4:4:172:LEU:HB2	2.10	0.51
4:4:252:LYS:HG3	4:4:332:UNK:CB	2.41	0.51
12:H:218:UNK:C	12:H:220:UNK:N	2.72	0.51
2:2:64:PHE:CE1	2:2:250:LEU:HD22	2.45	0.51
14:K:116:ILE:HG13	14:K:143:TRP:HB2	1.90	0.51
9:C:95:HIS:CD2	9:C:96:GLY:H	2.28	0.51
9:C:124:GLU:HB3	9:C:426:LYS:NZ	2.25	0.51
2:2:217:LEU:O	2:2:219:LYS:N	2.44	0.51
3:3:93:LEU:O	3:3:97:ILE:HD12	2.10	0.51
4:4:334:UNK:O	4:4:338:UNK:N	2.44	0.51
4:4:396:PHE:CE1	5:5:185:LEU:HB3	2.46	0.51
5:5:571:THR:O	5:5:575:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:281:UNK:CB	5:5:321:GLY:HA3	2.41	0.51
1:1:34:GLN:HE21	9:C:201:THR:HA	1.76	0.51
16:Z:13:UNK:O	16:Z:17:UNK:N	2.44	0.51
1:1:189:UNK:O	1:1:193:SER:OG	2.28	0.51
2:2:214:ILE:HD12	2:2:268:LEU:CD2	2.40	0.51
4:4:228:HIS:CE1	4:4:287:LEU:HD13	2.46	0.51
2:2:163:ILE:O	2:2:166:ILE:HG22	2.11	0.50
2:2:354:UNK:CA	2:2:361:VAL:HG21	2.40	0.50
1:1:198:ALA:HB3	1:1:235:ILE:HD11	1.93	0.50
3:3:72:THR:O	3:3:76:TYR:CD2	2.65	0.50
4:4:142:GLU:HA	4:4:145:LEU:HD13	1.93	0.50
13:I:179:CYS:HA	50:I:501:SF4:S2	2.51	0.50
2:2:57:GLU:O	2:2:121:ASN:HB3	2.12	0.50
5:5:112:HIS:O	5:5:114:VAL:N	2.45	0.50
9:C:180:ILE:HG13	9:C:347:ILE:HD12	1.93	0.50
3:3:69:GLU:HG2	3:3:95:LEU:HD22	1.94	0.50
4:4:225:PHE:CE1	4:4:287:LEU:HD12	2.46	0.50
9:C:388:TYR:HD1	13:I:139:ILE:HG21	1.77	0.50
5:5:136:TYR:H	5:5:196:UNK:HA	1.77	0.50
6:6:154:LEU:HD22	6:6:162:LEU:HB2	1.93	0.50
15:L:47:PHE:O	15:L:48:ASP:HB2	2.11	0.50
9:C:394:VAL:O	9:C:418:GLY:HA2	2.11	0.50
4:4:391:ASN:O	4:4:395:GLU:HB2	2.12	0.50
14:K:76:PHE:HB2	14:K:116:ILE:HD13	1.94	0.50
1:1:43:GLY:HA3	1:1:44:TYR:C	2.32	0.49
4:4:373:ALA:O	4:4:376:ILE:HG22	2.11	0.49
1:1:243:GLY:HA2	1:1:247:LEU:HB2	1.93	0.49
4:4:297:ASP:OD1	4:4:299:LYS:HG3	2.11	0.49
8:B:410:GLU:HA	8:B:413:MET:HB2	1.93	0.49
1:1:154:PHE:HZ	1:1:241:PHE:HE1	1.56	0.49
2:2:294:GLY:O	2:2:297:MET:HB2	2.13	0.49
2:2:296:MET:SD	2:2:313:ILE:HG12	2.52	0.49
9:C:279:GLY:H	9:C:445:HIS:HE1	1.57	0.49
15:L:39:ILE:HG13	15:L:40:LEU:N	2.27	0.49
1:1:145:SER:HB3	1:1:312:CYS:SG	2.52	0.49
1:1:281:ALA:O	1:1:285:LYS:HG2	2.12	0.49
2:2:235:TYR:O	2:2:239:ILE:HG13	2.12	0.49
5:5:92:ILE:CD1	5:5:127:MET:HG2	2.42	0.49
9:C:379:GLU:O	9:C:383:HIS:HB2	2.11	0.49
1:1:191:ILE:HG23	1:1:293:PHE:HE1	1.77	0.49
2:2:234:ILE:HG12	2:2:324:PHE:CD1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:350:UNK:O	2:2:420:UNK:HA	2.12	0.49
25:S:1133:UNK:O	25:S:1137:UNK:N	2.45	0.49
38:AN:3124:UNK:C	38:AN:3126:UNK:N	2.76	0.49
2:2:212:ILE:HG12	2:2:244:ILE:HG21	1.94	0.49
2:2:266:LEU:HD21	2:2:398:ILE:HG23	1.94	0.49
3:3:90:ILE:HA	3:3:93:LEU:HD12	1.93	0.49
14:K:126:LYS:O	14:K:129:PRO:HD2	2.13	0.49
1:1:151:THR:HA	1:1:154:PHE:HD2	1.78	0.49
2:2:118:UNK:HA	2:2:247:TYR:HB2	1.94	0.49
4:4:170:PHE:O	4:4:220:VAL:HG11	2.13	0.49
9:C:294:PRO:HA	9:C:297:ARG:HG3	1.95	0.49
1:1:143:LEU:HD23	1:1:197:THR:HG22	1.95	0.48
28:V:1417:UNK:C	28:V:1419:UNK:N	2.76	0.48
1:1:321:PHE:HA	1:1:324:PHE:CE2	2.47	0.48
3:3:96:LEU:O	3:3:100:ILE:HG13	2.13	0.48
4:4:290:LEU:HB3	5:5:573:GLY:HA2	1.95	0.48
5:5:173:MET:CB	5:5:235:TRP:HD1	2.18	0.48
9:C:446:PHE:HB3	9:C:448:PRO:HD2	1.95	0.48
1:1:321:PHE:HA	1:1:324:PHE:CD2	2.48	0.48
2:2:172:ILE:HD13	2:2:173:ASN:N	2.29	0.48
11:G:160:UNK:C	11:G:162:UNK:H	2.24	0.48
11:G:180:ARG:HH11	11:G:197:ARG:HB3	1.77	0.48
4:4:403:PHE:HA	4:4:410:UNK:CB	2.44	0.48
15:L:37:ASN:HD21	15:L:59:ILE:HB	1.78	0.48
25:S:1161:UNK:HA	25:S:1162:UNK:C	2.43	0.48
5:5:115:ARG:HB3	5:5:156:PHE:HZ	1.78	0.48
2:2:375:PRO:O	2:2:380:PHE:HB2	2.13	0.48
4:4:292:THR:CG2	4:4:304:TYR:HB3	2.44	0.48
8:B:385:THR:N	8:B:386:PRO:HD2	2.28	0.48
1:1:152:SER:HB3	1:1:324:PHE:CZ	2.47	0.48
6:6:165:LEU:HA	6:6:168:VAL:HG12	1.95	0.48
20:N:522:UNK:HA	20:N:524:UNK:N	2.28	0.48
2:2:1:MET:HG2	2:2:4:LEU:HD22	1.94	0.47
5:5:187:VAL:HG21	5:5:214:LEU:HD22	1.96	0.47
2:2:138:TYR:HB2	2:2:157:TYR:HB3	1.95	0.47
2:2:153:ALA:HB1	2:2:224:ILE:HG12	1.95	0.47
1:1:323:ILE:O	1:1:326:ILE:HG13	2.15	0.47
3:3:71:SER:O	3:3:75:PRO:HD3	2.13	0.47
4:4:225:PHE:CD1	4:4:283:LEU:HB3	2.49	0.47
4:4:292:THR:HG22	4:4:304:TYR:HB3	1.95	0.47
7:A:486:UNK:O	7:A:490:UNK:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:46:PHE:HB3	2:2:62:ASN:HB3	1.96	0.47
2:2:47:LEU:HB2	2:2:50:GLN:HG3	1.95	0.47
4:4:255:LEU:HG	4:4:317:VAL:HG21	1.97	0.47
9:C:293:GLY:HA2	9:C:296:LEU:N	2.26	0.47
1:1:295:TRP:HE3	13:I:87:LEU:HD22	1.78	0.47
2:2:295:TYR:CE1	2:2:402:LEU:HG	2.50	0.47
4:4:323:LEU:HD11	4:4:401:GLY:HA3	1.96	0.47
13:I:137:GLU:HA	13:I:144:ALA:HB3	1.96	0.47
1:1:226:PHE:HE1	3:3:16:PHE:HB3	1.79	0.47
2:2:67:TYR:HE1	2:2:314:THR:HG21	1.77	0.47
16:D:108:UNK:HA	16:D:109:UNK:HA	1.75	0.47
2:2:138:TYR:HE1	15:L:73:LEU:HD13	1.78	0.47
5:5:79:PHE:CE1	5:5:138:VAL:HG11	2.50	0.47
2:2:131:GLU:HB3	15:L:62:LEU:HD21	1.97	0.47
3:3:76:TYR:O	3:3:80:ILE:HG23	2.15	0.47
3:3:99:ILE:HA	3:3:102:PHE:HD2	1.80	0.47
6:6:29:PRO:O	6:6:33:ILE:HG13	2.15	0.47
4:4:228:HIS:O	4:4:231:LEU:HB2	2.15	0.46
5:5:153:LEU:HB3	5:5:246:VAL:HG11	1.97	0.46
1:1:30:LEU:HD23	1:1:298:ALA:HB2	1.97	0.46
2:2:245:LEU:O	2:2:249:VAL:HG23	2.15	0.46
2:2:279:ILE:HB	2:2:280:LYS:HE2	1.95	0.46
3:3:97:ILE:HG22	6:6:170:LEU:HD11	1.96	0.46
4:4:298:LEU:HD21	4:4:357:UNK:O	2.14	0.46
5:5:468:PHE:HA	5:5:472:ALA:HB3	1.96	0.46
9:C:92:PRO:HG2	9:C:98:LEU:HD13	1.97	0.46
2:2:295:TYR:O	2:2:298:LEU:HB2	2.16	0.46
4:4:312:ILE:HG12	4:4:399:LEU:HD13	1.97	0.46
5:5:99:VAL:HG11	5:5:249:LEU:HD13	1.96	0.46
11:G:168:ILE:HG23	11:G:171:LEU:HD23	1.98	0.46
2:2:372:ILE:HB	2:2:410:ALA:HB2	1.97	0.46
4:4:222:THR:HB	4:4:314:ILE:HD11	1.96	0.46
4:4:229:VAL:HG13	5:5:584:LEU:HG	1.98	0.46
4:4:263:LEU:O	4:4:267:CYS:SG	2.69	0.46
5:5:322:LEU:O	5:5:323:SER:HB2	2.14	0.46
13:I:171:TYR:HA	50:I:500:SF4:S1	2.55	0.46
5:5:589:PRO:HA	5:5:592:ILE:HB	1.97	0.46
13:I:179:CYS:SG	13:I:183:ALA:HB3	2.55	0.46
14:K:84:ALA:HB3	50:K:500:SF4:S4	2.56	0.46
1:1:28:LYS:HG2	1:1:39:PRO:HD2	1.97	0.46
1:1:196:GLU:HG3	1:1:308:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:301:UNK:C	9:C:198:GLY:HA2	2.46	0.46
2:2:239:ILE:HG13	2:2:239:ILE:H	1.48	0.46
4:4:178:MET:HB2	4:4:217:ALA:CB	2.43	0.46
4:4:294:ARG:O	4:4:296:ILE:N	2.49	0.46
4:4:456:ILE:HG23	4:4:457:LEU:HD23	1.98	0.46
5:5:221:ILE:HA	5:5:224:MET:HG2	1.98	0.46
9:C:190:VAL:HG21	9:C:340:PHE:HE2	1.81	0.46
14:K:93:VAL:HG21	14:K:187:LEU:HD23	1.98	0.46
3:3:98:LEU:HD22	6:6:170:LEU:HD22	1.97	0.46
5:5:33:UNK:CB	5:5:114:VAL:HG13	2.46	0.46
5:5:361:UNK:HA	5:5:434:LEU:HD23	1.96	0.46
9:C:200:LEU:HD23	9:C:200:LEU:H	1.80	0.46
15:L:16:VAL:HA	15:L:17:PHE:C	2.36	0.46
2:2:235:TYR:CE1	2:2:239:ILE:HG12	2.51	0.46
2:2:8:SER:O	2:2:12:PHE:HD2	1.98	0.46
2:2:351:UNK:HA	2:2:419:UNK:O	2.16	0.46
4:4:295:GLN:HG3	4:4:300:VAL:HG12	1.97	0.46
2:2:149:LYS:HB3	2:2:227:ASN:HA	1.97	0.45
2:2:384:LEU:O	2:2:388:MET:HB2	2.15	0.45
5:5:180:PHE:HB3	5:5:222:ALA:HB2	1.98	0.45
7:A:370:UNK:HA	7:A:371:UNK:CB	2.46	0.45
9:C:139:PHE:CZ	9:C:427:ILE:HG12	2.52	0.45
1:1:196:GLU:HA	1:1:201:PRO:HG3	1.98	0.45
5:5:62:UNK:N	5:5:79:PHE:O	2.49	0.45
5:5:83:ALA:O	5:5:86:ILE:HG13	2.16	0.45
1:1:166:ILE:HA	1:1:169:ILE:HD12	1.98	0.45
3:3:80:ILE:HB	3:3:81:TYR:H	1.56	0.45
4:4:230:TRP:CE3	4:4:234:VAL:HG21	2.51	0.45
5:5:143:TRP:HZ2	5:5:223:ALA:HA	1.80	0.45
8:B:94:SER:HA	8:B:97:LYS:HB3	1.98	0.45
3:3:53:UNK:O	3:3:55:UNK:N	2.49	0.45
5:5:478:UNK:HA	5:5:479:UNK:C	2.46	0.45
9:C:368:SER:C	9:C:370:PRO:HD3	2.37	0.45
14:K:112:ARG:HA	14:K:139:PRO:HD3	1.99	0.45
2:2:206:LEU:HA	2:2:209:LEU:HD12	1.98	0.45
3:3:19:UNK:O	3:3:21:UNK:N	2.50	0.45
3:3:60:ALA:O	6:6:70:LEU:HD21	2.17	0.45
4:4:224:LEU:HD23	4:4:284:THR:HG21	1.98	0.45
5:5:188:ILE:O	5:5:191:VAL:HG12	2.16	0.45
1:1:304:UNK:O	1:1:306:ASP:N	2.49	0.45
5:5:357:UNK:C	5:5:359:UNK:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:196:GLU:HA	1:1:201:PRO:CG	2.47	0.45
2:2:262:ILE:HG23	2:2:301:LEU:CD2	2.47	0.45
4:4:162:ARG:O	4:4:166:TYR:HB2	2.16	0.45
11:G:180:ARG:HB3	11:G:199:ILE:HD11	1.98	0.45
12:H:131:PRO:HD2	49:H:300:FES:S2	2.56	0.45
1:1:34:GLN:HB3	9:C:204:LEU:HD22	1.99	0.45
4:4:240:LEU:CD1	4:4:344:UNK:HA	2.46	0.45
6:6:44:ALA:HB1	6:6:56:SER:HB3	1.98	0.45
1:1:218:GLU:O	1:1:220:UNK:N	2.49	0.45
3:3:77:VAL:O	3:3:80:ILE:HG13	2.16	0.45
5:5:383:SER:HB3	5:5:391:THR:HG22	1.99	0.45
8:B:398:UNK:CB	8:B:414:LEU:HD22	2.47	0.45
2:2:298:LEU:HD21	2:2:398:ILE:HG22	1.99	0.45
4:4:323:LEU:CD1	4:4:401:GLY:HA3	2.47	0.45
5:5:189:ALA:O	5:5:193:GLY:N	2.48	0.45
9:C:212:LYS:HD3	9:C:250:TRP:HD1	1.82	0.45
3:3:106:UNK:O	3:3:107:UNK:O	2.35	0.44
9:C:279:GLY:HA2	9:C:453:ILE:HD11	1.99	0.44
1:1:230:ALA:O	1:1:234:ASN:HB2	2.17	0.44
2:2:64:PHE:CE2	2:2:250:LEU:HD13	2.52	0.44
5:5:228:ALA:HB2	5:5:235:TRP:HB3	1.99	0.44
9:C:183:VAL:HG11	9:C:250:TRP:HZ2	1.81	0.44
2:2:278:GLN:HG2	2:2:280:LYS:HE3	1.98	0.44
2:2:310:LEU:O	2:2:314:THR:HG23	2.16	0.44
4:4:161:GLU:O	4:4:165:PHE:CD1	2.69	0.44
4:4:265:LEU:CG	4:4:266:LEU:N	2.74	0.44
4:4:452:PHE:HA	4:4:455:ASN:HB2	1.98	0.44
5:5:101:ILE:HD12	5:5:461:PRO:HB3	1.99	0.44
11:G:99:UNK:CB	11:G:156:UNK:HA	2.47	0.44
5:5:123:PHE:CE1	5:5:253:ALA:HB2	2.53	0.44
1:1:29:THR:HB	1:1:294:ILE:HG21	1.99	0.44
1:1:210:GLU:HG2	1:1:211:LEU:HG	1.98	0.44
2:2:302:LEU:HD23	2:2:303:ASN:N	2.33	0.44
3:3:82:LEU:CB	3:3:83:VAL:HB	2.46	0.44
13:I:187:THR:HB	13:I:188:PRO:HD3	1.98	0.44
2:2:166:ILE:CD1	15:L:33:LEU:HG	2.48	0.44
5:5:166:SER:HB2	5:5:238:LEU:O	2.17	0.44
5:5:634:VAL:O	5:5:638:ASN:N	2.51	0.44
9:C:407:LYS:HE3	9:C:458:ASP:OD1	2.18	0.44
5:5:339:LYS:HD2	5:5:339:LYS:HA	1.73	0.44
5:5:480:UNK:HA	5:5:481:UNK:HA	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:33:LEU:O	15:L:36:ILE:HG22	2.18	0.44
6:6:147:LEU:C	6:6:149:THR:H	2.21	0.44
4:4:259:LEU:HD12	4:4:260:ARG:HD2	1.99	0.43
5:5:318:ILE:O	5:5:322:LEU:HB2	2.18	0.43
6:6:79:ASP:HB3	15:L:78:TYR:OH	2.18	0.43
13:I:160:THR:HG23	13:I:161:LYS:HG2	2.01	0.43
28:V:1403:UNK:C	28:V:1405:UNK:N	2.81	0.43
2:2:159:PHE:O	2:2:163:ILE:HG13	2.18	0.43
9:C:185:ASN:HB3	9:C:406:PRO:HG2	1.99	0.43
16:D:134:UNK:O	16:D:136:UNK:N	2.51	0.43
1:1:194:VAL:HG22	1:1:238:ILE:HG12	2.00	0.43
4:4:76:UNK:H	4:4:139:ILE:HD11	1.83	0.43
6:6:96:LEU:HD22	6:6:96:LEU:H	1.84	0.43
9:C:388:TYR:CD1	13:I:178:SER:HB3	2.52	0.43
6:6:71:PHE:HA	6:6:74:ILE:HG22	1.99	0.43
8:B:48:UNK:HA	8:B:132:ASP:OD1	2.18	0.43
2:2:211:LYS:O	2:2:221:LEU:HD11	2.18	0.43
2:2:310:LEU:HD13	2:2:310:LEU:HA	1.92	0.43
4:4:468:PRO:HB2	4:4:471:MET:HG2	2.00	0.43
6:6:13:ILE:H	6:6:13:ILE:HG13	1.63	0.43
6:6:27:LYS:HA	6:6:28:ASN:HA	1.42	0.43
15:L:23:ILE:H	15:L:23:ILE:HG13	1.56	0.43
30:BH:5106:UNK:O	30:BH:5108:UNK:N	2.52	0.43
2:2:287:PHE:O	2:2:291:THR:HG23	2.18	0.43
4:4:460:SER:HA	4:4:463:ILE:HD12	2.01	0.43
5:5:151:TYR:HB2	5:5:171:VAL:CG2	2.39	0.43
6:6:95:PRO:HG2	6:6:96:LEU:HD22	2.00	0.43
9:C:191:CYS:SG	9:C:206:GLY:HA3	2.59	0.43
14:K:61:LEU:HA	14:K:63:THR:N	2.31	0.43
16:D:107:UNK:HA	16:D:108:UNK:HA	1.72	0.43
45:AZ:4325:UNK:C	45:AZ:4327:UNK:H	2.30	0.43
2:2:211:LYS:HB2	2:2:244:ILE:HG21	2.01	0.43
3:3:62:LEU:C	3:3:65:PRO:HD2	2.38	0.43
4:4:165:PHE:CD1	4:4:165:PHE:N	2.86	0.43
5:5:175:ARG:HA	5:5:178:ASP:HB2	2.01	0.43
5:5:255:UNK:O	5:5:332:LEU:HD11	2.19	0.43
1:1:41:PHE:O	1:1:43:GLY:N	2.52	0.43
2:2:213:GLY:O	2:2:218:HIS:HA	2.19	0.43
8:B:409:ARG:O	8:B:413:MET:N	2.52	0.43
9:C:174:ARG:HH21	9:C:234:GLY:HA2	1.84	0.43
3:3:99:ILE:O	3:3:103:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:260:ARG:NE	4:4:260:ARG:HA	2.33	0.42
8:B:336:UNK:O	8:B:340:UNK:N	2.51	0.42
11:G:202:ASP:HA	14:K:126:LYS:HD2	2.01	0.42
20:N:519:UNK:HA	20:N:520:UNK:HA	1.84	0.42
2:2:7:ILE:HG13	2:2:7:ILE:H	1.50	0.42
2:2:399:SER:O	2:2:402:LEU:HB3	2.19	0.42
3:3:95:LEU:O	3:3:98:LEU:HB2	2.18	0.42
5:5:136:TYR:O	5:5:140:PHE:HD2	2.01	0.42
7:A:184:ILE:HG22	7:A:184:ILE:O	2.19	0.42
2:2:238:LEU:HD22	2:2:320:HIS:CE1	2.55	0.42
4:4:113:UNK:O	4:4:117:UNK:CB	2.68	0.42
11:G:165:VAL:O	11:G:190:PHE:HA	2.19	0.42
12:H:218:UNK:O	12:H:219:UNK:C	2.66	0.42
3:3:82:LEU:HB2	3:3:83:VAL:HB	2.01	0.42
4:4:180:LEU:O	4:4:184:VAL:HG23	2.19	0.42
8:B:385:THR:HG22	8:B:388:ARG:HH12	1.83	0.42
9:C:97:VAL:HG13	9:C:98:LEU:H	1.85	0.42
9:C:337:MET:O	9:C:340:PHE:HB2	2.19	0.42
1:1:21:TYR:HE2	1:1:47:LEU:HD22	1.84	0.42
1:1:326:ILE:CG2	23:Q:933:UNK:CB	2.97	0.42
2:2:66:PHE:HD2	2:2:70:MET:HE1	1.84	0.42
2:2:368:VAL:O	2:2:372:ILE:HG23	2.19	0.42
2:2:373:GLY:O	2:2:375:PRO:HD3	2.20	0.42
4:4:289:SER:O	4:4:292:THR:OG1	2.37	0.42
9:C:305:ILE:HB	9:C:404:GLU:HB2	2.01	0.42
2:2:74:PHE:O	2:2:78:VAL:HG23	2.19	0.42
4:4:208:THR:HA	4:4:269:ALA:HB2	2.02	0.42
9:C:311:TYR:HB2	9:C:312:ASP:H	1.73	0.42
9:C:337:MET:HA	9:C:340:PHE:CD2	2.43	0.42
11:G:123:UNK:HA	11:G:132:UNK:CB	2.49	0.42
21:O:615:UNK:C	21:O:617:UNK:N	2.83	0.42
1:1:152:SER:O	1:1:156:ILE:HG23	2.19	0.42
3:3:77:VAL:HA	3:3:88:PHE:HZ	1.85	0.42
11:G:193:HIS:HA	11:G:194:PRO:HD3	1.97	0.42
33:AC:2035:UNK:C	33:AC:2037:UNK:N	2.83	0.42
12:H:129:THR:HG21	12:H:168:CYS:HB2	2.01	0.42
29:W:1504:UNK:O	29:W:1506:UNK:N	2.53	0.42
2:2:71:LEU:O	2:2:75:ILE:HD12	2.19	0.42
4:4:214:LEU:HD23	4:4:261:LEU:HB3	2.01	0.42
6:6:63:TYR:HE2	15:L:34:LEU:HB2	1.85	0.42
9:C:465:ASP:HA	11:G:200:MET:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:140:ILE:HD13	2:2:235:TYR:HE2	1.85	0.42
2:2:153:ALA:HA	2:2:156:LEU:HB2	2.01	0.42
2:2:236:ILE:O	2:2:240:PRO:HD2	2.19	0.42
2:2:238:LEU:HD22	2:2:320:HIS:ND1	2.35	0.42
6:6:13:ILE:HG12	15:L:3:ILE:HG12	2.01	0.42
2:2:281:ILE:HD12	2:2:326:ILE:HD11	2.02	0.41
4:4:153:HIS:HB2	4:4:164:SER:OG	2.20	0.41
16:Z:55:UNK:N	16:Z:56:UNK:HA	2.35	0.41
1:1:148:LEU:HD21	3:3:70:ILE:HD13	2.01	0.41
2:2:61:PHE:HB3	2:2:64:PHE:HE2	1.85	0.41
6:6:145:THR:HA	6:6:146:LEU:HA	1.89	0.41
7:A:185:HIS:HB2	8:B:388:ARG:NH1	2.34	0.41
9:C:184:LEU:HD12	9:C:213:LEU:HB2	2.02	0.41
9:C:208:GLU:H	9:C:208:GLU:HG3	1.75	0.41
5:5:370:LEU:HB2	5:5:373:THR:OG1	2.19	0.41
7:A:188:ARG:HB2	50:A:902:SF4:S3	2.59	0.41
11:G:168:ILE:CG2	11:G:171:LEU:HB3	2.50	0.41
11:G:190:PHE:HB2	11:G:196:LEU:HD21	2.02	0.41
13:I:140:CYS:CB	13:I:144:ALA:HB2	2.50	0.41
1:1:56:LYS:HG3	14:K:72:ARG:HG2	2.02	0.41
2:2:180:ASN:HA	15:L:47:PHE:CE2	2.45	0.41
4:4:165:PHE:HD1	4:4:165:PHE:H	1.68	0.41
9:C:258:LEU:CD1	9:C:340:PHE:HB3	2.50	0.41
9:C:318:ASP:HB2	9:C:349:GLN:HE22	1.84	0.41
13:I:176:GLN:CA	13:I:184:ILE:HG23	2.46	0.41
2:2:75:ILE:HD13	2:2:242:ILE:CD1	2.50	0.41
2:2:139:LEU:HD23	6:6:179:ILE:HD12	2.01	0.41
4:4:171:THR:HG22	4:4:221:LYS:HE3	2.02	0.41
7:A:186:CYS:SG	7:A:188:ARG:HG3	2.60	0.41
9:C:216:PHE:HE1	9:C:243:LEU:HD12	1.86	0.41
9:C:343:SER:O	9:C:347:ILE:HG12	2.20	0.41
11:G:72:HIS:HA	11:G:89:PHE:HE2	1.84	0.41
21:O:647:UNK:O	21:O:651:UNK:N	2.53	0.41
1:1:27:ARG:HD2	1:1:39:PRO:HG3	2.01	0.41
2:2:209:LEU:HB3	2:2:214:ILE:HG12	2.03	0.41
11:G:190:PHE:O	11:G:196:LEU:HD11	2.21	0.41
13:I:132:ALA:HA	13:I:159:THR:HG23	2.02	0.41
3:3:91:VAL:HG13	6:6:166:ALA:HB2	2.03	0.41
4:4:468:PRO:CB	4:4:471:MET:HG2	2.51	0.41
5:5:494:UNK:O	5:5:497:UNK:O	2.38	0.41
19:M:414:UNK:C	19:M:416:UNK:N	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:M:421:UNK:O	19:M:426:UNK:N	2.54	0.41
1:1:199:ARG:HH21	1:1:231:GLU:HG2	1.86	0.41
3:3:40:UNK:HA	14:K:133:GLN:HB3	2.03	0.41
4:4:145:LEU:HD23	4:4:168:LEU:HD12	2.02	0.41
9:C:95:HIS:CG	9:C:96:GLY:N	2.84	0.41
16:D:114:UNK:C	16:D:116:UNK:N	2.84	0.41
1:1:152:SER:O	1:1:155:ILE:HG13	2.21	0.41
1:1:315:ILE:C	1:1:318:PRO:HD2	2.41	0.41
2:2:403:ILE:HD11	4:4:180:LEU:HB2	2.01	0.41
5:5:211:LEU:O	5:5:215:ILE:HD12	2.21	0.41
6:6:18:LEU:O	6:6:21:ILE:HG22	2.20	0.41
13:I:170:ILE:O	13:I:170:ILE:HG22	2.21	0.41
18:J:352:UNK:C	18:J:354:UNK:N	2.84	0.41
3:3:69:GLU:HG3	6:6:169:LEU:HD22	2.02	0.41
9:C:90:GLN:O	9:C:92:PRO:HD3	2.20	0.41
15:L:71:LEU:O	15:L:75:VAL:HG23	2.21	0.41
1:1:148:LEU:HD22	1:1:317:LEU:HD11	2.03	0.40
5:5:140:PHE:CD1	5:5:181:PHE:CD2	3.09	0.40
6:6:70:LEU:HB3	15:L:71:LEU:CD2	2.50	0.40
13:I:184:ILE:O	13:I:184:ILE:CG2	2.64	0.40
2:2:247:TYR:CA	2:2:250:LEU:HD23	2.32	0.40
8:B:97:LYS:HA	8:B:100:PHE:HD2	1.86	0.40
9:C:305:ILE:HD11	9:C:409:GLU:HG3	2.03	0.40
14:K:83:LEU:HB2	14:K:121:GLY:HA3	2.04	0.40
15:L:5:THR:HA	15:L:8:LEU:HD12	2.03	0.40
2:2:130:ILE:HG13	2:2:211:LYS:HE2	2.03	0.40
2:2:142:ALA:CB	6:6:179:ILE:HD11	2.50	0.40
6:6:165:LEU:HD23	6:6:168:VAL:HG11	2.02	0.40
9:C:148:MET:H	9:C:181:THR:HG21	1.85	0.40
9:C:287:LEU:HD22	11:G:117:UNK:CB	2.51	0.40
46:BC:4609:UNK:O	46:BC:4613:UNK:N	2.54	0.40
2:2:212:ILE:H	2:2:212:ILE:HG13	1.45	0.40
4:4:79:UNK:HA	4:4:131:UNK:HA	2.04	0.40
4:4:294:ARG:HB2	5:5:574:ASN:HA	2.02	0.40
6:6:92:ARG:O	6:6:95:PRO:HD2	2.22	0.40
9:C:342:GLN:O	9:C:346:ILE:HG12	2.22	0.40
2:2:266:LEU:HD22	2:2:401:VAL:HG11	2.02	0.40
4:4:236:SER:HB2	4:4:299:LYS:HD2	2.03	0.40
4:4:373:ALA:O	4:4:377:ILE:HG12	2.22	0.40
5:5:323:SER:O	5:5:325:TYR:N	2.55	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	202/327 (62%)	166 (82%)	30 (15%)	6 (3%)	4 33
2	2	320/438 (73%)	278 (87%)	31 (10%)	11 (3%)	3 31
3	3	64/89 (72%)	54 (84%)	7 (11%)	3 (5%)	2 22
4	4	243/470 (52%)	212 (87%)	24 (10%)	7 (3%)	4 33
5	5	356/619 (58%)	295 (83%)	46 (13%)	15 (4%)	3 25
6	6	141/185 (76%)	118 (84%)	14 (10%)	9 (6%)	1 17
7	A	63/628 (10%)	55 (87%)	5 (8%)	3 (5%)	2 22
8	B	72/370 (20%)	67 (93%)	5 (7%)	0	100 100
9	C	348/444 (78%)	303 (87%)	27 (8%)	18 (5%)	2 20
11	G	65/133 (49%)	55 (85%)	8 (12%)	2 (3%)	4 32
12	H	30/154 (20%)	28 (93%)	1 (3%)	1 (3%)	4 31
13	I	64/137 (47%)	47 (73%)	11 (17%)	6 (9%)	0 8
14	K	141/183 (77%)	126 (89%)	12 (8%)	3 (2%)	7 40
15	L	87/89 (98%)	72 (83%)	6 (7%)	9 (10%)	0 7
All	All	2196/4266 (52%)	1876 (85%)	227 (10%)	93 (4%)	3 25

All (93) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	42	VAL
1	1	44	TYR
1	1	45	TYR
1	1	199	ARG
1	1	212	VAL
1	1	217	THR
2	2	43	TYR
2	2	123	PHE
2	2	218	HIS

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Mol	Chain	Res	Type
3	3	83	VAL
4	4	158	SER
4	4	203	SER
4	4	208	THR
4	4	295	GLN
5	5	113	GLN
5	5	620	LEU
6	6	9	ILE
6	6	28	ASN
6	6	80	ILE
6	6	90	ASN
9	C	97	VAL
9	C	98	LEU
9	C	239	LEU
9	C	240	PRO
9	C	294	PRO
9	C	368	SER
11	G	191	GLU
13	I	139	ILE
13	I	140	CYS
13	I	179	CYS
13	I	182	ASP
14	K	57	VAL
14	K	60	THR
14	K	203	ILE
15	L	22	ILE
15	L	50	ILE
15	L	86	SER
2	2	51	THR
2	2	62	ASN
2	2	230	ILE
2	2	327	ILE
5	5	235	TRP
5	5	324	ALA
5	5	396	LYS
5	5	649	ILE
5	5	653	LEU
6	6	149	THR
6	6	150	ILE
7	A	133	CYS
7	A	187	THR
9	C	93	ALA

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Mol	Chain	Res	Type
9	C	327	GLY
11	G	83	PRO
13	I	81	ALA
13	I	171	TYR
15	L	87	TYR
2	2	52	TYR
2	2	300	LEU
3	3	4	PHE
4	4	202	LEU
4	4	229	VAL
5	5	209	THR
5	5	323	SER
5	5	619	MET
5	5	639	PHE
6	6	81	ASN
7	A	134	ALA
9	C	269	ARG
9	C	313	ALA
9	C	362	GLU
9	C	370	PRO
15	L	48	ASP
15	L	49	ASP
15	L	85	ASN
5	5	133	GLY
5	5	346	ALA
6	6	147	LEU
9	C	302	PRO
2	2	180	ASN
3	3	8	ILE
6	6	181	MET
9	C	101	ILE
9	C	201	THR
9	C	369	PRO
15	L	17	PHE
4	4	225	PHE
5	5	641	ILE
2	2	162	GLY
12	H	130	THR
9	C	234	GLY
9	C	355	PRO
5	5	634	VAL
15	L	88	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	175/186 (94%)	129 (74%)	46 (26%)	0 4
2	2	291/291 (100%)	220 (76%)	71 (24%)	0 4
3	3	60/60 (100%)	42 (70%)	18 (30%)	0 2
4	4	215/215 (100%)	163 (76%)	52 (24%)	0 4
5	5	301/305 (99%)	225 (75%)	76 (25%)	0 4
6	6	110/167 (66%)	73 (66%)	37 (34%)	0 1
7	A	39/40 (98%)	36 (92%)	3 (8%)	13 45
8	B	53/56 (95%)	50 (94%)	3 (6%)	20 55
9	C	238/371 (64%)	203 (85%)	35 (15%)	3 20
11	G	55/55 (100%)	53 (96%)	2 (4%)	35 67
12	H	19/19 (100%)	18 (95%)	1 (5%)	22 58
13	I	55/55 (100%)	44 (80%)	11 (20%)	1 8
14	K	91/157 (58%)	74 (81%)	17 (19%)	1 10
15	L	69/77 (90%)	46 (67%)	23 (33%)	0 2
All	All	1771/2054 (86%)	1376 (78%)	395 (22%)	1 6

All (395) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	3	ILE
1	1	11	PHE
1	1	14	CYS
1	1	22	LEU
1	1	33	MET
1	1	35	ARG
1	1	42	VAL
1	1	53	ASP
1	1	137	ILE
1	1	142	GLN
1	1	144	ILE

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Mol	Chain	Res	Type
1	1	147	GLU
1	1	150	LEU
1	1	151	THR
1	1	152	SER
1	1	155	ILE
1	1	156	ILE
1	1	157	ILE
1	1	162	SER
1	1	164	LEU
1	1	165	ASN
1	1	193	SER
1	1	196	GLU
1	1	197	THR
1	1	199	ARG
1	1	204	LEU
1	1	206	GLU
1	1	208	GLU
1	1	211	LEU
1	1	215	TYR
1	1	217	THR
1	1	229	LEU
1	1	241	PHE
1	1	247	LEU
1	1	276	LEU
1	1	277	ILE
1	1	278	ASN
1	1	279	SER
1	1	284	ILE
1	1	289	LEU
1	1	291	PHE
1	1	295	TRP
1	1	312	CYS
1	1	319	LEU
1	1	321	PHE
1	1	323	ILE
2	2	1	MET
2	2	2	LEU
2	2	3	ILE
2	2	7	ILE
2	2	8	SER
2	2	16	SER
2	2	17	LYS

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Mol	Chain	Res	Type
2	2	18	LEU
2	2	25	ILE
2	2	45	LEU
2	2	48	ASN
2	2	49	ASN
2	2	58	LEU
2	2	67	TYR
2	2	68	ILE
2	2	80	SER
2	2	125	THR
2	2	132	LEU
2	2	138	TYR
2	2	141	THR
2	2	143	ILE
2	2	145	ASN
2	2	156	LEU
2	2	171	SER
2	2	172	ILE
2	2	173	ASN
2	2	174	THR
2	2	178	VAL
2	2	187	LEU
2	2	188	ASP
2	2	196	ASP
2	2	197	LEU
2	2	204	LEU
2	2	212	ILE
2	2	219	LYS
2	2	224	ILE
2	2	232	ILE
2	2	233	THR
2	2	239	ILE
2	2	241	LYS
2	2	242	ILE
2	2	250	LEU
2	2	261	SER
2	2	267	THR
2	2	269	LEU
2	2	276	LEU
2	2	277	LEU
2	2	278	GLN
2	2	280	LYS

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Mol	Chain	Res	Type
2	2	282	LYS
2	2	283	ARG
2	2	288	SER
2	2	298	LEU
2	2	300	LEU
2	2	304	ASN
2	2	307	PHE
2	2	310	LEU
2	2	311	TYR
2	2	314	THR
2	2	319	SER
2	2	321	LEU
2	2	328	ILE
2	2	362	LEU
2	2	363	SER
2	2	367	VAL
2	2	370	SER
2	2	371	PHE
2	2	377	LEU
2	2	378	LEU
2	2	412	TYR
2	2	413	TYR
3	3	2	ASN
3	3	5	ILE
3	3	6	ILE
3	3	7	PHE
3	3	57	ILE
3	3	58	LEU
3	3	68	LEU
3	3	73	LEU
3	3	74	LEU
3	3	77	VAL
3	3	78	MET
3	3	81	TYR
3	3	83	VAL
3	3	85	ASN
3	3	88	PHE
3	3	90	ILE
3	3	98	LEU
3	3	102	PHE
4	4	136	SER
4	4	139	ILE

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Mol	Chain	Res	Type
4	4	144	THR
4	4	150	ILE
4	4	166	TYR
4	4	169	MET
4	4	172	LEU
4	4	180	LEU
4	4	182	ILE
4	4	185	ILE
4	4	201	VAL
4	4	203	SER
4	4	205	ASP
4	4	206	LEU
4	4	216	ILE
4	4	227	ILE
4	4	231	LEU
4	4	233	VAL
4	4	237	GLU
4	4	259	LEU
4	4	260	ARG
4	4	263	LEU
4	4	265	LEU
4	4	267	CYS
4	4	276	MET
4	4	280	ILE
4	4	281	SER
4	4	282	LEU
4	4	286	ILE
4	4	287	LEU
4	4	296	ILE
4	4	298	LEU
4	4	299	LYS
4	4	301	ILE
4	4	302	ILE
4	4	306	SER
4	4	307	ILE
4	4	320	ASN
4	4	323	LEU
4	4	325	ILE
4	4	372	LEU
4	4	397	LEU
4	4	404	ILE
4	4	405	ARG

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Mol	Chain	Res	Type
4	4	454	MET
4	4	455	ASN
4	4	457	LEU
4	4	458	ILE
4	4	461	THR
4	4	464	ILE
4	4	466	ILE
4	4	467	CYS
5	5	82	ASP
5	5	84	LEU
5	5	86	ILE
5	5	88	MET
5	5	89	LEU
5	5	103	SER
5	5	104	ILE
5	5	108	GLU
5	5	112	HIS
5	5	116	PHE
5	5	120	LEU
5	5	124	THR
5	5	136	TYR
5	5	137	PHE
5	5	138	VAL
5	5	139	LEU
5	5	143	TRP
5	5	145	PHE
5	5	160	ARG
5	5	161	LEU
5	5	162	GLN
5	5	176	PHE
5	5	181	PHE
5	5	185	LEU
5	5	188	ILE
5	5	191	VAL
5	5	209	THR
5	5	210	ASP
5	5	212	LEU
5	5	215	ILE
5	5	216	MET
5	5	217	LEU
5	5	230	PHE
5	5	233	HIS

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Mol	Chain	Res	Type
5	5	234	ASN
5	5	236	LEU
5	5	313	LEU
5	5	318	ILE
5	5	320	ILE
5	5	322	LEU
5	5	327	LEU
5	5	329	LEU
5	5	330	PHE
5	5	331	HIS
5	5	332	LEU
5	5	342	LEU
5	5	372	TYR
5	5	383	SER
5	5	390	LEU
5	5	394	TYR
5	5	399	ILE
5	5	418	TYR
5	5	432	LEU
5	5	434	LEU
5	5	460	LEU
5	5	462	MET
5	5	471	PHE
5	5	474	TRP
5	5	578	HIS
5	5	580	ASP
5	5	584	LEU
5	5	587	LEU
5	5	589	PRO
5	5	616	MET
5	5	619	MET
5	5	621	ILE
5	5	622	LEU
5	5	628	LEU
5	5	629	LEU
5	5	630	LEU
5	5	636	ASN
5	5	637	VAL
5	5	640	ILE
5	5	643	ILE
5	5	645	VAL
5	5	653	LEU

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Mol	Chain	Res	Type
6	6	11	ILE
6	6	13	ILE
6	6	15	LEU
6	6	23	ILE
6	6	28	ASN
6	6	41	VAL
6	6	42	ILE
6	6	58	LEU
6	6	59	TYR
6	6	70	LEU
6	6	72	LEU
6	6	74	ILE
6	6	77	LEU
6	6	80	ILE
6	6	83	THR
6	6	98	LEU
6	6	100	SER
6	6	102	ILE
6	6	104	LEU
6	6	109	LEU
6	6	110	MET
6	6	112	TYR
6	6	149	THR
6	6	150	ILE
6	6	154	LEU
6	6	155	LEU
6	6	156	THR
6	6	160	PHE
6	6	161	ILE
6	6	167	ILE
6	6	168	VAL
6	6	169	LEU
6	6	170	LEU
6	6	171	LEU
6	6	173	ILE
6	6	174	ILE
6	6	180	THR
7	A	124	MET
7	A	142	CYS
7	A	186	CYS
8	B	388	ARG
8	B	427	CYS

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Mol	Chain	Res	Type
8	B	429	LEU
9	C	102	LEU
9	C	139	PHE
9	C	144	TYR
9	C	145	VAL
9	C	147	MET
9	C	162	LEU
9	C	176	MET
9	C	180	ILE
9	C	186	HIS
9	C	189	SER
9	C	200	LEU
9	C	201	THR
9	C	204	LEU
9	C	207	PHE
9	C	208	GLU
9	C	214	MET
9	C	216	PHE
9	C	217	TYR
9	C	247	ILE
9	C	248	TYR
9	C	257	ARG
9	C	266	THR
9	C	278	ILE
9	C	284	GLN
9	C	285	ASP
9	C	291	LEU
9	C	297	ARG
9	C	308	ASN
9	C	311	TYR
9	C	344	LEU
9	C	351	CYS
9	C	359	VAL
9	C	377	ASP
9	C	387	LEU
9	C	425	CYS
11	G	84	LYS
11	G	177	TRP
12	H	130	THR
13	I	78	PHE
13	I	82	GLU
13	I	83	MET

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Mol	Chain	Res	Type
13	I	84	PHE
13	I	130	CYS
13	I	137	GLU
13	I	139	ILE
13	I	143	LEU
13	I	172	CYS
13	I	190	VAL
13	I	192	TYR
14	K	73	GLN
14	K	79	VAL
14	K	81	PHE
14	K	85	CYS
14	K	112	ARG
14	K	123	LEU
14	K	124	THR
14	K	125	ASN
14	K	131	LEU
14	K	132	ARG
14	K	140	GLU
14	K	168	ASP
14	K	177	VAL
14	K	180	CYS
14	K	193	GLN
14	K	194	LEU
14	K	196	ARG
15	L	2	PHE
15	L	3	ILE
15	L	12	PHE
15	L	19	ARG
15	L	20	ARG
15	L	24	LEU
15	L	28	CYS
15	L	29	LEU
15	L	36	ILE
15	L	39	ILE
15	L	41	LEU
15	L	42	ARG
15	L	46	LEU
15	L	48	ASP
15	L	49	ASP
15	L	51	SER
15	L	57	ILE

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Mol	Chain	Res	Type
15	L	62	LEU
15	L	71	LEU
15	L	74	LEU
15	L	78	TYR
15	L	79	ARG
15	L	84	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	165	ASN
2	2	62	ASN
2	2	173	ASN
4	4	400	GLN
4	4	455	ASN
4	4	469	GLN
5	5	113	GLN
5	5	162	GLN
7	A	185	HIS
9	C	185	ASN
9	C	445	HIS
11	G	193	HIS
13	I	189	ASN
14	K	113	GLN
14	K	133	GLN
14	K	152	ASN
15	L	37	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides 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	H	300	12	0,4,4	-	-	-		
50	SF4	B	500	8	0,12,12	-	-	-		
50	SF4	K	500	14	0,12,12	-	-	-		
49	FES	A	900	7	0,4,4	-	-	-		
50	SF4	I	500	13	0,12,12	-	-	-		
50	SF4	A	902	7	0,12,12	-	-	-		
50	SF4	A	901	7	0,12,12	-	-	-		
50	SF4	I	501	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	H	300	12	-	-	0/1/1/1
50	SF4	B	500	8	-	-	0/6/5/5
50	SF4	K	500	14	-	-	0/6/5/5
49	FES	A	900	7	-	-	0/1/1/1
50	SF4	I	500	13	-	-	0/6/5/5
50	SF4	A	902	7	-	-	0/6/5/5
50	SF4	A	901	7	-	-	0/6/5/5
50	SF4	I	501	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.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	H	300	FES	1	0
50	K	500	SF4	2	0
50	I	500	SF4	1	0
50	A	902	SF4	1	0
50	I	501	SF4	1	0

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	30
8	B	11
10	E	10
5	5	8
13	I	5
12	H	5
2	2	4
4	4	4
1	1	3
3	3	2
11	G	2
22	P	1
16	Z	1
37	AL	1
21	O	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	48.62
1	B	270:UNK	C	279:UNK	N	26.71
1	E	513:UNK	C	604:UNK	N	26.57
1	A	148:UNK	C	152:UNK	N	24.97
1	I	92:UNK	C	103:UNK	N	24.67
1	3	21:UNK	C	38:UNK	N	22.87

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	325:UNK	C	404:UNK	N	22.86
1	2	422:UNK	C	446:UNK	N	21.69
1	A	358:UNK	C	360:UNK	N	17.83
1	E	637:UNK	C	785:UNK	N	17.21
1	H	121:UNK	C	127:CYS	N	16.50
1	E	65:UNK	C	83:UNK	N	16.40
1	E	109:UNK	C	161:UNK	N	16.24
1	B	109:UNK	C	115:UNK	N	16.14
1	A	560:UNK	C	565:UNK	N	16.08
1	E	180:UNK	C	235:UNK	N	15.93
1	I	212:UNK	C	233:UNK	N	15.00
1	B	195:UNK	C	201:UNK	N	14.93
1	E	795:UNK	C	887:UNK	N	14.77
1	H	174:UNK	C	181:UNK	N	14.49
1	A	510:UNK	C	515:UNK	N	12.92
1	A	81:UNK	C	84:UNK	N	12.79
1	A	363:UNK	C	367:UNK	N	12.10
1	3	44:UNK	C	51:UNK	N	12.08
1	B	343:UNK	C	356:UNK	N	11.74
1	A	642:UNK	C	647:UNK	N	11.45
1	H	109:UNK	C	117:UNK	N	11.18
1	A	708:UNK	C	712:UNK	N	10.79
1	H	90:UNK	C	94:UNK	N	10.68
1	4	52:UNK	C	57:UNK	N	10.67
1	G	138:UNK	C	145:UNK	N	10.57
1	2	84:GLY	C	97:UNK	N	10.44
1	2	255:UNK	C	256:UNK	N	10.18
1	G	125:UNK	C	128:UNK	N	9.87
1	B	155:UNK	C	159:UNK	N	9.83
1	4	67:UNK	C	76:UNK	N	9.82
1	B	120:UNK	C	125:UNK	N	9.82
1	A	414:UNK	C	416:UNK	N	9.79
1	B	245:UNK	C	251:UNK	N	9.67
1	P	727:UNK	C	728:UNK	N	9.66
1	I	153:UNK	C	157:UNK	N	9.61
1	5	297:UNK	C	301:UNK	N	9.57
1	H	162:UNK	C	165:UNK	N	9.53
1	A	530:UNK	C	534:UNK	N	9.36
1	A	427:UNK	C	432:UNK	N	9.27
1	A	541:UNK	C	543:UNK	N	9.20
1	I	120:UNK	C	128:UNK	N	9.06
1	A	127:ALA	C	131:ALA	N	8.89

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	457:UNK	C	464:UNK	N	8.88
1	A	435:UNK	C	438:UNK	N	8.86
1	B	87:UNK	C	92:UNK	N	8.74
1	4	18:UNK	C	22:UNK	N	8.73
1	E	242:UNK	C	316:UNK	N	8.00
1	1	120:UNK	C	129:UNK	N	7.81
1	A	704:UNK	C	707:UNK	N	7.59
1	1	62:UNK	C	66:UNK	N	7.54
1	A	87:UNK	C	89:UNK	N	7.53
1	5	24:UNK	C	27:UNK	N	7.47
1	Z	17:UNK	C	18:UNK	N	7.27
1	A	492:UNK	C	496:UNK	N	7.13
1	I	235:UNK	C	238:UNK	N	7.03
1	A	273:UNK	C	276:UNK	N	6.99
1	4	435:UNK	C	437:UNK	N	6.95
1	A	293:UNK	C	297:UNK	N	6.62
1	A	257:UNK	C	260:UNK	N	6.51
1	A	246:UNK	C	248:UNK	N	6.34
1	A	408:UNK	C	409:UNK	N	6.33
1	A	580:UNK	C	586:UNK	N	6.31
1	5	604:UNK	C	613:UNK	N	6.10
1	B	303:UNK	C	306:UNK	N	5.89
1	A	236:GLY	C	240:UNK	N	5.83
1	5	447:UNK	C	455:UNK	N	5.76
1	A	181:UNK	C	183:CYS	N	5.74
1	A	309:UNK	C	313:UNK	N	5.28
1	E	57:UNK	C	59:UNK	N	5.13
1	5	437:UNK	C	439:UNK	N	5.04
1	B	406:UNK	C	407:UNK	N	4.53
1	B	238:UNK	C	240:UNK	N	4.43
1	AL	2916:UNK	C	2917:UNK	N	4.25
1	2	332:UNK	C	339:UNK	N	4.23
1	5	412:UNK	C	416:UNK	N	4.21
1	1	173:UNK	C	177:UNK	N	4.18
1	A	443:UNK	C	445:UNK	N	3.87
1	5	205:UNK	C	208:UNK	N	3.82
1	5	550:UNK	C	560:UNK	N	3.79
1	O	639:UNK	C	640:UNK	N	3.76
1	A	397:UNK	C	400:UNK	N	3.56
1	A	334:UNK	C	336:UNK	N	3.40

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.