



## wwPDB EM Map/Model Validation Report ⓘ

Sep 19, 2016 – 01:14 PM EDT

PDB ID : 5LDX  
EMDB ID: : EMD-4041  
Title : Structure of mammalian respiratory Complex I, class3.  
Authors : Vinothkumar, K.R.; Zhu, J.; Hirst, J.  
Deposited on : 2016-06-28  
Resolution : 5.60 Å(reported)

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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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) : rb-20027939

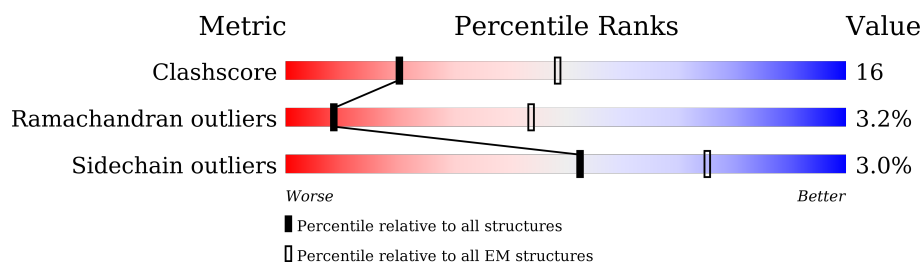
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.60 Å.

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




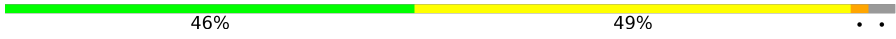
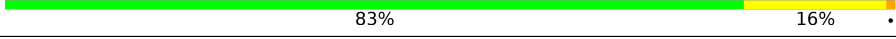

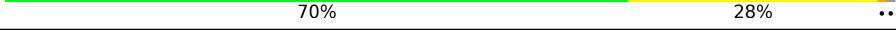
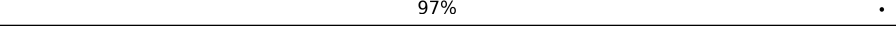
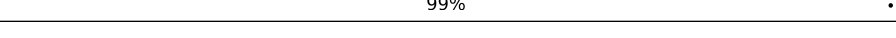
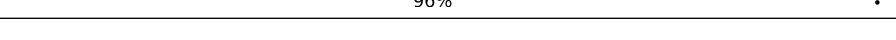
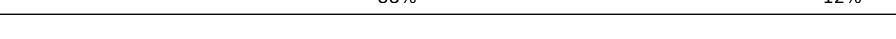
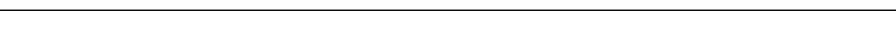







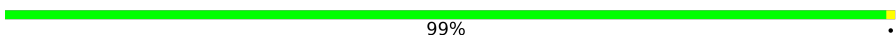

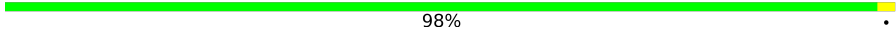



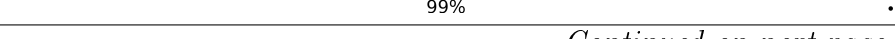

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	115	
2	B	179	
3	C	228	
4	D	429	
5	E	217	
6	F	444	
7	G	700	
8	H	318	
9	I	176	

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Mol	Chain	Length	Quality of chain
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	314	
16	P	283	
17	Q	113	
18	R	89	
19	S	99	
20	T	88	
20	U	88	
21	V	115	
22	W	127	
23	X	164	
24	Y	140	
25	Z	138	
26	a	70	
27	b	80	
28	c	49	
29	d	114	
30	e	106	
31	f	57	
32	g	125	
33	h	134	

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Mol	Chain	Length	Quality of chain
34	i	106	 99% .
35	j	52	 100%
36	k	74	 100%
37	l	118	 100%
38	m	118	 95% 5%
39	n	166	 98% .
40	o	58	 98% .
41	p	169	 97% .
42	q	138	 96% .
43	r	87	 100%
44	s	35	 100%

## 2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 51181 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-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	88	Total	C	N	O	S	0	0
			687	472	99	113	3		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	147	Total	C	N	O	S	0	0
			1159	740	203	202	14		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1684	1091	285	305	3		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	416	Total	C	N	O	S	0	0
			3229	2056	560	589	24		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	conflict	UNP P17694

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	186	Total	C	N	O	S	0	0
			959	583	186	186	4		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	425	Total	C	N	O	S	0	0
			2356	1432	463	455	6		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial, NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial, NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial, NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	685	Total	C	N	O	S	0	0
			3614	2172	715	712	15		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	296	Total	C	N	O	S	0	0
			2306	1551	357	376	22		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	176	Total	C	N	O	S	0	0
			1366	857	238	261	10		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	171	Total	C	N	O	S	0	0
			1211	814	179	207	11		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	95	Total	C	N	O	S	0	0
			720	472	108	126	14		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	604	Total	C	N	O	S	0	0
			4538	3005	708	787	38		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	457	Total	C	N	O	S	0	0
			3536	2352	555	591	38		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	344	Total	C	N	O	S	0	0
			2592	1713	405	440	34		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	314	Total	C	N	O	S	0	0
			1851	1148	347	353	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, NDUFA9.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	283	Total	C	N	O	0	0
			1415	849	283	283		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, NDUFS4.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	113	Total	C	N	O	0	0
			565	339	113	113		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial,NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial,NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	89	Total	C	N	O	S	0	0
			501	304	99	95	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	80	Total	C	N	O		0	0
			405	245	80	80			

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	75	Total	C	N	O		0	0
			378	228	75	75			
20	U	85	Total	C	N	O		0	0
			432	262	85	85			

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	106	Total	C	N	O	S	0	0
			685	430	126	128	1		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	111	Total	C	N	O	S	0	0
			817	516	154	144	3		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	164	Total	C	N	O	S	0	0
			1133	703	213	208	9		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	138	Total	C	N	O	S	0	0
			1011	644	173	188	6		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	138	Total	C	N	O	S	0	0
			921	573	172	170	6		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	64	Total	C	N	O	S	0	0
			480	312	86	77	5		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	80	Total	C	N	O	S	0	0
			519	336	89	93	1		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	46	Total	C	N	O	0	0
			320	211	56	53		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	114	Total	C	N	O	S	0	0
			790	504	146	137	3		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	89	Total	C	N	O	S	0	0
			616	382	121	108	5		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	54	Total	C	N	O	S	0	0
			350	223	62	64	1		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	97	Total	C	N	O	S	0	0
			677	438	120	117	2		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	134	Total	C	N	O		0	0
			770	486	143	141			

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	106	Total	C	N	O		0	0
			616	376	126	114			

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, NDUF2.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	j	52	Total	C	N	O	0	0
			260	156	52	52		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3, NDUF3.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	k	74	Total	C	N	O	0	0
			370	222	74	74		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, NDUF8.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	l	118	Total	C	N	O	0	0
			590	354	118	118		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	m	118	Total	C	N	O	0	0
			887	566	165	156		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	166	Total	C	N	O	S	0	0
			1088	677	212	196	3		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	58	Total	C	N	O	S	0	0
			296	176	58	58	4		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1

beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	169	Total	C	N	O	S	0	0
			1039	633	198	202	6		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	q	138	Total	C	N	O	0	0
			696	420	138	138		

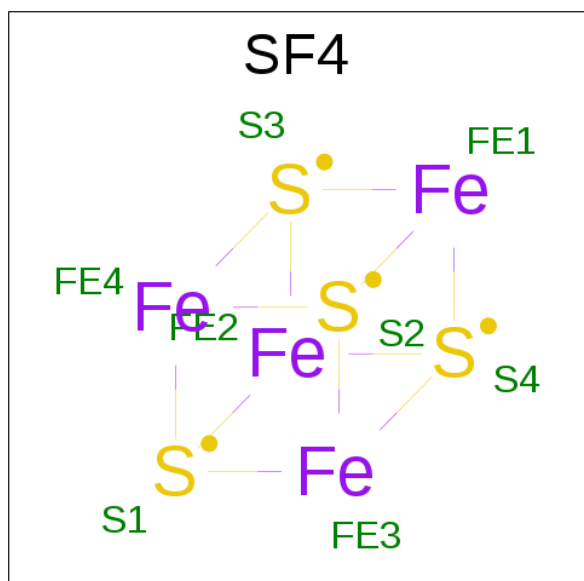
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7, NDUFA7.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	r	87	Total	C	N	O	0	0
			435	261	87	87		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, NDUFV3.

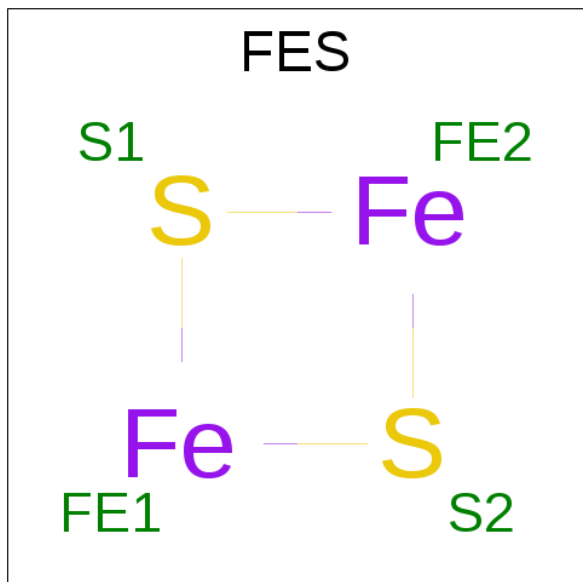
Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	35	Total	C	N	O	0	0
			175	105	35	35		

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



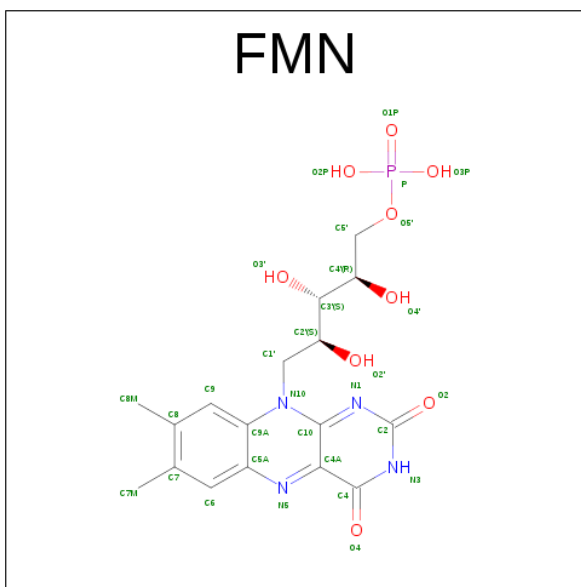
Mol	Chain	Residues	Atoms			AltConf
45	B	1	Total	Fe	S	0
			8	4	4	
45	F	1	Total	Fe	S	0
			8	4	4	
45	G	1	Total	Fe	S	0
			16	8	8	
45	G	1	Total	Fe	S	0
			16	8	8	
45	I	1	Total	Fe	S	0
			16	8	8	
45	I	1	Total	Fe	S	0
			16	8	8	

- Molecule 46 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



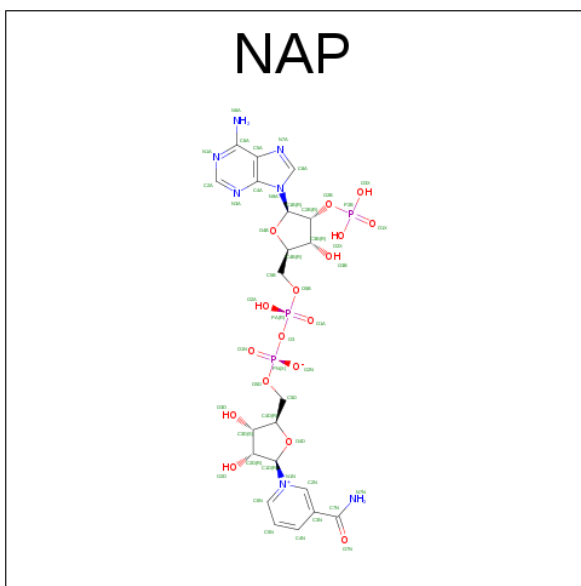
Mol	Chain	Residues	Atoms			AltConf
46	E	1	Total	Fe	S	0
			4	2	2	
46	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 47 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



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

- Molecule 48 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
48	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

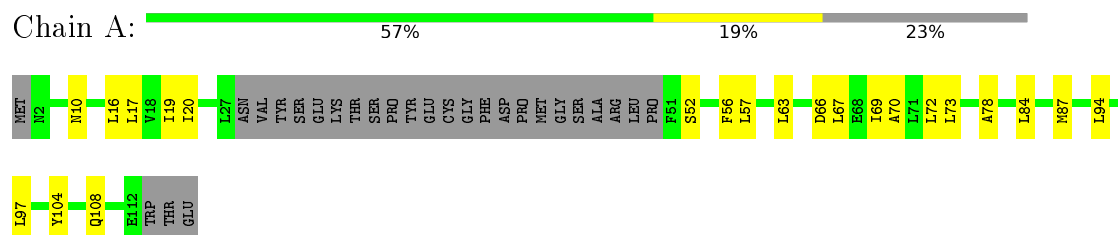
- Molecule 49 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

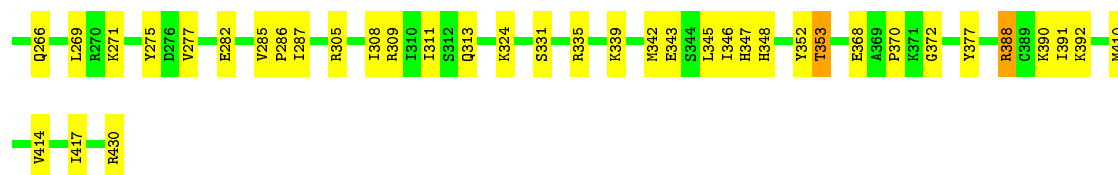
Mol	Chain	Residues	Atoms		AltConf
49	R	1	Total	Zn	0
			1	1	

### 3 Residue-property plots

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.

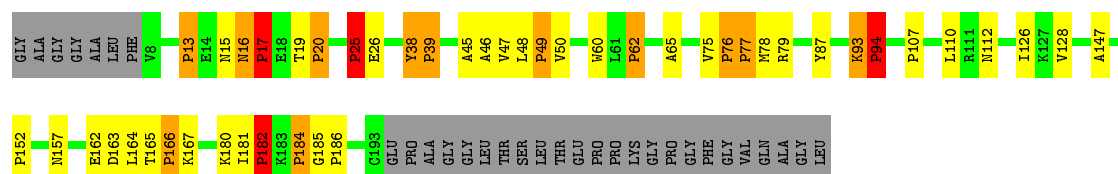
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3





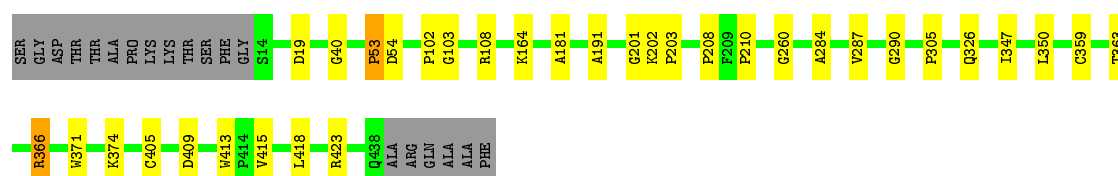
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E: 64% 14% 6% 14%



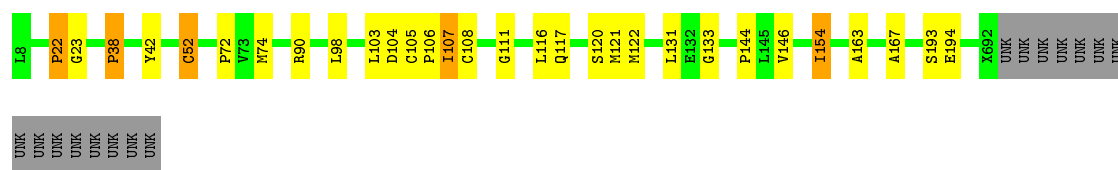
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F: 88% 7%



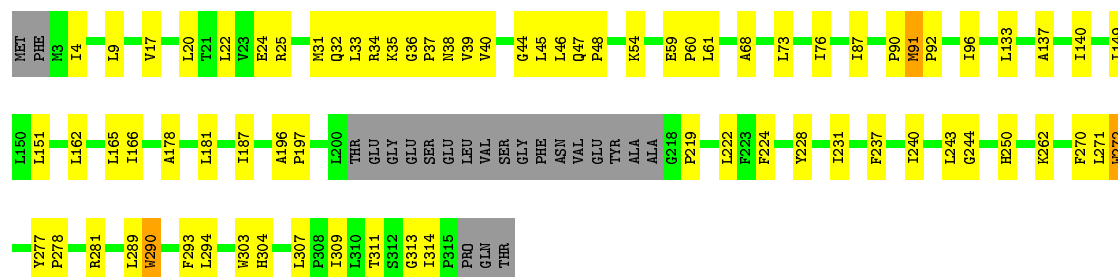
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial, NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial, NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial, NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G: 94%

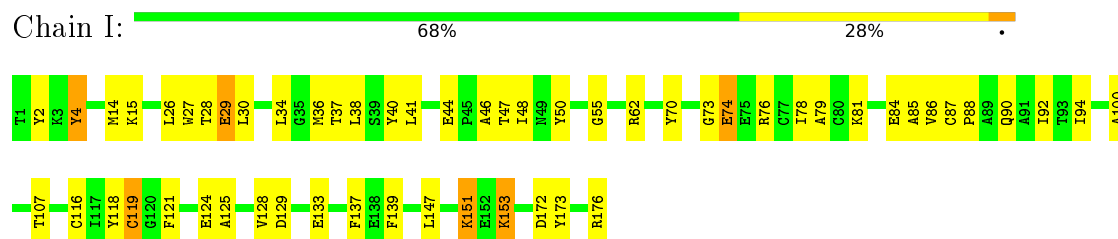


- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

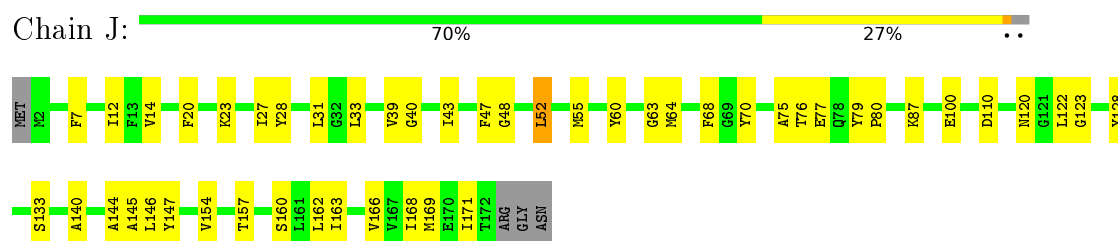
Chain H: 69% 23% 7%



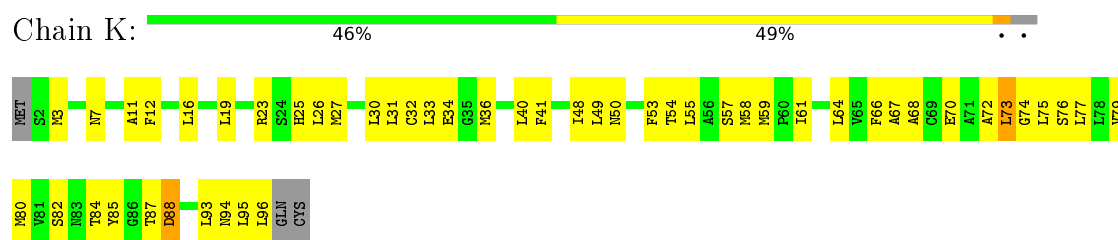
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



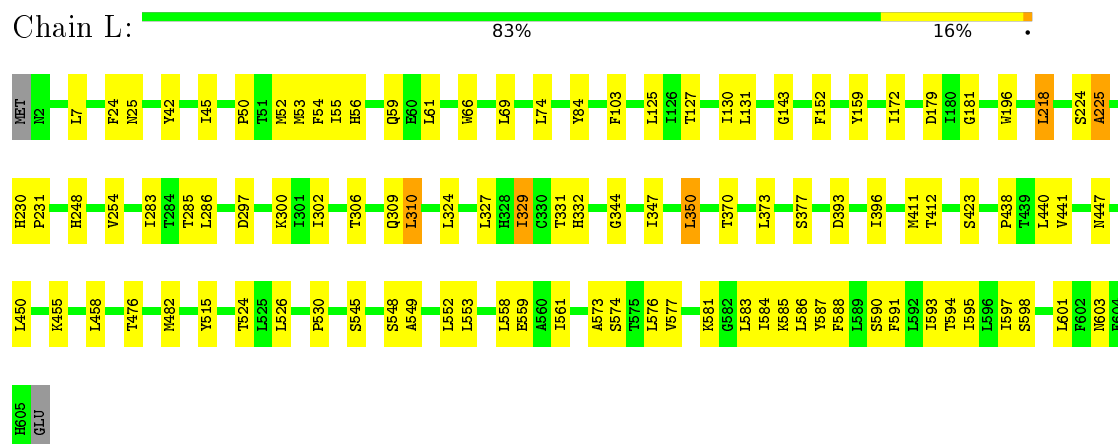
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

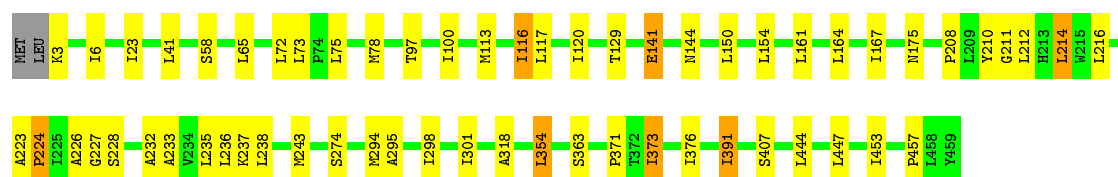


- Molecule 12: NADH-ubiquinone oxidoreductase chain 5



- Molecule 13: NADH-ubiquinone oxidoreductase chain 4





- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N: 70% 28% ..



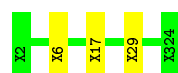
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O: 97% .



- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, NDUF9A9

Chain P: 99% .



- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, NDUF54

Chain Q: 96% .



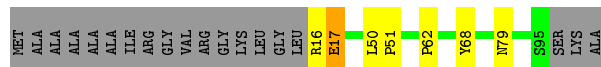
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial,NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial,NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R: 88% 12%




- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:  74% 6% 19%



- Molecule 20: Acyl carrier protein, mitochondrial

Chain T:  83% 15%



- Molecule 20: Acyl carrier protein, mitochondrial

Chain U:  91% 6%



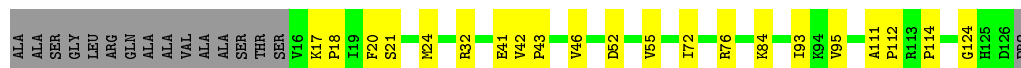
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:  75% 13% 8%



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:  71% 17% 13%




- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:  93% 7%




- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:  79% 18%




- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:  88% 12%



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:  84% 7% 9%




- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:  99%



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c:  88% 6% 6%




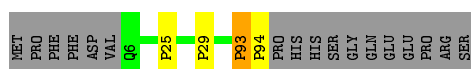
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:  98%



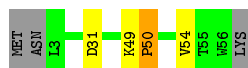
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:  80% 16%



- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f: 88% 5% • 5%



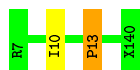
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g: 63% 13% • 22%



- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h: 99% ..



- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i: 99% .



- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, NDUFB2

Chain j: 100%

There are no outlier residues recorded for this chain.

- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3, NDUFB3

Chain k: 100%

There are no outlier residues recorded for this chain.

- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, NDUFB8

Chain l: 100%

There are no outlier residues recorded for this chain.

- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain m:  95% 5%



- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n:  98% .



- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:  98% .



- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p:  97% .



- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:  96% .



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7, NDUFA7

Chain r:  100%

There are no outlier residues recorded for this chain.

- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, NDUFV3

Chain s:  100%

There are no outlier residues recorded for this chain.

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	19306	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	per particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	5500	Depositor
Magnification	59000	Depositor
Image detector	Not provided	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	A	0.43	0/702	0.63	0/962
10	J	0.45	0/1239	0.55	0/1688
11	K	0.38	0/730	0.63	0/988
12	L	0.41	0/4653	0.57	0/6350
13	M	0.40	0/3624	0.60	0/4949
14	N	0.41	0/2656	0.61	0/3630
15	O	0.36	0/1446	0.53	0/1997
18	R	0.37	0/235	0.52	0/316
19	S	0.44	0/408	0.84	1/571 (0.2%)
2	B	0.39	0/1187	0.62	0/1607
20	T	0.31	0/380	0.52	0/531
20	U	0.30	0/436	0.50	0/610
21	V	0.51	0/696	0.86	5/954 (0.5%)
22	W	0.50	0/831	0.70	0/1128
23	X	0.43	0/877	0.63	1/1181 (0.1%)
24	Y	0.41	0/1031	0.55	0/1400
25	Z	0.37	0/585	0.54	0/781
26	a	0.45	0/494	0.57	0/669
27	b	0.42	0/352	0.53	0/481
28	c	0.46	0/330	0.61	0/455
29	d	0.40	0/581	0.50	0/782
3	C	0.43	0/1735	0.66	2/2365 (0.1%)
30	e	0.49	0/627	0.84	4/848 (0.5%)
31	f	0.50	0/356	0.70	1/488 (0.2%)
32	g	0.55	0/696	0.94	6/957 (0.6%)
33	h	0.49	0/301	0.71	1/409 (0.2%)
34	i	0.54	0/224	0.87	1/300 (0.3%)
38	m	0.42	0/801	0.56	0/1085
39	n	0.37	0/914	0.55	0/1247
4	D	0.42	0/3304	0.67	6/4478 (0.1%)
40	o	0.32	0/296	0.50	0/412
41	p	0.37	0/535	0.53	0/718

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
42	q	0.36	0/704	0.56	0/984
5	E	0.63	0/975	1.06	12/1370 (0.9%)
6	F	0.37	0/2389	0.55	1/3299 (0.0%)
7	G	0.40	0/1213	0.66	2/1658 (0.1%)
8	H	0.40	0/2371	0.58	0/3241
9	I	0.38	0/1395	0.62	0/1893
All	All	0.42	0/42309	0.63	43/57782 (0.1%)

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	S	1	0
2	B	0	1
All	All	1	1

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S	17	GLU	N-CA-C	14.07	148.98	111.00
7	G	22	PRO	CA-N-CD	-9.25	98.55	111.50
5	E	77	PRO	CA-N-CD	-9.12	98.73	111.50
6	F	53	PRO	CA-N-CD	-9.12	98.73	111.50
4	D	32	PRO	CA-N-CD	-9.06	98.81	111.50
5	E	166	PRO	CA-N-CD	-9.03	98.86	111.50
30	e	25	PRO	CA-N-CD	-8.98	98.93	111.50
32	g	32	PRO	CA-N-CD	-8.95	98.98	111.50
5	E	25	PRO	CA-N-CD	-8.94	98.98	111.50
5	E	49	PRO	CA-N-CD	-8.92	99.02	111.50
5	E	94	PRO	CA-N-CD	-8.92	99.01	111.50
34	i	29	PRO	CA-N-CD	-8.90	99.04	111.50
30	e	93	PRO	CA-N-CD	-8.89	99.06	111.50
21	V	107	PRO	CA-N-CD	-8.88	99.07	111.50
31	f	50	PRO	CA-N-CD	-8.85	99.11	111.50
5	E	39	PRO	CA-N-CD	-8.84	99.13	111.50
21	V	101	PRO	CA-N-CD	-8.84	99.13	111.50
32	g	42	PRO	CA-N-CD	-8.84	99.13	111.50
3	C	9	PRO	CA-N-CD	-8.82	99.15	111.50
30	e	29	PRO	CA-N-CD	-8.80	99.18	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	30	PRO	CA-N-CD	-8.79	99.19	111.50
5	E	13	PRO	CA-N-CD	-8.79	99.20	111.50
5	E	76	PRO	CA-N-CD	-8.78	99.21	111.50
4	D	31	PRO	CA-N-CD	-8.77	99.22	111.50
21	V	98	PRO	CA-N-CD	-8.74	99.26	111.50
21	V	106	PRO	CA-N-CD	-8.74	99.26	111.50
23	X	7	PRO	CA-N-CD	-8.73	99.28	111.50
32	g	121	PRO	CA-N-CD	-8.73	99.28	111.50
5	E	20	PRO	CA-N-CD	-8.71	99.31	111.50
5	E	17	PRO	CA-N-CD	-8.70	99.32	111.50
7	G	38	PRO	CA-N-CD	-8.69	99.33	111.50
5	E	62	PRO	CA-N-CD	-8.69	99.34	111.50
32	g	106	PRO	CA-N-CD	-8.66	99.37	111.50
32	g	30	PRO	CA-N-CD	-8.66	99.38	111.50
3	C	13	PRO	CA-N-CD	-8.65	99.39	111.50
4	D	6	PRO	CA-N-CD	-8.63	99.42	111.50
30	e	94	PRO	CA-N-CD	-8.58	99.49	111.50
21	V	19	PRO	CA-N-CD	-8.55	99.52	111.50
32	g	115	PRO	CA-N-CD	-8.38	99.76	111.50
33	h	13	PRO	CA-N-CD	-8.34	99.82	111.50
5	E	182	PRO	CA-N-CD	-7.89	100.45	111.50
4	D	38	PRO	C-N-CD	5.87	140.72	128.40
4	D	37	ASP	C-N-CD	5.40	139.74	128.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	S	17	GLU	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	149	CYS	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	A	687	0	722	21	0
2	B	1159	0	1166	42	0
3	C	1684	0	1610	48	0
4	D	3229	0	3123	179	0
5	E	959	0	509	97	0
6	F	2356	0	1535	19	0
7	G	3614	0	1341	29	0
8	H	2306	0	2419	92	0
9	I	1366	0	1286	57	0
10	J	1211	0	1165	109	0
11	K	720	0	760	191	0
12	L	4538	0	4480	204	0
13	M	3536	0	3652	46	0
14	N	2592	0	2630	266	0
15	O	1851	0	1131	1	0
16	P	1415	0	302	2	0
17	Q	565	0	122	3	0
18	R	501	0	246	19	0
19	S	405	0	197	4	0
20	T	378	0	176	1	0
20	U	432	0	207	2	0
21	V	685	0	563	24	0
22	W	817	0	743	29	0
23	X	1133	0	837	9	0
24	Y	1011	0	1018	69	0
25	Z	921	0	655	23	0
26	a	480	0	440	0	0
27	b	519	0	408	0	0
28	c	320	0	277	0	0
29	d	790	0	597	0	0
30	e	616	0	506	0	0
31	f	350	0	260	0	0
32	g	677	0	559	0	0
33	h	770	0	403	0	0
34	i	616	0	301	0	0
35	j	260	0	57	0	0
36	k	370	0	78	0	0
37	l	590	0	125	0	0
38	m	887	0	781	0	0
39	n	1088	0	769	0	0
40	o	296	0	134	0	0
41	p	1039	0	583	0	0
42	q	696	0	338	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	r	435	0	96	0	0
44	s	175	0	40	0	0
45	B	8	0	0	0	0
45	F	8	0	0	0	0
45	G	16	0	0	0	0
45	I	16	0	0	0	0
46	E	4	0	0	0	0
46	G	4	0	0	0	0
47	F	31	0	19	0	0
48	P	48	0	25	0	0
49	R	1	0	0	0	0
All	All	51181	0	39391	977	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 16.

All (977) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:38:PRO:HG3	14:N:50:PRO:CB	1.27	1.63
12:L:577:VAL:CG1	14:N:171:ASN:HB2	1.16	1.61
12:L:577:VAL:CB	14:N:171:ASN:HB2	1.21	1.59
11:K:93:LEU:HD13	12:L:584:ILE:CD1	1.27	1.57
12:L:576:LEU:CD1	14:N:167:TRP:HB2	1.37	1.55
11:K:93:LEU:CD1	12:L:584:ILE:HD12	1.08	1.54
12:L:591:PHE:CZ	14:N:113:PHE:HD2	1.23	1.51
12:L:576:LEU:HD12	14:N:167:TRP:CB	1.43	1.49
12:L:577:VAL:CG1	14:N:171:ASN:CB	1.86	1.49
12:L:576:LEU:HD11	14:N:167:TRP:CE3	1.50	1.45
12:L:591:PHE:CZ	14:N:113:PHE:CD2	2.00	1.44
4:D:25:THR:CB	12:L:581:LYS:HG3	1.46	1.44
12:L:577:VAL:HG11	14:N:171:ASN:CA	1.45	1.44
12:L:591:PHE:CE1	14:N:113:PHE:CE2	2.05	1.44
4:D:38:PRO:CG	14:N:50:PRO:HB3	1.47	1.43
12:L:591:PHE:CE1	14:N:113:PHE:CD2	2.08	1.41
12:L:577:VAL:HG11	14:N:171:ASN:CB	1.47	1.39
11:K:93:LEU:CD1	12:L:584:ILE:CD1	1.86	1.37
4:D:38:PRO:HG3	14:N:50:PRO:CG	1.52	1.37
12:L:576:LEU:CD1	14:N:167:TRP:CB	1.98	1.33
5:E:46:ALA:O	5:E:49:PRO:CD	1.76	1.32
5:E:15:ASN:C	5:E:17:PRO:HD3	1.48	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:25:THR:CB	12:L:581:LYS:CG	2.09	1.31
8:H:22:LEU:HD11	13:M:354:LEU:CD1	139.03	1.29
21:V:17:GLU:O	21:V:19:PRO:HD3	1.19	1.29
14:N:273:ASN:ND2	24:Y:137:GLU:O	1.62	1.29
22:W:18:PRO:HD3	22:W:76:ARG:CZ	1.62	1.27
22:W:18:PRO:HD3	22:W:76:ARG:NH2	1.51	1.26
5:E:15:ASN:O	5:E:17:PRO:HD3	1.07	1.24
10:J:68:PHE:CZ	11:K:75:LEU:HD13	1.73	1.24
14:N:277:ILE:CG2	24:Y:134:VAL:HA	1.68	1.23
4:D:38:PRO:CG	14:N:50:PRO:CG	2.17	1.23
5:E:46:ALA:O	5:E:49:PRO:HD2	1.31	1.20
12:L:585:LYS:HZ2	24:Y:43:LYS:NZ	1.37	1.19
12:L:593:ILE:HG12	24:Y:37:ALA:HB1	1.16	1.16
12:L:577:VAL:CB	14:N:171:ASN:CB	2.13	1.15
5:E:77:PRO:HD2	5:E:78:MET:H	1.09	1.15
4:D:38:PRO:CD	14:N:50:PRO:HG3	1.77	1.15
4:D:25:THR:CB	12:L:581:LYS:CD	2.25	1.15
11:K:73:LEU:HD13	14:N:38:LEU:HD22	1.23	1.15
12:L:577:VAL:HG21	14:N:171:ASN:H	1.05	1.14
4:D:38:PRO:CG	14:N:50:PRO:HG3	1.78	1.13
12:L:577:VAL:HG11	14:N:171:ASN:C	1.68	1.13
5:E:62:PRO:HD2	5:E:65:ALA:HB3	1.15	1.12
3:C:9:PRO:HD2	3:C:10:THR:H	1.07	1.11
12:L:577:VAL:HB	14:N:171:ASN:HB2	1.14	1.11
5:E:25:PRO:HD2	5:E:26:GLU:H	1.06	1.11
5:E:49:PRO:HD2	5:E:50:VAL:H	1.08	1.11
5:E:15:ASN:O	5:E:17:PRO:CD	1.98	1.10
11:K:93:LEU:HD11	12:L:584:ILE:HD12	1.23	1.10
4:D:38:PRO:CG	14:N:50:PRO:CB	2.09	1.10
11:K:93:LEU:HD13	12:L:584:ILE:HD11	1.25	1.10
21:V:98:PRO:HD2	21:V:99:TRP:H	1.03	1.10
4:D:32:PRO:HG3	4:D:36:VAL:CB	1.80	1.10
12:L:584:ILE:CD1	14:N:58:LYS:HE2	1.79	1.10
12:L:584:ILE:HD11	14:N:58:LYS:HE2	1.28	1.10
4:D:20:TYR:CB	14:N:171:ASN:OD1	2.01	1.09
12:L:587:TYR:HB3	14:N:113:PHE:CG	1.86	1.09
12:L:584:ILE:CG1	14:N:58:LYS:HE2	1.83	1.09
6:F:53:PRO:HD2	6:F:54:ASP:H	1.11	1.08
12:L:577:VAL:HB	14:N:171:ASN:ND2	1.67	1.08
5:E:166:PRO:HD2	5:E:167:LYS:H	1.08	1.08
12:L:576:LEU:HD12	14:N:167:TRP:HB3	1.21	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:577:VAL:HB	14:N:171:ASN:HD22	1.17	1.08
12:L:573:ALA:CB	14:N:170:LEU:HD13	1.84	1.08
5:E:62:PRO:CD	5:E:65:ALA:HB3	1.82	1.07
10:J:144:ALA:HB1	11:K:61:ILE:HD11	1.36	1.07
5:E:62:PRO:HG2	5:E:65:ALA:HB2	1.15	1.07
4:D:339:LYS:CE	18:R:67:GLY:HA2	1.85	1.06
12:L:577:VAL:HB	14:N:171:ASN:CB	1.76	1.06
5:E:46:ALA:C	5:E:49:PRO:CD	2.24	1.05
4:D:7:ASP:HA	14:N:305:PHE:CB	1.86	1.05
4:D:339:LYS:NZ	18:R:67:GLY:HA2	1.70	1.05
12:L:584:ILE:HD11	14:N:58:LYS:CE	1.87	1.05
5:E:46:ALA:C	5:E:49:PRO:HD3	1.76	1.05
7:G:22:PRO:HD2	7:G:23:GLY:H	1.15	1.04
12:L:594:THR:CG2	24:Y:38:TYR:OH	2.06	1.04
2:B:77:ARG:HE	8:H:25:ARG:NH2	1.56	1.03
4:D:25:THR:HA	12:L:581:LYS:CE	1.88	1.03
10:J:68:PHE:CE1	11:K:75:LEU:HD13	1.92	1.03
12:L:576:LEU:CD1	14:N:167:TRP:CE3	2.40	1.03
11:K:93:LEU:HD12	12:L:584:ILE:HD12	1.39	1.03
8:H:22:LEU:HD11	13:M:354:LEU:HD11	139.37	1.03
10:J:76:THR:HG22	11:K:87:THR:HB	1.37	1.02
14:N:277:ILE:HG22	24:Y:134:VAL:HA	1.41	1.02
10:J:145:ALA:HA	11:K:58:MET:HG3	1.35	1.02
12:L:585:LYS:NZ	24:Y:43:LYS:NZ	2.07	1.02
5:E:62:PRO:HG2	5:E:65:ALA:CB	1.90	1.02
10:J:76:THR:CG2	11:K:87:THR:HB	1.88	1.01
12:L:594:THR:HG22	24:Y:38:TYR:OH	1.58	1.01
12:L:577:VAL:HG21	14:N:171:ASN:N	1.75	1.01
12:L:593:ILE:HD11	24:Y:37:ALA:O	1.60	1.00
14:N:196:TYR:HE1	24:Y:136:ALA:O	1.42	1.00
3:C:13:PRO:HD2	3:C:14:ARG:H	1.24	1.00
12:L:591:PHE:CE1	14:N:110:PRO:O	2.15	1.00
22:W:18:PRO:HD3	22:W:76:ARG:NE	1.75	1.00
4:D:339:LYS:HE2	18:R:67:GLY:HA2	1.43	1.00
21:V:17:GLU:O	21:V:19:PRO:CD	2.08	1.00
11:K:94:ASN:OD1	14:N:51:ARG:NE	1.94	0.99
12:L:591:PHE:CE1	14:N:113:PHE:HE2	1.62	0.98
4:D:38:PRO:N	14:N:50:PRO:HG3	1.79	0.98
2:B:77:ARG:NE	8:H:25:ARG:HH22	1.59	0.98
12:L:576:LEU:CD1	14:N:167:TRP:HE3	1.75	0.98
5:E:93:LYS:CB	5:E:94:PRO:HD3	1.95	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:12:PHE:CE1	14:N:72:MET:HE2	2.00	0.97
5:E:62:PRO:CG	5:E:65:ALA:HB2	1.95	0.97
22:W:18:PRO:CD	22:W:76:ARG:NE	2.28	0.96
11:K:94:ASN:HB2	14:N:54:GLU:OE2	1.63	0.96
4:D:38:PRO:HB2	4:D:39:PRO:HD3	1.47	0.96
11:K:33:LEU:HD23	14:N:68:MET:SD	2.05	0.96
12:L:601:LEU:HD13	24:Y:34:VAL:CG2	1.95	0.96
11:K:96:LEU:O	14:N:117:GLU:HG3	1.64	0.96
22:W:18:PRO:HD2	22:W:76:ARG:HE	1.31	0.96
14:N:273:ASN:O	24:Y:136:ALA:CB	2.13	0.95
4:D:32:PRO:HG2	4:D:36:VAL:N	1.81	0.95
5:E:38:TYR:CB	5:E:39:PRO:HD3	1.97	0.95
4:D:38:PRO:CB	14:N:50:PRO:HB3	1.96	0.95
4:D:353:THR:HG22	9:I:85:ALA:HB3	1.46	0.95
12:L:576:LEU:HD12	14:N:167:TRP:CG	2.02	0.95
11:K:95:LEU:HD11	14:N:55:ALA:CA	1.98	0.94
22:W:18:PRO:CD	22:W:76:ARG:HE	1.81	0.94
12:L:593:ILE:HG21	24:Y:37:ALA:HB3	1.48	0.93
3:C:115:THR:HG21	22:W:18:PRO:CG	1.98	0.93
10:J:52:LEU:HD21	11:K:41:PHE:CZ	2.04	0.92
11:K:95:LEU:HD11	14:N:55:ALA:HB2	1.49	0.92
12:L:585:LYS:HZ2	24:Y:43:LYS:HZ3	0.92	0.92
11:K:73:LEU:CD1	14:N:38:LEU:HD22	1.99	0.92
12:L:593:ILE:CG1	24:Y:37:ALA:HB1	1.98	0.92
10:J:52:LEU:CD2	11:K:41:PHE:CZ	2.53	0.92
12:L:591:PHE:CE1	14:N:113:PHE:HD2	1.66	0.92
14:N:273:ASN:HA	24:Y:138:PRO:C	1.90	0.92
21:V:98:PRO:HD2	21:V:99:TRP:N	1.83	0.92
4:D:19:MET:CA	14:N:173:THR:HG23	1.99	0.91
11:K:95:LEU:HD22	14:N:117:GLU:O	1.69	0.91
3:C:9:PRO:HD2	3:C:10:THR:N	1.85	0.91
4:D:5:GLN:HA	14:N:303:THR:OG1	1.70	0.91
11:K:26:LEU:HD11	14:N:61:LEU:HD11	1.53	0.91
22:W:18:PRO:CD	22:W:76:ARG:NH2	2.34	0.91
1:A:78:ALA:HB1	10:J:146:LEU:HD23	1.53	0.91
12:L:573:ALA:HB1	14:N:170:LEU:HD13	1.51	0.91
4:D:31:PRO:HB3	14:N:51:ARG:HH12	1.35	0.91
4:D:25:THR:CB	12:L:581:LYS:HD2	2.01	0.91
10:J:144:ALA:HB1	11:K:61:ILE:CD1	2.00	0.90
10:J:47:PHE:HB2	11:K:49:LEU:HD23	1.50	0.90
4:D:38:PRO:HG3	14:N:50:PRO:HB3	0.95	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:577:VAL:HG12	14:N:171:ASN:HB2	1.53	0.90
14:N:196:TYR:CE1	24:Y:136:ALA:O	2.23	0.90
12:L:591:PHE:HE1	14:N:113:PHE:CE2	1.60	0.90
12:L:576:LEU:HD13	14:N:167:TRP:HB2	0.92	0.90
12:L:601:LEU:CD1	24:Y:34:VAL:HG22	2.02	0.89
5:E:15:ASN:C	5:E:17:PRO:CD	2.38	0.89
12:L:577:VAL:CG2	14:N:171:ASN:H	1.86	0.89
4:D:38:PRO:HD3	14:N:50:PRO:HD3	1.55	0.89
4:D:38:PRO:CB	14:N:50:PRO:CB	2.50	0.89
5:E:25:PRO:HD2	5:E:26:GLU:N	1.85	0.89
5:E:62:PRO:CD	5:E:65:ALA:CB	2.50	0.89
2:B:72:PHE:HD2	8:H:39:VAL:HG23	1.38	0.89
12:L:577:VAL:HG12	14:N:171:ASN:CB	2.02	0.88
4:D:19:MET:CB	14:N:173:THR:HG23	2.03	0.88
8:H:22:LEU:CD1	13:M:354:LEU:CD1	138.29	0.88
5:E:49:PRO:HD2	5:E:50:VAL:N	1.86	0.88
12:L:573:ALA:HB2	14:N:170:LEU:HD13	1.51	0.88
5:E:77:PRO:HD2	5:E:78:MET:N	1.87	0.88
11:K:93:LEU:HD11	12:L:584:ILE:CD1	1.82	0.88
5:E:166:PRO:HD2	5:E:167:LYS:N	1.87	0.88
10:J:128:TYR:O	11:K:50:ASN:OD1	1.91	0.88
11:K:84:THR:HG21	14:N:53:THR:HG21	1.56	0.88
11:K:95:LEU:HD11	14:N:55:ALA:CB	2.02	0.88
12:L:577:VAL:HB	14:N:171:ASN:CG	1.95	0.87
12:L:586:LEU:HD21	24:Y:43:LYS:HG3	1.57	0.87
4:D:25:THR:CA	12:L:581:LYS:HE3	2.04	0.87
4:D:18:VAL:O	4:D:20:TYR:N	2.07	0.87
2:B:67:TYR:HE1	9:I:55:GLY:HA3	1.40	0.87
12:L:593:ILE:HD13	24:Y:37:ALA:C	1.95	0.87
6:F:53:PRO:HD2	6:F:54:ASP:N	1.88	0.86
4:D:38:PRO:HG3	14:N:50:PRO:CD	2.05	0.86
22:W:18:PRO:HD3	22:W:76:ARG:HH21	1.39	0.85
4:D:19:MET:HA	14:N:173:THR:HG23	1.56	0.85
5:E:46:ALA:HA	5:E:49:PRO:CG	2.07	0.85
4:D:7:ASP:CA	14:N:305:PHE:CB	2.54	0.85
12:L:601:LEU:HD13	24:Y:34:VAL:HG22	1.54	0.85
3:C:13:PRO:HD2	3:C:14:ARG:N	1.91	0.85
7:G:22:PRO:HD2	7:G:23:GLY:N	1.90	0.85
4:D:25:THR:CA	12:L:581:LYS:HD2	2.07	0.85
2:B:77:ARG:HE	8:H:25:ARG:HH22	0.85	0.84
3:C:9:PRO:CD	3:C:10:THR:H	1.89	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:94:ASN:CB	14:N:54:GLU:OE2	2.25	0.84
4:D:32:PRO:CG	4:D:36:VAL:CA	2.54	0.84
12:L:591:PHE:CD1	14:N:110:PRO:O	2.30	0.84
4:D:25:THR:CA	12:L:581:LYS:CE	2.55	0.84
11:K:12:PHE:CE2	14:N:72:MET:HG2	2.13	0.84
11:K:95:LEU:CD1	14:N:55:ALA:HA	2.06	0.84
12:L:577:VAL:CB	14:N:171:ASN:HD22	1.90	0.83
21:V:98:PRO:CD	21:V:99:TRP:H	1.87	0.83
4:D:38:PRO:CD	14:N:50:PRO:CG	2.50	0.83
12:L:598:SER:CB	14:N:153:LEU:HD22	2.09	0.83
12:L:576:LEU:CD1	14:N:167:TRP:CG	2.58	0.83
14:N:273:ASN:O	24:Y:136:ALA:HB1	1.78	0.82
5:E:62:PRO:CG	5:E:65:ALA:CB	2.53	0.82
12:L:598:SER:CB	14:N:153:LEU:CD2	2.57	0.82
12:L:593:ILE:CD1	24:Y:37:ALA:C	2.48	0.82
5:E:49:PRO:CD	5:E:50:VAL:H	1.92	0.82
14:N:273:ASN:O	24:Y:136:ALA:HB3	1.77	0.82
12:L:576:LEU:HD13	14:N:167:TRP:CB	1.85	0.82
4:D:25:THR:HA	12:L:581:LYS:CD	2.08	0.82
4:D:32:PRO:CG	4:D:36:VAL:CB	2.56	0.82
11:K:33:LEU:CD2	14:N:68:MET:SD	2.67	0.82
22:W:18:PRO:CD	22:W:76:ARG:HH21	1.90	0.82
3:C:115:THR:HG21	22:W:18:PRO:HG2	1.59	0.82
4:D:38:PRO:HB3	14:N:50:PRO:CB	2.09	0.82
5:E:76:PRO:HG2	5:E:79:ARG:CB	2.10	0.81
4:D:38:PRO:HD3	14:N:50:PRO:CD	2.10	0.81
12:L:598:SER:HB2	14:N:153:LEU:HD22	1.62	0.81
4:D:38:PRO:HB2	4:D:39:PRO:CD	2.10	0.81
4:D:339:LYS:HZ1	18:R:67:GLY:HA2	1.44	0.81
5:E:25:PRO:CD	5:E:26:GLU:H	1.90	0.81
12:L:577:VAL:CG1	14:N:171:ASN:C	2.48	0.81
4:D:32:PRO:HG2	4:D:36:VAL:CA	2.10	0.81
11:K:77:LEU:HD11	14:N:41:ILE:HD13	1.62	0.81
12:L:576:LEU:HD11	14:N:167:TRP:CD2	2.15	0.81
5:E:166:PRO:CD	5:E:167:LYS:H	1.92	0.80
11:K:96:LEU:O	14:N:117:GLU:CG	2.29	0.80
4:D:6:PRO:O	14:N:305:PHE:CB	2.30	0.80
10:J:144:ALA:CB	11:K:61:ILE:HD11	2.11	0.80
10:J:23:LYS:HD3	11:K:23:ARG:O	1.81	0.80
9:I:74:GLU:OE2	18:R:44:UNK:HA	1.81	0.80
11:K:70:GLU:HG3	14:N:34:GLU:CD	2.01	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:33:LEU:HD22	14:N:68:MET:CE	2.12	0.80
4:D:6:PRO:O	14:N:305:PHE:N	2.15	0.80
5:E:77:PRO:CD	5:E:78:MET:H	1.93	0.79
4:D:25:THR:CA	12:L:581:LYS:CD	2.60	0.79
3:C:115:THR:HG21	22:W:18:PRO:HG3	1.64	0.79
4:D:345:LEU:HD21	7:G:106:PRO:HD3	1.65	0.79
12:L:591:PHE:HZ	14:N:113:PHE:HD2	0.88	0.79
10:J:68:PHE:CZ	11:K:75:LEU:CD1	2.61	0.79
5:E:46:ALA:O	5:E:49:PRO:CG	2.30	0.79
10:J:68:PHE:CE1	11:K:75:LEU:CD1	2.65	0.79
11:K:12:PHE:CE1	14:N:72:MET:CE	2.66	0.78
14:N:277:ILE:CG2	24:Y:134:VAL:CA	2.56	0.78
5:E:162:GLU:O	5:E:186:PRO:HD2	1.82	0.78
11:K:12:PHE:CG	14:N:72:MET:HE3	2.18	0.78
12:L:593:ILE:CD1	24:Y:37:ALA:O	2.31	0.78
14:N:274:ASN:HB3	24:Y:133:GLN:OE1	1.84	0.78
11:K:94:ASN:CB	14:N:54:GLU:CD	2.51	0.78
10:J:52:LEU:HD12	11:K:61:ILE:HG13	1.64	0.78
11:K:40:LEU:HD22	14:N:75:ILE:HD12	1.65	0.78
5:E:38:TYR:CB	5:E:39:PRO:CD	2.61	0.78
12:L:576:LEU:CD1	14:N:167:TRP:CD2	2.67	0.78
12:L:601:LEU:CD1	24:Y:34:VAL:CG2	2.59	0.78
4:D:32:PRO:HG3	4:D:36:VAL:CA	2.13	0.77
10:J:47:PHE:C	11:K:49:LEU:HD21	2.04	0.77
5:E:48:LEU:N	5:E:49:PRO:HD3	1.99	0.77
9:I:73:GLY:HA3	18:R:43:UNK:CB	2.15	0.77
11:K:95:LEU:CD1	14:N:55:ALA:CA	2.63	0.77
12:L:577:VAL:CG1	14:N:171:ASN:HB3	2.13	0.77
12:L:598:SER:HB2	14:N:153:LEU:CD2	2.15	0.76
6:F:53:PRO:CD	6:F:54:ASP:H	1.94	0.76
12:L:587:TYR:CD1	14:N:113:PHE:CD1	2.73	0.76
3:C:13:PRO:HG3	4:D:127:ASN:C	2.06	0.76
12:L:574:SER:HA	14:N:171:ASN:HD21	1.49	0.76
4:D:25:THR:HA	12:L:581:LYS:HD2	1.63	0.76
10:J:7:PHE:HE1	11:K:7:ASN:HD21	1.33	0.76
1:A:56:PHE:CE1	11:K:79:VAL:HG21	2.21	0.75
5:E:25:PRO:N	11:K:55:LEU:HD21	169.42	0.75
12:L:587:TYR:HB3	14:N:113:PHE:CD1	2.20	0.75
12:L:587:TYR:HB3	14:N:113:PHE:CB	2.16	0.75
3:C:115:THR:CG2	22:W:18:PRO:HG2	2.15	0.75
12:L:587:TYR:CD1	14:N:113:PHE:HD1	2.05	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:15:GLY:HA2	14:N:227:THR:HG21	1.68	0.75
8:H:22:LEU:HD11	13:M:354:LEU:HD12	139.76	0.75
5:E:165:THR:CB	5:E:166:PRO:HD3	2.17	0.75
5:E:19:THR:H	5:E:20:PRO:HD3	1.49	0.74
14:N:277:ILE:HG21	24:Y:134:VAL:HG22	1.68	0.74
5:E:94:PRO:HB3	25:Z:87:ARG:HD3	158.99	0.74
12:L:603:ASN:CB	24:Y:2:LYS:H	2.01	0.74
12:L:584:ILE:HG12	14:N:58:LYS:HE2	1.69	0.74
11:K:12:PHE:CZ	14:N:72:MET:HE2	2.23	0.74
11:K:73:LEU:HD22	14:N:38:LEU:HD23	1.70	0.73
4:D:339:LYS:NZ	18:R:67:GLY:CA	2.51	0.73
4:D:234:ILE:HG21	8:H:278:PRO:HG2	1.70	0.73
2:B:71:ARG:HB3	8:H:36:GLY:C	2.08	0.73
4:D:19:MET:HA	14:N:173:THR:CG2	2.17	0.73
12:L:558:LEU:HD22	13:M:211:GLY:HA2	1.70	0.73
5:E:94:PRO:HB3	25:Z:87:ARG:HH11	157.11	0.73
3:C:13:PRO:CD	3:C:14:ARG:H	1.98	0.73
10:J:157:THR:HG22	11:K:66:PHE:CE2	2.23	0.73
12:L:597:ILE:HD11	24:Y:34:VAL:HG13	1.69	0.73
11:K:73:LEU:HD13	14:N:38:LEU:CD2	2.13	0.73
10:J:52:LEU:HD12	11:K:61:ILE:CG1	2.19	0.73
12:L:545:SER:HB2	13:M:274:SER:HB2	1.69	0.73
12:L:593:ILE:HG12	24:Y:37:ALA:CB	2.10	0.72
6:F:371:TRP:HE1	7:G:131:LEU:HA	1.54	0.72
4:D:25:THR:CB	12:L:581:LYS:CE	2.67	0.72
11:K:59:MET:HG3	14:N:84:TRP:CZ3	2.25	0.72
10:J:75:ALA:HB2	11:K:82:SER:CB	2.20	0.72
5:E:162:GLU:O	5:E:185:GLY:HA2	1.89	0.72
8:H:22:LEU:CD1	13:M:354:LEU:HD11	138.62	0.72
14:N:277:ILE:HG23	24:Y:134:VAL:HA	1.66	0.72
5:E:147:ALA:HB2	6:F:108:ARG:CB	2.20	0.72
7:G:38:PRO:HD3	7:G:90:ARG:HH21	1.53	0.72
8:H:250:HIS:HA	23:X:90:TYR:HE2	1.55	0.71
10:J:120:ASN:O	11:K:3:MET:SD	2.48	0.71
12:L:248:HIS:HB3	12:L:306:THR:HG21	1.71	0.71
10:J:52:LEU:HD23	11:K:41:PHE:CE2	2.26	0.71
2:B:71:ARG:HG3	8:H:37:PRO:HG3	1.73	0.71
12:L:595:ILE:HG12	14:N:100:MET:CE	2.21	0.71
4:D:346:ILE:HG23	7:G:117:GLN:HG3	1.73	0.70
7:G:22:PRO:CD	7:G:23:GLY:H	1.97	0.70
10:J:20:PHE:HE1	11:K:31:LEU:HB3	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:13:PRO:HG3	4:D:127:ASN:O	1.92	0.70
21:V:98:PRO:CD	21:V:99:TRP:N	2.52	0.70
10:J:76:THR:HG23	11:K:87:THR:HB	1.74	0.70
12:L:594:THR:HG21	14:N:110:PRO:HB3	1.73	0.70
12:L:577:VAL:CG1	14:N:171:ASN:CA	2.39	0.70
5:E:184:PRO:CG	5:E:185:GLY:H	2.05	0.70
4:D:25:THR:CB	12:L:581:LYS:HE3	2.21	0.69
4:D:32:PRO:CG	4:D:36:VAL:HA	2.21	0.69
10:J:140:ALA:O	11:K:57:SER:OG	2.06	0.69
11:K:12:PHE:CD1	14:N:72:MET:HE3	2.27	0.69
5:E:46:ALA:HA	5:E:49:PRO:HG2	1.74	0.69
8:H:91:MET:HB3	8:H:92:PRO:HD2	1.75	0.69
10:J:68:PHE:CE1	11:K:75:LEU:HD22	2.27	0.69
8:H:22:LEU:HD21	13:M:354:LEU:HD11	139.97	0.69
12:L:590:SER:OG	14:N:113:PHE:CZ	2.45	0.69
5:E:46:ALA:HA	5:E:49:PRO:HG3	1.75	0.69
8:H:35:LYS:HB2	9:I:47:THR:HG21	1.74	0.69
4:D:339:LYS:HZ1	18:R:67:GLY:CA	2.06	0.69
12:L:597:ILE:CD1	24:Y:34:VAL:HG13	2.22	0.68
4:D:38:PRO:CB	14:N:50:PRO:HG3	2.22	0.68
5:E:25:PRO:CD	5:E:26:GLU:N	2.54	0.68
19:S:16:ARG:O	19:S:68:TYR:O	2.11	0.68
12:L:584:ILE:HD11	14:N:58:LYS:HE3	1.75	0.68
12:L:593:ILE:CG2	24:Y:37:ALA:HB3	2.21	0.68
8:H:272:TRP:CD1	9:I:34:LEU:HG	2.29	0.68
4:D:5:GLN:CA	14:N:303:THR:OG1	2.40	0.68
3:C:13:PRO:CD	3:C:14:ARG:N	2.56	0.68
10:J:146:LEU:N	11:K:58:MET:HE3	2.08	0.68
11:K:12:PHE:CZ	14:N:72:MET:HB2	2.28	0.68
3:C:13:PRO:HG3	4:D:127:ASN:CA	2.23	0.68
3:C:9:PRO:CD	3:C:10:THR:N	2.53	0.68
2:B:71:ARG:O	8:H:37:PRO:HA	1.94	0.68
11:K:73:LEU:HD22	14:N:38:LEU:CD2	2.24	0.67
5:E:166:PRO:CD	5:E:167:LYS:N	2.56	0.67
14:N:278:LEU:CD1	24:Y:135:PHE:CE1	2.77	0.67
4:D:15:GLY:HA2	14:N:227:THR:CG2	2.25	0.67
8:H:187:ILE:HD11	9:I:27:TRP:HE1	1.58	0.67
11:K:12:PHE:CD1	14:N:72:MET:CE	2.77	0.67
10:J:64:MET:HB3	11:K:34:GLU:OE2	1.95	0.67
10:J:122:LEU:O	11:K:3:MET:HG2	1.95	0.67
11:K:77:LEU:HD21	14:N:41:ILE:HG21	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:38:PRO:CD	14:N:50:PRO:HD3	2.25	0.66
10:J:145:ALA:HA	11:K:58:MET:CG	2.17	0.66
10:J:52:LEU:HD23	11:K:41:PHE:CZ	2.30	0.66
1:A:84:LEU:HD22	8:H:309:ILE:HG12	1.76	0.66
10:J:144:ALA:O	11:K:58:MET:HB2	1.95	0.66
6:F:53:PRO:CD	6:F:54:ASP:N	2.57	0.66
4:D:339:LYS:O	18:R:69:PRO:HA	1.95	0.66
10:J:23:LYS:CE	11:K:23:ARG:O	2.43	0.66
10:J:23:LYS:HE2	11:K:25:HIS:HB2	1.75	0.66
12:L:553:LEU:HD13	13:M:210:TYR:OH	1.96	0.66
5:E:39:PRO:HD2	5:E:39:PRO:O	1.95	0.66
11:K:70:GLU:HG3	14:N:34:GLU:OE1	1.95	0.66
11:K:16:LEU:HD21	14:N:69:LEU:HD21	1.76	0.66
4:D:25:THR:HA	12:L:581:LYS:NZ	2.09	0.66
7:G:38:PRO:HG3	7:G:90:ARG:NE	2.11	0.66
11:K:95:LEU:HB3	14:N:117:GLU:HB3	1.76	0.66
12:L:593:ILE:HD13	24:Y:38:TYR:N	2.11	0.66
10:J:55:MET:HB3	11:K:64:LEU:HD11	1.77	0.66
12:L:598:SER:CB	14:N:153:LEU:HD21	2.25	0.65
8:H:22:LEU:HD11	13:M:354:LEU:HD13	138.59	0.65
10:J:47:PHE:CB	11:K:49:LEU:HD23	2.25	0.65
5:E:25:PRO:N	11:K:55:LEU:CD2	168.80	0.65
5:E:93:LYS:CB	5:E:94:PRO:CD	2.73	0.65
12:L:598:SER:HA	14:N:153:LEU:HD21	1.78	0.65
14:N:4:ILE:HD11	15:O:9:UNK:N	2.10	0.65
10:J:52:LEU:CD2	11:K:41:PHE:CE2	2.79	0.65
10:J:64:MET:HE1	11:K:34:GLU:HG2	1.79	0.65
4:D:22:THR:CB	4:D:25:THR:O	2.45	0.65
5:E:107:PRO:HG2	6:F:103:GLY:N	2.11	0.65
3:C:186:GLU:H	3:C:187:PRO:HD2	1.61	0.65
7:G:106:PRO:O	7:G:106:PRO:HD2	5.24	0.65
8:H:33:LEU:HB2	9:I:40:TYR:CE2	2.32	0.65
8:H:33:LEU:HB2	9:I:40:TYR:HE2	1.62	0.65
2:B:71:ARG:HG3	8:H:37:PRO:CG	2.27	0.65
12:L:593:ILE:CG2	24:Y:37:ALA:CB	2.75	0.65
2:B:157:LEU:HD22	9:I:50:TYR:HB2	1.78	0.64
5:E:16:ASN:N	5:E:17:PRO:HD3	2.12	0.64
5:E:76:PRO:HD2	5:E:76:PRO:O	1.96	0.64
8:H:313:GLY:HA2	25:Z:53:ASN:HB3	1.79	0.64
10:J:23:LYS:CE	11:K:25:HIS:HB2	2.27	0.64
10:J:23:LYS:CD	11:K:23:ARG:O	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:585:LYS:NZ	24:Y:43:LYS:HZ1	1.93	0.64
5:E:13:PRO:O	5:E:13:PRO:HD2	1.96	0.64
5:E:165:THR:CB	5:E:166:PRO:CD	2.76	0.64
1:A:63:LEU:HD22	11:K:72:ALA:CB	2.27	0.64
14:N:273:ASN:HD22	24:Y:137:GLU:C	1.96	0.64
2:B:72:PHE:CD2	8:H:39:VAL:HG23	2.28	0.64
12:L:598:SER:HB3	14:N:153:LEU:HD22	1.80	0.64
10:J:48:GLY:N	11:K:49:LEU:HD21	2.12	0.64
21:V:101:PRO:HD2	21:V:101:PRO:O	1.97	0.64
5:E:46:ALA:CA	5:E:49:PRO:CG	2.76	0.64
10:J:23:LYS:HE2	11:K:23:ARG:O	1.98	0.64
21:V:96:TRP:O	21:V:98:PRO:HD3	1.97	0.64
4:D:7:ASP:C	14:N:305:PHE:CB	2.67	0.63
5:E:46:ALA:C	5:E:49:PRO:CG	2.66	0.63
10:J:75:ALA:CB	11:K:82:SER:HB3	2.28	0.63
10:J:144:ALA:CB	11:K:61:ILE:CD1	2.75	0.63
12:L:577:VAL:HG11	14:N:171:ASN:N	2.10	0.63
4:D:38:PRO:CD	14:N:50:PRO:CD	2.75	0.63
4:D:168:PHE:CE2	8:H:34:ARG:HD3	2.33	0.63
4:D:31:PRO:HB3	14:N:51:ARG:NH1	2.12	0.63
14:N:277:ILE:HG22	24:Y:133:GLN:O	1.99	0.63
4:D:6:PRO:HG3	14:N:303:THR:N	2.13	0.63
5:E:48:LEU:N	5:E:49:PRO:CD	2.61	0.63
12:L:152:PHE:HB2	12:L:172:ILE:HD11	1.80	0.63
2:B:119:CYS:HA	2:B:124:GLY:H	1.63	0.63
4:D:345:LEU:HD13	7:G:103:LEU:HD21	1.81	0.63
4:D:335:ARG:NH2	9:I:124:GLU:HA	2.14	0.63
4:D:30:PRO:O	4:D:30:PRO:HD2	1.96	0.63
10:J:23:LYS:NZ	11:K:25:HIS:O	2.27	0.63
2:B:82:GLN:HE22	8:H:224:PHE:HE2	1.47	0.63
11:K:94:ASN:HB3	14:N:54:GLU:CD	2.18	0.63
5:E:49:PRO:CD	5:E:50:VAL:N	2.55	0.63
5:E:77:PRO:CD	5:E:78:MET:N	2.56	0.62
21:V:106:PRO:O	21:V:106:PRO:HD2	1.99	0.62
5:E:94:PRO:HD2	5:E:94:PRO:O	1.97	0.62
10:J:23:LYS:HE2	11:K:25:HIS:H	1.65	0.62
11:K:12:PHE:CD2	14:N:72:MET:HE3	2.34	0.62
12:L:594:THR:HG23	24:Y:38:TYR:OH	1.98	0.62
5:E:19:THR:N	5:E:20:PRO:HD3	2.14	0.61
4:D:14:TYR:O	14:N:227:THR:HG23	1.99	0.61
11:K:12:PHE:CZ	14:N:72:MET:CE	2.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:71:MET:H	25:Z:72:PRO:HD2	1.64	0.61
4:D:31:PRO:HD2	4:D:31:PRO:O	2.01	0.61
10:J:144:ALA:O	11:K:58:MET:CB	2.47	0.61
12:L:593:ILE:HG21	24:Y:37:ALA:CB	2.25	0.61
4:D:6:PRO:HD2	4:D:6:PRO:O	1.98	0.61
3:C:52:ILE:HD13	3:C:107:VAL:HG13	1.83	0.61
12:L:591:PHE:HZ	14:N:113:PHE:CD2	1.74	0.61
12:L:601:LEU:HD13	24:Y:34:VAL:HG21	1.83	0.61
12:L:230:HIS:N	12:L:231:PRO:HD3	2.16	0.61
12:L:558:LEU:HD13	13:M:210:TYR:O	2.02	0.60
2:B:44:SER:HB3	8:H:47:GLN:HE21	1.65	0.60
5:E:184:PRO:HG2	5:E:185:GLY:H	1.64	0.60
10:J:52:LEU:CD1	11:K:61:ILE:HG13	2.32	0.60
12:L:598:SER:HB3	14:N:153:LEU:CD2	2.30	0.60
3:C:152:LEU:HB3	4:D:84:HIS:CG	2.36	0.60
3:C:13:PRO:HA	4:D:129:ARG:HB2	1.81	0.60
14:N:274:ASN:CB	24:Y:133:GLN:OE1	2.49	0.60
12:L:559:GLU:HB2	13:M:214:LEU:HD13	1.84	0.60
5:E:47:VAL:N	5:E:49:PRO:HD3	2.16	0.60
10:J:140:ALA:HB1	11:K:54:THR:H	1.65	0.60
10:J:68:PHE:HD2	11:K:27:MET:CE	2.15	0.60
11:K:73:LEU:CG	14:N:38:LEU:HD22	2.30	0.60
2:B:82:GLN:NE2	8:H:224:PHE:HE2	2.00	0.60
7:G:38:PRO:O	7:G:38:PRO:HD2	2.03	0.59
4:D:204:PRO:HD3	9:I:176:ARG:HD3	1.84	0.59
12:L:587:TYR:CB	14:N:113:PHE:CD1	2.84	0.59
4:D:234:ILE:HD13	8:H:278:PRO:HD2	1.84	0.59
10:J:171:ILE:HG22	11:K:80:MET:CE	2.32	0.59
22:W:111:ALA:HB3	22:W:112:PRO:HA	1.83	0.59
22:W:17:LYS:O	22:W:76:ARG:NH2	2.35	0.59
5:E:62:PRO:O	5:E:62:PRO:HD2	2.02	0.59
10:J:55:MET:HE2	11:K:64:LEU:HD22	1.84	0.59
11:K:12:PHE:HZ	14:N:72:MET:HB2	1.65	0.59
5:E:94:PRO:HB3	25:Z:87:ARG:NH1	157.24	0.59
12:L:590:SER:HB2	24:Y:38:TYR:CE1	2.38	0.59
4:D:335:ARG:HH22	9:I:124:GLU:HA	1.68	0.58
4:D:234:ILE:CG2	8:H:278:PRO:HG2	2.33	0.58
14:N:277:ILE:HG22	24:Y:134:VAL:CA	2.23	0.58
5:E:20:PRO:HD2	5:E:20:PRO:O	2.02	0.58
11:K:26:LEU:HD11	14:N:61:LEU:CD1	2.29	0.58
11:K:74:GLY:HA3	14:N:60:PHE:CZ	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:145:ALA:CA	11:K:58:MET:HG3	2.21	0.58
2:B:147:PRO:HG3	9:I:139:PHE:HB3	1.84	0.58
5:E:107:PRO:HG2	6:F:102:PRO:C	2.24	0.58
11:K:40:LEU:HD22	14:N:75:ILE:CD1	2.32	0.57
12:L:561:ILE:HG21	13:M:212:LEU:HD21	1.86	0.57
4:D:245:VAL:HG12	4:D:250:ALA:HB2	1.87	0.57
5:E:180:LYS:C	5:E:182:PRO:HD2	2.25	0.57
11:K:85:TYR:OH	14:N:54:GLU:OE2	2.23	0.57
11:K:70:GLU:CG	14:N:34:GLU:CD	2.73	0.57
4:D:347:HIS:ND1	7:G:121:MET:SD	2.77	0.57
1:A:63:LEU:HD22	11:K:72:ALA:HB2	1.86	0.57
4:D:352:TYR:HB3	9:I:86:VAL:CG2	2.34	0.57
2:B:65:PRO:O	9:I:47:THR:HA	2.05	0.56
12:L:591:PHE:CD1	14:N:113:PHE:HE2	2.20	0.56
4:D:339:LYS:HE2	18:R:67:GLY:CA	2.26	0.56
4:D:38:PRO:HB3	14:N:50:PRO:HB2	1.86	0.56
12:L:590:SER:HB2	24:Y:38:TYR:CD1	2.41	0.56
4:D:269:LEU:HB2	4:D:368:GLU:HG3	1.87	0.56
9:I:15:LYS:HG2	25:Z:32:TYR:HE2	1.70	0.56
2:B:67:TYR:CE1	9:I:55:GLY:HA3	2.31	0.56
10:J:64:MET:CE	11:K:34:GLU:HG2	2.35	0.56
12:L:598:SER:CA	14:N:153:LEU:HD21	2.36	0.56
2:B:149:CYS:SG	2:B:150:PRO:HD2	2.46	0.56
1:A:63:LEU:CD2	11:K:72:ALA:HB2	2.36	0.56
10:J:52:LEU:CD2	11:K:41:PHE:HZ	2.17	0.56
12:L:577:VAL:CG1	14:N:171:ASN:O	2.53	0.56
11:K:93:LEU:CD1	12:L:584:ILE:HD11	1.99	0.56
9:I:15:LYS:HG2	25:Z:32:TYR:CE2	2.40	0.56
10:J:76:THR:H	11:K:87:THR:HG22	1.71	0.56
4:D:116:GLN:HE22	4:D:138:ARG:HD3	1.70	0.56
13:M:65:LEU:HD21	13:M:238:LEU:HB2	1.87	0.56
23:X:7:PRO:HD2	23:X:7:PRO:O	2.06	0.56
10:J:68:PHE:HZ	11:K:30:LEU:HB3	1.71	0.55
10:J:68:PHE:CE1	11:K:75:LEU:CD2	2.89	0.55
4:D:339:LYS:O	18:R:70:ARG:N	2.35	0.55
11:K:70:GLU:HG3	14:N:34:GLU:OE2	2.06	0.55
12:L:587:TYR:CG	14:N:113:PHE:CD1	2.94	0.55
21:V:107:PRO:O	21:V:107:PRO:HD2	2.04	0.55
3:C:152:LEU:HD22	4:D:84:HIS:CD2	2.42	0.55
21:V:17:GLU:C	21:V:19:PRO:HD3	2.18	0.55
4:D:282:GLU:HB2	4:D:313:GLN:HE22	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:343:GLU:OE1	7:G:120:SER:HB2	2.06	0.55
10:J:47:PHE:HB2	11:K:49:LEU:CD2	2.30	0.55
1:A:70:ALA:HA	1:A:73:LEU:HD12	1.89	0.55
5:E:46:ALA:O	5:E:49:PRO:HG2	2.03	0.55
10:J:146:LEU:H	11:K:58:MET:HE3	1.71	0.55
13:M:233:ALA:HA	13:M:236:LEU:HD12	1.89	0.55
21:V:19:PRO:HD2	21:V:19:PRO:O	2.06	0.55
4:D:168:PHE:HB3	8:H:32:GLN:O	2.06	0.54
2:B:71:ARG:HB3	8:H:36:GLY:CA	2.37	0.54
12:L:587:TYR:CG	14:N:113:PHE:HB3	2.42	0.54
14:N:278:LEU:HD12	24:Y:135:PHE:CE1	2.42	0.54
3:C:79:THR:HG22	4:D:390:LYS:HD2	1.89	0.54
8:H:277:TYR:OH	9:I:30:LEU:O	2.18	0.54
12:L:587:TYR:CB	14:N:113:PHE:HB3	2.37	0.54
5:E:152:PRO:HG2	5:E:164:LEU:H	1.71	0.54
7:G:22:PRO:CD	7:G:23:GLY:N	2.59	0.54
10:J:60:TYR:OH	11:K:67:ALA:CB	2.55	0.54
4:D:324:LYS:HD3	4:D:331:SER:HB2	1.90	0.54
4:D:32:PRO:HD2	4:D:32:PRO:O	2.06	0.54
9:I:70:TYR:HA	9:I:76:ARG:HH21	1.73	0.54
10:J:68:PHE:CZ	11:K:30:LEU:HB3	2.43	0.54
11:K:33:LEU:HD22	14:N:68:MET:SD	2.47	0.54
10:J:20:PHE:HB3	11:K:32:CYS:SG	2.48	0.54
7:G:38:PRO:HG3	7:G:90:ARG:HE	1.72	0.54
4:D:165:THR:HG21	9:I:37:THR:CG2	2.37	0.54
8:H:289:LEU:HA	8:H:293:PHE:HB2	1.90	0.54
2:B:157:LEU:HD13	9:I:50:TYR:CD1	2.42	0.54
12:L:344:GLY:HA2	12:L:347:ILE:HD12	1.90	0.54
4:D:172:GLU:OE1	9:I:46:ALA:HB3	2.07	0.54
3:C:186:GLU:H	3:C:187:PRO:CD	2.20	0.53
3:C:129:TRP:HZ3	4:D:80:ILE:HD11	1.74	0.53
2:B:72:PHE:CE2	8:H:38:ASN:HB3	2.43	0.53
10:J:76:THR:HG23	11:K:88:ASP:H	1.72	0.53
12:L:577:VAL:HG12	14:N:171:ASN:HB3	1.82	0.53
4:D:26:ALA:H	12:L:581:LYS:HZ1	1.56	0.53
8:H:303:TRP:HE1	25:Z:46:TYR:HH	1.57	0.53
5:E:87:TYR:HA	6:F:181:ALA:HB1	1.91	0.53
10:J:160:SER:HA	10:J:163:ILE:HD12	1.89	0.53
10:J:76:THR:HG22	11:K:87:THR:CB	2.25	0.53
12:L:601:LEU:HD21	24:Y:30:ALA:O	2.07	0.53
22:W:18:PRO:N	22:W:76:ARG:HH21	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:594:THR:HG21	14:N:110:PRO:CB	2.38	0.53
10:J:55:MET:HB3	11:K:64:LEU:CD1	2.39	0.53
13:M:161:LEU:HD11	14:N:260:PHE:HZ	1.74	0.53
23:X:52:PRO:HB3	25:Z:78:LYS:HD3	1.89	0.53
11:K:40:LEU:HD13	14:N:71:MET:HG3	1.91	0.53
12:L:577:VAL:CB	14:N:171:ASN:ND2	2.54	0.53
10:J:23:LYS:NZ	11:K:23:ARG:H	2.07	0.52
2:B:43:SER:OG	8:H:40:VAL:HG11	2.10	0.52
3:C:34:PRO:HD2	3:C:38:GLN:HB2	1.91	0.52
5:E:184:PRO:CD	5:E:185:GLY:N	2.72	0.52
11:K:33:LEU:CD2	14:N:68:MET:CE	2.86	0.52
12:L:587:TYR:HB3	14:N:113:PHE:HB3	1.88	0.52
11:K:95:LEU:HD11	14:N:55:ALA:N	2.23	0.52
5:E:184:PRO:CG	5:E:185:GLY:N	2.72	0.52
10:J:68:PHE:CD2	11:K:27:MET:CE	2.93	0.52
22:W:111:ALA:N	22:W:112:PRO:HA	2.24	0.52
9:I:173:TYR:HB2	18:R:65:ALA:HA	1.91	0.52
10:J:171:ILE:HG22	11:K:80:MET:HE1	1.92	0.52
12:L:53:MET:SD	16:P:29:UNK:CB	163.88	0.52
4:D:347:HIS:CE1	7:G:121:MET:HA	2.46	0.52
11:K:33:LEU:HD22	14:N:68:MET:HE1	1.92	0.52
12:L:574:SER:HA	14:N:171:ASN:ND2	2.23	0.52
11:K:77:LEU:HD21	14:N:41:ILE:CG2	2.38	0.51
12:L:447:ASN:H	12:L:450:LEU:HD12	1.75	0.51
6:F:305:PRO:HD3	6:F:413:TRP:HB3	1.91	0.51
10:J:20:PHE:CE1	11:K:31:LEU:HB3	2.42	0.51
4:D:339:LYS:HZ3	18:R:66:LEU:C	2.12	0.51
22:W:18:PRO:HD2	22:W:76:ARG:NE	2.03	0.51
4:D:126:LEU:HB3	4:D:128:ILE:HD12	1.93	0.51
5:E:25:PRO:HG2	11:K:54:THR:HG22	168.30	0.51
10:J:75:ALA:HB2	11:K:82:SER:OG	2.11	0.51
12:L:548:SER:HA	12:L:552:LEU:HD12	1.91	0.51
10:J:75:ALA:HB2	11:K:82:SER:HB3	1.86	0.51
11:K:12:PHE:CZ	14:N:72:MET:HG2	2.44	0.51
2:B:71:ARG:HB3	8:H:36:GLY:HA2	1.93	0.51
10:J:146:LEU:H	11:K:58:MET:CE	2.23	0.51
14:N:89:LEU:HD21	14:N:98:MET:HG2	1.93	0.51
3:C:115:THR:CG2	22:W:18:PRO:CG	2.77	0.51
5:E:19:THR:N	5:E:20:PRO:CD	2.74	0.51
8:H:37:PRO:HB2	8:H:44:GLY:HA3	1.92	0.51
5:E:162:GLU:O	5:E:186:PRO:CD	2.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:295:ALA:HA	13:M:298:ILE:HD12	1.93	0.50
9:I:173:TYR:CB	18:R:65:ALA:HA	2.41	0.50
2:B:39:TRP:CH2	8:H:46:LEU:HB3	2.46	0.50
8:H:22:LEU:CD2	13:M:354:LEU:HD11	139.24	0.50
10:J:68:PHE:HD2	11:K:27:MET:HE1	1.76	0.50
1:A:56:PHE:HZ	11:K:76:SER:HA	1.75	0.50
8:H:311:THR:OG1	25:Z:50:MET:HG3	2.12	0.50
12:L:591:PHE:HE1	14:N:110:PRO:O	1.87	0.50
2:B:69:MET:HG2	2:B:157:LEU:HD23	1.92	0.50
4:D:32:PRO:HG2	4:D:36:VAL:HA	1.85	0.50
2:B:72:PHE:HZ	8:H:35:LYS:HD2	1.76	0.50
2:B:39:TRP:HH2	8:H:46:LEU:HB3	1.76	0.50
2:B:66:ARG:O	9:I:48:ILE:HB	2.11	0.50
11:K:70:GLU:OE1	14:N:30:TRP:CH2	2.64	0.50
25:Z:71:MET:N	25:Z:72:PRO:HD2	2.26	0.50
3:C:75:LEU:HD12	3:C:124:TYR:HB2	1.93	0.50
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.94	0.50
10:J:75:ALA:HB1	11:K:82:SER:HB3	1.93	0.50
4:D:38:PRO:CB	4:D:39:PRO:CD	2.85	0.50
5:E:75:VAL:CB	5:E:76:PRO:HD3	2.42	0.50
4:D:25:THR:C	12:L:581:LYS:HE3	2.32	0.50
11:K:96:LEU:C	14:N:117:GLU:HG2	2.32	0.50
12:L:601:LEU:HD11	24:Y:34:VAL:HG22	1.92	0.50
6:F:363:THR:HG22	6:F:366:ARG:HH21	1.77	0.50
8:H:22:LEU:CD1	13:M:354:LEU:HD13	137.85	0.50
12:L:309:GLN:HE21	12:L:332:HIS:HD2	1.59	0.50
1:A:72:LEU:HA	10:J:147:TYR:OH	2.11	0.50
3:C:34:PRO:HB3	21:V:98:PRO:O	2.11	0.49
3:C:94:TYR:HB2	3:C:107:VAL:HB	1.93	0.49
4:D:38:PRO:HG3	14:N:50:PRO:CA	2.28	0.49
5:E:184:PRO:HD2	5:E:185:GLY:N	2.27	0.49
9:I:173:TYR:CD2	18:R:65:ALA:HB2	2.47	0.49
22:W:46:VAL:HG21	22:W:55:VAL:HG22	1.94	0.49
4:D:410:MET:HG3	8:H:281:ARG:HH21	1.77	0.49
2:B:155:ALA:HB2	9:I:137:PHE:HD1	1.76	0.49
1:A:87:MET:HG3	10:J:147:TYR:HB2	1.95	0.49
11:K:58:MET:HA	11:K:61:ILE:HD12	1.94	0.49
10:J:68:PHE:HE1	11:K:75:LEU:HD22	1.75	0.49
4:D:391:ILE:H	4:D:430:ARG:HD3	1.78	0.49
8:H:313:GLY:HA2	25:Z:53:ASN:CB	2.42	0.49
3:C:93:VAL:HG22	3:C:108:LYS:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:31:MET:SD	9:I:37:THR:HB	2.52	0.49
4:D:169:TRP:CD1	9:I:40:TYR:CE2	3.00	0.49
1:A:56:PHE:CZ	11:K:79:VAL:HG21	2.46	0.49
13:M:235:LEU:HD23	13:M:238:LEU:HD11	1.93	0.49
12:L:586:LEU:O	24:Y:41:ALA:HB1	2.13	0.49
4:D:169:TRP:HA	9:I:40:TYR:OH	2.13	0.49
8:H:22:LEU:HD11	8:H:45:LEU:HA	1.95	0.49
10:J:33:LEU:HD12	11:K:31:LEU:CD2	2.42	0.49
4:D:38:PRO:CG	14:N:50:PRO:CD	2.74	0.49
21:V:21:GLU:HG3	21:V:24:LYS:HD3	1.95	0.49
4:D:343:GLU:HG2	7:G:98:LEU:HD13	1.94	0.49
8:H:90:PRO:HB2	8:H:166:ILE:HD11	1.95	0.49
10:J:75:ALA:CB	11:K:82:SER:CB	2.87	0.49
12:L:74:LEU:HD21	12:L:196:TRP:HB3	1.95	0.49
12:L:455:LYS:HA	12:L:458:LEU:HD12	1.94	0.49
14:N:16:GLY:HA2	14:N:19:ILE:HD12	1.95	0.49
21:V:34:LEU:HB3	21:V:44:ARG:HG3	1.94	0.49
12:L:285:THR:HG21	12:L:412:THR:HG22	1.94	0.49
14:N:151:LEU:HD22	14:N:195:PRO:HB3	1.95	0.49
4:D:19:MET:CA	14:N:173:THR:CG2	2.80	0.48
13:M:444:LEU:HA	13:M:447:LEU:HD12	1.94	0.48
12:L:591:PHE:HE1	14:N:113:PHE:CD2	1.88	0.48
5:E:39:PRO:O	5:E:39:PRO:CD	2.61	0.48
6:F:347:ILE:HA	6:F:350:LEU:HD12	1.96	0.48
2:B:157:LEU:HD13	9:I:50:TYR:HB2	1.96	0.48
13:M:373:ILE:HG21	13:M:444:LEU:HD22	1.94	0.48
17:Q:66:UNK:HA	17:Q:73:UNK:HA	1.95	0.48
4:D:6:PRO:O	14:N:305:PHE:CA	2.61	0.48
9:I:119:CYS:HB2	9:I:121:PHE:H	1.77	0.48
10:J:14:VAL:HG11	10:J:100:GLU:HG3	1.95	0.48
10:J:157:THR:HG22	11:K:66:PHE:HE2	1.77	0.48
5:E:75:VAL:CB	5:E:76:PRO:CD	2.91	0.48
7:G:106:PRO:O	7:G:106:PRO:CD	4.69	0.48
8:H:31:MET:HG2	9:I:41:LEU:HD12	1.95	0.48
12:L:593:ILE:CG1	24:Y:37:ALA:CB	2.80	0.48
13:M:243:MET:HG2	13:M:301:ILE:HG21	1.94	0.48
11:K:94:ASN:HB3	14:N:54:GLU:OE2	2.08	0.48
1:A:17:LEU:HA	1:A:20:ILE:HD12	1.95	0.48
4:D:144:ILE:HG13	4:D:147:LEU:HD12	1.95	0.48
8:H:137:ALA:HA	8:H:140:ILE:HG22	1.95	0.48
10:J:23:LYS:HE2	11:K:25:HIS:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:74:GLY:HA3	14:N:60:PHE:CE1	2.49	0.48
3:C:93:VAL:HG11	4:D:377:TYR:CZ	2.49	0.48
4:D:88:GLU:HG2	4:D:430:ARG:HG2	1.95	0.48
4:D:169:TRP:CZ2	9:I:40:TYR:CD1	3.01	0.48
14:N:176:ARG:HE	14:N:224:THR:HG22	1.79	0.48
4:D:97:LEU:HA	4:D:100:LEU:HD12	1.96	0.48
13:M:208:PRO:HG2	13:M:216:LEU:HD22	1.95	0.48
23:X:52:PRO:HG3	25:Z:78:LYS:HE3	1.96	0.48
5:E:76:PRO:CD	5:E:76:PRO:O	2.61	0.48
12:L:224:SER:HB3	12:L:310:LEU:HD11	1.95	0.48
12:L:598:SER:O	14:N:153:LEU:HD11	2.14	0.48
22:W:17:LYS:HA	22:W:18:PRO:HA	1.66	0.48
8:H:73:LEU:HA	8:H:76:ILE:HD12	1.96	0.48
11:K:48:ILE:HG23	11:K:53:PHE:HB2	1.95	0.48
4:D:309:ARG:HE	25:Z:19:UNK:CB	2.28	0.47
8:H:314:ILE:HD12	25:Z:57:ARG:HH22	1.79	0.47
11:K:93:LEU:HD13	12:L:584:ILE:CG1	2.27	0.47
14:N:191:THR:HA	14:N:194:LEU:HD12	1.96	0.47
3:C:13:PRO:HG3	4:D:127:ASN:HA	1.95	0.47
4:D:6:PRO:O	4:D:6:PRO:CD	2.62	0.47
5:E:45:ALA:O	5:E:49:PRO:HG3	2.14	0.47
4:D:348:HIS:HE1	9:I:125:ALA:O	1.96	0.47
12:L:254:VAL:HG23	12:L:329:ILE:HG21	1.95	0.47
14:N:181:TYR:HA	14:N:184:ILE:HD12	1.96	0.47
11:K:66:PHE:CZ	14:N:31:ILE:HG12	2.49	0.47
25:Z:39:ILE:HA	25:Z:42:LEU:HD12	1.95	0.47
2:B:126:TYR:O	2:B:128:TYR:N	2.47	0.47
2:B:71:ARG:HG3	8:H:37:PRO:CD	2.44	0.47
3:C:13:PRO:CG	4:D:127:ASN:O	2.62	0.47
10:J:14:VAL:HG22	11:K:11:ALA:HB2	1.95	0.47
3:C:35:LYS:H	21:V:102:LEU:CB	2.27	0.47
3:C:197:PHE:HE2	9:I:90:GLN:NE2	2.12	0.47
10:J:40:GLY:HA2	10:J:43:ILE:HD12	1.96	0.47
8:H:17:VAL:HA	8:H:20:LEU:HD12	1.96	0.47
2:B:71:ARG:CG	8:H:37:PRO:HG3	2.42	0.47
8:H:277:TYR:CE1	9:I:30:LEU:HG	2.50	0.47
12:L:297:ASP:HB2	12:L:300:LYS:HB2	1.96	0.47
12:L:573:ALA:HB1	14:N:170:LEU:CD1	2.34	0.47
4:D:107:ASP:HB2	4:D:114:ASN:HD21	1.80	0.47
4:D:32:PRO:HG3	4:D:36:VAL:HA	1.90	0.47
13:M:363:SER:HB2	13:M:407:SER:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:111:ALA:HB3	22:W:112:PRO:CA	2.44	0.47
4:D:30:PRO:CD	4:D:30:PRO:O	2.62	0.47
6:F:415:VAL:HA	6:F:418:LEU:HD12	1.97	0.47
10:J:55:MET:CE	11:K:64:LEU:HD22	2.44	0.47
4:D:305:ARG:HG2	25:Z:20:UNK:HA	1.97	0.47
4:D:343:GLU:HA	4:D:346:ILE:HD12	1.97	0.47
14:N:139:MET:HG3	14:N:205:LEU:HD21	1.97	0.47
4:D:25:THR:HA	12:L:581:LYS:HE3	1.69	0.47
8:H:24:GLU:HG2	8:H:271:LEU:HD21	1.96	0.47
10:J:76:THR:HG23	11:K:88:ASP:N	2.29	0.47
13:M:3:LYS:HD3	13:M:41:LEU:HD13	1.97	0.47
12:L:591:PHE:CD1	14:N:113:PHE:CE2	2.90	0.47
11:K:40:LEU:HB3	14:N:75:ILE:CD1	2.45	0.47
8:H:22:LEU:CG	13:M:354:LEU:HD11	138.11	0.46
14:N:277:ILE:HG21	24:Y:134:VAL:CG2	2.43	0.46
1:A:73:LEU:HD23	8:H:151:LEU:HD21	1.97	0.46
2:B:116:MET:HA	2:B:146:VAL:HB	1.98	0.46
8:H:304:HIS:HA	8:H:307:LEU:HD12	1.98	0.46
12:L:558:LEU:HD22	13:M:211:GLY:CA	2.42	0.46
11:K:40:LEU:HB3	14:N:75:ILE:HD13	1.97	0.46
22:W:17:LYS:C	22:W:76:ARG:HH21	2.18	0.46
4:D:308:ILE:HA	4:D:311:ILE:HD12	1.96	0.46
8:H:91:MET:HB3	8:H:92:PRO:CD	2.45	0.46
12:L:526:LEU:HD13	12:L:530:PRO:HG2	1.97	0.46
22:W:42:VAL:HG23	22:W:43:PRO:HD3	1.97	0.46
24:Y:62:ALA:HA	24:Y:65:ILE:HD12	1.96	0.46
8:H:35:LYS:HE3	9:I:47:THR:OG1	2.15	0.46
3:C:85:THR:HG22	17:Q:86:UNK:HA	1.98	0.46
10:J:28:TYR:HA	10:J:31:LEU:HD12	1.97	0.46
14:N:241:THR:HA	14:N:244:ILE:HD12	1.97	0.46
23:X:88:ILE:HD11	23:X:95:LEU:HD23	1.98	0.46
4:D:228:MET:SD	9:I:36:MET:HB2	2.56	0.46
4:D:38:PRO:CB	14:N:50:PRO:CG	2.76	0.46
5:E:13:PRO:O	5:E:13:PRO:CD	2.62	0.46
4:D:165:THR:HG21	9:I:37:THR:HG22	1.97	0.46
10:J:23:LYS:HE3	11:K:25:HIS:HB2	1.98	0.46
14:N:103:ALA:HA	14:N:107:GLY:H	1.81	0.46
3:C:32:ILE:HA	21:V:42:ALA:HB3	1.98	0.46
4:D:234:ILE:HD11	8:H:277:TYR:CD1	2.50	0.46
12:L:594:THR:HG22	24:Y:38:TYR:HH	1.73	0.46
4:D:38:PRO:CG	14:N:50:PRO:HD3	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:45:PRO:HG2	24:Y:50:GLU:HG2	1.98	0.46
7:G:38:PRO:HD3	7:G:90:ARG:NH2	2.27	0.46
2:B:71:ARG:HG3	8:H:37:PRO:N	2.30	0.46
4:D:287:ILE:O	9:I:4:TYR:HA	2.15	0.46
19:S:16:ARG:N	19:S:68:TYR:O	2.49	0.46
14:N:340:THR:N	14:N:341:PRO:HD2	2.31	0.46
4:D:38:PRO:HD3	14:N:50:PRO:HG3	1.84	0.46
3:C:57:VAL:HG21	3:C:117:ILE:HD11	1.97	0.45
12:L:131:LEU:HB2	12:L:143:GLY:HA3	1.98	0.45
14:N:248:LEU:HD21	14:N:296:LEU:HD23	1.98	0.45
21:V:101:PRO:CD	21:V:101:PRO:O	2.63	0.45
13:M:72:LEU:HA	13:M:75:LEU:HB2	1.97	0.45
4:D:38:PRO:HD3	14:N:50:PRO:CG	2.32	0.45
8:H:59:GLU:HA	8:H:60:PRO:HD3	1.85	0.45
21:V:106:PRO:O	21:V:106:PRO:CD	2.64	0.45
3:C:152:LEU:HB3	4:D:84:HIS:CD2	2.51	0.45
4:D:234:ILE:HD11	8:H:277:TYR:HD1	1.81	0.45
11:K:19:LEU:HD11	11:K:36:MET:HG3	1.99	0.45
11:K:93:LEU:HD13	12:L:584:ILE:HD12	0.93	0.45
12:L:594:THR:HA	12:L:597:ILE:HD12	1.97	0.45
1:A:10:ASN:ND2	8:H:87:ILE:HD11	2.32	0.45
6:F:191:ALA:HB2	6:F:203:PRO:HG3	1.98	0.45
8:H:22:LEU:HD23	8:H:37:PRO:HG2	1.98	0.45
11:K:40:LEU:HD21	14:N:72:MET:HA	1.99	0.45
13:M:129:THR:HG21	13:M:236:LEU:HD11	1.98	0.45
3:C:116:PRO:HG2	22:W:20:PHE:HA	1.98	0.45
5:E:94:PRO:HB3	25:Z:87:ARG:CD	159.46	0.45
10:J:157:THR:CG2	11:K:66:PHE:HE2	2.30	0.45
12:L:7:LEU:HD23	12:L:50:PRO:HD3	1.99	0.45
3:C:154:ASP:HB2	3:C:157:PHE:HB2	1.98	0.45
14:N:95:SER:HB2	14:N:149:ILE:HG22	1.97	0.45
10:J:27:ILE:HG13	10:J:80:PRO:HG3	1.99	0.45
14:N:277:ILE:HG21	24:Y:134:VAL:CA	2.46	0.45
24:Y:24:THR:HA	24:Y:27:ILE:HD12	1.99	0.45
8:H:290:TRP:HA	8:H:294:LEU:HD12	1.98	0.44
4:D:164:MET:HB3	8:H:32:GLN:NE2	2.32	0.44
4:D:169:TRP:CE2	9:I:40:TYR:CD1	3.05	0.44
10:J:157:THR:CG2	11:K:66:PHE:CE2	2.98	0.44
20:U:4:PRO:HA	20:U:5:PRO:HD3	1.90	0.44
4:D:352:TYR:HB3	9:I:86:VAL:HG22	1.99	0.44
8:H:162:LEU:HA	8:H:165:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:ASP:OD1	8:H:54:LYS:HE2	2.17	0.44
11:K:73:LEU:CB	14:N:38:LEU:HD22	2.47	0.44
13:M:232:ALA:HA	13:M:235:LEU:HD12	1.99	0.44
5:E:94:PRO:O	5:E:94:PRO:CD	2.63	0.44
7:G:38:PRO:O	7:G:38:PRO:CD	2.66	0.44
1:A:97:LEU:HD22	10:J:162:LEU:HD11	2.00	0.44
10:J:12:ILE:HB	10:J:39:VAL:HG11	1.99	0.44
1:A:10:ASN:HD21	8:H:87:ILE:HD11	1.82	0.44
4:D:410:MET:CG	8:H:281:ARG:HH21	2.31	0.44
11:K:94:ASN:HB2	14:N:54:GLU:CD	2.19	0.44
11:K:96:LEU:C	14:N:117:GLU:CG	2.86	0.44
14:N:15:LEU:HA	14:N:18:ILE:HD12	2.00	0.44
12:L:377:SER:HB2	12:L:423:SER:HB2	2.00	0.44
12:L:393:ASP:HA	12:L:396:ILE:HD12	1.98	0.44
12:L:601:LEU:HD21	24:Y:30:ALA:HB1	2.00	0.44
13:M:237:LYS:HD2	13:M:294:MET:HG3	1.99	0.44
14:N:26:TRP:HB2	14:N:84:TRP:CD1	2.53	0.44
17:Q:22:UNK:O	22:W:84:LYS:HE3	2.17	0.44
24:Y:120:THR:HA	24:Y:123:LEU:HD12	1.99	0.44
4:D:113:CYS:H	4:D:145:THR:HG21	1.82	0.44
5:E:47:VAL:C	5:E:49:PRO:HD3	2.38	0.44
10:J:144:ALA:O	11:K:58:MET:CA	2.66	0.44
10:J:33:LEU:HD12	11:K:31:LEU:HD22	2.00	0.44
8:H:133:LEU:HD22	10:J:70:TYR:CD2	2.53	0.44
14:N:203:LEU:HA	14:N:206:ILE:HD12	2.00	0.44
14:N:326:LEU:N	14:N:327:PRO:HD2	2.32	0.44
12:L:601:LEU:HD11	24:Y:34:VAL:CG2	2.43	0.44
12:L:561:ILE:HD13	13:M:212:LEU:HG	2.00	0.44
14:N:160:LEU:HA	14:N:163:LEU:HD12	2.00	0.44
8:H:149:ILE:HG23	8:H:181:LEU:HD22	1.99	0.44
14:N:125:SER:HA	14:N:128:LEU:HD12	1.99	0.44
14:N:167:TRP:HA	14:N:170:LEU:HD12	1.99	0.44
4:D:31:PRO:CD	4:D:31:PRO:O	2.65	0.43
7:G:98:LEU:HD21	7:G:116:LEU:HD21	2.00	0.43
10:J:47:PHE:CB	11:K:49:LEU:CD2	2.93	0.43
19:S:50:LEU:HA	19:S:51:PRO:HD3	1.91	0.43
19:S:62:PRO:HG2	19:S:79:ASN:HA	1.99	0.43
11:K:12:PHE:CZ	14:N:72:MET:CG	3.01	0.43
13:M:318:ALA:HB2	13:M:373:ILE:HG12	1.99	0.43
12:L:577:VAL:CG2	14:N:171:ASN:HD22	2.29	0.43
14:N:277:ILE:HG22	24:Y:133:GLN:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:27:HIS:H	12:L:581:LYS:HZ1	1.66	0.43
5:E:20:PRO:CD	5:E:20:PRO:O	2.66	0.43
11:K:30:LEU:HA	11:K:33:LEU:HD12	1.99	0.43
10:J:140:ALA:HB1	11:K:54:THR:HA	2.01	0.43
5:E:107:PRO:HB3	6:F:103:GLY:HA2	2.00	0.43
7:G:154:ILE:HG13	7:G:154:ILE:H	1.68	0.43
8:H:237:PHE:HA	8:H:240:ILE:HD12	2.00	0.43
12:L:52:MET:HA	12:L:55:ILE:HD12	1.99	0.43
4:D:169:TRP:NE1	9:I:40:TYR:CD2	2.87	0.43
9:I:62:ARG:HA	9:I:133:GLU:HB3	2.00	0.43
9:I:76:ARG:HH12	18:R:66:LEU:HD22	1.83	0.43
11:K:96:LEU:O	14:N:117:GLU:HG2	2.17	0.43
12:L:127:THR:HA	12:L:130:ILE:HD12	2.00	0.43
20:T:48:VAL:O	22:W:32:ARG:NH2	2.52	0.43
6:F:202:LYS:HA	6:F:203:PRO:HD3	1.92	0.43
8:H:178:ALA:HB1	8:H:181:LEU:HB2	2.01	0.43
12:L:601:LEU:HD21	24:Y:30:ALA:C	2.39	0.43
8:H:313:GLY:HA2	25:Z:53:ASN:ND2	2.33	0.43
8:H:47:GLN:N	8:H:48:PRO:HD2	2.33	0.43
12:L:594:THR:CG2	14:N:110:PRO:HB3	2.45	0.43
3:C:77:ASP:HB3	4:D:392:LYS:HG3	2.01	0.43
8:H:243:LEU:HD13	8:H:262:LYS:HB3	2.01	0.43
23:X:46:ARG:HD2	25:Z:78:LYS:HE2	2.00	0.43
2:B:118:SER:HA	2:B:121:ASN:HD22	1.84	0.43
2:B:43:SER:OG	8:H:40:VAL:CG1	2.66	0.43
3:C:67:HIS:HD2	3:C:70:ALA:H	1.67	0.43
4:D:100:LEU:HD21	4:D:196:PRO:HD3	1.99	0.43
9:I:151:LYS:HE2	9:I:153:LYS:HD2	2.01	0.43
10:J:68:PHE:CD2	11:K:27:MET:HE1	2.54	0.43
11:K:95:LEU:CD1	14:N:55:ALA:N	2.81	0.43
5:E:184:PRO:CD	5:E:185:GLY:H	2.30	0.42
8:H:219:PRO:HA	8:H:222:LEU:HD12	2.01	0.42
12:L:577:VAL:CG2	14:N:171:ASN:HB2	2.26	0.42
11:K:96:LEU:CA	14:N:117:GLU:HG2	2.49	0.42
13:M:141:GLU:HB2	13:M:144:ASN:HB2	2.01	0.42
22:W:41:GLU:HG3	22:W:93:ILE:HG12	2.01	0.42
1:A:57:LEU:HD22	10:J:169:MET:SD	2.58	0.42
3:C:205:ALA:HA	7:G:122:MET:SD	2.59	0.42
4:D:414:VAL:HA	4:D:417:ILE:HD12	2.00	0.42
10:J:47:PHE:C	11:K:49:LEU:CD2	2.82	0.42
11:K:59:MET:HG3	14:N:84:TRP:HZ3	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:373:ILE:HA	13:M:376:ILE:HD12	2.02	0.42
16:P:6:UNK:HA	16:P:17:UNK:HA	2.01	0.42
4:D:204:PRO:HA	9:I:176:ARG:HB3	2.01	0.42
4:D:232:ASN:HA	9:I:29:GLU:HG2	2.02	0.42
12:L:225:ALA:HB3	12:L:310:LEU:HD13	2.01	0.42
14:N:170:LEU:HG	14:N:292:PHE:HE1	1.85	0.42
7:G:107:ILE:HD11	18:R:86:TYR:CZ	2.54	0.42
12:L:54:PHE:HE1	12:L:59:GLN:HG2	1.84	0.42
25:Z:65:GLU:HA	25:Z:68:ILE:HD12	2.02	0.42
4:D:18:VAL:C	4:D:20:TYR:N	2.67	0.42
4:D:25:THR:CB	12:L:581:LYS:CB	2.93	0.42
10:J:7:PHE:CE1	11:K:7:ASN:ND2	2.77	0.42
13:M:223:ALA:HA	13:M:224:PRO:HD2	1.91	0.42
13:M:75:LEU:HA	13:M:78:MET:HG2	2.02	0.42
12:L:576:LEU:HD11	14:N:167:TRP:HE3	0.78	0.42
4:D:158:ALA:HB1	4:D:163:ALA:HB3	2.02	0.42
4:D:92:GLU:HG2	4:D:388:ARG:H	1.84	0.42
5:E:62:PRO:O	5:E:62:PRO:CD	2.66	0.42
7:G:107:ILE:HD13	18:R:85:GLY:HA3	2.02	0.42
13:M:97:THR:HA	13:M:100:ILE:HD12	2.02	0.42
4:D:165:THR:HA	8:H:32:GLN:HG2	2.00	0.42
6:F:374:LYS:HE3	7:G:133:GLY:HA3	2.00	0.42
5:E:16:ASN:N	5:E:17:PRO:CD	2.76	0.42
12:L:181:GLY:HA3	12:L:218:LEU:HB3	2.02	0.42
12:L:329:ILE:H	12:L:329:ILE:HG13	1.69	0.42
12:L:545:SER:OG	13:M:274:SER:O	2.32	0.42
4:D:227:GLU:HA	4:D:231:ASN:HD22	1.85	0.41
7:G:163:ALA:HA	7:G:167:ALA:HB3	2.02	0.41
12:L:440:LEU:H	20:U:57:GLU:HA	1.84	0.41
12:L:588:PHE:CZ	14:N:62:THR:HG23	2.55	0.41
13:M:164:LEU:HA	13:M:167:ILE:HD12	2.02	0.41
4:D:339:LYS:NZ	18:R:66:LEU:C	2.73	0.41
8:H:272:TRP:CZ2	9:I:38:LEU:HD12	2.55	0.41
11:K:12:PHE:CZ	14:N:72:MET:CB	3.02	0.41
12:L:42:TYR:HA	12:L:45:ILE:HD12	2.02	0.41
14:N:254:LEU:HA	14:N:255:PRO:HD3	1.83	0.41
14:N:273:ASN:CA	24:Y:138:PRO:C	2.76	0.41
5:E:15:ASN:O	5:E:17:PRO:CG	2.64	0.41
5:E:46:ALA:CA	5:E:49:PRO:HG2	2.44	0.41
12:L:350:LEU:HD22	12:L:438:PRO:HG3	2.01	0.41
21:V:33:VAL:HA	21:V:36:HIS:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:PHE:HE1	21:V:43:TYR:HE1	1.68	0.41
4:D:146:ARG:HG2	4:D:370:PRO:HG3	2.01	0.41
14:N:175:LEU:HA	14:N:178:ILE:HD12	2.01	0.41
3:C:31:GLU:CD	21:V:46:TYR:HH	2.23	0.41
1:A:104:TYR:CZ	10:J:166:VAL:HG13	2.55	0.41
2:B:126:TYR:HA	4:D:90:LEU:HD21	2.02	0.41
13:M:116:ILE:H	13:M:116:ILE:HG13	1.66	0.41
21:V:107:PRO:O	21:V:107:PRO:CD	2.68	0.41
22:W:112:PRO:O	22:W:112:PRO:HD2	2.20	0.41
1:A:67:LEU:HD21	11:K:68:ALA:HB3	2.02	0.41
1:A:94:LEU:HD11	10:J:154:VAL:HG13	2.01	0.41
10:J:168:ILE:HA	10:J:171:ILE:HD12	2.01	0.41
13:M:58:SER:HB3	13:M:113:MET:H	1.84	0.41
21:V:19:PRO:O	21:V:19:PRO:CD	2.68	0.41
9:I:81:LYS:HG2	9:I:94:ILE:HG23	2.01	0.41
9:I:87:CYS:HA	9:I:88:PRO:HD3	1.85	0.41
13:M:117:LEU:HG	13:M:120:ILE:HD11	2.02	0.41
12:L:585:LYS:HZ3	24:Y:43:LYS:NZ	2.11	0.41
12:L:286:LEU:HD12	12:L:411:MET:HG3	2.02	0.41
14:N:20:VAL:HA	14:N:29:VAL:HG12	2.03	0.41
6:F:208:PRO:HB3	7:G:72:PRO:HD3	2.01	0.41
8:H:162:LEU:HD21	8:H:237:PHE:HE1	1.86	0.41
12:L:370:THR:HA	12:L:373:LEU:HD12	2.02	0.41
14:N:151:LEU:HA	14:N:154:ILE:HD12	2.02	0.41
24:Y:82:LYS:HA	24:Y:83:PRO:HD3	1.86	0.41
5:E:110:LEU:CB	6:F:260:GLY:CA	2.99	0.41
23:X:10:GLU:HA	25:Z:86:LEU:HD13	2.03	0.41
4:D:266:GLN:HG2	4:D:287:ILE:HD13	2.02	0.41
5:E:47:VAL:C	5:E:49:PRO:CD	2.89	0.41
13:M:391:ILE:HG13	13:M:391:ILE:H	1.67	0.41
3:C:88:ASN:HA	3:C:112:ASP:HB3	2.02	0.40
4:D:165:THR:HG21	9:I:37:THR:HG21	2.01	0.40
24:Y:44:THR:HG22	24:Y:54:ARG:HH11	1.86	0.40
5:E:94:PRO:CB	25:Z:87:ARG:HH11	157.23	0.40
2:B:138:ARG:CZ	3:C:174:LEU:HD11	2.52	0.40
4:D:285:VAL:HA	4:D:286:PRO:HD3	1.92	0.40
3:C:81:VAL:HG22	4:D:388:ARG:HH21	1.87	0.40
1:A:16:LEU:HA	1:A:19:ILE:HD12	2.03	0.40
14:N:224:THR:H	14:N:228:LEU:HD23	1.85	0.40
23:X:7:PRO:O	23:X:7:PRO:CD	2.69	0.40
23:X:94:GLN:HB3	23:X:97:ARG:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:169:TRP:CZ2	9:I:40:TYR:CG	3.09	0.40
4:D:342:MET:HG3	4:D:346:ILE:HD11	2.03	0.40
4:D:347:HIS:CE1	7:G:121:MET:SD	3.15	0.40
12:L:590:SER:HA	12:L:593:ILE:HD12	2.04	0.40
13:M:150:LEU:HB3	13:M:154:LEU:HD12	2.04	0.40
14:N:74:VAL:HG13	14:N:84:TRP:HE1	1.86	0.40
14:N:278:LEU:HD11	24:Y:135:PHE:CE1	2.56	0.40
4:D:197:GLY:HA3	4:D:331:SER:HB3	2.04	0.40
2:B:39:TRP:CH2	8:H:46:LEU:HD22	2.57	0.40
9:I:84:GLU:HA	9:I:92:ILE:HG23	2.03	0.40
12:L:324:LEU:HA	12:L:327:LEU:HD12	2.04	0.40
14:N:214:THR:O	14:N:218:MET:HG2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	A	84/115 (73%)	79 (94%)	3 (4%)	2 (2%)	7	47
2	B	145/179 (81%)	128 (88%)	10 (7%)	7 (5%)	3	31
3	C	204/228 (90%)	174 (85%)	23 (11%)	7 (3%)	5	40
4	D	412/429 (96%)	360 (87%)	37 (9%)	15 (4%)	4	38
5	E	184/217 (85%)	151 (82%)	18 (10%)	15 (8%)	1	18
6	F	423/444 (95%)	375 (89%)	38 (9%)	10 (2%)	7	47
7	G	201/700 (29%)	168 (84%)	26 (13%)	7 (4%)	4	39
8	H	292/318 (92%)	270 (92%)	16 (6%)	6 (2%)	9	50
9	I	174/176 (99%)	144 (83%)	19 (11%)	11 (6%)	2	25
10	J	169/175 (97%)	150 (89%)	14 (8%)	5 (3%)	5	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	93/98 (95%)	88 (95%)	5 (5%)	0	100	100
12	L	602/606 (99%)	539 (90%)	52 (9%)	11 (2%)	11	53
13	M	455/459 (99%)	411 (90%)	34 (8%)	10 (2%)	8	49
14	N	342/347 (99%)	309 (90%)	26 (8%)	7 (2%)	9	51
15	O	227/314 (72%)	199 (88%)	20 (9%)	8 (4%)	4	39
18	R	34/89 (38%)	30 (88%)	3 (9%)	1 (3%)	6	43
19	S	78/99 (79%)	72 (92%)	5 (6%)	1 (1%)	15	60
20	T	73/88 (83%)	69 (94%)	3 (4%)	1 (1%)	14	58
20	U	83/88 (94%)	74 (89%)	7 (8%)	2 (2%)	7	47
21	V	104/115 (90%)	91 (88%)	8 (8%)	5 (5%)	3	31
22	W	109/127 (86%)	90 (83%)	12 (11%)	7 (6%)	2	25
23	X	108/164 (66%)	94 (87%)	11 (10%)	3 (3%)	6	44
24	Y	136/140 (97%)	124 (91%)	8 (6%)	4 (3%)	6	43
25	Z	69/138 (50%)	65 (94%)	4 (6%)	0	100	100
26	a	62/70 (89%)	54 (87%)	4 (6%)	4 (6%)	1	25
27	b	44/80 (55%)	40 (91%)	4 (9%)	0	100	100
28	c	44/49 (90%)	39 (89%)	2 (4%)	3 (7%)	1	23
29	d	69/114 (60%)	64 (93%)	4 (6%)	1 (1%)	14	58
30	e	87/106 (82%)	76 (87%)	10 (12%)	1 (1%)	17	63
31	f	52/57 (91%)	44 (85%)	5 (10%)	3 (6%)	2	27
32	g	95/125 (76%)	67 (70%)	15 (16%)	13 (14%)	0	6
33	h	38/134 (28%)	35 (92%)	1 (3%)	2 (5%)	2	29
34	i	25/106 (24%)	24 (96%)	1 (4%)	0	100	100
38	m	96/118 (81%)	84 (88%)	8 (8%)	4 (4%)	3	34
39	n	126/166 (76%)	113 (90%)	10 (8%)	3 (2%)	7	47
40	o	56/58 (97%)	52 (93%)	3 (5%)	1 (2%)	11	53
41	p	67/169 (40%)	60 (90%)	4 (6%)	3 (4%)	3	33
42	q	136/138 (99%)	110 (81%)	21 (15%)	5 (4%)	4	38
All	All	5798/7343 (79%)	5116 (88%)	494 (8%)	188 (3%)	8	41

All (188) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	127	HIS
2	B	150	PRO
3	C	9	PRO
4	D	38	PRO
5	E	16	ASN
5	E	17	PRO
5	E	94	PRO
5	E	126	ILE
5	E	182	PRO
5	E	184	PRO
6	F	423	ARG
9	I	153	LYS
12	L	84	TYR
13	M	6	ILE
14	N	3	PRO
14	N	306	PRO
15	O	166	PRO
21	V	19	PRO
21	V	98	PRO
28	c	11	SER
30	e	93	PRO
31	f	50	PRO
32	g	31	GLU
32	g	42	PRO
32	g	80	LEU
32	g	115	PRO
33	h	10	ILE
39	n	81	PHE
3	C	67	HIS
4	D	258	VAL
4	D	259	MET
6	F	164	LYS
7	G	74	MET
7	G	194	GLU
8	H	68	ALA
8	H	91	MET
9	I	14	MET
9	I	74	GLU
9	I	100	ALA
9	I	151	LYS
10	J	79	TYR
12	L	24	PHE
12	L	25	ASN

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Mol	Chain	Res	Type
13	M	175	ASN
13	M	224	PRO
13	M	226	ALA
14	N	46	LYS
15	O	93	SER
15	O	118	THR
15	O	303	LYS
20	T	32	VAL
22	W	21	SER
22	W	24	MET
22	W	52	ASP
26	a	40	HIS
29	d	53	VAL
31	f	54	VAL
39	n	82	PRO
41	p	120	HIS
42	q	54	GLN
42	q	63	ILE
42	q	84	PRO
2	B	122	GLY
2	B	126	TYR
3	C	178	ASP
3	C	186	GLU
4	D	35	ASP
4	D	45	SER
4	D	353	THR
4	D	388	ARG
5	E	25	PRO
5	E	38	TYR
5	E	157	ASN
6	F	19	ASP
6	F	284	ALA
6	F	326	GLN
7	G	193	SER
9	I	2	TYR
9	I	4	TYR
10	J	110	ASP
10	J	133	SER
12	L	476	THR
12	L	549	ALA
12	L	583	LEU
13	M	371	PRO

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Mol	Chain	Res	Type
13	M	373	ILE
19	S	17	GLU
22	W	114	PRO
22	W	124	GLY
28	c	6	GLU
32	g	38	TYR
32	g	43	ASP
32	g	76	PHE
32	g	108	MET
32	g	120	LEU
41	p	124	CYS
1	A	52	SER
1	A	108	GLN
2	B	73	GLY
2	B	79	SER
2	B	171	LYS
4	D	46	ASN
4	D	64	LEU
4	D	256	SER
5	E	60	TRP
5	E	93	LYS
5	E	112	ASN
5	E	163	ASP
6	F	40	GLY
7	G	144	PRO
8	H	196	ALA
9	I	116	CYS
9	I	118	TYR
12	L	56	HIS
12	L	225	ALA
12	L	515	TYR
13	M	227	GLY
14	N	48	HIS
14	N	90	PHE
14	N	197	ASN
14	N	338	PRO
15	O	126	ARG
15	O	314	ASP
18	R	80	LYS
20	U	87	TYR
22	W	72	ILE
24	Y	43	LYS

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Mol	Chain	Res	Type
24	Y	82	LYS
32	g	50	ASP
32	g	77	VAL
32	g	83	TYR
33	h	13	PRO
38	m	61	ASP
41	p	78	GLU
42	q	82	VAL
3	C	13	PRO
3	C	203	TRP
4	D	18	VAL
6	F	287	VAL
7	G	52	CYS
7	G	146	VAL
9	I	28	THR
9	I	79	ALA
10	J	63	GLY
20	U	32	VAL
21	V	101	PRO
22	W	95	VAL
23	X	14	VAL
26	a	42	PRO
38	m	56	ARG
38	m	118	GLY
3	C	39	GLN
5	E	128	VAL
8	H	244	GLY
13	M	457	PRO
21	V	37	ILE
21	V	103	VAL
23	X	92	GLY
26	a	56	GLY
26	a	57	VAL
28	c	12	PRO
31	f	49	LYS
32	g	49	LYS
38	m	81	PRO
39	n	76	PRO
4	D	6	PRO
6	F	290	GLY
8	H	96	ILE
12	L	441	VAL

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Mol	Chain	Res	Type
12	L	482	MET
23	X	23	VAL
40	o	73	PHE
4	D	277	VAL
5	E	181	ILE
8	H	197	PRO
42	q	70	GLY
6	F	201	GLY
6	F	210	PRO
7	G	111	GLY
10	J	123	GLY
13	M	23	ILE
15	O	312	VAL
24	Y	83	PRO
4	D	39	PRO
13	M	453	ILE
15	O	301	GLY
24	Y	109	ILE
4	D	372	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	A	72/101 (71%)	70 (97%)	2 (3%)	51	78
2	B	124/150 (83%)	117 (94%)	7 (6%)	26	63
3	C	179/204 (88%)	173 (97%)	6 (3%)	44	76
4	D	332/371 (90%)	321 (97%)	11 (3%)	45	76
5	E	21/183 (12%)	20 (95%)	1 (5%)	31	67
6	F	84/353 (24%)	80 (95%)	4 (5%)	31	67
7	G	64/172 (37%)	57 (89%)	7 (11%)	8	35
8	H	249/275 (90%)	243 (98%)	6 (2%)	57	82
9	I	138/151 (91%)	128 (93%)	10 (7%)	18	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	112/142 (79%)	109 (97%)	3 (3%)	52	79
11	K	83/86 (96%)	81 (98%)	2 (2%)	57	82
12	L	463/534 (87%)	448 (97%)	15 (3%)	46	77
13	M	384/413 (93%)	377 (98%)	7 (2%)	66	87
14	N	277/316 (88%)	264 (95%)	13 (5%)	32	68
15	O	83/205 (40%)	82 (99%)	1 (1%)	78	90
18	R	17/26 (65%)	16 (94%)	1 (6%)	24	61
19	S	4/82 (5%)	4 (100%)	0	100	100
20	T	3/81 (4%)	3 (100%)	0	100	100
20	U	5/81 (6%)	5 (100%)	0	100	100
21	V	47/101 (46%)	47 (100%)	0	100	100
22	W	71/113 (63%)	71 (100%)	0	100	100
23	X	83/99 (84%)	83 (100%)	0	100	100
24	Y	99/101 (98%)	97 (98%)	2 (2%)	63	85
25	Z	59/59 (100%)	59 (100%)	0	100	100
26	a	41/59 (70%)	40 (98%)	1 (2%)	57	82
27	b	36/36 (100%)	35 (97%)	1 (3%)	51	78
28	c	26/45 (58%)	26 (100%)	0	100	100
29	d	56/60 (93%)	55 (98%)	1 (2%)	66	87
30	e	45/96 (47%)	45 (100%)	0	100	100
31	f	22/54 (41%)	21 (96%)	1 (4%)	34	69
32	g	51/112 (46%)	50 (98%)	1 (2%)	63	85
33	h	28/35 (80%)	28 (100%)	0	100	100
34	i	20/27 (74%)	20 (100%)	0	100	100
38	m	75/86 (87%)	73 (97%)	2 (3%)	52	79
39	n	65/117 (56%)	64 (98%)	1 (2%)	72	89
40	o	5/56 (9%)	5 (100%)	0	100	100
41	p	50/62 (81%)	48 (96%)	2 (4%)	38	71
42	q	9/124 (7%)	9 (100%)	0	100	100
All	All	3582/5368 (67%)	3474 (97%)	108 (3%)	52	77

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ASP
1	A	69	ILE
2	B	35	ASP
2	B	54	CYS
2	B	68	ASP
2	B	71	ARG
2	B	125	TYR
2	B	126	TYR
2	B	156	LEU
3	C	65	ARG
3	C	78	LEU
3	C	117	ILE
3	C	165	ASP
3	C	199	LEU
3	C	211	GLN
4	D	39	PRO
4	D	83	LEU
4	D	88	GLU
4	D	104	ASP
4	D	106	LEU
4	D	107	ASP
4	D	223	ASP
4	D	234	ILE
4	D	251	LEU
4	D	271	LYS
4	D	275	TYR
5	E	182	PRO
6	F	359	CYS
6	F	366	ARG
6	F	405	CYS
6	F	409	ASP
7	G	42	TYR
7	G	52	CYS
7	G	104	ASP
7	G	105	CYS
7	G	107	ILE
7	G	108	CYS
7	G	154	ILE
8	H	4	ILE
8	H	9	LEU
8	H	61	LEU
8	H	270	PHE
8	H	272	TRP

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Mol	Chain	Res	Type
8	H	290	TRP
9	I	26	LEU
9	I	29	GLU
9	I	44	GLU
9	I	78	ILE
9	I	107	THR
9	I	119	CYS
9	I	128	VAL
9	I	129	ASP
9	I	147	LEU
9	I	172	ASP
10	J	52	LEU
10	J	77	GLU
10	J	87	LYS
11	K	73	LEU
11	K	88	ASP
12	L	61	LEU
12	L	66	TRP
12	L	69	LEU
12	L	103	PHE
12	L	125	LEU
12	L	159	TYR
12	L	179	ASP
12	L	218	LEU
12	L	283	ILE
12	L	302	ILE
12	L	310	LEU
12	L	329	ILE
12	L	331	THR
12	L	350	LEU
12	L	524	THR
13	M	73	LEU
13	M	116	ILE
13	M	141	GLU
13	M	214	LEU
13	M	228	SER
13	M	354	LEU
13	M	391	ILE
14	N	27	LEU
14	N	62	THR
14	N	63	GLN
14	N	70	LEU

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Mol	Chain	Res	Type
14	N	84	TRP
14	N	87	MET
14	N	89	LEU
14	N	91	ASN
14	N	201	THR
14	N	203	LEU
14	N	204	ASN
14	N	239	ILE
14	N	302	LEU
15	O	110	ASP
18	R	84	CYS
24	Y	105	ARG
24	Y	107	TYR
26	a	16	LEU
27	b	44	ILE
29	d	75	LEU
31	f	31	ASP
32	g	64	PHE
38	m	108	ARG
38	m	109	ASP
39	n	53	GLU
41	p	98	ASP
41	p	140	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
3	C	67	HIS
4	D	79	HIS
4	D	114	ASN
4	D	116	GLN
4	D	200	HIS
4	D	231	ASN
4	D	348	HIS
4	D	398	HIS
6	F	398	GLN
6	F	402	HIS
7	G	100	ASN
8	H	5	ASN
8	H	169	GLN
8	H	247	HIS

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Mol	Chain	Res	Type
9	I	90	GLN
9	I	168	ASN
12	L	72	GLN
12	L	170	GLN
12	L	295	GLN
12	L	309	GLN
12	L	320	ASN
13	M	279	GLN
14	N	36	ASN
21	V	36	HIS
21	V	49	GLN
25	Z	53	ASN
27	b	45	ASN
28	c	34	GLN
29	d	59	HIS
30	e	69	GLN
38	m	74	ASN
39	n	13	GLN
39	n	72	HIS
41	p	106	GLN

### 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 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\# Z  > 2$
45	SF4	B	201	2	0,12,12	0.00	-	0,24,24	0.00	-
46	FES	E	301	5	0,4,4	0.00	-	0,4,4	0.00	-
47	FMN	F	501	-	32,33,33	1.78	6 (18%)	34,50,50	2.22	8 (23%)
45	SF4	F	502	6	0,12,12	0.00	-	0,24,24	0.00	-
45	SF4	G	801	7	0,12,12	0.00	-	0,24,24	0.00	-
45	SF4	G	802	7	0,12,12	0.00	-	0,24,24	0.00	-
46	FES	G	803	7	0,4,4	0.00	-	0,4,4	0.00	-
45	SF4	I	201	9	0,12,12	0.00	-	0,24,24	0.00	-
45	SF4	I	202	9	0,12,12	0.00	-	0,24,24	0.00	-
48	NAP	P	501	-	45,52,52	0.90	1 (2%)	55,80,80	1.48	4 (7%)

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
45	SF4	B	201	2	-	0/0/48/48	0/6/5/5
46	FES	E	301	5	-	0/0/4/4	0/1/1/1
47	FMN	F	501	-	-	0/18/18/18	0/3/3/3
45	SF4	F	502	6	-	0/0/48/48	0/6/5/5
45	SF4	G	801	7	-	0/0/48/48	0/6/5/5
45	SF4	G	802	7	-	0/0/48/48	0/6/5/5
46	FES	G	803	7	-	0/0/4/4	0/1/1/1
45	SF4	I	201	9	-	0/0/48/48	0/6/5/5
45	SF4	I	202	9	-	0/0/48/48	0/6/5/5
48	NAP	P	501	-	-	0/27/67/67	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	F	501	FMN	C10-N10	3.29	1.43	1.39
47	F	501	FMN	C9A-N10	3.32	1.43	1.38
48	P	501	NAP	C5A-C4A	3.32	1.48	1.40
47	F	501	FMN	C8-C7	3.68	1.50	1.41
47	F	501	FMN	C4-C4A	3.91	1.49	1.41
47	F	501	FMN	C9A-C5A	3.92	1.50	1.42
47	F	501	FMN	C4A-C10	4.69	1.49	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	P	501	NAP	N3A-C2A-N1A	-7.44	123.03	128.87
47	F	501	FMN	C4-C4A-C10	-4.43	117.11	119.94
47	F	501	FMN	C4A-C4-N3	-3.72	118.66	123.52
47	F	501	FMN	N3-C2-N1	-3.03	122.59	127.69
48	P	501	NAP	C4B-O4B-C1B	2.01	111.77	109.64
47	F	501	FMN	C5A-C9A-N10	2.04	119.10	117.58
48	P	501	NAP	C4D-O4D-C1D	2.41	112.20	109.64
47	F	501	FMN	C4-C4A-N5	2.46	121.69	118.70
47	F	501	FMN	C1'-N10-C9A	2.65	121.90	118.83
48	P	501	NAP	O4D-C1D-N1N	3.30	111.66	108.10
47	F	501	FMN	C4A-N5-C5A	3.99	121.43	116.72
47	F	501	FMN	C4-N3-C2	8.23	122.03	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
16	P	2
43	r	1
34	i	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	70:UNK	C	100:UNK	N	22.99
1	P	252:UNK	C	280:UNK	N	21.70
1	P	186:UNK	C	200:UNK	N	21.19
1	i	32:PRO	C	40:UNK	N	15.55