wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:32 PM BST

PDB ID	:	2YBB
EMDB ID:	:	EMD-1876
Title	:	Fitted model for bovine mitochondrial supercomplex I1III2IV1 by single particle cryo-EM (EMD-1876)
Authors	:	Althoff, T.; Mills, D.J.; Popot, J.-L.; Kuehlbrandt, W.
Deposited on	:	2011-03-02
Resolution	:	19.00 Å(reported)
Based on PDB ID	:	3IAM,3M9C,1PP9,1BGY,1OCC,2B4Z

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

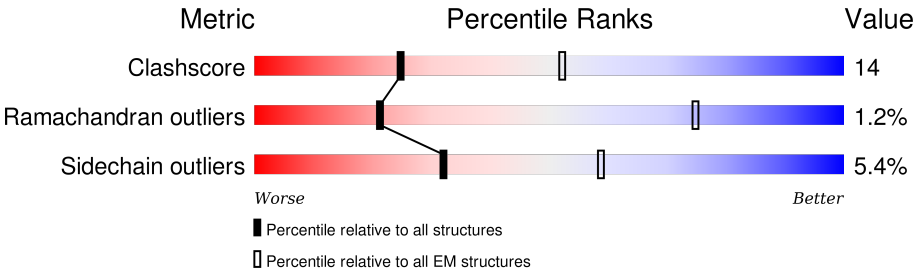
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 19.00 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	438	55% 39% 6%
2	2	181	56% 38% 5% •
3	3	783	49% 41% 6% •
4	4	409	44% 41% 7% 8%
5	5	207	52% 37% 6% 5%
6	6	181	40% 34% 6% 20%
7	7	129	63% 33% • •
8	8	182	42% 38% • 15%
9	A	446	78% 21% ••

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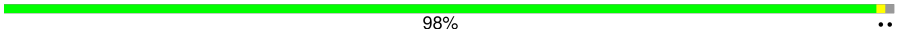
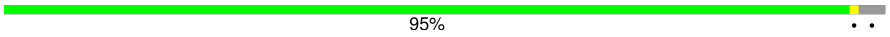
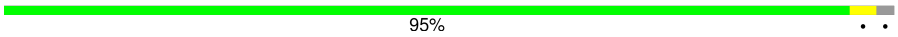
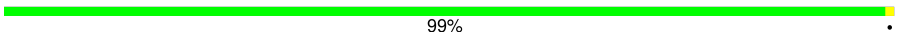
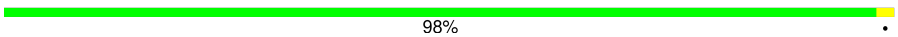
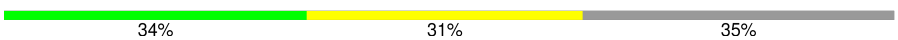
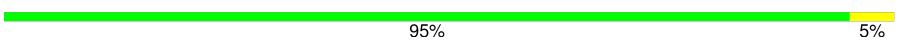
Mol	Chain	Length	Quality of chain
9	a	446	
10	B	439	
10	b	439	
11	C	379	
11	c	379	
12	D	241	
12	d	241	
13	E	196	
13	e	196	
14	F	110	
14	f	110	
15	G	81	
15	g	81	
16	H	78	
16	h	78	
17	I	65	
17	i	65	
18	J	62	
18	j	62	
19	K	56	
19	k	56	
20	L	514	
21	M	227	
22	N	261	
23	O	147	

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Mol	Chain	Length	Quality of chain
24	P	109	78% 19%
25	Q	98	63% 31% 6%
26	R	84	58% 32% 8%
27	S	85	60% 22% 6% 12%
28	T	73	75% 21%
29	U	59	68% 20% 5%
30	V	56	64% 23% 13%
31	W	47	81% 17%
32	X	46	67% 24% 7%
33	Y	104	80% 19%
34	m	474	100%
35	n	391	100%
36	o	378	100%
37	p	281	100%

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
38	SF4	8	183	-	-	X	-
49	HEA	L	515	X	-	-	-
49	HEA	L	516	X	-	-	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 72626 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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-QUINONE OXIDOREDUCTASE SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	437	3417	2180	595	624	18	0	0

- Molecule 2 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	179	1410	897	239	266	8	0	0

- Molecule 3 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	754	5880	3743	1055	1051	31	0	0

- Molecule 4 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	378	3018	1946	511	550	11	0	0

- Molecule 5 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	196	1607	1043	273	288	3	0	0

- Molecule 6 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	144	1102	700	192	197	13	0	0

- Molecule 7 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	127	Total	C	N	O	S	0	0
			1031	664	183	181	3		

- Molecule 8 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	154	Total	C	N	O	S	0	0
			1193	759	201	222	11		

- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	443	Total	C	N	O	S	0	1
			3403	2121	602	660	20		
9	a	443	Total	C	N	O	S	0	1
			3403	2121	602	660	20		

- Molecule 10 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	424	Total	C	N	O	S	0	1
			3177	1996	562	612	7		
10	b	424	Total	C	N	O	S	0	0
			3180	1998	562	613	7		

- Molecule 11 is a protein called CYTOCHROME B.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	365	Total	C	N	O	S	0	0
			2892	1940	450	485	17		
11	c	370	Total	C	N	O	S	0	0
			2931	1968	455	490	18		

- Molecule 12 is a protein called CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	241	Total	C	N	O	S	0	0
			1919	1225	330	349	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	241	Total	C	N	O	S	0	0
			1919	1225	330	349	15		

- Molecule 13 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	196	Total	C	N	O	S	0	0
			1519	957	263	291	8		
13	e	196	Total	C	N	O	S	0	0
			1519	957	263	291	8		

- Molecule 14 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	99	Total	C	N	O	S	0	0
			861	545	155	159	2		
14	f	99	Total	C	N	O	S	0	0
			861	545	155	159	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	56	ASP	ASN	ENGINEERED MUTATION	UNP P00129
f	56	ASP	ASN	ENGINEERED MUTATION	UNP P00129

- Molecule 15 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	75	Total	C	N	O	S	0	2
			621	406	117	97	1		
15	g	76	Total	C	N	O	S	0	2
			626	409	118	98	1		

- Molecule 16 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	66	Total	C	N	O	S	0	0
			539	327	98	109	5		
16	h	66	Total	C	N	O	S	0	0
			539	327	98	109	5		

- Molecule 17 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	42	Total	C	N	O	S	0	0
			285	174	55	55	1		
17	i	42	Total	C	N	O	S	0	0
			285	174	55	55	1		

- Molecule 18 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	J	62	Total	C	N	O	0	0
			507	333	88	86		
18	j	62	Total	C	N	O	0	0
			507	333	88	86		

- Molecule 19 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	K	22	Total	C	N	O	0	0
			159	103	29	27		
19	k	22	Total	C	N	O	0	0
			159	103	29	27		

- Molecule 20 is a protein called CYTOCHROME C OXIDASE SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	514	Total	C	N	O	S	0	0
			4025	2690	623	677	35		

- Molecule 21 is a protein called CYTOCHROME C OXIDASE SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	227	Total	C	N	O	S	0	0
			1822	1184	281	339	18		

- Molecule 22 is a protein called CYTOCHROME C OXIDASE SUBUNIT 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	261	Total	C	N	O	S	0	0
			2124	1420	338	353	13		

- Molecule 23 is a protein called CYTOCHROME C OXIDASE SUBUNIT 4 ISOFORM 1,

MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	144	Total	C	N	O	S	0	0
			1195	777	196	218	4		

- Molecule 24 is a protein called CYTOCHROME C OXIDASE SUBUNIT 5A, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	109	Total	C	N	O	S	0	0
			878	558	150	168	2		

- Molecule 25 is a protein called CYTOCHROME C OXIDASE SUBUNIT 5B, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	98	Total	C	N	O	S	0	0
			748	464	134	145	5		

- Molecule 26 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE VIA, CYTOCHROME C OXIDASE POLYPEPTIDE VB.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	84	Total	C	N	O	S	0	0
			672	431	129	111	1		

- Molecule 27 is a protein called CYTOCHROME C OXIDASE SUBUNIT 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	75	Total	C	N	O	S	0	0
			628	395	114	114	5		

- Molecule 28 is a protein called CYTOCHROME C OXIDASE SUBUNIT 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	73	Total	C	N	O	S	0	0
			598	388	107	99	4		

- Molecule 29 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7A1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	57	Total	C	N	O	S	0	1
			442	285	74	80	3		

- Molecule 30 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7B, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	49	Total	C	N	O	S	0	0
			384	250	65	67	2		

- Molecule 31 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7C, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	47	Total	C	N	O	S	0	0
			386	257	65	62	2		

- Molecule 32 is a protein called CYTOCHROME C OXIDASE SUBUNIT 8B, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	X	43	Total	C	N	O	0	0
			335	223	53	59		

- Molecule 33 is a protein called CYTOCHROME C.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Y	104	Total	C	N	O	S	7	0
			875	552	155	163	5		

- Molecule 34 is a protein called NADH\: UBIQUINONE OXIDOREDUCTASE, MEMBRANE SUBUNIT L,.

Mol	Chain	Residues	Atoms			AltConf	Trace
34	m	474	Total	C	N	0	0
			1422	948	474		

- Molecule 35 is a protein called NADH\: UBIQUINONE OXIDOREDUCTASE, MEMBRANE SUBUNIT M,.

Mol	Chain	Residues	Atoms			AltConf	Trace
35	n	391	Total	C	N	0	0
			1173	782	391		

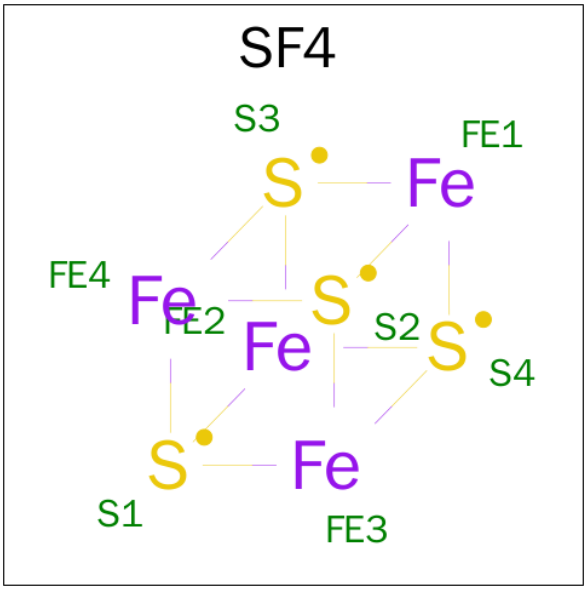
- Molecule 36 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT N.

Mol	Chain	Residues	Atoms			AltConf	Trace
36	o	378	Total	C	N	0	0
			1134	756	378		

- Molecule 37 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT K.

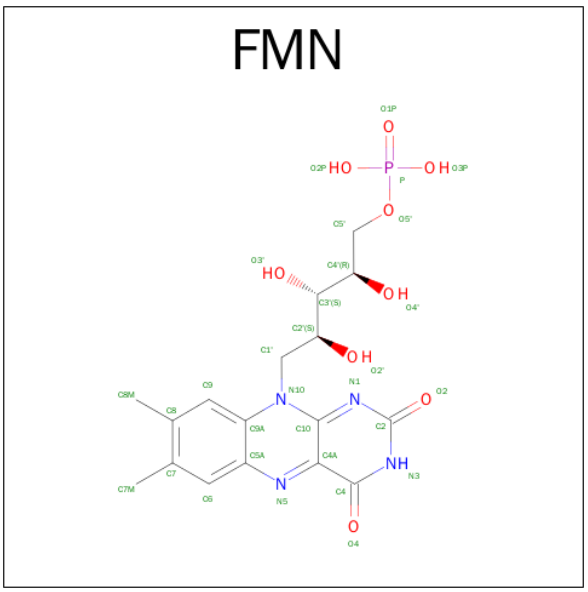
Mol	Chain	Residues	Atoms			AltConf	Trace
37	p	281	Total	C	N	0	0
			843	562	281		

- Molecule 38 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



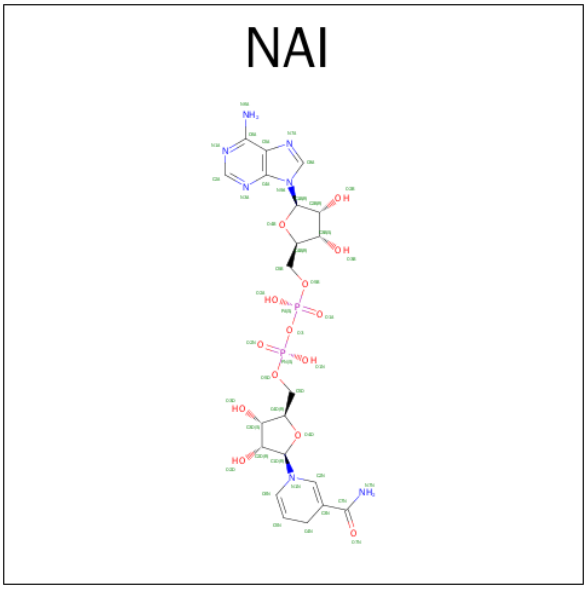
Mol	Chain	Residues	Atoms			AltConf
38	1	1	Total	Fe	S	0
			8	4	4	
38	3	1	Total	Fe	S	0
			24	12	12	
38	3	1	Total	Fe	S	0
			24	12	12	
38	3	1	Total	Fe	S	0
			24	12	12	
38	6	1	Total	Fe	S	0
			8	4	4	
38	8	1	Total	Fe	S	0
			16	8	8	
38	8	1	Total	Fe	S	0
			16	8	8	

- Molecule 39 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
39	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 40 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).

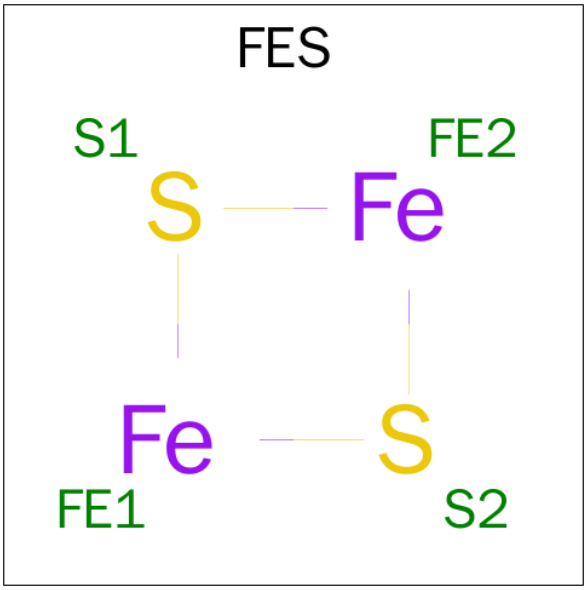


Mol	Chain	Residues	Atoms					AltConf
40	1	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 41 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
41	1	1	Total Mg 1 1	0
41	4	1	Total Mg 1 1	0
41	5	1	Total Mg 1 1	0
41	2	1	Total Mg 1 1	0
41	L	1	Total Mg 1 1	0
41	3	2	Total Mg 2 2	0

- Molecule 42 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

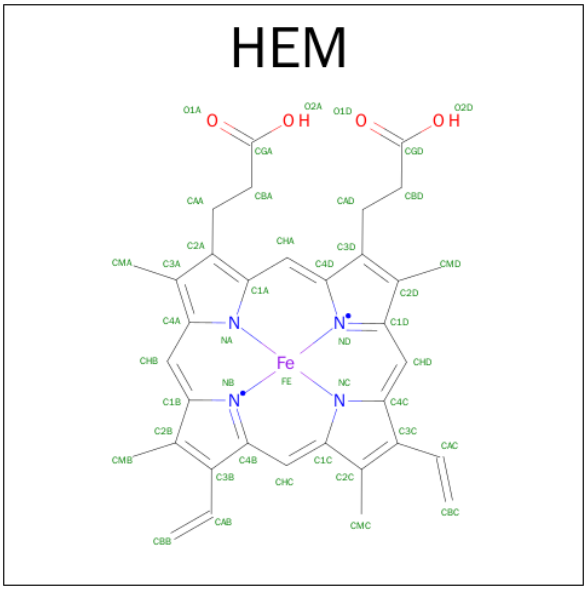


Mol	Chain	Residues	Atoms	AltConf
42	2	1	Total Fe S 4 2 2	0
42	3	1	Total Fe S 4 2 2	0
42	E	1	Total Fe S 4 2 2	0
42	e	1	Total Fe S 4 2 2	0

- Molecule 43 is CALCIUM ION (three-letter code: CA) (formula: Ca).

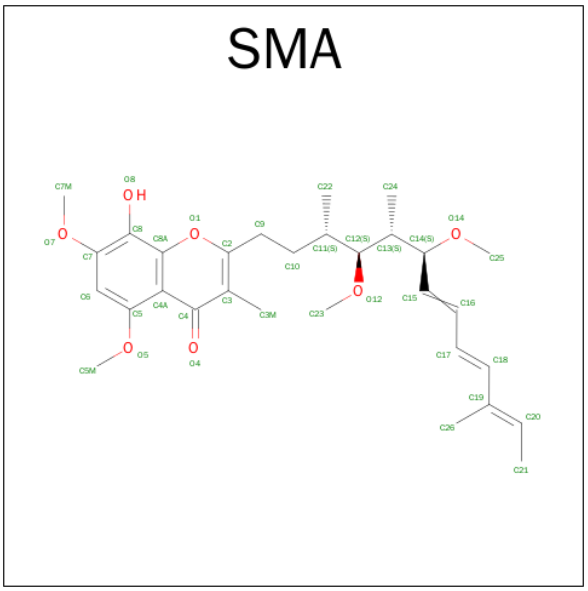
Mol	Chain	Residues	Atoms		AltConf
43	7	1	Total	Ca	0
			1	1	

- Molecule 44 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



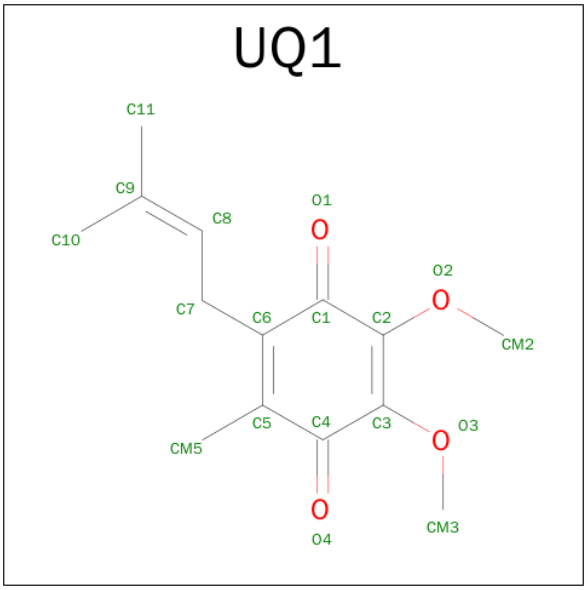
Mol	Chain	Residues	Atoms					AltConf
44	C	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
44	C	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
44	Y	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
44	c	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
44	c	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

- Molecule 45 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



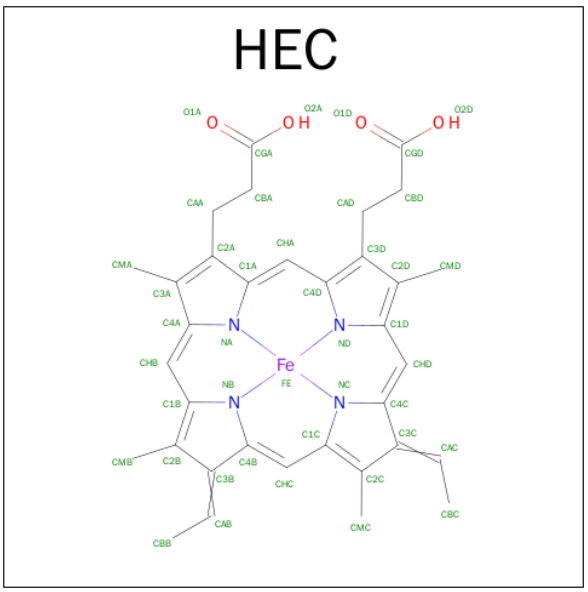
Mol	Chain	Residues	Atoms	AltConf
45	C	1	Total C O 37 30 7	0
45	c	1	Total C O 37 30 7	0

- Molecule 46 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$).



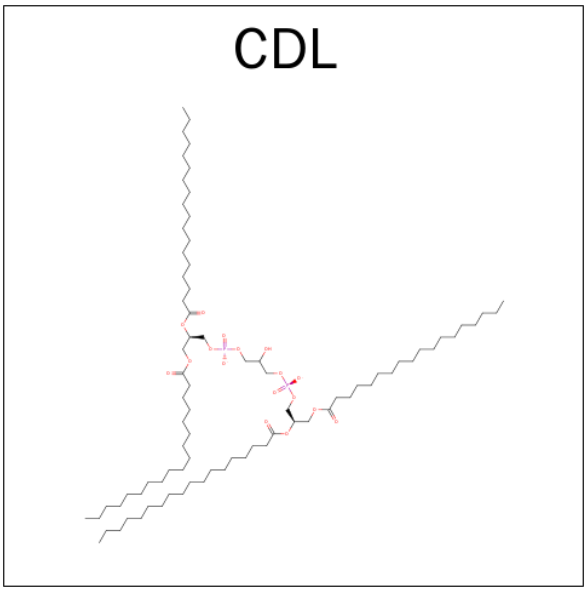
Mol	Chain	Residues	Atoms	AltConf
46	C	1	Total C O 14 10 4	0
46	c	1	Total C O 14 10 4	0

- Molecule 47 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
47	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
47	d	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 48 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
48	G	1	Total	C	O	P	0
			94	56	34	4	

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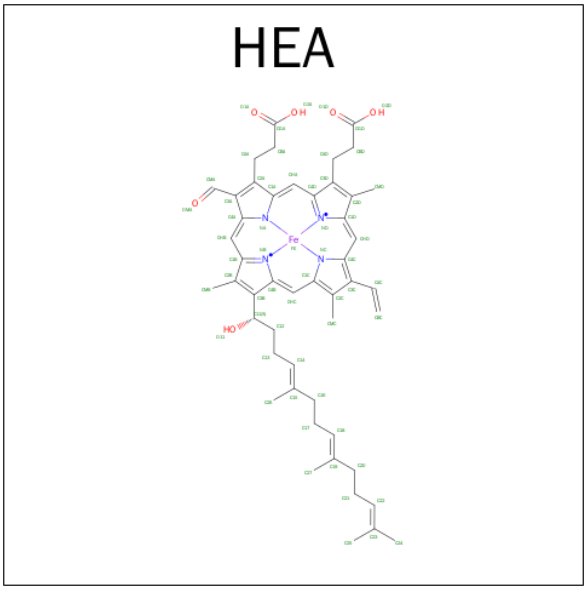
Mol	Chain	Residues	Atoms				AltConf
48	G	1	Total	C	O	P	0
			94	56	34	4	
48	d	1	Total	C	O	P	0
			50	31	17	2	
48	g	1	Total	C	O	P	0
			49	30	17	2	

- Molecule 49 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
49	L	1	Total	C	Fe	N	O	0
			120	98	2	8	12	
49	L	1	Total	C	Fe	N	O	0
			120	98	2	8	12	

- Molecule 50 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
50	L	1	Total	Cu	0
			1	1	
50	M	2	Total	Cu	0
			2	2	

- Molecule 51 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
51	Q	1	Total Zn 1 1	0

- Molecule 52 is water.

Mol	Chain	Residues	Atoms	AltConf
52	A	187	Total O 187 187	0
52	B	149	Total O 149 149	0
52	C	125	Total O 125 125	0
52	D	118	Total O 118 118	0
52	E	54	Total O 54 54	0
52	F	57	Total O 57 57	0
52	G	24	Total O 24 24	0
52	H	14	Total O 14 14	0
52	I	16	Total O 16 16	0
52	J	5	Total O 5 5	0
52	Y	161	Total O 161 161	0
52	a	134	Total O 134 134	0
52	b	130	Total O 130 130	0
52	c	122	Total O 122 122	0
52	d	109	Total O 109 109	0
52	e	64	Total O 64 64	0
52	f	73	Total O 73 73	0
52	g	21	Total O 21 21	0
52	h	16	Total O 16 16	0

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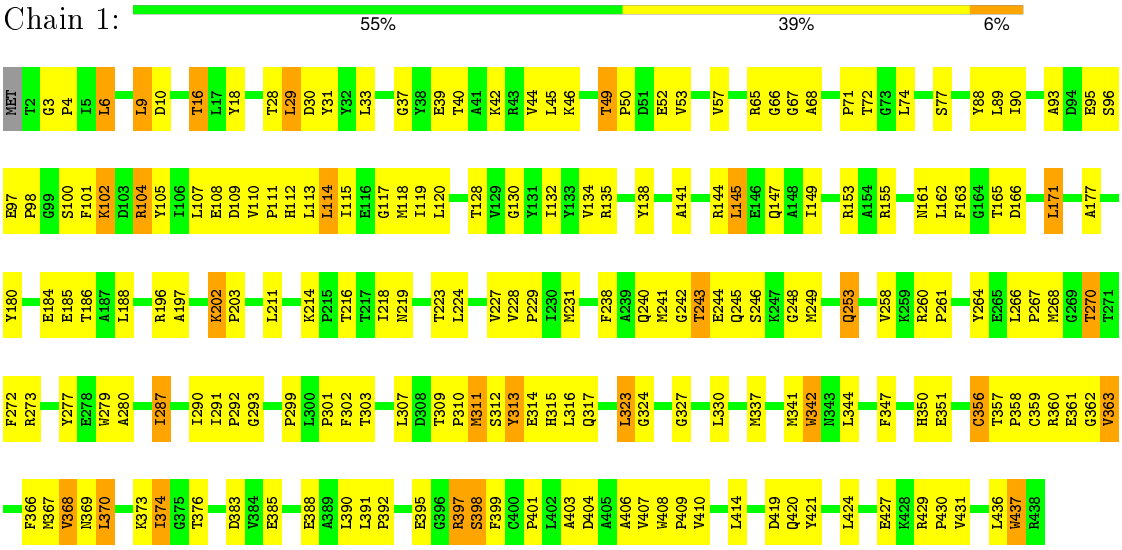
Mol	Chain	Residues	Atoms	AltConf
52	i	10	Total O 10 10	0
52	j	9	Total O 9 9	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

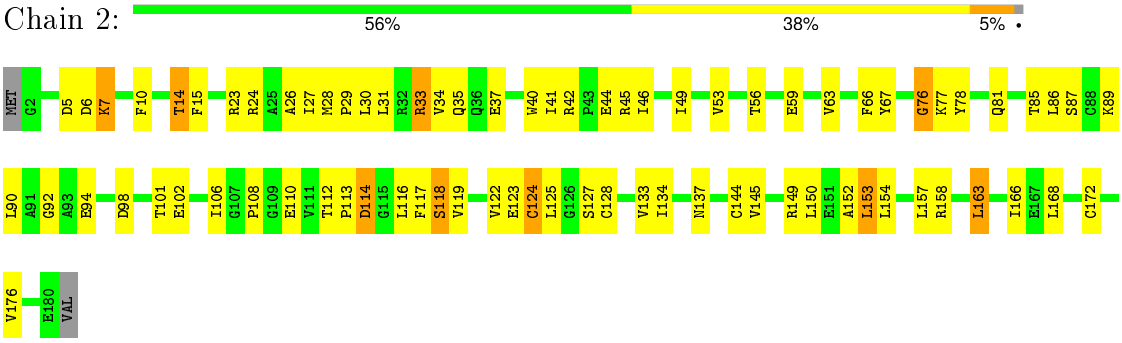
- Molecule 1: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 1

Chain 1:



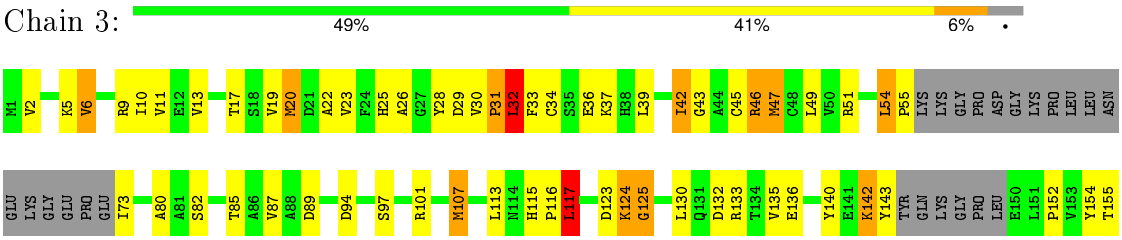
- Molecule 2: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 2

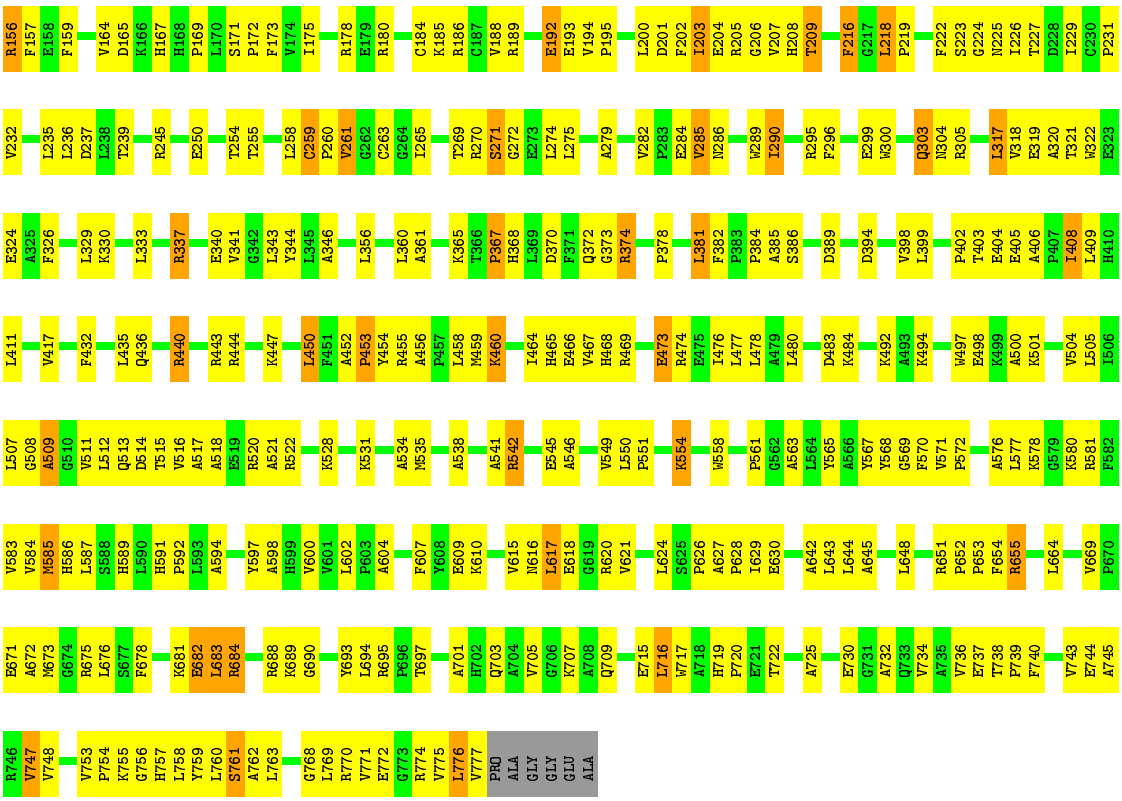
Chain 2:



- Molecule 3: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 3

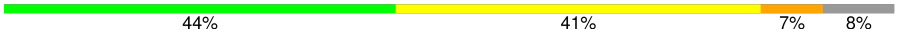
Chain 3:

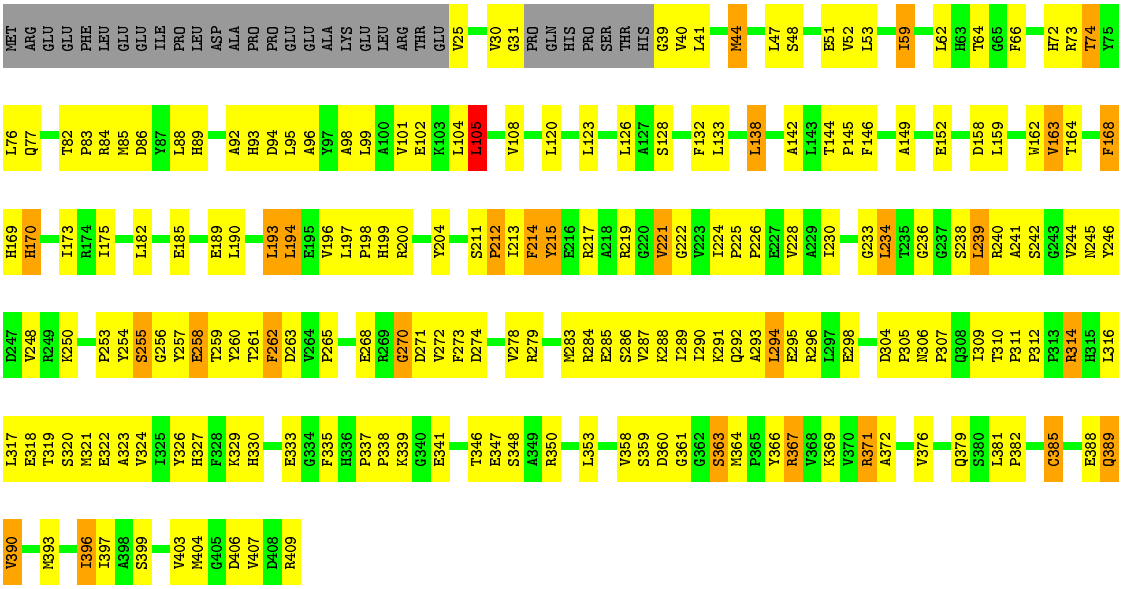




- Molecule 4: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 4

Chain 4:

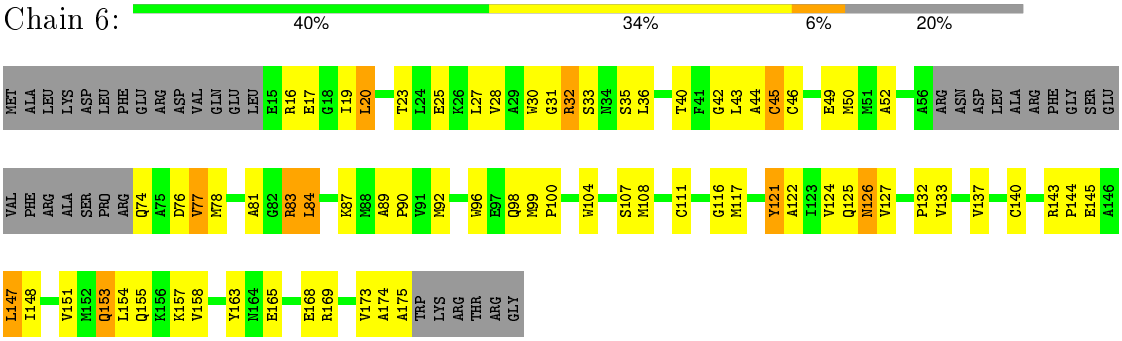




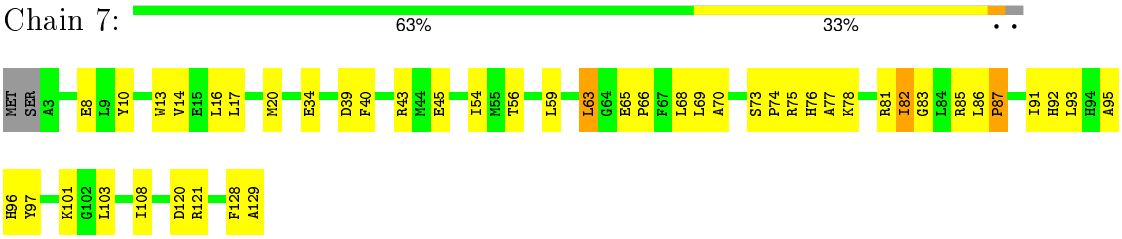
- Molecule 5: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 5

Chain 5:

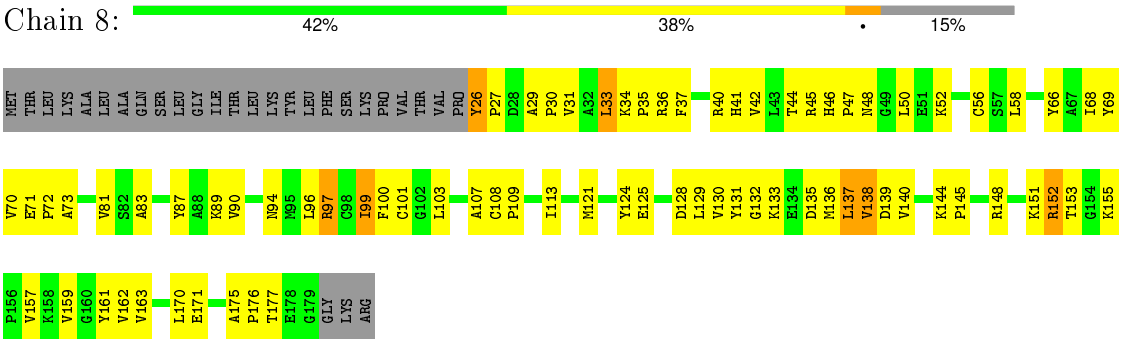
• Molecule 6: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 6



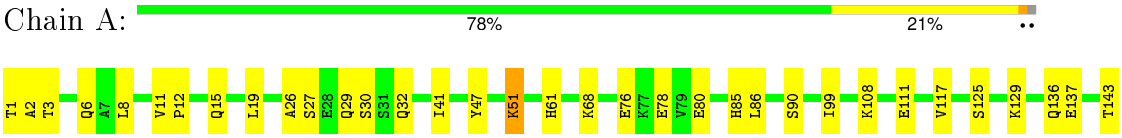
• Molecule 7: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 15

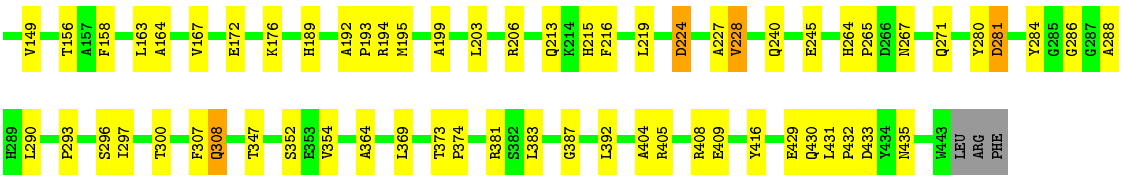


• Molecule 8: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 9



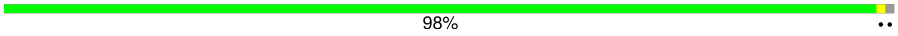
• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL

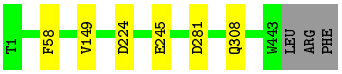




• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL

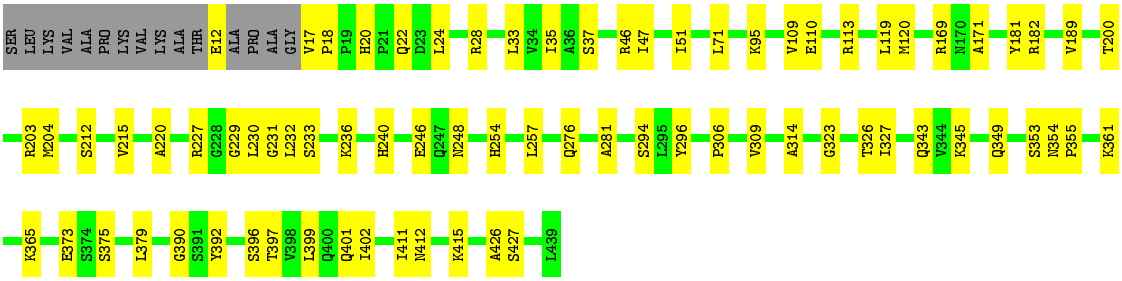
Chain a:





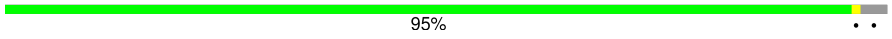
• Molecule 10: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL

Chain B:



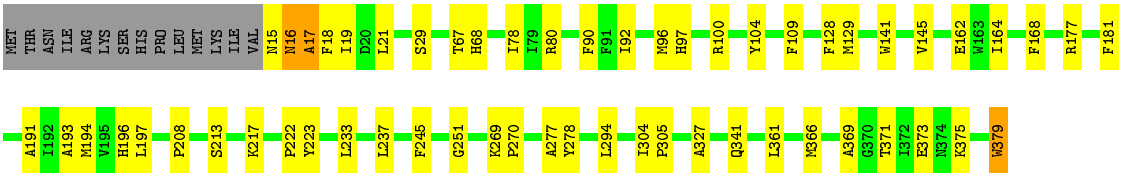
• Molecule 10: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL

Chain b:



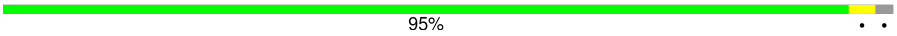
• Molecule 11: CYTOCHROME B

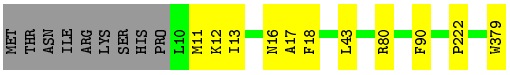
Chain C:



• Molecule 11: CYTOCHROME B

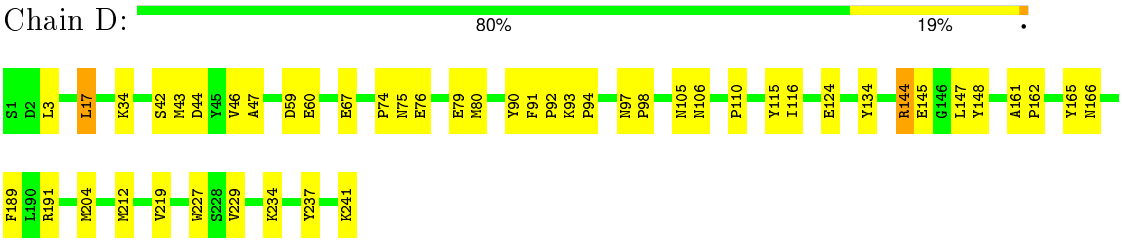
Chain c:





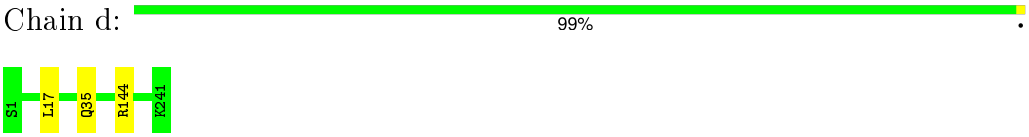
• Molecule 12: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL

Chain D:



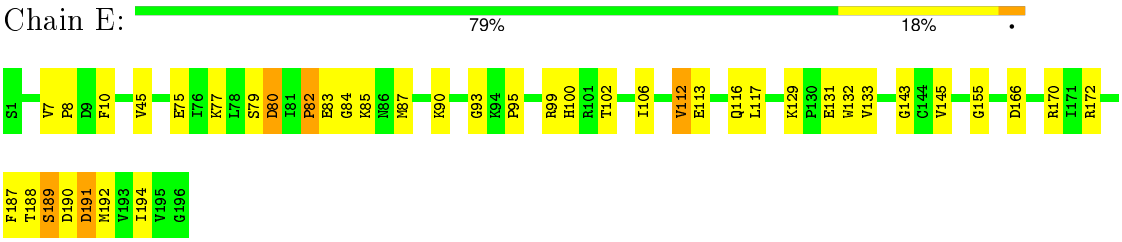
• Molecule 12: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL

Chain d:



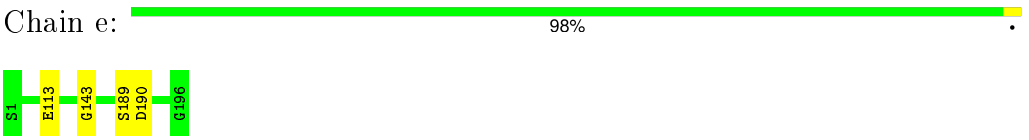
• Molecule 13: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

Chain E:



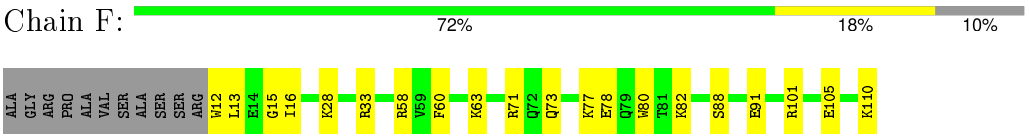
• Molecule 13: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

Chain e:



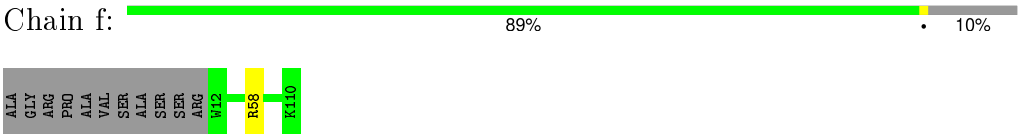
• Molecule 14: CYTOCHROME B-C1 COMPLEX SUBUNIT 7

Chain F:



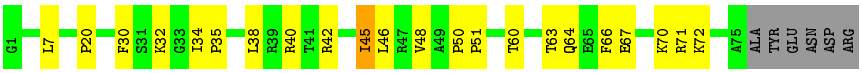
• Molecule 14: CYTOCHROME B-C1 COMPLEX SUBUNIT 7

Chain f:



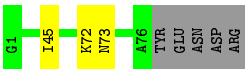
• Molecule 15: CYTOCHROME B-C1 COMPLEX SUBUNIT 8

Chain G:



• Molecule 15: CYTOCHROME B-C1 COMPLEX SUBUNIT 8

Chain g:



• Molecule 16: CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL

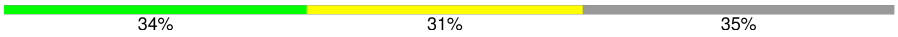
Chain H:

• Molecule 16: CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL

Chain h:

• Molecule 17: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

Chain I:

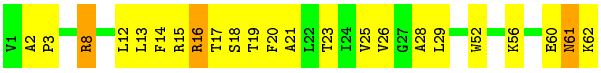


• Molecule 17: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

Chain i:

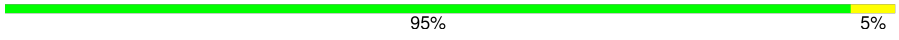
• Molecule 18: CYTOCHROME B-C1 COMPLEX SUBUNIT 9

Chain J:



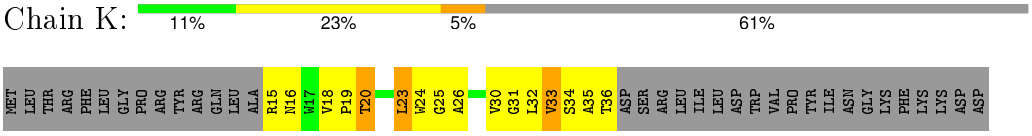
• Molecule 18: CYTOCHROME B-C1 COMPLEX SUBUNIT 9

Chain j:



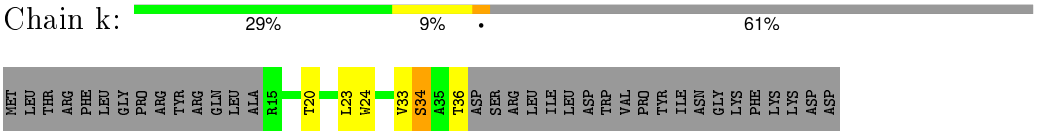
• Molecule 19: CYTOCHROME B-C1 COMPLEX SUBUNIT 10

Chain K:



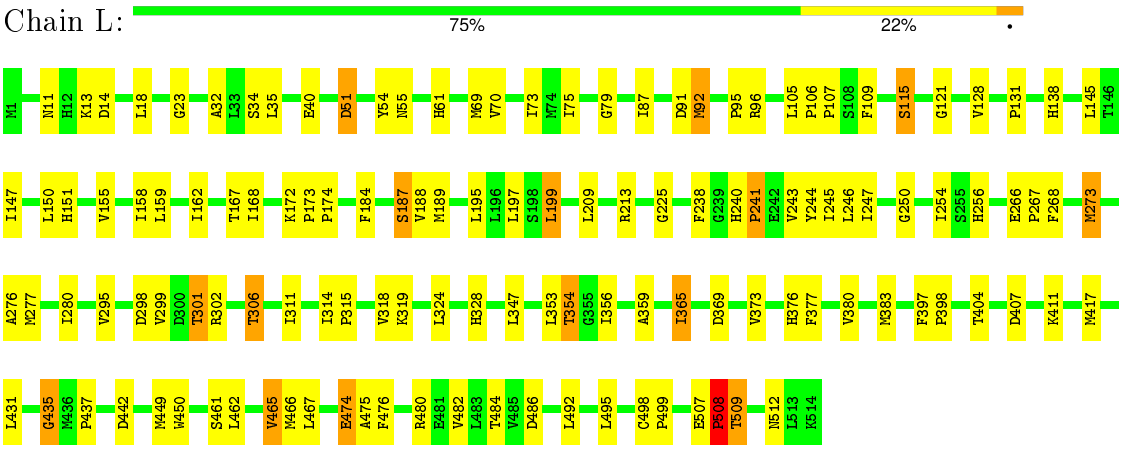
• Molecule 19: CYTOCHROME B-C1 COMPLEX SUBUNIT 10

Chain k:



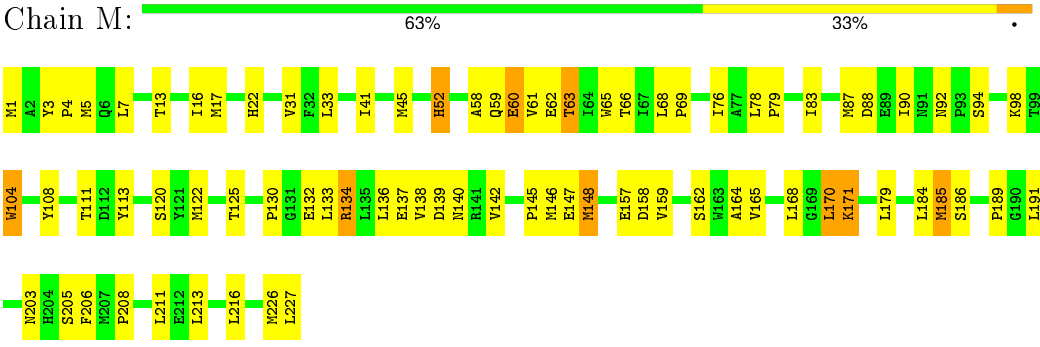
• Molecule 20: CYTOCHROME C OXIDASE SUBUNIT 1

Chain L:



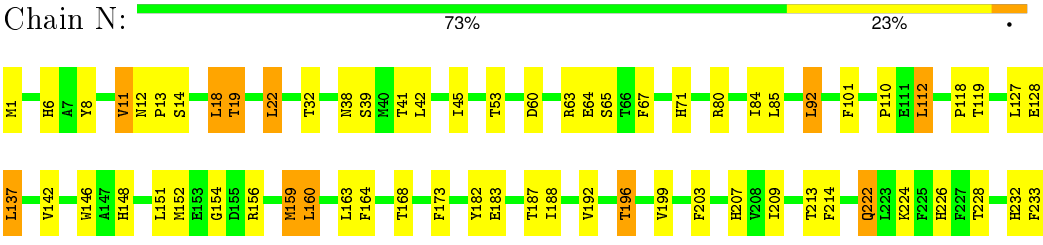
• Molecule 21: CYTOCHROME C OXIDASE SUBUNIT 2

Chain M:



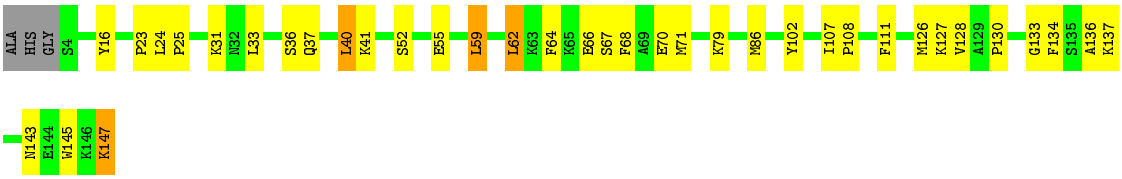
• Molecule 22: CYTOCHROME C OXIDASE SUBUNIT 3

Chain N:



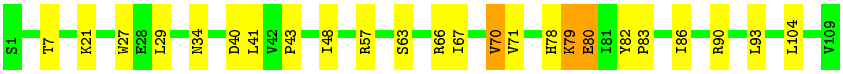
• Molecule 23: CYTOCHROME C OXIDASE SUBUNIT 4 ISOFORM 1, MITOCHONDRIAL

Chain O:



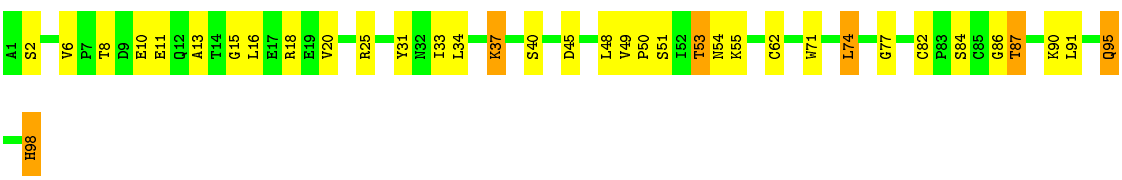
• Molecule 24: CYTOCHROME C OXIDASE SUBUNIT 5A, MITOCHONDRIAL

Chain P:



• Molecule 25: CYTOCHROME C OXIDASE SUBUNIT 5B, MITOCHONDRIAL

Chain Q:



• Molecule 26: CYTOCHROME C OXIDASE POLYPEPTIDE VIA, CYTOCHROME C OXIDASE POLYPEPTIDE VB

Chain R:

• Molecule 27: CYTOCHROME C OXIDASE SUBUNIT 6B1

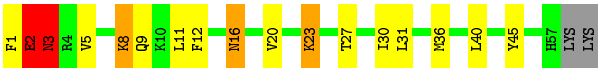
Chain S:

• Molecule 28: CYTOCHROME C OXIDASE SUBUNIT 6C

Chain T:

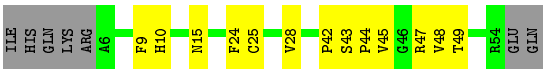
• Molecule 29: CYTOCHROME C OXIDASE SUBUNIT 7A1, MITOCHONDRIAL

Chain U:



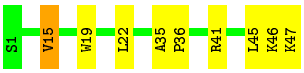
• Molecule 30: CYTOCHROME C OXIDASE SUBUNIT 7B, MITOCHONDRIAL

Chain V:



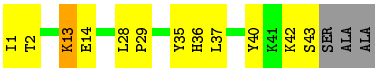
• Molecule 31: CYTOCHROME C OXIDASE SUBUNIT 7C, MITOCHONDRIAL

Chain W:



• Molecule 32: CYTOCHROME C OXIDASE SUBUNIT 8B, MITOCHONDRIAL

Chain X:

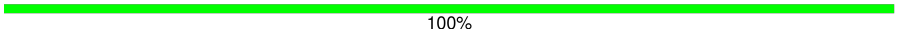


• Molecule 33: CYTOCHROME C

Chain Y:

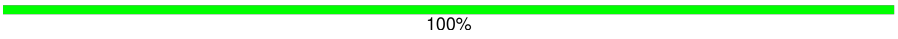
• Molecule 34: NADH\: UBIQUINONE OXIDOREDUCTASE, MEMBRANE SUBUNIT L,

Chain m:



• Molecule 35: NADH\: UBIQUINONE OXIDOREDUCTASE, MEMBRANE SUBUNIT M,

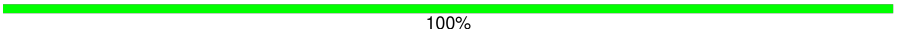
Chain n:



There are no outlier residues recorded for this chain.

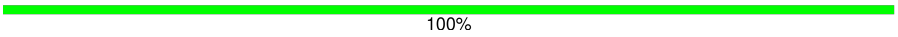
• Molecule 36: NADH-QUINONE OXIDOREDUCTASE SUBUNIT N

Chain o:



There are no outlier residues recorded for this chain.

- Molecule 37: NADH-QUINONE OXIDOREDUCTASE SUBUNIT K

Chain p: 

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE-FLIPPPING ON EACH PARTICLE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CDL, SF4, NAI, ZN, FMN, SMA, FES, HEC, UQ1, HEM, CA, CU, HEA

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	1	0.45	1/3506 (0.0%)	0.63	2/4745 (0.0%)
10	B	0.32	0/3235	0.65	0/4387
10	b	0.31	0/3239	0.65	1/4393 (0.0%)
11	C	0.37	0/2986	0.65	1/4089 (0.0%)
11	c	0.35	0/3024	0.64	0/4137
12	D	0.34	0/1978	0.65	0/2684
12	d	0.34	0/1978	0.65	0/2684
13	E	0.32	0/1553	0.67	1/2100 (0.0%)
13	e	0.35	0/1553	0.69	1/2100 (0.0%)
14	F	0.32	0/878	0.64	0/1175
14	f	0.32	0/878	0.65	0/1175
15	G	0.32	0/642	0.65	0/869
15	g	0.34	0/647	0.68	0/876
16	H	0.31	0/544	0.60	0/729
16	h	0.31	0/544	0.56	0/729
17	I	0.32	0/285	0.66	0/384
17	i	0.32	0/285	0.69	0/384
18	J	0.37	0/520	0.65	0/699
18	j	0.36	0/520	0.65	0/699
19	K	0.42	0/163	1.01	0/225
19	k	0.46	0/163	1.17	0/225
2	2	0.45	0/1443	0.64	0/1958
20	L	0.60	0/4164	0.76	1/5688 (0.0%)
21	M	0.57	0/1868	0.79	0/2544
22	N	0.56	0/2211	0.68	0/3023
23	O	0.57	0/1229	0.64	1/1658 (0.1%)
24	P	0.50	0/898	0.66	0/1218
25	Q	0.56	0/765	0.81	0/1038
26	R	0.54	0/699	0.73	1/950 (0.1%)
27	S	0.55	0/648	0.73	0/877
28	T	0.60	0/611	0.65	0/810
29	U	0.61	0/451	0.72	0/610

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
3	3	0.43	0/6019	0.61	1/8163 (0.0%)
30	V	0.57	0/398	0.66	0/546
31	W	0.63	0/399	0.62	0/534
32	X	0.51	0/345	0.65	0/470
33	Y	0.31	0/891	0.60	0/1186
4	4	0.40	0/3096	0.59	2/4207 (0.0%)
5	5	0.44	0/1656	0.61	0/2246
6	6	0.48	0/1126	0.64	0/1528
7	7	0.43	0/1059	0.60	0/1429
8	8	0.48	0/1224	0.66	0/1663
9	A	0.32	0/3472	0.66	0/4714
9	a	0.33	0/3472	0.67	0/4714
All	All	0.43	1/67265 (0.0%)	0.66	12/91262 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
19	k	0	1
34	m	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	356	CYS	CB-SG	-5.05	1.73	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	4	39	GLY	N-CA-C	-7.72	93.79	113.10
4	4	105	LEU	CA-CB-CG	7.21	131.89	115.30
10	b	228	GLY	N-CA-C	-6.96	95.71	113.10
23	O	133	GLY	N-CA-C	6.43	129.19	113.10
3	3	32	LEU	CA-CB-CG	5.91	128.89	115.30
13	e	143	GLY	N-CA-C	5.69	127.33	113.10
13	E	143	GLY	N-CA-C	5.38	126.54	113.10
26	R	5	LYS	N-CA-C	5.22	125.09	111.00
11	C	109	PHE	N-CA-C	-5.21	96.93	111.00
20	L	435	GLY	N-CA-C	5.16	125.99	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	356	CYS	CB-CA-C	-5.16	100.09	110.40
1	1	342	TRP	CA-CB-CG	5.09	123.36	113.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	k	24	TRP	Mainchain
34	m	1212	UNK	Peptide

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	3417	0	3388	169	0
2	2	1410	0	1376	70	0
3	3	5880	0	5911	354	0
4	4	3018	0	3009	195	0
5	5	1607	0	1574	95	0
6	6	1102	0	1108	79	0
7	7	1031	0	1029	39	0
8	8	1193	0	1160	69	0
9	A	3403	0	3301	95	0
9	a	3403	0	3302	0	0
10	B	3177	0	3152	85	0
10	b	3180	0	3156	0	0
11	C	2892	0	2938	48	0
11	c	2931	0	2989	0	0
12	D	1919	0	1868	63	0
12	d	1919	0	1867	0	0
13	E	1519	0	1503	38	0
13	e	1519	0	1503	0	0
14	F	861	0	854	22	0
14	f	861	0	854	0	0
15	G	621	0	626	29	0
15	g	626	0	631	0	0
16	H	539	0	524	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	h	539	0	524	0	0
17	I	285	0	288	46	0
17	i	285	0	288	0	0
18	J	507	0	512	71	0
18	j	507	0	512	0	0
19	K	159	0	159	61	0
19	k	159	0	159	0	0
20	L	4025	0	4003	82	0
21	M	1822	0	1834	72	0
22	N	2124	0	2042	47	0
23	O	1195	0	1183	33	0
24	P	878	0	868	21	0
25	Q	748	0	728	26	0
26	R	672	0	645	30	0
27	S	628	0	582	22	0
28	T	598	0	612	14	0
29	U	442	0	439	14	0
30	V	384	0	366	9	0
31	W	386	0	388	8	0
32	X	335	0	352	12	0
33	Y	875	0	885	39	0
34	m	1422	0	52	0	0
35	n	1173	0	37	0	0
36	o	1134	0	36	0	0
37	p	843	0	24	0	0
38	1	8	0	0	0	0
38	3	24	0	0	3	0
38	6	8	0	0	1	0
38	8	16	0	0	2	0
39	1	31	0	19	6	0
40	1	44	0	27	6	0
41	1	1	0	0	0	0
41	2	1	0	0	0	0
41	3	2	0	0	0	0
41	4	1	0	0	0	0
41	5	1	0	0	0	0
41	L	1	0	0	0	0
42	2	4	0	0	0	0
42	3	4	0	0	1	0
42	E	4	0	0	0	0
42	e	4	0	0	0	0
43	7	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	C	86	0	60	5	0
44	Y	43	0	30	7	0
44	c	86	0	60	0	0
45	C	37	0	42	1	0
45	c	37	0	42	0	0
46	C	14	0	9	2	0
46	c	14	0	9	0	0
47	D	43	0	30	6	0
47	d	43	0	30	0	0
48	G	94	0	76	5	0
48	d	50	0	44	0	0
48	g	49	0	42	0	0
49	L	120	0	108	7	0
50	L	1	0	0	0	0
50	M	2	0	0	0	0
51	Q	1	0	0	0	0
52	A	187	0	0	11	0
52	B	149	0	0	3	0
52	C	125	0	0	4	0
52	D	118	0	0	2	0
52	E	54	0	0	2	0
52	F	57	0	0	3	0
52	G	24	0	0	1	0
52	H	14	0	0	0	0
52	I	16	0	0	2	0
52	J	5	0	0	0	0
52	Y	161	0	0	18	0
52	a	134	0	0	0	0
52	b	130	0	0	0	0
52	c	122	0	0	0	0
52	d	109	0	0	0	0
52	e	64	0	0	0	0
52	f	73	0	0	0	0
52	g	21	0	0	0	0
52	h	16	0	0	0	0
52	i	10	0	0	0	0
52	j	9	0	0	0	0
All	All	72626	0	65769	1833	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 14.

All (1833) 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)
18:J:29:LEU:HD21	19:K:34:SER:CB	69.19	1.63
18:J:29:LEU:CD2	19:K:34:SER:HB2	70.77	1.42
9:A:408:ARG:NH2	19:K:15:ARG:HG2	78.17	1.38
12:D:106:ASN:HB2	52:Y:350:HOH:O	51.68	1.29
12:D:145:GLU:OE1	33:Y:27:LYS:HD3	63.63	1.28
18:J:29:LEU:HD21	19:K:34:SER:OG	68.69	1.25
18:J:29:LEU:CD2	19:K:34:SER:CB	69.80	1.25
9:A:408:ARG:HH22	19:K:15:ARG:CG	78.54	1.20
33:Y:14:CYS:SG	44:Y:500:HEM:HAB	1.85	1.16
10:B:95:LYS:HB2	17:I:32:ALA:HB2	1.57	1.16
1:1:104:ARG:HH21	2:2:127:SER:HB3	1.04	1.15
3:3:31:PRO:HB3	3:3:47:MET:HE3	1.29	1.15
18:J:17:THR:HG22	19:K:24:TRP:HZ2	63.68	1.13
12:D:145:GLU:CD	52:Y:269:HOH:O	67.66	1.13
3:3:474:ARG:HH21	3:3:516:VAL:HG21	1.03	1.11
18:J:17:THR:HG22	19:K:24:TRP:CZ2	63.76	1.11
15:G:45:ILE:HG22	15:G:46:LEU:HD22	5.35	1.11
33:Y:14:CYS:SG	44:Y:500:HEM:CAB	2.40	1.10
6:6:83:ARG:HH11	6:6:83:ARG:HG3	1.13	1.07
10:B:12:GLU:HG2	10:B:17:VAL:H	1.15	1.07
12:D:145:GLU:OE2	33:Y:25:LYS:HE2	66.52	1.06
3:3:11:VAL:HG11	3:3:25:HIS:HD2	1.16	1.05
18:J:18:SER:HB2	19:K:23:LEU:HB2	73.83	1.05
1:1:97:GLU:HB2	40:1:441:NAI:H42N	1.37	1.04
1:1:104:ARG:NH2	2:2:127:SER:HB3	1.73	1.04
1:1:358:PRO:HD3	3:3:107:MET:HE3	1.41	1.03
52:A:4099:HOH:O	19:K:15:ARG:NE	83.91	1.02
3:3:474:ARG:NH2	3:3:516:VAL:HG21	1.75	1.01
10:B:200:THR:HB	10:B:229:GLY:HA2	5.90	1.01
18:J:18:SER:CB	19:K:23:LEU:HB2	73.85	1.01
13:E:166:ASP:HA	52:E:541:HOH:O	1.59	1.00
5:5:66:GLU:HG2	5:5:95:PRO:HA	1.40	1.00
5:5:52:ILE:CG2	5:5:114:LEU:HB3	1.92	0.99
5:5:175:THR:HG23	5:5:178:ASP:HB2	1.42	0.99
18:J:25:VAL:HG11	19:K:30:VAL:HB	71.04	0.97
12:D:145:GLU:OE1	33:Y:27:LYS:CD	62.88	0.96
1:1:337:MET:HA	1:1:337:MET:HE2	1.43	0.96
3:3:373:GLY:HA3	3:3:538:ALA:HB2	1.48	0.96
18:J:18:SER:HB2	19:K:23:LEU:CB	74.68	0.95
12:D:165:TYR:OH	33:Y:83:ALA:HB3	64.41	0.95
26:R:5:LYS:HZ3	26:R:6:GLY:H	0.94	0.94
4:4:341:GLU:HG2	4:4:358:VAL:HG22	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:405:GLU:HB2	3:3:535:MET:HE2	1.49	0.94
3:3:117:LEU:HD12	4:4:321:MET:HE1	1.50	0.93
1:1:16:THR:HG21	1:1:229:PRO:HB3	1.50	0.93
18:J:29:LEU:CD2	19:K:34:SER:OG	69.31	0.92
20:L:365:ILE:HD12	21:M:87:MET:HE1	1.51	0.92
3:3:701:ALA:HB2	3:3:763:LEU:HB2	1.49	0.92
9:A:136:GLN:HE21	17:I:51:CYS:HB3	1.34	0.92
1:1:184:GLU:OE1	1:1:186:THR:HG22	1.69	0.92
2:2:114:ASP:HB2	2:2:116:LEU:HD22	1.52	0.92
3:3:522:ARG:HH12	3:3:681:LYS:HE3	1.35	0.91
47:D:501:HEC:CBC	52:Y:308:HOH:O	51.48	0.91
12:D:59:ASP:OD2	18:J:62:LYS:HB3	7.65	0.91
5:5:121:LEU:HB3	5:5:146:LEU:HB2	1.52	0.91
3:3:165:ASP:HB3	3:3:178:ARG:HD2	1.52	0.91
4:4:40:VAL:HG13	4:4:404:MET:HG3	1.52	0.90
3:3:11:VAL:HG11	3:3:25:HIS:CD2	2.06	0.90
14:F:13:LEU:HD12	14:F:16:ILE:HD11	2.31	0.90
4:4:250:LYS:HE2	4:4:262:PHE:HB3	1.54	0.90
9:A:293:PRO:O	9:A:297:ILE:HG12	1.71	0.89
3:3:115:HIS:CG	3:3:116:PRO:HD2	2.07	0.89
17:I:32:ALA:N	17:I:72:VAL:HG23	1.88	0.89
9:A:1:THR:HG21	10:B:212:SER:HB3	1.54	0.89
1:1:437:TRP:HB3	2:2:92:GLY:HA3	1.55	0.88
3:3:738:THR:HG22	3:3:740:PHE:H	1.39	0.88
22:N:112:LEU:HG	22:N:118:PRO:HB3	1.55	0.88
17:I:64:LEU:HD12	17:I:77:ARG:O	1.78	0.88
12:D:161:ALA:HB3	52:Y:236:HOH:O	59.38	0.88
3:3:186:ARG:HD3	3:3:229:ILE:HG22	1.55	0.88
18:J:16:ARG:HB2	18:J:19:THR:HG22	1.58	0.87
5:5:5:ARG:HG3	5:5:5:ARG:HH11	1.37	0.87
10:B:12:GLU:HG2	10:B:17:VAL:N	1.90	0.87
11:C:129:MET:HE1	11:C:181:PHE:HD2	1.39	0.87
18:J:29:LEU:HD21	19:K:34:SER:HB2	70.16	0.86
1:1:149:ILE:HD13	1:1:171:LEU:HB3	1.57	0.86
4:4:96:ALA:HB2	4:4:346:THR:HG21	1.58	0.86
3:3:237:ASP:OD1	3:3:239:THR:HG22	1.75	0.86
17:I:52:ARG:HB3	17:I:52:ARG:HH11	4.57	0.86
18:J:17:THR:CG2	19:K:24:TRP:HZ2	63.38	0.85
1:1:242:GLY:HA2	1:1:268:MET:O	1.76	0.85
3:3:561:PRO:HB3	3:3:576:ALA:HA	1.58	0.85
6:6:46:CYS:HB3	6:6:81:ALA:HB1	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:145:GLU:CD	33:Y:25:LYS:HE2	65.92	0.85
21:M:78:LEU:HB2	21:M:79:PRO:HD3	1.58	0.85
3:3:494:LYS:O	3:3:498:GLU:HG2	1.76	0.84
3:3:116:PRO:O	3:3:117:LEU:HB2	1.78	0.84
4:4:367:ARG:HH11	4:4:367:ARG:HG2	1.43	0.84
33:Y:65[B]:MET:HE1	33:Y:92:GLU:HA	1.59	0.84
47:D:501:HEC:HBC3	52:Y:308:HOH:O	51.70	0.84
1:1:293:GLY:HA3	1:1:324:GLY:H	1.42	0.84
3:3:522:ARG:NH1	3:3:681:LYS:HE3	1.92	0.84
1:1:118:MET:HG2	1:1:224:LEU:HD13	1.60	0.83
9:A:408:ARG:CZ	19:K:15:ARG:HG2	78.64	0.83
5:5:52:ILE:HG21	5:5:114:LEU:HB3	1.57	0.83
6:6:83:ARG:NH1	6:6:83:ARG:HG3	1.93	0.83
10:B:236:LYS:HD2	10:B:236:LYS:H	4.86	0.83
52:A:4099:HOH:O	19:K:15:ARG:CZ	84.88	0.82
7:7:101:LYS:HE2	7:7:101:LYS:HA	1.60	0.82
1:1:185:GLU:HB2	1:1:218:ILE:HD12	1.62	0.82
3:3:515:THR:HG23	3:3:683:LEU:HD12	1.60	0.82
17:I:36:ALA:HB2	17:I:73:PRO:HD2	1.61	0.82
1:1:246:SER:HB3	1:1:268:MET:HG2	1.62	0.82
17:I:52:ARG:HB3	17:I:52:ARG:NH1	4.82	0.82
10:B:95:LYS:CB	17:I:32:ALA:HB2	2.26	0.81
9:A:29:GLN:HB3	10:B:12:GLU:O	2.16	0.81
33:Y:72:LYS:HD2	52:Y:358:HOH:O	1.79	0.81
15:G:72:LYS:HG3	16:H:56:GLU:OE2	3.82	0.81
26:R:5:LYS:HZ3	26:R:6:GLY:N	1.77	0.81
12:D:145:GLU:CG	52:Y:269:HOH:O	68.28	0.81
3:3:501:LYS:HD2	3:3:501:LYS:H	1.43	0.81
18:J:25:VAL:HG11	19:K:30:VAL:HG11	72.68	0.81
3:3:642:ALA:HB1	3:3:652:PRO:HG3	1.63	0.81
3:3:384:PRO:HG3	3:3:542:ARG:HH21	1.45	0.81
4:4:212:PRO:HB2	4:4:213:ILE:HD12	1.63	0.80
4:4:363:SER:HB2	5:5:174:LEU:H	1.46	0.80
12:D:74:PRO:HG3	12:D:80:MET:HE1	1.62	0.80
1:1:344:LEU:O	1:1:347:PHE:HB3	1.80	0.80
52:A:4099:HOH:O	19:K:15:ARG:NH2	85.64	0.80
27:S:39:CYS:SG	27:S:53:CYS:HB3	2.22	0.79
4:4:310:THR:HG22	4:4:311:PRO:O	1.83	0.79
3:3:279:ALA:HB2	3:3:290:ILE:HG12	1.64	0.79
4:4:254:TYR:HD1	4:4:255:SER:H	1.30	0.79
27:S:75:ARG:HG2	27:S:75:ARG:HH11	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:171:SER:HB2	3:3:172:PRO:HD2	1.64	0.79
9:A:2:ALA:HB1	9:A:6:GLN:HB2	1.65	0.79
5:5:186:GLY:HA2	5:5:190:LYS:HD3	1.65	0.79
27:S:39:CYS:SG	27:S:53:CYS:CB	2.70	0.79
10:B:200:THR:CB	10:B:229:GLY:HA2	5.62	0.79
3:3:370:ASP:OD1	3:3:551:PRO:HD3	1.82	0.79
5:5:47:ASN:ND2	5:5:47:ASN:H	1.80	0.79
4:4:222:GLY:HA3	4:4:396:ILE:HD11	1.63	0.78
12:D:110:PRO:HG3	47:D:501:HEC:HMD3	1.95	0.78
18:J:16:ARG:NH1	18:J:19:THR:HG21	1.99	0.78
5:5:47:ASN:H	5:5:47:ASN:HD22	1.32	0.78
4:4:104:LEU:O	5:5:193:ARG:HD2	1.84	0.78
9:A:1:THR:HG21	10:B:212:SER:CB	2.13	0.78
1:1:162:LEU:O	1:1:165:THR:HG22	1.84	0.78
18:J:13:LEU:O	18:J:19:THR:HG23	1.90	0.78
3:3:55:PRO:HB3	3:3:73:ILE:HA	1.66	0.78
33:Y:17:CYS:HG	44:Y:500:HEM:CAC	1.98	0.77
3:3:194:VAL:HB	3:3:195:PRO:HD3	1.66	0.77
12:D:145:GLU:OE2	52:Y:247:HOH:O	68.87	0.77
8:8:26:TYR:N	8:8:27:PRO:HD3	1.98	0.77
4:4:213:ILE:H	4:4:213:ILE:HD12	1.48	0.77
7:7:8:GLU:HG2	7:7:97:TYR:CZ	2.19	0.77
26:R:5:LYS:NZ	26:R:6:GLY:H	1.78	0.77
3:3:655:ARG:HB2	3:3:655:ARG:HH11	1.47	0.77
17:I:32:ALA:N	17:I:71:ASN:HB3	1.99	0.76
10:B:47:ILE:HG21	10:B:120:MET:HE3	1.68	0.76
3:3:542:ARG:HH11	3:3:542:ARG:HB2	1.51	0.76
18:J:29:LEU:HD22	19:K:34:SER:HB2	71.25	0.76
4:4:261:THR:N	4:4:292:GLN:HE22	1.83	0.76
7:7:121:ARG:HH11	7:7:121:ARG:HG3	1.50	0.76
4:4:105:LEU:HD13	4:4:309:ILE:HD13	1.67	0.76
22:N:187:THR:HG21	26:R:68:THR:HG21	1.68	0.76
21:M:59:GLN:H	21:M:62:GLU:HG3	1.51	0.75
1:1:358:PRO:HD3	3:3:107:MET:CE	2.16	0.75
3:3:194:VAL:HG12	3:3:411:LEU:HD22	1.66	0.75
3:3:184:CYS:SG	3:3:184:CYS:O	2.45	0.75
4:4:346:THR:HG23	4:4:353:LEU:HB3	1.69	0.75
3:3:218:LEU:N	3:3:219:PRO:HD3	2.01	0.75
5:5:5:ARG:HG3	5:5:5:ARG:NH1	2.00	0.75
3:3:509:ALA:HB1	3:3:768:GLY:HA3	1.68	0.75
5:5:66:GLU:HG2	5:5:95:PRO:CA	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:402:PRO:HA	3:3:535:MET:CE	2.17	0.74
4:4:274:ASP:O	4:4:278:VAL:HG23	1.87	0.74
11:C:379:TRP:CZ3	14:F:33:ARG:HD3	2.28	0.74
3:3:101:ARG:NH1	3:3:140:TYR:CD1	2.55	0.74
4:4:261:THR:H	4:4:292:GLN:HE22	1.34	0.74
3:3:384:PRO:HG3	3:3:542:ARG:NH2	2.01	0.74
18:J:3:PRO:HB2	18:J:8:ARG:NH1	3.25	0.74
21:M:184:LEU:HD11	21:M:211:LEU:HD21	1.69	0.74
9:A:408:ARG:NH2	19:K:15:ARG:CG	78.57	0.74
3:3:405:GLU:HB2	3:3:535:MET:CE	2.17	0.74
9:A:3:THR:OG1	9:A:6:GLN:HG3	1.87	0.74
2:2:101:THR:HG22	7:7:108:ILE:HD11	1.69	0.74
1:1:40:THR:O	1:1:44:VAL:HG23	1.87	0.74
10:B:71:LEU:HD23	17:I:68:VAL:HG21	1.70	0.73
4:4:47:LEU:HD12	4:4:48:SER:N	2.03	0.73
2:2:101:THR:HG23	2:2:106:ILE:O	1.87	0.73
3:3:156:ARG:HG3	3:3:156:ARG:HH11	1.53	0.73
3:3:567:TYR:HA	3:3:584:VAL:HG23	1.69	0.73
23:O:23:PRO:O	24:P:66:ARG:HD3	1.89	0.73
17:I:32:ALA:N	17:I:71:ASN:CB	2.51	0.73
6:6:77:VAL:HG22	6:6:104:TRP:HB2	1.69	0.73
11:C:129:MET:HE1	11:C:181:PHE:CD2	2.24	0.73
11:C:129:MET:CE	11:C:181:PHE:HD2	2.02	0.73
1:1:50:PRO:O	1:1:53:VAL:HG12	1.89	0.73
26:R:54:ARG:HD3	26:R:54:ARG:N	2.04	0.73
6:6:148:ILE:HG21	8:8:27:PRO:HG3	1.71	0.72
3:3:20:MET:CE	3:3:432:PHE:HB2	2.18	0.72
18:J:16:ARG:HH11	18:J:19:THR:HG21	1.92	0.72
2:2:81:GLN:HB3	2:2:122:VAL:HG21	1.70	0.72
5:5:10:ALA:HB1	5:5:15:TYR:HB2	1.72	0.72
16:H:28:GLU:O	16:H:31:VAL:HG22	1.92	0.72
4:4:126:LEU:HD21	4:4:286:SER:HB2	1.71	0.72
47:D:501:HEC:HBC2	52:Y:308:HOH:O	52.30	0.72
4:4:262:PHE:CE1	4:4:289:ILE:HD11	2.24	0.72
9:A:352:SER:HB3	14:F:110:LYS:HD2	77.71	0.72
1:1:253:GLN:HE21	1:1:253:GLN:N	1.87	0.72
19:K:18:VAL:HB	19:K:19:PRO:HD3	1.95	0.72
8:8:96:LEU:HD21	8:8:129:LEU:HD13	1.71	0.72
6:6:163:TYR:HB2	8:8:152:ARG:NH1	2.05	0.72
3:3:55:PRO:HB3	3:3:73:ILE:CA	2.18	0.71
14:F:13:LEU:O	14:F:16:ILE:HG12	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:J:16:ARG:HB2	18:J:16:ARG:HH11	1.55	0.71
1:1:253:GLN:HE21	1:1:253:GLN:H	1.39	0.71
33:Y:17:CYS:SG	44:Y:500:HEM:CAC	2.78	0.71
8:8:40:ARG:HB2	8:8:121:MET:HE1	1.73	0.71
13:E:113:GLU:HB3	13:E:116:GLN:NE2	2.05	0.71
9:A:408:ARG:HH22	19:K:15:ARG:HB2	77.27	0.71
39:1:440:FMN:N1	39:1:440:FMN:O3'	2.20	0.71
16:H:43:ARG:O	16:H:47:ARG:HD2	1.89	0.71
3:3:583:VAL:CG2	3:3:598:ALA:HA	2.21	0.71
6:6:108:MET:HA	6:6:137:VAL:CG1	2.21	0.71
4:4:371:ARG:NH1	5:5:50:ALA:O	2.24	0.71
3:3:11:VAL:CG1	3:3:25:HIS:HD2	2.00	0.71
1:1:90:ILE:HD11	1:1:211:LEU:HD22	1.72	0.71
23:O:147:LYS:HE3	23:O:147:LYS:HA	1.72	0.70
20:L:11:ASN:HD22	20:L:14:ASP:H	1.39	0.70
4:4:318:GLU:HB2	7:7:39:ASP:HA	1.73	0.70
1:1:395:GLU:HB2	1:1:407:VAL:HG21	1.72	0.70
10:B:231:GLY:N	10:B:233:SER:H	1.90	0.70
2:2:106:ILE:HG23	2:2:110:GLU:HB2	1.73	0.70
21:M:13:THR:HB	21:M:168:LEU:HD23	1.74	0.70
3:3:386:SER:HB2	3:3:675:ARG:HH12	1.57	0.70
12:D:145:GLU:HG2	52:Y:269:HOH:O	68.55	0.69
9:A:136:GLN:HE21	17:I:51:CYS:CB	2.04	0.69
6:6:77:VAL:HA	6:6:104:TRP:O	1.92	0.69
2:2:27:ILE:O	2:2:31:LEU:HD23	1.92	0.69
3:3:402:PRO:HA	3:3:535:MET:HE1	1.74	0.69
12:D:74:PRO:HG3	12:D:80:MET:CE	2.27	0.69
9:A:352:SER:HB3	14:F:110:LYS:CD	78.62	0.69
1:1:267:PRO:O	1:1:270:THR:HG23	1.93	0.69
2:2:144:CYS:O	2:2:149:ARG:HD2	1.93	0.69
4:4:254:TYR:CE2	4:4:346:THR:HA	2.27	0.69
5:5:29:LEU:O	5:5:92:VAL:HG12	1.93	0.69
3:3:737:GLU:HB2	3:3:776:LEU:HD21	1.74	0.68
4:4:272:VAL:HG23	4:4:399:SER:HB3	1.74	0.68
3:3:261:VAL:HG22	38:3:786:SF4:S2	2.33	0.68
22:N:154:GLY:HA2	25:Q:6:VAL:HG22	1.75	0.68
22:N:156:ARG:HH11	22:N:156:ARG:HG3	1.56	0.68
10:B:229:GLY:C	10:B:231:GLY:N	4.49	0.68
10:B:353:SER:HB3	10:B:355:PRO:HD2	1.76	0.68
8:8:71:GLU:HB2	8:8:90:VAL:HB	1.74	0.68
1:1:219:ASN:ND2	39:1:440:FMN:O2P	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:49:THR:HG23	1:1:52:GLU:HG3	1.75	0.68
1:1:18:TYR:OH	1:1:105:TYR:HB2	1.94	0.68
13:E:79:SER:HB3	13:E:191:ASP:OD2	2.15	0.68
22:N:12:ASN:HD22	29:U:20:VAL:H	1.39	0.68
9:A:29:GLN:HG3	9:A:203:LEU:O	2.00	0.68
5:5:47:ASN:N	5:5:47:ASN:HD22	1.87	0.68
3:3:2:VAL:CG1	3:3:89:ASP:HA	2.24	0.68
5:5:123:GLY:H	5:5:147:ARG:NH1	1.92	0.68
10:B:236:LYS:CD	10:B:236:LYS:H	4.10	0.68
1:1:363:VAL:HA	1:1:367:MET:HB2	1.76	0.68
5:5:145:PRO:HA	5:5:150:TYR:CD1	2.27	0.68
17:I:36:ALA:CB	17:I:73:PRO:HD2	2.23	0.68
2:2:110:GLU:HA	7:7:121:ARG:HH12	1.59	0.68
1:1:104:ARG:HD2	1:1:108:GLU:OE2	1.94	0.67
6:6:108:MET:HA	6:6:137:VAL:HG13	1.75	0.67
9:A:32:GLN:OE1	10:B:373:GLU:HB2	2.56	0.67
27:S:38:ARG:HG2	27:S:85:ILE:HG23	1.77	0.67
4:4:85:MET:CE	4:4:409:ARG:HB2	2.24	0.67
20:L:151:HIS:O	20:L:155:VAL:HG23	1.95	0.67
13:E:113:GLU:HB3	13:E:116:GLN:HE21	1.55	0.67
4:4:372:ALA:HB1	4:4:406:ASP:OD1	1.94	0.67
10:B:95:LYS:HB2	17:I:32:ALA:CB	2.41	0.67
2:2:134:ILE:HG13	2:2:145:VAL:HG21	1.77	0.67
1:1:16:THR:CG2	1:1:229:PRO:HB3	2.22	0.67
24:P:43:PRO:HB2	24:P:48:ILE:HD11	1.76	0.67
3:3:378:PRO:O	3:3:381:LEU:HB2	1.93	0.67
10:B:169:ARG:HG3	10:B:240:HIS:HB2	1.84	0.67
18:J:25:VAL:CG1	19:K:30:VAL:HG11	72.61	0.67
33:Y:65[B]:MET:CE	33:Y:92:GLU:HA	2.24	0.67
9:A:2:ALA:O	10:B:113:ARG:NE	2.28	0.67
8:8:40:ARG:HB2	8:8:121:MET:CE	2.25	0.67
15:G:60:THR:O	15:G:64:GLN:HG3	1.95	0.67
12:D:161:ALA:CB	52:Y:236:HOH:O	60.08	0.67
3:3:216:PHE:CZ	7:7:128:PHE:HD2	2.13	0.66
52:A:4185:HOH:O	17:I:73:PRO:HG3	1.94	0.66
1:1:110:VAL:N	1:1:111:PRO:HD3	2.11	0.66
3:3:42:ILE:HD11	3:3:189:ARG:CD	2.26	0.66
12:D:75:ASN:HD21	12:D:79:GLU:HG2	5.37	0.66
18:J:29:LEU:CG	19:K:34:SER:HB2	71.78	0.66
10:B:95:LYS:HD3	10:B:110:GLU:OE2	1.94	0.66
31:W:19:TRP:HZ2	32:X:14:GLU:HG2	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:298:ASP:HB2	20:L:301:THR:HG23	1.77	0.66
3:3:405:GLU:OE1	3:3:508:GLY:HA3	1.95	0.66
1:1:437:TRP:CB	2:2:92:GLY:HA3	2.25	0.66
23:O:24:LEU:H	24:P:34:ASN:HD21	1.44	0.66
18:J:8:ARG:HH11	18:J:8:ARG:HG2	2.08	0.66
3:3:538:ALA:HB3	3:3:541:ALA:HB2	1.75	0.66
12:D:145:GLU:CD	33:Y:25:LYS:CE	65.14	0.66
21:M:186:SER:HB3	21:M:213:LEU:HD22	1.76	0.66
22:N:209:ILE:O	22:N:213:THR:HG23	1.95	0.66
5:5:66:GLU:CG	5:5:95:PRO:HA	2.19	0.66
3:3:738:THR:HG23	3:3:739:PRO:HD2	1.77	0.66
9:A:86:LEU:HD13	9:A:99:ILE:HG12	1.77	0.66
22:N:101:PHE:HZ	22:N:260:GLY:HA3	1.61	0.65
3:3:591:HIS:ND1	3:3:592:PRO:HD2	2.11	0.65
1:1:370:LEU:O	1:1:374:ILE:HG22	1.96	0.65
22:N:160:LEU:HD13	22:N:222:GLN:HG2	1.78	0.65
3:3:578:LYS:HG2	3:3:597:TYR:HE2	1.62	0.65
14:F:13:LEU:HA	14:F:16:ILE:HG12	2.68	0.65
3:3:54:LEU:N	3:3:55:PRO:CD	2.60	0.65
4:4:279:ARG:HH11	4:4:279:ARG:HG3	1.60	0.65
1:1:115:ILE:O	1:1:119:ILE:HG13	1.97	0.65
9:A:408:ARG:HH22	19:K:15:ARG:CB	77.53	0.65
31:W:45:LEU:HD21	32:X:40:TYR:HA	1.78	0.65
20:L:172:LYS:NZ	20:L:172:LYS:HB2	2.12	0.65
3:3:285:VAL:HG22	3:3:286:ASN:H	1.61	0.65
10:B:365:LYS:HG2	10:B:399:LEU:HD22	1.86	0.65
10:B:95:LYS:HD2	17:I:32:ALA:HB2	1.79	0.65
3:3:739:PRO:HG2	3:3:771:VAL:CG1	2.27	0.65
18:J:16:ARG:HH11	18:J:16:ARG:CB	2.10	0.65
3:3:20:MET:HE1	3:3:432:PHE:HB2	1.78	0.64
4:4:85:MET:HE3	4:4:409:ARG:HB2	1.78	0.64
4:4:98:ALA:O	4:4:102:GLU:HG3	1.97	0.64
27:S:39:CYS:HG	27:S:53:CYS:HG	0.71	0.64
3:3:722:THR:HG21	3:3:756:GLY:N	2.12	0.64
3:3:206:GLY:O	3:3:209:THR:HG23	1.98	0.64
17:I:36:ALA:HB3	17:I:73:PRO:HG2	1.78	0.64
15:G:71:ARG:HH11	15:G:72:LYS:HZ2	8.53	0.64
3:3:671:GLU:HG2	3:3:672:ALA:H	1.62	0.64
18:J:16:ARG:HB2	18:J:19:THR:CG2	2.26	0.64
21:M:120:SER:OG	21:M:138:VAL:HG21	1.97	0.64
10:B:231:GLY:N	10:B:232:LEU:N	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:16:THR:HG21	1:1:229:PRO:CB	2.25	0.64
3:3:279:ALA:CB	3:3:290:ILE:HG12	2.28	0.64
5:5:47:ASN:HD21	5:5:76:SER:HA	1.61	0.64
1:1:299:PRO:HG3	1:1:341:MET:HE3	1.80	0.64
2:2:26:ALA:O	2:2:29:PRO:HG2	1.97	0.64
1:1:350:HIS:O	3:3:205:ARG:NH1	2.31	0.64
10:B:412:ASN:HA	10:B:415:LYS:HD2	1.80	0.64
2:2:122:VAL:HG12	2:2:123:GLU:N	2.12	0.64
2:2:106:ILE:CG2	2:2:110:GLU:HB2	2.27	0.64
12:D:75:ASN:ND2	12:D:79:GLU:HG2	5.99	0.64
13:E:45:VAL:HG13	18:J:28:ALA:HA	1.80	0.64
16:H:25:GLU:HG2	16:H:34:ARG:HH22	1.62	0.64
5:5:18:GLU:HB2	5:5:26:TRP:HB2	1.80	0.63
1:1:120:LEU:HD13	1:1:227:VAL:HG12	1.79	0.63
20:L:195:LEU:HD23	20:L:245:ILE:HD13	1.79	0.63
7:7:10:TYR:O	7:7:14:VAL:HG23	1.98	0.63
1:1:357:THR:N	1:1:358:PRO:HD2	2.12	0.63
3:3:739:PRO:HG2	3:3:771:VAL:HG12	1.79	0.63
6:6:36:LEU:HD22	6:6:77:VAL:HG21	1.79	0.63
13:E:190:ASP:HB2	13:E:192:MET:HG2	3.72	0.63
3:3:30:VAL:CG2	3:3:31:PRO:HD2	2.28	0.63
3:3:184:CYS:O	38:3:785:SF4:S3	2.57	0.63
24:P:82:TYR:HB3	24:P:83:PRO:HD3	1.81	0.63
9:A:136:GLN:NE2	17:I:51:CYS:HB3	2.15	0.63
4:4:59:ILE:HD11	5:5:135:ILE:HG23	1.79	0.63
8:8:56:CYS:SG	8:8:58:LEU:HB2	2.39	0.63
27:S:57:ARG:HH11	27:S:57:ARG:HB3	1.64	0.63
3:3:55:PRO:CB	3:3:73:ILE:HA	2.29	0.63
23:O:16:TYR:CE1	23:O:25:PRO:HG3	2.34	0.63
6:6:96:TRP:HA	6:6:99:MET:HE3	1.80	0.63
3:3:101:ARG:NH1	3:3:140:TYR:CE1	2.67	0.62
3:3:285:VAL:HG22	3:3:286:ASN:N	2.14	0.62
14:F:28:LYS:HE3	52:F:4052:HOH:O	1.98	0.62
11:C:29:SER:HB2	48:G:2004:CDL:HA31	1.81	0.62
4:4:230:ILE:O	4:4:230:ILE:HG22	2.00	0.62
9:A:51:LYS:H	9:A:51:LYS:HZ1	1.47	0.62
19:K:26:ALA:O	19:K:30:VAL:HG23	2.25	0.62
3:3:117:LEU:HD12	4:4:321:MET:CE	2.28	0.62
4:4:367:ARG:HG2	4:4:367:ARG:NH1	2.10	0.62
1:1:253:GLN:HG2	1:1:327:GLY:HA2	1.81	0.62
2:2:33:ARG:HH21	2:2:37:GLU:HG2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:397:ARG:HD2	1:1:397:ARG:N	2.14	0.62
3:3:154:TYR:CZ	4:4:312:PRO:HB3	2.34	0.62
5:5:59:THR:HG22	5:5:59:THR:O	1.99	0.62
4:4:47:LEU:HD12	4:4:48:SER:H	1.63	0.62
8:8:44:THR:HA	8:8:138:VAL:HG13	1.80	0.62
21:M:16:ILE:HD12	21:M:17:MET:N	2.15	0.62
3:3:736:VAL:HG22	3:3:775:VAL:HG22	1.80	0.62
4:4:190:LEU:O	4:4:194:LEU:HB2	1.99	0.62
2:2:114:ASP:HB2	2:2:116:LEU:CD2	2.26	0.62
33:Y:72:LYS:HD3	33:Y:78:THR:HG22	1.82	0.62
4:4:393:MET:HA	4:4:396:ILE:HG22	1.81	0.62
2:2:10:PHE:CZ	2:2:33:ARG:HG3	2.34	0.62
3:3:545:GLU:HA	3:3:550:LEU:HD11	1.81	0.62
6:6:76:ASP:O	6:6:77:VAL:HB	2.00	0.62
3:3:583:VAL:HG21	3:3:598:ALA:HA	1.80	0.62
20:L:128:VAL:O	20:L:128:VAL:HG22	1.99	0.62
1:1:104:ARG:NH2	2:2:127:SER:CB	2.57	0.62
18:J:3:PRO:HD2	18:J:8:ARG:CZ	2.30	0.62
6:6:154:LEU:O	6:6:158:VAL:HG13	1.99	0.62
4:4:89:HIS:CE1	4:4:92:ALA:HB2	2.35	0.62
12:D:60:GLU:HG3	18:J:62:LYS:NZ	9.91	0.61
3:3:346:ALA:HB2	3:3:569:GLY:O	1.99	0.61
9:A:408:ARG:NH1	19:K:15:ARG:CG	79.44	0.61
4:4:64:THR:OG1	6:6:83:ARG:NH1	2.33	0.61
6:6:143:ARG:HG2	6:6:144:PRO:HD2	1.82	0.61
13:E:113:GLU:CB	13:E:116:GLN:HE21	2.13	0.61
3:3:185:LYS:HG3	3:3:202:PHE:HE2	1.65	0.61
10:B:296:TYR:OH	17:I:52:ARG:NE	4.56	0.61
1:1:266:LEU:HB3	1:1:270:THR:HG21	1.83	0.61
18:J:14:PHE:HA	18:J:20:PHE:HD1	1.64	0.61
6:6:153:GLN:HG3	8:8:124:TYR:OH	2.00	0.61
3:3:333:LEU:HB3	3:3:648:LEU:HD21	1.82	0.61
32:X:13:LYS:H	32:X:13:LYS:HD3	1.65	0.61
33:Y:65[B]:MET:SD	33:Y:95:ILE:HD12	2.40	0.61
20:L:11:ASN:HD21	20:L:13:LYS:HB2	1.64	0.61
3:3:259:CYS:SG	3:3:261:VAL:HG13	2.40	0.61
22:N:154:GLY:HA2	25:Q:6:VAL:CG2	2.30	0.61
3:3:282:VAL:HG22	3:3:285:VAL:HG12	1.80	0.61
4:4:83:PRO:HB2	4:4:169:HIS:HA	1.82	0.61
3:3:305:ARG:HH22	3:3:609:GLU:CD	2.04	0.61
21:M:122:MET:HB2	21:M:208:PRO:HD2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:92:MET:CE	20:L:167:THR:HG21	2.31	0.61
3:3:435:LEU:H	3:3:435:LEU:HD22	1.65	0.61
1:1:66:GLY:O	40:1:441:NAI:H2N	2.01	0.61
3:3:722:THR:HG21	3:3:756:GLY:H	1.66	0.61
7:7:34:GLU:HB3	7:7:56:THR:HG22	1.83	0.61
10:B:47:ILE:HG21	10:B:120:MET:CE	2.30	0.61
8:8:73:ALA:HB2	8:8:89:LYS:HB2	1.80	0.61
12:D:116:ILE:HG12	47:D:501:HEC:HMA3	1.83	0.61
1:1:270:THR:O	1:1:311:MET:HG3	2.00	0.61
1:1:385:GLU:O	1:1:388:GLU:HB3	2.00	0.61
3:3:304:ASN:O	3:3:589:HIS:CD2	2.54	0.61
22:N:192:VAL:O	22:N:196:THR:HB	2.01	0.61
10:B:397:THR:O	10:B:401:GLN:HG3	2.00	0.61
1:1:356:CYS:HB3	1:1:358:PRO:HD2	1.83	0.61
3:3:453:PRO:HD3	3:3:468:HIS:CE1	2.36	0.61
22:N:148:HIS:O	22:N:152:MET:HG3	2.01	0.61
25:Q:13:ALA:O	25:Q:18:ARG:HD2	2.00	0.61
10:B:227:ARG:C	10:B:229:GLY:N	4.24	0.60
1:1:267:PRO:HG2	1:1:270:THR:HG22	1.83	0.60
3:3:615:VAL:HG22	3:3:621:VAL:HG12	1.82	0.60
2:2:78:TYR:HA	2:2:137:ASN:HD21	1.66	0.60
1:1:145:LEU:O	1:1:149:ILE:HG13	2.01	0.60
21:M:59:GLN:HA	21:M:62:GLU:HB2	1.83	0.60
33:Y:52[B]:ASN:C	33:Y:52[B]:ASN:HD22	2.04	0.60
27:S:39:CYS:HG	27:S:53:CYS:CB	2.07	0.60
17:I:36:ALA:HB3	17:I:73:PRO:CG	2.31	0.60
3:3:655:ARG:HB2	3:3:655:ARG:NH1	2.16	0.60
5:5:37:GLU:O	5:5:41:TYR:HD1	1.84	0.60
18:J:16:ARG:CG	18:J:16:ARG:HH11	2.12	0.60
10:B:35:ILE:HD12	10:B:35:ILE:N	2.27	0.60
6:6:83:ARG:HH11	6:6:83:ARG:CG	1.97	0.60
18:J:25:VAL:HG12	19:K:30:VAL:CG1	73.01	0.60
3:3:116:PRO:O	3:3:117:LEU:CB	2.49	0.60
4:4:250:LYS:CE	4:4:262:PHE:HB3	2.31	0.60
1:1:88:TYR:HB2	1:1:216:THR:HG22	1.84	0.60
3:3:2:VAL:HG13	3:3:89:ASP:HA	1.83	0.60
20:L:92:MET:HE2	20:L:167:THR:HG21	1.84	0.60
9:A:296:SER:O	9:A:300:THR:HG23	2.02	0.60
49:L:516:HEA:HBC1	49:L:516:HEA:HMC1	1.83	0.60
10:B:203:ARG:HH12	10:B:233:SER:HA	4.51	0.60
3:3:216:PHE:HZ	7:7:128:PHE:HD2	1.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:200:ARG:HG3	4:4:204:TYR:HE1	1.67	0.60
39:1:440:FMN:HO3'	39:1:440:FMN:C2	2.13	0.60
4:4:234:LEU:HD21	4:4:238:SER:HB2	1.84	0.60
4:4:226:PRO:HG3	4:4:242:SER:O	2.02	0.60
4:4:164:THR:OG1	4:4:170:HIS:HB3	2.02	0.60
3:3:385:ALA:HB2	3:3:531:LYS:HB3	1.84	0.60
3:3:513:GLN:HG2	3:3:769:LEU:HD23	1.84	0.60
9:A:41:ILE:HG12	9:A:195:MET:HG2	1.89	0.60
3:3:722:THR:HA	3:3:725:ALA:HB3	1.84	0.60
6:6:99:MET:HG2	6:6:100:PRO:HD2	1.84	0.60
4:4:149:ALA:HA	4:4:152:GLU:OE1	2.00	0.60
18:J:29:LEU:HD21	19:K:34:SER:HG	68.41	0.60
17:I:32:ALA:N	17:I:71:ASN:HB2	2.19	0.60
15:G:71:ARG:HH11	15:G:72:LYS:NZ	8.99	0.60
4:4:222:GLY:CA	4:4:396:ILE:HD11	2.32	0.60
32:X:28:LEU:HB2	32:X:29:PRO:HD3	1.84	0.60
21:M:193:TYR:HE1	23:O:126:MET:HE1	1.66	0.60
4:4:389:GLN:HG3	4:4:390:VAL:H	1.67	0.60
4:4:236:GLY:C	4:4:238:SER:H	2.05	0.59
25:Q:62:CYS:SG	25:Q:84:SER:OG	2.60	0.59
22:N:119:THR:O	26:R:52:HIS:HE1	1.84	0.59
4:4:221:VAL:O	4:4:272:VAL:HG12	2.02	0.59
3:3:337:ARG:HH12	3:3:581:ARG:NH1	2.00	0.59
1:1:138:TYR:HB3	1:1:141:ALA:HB3	1.84	0.59
3:3:515:THR:HG23	3:3:683:LEU:CD1	2.31	0.59
21:M:179:LEU:HD21	27:S:65:PRO:HD3	1.85	0.59
8:8:175:ALA:O	8:8:177:THR:HG23	2.02	0.59
3:3:583:VAL:HG21	3:3:597:TYR:O	2.02	0.59
2:2:149:ARG:NH1	2:2:168:LEU:HD13	2.16	0.59
3:3:586:HIS:CD2	3:3:604:ALA:HB2	2.37	0.59
9:A:172:GLU:OE2	9:A:176:LYS:HE3	2.06	0.59
1:1:374:ILE:HG12	1:1:374:ILE:O	2.02	0.59
1:1:301:PRO:HB2	1:1:303:THR:HG23	1.85	0.59
13:E:85:LYS:NZ	13:E:87:MET:SD	2.75	0.59
3:3:343:LEU:HD12	3:3:361:ALA:HB2	1.84	0.59
9:A:216:PHE:HD2	9:A:219:LEU:HD22	1.71	0.59
27:S:57:ARG:HG3	27:S:60:TYR:CE2	2.38	0.59
3:3:132:ASP:OD1	4:4:329:LYS:HE2	2.02	0.59
21:M:226:MET:O	21:M:227:LEU:HB2	2.02	0.59
4:4:163:VAL:HG22	4:4:164:THR:HG22	1.85	0.59
5:5:80:TRP:CE3	5:5:80:TRP:HA	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:N:6:HIS:HD2	22:N:8:TYR:H	1.49	0.59
12:D:43:MET:HE2	12:D:46:VAL:HG21	1.90	0.59
3:3:511:VAL:O	3:3:518:ALA:HB2	2.03	0.59
9:A:8:LEU:HD22	9:A:392:LEU:HB3	2.25	0.59
4:4:74:THR:HB	4:4:77:GLN:H	1.67	0.59
26:R:5:LYS:HZ3	26:R:5:LYS:HB3	1.66	0.59
4:4:40:VAL:O	4:4:40:VAL:HG22	2.03	0.59
18:J:3:PRO:HD2	18:J:8:ARG:NH2	2.18	0.59
13:E:77:LYS:HE3	13:E:79:SER:OG	2.03	0.59
11:C:145:VAL:HG21	45:C:2001:SMA:H6	1.84	0.59
15:G:45:ILE:HG22	15:G:46:LEU:HD12	1.85	0.58
3:3:156:ARG:HG3	3:3:156:ARG:NH1	2.15	0.58
31:W:46:LYS:O	31:W:47:LYS:HB2	2.02	0.58
20:L:273:MET:HG3	20:L:319:LYS:HZ1	1.67	0.58
5:5:34:PHE:HE1	5:5:38:MET:HE1	1.67	0.58
10:B:20:HIS:HB2	10:B:22:GLN:HG3	1.84	0.58
4:4:225:PRO:HG2	4:4:228:VAL:HB	1.85	0.58
3:3:123:ASP:HB2	3:3:236:LEU:HD13	1.85	0.58
7:7:121:ARG:NH1	7:7:121:ARG:HG3	2.18	0.58
1:1:397:ARG:HD2	1:1:397:ARG:H	1.68	0.58
1:1:33:LEU:HA	1:1:37:GLY:HA2	1.86	0.58
15:G:66:PHE:CZ	15:G:70:LYS:HD2	2.47	0.58
3:3:227:THR:HG21	3:3:237:ASP:HB2	1.86	0.58
6:6:163:TYR:HB2	8:8:152:ARG:HH11	1.68	0.58
30:V:43:SER:OG	30:V:45:VAL:HG12	2.04	0.58
9:A:373:THR:HB	9:A:374:PRO:HD3	1.92	0.58
3:3:279:ALA:HB2	3:3:290:ILE:CG1	2.31	0.58
10:B:309:VAL:HG23	10:B:326:THR:HG22	1.85	0.58
10:B:227:ARG:C	10:B:229:GLY:H	4.39	0.58
5:5:123:GLY:H	5:5:147:ARG:HH11	1.51	0.58
10:B:412:ASN:HD22	10:B:415:LYS:HD2	1.67	0.58
3:3:205:ARG:C	3:3:209:THR:HG22	2.24	0.58
9:A:347:THR:O	19:K:16:ASN:ND2	75.13	0.58
3:3:185:LYS:HG2	3:3:188:VAL:HG22	1.86	0.58
13:E:99:ARG:HB3	13:E:133:VAL:CG1	2.33	0.58
10:B:354:ASN:N	10:B:355:PRO:CD	2.66	0.58
3:3:42:ILE:HD11	3:3:189:ARG:HD2	1.85	0.58
20:L:184:PHE:H	20:L:256:HIS:HE1	1.52	0.58
20:L:404:THR:O	20:L:480:ARG:NH1	2.37	0.58
3:3:440:ARG:HG2	3:3:440:ARG:HH11	1.67	0.58
4:4:363:SER:HB2	5:5:174:LEU:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:189:VAL:HG23	52:B:3089:HOH:O	2.03	0.57
6:6:78:MET:HG3	6:6:78:MET:O	2.03	0.57
2:2:77:LYS:H	2:2:116:LEU:HA	1.68	0.57
3:3:370:ASP:OD1	3:3:374:ARG:HD3	2.03	0.57
33:Y:65[B]:MET:HE3	33:Y:92:GLU:HG2	1.85	0.57
1:1:214:LYS:O	1:1:216:THR:HG23	2.03	0.57
13:E:190:ASP:O	13:E:192:MET:HG2	2.05	0.57
9:A:51:LYS:H	9:A:51:LYS:NZ	2.03	0.57
3:3:398:VAL:HB	3:3:450:LEU:HD22	1.87	0.57
1:1:177:ALA:O	2:2:67:TYR:HB3	2.05	0.57
4:4:95:LEU:HG	4:4:99:LEU:HD23	1.87	0.57
18:J:29:LEU:CD1	19:K:34:SER:HB2	72.57	0.57
3:3:394:ASP:OD2	3:3:501:LYS:HB2	2.05	0.57
4:4:288:LYS:O	4:4:292:GLN:HB2	2.05	0.57
4:4:239:LEU:HD22	4:4:244:VAL:HB	1.87	0.57
1:1:6:LEU:HB2	1:1:241:MET:HA	1.86	0.57
3:3:689:LYS:HB2	3:3:772:GLU:HG2	1.85	0.57
9:A:30:SER:HA	10:B:18:PRO:HG3	2.88	0.57
3:3:583:VAL:HG23	3:3:598:ALA:HA	1.87	0.57
31:W:41:ARG:HG3	32:X:40:TYR:CE2	2.40	0.57
3:3:385:ALA:HB2	3:3:531:LYS:CB	2.35	0.57
5:5:34:PHE:HE1	5:5:38:MET:CE	2.18	0.57
4:4:144:THR:HB	4:4:145:PRO:HD3	1.84	0.57
21:M:189:PRO:HD2	28:T:54:TYR:OH	2.05	0.57
3:3:167:HIS:O	3:3:167:HIS:ND1	2.36	0.57
18:J:12:LEU:O	18:J:13:LEU:HD23	2.04	0.57
3:3:469:ARG:HG2	3:3:754:PRO:HB3	1.85	0.57
9:A:286:GLY:HA3	9:A:290:LEU:HD21	1.95	0.57
14:F:82:LYS:HE3	52:F:4032:HOH:O	2.04	0.57
27:S:71:THR:O	27:S:75:ARG:HD3	2.05	0.57
18:J:3:PRO:HB2	18:J:8:ARG:HD3	1.86	0.57
15:G:40:ARG:HB3	48:G:2004:CDL:HB32	1.85	0.57
3:3:607:PHE:HA	3:3:610:LYS:HE2	1.87	0.57
29:U:3:ASN:C	29:U:3:ASN:HD22	2.08	0.57
9:A:136:GLN:NE2	17:I:51:CYS:CB	2.67	0.56
17:I:62:ARG:O	17:I:78:TYR:HB3	2.07	0.56
3:3:567:TYR:HA	3:3:584:VAL:CG2	2.36	0.56
3:3:226:ILE:HD12	3:3:235:LEU:HD13	1.85	0.56
22:N:203:PHE:O	22:N:207:HIS:HD2	1.88	0.56
2:2:44:GLU:CD	2:2:44:GLU:H	2.09	0.56
3:3:140:TYR:CE2	3:3:142:LYS:HB3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:93:ALA:O	1:1:134:VAL:HA	2.05	0.56
21:M:132:GLU:HB3	21:M:137:GLU:HG3	1.87	0.56
10:B:95:LYS:CG	17:I:32:ALA:HB2	2.35	0.56
6:6:83:ARG:HD3	38:6:182:SF4:S4	2.46	0.56
4:4:211:SER:HB2	4:4:214:PHE:HB3	1.87	0.56
5:5:37:GLU:O	5:5:41:TYR:CD1	2.58	0.56
33:Y:69:GLU:HB2	33:Y:91[B]:ARG:NH1	2.20	0.56
3:3:6:VAL:HG13	3:3:23:VAL:HG22	1.88	0.56
3:3:204:GLU:O	3:3:209:THR:HB	2.06	0.56
3:3:440:ARG:HH11	3:3:440:ARG:CG	2.19	0.56
6:6:121:TYR:H	6:6:121:TYR:HD1	1.52	0.56
3:3:320:ALA:HB1	3:3:324:GLU:HB2	1.87	0.56
7:7:63:LEU:HD13	7:7:129:ALA:HB3	1.86	0.56
24:P:78:HIS:ND1	28:T:12:LEU:HD22	2.21	0.56
26:R:5:LYS:HD2	26:R:6:GLY:N	2.21	0.56
3:3:469:ARG:HG2	3:3:754:PRO:CB	2.35	0.56
8:8:41:HIS:HB3	8:8:113:ILE:HD11	1.88	0.56
1:1:28:THR:HG22	1:1:30:ASP:H	1.70	0.56
3:3:550:LEU:N	3:3:550:LEU:HD12	2.20	0.56
10:B:20:HIS:HB2	10:B:22:GLN:CG	2.36	0.56
3:3:11:VAL:CG1	3:3:25:HIS:CD2	2.81	0.56
15:G:71:ARG:HD3	15:G:72:LYS:HZ3	9.61	0.56
6:6:49:GLU:HA	6:6:49:GLU:OE1	2.05	0.56
18:J:25:VAL:HG11	19:K:30:VAL:CB	71.74	0.56
18:J:8:ARG:HH11	18:J:8:ARG:CG	2.37	0.56
15:G:30:PHE:O	15:G:34:ILE:HG12	2.06	0.56
4:4:138:LEU:HD13	4:4:146:PHE:CD1	2.41	0.56
6:6:83:ARG:H	6:6:83:ARG:HD3	1.71	0.55
4:4:25:VAL:HA	4:4:48:SER:HB3	1.88	0.55
3:3:694:LEU:HB3	3:3:762:ALA:HB2	1.88	0.55
13:E:90:LYS:HE2	13:E:93:GLY:HA2	1.87	0.55
3:3:474:ARG:HA	3:3:517:ALA:HB2	1.89	0.55
5:5:52:ILE:HG22	5:5:114:LEU:HB3	1.86	0.55
4:4:254:TYR:O	4:4:256:GLY:N	2.35	0.55
1:1:359:CYS:HA	1:1:363:VAL:HG13	1.87	0.55
15:G:34:ILE:HB	15:G:35:PRO:HD3	1.95	0.55
11:C:217:LYS:HG3	15:G:7:LEU:HD13	1.88	0.55
12:D:241:LYS:OXT	12:D:241:LYS:HD3	4.79	0.55
12:D:165:TYR:OH	33:Y:83:ALA:CB	63.67	0.55
5:5:53:VAL:HG13	5:5:71:VAL:HB	1.86	0.55
3:3:115:HIS:ND1	3:3:116:PRO:HD2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:112:THR:OG1	2:2:113:PRO:HD2	2.05	0.55
3:3:270:ARG:O	3:3:271:SER:HB2	2.06	0.55
22:N:42:LEU:HD13	29:U:45:TYR:CD2	2.41	0.55
21:M:111:THR:HG21	27:S:66:ILE:HD11	1.88	0.55
15:G:63:THR:O	15:G:67:GLU:HG2	2.06	0.55
1:1:373:LYS:HD3	1:1:383:ASP:OD2	2.06	0.55
3:3:47:MET:SD	3:3:107:MET:HB3	2.46	0.55
3:3:225:ASN:ND2	3:3:289:TRP:HB3	2.21	0.55
4:4:246:TYR:CD1	5:5:77:LEU:HD22	2.42	0.55
11:C:245:PHE:CD1	12:D:17:LEU:HD13	2.41	0.55
7:7:108:ILE:HD12	7:7:108:ILE:N	2.22	0.55
4:4:193:LEU:HD22	4:4:197:LEU:HG	1.88	0.55
14:F:63:LYS:HE2	52:G:1280:HOH:O	2.06	0.55
5:5:175:THR:HG23	5:5:178:ASP:CB	2.26	0.55
18:J:25:VAL:HG12	18:J:26:VAL:N	2.73	0.55
22:N:222:GLN:HA	22:N:222:GLN:HE21	1.72	0.55
3:3:507:LEU:HD22	3:3:511:VAL:HG11	1.88	0.55
13:E:188:THR:HG21	13:E:194:ILE:CD1	2.97	0.55
2:2:98:ASP:O	2:2:102:GLU:HB2	2.07	0.55
8:8:131:TYR:HB2	8:8:136:MET:HE2	1.87	0.55
20:L:95:PRO:HB2	22:N:11:VAL:HG13	1.87	0.55
3:3:30:VAL:HG22	3:3:31:PRO:HD2	1.87	0.55
4:4:263:ASP:O	4:4:265:PRO:HD3	2.07	0.55
9:A:364:ALA:HB2	17:I:33:ALA:HB1	1.95	0.55
4:4:320:SER:O	4:4:324:VAL:HG23	2.07	0.55
3:3:101:ARG:NH1	3:3:140:TYR:HD1	2.00	0.55
10:B:95:LYS:HD2	17:I:32:ALA:CB	2.36	0.55
7:7:8:GLU:HG2	7:7:97:TYR:CE2	2.42	0.55
3:3:34:CYS:HA	3:3:184:CYS:HB2	1.89	0.55
6:6:92:MET:HE1	6:6:127:VAL:HG13	1.89	0.55
10:B:229:GLY:O	10:B:230:LEU:HB2	4.57	0.55
4:4:213:ILE:N	4:4:213:ILE:HD12	2.20	0.55
19:K:32:LEU:O	19:K:33:VAL:C	2.46	0.55
3:3:456:ALA:HB3	3:3:459:MET:HG3	1.88	0.55
6:6:83:ARG:NH1	6:6:83:ARG:CG	2.64	0.54
3:3:402:PRO:HA	3:3:535:MET:HE3	1.90	0.54
1:1:184:GLU:CD	1:1:186:THR:HG22	2.28	0.54
16:H:25:GLU:CG	16:H:34:ARG:HH22	2.19	0.54
8:8:48:ASN:HB2	8:8:50:LEU:HD23	1.89	0.54
18:J:56:LYS:HG2	18:J:60:GLU:CD	2.39	0.54
22:N:151:LEU:HB2	22:N:159:MET:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:550:LEU:HD23	3:3:684:ARG:HH21	1.73	0.54
20:L:407:ASP:O	20:L:411:LYS:HG3	2.07	0.54
9:A:76:GLU:HG2	9:A:80:GLU:OE2	2.07	0.54
8:8:137:LEU:O	8:8:140:VAL:HG12	2.08	0.54
24:P:80:GLU:CD	24:P:80:GLU:H	2.10	0.54
13:E:191:ASP:N	13:E:191:ASP:OD1	2.99	0.54
4:4:233:GLY:HA2	5:5:48:PHE:HE1	1.71	0.54
6:6:165:GLU:HG2	8:8:148:ARG:NH1	2.22	0.54
4:4:409:ARG:NH2	5:5:117:GLU:OE2	2.40	0.54
33:Y:41:GLY:N	33:Y:52[A]:ASN:HD21	2.05	0.54
4:4:193:LEU:CD2	4:4:197:LEU:HG	2.38	0.54
3:3:715:GLU:H	3:3:761:SER:HB2	1.72	0.54
23:O:108:PRO:HG2	23:O:111:PHE:CE2	2.42	0.54
4:4:248:VAL:HB	4:4:347:GLU:HB2	1.89	0.54
7:7:82:ILE:HG23	7:7:95:ALA:HB3	1.90	0.54
3:3:113:LEU:HD12	3:3:157:PHE:HB2	1.90	0.54
11:C:100:ARG:HD2	11:C:100:ARG:C	2.35	0.54
5:5:53:VAL:CG1	5:5:71:VAL:HB	2.37	0.54
3:3:444:ARG:NH2	3:3:447:LYS:HG3	2.22	0.54
4:4:241:ALA:HB2	4:4:278:VAL:HG21	1.90	0.54
11:C:341:GLN:NE2	52:C:2099:HOH:O	2.39	0.54
3:3:629:ILE:HG22	3:3:630:GLU:N	2.23	0.54
1:1:98:PRO:HA	2:2:124:CYS:SG	2.48	0.54
3:3:546:ALA:HA	3:3:678:PHE:CE2	2.43	0.54
25:Q:55:LYS:HA	25:Q:74:LEU:O	2.08	0.54
3:3:318:VAL:HG12	3:3:319:GLU:N	2.23	0.54
1:1:376:THR:HG22	1:1:376:THR:O	2.07	0.54
10:B:314:ALA:HA	17:I:63:PRO:HD3	1.90	0.54
33:Y:65[B]:MET:CE	33:Y:95:ILE:HD12	2.38	0.54
6:6:163:TYR:HD2	8:8:152:ARG:NH1	2.05	0.54
28:T:63:MET:HB3	28:T:68:ILE:HD11	1.89	0.54
3:3:664:LEU:O	3:3:669:VAL:HG12	2.08	0.54
10:B:12:GLU:O	10:B:18:PRO:HD3	2.08	0.54
4:4:369:LYS:HG3	5:5:53:VAL:HG23	1.90	0.54
21:M:165:VAL:HB	21:M:170:LEU:HD12	1.90	0.54
4:4:337:PRO:O	4:4:361:GLY:HA2	2.07	0.54
1:1:406:ALA:O	1:1:410:VAL:HG23	2.08	0.54
21:M:136:LEU:HB3	21:M:193:TYR:HD2	1.73	0.53
6:6:42:GLY:O	6:6:43:LEU:HD23	2.07	0.53
9:A:30:SER:CA	10:B:18:PRO:HG3	3.40	0.53
3:3:55:PRO:HB3	3:3:73:ILE:N	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:452:ALA:O	3:3:454:TYR:N	2.42	0.53
25:Q:48:LEU:O	25:Q:50:PRO:HD3	2.08	0.53
24:P:41:LEU:HD12	24:P:41:LEU:O	2.08	0.53
5:5:121:LEU:HD13	5:5:146:LEU:HD23	1.91	0.53
2:2:28:MET:HB2	2:2:29:PRO:CD	2.38	0.53
21:M:203:ASN:HD22	21:M:206:PHE:HD2	1.55	0.53
17:I:72:VAL:HG13	17:I:73:PRO:HD2	1.92	0.53
18:J:25:VAL:CG1	19:K:30:VAL:CG1	72.19	0.53
18:J:25:VAL:CG1	19:K:30:VAL:HB	70.96	0.53
3:3:501:LYS:HD2	3:3:501:LYS:N	2.19	0.53
3:3:356:LEU:HD13	3:3:654:PHE:HB2	1.91	0.53
2:2:153:LEU:O	2:2:153:LEU:HD22	2.09	0.53
18:J:25:VAL:HG11	19:K:30:VAL:CG1	72.27	0.53
10:B:411:ILE:O	10:B:415:LYS:HG3	2.77	0.53
1:1:74:LEU:O	1:1:77:SER:HB3	2.09	0.53
1:1:161:ASN:ND2	1:1:166:ASP:HA	2.23	0.53
3:3:572:PRO:HG2	3:3:577:LEU:HD21	1.91	0.53
3:3:205:ARG:HG3	3:3:205:ARG:HH11	1.72	0.53
23:O:128:VAL:O	23:O:134:PHE:HB3	2.09	0.53
1:1:313:TYR:CE1	1:1:323:LEU:HD13	2.44	0.53
8:8:132:GLY:H	8:8:135:ASP:HB2	1.74	0.53
27:S:75:ARG:NH1	27:S:75:ARG:HG2	2.19	0.53
3:3:386:SER:HB2	3:3:675:ARG:NH1	2.22	0.53
10:B:353:SER:CB	10:B:355:PRO:HD2	2.38	0.53
4:4:283:MET:O	4:4:287:VAL:HG23	2.08	0.53
23:O:40:LEU:HD13	23:O:59:LEU:HD13	1.90	0.53
20:L:302:ARG:O	20:L:306:THR:HG23	2.09	0.53
16:H:41:ASP:O	16:H:45:SER:HB2	2.09	0.53
10:B:95:LYS:HG3	17:I:32:ALA:N	2.88	0.53
33:Y:41:GLY:HA2	33:Y:48:TYR:CZ	2.43	0.53
5:5:37:GLU:O	5:5:40:HIS:HB3	2.08	0.53
10:B:276:GLN:HG2	10:B:281:ALA:HB2	1.91	0.53
6:6:74:GLN:OE1	6:6:74:GLN:HA	2.09	0.53
4:4:213:ILE:H	4:4:213:ILE:CD1	2.20	0.53
5:5:87:ARG:O	5:5:88:PHE:HB3	2.09	0.53
3:3:136:GLU:HG2	5:5:189:ARG:HG3	1.91	0.53
25:Q:82:CYS:N	25:Q:86:GLY:O	2.41	0.53
7:7:20:MET:HE3	7:7:59:LEU:HG	1.89	0.53
3:3:645:ALA:HB3	3:3:652:PRO:HD3	1.91	0.53
6:6:96:TRP:O	6:6:99:MET:HB2	2.09	0.53
21:M:104:TRP:CG	21:M:203:ASN:HB2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:398:PRO:O	20:L:498:CYS:HB3	2.08	0.53
12:D:166:ASN:HB3	16:H:13:LEU:HD23	1.91	0.53
23:O:52:SER:OG	23:O:55:GLU:HG3	2.08	0.53
1:1:397:ARG:HG3	3:3:49:LEU:HD13	1.91	0.52
13:E:188:THR:HG21	13:E:194:ILE:HD12	2.92	0.52
4:4:327:HIS:HE1	8:8:107:ALA:O	1.92	0.52
10:B:294:SER:OG	10:B:343:GLN:NE2	2.42	0.52
3:3:31:PRO:HB3	3:3:47:MET:CE	2.20	0.52
5:5:5:ARG:CG	5:5:5:ARG:HH11	2.15	0.52
21:M:59:GLN:N	21:M:62:GLU:HG3	2.24	0.52
5:5:80:TRP:CD1	5:5:81:LYS:HG2	2.45	0.52
2:2:40:TRP:CH2	2:2:42:ARG:HG2	2.45	0.52
25:Q:8:THR:OG1	25:Q:11:GLU:HG2	2.10	0.52
9:A:206:ARG:HH11	9:A:206:ARG:HG3	1.76	0.52
6:6:163:TYR:CD1	6:6:169:ARG:HA	2.44	0.52
7:7:34:GLU:HB3	7:7:56:THR:CG2	2.40	0.52
13:E:90:LYS:CE	13:E:93:GLY:HA2	2.40	0.52
1:1:196:ARG:NH2	3:3:203:ILE:O	2.42	0.52
23:O:67:SER:OG	23:O:70:GLU:HG3	2.08	0.52
11:C:162:GLU:OE2	11:C:168:PHE:HD1	1.98	0.52
4:4:381:LEU:HD11	4:4:397:ILE:HG12	1.91	0.52
12:D:60:GLU:HG3	18:J:62:LYS:HZ3	9.25	0.52
3:3:466:GLU:CD	3:3:467:VAL:H	2.13	0.52
5:5:32:GLU:CD	5:5:32:GLU:H	2.13	0.52
12:D:145:GLU:OE1	52:Y:269:HOH:O	66.63	0.52
1:1:358:PRO:O	1:1:362:GLY:HA3	2.08	0.52
11:C:379:TRP:CE3	14:F:33:ARG:HD3	2.47	0.52
25:Q:51:SER:HB2	25:Q:91:LEU:HD11	1.90	0.52
6:6:116:GLY:O	8:8:97:ARG:NH1	2.42	0.52
22:N:18:LEU:HD22	22:N:22:LEU:HD22	1.92	0.52
20:L:225:GLY:HA3	22:N:112:LEU:HD13	1.92	0.52
26:R:8:HIS:O	26:R:10:GLY:N	2.42	0.52
3:3:600:VAL:HG12	3:3:602:LEU:CD1	2.40	0.52
5:5:161:GLU:CG	5:5:163:ARG:HH22	2.23	0.52
26:R:42:ARG:HH11	26:R:42:ARG:HG3	1.74	0.52
20:L:268:PHE:CZ	21:M:58:ALA:HA	2.44	0.52
8:8:144:LYS:HB2	8:8:145:PRO:HD2	1.92	0.52
4:4:123:LEU:HD13	4:4:290:ILE:HD12	1.92	0.52
3:3:31:PRO:CB	3:3:47:MET:HE3	2.21	0.52
10:B:46:ARG:HG2	10:B:379:LEU:HD22	3.88	0.52
3:3:218:LEU:H	3:3:219:PRO:HD3	1.71	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:363:VAL:O	1:1:368:VAL:HG12	2.09	0.52
1:1:29:LEU:HD23	1:1:112:HIS:CE1	2.45	0.52
24:P:63:SER:O	24:P:67:ILE:HG13	2.10	0.52
20:L:187:SER:HB2	20:L:277:MET:HE1	1.92	0.52
3:3:688:ARG:HB3	3:3:770:ARG:HB2	1.91	0.52
4:4:404:MET:HA	4:4:407:VAL:CG1	2.40	0.52
23:O:23:PRO:HD2	24:P:34:ASN:HD22	1.74	0.52
21:M:102:HIS:O	21:M:104:TRP:N	2.42	0.52
20:L:240:HIS:HB3	20:L:241:PRO:HD3	1.92	0.52
12:D:34:LYS:HE3	52:D:4097:HOH:O	2.09	0.52
2:2:76:GLY:H	2:2:118:SER:HB2	1.74	0.52
13:E:102:THR:O	13:E:106:ILE:HG13	2.09	0.52
13:E:77:LYS:HD3	13:E:80:ASP:OD2	2.31	0.52
3:3:42:ILE:HG22	3:3:43:GLY:H	1.75	0.52
4:4:245:ASN:O	5:5:79:GLY:HA3	2.09	0.52
26:R:2:SER:OG	26:R:3:ALA:N	2.41	0.52
3:3:51:ARG:HB3	3:3:94:ASP:HB3	1.91	0.52
10:B:306:PRO:HA	17:I:52:ARG:HE	1.74	0.51
13:E:189:SER:C	13:E:190:ASP:OD1	2.49	0.51
9:A:308:GLN:HG2	52:A:4140:HOH:O	2.10	0.51
14:F:88:SER:OG	14:F:91:GLU:HB2	2.12	0.51
21:M:33:LEU:HD23	28:T:28:SER:HB2	1.91	0.51
14:F:71:ARG:O	14:F:73:GLN:HG3	3.90	0.51
21:M:68:LEU:HB3	21:M:69:PRO:HD3	1.91	0.51
2:2:27:ILE:HG12	2:2:53:VAL:HG21	1.91	0.51
5:5:36:GLU:HG3	5:5:37:GLU:N	2.24	0.51
22:N:119:THR:O	26:R:52:HIS:CE1	2.63	0.51
10:B:189:VAL:HG23	52:B:3052:HOH:O	41.84	0.51
1:1:310:PRO:O	1:1:315:HIS:HB2	2.10	0.51
1:1:258:VAL:HG21	1:1:280:ALA:HB1	1.91	0.51
8:8:26:TYR:N	8:8:27:PRO:CD	2.69	0.51
3:3:132:ASP:O	3:3:135:VAL:HG12	2.09	0.51
1:1:93:ALA:HB1	1:1:107:LEU:HD11	1.91	0.51
20:L:449:MET:SD	21:M:5:MET:HE2	2.51	0.51
7:7:66:PRO:O	7:7:87:PRO:HG2	2.11	0.51
21:M:1:MET:SD	21:M:133:LEU:CD1	2.98	0.51
3:3:568:TYR:CD1	3:3:572:PRO:HG3	2.46	0.51
1:1:96:SER:HA	1:1:135:ARG:NH1	2.26	0.51
20:L:75:ILE:O	20:L:79:GLY:HA3	2.11	0.51
2:2:31:LEU:HD12	2:2:41:ILE:HD13	1.92	0.51
8:8:45:ARG:NH2	8:8:137:LEU:HD23	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:O:40:LEU:HD22	23:O:59:LEU:HD13	1.92	0.51
20:L:250:GLY:O	20:L:254:ILE:HG12	2.11	0.51
21:M:100:MET:CE	21:M:157:GLU:HG3	2.40	0.51
12:D:229:VAL:CG2	15:G:20:PRO:HD3	2.49	0.51
10:B:181:TYR:CE1	10:B:182:ARG:HG2	2.54	0.51
1:1:437:TRP:C	1:1:437:TRP:CD1	2.84	0.51
1:1:197:ALA:HB3	2:2:66:PHE:CE1	2.46	0.51
6:6:23:THR:O	6:6:27:LEU:HD13	2.09	0.51
6:6:46:CYS:HB3	6:6:108:MET:HE2	1.92	0.51
15:G:71:ARG:HB2	15:G:72:LYS:HD3	6.50	0.51
1:1:292:PRO:HB2	1:1:316:LEU:CD2	2.41	0.51
9:A:227:ALA:O	9:A:228:VAL:C	2.49	0.51
6:6:50:MET:C	6:6:52:ALA:H	2.12	0.51
11:C:369:ALA:O	11:C:373:GLU:HG3	2.10	0.51
10:B:229:GLY:O	10:B:231:GLY:N	4.52	0.51
18:J:13:LEU:HB3	18:J:23:THR:OG1	2.10	0.51
44:C:502:HEM:HBA1	46:C:2002:UQ1:O2	2.11	0.51
4:4:133:LEU:HD21	4:4:204:TYR:CD2	2.46	0.51
3:3:337:ARG:HD3	3:3:340:GLU:HG3	1.92	0.51
8:8:153:THR:HG22	8:8:155:LYS:H	1.76	0.51
1:1:260:ARG:HG3	1:1:264:TYR:OH	2.11	0.51
9:A:408:ARG:NH2	19:K:15:ARG:CB	77.57	0.51
1:1:114:LEU:HD22	1:1:118:MET:HG3	1.93	0.51
3:3:94:ASP:OD2	3:3:97:SER:HB2	2.10	0.51
20:L:365:ILE:HD12	21:M:87:MET:CE	2.34	0.51
1:1:149:ILE:O	1:1:153:ARG:HG3	2.11	0.51
18:J:56:LYS:O	18:J:60:GLU:HG3	2.63	0.51
4:4:381:LEU:N	4:4:382:PRO:CD	2.74	0.51
1:1:29:LEU:HD22	1:1:29:LEU:O	2.10	0.51
3:3:617:LEU:HD23	3:3:618:GLU:N	2.26	0.51
12:D:234:LYS:HD3	13:E:8:PRO:HB2	1.91	0.51
6:6:117:MET:CE	8:8:99:ILE:HG12	2.41	0.51
3:3:224:GLY:O	3:3:227:THR:HB	2.09	0.50
3:3:642:ALA:CB	3:3:652:PRO:HG3	2.39	0.50
3:3:20:MET:HE2	3:3:432:PHE:HB2	1.91	0.50
15:G:40:ARG:CB	48:G:2004:CDL:HB32	2.41	0.50
8:8:73:ALA:HB3	8:8:87:TYR:CE1	2.46	0.50
9:A:117:VAL:HG11	9:A:195:MET:HE1	1.98	0.50
4:4:333:GLU:OE2	5:5:189:ARG:HD2	2.11	0.50
12:D:34:LYS:NZ	12:D:67:GLU:OE1	2.31	0.50
9:A:381:ARG:HH11	9:A:381:ARG:HG2	1.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:101:LEU:O	5:5:126:PHE:HA	2.11	0.50
4:4:346:THR:CG2	4:4:353:LEU:HB3	2.40	0.50
4:4:261:THR:H	4:4:292:GLN:NE2	2.04	0.50
4:4:126:LEU:HD21	4:4:286:SER:CB	2.40	0.50
6:6:163:TYR:HD2	8:8:152:ARG:HH11	1.59	0.50
4:4:371:ARG:HH22	4:4:376:VAL:HG21	1.76	0.50
2:2:149:ARG:O	2:2:152:ALA:HB3	2.11	0.50
3:3:43:GLY:HA2	42:3:787:FES:S2	2.52	0.50
10:B:33:LEU:CD2	10:B:220:ALA:HB1	2.41	0.50
20:L:40:GLU:HG2	20:L:54:TYR:CD1	2.47	0.50
6:6:83:ARG:HA	6:6:111:CYS:HB3	1.92	0.50
1:1:97:GLU:O	1:1:100:SER:HB3	2.11	0.50
3:3:20:MET:HE1	3:3:432:PHE:CB	2.41	0.50
13:E:80:ASP:O	13:E:82:PRO:HD3	2.21	0.50
33:Y:41:GLY:CA	33:Y:52[A]:ASN:ND2	2.74	0.50
5:5:7:LEU:HD22	5:5:17:ILE:HD12	1.93	0.50
1:1:312:SER:C	1:1:314:GLU:H	2.15	0.50
2:2:89:LYS:HE3	2:2:94:GLU:OE1	2.11	0.50
6:6:30:TRP:CD1	6:6:30:TRP:O	2.65	0.50
3:3:405:GLU:CB	3:3:535:MET:HE2	2.33	0.50
1:1:437:TRP:O	1:1:437:TRP:CD1	2.64	0.50
1:1:132:ILE:HG21	1:1:145:LEU:HD11	1.94	0.50
20:L:184:PHE:H	20:L:256:HIS:CE1	2.29	0.50
18:J:52:TRP:O	18:J:56:LYS:HB2	2.13	0.50
4:4:233:GLY:HA2	5:5:48:PHE:CE1	2.46	0.50
26:R:44:ARG:HD2	26:R:74:ARG:O	2.12	0.50
1:1:243:THR:HG21	1:1:315:HIS:HE1	1.77	0.50
12:D:234:LYS:HE2	13:E:10:PHE:CE1	2.46	0.50
21:M:145:PRO:CG	21:M:148:MET:HE2	2.41	0.50
2:2:6:ASP:HB3	2:2:7:LYS:HD2	1.92	0.50
11:C:191:ALA:HA	11:C:194:MET:HE2	1.97	0.50
9:A:68:LYS:HA	9:A:68:LYS:HE3	5.21	0.50
21:M:139:ASP:OD1	21:M:140:ASN:N	2.44	0.50
1:1:358:PRO:CD	3:3:107:MET:HE3	2.29	0.50
1:1:401:PRO:O	1:1:404:ASP:HB2	2.12	0.50
12:D:43:MET:HE1	12:D:189:PHE:HZ	1.76	0.50
13:E:99:ARG:HB3	13:E:133:VAL:HG12	1.91	0.50
8:8:68:ILE:HD11	38:8:183:SF4:S1	2.51	0.50
3:3:326:PHE:CZ	3:3:330:LYS:HE3	2.47	0.50
6:6:32:ARG:HA	6:6:35:SER:OG	2.10	0.50
4:4:73:ARG:O	4:4:364:MET:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:549:VAL:HG12	3:3:549:VAL:O	2.12	0.50
7:7:40:PHE:HE1	8:8:83:ALA:HB2	1.76	0.50
2:2:113:PRO:HG2	2:2:114:ASP:OD1	2.11	0.50
4:4:271:ASP:OD1	4:4:274:ASP:N	2.39	0.50
11:C:245:PHE:CG	12:D:17:LEU:HD13	2.50	0.50
12:D:124:GLU:OE2	12:D:191:ARG:CD	2.63	0.50
9:A:125:SER:O	9:A:129:LYS:HG3	2.12	0.50
3:3:550:LEU:HB3	3:3:684:ARG:HH21	1.77	0.50
11:C:15:ASN:O	11:C:17:ALA:N	2.60	0.50
2:2:122:VAL:CG1	2:2:123:GLU:N	2.75	0.50
20:L:172:LYS:HZ3	20:L:172:LYS:HB2	1.75	0.50
21:M:136:LEU:HB3	21:M:193:TYR:CD2	2.46	0.50
12:D:43:MET:HE1	12:D:189:PHE:CZ	2.47	0.50
5:5:163:ARG:HD2	8:8:69:TYR:CD1	2.47	0.50
26:R:42:ARG:NH1	26:R:74:ARG:HH21	2.10	0.50
10:B:109:VAL:HB	10:B:119:LEU:HD12	1.94	0.50
25:Q:37:LYS:N	25:Q:37:LYS:HD3	2.27	0.50
18:J:16:ARG:CG	18:J:16:ARG:NH1	2.75	0.50
23:O:64:PHE:CE1	24:P:66:ARG:HD2	2.46	0.50
1:1:272:PHE:HZ	1:1:316:LEU:HD21	1.77	0.50
11:C:68:HIS:HD2	52:C:2126:HOH:O	1.95	0.50
21:M:186:SER:CB	21:M:213:LEU:HD22	2.40	0.50
8:8:151:LYS:C	8:8:153:THR:H	2.16	0.50
3:3:192:GLU:HG3	3:3:193:GLU:HG3	1.92	0.50
3:3:697:THR:OG1	3:3:763:LEU:HD23	2.11	0.50
3:3:171:SER:CB	3:3:172:PRO:HD2	2.39	0.50
5:5:30:PRO:HG2	5:5:33:ARG:HB2	1.93	0.50
22:N:156:ARG:NH1	22:N:156:ARG:HG3	2.22	0.50
22:N:42:LEU:HD13	29:U:45:TYR:HD2	1.77	0.50
3:3:474:ARG:NH2	3:3:516:VAL:CG2	2.64	0.49
3:3:55:PRO:HG3	3:3:73:ILE:HA	1.92	0.49
3:3:135:VAL:HG23	4:4:326:TYR:CE2	2.46	0.49
1:1:238:PHE:CZ	1:1:248:GLY:HA3	2.47	0.49
11:C:164:ILE:O	11:C:177:ARG:HD2	2.22	0.49
14:F:78:GLU:CD	14:F:78:GLU:H	2.15	0.49
26:R:5:LYS:NZ	26:R:5:LYS:HB3	2.27	0.49
2:2:112:THR:HG22	2:2:117:PHE:H	1.76	0.49
11:C:129:MET:HE2	11:C:181:PHE:HB2	1.94	0.49
4:4:385:CYS:HB3	4:4:396:ILE:HG21	1.94	0.49
2:2:122:VAL:HG12	2:2:123:GLU:H	1.77	0.49
4:4:132:PHE:CE2	4:4:279:ARG:HG3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:508:PRO:HG3	22:N:6:HIS:HB3	1.94	0.49
20:L:266:GLU:HB2	20:L:267:PRO:HD2	1.94	0.49
10:B:95:LYS:CD	17:I:32:ALA:HB2	2.41	0.49
1:1:219:ASN:ND2	1:1:223:THR:HG21	2.27	0.49
10:B:200:THR:O	10:B:204:MET:HG3	2.52	0.49
20:L:11:ASN:ND2	20:L:14:ASP:H	2.07	0.49
2:2:24:ARG:HA	2:2:53:VAL:CG1	2.42	0.49
3:3:42:ILE:HG22	3:3:43:GLY:N	2.27	0.49
33:Y:41:GLY:CA	33:Y:52[A]:ASN:HD21	2.24	0.49
3:3:19:VAL:O	3:3:22:ALA:HB3	2.12	0.49
3:3:693:TYR:HB3	3:3:759:TYR:CD1	2.48	0.49
3:3:208:HIS:ND1	7:7:92:HIS:CE1	2.80	0.49
18:J:18:SER:CB	19:K:23:LEU:CB	74.70	0.49
18:J:16:ARG:CB	18:J:19:THR:HG22	2.38	0.49
13:E:82:PRO:O	13:E:100:HIS:HB3	2.12	0.49
21:M:186:SER:HB3	21:M:213:LEU:CD2	2.42	0.49
20:L:377:PHE:HA	20:L:380:VAL:HG22	1.93	0.49
4:4:381:LEU:HB3	4:4:382:PRO:HD3	1.95	0.49
21:M:90:ILE:HD12	21:M:90:ILE:H	1.77	0.49
13:E:155:GLY:N	52:E:541:HOH:O	2.46	0.49
10:B:365:LYS:HG2	10:B:399:LEU:CD2	2.45	0.49
2:2:28:MET:HB2	2:2:29:PRO:HD2	1.95	0.49
3:3:188:VAL:CG1	3:3:201:ASP:HA	2.42	0.49
5:5:161:GLU:HB2	5:5:163:ARG:CZ	2.43	0.49
3:3:707:LYS:C	3:3:709:GLN:H	2.14	0.49
3:3:367:PRO:CG	3:3:554:LYS:HB2	2.43	0.49
11:C:371:THR:O	11:C:375:LYS:HG2	2.13	0.49
20:L:168:ILE:HG21	20:L:189:MET:HG3	1.94	0.49
4:4:320:SER:HB3	4:4:323:ALA:HB3	1.95	0.49
21:M:13:THR:HG22	21:M:13:THR:O	2.12	0.49
16:H:28:GLU:O	16:H:32:LYS:HG2	2.13	0.49
21:M:16:ILE:HD12	21:M:17:MET:H	1.78	0.49
3:3:734:VAL:HG12	3:3:736:VAL:HG23	1.94	0.49
3:3:477:LEU:CD2	3:3:521:ALA:HB2	2.42	0.49
26:R:42:ARG:O	26:R:42:ARG:HD2	2.13	0.49
13:E:129:LYS:HG3	13:E:187:PHE:CE2	3.96	0.49
9:A:189:HIS:ND1	9:A:194:ARG:NH2	2.59	0.49
20:L:145:LEU:HD21	22:N:32:THR:HG21	1.93	0.49
4:4:284:ARG:HH11	4:4:284:ARG:HG3	1.77	0.49
17:I:32:ALA:HA	17:I:71:ASN:HD22	1.98	0.49
26:R:5:LYS:C	26:R:5:LYS:HD2	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Y:41:GLY:HA2	33:Y:48:TYR:CE1	2.47	0.49
9:A:90:SER:HB3	52:A:4116:HOH:O	2.11	0.49
3:3:130:LEU:HD23	38:3:784:SF4:S4	2.52	0.49
18:J:3:PRO:HB2	18:J:8:ARG:HH11	3.11	0.49
4:4:234:LEU:O	4:4:239:LEU:HG	2.12	0.49
22:N:224:LYS:HZ2	22:N:226:HIS:HE2	1.59	0.49
20:L:87:ILE:O	20:L:173:PRO:HD3	2.13	0.49
9:A:408:ARG:NH1	19:K:15:ARG:HG2	79.06	0.49
3:3:218:LEU:N	3:3:219:PRO:CD	2.75	0.49
1:1:359:CYS:HB2	1:1:403:ALA:HB2	1.93	0.49
9:A:405:ARG:O	9:A:409:GLU:HG3	2.20	0.49
11:C:15:ASN:O	11:C:16:ASN:C	2.50	0.49
2:2:33:ARG:HH21	2:2:37:GLU:CG	2.26	0.49
9:A:172:GLU:HG3	9:A:176:LYS:HE3	1.95	0.49
22:N:65:SER:HB3	22:N:71:HIS:CE1	2.48	0.49
20:L:509:THR:HG1	25:Q:71:TRP:HZ3	1.60	0.49
4:4:168:PHE:CD1	4:4:168:PHE:N	2.81	0.49
4:4:62:LEU:HD23	4:4:62:LEU:HA	1.65	0.49
33:Y:70:ASN:HD22	33:Y:70:ASN:C	2.16	0.49
5:5:175:THR:OG1	5:5:175:THR:O	2.31	0.48
3:3:719:HIS:ND1	3:3:720:PRO:HD2	2.28	0.48
1:1:9:LEU:HD13	1:1:279:TRP:CZ2	2.48	0.48
9:A:143:THR:OG1	17:I:48:SER:HB3	2.13	0.48
20:L:197:LEU:O	22:N:92:LEU:HD22	2.13	0.48
9:A:264:HIS:ND1	9:A:265:PRO:HD2	2.36	0.48
11:C:251:GLY:HA3	52:C:2091:HOH:O	2.13	0.48
7:7:39:ASP:OD2	7:7:75:ARG:HD3	2.14	0.48
1:1:299:PRO:HG3	1:1:341:MET:CE	2.43	0.48
3:3:518:ALA:O	3:3:521:ALA:HB3	2.13	0.48
3:3:629:ILE:HG22	3:3:630:GLU:H	1.77	0.48
4:4:341:GLU:OE1	5:5:91:ARG:NH2	2.46	0.48
3:3:508:GLY:O	3:3:512:LEU:HB2	2.13	0.48
4:4:53:LEU:HD22	4:4:53:LEU:N	2.28	0.48
4:4:82:THR:N	4:4:83:PRO:HD2	2.29	0.48
5:5:31:ARG:O	5:5:34:PHE:HB3	2.12	0.48
5:5:163:ARG:HD2	8:8:69:TYR:CE1	2.48	0.48
9:A:227:ALA:O	9:A:228:VAL:HB	3.86	0.48
1:1:9:LEU:HD13	1:1:279:TRP:HZ2	1.78	0.48
12:D:3:LEU:HD12	16:H:55:THR:HG22	2.08	0.48
3:3:584:VAL:HG12	3:3:600:VAL:HB	1.94	0.48
4:4:102:GLU:HG2	4:4:175:ILE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:21:LEU:HD21	46:C:2002:UQ1:HM32	1.95	0.48
3:3:333:LEU:HB3	3:3:648:LEU:CD2	2.43	0.48
3:3:321:THR:HG22	3:3:322:TRP:N	2.29	0.48
29:U:16:ASN:ND2	29:U:16:ASN:H	2.12	0.48
1:1:72:THR:HG21	1:1:223:THR:HG23	1.94	0.48
21:M:78:LEU:HB2	21:M:79:PRO:CD	2.38	0.48
20:L:11:ASN:ND2	20:L:13:LYS:HB2	2.28	0.48
2:2:24:ARG:HA	2:2:53:VAL:HG13	1.94	0.48
4:4:219:ARG:NH1	4:4:273:PHE:CD2	2.81	0.48
3:3:719:HIS:HB2	3:3:753:VAL:O	2.12	0.48
7:7:14:VAL:HA	7:7:17:LEU:HD12	1.95	0.48
4:4:163:VAL:HG22	4:4:164:THR:CG2	2.43	0.48
11:C:191:ALA:HA	11:C:194:MET:CE	2.43	0.48
1:1:273:ARG:HB2	1:1:307:LEU:O	2.13	0.48
5:5:167:PRO:HB3	8:8:66:TYR:CE2	2.48	0.48
27:S:24:ASN:ND2	27:S:26:THR:H	2.11	0.48
10:B:396:SER:HB3	52:B:3031:HOH:O	2.14	0.48
10:B:51:ILE:HG12	10:B:204:MET:HG2	1.95	0.48
11:C:97:HIS:CD2	44:C:502:HEM:NC	2.81	0.48
1:1:420:GLN:O	1:1:424:LEU:HD13	2.14	0.48
21:M:22:HIS:CE1	28:T:44:LYS:HD3	2.49	0.48
1:1:311:MET:HA	1:1:316:LEU:HD11	1.94	0.48
13:E:83:GLU:HG2	13:E:102:THR:HG22	4.45	0.48
28:T:39:VAL:O	28:T:42:LYS:HE2	2.14	0.48
20:L:115:SER:O	20:L:121:GLY:HA2	2.14	0.48
17:I:36:ALA:HB2	17:I:73:PRO:CD	2.40	0.48
9:A:15:GLN:NE2	10:B:12:GLU:HB2	2.29	0.48
47:D:501:HEC:HMC1	47:D:501:HEC:HBC3	1.94	0.48
13:E:79:SER:CB	13:E:191:ASP:OD2	2.99	0.48
6:6:121:TYR:CG	6:6:122:ALA:N	2.81	0.48
4:4:88:LEU:HD12	4:4:403:VAL:HG22	1.94	0.48
7:7:86:LEU:HD12	7:7:91:ILE:HD12	1.95	0.48
1:1:188:LEU:HD23	1:1:188:LEU:O	2.13	0.48
4:4:94:ASP:HB3	4:4:173:ILE:HG21	1.96	0.48
12:D:59:ASP:OD2	18:J:62:LYS:CB	6.70	0.48
4:4:250:LYS:HE2	4:4:262:PHE:CB	2.33	0.48
21:M:59:GLN:O	21:M:62:GLU:HB2	2.13	0.48
1:1:120:LEU:HD22	1:1:231:MET:HG3	1.96	0.48
21:M:4:PRO:HB2	30:V:43:SER:HA	1.96	0.48
3:3:113:LEU:CD1	3:3:157:PHE:HB2	2.43	0.48
4:4:86:ASP:OD2	4:4:350:ARG:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:254:THR:OG1	3:3:624:LEU:HD12	2.12	0.48
11:C:78:ILE:CD1	12:D:204:MET:HE1	2.50	0.48
3:3:341:VAL:HA	3:3:565:TYR:O	2.13	0.48
10:B:24:LEU:HD13	10:B:392:TYR:CD2	2.49	0.48
1:1:356:CYS:SG	1:1:399:PHE:HB2	2.53	0.48
18:J:16:ARG:HH12	18:J:19:THR:HG21	1.76	0.48
6:6:104:TRP:NE1	6:6:173:VAL:HG22	2.29	0.48
2:2:145:VAL:CG1	2:2:150:LEU:HB2	2.44	0.48
8:8:44:THR:HA	8:8:138:VAL:CG1	2.44	0.48
20:L:397:PHE:HB3	20:L:398:PRO:HD3	1.95	0.48
6:6:140:CYS:SG	8:8:99:ILE:HG13	2.54	0.48
8:8:100:PHE:HA	38:8:183:SF4:S4	2.54	0.48
29:U:8:LYS:HB3	29:U:8:LYS:NZ	2.29	0.48
18:J:61:ASN:C	18:J:62:LYS:HG3	5.20	0.47
18:J:16:ARG:O	18:J:19:THR:HG22	2.14	0.47
3:3:465:HIS:CG	3:3:465:HIS:O	2.66	0.47
12:D:124:GLU:OE2	12:D:191:ARG:HD2	2.14	0.47
3:3:382:PHE:CD1	3:3:382:PHE:N	2.81	0.47
3:3:117:LEU:HG	4:4:324:VAL:HG21	1.96	0.47
10:B:46:ARG:HD2	10:B:375:SER:OG	2.14	0.47
4:4:215:TYR:CE1	4:4:219:ARG:HG2	2.49	0.47
1:1:109:ASP:O	1:1:110:VAL:HG13	2.13	0.47
3:3:571:VAL:HG11	3:3:591:HIS:CD2	2.50	0.47
4:4:238:SER:OG	4:4:279:ARG:NH2	2.47	0.47
3:3:473:GLU:O	3:3:477:LEU:HD12	2.14	0.47
25:Q:49:VAL:HG21	25:Q:74:LEU:HD12	1.95	0.47
20:L:449:MET:SD	21:M:5:MET:CE	3.02	0.47
10:B:361:LYS:HE2	10:B:402:ILE:O	2.18	0.47
22:N:164:PHE:O	22:N:168:THR:HG23	2.14	0.47
10:B:345:LYS:O	10:B:349:GLN:HG3	2.14	0.47
13:E:131:GLU:HG2	13:E:132:TRP:CD1	2.49	0.47
15:G:45:ILE:HG22	15:G:46:LEU:CD2	5.13	0.47
4:4:93:HIS:CE1	4:4:353:LEU:HD11	2.49	0.47
8:8:133:LYS:O	8:8:137:LEU:HD13	2.14	0.47
1:1:188:LEU:C	1:1:188:LEU:HD23	2.34	0.47
23:O:68:PHE:HA	23:O:71:MET:HG2	1.95	0.47
4:4:366:TYR:CZ	5:5:148:LYS:HE3	2.49	0.47
20:L:476:PHE:CD1	31:W:15:VAL:HG21	2.48	0.47
5:5:25:LEU:N	5:5:25:LEU:CD2	2.78	0.47
3:3:512:LEU:HD21	3:3:534:ALA:HB1	1.96	0.47
3:3:224:GLY:HA3	3:3:295:ARG:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A:4072:HOH:O	14:F:110:LYS:HD2	77.94	0.47
4:4:194:LEU:HD12	4:4:194:LEU:HA	1.71	0.47
3:3:440:ARG:NH1	3:3:440:ARG:CG	2.77	0.47
9:A:429:GLU:OE2	15:G:7:LEU:HB2	2.14	0.47
1:1:391:LEU:HB2	1:1:392:PRO:CD	2.43	0.47
25:Q:31:TYR:HE1	25:Q:98:HIS:HE1	1.62	0.47
18:J:17:THR:CG2	19:K:24:TRP:CZ2	63.46	0.47
1:1:37:GLY:C	1:1:39:GLU:H	2.18	0.47
9:A:431:LEU:HD12	9:A:432:PRO:HD2	1.96	0.47
10:B:246:GLU:O	10:B:427:SER:HA	2.14	0.47
4:4:30:VAL:HG12	4:4:31:GLY:N	2.29	0.47
21:M:63:THR:O	21:M:66:THR:HG22	2.15	0.47
3:3:591:HIS:ND1	3:3:592:PRO:CD	2.76	0.47
21:M:108:TYR:CD1	21:M:108:TYR:N	2.83	0.47
15:G:46:LEU:HD22	15:G:46:LEU:N	4.83	0.47
10:B:12:GLU:CG	10:B:17:VAL:H	2.04	0.47
10:B:17:VAL:HG13	10:B:18:PRO:HD2	3.34	0.47
1:1:219:ASN:HD22	1:1:223:THR:HG21	1.78	0.47
21:M:83:ILE:O	21:M:87:MET:HG3	2.14	0.47
1:1:49:THR:HG23	1:1:52:GLU:CG	2.43	0.47
3:3:717:TRP:HB2	3:3:759:TYR:HB2	1.97	0.47
11:C:141:TRP:CH2	13:E:145:VAL:HG23	46.44	0.47
9:A:213:GLN:HG2	52:A:4055:HOH:O	2.15	0.47
11:C:361:LEU:O	11:C:366:MET:HG3	2.24	0.47
11:C:277:ALA:HB1	11:C:294:LEU:CD1	2.44	0.47
5:5:3:LEU:HB2	5:5:86:SER:HB3	1.96	0.47
3:3:732:ALA:O	3:3:747:VAL:HG12	2.15	0.47
19:K:19:PRO:O	19:K:23:LEU:HG	2.14	0.47
10:B:212:SER:OG	10:B:215:VAL:HG23	2.15	0.47
6:6:163:TYR:CD2	8:8:152:ARG:HD2	2.50	0.47
27:S:60:TYR:CD1	27:S:60:TYR:C	2.88	0.47
20:L:507:GLU:O	20:L:508:PRO:O	2.32	0.47
6:6:28:VAL:O	6:6:32:ARG:HG2	2.15	0.47
4:4:88:LEU:HD12	4:4:403:VAL:CG2	2.45	0.47
8:8:29:ALA:HA	8:8:30:PRO:HD2	1.72	0.47
4:4:257:TYR:C	4:4:259:THR:H	2.18	0.47
3:3:124:LYS:HD3	3:3:124:LYS:HA	1.75	0.47
19:K:31:GLY:O	19:K:35:ALA:N	2.46	0.47
10:B:95:LYS:HE3	17:I:72:VAL:HG21	1.97	0.47
1:1:356:CYS:SG	1:1:399:PHE:CB	3.03	0.47
4:4:234:LEU:CD2	4:4:238:SER:HB2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:279:ARG:HG3	4:4:279:ARG:NH1	2.29	0.47
6:6:117:MET:HE2	8:8:99:ILE:HG12	1.97	0.47
11:C:375:LYS:HD2	11:C:375:LYS:N	4.17	0.47
33:Y:12[A]:GLN:HG3	52:Y:351:HOH:O	2.14	0.47
3:3:54:LEU:N	3:3:55:PRO:HD3	2.30	0.47
4:4:211:SER:OG	4:4:215:TYR:HB2	2.15	0.47
6:6:99:MET:CG	6:6:100:PRO:HD2	2.44	0.47
2:2:153:LEU:O	2:2:157:LEU:HG	2.15	0.47
23:O:41:LYS:HD3	23:O:62:LEU:HD23	1.97	0.47
3:3:458:LEU:C	3:3:460:LYS:H	2.18	0.47
26:R:67:HIS:CD2	26:R:78:LEU:HD11	2.50	0.47
29:U:11:LEU:HD23	29:U:11:LEU:O	2.15	0.47
12:D:105:ASN:C	52:Y:350:HOH:O	49.11	0.46
3:3:370:ASP:OD2	3:3:558:TRP:HD1	1.98	0.46
16:H:31:VAL:HG23	16:H:32:LYS:N	2.30	0.46
2:2:10:PHE:O	2:2:14:THR:OG1	2.34	0.46
3:3:113:LEU:HD12	3:3:157:PHE:CB	2.44	0.46
21:M:1:MET:SD	21:M:133:LEU:HD11	2.56	0.46
3:3:19:VAL:HG23	3:3:85:THR:O	2.15	0.46
1:1:42:LYS:O	1:1:46:LYS:HG3	2.15	0.46
4:4:108:VAL:HG23	4:4:108:VAL:O	2.15	0.46
21:M:5:MET:CE	30:V:42:PRO:HA	2.45	0.46
1:1:245:GLN:HB2	1:1:314:GLU:OE2	2.15	0.46
22:N:80:ARG:O	22:N:84:ILE:HG12	2.14	0.46
23:O:102:TYR:CD2	32:X:35:TYR:HE1	2.33	0.46
20:L:484:THR:HB	32:X:2:THR:OG1	2.15	0.46
12:D:44:ASP:OD1	12:D:93:LYS:HE2	2.15	0.46
12:D:97:ASN:HB2	12:D:98:PRO:HD2	2.01	0.46
4:4:291:LYS:O	4:4:295:GLU:HG3	2.14	0.46
9:A:15:GLN:O	9:A:26:ALA:HA	2.16	0.46
5:5:71:VAL:HG22	5:5:91:ARG:HB2	1.97	0.46
13:E:85:LYS:HZ3	13:E:87:MET:HA	1.80	0.46
23:O:108:PRO:HG2	23:O:111:PHE:CD2	2.50	0.46
1:1:161:ASN:HD22	1:1:166:ASP:HA	1.80	0.46
1:1:243:THR:HG22	1:1:244:GLU:H	1.79	0.46
3:3:269:THR:HG22	3:3:274:LEU:HA	1.97	0.46
11:C:92:ILE:O	11:C:96:MET:HG2	2.17	0.46
18:J:8:ARG:NH1	18:J:8:ARG:CG	2.93	0.46
6:6:104:TRP:NE1	6:6:158:VAL:HG12	2.30	0.46
1:1:53:VAL:HG23	1:1:231:MET:CE	2.45	0.46
20:L:273:MET:HG3	20:L:319:LYS:NZ	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:299:VAL:HA	20:L:302:ARG:NH1	2.31	0.46
20:L:435:GLY:O	20:L:437:PRO:HD3	2.15	0.46
9:A:167:VAL:HG13	52:A:4111:HOH:O	2.15	0.46
11:C:193:ALA:O	11:C:196:HIS:HB3	2.16	0.46
4:4:262:PHE:CD1	4:4:289:ILE:HD11	2.51	0.46
3:3:33:PHE:O	3:3:186:ARG:NH2	2.48	0.46
10:B:354:ASN:HB3	10:B:355:PRO:HD3	2.19	0.46
1:1:110:VAL:O	1:1:113:LEU:HB3	2.15	0.46
4:4:200:ARG:O	4:4:204:TYR:HD1	1.99	0.46
9:A:369:LEU:HD12	9:A:392:LEU:HD21	1.98	0.46
3:3:326:PHE:CD1	3:3:643:LEU:HG	2.49	0.46
25:Q:40:SER:OG	25:Q:45:ASP:HB3	2.16	0.46
49:L:515:HEA:HMC1	49:L:515:HEA:CBC	2.46	0.46
4:4:320:SER:HB3	4:4:323:ALA:CB	2.46	0.46
3:3:695:ARG:O	3:3:697:THR:HG23	2.14	0.46
4:4:393:MET:HA	4:4:396:ILE:CG2	2.44	0.46
23:O:66:GLU:O	24:P:66:ARG:NH2	2.49	0.46
3:3:571:VAL:HA	3:3:572:PRO:HD3	1.73	0.46
18:J:56:LYS:HG2	18:J:60:GLU:CG	3.13	0.46
11:C:104:TYR:CD1	11:C:208:PRO:HA	2.51	0.46
19:K:34:SER:OG	19:K:35:ALA:N	2.97	0.46
19:K:18:VAL:CB	19:K:19:PRO:HD3	2.68	0.46
3:3:561:PRO:CB	3:3:576:ALA:HA	2.37	0.46
9:A:86:LEU:HD13	9:A:99:ILE:CG1	2.45	0.46
20:L:195:LEU:CD2	20:L:245:ILE:HD13	2.45	0.46
3:3:587:LEU:HD13	3:3:589:HIS:O	2.16	0.46
3:3:715:GLU:HA	3:3:745:ALA:HB1	1.97	0.46
11:C:233:LEU:HD11	12:D:219:VAL:HG21	1.98	0.46
23:O:23:PRO:HB3	24:P:70:VAL:CG2	2.45	0.46
1:1:53:VAL:O	1:1:57:VAL:HG23	2.16	0.46
1:1:211:LEU:H	1:1:216:THR:HG21	1.78	0.46
5:5:116:ARG:HB3	5:5:135:ILE:HG13	1.97	0.46
1:1:28:THR:HB	1:1:31:TYR:H	1.80	0.46
9:A:47:TYR:HB3	9:A:189:HIS:CE1	2.82	0.46
3:3:478:LEU:HD22	3:3:484:LYS:HB2	1.97	0.46
20:L:147:ILE:HD11	20:L:209:LEU:HD23	1.98	0.46
30:V:9:PHE:HD1	30:V:10:HIS:HD2	1.64	0.46
17:I:36:ALA:CB	17:I:73:PRO:HB2	2.46	0.46
7:7:121:ARG:CG	7:7:121:ARG:NH1	2.78	0.46
3:3:192:GLU:HG3	3:3:193:GLU:N	2.31	0.46
9:A:264:HIS:HA	9:A:265:PRO:HD3	1.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:24:LEU:HD12	10:B:37:SER:O	5.35	0.46
12:D:134:TYR:CG	12:D:162:PRO:HG3	2.51	0.46
32:X:1:ILE:HG23	32:X:1:ILE:O	2.15	0.46
9:A:408:ARG:CZ	19:K:15:ARG:CG	79.04	0.46
1:1:228:VAL:HB	1:1:229:PRO:CD	2.45	0.46
14:F:12:TRP:O	14:F:16:ILE:N	3.46	0.46
3:3:101:ARG:HB3	3:3:101:ARG:NH1	2.31	0.46
1:1:101:PHE:CZ	1:1:253:GLN:HB2	2.51	0.46
6:6:163:TYR:HD1	6:6:168:GLU:O	1.99	0.46
3:3:722:THR:CG2	3:3:755:LYS:HB3	2.45	0.46
3:3:337:ARG:H	3:3:337:ARG:HD2	1.80	0.46
17:I:70:LEU:HB3	52:I:1016:HOH:O	2.16	0.46
9:A:111:GLU:HG3	9:A:215:HIS:CE1	2.54	0.46
8:8:33:LEU:HD11	8:8:161:TYR:HB2	1.98	0.46
4:4:44:MET:HA	4:4:44:MET:CE	2.46	0.46
9:A:15:GLN:HE21	10:B:12:GLU:HB2	1.81	0.45
15:G:40:ARG:NH2	48:G:2004:CDL:HB31	2.32	0.45
9:A:354:VAL:HG21	9:A:404:ALA:HA	1.98	0.45
20:L:431:LEU:HD21	20:L:450:TRP:HB2	1.99	0.45
10:B:257:LEU:O	10:B:323:GLY:HA3	2.15	0.45
3:3:476:ILE:O	3:3:480:LEU:HG	2.16	0.45
32:X:37:LEU:HA	32:X:37:LEU:HD23	1.83	0.45
5:5:195:LEU:HD22	5:5:195:LEU:N	2.30	0.45
5:5:15:TYR:OH	5:5:33:ARG:HD3	2.15	0.45
8:8:34:LYS:HB3	8:8:35:PRO:HD2	1.97	0.45
6:6:89:ALA:N	6:6:90:PRO:HD2	2.31	0.45
5:5:47:ASN:ND2	5:5:76:SER:HA	2.31	0.45
9:A:85:HIS:O	9:A:99:ILE:HA	2.16	0.45
9:A:51:LYS:HB2	9:A:51:LYS:HZ2	1.82	0.45
4:4:200:ARG:O	4:4:204:TYR:CD1	2.70	0.45
23:O:33:LEU:HD13	23:O:41:LYS:HG3	1.97	0.45
12:D:144:ARG:HG3	12:D:147:LEU:HD12	2.09	0.45
39:1:440:FMN:H1'1	39:1:440:FMN:H9	1.62	0.45
21:M:76:ILE:O	21:M:79:PRO:HD2	2.16	0.45
3:3:55:PRO:CG	3:3:73:ILE:HA	2.45	0.45
6:6:145:GLU:HG2	8:8:31:VAL:HG21	1.98	0.45
24:P:70:VAL:HG12	24:P:71:VAL:N	2.31	0.45
3:3:2:VAL:HG13	3:3:89:ASP:CA	2.47	0.45
4:4:142:ALA:HB1	4:4:145:PRO:HD2	1.99	0.45
29:U:2:GLU:CG	29:U:3:ASN:H	2.30	0.45
25:Q:98:HIS:N	25:Q:98:HIS:ND1	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:8:125:GLU:O	8:8:128:ASP:HB2	2.16	0.45
17:I:76:VAL:HG13	17:I:76:VAL:O	2.16	0.45
3:3:469:ARG:HG2	3:3:754:PRO:HG3	1.97	0.45
3:3:123:ASP:C	3:3:125:GLY:H	2.19	0.45
6:6:84:LEU:HD11	6:6:89:ALA:HA	1.98	0.45
3:3:616:ASN:HB3	3:3:620:ARG:H	1.81	0.45
21:M:41:ILE:O	21:M:45:MET:HG2	2.16	0.45
3:3:200:LEU:HA	3:3:200:LEU:HD12	1.80	0.45
5:5:75:VAL:HG12	5:5:76:SER:N	2.31	0.45
5:5:161:GLU:CG	5:5:163:ARG:NH2	2.79	0.45
20:L:240:HIS:O	20:L:243:VAL:HG22	2.16	0.45
4:4:350:ARG:NE	4:4:403:VAL:HG23	2.32	0.45
1:1:45:LEU:HD12	1:1:163:PHE:HD2	1.81	0.45
3:3:417:VAL:CG1	3:3:443:ARG:HB3	2.46	0.45
23:O:79:LYS:NZ	30:V:15:ASN:HD21	2.15	0.45
19:K:23:LEU:HD23	19:K:23:LEU:N	2.63	0.45
3:3:541:ALA:O	3:3:545:GLU:HG3	2.15	0.45
15:G:71:ARG:NH1	15:G:72:LYS:HD2	6.85	0.45
10:B:120:MET:HB2	10:B:120:MET:HE2	1.80	0.45
4:4:105:LEU:HD13	4:4:309:ILE:CD1	2.44	0.45
1:1:397:ARG:O	1:1:397:ARG:HG2	2.16	0.45
3:3:452:ALA:C	3:3:454:TYR:H	2.20	0.45
4:4:158:ASP:OD1	8:8:34:LYS:HE3	2.17	0.45
5:5:72:TYR:HB2	5:5:90:VAL:HG13	1.98	0.45
6:6:125:GLN:O	6:6:126:ASN:CB	2.64	0.45
33:Y:17:CYS:SG	44:Y:500:HEM:C3C	3.10	0.45
21:M:58:ALA:O	21:M:60:GLU:HG3	2.16	0.45
21:M:94:SER:OG	21:M:148:MET:HE3	2.16	0.45
21:M:162:SER:HB2	21:M:198:GLU:HB2	1.99	0.45
4:4:101:VAL:HG11	4:4:175:ILE:HD12	1.98	0.45
23:O:33:LEU:HD22	23:O:37:GLN:HB3	1.97	0.45
10:B:327:ILE:HG21	17:I:55:LEU:HD11	1.98	0.45
4:4:314:ARG:NH2	8:8:108:CYS:O	2.50	0.45
12:D:145:GLU:OE1	33:Y:25:LYS:HE2	64.87	0.45
18:J:16:ARG:HG3	18:J:16:ARG:NH1	2.32	0.45
3:3:29:ASP:OD2	5:5:186:GLY:HA3	2.17	0.45
10:B:71:LEU:CD2	17:I:68:VAL:HG21	2.44	0.45
4:4:221:VAL:HG12	4:4:388:GLU:OE1	2.17	0.45
3:3:694:LEU:HD23	3:3:760:LEU:HB3	1.98	0.45
20:L:306:THR:HB	20:L:359:ALA:O	2.15	0.45
25:Q:31:TYR:HE1	25:Q:98:HIS:CE1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:51:ASP:O	20:L:55:ASN:HB2	2.17	0.45
10:B:28:ARG:HH21	10:B:390:GLY:HA3	1.81	0.45
11:C:327:ALA:HA	15:G:51:PRO:HB3	2.08	0.45
16:H:31:VAL:O	16:H:35:GLU:HG3	2.18	0.44
4:4:101:VAL:CG1	4:4:175:ILE:HD12	2.47	0.44
20:L:158:ILE:O	20:L:162:ILE:HG13	2.17	0.44
20:L:131:PRO:HB2	21:M:159:VAL:HA	1.99	0.44
5:5:103:THR:HG22	5:5:127:GLU:O	2.17	0.44
1:1:68:ALA:HB1	40:1:441:NAI:H51A	1.98	0.44
1:1:149:ILE:HD13	1:1:171:LEU:CB	2.37	0.44
15:G:40:ARG:CZ	48:G:2004:CDL:HB31	2.47	0.44
4:4:190:LEU:HG	4:4:194:LEU:HD22	1.98	0.44
24:P:78:HIS:CE1	28:T:12:LEU:HD22	2.52	0.44
11:C:213:SER:OG	11:C:217:LYS:NZ	2.67	0.44
4:4:197:LEU:O	4:4:198:PRO:C	2.56	0.44
4:4:263:ASP:HB2	4:4:285:GLU:OE1	2.16	0.44
3:3:459:MET:CE	3:3:465:HIS:HB2	2.46	0.44
3:3:497:TRP:O	3:3:500:ALA:HB3	2.17	0.44
3:3:13:VAL:HG21	3:3:17:THR:HG21	1.99	0.44
4:4:253:PRO:HB2	4:4:258:GLU:HG3	1.99	0.44
4:4:185:GLU:O	4:4:189:GLU:HG2	2.17	0.44
3:3:117:LEU:N	4:4:321:MET:CE	2.80	0.44
6:6:145:GLU:HG2	8:8:31:VAL:CG2	2.47	0.44
18:J:8:ARG:HD2	18:J:8:ARG:HA	1.76	0.44
4:4:240:ARG:C	4:4:242:SER:H	2.19	0.44
26:R:42:ARG:NH1	26:R:42:ARG:HG3	2.32	0.44
6:6:84:LEU:HD12	6:6:124:VAL:HG21	1.99	0.44
5:5:111:ALA:O	5:5:115:GLU:HG3	2.17	0.44
5:5:119:TYR:O	5:5:122:PHE:O	2.35	0.44
3:3:36:GLU:HG3	3:3:37:LYS:N	2.32	0.44
11:C:304:ILE:HB	11:C:305:PRO:HD3	1.99	0.44
4:4:339:LYS:HA	4:4:359:SER:O	2.17	0.44
13:E:112:VAL:CG2	13:E:172:ARG:NH2	2.93	0.44
2:2:87:SER:HB3	2:2:128:CYS:HB3	2.00	0.44
1:1:414:LEU:HD13	1:1:421:TYR:CE2	2.53	0.44
29:U:30:ILE:HG13	29:U:31:LEU:N	2.33	0.44
33:Y:72:LYS:HE2	52:Y:273:HOH:O	2.17	0.44
3:3:736:VAL:HG11	3:3:760:LEU:HD22	1.98	0.44
13:E:75:GLU:HG2	13:E:194:ILE:HG12	2.00	0.44
26:R:3:ALA:O	26:R:4:ALA:HB2	2.17	0.44
13:E:95:PRO:HG2	13:E:145:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:19:LEU:HD22	9:A:213:GLN:HG3	2.16	0.44
3:3:36:GLU:HB3	3:3:39:LEU:HD12	1.99	0.44
25:Q:33:ILE:HG22	25:Q:34:LEU:HD12	1.98	0.44
22:N:63:ARG:HA	22:N:67:PHE:CD2	2.53	0.44
1:1:408:TRP:HB2	1:1:409:PRO:HD2	1.99	0.44
22:N:41:THR:O	22:N:45:ILE:HG13	2.18	0.44
4:4:363:SER:CB	5:5:174:LEU:H	2.25	0.44
49:L:516:HEA:O11	49:L:516:HEA:HHC	2.17	0.44
22:N:183:GLU:O	26:R:42:ARG:NH2	2.50	0.44
1:1:391:LEU:HB2	1:1:392:PRO:HD3	2.00	0.44
1:1:97:GLU:HB2	40:1:441:NAI:C4N	2.27	0.44
17:I:62:ARG:HB3	17:I:63:PRO:HD2	2.02	0.44
6:6:145:GLU:HA	6:6:148:ILE:HD13	1.99	0.44
4:4:47:LEU:HD13	4:4:52:VAL:HA	1.98	0.44
2:2:26:ALA:O	2:2:30:LEU:HG	2.18	0.44
1:1:42:LYS:HG3	1:1:163:PHE:CD1	2.53	0.44
20:L:32:ALA:HB3	31:W:36:PRO:HG2	1.98	0.44
7:7:74:PRO:HG2	7:7:77:ALA:HB2	1.99	0.44
7:7:70:ALA:HA	7:7:83:GLY:O	2.17	0.44
15:G:38:LEU:HB3	15:G:42:ARG:NH1	2.32	0.44
11:C:270:PRO:HG2	11:C:278:TYR:CG	2.54	0.44
1:1:184:GLU:OE1	1:1:186:THR:CG2	2.52	0.44
21:M:122:MET:HB2	21:M:208:PRO:CD	2.47	0.44
14:F:110:LYS:HG3	14:F:110:LYS:O	4.85	0.44
2:2:31:LEU:HD22	2:2:49:ILE:HD12	1.99	0.44
2:2:45:ARG:O	2:2:49:ILE:HG13	2.18	0.44
11:C:197:LEU:HD21	44:C:502:HEM:HMA1	2.00	0.44
52:D:4077:HOH:O	14:F:71:ARG:HD3	2.18	0.44
6:6:25:GLU:HA	6:6:28:VAL:HG23	1.98	0.44
21:M:63:THR:HA	21:M:66:THR:HG22	2.00	0.44
13:E:112:VAL:HG22	13:E:172:ARG:NH2	2.34	0.44
5:5:39:ALA:HA	5:5:107:LEU:HD13	1.99	0.44
28:T:61:GLU:OE1	28:T:64:ARG:NH1	2.51	0.44
17:I:36:ALA:CB	17:I:73:PRO:CD	2.95	0.44
5:5:144:HIS:O	5:5:147:ARG:HG2	2.17	0.44
3:3:753:VAL:HA	3:3:754:PRO:HD2	1.84	0.44
1:1:398:SER:C	3:3:46:ARG:HD2	2.38	0.44
12:D:42:SER:HB3	12:D:94:PRO:HD2	2.30	0.44
6:6:132:PRO:HB3	6:6:174:ALA:HB1	2.00	0.44
8:8:103:LEU:HD23	8:8:103:LEU:HA	1.78	0.44
9:A:27:SER:HA	9:A:199:ALA:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:U:36:MET:O	29:U:40:LEU:HG	2.18	0.44
3:3:317:LEU:HD22	3:3:317:LEU:N	2.32	0.44
7:7:13:TRP:O	7:7:17:LEU:HG	2.16	0.44
3:3:587:LEU:O	3:3:604:ALA:HB3	2.17	0.44
1:1:260:ARG:HA	1:1:261:PRO:HD2	1.75	0.44
9:A:433:ASP:OD2	9:A:435:ASN:HB2	2.23	0.44
2:2:125:LEU:HD12	2:2:133:VAL:HG12	2.00	0.44
21:M:98:LYS:HB2	21:M:98:LYS:HE3	1.80	0.44
1:1:171:LEU:HA	1:1:171:LEU:HD12	1.73	0.43
21:M:59:GLN:CA	21:M:62:GLU:HB2	2.46	0.43
1:1:397:ARG:O	3:3:46:ARG:HD3	2.18	0.43
15:G:32:LYS:C	15:G:35:PRO:HD2	2.39	0.43
3:3:368:HIS:CE1	3:3:563:ALA:HA	2.53	0.43
9:A:416:TYR:HB3	18:J:15:ARG:NH2	2.66	0.43
3:3:152:PRO:HG3	4:4:305:PRO:O	2.18	0.43
16:H:51:GLU:HG3	16:H:52:GLU:N	2.32	0.43
44:C:501:HEM:HMC1	44:C:501:HEM:HBC2	2.00	0.43
3:3:514:ASP:OD1	3:3:516:VAL:HB	2.17	0.43
6:6:36:LEU:HD22	6:6:77:VAL:CG2	2.46	0.43
26:R:54:ARG:CD	26:R:54:ARG:N	2.80	0.43
4:4:257:TYR:C	4:4:259:THR:N	2.72	0.43
3:3:250:GLU:CD	3:3:628:PRO:HG2	2.39	0.43
5:5:138:PRO:HA	6:6:87:LYS:HD2	2.00	0.43
9:A:240:GLN:NE2	52:A:4184:HOH:O	2.51	0.43
22:N:137:LEU:HD12	22:N:137:LEU:HA	1.69	0.43
3:3:117:LEU:N	4:4:321:MET:HE3	2.34	0.43
3:3:222:PHE:CD1	3:3:411:LEU:HD11	2.52	0.43
2:2:122:VAL:CG1	2:2:123:GLU:H	2.31	0.43
3:3:344:TYR:CD2	3:3:568:TYR:CE1	3.07	0.43
20:L:377:PHE:CD2	49:L:516:HEA:HAD1	2.54	0.43
3:3:505:LEU:HD21	3:3:507:LEU:CD2	2.48	0.43
28:T:68:ILE:HG13	28:T:69:PHE:N	2.33	0.43
9:A:224:ASP:OD1	9:A:227:ALA:HB2	2.99	0.43
31:W:35:ALA:HB3	31:W:36:PRO:HD3	1.99	0.43
9:A:267:ASN:O	9:A:271:GLN:HG2	2.20	0.43
4:4:260:TYR:HE2	4:4:293:ALA:HB2	1.82	0.43
12:D:106:ASN:CB	52:Y:350:HOH:O	51.52	0.43
3:3:49:LEU:HA	3:3:80:ALA:O	2.18	0.43
8:8:73:ALA:HB3	8:8:87:TYR:CZ	2.53	0.43
4:4:200:ARG:HD2	4:4:200:ARG:HA	1.86	0.43
3:3:223:SER:O	3:3:226:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:M:1:MET:SD	21:M:133:LEU:HD13	2.58	0.43
6:6:50:MET:C	6:6:52:ALA:N	2.71	0.43
3:3:716:LEU:HD21	3:3:758:LEU:HB3	1.99	0.43
3:3:173:PHE:HB3	3:3:296:PHE:CE2	2.54	0.43
3:3:9:ARG:HD2	3:3:26:ALA:O	2.19	0.43
9:A:383:LEU:O	9:A:387:GLY:HA2	2.18	0.43
33:Y:61[A]:GLU:HG3	52:Y:280:HOH:O	2.17	0.43
14:F:77:LYS:HA	14:F:80:TRP:CE2	2.55	0.43
1:1:361:GLU:H	1:1:361:GLU:HG2	1.53	0.43
9:A:408:ARG:NH1	19:K:15:ARG:HG3	79.73	0.43
12:D:145:GLU:OE1	33:Y:25:LYS:CE	64.08	0.43
1:1:180:TYR:N	1:1:351:GLU:OE1	2.47	0.43
3:3:117:LEU:CD1	4:4:321:MET:HE1	2.35	0.43
3:3:719:HIS:CD2	3:3:755:LYS:HG2	2.54	0.43
3:3:305:ARG:NH2	3:3:609:GLU:OE1	2.51	0.43
3:3:125:GLY:HA2	3:3:245:ARG:HH21	1.84	0.43
29:U:3:ASN:ND2	29:U:5:VAL:HG13	2.33	0.43
23:O:40:LEU:HD22	23:O:59:LEU:CD1	2.47	0.43
9:A:381:ARG:HG2	52:A:4120:HOH:O	2.19	0.43
11:C:78:ILE:HD12	12:D:204:MET:CE	2.56	0.43
11:C:269:LYS:HA	11:C:270:PRO:HD3	1.82	0.43
22:N:19:THR:CG2	22:N:53:THR:OG1	2.66	0.43
3:3:300:TRP:N	3:3:705:VAL:HG21	2.33	0.43
19:K:20:THR:HG23	19:K:24:TRP:HD1	1.83	0.43
10:B:230:LEU:HB3	10:B:233:SER:OG	2.17	0.43
33:Y:72:LYS:HG2	52:Y:273:HOH:O	2.17	0.43
2:2:81:GLN:HB3	2:2:122:VAL:CG2	2.43	0.43
6:6:163:TYR:CD2	8:8:152:ARG:NH1	2.85	0.43
3:3:504:VAL:HG12	3:3:505:LEU:N	2.34	0.43
4:4:257:TYR:O	4:4:259:THR:N	2.51	0.43
22:N:80:ARG:HG2	22:N:233:PHE:CE1	2.54	0.43
15:G:48:VAL:O	15:G:51:PRO:HD2	2.18	0.43
8:8:101:CYS:SG	8:8:103:LEU:HB2	2.58	0.43
28:T:26:MET:SD	28:T:26:MET:N	2.91	0.43
12:D:145:GLU:OE2	33:Y:25:LYS:CE	65.75	0.43
3:3:550:LEU:CD2	3:3:684:ARG:HH21	2.31	0.43
4:4:241:ALA:O	4:4:270:GLY:HA2	2.18	0.43
23:O:24:LEU:HA	23:O:25:PRO:HD2	1.93	0.43
3:3:594:ALA:O	3:3:598:ALA:HB3	2.19	0.43
8:8:71:GLU:HA	8:8:72:PRO:HD3	1.80	0.43
27:S:57:ARG:HB3	27:S:57:ARG:NH1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:288:ALA:HB2	9:A:300:THR:HG22	2.02	0.43
3:3:343:LEU:CD1	3:3:360:LEU:HD23	2.49	0.43
20:L:240:HIS:NE2	20:L:244:TYR:CE2	2.81	0.43
1:1:314:GLU:HA	1:1:317:GLN:HB3	1.99	0.43
15:G:50:PRO:HB2	15:G:51:PRO:HD3	2.01	0.43
1:1:401:PRO:HG2	39:1:440:FMN:C8M	2.49	0.43
5:5:178:ASP:HA	5:5:179:PRO:HD2	1.84	0.43
18:J:25:VAL:HG12	19:K:30:VAL:HG12	72.30	0.43
6:6:76:ASP:O	6:6:77:VAL:CB	2.65	0.43
9:A:117:VAL:HG11	9:A:195:MET:CE	2.49	0.43
9:A:286:GLY:HA3	9:A:290:LEU:CD2	2.58	0.43
21:M:100:MET:HE2	21:M:157:GLU:HG3	1.99	0.43
5:5:25:LEU:HD23	5:5:25:LEU:N	2.34	0.43
30:V:44:PRO:HA	30:V:47:ARG:NH1	2.34	0.43
9:A:61:HIS:CE1	9:A:137:GLU:OE1	2.72	0.43
28:T:21:ILE:O	28:T:25:PHE:HD2	2.02	0.43
7:7:45:GLU:H	7:7:45:GLU:CD	2.21	0.43
33:Y:14:CYS:CB	44:Y:500:HEM:HAB	2.47	0.43
5:5:178:ASP:OD1	5:5:179:PRO:HD2	2.19	0.43
3:3:585:MET:HG3	3:3:598:ALA:CB	2.48	0.43
31:W:41:ARG:HD2	32:X:40:TYR:CZ	2.54	0.43
10:B:181:TYR:CD2	10:B:248:ASN:HA	20.25	0.43
3:3:254:THR:HG23	3:3:255:THR:N	2.34	0.43
26:R:78:LEU:HA	26:R:78:LEU:HD12	1.75	0.43
6:6:174:ALA:O	6:6:175:ALA:HB2	2.19	0.43
22:N:60:ASP:O	22:N:64:GLU:HG3	2.19	0.43
21:M:52:HIS:CD2	24:P:40:ASP:HB2	2.54	0.43
3:3:186:ARG:HD2	3:3:231:PRO:HD3	1.99	0.43
3:3:225:ASN:HD21	3:3:289:TRP:HB3	1.84	0.43
3:3:33:PHE:HB2	3:3:45:CYS:SG	2.59	0.43
3:3:194:VAL:HB	3:3:195:PRO:CD	2.44	0.43
3:3:672:ALA:O	3:3:673:MET:HB2	2.19	0.43
21:M:5:MET:HE3	30:V:42:PRO:HA	2.01	0.43
1:1:45:LEU:HD12	1:1:163:PHE:CD2	2.54	0.43
3:3:483:ASP:O	3:3:484:LYS:HG2	2.19	0.43
2:2:15:PHE:HE1	2:2:23:ARG:HB3	1.84	0.43
12:D:47:ALA:HA	12:D:90:TYR:HA	2.01	0.43
26:R:5:LYS:CD	26:R:6:GLY:N	2.81	0.42
3:3:225:ASN:O	3:3:229:ILE:HG13	2.19	0.42
4:4:338:PRO:HG2	5:5:193:ARG:HD3	2.01	0.42
13:E:117:LEU:HD13	13:E:170:ARG:HD2	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:106:PRO:HB2	20:L:107:PRO:HD3	2.01	0.42
20:L:356:ILE:HD13	20:L:356:ILE:HA	1.90	0.42
4:4:369:LYS:HD3	4:4:369:LYS:C	2.40	0.42
5:5:74:LEU:O	5:5:87:ARG:HA	2.19	0.42
3:3:386:SER:HB3	3:3:389:ASP:CG	2.40	0.42
7:7:17:LEU:HD22	7:7:54:ILE:HD11	2.00	0.42
20:L:247:ILE:HB	49:L:516:HEA:HBC1	2.01	0.42
3:3:513:GLN:NE2	3:3:769:LEU:HD21	2.34	0.42
21:M:193:TYR:CE1	23:O:126:MET:HE1	2.51	0.42
3:3:689:LYS:H	3:3:689:LYS:HG2	1.44	0.42
5:5:77:LEU:HA	5:5:78:PRO:HD3	1.61	0.42
6:6:140:CYS:O	6:6:140:CYS:SG	2.77	0.42
3:3:326:PHE:CE2	3:3:330:LYS:HE3	2.55	0.42
3:3:258:LEU:HD11	3:3:703:GLN:NE2	2.34	0.42
4:4:159:LEU:O	4:4:162:TRP:HB2	2.19	0.42
20:L:70:VAL:HG11	20:L:246:LEU:HD22	1.99	0.42
8:8:170:LEU:O	8:8:171:GLU:C	2.56	0.42
3:3:403:THR:HG22	3:3:404:GLU:OE2	2.19	0.42
1:1:67:GLY:HA2	1:1:324:GLY:O	2.20	0.42
24:P:27:TRP:CH2	25:Q:86:GLY:HA2	2.54	0.42
4:4:304:ASP:HA	4:4:305:PRO:HD2	1.87	0.42
22:N:19:THR:HG22	22:N:53:THR:OG1	2.18	0.42
16:H:19:THR:O	16:H:23:GLN:HG3	2.19	0.42
16:H:31:VAL:CG2	16:H:32:LYS:N	2.82	0.42
1:1:291:ILE:HA	1:1:292:PRO:HD2	1.84	0.42
3:3:206:GLY:O	3:3:209:THR:CG2	2.67	0.42
20:L:173:PRO:HA	20:L:174:PRO:HD3	1.96	0.42
23:O:37:GLN:O	23:O:41:LYS:HG2	2.18	0.42
10:B:28:ARG:HB2	10:B:28:ARG:NH1	4.73	0.42
4:4:339:LYS:HG2	4:4:360:ASP:HA	2.01	0.42
11:C:67:THR:HB	12:D:115:TYR:OH	2.29	0.42
3:3:329:LEU:HD21	3:3:644:LEU:HD12	2.01	0.42
20:L:462:LEU:O	20:L:466:MET:HG3	2.20	0.42
19:K:20:THR:HG23	19:K:24:TRP:CD1	2.54	0.42
17:I:77:ARG:O	17:I:78:TYR:HB2	2.19	0.42
2:2:101:THR:HG22	7:7:108:ILE:CD1	2.46	0.42
25:Q:74:LEU:HA	25:Q:74:LEU:HD23	1.87	0.42
8:8:100:PHE:N	8:8:100:PHE:CD1	2.87	0.42
3:3:717:TRP:CD1	3:3:748:VAL:HB	2.54	0.42
49:L:515:HEA:H122	49:L:515:HEA:HHC	2.02	0.42
3:3:258:LEU:HD23	3:3:258:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:96:HIS:O	7:7:103:LEU:HD12	2.19	0.42
9:A:156:THR:HA	13:E:7:VAL:HG21	2.05	0.42
22:N:110:PRO:HB3	27:S:30:TRP:CD2	2.54	0.42
4:4:317:LEU:HD12	4:4:317:LEU:HA	1.91	0.42
22:N:173:PHE:CD1	22:N:173:PHE:C	2.92	0.42
21:M:3:TYR:N	21:M:3:TYR:CD1	2.87	0.42
19:K:24:TRP:CE3	19:K:24:TRP:HA	2.56	0.42
3:3:681:LYS:O	3:3:682:GLU:HB3	2.20	0.42
1:1:437:TRP:O	1:1:437:TRP:HD1	2.03	0.42
6:6:163:TYR:OH	6:6:169:ARG:NH2	2.52	0.42
11:C:68:HIS:HE1	52:C:2049:HOH:O	2.01	0.42
3:3:473:GLU:HG2	3:3:473:GLU:H	1.67	0.42
1:1:6:LEU:HD12	1:1:240:GLN:HG3	2.01	0.42
20:L:187:SER:HB2	20:L:277:MET:CE	2.50	0.42
20:L:495:LEU:HD23	20:L:495:LEU:HA	1.68	0.42
39:1:440:FMN:HM81	40:1:441:NAI:O1N	2.19	0.42
3:3:586:HIS:NE2	3:3:604:ALA:HB2	2.34	0.42
20:L:498:CYS:HA	20:L:499:PRO:HA	1.78	0.42
4:4:350:ARG:HE	4:4:403:VAL:HG23	1.85	0.42
8:8:170:LEU:HD23	8:8:170:LEU:HA	1.88	0.42
16:H:23:GLN:O	16:H:26:GLN:HG2	2.20	0.42
3:3:5:LYS:HB2	3:3:10:ILE:HG13	2.01	0.42
25:Q:53:THR:HG22	25:Q:54:ASN:OD1	2.19	0.42
3:3:155:THR:HB	4:4:322:GLU:OE1	2.19	0.42
4:4:213:ILE:HG22	4:4:217:ARG:CG	2.49	0.42
3:3:20:MET:HG3	3:3:82:SER:OG	2.20	0.42
6:6:163:TYR:HD1	6:6:169:ARG:HA	1.85	0.42
4:4:88:LEU:HD23	4:4:88:LEU:HA	1.95	0.42
44:C:501:HEM:O2D	44:C:501:HEM:O2A	2.37	0.42
4:4:306:ASN:HA	4:4:307:PRO:HD3	1.81	0.42
1:1:390:LEU:HA	1:1:390:LEU:HD23	1.84	0.42
3:3:370:ASP:OD2	3:3:558:TRP:CD1	2.73	0.42
6:6:143:ARG:HG2	6:6:145:GLU:OE1	2.20	0.42
4:4:52:VAL:HG23	4:4:388:GLU:O	2.20	0.42
1:1:110:VAL:N	1:1:111:PRO:CD	2.82	0.42
5:5:116:ARG:CG	5:5:129:HIS:CE1	3.02	0.42
4:4:72:HIS:O	4:4:73:ARG:HD3	2.19	0.42
27:S:24:ASN:HD22	27:S:25:GLN:N	2.18	0.42
3:3:497:TRP:O	3:3:528:LYS:HE3	2.20	0.42
1:1:408:TRP:CB	1:1:409:PRO:CD	2.98	0.42
28:T:21:ILE:HD12	28:T:21:ILE:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:P:21:LYS:O	24:P:57:ARG:NH1	2.53	0.42
8:8:46:HIS:HB3	8:8:47:PRO:HD2	2.01	0.42
9:A:11:VAL:HA	9:A:12:PRO:HD3	1.93	0.42
9:A:280:TYR:HA	9:A:284:TYR:CE2	2.56	0.42
9:A:78:GLU:OE2	9:A:108:LYS:HD2	2.20	0.42
9:A:281:ASP:C	9:A:281:ASP:OD1	2.63	0.42
3:3:116:PRO:HG3	3:3:180:ARG:HG2	2.02	0.42
14:F:12:TRP:O	14:F:15:GLY:N	2.83	0.42
2:2:30:LEU:O	2:2:34:VAL:HG23	2.20	0.42
8:8:81:VAL:HG11	8:8:87:TYR:CD2	2.54	0.42
3:3:157:PHE:CZ	3:3:159:PHE:HB2	2.55	0.42
26:R:42:ARG:NH1	26:R:74:ARG:NH2	2.68	0.42
3:3:368:HIS:HE2	3:3:554:LYS:HG2	1.85	0.42
3:3:563:ALA:HB3	3:3:580:LYS:HE3	2.01	0.42
23:O:86:MET:O	30:V:25:CYS:HB2	2.20	0.42
9:A:158:PHE:O	9:A:164:ALA:HB2	2.20	0.42
3:3:743:VAL:HG12	3:3:744:GLU:N	2.34	0.42
12:D:91:PHE:HA	12:D:92:PRO:HD3	1.93	0.42
27:S:57:ARG:HA	27:S:60:TYR:CD2	2.55	0.41
9:A:347:THR:HA	19:K:16:ASN:HD22	74.39	0.41
2:2:59:GLU:O	2:2:63:VAL:HG23	2.21	0.41
20:L:474:GLU:HG3	20:L:475:ALA:N	2.34	0.41
4:4:296:ARG:O	4:4:298:GLU:HG3	2.20	0.41
6:6:31:GLY:C	6:6:33:SER:N	2.73	0.41
1:1:65:ARG:HH11	1:1:65:ARG:HG3	1.85	0.41
20:L:311:ILE:HD13	20:L:311:ILE:HG21	1.75	0.41
3:3:229:ILE:HD13	3:3:229:ILE:HG21	1.85	0.41
12:D:74:PRO:HG3	12:D:80:MET:HE2	2.19	0.41
4:4:53:LEU:CD2	4:4:53:LEU:N	2.83	0.41
3:3:469:ARG:HD2	3:3:757:HIS:HE1	1.85	0.41
29:U:5:VAL:O	29:U:9:GLN:HG3	2.21	0.41
7:7:16:LEU:HD13	7:7:20:MET:HG3	2.03	0.41
28:T:35:TYR:O	28:T:39:VAL:HB	2.19	0.41
3:3:317:LEU:HD22	3:3:317:LEU:H	1.85	0.41
22:N:146:TRP:CE2	26:R:17:ARG:HB2	2.56	0.41
23:O:127:LYS:O	23:O:130:PRO:HD3	2.20	0.41
1:1:427:GLU:OE1	1:1:429:ARG:HD3	2.20	0.41
20:L:199:LEU:HD12	20:L:199:LEU:HA	1.91	0.41
21:M:185:MET:SD	21:M:185:MET:C	2.99	0.41
2:2:112:THR:HG21	2:2:116:LEU:HD23	2.03	0.41
8:8:96:LEU:CD2	8:8:129:LEU:HD13	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:145:VAL:HG12	2:2:150:LEU:HB2	2.03	0.41
23:O:126:MET:HG3	23:O:128:VAL:HG23	2.01	0.41
22:N:224:LYS:NZ	22:N:226:HIS:HE2	2.18	0.41
2:2:87:SER:CB	2:2:128:CYS:HB3	2.50	0.41
23:O:130:PRO:O	23:O:136:ALA:HB2	2.20	0.41
5:5:67:ARG:HB3	5:5:96:GLU:HB2	2.02	0.41
21:M:164:ALA:HB2	21:M:171:LYS:HD3	2.03	0.41
2:2:163:LEU:HA	2:2:166:ILE:HD11	2.00	0.41
29:U:12:PHE:O	29:U:23:LYS:HE2	2.21	0.41
11:C:19:ILE:HA	11:C:19:ILE:HD13	1.88	0.41
18:J:29:LEU:HD11	19:K:34:SER:HB2	71.97	0.41
1:1:357:THR:N	1:1:358:PRO:CD	2.80	0.41
3:3:683:LEU:HD23	3:3:683:LEU:N	2.35	0.41
10:B:46:ARG:O	10:B:47:ILE:HD13	2.21	0.41
1:1:109:ASP:O	1:1:110:VAL:CG1	2.69	0.41
4:4:279:ARG:O	4:4:283:MET:HG3	2.20	0.41
21:M:193:TYR:CD1	21:M:193:TYR:N	2.88	0.41
4:4:233:GLY:CA	5:5:48:PHE:HE1	2.33	0.41
7:7:59:LEU:HB2	7:7:68:LEU:HB3	2.02	0.41
4:4:379:GLN:O	4:4:382:PRO:HD2	2.21	0.41
1:1:309:THR:HA	1:1:310:PRO:HD3	1.92	0.41
7:7:65:GLU:HA	7:7:66:PRO:HD3	1.73	0.41
4:4:128:SER:OG	4:4:350:ARG:NH1	2.47	0.41
23:O:137:LYS:O	23:O:145:TRP:HE3	2.03	0.41
22:N:182:TYR:O	26:R:72:ASN:HB2	2.21	0.41
8:8:162:VAL:HA	8:8:176:PRO:O	2.21	0.41
24:P:93:LEU:HD23	24:P:93:LEU:HA	1.88	0.41
6:6:44:ALA:O	6:6:46:CYS:N	2.53	0.41
33:Y:72:LYS:HD3	33:Y:78:THR:CG2	2.48	0.41
18:J:2:ALA:HA	18:J:3:PRO:HD3	1.96	0.41
20:L:298:ASP:HB2	20:L:301:THR:CG2	2.49	0.41
2:2:33:ARG:NH2	2:2:37:GLU:CG	2.83	0.41
21:M:191:LEU:HB2	23:O:126:MET:HE1	2.03	0.41
14:F:63:LYS:HG3	52:F:4045:HOH:O	2.20	0.41
4:4:290:ILE:O	4:4:294:LEU:HB2	2.20	0.41
8:8:153:THR:HG22	8:8:155:LYS:N	2.36	0.41
3:3:458:LEU:C	3:3:460:LYS:N	2.73	0.41
6:6:31:GLY:C	6:6:33:SER:H	2.24	0.41
1:1:95:GLU:OE2	1:1:102:LYS:HD3	2.20	0.41
1:1:287:ILE:HG22	1:1:302:PHE:HB2	2.03	0.41
20:L:314:ILE:HB	20:L:315:PRO:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:P:104:LEU:HA	24:P:104:LEU:HD23	1.87	0.41
18:J:21:ALA:CB	19:K:24:TRP:CZ3	64.63	0.41
4:4:84:ARG:O	6:6:83:ARG:NH2	2.54	0.41
6:6:143:ARG:CG	6:6:144:PRO:HD2	2.50	0.41
4:4:221:VAL:HG23	4:4:272:VAL:CG1	2.50	0.41
12:D:43:MET:HE2	12:D:46:VAL:CG2	2.51	0.41
8:8:48:ASN:HB2	8:8:50:LEU:CD2	2.50	0.41
22:N:146:TRP:NE1	26:R:17:ARG:HB2	2.35	0.41
20:L:354:THR:HG21	20:L:376:HIS:HA	2.03	0.41
25:Q:16:LEU:O	25:Q:20:VAL:HG13	2.21	0.41
2:2:154:LEU:O	2:2:158:ARG:HB2	2.21	0.41
3:3:464:ILE:H	3:3:464:ILE:HG12	1.69	0.41
3:3:408:ILE:HG23	3:3:408:ILE:O	2.21	0.41
17:I:36:ALA:HB3	17:I:73:PRO:HB2	2.02	0.41
18:J:25:VAL:CG1	19:K:30:VAL:HG12	71.47	0.41
7:7:75:ARG:HE	7:7:76:HIS:CE1	2.39	0.41
3:3:261:VAL:HG12	3:3:406:ALA:HB1	2.02	0.41
4:4:163:VAL:HG13	4:4:164:THR:HG23	2.02	0.41
3:3:473:GLU:O	3:3:477:LEU:CD1	2.69	0.41
3:3:398:VAL:C	3:3:399:LEU:HD12	2.41	0.41
49:L:515:HEA:HMC1	49:L:515:HEA:HBC1	2.03	0.41
3:3:272:GLY:HA2	3:3:628:PRO:O	2.20	0.41
3:3:169:PRO:HA	3:3:175:ILE:HA	2.03	0.41
20:L:442:ASP:OD2	21:M:134:ARG:NH2	2.54	0.41
11:C:223:TYR:HB3	12:D:227:TRP:CZ2	2.64	0.41
26:R:77:PRO:HA	26:R:82:TYR:HA	2.02	0.41
30:V:24:PHE:CE1	30:V:28:VAL:HG21	2.56	0.41
3:3:409:LEU:HD23	3:3:409:LEU:HA	1.80	0.41
18:J:29:LEU:HD11	19:K:34:SER:CB	71.01	0.41
3:3:651:ARG:NH1	3:3:653:PRO:HA	2.36	0.41
3:3:259:CYS:CB	3:3:260:PRO:CD	2.98	0.41
3:3:285:VAL:HG13	3:3:286:ASN:H	1.86	0.41
20:L:398:PRO:HB3	20:L:482:VAL:HG21	2.03	0.41
11:C:162:GLU:OE2	11:C:168:PHE:CD1	2.76	0.41
8:8:144:LYS:HB2	8:8:145:PRO:CD	2.50	0.41
1:1:102:LYS:H	1:1:102:LYS:HD3	1.84	0.41
1:1:287:ILE:HG13	1:1:330:LEU:HB3	2.03	0.41
12:D:237:TYR:HB2	14:F:60:PHE:CD1	2.56	0.41
9:A:430:GLN:HG2	9:A:430:GLN:O	2.21	0.41
24:P:86:ILE:HD13	24:P:86:ILE:HA	1.88	0.41
18:J:29:LEU:CG	19:K:34:SER:CB	70.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:52:ILE:O	5:5:52:ILE:HG23	2.20	0.41
3:3:501:LYS:H	3:3:501:LYS:CD	2.21	0.41
4:4:48:SER:H	4:4:53:LEU:HD23	1.85	0.41
6:6:163:TYR:HB3	6:6:168:GLU:O	2.21	0.41
4:4:318:GLU:OE2	7:7:75:ARG:NH2	2.54	0.41
7:7:75:ARG:HE	7:7:76:HIS:CD2	2.39	0.41
3:3:205:ARG:CG	3:3:205:ARG:HH11	2.33	0.41
5:5:116:ARG:HG3	5:5:129:HIS:CE1	2.56	0.41
12:D:43:MET:CE	12:D:46:VAL:HG21	2.50	0.41
7:7:68:LEU:HD13	7:7:69:LEU:N	2.36	0.41
20:L:168:ILE:CG2	20:L:189:MET:HG3	2.51	0.41
4:4:30:VAL:CG1	4:4:31:GLY:N	2.83	0.41
8:8:33:LEU:HD22	8:8:37:PHE:CD2	2.55	0.41
29:U:31:LEU:HA	29:U:31:LEU:HD23	1.83	0.41
16:H:51:GLU:HG3	16:H:52:GLU:H	1.86	0.41
3:3:627:ALA:HA	3:3:628:PRO:HD3	1.82	0.41
20:L:69:MET:HE1	20:L:70:VAL:HG23	2.03	0.41
3:3:5:LYS:HA	3:3:10:ILE:HA	2.03	0.41
1:1:65:ARG:HD3	1:1:65:ARG:HA	1.76	0.41
22:N:228:THR:O	22:N:232:HIS:HD2	2.04	0.41
1:1:202:LYS:N	1:1:203:PRO:CD	2.84	0.41
3:3:436:GLN:HE21	3:3:436:GLN:HB3	1.65	0.41
33:Y:57:ILE:C	33:Y:57:ILE:HD12	2.41	0.41
27:S:20:PHE:N	27:S:21:PRO:HD3	2.35	0.41
28:T:19:PHE:CD1	28:T:19:PHE:C	2.94	0.41
27:S:58:ARG:HD2	27:S:58:ARG:HA	1.74	0.41
6:6:107:SER:HB2	6:6:133:VAL:HG11	2.03	0.41
3:3:87:VAL:O	3:3:87:VAL:HG23	2.21	0.41
33:Y:68:LEU:HD21	44:Y:500:HEM:HMB2	2.02	0.41
19:K:24:TRP:O	19:K:25:GLY:C	2.75	0.41
1:1:141:ALA:O	1:1:145:LEU:HB2	2.21	0.41
3:3:652:PRO:HA	3:3:653:PRO:HD3	1.82	0.41
4:4:311:PRO:HD3	4:4:330:HIS:CE1	2.56	0.41
2:2:24:ARG:HG2	2:2:53:VAL:HG11	2.03	0.41
13:E:84:GLY:N	13:E:100:HIS:O	2.54	0.41
4:4:329:LYS:O	4:4:333:GLU:O	2.39	0.41
22:N:6:HIS:CD2	22:N:8:TYR:HB2	2.55	0.41
3:3:504:VAL:CG1	3:3:505:LEU:N	2.84	0.41
21:M:146:MET:SD	21:M:189:PRO:HB3	2.60	0.41
25:Q:49:VAL:O	25:Q:91:LEU:HD12	2.21	0.41
25:Q:86:GLY:O	25:Q:87:THR:O	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:M:60:GLU:CD	21:M:61:VAL:H	2.24	0.41
21:M:145:PRO:HG2	21:M:148:MET:HE2	2.03	0.41
4:4:348:SER:C	4:4:350:ARG:H	2.22	0.41
20:L:69:MET:CE	20:L:70:VAL:HG23	2.51	0.41
20:L:276:ALA:O	20:L:280:ILE:HG13	2.21	0.41
6:6:147:LEU:O	6:6:151:VAL:HG13	2.21	0.41
6:6:155:GLN:C	6:6:157:LYS:N	2.75	0.41
9:A:307:PHE:C	9:A:307:PHE:CD1	2.96	0.41
11:C:129:MET:CE	11:C:181:PHE:CD2	2.90	0.40
5:5:75:VAL:HG22	5:5:87:ARG:HG3	2.03	0.40
4:4:241:ALA:CB	4:4:278:VAL:HG21	2.51	0.40
3:3:156:ARG:HH11	3:3:156:ARG:CG	2.28	0.40
22:N:42:LEU:HA	22:N:42:LEU:HD12	1.66	0.40
3:3:478:LEU:HD12	3:3:520:ARG:CZ	2.52	0.40
14:F:101:ARG:O	14:F:105:GLU:HG3	2.21	0.40
1:1:180:TYR:OH	40:1:441:NAI:H5N	2.21	0.40
18:J:25:VAL:HG12	19:K:30:VAL:HG11	73.44	0.40
3:3:550:LEU:N	3:3:550:LEU:CD1	2.83	0.40
4:4:404:MET:HA	4:4:407:VAL:HG12	2.02	0.40
8:8:44:THR:OG1	8:8:52:LYS:HD2	2.21	0.40
4:4:196:VAL:O	4:4:200:ARG:HB2	2.21	0.40
27:S:65:PRO:HG2	27:S:68:TRP:CG	2.55	0.40
5:5:161:GLU:HG3	5:5:163:ARG:HH22	1.84	0.40
32:X:35:TYR:HD2	32:X:36:HIS:CE1	2.39	0.40
5:5:49:LEU:HD23	5:5:111:ALA:HB2	2.02	0.40
7:7:73:SER:HA	7:7:74:PRO:HD2	1.90	0.40
12:D:148:TYR:HE2	33:Y:16:GLN:HB3	66.63	0.40
3:3:299:GLU:O	3:3:303:GLN:HG3	2.21	0.40
9:A:163:LEU:HA	9:A:163:LEU:HD23	1.92	0.40
17:I:62:ARG:HB2	17:I:78:TYR:CG	2.60	0.40
1:1:117:GLY:O	1:1:120:LEU:HB2	2.21	0.40
3:3:689:LYS:HD2	3:3:772:GLU:CG	2.51	0.40
25:Q:91:LEU:HA	25:Q:91:LEU:HD12	1.89	0.40
4:4:327:HIS:CE1	8:8:107:ALA:O	2.74	0.40
1:1:196:ARG:HG2	2:2:63:VAL:HA	2.04	0.40
8:8:99:ILE:HA	8:8:99:ILE:HD12	1.84	0.40
1:1:273:ARG:O	1:1:277:TYR:HB2	2.21	0.40
9:A:19:LEU:CD2	9:A:213:GLN:HG3	2.57	0.40
23:O:102:TYR:HD2	32:X:35:TYR:HE1	1.68	0.40
1:1:89:LEU:O	1:1:130:GLY:HA2	2.21	0.40
3:3:372:GLN:HB2	3:3:570:PHE:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:64:THR:HB	4:4:66:PHE:CE1	2.57	0.40
17:I:62:ARG:NH2	52:I:1591:HOH:O	2.54	0.40
21:M:168:LEU:HD13	21:M:184:LEU:HG	2.03	0.40
3:3:469:ARG:HG2	3:3:754:PRO:CG	2.52	0.40
4:4:224:ILE:HA	4:4:225:PRO:HD2	1.87	0.40
1:1:429:ARG:HA	1:1:430:PRO:HD2	1.92	0.40
2:2:163:LEU:HA	2:2:166:ILE:CD1	2.52	0.40
5:5:2:ARG:HB2	5:5:84:ASP:OD2	2.21	0.40
26:R:15:THR:O	26:R:19:LEU:HG	2.22	0.40
20:L:23:GLY:HA3	20:L:73:ILE:HG13	2.03	0.40
25:Q:10:GLU:HG2	25:Q:25:ARG:HH22	1.86	0.40
11:C:237:LEU:HD13	12:D:212:MET:HG3	2.04	0.40
10:B:254:HIS:O	10:B:426:ALA:HA	2.21	0.40
25:Q:77:GLY:O	25:Q:90:LYS:NZ	2.54	0.40
6:6:16:ARG:NH1	6:6:17:GLU:OE2	2.54	0.40
27:S:84:LYS:HD2	27:S:84:LYS:HA	1.83	0.40
24:P:79:LYS:HD3	24:P:79:LYS:H	1.87	0.40
15:G:45:ILE:HG22	15:G:46:LEU:N	2.40	0.40
15:G:71:ARG:NH1	15:G:72:LYS:HZ2	8.29	0.40
4:4:230:ILE:O	4:4:230:ILE:CG2	2.67	0.40
16:H:41:ASP:O	16:H:45:SER:CB	2.70	0.40
3:3:688:ARG:CB	3:3:770:ARG:HD3	2.51	0.40
3:3:274:LEU:HD12	3:3:274:LEU:HA	1.82	0.40
8:8:108:CYS:HA	8:8:109:PRO:HD2	1.78	0.40
20:L:461:SER:O	20:L:465:VAL:HG13	2.21	0.40
20:L:34:SER:HB3	20:L:61:HIS:CE1	2.57	0.40
9:A:192:ALA:HB3	9:A:193:PRO:HD3	2.11	0.40
1:1:436:LEU:HD23	2:2:90:LEU:HA	2.03	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 PDB entries followed by that with respect to all EM entries.

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	435/438 (99%)	380 (87%)	48 (11%)	7 (2%)	12 56
2	2	177/181 (98%)	151 (85%)	22 (12%)	4 (2%)	8 48
3	3	748/783 (96%)	624 (83%)	101 (14%)	23 (3%)	5 42
4	4	374/409 (91%)	331 (88%)	34 (9%)	9 (2%)	7 47
5	5	194/207 (94%)	166 (86%)	24 (12%)	4 (2%)	9 50
6	6	140/181 (77%)	114 (81%)	21 (15%)	5 (4%)	4 38
7	7	125/129 (97%)	111 (89%)	13 (10%)	1 (1%)	24 69
8	8	152/182 (84%)	129 (85%)	22 (14%)	1 (1%)	26 71
9	A	441/446 (99%)	425 (96%)	14 (3%)	2 (0%)	34 77
9	a	441/446 (99%)	424 (96%)	16 (4%)	1 (0%)	52 86
10	B	418/439 (95%)	409 (98%)	8 (2%)	1 (0%)	52 86
10	b	420/439 (96%)	406 (97%)	12 (3%)	2 (0%)	34 77
11	C	363/379 (96%)	354 (98%)	6 (2%)	3 (1%)	24 69
11	c	366/379 (97%)	353 (96%)	8 (2%)	5 (1%)	14 58
12	D	239/241 (99%)	234 (98%)	5 (2%)	0	100 100
12	d	239/241 (99%)	235 (98%)	4 (2%)	0	100 100
13	E	194/196 (99%)	183 (94%)	7 (4%)	4 (2%)	9 50
13	e	194/196 (99%)	184 (95%)	9 (5%)	1 (0%)	34 77
14	F	97/110 (88%)	96 (99%)	1 (1%)	0	100 100
14	f	97/110 (88%)	96 (99%)	1 (1%)	0	100 100
15	G	73/81 (90%)	72 (99%)	1 (1%)	0	100 100
15	g	74/81 (91%)	69 (93%)	4 (5%)	1 (1%)	14 58
16	H	64/78 (82%)	61 (95%)	3 (5%)	0	100 100
16	h	64/78 (82%)	62 (97%)	1 (2%)	1 (2%)	12 56
17	I	38/65 (58%)	36 (95%)	1 (3%)	1 (3%)	7 45
17	i	38/65 (58%)	36 (95%)	1 (3%)	1 (3%)	7 45
18	J	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	11 55
18	j	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	11 55
19	K	20/56 (36%)	17 (85%)	2 (10%)	1 (5%)	3 31
19	k	20/56 (36%)	15 (75%)	3 (15%)	2 (10%)	1 14
20	L	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	24 69
21	M	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	15 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
22	N	259/261 (99%)	249 (96%)	10 (4%)	0	100 100
23	O	142/147 (97%)	135 (95%)	7 (5%)	0	100 100
24	P	107/109 (98%)	104 (97%)	3 (3%)	0	100 100
25	Q	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	3 34
26	R	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	2 26
27	S	73/85 (86%)	64 (88%)	8 (11%)	1 (1%)	14 58
28	T	71/73 (97%)	65 (92%)	6 (8%)	0	100 100
29	U	54/59 (92%)	48 (89%)	4 (7%)	2 (4%)	4 38
30	V	47/56 (84%)	41 (87%)	6 (13%)	0	100 100
31	W	45/47 (96%)	42 (93%)	3 (7%)	0	100 100
32	X	41/46 (89%)	39 (95%)	2 (5%)	0	100 100
33	Y	109/104 (105%)	106 (97%)	3 (3%)	0	100 100
All	All	8228/8726 (94%)	7616 (93%)	511 (6%)	101 (1%)	21 61

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	4	PRO
2	2	108	PRO
3	3	6	VAL
3	3	117	LEU
3	3	216	PHE
3	3	367	PRO
3	3	509	ALA
4	4	212	PRO
4	4	255	SER
5	5	81	LYS
7	7	87	PRO
9	A	224	ASP
11	C	16	ASN
11	C	17	ALA
17	I	41	PRO
18	J	61	ASN
20	L	328	HIS
20	L	508	PRO
25	Q	2	SER
25	Q	87	THR
25	Q	95	GLN

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Mol	Chain	Res	Type
26	R	4	ALA
26	R	9	GLY
27	S	46	LYS
29	U	2	GLU
9	a	224	ASP
11	c	17	ALA
15	g	72	LYS
17	i	41	PRO
18	j	61	ASN
1	1	360	ARG
2	2	86	LEU
2	2	124	CYS
3	3	31	PRO
3	3	32	LEU
3	3	125	GLY
3	3	164	VAL
3	3	263	CYS
3	3	453	PRO
3	3	554	LYS
4	4	51	GLU
4	4	258	GLU
5	5	83	GLY
6	6	45	CYS
8	8	152	ARG
10	B	171	ALA
13	E	112	VAL
26	R	5	LYS
10	b	171	ALA
10	b	231	GLY
11	c	16	ASN
16	h	48	SER
1	1	71	PRO
2	2	76	GLY
3	3	28	TYR
3	3	271	SER
3	3	285	VAL
3	3	365	LYS
3	3	374	ARG
3	3	690	GLY
4	4	214	PHE
4	4	389	GLN
6	6	98	GLN

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Mol	Chain	Res	Type
6	6	126	ASN
21	M	104	TRP
26	R	61	SER
13	e	189	SER
19	k	33	VAL
1	1	313	TYR
3	3	682	GLU
3	3	730	GLU
4	4	268	GLU
4	4	270	GLY
6	6	77	VAL
20	L	51	ASP
3	3	203	ILE
3	3	455	ARG
5	5	127	GLU
9	A	228	VAL
11	C	18	PHE
13	E	189	SER
13	E	191	ASP
21	M	103	GLN
29	U	3	ASN
11	c	11	MET
19	k	34	SER
1	1	311	MET
4	4	390	VAL
6	6	20	LEU
20	L	91	ASP
21	M	158	ASP
26	R	49	PRO
11	c	18	PHE
1	1	202	LYS
5	5	52	ILE
13	E	82	PRO
1	1	3	GLY
11	c	13	ILE
25	Q	15	GLY
3	3	626	PRO
19	K	33	VAL

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 PDB entries followed by that with respect to all EM entries.

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	355/356 (100%)	321 (90%)	34 (10%)	10 40
2	2	150/152 (99%)	135 (90%)	15 (10%)	9 38
3	3	607/628 (97%)	560 (92%)	47 (8%)	16 52
4	4	326/355 (92%)	296 (91%)	30 (9%)	11 43
5	5	167/175 (95%)	155 (93%)	12 (7%)	18 55
6	6	117/149 (78%)	107 (92%)	10 (8%)	13 48
7	7	104/106 (98%)	96 (92%)	8 (8%)	16 52
8	8	126/150 (84%)	111 (88%)	15 (12%)	6 31
9	A	364/370 (98%)	359 (99%)	5 (1%)	74 89
9	a	364/370 (98%)	359 (99%)	5 (1%)	74 89
10	B	332/343 (97%)	332 (100%)	0	100 100
10	b	332/343 (97%)	330 (99%)	2 (1%)	90 95
11	C	312/327 (95%)	307 (98%)	5 (2%)	70 88
11	c	316/327 (97%)	310 (98%)	6 (2%)	65 86
12	D	206/206 (100%)	203 (98%)	3 (2%)	72 88
12	d	206/206 (100%)	203 (98%)	3 (2%)	72 88
13	E	168/168 (100%)	167 (99%)	1 (1%)	90 95
13	e	168/168 (100%)	166 (99%)	2 (1%)	78 90
14	F	90/98 (92%)	89 (99%)	1 (1%)	80 91
14	f	90/98 (92%)	89 (99%)	1 (1%)	80 91
15	G	66/71 (93%)	65 (98%)	1 (2%)	72 88
15	g	66/71 (93%)	64 (97%)	2 (3%)	48 77
16	H	63/74 (85%)	61 (97%)	2 (3%)	46 76
16	h	63/74 (85%)	62 (98%)	1 (2%)	70 88
17	I	28/51 (55%)	27 (96%)	1 (4%)	42 74
17	i	28/51 (55%)	26 (93%)	2 (7%)	18 55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	J	51/52 (98%)	49 (96%)	2 (4%)	39 72
18	j	51/52 (98%)	49 (96%)	2 (4%)	39 72
19	K	15/46 (33%)	12 (80%)	3 (20%)	1 11
19	k	15/46 (33%)	11 (73%)	4 (27%)	0 5
20	L	427/427 (100%)	389 (91%)	38 (9%)	12 44
21	M	211/211 (100%)	191 (90%)	20 (10%)	11 41
22	N	226/226 (100%)	199 (88%)	27 (12%)	6 31
23	O	128/129 (99%)	120 (94%)	8 (6%)	22 59
24	P	95/95 (100%)	89 (94%)	6 (6%)	22 59
25	Q	81/81 (100%)	76 (94%)	5 (6%)	23 60
26	R	68/68 (100%)	50 (74%)	18 (26%)	0 5
27	S	67/75 (89%)	58 (87%)	9 (13%)	5 27
28	T	58/58 (100%)	53 (91%)	5 (9%)	13 47
29	U	47/50 (94%)	40 (85%)	7 (15%)	4 23
30	V	39/46 (85%)	37 (95%)	2 (5%)	29 66
31	W	40/40 (100%)	38 (95%)	2 (5%)	30 66
32	X	37/38 (97%)	34 (92%)	3 (8%)	15 50
33	Y	91/84 (108%)	90 (99%)	1 (1%)	80 91
All	All	6961/7311 (95%)	6585 (95%)	376 (5%)	32 64

All (376) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	6	LEU
1	1	9	LEU
1	1	10	ASP
1	1	16	THR
1	1	29	LEU
1	1	49	THR
1	1	102	LYS
1	1	104	ARG
1	1	114	LEU
1	1	128	THR
1	1	144	ARG
1	1	145	LEU
1	1	147	GLN

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Mol	Chain	Res	Type
1	1	155	ARG
1	1	171	LEU
1	1	243	THR
1	1	249	MET
1	1	253	GLN
1	1	270	THR
1	1	287	ILE
1	1	290	ILE
1	1	323	LEU
1	1	342	TRP
1	1	363	VAL
1	1	366	PHE
1	1	368	VAL
1	1	369	ASN
1	1	370	LEU
1	1	374	ILE
1	1	397	ARG
1	1	398	SER
1	1	419	ASP
1	1	431	VAL
1	1	437	TRP
2	2	5	ASP
2	2	7	LYS
2	2	14	THR
2	2	33	ARG
2	2	35	GLN
2	2	46	ILE
2	2	56	THR
2	2	85	THR
2	2	114	ASP
2	2	118	SER
2	2	119	VAL
2	2	153	LEU
2	2	163	LEU
2	2	172	CYS
2	2	176	VAL
3	3	20	MET
3	3	32	LEU
3	3	42	ILE
3	3	46	ARG
3	3	47	MET
3	3	54	LEU

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Mol	Chain	Res	Type
3	3	107	MET
3	3	117	LEU
3	3	124	LYS
3	3	133	ARG
3	3	142	LYS
3	3	143	TYR
3	3	156	ARG
3	3	192	GLU
3	3	207	VAL
3	3	209	THR
3	3	218	LEU
3	3	232	VAL
3	3	259	CYS
3	3	261	VAL
3	3	265	ILE
3	3	275	LEU
3	3	284	GLU
3	3	290	ILE
3	3	303	GLN
3	3	317	LEU
3	3	337	ARG
3	3	381	LEU
3	3	408	ILE
3	3	440	ARG
3	3	450	LEU
3	3	460	LYS
3	3	473	GLU
3	3	492	LYS
3	3	542	ARG
3	3	585	MET
3	3	617	LEU
3	3	655	ARG
3	3	676	LEU
3	3	683	LEU
3	3	684	ARG
3	3	716	LEU
3	3	747	VAL
3	3	761	SER
3	3	774	ARG
3	3	776	LEU
3	3	777	VAL
4	4	41	LEU

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Mol	Chain	Res	Type
4	4	44	MET
4	4	59	ILE
4	4	74	THR
4	4	76	LEU
4	4	105	LEU
4	4	120	LEU
4	4	138	LEU
4	4	163	VAL
4	4	168	PHE
4	4	170	HIS
4	4	182	LEU
4	4	193	LEU
4	4	194	LEU
4	4	199	HIS
4	4	215	TYR
4	4	221	VAL
4	4	234	LEU
4	4	239	LEU
4	4	262	PHE
4	4	294	LEU
4	4	314	ARG
4	4	316	LEU
4	4	319	THR
4	4	335	PHE
4	4	363	SER
4	4	367	ARG
4	4	371	ARG
4	4	385	CYS
4	4	396	ILE
5	5	1	MET
5	5	25	LEU
5	5	27	VAL
5	5	47	ASN
5	5	84	ASP
5	5	90	VAL
5	5	91	ARG
5	5	100	ARG
5	5	103	THR
5	5	135	ILE
5	5	146	LEU
5	5	175	THR
6	6	19	ILE

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Mol	Chain	Res	Type
6	6	20	LEU
6	6	32	ARG
6	6	40	THR
6	6	45	CYS
6	6	83	ARG
6	6	84	LEU
6	6	121	TYR
6	6	147	LEU
6	6	153	GLN
7	7	43	ARG
7	7	63	LEU
7	7	78	LYS
7	7	81	ARG
7	7	82	ILE
7	7	85	ARG
7	7	93	LEU
7	7	120	ASP
8	8	26	TYR
8	8	33	LEU
8	8	36	ARG
8	8	42	VAL
8	8	70	VAL
8	8	94	ASN
8	8	97	ARG
8	8	99	ILE
8	8	130	VAL
8	8	137	LEU
8	8	138	VAL
8	8	139	ASP
8	8	157	VAL
8	8	159	VAL
8	8	163	VAL
9	A	51	LYS
9	A	149	VAL
9	A	245	GLU
9	A	281	ASP
9	A	308	GLN
11	C	80	ARG
11	C	90	PHE
11	C	128	PHE
11	C	222	PRO
11	C	379	TRP

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Mol	Chain	Res	Type
12	D	17	LEU
12	D	76	GLU
12	D	144	ARG
13	E	80	ASP
14	F	58	ARG
15	G	45	ILE
16	H	47	ARG
16	H	51	GLU
17	I	42	VAL
18	J	8	ARG
18	J	16	ARG
19	K	20	THR
19	K	23	LEU
19	K	36	THR
20	L	18	LEU
20	L	35	LEU
20	L	92	MET
20	L	96	ARG
20	L	105	LEU
20	L	109	PHE
20	L	115	SER
20	L	138	HIS
20	L	150	LEU
20	L	159	LEU
20	L	187	SER
20	L	188	VAL
20	L	199	LEU
20	L	213	ARG
20	L	238	PHE
20	L	241	PRO
20	L	273	MET
20	L	295	VAL
20	L	301	THR
20	L	306	THR
20	L	318	VAL
20	L	324	LEU
20	L	347	LEU
20	L	353	LEU
20	L	354	THR
20	L	365	ILE
20	L	369	ASP
20	L	373	VAL

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Mol	Chain	Res	Type
20	L	383	MET
20	L	417	MET
20	L	465	VAL
20	L	467	LEU
20	L	474	GLU
20	L	486	ASP
20	L	492	LEU
20	L	508	PRO
20	L	509	THR
20	L	512	ASN
21	M	7	LEU
21	M	31	VAL
21	M	52	HIS
21	M	60	GLU
21	M	63	THR
21	M	65	TRP
21	M	88	ASP
21	M	92	ASN
21	M	113	TYR
21	M	125	THR
21	M	130	PRO
21	M	134	ARG
21	M	142	VAL
21	M	147	GLU
21	M	148	MET
21	M	170	LEU
21	M	171	LYS
21	M	185	MET
21	M	205	SER
21	M	216	LEU
22	N	1	MET
22	N	11	VAL
22	N	13	PRO
22	N	14	SER
22	N	18	LEU
22	N	19	THR
22	N	22	LEU
22	N	38	ASN
22	N	39	SER
22	N	85	LEU
22	N	92	LEU
22	N	112	LEU

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Mol	Chain	Res	Type
22	N	127	LEU
22	N	128	GLU
22	N	131	LEU
22	N	132	LEU
22	N	137	LEU
22	N	142	VAL
22	N	159	MET
22	N	160	LEU
22	N	163	LEU
22	N	188	ILE
22	N	196	THR
22	N	199	VAL
22	N	214	PHE
22	N	222	GLN
22	N	258	TRP
23	O	31	LYS
23	O	36	SER
23	O	40	LEU
23	O	59	LEU
23	O	62	LEU
23	O	107	ILE
23	O	143	ASN
23	O	147	LYS
24	P	7	THR
24	P	29	LEU
24	P	70	VAL
24	P	79	LYS
24	P	80	GLU
24	P	90	ARG
25	Q	37	LYS
25	Q	53	THR
25	Q	74	LEU
25	Q	95	GLN
25	Q	98	HIS
26	R	5	LYS
26	R	7	ASP
26	R	8	HIS
26	R	14	ARG
26	R	17	ARG
26	R	33	LEU
26	R	34	ASN
26	R	37	LEU

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Mol	Chain	Res	Type
26	R	38	HIS
26	R	41	HIS
26	R	42	ARG
26	R	43	GLU
26	R	48	ILE
26	R	54	ARG
26	R	56	ARG
26	R	68	THR
26	R	69	PHE
26	R	78	LEU
27	S	19	ARG
27	S	24	ASN
27	S	28	ASN
27	S	29	CYS
27	S	51	SER
27	S	53	CYS
27	S	57	ARG
27	S	60	TYR
27	S	75	ARG
28	T	2	THR
28	T	8	GLN
28	T	26	MET
28	T	44	LYS
28	T	64	ARG
29	U	1	PHE
29	U	2	GLU
29	U	3	ASN
29	U	8	LYS
29	U	16	ASN
29	U	23	LYS
29	U	27	THR
30	V	48	VAL
30	V	49	THR
31	W	15	VAL
31	W	22	LEU
32	X	13	LYS
32	X	42	LYS
32	X	43	SER
33	Y	70	ASN
9	a	58	PHE
9	a	149	VAL
9	a	245	GLU

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Mol	Chain	Res	Type
9	a	281	ASP
9	a	308	GLN
10	b	212	SER
10	b	236	LYS
11	c	12	LYS
11	c	43	LEU
11	c	80	ARG
11	c	90	PHE
11	c	222	PRO
11	c	379	TRP
12	d	17	LEU
12	d	35	GLN
12	d	144	ARG
13	e	113	GLU
13	e	190	ASP
14	f	58	ARG
15	g	45	ILE
15	g	73	ASN
16	h	46	SER
17	i	42	VAL
17	i	52	ARG
18	j	8	ARG
18	j	25	VAL
19	k	20	THR
19	k	23	LEU
19	k	34	SER
19	k	36	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	87	HIS
1	1	161	ASN
1	1	219	ASN
1	1	369	ASN
2	2	137	ASN
3	3	303	GLN
3	3	757	HIS
4	4	292	GLN
4	4	327	HIS
4	4	330	HIS
5	5	40	HIS

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Mol	Chain	Res	Type
5	5	47	ASN
5	5	112	ASN
7	7	92	HIS
8	8	94	ASN
9	A	15	GLN
9	A	61	HIS
9	A	136	GLN
9	A	213	GLN
9	A	271	GLN
10	B	22	GLN
10	B	104	ASN
10	B	343	GLN
10	B	412	ASN
11	C	68	HIS
11	C	159	ASN
12	D	106	ASN
13	E	57	GLN
13	E	116	GLN
15	G	28	HIS
15	G	73	ASN
20	L	11	ASN
20	L	12	HIS
20	L	43	GLN
20	L	99	ASN
20	L	170	ASN
20	L	256	HIS
20	L	360	ASN
20	L	413	HIS
20	L	512	ASN
21	M	103	GLN
21	M	203	ASN
22	N	6	HIS
22	N	12	ASN
22	N	133	ASN
22	N	148	HIS
22	N	158	HIS
22	N	207	HIS
22	N	222	GLN
22	N	232	HIS
23	O	109	HIS
24	P	34	ASN
25	Q	66	ASN

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Mol	Chain	Res	Type
26	R	52	HIS
27	S	23	GLN
27	S	24	ASN
27	S	25	GLN
27	S	28	ASN
27	S	37	HIS
28	T	8	GLN
29	U	3	ASN
29	U	16	ASN
30	V	10	HIS
30	V	15	ASN
30	V	41	ASN
32	X	39	ASN
33	Y	54	ASN
33	Y	70	ASN
9	a	15	GLN
9	a	61	HIS
9	a	136	GLN
9	a	165	GLN
9	a	213	GLN
9	a	271	GLN
10	b	104	ASN
10	b	240	HIS
10	b	343	GLN
10	b	412	ASN
11	c	68	HIS
11	c	159	ASN
13	e	57	GLN
14	f	73	GLN
15	g	28	HIS
17	i	71	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 42 ligands modelled in this entry, 12 are monoatomic - leaving 30 for Mogul analysis.

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	$\#\|Z\| > 2$
38	SF4	1	439	1	0,12,12	0.00	-	0,24,24	0.00	-
39	FMN	1	440	-	32,33,33	1.44	4 (12%)	34,50,50	1.99	6 (17%)
40	NAI	1	441	-	41,48,48	3.78	27 (65%)	46,73,73	1.92	4 (8%)
42	FES	2	182	2	0,4,4	0.00	-	0,4,4	0.00	-
38	SF4	3	784	3	0,12,12	0.00	-	0,24,24	0.00	-
38	SF4	3	785	3	0,12,12	0.00	-	0,24,24	0.00	-
38	SF4	3	786	3	0,12,12	0.00	-	0,24,24	0.00	-
42	FES	3	787	3	0,4,4	0.00	-	0,4,4	0.00	-
38	SF4	6	182	6	0,12,12	0.00	-	0,24,24	0.00	-
38	SF4	8	183	8	0,12,12	0.00	-	0,24,24	0.00	-
38	SF4	8	184	8	0,12,12	0.00	-	0,24,24	0.00	-
45	SMA	C	2001	-	35,38,38	1.82	6 (17%)	39,52,52	1.81	3 (7%)
46	UQ1	C	2002	-	14,14,18	2.13	8 (57%)	18,20,25	0.52	0
44	HEM	C	501	11	24,50,50	2.07	6 (25%)	16,82,82	1.49	4 (25%)
44	HEM	C	502	11	24,50,50	2.13	7 (29%)	16,82,82	2.11	5 (31%)
47	HEC	D	501	12	24,50,50	2.00	5 (20%)	19,82,82	3.04	5 (26%)
42	FES	E	501	13	0,4,4	0.00	-	0,4,4	0.00	-
48	CDL	G	2003	-	49,49,99	1.09	4 (8%)	51,61,111	1.12	4 (7%)
48	CDL	G	2004	-	43,43,99	1.12	2 (4%)	45,55,111	1.25	4 (8%)
49	HEA	L	515	20	40,67,67	1.49	5 (12%)	36,103,103	1.66	8 (22%)
49	HEA	L	516	20	40,67,67	1.58	4 (10%)	36,103,103	1.48	9 (25%)
44	HEM	Y	500	33	24,50,50	1.66	4 (16%)	16,82,82	2.87	8 (50%)
45	SMA	c	3001	-	35,38,38	2.02	8 (22%)	39,52,52	1.84	3 (7%)
46	UQ1	c	3002	-	14,14,18	1.94	8 (57%)	18,20,25	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	HEM	c	501	11	24,50,50	2.24	7 (29%)	16,82,82	1.24	2 (12%)
44	HEM	c	502	11	24,50,50	2.32	8 (33%)	16,82,82	1.72	4 (25%)
48	CDL	d	3003	-	49,49,99	1.08	4 (8%)	51,61,111	1.18	4 (7%)
47	HEC	d	501	12	24,50,50	2.04	4 (16%)	19,82,82	2.58	3 (15%)
42	FES	e	501	13	0,4,4	0.00	-	0,4,4	0.00	-
48	CDL	g	3004	-	48,48,99	1.14	4 (8%)	50,60,111	1.14	2 (4%)

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
38	SF4	1	439	1	-	0/0/48/48	0/6/5/5
39	FMN	1	440	-	-	0/18/18/18	0/3/3/3
40	NAI	1	441	-	-	0/25/72/72	0/5/5/5
42	FES	2	182	2	-	0/0/4/4	0/1/1/1
38	SF4	3	784	3	-	0/0/48/48	0/6/5/5
38	SF4	3	785	3	-	0/0/48/48	0/6/5/5
38	SF4	3	786	3	-	0/0/48/48	0/6/5/5
42	FES	3	787	3	-	0/0/4/4	0/1/1/1
38	SF4	6	182	6	-	0/0/48/48	0/6/5/5
38	SF4	8	183	8	-	0/0/48/48	0/6/5/5
38	SF4	8	184	8	-	0/0/48/48	0/6/5/5
45	SMA	C	2001	-	-	0/33/34/34	0/2/2/2
46	UQ1	C	2002	-	-	0/4/28/33	0/1/1/1
44	HEM	C	501	11	-	0/6/54/54	0/0/8/8
44	HEM	C	502	11	-	0/6/54/54	0/0/8/8
47	HEC	D	501	12	-	0/6/54/54	0/0/8/8
42	FES	E	501	13	-	0/0/4/4	0/1/1/1
48	CDL	G	2003	-	-	0/58/58/110	0/0/0/0
48	CDL	G	2004	-	-	0/52/52/110	0/0/0/0
49	HEA	L	515	20	3/3/7/16	0/24/76/76	0/0/8/8
49	HEA	L	516	20	3/3/7/16	0/24/76/76	0/0/8/8
44	HEM	Y	500	33	-	0/6/54/54	0/0/8/8
45	SMA	c	3001	-	-	0/33/34/34	0/2/2/2
46	UQ1	c	3002	-	-	0/4/28/33	0/1/1/1
44	HEM	c	501	11	-	0/6/54/54	0/0/8/8
44	HEM	c	502	11	-	0/6/54/54	0/0/8/8
48	CDL	d	3003	-	-	0/58/58/110	0/0/0/0
47	HEC	d	501	12	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	FES	e	501	13	-	0/0/4/4	0/1/1/1
48	CDL	g	3004	-	-	0/57/57/110	0/0/0/0

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	1	441	NAI	C2B-C1B	-9.32	1.38	1.53
49	L	516	HEA	C3A-C2A	-7.06	1.31	1.40
47	d	501	HEC	C3C-C2C	-6.16	1.34	1.40
47	D	501	HEC	C3B-C2B	-5.94	1.34	1.40
40	1	441	NAI	C2B-C3B	-5.72	1.38	1.53
40	1	441	NAI	C3D-C4D	-5.51	1.38	1.53
44	c	501	HEM	C3B-CAB	-5.44	1.36	1.47
44	C	501	HEM	C3C-CAC	-5.32	1.36	1.47
40	1	441	NAI	C2D-C1D	-5.14	1.37	1.53
40	1	441	NAI	C3B-C4B	-5.02	1.39	1.53
47	D	501	HEC	C3C-C2C	-4.90	1.35	1.40
44	c	502	HEM	C3B-CAB	-4.87	1.37	1.47
44	c	501	HEM	C3C-CAC	-4.85	1.37	1.47
44	C	502	HEM	C3C-CAC	-4.83	1.37	1.47
44	Y	500	HEM	C3C-CAC	-4.83	1.37	1.47
44	c	502	HEM	C3C-CAC	-4.74	1.37	1.47
44	C	501	HEM	C3B-CAB	-4.57	1.38	1.47
49	L	516	HEA	C3A-CMA	-3.84	1.37	1.46
49	L	515	HEA	C3C-C2C	-3.59	1.35	1.40
47	d	501	HEC	C3B-C2B	-3.49	1.37	1.40
40	1	441	NAI	O4B-C1B	-3.44	1.36	1.41
40	1	441	NAI	C2D-C3D	-3.33	1.44	1.53
40	1	441	NAI	O4D-C4D	-3.17	1.37	1.45
40	1	441	NAI	C6A-N1A	-3.07	1.23	1.37
49	L	515	HEA	C3A-CMA	-2.97	1.39	1.46
40	1	441	NAI	O4B-C4B	-2.96	1.38	1.45
44	c	501	HEM	C3B-C2B	-2.87	1.36	1.40
49	L	516	HEA	C3C-C2C	-2.82	1.36	1.40
44	Y	500	HEM	C3B-CAB	-2.71	1.42	1.47
40	1	441	NAI	PN-O1N	-2.67	1.43	1.55
40	1	441	NAI	O3B-C3B	-2.56	1.36	1.43
44	c	502	HEM	C3B-C2B	-2.54	1.37	1.40
44	Y	500	HEM	C4A-CHB	-2.54	1.33	1.40
48	g	3004	CDL	OA8-CA6	-2.53	1.39	1.45
40	1	441	NAI	C1D-N1N	-2.52	1.38	1.46
48	g	3004	CDL	OB8-CB6	-2.41	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	1	441	NAI	O4D-C1D	-2.41	1.36	1.42
44	C	502	HEM	C3B-CAB	-2.40	1.42	1.47
49	L	515	HEA	C3A-C2A	-2.40	1.37	1.40
40	1	441	NAI	PA-O2A	-2.38	1.45	1.55
45	c	3001	SMA	C9-C2	-2.28	1.48	1.51
39	1	440	FMN	C10-N10	-2.24	1.36	1.39
40	1	441	NAI	O2B-C2B	-2.24	1.37	1.43
48	G	2004	CDL	OA8-CA6	-2.13	1.40	1.45
48	d	3003	CDL	OA8-CA6	-2.12	1.40	1.45
48	d	3003	CDL	OB8-CB6	-2.12	1.40	1.45
44	C	501	HEM	C3B-C2B	-2.12	1.37	1.40
48	G	2003	CDL	OB8-CB6	-2.08	1.40	1.45
48	G	2003	CDL	OA8-CA6	-2.02	1.40	1.45
49	L	516	HEA	CAA-C2A	2.09	1.55	1.52
47	D	501	HEC	C4C-NC	2.10	1.39	1.36
44	c	501	HEM	C1C-NC	2.15	1.39	1.36
46	C	2002	UQ1	C5-C4	2.16	1.55	1.47
46	c	3002	UQ1	C3-C4	2.16	1.55	1.49
48	d	3003	CDL	CB3-CB4	2.18	1.57	1.50
46	c	3002	UQ1	C5-C4	2.19	1.55	1.47
48	G	2003	CDL	CA3-CA4	2.20	1.57	1.50
46	C	2002	UQ1	C6-C1	2.22	1.55	1.47
48	G	2003	CDL	O1-C1	2.25	1.50	1.43
40	1	441	NAI	C4A-N3A	2.26	1.38	1.35
48	d	3003	CDL	O1-C1	2.27	1.50	1.43
46	c	3002	UQ1	C6-C1	2.30	1.56	1.47
45	c	3001	SMA	C6-C5	2.32	1.45	1.37
44	c	502	HEM	CMC-C2C	2.33	1.56	1.51
40	1	441	NAI	PN-O5D	2.33	1.69	1.59
46	c	3002	UQ1	O3-C3	2.35	1.43	1.36
40	1	441	NAI	C6A-C5A	2.37	1.55	1.42
46	c	3002	UQ1	O2-C2	2.38	1.43	1.36
46	c	3002	UQ1	C2-C1	2.38	1.56	1.49
47	D	501	HEC	C3B-C4B	2.42	1.47	1.43
45	C	2001	SMA	C4A-C8A	2.45	1.44	1.41
48	g	3004	CDL	CA3-CA4	2.46	1.57	1.50
48	g	3004	CDL	O1-C1	2.47	1.50	1.43
48	G	2004	CDL	O1-C1	2.61	1.51	1.43
45	c	3001	SMA	C7-C8	2.63	1.43	1.40
44	C	501	HEM	C1B-NB	2.70	1.40	1.36
46	C	2002	UQ1	O2-C2	2.71	1.44	1.36
46	c	3002	UQ1	CM5-C5	2.75	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	C	2002	UQ1	C2-C1	2.77	1.57	1.49
46	C	2002	UQ1	C3-C4	2.78	1.57	1.49
46	C	2002	UQ1	CM5-C5	2.81	1.56	1.50
47	d	501	HEC	C3C-C4C	2.83	1.48	1.43
39	1	440	FMN	C5A-N5	2.83	1.39	1.35
45	C	2001	SMA	C7-C8	2.89	1.44	1.40
46	c	3002	UQ1	C7-C6	2.93	1.57	1.50
46	C	2002	UQ1	C7-C6	2.93	1.57	1.50
45	C	2001	SMA	C6-C7	2.96	1.44	1.38
46	C	2002	UQ1	O3-C3	2.99	1.44	1.36
45	c	3001	SMA	C4A-C8A	3.04	1.45	1.41
45	c	3001	SMA	C6-C7	3.08	1.44	1.38
44	c	501	HEM	CBC-CAC	3.09	1.52	1.28
44	c	502	HEM	CBC-CAC	3.15	1.52	1.28
47	D	501	HEC	C3C-C4C	3.20	1.49	1.43
40	1	441	NAI	C6A-N6A	3.26	1.47	1.34
44	C	502	HEM	CBC-CAC	3.28	1.53	1.28
45	C	2001	SMA	O1-C2	3.30	1.39	1.35
44	C	502	HEM	CBB-CAB	3.32	1.53	1.28
44	C	501	HEM	CBC-CAC	3.36	1.54	1.28
45	c	3001	SMA	C4-C3	3.42	1.51	1.41
44	C	501	HEM	CBB-CAB	3.42	1.54	1.28
45	C	2001	SMA	C4-C3	3.52	1.51	1.41
39	1	440	FMN	C4A-N5	3.61	1.38	1.33
44	c	501	HEM	CBB-CAB	3.69	1.56	1.28
44	C	502	HEM	C1C-NC	3.69	1.41	1.36
44	Y	500	HEM	C3B-C2B	3.69	1.45	1.40
44	C	502	HEM	C1B-NB	3.71	1.41	1.36
44	c	502	HEM	CBB-CAB	3.75	1.57	1.28
40	1	441	NAI	C5A-N7A	3.76	1.52	1.39
39	1	440	FMN	C4-N3	3.82	1.39	1.33
40	1	441	NAI	PN-O2N	3.83	1.65	1.51
40	1	441	NAI	PA-O1A	3.93	1.65	1.51
44	C	502	HEM	C4D-ND	3.97	1.42	1.36
44	c	501	HEM	C4C-NC	4.04	1.42	1.36
40	1	441	NAI	C7N-N7N	4.12	1.45	1.33
49	L	515	HEA	C1A-NA	4.18	1.42	1.36
44	c	502	HEM	C1C-NC	4.19	1.42	1.36
45	c	3001	SMA	O1-C2	4.31	1.40	1.35
40	1	441	NAI	C4N-C5N	4.33	1.58	1.49
44	c	502	HEM	C4C-NC	4.37	1.42	1.36
49	L	515	HEA	C4B-NB	4.42	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	d	501	HEC	C3B-C4B	4.45	1.51	1.43
45	C	2001	SMA	C4-C4A	6.74	1.50	1.41
40	1	441	NAI	C2N-N1N	6.81	1.50	1.37
45	c	3001	SMA	C4-C4A	7.64	1.52	1.41
40	1	441	NAI	C2A-N1A	11.02	1.55	1.33

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	1	441	NAI	N3A-C2A-N1A	-9.78	121.19	128.87
47	D	501	HEC	CBB-CAB-C3B	-8.90	107.89	127.34
47	d	501	HEC	CBB-CAB-C3B	-8.75	108.22	127.34
47	D	501	HEC	CBC-CAC-C3C	-8.03	109.79	127.34
45	c	3001	SMA	C9-C10-C11	-7.19	105.90	114.79
45	C	2001	SMA	C9-C10-C11	-6.51	106.74	114.79
47	d	501	HEC	CBC-CAC-C3C	-5.74	114.79	127.34
44	Y	500	HEM	CBD-CAD-C3D	-4.76	104.11	112.47
44	C	502	HEM	CBD-CAD-C3D	-4.68	104.26	112.47
39	1	440	FMN	N3-C2-N1	-4.42	120.24	127.69
49	L	515	HEA	C17-C18-C19	-4.39	118.07	127.75
48	G	2004	CDL	CB4-OB6-CB5	-4.29	109.85	117.93
44	c	502	HEM	CMA-C3A-C4A	-4.02	121.47	128.31
40	1	441	NAI	C4D-O4D-C1D	-3.88	100.98	109.52
48	d	3003	CDL	CB4-OB6-CB5	-3.81	110.77	117.93
48	g	3004	CDL	CA4-OA6-CA5	-3.77	110.84	117.93
48	G	2003	CDL	CA4-OA6-CA5	-3.54	111.26	117.93
49	L	515	HEA	C13-C14-C15	-3.52	119.98	127.75
39	1	440	FMN	C4A-C4-N3	-3.44	119.02	123.52
49	L	515	HEA	CMB-C2B-C1B	-3.40	122.53	128.31
39	1	440	FMN	C1'-C2'-C3'	-3.39	100.13	109.82
44	C	501	HEM	CBA-CAA-C2A	-3.08	107.07	112.49
48	d	3003	CDL	CA6-CA4-CA3	-3.07	104.92	112.08
48	g	3004	CDL	CB4-OB6-CB5	-3.03	110.42	117.91
47	D	501	HEC	CMD-C2D-C1D	-2.95	123.29	128.31
48	G	2004	CDL	CA6-CA4-CA3	-2.89	105.34	112.08
49	L	515	HEA	C16-C17-C18	-2.83	104.19	111.61
44	Y	500	HEM	CMA-C3A-C4A	-2.76	123.62	128.31
48	G	2003	CDL	CB4-OB6-CB5	-2.74	111.14	117.91
49	L	515	HEA	C27-C19-C18	-2.68	118.39	123.58
48	d	3003	CDL	CA4-OA6-CA5	-2.62	111.43	117.91
49	L	516	HEA	C13-C14-C15	-2.53	122.17	127.75
48	G	2003	CDL	CB6-CB4-CB3	-2.53	106.19	112.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	C	2001	SMA	C3M-C3-C4	-2.49	117.00	121.22
44	Y	500	HEM	CMD-C2D-C1D	-2.39	124.24	128.31
45	c	3001	SMA	C3M-C3-C4	-2.39	117.16	121.22
44	C	502	HEM	CMA-C3A-C4A	-2.33	124.35	128.31
44	C	501	HEM	CAA-C2A-C3A	-2.29	122.46	129.00
49	L	515	HEA	C17-C16-C15	-2.28	105.06	112.61
48	G	2004	CDL	CB6-CB4-CB3	-2.25	106.85	112.08
48	G	2004	CDL	CA4-OA6-CA5	-2.24	112.38	117.91
48	d	3003	CDL	CB6-OB8-CB7	-2.21	111.57	117.12
48	G	2003	CDL	CA6-OA8-CA7	-2.10	111.85	117.12
47	d	501	HEC	CMC-C2C-C1C	-2.10	124.74	128.31
49	L	515	HEA	C12-C13-C14	-2.07	106.54	112.42
49	L	516	HEA	C26-C15-C14	-2.06	119.59	123.58
49	L	516	HEA	C1A-C2A-C3A	-2.00	105.07	107.07
44	c	501	HEM	CMA-C3A-C2A	2.01	129.43	125.24
49	L	516	HEA	C27-C19-C20	2.04	118.48	115.37
44	C	501	HEM	CMD-C2D-C3D	2.07	129.56	125.24
49	L	516	HEA	C25-C23-C24	2.11	119.73	114.61
49	L	516	HEA	CMC-C2C-C3C	2.14	129.28	125.09
44	c	502	HEM	C3B-CAB-CBB	2.15	130.72	126.40
39	1	440	FMN	C4A-N5-C5A	2.15	119.26	116.72
47	D	501	HEC	CMA-C3A-C2A	2.20	129.85	125.24
44	Y	500	HEM	C3B-C4B-NB	2.23	112.09	109.21
47	D	501	HEC	C4B-C3B-C2B	2.27	108.87	106.19
44	C	502	HEM	CMA-C3A-C2A	2.33	130.11	125.24
49	L	516	HEA	C26-C15-C16	2.36	118.97	115.37
44	Y	500	HEM	CMB-C2B-C3B	2.37	129.73	125.09
44	c	502	HEM	CMA-C3A-C2A	2.53	130.53	125.24
49	L	515	HEA	C20-C19-C18	2.64	125.89	120.98
44	c	501	HEM	CMC-C2C-C3C	2.65	130.26	125.09
40	1	441	NAI	O5B-C5B-C4B	2.69	118.80	109.09
44	Y	500	HEM	CMD-C2D-C3D	2.75	131.00	125.24
44	C	502	HEM	CMC-C2C-C3C	2.78	130.52	125.09
44	C	501	HEM	C3B-C4B-NB	2.80	112.83	109.21
49	L	516	HEA	CBA-CAA-C2A	2.84	117.45	112.47
40	1	441	NAI	O4D-C1D-N1N	3.11	114.02	108.09
44	c	502	HEM	CMC-C2C-C3C	3.28	131.51	125.09
49	L	516	HEA	CBD-CAD-C3D	3.32	118.32	112.49
44	Y	500	HEM	CAD-CBD-CGD	3.88	120.33	112.78
44	C	502	HEM	C3B-C4B-NB	3.95	114.32	109.21
39	1	440	FMN	O2'-C2'-C3'	4.88	121.51	108.96
39	1	440	FMN	C4-N3-C2	6.10	120.24	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	Y	500	HEM	C3C-CAC-CBC	7.13	140.73	126.40
45	C	2001	SMA	C9-C2-C3	7.22	130.08	120.56
45	c	3001	SMA	C9-C2-C3	7.24	130.11	120.56

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
49	L	516	HEA	ND
49	L	516	HEA	NA
49	L	516	HEA	NB
49	L	515	HEA	ND
49	L	515	HEA	NA
49	L	515	HEA	NB

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	1	440	FMN	6	0
40	1	441	NAI	6	0
38	3	784	SF4	1	0
38	3	785	SF4	1	0
38	3	786	SF4	1	0
42	3	787	FES	1	0
38	6	182	SF4	1	0
38	8	183	SF4	2	0
45	C	2001	SMA	1	0
46	C	2002	UQ1	2	0
44	C	501	HEM	2	0
44	C	502	HEM	3	0
47	D	501	HEC	6	0
48	G	2004	CDL	5	0
49	L	515	HEA	3	0
49	L	516	HEA	4	0
44	Y	500	HEM	7	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.