Full wwPDB EM Validation Report ⓘ

Aug 27, 2026 – 12:47 pm BST

PDB ID	:	7A23 / pdb_00007a23
EMDB ID	:	EMD-11614
Title	:	Plant mitochondrial respiratory complex I
Authors	:	Soufari, H.; Waltz, F.; Hashem, Y.
Deposited on	:	2020-08-15
Resolution	:	3.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

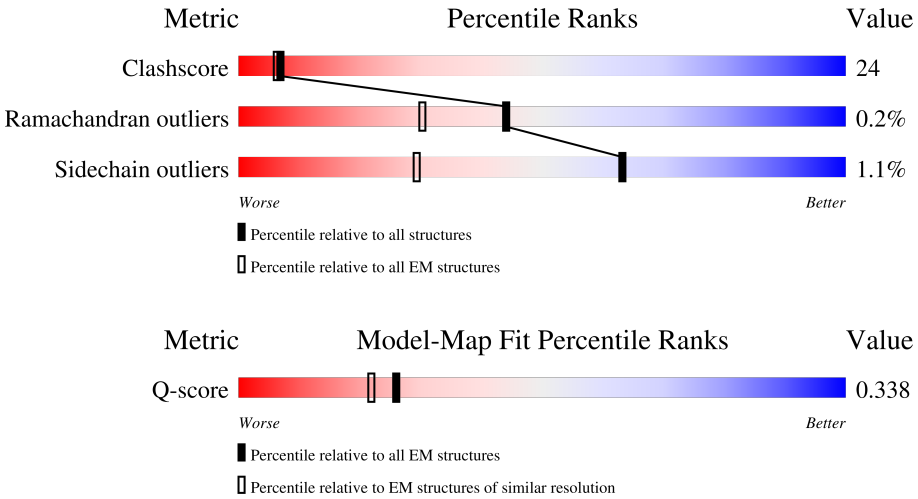
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.70 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.



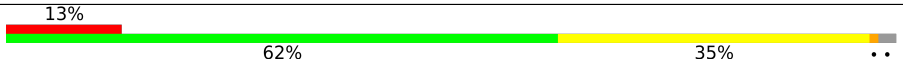
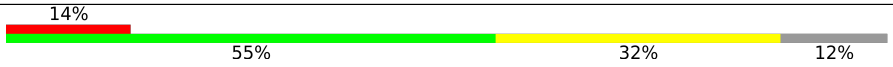
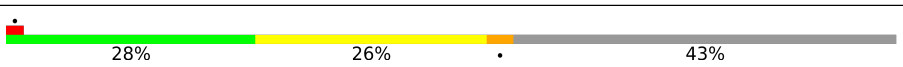
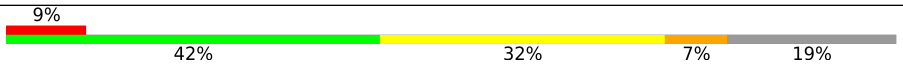
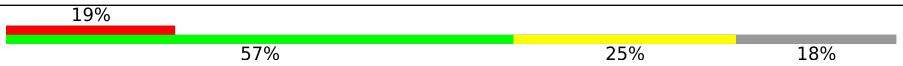
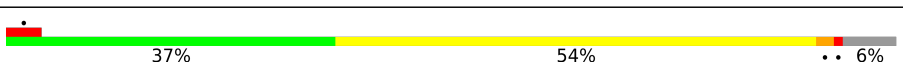
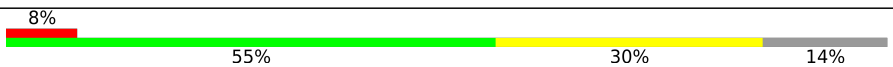
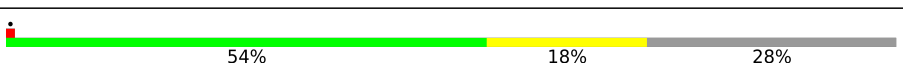
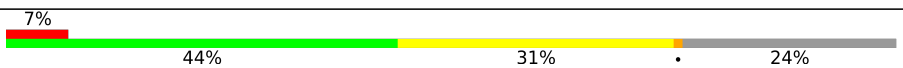
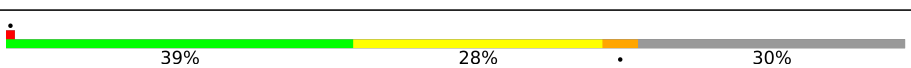
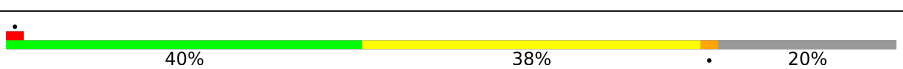
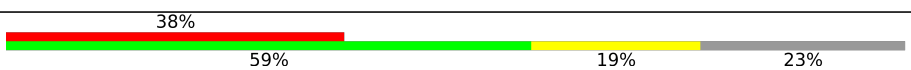
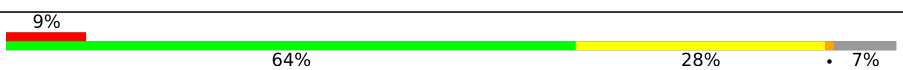
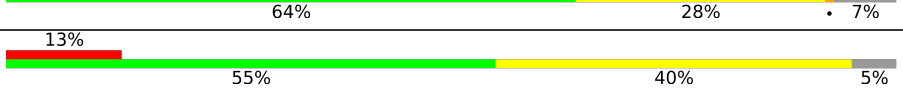
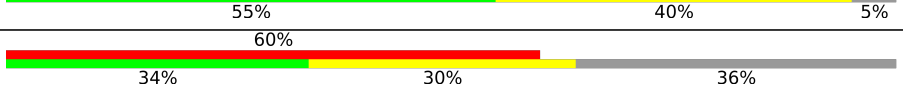
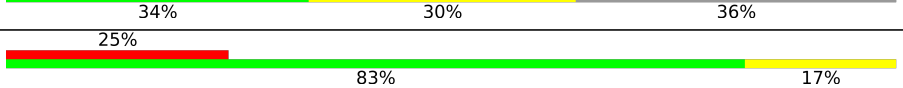
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	486	5% 48% 40% 12%
2	I	499	14% 54% 41%
3	J	119	32% 45% 36% 19%
4	N	205	20% 44% 29% 27%

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Mol	Chain	Length	Quality of chain
5	H	325	
6	K	100	
7	Y	106	
8	Z	143	
9	V	65	
10	W	65	
11	S	131	
12	i	81	
13	j	83	
14	G	394	
15	C	748	
16	T	402	
17	F	190	
18	B	255	
19	O	154	
20	P	110	
21	R	169	
22	U	159	
23	E	218	
24	D	222	
25	X	133	
26	c	106	
27	Q	97	
28	k	122	
29	r	24	

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Mol	Chain	Length	Quality of chain
30	n	113	8% 17% 6% 76%
31	o	252	21% 42% 38% 20%
32	p	275	34% 41% 38% 19%
32	q	275	34% 47% 33% 17%
33	M	495	37% 37% 59%
34	f	107	28% 37% 34% 29%
35	g	114	25% 24% 18% 59%
36	d	117	56% 53% 44%
37	a	669	80% 48% 41% 10%
38	b	103	56% 34% 27% 39%
39	h	69	39% 35% 6% 59%
40	e	126	67% 65% 33%
41	l	71	8% 31% 68%
42	s	20	80% 65% 35%
43	m	98	16% 36% 34% 30%
44	t	73	42% 33% 8% 58%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	A	501	-	-	X	-
45	SF4	D	301	-	-	X	-
45	SF4	E	301	-	-	X	-
47	T7X	I	501	X	-	-	-
48	CDL	I	502	-	-	X	-
48	CDL	I	503	-	-	X	-
48	CDL	J	401	-	-	X	-
49	U10	H	501	-	-	X	-
51	FES	B	301	-	-	X	-

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 57959 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 51kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	429	3328	2100	593	610	25	0	0

- Molecule 2 is a protein called Nad2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	I	481	3754	2525	569	633	27	0	0

- Molecule 3 is a protein called Nad3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	96	800	559	112	126	3	0	0

- Molecule 4 is a protein called Nad6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	N	149	1201	810	194	189	8	0	0

- Molecule 5 is a protein called Nad1m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	318	2493	1691	378	409	15	0	0

- Molecule 6 is a protein called Nad4Lm.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	K	85	667	450	101	110	6	0	0

- Molecule 7 is a protein called PGIV.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	98	Total	C	N	O	S	0	0
			774	484	133	145	12		

- Molecule 8 is a protein called B16.6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	140	Total	C	N	O	S	0	0
			1103	701	195	199	8		

- Molecule 9 is a protein called MWFE.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	57	Total	C	N	O	S	0	0
			461	296	82	78	5		

- Molecule 10 is a protein called B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	37	Total	C	N	O	S	0	0
			273	179	45	46	3		

- Molecule 11 is a protein called B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	101	Total	C	N	O	S	0	0
			821	513	143	161	4		

- Molecule 12 is a protein called B14.5b.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	i	66	Total	C	N	O	S	0	0
			514	331	91	87	5		

- Molecule 13 is a protein called 15kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	j	68	Total	C	N	O	S	0	0
			582	359	113	103	7		

- Molecule 14 is a protein called Nad7m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	382	Total	C	N	O	S	0	0
			3049	1939	535	551	24		

- Molecule 15 is a protein called 75kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	693	Total	C	N	O	S	0	0
			5288	3315	926	1008	39		

- Molecule 16 is a protein called 39kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	328	Total	C	N	O	S	0	0
			2535	1628	433	459	15		

- Molecule 17 is a protein called Nad9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	F	178	Total	C	N	O	S	0	0
			1518	979	262	272	5		

- Molecule 18 is a protein called 24kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B	219	Total	C	N	O	S	0	0
			1702	1081	286	323	12		

- Molecule 19 is a protein called 18kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	111	Total	C	N	O	S	0	0
			874	561	150	162	1		

- Molecule 20 is a protein called 13kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	71	Total	C	N	O	S	0	0
			554	348	97	103	6		

- Molecule 21 is a protein called B13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	129	Total	C	N	O	S	0	0
			1039	656	174	204	5		

- Molecule 22 is a protein called B17.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	122	Total	C	N	O	S	0	0
			1011	643	184	183	1		

- Molecule 23 is a protein called PSST.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	E	153	Total	C	N	O	S	0	0
			1215	779	212	210	14		

- Molecule 24 is a protein called TYKY.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	D	177	Total	C	N	O	S	0	0
			1438	901	239	287	11		

- Molecule 25 is a protein called B14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	103	Total	C	N	O	S	0	0
			843	537	151	152	3		

- Molecule 26 is a protein called 20.9kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	99	Total	C	N	O	S	0	0
			744	479	121	140	4		

- Molecule 27 is a protein called B8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Q	92	Total	C	N	O	S	0	0
			722	456	128	132	6		

- Molecule 28 is a protein called ACPM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	k	78	Total	C	N	O	S	0	0
			614	390	94	127	3		

- Molecule 29 is a protein called Unk1.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	r	24	Total	C	N	O	0	0
			120	72	24	24		

- Molecule 30 is a protein called P2.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	n	27	Total	C	N	O	0	0
			205	133	35	37		

- Molecule 31 is a protein called CAL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	o	202	Total	C	N	O	S	0	0
			1568	1006	270	287	5		

- Molecule 32 is a protein called CA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	q	228	Total	C	N	O	S	0	0
			1736	1088	318	324	6		
32	p	224	Total	C	N	O	S	0	0
			1705	1068	311	320	6		

- Molecule 33 is a protein called Nad4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	M	482	Total	C	N	O	S	0	0
			3825	2579	593	630	23		

- Molecule 34 is a protein called PDSW.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	76	Total	C	N	O	S	0	0
			640	407	116	113	4		

- Molecule 35 is a protein called ESSS.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	47	Total	C	N	O	S	0	0
			386	253	60	71	2		

- Molecule 36 is a protein called B22.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	d	66	Total	C	N	O	0	0
			329	197	66	66		

- Molecule 37 is a protein called Nad5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	a	600	Total	C	N	O	S	0	0
			4677	3106	725	813	33		

- Molecule 38 is a protein called B18.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	b	63	Total	C	N	O	S	0	0
			519	327	89	94	9		

- Molecule 39 is a protein called AGGG.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	28	Total	C	N	O	S	0	0
			232	155	40	35	2		

- Molecule 40 is a protein called ACPM2.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	e	84	Total	C	N	O	0	0
			417	249	84	84		

- Molecule 41 is a protein called B15.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	l	23	Total	C	N	O	0	0
			112	66	23	23		

- Molecule 42 is a protein called Unk2.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	s	20	Total	C	N	O	0	0
			100	60	20	20		

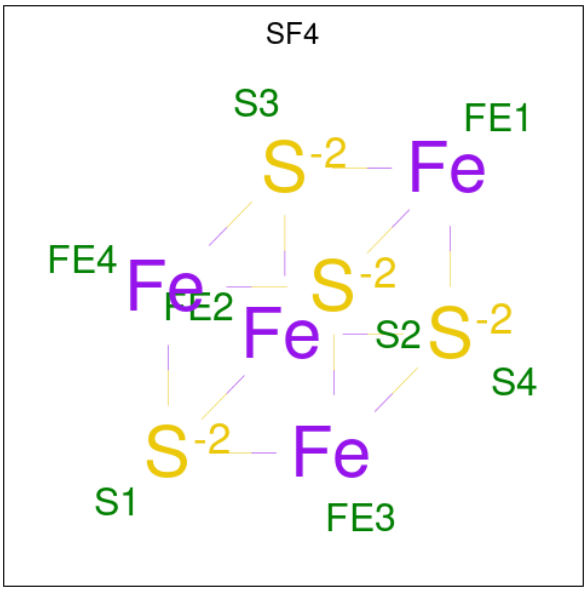
- Molecule 43 is a protein called P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	69	Total	C	N	O	S	0	0
			605	385	112	103	5		

- Molecule 44 is a protein called B12-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	31	Total	C	N	O	S	0	0
			232	149	42	38	3		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



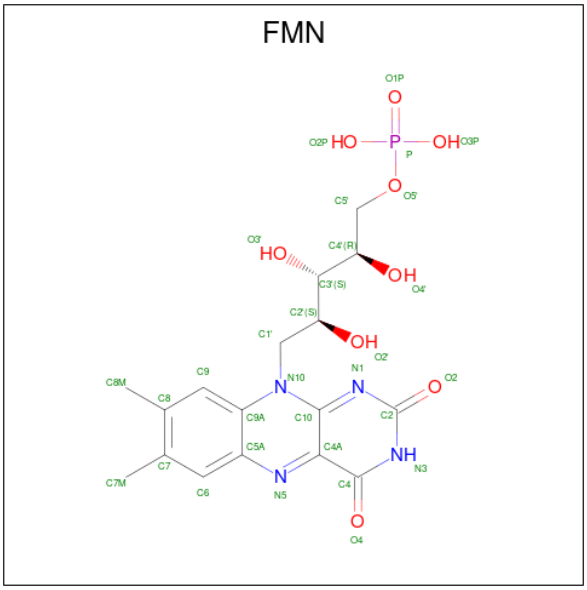
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	E	1	Total	Fe	S	0
			8	4	4	

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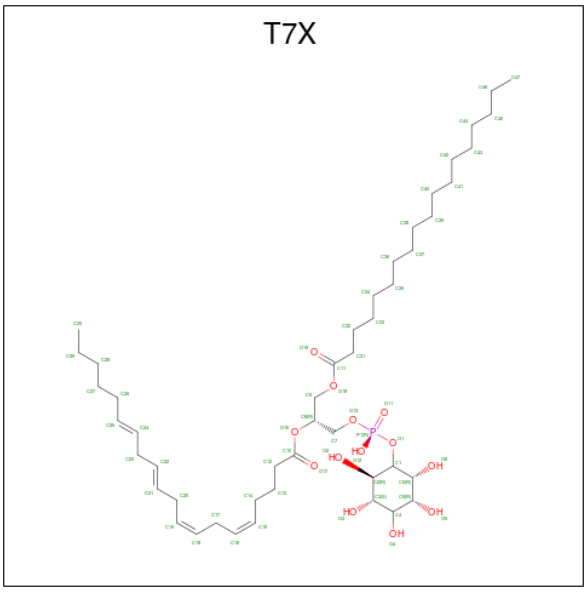
Mol	Chain	Residues	Atoms	AltConf
45	D	1	Total Fe S 8 4 4	0
45	D	1	Total Fe S 8 4 4	0

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



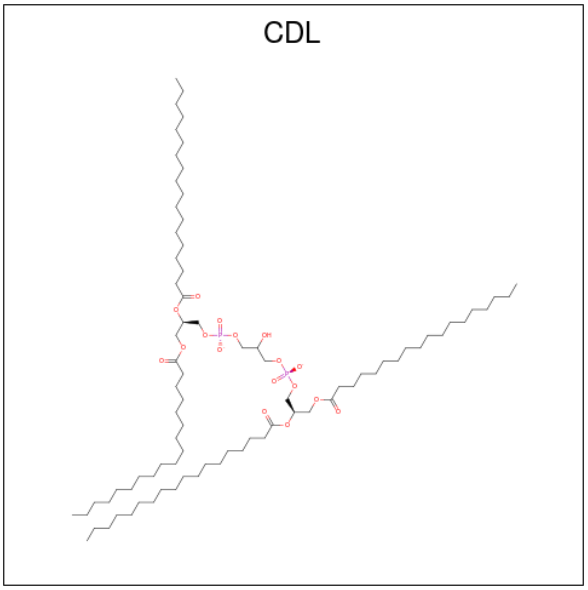
Mol	Chain	Residues	Atoms	AltConf
46	A	1	Total C N O P 31 17 4 9 1	0

- Molecule 47 is Phosphatidylinositol (CCD ID: T7X) (formula: $C_{47}H_{83}O_{13}P$).



Mol	Chain	Residues	Atoms				AltConf
47	I	1	Total 54	C 40	O 13	P 1	0
47	p	1	Total 61	C 47	O 13	P 1	0

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



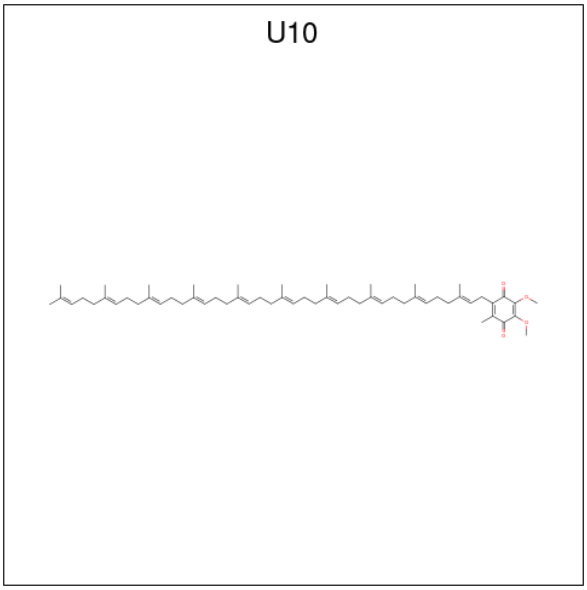
Mol	Chain	Residues	Atoms				AltConf
48	I	1	Total 100	C 81	O 17	P 2	0
48	I	1	Total 98	C 79	O 17	P 2	0

Continued on next page...

Continued from previous page...

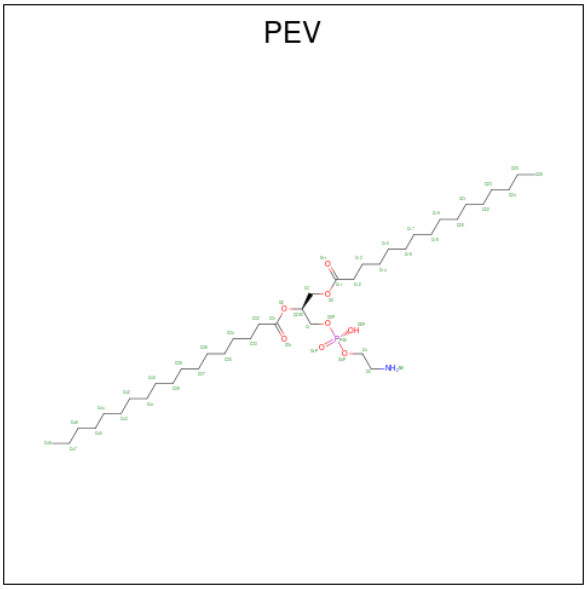
Mol	Chain	Residues	Atoms				AltConf
48	J	1	Total	C	O	P	0
			87	68	17	2	

- Molecule 49 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



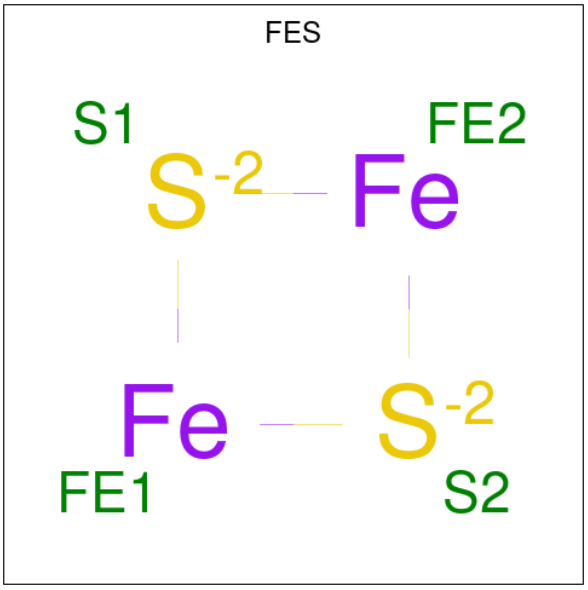
Mol	Chain	Residues	Atoms			AltConf
49	H	1	Total	C	O	0
			44	40	4	

- Molecule 50 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PEV) (formula: $C_{39}H_{78}NO_8P$).



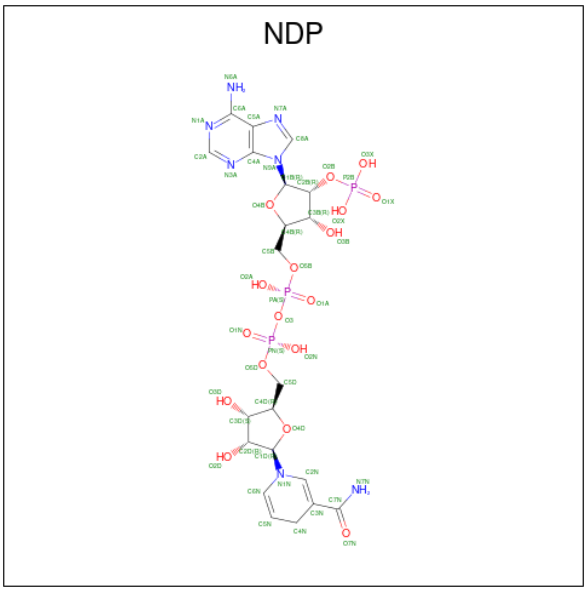
Mol	Chain	Residues	Atoms					AltConf
50	H	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 51 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms				AltConf
51	C	1	Total	Fe	S		0
			4	2	2		
51	B	1	Total	Fe	S		0
			4	2	2		

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

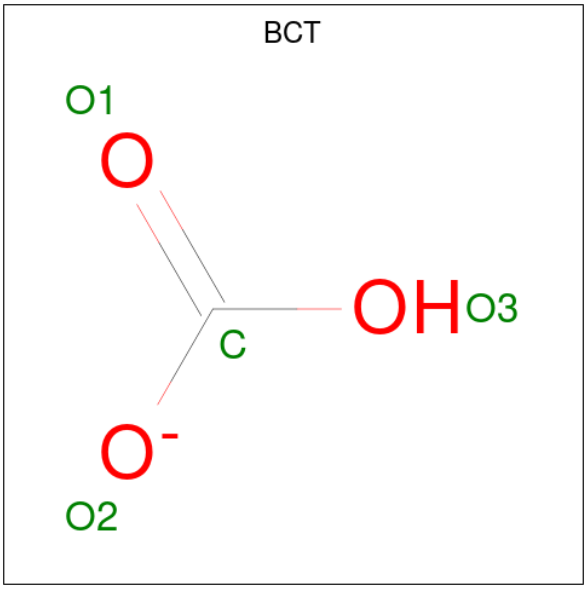


Mol	Chain	Residues	Atoms					AltConf
52	T	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	P	1	Total	Zn	0
			1	1	
53	q	1	Total	Zn	0
			1	1	

- Molecule 54 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
54	q	1	4	1	3	0

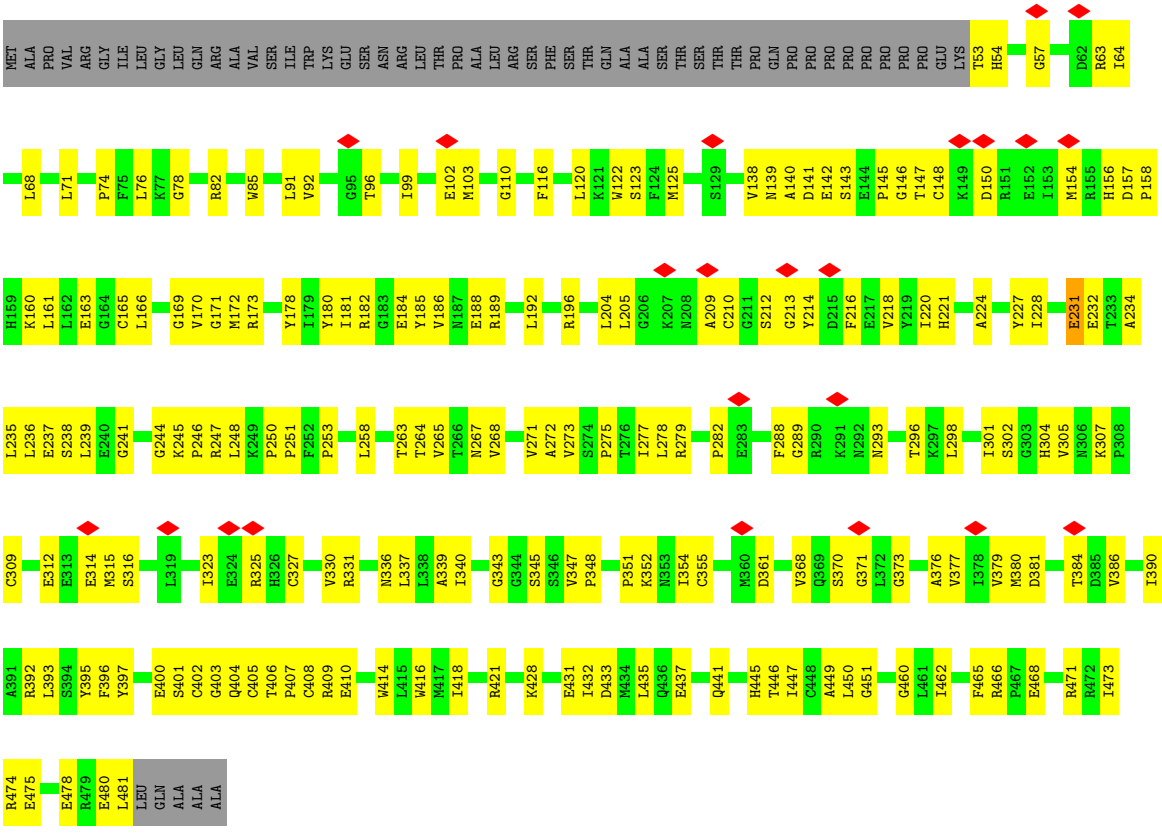
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: 51kDa

Chain A:

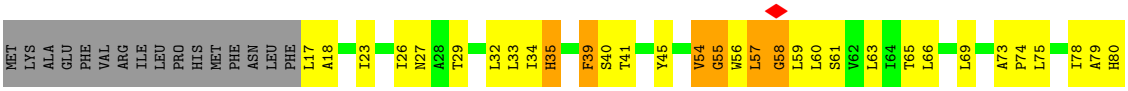


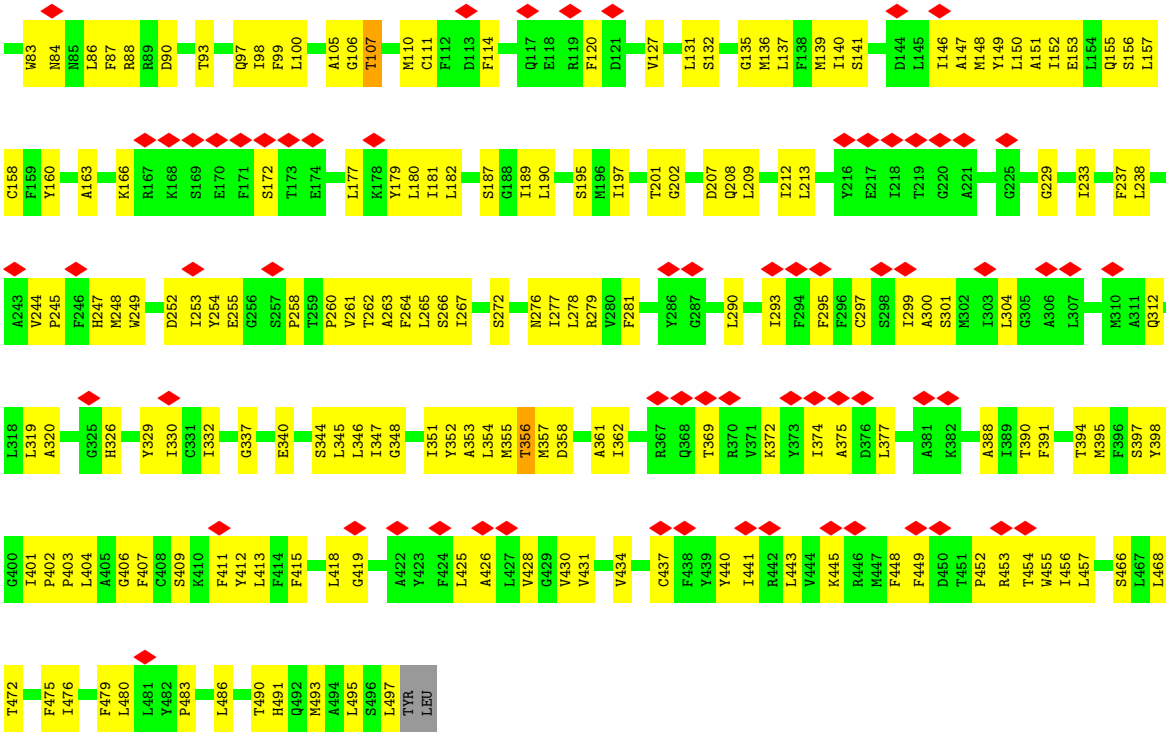


- Molecule 2: Nad2m

Chain I:



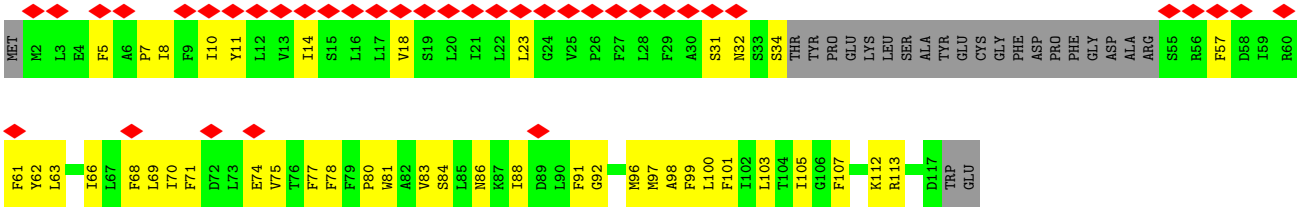




• Molecule 3: Nad3m

Chain J:

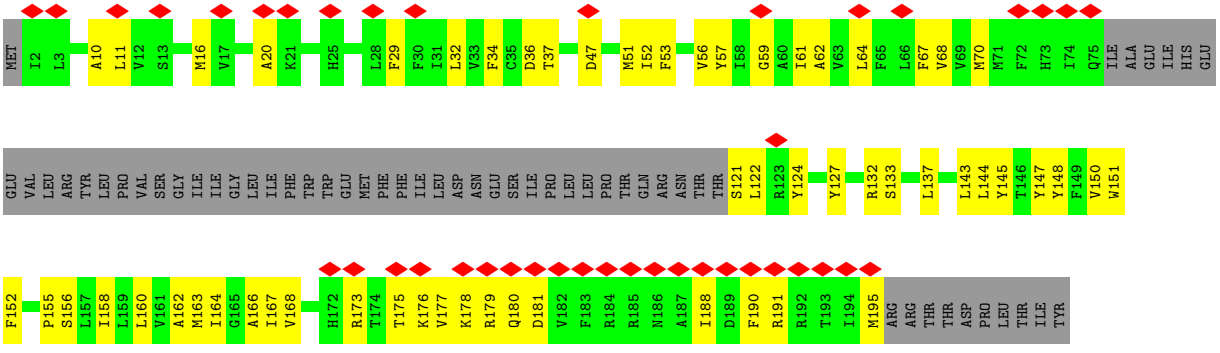




• Molecule 4: Nad6m

Chain N:

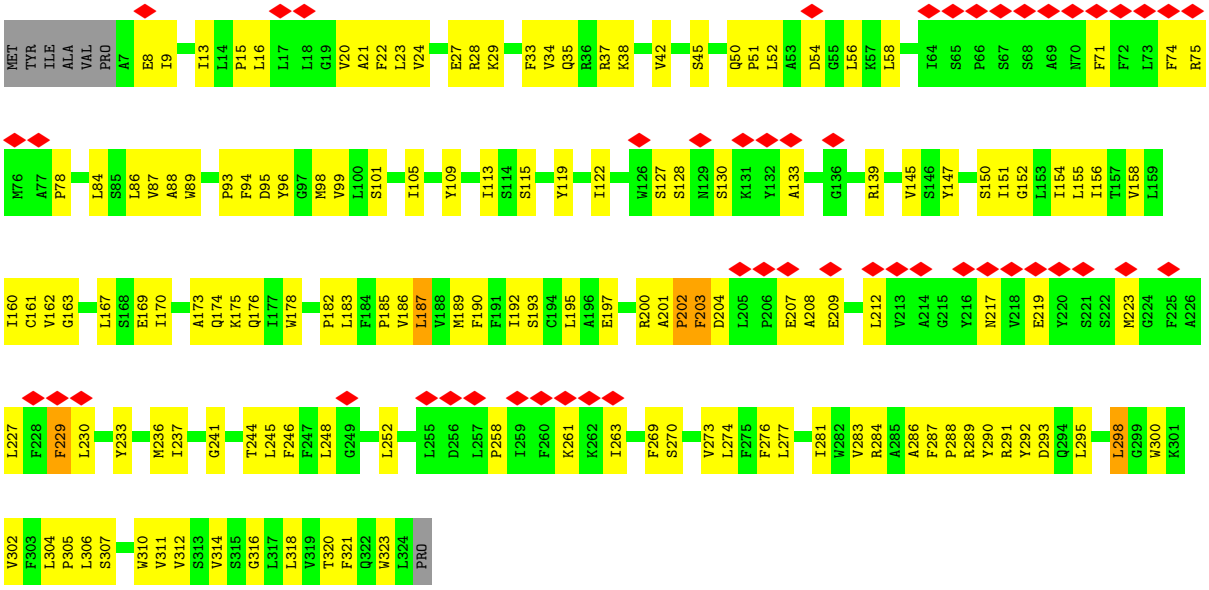




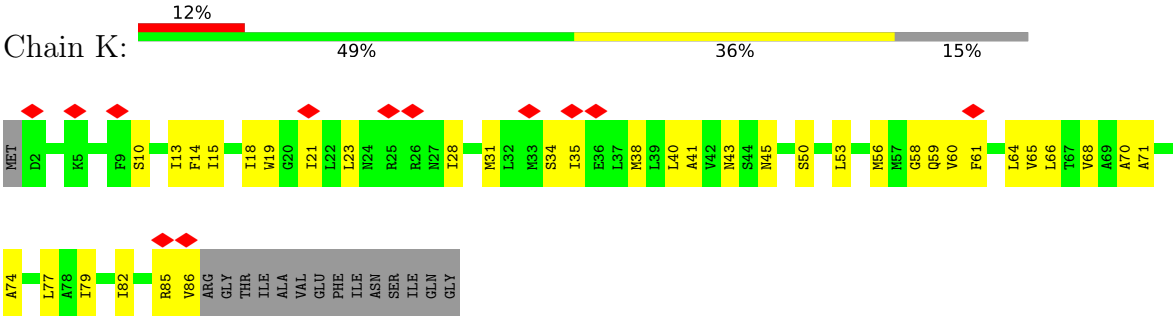
• Molecule 5: Nad1m

Chain H:

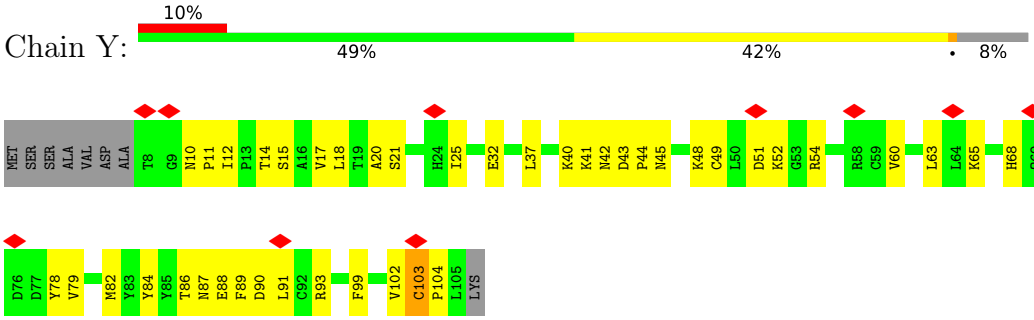




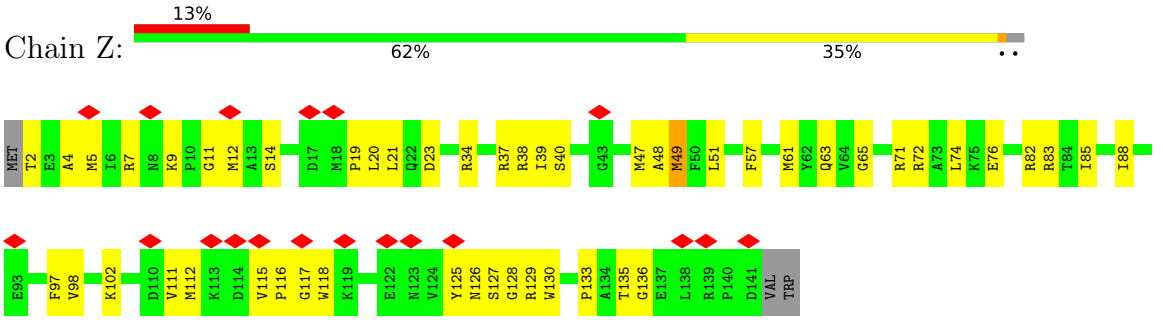
• Molecule 6: Nad4Lm



• Molecule 7: PGIV

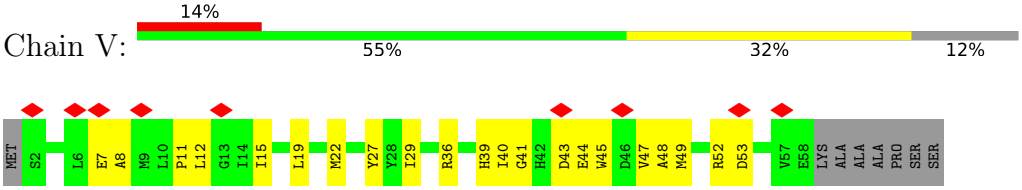


• Molecule 8: B16.6



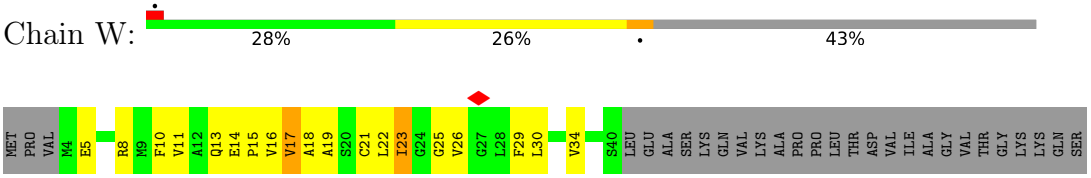
• Molecule 9: MWFE

Chain V:



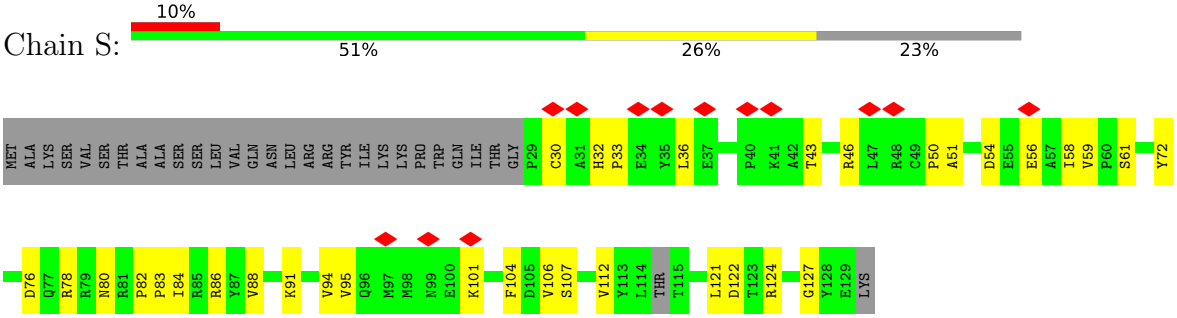
• Molecule 10: B9

Chain W:



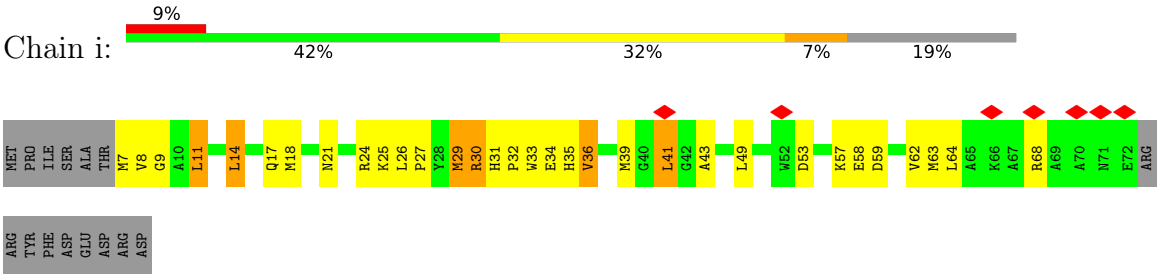
• Molecule 11: B14.5a

Chain S:



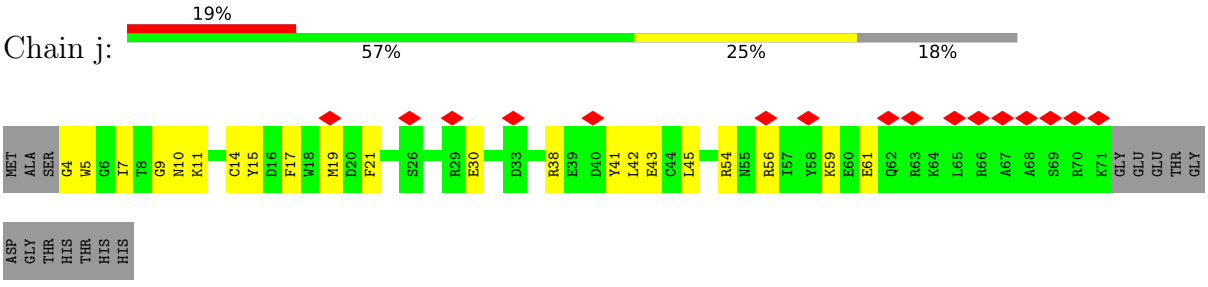
• Molecule 12: B14.5b

Chain i:



• Molecule 13: 15kDa

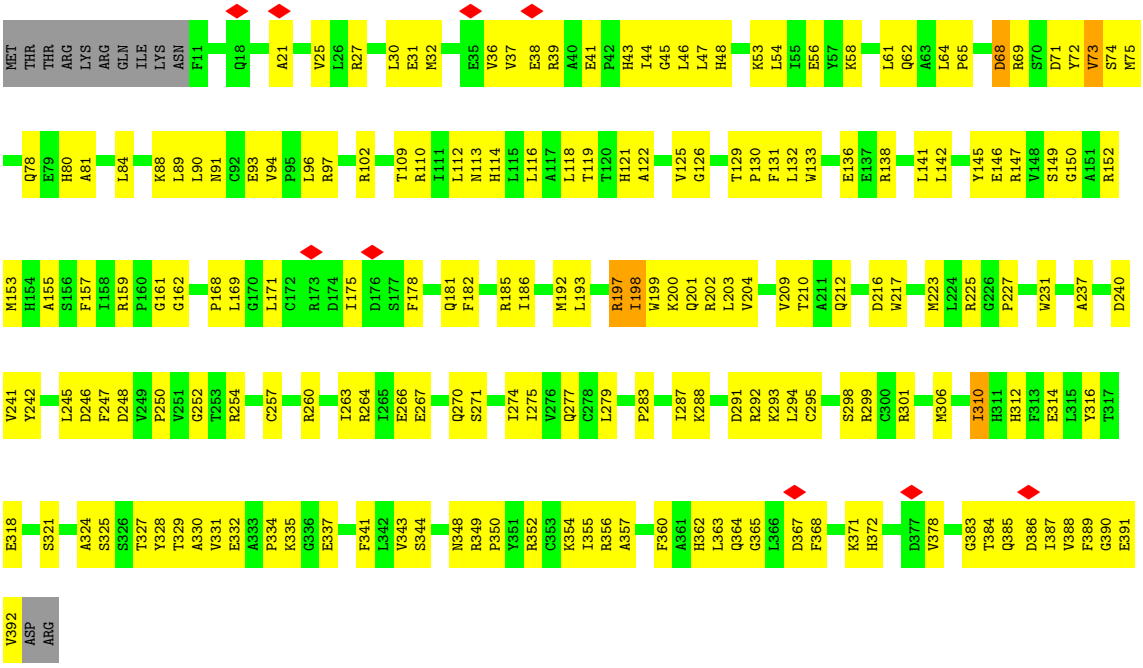
Chain j:



• Molecule 14: Nad7m

Chain G:

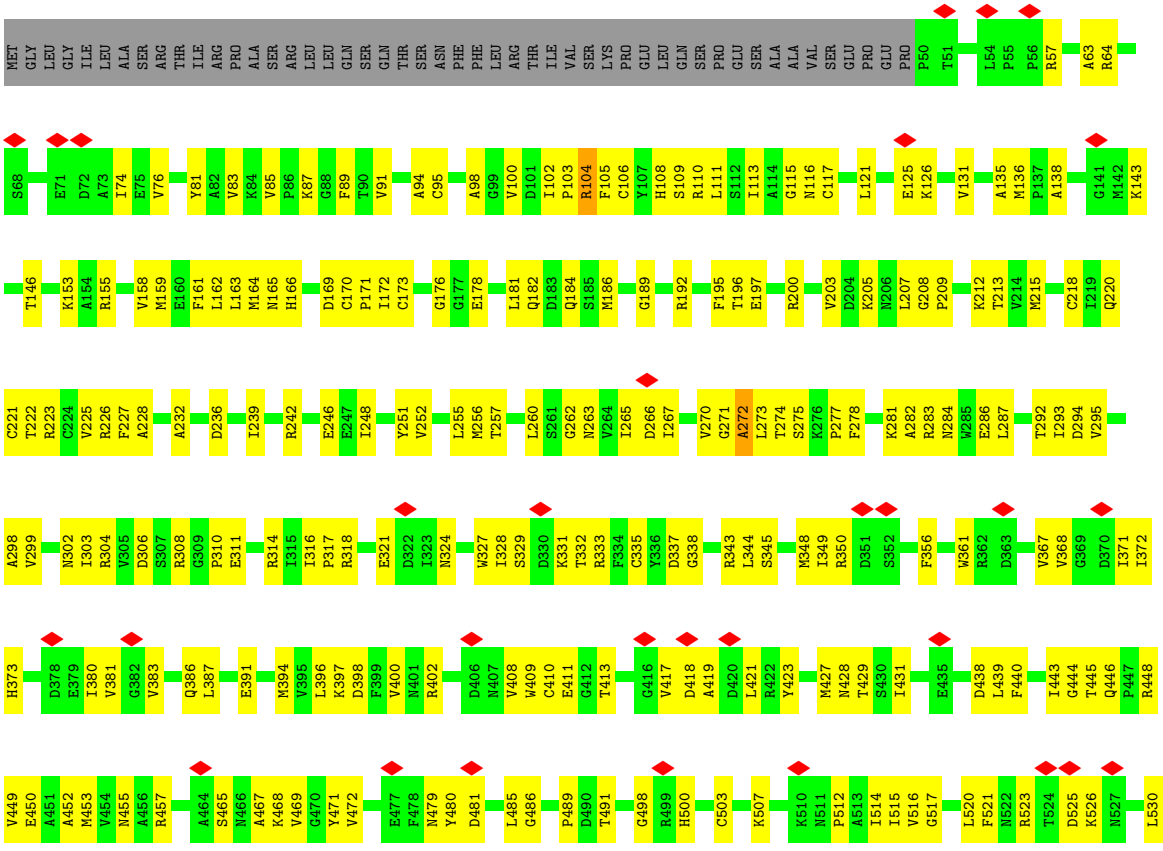


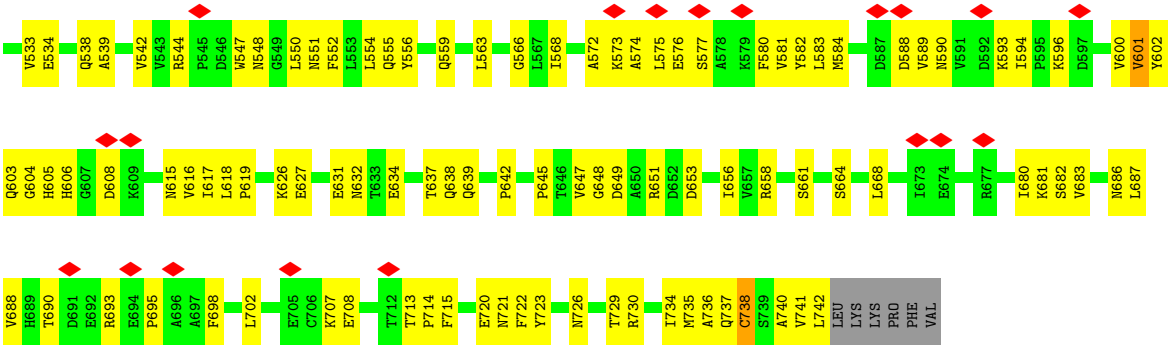


• Molecule 15: 75kDa

Chain C:



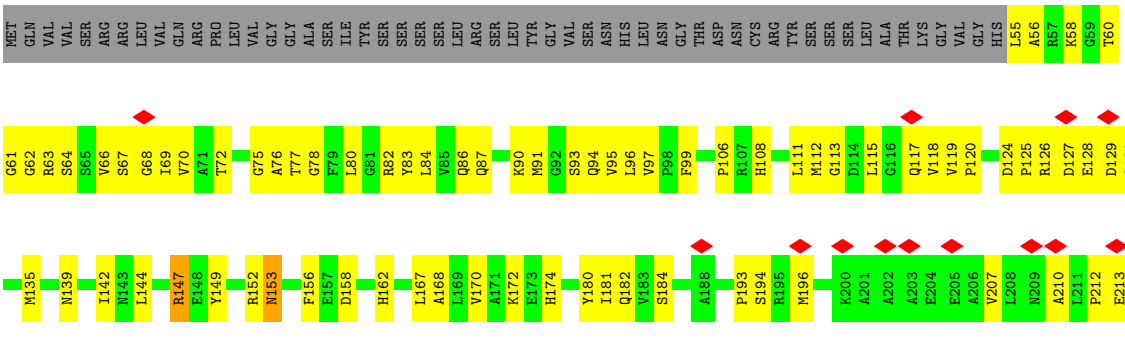




• Molecule 16: 39kDa

Chain T:

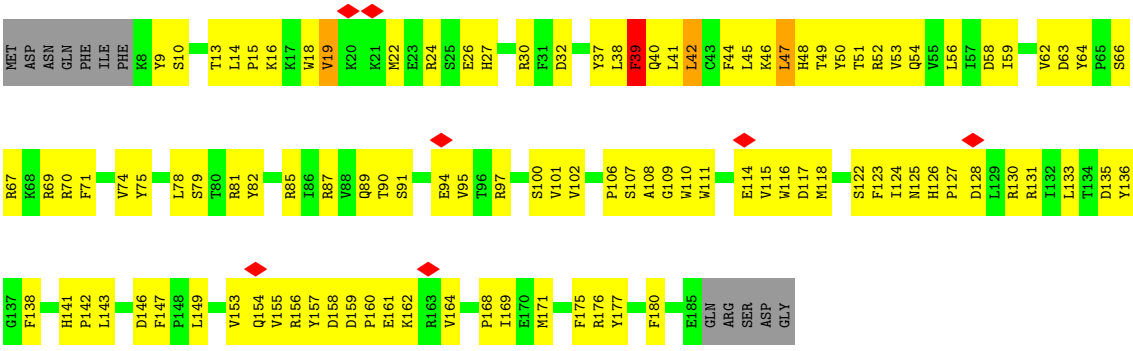




• Molecule 17: Nad9m

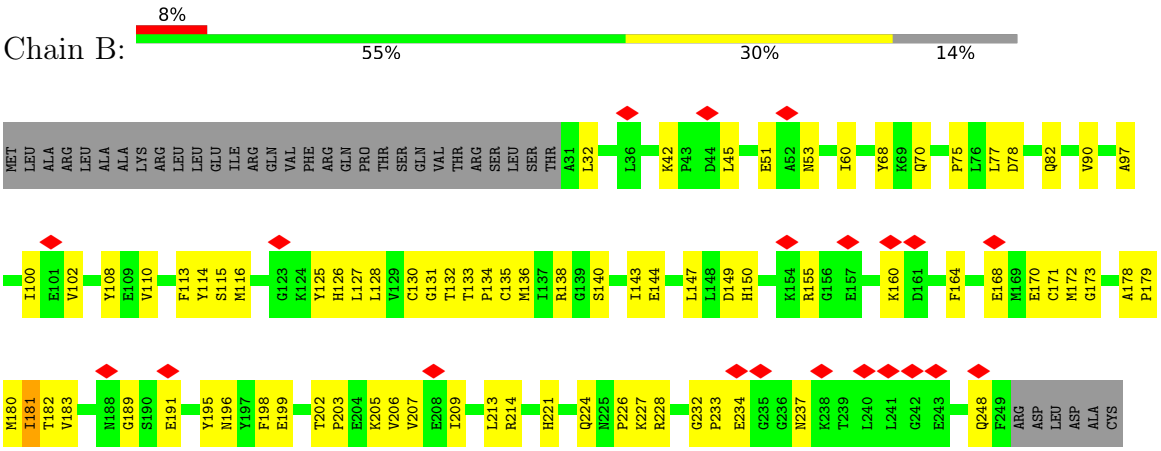
Chain F:





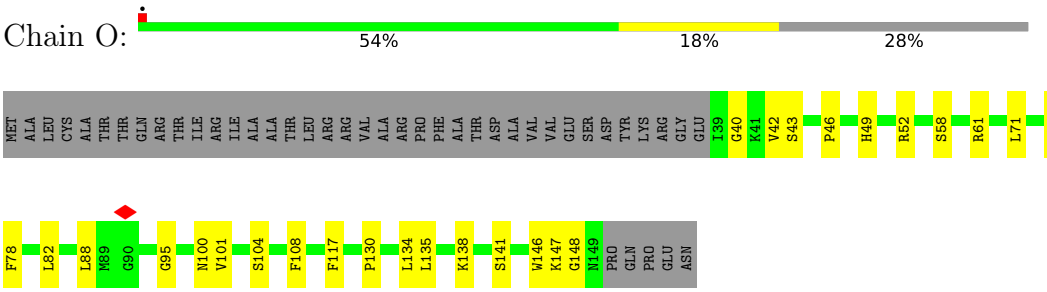
- Molecule 18: 24kDa

Chain B:



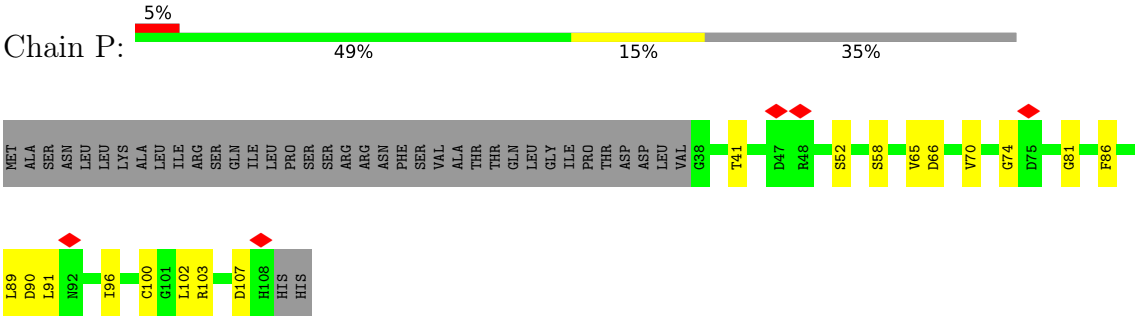
- Molecule 19: 18kDa

Chain O:



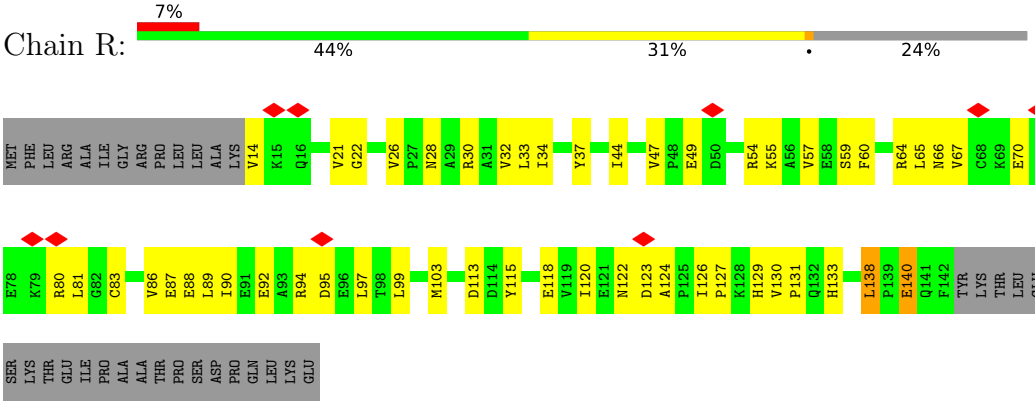
- Molecule 20: 13kDa

Chain P:



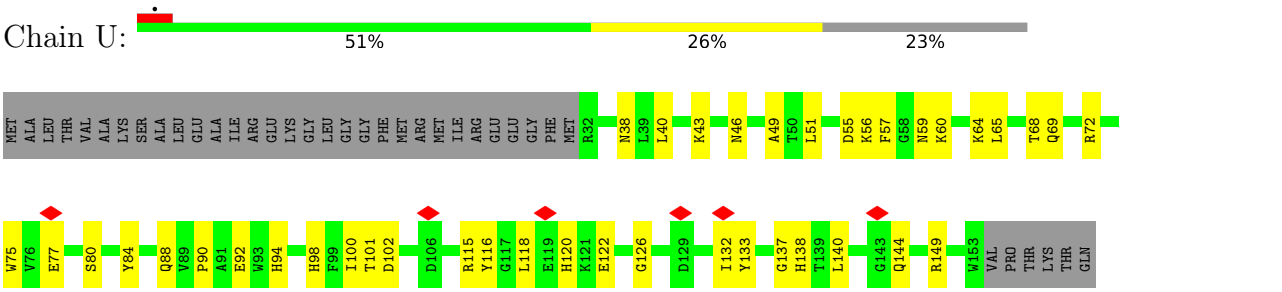
- Molecule 21: B13

Chain R:



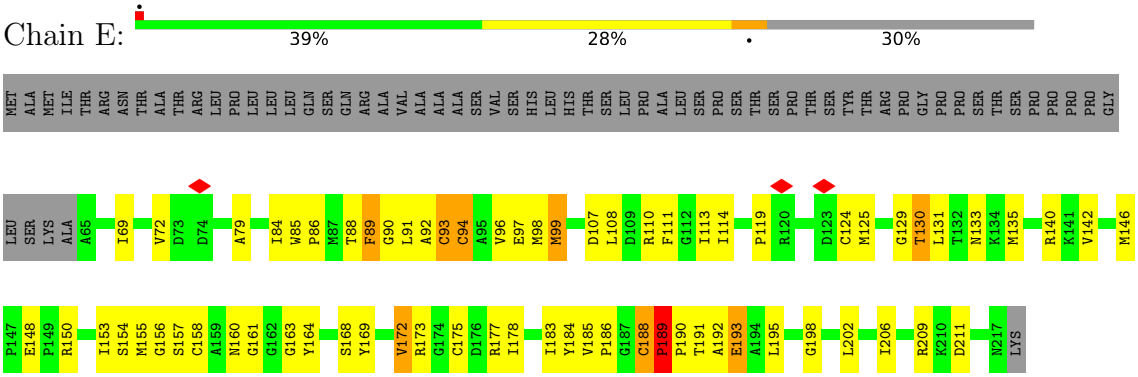
- Molecule 22: B17.2

Chain U:



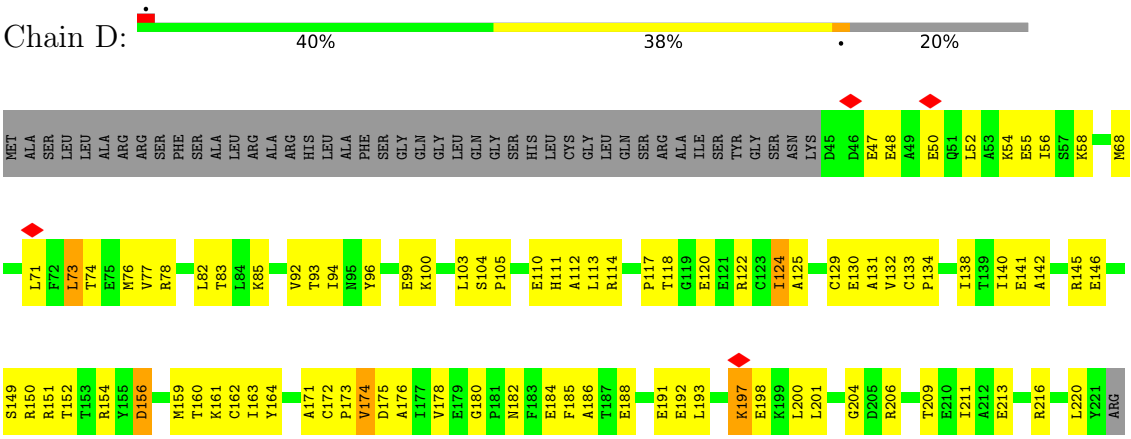
• Molecule 23: PSST

Chain E:



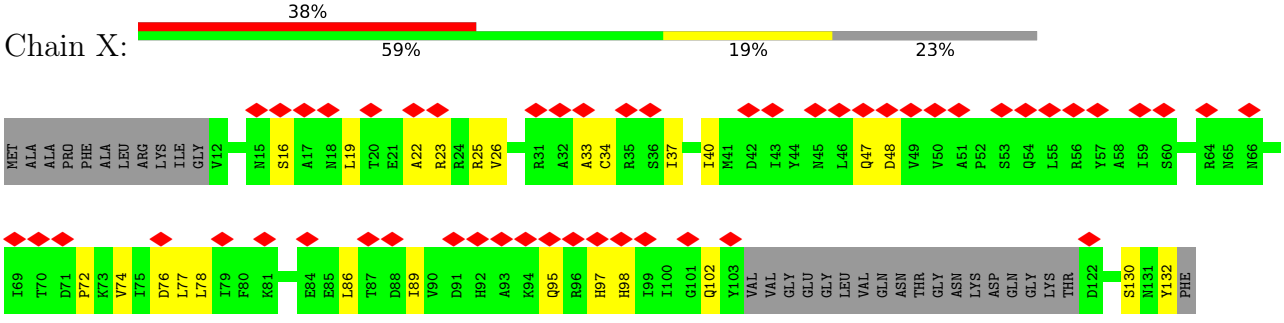
• Molecule 24: TYKY

Chain D:



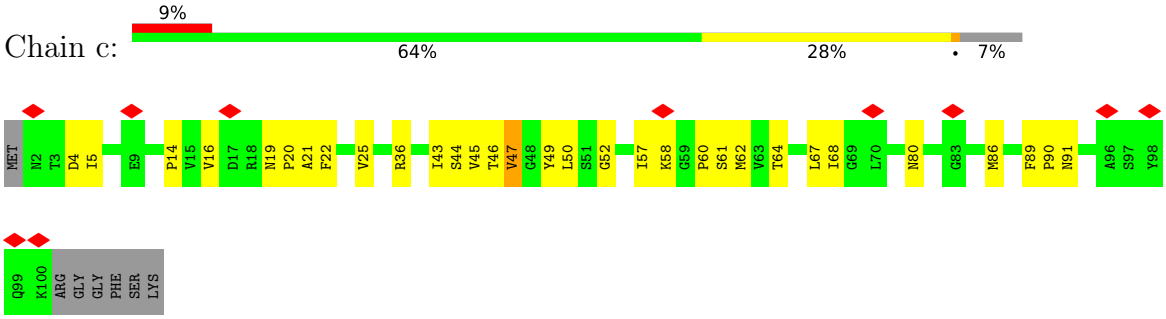
• Molecule 25: B14

Chain X:



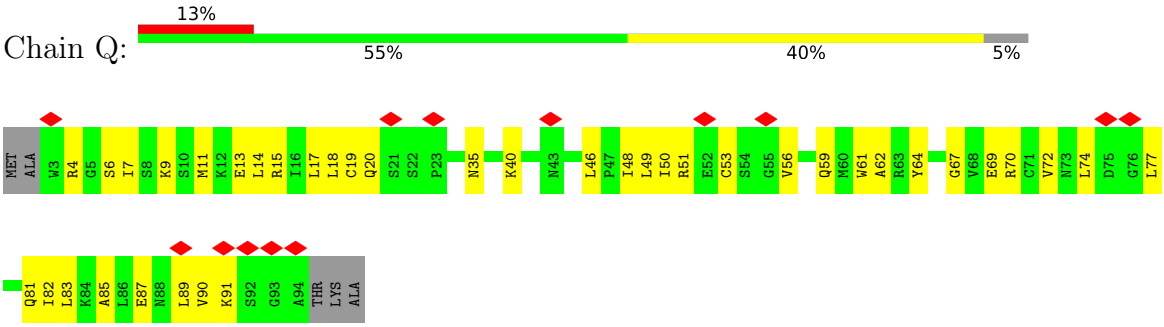
• Molecule 26: 20.9kDa

Chain c:



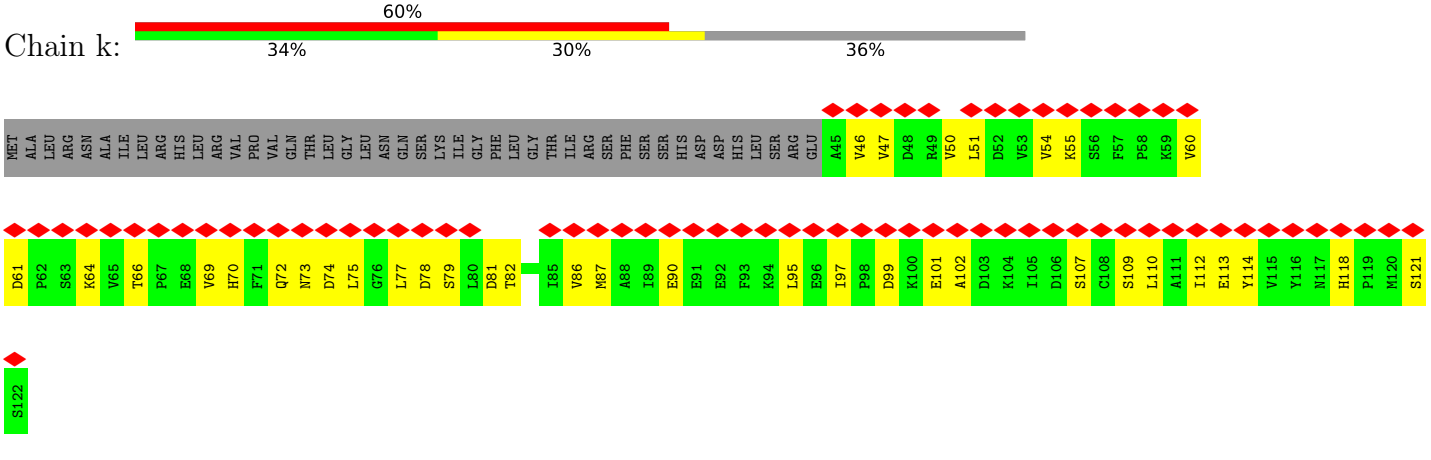
• Molecule 27: B8

Chain Q:



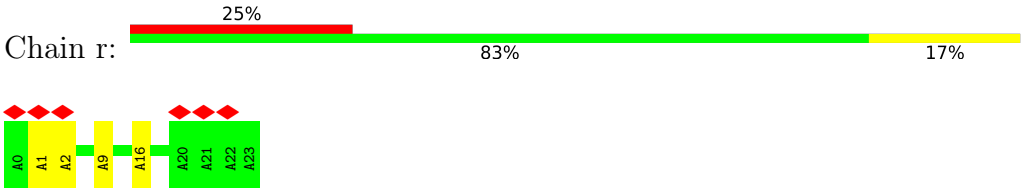
• Molecule 28: ACPM1

Chain k:



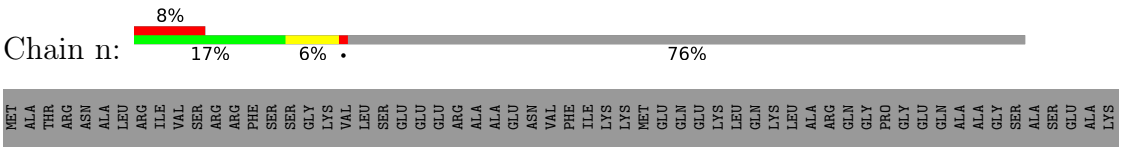
• Molecule 29: Unk1

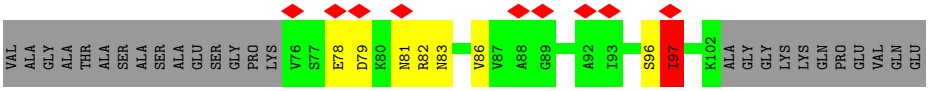
Chain r:



• Molecule 30: P2

Chain n:

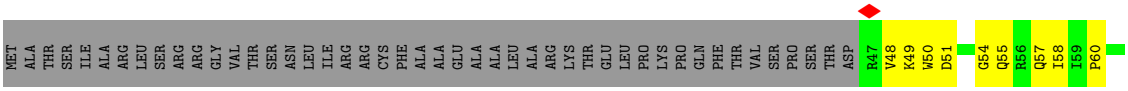


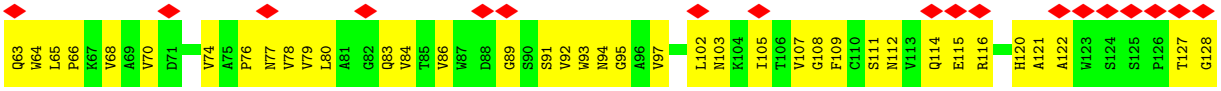


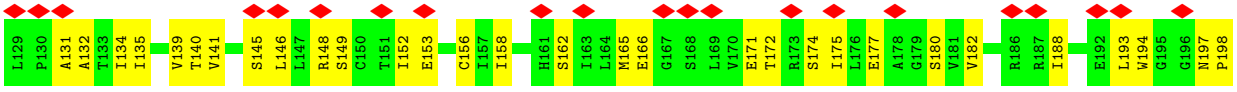
• Molecule 31: CAL1

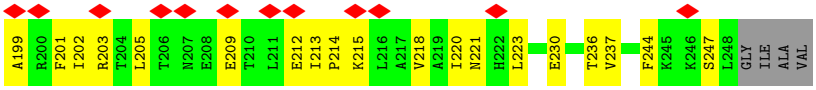
Chain o:









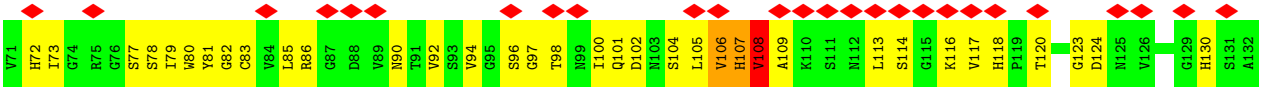


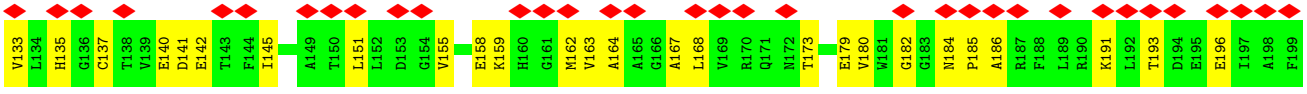
• Molecule 32: CA1

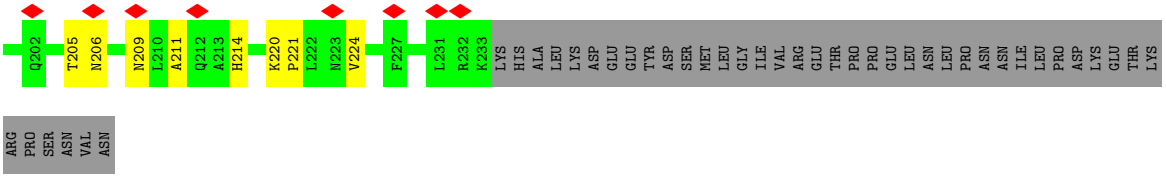
Chain q:







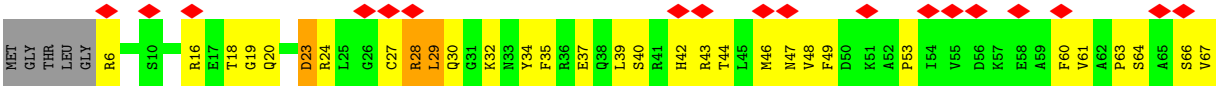


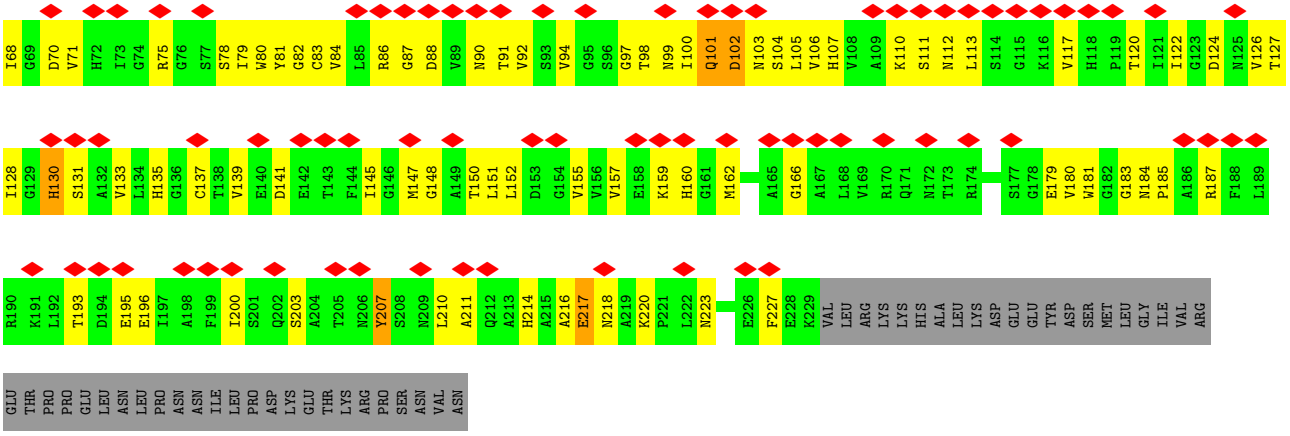


• Molecule 32: CA1

Chain p:



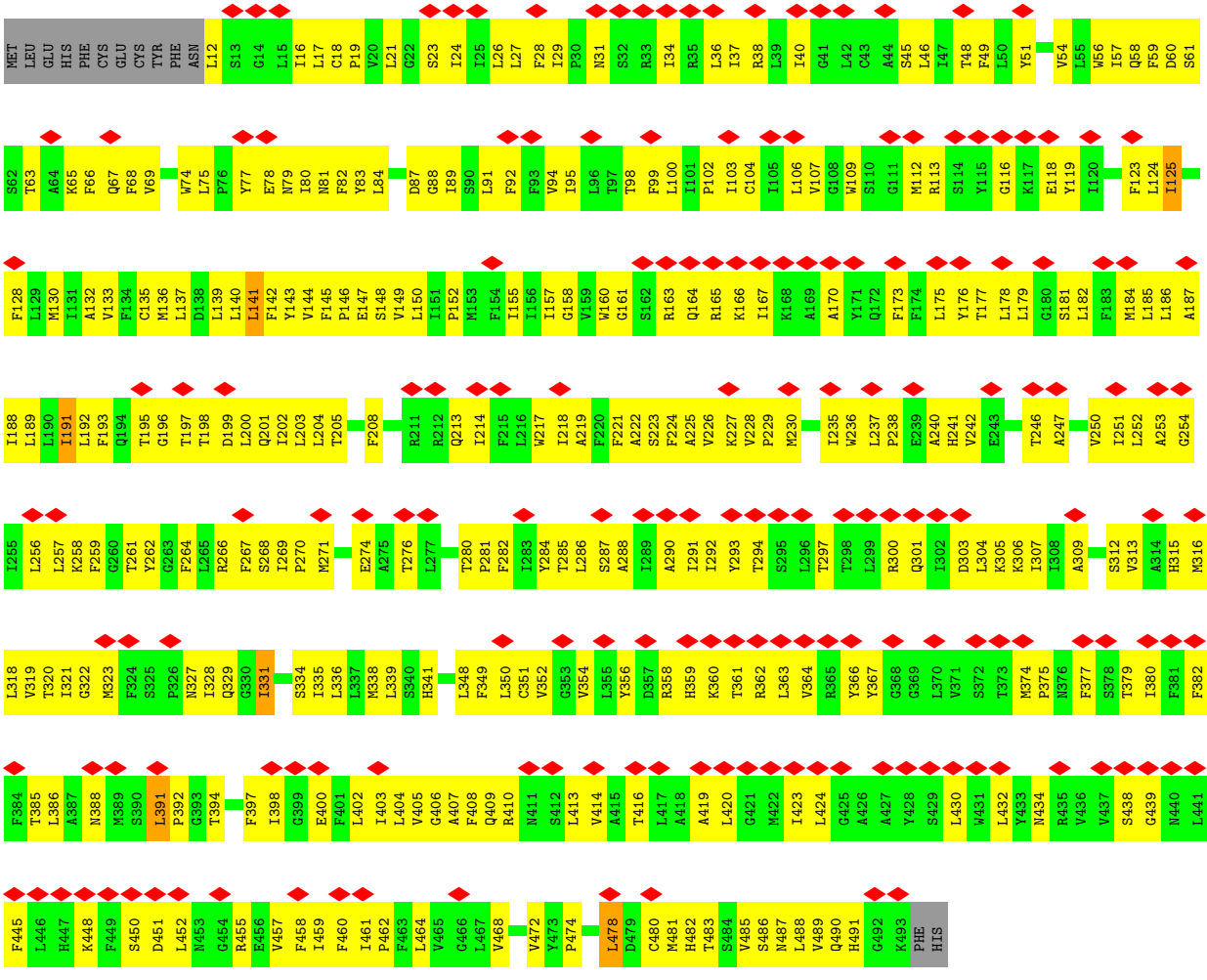




• Molecule 33: Nad4m

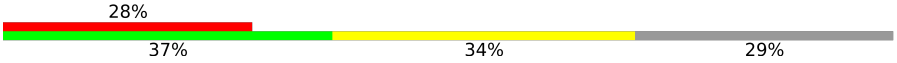
Chain M:

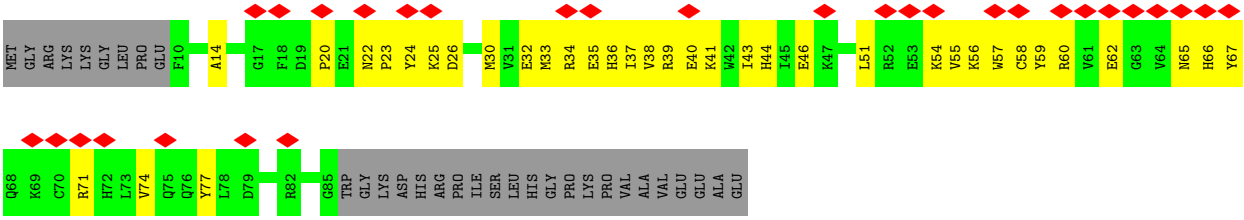




• Molecule 34: PDSW

Chain f:

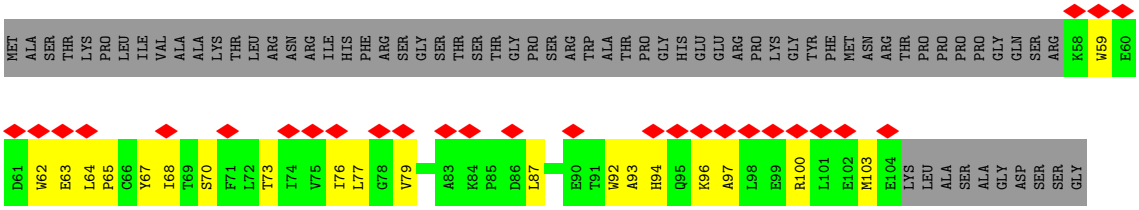




• Molecule 35: ESSS

Chain g:

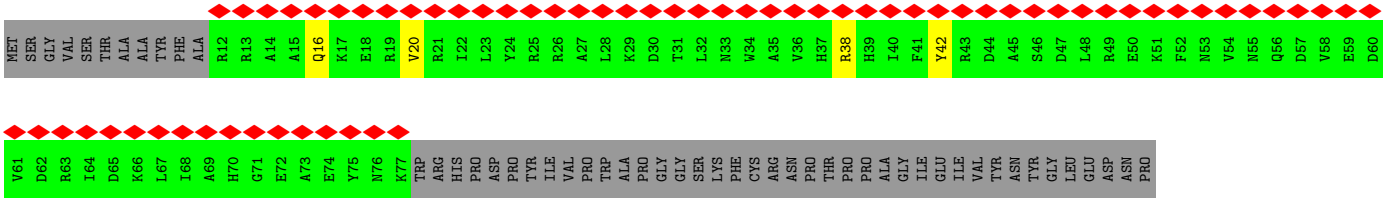




• Molecule 36: B22

Chain d:

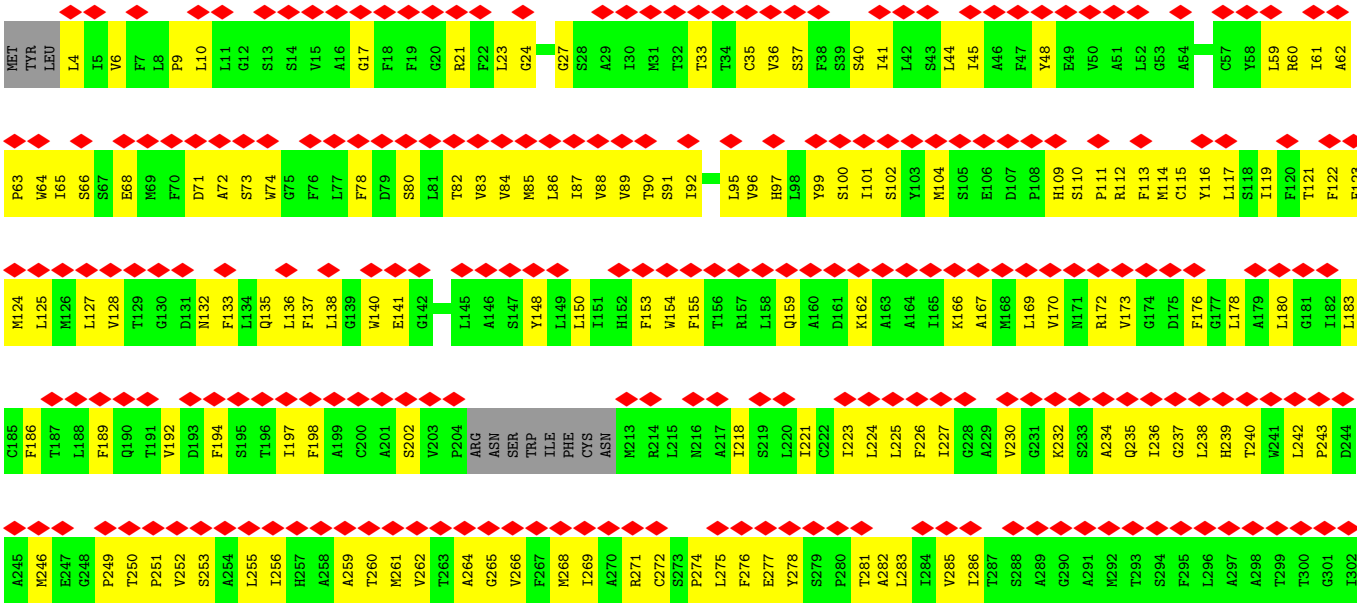


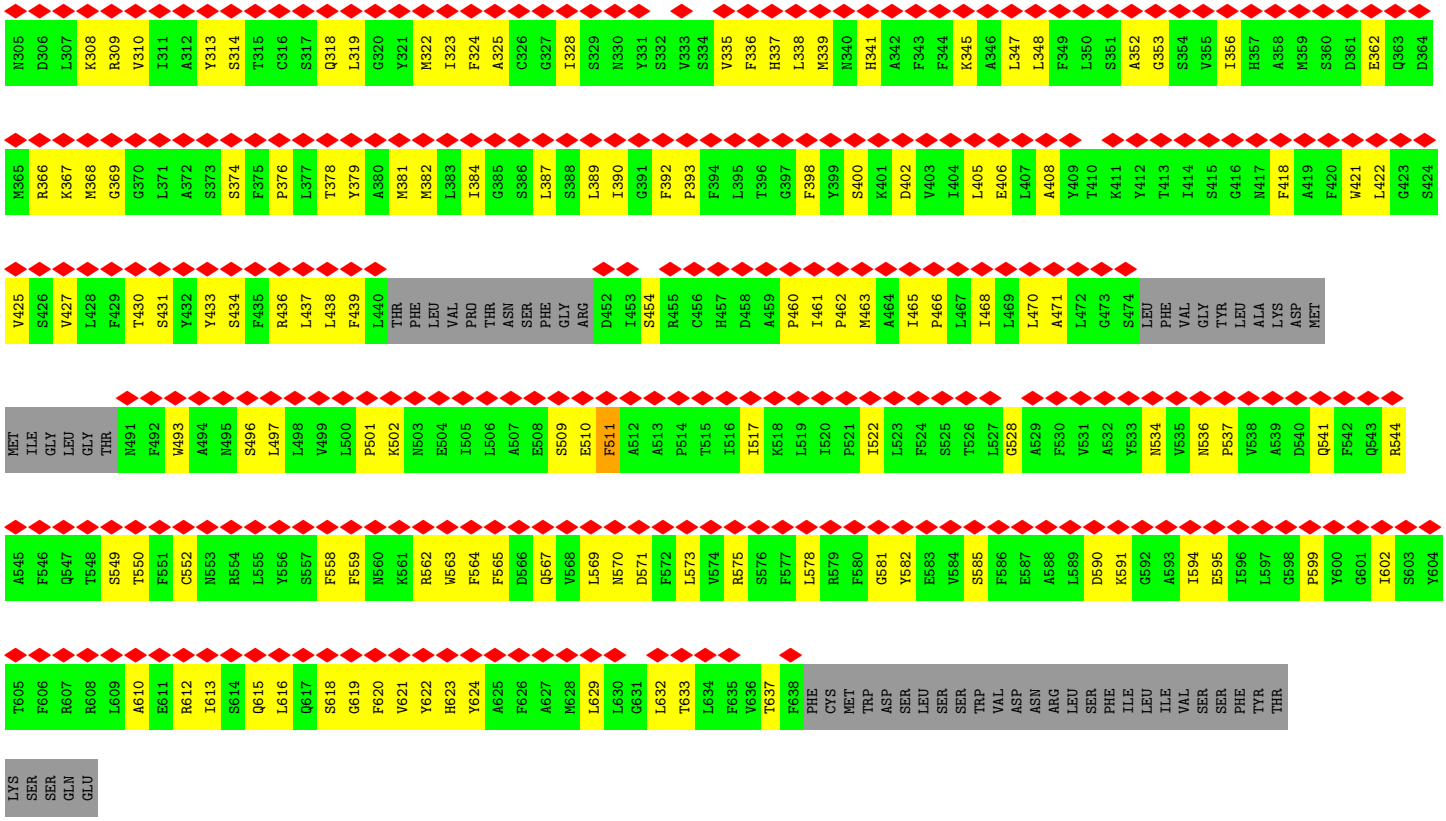


• Molecule 37: Nad5m

Chain a:

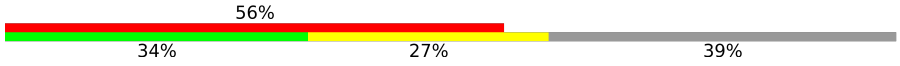


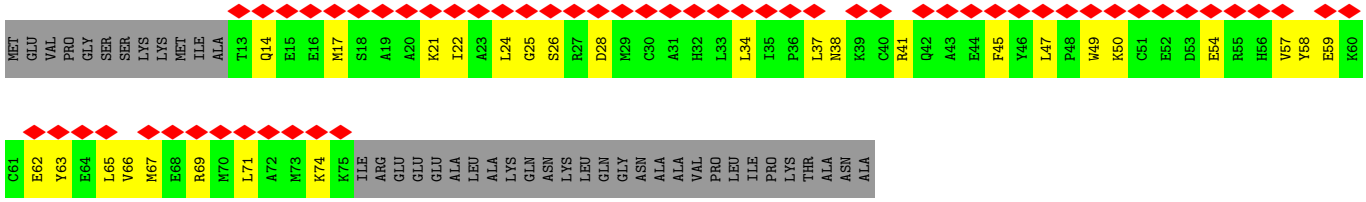




• Molecule 38: B18

Chain b:

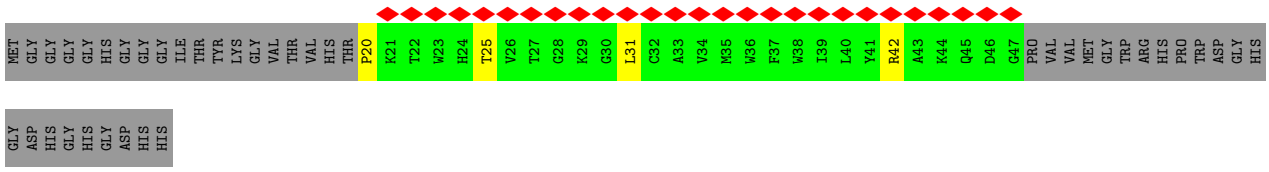




• Molecule 39: AGGG

Chain h:

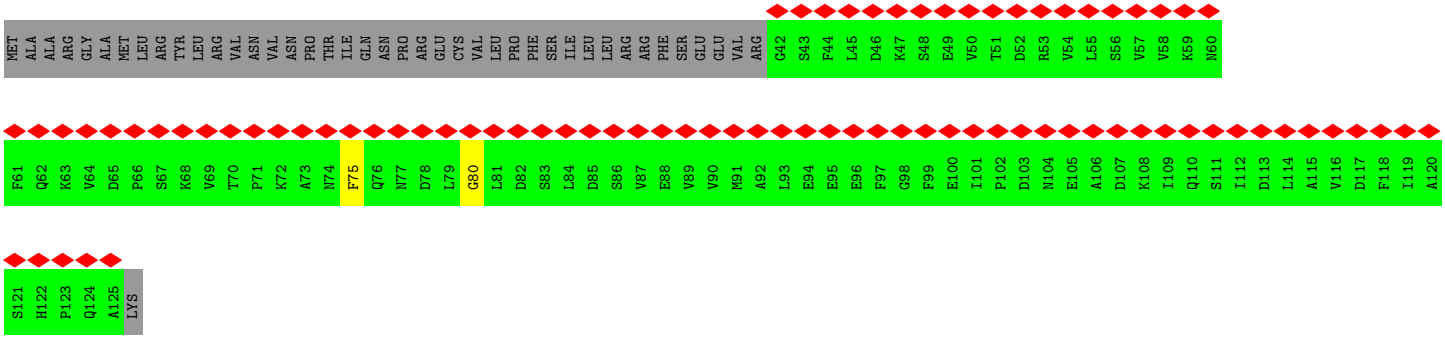




• Molecule 40: ACPM2

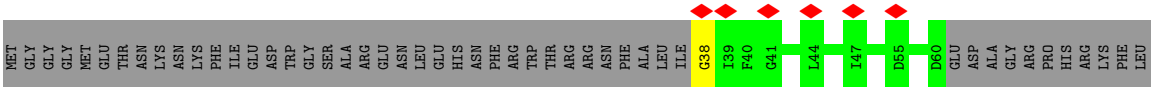
Chain e:



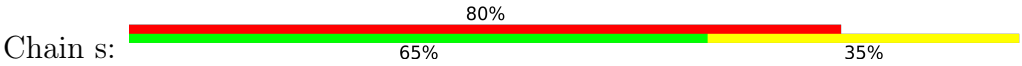


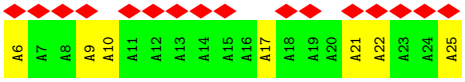
• Molecule 41: B15





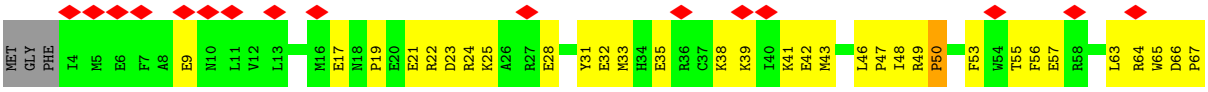
• Molecule 42: Unk2





• Molecule 43: P1





• Molecule 44: B12-1





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65018	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.257	Depositor
Minimum map value	-0.079	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0235	Depositor
Map size (Å)	399.6, 399.6, 399.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, FES, NDP, T7X, CDL, BCT, U10, PEV, ZN, FMN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.40	0/3401	0.59	0/4588
2	I	0.46	0/3855	0.76	10/5234 (0.2%)
3	J	0.31	0/826	0.41	0/1120
4	N	0.29	0/1227	0.44	0/1664
5	H	0.57	2/2565 (0.1%)	0.81	9/3492 (0.3%)
6	K	0.40	0/677	0.55	0/916
7	Y	0.40	0/788	0.59	0/1059
8	Z	0.34	0/1132	0.62	1/1530 (0.1%)
9	V	0.26	0/473	0.39	0/636
10	W	0.70	0/277	0.99	2/375 (0.5%)
11	S	0.25	0/840	0.47	0/1141
12	i	0.62	0/524	1.12	4/706 (0.6%)
13	j	0.23	0/595	0.45	0/791
14	G	0.52	0/3120	0.69	2/4221 (0.0%)
15	C	0.48	0/5386	0.69	5/7299 (0.1%)
16	T	0.44	0/2591	0.63	0/3509
17	F	0.47	0/1564	0.71	2/2120 (0.1%)
18	B	0.31	0/1743	0.48	0/2364
19	O	0.41	0/899	0.46	0/1215
20	P	0.46	0/567	0.64	0/768
21	R	0.56	0/1061	0.93	1/1441 (0.1%)
22	U	0.40	0/1044	0.52	0/1413
23	E	0.61	0/1250	0.96	4/1697 (0.2%)
24	D	0.70	0/1467	1.01	3/1981 (0.2%)
25	X	0.19	0/861	0.35	0/1166
26	c	0.48	1/760 (0.1%)	0.64	1/1028 (0.1%)
27	Q	0.23	0/734	0.37	0/989
28	k	0.13	0/625	0.33	0/848
29	r	0.16	0/119	0.31	0/165
30	n	0.49	0/208	0.92	1/282 (0.4%)
31	o	0.25	0/1606	0.46	0/2192
32	p	0.45	0/1737	0.83	5/2353 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	q	0.34	0/1768	0.70	3/2395 (0.1%)
33	M	0.39	0/3930	0.69	2/5344 (0.0%)
34	f	0.23	0/657	0.54	0/885
35	g	0.41	0/396	0.69	0/539
36	d	0.16	0/328	0.46	0/457
37	a	0.22	0/4802	0.54	0/6520
38	b	0.19	0/528	0.54	0/705
39	h	0.89	0/241	1.18	0/326
40	e	0.17	0/416	0.43	0/579
41	l	0.15	0/111	0.32	0/152
42	s	0.15	0/99	0.33	0/137
43	m	0.24	0/621	0.65	1/834 (0.1%)
44	t	0.94	0/237	1.20	0/319
All	All	0.42	3/58656 (0.0%)	0.67	56/79495 (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
32	q	0	1
33	M	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	288	PRO	C-O	-6.29	1.16	1.23
26	c	44	SER	CA-CB	-5.82	1.44	1.53
5	H	307	SER	CA-CB	-5.09	1.45	1.53

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	202	PRO	N-CA-C	-11.71	98.61	113.84
23	E	189	PRO	N-CA-C	-10.57	97.81	110.70
2	I	57	LEU	N-CA-C	-9.71	99.99	112.23
2	I	54	VAL	N-CA-C	-9.39	99.45	112.50
32	q	9	TYR	N-CA-C	-9.16	102.11	113.38
5	H	229	PHE	CB-CA-C	8.59	125.45	110.85
10	W	23	ILE	N-CA-C	-8.43	101.52	113.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	R	140	GLU	N-CA-C	-8.41	101.48	112.41
30	n	97	ILE	N-CA-C	-8.21	102.54	110.42
15	C	737	GLN	CB-CA-C	7.75	117.50	109.83
33	M	166	LYS	N-CA-C	-7.69	98.29	109.59
15	C	738	CYS	N-CA-C	-7.66	103.66	113.16
2	I	60	LEU	N-CA-C	-7.62	103.60	113.12
12	i	25	LYS	CB-CA-C	7.50	117.25	109.83
2	I	58	GLY	CA-C-O	-7.31	114.84	120.76
2	I	107	THR	CB-CA-C	7.26	123.19	110.85
14	G	198	ILE	N-CA-C	-7.15	102.50	113.16
2	I	39	PHE	CA-CB-CG	-6.94	106.86	113.80
32	p	185	PRO	N-CA-C	-6.80	98.46	112.47
32	p	28	ARG	N-CA-C	-6.70	105.10	113.20
12	i	14	LEU	N-CA-C	-6.68	104.00	111.28
32	p	23	ASP	CB-CA-C	-6.57	100.52	110.90
43	m	47	PRO	N-CA-CB	6.54	110.12	103.25
5	H	202	PRO	CB-CA-C	-6.53	102.58	111.85
10	W	17	VAL	N-CA-C	-6.50	106.34	113.43
2	I	55	GLY	N-CA-C	-6.35	102.37	112.66
23	E	94	CYS	CB-CA-C	6.20	123.78	110.21
14	G	197	ARG	N-CA-C	-5.99	105.97	113.28
5	H	286	ALA	N-CA-C	5.91	120.35	113.20
5	H	229	PHE	CA-CB-CG	-5.89	107.91	113.80
33	M	125	ILE	N-CA-C	-5.86	107.10	112.96
32	q	10	SER	N-CA-C	-5.83	106.22	113.15
17	F	50	TYR	CB-CA-C	5.74	120.73	109.72
5	H	298	LEU	N-CA-C	-5.70	106.20	114.12
2	I	356	THR	CB-CA-C	5.59	120.35	110.85
26	c	47	VAL	N-CA-C	-5.57	105.77	113.00
15	C	736	ALA	N-CA-C	-5.53	102.10	110.28
15	C	236	ASP	N-CA-C	-5.44	106.58	113.43
17	F	39	PHE	N-CA-C	-5.37	105.53	111.71
23	E	99	MET	N-CA-C	-5.37	105.51	111.36
8	Z	49	MET	N-CA-C	-5.30	105.63	112.68
5	H	187	LEU	N-CA-C	-5.26	105.54	111.28
5	H	284	ARG	N-CA-C	-5.26	105.14	112.45
5	H	203	PHE	CB-CA-C	-5.25	104.25	112.12
12	i	18	MET	N-CA-C	-5.24	105.65	111.36
2	I	61	SER	N-CA-C	-5.18	106.06	112.38
24	D	124	ILE	N-CA-C	-5.17	102.92	109.58
12	i	29	MET	CA-C-O	-5.16	114.19	120.54
32	p	130	HIS	CB-CA-C	-5.16	100.04	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	q	11	VAL	N-CA-C	-5.11	106.27	112.76
15	C	736	ALA	CA-C-O	-5.08	115.47	121.16
23	E	156	GLY	CA-C-O	-5.08	118.17	122.29
24	D	130	GLU	N-CA-C	-5.08	105.74	111.28
24	D	201	LEU	N-CA-C	-5.06	106.94	113.01
32	p	101	GLN	CA-C-O	-5.04	113.96	119.00
2	I	26	ILE	N-CA-C	-5.02	106.78	111.45

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	M	478	LEU	Peptide
32	q	109	ALA	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	3328	0	3314	170	0
2	I	3754	0	3862	213	0
3	J	800	0	816	56	0
4	N	1201	0	1284	62	0
5	H	2493	0	2590	157	0
6	K	667	0	719	47	0
7	Y	774	0	767	42	0
8	Z	1103	0	1093	52	0
9	V	461	0	459	25	0
10	W	273	0	294	18	0
11	S	821	0	795	41	0
12	i	514	0	530	37	0
13	j	582	0	553	43	0
14	G	3049	0	3016	193	0
15	C	5288	0	5278	269	0
16	T	2535	0	2583	104	0
17	F	1518	0	1470	103	0
18	B	1702	0	1685	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	O	874	0	865	28	0
20	P	554	0	544	13	0
21	R	1039	0	1018	74	0
22	U	1011	0	952	44	0
23	E	1215	0	1195	90	0
24	D	1438	0	1368	98	0
25	X	843	0	834	19	0
26	c	744	0	742	32	0
27	Q	722	0	752	26	0
28	k	614	0	603	30	0
29	r	120	0	122	4	0
30	n	205	0	209	8	0
31	o	1568	0	1579	87	0
32	p	1705	0	1688	120	0
32	q	1736	0	1723	127	0
33	M	3825	0	3987	321	0
34	f	640	0	623	41	0
35	g	386	0	383	26	0
36	d	329	0	153	2	0
37	a	4677	0	4708	239	0
38	b	519	0	517	28	0
39	h	232	0	231	3	0
40	e	417	0	184	1	0
41	l	112	0	50	1	0
42	s	100	0	99	5	0
43	m	605	0	587	78	0
44	t	232	0	236	9	0
45	A	8	0	0	3	0
45	C	16	0	0	1	0
45	D	16	0	0	3	0
45	E	8	0	0	6	0
46	A	31	0	19	3	0
47	I	54	0	0	3	0
47	p	61	0	0	0	0
48	I	198	0	305	82	0
48	J	87	0	124	39	0
49	H	44	0	57	25	0
50	H	49	0	77	10	0
51	B	4	0	0	2	0
51	C	4	0	0	0	0
52	T	48	0	26	4	0
53	P	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	q	1	0	0	0	0
54	q	4	0	1	1	0
All	All	57959	0	57669	2814	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 24.

All (2814) 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)
15:C:227:PHE:CD2	15:C:267:ILE:HD11	1.60	1.37
11:S:84:ILE:CG1	21:R:122:ASN:OD1	1.71	1.36
33:M:140:LEU:HD23	33:M:188:ILE:CG2	1.61	1.30
15:C:227:PHE:CD2	15:C:267:ILE:CD1	2.14	1.29
32:q:17:GLU:HG2	32:p:19:GLY:O	1.27	1.27
33:M:140:LEU:CD2	33:M:188:ILE:CG2	2.17	1.20
2:I:340:GLU:OE1	43:m:39:LYS:HB3	1.42	1.20
33:M:140:LEU:HD11	33:M:192:LEU:HD22	1.22	1.16
15:C:227:PHE:CE2	15:C:267:ILE:HD11	1.81	1.14
33:M:140:LEU:HD23	33:M:188:ILE:HG21	1.21	1.10
48:I:502:CDL:H371	48:I:502:CDL:H192	1.15	1.10
49:H:501:U10:H102	23:E:85:TRP:CH2	1.86	1.10
11:S:84:ILE:HG13	21:R:122:ASN:OD1	1.31	1.10
21:R:138:LEU:HD23	21:R:138:LEU:H	1.14	1.08
32:q:17:GLU:CG	32:p:19:GLY:O	2.03	1.07
48:J:401:CDL:HA61	48:J:401:CDL:H112	1.37	1.06
23:E:129:GLY:HA2	45:E:301:SF4:S4	1.94	1.06
24:D:73:LEU:H	24:D:73:LEU:HD12	1.19	1.05
14:G:306:MET:HE1	15:C:170:CYS:SG	1.96	1.05
48:I:502:CDL:H742	48:I:502:CDL:H221	1.34	1.04
5:H:204:ASP:HB2	5:H:207:GLU:HB3	1.37	1.04
1:A:228:ILE:HD13	1:A:402:CYS:HB3	1.38	1.04
11:S:84:ILE:HG12	21:R:122:ASN:OD1	1.51	1.04
15:C:212:LYS:HZ1	15:C:274:THR:HG21	1.19	1.04
14:G:47:LEU:CD2	14:G:390:GLY:HA2	1.88	1.04
2:I:84:ASN:ND2	43:m:56:PHE:CB	2.21	1.03
13:j:11:LYS:HD2	43:m:67:PRO:HD3	1.42	1.01
44:t:32:LEU:HD12	44:t:35:LEU:HD13	1.39	1.01
14:G:94:VAL:H	21:R:129:HIS:CE1	1.79	1.01
15:C:227:PHE:CG	15:C:267:ILE:CD1	2.45	1.00
48:J:401:CDL:HB22	26:c:21:ALA:HB1	1.44	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:47:LEU:O	14:G:47:LEU:HD23	1.60	1.00
33:M:140:LEU:CD2	33:M:188:ILE:HG22	1.92	0.99
49:H:501:U10:H1M1	49:H:501:U10:H112	1.42	0.99
48:I:503:CDL:H792	48:I:503:CDL:H631	1.42	0.98
14:G:47:LEU:HD21	14:G:390:GLY:HA2	1.44	0.98
48:J:401:CDL:HB31	48:J:401:CDL:HA31	1.44	0.98
7:Y:71:CYS:SG	7:Y:102:VAL:HG23	2.03	0.97
32:q:18:THR:O	32:q:22:LEU:HD13	1.62	0.97
14:G:88:LYS:NZ	21:R:126:ILE:HD13	1.78	0.97
33:M:140:LEU:CD1	33:M:192:LEU:HD22	1.94	0.97
3:J:97:MET:SD	5:H:312:VAL:HG12	2.04	0.97
14:G:93:GLU:HA	21:R:129:HIS:HE1	1.30	0.96
49:H:501:U10:H102	23:E:85:TRP:HH2	1.24	0.96
15:C:227:PHE:CD2	15:C:267:ILE:HD13	2.01	0.94
2:I:495:LEU:HD22	12:i:64:LEU:HD11	1.49	0.94
48:I:502:CDL:H192	48:I:502:CDL:C37	1.98	0.94
2:I:107:THR:CG2	2:I:267:ILE:HD11	1.97	0.93
14:G:88:LYS:NZ	21:R:126:ILE:CD1	2.29	0.93
48:I:502:CDL:H792	48:I:502:CDL:C62	1.98	0.93
13:j:15:TYR:OH	43:m:57:GLU:HB3	1.68	0.93
15:C:212:LYS:NZ	15:C:274:THR:HG21	1.83	0.92
2:I:84:ASN:ND2	43:m:56:PHE:CG	2.36	0.92
3:J:101:PHE:CE2	48:J:401:CDL:C62	2.53	0.92
2:I:84:ASN:ND2	43:m:56:PHE:HB2	1.85	0.91
5:H:154:ILE:HD12	5:H:186:VAL:HG13	1.52	0.91
44:t:32:LEU:CD1	44:t:35:LEU:HD13	2.00	0.91
48:I:503:CDL:H121	48:I:503:CDL:CB7	2.01	0.90
48:I:502:CDL:H792	48:I:502:CDL:H622	1.52	0.90
1:A:228:ILE:HD11	18:B:113:PHE:CZ	2.07	0.90
2:I:107:THR:HG21	2:I:267:ILE:HD11	1.50	0.90
37:a:261:MET:HG2	37:a:262:VAL:HG13	1.54	0.89
2:I:415:PHE:HZ	43:m:38:LYS:HE3	1.34	0.89
14:G:94:VAL:HG22	21:R:129:HIS:CD2	2.08	0.88
33:M:140:LEU:HD21	33:M:188:ILE:CG2	2.02	0.88
13:j:5:TRP:CE3	43:m:65:TRP:HB3	2.08	0.88
1:A:125:MET:SD	1:A:264:THR:HG23	2.13	0.88
1:A:182:ARG:NH1	18:B:171:CYS:O	2.05	0.88
14:G:69:ARG:HD3	45:E:301:SF4:S2	2.13	0.88
48:I:503:CDL:H812	48:I:503:CDL:H212	1.54	0.88
15:C:227:PHE:CG	15:C:267:ILE:HD13	2.07	0.88
48:J:401:CDL:H231	48:J:401:CDL:H751	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:a:96:VAL:HG13	37:a:251:PRO:HB2	1.55	0.87
48:I:502:CDL:H841	48:I:502:CDL:H641	1.56	0.87
7:Y:71:CYS:SG	7:Y:103:CYS:CB	2.62	0.87
32:q:17:GLU:HG3	32:p:23:ASP:HB2	1.56	0.87
33:M:140:LEU:HD21	33:M:188:ILE:HG22	1.52	0.87
18:B:228:ARG:HB3	18:B:234:GLU:HA	1.55	0.87
48:I:503:CDL:OB3	30:n:81:ASN:ND2	2.06	0.87
32:q:17:GLU:HG2	32:p:19:GLY:C	1.99	0.86
48:I:502:CDL:OA7	48:I:502:CDL:HB22	1.74	0.86
1:A:228:ILE:HD11	18:B:113:PHE:HZ	1.39	0.86
14:G:91:ASN:HA	21:R:127:PRO:HD3	1.56	0.86
12:i:30:ARG:HB3	12:i:32:PRO:HD2	1.54	0.86
37:a:502:LYS:HE2	38:b:26:SER:HB3	1.57	0.85
13:j:10:ASN:H	43:m:64:ARG:HH22	1.21	0.85
14:G:110:ARG:NH2	14:G:332:GLU:O	2.10	0.85
21:R:138:LEU:H	21:R:138:LEU:CD2	1.89	0.85
17:F:118:MET:HB3	17:F:143:LEU:HB2	1.59	0.85
37:a:246:MET:HB2	37:a:309:ARG:HE	1.41	0.85
4:N:64:LEU:HB3	6:K:77:LEU:HD12	1.57	0.84
13:j:5:TRP:CZ3	43:m:65:TRP:CD1	2.65	0.84
14:G:88:LYS:HZ2	21:R:126:ILE:CD1	1.87	0.84
14:G:47:LEU:HD22	14:G:389:PHE:O	1.76	0.84
3:J:91:PHE:CE1	48:J:401:CDL:H161	2.13	0.84
7:Y:71:CYS:SG	7:Y:103:CYS:HB2	2.17	0.84
2:I:84:ASN:HD21	43:m:56:PHE:CB	1.88	0.83
1:A:228:ILE:HG22	1:A:450:LEU:CD1	2.09	0.83
48:I:503:CDL:H632	26:c:67:LEU:HD13	1.60	0.83
14:G:88:LYS:HZ1	21:R:126:ILE:HD13	1.44	0.83
15:C:212:LYS:NZ	15:C:274:THR:CG2	2.42	0.82
2:I:59:LEU:CD1	2:I:105:ALA:HA	2.09	0.82
48:I:502:CDL:H392	48:I:502:CDL:H212	1.60	0.82
17:F:41:LEU:HD12	17:F:41:LEU:O	1.79	0.82
37:a:24:GLY:HA3	37:a:33:THR:H	1.45	0.82
48:J:401:CDL:HB31	48:J:401:CDL:CA3	2.10	0.82
4:N:61:ILE:HD11	6:K:70:ALA:HA	1.60	0.82
49:H:501:U10:H1M1	49:H:501:U10:C11	2.09	0.82
37:a:198:PHE:O	37:a:202:SER:HB3	1.79	0.82
1:A:228:ILE:HG22	1:A:450:LEU:HD13	1.60	0.81
10:W:19:ALA:O	10:W:23:ILE:HG12	1.81	0.81
14:G:94:VAL:HG22	21:R:129:HIS:NE2	1.96	0.81
2:I:23:ILE:HD13	48:J:401:CDL:H741	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:M:261:THR:OG1	33:M:338:MET:SD	2.39	0.80
8:Z:129:ARG:HE	8:Z:130:TRP:H	1.29	0.80
2:I:100:LEU:HD23	2:I:137:LEU:HD23	1.64	0.80
6:K:43:ASN:HD21	6:K:66:LEU:HG	1.46	0.80
2:I:340:GLU:OE1	43:m:39:LYS:CB	2.26	0.80
13:j:11:LYS:HD2	43:m:67:PRO:CD	2.11	0.80
33:M:490:GLN:HE22	34:f:37:ILE:HB	1.46	0.80
14:G:152:ARG:HH12	23:E:192:ALA:CB	1.94	0.80
14:G:329:THR:HG23	21:R:131:PRO:HG2	1.64	0.79
2:I:402:PRO:HG2	33:M:147:GLU:HB3	1.63	0.79
2:I:415:PHE:HB2	33:M:189:LEU:HD22	1.63	0.79
14:G:47:LEU:HD22	14:G:390:GLY:HA2	1.64	0.79
2:I:352:TYR:O	2:I:356:THR:HG22	1.81	0.79
48:I:502:CDL:H112	48:I:502:CDL:OA8	1.81	0.79
12:i:17:GLN:NE2	12:i:17:GLN:HA	1.98	0.79
10:W:22:LEU:O	10:W:22:LEU:HD23	1.82	0.79
37:a:369:GLY:HA3	44:t:24:LEU:HA	1.65	0.79
31:o:48:VAL:HB	32:p:223:ASN:HD22	1.48	0.79
33:M:140:LEU:HD11	33:M:192:LEU:CD2	2.08	0.79
2:I:181:ILE:HD11	6:K:28:ILE:HG23	1.66	0.78
48:J:401:CDL:H112	48:J:401:CDL:CA6	2.14	0.78
32:q:81:TYR:HH	32:q:214:HIS:HD1	1.29	0.78
1:A:181:ILE:HG21	1:A:189:ARG:HB3	1.66	0.78
3:J:101:PHE:CZ	48:J:401:CDL:C62	2.67	0.78
12:i:29:MET:HG3	12:i:29:MET:O	1.83	0.78
15:C:173:CYS:SG	15:C:271:GLY:HA3	2.24	0.78
32:q:18:THR:O	32:q:22:LEU:CD1	2.31	0.77
14:G:74:SER:HB3	14:G:113:ASN:HD22	1.48	0.77
5:H:88:ALA:HB2	5:H:113:ILE:HG21	1.66	0.77
15:C:299:VAL:HG21	15:C:453:MET:HB2	1.65	0.77
48:I:503:CDL:PB2	30:n:81:ASN:HD21	2.07	0.77
33:M:184:MET:HE2	33:M:188:ILE:HD11	1.66	0.76
7:Y:71:CYS:SG	7:Y:103:CYS:HB3	2.24	0.76
15:C:159:MET:HG2	15:C:189:GLY:HA3	1.67	0.76
33:M:386:LEU:HD13	33:M:391:LEU:HD23	1.67	0.76
1:A:166:LEU:HD12	1:A:205:LEU:HD23	1.68	0.76
37:a:132:ASN:HA	37:a:194:PHE:HE1	1.48	0.76
48:I:502:CDL:OA6	48:I:502:CDL:HA22	1.85	0.76
32:p:99:ASN:HD22	32:p:207:TYR:HB2	1.51	0.76
48:I:503:CDL:OB4	48:I:503:CDL:HA22	1.85	0.76
14:G:152:ARG:HH12	23:E:192:ALA:HB3	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:I:503:CDL:H641	48:I:503:CDL:H832	1.67	0.76
17:F:128:ASP:OD1	17:F:130:ARG:NH1	2.19	0.76
32:p:16:ARG:HH21	32:p:16:ARG:HG2	1.49	0.76
3:J:98:ALA:HB2	48:J:401:CDL:H401	1.68	0.76
12:i:26:LEU:HD23	31:o:70:VAL:HG11	1.68	0.76
31:o:112:ASN:HD21	31:o:140:THR:HG23	1.51	0.76
17:F:97:ARG:HH22	25:X:76:ASP:HB3	1.48	0.75
33:M:139:LEU:HA	33:M:142:PHE:HB3	1.66	0.75
33:M:98:THR:O	33:M:102:PRO:HD2	1.85	0.75
33:M:382:PHE:HA	33:M:385:THR:HG22	1.69	0.75
37:a:95:LEU:HD12	37:a:466:PRO:HB3	1.67	0.75
2:I:208:GLN:NE2	43:m:53:PHE:CE1	2.54	0.75
24:D:73:LEU:H	24:D:73:LEU:CD1	1.97	0.75
15:C:316:ILE:HG13	15:C:317:PRO:HD2	1.68	0.75
1:A:185:TYR:HB3	1:A:188:GLU:HB2	1.69	0.74
37:a:237:GLY:O	37:a:562:ARG:NH1	2.20	0.74
37:a:501:PRO:HG2	38:b:21:LYS:HE2	1.70	0.74
2:I:23:ILE:CD1	48:J:401:CDL:H741	2.17	0.74
16:T:72:THR:HG22	16:T:96:LEU:HB2	1.67	0.74
16:T:75:GLY:HA3	16:T:144:LEU:HB2	1.68	0.74
48:I:502:CDL:H822	48:I:502:CDL:H621	1.68	0.74
5:H:320:THR:HG21	10:W:30:LEU:HB3	1.68	0.74
14:G:88:LYS:HZ2	21:R:126:ILE:HD12	1.51	0.74
17:F:30:ARG:NH2	17:F:89:GLN:OE1	2.21	0.74
33:M:253:ALA:O	33:M:258:LYS:NZ	2.19	0.74
2:I:340:GLU:CD	43:m:39:LYS:HB3	2.11	0.74
2:I:244:VAL:O	2:I:247:HIS:ND1	2.19	0.74
33:M:54:VAL:HA	33:M:57:ILE:HD12	1.70	0.74
48:I:503:CDL:H792	48:I:503:CDL:C63	2.17	0.74
37:a:135:GLN:HA	37:a:138:LEU:HD12	1.70	0.74
2:I:45:TYR:HE2	48:I:503:CDL:HA61	1.53	0.74
48:J:401:CDL:H381	48:J:401:CDL:H421	1.69	0.74
15:C:260:LEU:HD13	15:C:453:MET:HE1	1.69	0.73
21:R:49:GLU:HA	21:R:54:ARG:HD3	1.68	0.73
15:C:512:PRO:O	15:C:547:TRP:NE1	2.19	0.73
28:k:61:ASP:HB3	28:k:64:LYS:HE3	1.68	0.73
16:T:76:ALA:HB3	16:T:97:VAL:HG13	1.70	0.73
17:F:135:ASP:OD1	17:F:136:TYR:N	2.21	0.73
18:B:144:GLU:OE2	18:B:155:ARG:NH2	2.21	0.73
15:C:205:LYS:O	15:C:213:THR:OG1	2.06	0.73
27:Q:50:ILE:O	27:Q:51:ARG:NH1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:R:64:ARG:NH2	21:R:83:CYS:SG	2.62	0.73
33:M:315:HIS:HA	33:M:318:LEU:HD12	1.71	0.73
37:a:71:ASP:O	37:a:74:TRP:NE1	2.21	0.73
1:A:228:ILE:CD1	18:B:113:PHE:HZ	2.01	0.72
15:C:106:CYS:HB3	15:C:221:CYS:HB2	1.71	0.72
5:H:24:VAL:HG11	49:H:501:U10:H13	1.72	0.72
5:H:273:VAL:HG11	9:V:19:LEU:HD22	1.71	0.72
14:G:152:ARG:NH1	23:E:192:ALA:H	1.87	0.72
2:I:33:LEU:HD13	2:I:127:VAL:HG21	1.71	0.72
14:G:310:ILE:HD13	15:C:182:GLN:HA	1.72	0.72
23:E:119:PRO:HB3	23:E:142:VAL:HG13	1.72	0.72
2:I:403:PRO:HD3	33:M:148:SER:HA	1.71	0.72
14:G:352:ARG:HH22	14:G:354:LYS:HD3	1.53	0.72
21:R:67:VAL:HG11	21:R:81:LEU:HB2	1.71	0.72
5:H:56:LEU:HD13	49:H:501:U10:H303	1.70	0.72
13:j:5:TRP:CH2	43:m:65:TRP:CD1	2.78	0.72
21:R:138:LEU:HD23	21:R:138:LEU:N	1.99	0.72
24:D:154:ARG:HG2	24:D:197:LYS:HE3	1.71	0.72
37:a:310:VAL:HB	37:a:437:LEU:HD22	1.72	0.72
18:B:172:MET:N	51:B:301:FES:S1	2.62	0.72
20:P:74:GLY:HA3	20:P:81:GLY:HA3	1.71	0.72
17:F:124:ILE:HG22	17:F:125:ASN:HD22	1.55	0.72
33:M:17:LEU:HD12	33:M:21:LEU:HD23	1.72	0.72
24:D:172:CYS:SG	24:D:176:ALA:N	2.64	0.71
48:I:503:CDL:H812	48:I:503:CDL:C21	2.19	0.71
11:S:84:ILE:HG13	21:R:122:ASN:CG	2.15	0.71
21:R:127:PRO:O	21:R:130:VAL:HG12	1.90	0.71
33:M:304:LEU:HA	33:M:307:ILE:HD12	1.73	0.71
33:M:51:TYR:HA	33:M:54:VAL:HG12	1.71	0.71
37:a:170:VAL:HA	37:a:173:VAL:HG22	1.73	0.71
1:A:181:ILE:HD11	1:A:192:LEU:HD23	1.72	0.71
22:U:43:LYS:NZ	22:U:77:GLU:OE2	2.22	0.71
33:M:63:THR:HB	33:M:65:LYS:HG2	1.72	0.71
33:M:217:TRP:NE1	33:M:268:SER:OG	2.23	0.71
1:A:337:LEU:HB3	1:A:352:LYS:HG3	1.72	0.71
2:I:411:PHE:CZ	33:M:189:LEU:HD21	2.26	0.71
37:a:239:HIS:HB2	37:a:242:LEU:HD13	1.73	0.71
2:I:41:THR:HG22	2:I:41:THR:O	1.90	0.71
48:I:503:CDL:H271	48:I:503:CDL:H231	1.72	0.71
31:o:49:LYS:HG3	32:q:45:LEU:HG	1.72	0.71
5:H:15:PRO:HB2	9:V:22:MET:HG3	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:534:GLU:O	15:C:538:GLN:NE2	2.23	0.70
23:E:191:THR:HG22	23:E:193:GLU:CG	2.20	0.70
33:M:149:VAL:HG21	33:M:259:PHE:HE2	1.56	0.70
26:c:45:VAL:HG13	26:c:62:MET:HG3	1.71	0.70
32:p:16:ARG:HG2	32:p:16:ARG:NH2	2.04	0.70
34:f:55:VAL:HG22	34:f:74:VAL:HG22	1.72	0.70
37:a:368:MET:HE1	37:a:439:PHE:HB3	1.72	0.70
15:C:523:ARG:NH2	15:C:713:THR:O	2.24	0.70
33:M:262:TYR:OH	33:M:266:ARG:NH2	2.24	0.70
1:A:449:ALA:HB3	46:A:502:FMN:HM83	1.73	0.70
33:M:204:LEU:HD11	33:M:270:PRO:HB2	1.74	0.70
4:N:124:TYR:OH	7:Y:40:LYS:NZ	2.25	0.70
33:M:163:ARG:HA	33:M:167:ILE:HD11	1.74	0.70
7:Y:51:ASP:HA	7:Y:54:ARG:HD2	1.72	0.70
3:J:11:TYR:HA	5:H:9:ILE:HD13	1.74	0.69
22:U:75:TRP:HB3	24:D:99:GLU:HB3	1.73	0.69
31:o:223:LEU:HD22	32:p:110:LYS:HB3	1.73	0.69
33:M:356:TYR:O	33:M:360:LYS:N	2.25	0.69
33:M:407:ALA:HB3	37:a:183:LEU:HD21	1.73	0.69
1:A:293:ASN:ND2	1:A:315:MET:SD	2.64	0.69
43:m:42:GLU:HG3	43:m:43:MET:H	1.57	0.69
17:F:117:ASP:OD1	17:F:131:ARG:NH1	2.24	0.69
33:M:358:ARG:NH2	33:M:451:ASP:O	2.25	0.69
13:j:5:TRP:CZ3	43:m:65:TRP:HB3	2.27	0.69
38:b:34:LEU:O	38:b:38:ASN:ND2	2.26	0.69
1:A:288:PHE:HB3	1:A:314:GLU:HG3	1.73	0.69
15:C:400:VAL:HG21	15:C:408:VAL:HB	1.73	0.69
37:a:239:HIS:O	37:a:562:ARG:NH2	2.25	0.69
5:H:200:ARG:HH22	5:H:281:ILE:HA	1.57	0.69
14:G:88:LYS:NZ	21:R:126:ILE:HD12	2.03	0.69
15:C:302:ASN:OD1	15:C:318:ARG:NH1	2.26	0.69
37:a:398:PHE:HA	37:a:402:ASP:HB3	1.73	0.69
15:C:76:VAL:HG11	15:C:138:ALA:HB1	1.75	0.69
17:F:81:ARG:NH2	21:R:83:CYS:O	2.25	0.69
48:I:503:CDL:H182	48:I:503:CDL:H391	1.75	0.68
14:G:152:ARG:HH11	23:E:192:ALA:H	1.39	0.68
23:E:154:SER:OG	23:E:175:CYS:SG	2.49	0.68
37:a:186:PHE:HZ	37:a:192:VAL:HG12	1.57	0.68
48:I:502:CDL:H402	48:I:502:CDL:H441	1.73	0.68
48:J:401:CDL:HA61	48:J:401:CDL:C11	2.18	0.68
37:a:159:GLN:HA	37:a:162:LYS:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:m:49:ARG:HH12	43:m:55:THR:HG21	1.57	0.68
2:I:395:MET:HB3	2:I:440:TYR:HD2	1.58	0.68
20:P:65:VAL:HG21	20:P:70:VAL:HG12	1.76	0.68
33:M:478:LEU:HA	33:M:481:MET:HE3	1.75	0.68
13:j:19:MET:CE	43:m:57:GLU:HG3	2.23	0.68
2:I:148:MET:HG3	2:I:276:ASN:HD21	1.58	0.68
3:J:91:PHE:HE1	48:J:401:CDL:H161	1.59	0.68
2:I:79:ALA:O	2:I:83:TRP:NE1	2.26	0.68
17:F:81:ARG:NH2	21:R:83:CYS:SG	2.67	0.68
13:j:19:MET:HE1	43:m:57:GLU:HG3	1.76	0.68
33:M:229:PRO:HB2	33:M:313:VAL:HG13	1.74	0.68
37:a:23:LEU:HD12	37:a:27:GLY:HA2	1.76	0.68
14:G:109:THR:OG1	14:G:145:TYR:OH	2.11	0.68
15:C:207:LEU:HD12	15:C:213:THR:HG21	1.76	0.68
12:i:17:GLN:HA	12:i:17:GLN:HE21	1.58	0.67
33:M:99:PHE:CE1	33:M:462:PRO:HB2	2.30	0.67
15:C:449:VAL:HG13	15:C:722:PHE:HB2	1.76	0.67
33:M:140:LEU:CD2	33:M:188:ILE:HG23	2.22	0.67
37:a:96:VAL:HG21	37:a:255:LEU:HG	1.76	0.67
2:I:430:VAL:CG1	33:M:182:LEU:HB3	2.24	0.67
31:o:230:GLU:O	32:q:36:ARG:NH1	2.27	0.67
33:M:335:ILE:HA	33:M:338:MET:HE3	1.76	0.67
34:f:39:ARG:HH22	35:g:93:ALA:HA	1.58	0.67
3:J:34:SER:OG	23:E:148:GLU:OE2	2.12	0.67
15:C:225:VAL:CG2	15:C:248:ILE:HG23	2.24	0.67
37:a:62:ALA:O	37:a:74:TRP:N	2.27	0.67
37:a:202:SER:HA	37:a:278:TYR:HB2	1.77	0.67
1:A:163:GLU:OE2	1:A:279:ARG:NH1	2.27	0.67
1:A:304:HIS:H	18:B:138:ARG:HD3	1.60	0.67
3:J:99:PHE:CD2	4:N:156:SER:HB2	2.30	0.67
4:N:155:PRO:HG2	6:K:64:LEU:HD22	1.77	0.67
23:E:191:THR:HG22	23:E:193:GLU:HG2	1.76	0.67
7:Y:25:ILE:HD13	7:Y:63:LEU:HD23	1.75	0.67
7:Y:11:PRO:HG3	7:Y:65:LYS:HD3	1.76	0.67
22:U:92:GLU:HG3	24:D:209:THR:HG21	1.76	0.67
33:M:139:LEU:HD13	33:M:188:ILE:HG12	1.74	0.67
2:I:29:THR:HG21	2:I:131:LEU:HG	1.76	0.67
17:F:47:LEU:HA	21:R:95:ASP:HB3	1.75	0.67
23:E:146:MET:HE2	23:E:150:ARG:HB2	1.77	0.67
12:i:39:MET:O	12:i:39:MET:SD	2.53	0.67
16:T:359:LYS:HG2	16:T:360:PHE:H	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:10:ALA:HB2	4:N:36:ASP:HB2	1.77	0.67
16:T:225:THR:HG21	17:F:162:LYS:HD3	1.77	0.67
17:F:100:SER:HB2	17:F:123:PHE:HB3	1.77	0.67
2:I:263:ALA:O	2:I:267:ILE:HG12	1.94	0.66
14:G:125:VAL:HG13	14:G:202:ARG:HG2	1.77	0.66
7:Y:43:ASP:HB2	8:Z:129:ARG:HH22	1.59	0.66
12:i:41:LEU:C	12:i:41:LEU:HD23	2.20	0.66
32:p:29:LEU:O	32:p:29:LEU:HD23	1.96	0.66
14:G:36:VAL:HG13	14:G:372:HIS:HA	1.76	0.66
32:p:24:ARG:O	32:p:28:ARG:HB2	1.96	0.66
33:M:439:GLY:H	37:a:155:PHE:HE2	1.43	0.66
14:G:102:ARG:NH2	14:G:162:GLY:O	2.23	0.66
32:q:17:GLU:CG	32:p:23:ASP:HB2	2.24	0.66
48:J:401:CDL:H441	48:J:401:CDL:H591	1.77	0.66
22:U:88:GLN:HG2	22:U:122:GLU:HG2	1.76	0.66
15:C:64:ARG:HH21	19:O:134:LEU:HG	1.61	0.66
1:A:330:VAL:HG21	1:A:337:LEU:HD12	1.78	0.66
32:q:35:PHE:H	32:p:48:VAL:HG21	1.60	0.66
32:p:130:HIS:N	32:p:130:HIS:CD2	2.62	0.66
7:Y:60:VAL:HG11	8:Z:88:ILE:HG12	1.77	0.66
15:C:486:GLY:HA3	15:C:491:THR:HG21	1.78	0.66
30:n:79:ASP:O	30:n:83:ASN:ND2	2.29	0.66
33:M:358:ARG:O	33:M:448:LYS:NZ	2.29	0.66
7:Y:71:CYS:SG	7:Y:102:VAL:CG2	2.82	0.66
15:C:583:LEU:HD22	15:C:589:VAL:HG11	1.76	0.66
31:o:131:ALA:HB1	31:o:149:SER:HB3	1.79	0.65
32:q:98:THR:OG1	32:q:123:GLY:O	2.12	0.65
33:M:483:THR:O	33:M:487:ASN:ND2	2.30	0.65
37:a:232:LYS:NZ	37:a:260:THR:O	2.27	0.65
2:I:401:ILE:HG22	2:I:403:PRO:HD2	1.79	0.65
17:F:81:ARG:NE	21:R:92:GLU:OE2	2.29	0.65
32:q:17:GLU:HG3	32:p:23:ASP:H	1.61	0.65
32:p:159:LYS:HB3	32:p:160:HIS:HD2	1.61	0.65
37:a:266:VAL:HA	37:a:269:ILE:HG12	1.78	0.65
2:I:411:PHE:CE1	33:M:185:LEU:HD11	2.30	0.65
5:H:128:SER:HB2	5:H:217:ASN:HA	1.77	0.65
6:K:50:SER:HB2	6:K:58:GLY:HA3	1.79	0.65
15:C:594:ILE:HD12	15:C:600:VAL:HG21	1.77	0.65
1:A:228:ILE:CD1	1:A:402:CYS:HB3	2.21	0.65
17:F:22:MET:HB2	17:F:32:ASP:HB3	1.78	0.65
37:a:82:THR:HG22	37:a:271:ARG:HH22	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:357:ALA:HB1	14:G:391:GLU:HB3	1.79	0.65
48:I:503:CDL:H632	26:c:67:LEU:CD1	2.27	0.65
33:M:301:GLN:HE21	33:M:306:LYS:HD3	1.61	0.65
35:g:59:TRP:O	35:g:67:TYR:OH	2.15	0.65
14:G:31:GLU:HB3	14:G:39:ARG:HG2	1.79	0.65
23:E:191:THR:CG2	23:E:193:GLU:HG3	2.27	0.65
37:a:127:LEU:HD13	37:a:264:ALA:HB1	1.78	0.65
37:a:184:GLY:HA3	37:a:221:ILE:HD11	1.78	0.65
5:H:291:ARG:HG2	5:H:291:ARG:HH11	1.62	0.65
2:I:267:ILE:HG22	2:I:356:THR:HG23	1.80	0.65
24:D:156:ASP:N	24:D:156:ASP:OD1	2.30	0.65
26:c:14:PRO:O	26:c:91:ASN:ND2	2.30	0.65
31:o:223:LEU:HB2	32:p:110:LYS:HD3	1.79	0.65
33:M:104:CYS:HB3	33:M:247:ALA:HB1	1.79	0.65
33:M:322:GLY:HA3	33:M:403:ILE:HD13	1.78	0.65
37:a:63:PRO:HA	37:a:73:SER:H	1.62	0.65
1:A:441:GLN:O	1:A:445:HIS:ND1	2.30	0.64
2:I:434:VAL:HG21	33:M:179:LEU:HA	1.79	0.64
48:I:502:CDL:H402	48:I:502:CDL:C44	2.28	0.64
48:I:503:CDL:H382	48:I:503:CDL:H151	1.78	0.64
3:J:98:ALA:CA	48:J:401:CDL:H401	2.27	0.64
15:C:111:LEU:O	19:O:138:LYS:NZ	2.30	0.64
37:a:234:ALA:HA	37:a:239:HIS:HA	1.77	0.64
14:G:318:GLU:HA	17:F:180:PHE:HB3	1.79	0.64
31:o:77:ASN:ND2	32:p:66:SER:OG	2.29	0.64
37:a:41:ILE:HD12	37:a:101:ILE:HB	1.79	0.64
37:a:44:LEU:O	37:a:48:TYR:HB2	1.97	0.64
15:C:380:ILE:HG23	15:C:580:PHE:HD2	1.60	0.64
21:R:67:VAL:HG23	21:R:80:ARG:HD2	1.79	0.64
28:k:95:LEU:HD21	28:k:121:SER:HA	1.79	0.64
2:I:449:PHE:HE2	33:M:158:GLY:HA3	1.61	0.64
1:A:180:TYR:HH	1:A:238:SER:HG	1.45	0.64
33:M:56:TRP:HA	33:M:91:LEU:HD11	1.79	0.64
37:a:282:ALA:O	37:a:286:ILE:HG13	1.96	0.64
1:A:138:VAL:HG21	1:A:165:CYS:SG	2.37	0.64
2:I:66:LEU:HD11	2:I:98:ILE:HG23	1.80	0.64
14:G:298:SER:HB2	14:G:301:ARG:HD3	1.78	0.64
4:N:53:PHE:O	4:N:57:TYR:HB2	1.97	0.64
8:Z:133:PRO:HB2	13:j:54:ARG:HH11	1.63	0.64
15:C:631:GLU:OE2	15:C:686:ASN:ND2	2.30	0.64
16:T:221:THR:HA	52:T:501:NDP:H42N	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:k:64:LYS:HZ2	28:k:75:LEU:HD23	1.63	0.64
43:m:19:PRO:O	43:m:22:ARG:NH2	2.29	0.64
2:I:201:THR:HG23	2:I:212:ILE:HG21	1.78	0.64
48:I:502:CDL:H621	48:I:502:CDL:C82	2.28	0.64
15:C:85:VAL:HG11	15:C:94:ALA:HA	1.78	0.64
17:F:74:VAL:HG13	17:F:89:GLN:HG2	1.80	0.64
33:M:402:LEU:HA	33:M:405:VAL:HG12	1.79	0.64
37:a:510:GLU:CD	37:a:510:GLU:H	2.06	0.64
1:A:63:ARG:NH1	1:A:312:GLU:O	2.31	0.64
1:A:224:ALA:HB1	18:B:116:MET:HB2	1.78	0.64
25:X:23:ARG:NH1	28:k:79:SER:OG	2.31	0.64
2:I:457:LEU:HD21	31:o:109:PHE:HB2	1.81	0.63
11:S:84:ILE:CG1	21:R:122:ASN:CG	2.69	0.63
14:G:94:VAL:N	21:R:129:HIS:CE1	2.61	0.63
15:C:321:GLU:O	15:C:457:ARG:NH2	2.31	0.63
16:T:182:GLN:HB3	16:T:216:ILE:HG12	1.80	0.63
23:E:164:TYR:CG	24:D:163:ILE:HG21	2.32	0.63
25:X:47:GLN:NE2	25:X:48:ASP:OD1	2.31	0.63
32:p:29:LEU:HD23	32:p:29:LEU:C	2.23	0.63
3:J:98:ALA:CB	48:J:401:CDL:H401	2.28	0.63
7:Y:45:ASN:HB3	7:Y:48:LYS:HG2	1.80	0.63
14:G:56:GLU:HG2	14:G:352:ARG:H	1.62	0.63
15:C:387:LEU:HD11	15:C:726:ASN:HD22	1.62	0.63
33:M:83:TYR:OH	33:M:201:GLN:NE2	2.30	0.63
37:a:41:ILE:HD11	37:a:114:MET:HG2	1.80	0.63
1:A:309:CYS:HB3	18:B:233:PRO:HA	1.81	0.63
2:I:495:LEU:HD22	12:i:64:LEU:CD1	2.27	0.63
48:I:503:CDL:H442	10:W:21:CYS:SG	2.38	0.63
15:C:207:LEU:HD22	15:C:256:MET:HG3	1.81	0.63
1:A:248:LEU:HD22	15:C:135:ALA:HB3	1.81	0.63
2:I:59:LEU:HD13	2:I:105:ALA:HA	1.81	0.63
12:i:14:LEU:HD22	33:M:28:PHE:CZ	2.33	0.63
32:q:68:ILE:HB	32:q:86:ARG:HA	1.80	0.63
33:M:145:PHE:HA	33:M:148:SER:HB3	1.81	0.63
33:M:304:LEU:H	33:M:364:VAL:HG21	1.62	0.63
48:I:503:CDL:H221	48:I:503:CDL:H452	1.79	0.63
5:H:155:LEU:HA	5:H:158:VAL:HG12	1.81	0.63
5:H:291:ARG:HD3	14:G:202:ARG:HE	1.64	0.63
13:j:11:LYS:CD	43:m:67:PRO:HD3	2.22	0.63
2:I:326:HIS:O	2:I:330:ILE:HG12	1.98	0.63
17:F:52:ARG:HD2	21:R:92:GLU:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:D:94:ILE:HG23	24:D:99:GLU:HG3	1.80	0.63
33:M:257:LEU:HD23	33:M:316:MET:HG3	1.81	0.63
2:I:415:PHE:CZ	43:m:38:LYS:HE3	2.25	0.63
5:H:320:THR:OG1	5:H:321:PHE:N	2.30	0.63
14:G:94:VAL:HG13	21:R:129:HIS:NE2	2.14	0.63
37:a:198:PHE:HB2	37:a:274:PRO:HB2	1.79	0.63
2:I:430:VAL:HG13	33:M:182:LEU:HB3	1.80	0.63
12:i:11:LEU:HD21	33:M:24:ILE:HG21	1.79	0.63
24:D:154:ARG:HA	24:D:197:LYS:HB3	1.81	0.63
24:D:161:LYS:HG2	24:D:161:LYS:O	1.99	0.63
32:q:43:ARG:HD2	32:p:216:ALA:HA	1.79	0.63
33:M:327:ASN:HD22	33:M:406:GLY:HA2	1.64	0.63
35:g:100:ARG:HA	35:g:103:MET:HG2	1.81	0.63
42:s:6:ALA:O	42:s:10:ALA:N	2.29	0.63
43:m:67:PRO:O	43:m:71:GLN:NE2	2.32	0.63
14:G:225:ARG:NH1	14:G:267:GLU:OE2	2.29	0.63
14:G:25:VAL:HG21	14:G:47:LEU:HB2	1.81	0.62
15:C:125:GLU:HB2	15:C:143:LYS:HB2	1.80	0.62
23:E:124:CYS:SG	23:E:125:MET:N	2.72	0.62
32:q:105:LEU:HG	32:p:130:HIS:HB3	1.80	0.62
37:a:314:SER:OG	37:a:345:LYS:NZ	2.30	0.62
5:H:50:GLN:NE2	5:H:54:ASP:OD1	2.32	0.62
37:a:166:LYS:HA	37:a:169:LEU:HD23	1.81	0.62
1:A:182:ARG:NE	1:A:184:GLU:OE1	2.31	0.62
48:I:503:CDL:H151	48:I:503:CDL:C38	2.29	0.62
8:Z:11:GLY:O	8:Z:12:MET:HG2	1.98	0.62
15:C:626:LYS:NZ	15:C:653:ASP:OD2	2.26	0.62
37:a:95:LEU:HD21	37:a:470:LEU:HD22	1.80	0.62
1:A:228:ILE:CD1	1:A:244:GLY:O	2.48	0.62
48:J:401:CDL:HA31	48:J:401:CDL:CB3	2.24	0.62
15:C:165:ASN:HB3	15:C:200:ARG:HG3	1.81	0.62
17:F:156:ARG:NH1	23:E:133:ASN:O	2.33	0.62
18:B:78:ASP:OD1	18:B:82:GLN:NE2	2.31	0.62
48:I:502:CDL:H792	48:I:502:CDL:C61	2.29	0.62
15:C:507:LYS:NZ	15:C:539:ALA:O	2.29	0.62
32:q:35:PHE:N	32:p:48:VAL:HG21	2.14	0.62
33:M:253:ALA:HA	33:M:257:LEU:HD13	1.82	0.62
37:a:366:ARG:NH2	44:t:20:LYS:HG3	2.14	0.62
6:K:79:ILE:HA	6:K:82:ILE:HG22	1.81	0.62
32:p:99:ASN:ND2	32:p:207:TYR:HB2	2.15	0.62
37:a:336:PHE:HA	37:a:339:MET:HE2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:MET:HG3	1:A:172:MET:HB2	1.80	0.62
48:J:401:CDL:HB21	26:c:22:PHE:N	2.14	0.62
49:H:501:U10:O2	49:H:501:U10:H3M2	1.98	0.62
28:k:110:LEU:HA	28:k:113:GLU:HG3	1.80	0.62
31:o:237:VAL:HG21	32:p:39:LEU:HB2	1.82	0.62
37:a:4:LEU:HD13	42:s:17:ALA:HA	1.82	0.62
31:o:74:VAL:HG12	31:o:78:VAL:HG21	1.80	0.62
31:o:103:ASN:ND2	31:o:131:ALA:O	2.32	0.62
32:q:85:LEU:HG	32:q:106:VAL:HB	1.81	0.62
32:p:70:ASP:HB3	32:p:91:THR:HA	1.82	0.62
5:H:302:VAL:HG22	10:W:16:VAL:HG21	1.80	0.62
15:C:443:ILE:HA	15:C:472:VAL:HG23	1.80	0.62
15:C:469:VAL:HG21	15:C:480:TYR:HE1	1.63	0.62
33:M:78:GLU:OE1	43:m:38:LYS:NZ	2.31	0.62
43:m:71:GLN:N	43:m:71:GLN:OE1	2.32	0.62
5:H:154:ILE:HG23	5:H:186:VAL:CG1	2.30	0.61
7:Y:42:ASN:ND2	7:Y:43:ASP:OD1	2.33	0.61
31:o:86:VAL:HA	31:o:107:VAL:HG22	1.82	0.61
37:a:256:ILE:HA	37:a:260:THR:HG22	1.81	0.61
37:a:564:PHE:HE1	37:a:570:ASN:H	1.47	0.61
5:H:277:LEU:O	5:H:281:ILE:HG12	2.00	0.61
17:F:159:ASP:OD1	17:F:159:ASP:N	2.32	0.61
37:a:559:PHE:HA	37:a:563:TRP:HA	1.81	0.61
1:A:337:LEU:HD22	1:A:352:LYS:HB2	1.81	0.61
48:I:503:CDL:H121	48:I:503:CDL:OB8	2.00	0.61
48:I:503:CDL:H772	48:I:503:CDL:H162	1.81	0.61
5:H:23:LEU:HD11	5:H:236:MET:HE2	1.82	0.61
31:o:202:ILE:HG22	31:o:203:ARG:HG3	1.82	0.61
14:G:80:HIS:CD2	14:G:102:ARG:HD3	2.36	0.61
32:p:162:MET:HE1	32:p:196:GLU:HB3	1.80	0.61
33:M:124:LEU:HD12	33:M:160:TRP:HH2	1.65	0.61
37:a:170:VAL:HG21	37:a:562:ARG:CZ	2.30	0.61
37:a:197:ILE:HD12	37:a:275:LEU:HD21	1.82	0.61
15:C:227:PHE:CB	15:C:267:ILE:HD13	2.31	0.61
15:C:368:VAL:O	15:C:372:ILE:HG23	2.00	0.61
31:o:66:PRO:HB2	31:o:80:LEU:HD23	1.83	0.61
2:I:480:LEU:O	33:M:74:TRP:NE1	2.34	0.61
48:I:502:CDL:H151	26:c:50:LEU:HD13	1.81	0.61
3:J:23:LEU:HD11	5:H:75:ARG:HG2	1.81	0.61
15:C:286:GLU:OE2	15:C:308:ARG:NH2	2.34	0.61
23:E:202:LEU:O	23:E:206:ILE:HG12	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:k:72:GLN:NE2	28:k:77:LEU:O	2.34	0.61
33:M:60:ASP:HB3	33:M:67:GLN:HE22	1.65	0.61
1:A:140:ALA:HA	1:A:268:VAL:HG13	1.83	0.61
10:W:13:GLN:HG2	24:D:54:LYS:HG3	1.81	0.61
13:j:11:LYS:HB2	43:m:67:PRO:HD3	1.82	0.61
14:G:337:GLU:OE2	17:F:85:ARG:NH2	2.34	0.61
40:e:75:PHE:O	40:e:80:GLY:N	2.34	0.61
2:I:267:ILE:HG22	2:I:356:THR:CG2	2.30	0.60
48:I:502:CDL:HA22	48:I:502:CDL:CA5	2.31	0.60
48:I:503:CDL:H841	3:J:101:PHE:HZ	1.66	0.60
8:Z:40:SER:HB3	11:S:33:PRO:HB3	1.83	0.60
24:D:191:GLU:OE1	24:D:191:GLU:N	2.27	0.60
49:H:501:U10:H4M3	49:H:501:U10:O5	2.01	0.60
28:k:70:HIS:HB3	28:k:73:ASN:HB2	1.83	0.60
32:q:86:ARG:HB2	32:q:107:HIS:HB2	1.82	0.60
33:M:181:SER:HA	33:M:223:SER:HB2	1.83	0.60
3:J:88:ILE:HD12	3:J:92:GLY:HA3	1.82	0.60
3:J:97:MET:SD	5:H:312:VAL:CG1	2.84	0.60
12:i:7:MET:HG3	12:i:8:VAL:H	1.66	0.60
14:G:47:LEU:HD22	14:G:390:GLY:CA	2.30	0.60
14:G:72:TYR:CZ	14:G:388:VAL:HG13	2.35	0.60
15:C:100:VAL:HG11	15:C:146:THR:HG21	1.83	0.60
2:I:86:LEU:HD22	4:N:150:VAL:HB	1.82	0.60
35:g:97:ALA:HA	35:g:100:ARG:HG3	1.83	0.60
37:a:132:ASN:HA	37:a:194:PHE:CE1	2.35	0.60
2:I:411:PHE:CE1	33:M:189:LEU:HD21	2.36	0.60
23:E:94:CYS:SG	23:E:190:PRO:HD3	2.42	0.60
27:Q:53:CYS:SG	27:Q:56:VAL:HB	2.42	0.60
33:M:264:PHE:HB3	33:M:323:MET:HE3	1.82	0.60
2:I:449:PHE:CE2	33:M:158:GLY:HA3	2.37	0.60
3:J:77:PHE:O	4:N:145:TYR:OH	2.12	0.60
4:N:179:ARG:HD2	29:r:1:ALA:HB2	1.84	0.60
12:i:33:TRP:HE3	12:i:33:TRP:H	1.49	0.60
15:C:172:ILE:HG13	24:D:150:ARG:HD2	1.84	0.60
17:F:154:GLN:OE1	23:E:133:ASN:ND2	2.33	0.60
32:p:86:ARG:NH2	32:p:88:ASP:H	1.99	0.60
37:a:80:SER:HB3	37:a:493:TRP:HH2	1.67	0.60
2:I:41:THR:OG1	4:N:176:LYS:HG2	2.01	0.60
2:I:247:HIS:CG	2:I:248:MET:H	2.19	0.60
5:H:151:ILE:HG23	5:H:190:PHE:HE1	1.66	0.60
32:q:18:THR:C	32:q:22:LEU:HD13	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:q:113:LEU:HD11	32:p:195:GLU:HG3	1.82	0.60
2:I:55:GLY:O	2:I:57:LEU:N	2.32	0.60
12:i:14:LEU:HG	12:i:33:TRP:HD1	1.65	0.60
14:G:216:ASP:HB3	17:F:106:PRO:HD2	1.84	0.60
26:c:52:GLY:HA3	26:c:57:ILE:O	2.02	0.60
32:q:193:THR:HG23	32:q:196:GLU:H	1.66	0.60
37:a:235:GLN:HG2	37:a:261:MET:HE3	1.83	0.60
1:A:380:MET:HB3	1:A:384:THR:HG21	1.84	0.60
1:A:445:HIS:HB3	15:C:121:LEU:HD11	1.82	0.60
2:I:148:MET:HE3	2:I:190:LEU:HD21	1.83	0.60
7:Y:74:GLU:HB3	7:Y:99:PHE:HA	1.83	0.60
32:q:100:ILE:HD13	32:q:106:VAL:HG21	1.84	0.60
33:M:132:ALA:O	33:M:136:MET:N	2.33	0.60
2:I:402:PRO:HA	2:I:407:PHE:CG	2.36	0.59
5:H:23:LEU:HD22	5:H:233:TYR:HB3	1.84	0.59
2:I:177:LEU:HD21	6:K:28:ILE:HG21	1.84	0.59
3:J:66:ILE:HG23	6:K:74:ALA:HB1	1.83	0.59
17:F:53:VAL:HA	17:F:79:SER:HA	1.85	0.59
22:U:98:HIS:CE1	24:D:100:LYS:HD2	2.37	0.59
24:D:96:TYR:OH	24:D:184:GLU:OE2	2.19	0.59
2:I:197:ILE:HD12	2:I:233:ILE:HD12	1.84	0.59
3:J:91:PHE:CD1	48:J:401:CDL:H161	2.36	0.59
5:H:20:VAL:HG11	5:H:230:LEU:HA	1.84	0.59
14:G:264:ARG:NH2	14:G:384:THR:O	2.34	0.59
16:T:168:ALA:HB2	16:T:207:VAL:HG23	1.84	0.59
22:U:133:TYR:HB3	24:D:192:GLU:HG3	1.82	0.59
43:m:64:ARG:HG3	43:m:65:TRP:H	1.67	0.59
1:A:251:PRO:HB3	19:O:141:SER:HB3	1.83	0.59
34:f:39:ARG:HE	35:g:96:LYS:HD3	1.66	0.59
37:a:35:CYS:SG	37:a:36:VAL:N	2.75	0.59
9:V:40:ILE:HG13	9:V:41:GLY:H	1.68	0.59
23:E:157:SER:H	23:E:188:CYS:HA	1.67	0.59
24:D:129:CYS:HA	24:D:132:VAL:HG12	1.84	0.59
2:I:244:VAL:HG23	2:I:304:LEU:HD22	1.83	0.59
16:T:64:SER:OG	17:F:171:MET:HB3	2.03	0.59
18:B:143:ILE:HG23	18:B:206:VAL:HG21	1.84	0.59
25:X:34:CYS:HB3	28:k:87:MET:HE2	1.85	0.59
37:a:341:HIS:CE1	37:a:345:LYS:HE2	2.38	0.59
13:j:5:TRP:CZ3	43:m:65:TRP:CG	2.91	0.59
14:G:61:LEU:HD21	14:G:316:TYR:CE1	2.37	0.59
1:A:409:ARG:HE	1:A:410:GLU:HG2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:41:GLU:OE2	14:G:43:HIS:NE2	2.35	0.59
23:E:191:THR:CG2	23:E:193:GLU:CG	2.79	0.59
33:M:24:ILE:HA	33:M:27:LEU:HD12	1.83	0.59
37:a:461:ILE:O	37:a:465:ILE:HG12	2.03	0.59
5:H:212:LEU:HD21	5:H:229:PHE:CE1	2.37	0.59
11:S:43:THR:HG22	22:U:69:GLN:H	1.67	0.59
31:o:237:VAL:HG23	32:p:39:LEU:HD12	1.83	0.59
32:p:83:CYS:SG	32:p:100:ILE:HG21	2.43	0.59
14:G:328:TYR:HD1	14:G:341:PHE:HB2	1.68	0.59
14:G:352:ARG:NH2	14:G:354:LYS:HD3	2.17	0.59
15:C:521:PHE:HE1	15:C:530:LEU:HD21	1.67	0.59
18:B:126:HIS:CE1	18:B:128:LEU:HD21	2.38	0.59
20:P:65:VAL:HG22	20:P:66:ASP:H	1.68	0.59
33:M:222:ALA:O	33:M:226:VAL:HG23	2.03	0.59
33:M:224:PHE:O	33:M:228:VAL:N	2.25	0.59
37:a:100:SER:O	37:a:104:MET:N	2.34	0.59
5:H:203:PHE:HD1	5:H:295:LEU:HG	1.68	0.58
16:T:249:GLY:O	16:T:289:THR:OG1	2.20	0.58
31:o:165:MET:HE3	31:o:166:GLU:H	1.68	0.58
33:M:334:SER:HA	33:M:403:ILE:HD11	1.83	0.58
33:M:392:PRO:HA	33:M:397:PHE:CG	2.38	0.58
16:T:60:THR:HB	19:O:82:LEU:HD21	1.84	0.58
22:U:46:ASN:HD21	22:U:75:TRP:HE1	1.51	0.58
33:M:309:ALA:O	33:M:313:VAL:HG23	2.03	0.58
3:J:31:SER:OG	3:J:32:ASN:N	2.32	0.58
5:H:56:LEU:HD23	23:E:79:ALA:HB2	1.86	0.58
5:H:38:LYS:HE2	24:D:93:THR:HG21	1.85	0.58
5:H:207:GLU:HA	5:H:212:LEU:HB2	1.84	0.58
12:i:14:LEU:HA	12:i:36:VAL:HG11	1.85	0.58
14:G:25:VAL:HG12	23:E:135:MET:HE2	1.84	0.58
18:B:132:THR:HG22	18:B:133:THR:H	1.68	0.58
31:o:58:ILE:HG23	31:o:66:PRO:HG2	1.84	0.58
33:M:491:HIS:HE1	34:f:30:MET:HE1	1.68	0.58
34:f:56:LYS:NZ	37:a:71:ASP:OD2	2.35	0.58
16:T:193:PRO:HB2	16:T:345:ASN:HB3	1.85	0.58
33:M:443:PRO:HD2	33:M:445:PHE:HE1	1.68	0.58
39:h:31:LEU:HD22	44:t:37:ILE:HB	1.86	0.58
1:A:236:LEU:HD11	1:A:253:PRO:HB3	1.85	0.58
7:Y:89:PHE:HB3	7:Y:93:ARG:HH12	1.68	0.58
9:V:12:LEU:HA	9:V:15:ILE:HG22	1.85	0.58
32:p:67:VAL:HG12	32:p:71:VAL:HG21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:361:ALA:HB3	2:I:469:LEU:HD13	1.84	0.58
5:H:292:TYR:HA	5:H:295:LEU:HB3	1.86	0.58
14:G:237:ALA:HB2	21:R:133:HIS:ND1	2.19	0.58
32:p:27:CYS:O	32:p:27:CYS:SG	2.61	0.58
33:M:100:LEU:HD21	33:M:250:VAL:HG12	1.86	0.58
2:I:332:ILE:HD11	2:I:413:LEU:HB3	1.85	0.58
3:J:78:PHE:CE1	5:H:311:VAL:HG11	2.39	0.58
15:C:293:ILE:HG13	15:C:638:GLN:HB3	1.85	0.58
24:D:73:LEU:HB3	24:D:76:MET:HB2	1.85	0.58
28:k:86:VAL:HG11	28:k:102:ALA:HB1	1.84	0.58
33:M:269:ILE:HA	33:M:276:THR:HG21	1.84	0.58
2:I:358:ASP:HB2	2:I:472:THR:HG21	1.86	0.58
2:I:374:ILE:HG21	2:I:443:LEU:HD11	1.85	0.58
11:S:46:ARG:HD3	11:S:50:PRO:HD3	1.85	0.58
14:G:328:TYR:CE2	14:G:330:ALA:HB2	2.39	0.58
17:F:38:LEU:HD22	17:F:90:THR:HG21	1.84	0.58
32:q:80:TRP:HD1	32:q:101:GLN:HA	1.68	0.58
43:m:31:TYR:O	43:m:35:GLU:HG2	2.04	0.58
14:G:225:ARG:O	14:G:252:GLY:N	2.33	0.58
31:o:145:SER:OG	31:o:162:SER:O	2.21	0.58
37:a:115:CYS:O	37:a:119:ILE:HG13	2.03	0.58
37:a:236:ILE:O	37:a:239:HIS:ND1	2.25	0.58
10:W:14:GLU:HB3	10:W:17:VAL:HG12	1.86	0.57
27:Q:20:GLN:NE2	27:Q:53:CYS:O	2.37	0.57
32:q:17:GLU:HG3	32:p:23:ASP:CB	2.29	0.57
32:p:151:LEU:HD23	32:p:155:VAL:HG11	1.86	0.57
37:a:250:THR:HG21	37:a:353:GLY:HA2	1.86	0.57
2:I:147:ALA:HB2	4:N:151:TRP:NE1	2.19	0.57
5:H:42:VAL:HG23	22:U:38:ASN:H	1.68	0.57
5:H:318:LEU:HD22	5:H:323:TRP:HB2	1.85	0.57
15:C:103:PRO:HG3	15:C:155:ARG:HD3	1.86	0.57
15:C:603:GLN:HG3	15:C:656:ILE:HG21	1.85	0.57
33:M:203:LEU:HD22	33:M:271:MET:HE1	1.86	0.57
33:M:287:SER:O	33:M:291:ILE:HG13	2.03	0.57
33:M:461:ILE:O	33:M:464:LEU:HG	2.04	0.57
15:C:418:ASP:OD2	27:Q:40:LYS:NZ	2.29	0.57
16:T:80:LEU:HB2	16:T:222:MET:HE1	1.85	0.57
17:F:59:ILE:HG22	17:F:115:VAL:HG21	1.86	0.57
18:B:233:PRO:HD2	18:B:237:ASN:HA	1.85	0.57
21:R:26:VAL:HG22	21:R:87:GLU:HG3	1.85	0.57
27:Q:74:LEU:HD13	27:Q:82:ILE:HG12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:p:105:LEU:HB3	32:p:107:HIS:NE2	2.19	0.57
33:M:335:ILE:HD11	33:M:481:MET:HE2	1.87	0.57
34:f:39:ARG:O	34:f:43:ILE:HG12	2.04	0.57
32:q:117:VAL:HG13	32:q:118:HIS:H	1.69	0.57
32:p:135:HIS:N	32:p:137:CYS:SG	2.76	0.57
33:M:56:TRP:HB2	33:M:95:ILE:HD11	1.85	0.57
33:M:140:LEU:CD2	33:M:188:ILE:HG21	2.06	0.57
37:a:59:LEU:HB2	37:a:78:PHE:CE1	2.39	0.57
8:Z:21:LEU:H	11:S:58:ILE:HB	1.68	0.57
21:R:14:VAL:HG12	21:R:74:TRP:HE1	1.70	0.57
32:q:36:ARG:HB2	32:p:44:THR:HB	1.86	0.57
2:I:399:ALA:HB1	2:I:437:CYS:HA	1.87	0.57
17:F:157:TYR:HE1	17:F:168:PRO:HG3	1.70	0.57
23:E:130:THR:HG22	23:E:130:THR:O	2.05	0.57
23:E:158:CYS:N	45:E:301:SF4:S3	2.64	0.57
26:c:5:ILE:HG21	26:c:19:ASN:HB2	1.86	0.57
33:M:297:THR:O	33:M:300:ARG:N	2.36	0.57
33:M:319:VAL:HG11	33:M:338:MET:HG3	1.86	0.57
1:A:228:ILE:HD12	1:A:244:GLY:O	2.04	0.57
2:I:434:VAL:HG11	33:M:179:LEU:HB2	1.86	0.57
5:H:291:ARG:HG2	5:H:291:ARG:NH1	2.18	0.57
15:C:292:THR:HG22	15:C:293:ILE:H	1.70	0.57
15:C:445:THR:HG21	15:C:515:ILE:HG22	1.85	0.57
31:o:65:LEU:HD12	31:o:66:PRO:HD2	1.87	0.57
33:M:423:ILE:HG13	33:M:424:LEU:HD12	1.85	0.57
8:Z:34:ARG:HD2	8:Z:38:ARG:HG2	1.87	0.57
15:C:277:PRO:HB3	15:C:734:ILE:HD13	1.86	0.57
2:I:148:MET:HG3	2:I:276:ASN:ND2	2.19	0.57
2:I:419:GLY:O	43:m:39:LYS:NZ	2.30	0.57
13:j:14:CYS:HB2	13:j:17:PHE:HB2	1.87	0.57
14:G:90:LEU:HD13	14:G:294:LEU:HD13	1.85	0.57
1:A:64:ILE:O	1:A:160:LYS:NZ	2.35	0.57
32:q:80:TRP:CD1	32:q:101:GLN:HA	2.40	0.57
34:f:30:MET:O	34:f:33:MET:HG2	2.05	0.57
4:N:175:THR:HG22	4:N:176:LYS:H	1.70	0.56
5:H:204:ASP:HB2	5:H:207:GLU:CB	2.24	0.56
32:q:14:TRP:CD1	32:q:14:TRP:C	2.83	0.56
33:M:320:THR:HA	33:M:323:MET:HG3	1.86	0.56
37:a:125:LEU:HA	37:a:128:VAL:HG22	1.88	0.56
1:A:468:GLU:OE1	1:A:471:ARG:NH2	2.37	0.56
14:G:250:PRO:HB3	14:G:266:GLU:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:306:MET:HG3	15:C:163:LEU:HD22	1.87	0.56
15:C:131:VAL:HB	15:C:136:MET:HE3	1.87	0.56
15:C:397:LYS:NZ	27:Q:13:GLU:OE2	2.37	0.56
27:Q:14:LEU:HD23	27:Q:48:ILE:HG23	1.87	0.56
31:o:91:SER:HG	31:o:93:TRP:NE1	2.04	0.56
1:A:148:CYS:HB3	18:B:173:GLY:O	2.05	0.56
15:C:627:GLU:HB2	15:C:642:PRO:HD3	1.86	0.56
17:F:175:PHE:HB3	19:O:100:ASN:HD22	1.69	0.56
24:D:145:ARG:CZ	24:D:151:ARG:HG3	2.36	0.56
24:D:174:VAL:HG23	24:D:174:VAL:O	2.04	0.56
32:q:50:ASP:OD1	32:q:51:LYS:NZ	2.31	0.56
37:a:367:LYS:HB2	44:t:24:LEU:HD13	1.87	0.56
2:I:208:GLN:NE2	43:m:53:PHE:CZ	2.74	0.56
5:H:35:GLN:HG2	14:G:129:THR:HA	1.88	0.56
17:F:153:VAL:HG12	17:F:169:ILE:HA	1.87	0.56
32:q:66:SER:HG	32:p:64:SER:HG	1.52	0.56
33:M:349:PHE:HA	33:M:352:VAL:HG22	1.87	0.56
34:f:59:TYR:HD1	34:f:66:HIS:HB2	1.71	0.56
37:a:99:TYR:CE1	37:a:463:MET:HG3	2.41	0.56
37:a:178:LEU:HD13	37:a:268:MET:HE2	1.87	0.56
2:I:132:SER:HB2	2:I:158:CYS:HB2	1.87	0.56
2:I:415:PHE:HB2	33:M:189:LEU:CD2	2.35	0.56
32:p:46:MET:HB3	32:p:53:PRO:HG2	1.86	0.56
37:a:465:ILE:HA	37:a:468:ILE:HD12	1.86	0.56
1:A:158:PRO:HB2	1:A:192:LEU:HD13	1.88	0.56
14:G:47:LEU:HD22	14:G:389:PHE:C	2.30	0.56
15:C:161:PHE:HA	15:C:164:MET:HE3	1.87	0.56
16:T:328:LYS:HE2	16:T:331:PHE:HB3	1.87	0.56
17:F:48:HIS:HD2	17:F:51:THR:H	1.53	0.56
23:E:97:GLU:HG2	23:E:190:PRO:O	2.06	0.56
2:I:295:PHE:CZ	2:I:299:ILE:HD11	2.41	0.56
14:G:250:PRO:HG2	14:G:263:ILE:HG23	1.86	0.56
15:C:427:MET:HA	15:C:551:ASN:HB2	1.87	0.56
32:q:73:ILE:HG12	32:q:79:ILE:HD11	1.88	0.56
14:G:56:GLU:O	14:G:349:ARG:NH1	2.39	0.56
14:G:318:GLU:O	14:G:348:ASN:ND2	2.31	0.56
38:b:47:LEU:H	38:b:50:LYS:HE3	1.69	0.56
2:I:17:LEU:HB2	2:I:78:ILE:HG21	1.87	0.56
2:I:369:THR:HG22	2:I:456:ILE:HD13	1.88	0.56
48:I:502:CDL:H321	26:c:47:VAL:HG22	1.88	0.56
49:H:501:U10:C25	49:H:501:U10:H211	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:741:VAL:O	15:C:741:VAL:HG12	2.06	0.56
31:o:91:SER:OG	31:o:93:TRP:NE1	2.39	0.56
33:M:66:PHE:HA	33:M:87:ASP:HB3	1.88	0.56
37:a:84:VAL:O	37:a:88:VAL:HG23	2.05	0.56
37:a:117:LEU:O	37:a:121:THR:HG23	2.06	0.56
1:A:92:VAL:HG13	1:A:170:VAL:HG21	1.88	0.56
1:A:178:TYR:HB3	1:A:239:LEU:HD11	1.88	0.56
1:A:228:ILE:HD13	1:A:402:CYS:CB	2.24	0.56
2:I:362:ILE:HG13	2:I:469:LEU:HD11	1.87	0.56
48:I:502:CDL:H631	32:p:18:THR:HG21	1.88	0.56
14:G:168:PRO:HG2	14:G:171:LEU:HB2	1.87	0.56
23:E:131:LEU:HD23	23:E:172:VAL:HG21	1.88	0.56
36:d:16:GLN:O	36:d:20:VAL:N	2.25	0.56
43:m:66:ASP:OD1	43:m:66:ASP:N	2.39	0.56
14:G:93:GLU:HA	21:R:129:HIS:CE1	2.22	0.55
14:G:217:TRP:HA	17:F:107:SER:HB3	1.87	0.55
16:T:83:TYR:CE2	17:F:160:PRO:HB3	2.41	0.55
32:p:75:ARG:O	32:p:97:GLY:N	2.36	0.55
32:p:131:SER:HB2	32:p:148:GLY:HA2	1.88	0.55
6:K:56:MET:HE2	13:j:7:ILE:HA	1.88	0.55
15:C:212:LYS:HZ2	15:C:274:THR:CG2	2.19	0.55
15:C:257:THR:HA	15:C:741:VAL:HG13	1.87	0.55
19:O:76:ILE:HG13	19:O:108:PHE:HE2	1.69	0.55
1:A:180:TYR:CG	1:A:235:LEU:HD11	2.42	0.55
3:J:10:ILE:O	3:J:14:ILE:HG12	2.07	0.55
14:G:209:VAL:HG23	14:G:227:PRO:HG3	1.89	0.55
15:C:681:LYS:HB2	15:C:688:VAL:HG21	1.88	0.55
27:Q:15:ARG:NH1	27:Q:69:GLU:OE1	2.37	0.55
31:o:177:GLU:O	31:o:180:SER:OG	2.21	0.55
32:q:90:ASN:ND2	32:q:117:VAL:O	2.39	0.55
37:a:62:ALA:N	37:a:74:TRP:O	2.33	0.55
37:a:430:THR:HA	37:a:433:TYR:CZ	2.40	0.55
2:I:237:PHE:HB3	2:I:277:ILE:HD11	1.89	0.55
4:N:160:LEU:HA	4:N:163:MET:HE3	1.88	0.55
5:H:20:VAL:HG13	5:H:233:TYR:HB2	1.88	0.55
5:H:96:TYR:CZ	7:Y:91:LEU:HD21	2.42	0.55
28:k:109:SER:HA	28:k:112:ILE:HD12	1.87	0.55
1:A:172:MET:SD	1:A:264:THR:OG1	2.65	0.55
4:N:162:ALA:HB2	6:K:71:ALA:HB1	1.88	0.55
14:G:130:PRO:HG2	14:G:193:LEU:HD21	1.88	0.55
31:o:182:VAL:HA	31:o:199:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:f:51:LEU:HB3	34:f:77:TYR:HD1	1.70	0.55
5:H:270:SER:O	5:H:274:LEU:HG	2.06	0.55
15:C:608:ASP:OD2	15:C:730:ARG:NH2	2.38	0.55
37:a:281:THR:O	37:a:285:VAL:HG23	2.06	0.55
2:I:262:THR:O	2:I:266:SER:HB3	2.06	0.55
48:I:503:CDL:CB7	48:I:503:CDL:H742	2.37	0.55
15:C:207:LEU:HD12	15:C:213:THR:CG2	2.37	0.55
15:C:271:GLY:O	15:C:272:ALA:C	2.50	0.55
5:H:174:GLN:NE2	5:H:246:PHE:O	2.39	0.55
16:T:316:LYS:NZ	16:T:345:ASN:OD1	2.33	0.55
32:q:163:VAL:HG12	32:q:167:ALA:HB3	1.89	0.55
32:q:167:ALA:HB1	32:q:182:GLY:HA2	1.89	0.55
33:M:92:PHE:HA	33:M:95:ILE:HB	1.87	0.55
33:M:458:PHE:CZ	35:g:70:SER:HB3	2.42	0.55
48:I:503:CDL:C63	26:c:67:LEU:HD13	2.35	0.55
5:H:93:PRO:HB3	5:H:99:VAL:HB	1.88	0.55
14:G:68:ASP:OD1	14:G:68:ASP:N	2.28	0.55
14:G:385:GLN:HB2	14:G:387:ILE:HG12	1.88	0.55
15:C:225:VAL:HG23	15:C:248:ILE:HG23	1.87	0.55
18:B:138:ARG:HG3	18:B:178:ALA:HB1	1.88	0.55
19:O:46:PRO:HG2	19:O:49:HIS:HD2	1.72	0.55
43:m:17:GLU:HG3	43:m:19:PRO:HG3	1.88	0.55
1:A:145:PRO:HD2	1:A:345:SER:HB3	1.89	0.55
1:A:435:LEU:HB3	1:A:462:ILE:HD11	1.88	0.55
14:G:74:SER:OG	14:G:74:SER:O	2.21	0.55
14:G:310:ILE:HD12	15:C:163:LEU:HD11	1.89	0.55
31:o:146:LEU:HD11	32:q:130:HIS:HB2	1.89	0.55
48:I:502:CDL:OB7	48:I:502:CDL:H532	2.06	0.54
6:K:79:ILE:O	6:K:82:ILE:HG22	2.07	0.54
7:Y:103:CYS:HB3	7:Y:104:PRO:HD3	1.90	0.54
12:i:49:LEU:O	12:i:53:ASP:HB2	2.06	0.54
15:C:651:ARG:NE	25:X:130:SER:O	2.41	0.54
30:n:78:GLU:OE2	32:q:8:PHE:HB2	2.07	0.54
32:q:47:ASN:ND2	32:p:81:TYR:OH	2.41	0.54
37:a:104:MET:HG3	37:a:114:MET:SD	2.47	0.54
37:a:238:LEU:HA	37:a:562:ARG:HH12	1.72	0.54
37:a:433:TYR:HA	37:a:436:ARG:HB3	1.89	0.54
1:A:78:GLY:O	1:A:82:ARG:NH1	2.41	0.54
2:I:252:ASP:OD1	2:I:317:ARG:NH2	2.40	0.54
4:N:16:MET:HE3	4:N:20:ALA:HB2	1.88	0.54
5:H:21:ALA:O	5:H:24:VAL:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:34:VAL:HG13	24:D:83:THR:HG23	1.89	0.54
5:H:84:LEU:HA	5:H:87:VAL:HG12	1.90	0.54
13:j:15:TYR:CZ	43:m:65:TRP:CH2	2.96	0.54
14:G:72:TYR:CE2	23:E:92:ALA:HA	2.41	0.54
14:G:360:PHE:CE1	17:F:110:TRP:HB3	2.42	0.54
16:T:128:GLU:C	16:T:130:SER:H	2.13	0.54
33:M:109:TRP:HH2	35:g:67:TYR:HA	1.72	0.54
33:M:181:SER:HA	33:M:223:SER:CB	2.37	0.54
33:M:241:HIS:CE1	33:M:252:LEU:HB3	2.42	0.54
33:M:490:GLN:HG2	34:f:34:ARG:HH21	1.73	0.54
2:I:267:ILE:CG2	2:I:356:THR:HG23	2.37	0.54
48:I:503:CDL:H742	48:I:503:CDL:OB9	2.07	0.54
5:H:283:VAL:O	5:H:283:VAL:HG12	2.06	0.54
14:G:110:ARG:HA	14:G:334:PRO:HG3	1.89	0.54
15:C:109:SER:O	19:O:138:LYS:NZ	2.41	0.54
17:F:97:ARG:HG2	17:F:122:SER:HB2	1.87	0.54
22:U:46:ASN:HA	22:U:49:ALA:HB3	1.88	0.54
32:q:140:GLU:HG3	32:q:158:GLU:HA	1.89	0.54
1:A:122:TRP:N	1:A:122:TRP:CD1	2.75	0.54
14:G:69:ARG:CD	45:E:301:SF4:S2	2.92	0.54
20:P:58:SER:HA	20:P:103:ARG:HH22	1.72	0.54
33:M:125:ILE:HG23	33:M:251:ILE:HD11	1.90	0.54
33:M:281:PRO:HA	33:M:284:TYR:HD2	1.72	0.54
1:A:141:ASP:HA	1:A:182:ARG:HB2	1.89	0.54
1:A:446:THR:HB	45:A:501:SF4:S3	2.48	0.54
2:I:419:GLY:O	43:m:39:LYS:CD	2.56	0.54
49:H:501:U10:H101	49:H:501:U10:H153	1.89	0.54
32:q:43:ARG:O	32:q:47:ASN:ND2	2.38	0.54
32:q:135:HIS:CG	32:p:147:MET:HE3	2.43	0.54
33:M:49:PHE:CE2	35:g:77:LEU:HD21	2.42	0.54
33:M:410:ARG:HH12	33:M:413:LEU:HG	1.72	0.54
1:A:301:ILE:HA	1:A:377:VAL:HG13	1.88	0.54
3:J:81:TRP:CD2	3:J:96:MET:HG2	2.42	0.54
5:H:170:ILE:O	5:H:174:GLN:NE2	2.41	0.54
15:C:720:GLU:N	15:C:720:GLU:OE2	2.39	0.54
18:B:196:ASN:HB3	18:B:221:HIS:HB3	1.89	0.54
31:o:78:VAL:HG11	31:o:92:VAL:HG12	1.90	0.54
1:A:301:ILE:HG21	1:A:327:CYS:SG	2.48	0.54
4:N:144:LEU:HD11	6:K:64:LEU:HD21	1.90	0.54
17:F:38:LEU:HD21	17:F:75:TYR:CZ	2.43	0.54
32:q:107:HIS:HD2	32:p:130:HIS:CE1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:a:398:PHE:HZ	37:a:522:ILE:HD11	1.73	0.54
15:C:368:VAL:HG22	15:C:616:VAL:HG11	1.90	0.54
22:U:115:ARG:HD3	24:D:118:THR:HA	1.90	0.54
23:E:89:PHE:CE2	23:E:135:MET:HE3	2.43	0.54
32:q:18:THR:HG22	32:q:22:LEU:CD1	2.38	0.54
33:M:45:SER:O	33:M:48:THR:HG22	2.08	0.54
37:a:116:TYR:HA	37:a:119:ILE:HD12	1.89	0.54
37:a:283:LEU:HA	37:a:286:ILE:HD12	1.88	0.54
1:A:370:SER:OG	1:A:371:GLY:N	2.41	0.54
2:I:97:GLN:NE2	2:I:137:LEU:O	2.41	0.54
2:I:146:ILE:HG23	6:K:61:PHE:CD1	2.43	0.54
48:I:503:CDL:H162	48:I:503:CDL:C76	2.37	0.54
49:H:501:U10:C10	23:E:85:TRP:CH2	2.77	0.54
13:j:11:LYS:HD2	43:m:67:PRO:CG	2.37	0.54
18:B:228:ARG:NH1	18:B:232:GLY:O	2.41	0.54
37:a:620:PHE:HA	37:a:623:HIS:HB3	1.90	0.54
1:A:228:ILE:HG23	1:A:400:GLU:O	2.09	0.54
2:I:483:PRO:HG2	33:M:74:TRP:O	2.08	0.54
3:J:83:VAL:HG21	4:N:137:LEU:HB3	1.89	0.54
15:C:104:ARG:HG2	15:C:104:ARG:O	2.08	0.54
15:C:317:PRO:HB3	15:C:328:ILE:HG12	1.89	0.54
15:C:398:ASP:HB3	15:C:668:LEU:HD11	1.89	0.54
15:C:581:VAL:HB	15:C:600:VAL:HG22	1.89	0.54
32:p:126:VAL:HG12	32:p:128:ILE:HG13	1.89	0.54
1:A:74:PRO:HB3	1:A:157:ASP:H	1.72	0.53
1:A:138:VAL:HG11	1:A:161:LEU:HD11	1.90	0.53
2:I:32:LEU:HD21	2:I:57:LEU:HB3	1.89	0.53
13:j:11:LYS:HD2	43:m:67:PRO:HG3	1.89	0.53
18:B:178:ALA:HB3	18:B:179:PRO:HD3	1.90	0.53
22:U:38:ASN:HD22	23:E:110:ARG:HH22	1.54	0.53
32:q:42:HIS:CD2	32:p:43:ARG:HH11	2.26	0.53
37:a:569:LEU:O	37:a:573:LEU:HG	2.08	0.53
5:H:316:GLY:O	5:H:320:THR:HG23	2.08	0.53
21:R:129:HIS:CG	21:R:129:HIS:O	2.59	0.53
24:D:140:ILE:HA	24:D:154:ARG:O	2.08	0.53
33:M:328:ILE:HG13	33:M:329:GLN:N	2.24	0.53
37:a:198:PHE:O	37:a:202:SER:CB	2.53	0.53
37:a:599:PRO:HA	37:a:602:ILE:HB	1.91	0.53
2:I:397:SER:O	2:I:406:GLY:HA3	2.08	0.53
49:H:501:U10:C25	49:H:501:U10:C21	2.87	0.53
12:i:30:ARG:HH21	12:i:30:ARG:HG2	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:83:VAL:HG11	15:C:98:ALA:HB2	1.90	0.53
16:T:219:PRO:HG2	52:T:501:NDP:H6N	1.89	0.53
18:B:135:CYS:HB3	18:B:140:SER:HB2	1.90	0.53
22:U:126:GLY:HA3	24:D:188:GLU:HG3	1.89	0.53
24:D:178:VAL:HG21	24:D:211:ILE:HG21	1.90	0.53
43:m:28:GLU:O	43:m:31:TYR:HB2	2.09	0.53
2:I:197:ILE:HG13	2:I:229:GLY:HA3	1.90	0.53
48:I:502:CDL:H371	48:I:502:CDL:C19	2.10	0.53
48:J:401:CDL:C55	48:J:401:CDL:H711	2.38	0.53
5:H:42:VAL:CG1	23:E:111:PHE:HA	2.39	0.53
12:i:68:ARG:HG3	12:i:68:ARG:O	2.08	0.53
26:c:43:ILE:HG22	26:c:43:ILE:O	2.08	0.53
32:p:130:HIS:CD2	32:p:130:HIS:H	2.26	0.53
33:M:214:ILE:O	33:M:218:ILE:HG23	2.08	0.53
42:s:6:ALA:HB1	42:s:9:ALA:HB3	1.90	0.53
48:J:401:CDL:CA6	48:J:401:CDL:C11	2.78	0.53
4:N:133:SER:OG	9:V:44:GLU:OE1	2.23	0.53
5:H:130:SER:HB2	5:H:133:ALA:HB3	1.90	0.53
12:i:21:ASN:ND2	12:i:33:TRP:HH2	2.06	0.53
14:G:47:LEU:CD2	14:G:47:LEU:O	2.46	0.53
28:k:101:GLU:HG2	28:k:114:TYR:CZ	2.44	0.53
33:M:270:PRO:HB3	33:M:488:LEU:HG	1.89	0.53
33:M:362:ARG:HA	33:M:362:ARG:HE	1.72	0.53
1:A:289:GLY:HA2	1:A:316:SER:HB2	1.90	0.53
47:I:501:T7X:O6	47:I:501:T7X:O11	2.27	0.53
48:I:502:CDL:C62	48:I:502:CDL:H822	2.38	0.53
21:R:66:ASN:O	21:R:70:GLU:HG2	2.09	0.53
21:R:129:HIS:CD2	21:R:129:HIS:O	2.62	0.53
32:q:17:GLU:OE2	32:p:20:GLN:HA	2.09	0.53
32:q:68:ILE:HG21	32:p:214:HIS:HE1	1.74	0.53
32:q:105:LEU:HD23	32:q:133:VAL:HG22	1.91	0.53
32:q:105:LEU:O	32:q:107:HIS:N	2.33	0.53
32:p:92:VAL:HG12	32:p:94:VAL:HG23	1.90	0.53
33:M:116:GLY:HA2	33:M:160:TRP:HD1	1.74	0.53
33:M:230:MET:HA	33:M:317:ASN:HD21	1.74	0.53
33:M:478:LEU:HB3	33:M:482:HIS:CE1	2.44	0.53
5:H:24:VAL:HG12	5:H:233:TYR:CD2	2.44	0.53
5:H:167:LEU:HD23	5:H:245:LEU:HD13	1.91	0.53
16:T:68:GLY:O	16:T:139:ASN:ND2	2.42	0.53
31:o:89:GLY:O	31:o:221:ASN:ND2	2.42	0.53
35:g:62:TRP:CD1	35:g:64:LEU:HD22	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:a:24:GLY:HA2	37:a:37:SER:HA	1.90	0.53
2:I:207:ASP:OD1	43:m:50:PRO:O	2.27	0.53
14:G:84:LEU:HD13	21:R:131:PRO:HD3	1.91	0.53
14:G:245:LEU:HD13	14:G:274:ILE:HG23	1.91	0.53
17:F:102:VAL:HG11	17:F:127:PRO:HD2	1.90	0.53
17:F:135:ASP:OD2	17:F:156:ARG:NH1	2.42	0.53
19:O:42:VAL:HB	25:X:77:LEU:HD23	1.91	0.53
19:O:61:ARG:HB2	19:O:71:LEU:HD11	1.91	0.53
33:M:23:SER:HB2	33:M:123:PHE:CD1	2.43	0.53
37:a:322:MET:HE1	37:a:338:LEU:CA	2.39	0.53
5:H:21:ALA:HB2	49:H:501:U10:H202	1.91	0.53
5:H:306:LEU:O	5:H:310:TRP:HD1	1.91	0.53
13:j:11:LYS:HB2	43:m:66:ASP:HA	1.91	0.53
15:C:227:PHE:HB2	15:C:267:ILE:HD13	1.90	0.53
16:T:83:TYR:O	16:T:87:GLN:HG2	2.09	0.53
23:E:130:THR:HA	23:E:158:CYS:HB3	1.91	0.53
24:D:73:LEU:HD12	24:D:73:LEU:N	2.05	0.53
33:M:92:PHE:CZ	33:M:335:ILE:HD12	2.44	0.53
34:f:59:TYR:CD1	34:f:66:HIS:HB2	2.44	0.53
37:a:102:SER:OG	37:a:463:MET:HB2	2.08	0.53
3:J:71:PHE:CE1	5:H:304:LEU:HD21	2.44	0.53
9:V:44:GLU:HA	9:V:47:VAL:HG22	1.91	0.53
15:C:554:LEU:HD23	15:C:559:GLN:HB3	1.91	0.53
16:T:311:PRO:HD2	16:T:314:ILE:HD12	1.90	0.53
16:T:322:ARG:HD3	16:T:336:PRO:HB3	1.90	0.53
16:T:355:ASP:N	16:T:355:ASP:OD1	2.42	0.53
18:B:155:ARG:NH2	18:B:168:GLU:HB2	2.24	0.53
23:E:157:SER:N	45:E:301:SF4:S3	2.82	0.53
31:o:108:GLY:N	31:o:111:SER:OG	2.42	0.53
33:M:140:LEU:HD23	33:M:188:ILE:HG23	1.74	0.53
33:M:288:ALA:O	33:M:292:ILE:HG12	2.08	0.53
33:M:407:ALA:HA	33:M:410:ARG:HB2	1.89	0.53
33:M:455:ARG:O	33:M:459:ILE:HG23	2.09	0.53
37:a:304:GLN:H	37:a:436:ARG:NH1	2.06	0.53
1:A:405:CYS:HB3	1:A:447:ILE:HG13	1.91	0.52
2:I:244:VAL:HG11	2:I:300:ALA:HB3	1.91	0.52
48:J:401:CDL:C42	48:J:401:CDL:H612	2.39	0.52
49:H:501:U10:H211	49:H:501:U10:H252	1.91	0.52
7:Y:90:ASP:OD2	8:Z:74:LEU:HD21	2.09	0.52
10:W:5:GLU:HA	10:W:8:ARG:HH11	1.73	0.52
14:G:58:LYS:O	14:G:350:PRO:HD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:75:MET:N	14:G:75:MET:SD	2.82	0.52
15:C:110:ARG:HB2	15:C:327:TRP:HZ2	1.73	0.52
27:Q:59:GLN:OE1	27:Q:61:TRP:NE1	2.36	0.52
33:M:218:ILE:HA	33:M:221:PHE:HB3	1.91	0.52
33:M:315:HIS:O	33:M:319:VAL:HG23	2.09	0.52
34:f:60:ARG:HH22	37:a:60:ARG:HD2	1.73	0.52
14:G:299:ARG:NH2	24:D:172:CYS:O	2.42	0.52
17:F:95:VAL:HG11	25:X:74:VAL:HG22	1.92	0.52
24:D:111:HIS:H	24:D:159:MET:HE1	1.74	0.52
33:M:230:MET:HE2	33:M:320:THR:HG21	1.90	0.52
37:a:133:PHE:HA	37:a:136:LEU:HB3	1.91	0.52
2:I:39:PHE:CZ	26:c:60:PRO:HB2	2.44	0.52
50:H:502:PEV:H241	10:W:23:ILE:HD12	1.92	0.52
8:Z:7:ARG:HB3	8:Z:19:PRO:HD2	1.91	0.52
15:C:602:TYR:CZ	15:C:604:GLY:HA3	2.45	0.52
15:C:605:HIS:CD2	15:C:606:HIS:HD2	2.26	0.52
28:k:50:VAL:O	28:k:54:VAL:HG23	2.10	0.52
32:q:94:VAL:HG13	32:q:98:THR:HB	1.91	0.52
32:q:184:ASN:HD21	32:p:183:GLY:HA2	1.74	0.52
33:M:113:ARG:HG2	33:M:118:GLU:OE1	2.09	0.52
2:I:362:ILE:HD11	2:I:390:THR:HG22	1.92	0.52
48:I:503:CDL:HA4	48:I:503:CDL:OA9	2.10	0.52
5:H:176:GLN:HE21	8:Z:63:GLN:HE22	1.58	0.52
31:o:64:TRP:HB3	31:o:83:GLN:HG3	1.89	0.52
31:o:112:ASN:CG	31:o:220:ILE:HG21	2.33	0.52
33:M:87:ASP:OD1	33:M:266:ARG:NH1	2.43	0.52
33:M:92:PHE:HD1	33:M:339:LEU:HD21	1.73	0.52
33:M:276:THR:O	33:M:280:THR:HG23	2.10	0.52
37:a:352:ALA:O	37:a:356:ILE:HG13	2.10	0.52
37:a:578:LEU:HB3	37:a:582:TYR:CZ	2.44	0.52
1:A:323:ILE:HA	1:A:327:CYS:SG	2.49	0.52
50:H:502:PEV:H181	24:D:71:LEU:HD13	1.91	0.52
14:G:152:ARG:NH1	23:E:192:ALA:CB	2.70	0.52
33:M:109:TRP:CE3	35:g:65:PRO:HB2	2.44	0.52
2:I:312:GLN:NE2	2:I:317:ARG:HD2	2.24	0.52
48:J:401:CDL:H731	48:J:401:CDL:H562	1.91	0.52
8:Z:9:LYS:HB2	8:Z:19:PRO:HG3	1.90	0.52
8:Z:20:LEU:H	11:S:58:ILE:HG21	1.73	0.52
16:T:113:GLY:HA3	16:T:118:VAL:HG23	1.92	0.52
18:B:209:ILE:HD11	18:B:224:GLN:HG3	1.92	0.52
24:D:124:ILE:O	24:D:124:ILE:HD12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:o:91:SER:HG	31:o:93:TRP:CD1	2.27	0.52
31:o:152:ILE:HD13	31:o:158:ILE:HG13	1.91	0.52
32:q:22:LEU:C	32:q:24:ARG:N	2.67	0.52
1:A:180:TYR:CD1	1:A:235:LEU:HD11	2.45	0.52
2:I:59:LEU:O	2:I:63:LEU:HG	2.08	0.52
2:I:346:LEU:HD13	2:I:493:MET:HE2	1.92	0.52
8:Z:82:ARG:NH1	9:V:43:ASP:OD2	2.33	0.52
8:Z:115:VAL:CG1	8:Z:116:PRO:HD3	2.40	0.52
8:Z:126:ASN:HD22	13:j:43:GLU:HG3	1.75	0.52
15:C:176:GLY:HA2	45:C:801:SF4:S3	2.50	0.52
18:B:202:THR:H	18:B:205:LYS:HB2	1.74	0.52
23:E:185:VAL:HG22	23:E:198:GLY:HA3	1.91	0.52
25:X:16:SER:OG	25:X:76:ASP:OD2	2.23	0.52
32:q:135:HIS:HB2	32:p:147:MET:HG2	1.92	0.52
33:M:356:TYR:HB2	33:M:362:ARG:NH1	2.24	0.52
37:a:629:LEU:O	37:a:633:THR:HG23	2.09	0.52
38:b:37:LEU:HG	38:b:41:ARG:HE	1.74	0.52
1:A:110:GLY:N	1:A:116:PHE:O	2.43	0.52
4:N:62:ALA:HB3	5:H:119:TYR:OH	2.10	0.52
5:H:192:ILE:HG22	5:H:192:ILE:O	2.10	0.52
14:G:212:GLN:NE2	14:G:216:ASP:OD1	2.43	0.52
15:C:391:GLU:HA	15:C:680:ILE:HD11	1.92	0.52
15:C:443:ILE:HD12	15:C:533:VAL:HG22	1.92	0.52
31:o:108:GLY:N	31:o:135:ILE:O	2.41	0.52
32:q:184:ASN:ND2	32:p:184:ASN:H	2.08	0.52
37:a:246:MET:HG2	37:a:308:LYS:HB2	1.91	0.52
1:A:471:ARG:NH1	1:A:475:GLU:OE1	2.43	0.52
48:J:401:CDL:H751	48:J:401:CDL:C23	2.36	0.52
5:H:42:VAL:HG11	23:E:111:PHE:HA	1.90	0.52
50:H:502:PEV:HN61	10:W:15:PRO:HD2	1.74	0.52
12:i:35:HIS:CG	12:i:35:HIS:O	2.63	0.52
16:T:149:TYR:HB3	16:T:340:ASN:HD21	1.74	0.52
27:Q:72:VAL:HG11	27:Q:85:ALA:HB1	1.91	0.52
37:a:17:GLY:O	37:a:21:ARG:NH1	2.43	0.52
22:U:75:TRP:CB	24:D:99:GLU:HB3	2.39	0.52
37:a:595:GLU:O	37:a:599:PRO:HD2	2.09	0.52
38:b:14:GLN:HA	38:b:24:LEU:HD21	1.91	0.52
1:A:221:HIS:CD2	1:A:239:LEU:HG	2.45	0.51
2:I:32:LEU:HB3	2:I:54:VAL:HG13	1.92	0.51
2:I:491:HIS:O	2:I:495:LEU:HG	2.10	0.51
3:J:69:LEU:HD23	6:K:74:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:233:TYR:O	5:H:237:ILE:HG13	2.09	0.51
6:K:59:GLN:HE22	13:j:7:ILE:HG23	1.75	0.51
14:G:81:ALA:HB2	14:G:331:VAL:HG22	1.90	0.51
15:C:402:ARG:NH2	27:Q:67:GLY:O	2.44	0.51
20:P:70:VAL:HG13	20:P:89:LEU:HD11	1.93	0.51
23:E:161:GLY:HA3	24:D:160:THR:HB	1.92	0.51
24:D:125:ALA:HB2	24:D:152:THR:HG22	1.90	0.51
33:M:60:ASP:OD1	35:g:87:LEU:HB3	2.10	0.51
37:a:74:TRP:HZ3	37:a:135:GLN:H	1.58	0.51
37:a:89:VAL:HA	37:a:92:ILE:HD12	1.92	0.51
48:I:502:CDL:H402	48:I:502:CDL:C45	2.40	0.51
5:H:323:TRP:HB3	8:Z:65:GLY:HA2	1.92	0.51
13:j:5:TRP:CE3	43:m:65:TRP:CB	2.86	0.51
15:C:146:THR:O	15:C:155:ARG:NH2	2.43	0.51
15:C:427:MET:HG3	15:C:551:ASN:HB2	1.93	0.51
16:T:62:GLY:HA3	16:T:90:LYS:O	2.10	0.51
16:T:237:VAL:HG13	16:T:241:GLY:HA2	1.92	0.51
32:q:22:LEU:C	32:q:24:ARG:H	2.17	0.51
33:M:139:LEU:HB3	33:M:267:PHE:CD2	2.45	0.51
33:M:264:PHE:O	33:M:268:SER:HB3	2.09	0.51
37:a:124:MET:SD	37:a:259:ALA:HB1	2.50	0.51
37:a:137:PHE:HD1	37:a:178:LEU:HD23	1.76	0.51
43:m:48:ILE:HG13	43:m:50:PRO:HD2	1.91	0.51
1:A:231:GLU:N	1:A:231:GLU:OE2	2.44	0.51
1:A:248:LEU:HD11	15:C:115:GLY:HA3	1.91	0.51
48:I:502:CDL:H402	48:I:502:CDL:H452	1.92	0.51
5:H:28:ARG:CZ	23:E:114:ILE:HD11	2.40	0.51
5:H:29:LYS:NZ	9:V:7:GLU:OE2	2.42	0.51
5:H:201:ALA:HB1	5:H:202:PRO:HD2	1.93	0.51
15:C:338:GLY:O	15:C:606:HIS:HE1	1.93	0.51
15:C:627:GLU:OE2	15:C:639:GLN:NE2	2.43	0.51
15:C:649:ASP:OD1	15:C:651:ARG:NH1	2.31	0.51
33:M:170:ALA:HB3	33:M:173:PHE:HB3	1.92	0.51
34:f:41:LYS:HA	34:f:44:HIS:CE1	2.44	0.51
37:a:218:ILE:HB	37:a:278:TYR:HE1	1.75	0.51
37:a:234:ALA:CA	37:a:239:HIS:HA	2.40	0.51
1:A:237:GLU:HG2	1:A:247:ARG:HH21	1.74	0.51
2:I:59:LEU:CD1	2:I:105:ALA:CA	2.87	0.51
48:I:503:CDL:PB2	30:n:81:ASN:ND2	2.79	0.51
5:H:95:ASP:OD1	5:H:96:TYR:N	2.42	0.51
5:H:195:LEU:HD13	5:H:202:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:S:61:SER:OG	14:G:292:ARG:NH1	2.31	0.51
14:G:21:ALA:HA	23:E:90:GLY:HA3	1.93	0.51
17:F:63:ASP:CG	17:F:70:ARG:HH21	2.18	0.51
24:D:77:VAL:O	24:D:77:VAL:HG12	2.10	0.51
10:W:11:VAL:HG22	10:W:18:ALA:HB1	1.92	0.51
15:C:105:PHE:HZ	15:C:181:LEU:HA	1.76	0.51
16:T:225:THR:O	16:T:226:GLU:HG2	2.10	0.51
17:F:53:VAL:HG23	17:F:54:GLN:H	1.76	0.51
22:U:137:GLY:HA2	22:U:144:GLN:HG3	1.92	0.51
33:M:235:ILE:O	33:M:238:PRO:HD2	2.10	0.51
37:a:236:ILE:HG23	37:a:237:GLY:H	1.76	0.51
37:a:322:MET:HE1	37:a:338:LEU:HA	1.93	0.51
38:b:47:LEU:N	38:b:50:LYS:HE3	2.26	0.51
48:J:401:CDL:H591	48:J:401:CDL:C44	2.40	0.51
14:G:27:ARG:NE	14:G:46:LEU:HD21	2.25	0.51
14:G:44:ILE:HD11	14:G:363:LEU:HD23	1.93	0.51
14:G:138:ARG:O	14:G:142:LEU:HG	2.11	0.51
14:G:257:CYS:SG	14:G:260:ARG:NH2	2.84	0.51
15:C:239:ILE:HD11	15:C:246:GLU:CD	2.35	0.51
21:R:30:ARG:O	21:R:34:ILE:HG12	2.11	0.51
26:c:36:ARG:NH1	26:c:80:ASN:OD1	2.43	0.51
32:q:72:HIS:O	32:q:94:VAL:N	2.43	0.51
32:q:77:SER:HB2	32:q:97:GLY:H	1.74	0.51
37:a:550:THR:HG22	37:a:552:CYS:H	1.75	0.51
1:A:228:ILE:HD11	18:B:113:PHE:CE2	2.45	0.51
1:A:248:LEU:HB3	1:A:250:PRO:HD2	1.93	0.51
9:V:43:ASP:OD1	9:V:43:ASP:N	2.43	0.51
12:i:17:GLN:NE2	12:i:17:GLN:CA	2.72	0.51
15:C:367:VAL:O	15:C:371:ILE:HG12	2.11	0.51
16:T:300:MET:O	16:T:382:ARG:NE	2.40	0.51
17:F:24:ARG:NH1	17:F:87:ARG:HH21	2.08	0.51
32:p:207:TYR:HA	32:p:210:LEU:HB3	1.91	0.51
33:M:223:SER:O	33:M:227:LYS:HG2	2.11	0.51
37:a:97:HIS:CE1	37:a:117:LEU:HD23	2.45	0.51
37:a:150:LEU:HB3	37:a:252:VAL:HG13	1.92	0.51
2:I:189:ILE:HD13	6:K:14:PHE:HZ	1.75	0.51
3:J:99:PHE:HD2	4:N:156:SER:HB2	1.75	0.51
4:N:195:MET:C	31:o:102:LEU:HD13	2.36	0.51
5:H:283:VAL:O	5:H:283:VAL:CG1	2.59	0.51
15:C:574:ALA:C	15:C:576:GLU:H	2.19	0.51
17:F:157:TYR:CE1	17:F:168:PRO:HG3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:E:173:ARG:N	23:E:173:ARG:HD2	2.26	0.51
32:p:29:LEU:C	32:p:29:LEU:CD2	2.84	0.51
33:M:82:PHE:CD1	33:M:141:LEU:HD23	2.46	0.51
37:a:341:HIS:NE2	37:a:345:LYS:HE2	2.26	0.51
37:a:366:ARG:HH22	44:t:20:LYS:HG3	1.75	0.51
37:a:613:ILE:HA	37:a:616:LEU:HD13	1.93	0.51
2:I:18:ALA:HB2	2:I:78:ILE:HG22	1.92	0.51
2:I:244:VAL:HB	2:I:301:SER:HA	1.93	0.51
14:G:321:SER:O	14:G:321:SER:OG	2.28	0.51
22:U:115:ARG:NH2	22:U:115:ARG:HB3	2.26	0.51
26:c:62:MET:HE1	30:n:81:ASN:HA	1.92	0.51
32:q:22:LEU:O	32:q:24:ARG:N	2.43	0.51
32:q:96:SER:N	32:q:124:ASP:OD1	2.44	0.51
33:M:38:ARG:HG3	33:M:118:GLU:HG2	1.92	0.51
33:M:377:PHE:HA	33:M:380:ILE:HG22	1.93	0.51
38:b:47:LEU:O	38:b:50:LYS:HG2	2.11	0.51
2:I:84:ASN:ND2	43:m:56:PHE:HB3	2.20	0.51
2:I:146:ILE:HG12	6:K:61:PHE:CD2	2.45	0.51
13:j:15:TYR:CD1	43:m:65:TRP:HZ3	2.29	0.51
14:G:136:GLU:HG2	24:D:92:VAL:HG21	1.92	0.51
15:C:213:THR:HG22	15:C:273:LEU:HD22	1.93	0.51
15:C:411:GLU:OE1	15:C:588:ASP:N	2.44	0.51
22:U:38:ASN:HD22	23:E:110:ARG:NH2	2.09	0.51
27:Q:35:ASN:HD21	27:Q:83:LEU:HD13	1.76	0.51
33:M:37:ILE:HG13	33:M:38:ARG:N	2.26	0.51
33:M:136:MET:HE3	33:M:145:PHE:CE2	2.46	0.51
8:Z:111:VAL:HG21	13:j:61:GLU:HB2	1.92	0.50
15:C:304:ARG:HB2	15:C:316:ILE:HG22	1.92	0.50
16:T:97:VAL:O	16:T:120:PRO:HA	2.11	0.50
17:F:9:TYR:CZ	17:F:13:THR:HG21	2.45	0.50
33:M:23:SER:HB2	33:M:123:PHE:HD1	1.75	0.50
33:M:143:TYR:HB2	33:M:188:ILE:HD13	1.92	0.50
33:M:350:LEU:HD11	33:M:459:ILE:HG13	1.93	0.50
37:a:218:ILE:HB	37:a:278:TYR:CE1	2.46	0.50
37:a:230:VAL:HG12	37:a:238:LEU:HG	1.93	0.50
1:A:186:VAL:HB	18:B:195:TYR:HB3	1.94	0.50
2:I:75:LEU:O	2:I:78:ILE:HB	2.11	0.50
2:I:179:TYR:HB2	2:I:253:ILE:HG23	1.93	0.50
14:G:48:HIS:CG	14:G:48:HIS:O	2.61	0.50
24:D:112:ALA:HB1	24:D:204:GLY:HA3	1.94	0.50
32:q:64:SER:OG	32:q:82:GLY:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:q:179:GLU:HA	32:q:191:LYS:HD3	1.92	0.50
37:a:405:LEU:HD13	37:a:425:VAL:HB	1.93	0.50
37:a:408:ALA:HB1	37:a:421:TRP:HB3	1.93	0.50
1:A:228:ILE:HG21	1:A:402:CYS:H	1.76	0.50
2:I:202:GLY:HA2	6:K:53:LEU:HD13	1.93	0.50
47:I:501:T7X:O4	48:I:502:CDL:HA21	2.11	0.50
3:J:69:LEU:HD11	6:K:70:ALA:HB1	1.93	0.50
12:i:11:LEU:O	12:i:11:LEU:HD12	2.11	0.50
23:E:188:CYS:O	45:E:301:SF4:S1	2.69	0.50
32:p:207:TYR:N	32:p:207:TYR:CD1	2.76	0.50
37:a:392:PHE:CG	37:a:393:PRO:HD2	2.46	0.50
2:I:114:PHE:CG	2:I:260:PRO:HG3	2.46	0.50
48:I:503:CDL:H792	48:I:503:CDL:C64	2.41	0.50
15:C:465:SER:O	15:C:467:ALA:N	2.44	0.50
32:q:42:HIS:CD2	32:p:43:ARG:HD3	2.47	0.50
33:M:27:LEU:HA	33:M:119:TYR:CE2	2.46	0.50
1:A:227:TYR:HB3	1:A:400:GLU:HB3	1.93	0.50
2:I:140:ILE:HD11	2:I:272:SER:HA	1.93	0.50
50:H:502:PEV:H441	24:D:73:LEU:HD13	1.94	0.50
14:G:362:HIS:O	14:G:385:GLN:NE2	2.44	0.50
15:C:222:THR:O	15:C:226:ARG:HG3	2.12	0.50
15:C:284:ASN:ND2	15:C:284:ASN:O	2.45	0.50
15:C:348:MET:HB3	15:C:356:PHE:HB3	1.93	0.50
21:R:130:VAL:HG22	21:R:131:PRO:HD2	1.93	0.50
23:E:84:ILE:HG23	23:E:113:ILE:HG13	1.93	0.50
25:X:40:ILE:HD12	25:X:89:ILE:HG22	1.92	0.50
31:o:79:VAL:HG11	32:q:81:TYR:CG	2.46	0.50
33:M:485:VAL:O	33:M:489:VAL:HG23	2.10	0.50
1:A:480:GLU:O	1:A:481:LEU:HG	2.12	0.50
2:I:437:CYS:HB3	33:M:178:LEU:CD2	2.41	0.50
48:J:401:CDL:H612	48:J:401:CDL:H422	1.93	0.50
15:C:57:ARG:CZ	15:C:81:TYR:HB3	2.41	0.50
20:P:65:VAL:O	20:P:107:ASP:HB3	2.11	0.50
27:Q:14:LEU:O	27:Q:49:LEU:N	2.43	0.50
31:o:50:TRP:CD1	32:q:43:ARG:HA	2.47	0.50
33:M:225:ALA:HA	33:M:228:VAL:HB	1.94	0.50
37:a:83:VAL:HA	37:a:86:LEU:HD12	1.94	0.50
37:a:534:ASN:HD21	37:a:537:PRO:HA	1.75	0.50
38:b:62:GLU:HA	38:b:65:LEU:HB2	1.93	0.50
2:I:290:LEU:O	2:I:293:ILE:HG22	2.12	0.50
48:I:502:CDL:H592	48:I:502:CDL:H782	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:I:503:CDL:H162	48:I:503:CDL:C77	2.42	0.50
5:H:154:ILE:HG23	5:H:186:VAL:HG12	1.94	0.50
8:Z:47:MET:C	8:Z:49:MET:H	2.17	0.50
14:G:264:ARG:NE	14:G:386:ASP:OD2	2.45	0.50
20:P:100:CYS:O	20:P:100:CYS:SG	2.69	0.50
32:p:60:PHE:HB3	32:p:211:ALA:HB1	1.94	0.50
32:p:98:THR:HG22	32:p:126:VAL:H	1.77	0.50
33:M:262:TYR:CZ	33:M:266:ARG:HG3	2.47	0.50
37:a:318:GLN:HB3	37:a:341:HIS:CE1	2.46	0.50
38:b:34:LEU:HD11	38:b:58:TYR:CZ	2.46	0.50
12:i:39:MET:HE3	12:i:43:ALA:HB2	1.93	0.50
13:j:15:TYR:CZ	43:m:65:TRP:CZ3	3.00	0.50
14:G:53:LYS:HE3	17:F:149:LEU:HA	1.94	0.50
15:C:485:LEU:HD22	15:C:500:HIS:HE2	1.76	0.50
16:T:261:VAL:HG13	16:T:282:LEU:HD12	1.93	0.50
17:F:44:PHE:O	17:F:45:LEU:HB2	2.11	0.50
32:q:168:LEU:HD22	32:p:166:GLY:HA3	1.92	0.50
33:M:176:TYR:CD1	33:M:176:TYR:C	2.90	0.50
33:M:318:LEU:O	33:M:321:ILE:HG22	2.12	0.50
2:I:437:CYS:HB3	33:M:178:LEU:HD21	1.94	0.50
5:H:22:PHE:CD1	5:H:51:PRO:HG2	2.46	0.50
5:H:323:TRP:HB3	8:Z:65:GLY:CA	2.42	0.50
8:Z:37:ARG:HD2	8:Z:39:ILE:HD12	1.94	0.50
15:C:186:MET:HG3	15:C:186:MET:O	2.12	0.50
18:B:149:ASP:OD1	18:B:150:HIS:N	2.45	0.50
18:B:226:PRO:O	18:B:227:LYS:NZ	2.34	0.50
25:X:95:GLN:OE1	25:X:97:HIS:N	2.45	0.50
31:o:50:TRP:HZ2	32:q:41:ARG:HA	1.77	0.50
31:o:79:VAL:HG11	32:q:81:TYR:CD1	2.46	0.50
31:o:188:ILE:HG23	31:o:194:TRP:CD1	2.46	0.50
37:a:9:PRO:HG3	37:a:48:TYR:CE1	2.46	0.50
37:a:310:VAL:HA	37:a:313:TYR:CD2	2.46	0.50
38:b:49:TRP:CD1	38:b:49:TRP:H	2.30	0.50
1:A:337:LEU:HD21	1:A:340:ILE:HG13	1.93	0.49
1:A:340:ILE:HD12	1:A:355:CYS:SG	2.51	0.49
5:H:74:PHE:HE2	5:H:219:GLU:HB3	1.77	0.49
14:G:146:GLU:OE1	24:D:104:SER:OG	2.19	0.49
15:C:105:PHE:CZ	15:C:181:LEU:HA	2.47	0.49
16:T:174:HIS:ND1	16:T:174:HIS:O	2.45	0.49
32:q:68:ILE:HG21	32:p:214:HIS:CE1	2.46	0.49
33:M:143:TYR:CD2	33:M:185:LEU:HD13	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ILE:HG21	1:A:402:CYS:N	2.27	0.49
1:A:343:GLY:H	1:A:347:VAL:HG21	1.77	0.49
3:J:98:ALA:HA	48:J:401:CDL:H401	1.94	0.49
7:Y:86:THR:OG1	7:Y:86:THR:O	2.28	0.49
13:j:11:LYS:H	43:m:65:TRP:C	2.20	0.49
14:G:53:LYS:HE2	17:F:147:PHE:HD2	1.77	0.49
15:C:295:VAL:HG23	15:C:387:LEU:HD22	1.94	0.49
15:C:680:ILE:HA	15:C:683:VAL:HG12	1.94	0.49
16:T:78:GLY:HA3	52:T:501:NDP:H52A	1.95	0.49
16:T:182:GLN:HG2	16:T:207:VAL:HG11	1.94	0.49
22:U:94:HIS:ND1	22:U:94:HIS:O	2.45	0.49
24:D:213:GLU:OE1	24:D:216:ARG:NH1	2.45	0.49
31:o:60:PRO:HB3	31:o:65:LEU:HD13	1.94	0.49
33:M:94:VAL:HG11	33:M:135:CYS:SG	2.53	0.49
33:M:335:ILE:CD1	33:M:481:MET:HG3	2.42	0.49
33:M:392:PRO:HG2	37:a:141:GLU:HB3	1.94	0.49
2:I:40:SER:HB3	4:N:176:LYS:NZ	2.27	0.49
4:N:188:ILE:HG13	31:o:63:GLN:HG2	1.93	0.49
5:H:207:GLU:HG3	5:H:212:LEU:HD13	1.93	0.49
17:F:58:ASP:OD1	17:F:59:ILE:N	2.45	0.49
32:p:187:ARG:HG3	32:p:187:ARG:O	2.12	0.49
37:a:558:PHE:HA	37:a:564:PHE:HB3	1.94	0.49
38:b:14:GLN:O	38:b:24:LEU:HD11	2.12	0.49
1:A:154:MET:O	1:A:158:PRO:HB3	2.11	0.49
1:A:433:ASP:CG	1:A:466:ARG:HH22	2.19	0.49
2:I:39:PHE:CZ	26:c:60:PRO:CB	2.95	0.49
8:Z:135:THR:OG1	8:Z:136:GLY:N	2.45	0.49
15:C:196:THR:O	15:C:197:GLU:HG3	2.12	0.49
15:C:281:LYS:HA	24:D:142:ALA:O	2.11	0.49
16:T:60:THR:HG23	16:T:61:GLY:H	1.77	0.49
26:c:47:VAL:O	26:c:47:VAL:HG12	2.11	0.49
32:p:124:ASP:H	32:p:141:ASP:HA	1.78	0.49
33:M:78:GLU:HA	43:m:35:GLU:HG3	1.94	0.49
33:M:312:SER:HB3	33:M:341:HIS:HE2	1.78	0.49
37:a:109:HIS:HB2	37:a:153:PHE:HE1	1.77	0.49
37:a:124:MET:HA	37:a:127:LEU:HD12	1.95	0.49
37:a:276:PHE:HD2	37:a:286:ILE:HD11	1.77	0.49
1:A:302:SER:OG	18:B:134:PRO:HB3	2.11	0.49
2:I:147:ALA:HB2	4:N:151:TRP:HE1	1.75	0.49
48:I:503:CDL:H841	3:J:101:PHE:CZ	2.46	0.49
6:K:79:ILE:O	6:K:82:ILE:CG2	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:10:ASN:OD1	7:Y:10:ASN:N	2.45	0.49
11:S:121:LEU:HD23	11:S:121:LEU:H	1.77	0.49
12:i:14:LEU:HG	12:i:33:TRP:CD1	2.45	0.49
14:G:152:ARG:HH12	23:E:192:ALA:HB2	1.77	0.49
16:T:95:VAL:N	16:T:117:GLN:O	2.43	0.49
17:F:39:PHE:CD1	17:F:39:PHE:C	2.90	0.49
21:R:30:ARG:HG3	21:R:77:ILE:HD11	1.94	0.49
37:a:150:LEU:HB3	37:a:252:VAL:CG1	2.43	0.49
6:K:19:TRP:O	6:K:23:LEU:HG	2.12	0.49
16:T:312:PHE:CZ	16:T:348:THR:HA	2.47	0.49
22:U:56:LYS:NZ	22:U:92:GLU:OE1	2.44	0.49
32:q:173:THR:HG21	32:q:186:ALA:HB1	1.95	0.49
32:p:113:LEU:HD22	33:M:112:MET:HE2	1.94	0.49
33:M:348:LEU:O	33:M:352:VAL:HG13	2.13	0.49
37:a:336:PHE:HE2	37:a:496:SER:HB3	1.76	0.49
48:I:503:CDL:H721	48:I:503:CDL:H761	1.94	0.49
48:J:401:CDL:H711	48:J:401:CDL:H551	1.93	0.49
5:H:248:LEU:HD22	5:H:276:PHE:HE2	1.77	0.49
15:C:239:ILE:HG23	15:C:239:ILE:O	2.13	0.49
16:T:111:LEU:O	16:T:112:MET:HG2	2.12	0.49
16:T:360:PHE:CE2	16:T:367:PRO:HB3	2.48	0.49
17:F:48:HIS:O	17:F:52:ARG:HG2	2.12	0.49
33:M:92:PHE:HA	33:M:95:ILE:HD12	1.93	0.49
35:g:73:THR:O	35:g:76:ILE:HG22	2.12	0.49
11:S:50:PRO:HB2	24:D:105:PRO:CD	2.42	0.49
33:M:56:TRP:CD1	33:M:91:LEU:HD21	2.48	0.49
33:M:356:TYR:OH	33:M:360:LYS:NZ	2.34	0.49
34:f:58:CYS:O	34:f:62:GLU:HG2	2.13	0.49
1:A:408:CYS:HB3	45:A:501:SF4:S4	2.53	0.49
48:I:502:CDL:H371	48:I:502:CDL:H161	1.95	0.49
13:j:15:TYR:CE1	43:m:65:TRP:CZ3	3.01	0.49
14:G:352:ARG:HG2	17:F:62:VAL:HG22	1.95	0.49
15:C:212:LYS:HE3	15:C:274:THR:HG23	1.95	0.49
16:T:58:LYS:HE3	16:T:66:VAL:HG21	1.95	0.49
18:B:100:ILE:HG23	18:B:102:VAL:HG22	1.95	0.49
19:O:100:ASN:OD1	19:O:101:VAL:N	2.46	0.49
22:U:116:TYR:HE1	24:D:117:PRO:HA	1.78	0.49
24:D:52:LEU:O	24:D:56:ILE:HG12	2.13	0.49
31:o:209:GLU:O	31:o:213:ILE:HG13	2.12	0.49
1:A:381:ASP:O	1:A:384:THR:HG22	2.11	0.49
48:I:502:CDL:HB22	48:I:502:CDL:CA5	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:80:PRO:HB2	4:N:145:TYR:HE2	1.77	0.49
5:H:37:ARG:HB2	23:E:107:ASP:OD2	2.13	0.49
5:H:37:ARG:HD2	23:E:107:ASP:OD1	2.12	0.49
15:C:277:PRO:HB3	15:C:734:ILE:CD1	2.43	0.49
15:C:349:ILE:HG22	15:C:616:VAL:HG23	1.94	0.49
24:D:172:CYS:SG	24:D:175:ASP:N	2.85	0.49
31:o:103:ASN:ND2	31:o:122:ALA:O	2.44	0.49
32:q:18:THR:CG2	32:q:22:LEU:CD1	2.91	0.49
32:q:141:ASP:OD1	32:q:142:GLU:N	2.46	0.49
32:p:179:GLU:HB3	32:p:181:TRP:HE1	1.77	0.49
1:A:361:ASP:OD1	1:A:361:ASP:N	2.45	0.48
2:I:426:ALA:O	2:I:430:VAL:HG23	2.12	0.48
16:T:152:ARG:HH11	16:T:332:PRO:HG3	1.78	0.48
16:T:282:LEU:HD22	16:T:360:PHE:HE1	1.78	0.48
27:Q:7:ILE:HG12	27:Q:90:VAL:HG21	1.94	0.48
32:p:139:VAL:HG23	32:p:157:VAL:HB	1.95	0.48
33:M:304:LEU:N	33:M:364:VAL:HG21	2.27	0.48
37:a:225:LEU:HD12	37:a:268:MET:SD	2.53	0.48
1:A:71:LEU:HD11	18:B:237:ASN:HD21	1.78	0.48
2:I:326:HIS:HA	2:I:329:TYR:HD2	1.78	0.48
48:I:502:CDL:H742	48:I:502:CDL:C22	2.24	0.48
8:Z:112:MET:O	8:Z:116:PRO:HD2	2.12	0.48
14:G:94:VAL:CG2	21:R:129:HIS:CD2	2.90	0.48
15:C:550:LEU:HD11	15:C:552:PHE:HE1	1.78	0.48
16:T:84:LEU:HD23	16:T:144:LEU:HD11	1.95	0.48
18:B:68:TYR:CZ	19:O:147:LYS:HG2	2.48	0.48
19:O:58:SER:HB3	19:O:130:PRO:HB3	1.94	0.48
27:Q:11:MET:HE1	27:Q:14:LEU:HB2	1.95	0.48
31:o:50:TRP:H	32:q:45:LEU:HB3	1.78	0.48
33:M:188:ILE:O	33:M:191:ILE:HG12	2.12	0.48
37:a:497:LEU:O	37:a:501:PRO:HB3	2.13	0.48
1:A:57:GLY:HA2	1:A:325:ARG:HH12	1.78	0.48
5:H:52:LEU:HG	49:H:501:U10:H251	1.94	0.48
8:Z:118:TRP:HH2	13:j:56:ARG:HD3	1.78	0.48
15:C:409:TRP:HD1	15:C:410:CYS:O	1.95	0.48
31:o:54:GLY:HA2	32:q:42:HIS:CE1	2.48	0.48
32:p:94:VAL:HG22	32:p:122:ILE:HD12	1.95	0.48
33:M:31:ASN:ND2	33:M:36:LEU:HB3	2.27	0.48
33:M:307:ILE:HG21	33:M:432:LEU:HG	1.94	0.48
33:M:413:LEU:O	33:M:416:THR:OG1	2.31	0.48
37:a:41:ILE:CD1	37:a:114:MET:HG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:m:63:LEU:HD12	43:m:64:ARG:N	2.28	0.48
4:N:67:PHE:HA	4:N:70:MET:HE2	1.95	0.48
5:H:74:PHE:HB3	5:H:127:SER:CB	2.42	0.48
14:G:175:ILE:HG22	14:G:279:LEU:HD11	1.96	0.48
16:T:172:LYS:HD2	16:T:210:ALA:O	2.14	0.48
32:q:18:THR:HG22	32:q:22:LEU:HD13	1.94	0.48
32:p:216:ALA:N	32:p:217:GLU:OE1	2.46	0.48
33:M:490:GLN:OE1	34:f:38:VAL:N	2.46	0.48
37:a:6:VAL:HG23	37:a:125:LEU:HD22	1.94	0.48
2:I:180:LEU:HD13	6:K:79:ILE:HD12	1.95	0.48
5:H:185:PRO:HB3	50:H:502:PEV:H162	1.96	0.48
8:Z:98:VAL:O	8:Z:102:LYS:HG2	2.13	0.48
11:S:50:PRO:HB2	24:D:105:PRO:HD2	1.94	0.48
13:j:11:LYS:CB	43:m:67:PRO:HD3	2.44	0.48
15:C:383:VAL:HB	15:C:583:LEU:HD23	1.95	0.48
15:C:582:TYR:HD1	15:C:601:VAL:HG13	1.77	0.48
25:X:22:ALA:O	25:X:26:VAL:HG23	2.14	0.48
31:o:49:LYS:HB2	32:q:46:MET:HE3	1.96	0.48
32:q:18:THR:CG2	32:q:22:LEU:HD11	2.43	0.48
33:M:354:VAL:O	33:M:358:ARG:HG2	2.13	0.48
1:A:85:TRP:CD2	1:A:204:LEU:HD13	2.49	0.48
1:A:139:ASN:ND2	46:A:502:FMN:H1'1	2.28	0.48
2:I:254:TYR:HD2	2:I:320:ALA:HA	1.79	0.48
2:I:374:ILE:HG23	2:I:377:LEU:HD23	1.96	0.48
2:I:375:ALA:HB1	2:I:453:ARG:HD3	1.96	0.48
13:j:15:TYR:CE1	43:m:65:TRP:HZ3	2.32	0.48
14:G:181:GLN:OE1	14:G:185:ARG:NH2	2.45	0.48
15:C:292:THR:C	15:C:303:ILE:HG22	2.38	0.48
15:C:729:THR:HG23	15:C:735:MET:HG3	1.96	0.48
18:B:125:TYR:CE1	18:B:213:LEU:HD22	2.49	0.48
25:X:33:ALA:HA	25:X:86:LEU:HD21	1.95	0.48
26:c:4:ASP:OD1	26:c:4:ASP:N	2.45	0.48
27:Q:4:ARG:HH21	27:Q:83:LEU:HG	1.79	0.48
31:o:135:ILE:HD13	31:o:141:VAL:HG21	1.94	0.48
32:p:106:VAL:HG12	32:p:120:THR:HG21	1.95	0.48
37:a:140:TRP:CD2	37:a:178:LEU:HD22	2.49	0.48
37:a:226:PHE:O	37:a:230:VAL:HG23	2.12	0.48
37:a:253:SER:HA	37:a:256:ILE:HG12	1.95	0.48
37:a:322:MET:HE3	37:a:337:HIS:HB3	1.95	0.48
42:s:22:ALA:HA	42:s:25:ALA:HB3	1.94	0.48
4:N:67:PHE:HE1	5:H:122:ILE:HD13	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:189:MET:HE3	5:H:189:MET:HB2	1.75	0.48
14:G:365:GLY:HA2	14:G:368:PHE:CE2	2.48	0.48
15:C:103:PRO:HB2	15:C:184:GLN:HE21	1.77	0.48
15:C:440:PHE:CD2	15:C:469:VAL:HG12	2.49	0.48
23:E:86:PRO:HD3	23:E:113:ILE:HG23	1.96	0.48
31:o:120:HIS:CG	31:o:121:ALA:H	2.31	0.48
32:p:61:VAL:HG22	32:p:79:ILE:HD13	1.96	0.48
37:a:113:PHE:HB2	37:a:153:PHE:CD1	2.49	0.48
37:a:581:GLY:O	37:a:585:SER:HB3	2.14	0.48
44:t:29:ARG:HH11	44:t:30:HIS:HB2	1.77	0.48
1:A:339:ALA:HB2	1:A:465:PHE:CZ	2.49	0.48
2:I:418:LEU:HD12	33:M:189:LEU:HB2	1.95	0.48
2:I:452:PRO:HB3	2:I:455:TRP:HE1	1.79	0.48
48:I:503:CDL:H342	3:J:112:LYS:NZ	2.29	0.48
4:N:132:ARG:HH21	8:Z:83:ARG:HH22	1.61	0.48
15:C:292:THR:HG22	15:C:293:ILE:N	2.27	0.48
15:C:423:TYR:HA	15:C:428:ASN:HD21	1.79	0.48
17:F:56:LEU:HD22	17:F:108:ALA:HB2	1.95	0.48
28:k:90:GLU:HB3	28:k:97:ILE:HD12	1.95	0.48
32:q:105:LEU:C	32:q:107:HIS:H	2.19	0.48
33:M:201:GLN:OE1	43:m:25:LYS:HD2	2.14	0.48
34:f:14:ALA:HA	34:f:36:HIS:CD2	2.48	0.48
37:a:376:PRO:HG2	37:a:379:TYR:HB3	1.95	0.48
13:j:11:LYS:HB2	43:m:67:PRO:CD	2.43	0.48
15:C:293:ILE:HG22	15:C:294:ASP:H	1.77	0.48
15:C:344:LEU:HD22	15:C:617:ILE:HG21	1.96	0.48
15:C:429:THR:HG23	15:C:548:ASN:O	2.14	0.48
15:C:445:THR:OG1	15:C:517:GLY:N	2.38	0.48
15:C:566:GLY:HA3	27:Q:49:LEU:HD21	1.94	0.48
23:E:173:ARG:N	23:E:173:ARG:CD	2.77	0.48
38:b:54:GLU:HA	38:b:57:VAL:HG12	1.96	0.48
2:I:150:LEU:HD11	6:K:64:LEU:HD13	1.96	0.48
6:K:79:ILE:HA	6:K:82:ILE:CG2	2.44	0.48
15:C:222:THR:O	15:C:222:THR:HG22	2.14	0.48
15:C:431:ILE:HG13	15:C:634:GLU:HB3	1.96	0.48
15:C:637:THR:HG21	15:C:687:LEU:HA	1.96	0.48
28:k:51:LEU:O	28:k:55:LYS:HG2	2.14	0.48
3:J:71:PHE:O	3:J:75:VAL:HG23	2.14	0.47
5:H:230:LEU:HD11	49:H:501:U10:H171	1.95	0.47
8:Z:2:THR:C	8:Z:4:ALA:H	2.22	0.47
11:S:30:CYS:HB3	11:S:32:HIS:HD1	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:S:94:VAL:HG11	21:R:115:TYR:HE2	1.79	0.47
15:C:125:GLU:HG3	15:C:126:LYS:HG3	1.95	0.47
22:U:51:LEU:HD11	22:U:60:LYS:HG2	1.96	0.47
28:k:97:ILE:HG23	28:k:114:TYR:HE2	1.77	0.47
33:M:197:THR:HG22	33:M:202:ILE:HG22	1.94	0.47
33:M:457:VAL:O	33:M:461:ILE:HG13	2.14	0.47
33:M:490:GLN:O	34:f:34:ARG:NH2	2.47	0.47
37:a:408:ALA:HB1	37:a:421:TRP:CD1	2.48	0.47
2:I:195:SER:OG	6:K:45:ASN:ND2	2.46	0.47
2:I:377:LEU:HD21	2:I:391:PHE:CE2	2.49	0.47
7:Y:15:SER:OG	9:V:53:ASP:OD2	2.28	0.47
15:C:582:TYR:CD1	15:C:601:VAL:HG13	2.49	0.47
15:C:740:ALA:C	15:C:742:LEU:H	2.21	0.47
16:T:99:PHE:CD1	16:T:106:PRO:HG3	2.49	0.47
17:F:161:GLU:O	17:F:164:VAL:HB	2.14	0.47
21:R:64:ARG:HA	21:R:67:VAL:HG12	1.96	0.47
32:q:9:TYR:C	32:q:11:VAL:H	2.22	0.47
33:M:196:GLY:O	43:m:32:GLU:HG2	2.14	0.47
37:a:24:GLY:HA3	37:a:33:THR:N	2.22	0.47
37:a:242:LEU:O	37:a:309:ARG:NH2	2.47	0.47
14:G:197:ARG:O	14:G:201:GLN:HB2	2.15	0.47
15:C:287:LEU:HB3	15:C:306:ASP:HB3	1.96	0.47
16:T:86:GLN:HG3	17:F:160:PRO:HD3	1.95	0.47
16:T:135:MET:HE1	16:T:170:VAL:HG23	1.95	0.47
16:T:181:ILE:HG12	16:T:215:THR:HB	1.96	0.47
16:T:216:ILE:HB	16:T:279:THR:HG22	1.96	0.47
16:T:251:THR:HG21	16:T:347:LEU:HD12	1.95	0.47
23:E:163:GLY:H	24:D:161:LYS:HA	1.78	0.47
27:Q:64:TYR:HE2	27:Q:70:ARG:HG2	1.79	0.47
28:k:114:TYR:O	28:k:118:HIS:ND1	2.46	0.47
33:M:143:TYR:CE2	33:M:185:LEU:HD13	2.49	0.47
35:g:92:TRP:CE2	35:g:96:LYS:HD2	2.50	0.47
3:J:66:ILE:HG21	4:N:166:ALA:HB2	1.97	0.47
3:J:84:SER:O	3:J:84:SER:OG	2.26	0.47
4:N:173:ARG:HD2	4:N:178:LYS:HG2	1.97	0.47
15:C:169:ASP:O	15:C:173:CYS:N	2.47	0.47
22:U:100:ILE:HG22	24:D:103:LEU:HB2	1.96	0.47
32:q:17:GLU:HG3	32:p:23:ASP:N	2.29	0.47
32:q:184:ASN:HB3	32:q:185:PRO:HD3	1.97	0.47
33:M:164:GLN:O	33:M:165:ARG:NE	2.44	0.47
1:A:273:VAL:O	1:A:277:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:TYR:HB2	1:A:416:TRP:CD1	2.50	0.47
2:I:475:PHE:O	2:I:479:PHE:HB2	2.14	0.47
4:N:52:ILE:O	4:N:56:VAL:HG22	2.13	0.47
5:H:150:SER:O	5:H:154:ILE:HG12	2.13	0.47
14:G:96:LEU:HB3	14:G:283:PRO:HG2	1.97	0.47
14:G:247:PHE:CG	14:G:274:ILE:HD11	2.49	0.47
15:C:251:TYR:HB3	18:B:108:TYR:CD2	2.48	0.47
17:F:42:LEU:HD12	17:F:101:VAL:HG11	1.96	0.47
17:F:155:VAL:HG23	17:F:168:PRO:HG2	1.96	0.47
17:F:175:PHE:HB3	19:O:100:ASN:ND2	2.28	0.47
28:k:47:VAL:HG22	28:k:112:ILE:HG23	1.95	0.47
33:M:391:LEU:O	33:M:394:THR:HG22	2.15	0.47
34:f:65:ASN:C	34:f:67:TYR:H	2.21	0.47
37:a:460:PRO:HD2	37:a:463:MET:SD	2.54	0.47
1:A:343:GLY:HA3	1:A:373:GLY:H	1.80	0.47
1:A:428:LYS:NZ	8:Z:12:MET:SD	2.85	0.47
2:I:107:THR:HA	2:I:110:MET:HE2	1.96	0.47
3:J:70:ILE:O	3:J:74:GLU:HG3	2.15	0.47
5:H:291:ARG:CG	5:H:291:ARG:O	2.62	0.47
8:Z:38:ARG:NH2	11:S:127:GLY:HA3	2.29	0.47
11:S:106:VAL:O	11:S:107:SER:OG	2.25	0.47
13:j:21:PHE:CE1	13:j:38:ARG:HB2	2.49	0.47
14:G:153:MET:HG2	23:E:97:GLU:OE2	2.15	0.47
32:p:84:VAL:HG12	32:p:86:ARG:HB2	1.97	0.47
33:M:147:GLU:OE1	33:M:147:GLU:N	2.47	0.47
33:M:237:LEU:HD12	33:M:313:VAL:HG22	1.96	0.47
37:a:563:TRP:CE2	37:a:565:PHE:HB2	2.50	0.47
1:A:267:ASN:OD1	1:A:268:VAL:N	2.48	0.47
2:I:233:ILE:HG22	2:I:281:PHE:CZ	2.50	0.47
47:I:501:T7X:O16	47:I:501:T7X:P1	2.72	0.47
49:H:501:U10:O2	49:H:501:U10:C3M	2.63	0.47
7:Y:10:ASN:O	7:Y:12:ILE:N	2.42	0.47
7:Y:32:GLU:N	7:Y:32:GLU:OE2	2.47	0.47
10:W:19:ALA:O	10:W:23:ILE:CG1	2.58	0.47
10:W:25:GLY:O	10:W:29:PHE:N	2.48	0.47
10:W:30:LEU:O	10:W:34:VAL:HB	2.15	0.47
14:G:74:SER:HB2	14:G:334:PRO:HG2	1.97	0.47
14:G:372:HIS:HB3	29:r:2:ALA:HB1	1.96	0.47
15:C:228:ALA:HA	15:C:232:ALA:HB3	1.95	0.47
15:C:639:GLN:OE1	15:C:690:THR:HG21	2.15	0.47
22:U:118:LEU:HB3	24:D:206:ARG:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:E:209:ARG:NH1	23:E:211:ASP:OD2	2.44	0.47
31:o:212:GLU:HA	31:o:215:LYS:HD3	1.96	0.47
32:q:137:CYS:SG	32:q:151:LEU:HB3	2.54	0.47
33:M:26:LEU:HB3	33:M:119:TYR:CE1	2.50	0.47
33:M:38:ARG:NH1	33:M:109:TRP:O	2.48	0.47
33:M:46:LEU:HD22	35:g:73:THR:HG21	1.97	0.47
33:M:200:LEU:O	33:M:204:LEU:HD23	2.15	0.47
33:M:490:GLN:NE2	34:f:34:ARG:HA	2.30	0.47
37:a:337:HIS:CG	37:a:400:SER:HB3	2.50	0.47
37:a:612:ARG:O	37:a:615:GLN:HB3	2.14	0.47
1:A:480:GLU:OE1	8:Z:11:GLY:N	2.47	0.47
7:Y:78:TYR:O	7:Y:82:MET:HG2	2.15	0.47
14:G:71:ASP:HB3	14:G:78:GLN:NE2	2.29	0.47
15:C:262:GLY:O	15:C:265:ILE:HD12	2.15	0.47
18:B:248:GLN:OE1	18:B:248:GLN:N	2.44	0.47
23:E:155:MET:HG2	23:E:190:PRO:HG2	1.97	0.47
31:o:94:ASN:O	31:o:116:ARG:N	2.47	0.47
33:M:177:THR:HG23	33:M:226:VAL:HG11	1.96	0.47
1:A:245:LYS:HE3	15:C:239:ILE:HD13	1.95	0.47
1:A:340:ILE:HG12	1:A:379:VAL:HA	1.97	0.47
1:A:392:ARG:NH1	18:B:168:GLU:OE2	2.48	0.47
2:I:99:PHE:HZ	2:I:353:ALA:HB3	1.79	0.47
48:I:502:CDL:H792	48:I:502:CDL:H612	1.96	0.47
3:J:5:PHE:CD1	3:J:8:ILE:HD11	2.50	0.47
48:J:401:CDL:OB7	48:J:401:CDL:H312	2.14	0.47
7:Y:44:PRO:HD2	8:Z:129:ARG:CZ	2.45	0.47
12:i:14:LEU:HD22	33:M:28:PHE:CE1	2.50	0.47
15:C:343:ARG:HB3	15:C:647:VAL:HG21	1.97	0.47
18:B:42:LYS:HG2	18:B:45:LEU:HG	1.97	0.47
21:R:127:PRO:O	21:R:130:VAL:CG1	2.60	0.47
24:D:180:GLY:C	24:D:182:ASN:H	2.23	0.47
1:A:234:ALA:HB2	1:A:246:PRO:HG3	1.97	0.47
2:I:326:HIS:HD2	2:I:398:TYR:HD1	1.62	0.47
2:I:466:SER:OG	12:i:24:ARG:HG2	2.14	0.47
48:I:502:CDL:H161	48:I:502:CDL:H362	1.97	0.47
3:J:71:PHE:CE1	3:J:103:LEU:HD21	2.50	0.47
14:G:312:HIS:HE1	24:D:171:ALA:O	1.98	0.47
15:C:337:ASP:HB2	15:C:734:ILE:HD12	1.97	0.47
16:T:184:SER:O	16:T:219:PRO:HD2	2.15	0.47
22:U:49:ALA:HB2	22:U:64:LYS:HB2	1.96	0.47
23:E:186:PRO:HB2	24:D:185:PHE:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:E:188:CYS:SG	23:E:189:PRO:HD3	2.55	0.47
31:o:112:ASN:ND2	31:o:220:ILE:HG21	2.29	0.47
33:M:351:CYS:HG	33:M:460:PHE:HZ	1.63	0.47
37:a:621:VAL:HG23	37:a:622:TYR:CD1	2.50	0.47
1:A:337:LEU:HD11	1:A:340:ILE:HD11	1.96	0.46
1:A:354:ILE:HD12	1:A:368:VAL:HG22	1.97	0.46
2:I:34:ILE:HD11	3:J:105:ILE:HG23	1.96	0.46
2:I:369:THR:HB	2:I:372:LYS:HD2	1.97	0.46
5:H:175:LYS:HE2	5:H:175:LYS:HB3	1.76	0.46
49:H:501:U10:H102	23:E:85:TRP:CZ2	2.45	0.46
14:G:254:ARG:HD3	29:r:9:ALA:HB1	1.97	0.46
14:G:356:ARG:HB2	17:F:58:ASP:OD2	2.15	0.46
15:C:328:ILE:CD1	15:C:333:ARG:HG2	2.45	0.46
15:C:444:GLY:N	15:C:472:VAL:O	2.43	0.46
16:T:75:GLY:CA	16:T:144:LEU:HB2	2.42	0.46
27:Q:91:LYS:HD2	27:Q:91:LYS:HA	1.70	0.46
31:o:223:LEU:HD21	32:p:86:ARG:NH1	2.29	0.46
32:q:221:PRO:HB3	32:p:37:GLU:CD	2.41	0.46
37:a:104:MET:HB3	37:a:110:SER:OG	2.14	0.46
37:a:308:LYS:HB3	37:a:356:ILE:HD11	1.96	0.46
43:m:42:GLU:HG3	43:m:43:MET:N	2.28	0.46
1:A:99:ILE:HG23	1:A:278:LEU:HD11	1.96	0.46
2:I:153:GLU:HG2	6:K:68:VAL:CG1	2.45	0.46
2:I:418:LEU:HD12	33:M:189:LEU:CB	2.44	0.46
5:H:27:GLU:CD	5:H:200:ARG:HE	2.23	0.46
6:K:28:ILE:O	6:K:31:MET:HB2	2.15	0.46
6:K:41:ALA:O	6:K:45:ASN:HB2	2.15	0.46
11:S:78:ARG:HH22	15:C:186:MET:HE3	1.80	0.46
15:C:331:LYS:O	15:C:335:CYS:HB3	2.15	0.46
15:C:658:ARG:HD3	15:C:668:LEU:HD23	1.96	0.46
17:F:18:TRP:HZ3	17:F:44:PHE:HB2	1.79	0.46
17:F:26:GLU:CD	17:F:27:HIS:H	2.22	0.46
17:F:71:PHE:HE2	17:F:94:GLU:HA	1.80	0.46
17:F:158:ASP:OD2	23:E:140:ARG:NE	2.48	0.46
26:c:20:PRO:HD3	26:c:86:MET:HG3	1.96	0.46
33:M:69:VAL:HA	33:M:84:LEU:O	2.14	0.46
33:M:254:GLY:C	33:M:258:LYS:HZ3	2.23	0.46
2:I:172:SER:HB2	2:I:258:PRO:HD3	1.97	0.46
2:I:247:HIS:CD2	2:I:248:MET:H	2.33	0.46
2:I:412:TYR:HE2	33:M:77:TYR:HH	1.54	0.46
5:H:16:LEU:HD23	5:H:86:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:74:PHE:CE2	5:H:219:GLU:HB3	2.49	0.46
5:H:287:PHE:HB3	14:G:198:ILE:HD12	1.97	0.46
5:H:302:VAL:HG11	50:H:502:PEV:H32	1.96	0.46
8:Z:5:MET:HG3	15:C:196:THR:OG1	2.15	0.46
11:S:84:ILE:CB	21:R:122:ASN:OD1	2.55	0.46
13:j:41:TYR:HD2	13:j:42:LEU:HD12	1.81	0.46
14:G:58:LYS:HB3	14:G:62:GLN:HB2	1.96	0.46
14:G:116:LEU:HD12	14:G:138:ARG:NH2	2.29	0.46
14:G:161:GLY:HA3	14:G:295:CYS:SG	2.56	0.46
15:C:113:ILE:HD11	19:O:138:LYS:HG3	1.96	0.46
17:F:53:VAL:HG23	17:F:54:GLN:N	2.30	0.46
21:R:99:LEU:O	21:R:103:MET:HG2	2.14	0.46
32:p:128:ILE:HG12	32:p:145:ILE:HD13	1.96	0.46
35:g:92:TRP:NE1	35:g:96:LYS:HD2	2.30	0.46
37:a:274:PRO:HA	37:a:277:GLU:HB2	1.96	0.46
1:A:96:THR:OG1	1:A:171:GLY:O	2.33	0.46
1:A:401:SER:O	1:A:403:GLY:N	2.48	0.46
4:N:37:THR:HG21	6:K:40:LEU:HD11	1.98	0.46
4:N:59:GLY:HA3	5:H:115:SER:HB3	1.97	0.46
4:N:68:VAL:HG21	6:K:77:LEU:HD13	1.96	0.46
4:N:190:PHE:O	4:N:191:ARG:HG2	2.15	0.46
5:H:200:ARG:HD3	5:H:236:MET:SD	2.55	0.46
6:K:85:ARG:O	6:K:86:VAL:C	2.57	0.46
15:C:455:ASN:ND2	15:C:479:ASN:OD1	2.44	0.46
16:T:220:ALA:O	16:T:221:THR:C	2.59	0.46
22:U:68:THR:OG1	22:U:69:GLN:N	2.48	0.46
23:E:160:ASN:HB2	23:E:184:TYR:HD2	1.80	0.46
26:c:16:VAL:HG23	26:c:91:ASN:HD21	1.80	0.46
28:k:95:LEU:HD13	28:k:118:HIS:CG	2.50	0.46
37:a:347:LEU:HD11	37:a:471:ALA:HA	1.97	0.46
37:a:558:PHE:CD1	37:a:564:PHE:HD2	2.33	0.46
1:A:432:ILE:HD11	1:A:473:ILE:HD12	1.97	0.46
2:I:88:ARG:O	2:I:279:ARG:NH2	2.47	0.46
2:I:179:TYR:CE2	2:I:265:LEU:HD22	2.50	0.46
2:I:189:ILE:HD11	6:K:18:ILE:HD12	1.97	0.46
48:I:502:CDL:H161	48:I:502:CDL:C36	2.46	0.46
48:I:503:CDL:H641	48:I:503:CDL:C27	2.46	0.46
48:J:401:CDL:OB5	48:J:401:CDL:H1	2.16	0.46
5:H:78:PRO:HB2	5:H:227:LEU:HD23	1.97	0.46
7:Y:68:HIS:O	7:Y:72:GLN:HB3	2.15	0.46
14:G:155:ALA:O	14:G:157:PHE:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:379:ILE:HG23	16:T:382:ARG:HD2	1.97	0.46
24:D:133:CYS:HA	45:D:301:SF4:S2	2.55	0.46
27:Q:4:ARG:CZ	27:Q:87:GLU:HB2	2.46	0.46
33:M:89:ILE:H	33:M:89:ILE:HD12	1.80	0.46
33:M:201:GLN:O	33:M:205:THR:HG23	2.15	0.46
1:A:418:ILE:HG21	1:A:435:LEU:HD13	1.97	0.46
50:H:502:PEV:H262	8:Z:57:PHE:HD2	1.80	0.46
6:K:21:ILE:HA	6:K:31:MET:SD	2.56	0.46
8:Z:12:MET:O	8:Z:14:SER:N	2.48	0.46
14:G:266:GLU:OE1	14:G:270:GLN:NE2	2.49	0.46
19:O:82:LEU:HD13	25:X:132:TYR:CE1	2.51	0.46
24:D:68:MET:HE1	24:D:71:LEU:HD12	1.97	0.46
32:q:79:ILE:HG22	32:q:83:CYS:SG	2.55	0.46
32:p:47:ASN:HB3	32:p:68:ILE:HG23	1.97	0.46
33:M:92:PHE:CD1	33:M:339:LEU:HD11	2.51	0.46
33:M:252:LEU:HD12	33:M:256:LEU:HG	1.97	0.46
33:M:408:PHE:HD1	33:M:409:GLN:HG2	1.80	0.46
43:m:23:ASP:OD1	43:m:24:ARG:N	2.49	0.46
48:I:503:CDL:H622	48:I:503:CDL:H272	1.98	0.46
5:H:87:VAL:HG22	5:H:109:TYR:OH	2.16	0.46
11:S:94:VAL:HG11	21:R:115:TYR:CE2	2.50	0.46
14:G:112:LEU:HD21	14:G:141:LEU:HB2	1.98	0.46
14:G:367:ASP:O	14:G:371:LYS:HG3	2.15	0.46
15:C:171:PRO:HB3	24:D:173:PRO:HG3	1.97	0.46
15:C:514:ILE:HG22	15:C:542:VAL:HG11	1.98	0.46
17:F:10:SER:OG	17:F:45:LEU:HD21	2.16	0.46
18:B:130:CYS:SG	18:B:131:GLY:N	2.89	0.46
18:B:160:LYS:HE2	18:B:160:LYS:HB2	1.81	0.46
19:O:52:ARG:HD3	19:O:78:PHE:HB3	1.98	0.46
23:E:175:CYS:C	23:E:177:ARG:H	2.23	0.46
24:D:111:HIS:HE1	45:D:301:SF4:S4	2.37	0.46
32:p:86:ARG:HH22	32:p:88:ASP:H	1.61	0.46
33:M:74:TRP:HB2	33:M:81:ASN:HA	1.98	0.46
37:a:571:ASP:HB3	37:a:575:ARG:HE	1.81	0.46
39:h:42:ARG:O	39:h:42:ARG:NH2	2.48	0.46
2:I:65:THR:O	2:I:69:LEU:N	2.43	0.46
48:I:503:CDL:HA32	48:I:503:CDL:HB31	1.97	0.46
4:N:180:GLN:HG3	4:N:181:ASP:H	1.81	0.46
5:H:71:PHE:HB2	5:H:75:ARG:CZ	2.46	0.46
14:G:121:HIS:HE1	14:G:203:LEU:HD21	1.81	0.46
15:C:159:MET:O	15:C:159:MET:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:178:GLU:CD	15:C:314:ARG:HH22	2.23	0.46
15:C:242:ARG:NH2	18:B:115:SER:HB3	2.30	0.46
15:C:310:PRO:HA	15:C:645:PRO:HD2	1.97	0.46
15:C:381:VAL:HG11	15:C:575:LEU:H	1.81	0.46
32:q:83:CYS:HB3	32:q:104:SER:H	1.80	0.46
33:M:27:LEU:HD23	33:M:119:TYR:HE2	1.80	0.46
33:M:208:PHE:HB2	33:M:213:GLN:HG2	1.97	0.46
33:M:236:TRP:O	33:M:240:ALA:CB	2.64	0.46
37:a:335:VAL:O	37:a:339:MET:HG3	2.16	0.46
3:J:70:ILE:HG21	4:N:163:MET:HG3	1.98	0.46
7:Y:17:VAL:HG23	7:Y:79:VAL:HG11	1.98	0.46
8:Z:118:TRP:CH2	13:j:56:ARG:HD3	2.51	0.46
10:W:17:VAL:O	10:W:17:VAL:HG22	2.16	0.46
12:i:33:TRP:N	12:i:33:TRP:CE3	2.84	0.46
14:G:62:GLN:O	14:G:65:PRO:HD2	2.15	0.46
14:G:93:GLU:CA	21:R:129:HIS:HE1	2.16	0.46
16:T:253:PHE:O	16:T:255:PRO:HD3	2.16	0.46
32:q:8:PHE:N	32:p:30:GLN:HG2	2.31	0.46
32:p:90:ASN:ND2	32:p:117:VAL:O	2.49	0.46
33:M:137:LEU:HD21	33:M:266:ARG:NH2	2.31	0.46
33:M:303:ASP:O	33:M:307:ILE:HG13	2.15	0.46
34:f:46:GLU:OE2	35:g:94:HIS:NE2	2.49	0.46
35:g:64:LEU:HD23	35:g:65:PRO:HD3	1.97	0.46
37:a:140:TRP:CH2	37:a:265:GLY:HA2	2.50	0.46
2:I:86:LEU:HD21	4:N:148:TYR:HA	1.98	0.46
2:I:157:LEU:HD23	4:N:158:ILE:HG23	1.96	0.46
2:I:326:HIS:HD2	2:I:398:TYR:CD1	2.34	0.46
5:H:74:PHE:HB3	5:H:127:SER:HB3	1.97	0.46
14:G:113:ASN:HD21	14:G:335:LYS:CE	2.29	0.46
14:G:182:PHE:CE2	14:G:186:ILE:HD11	2.52	0.46
16:T:119:VAL:HG11	22:U:140:LEU:HG	1.97	0.46
16:T:253:PHE:HA	16:T:352:LEU:O	2.16	0.46
18:B:51:GLU:C	18:B:53:ASN:H	2.23	0.46
24:D:163:ILE:HG12	45:D:301:SF4:S3	2.56	0.46
32:p:6:ARG:HD2	32:p:6:ARG:HA	1.69	0.46
33:M:92:PHE:HZ	33:M:335:ILE:HD12	1.80	0.46
33:M:318:LEU:HA	33:M:321:ILE:HG22	1.98	0.46
33:M:400:GLU:O	33:M:403:ILE:HB	2.16	0.46
37:a:381:MET:HA	37:a:384:ILE:HD13	1.97	0.46
37:a:431:SER:OG	37:a:528:GLY:HA3	2.16	0.46
43:m:64:ARG:HD2	43:m:64:ARG:HA	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:404:LEU:HD22	2:I:476:ILE:HG22	1.97	0.45
48:I:502:CDL:H791	12:i:34:GLU:HB2	1.96	0.45
48:I:503:CDL:CB5	48:I:503:CDL:OB5	2.64	0.45
12:i:17:GLN:HG2	12:i:32:PRO:HB2	1.98	0.45
14:G:32:MET:HE2	14:G:32:MET:HB3	1.86	0.45
15:C:108:HIS:HB3	15:C:111:LEU:HB2	1.97	0.45
15:C:329:SER:HB3	15:C:452:ALA:HB3	1.98	0.45
16:T:253:PHE:CE2	16:T:255:PRO:HG3	2.51	0.45
31:o:120:HIS:CG	31:o:121:ALA:N	2.84	0.45
32:q:16:ARG:HD3	32:q:16:ARG:HA	1.53	0.45
32:p:216:ALA:O	32:p:218:ASN:N	2.50	0.45
33:M:140:LEU:O	33:M:143:TYR:HB3	2.16	0.45
37:a:549:SER:OG	37:a:550:THR:N	2.48	0.45
37:a:591:LYS:O	37:a:595:GLU:HG3	2.16	0.45
1:A:228:ILE:HG21	1:A:401:SER:HA	1.98	0.45
2:I:146:ILE:HG12	6:K:61:PHE:CG	2.52	0.45
6:K:10:SER:OG	6:K:41:ALA:O	2.34	0.45
14:G:119:THR:HA	14:G:122:ALA:HB3	1.98	0.45
15:C:192:ARG:CZ	15:C:192:ARG:HB2	2.46	0.45
15:C:361:TRP:CZ2	15:C:619:PRO:HD2	2.51	0.45
17:F:180:PHE:CZ	24:D:131:ALA:HB1	2.50	0.45
21:R:88:GLU:O	21:R:92:GLU:HG3	2.16	0.45
32:q:68:ILE:HG13	32:q:86:ARG:HG2	1.98	0.45
32:q:92:VAL:HG22	32:q:108:VAL:CG2	2.46	0.45
32:q:164:ALA:HB3	32:q:167:ALA:HB2	1.97	0.45
32:p:100:ILE:HG22	32:p:104:SER:HB3	1.99	0.45
34:f:46:GLU:HG2	35:g:93:ALA:HB1	1.99	0.45
37:a:406:GLU:HG2	37:a:517:ILE:HB	1.99	0.45
1:A:192:LEU:HG	1:A:220:ILE:HD11	1.98	0.45
1:A:406:THR:H	15:C:117:CYS:HA	1.81	0.45
2:I:340:GLU:OE1	43:m:39:LYS:CG	2.63	0.45
2:I:390:THR:HG21	2:I:469:LEU:HG	1.98	0.45
48:I:503:CDL:C76	48:I:503:CDL:H721	2.47	0.45
4:N:34:PHE:CD2	4:N:57:TYR:HB3	2.51	0.45
8:Z:51:LEU:HD23	8:Z:51:LEU:HA	1.84	0.45
14:G:141:LEU:HD21	14:G:178:PHE:CE2	2.52	0.45
14:G:341:PHE:CE2	14:G:343:VAL:HG23	2.52	0.45
15:C:386:GLN:NE2	15:C:588:ASP:OD1	2.49	0.45
15:C:413:THR:HB	15:C:417:VAL:HG21	1.98	0.45
15:C:572:ALA:C	15:C:574:ALA:H	2.22	0.45
17:F:177:TYR:CG	19:O:104:SER:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:o:112:ASN:HD22	31:o:114:GLN:HG2	1.81	0.45
31:o:120:HIS:CD2	31:o:121:ALA:H	2.34	0.45
32:p:113:LEU:HD22	33:M:112:MET:CE	2.47	0.45
33:M:364:VAL:HA	33:M:367:TYR:CE2	2.51	0.45
37:a:255:LEU:HD23	37:a:255:LEU:HA	1.80	0.45
1:A:396:PHE:CD1	18:B:170:GLU:HB3	2.51	0.45
2:I:182:LEU:HB2	2:I:249:TRP:HE3	1.80	0.45
2:I:255:GLU:OE1	2:I:317:ARG:NE	2.50	0.45
5:H:162:VAL:HG12	5:H:163:GLY:N	2.31	0.45
7:Y:41:LYS:HE3	43:m:69:ILE:HD13	1.99	0.45
10:W:30:LEU:HD23	10:W:34:VAL:HG21	1.98	0.45
14:G:69:ARG:NH2	23:E:188:CYS:SG	2.81	0.45
15:C:227:PHE:CE2	15:C:267:ILE:CD1	2.70	0.45
16:T:63:ARG:NH2	23:E:177:ARG:HD3	2.31	0.45
17:F:14:LEU:HD23	17:F:15:PRO:HD2	1.98	0.45
17:F:41:LEU:HD12	17:F:41:LEU:C	2.41	0.45
17:F:114:GLU:HG3	17:F:133:LEU:HD12	1.98	0.45
23:E:93:CYS:O	23:E:96:VAL:N	2.49	0.45
32:p:48:VAL:HG12	32:p:49:PHE:N	2.32	0.45
33:M:359:HIS:HB3	33:M:361:THR:HG22	1.98	0.45
37:a:239:HIS:HD2	37:a:243:PRO:HD3	1.82	0.45
37:a:387:LEU:O	37:a:390:ILE:HG22	2.16	0.45
2:I:402:PRO:HG2	33:M:147:GLU:CB	2.41	0.45
2:I:449:PHE:HD2	33:M:167:ILE:HB	1.80	0.45
5:H:58:LEU:CD1	49:H:501:U10:H153	2.46	0.45
14:G:146:GLU:OE1	24:D:104:SER:N	2.50	0.45
16:T:215:THR:OG1	16:T:275:SER:O	2.26	0.45
16:T:344:ILE:O	16:T:348:THR:HG23	2.16	0.45
23:E:191:THR:HG22	23:E:193:GLU:HG3	1.87	0.45
24:D:113:LEU:HD13	24:D:198:GLU:HG3	1.98	0.45
28:k:70:HIS:CD2	28:k:107:SER:HB2	2.51	0.45
30:n:82:ARG:O	30:n:86:VAL:HG23	2.17	0.45
33:M:282:PHE:CZ	33:M:286:LEU:HD11	2.51	0.45
37:a:465:ILE:HB	37:a:466:PRO:HD3	1.99	0.45
49:H:501:U10:H112	49:H:501:U10:C1M	2.30	0.45
50:H:502:PEV:H142	24:D:71:LEU:O	2.17	0.45
14:G:354:LYS:HD2	14:G:355:ILE:H	1.81	0.45
18:B:60:ILE:HG21	18:B:75:PRO:HB2	1.97	0.45
23:E:91:LEU:O	23:E:129:GLY:HA3	2.17	0.45
32:q:116:LYS:HB2	32:q:118:HIS:CD2	2.51	0.45
32:q:137:CYS:HB2	32:q:155:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:M:106:LEU:O	33:M:455:ARG:HD2	2.17	0.45
33:M:281:PRO:O	33:M:285:THR:HG23	2.16	0.45
1:A:142:GLU:OE1	1:A:147:THR:HG22	2.17	0.45
2:I:337:GLY:O	43:m:42:GLU:OE1	2.34	0.45
48:I:502:CDL:H171	48:I:502:CDL:H201	1.85	0.45
48:I:503:CDL:H602	48:I:503:CDL:H771	1.99	0.45
4:N:173:ARG:HA	4:N:177:VAL:HG13	1.98	0.45
5:H:98:MET:HG2	9:V:27:TYR:HB2	1.99	0.45
5:H:147:TYR:OH	5:H:295:LEU:O	2.32	0.45
5:H:202:PRO:O	5:H:289:ARG:HA	2.16	0.45
15:C:525:ASP:OD1	15:C:525:ASP:N	2.46	0.45
16:T:254:GLN:HG2	16:T:287:VAL:HA	1.98	0.45
22:U:72:ARG:HD2	24:D:93:THR:O	2.17	0.45
23:E:155:MET:HE3	23:E:195:LEU:HB2	1.98	0.45
28:k:107:SER:HB3	28:k:110:LEU:HD12	1.98	0.45
32:q:45:LEU:HD13	32:q:63:PRO:HA	1.98	0.45
33:M:139:LEU:HD21	33:M:203:LEU:HD13	1.99	0.45
33:M:203:LEU:HB3	33:M:271:MET:HE1	1.98	0.45
37:a:166:LYS:O	37:a:169:LEU:HB2	2.17	0.45
37:a:465:ILE:HD13	37:a:468:ILE:HD12	1.99	0.45
43:m:64:ARG:CG	43:m:65:TRP:H	2.30	0.45
1:A:407:PRO:HA	15:C:161:PHE:CD2	2.52	0.45
3:J:62:TYR:O	3:J:66:ILE:HG12	2.16	0.45
3:J:81:TRP:CZ3	5:H:160:ILE:HD11	2.52	0.45
48:J:401:CDL:OB7	48:J:401:CDL:HB32	2.16	0.45
50:H:502:PEV:H262	8:Z:57:PHE:CD2	2.52	0.45
8:Z:127:SER:OG	8:Z:128:GLY:N	2.50	0.45
13:j:19:MET:HE3	43:m:57:GLU:HG3	1.99	0.45
14:G:54:LEU:HD11	23:E:168:SER:HB2	1.99	0.45
15:C:361:TRP:CZ3	15:C:618:LEU:HD22	2.52	0.45
21:R:28:ASN:O	21:R:28:ASN:ND2	2.50	0.45
24:D:92:VAL:HG23	24:D:92:VAL:O	2.16	0.45
31:o:244:PHE:O	31:o:247:SER:OG	2.25	0.45
33:M:80:ILE:HG21	33:M:140:LEU:HD12	1.99	0.45
33:M:133:VAL:HG21	33:M:146:PRO:HG3	1.99	0.45
37:a:45:ILE:HD11	37:a:97:HIS:HB3	1.99	0.45
37:a:582:TYR:CD2	41:l:38:GLY:HA3	2.52	0.45
4:N:11:LEU:HB3	37:a:632:LEU:HD11	1.98	0.45
49:H:501:U10:H101	49:H:501:U10:H122	1.66	0.45
14:G:64:LEU:HD22	14:G:159:ARG:HD3	1.99	0.45
17:F:153:VAL:O	17:F:153:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:P:41:THR:HG21	20:P:52:SER:HB2	1.99	0.45
24:D:134:PRO:HG2	24:D:163:ILE:HD11	1.98	0.45
32:q:107:HIS:CE1	54:q:802:BCT:O2	2.45	0.45
33:M:88:GLY:O	33:M:91:LEU:HB3	2.16	0.45
1:A:421:ARG:NH1	1:A:431:GLU:OE1	2.49	0.45
48:I:503:CDL:H151	48:I:503:CDL:H381	1.99	0.45
4:N:64:LEU:O	4:N:68:VAL:HG23	2.17	0.45
5:H:186:VAL:HA	5:H:189:MET:HE3	1.98	0.45
12:i:58:GLU:O	12:i:62:VAL:HG13	2.16	0.45
14:G:202:ARG:O	14:G:203:LEU:HD12	2.17	0.45
15:C:208:GLY:HA2	15:C:255:LEU:HG	1.98	0.45
15:C:394:MET:SD	15:C:683:VAL:HG11	2.57	0.45
15:C:632:ASN:HD21	15:C:634:GLU:HG2	1.82	0.45
25:X:33:ALA:O	25:X:37:ILE:HG13	2.17	0.45
27:Q:6:SER:HA	27:Q:9:LYS:HE2	1.98	0.45
33:M:89:ILE:HA	33:M:92:PHE:CZ	2.52	0.45
33:M:419:ALA:HA	37:a:176:PHE:CE2	2.52	0.45
37:a:223:ILE:HD11	37:a:282:ALA:HA	1.99	0.45
2:I:486:LEU:O	2:I:490:THR:HG23	2.18	0.44
15:C:74:ILE:N	15:C:85:VAL:O	2.50	0.44
16:T:84:LEU:HD21	16:T:142:ILE:HD13	1.98	0.44
18:B:135:CYS:HB3	18:B:140:SER:CB	2.47	0.44
18:B:181:ILE:HG23	18:B:198:PHE:HB2	1.99	0.44
26:c:57:ILE:HG22	26:c:61:SER:H	1.81	0.44
32:q:81:TYR:OH	32:q:214:HIS:ND1	2.36	0.44
32:q:105:LEU:C	32:q:107:HIS:N	2.75	0.44
1:A:143:SER:HB3	1:A:227:TYR:HA	2.00	0.44
1:A:248:LEU:HD22	15:C:135:ALA:CB	2.48	0.44
2:I:468:LEU:HD12	2:I:468:LEU:O	2.18	0.44
4:N:124:TYR:HB2	8:Z:97:PHE:CD1	2.52	0.44
5:H:29:LYS:HD2	9:V:11:PRO:HG2	1.99	0.44
11:S:84:ILE:HG12	21:R:122:ASN:CG	2.35	0.44
11:S:104:PHE:O	21:R:59:SER:OG	2.32	0.44
11:S:121:LEU:HG	11:S:122:ASP:H	1.83	0.44
14:G:44:ILE:HG22	14:G:45:GLY:N	2.31	0.44
14:G:324:ALA:HA	14:G:344:SER:O	2.17	0.44
23:E:86:PRO:CD	23:E:113:ILE:HG23	2.48	0.44
27:Q:62:ALA:HB2	27:Q:89:LEU:HD13	1.98	0.44
32:p:16:ARG:HH21	32:p:16:ARG:CG	2.20	0.44
32:p:80:TRP:HZ3	32:p:214:HIS:CE1	2.35	0.44
32:p:111:SER:OG	32:p:112:ASN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:M:77:TYR:C	33:M:79:ASN:H	2.24	0.44
33:M:434:ASN:O	33:M:438:SER:N	2.49	0.44
1:A:91:LEU:HD11	1:A:279:ARG:HG2	2.00	0.44
2:I:73:ALA:HB3	2:I:74:PRO:HD3	1.99	0.44
5:H:182:PRO:HB2	8:Z:61:MET:HE2	1.98	0.44
5:H:291:ARG:C	5:H:293:ASP:H	2.25	0.44
7:Y:49:CYS:HB2	7:Y:52:LYS:HB2	1.99	0.44
13:j:59:LYS:HE2	13:j:59:LYS:HB3	1.81	0.44
14:G:209:VAL:HG12	14:G:368:PHE:HE1	1.82	0.44
15:C:556:TYR:HB2	15:C:559:GLN:HB2	1.98	0.44
15:C:721:ASN:O	15:C:722:PHE:HB3	2.17	0.44
17:F:177:TYR:CD1	19:O:104:SER:HB2	2.52	0.44
22:U:101:THR:OG1	22:U:102:ASP:N	2.51	0.44
31:o:132:ALA:O	31:o:134:ILE:HG12	2.18	0.44
32:q:62:ALA:O	32:q:65:ALA:N	2.37	0.44
33:M:203:LEU:HB3	33:M:271:MET:SD	2.58	0.44
37:a:223:ILE:O	37:a:227:ILE:HG12	2.17	0.44
1:A:235:LEU:HD12	1:A:235:LEU:HA	1.69	0.44
2:I:277:ILE:HG23	2:I:281:PHE:HD2	1.81	0.44
48:I:502:CDL:H392	48:I:502:CDL:C21	2.41	0.44
5:H:151:ILE:O	5:H:155:LEU:HG	2.17	0.44
7:Y:82:MET:HE3	7:Y:87:ASN:HA	1.98	0.44
11:S:91:LYS:O	11:S:95:VAL:HG22	2.18	0.44
12:i:41:LEU:C	12:i:41:LEU:CD2	2.90	0.44
14:G:71:ASP:HB3	14:G:78:GLN:CD	2.43	0.44
15:C:278:PHE:CZ	15:C:282:ALA:HB3	2.53	0.44
15:C:584:MET:HG3	15:C:603:GLN:OE1	2.18	0.44
31:o:55:GLN:H	32:p:40:SER:HB2	1.82	0.44
31:o:79:VAL:HB	31:o:97:VAL:HG13	1.98	0.44
32:q:220:LYS:O	32:q:224:VAL:HG23	2.18	0.44
33:M:281:PRO:HA	33:M:284:TYR:CD2	2.50	0.44
33:M:423:ILE:HG22	37:a:172:ARG:HE	1.81	0.44
37:a:402:ASP:OD2	37:a:517:ILE:HG22	2.17	0.44
37:a:610:ALA:HA	37:a:613:ILE:HG12	1.98	0.44
1:A:307:LYS:HB2	1:A:327:CYS:O	2.17	0.44
2:I:136:MET:O	2:I:140:ILE:HG12	2.17	0.44
3:J:88:ILE:HB	3:J:92:GLY:HA3	1.99	0.44
7:Y:18:LEU:HD23	7:Y:18:LEU:HA	1.72	0.44
15:C:582:TYR:HA	15:C:601:VAL:HG13	1.99	0.44
24:D:125:ALA:HB2	24:D:152:THR:CG2	2.47	0.44
32:q:43:ARG:NH2	32:p:214:HIS:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:q:46:MET:HG3	32:p:220:LYS:HZ3	1.83	0.44
33:M:404:LEU:HB3	37:a:183:LEU:HD12	2.00	0.44
34:f:22:ASN:HA	34:f:23:PRO:HD3	1.86	0.44
1:A:156:HIS:O	1:A:157:ASP:HB3	2.17	0.44
46:A:502:FMN:C9	46:A:502:FMN:O2'	2.66	0.44
2:I:56:TRP:HA	2:I:56:TRP:CE3	2.51	0.44
2:I:295:PHE:HD1	2:I:425:LEU:HD22	1.83	0.44
3:J:86:ASN:OD1	3:J:86:ASN:N	2.47	0.44
4:N:147:TYR:OH	43:m:63:LEU:HD11	2.16	0.44
11:S:32:HIS:CD2	11:S:36:LEU:HD22	2.53	0.44
15:C:520:LEU:HD22	15:C:715:PHE:HE1	1.82	0.44
15:C:698:PHE:HE2	27:Q:18:LEU:HD21	1.82	0.44
16:T:243:LEU:HB2	16:T:298:TYR:OH	2.17	0.44
17:F:118:MET:SD	17:F:143:LEU:HD13	2.57	0.44
31:o:194:TRP:NE1	31:o:201:PHE:HD1	2.16	0.44
32:q:120:THR:HG23	32:q:137:CYS:O	2.17	0.44
33:M:26:LEU:HD11	33:M:40:ILE:HG22	1.98	0.44
33:M:149:VAL:C	33:M:152:PRO:HD2	2.43	0.44
33:M:246:THR:O	33:M:250:VAL:HG23	2.18	0.44
33:M:375:PRO:O	33:M:379:THR:HG23	2.17	0.44
37:a:83:VAL:O	37:a:87:ILE:HG12	2.17	0.44
37:a:272:CYS:HB3	37:a:275:LEU:HD12	1.98	0.44
38:b:21:LYS:NZ	38:b:22:ILE:HG13	2.32	0.44
38:b:21:LYS:HE3	38:b:34:LEU:HD22	2.00	0.44
1:A:68:LEU:HD11	1:A:298:LEU:HD11	1.99	0.44
1:A:145:PRO:HB2	1:A:345:SER:HB2	2.00	0.44
1:A:146:GLY:C	1:A:376:ALA:HB1	2.42	0.44
1:A:212:SER:OG	1:A:213:GLY:N	2.51	0.44
1:A:307:LYS:HB3	18:B:233:PRO:O	2.17	0.44
2:I:35:HIS:CG	26:c:64:THR:HG21	2.53	0.44
2:I:418:LEU:CD1	33:M:189:LEU:HB2	2.47	0.44
2:I:428:VAL:HA	2:I:431:VAL:HG12	2.00	0.44
5:H:8:GLU:HB3	9:V:29:ILE:HG21	1.99	0.44
5:H:28:ARG:NE	23:E:114:ILE:HD11	2.33	0.44
5:H:300:TRP:O	5:H:305:PRO:HD3	2.18	0.44
6:K:56:MET:SD	6:K:59:GLN:HB2	2.58	0.44
7:Y:43:ASP:HB2	8:Z:129:ARG:NH2	2.29	0.44
11:S:112:VAL:HG22	17:F:82:TYR:CE1	2.53	0.44
14:G:200:LYS:O	14:G:204:VAL:HG23	2.18	0.44
14:G:321:SER:HA	14:G:348:ASN:HA	1.99	0.44
32:p:78:SER:O	32:p:100:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:p:99:ASN:HB2	32:p:127:THR:HA	2.00	0.44
33:M:59:PHE:HZ	33:M:88:GLY:H	1.65	0.44
33:M:253:ALA:HB2	33:M:349:PHE:HE2	1.83	0.44
33:M:335:ILE:HG13	33:M:336:LEU:N	2.32	0.44
33:M:377:PHE:HB2	33:M:452:LEU:HD11	1.99	0.44
33:M:443:PRO:HD2	33:M:445:PHE:CE1	2.50	0.44
33:M:486:SER:HB2	34:f:38:VAL:CG2	2.48	0.44
37:a:239:HIS:CE1	37:a:562:ARG:H	2.35	0.44
1:A:246:PRO:HD2	45:A:501:SF4:S2	2.58	0.44
1:A:345:SER:OG	1:A:393:LEU:HD22	2.18	0.44
3:J:18:VAL:HG11	5:H:13:ILE:HG21	1.98	0.44
3:J:113:ARG:HG2	4:N:167:ILE:CG2	2.48	0.44
4:N:29:PHE:HA	4:N:32:LEU:HB2	2.00	0.44
5:H:45:SER:O	22:U:40:LEU:HD23	2.18	0.44
5:H:178:TRP:O	5:H:182:PRO:HD2	2.18	0.44
6:K:79:ILE:CA	6:K:82:ILE:HG22	2.44	0.44
14:G:38:GLU:O	14:G:371:LYS:NZ	2.42	0.44
14:G:121:HIS:CD2	14:G:383:GLY:HA3	2.53	0.44
15:C:95:CYS:SG	15:C:102:ILE:HD11	2.58	0.44
15:C:281:LYS:O	15:C:308:ARG:NH1	2.50	0.44
15:C:572:ALA:O	15:C:573:LYS:HB2	2.18	0.44
16:T:288:PHE:CE2	16:T:370:LEU:HD12	2.53	0.44
17:F:24:ARG:HA	21:R:120:ILE:O	2.17	0.44
22:U:138:HIS:C	22:U:140:LEU:H	2.25	0.44
24:D:50:GLU:O	24:D:54:LYS:HG2	2.18	0.44
24:D:159:MET:O	24:D:162:CYS:HB3	2.16	0.44
26:c:20:PRO:HB2	26:c:25:VAL:HB	1.99	0.44
28:k:78:ASP:O	28:k:82:THR:HG23	2.18	0.44
31:o:194:TRP:CZ2	31:o:201:PHE:HB2	2.53	0.44
31:o:230:GLU:HB3	32:q:36:ARG:NH1	2.33	0.44
32:q:78:SER:HB2	32:q:211:ALA:CB	2.48	0.44
32:p:24:ARG:HG3	32:p:35:PHE:CD2	2.53	0.44
32:p:104:SER:OG	32:p:105:LEU:N	2.49	0.44
33:M:253:ALA:HB2	33:M:349:PHE:CE2	2.52	0.44
33:M:267:PHE:HA	33:M:271:MET:HG3	2.00	0.44
33:M:350:LEU:HD22	33:M:460:PHE:CZ	2.53	0.44
37:a:379:TYR:CZ	37:a:382:MET:HG2	2.53	0.44
38:b:17:MET:HE3	38:b:17:MET:HB2	1.86	0.44
1:A:145:PRO:HB3	18:B:132:THR:HG21	1.99	0.44
2:I:212:ILE:HG22	2:I:213:LEU:HD12	1.99	0.44
2:I:278:LEU:HD21	2:I:345:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:201:ALA:C	5:H:203:PHE:N	2.72	0.44
15:C:311:GLU:OE1	22:U:149:ARG:NH2	2.41	0.44
15:C:328:ILE:HB	15:C:332:THR:OG1	2.17	0.44
15:C:658:ARG:O	15:C:661:SER:OG	2.23	0.44
17:F:56:LEU:HD21	17:F:59:ILE:HG13	1.99	0.44
22:U:126:GLY:H	22:U:132:ILE:HD12	1.83	0.44
24:D:74:THR:O	24:D:78:ARG:HG3	2.17	0.44
31:o:68:VAL:HA	31:o:86:VAL:HG22	2.00	0.44
33:M:66:PHE:HE2	33:M:201:GLN:HG2	1.83	0.44
33:M:145:PHE:O	33:M:149:VAL:HG13	2.18	0.44
33:M:269:ILE:HD13	33:M:276:THR:HG21	2.00	0.44
33:M:486:SER:HB2	34:f:38:VAL:HG21	2.00	0.44
34:f:23:PRO:HB2	34:f:30:MET:HG3	2.00	0.44
34:f:32:GLU:O	34:f:35:GLU:HG3	2.18	0.44
37:a:61:ILE:HD12	37:a:73:SER:O	2.18	0.44
1:A:305:VAL:HG11	1:A:327:CYS:SG	2.58	0.43
1:A:351:PRO:HD2	1:A:354:ILE:HG12	2.00	0.43
2:I:249:TRP:O	2:I:253:ILE:HG12	2.18	0.43
2:I:344:SER:HB2	2:I:413:LEU:HA	2.00	0.43
2:I:362:ILE:HG21	2:I:391:PHE:HD1	1.82	0.43
3:J:113:ARG:CD	4:N:176:LYS:HE3	2.48	0.43
4:N:127:TYR:HE1	9:V:48:ALA:HB1	1.82	0.43
5:H:33:PHE:CD1	9:V:8:ALA:HB2	2.53	0.43
5:H:169:GLU:OE2	8:Z:71:ARG:NE	2.33	0.43
12:i:9:GLY:O	12:i:39:MET:HG3	2.17	0.43
13:j:9:GLY:HA3	43:m:64:ARG:NH1	2.33	0.43
14:G:197:ARG:HH12	24:D:73:LEU:HA	1.82	0.43
15:C:345:SER:HB2	15:C:648:GLY:HA3	2.00	0.43
15:C:373:HIS:NE2	15:C:664:SER:O	2.36	0.43
16:T:69:ILE:HD12	16:T:91:MET:HE1	1.99	0.43
17:F:46:LYS:C	17:F:47:LEU:HG	2.43	0.43
20:P:96:ILE:HG22	20:P:103:ARG:HG2	1.99	0.43
21:R:123:ASP:O	21:R:124:ALA:C	2.60	0.43
26:c:49:TYR:HE1	26:c:58:LYS:HD3	1.83	0.43
28:k:66:THR:O	28:k:69:VAL:HG12	2.18	0.43
32:q:114:SER:O	32:q:114:SER:OG	2.36	0.43
33:M:46:LEU:HD13	35:g:73:THR:OG1	2.18	0.43
33:M:49:PHE:HE2	35:g:77:LEU:HD21	1.81	0.43
33:M:49:PHE:HA	33:M:98:THR:HB	2.00	0.43
33:M:74:TRP:HB3	33:M:80:ILE:O	2.18	0.43
33:M:392:PRO:HA	33:M:397:PHE:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:M:490:GLN:NE2	34:f:37:ILE:HB	2.25	0.43
37:a:64:TRP:CD1	37:a:65:ILE:H	2.36	0.43
37:a:615:GLN:HA	37:a:618:SER:OG	2.18	0.43
2:I:87:PHE:HB2	2:I:141:SER:O	2.18	0.43
2:I:90:ASP:H	2:I:93:THR:HG1	1.64	0.43
2:I:156:SER:HB3	2:I:160:TYR:CZ	2.53	0.43
5:H:161:CYS:SG	5:H:314:VAL:HG11	2.58	0.43
7:Y:12:ILE:O	7:Y:14:THR:N	2.47	0.43
7:Y:51:ASP:OD1	7:Y:51:ASP:N	2.49	0.43
8:Z:47:MET:O	8:Z:48:ALA:HB3	2.18	0.43
15:C:111:LEU:HD12	15:C:223:ARG:HG2	2.00	0.43
15:C:209:PRO:HD3	15:C:255:LEU:HD23	2.00	0.43
16:T:305:PRO:HB3	16:T:307:TYR:CE2	2.54	0.43
19:O:74:TRP:CH2	19:O:130:PRO:HD3	2.53	0.43
20:P:70:VAL:O	20:P:86:PHE:HA	2.18	0.43
22:U:55:ASP:OD1	22:U:57:PHE:N	2.51	0.43
23:E:175:CYS:C	23:E:177:ARG:N	2.74	0.43
24:D:114:ARG:HB3	24:D:122:ARG:HD2	2.00	0.43
24:D:146:GLU:H	24:D:146:GLU:CD	2.26	0.43
28:k:99:ASP:N	28:k:99:ASP:OD1	2.49	0.43
31:o:127:THR:OG1	31:o:128:GLY:N	2.51	0.43
32:q:42:HIS:O	32:q:42:HIS:CG	2.72	0.43
32:p:32:LYS:HD2	32:p:34:TYR:CE2	2.53	0.43
32:p:82:GLY:HA3	32:p:103:ASN:OD1	2.18	0.43
32:p:193:THR:OG1	32:p:196:GLU:HG3	2.16	0.43
33:M:213:GLN:OE1	33:M:274:GLU:HB2	2.18	0.43
33:M:322:GLY:HA3	33:M:403:ILE:CD1	2.48	0.43
33:M:398:ILE:HD13	33:M:474:PRO:HG3	1.99	0.43
33:M:432:LEU:HD13	33:M:432:LEU:HA	1.82	0.43
37:a:322:MET:HG2	37:a:337:HIS:CE1	2.53	0.43
37:a:325:ALA:O	37:a:328:ILE:HG22	2.19	0.43
43:m:66:ASP:HB2	43:m:69:ILE:HG22	1.99	0.43
2:I:163:ALA:HA	2:I:261:VAL:HG21	1.99	0.43
2:I:238:LEU:HD13	2:I:297:CYS:SG	2.58	0.43
2:I:247:HIS:CG	2:I:248:MET:N	2.83	0.43
2:I:355:MET:HG2	2:I:394:THR:HG23	2.01	0.43
2:I:412:TYR:CE2	33:M:77:TYR:OH	2.64	0.43
8:Z:125:TYR:HB3	8:Z:127:SER:O	2.18	0.43
15:C:176:GLY:O	15:C:182:GLN:NE2	2.51	0.43
15:C:396:LEU:O	15:C:400:VAL:HG22	2.18	0.43
15:C:413:THR:HG21	15:C:563:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:431:ILE:HG22	15:C:457:ARG:HG3	1.98	0.43
16:T:60:THR:HG23	16:T:61:GLY:N	2.33	0.43
16:T:153:ASN:HD22	16:T:153:ASN:HA	1.59	0.43
17:F:66:SER:HB3	19:O:108:PHE:HA	2.00	0.43
23:E:155:MET:HA	23:E:185:VAL:HB	1.99	0.43
24:D:77:VAL:O	24:D:77:VAL:CG1	2.66	0.43
33:M:81:ASN:OD1	33:M:81:ASN:N	2.49	0.43
33:M:348:LEU:HD12	33:M:388:ASN:HD22	1.83	0.43
33:M:420:LEU:HA	33:M:423:ILE:HG12	1.99	0.43
1:A:241:GLY:HA3	18:B:70:GLN:HG2	2.01	0.43
1:A:296:THR:O	1:A:296:THR:OG1	2.35	0.43
1:A:406:THR:HG21	15:C:162:LEU:HG	2.00	0.43
8:Z:23:ASP:O	14:G:97:ARG:NH1	2.48	0.43
13:j:4:GLY:O	43:m:65:TRP:CE3	2.72	0.43
14:G:45:GLY:HA2	14:G:48:HIS:HB2	2.00	0.43
15:C:63:ALA:HB1	19:O:135:LEU:HG	2.00	0.43
15:C:220:GLN:HG2	15:C:246:GLU:HB3	2.01	0.43
15:C:251:TYR:HE2	18:B:90:VAL:HG22	1.83	0.43
16:T:251:THR:O	16:T:289:THR:OG1	2.36	0.43
16:T:252:LYS:H	16:T:350:ASP:CB	2.31	0.43
21:R:138:LEU:O	21:R:140:GLU:N	2.48	0.43
23:E:184:TYR:CD1	23:E:184:TYR:N	2.86	0.43
23:E:193:GLU:HG2	23:E:193:GLU:H	1.47	0.43
32:q:51:LYS:HD2	32:q:70:ASP:HB2	2.00	0.43
33:M:193:PHE:CD1	33:M:193:PHE:C	2.95	0.43
33:M:293:TYR:O	33:M:297:THR:HG23	2.18	0.43
33:M:294:THR:HG21	33:M:313:VAL:CG1	2.48	0.43
33:M:316:MET:HE3	33:M:316:MET:HB3	1.86	0.43
33:M:328:ILE:HG13	33:M:329:GLN:H	1.84	0.43
37:a:336:PHE:CE2	37:a:496:SER:HB3	2.53	0.43
1:A:348:PRO:HB3	1:A:460:GLY:HA3	2.00	0.43
1:A:396:PHE:HD1	18:B:170:GLU:HB3	1.83	0.43
2:I:80:HIS:CD2	2:I:83:TRP:HB2	2.53	0.43
2:I:425:LEU:HD12	2:I:425:LEU:HA	1.87	0.43
5:H:95:ASP:HB3	5:H:98:MET:SD	2.59	0.43
14:G:210:THR:HA	21:R:21:VAL:HG12	2.01	0.43
14:G:364:GLN:CD	17:F:110:TRP:HB2	2.43	0.43
15:C:170:CYS:HB2	15:C:171:PRO:HD3	2.00	0.43
18:B:164:PHE:HE2	18:B:214:ARG:HB3	1.83	0.43
21:R:130:VAL:O	21:R:131:PRO:C	2.62	0.43
23:E:108:LEU:HD13	23:E:113:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:E:135:MET:HG3	23:E:135:MET:O	2.18	0.43
27:Q:46:LEU:HD23	27:Q:48:ILE:HG12	2.00	0.43
31:o:77:ASN:HB2	31:o:95:GLY:H	1.84	0.43
32:p:203:SER:HB2	32:p:207:TYR:CZ	2.54	0.43
34:f:36:HIS:O	34:f:39:ARG:HB3	2.19	0.43
36:d:38:ARG:O	36:d:42:TYR:CB	2.66	0.43
37:a:262:VAL:O	37:a:266:VAL:HG22	2.18	0.43
1:A:232:GLU:HG3	1:A:265:VAL:HB	2.00	0.43
2:I:348:GLY:HA2	2:I:409:SER:OG	2.19	0.43
5:H:23:LEU:HD12	5:H:277:LEU:HD13	2.01	0.43
14:G:306:MET:O	14:G:306:MET:SD	2.77	0.43
15:C:443:ILE:O	15:C:445:THR:OG1	2.34	0.43
15:C:707:LYS:HG2	15:C:708:GLU:H	1.84	0.43
17:F:138:PHE:HE2	17:F:142:PRO:HD3	1.84	0.43
18:B:134:PRO:HB2	51:B:301:FES:S2	2.59	0.43
21:R:33:LEU:HD23	21:R:33:LEU:HA	1.82	0.43
21:R:86:VAL:HA	21:R:89:LEU:HB2	2.01	0.43
24:D:182:ASN:C	24:D:184:GLU:H	2.27	0.43
26:c:49:TYR:O	26:c:50:LEU:C	2.61	0.43
31:o:223:LEU:HD21	32:p:86:ARG:HH11	1.84	0.43
32:q:83:CYS:HB2	32:q:104:SER:HB2	1.99	0.43
33:M:18:CYS:O	33:M:21:LEU:HG	2.18	0.43
43:m:23:ASP:OD1	43:m:23:ASP:C	2.61	0.43
2:I:237:PHE:O	2:I:241:ILE:HG12	2.18	0.43
5:H:58:LEU:CD1	49:H:501:U10:C15	2.97	0.43
14:G:89:LEU:HD22	14:G:325:SER:HB2	2.01	0.43
15:C:74:ILE:HD12	15:C:87:LYS:HA	2.00	0.43
15:C:159:MET:HE2	15:C:159:MET:HB2	1.84	0.43
15:C:252:VAL:HG11	18:B:90:VAL:HG11	2.00	0.43
17:F:18:TRP:CD1	17:F:37:TYR:HB3	2.54	0.43
18:B:32:LEU:HD22	20:P:90:ASP:HB3	2.00	0.43
25:X:78:LEU:HD23	25:X:78:LEU:HA	1.85	0.43
31:o:139:VAL:HG13	31:o:156:CYS:HB2	2.01	0.43
31:o:158:ILE:HG22	31:o:162:SER:OG	2.18	0.43
32:q:104:SER:C	32:q:105:LEU:HD22	2.44	0.43
33:M:241:HIS:CE1	33:M:349:PHE:CE2	3.06	0.43
35:g:64:LEU:HG	35:g:65:PRO:HD3	1.99	0.43
37:a:80:SER:HB3	37:a:493:TRP:CH2	2.51	0.43
37:a:189:PHE:CE2	37:a:197:ILE:HB	2.53	0.43
1:A:407:PRO:HG3	15:C:158:VAL:HG22	2.01	0.43
2:I:27:ASN:HD21	48:J:401:CDL:H772	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:388:ALA:HB1	2:I:448:PHE:HE1	1.83	0.43
48:I:502:CDL:PA1	48:I:502:CDL:H1O1	2.42	0.43
5:H:175:LYS:HD2	5:H:252:LEU:HD22	2.01	0.43
15:C:91:VAL:HG23	15:C:136:MET:O	2.19	0.43
15:C:213:THR:HB	15:C:215:MET:SD	2.59	0.43
17:F:59:ILE:HB	17:F:111:TRP:HB3	2.01	0.43
19:O:146:TRP:CZ2	19:O:148:GLY:HA2	2.54	0.43
24:D:68:MET:HE2	24:D:68:MET:N	2.33	0.43
31:o:51:ASP:HB3	32:p:227:PHE:CE2	2.54	0.43
32:q:77:SER:OG	32:q:98:THR:O	2.26	0.43
32:p:133:VAL:HB	32:p:150:THR:HG23	2.00	0.43
33:M:331:ILE:H	33:M:331:ILE:HG12	1.68	0.43
37:a:88:VAL:HG12	37:a:92:ILE:HD11	2.00	0.43
37:a:567:GLN:HB3	37:a:570:ASN:HB3	2.01	0.43
1:A:228:ILE:CG2	1:A:400:GLU:O	2.67	0.43
2:I:166:LYS:HE3	2:I:166:LYS:HB3	1.88	0.43
2:I:244:VAL:HG11	2:I:300:ALA:C	2.44	0.43
2:I:491:HIS:CD2	12:i:57:LYS:HE3	2.54	0.43
5:H:227:LEU:HD12	5:H:227:LEU:HA	1.81	0.43
7:Y:73:LYS:H	7:Y:73:LYS:HG2	1.64	0.43
13:j:5:TRP:CZ3	43:m:65:TRP:CB	2.99	0.43
15:C:222:THR:HG22	15:C:226:ARG:HG3	2.01	0.43
17:F:146:ASP:HB3	19:O:117:PHE:CZ	2.54	0.43
21:R:57:VAL:HA	21:R:60:PHE:CE2	2.54	0.43
33:M:491:HIS:CE1	34:f:30:MET:HE1	2.52	0.43
37:a:154:TRP:HD1	37:a:249:PRO:HD3	1.84	0.43
37:a:541:GLN:HE22	37:a:544:ARG:NH1	2.16	0.43
44:t:32:LEU:HD13	44:t:35:LEU:HD13	1.95	0.43
2:I:45:TYR:CE2	48:I:503:CDL:HA61	2.44	0.43
5:H:101:SER:O	5:H:101:SER:OG	2.34	0.43
5:H:277:LEU:HD23	5:H:277:LEU:HA	1.86	0.43
17:F:109:GLY:HA2	17:F:126:HIS:HE1	1.84	0.43
17:F:155:VAL:O	17:F:168:PRO:HD2	2.19	0.43
17:F:171:MET:HG2	19:O:95:GLY:HA2	2.00	0.43
21:R:97:LEU:HD23	21:R:97:LEU:HA	1.84	0.43
31:o:112:ASN:HD22	31:o:114:GLN:HE21	1.66	0.43
37:a:119:ILE:HG22	37:a:123:PHE:CE2	2.53	0.43
38:b:66:VAL:HG22	38:b:69:ARG:HH11	1.84	0.43
2:I:58:GLY:O	2:I:59:LEU:HB3	2.19	0.42
2:I:362:ILE:HG21	2:I:391:PHE:CD1	2.53	0.42
3:J:100:LEU:HD12	3:J:100:LEU:HA	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:22:PHE:HD1	5:H:51:PRO:HG2	1.82	0.42
5:H:241:GLY:HA2	5:H:244:THR:HG22	2.01	0.42
7:Y:20:ALA:HB2	7:Y:82:MET:HG3	2.01	0.42
14:G:147:ARG:HG2	14:G:168:PRO:HG3	2.01	0.42
14:G:231:TRP:CZ2	17:F:78:LEU:HD21	2.54	0.42
15:C:448:ARG:HE	15:C:479:ASN:HD21	1.67	0.42
16:T:55:LEU:HB3	16:T:56:ALA:H	1.55	0.42
17:F:14:LEU:HD21	17:F:41:LEU:HD13	2.01	0.42
24:D:47:GLU:HG2	24:D:48:GLU:N	2.33	0.42
25:X:25:ARG:HD2	25:X:76:ASP:OD1	2.18	0.42
26:c:57:ILE:O	26:c:61:SER:HB3	2.19	0.42
28:k:54:VAL:O	28:k:60:VAL:HG21	2.18	0.42
28:k:69:VAL:HG23	28:k:74:ASP:OD2	2.18	0.42
33:M:419:ALA:O	33:M:423:ILE:HG12	2.19	0.42
1:A:145:PRO:HD2	1:A:345:SER:CB	2.49	0.42
1:A:245:LYS:HD3	1:A:404:GLN:HB2	2.00	0.42
2:I:135:GLY:O	2:I:151:ALA:HB1	2.18	0.42
2:I:418:LEU:HD11	33:M:186:LEU:HD22	2.01	0.42
14:G:287:ILE:HD12	14:G:287:ILE:HA	1.91	0.42
14:G:306:MET:HE2	15:C:166:HIS:CD2	2.54	0.42
23:E:185:VAL:HG11	23:E:195:LEU:HA	2.01	0.42
31:o:122:ALA:N	31:o:149:SER:OG	2.40	0.42
33:M:29:ILE:HG22	33:M:31:ASN:HB2	2.01	0.42
33:M:175:LEU:HD23	33:M:175:LEU:C	2.43	0.42
37:a:112:ARG:NH2	37:a:116:TYR:OH	2.52	0.42
43:m:53:PHE:O	43:m:57:GLU:HG2	2.19	0.42
1:A:103:MET:HE2	1:A:122:TRP:CH2	2.55	0.42
1:A:120:LEU:O	1:A:123:SER:OG	2.35	0.42
1:A:433:ASP:OD1	1:A:466:ARG:NH2	2.42	0.42
3:J:96:MET:SD	4:N:152:PHE:HZ	2.43	0.42
6:K:34:SER:O	6:K:38:MET:HG2	2.19	0.42
11:S:72:TYR:OH	14:G:291:ASP:OD1	2.27	0.42
14:G:65:PRO:HB2	23:E:164:TYR:CE2	2.54	0.42
15:C:576:GLU:O	15:C:577:SER:OG	2.33	0.42
15:C:721:ASN:C	15:C:723:TYR:H	2.27	0.42
16:T:111:LEU:HD11	17:F:158:ASP:HB3	2.01	0.42
16:T:212:PRO:C	16:T:213:GLU:HG3	2.44	0.42
17:F:19:VAL:O	17:F:19:VAL:HG22	2.19	0.42
24:D:193:LEU:HD12	24:D:193:LEU:HA	1.78	0.42
26:c:89:PHE:HB3	26:c:90:PRO:HD2	2.00	0.42
32:q:42:HIS:HB2	32:p:63:PRO:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:M:56:TRP:HD1	33:M:91:LEU:HD21	1.84	0.42
33:M:116:GLY:HA2	33:M:160:TRP:CD1	2.54	0.42
34:f:51:LEU:CB	34:f:77:TYR:HD1	2.33	0.42
37:a:99:TYR:CZ	37:a:463:MET:HE2	2.53	0.42
37:a:319:LEU:HA	37:a:319:LEU:HD13	1.80	0.42
37:a:348:LEU:HD21	37:a:389:LEU:HD13	2.00	0.42
2:I:32:LEU:HG	26:c:68:ILE:HD11	2.01	0.42
2:I:107:THR:OG1	2:I:264:PHE:CE1	2.65	0.42
48:I:502:CDL:H452	48:I:502:CDL:C40	2.49	0.42
4:N:51:MET:HE3	5:H:109:TYR:HB2	2.01	0.42
5:H:34:VAL:CG1	24:D:83:THR:HG23	2.48	0.42
5:H:89:TRP:HZ2	5:H:237:ILE:HG22	1.84	0.42
6:K:79:ILE:C	6:K:82:ILE:HG22	2.44	0.42
8:Z:72:ARG:O	8:Z:76:GLU:HG2	2.19	0.42
15:C:723:TYR:O	15:C:735:MET:HB3	2.19	0.42
16:T:194:SER:HB3	16:T:342:ASP:O	2.19	0.42
16:T:335:SER:O	16:T:335:SER:OG	2.31	0.42
17:F:158:ASP:OD1	17:F:159:ASP:N	2.53	0.42
18:B:170:GLU:O	18:B:171:CYS:C	2.62	0.42
23:E:69:ILE:HA	23:E:72:VAL:HG12	2.01	0.42
33:M:58:GLN:HB3	33:M:68:PHE:CZ	2.54	0.42
33:M:61:SER:OG	33:M:480:CYS:HA	2.18	0.42
33:M:130:MET:HG3	33:M:259:PHE:HZ	1.85	0.42
33:M:284:TYR:HA	33:M:321:ILE:HD12	2.01	0.42
43:m:33:MET:HE3	43:m:33:MET:HB3	1.82	0.42
2:I:146:ILE:HD12	4:N:151:TRP:CZ3	2.55	0.42
14:G:288:LYS:HE2	14:G:288:LYS:HB2	1.83	0.42
15:C:440:PHE:HD2	15:C:469:VAL:HG12	1.85	0.42
15:C:740:ALA:C	15:C:742:LEU:N	2.78	0.42
15:C:741:VAL:O	15:C:741:VAL:CG1	2.67	0.42
18:B:180:MET:HE2	18:B:180:MET:HB2	1.92	0.42
31:o:57:GLN:HG3	31:o:58:ILE:HG13	2.02	0.42
32:q:117:VAL:O	32:q:118:HIS:ND1	2.52	0.42
32:q:118:HIS:ND1	32:q:118:HIS:O	2.50	0.42
32:p:87:GLY:HA3	32:p:92:VAL:HG23	2.01	0.42
33:M:124:LEU:HD12	33:M:160:TRP:CH2	2.50	0.42
33:M:363:LEU:HB2	33:M:366:TYR:CD2	2.53	0.42
33:M:430:LEU:HD12	37:a:148:TYR:CE2	2.55	0.42
38:b:17:MET:HB3	38:b:24:LEU:HG	2.00	0.42
38:b:37:LEU:HD23	38:b:41:ARG:HH11	1.84	0.42
1:A:209:ALA:N	1:A:214:TYR:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:201:THR:HG21	2:I:209:LEU:HD12	2.02	0.42
48:I:503:CDL:H221	48:I:503:CDL:H471	2.01	0.42
3:J:57:PHE:CE2	6:K:86:VAL:HA	2.55	0.42
4:N:121:SER:OG	4:N:122:LEU:N	2.52	0.42
13:j:41:TYR:CZ	13:j:45:LEU:HD11	2.54	0.42
15:C:196:THR:O	15:C:196:THR:HG23	2.19	0.42
15:C:225:VAL:HG23	15:C:248:ILE:CG2	2.49	0.42
15:C:343:ARG:HA	15:C:343:ARG:HD2	1.82	0.42
15:C:603:GLN:NE2	15:C:653:ASP:HA	2.34	0.42
23:E:155:MET:SD	23:E:195:LEU:HD22	2.59	0.42
31:o:197:ASN:HB2	31:o:198:PRO:HD3	2.02	0.42
32:q:184:ASN:HD22	32:p:184:ASN:H	1.66	0.42
37:a:338:LEU:HA	37:a:338:LEU:HD12	1.81	0.42
43:m:38:LYS:HA	43:m:41:LYS:NZ	2.35	0.42
1:A:102:GLU:OE1	1:A:282:PRO:HG2	2.20	0.42
1:A:231:GLU:OE2	1:A:231:GLU:CA	2.67	0.42
2:I:351:ILE:HG22	2:I:351:ILE:O	2.19	0.42
48:I:502:CDL:OA7	48:I:502:CDL:C13	2.68	0.42
6:K:13:ILE:HG22	6:K:41:ALA:HB2	2.02	0.42
6:K:60:VAL:O	6:K:64:LEU:HG	2.20	0.42
7:Y:37:LEU:HD23	7:Y:37:LEU:HA	1.81	0.42
8:Z:85:ILE:HD11	9:V:45:TRP:HZ2	1.84	0.42
9:V:49:MET:HA	9:V:52:ARG:HG2	2.01	0.42
10:W:19:ALA:CB	24:D:71:LEU:HD11	2.50	0.42
11:S:54:ASP:OD1	11:S:54:ASP:N	2.53	0.42
11:S:59:VAL:HG13	11:S:59:VAL:O	2.20	0.42
12:i:30:ARG:HB3	12:i:32:PRO:CD	2.38	0.42
12:i:35:HIS:O	12:i:35:HIS:ND1	2.53	0.42
14:G:231:TRP:CZ2	17:F:78:LEU:HD11	2.55	0.42
15:C:329:SER:N	15:C:453:MET:HE3	2.35	0.42
16:T:348:THR:OG1	16:T:349:THR:N	2.52	0.42
17:F:97:ARG:NH2	25:X:76:ASP:HB3	2.27	0.42
17:F:100:SER:HB3	17:F:124:ILE:O	2.20	0.42
18:B:180:MET:HA	18:B:199:GLU:HA	2.00	0.42
22:U:65:LEU:HD23	22:U:65:LEU:H	1.84	0.42
26:c:61:SER:HA	26:c:64:THR:HG22	2.01	0.42
32:q:46:MET:HG3	32:p:220:LYS:NZ	2.34	0.42
32:q:86:ARG:NH2	32:p:101:GLN:O	2.53	0.42
32:q:162:MET:O	32:q:180:VAL:HA	2.20	0.42
32:p:102:ASP:HB3	32:p:103:ASN:H	1.65	0.42
32:p:152:LEU:HD23	32:p:152:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:M:27:LEU:N	33:M:119:TYR:OH	2.53	0.42
33:M:358:ARG:HE	33:M:450:SER:HB3	1.84	0.42
37:a:64:TRP:CD1	37:a:65:ILE:HG12	2.55	0.42
37:a:427:VAL:HA	37:a:430:THR:OG1	2.19	0.42
1:A:397:TYR:O	1:A:401:SER:HB3	2.20	0.42
1:A:406:THR:OG1	1:A:409:ARG:NH2	2.53	0.42
1:A:414:TRP:CE3	15:C:164:MET:HE2	2.55	0.42
2:I:39:PHE:HZ	26:c:60:PRO:HB3	1.85	0.42
2:I:139:MET:HE3	2:I:152:ILE:HG12	2.01	0.42
48:I:503:CDL:H411	10:W:10:PHE:CZ	2.55	0.42
48:J:401:CDL:OB5	48:J:401:CDL:OA2	2.37	0.42
4:N:47:ASP:N	4:N:47:ASP:OD1	2.50	0.42
5:H:23:LEU:HB2	9:V:15:ILE:HD12	2.02	0.42
5:H:192:ILE:HG12	50:H:502:PEV:H392	2.02	0.42
7:Y:43:ASP:OD1	7:Y:43:ASP:N	2.53	0.42
9:V:49:MET:O	9:V:53:ASP:HB2	2.20	0.42
14:G:114:HIS:O	14:G:118:LEU:HB2	2.19	0.42
15:C:165:ASN:HD22	15:C:165:ASN:HA	1.63	0.42
16:T:156:PHE:CE1	16:T:196:MET:HB3	2.55	0.42
18:B:77:LEU:HD23	18:B:77:LEU:HA	1.92	0.42
21:R:28:ASN:O	21:R:32:VAL:HG12	2.20	0.42
22:U:56:LYS:HG3	22:U:57:PHE:CD1	2.55	0.42
32:p:23:ASP:O	32:p:24:ARG:C	2.62	0.42
32:p:87:GLY:HA3	32:p:92:VAL:CG2	2.49	0.42
37:a:434:SER:O	37:a:438:LEU:HG	2.20	0.42
2:I:80:HIS:HE1	43:m:55:THR:HB	1.85	0.42
3:J:63:LEU:HD23	3:J:63:LEU:HA	1.76	0.42
5:H:152:GLY:O	5:H:156:ILE:HG12	2.20	0.42
5:H:169:GLU:O	5:H:173:ALA:N	2.53	0.42
5:H:187:LEU:HD11	5:H:276:PHE:CZ	2.55	0.42
12:i:21:ASN:ND2	12:i:27:PRO:O	2.45	0.42
14:G:248:ASP:O	14:G:270:GLN:HG3	2.20	0.42
16:T:82:ARG:HG2	16:T:108:HIS:NE2	2.35	0.42
16:T:83:TYR:CD2	17:F:160:PRO:HB3	2.54	0.42
16:T:233:TRP:HB3	16:T:297:MET:HE1	2.02	0.42
17:F:176:ARG:NH2	24:D:138:ILE:O	2.53	0.42
24:D:110:GLU:HB3	24:D:182:ASN:HB3	2.01	0.42
31:o:120:HIS:O	31:o:148:ARG:HA	2.19	0.42
31:o:171:GLU:O	31:o:174:SER:OG	2.19	0.42
32:q:17:GLU:HG3	32:p:19:GLY:O	2.07	0.42
32:q:67:VAL:HG23	32:q:67:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:a:110:SER:HB3	37:a:111:PRO:HD3	2.02	0.42
37:a:221:ILE:O	37:a:225:LEU:HD23	2.19	0.42
3:J:91:PHE:CD1	48:J:401:CDL:C16	3.03	0.42
3:J:113:ARG:HD3	4:N:176:LYS:HE3	2.02	0.42
8:Z:112:MET:HB3	8:Z:117:GLY:HA3	2.02	0.42
11:S:51:ALA:HB2	24:D:105:PRO:HB3	2.02	0.42
11:S:82:PRO:HA	11:S:83:PRO:HD3	1.93	0.42
15:C:596:LYS:HD3	15:C:596:LYS:HA	1.85	0.42
18:B:136:MET:HE2	18:B:136:MET:HB3	1.94	0.42
23:E:96:VAL:HA	23:E:99:MET:HE3	2.02	0.42
23:E:186:PRO:HD3	24:D:186:ALA:HA	2.01	0.42
24:D:55:GLU:O	24:D:58:LYS:HG2	2.20	0.42
28:k:46:VAL:O	28:k:50:VAL:HG13	2.20	0.42
31:o:84:VAL:HG22	31:o:105:ILE:HB	2.02	0.42
32:p:98:THR:HG21	32:p:122:ILE:HG22	2.02	0.42
33:M:104:CYS:O	33:M:107:VAL:HG12	2.19	0.42
34:f:67:TYR:O	34:f:71:ARG:HB3	2.19	0.42
35:g:63:GLU:OE1	35:g:68:ILE:HD12	2.20	0.42
37:a:345:LYS:HA	37:a:348:LEU:HG	2.00	0.42
37:a:590:ASP:O	37:a:594:ILE:HG12	2.19	0.42
43:m:21:GLU:O	43:m:24:ARG:HB2	2.19	0.42
2:I:403:PRO:HB3	33:M:148:SER:OG	2.19	0.41
48:J:401:CDL:HB21	26:c:22:PHE:H	1.84	0.41
14:G:45:GLY:HA2	14:G:48:HIS:CB	2.50	0.41
15:C:203:VAL:HG11	20:P:91:LEU:HG	2.02	0.41
18:B:127:LEU:HD22	18:B:183:VAL:HG12	2.02	0.41
21:R:37:TYR:HB2	21:R:65:LEU:HD13	2.01	0.41
22:U:98:HIS:NE2	24:D:100:LYS:HD2	2.35	0.41
22:U:100:ILE:CG2	24:D:103:LEU:HB2	2.49	0.41
24:D:111:HIS:CD2	24:D:111:HIS:N	2.87	0.41
25:X:98:HIS:O	25:X:102:GLN:N	2.42	0.41
31:o:55:GLN:OE1	32:q:64:SER:HB3	2.20	0.41
32:q:205:THR:O	32:q:209:ASN:ND2	2.53	0.41
33:M:187:ALA:HB2	33:M:219:ALA:CB	2.50	0.41
33:M:358:ARG:HA	33:M:358:ARG:HD2	1.91	0.41
37:a:250:THR:N	37:a:251:PRO:HD2	2.35	0.41
37:a:633:THR:O	37:a:637:THR:HG23	2.20	0.41
1:A:224:ALA:O	18:B:114:TYR:HB3	2.21	0.41
2:I:469:LEU:HD12	2:I:469:LEU:HA	1.65	0.41
48:J:401:CDL:H402	48:J:401:CDL:H371	1.87	0.41
5:H:321:PHE:O	5:H:323:TRP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:H:501:U10:C10	23:E:85:TRP:HH2	2.11	0.41
6:K:14:PHE:CE1	6:K:38:MET:HE3	2.55	0.41
14:G:223:MET:SD	14:G:385:GLN:HA	2.60	0.41
15:C:445:THR:O	15:C:446:GLN:C	2.64	0.41
15:C:544:ARG:HG2	15:C:547:TRP:HB3	2.01	0.41
16:T:84:LEU:HD21	16:T:142:ILE:HG21	2.01	0.41
16:T:282:LEU:HD22	16:T:360:PHE:CE1	2.54	0.41
18:B:97:ALA:HA	18:B:100:ILE:HG22	2.02	0.41
21:R:44:ILE:O	21:R:47:VAL:HG22	2.20	0.41
25:X:19:LEU:HD22	25:X:72:PRO:HG3	2.01	0.41
33:M:136:MET:HE3	33:M:145:PHE:HE2	1.85	0.41
33:M:198:THR:HG23	33:M:199:ASP:N	2.35	0.41
33:M:374:MET:HG3	33:M:377:PHE:HB3	2.02	0.41
33:M:468:VAL:O	33:M:472:VAL:HG22	2.20	0.41
34:f:22:ASN:HB2	34:f:24:TYR:HE1	1.85	0.41
34:f:26:ASP:O	34:f:30:MET:N	2.47	0.41
37:a:275:LEU:HA	37:a:278:TYR:CD2	2.55	0.41
37:a:323:ILE:HG13	37:a:324:PHE:N	2.35	0.41
37:a:345:LYS:HD3	37:a:348:LEU:HD11	2.00	0.41
1:A:142:GLU:CD	1:A:150:ASP:HB2	2.45	0.41
1:A:169:GLY:HA3	1:A:216:PHE:CE1	2.55	0.41
2:I:55:GLY:C	2:I:57:LEU:N	2.78	0.41
2:I:347:ILE:HD13	2:I:486:LEU:HG	2.02	0.41
2:I:412:TYR:CZ	33:M:77:TYR:OH	2.71	0.41
48:I:503:CDL:H191	48:I:503:CDL:H432	2.02	0.41
3:J:61:PHE:CZ	5:H:139:ARG:HG2	2.55	0.41
4:N:47:ASP:HB2	5:H:105:ILE:HD13	2.02	0.41
5:H:158:VAL:HG21	5:H:246:PHE:HB3	2.02	0.41
5:H:269:PHE:HE2	9:V:19:LEU:HD23	1.85	0.41
6:K:15:ILE:HA	6:K:18:ILE:HG22	2.02	0.41
8:Z:47:MET:C	8:Z:49:MET:N	2.78	0.41
11:S:86:ARG:HA	21:R:120:ILE:HA	2.01	0.41
14:G:248:ASP:HB3	29:r:16:ALA:HB1	2.02	0.41
15:C:164:MET:HG3	15:C:195:PHE:CD1	2.55	0.41
15:C:212:LYS:CE	15:C:274:THR:CG2	2.98	0.41
15:C:438:ASP:O	15:C:439:LEU:HD23	2.20	0.41
15:C:516:VAL:HB	15:C:552:PHE:CD1	2.54	0.41
15:C:723:TYR:HD1	15:C:735:MET:HE3	1.85	0.41
16:T:70:VAL:HA	16:T:94:GLN:HB3	2.02	0.41
16:T:289:THR:HG23	16:T:292:GLU:H	1.86	0.41
22:U:55:ASP:OD2	22:U:59:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:D:141:GLU:HB2	24:D:154:ARG:HB2	2.01	0.41
31:o:175:ILE:O	31:o:193:LEU:HA	2.19	0.41
32:q:117:VAL:HG13	32:q:118:HIS:N	2.35	0.41
33:M:17:LEU:HA	33:M:128:PHE:CZ	2.55	0.41
33:M:242:VAL:HG12	33:M:305:LYS:HB2	2.02	0.41
38:b:67:MET:O	38:b:71:LEU:HG	2.21	0.41
1:A:224:ALA:HB3	18:B:114:TYR:HB3	2.01	0.41
1:A:446:THR:HG21	1:A:451:GLY:HA3	2.02	0.41
48:I:503:CDL:HB61	48:I:503:CDL:OA6	2.19	0.41
4:N:61:ILE:O	4:N:64:LEU:HB2	2.20	0.41
4:N:167:ILE:HD13	4:N:167:ILE:HA	1.82	0.41
7:Y:21:SER:O	7:Y:25:ILE:HG12	2.20	0.41
7:Y:45:ASN:HA	8:Z:130:TRP:CD1	2.55	0.41
16:T:77:THR:O	16:T:77:THR:OG1	2.36	0.41
16:T:128:GLU:O	16:T:129:ASP:HB3	2.21	0.41
16:T:218:ARG:HB2	16:T:281:GLU:HA	2.01	0.41
17:F:109:GLY:HA2	17:F:126:HIS:CE1	2.55	0.41
21:R:55:LYS:HA	21:R:55:LYS:HD2	1.81	0.41
23:E:108:LEU:HA	23:E:108:LEU:HD23	1.71	0.41
28:k:77:LEU:HD13	28:k:81:ASP:HB3	2.02	0.41
31:o:76:PRO:HB2	32:p:42:HIS:N	2.35	0.41
33:M:290:ALA:O	33:M:294:THR:HG23	2.20	0.41
33:M:318:LEU:O	33:M:403:ILE:HD12	2.20	0.41
35:g:62:TRP:O	35:g:67:TYR:OH	2.37	0.41
37:a:63:PRO:HA	37:a:73:SER:N	2.33	0.41
38:b:74:LYS:HE2	38:b:74:LYS:HB2	1.94	0.41
1:A:272:ALA:O	1:A:275:PRO:HD2	2.20	0.41
1:A:410:GLU:HB2	15:C:161:PHE:HB3	2.01	0.41
1:A:474:ARG:O	1:A:478:GLU:HG2	2.20	0.41
5:H:24:VAL:HG12	5:H:233:TYR:HD2	1.83	0.41
5:H:289:ARG:HG3	14:G:126:GLY:HA3	2.02	0.41
11:S:76:ASP:HB3	11:S:80:ASN:HB2	2.02	0.41
14:G:30:LEU:HD11	14:G:378:VAL:HG11	2.01	0.41
14:G:210:THR:HG1	21:R:22:GLY:HA3	1.85	0.41
14:G:293:LYS:O	14:G:294:LEU:HD23	2.20	0.41
15:C:111:LEU:HD11	15:C:227:PHE:HB2	2.02	0.41
15:C:444:GLY:O	15:C:471:TYR:HE1	2.04	0.41
16:T:126:ARG:NH1	16:T:153:ASN:O	2.53	0.41
21:R:90:ILE:HG22	21:R:94:ARG:HH22	1.84	0.41
23:E:88:THR:HB	23:E:98:MET:SD	2.61	0.41
23:E:157:SER:HB2	23:E:188:CYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:k:90:GLU:HB2	28:k:95:LEU:O	2.20	0.41
28:k:110:LEU:HA	28:k:113:GLU:CG	2.48	0.41
32:q:130:HIS:CD2	32:q:130:HIS:H	2.38	0.41
32:q:206:ASN:HA	32:q:209:ASN:HD21	1.86	0.41
32:p:30:GLN:OE1	32:p:30:GLN:N	2.53	0.41
33:M:139:LEU:HB3	33:M:267:PHE:CE2	2.55	0.41
34:f:39:ARG:HH22	35:g:93:ALA:CA	2.28	0.41
37:a:362:GLU:HB3	37:a:454:SER:OG	2.20	0.41
37:a:374:SER:C	37:a:376:PRO:HD3	2.45	0.41
37:a:418:PHE:CZ	37:a:422:LEU:HD13	2.55	0.41
37:a:461:ILE:HB	37:a:462:PRO:HD3	2.02	0.41
43:m:9:GLU:H	43:m:9:GLU:CD	2.27	0.41
1:A:258:LEU:H	1:A:263:THR:HG21	1.84	0.41
48:J:401:CDL:H711	48:J:401:CDL:H552	2.03	0.41
5:H:38:LYS:HE2	24:D:93:THR:CG2	2.51	0.41
5:H:89:TRP:CZ2	5:H:237:ILE:HG22	2.55	0.41
5:H:208:ALA:O	5:H:209:GLU:C	2.63	0.41
5:H:304:LEU:HB3	5:H:305:PRO:HD3	2.01	0.41
7:Y:84:TYR:O	9:V:36:ARG:HB2	2.21	0.41
8:Z:129:ARG:NE	8:Z:130:TRP:H	2.08	0.41
11:S:56:GLU:HA	24:D:220:LEU:HD13	2.01	0.41
11:S:88:VAL:HA	21:R:118:GLU:HA	2.01	0.41
14:G:240:ASP:C	14:G:242:TYR:N	2.79	0.41
15:C:421:LEU:HD11	15:C:702:LEU:HB2	2.01	0.41
16:T:167:LEU:HB2	16:T:180:TYR:OH	2.20	0.41
18:B:189:GLY:C	18:B:191:GLU:H	2.28	0.41
26:c:49:TYR:CD1	26:c:58:LYS:HB2	2.56	0.41
31:o:214:PRO:O	31:o:218:VAL:HG22	2.20	0.41
32:q:145:ILE:HD12	32:q:151:LEU:HD21	2.02	0.41
33:M:12:LEU:HD21	33:M:16:ILE:HD12	2.01	0.41
37:a:262:VAL:HG11	37:a:319:LEU:HG	2.03	0.41
37:a:347:LEU:HD23	37:a:347:LEU:HA	1.88	0.41
1:A:268:VAL:HA	1:A:271:VAL:HG12	2.02	0.41
2:I:244:VAL:HG13	2:I:245:PRO:CD	2.50	0.41
2:I:453:ARG:O	2:I:454:THR:OG1	2.35	0.41
5:H:94:PHE:CZ	9:V:22:MET:HE2	2.56	0.41
5:H:183:LEU:HD21	5:H:314:VAL:HG21	2.02	0.41
11:S:78:ARG:HD3	14:G:294:LEU:HD21	2.02	0.41
14:G:149:SER:OG	14:G:150:GLY:N	2.54	0.41
15:C:419:ALA:HB3	15:C:568:ILE:HD11	2.02	0.41
15:C:489:PRO:HD3	15:C:714:PRO:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:590:ASN:HB3	15:C:593:LYS:HG3	2.02	0.41
15:C:722:PHE:O	15:C:722:PHE:CG	2.73	0.41
15:C:735:MET:O	15:C:738:CYS:HB2	2.20	0.41
16:T:67:SER:HB2	16:T:93:SER:HB3	2.02	0.41
16:T:125:PRO:HG3	52:T:501:NDP:H2A	2.02	0.41
16:T:234:SER:C	16:T:236:PHE:H	2.29	0.41
22:U:80:SER:O	22:U:84:TYR:HB3	2.20	0.41
30:n:96:SER:O	30:n:97:ILE:C	2.62	0.41
31:o:153:GLU:HB3	31:o:172:THR:HG22	2.03	0.41
32:q:73:ILE:HG21	32:q:79:ILE:HD11	2.01	0.41
32:q:140:GLU:HB3	32:q:159:LYS:HG2	2.02	0.41
33:M:19:PRO:HB2	33:M:128:PHE:CD1	2.55	0.41
33:M:423:ILE:HD12	37:a:173:VAL:HG12	2.03	0.41
34:f:20:PRO:HB2	34:f:22:ASN:OD1	2.20	0.41
37:a:66:SER:HB2	37:a:72:ALA:HB2	2.02	0.41
37:a:124:MET:SD	37:a:264:ALA:HB2	2.60	0.41
37:a:262:VAL:HG21	37:a:319:LEU:HG	2.03	0.41
37:a:378:THR:HG23	39:h:20:PRO:HB3	2.03	0.41
37:a:621:VAL:HA	37:a:624:TYR:CD2	2.55	0.41
1:A:437:GLU:OE2	15:C:153:LYS:NZ	2.54	0.41
2:I:106:GLY:HA3	2:I:357:MET:SD	2.60	0.41
5:H:58:LEU:HD12	49:H:501:U10:H153	2.02	0.41
5:H:237:ILE:HD11	9:V:15:ILE:HD11	2.03	0.41
5:H:258:PRO:HD2	5:H:263:ILE:HD11	2.02	0.41
13:j:30:GLU:OE1	13:j:30:GLU:N	2.54	0.41
14:G:199:TRP:O	14:G:200:LYS:C	2.62	0.41
14:G:240:ASP:HB3	14:G:241:VAL:H	1.73	0.41
15:C:173:CYS:O	15:C:283:ARG:NH2	2.53	0.41
15:C:682:SER:O	27:Q:17:LEU:HD11	2.21	0.41
16:T:80:LEU:HG	16:T:144:LEU:HD13	2.02	0.41
28:k:70:HIS:HA	28:k:107:SER:HA	2.02	0.41
34:f:22:ASN:HB2	34:f:24:TYR:CE1	2.56	0.41
37:a:59:LEU:C	37:a:60:ARG:HD3	2.46	0.41
37:a:180:LEU:HG	37:a:224:LEU:HD13	2.03	0.41
1:A:53:THR:OG1	1:A:54:HIS:N	2.53	0.41
1:A:204:LEU:O	1:A:210:CYS:N	2.47	0.41
1:A:386:VAL:O	1:A:390:ILE:HG12	2.21	0.41
1:A:401:SER:C	1:A:403:GLY:H	2.29	0.41
2:I:107:THR:O	2:I:111:CYS:SG	2.73	0.41
2:I:150:LEU:HD23	2:I:150:LEU:HA	1.81	0.41
2:I:244:VAL:HG13	2:I:245:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:7:PRO:O	3:J:10:ILE:HG13	2.21	0.41
4:N:143:LEU:HD23	4:N:148:TYR:HE2	1.86	0.41
8:Z:38:ARG:HD3	8:Z:38:ARG:HA	1.72	0.41
11:S:124:ARG:HA	11:S:124:ARG:HD2	1.74	0.41
13:j:10:ASN:HA	43:m:66:ASP:O	2.21	0.41
14:G:44:ILE:CG2	14:G:392:VAL:HG12	2.51	0.41
14:G:89:LEU:HD21	14:G:327:THR:HG22	2.03	0.41
14:G:119:THR:HB	14:G:131:PHE:HA	2.03	0.41
14:G:169:LEU:HA	14:G:169:LEU:HD23	1.76	0.41
14:G:271:SER:O	14:G:275:ILE:HG12	2.21	0.41
15:C:85:VAL:HB	15:C:89:PHE:CD2	2.55	0.41
15:C:324:ASN:HB2	15:C:327:TRP:O	2.20	0.41
15:C:350:ARG:HG3	15:C:615:ASN:HA	2.03	0.41
15:C:516:VAL:HG21	15:C:533:VAL:HG11	2.03	0.41
15:C:517:GLY:O	15:C:520:LEU:HG	2.21	0.41
15:C:693:ARG:CZ	15:C:695:PRO:HG3	2.51	0.41
16:T:80:LEU:HD12	16:T:80:LEU:O	2.20	0.41
16:T:90:LYS:O	16:T:90:LYS:HG2	2.21	0.41
16:T:221:THR:HB	16:T:229:ILE:HG13	2.03	0.41
17:F:16:LYS:HA	17:F:16:LYS:HD3	1.89	0.41
17:F:64:TYR:HB2	17:F:67:ARG:HD2	2.03	0.41
19:O:76:ILE:HG13	19:O:108:PHE:CE2	2.53	0.41
22:U:115:ARG:HB3	22:U:115:ARG:HH21	1.86	0.41
22:U:149:ARG:H	22:U:149:ARG:HG2	1.67	0.41
24:D:145:ARG:HG2	24:D:149:SER:O	2.20	0.41
24:D:159:MET:HB3	24:D:164:TYR:OH	2.21	0.41
27:Q:77:LEU:HB3	27:Q:81:GLN:HB2	2.02	0.41
31:o:175:ILE:HB	31:o:205:LEU:HD11	2.02	0.41
31:o:236:THR:HG22	32:q:38:GLN:NE2	2.36	0.41
32:p:113:LEU:HD13	33:M:112:MET:SD	2.61	0.41
32:p:162:MET:HE2	32:p:200:ILE:HG21	2.03	0.41
33:M:100:LEU:O	33:M:103:ILE:HB	2.21	0.41
33:M:143:TYR:HB2	33:M:188:ILE:CD1	2.51	0.41
35:g:59:TRP:HB3	35:g:62:TRP:HB3	2.02	0.41
37:a:10:LEU:HD13	37:a:122:PHE:CE2	2.56	0.41
37:a:87:ILE:HA	37:a:90:THR:HG22	2.03	0.41
37:a:236:ILE:HG23	37:a:237:GLY:N	2.35	0.41
37:a:322:MET:HE2	37:a:322:MET:HB3	1.57	0.41
37:a:502:LYS:O	38:b:25:GLY:HA2	2.20	0.41
43:m:24:ARG:HD3	43:m:24:ARG:HA	1.91	0.41
5:H:261:LYS:HG3	5:H:263:ILE:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:88:GLU:OE1	9:V:39:HIS:HE1	2.04	0.41
14:G:53:LYS:HD3	23:E:169:TYR:CE1	2.56	0.41
14:G:73:VAL:HG12	23:E:96:VAL:HG21	2.03	0.41
14:G:132:LEU:HD23	14:G:132:LEU:HA	1.80	0.41
18:B:147:LEU:HB2	18:B:206:VAL:HG11	2.03	0.41
23:E:131:LEU:HD21	23:E:178:ILE:HG13	2.03	0.41
23:E:154:SER:O	23:E:185:VAL:N	2.51	0.41
32:p:220:LYS:HB3	32:p:223:ASN:OD1	2.21	0.41
33:M:133:VAL:HB	33:M:145:PHE:HB2	2.03	0.41
33:M:157:ILE:O	33:M:161:GLY:HA3	2.19	0.41
33:M:464:LEU:O	33:M:468:VAL:HG12	2.21	0.41
38:b:21:LYS:HD2	38:b:22:ILE:H	1.85	0.41
38:b:62:GLU:HA	38:b:65:LEU:HD12	2.03	0.41
42:s:21:ALA:O	42:s:25:ALA:N	2.54	0.41
1:A:401:SER:C	1:A:403:GLY:N	2.79	0.40
2:I:35:HIS:CD2	2:I:54:VAL:HG22	2.56	0.40
2:I:319:LEU:HD23	2:I:319:LEU:HA	1.95	0.40
6:K:61:PHE:O	6:K:65:VAL:HG23	2.22	0.40
11:S:32:HIS:NE2	24:D:85:LYS:HE2	2.36	0.40
11:S:101:LYS:HA	11:S:101:LYS:HD3	1.89	0.40
14:G:133:TRP:CH2	14:G:192:MET:HE3	2.56	0.40
14:G:246:ASP:H	14:G:277:GLN:NE2	2.19	0.40
15:C:162:LEU:O	15:C:166:HIS:HB2	2.20	0.40
15:C:481:ASP:OD1	15:C:481:ASP:N	2.54	0.40
22:U:90:PRO:HA	22:U:120:HIS:CD2	2.55	0.40
24:D:145:ARG:NH2	24:D:151:ARG:HG3	2.36	0.40
33:M:23:SER:O	33:M:119:TYR:OH	2.39	0.40
33:M:34:ILE:HG22	33:M:38:ARG:HD3	2.02	0.40
33:M:193:PHE:CD1	33:M:193:PHE:O	2.74	0.40
33:M:284:TYR:CG	33:M:414:VAL:HG11	2.56	0.40
33:M:304:LEU:H	33:M:364:VAL:CG2	2.30	0.40
34:f:24:TYR:CZ	34:f:25:LYS:HG3	2.56	0.40
34:f:40:GLU:O	34:f:43:ILE:HB	2.20	0.40
34:f:54:LYS:HA	34:f:57:TRP:HB3	2.02	0.40
37:a:40:SER:HB3	37:a:101:ILE:HD11	2.03	0.40
37:a:85:MET:O	37:a:89:VAL:HG12	2.21	0.40
37:a:87:ILE:O	37:a:91:SER:OG	2.35	0.40
1:A:76:LEU:HD23	1:A:76:LEU:HA	1.92	0.40
2:I:17:LEU:HD13	2:I:78:ILE:HD13	2.03	0.40
2:I:149:TYR:HE1	2:I:187:SER:OG	2.04	0.40
2:I:441:ILE:CG2	2:I:445:LYS:HE3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:173:ARG:HD2	4:N:178:LYS:CG	2.51	0.40
5:H:195:LEU:HD23	5:H:195:LEU:HA	1.91	0.40
5:H:223:MET:HE3	5:H:223:MET:HB3	2.00	0.40
14:G:37:VAL:HG21	14:G:378:VAL:HG21	2.04	0.40
14:G:118:LEU:HD23	14:G:118:LEU:HA	1.82	0.40
15:C:450:GLU:OE2	15:C:555:GLN:HB3	2.21	0.40
16:T:124:ASP:HB2	16:T:127:ASP:HB3	2.03	0.40
16:T:275:SER:OG	16:T:280:TYR:OH	2.22	0.40
32:q:167:ALA:CB	32:q:182:GLY:HA2	2.50	0.40
32:p:130:HIS:O	32:p:148:GLY:N	2.54	0.40
32:p:162:MET:O	32:p:180:VAL:HG13	2.21	0.40
33:M:349:PHE:HA	33:M:349:PHE:HD1	1.76	0.40
33:M:482:HIS:CE1	37:a:68:GLU:HB2	2.56	0.40
37:a:167:ALA:C	37:a:240:THR:HG23	2.47	0.40
38:b:28:ASP:OD1	38:b:28:ASP:N	2.54	0.40
38:b:45:PHE:HB2	38:b:47:LEU:HD23	2.03	0.40
38:b:59:GLU:O	38:b:63:TYR:HB2	2.21	0.40
1:A:404:GLN:O	15:C:116:ASN:HA	2.20	0.40
2:I:152:ILE:O	2:I:155:GLN:HG3	2.21	0.40
3:J:107:PHE:HE2	5:H:305:PRO:HG3	1.86	0.40
4:N:164:ILE:O	4:N:168:VAL:HG12	2.21	0.40
5:H:139:ARG:HB3	5:H:292:TYR:CZ	2.56	0.40
9:V:15:ILE:HG21	9:V:15:ILE:HD13	1.80	0.40
11:S:43:THR:HG22	22:U:69:GLN:N	2.33	0.40
12:i:59:ASP:O	12:i:63:MET:HG2	2.21	0.40
14:G:192:MET:HE2	24:D:82:LEU:HD23	2.04	0.40
14:G:210:THR:OG1	21:R:22:GLY:HA3	2.21	0.40
15:C:260:LEU:HD12	15:C:263:ASN:ND2	2.36	0.40
15:C:298:ALA:HB3	15:C:554:LEU:O	2.20	0.40
15:C:439:LEU:HD22	15:C:468:LYS:HB2	2.03	0.40
15:C:498:GLY:HA2	15:C:503:CYS:SG	2.62	0.40
15:C:526:LYS:HE2	15:C:526:LYS:HB2	1.87	0.40
16:T:158:ASP:HA	16:T:162:HIS:HB2	2.02	0.40
18:B:182:THR:HG21	18:B:195:TYR:CE2	2.57	0.40
19:O:40:GLY:O	19:O:43:SER:OG	2.40	0.40
20:P:102:LEU:HA	20:P:102:LEU:HD23	1.84	0.40
22:U:133:TYR:CD2	24:D:200:LEU:HD22	2.56	0.40
24:D:164:TYR:N	24:D:164:TYR:CD1	2.89	0.40
31:o:141:VAL:HA	31:o:158:ILE:HB	2.02	0.40
37:a:619:GLY:O	37:a:623:HIS:N	2.49	0.40
38:b:62:GLU:O	38:b:66:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ARG:HD2	1:A:218:VAL:O	2.22	0.40
3:J:68:PHE:CD1	5:H:145:VAL:HG22	2.56	0.40
5:H:193:SER:O	5:H:197:GLU:N	2.45	0.40
6:K:31:MET:O	6:K:35:ILE:HG12	2.22	0.40
14:G:46:LEU:HD23	23:E:135:MET:SD	2.61	0.40
14:G:314:GLU:O	14:G:318:GLU:HB3	2.21	0.40
16:T:115:LEU:O	19:O:88:LEU:HD22	2.21	0.40
16:T:218:ARG:HB2	16:T:280:TYR:O	2.22	0.40
16:T:358:LEU:HD12	16:T:358:LEU:H	1.85	0.40
17:F:69:ARG:NH1	17:F:91:SER:O	2.55	0.40
17:F:116:TRP:HZ3	17:F:131:ARG:HG3	1.87	0.40
18:B:203:PRO:O	18:B:207:VAL:HG22	2.21	0.40
21:R:60:PHE:O	21:R:64:ARG:HG3	2.21	0.40
31:o:114:GLN:HB3	31:o:115:GLU:OE2	2.20	0.40
33:M:45:SER:OG	33:M:102:PRO:HG3	2.22	0.40
33:M:75:LEU:HD11	33:M:80:ILE:HG12	2.03	0.40
33:M:335:ILE:HD11	33:M:481:MET:HG3	2.03	0.40
33:M:362:ARG:HA	33:M:362:ARG:NE	2.35	0.40
37:a:41:ILE:HG23	37:a:44:LEU:HD13	2.03	0.40
37:a:534:ASN:ND2	37:a:536:ASN:O	2.55	0.40
1:A:96:THR:HG21	1:A:173:ARG:NE	2.36	0.40
1:A:331:ARG:O	1:A:336:ASN:ND2	2.41	0.40
49:H:501:U10:O5	49:H:501:U10:C4M	2.67	0.40
14:G:225:ARG:NH2	14:G:332:GLU:OE2	2.54	0.40
14:G:266:GLU:CD	14:G:270:GLN:HE21	2.30	0.40
16:T:147:ARG:HA	16:T:147:ARG:HD3	1.77	0.40
17:F:18:TRP:CZ2	17:F:40:GLN:HB3	2.57	0.40
17:F:44:PHE:C	17:F:46:LYS:H	2.29	0.40
17:F:118:MET:O	17:F:141:HIS:HB3	2.21	0.40
24:D:47:GLU:HG2	24:D:48:GLU:H	1.86	0.40
31:o:54:GLY:HA2	32:q:42:HIS:NE2	2.36	0.40
33:M:74:TRP:CZ3	33:M:141:LEU:HD11	2.56	0.40
33:M:143:TYR:O	33:M:144:VAL:C	2.62	0.40
33:M:392:PRO:HB2	37:a:138:LEU:HA	2.03	0.40
34:f:36:HIS:O	34:f:40:GLU:HG2	2.21	0.40
35:g:76:ILE:HA	35:g:79:VAL:HG12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	427/486 (88%)	381 (89%)	46 (11%)	0	100	100
2	I	479/499 (96%)	440 (92%)	39 (8%)	0	100	100
3	J	92/119 (77%)	86 (94%)	6 (6%)	0	100	100
4	N	145/205 (71%)	125 (86%)	20 (14%)	0	100	100
5	H	316/325 (97%)	283 (90%)	33 (10%)	0	100	100
6	K	83/100 (83%)	81 (98%)	2 (2%)	0	100	100
7	Y	96/106 (91%)	87 (91%)	8 (8%)	1 (1%)	12	43
8	Z	138/143 (96%)	112 (81%)	26 (19%)	0	100	100
9	V	55/65 (85%)	52 (94%)	3 (6%)	0	100	100
10	W	35/65 (54%)	31 (89%)	4 (11%)	0	100	100
11	S	99/131 (76%)	86 (87%)	13 (13%)	0	100	100
12	i	64/81 (79%)	59 (92%)	4 (6%)	1 (2%)	7	35
13	j	66/83 (80%)	63 (96%)	3 (4%)	0	100	100
14	G	380/394 (96%)	348 (92%)	32 (8%)	0	100	100
15	C	691/748 (92%)	618 (89%)	72 (10%)	1 (0%)	48	78
16	T	326/402 (81%)	281 (86%)	45 (14%)	0	100	100
17	F	176/190 (93%)	151 (86%)	25 (14%)	0	100	100
18	B	217/255 (85%)	184 (85%)	33 (15%)	0	100	100
19	O	109/154 (71%)	102 (94%)	7 (6%)	0	100	100
20	P	69/110 (63%)	64 (93%)	5 (7%)	0	100	100
21	R	127/169 (75%)	119 (94%)	8 (6%)	0	100	100
22	U	120/159 (76%)	98 (82%)	22 (18%)	0	100	100
23	E	151/218 (69%)	134 (89%)	16 (11%)	1 (1%)	18	50
24	D	175/222 (79%)	160 (91%)	14 (8%)	1 (1%)	21	52
25	X	99/133 (74%)	92 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	c	97/106 (92%)	91 (94%)	6 (6%)	0	100	100
27	Q	90/97 (93%)	81 (90%)	9 (10%)	0	100	100
28	k	76/122 (62%)	74 (97%)	2 (3%)	0	100	100
29	r	22/24 (92%)	18 (82%)	4 (18%)	0	100	100
30	n	25/113 (22%)	22 (88%)	3 (12%)	0	100	100
31	o	200/252 (79%)	172 (86%)	28 (14%)	0	100	100
32	p	222/275 (81%)	190 (86%)	30 (14%)	2 (1%)	14	45
32	q	226/275 (82%)	195 (86%)	28 (12%)	3 (1%)	9	38
33	M	480/495 (97%)	433 (90%)	47 (10%)	0	100	100
34	f	74/107 (69%)	67 (90%)	7 (10%)	0	100	100
35	g	45/114 (40%)	39 (87%)	6 (13%)	0	100	100
36	d	64/117 (55%)	60 (94%)	4 (6%)	0	100	100
37	a	592/669 (88%)	524 (88%)	66 (11%)	2 (0%)	36	65
38	b	61/103 (59%)	50 (82%)	11 (18%)	0	100	100
39	h	26/69 (38%)	26 (100%)	0	0	100	100
40	e	82/126 (65%)	80 (98%)	2 (2%)	0	100	100
41	l	21/71 (30%)	21 (100%)	0	0	100	100
42	s	18/20 (90%)	18 (100%)	0	0	100	100
43	m	67/98 (68%)	48 (72%)	17 (25%)	2 (3%)	3	26
44	t	29/73 (40%)	28 (97%)	1 (3%)	0	100	100
All	All	7252/8888 (82%)	6474 (89%)	764 (10%)	14 (0%)	44	72

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	i	30	ARG
32	q	108	VAL
15	C	272	ALA
24	D	120	GLU
32	q	23	ASP
32	q	106	VAL
32	p	102	ASP
32	p	217	GLU
37	a	509	SER
7	Y	103	CYS

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Mol	Chain	Res	Type
23	E	189	PRO
37	a	511	PHE
43	m	46	LEU
43	m	50	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	349/396 (88%)	348 (100%)	1 (0%)	86	83
2	I	399/416 (96%)	394 (99%)	5 (1%)	61	71
3	J	87/106 (82%)	87 (100%)	0	100	100
4	N	133/186 (72%)	133 (100%)	0	100	100
5	H	266/272 (98%)	264 (99%)	2 (1%)	73	76
6	K	74/86 (86%)	74 (100%)	0	100	100
7	Y	88/94 (94%)	88 (100%)	0	100	100
8	Z	112/115 (97%)	112 (100%)	0	100	100
9	V	48/53 (91%)	48 (100%)	0	100	100
10	W	30/53 (57%)	29 (97%)	1 (3%)	33	55
11	S	92/118 (78%)	92 (100%)	0	100	100
12	i	52/66 (79%)	48 (92%)	4 (8%)	12	38
13	j	62/73 (85%)	62 (100%)	0	100	100
14	G	328/340 (96%)	325 (99%)	3 (1%)	70	75
15	C	576/625 (92%)	570 (99%)	6 (1%)	68	74
16	T	271/334 (81%)	269 (99%)	2 (1%)	76	77
17	F	168/179 (94%)	163 (97%)	5 (3%)	36	57
18	B	188/220 (86%)	186 (99%)	2 (1%)	65	73
19	O	93/128 (73%)	93 (100%)	0	100	100
20	P	62/97 (64%)	62 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	R	115/148 (78%)	113 (98%)	2 (2%)	53 67
22	U	104/133 (78%)	104 (100%)	0	100 100
23	E	129/184 (70%)	121 (94%)	8 (6%)	16 44
24	D	157/191 (82%)	153 (98%)	4 (2%)	42 61
25	X	92/114 (81%)	92 (100%)	0	100 100
26	c	79/84 (94%)	78 (99%)	1 (1%)	61 71
27	Q	82/85 (96%)	81 (99%)	1 (1%)	63 72
28	k	73/112 (65%)	73 (100%)	0	100 100
30	n	21/84 (25%)	20 (95%)	1 (5%)	23 48
31	o	171/211 (81%)	171 (100%)	0	100 100
32	p	181/228 (79%)	179 (99%)	2 (1%)	65 73
32	q	184/228 (81%)	179 (97%)	5 (3%)	39 59
33	M	421/434 (97%)	414 (98%)	7 (2%)	53 67
34	f	68/93 (73%)	68 (100%)	0	100 100
35	g	42/96 (44%)	42 (100%)	0	100 100
37	a	504/568 (89%)	503 (100%)	1 (0%)	87 86
38	b	56/87 (64%)	56 (100%)	0	100 100
39	h	23/51 (45%)	22 (96%)	1 (4%)	26 50
43	m	63/90 (70%)	63 (100%)	0	100 100
44	t	24/60 (40%)	23 (96%)	1 (4%)	26 51
All	All	6067/7238 (84%)	6002 (99%)	65 (1%)	63 73

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	GLU
2	I	35	HIS
2	I	120	PHE
2	I	354	LEU
2	I	469	LEU
2	I	497	LEU
5	H	290	TYR
5	H	298	LEU
10	W	26	VAL
12	i	11	LEU

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Mol	Chain	Res	Type
12	i	31	HIS
12	i	36	VAL
12	i	41	LEU
14	G	68	ASP
14	G	73	VAL
14	G	310	ILE
15	C	104	ARG
15	C	218	CYS
15	C	266	ASP
15	C	270	VAL
15	C	275	SER
15	C	601	VAL
16	T	147	ARG
16	T	153	ASN
17	F	19	VAL
17	F	39	PHE
17	F	42	LEU
17	F	47	LEU
17	F	49	THR
18	B	110	VAL
18	B	181	ILE
21	R	113	ASP
21	R	138	LEU
23	E	89	PHE
23	E	93	CYS
23	E	130	THR
23	E	153	ILE
23	E	172	VAL
23	E	183	ILE
23	E	188	CYS
23	E	193	GLU
24	D	73	LEU
24	D	156	ASP
24	D	174	VAL
24	D	197	LYS
26	c	46	THR
27	Q	19	CYS
30	n	97	ILE
32	q	14	TRP
32	q	16	ARG
32	q	102	ASP
32	q	107	HIS

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Mol	Chain	Res	Type
32	q	108	VAL
32	p	29	LEU
32	p	207	TYR
33	M	141	LEU
33	M	150	LEU
33	M	155	ILE
33	M	191	ILE
33	M	195	THR
33	M	331	ILE
33	M	391	LEU
37	a	511	PHE
39	h	25	THR
44	t	37	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	441	GLN
2	I	80	HIS
2	I	84	ASN
2	I	117	GLN
2	I	292	GLN
2	I	312	GLN
2	I	326	HIS
2	I	464	ASN
4	N	25	HIS
4	N	73	HIS
4	N	180	GLN
5	H	143	GLN
6	K	27	ASN
6	K	43	ASN
6	K	45	ASN
7	Y	45	ASN
7	Y	87	ASN
8	Z	63	GLN
8	Z	126	ASN
9	V	34	HIS
9	V	39	HIS
9	V	42	HIS
11	S	69	ASN
12	i	17	GLN
14	G	23	HIS

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Mol	Chain	Res	Type
14	G	78	GLN
14	G	99	GLN
14	G	113	ASN
14	G	121	HIS
14	G	277	GLN
14	G	385	GLN
15	C	93	GLN
15	C	165	ASN
15	C	182	GLN
15	C	184	GLN
15	C	284	ASN
15	C	508	ASN
15	C	522	ASN
15	C	538	GLN
15	C	605	HIS
15	C	606	HIS
15	C	716	GLN
16	T	117	GLN
16	T	153	ASN
16	T	182	GLN
16	T	209	ASN
16	T	291	HIS
16	T	340	ASN
17	F	27	HIS
17	F	40	GLN
17	F	76	ASN
17	F	125	ASN
18	B	33	ASN
18	B	81	GLN
18	B	84	ASN
18	B	118	ASN
18	B	126	HIS
18	B	196	ASN
18	B	221	HIS
19	O	49	HIS
19	O	77	ASN
20	P	92	ASN
20	P	106	GLN
20	P	108	HIS
21	R	66	ASN
21	R	129	HIS
22	U	41	GLN

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Mol	Chain	Res	Type
22	U	46	ASN
22	U	69	GLN
22	U	134	HIS
22	U	138	HIS
23	E	100	HIS
23	E	145	GLN
23	E	166	HIS
23	E	217	ASN
24	D	111	HIS
24	D	190	HIS
25	X	97	HIS
25	X	102	GLN
25	X	131	ASN
26	c	28	ASN
26	c	91	ASN
27	Q	35	ASN
27	Q	88	ASN
30	n	81	ASN
30	n	83	ASN
31	o	77	ASN
31	o	94	ASN
31	o	112	ASN
31	o	120	HIS
32	q	33	ASN
32	q	38	GLN
32	q	47	ASN
32	q	135	HIS
32	q	184	ASN
32	q	206	ASN
32	q	209	ASN
32	q	218	ASN
32	q	223	ASN
32	p	99	ASN
32	p	130	HIS
32	p	160	HIS
32	p	214	HIS
32	p	223	ASN
33	M	67	GLN
33	M	201	GLN
33	M	241	HIS
33	M	301	GLN
33	M	317	ASN

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Mol	Chain	Res	Type
33	M	434	ASN
33	M	491	HIS
34	f	36	HIS
34	f	65	ASN
34	f	66	HIS
37	a	171	ASN
37	a	417	ASN
37	a	534	ASN
37	a	541	GLN
37	a	560	ASN
37	a	567	GLN
38	b	56	HIS
43	m	68	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	$\#\|Z\| > 2$
50	PEV	H	502	-	48,48,48	0.38	0	51,53,53	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	CDL	I	503	-	97,97,99	0.27	0	103,109,111	0.34	0
47	T7X	I	501	-	54,54,61	0.28	0	64,66,73	0.77	3 (4%)
45	SF4	C	801	15	0,12,12	-	-	-		
51	FES	C	803	15	0,4,4	-	-	-		
51	FES	B	301	-	0,4,4	-	-	-		
45	SF4	D	301	24	0,12,12	-	-	-		
54	BCT	q	802	53	2,3,3	0.60	0	2,3,3	0.26	0
46	FMN	A	502	-	33,33,33	0.62	0	48,50,50	0.72	1 (2%)
47	T7X	p	301	-	61,61,61	0.26	0	71,73,73	0.39	0
48	CDL	J	401	-	86,86,99	0.31	0	92,98,111	0.52	1 (1%)
45	SF4	D	302	24	0,12,12	-	-	-		
48	CDL	I	502	-	99,99,99	0.27	0	105,111,111	0.43	0
52	NDP	T	501	-	49,52,52	0.49	0	66,80,80	0.69	1 (1%)
45	SF4	E	301	23	0,12,12	-	-	-		
45	SF4	C	802	15	0,12,12	-	-	-		
49	U10	H	501	-	44,44,63	0.72	2 (4%)	53,56,79	0.57	0
45	SF4	A	501	1	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	PEV	H	502	-	-	25/52/52/52	-
48	CDL	I	503	-	-	32/108/108/110	-
47	T7X	I	501	-	1/1/10/18	16/49/73/80	0/1/1/1
45	SF4	C	801	15	-	-	0/6/5/5
51	FES	C	803	15	-	-	0/1/1/1
51	FES	B	301	-	-	-	0/1/1/1
45	SF4	D	301	24	-	-	0/6/5/5
46	FMN	A	502	-	-	6/18/18/18	0/3/3/3
47	T7X	p	301	-	-	16/56/80/80	0/1/1/1
48	CDL	J	401	-	-	33/97/97/110	-
45	SF4	D	302	24	-	-	0/6/5/5
48	CDL	I	502	-	-	33/110/110/110	-
52	NDP	T	501	-	-	6/34/77/77	0/5/5/5
45	SF4	E	301	23	-	-	0/6/5/5
45	SF4	C	802	15	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	U10	H	501	-	-	18/41/65/87	0/1/1/1
45	SF4	A	501	1	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	H	501	U10	C4-C5	-2.41	1.41	1.48
49	H	501	U10	C3-C2	-2.38	1.42	1.48

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	I	501	T7X	C4-C3-C2	3.29	116.58	110.82
48	J	401	CDL	OA6-CA4-CA6	2.84	118.69	108.40
47	I	501	T7X	O3-C3-C4	2.55	116.24	110.35
47	I	501	T7X	O3-C3-C2	2.41	115.92	110.35
52	T	501	NDP	O4D-C1D-C2D	-2.39	101.42	106.64
46	A	502	FMN	C4-N3-C2	-2.09	121.78	125.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
47	I	501	T7X	C3

All (185) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	O3'-C3'-C4'-C5'
47	I	501	T7X	C2-C1-O1-P1
47	I	501	T7X	C6-C1-O1-P1
47	I	501	T7X	C8-C7-O13-P1
47	I	501	T7X	C12-C10-O16-C8
47	I	501	T7X	O17-C10-O16-C8
48	I	502	CDL	CA2-OA2-PA1-OA3
48	I	502	CDL	OA7-CA5-OA6-CA4
48	I	502	CDL	C11-CA5-OA6-CA4
48	I	502	CDL	CB3-OB5-PB2-OB3
48	I	502	CDL	CB4-CB3-OB5-PB2
48	I	503	CDL	C1-CA2-OA2-PA1
48	I	503	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
48	I	503	CDL	OB9-CB7-OB8-CB6
48	I	503	CDL	C71-CB7-OB8-CB6
48	J	401	CDL	OA7-CA5-OA6-CA4
48	J	401	CDL	C1-CB2-OB2-PB2
48	J	401	CDL	CB3-OB5-PB2-OB2
48	J	401	CDL	CB4-CB3-OB5-PB2
49	H	501	U10	C12-C11-C9-C10
49	H	501	U10	C17-C18-C19-C20
49	H	501	U10	C17-C18-C19-C21
49	H	501	U10	C21-C22-C23-C24
49	H	501	U10	C26-C27-C28-C29
49	H	501	U10	C35-C34-C36-C37
50	H	502	PEV	C1-O3P-P-O1P
50	H	502	PEV	C1-O3P-P-O4P
50	H	502	PEV	C4-O4P-P-O1P
50	H	502	PEV	C5-C4-O4P-P
48	J	401	CDL	C11-CA5-OA6-CA4
49	H	501	U10	C12-C11-C9-C8
48	I	502	CDL	O1-C1-CA2-OA2
49	H	501	U10	C14-C16-C17-C18
49	H	501	U10	C24-C26-C27-C28
46	A	502	FMN	C2'-C3'-C4'-C5'
50	H	502	PEV	C16-C17-C18-C19
50	H	502	PEV	C11-C12-C13-C14
46	A	502	FMN	O3'-C3'-C4'-O4'
46	A	502	FMN	C2'-C3'-C4'-O4'
49	H	501	U10	C4-C3-O3-C3M
48	I	502	CDL	CA2-OA2-PA1-OA5
48	I	502	CDL	CA7-C31-C32-C33
52	T	501	NDP	C2D-C1D-N1N-C6N
48	I	502	CDL	C79-C80-C81-C82
47	p	301	T7X	C12-C10-O16-C8
50	H	502	PEV	C22-C23-C24-C25
49	H	501	U10	C3-C4-O4-C4M
48	I	503	CDL	C34-C35-C36-C37
47	p	301	T7X	O17-C10-O16-C8
48	J	401	CDL	C35-C36-C37-C38
48	I	503	CDL	CB2-OB2-PB2-OB5
52	T	501	NDP	C2D-C1D-N1N-C2N
48	I	503	CDL	C1-CB2-OB2-PB2
48	I	502	CDL	CA5-C11-C12-C13
49	H	501	U10	C7-C8-C9-C11

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Mol	Chain	Res	Type	Atoms
50	H	502	PEV	C23-C24-C25-C26
50	H	502	PEV	C35-C36-C37-C38
47	I	501	T7X	C39-C40-C41-C42
48	J	401	CDL	CA6-CA4-OA6-CA5
48	I	503	CDL	C36-C37-C38-C39
48	I	502	CDL	C77-C78-C79-C80
48	I	503	CDL	OB6-CB4-CB6-OB8
48	I	503	CDL	C53-C54-C55-C56
48	J	401	CDL	C19-C20-C21-C22
48	I	502	CDL	CB2-C1-CA2-OA2
48	J	401	CDL	C17-C18-C19-C20
50	H	502	PEV	O3P-C1-C2-C3
48	J	401	CDL	C51-C52-C53-C54
47	p	301	T7X	C31-C11-O18-C9
48	I	502	CDL	C1-CA2-OA2-PA1
48	J	401	CDL	CA4-CA3-OA5-PA1
48	I	502	CDL	C15-C16-C17-C18
48	I	503	CDL	CB3-CB4-CB6-OB8
47	I	501	T7X	C15-C16-C17-C18
47	I	501	T7X	C18-C19-C20-C21
47	p	301	T7X	C19-C20-C21-C22
47	p	301	T7X	C22-C23-C24-C25
50	H	502	PEV	O3P-C1-C2-O2
50	H	502	PEV	C2-C1-O3P-P
48	I	502	CDL	C75-C76-C77-C78
48	I	502	CDL	C18-C19-C20-C21
48	J	401	CDL	OA5-CA3-CA4-CA6
48	I	503	CDL	C73-C74-C75-C76
48	J	401	CDL	C21-C22-C23-C24
47	I	501	T7X	C7-C8-C9-O18
48	J	401	CDL	OA5-CA3-CA4-OA6
47	I	501	T7X	O16-C8-C9-O18
48	I	503	CDL	C80-C81-C82-C83
48	J	401	CDL	C51-CB5-OB6-CB4
48	I	503	CDL	C20-C21-C22-C23
48	J	401	CDL	C72-C73-C74-C75
48	I	503	CDL	C57-C58-C59-C60
48	I	503	CDL	CB5-C51-C52-C53
48	I	502	CDL	CA2-OA2-PA1-OA4
48	J	401	CDL	CB3-OB5-PB2-OB4
48	J	401	CDL	C53-C54-C55-C56
49	H	501	U10	C25-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
48	J	401	CDL	CB7-C71-C72-C73
52	T	501	NDP	O4D-C1D-N1N-C6N
48	I	502	CDL	C33-C34-C35-C36
48	I	503	CDL	C72-C73-C74-C75
48	I	503	CDL	C31-CA7-OA8-CA6
47	p	301	T7X	O19-C11-O18-C9
46	A	502	FMN	C5'-O5'-P-O1P
48	I	503	CDL	CA4-CA6-OA8-CA7
47	I	501	T7X	C7-O13-P1-O1
48	I	502	CDL	CB3-OB5-PB2-OB2
48	I	503	CDL	CA2-OA2-PA1-OA5
48	I	503	CDL	CB3-OB5-PB2-OB2
48	J	401	CDL	CA2-OA2-PA1-OA5
50	H	502	PEV	C36-C37-C38-C39
48	J	401	CDL	C16-C17-C18-C19
47	p	301	T7X	C24-C25-C26-C27
48	I	502	CDL	C59-C60-C61-C62
48	J	401	CDL	C31-C32-C33-C34
48	I	503	CDL	C17-C18-C19-C20
48	I	502	CDL	CA2-C1-CB2-OB2
48	I	503	CDL	C16-C17-C18-C19
47	p	301	T7X	C13-C14-C15-C16
50	H	502	PEV	C33-C34-C35-C36
48	I	503	CDL	OA9-CA7-OA8-CA6
50	H	502	PEV	O2-C2-C3-O3
50	H	502	PEV	C13-C14-C15-C16
49	H	501	U10	C23-C24-C26-C27
48	I	502	CDL	C11-C12-C13-C14
48	I	502	CDL	CB3-CB4-CB6-OB8
48	J	401	CDL	OB7-CB5-OB6-CB4
49	H	501	U10	C7-C8-C9-C10
47	p	301	T7X	C36-C37-C38-C39
48	J	401	CDL	C33-C34-C35-C36
47	p	301	T7X	C1-O1-P1-O12
47	p	301	T7X	C37-C38-C39-C40
48	J	401	CDL	C34-C35-C36-C37
48	J	401	CDL	CB6-CB4-OB6-CB5
50	H	502	PEV	C3-C2-O2-C31
47	p	301	T7X	C43-C44-C45-C46
47	I	501	T7X	C21-C22-C23-C24
52	T	501	NDP	O4D-C1D-N1N-C2N
48	J	401	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
50	H	502	PEV	C41-C42-C43-C44
52	T	501	NDP	PN-O3-PA-O1A
48	I	502	CDL	C57-C58-C59-C60
48	I	503	CDL	C75-C76-C77-C78
48	J	401	CDL	C75-C76-C77-C78
50	H	502	PEV	C21-C22-C23-C24
48	I	502	CDL	C31-CA7-OA8-CA6
50	H	502	PEV	C14-C15-C16-C17
48	J	401	CDL	C31-CA7-OA8-CA6
48	J	401	CDL	C24-C25-C26-C27
50	H	502	PEV	C4-O4P-P-O3P
48	J	401	CDL	C52-C53-C54-C55
48	I	502	CDL	C78-C79-C80-C81
48	I	503	CDL	C44-C45-C46-C47
48	I	502	CDL	C20-C21-C22-C23
48	I	503	CDL	C15-C16-C17-C18
52	T	501	NDP	O4D-C4D-C5D-O5D
48	I	502	CDL	C51-CB5-OB6-CB4
48	I	502	CDL	C32-C33-C34-C35
48	I	502	CDL	C73-C74-C75-C76
48	J	401	CDL	C32-C31-CA7-OA8
47	p	301	T7X	C32-C33-C34-C35
47	p	301	T7X	C1-O1-P1-O13
49	H	501	U10	C16-C17-C18-C19
47	I	501	T7X	C31-C11-O18-C9
48	I	502	CDL	OB7-CB5-OB6-CB4
47	I	501	T7X	C38-C39-C40-C41
48	I	503	CDL	CB2-OB2-PB2-OB3
48	I	503	CDL	CB3-OB5-PB2-OB3
48	I	502	CDL	C51-C52-C53-C54
49	H	501	U10	C33-C34-C36-C37
50	H	502	PEV	C1-C2-O2-C31
47	I	501	T7X	O18-C11-C31-C32
49	H	501	U10	C27-C28-C29-C30
47	p	301	T7X	C34-C35-C36-C37
48	I	502	CDL	C36-C37-C38-C39
48	I	503	CDL	C52-C51-CB5-OB6
48	I	503	CDL	C12-C11-CA5-OA7
48	I	503	CDL	C12-C11-CA5-OA6
48	J	401	CDL	C32-C31-CA7-OA9
50	H	502	PEV	C12-C13-C14-C15
47	I	501	T7X	O19-C11-C31-C32

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Mol	Chain	Res	Type	Atoms
50	H	502	PEV	C37-C38-C39-C40
47	p	301	T7X	C42-C43-C44-C45
50	H	502	PEV	O2-C31-C32-C33

There are no ring outliers.

14 monomers are involved in 181 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	H	502	PEV	10	0
48	I	503	CDL	44	0
47	I	501	T7X	3	0
45	C	801	SF4	1	0
51	B	301	FES	2	0
45	D	301	SF4	3	0
54	q	802	BCT	1	0
46	A	502	FMN	3	0
48	J	401	CDL	39	0
48	I	502	CDL	38	0
52	T	501	NDP	4	0
45	E	301	SF4	6	0
49	H	501	U10	25	0
45	A	501	SF4	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

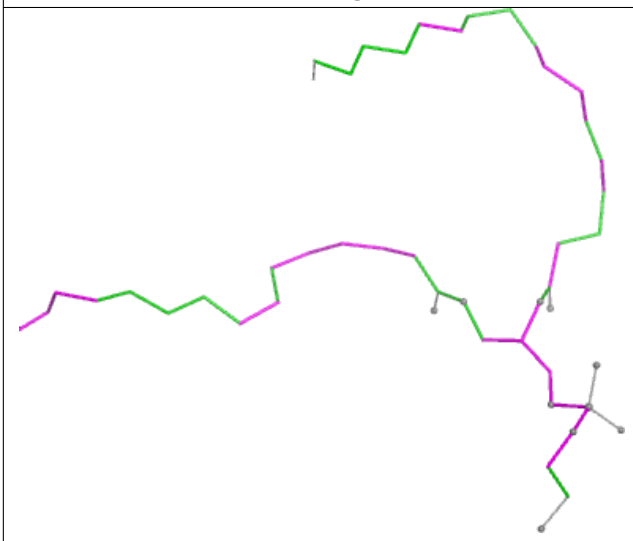
Ligand PEV H 502



Bond lengths



Bond angles

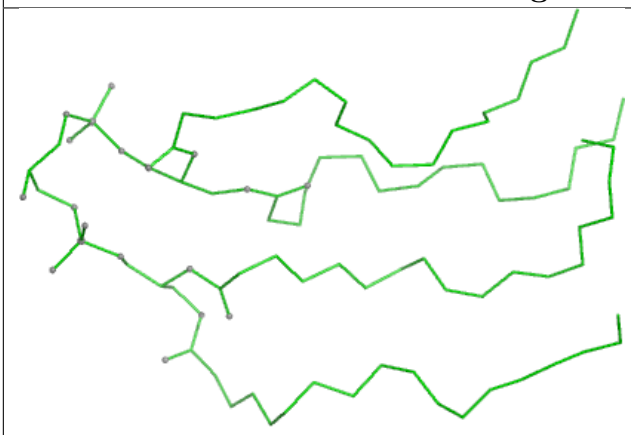


Torsions

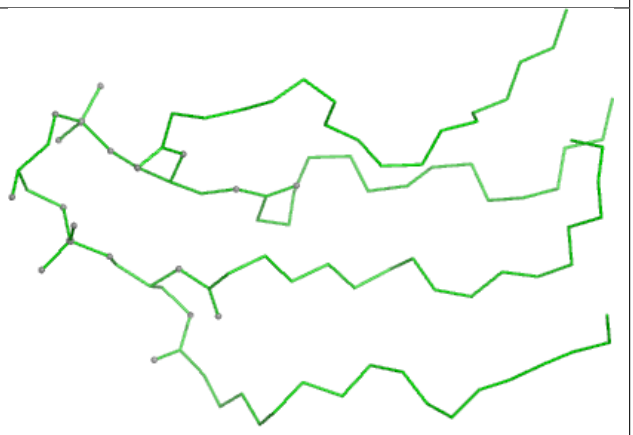


Rings

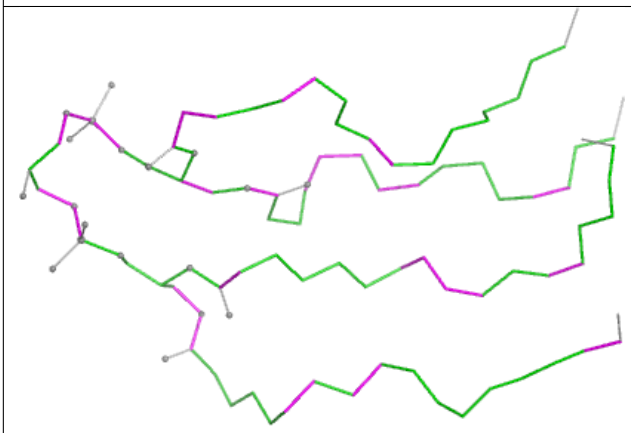
Ligand CDL I 503



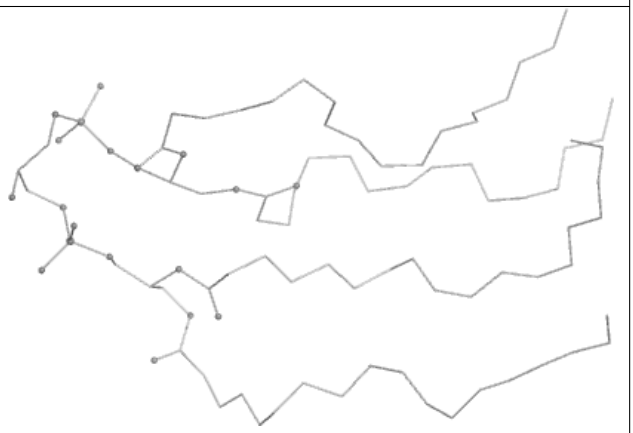
Bond lengths



Bond angles

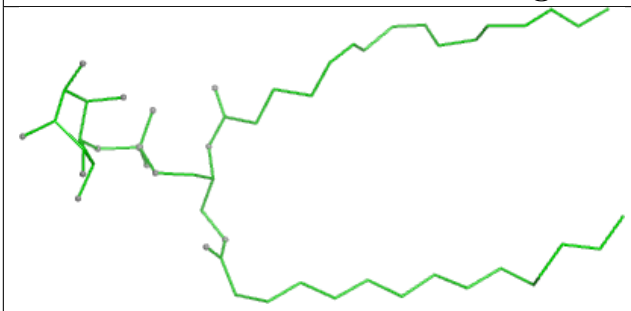


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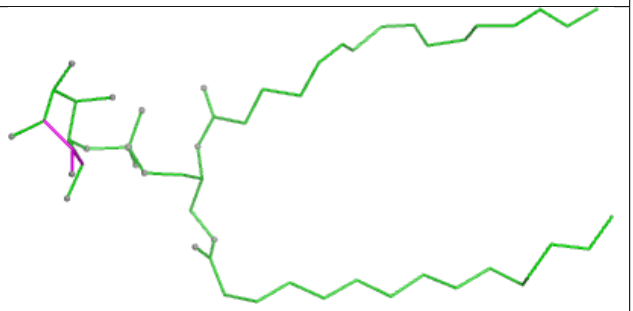


Rings

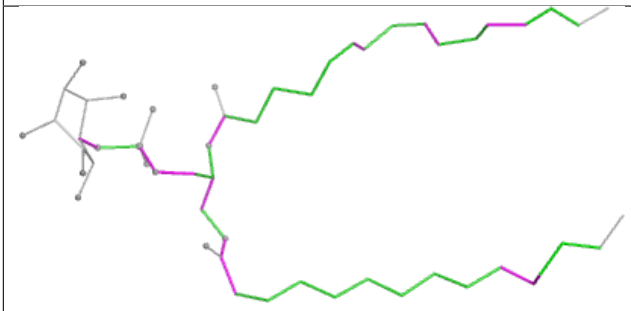
Ligand T7X I 501



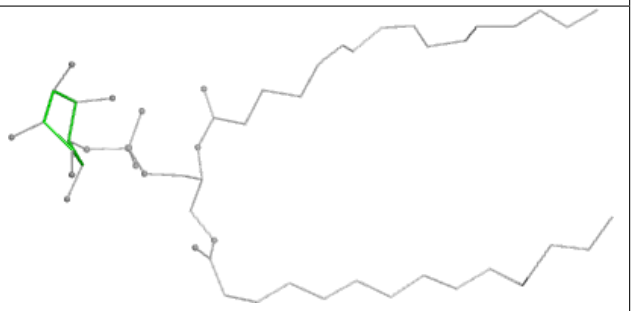
Bond lengths



Bond angles

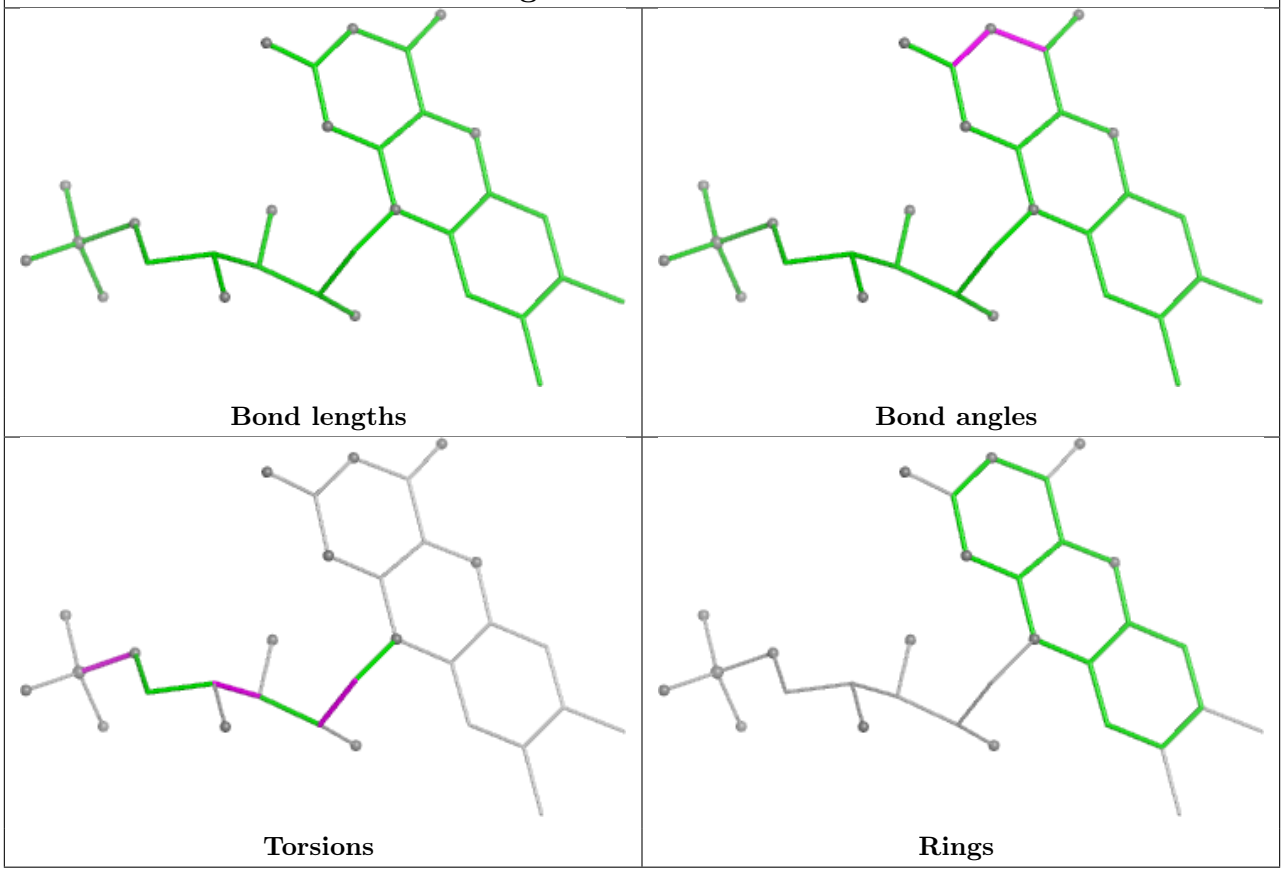


Torsions

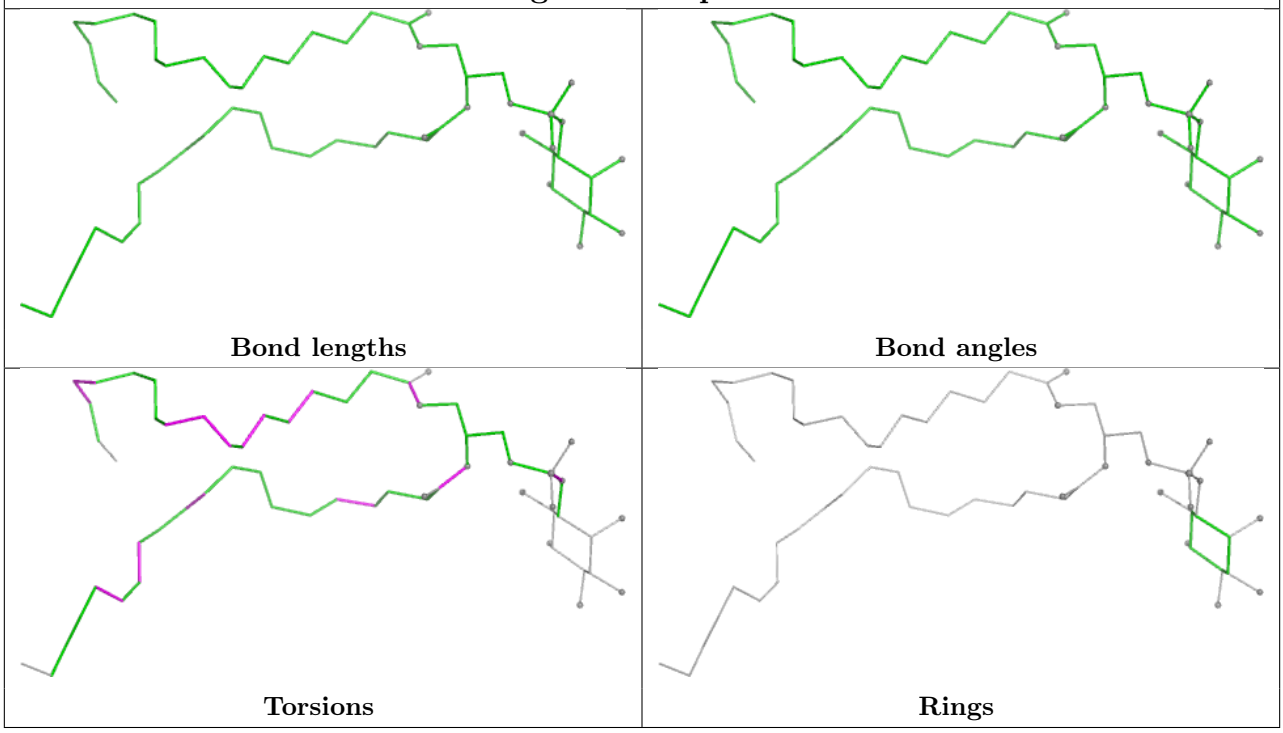


Rings

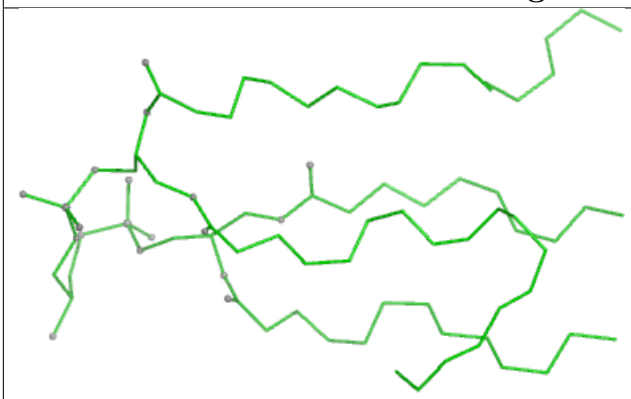
Ligand FMN A 502



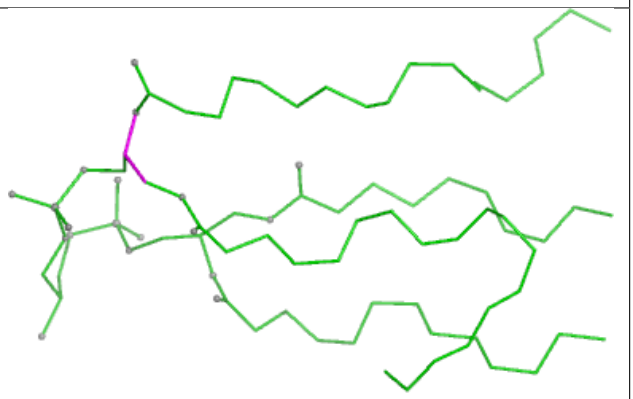
Ligand T7X p 301



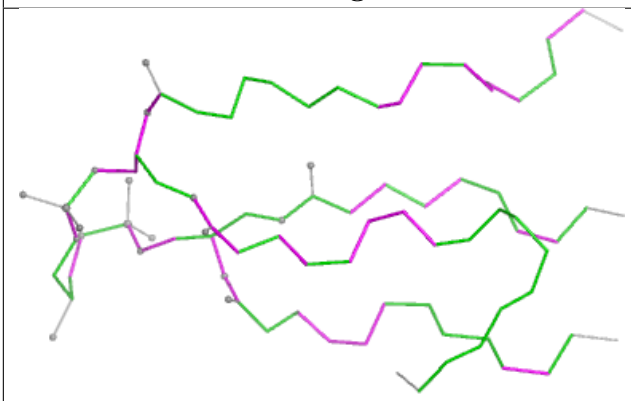
Ligand CDL J 401



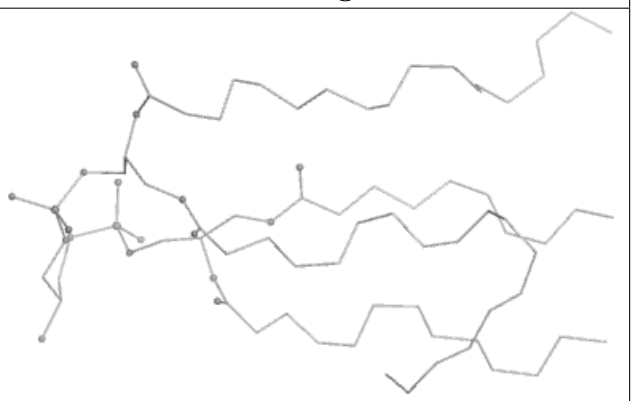
Bond lengths



Bond angles

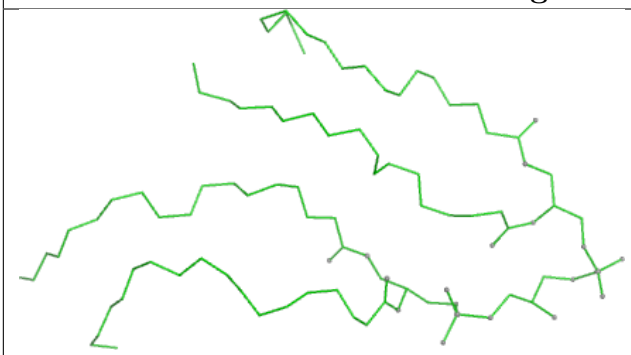


Torsions

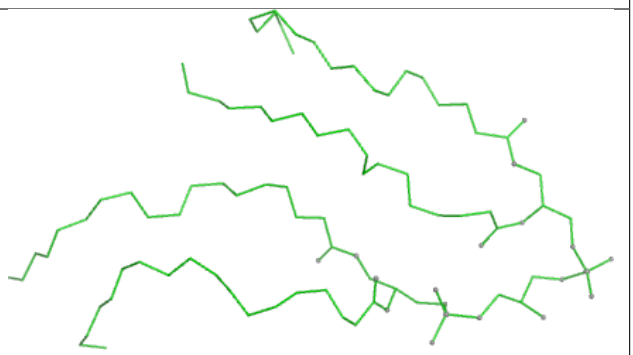


Rings

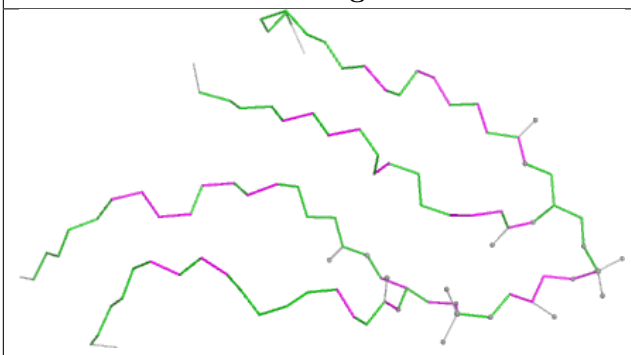
Ligand CDL I 502



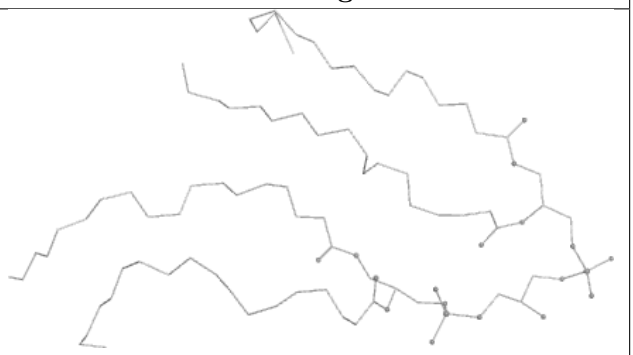
Bond lengths



Bond angles

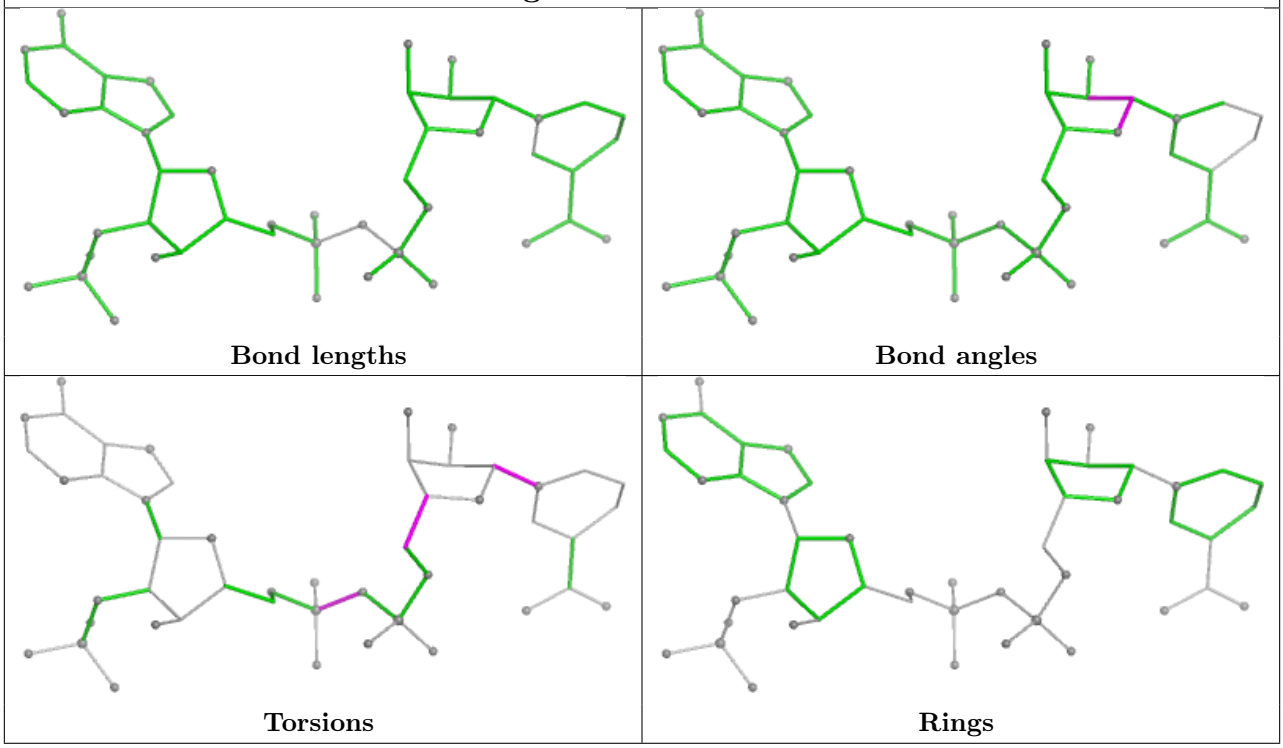


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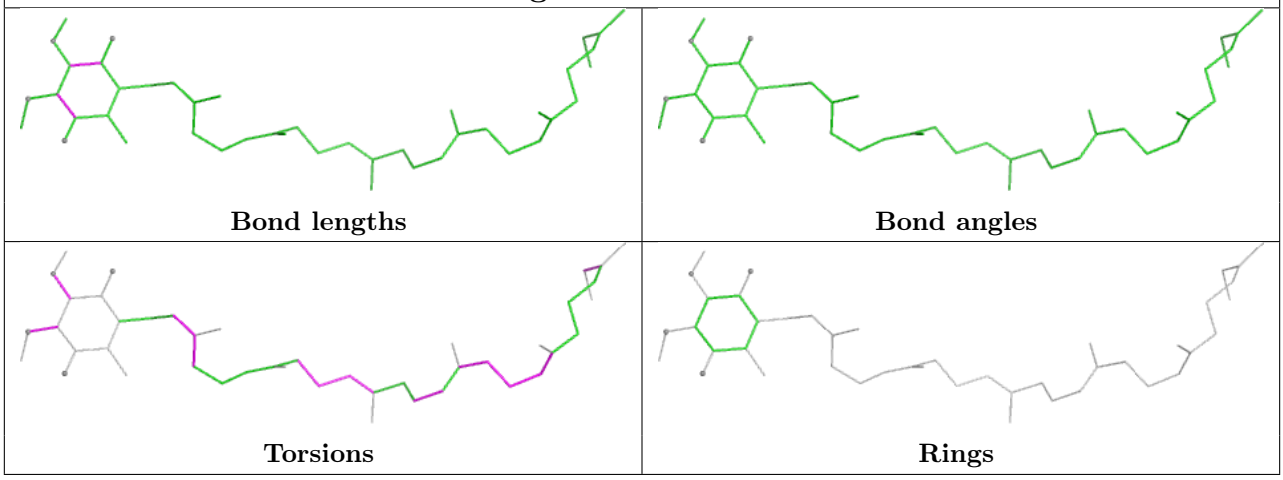


Rings

Ligand NDP T 501



Ligand U10 H 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

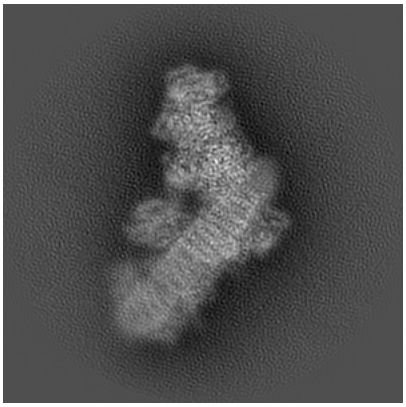
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11614. These allow visual inspection of the internal detail of the map and identification of artifacts.

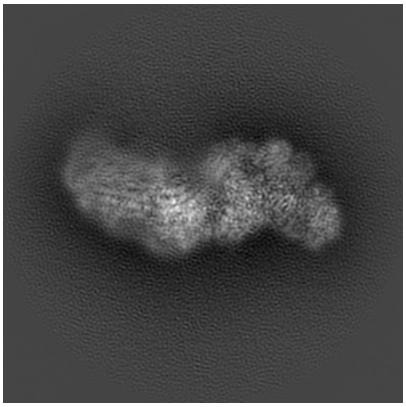
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

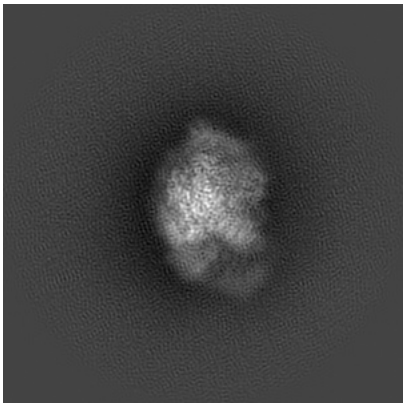
6.1.1 Primary map



X



Y

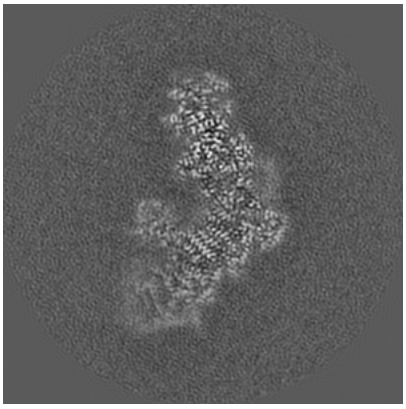


Z

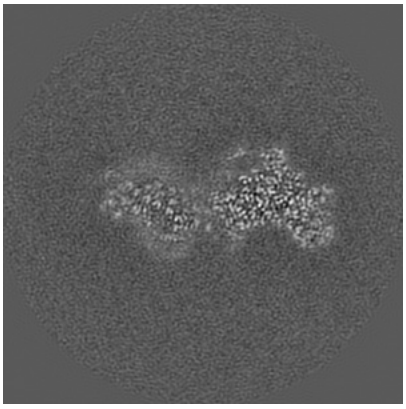
The images above show the map projected in three orthogonal directions.

6.2 Central slices

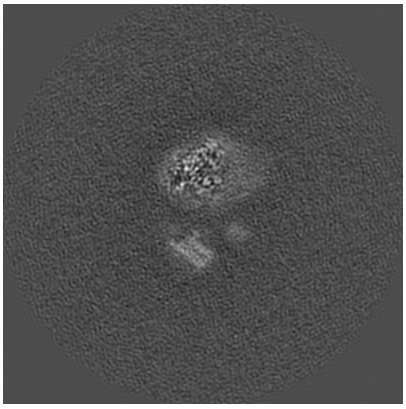
6.2.1 Primary map



X Index: 180



Y Index: 180

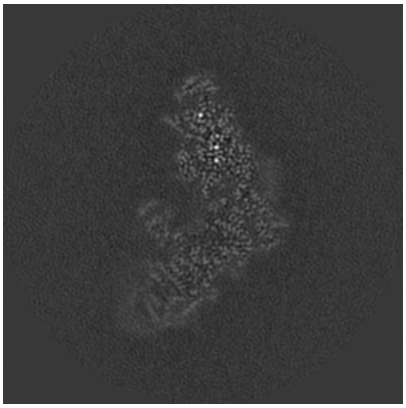


Z Index: 180

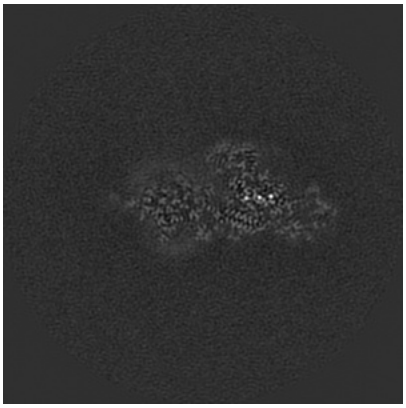
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

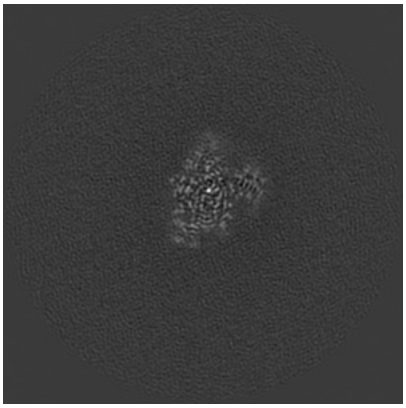
6.3.1 Primary map



X Index: 185



Y Index: 192

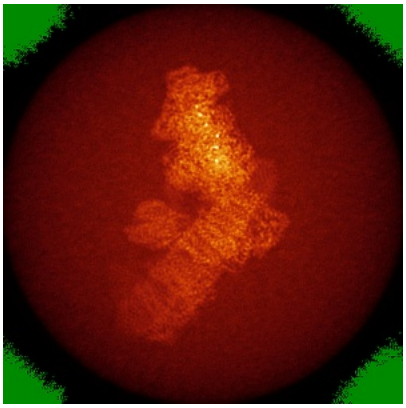


Z Index: 218

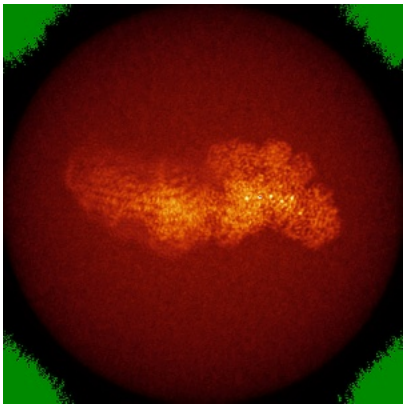
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

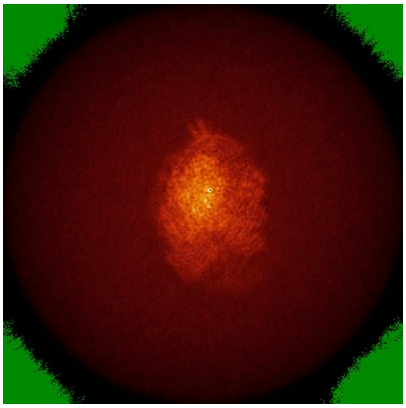
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0235. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

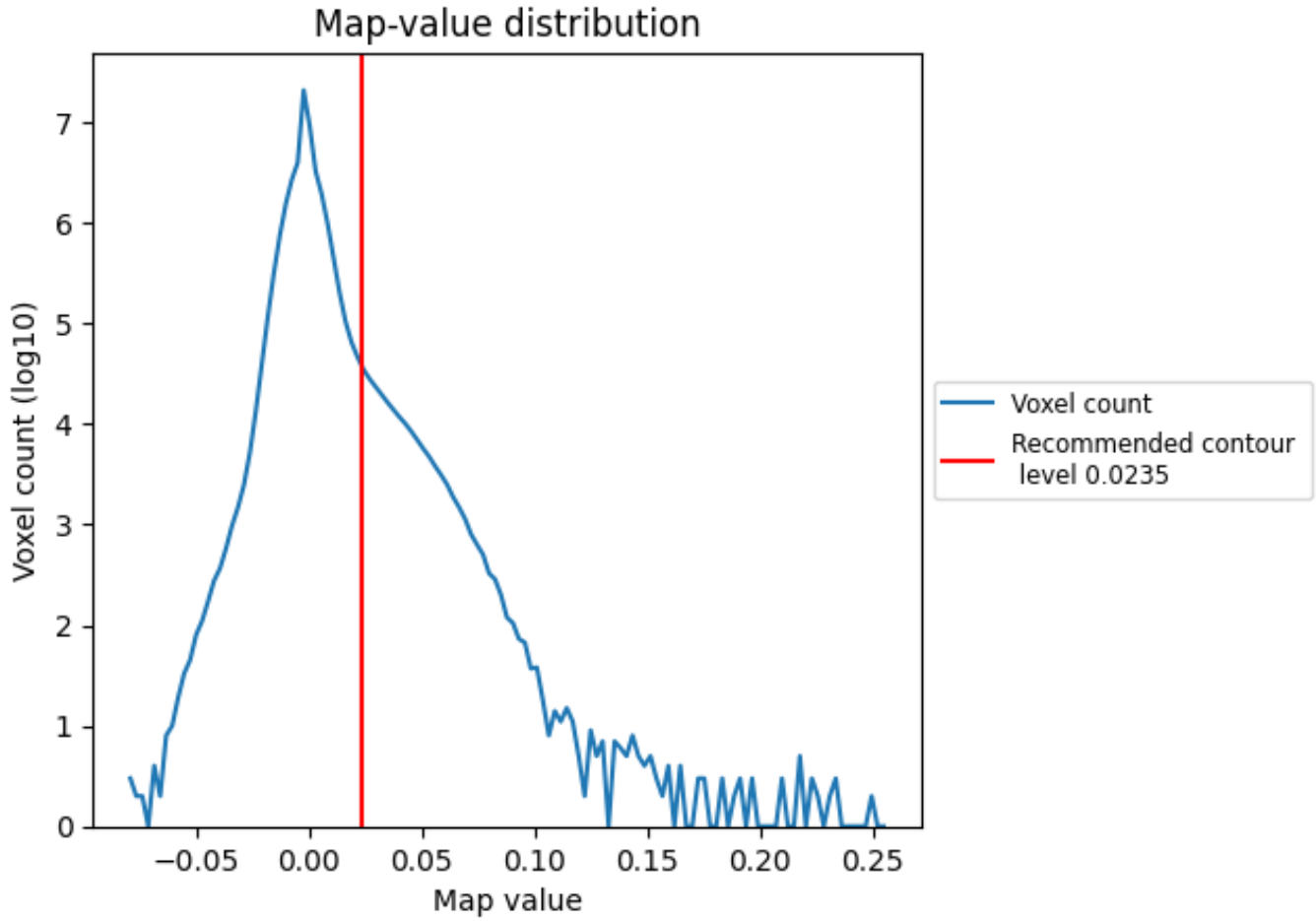
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

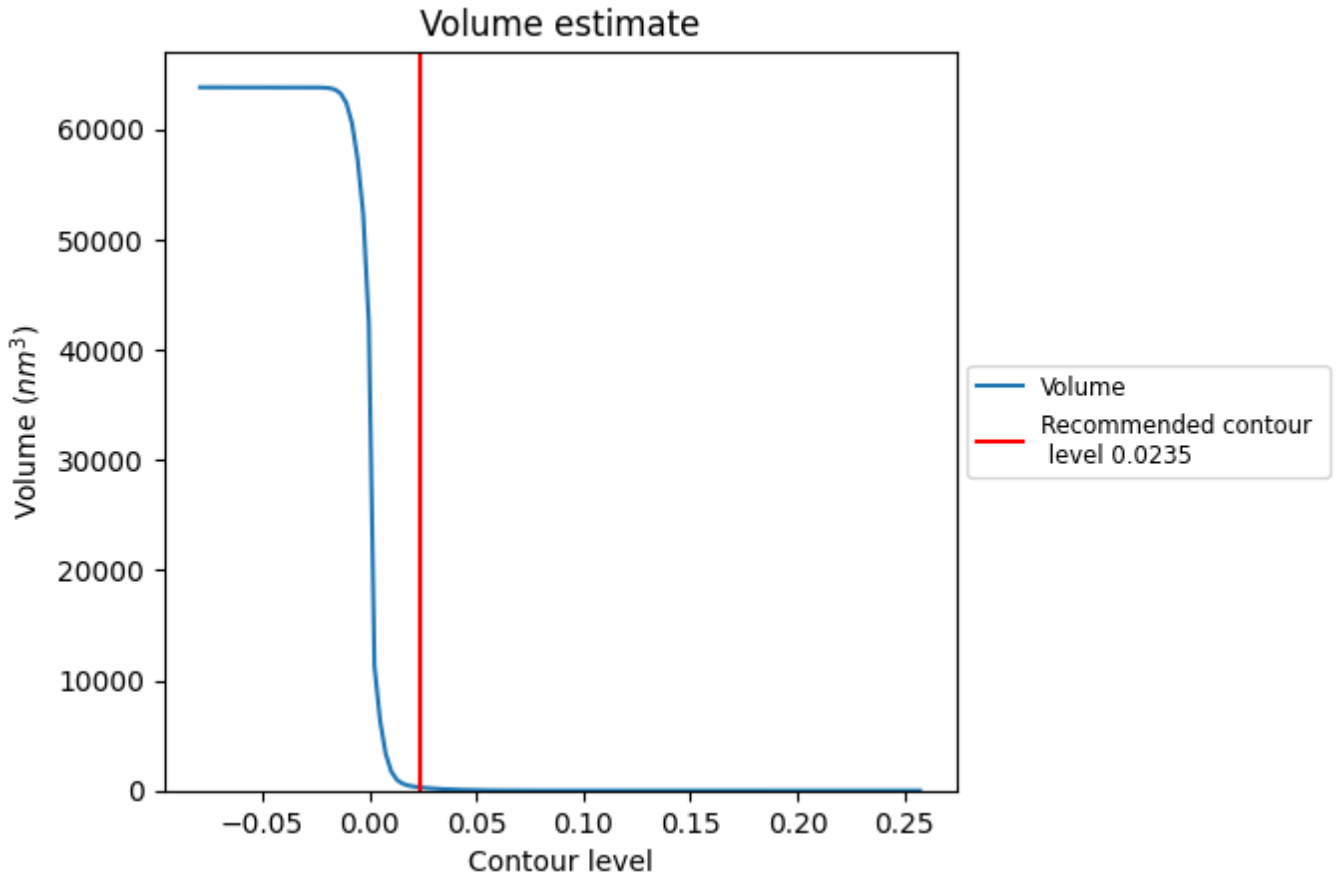
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

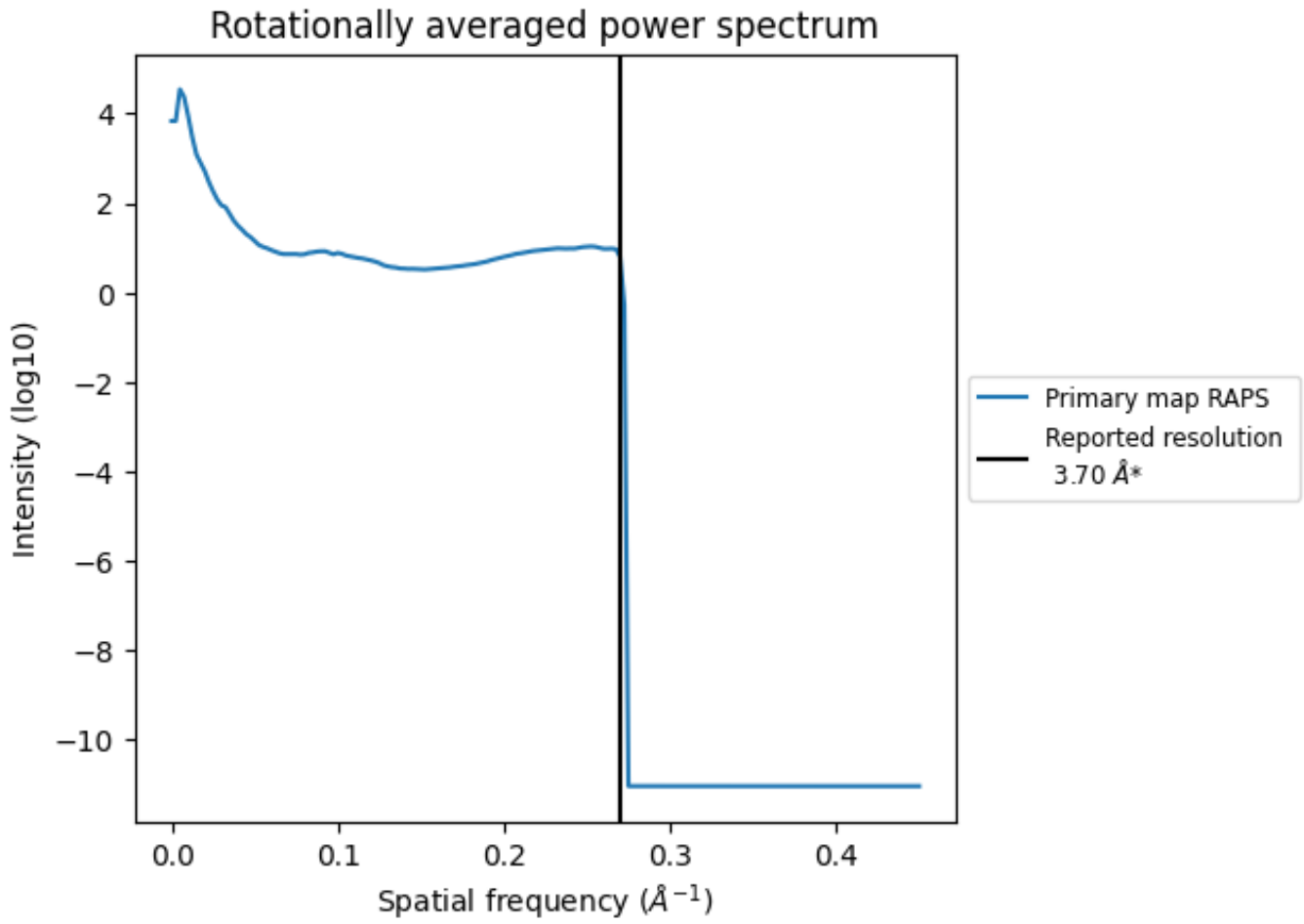
7.2 Volume estimate



The volume at the recommended contour level is 289 nm^3; this corresponds to an approximate mass of 261 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

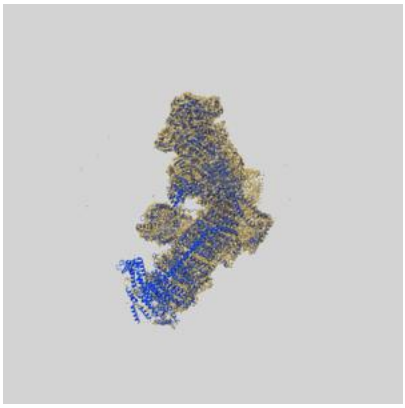
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

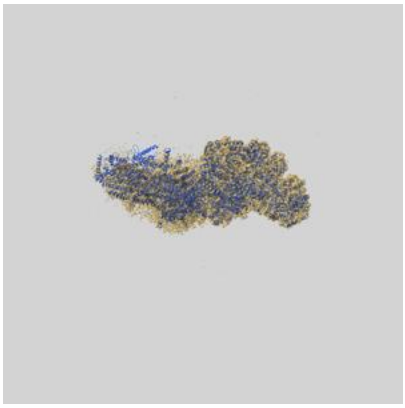
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11614 and PDB model 7A23. Per-residue inclusion information can be found in section 3 on page 18.

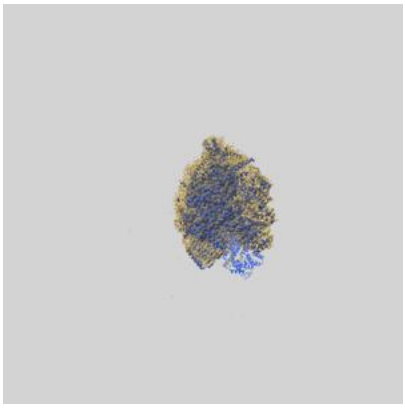
9.1 Map-model overlay



X



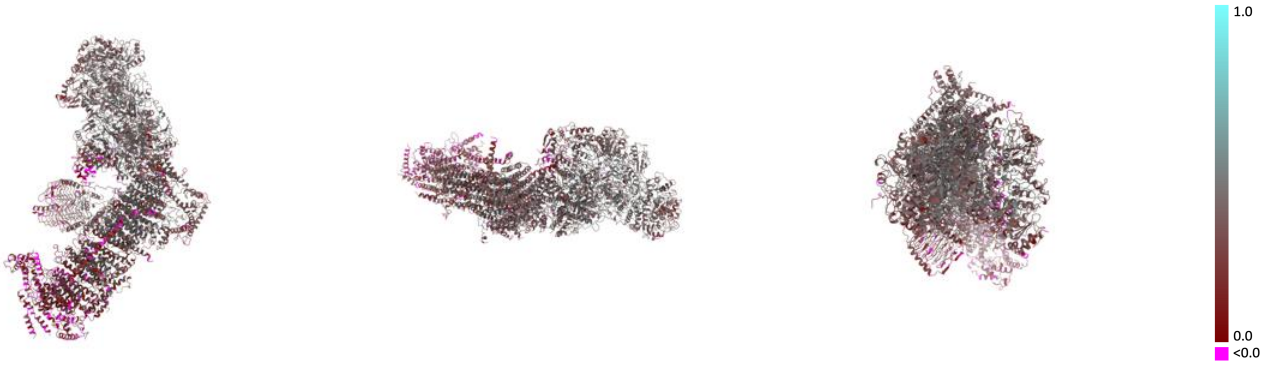
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0235 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

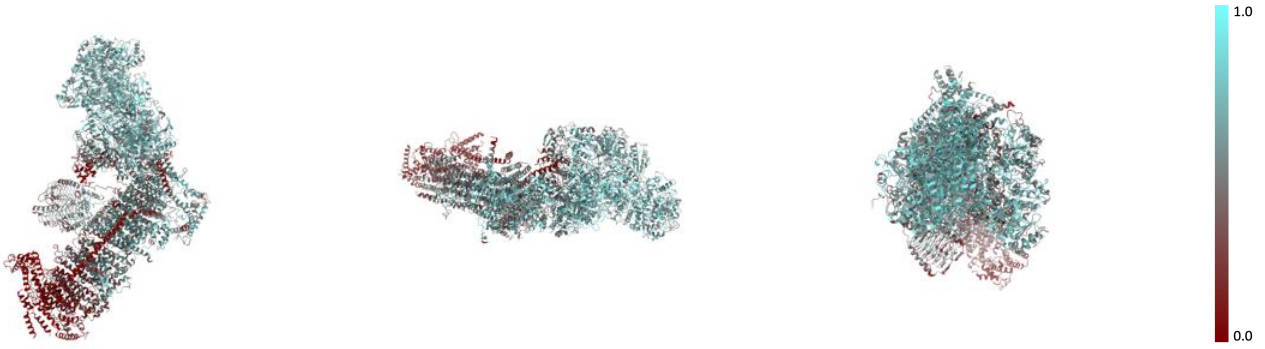
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

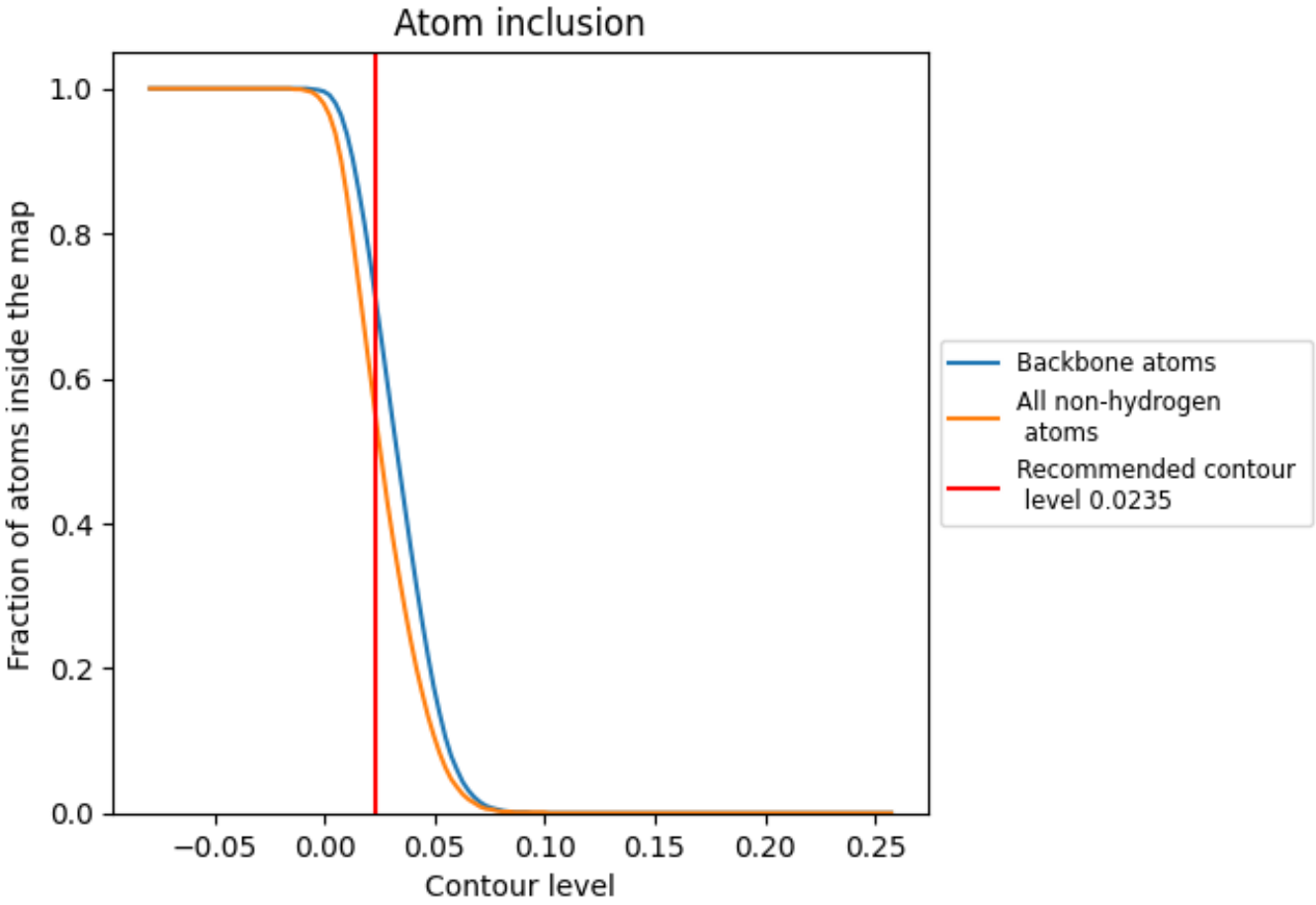
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0235).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0235) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5400	0.3380
A	0.6630	0.3770
B	0.6470	0.3780
C	0.6700	0.4080
D	0.7190	0.4150
E	0.7260	0.4370
F	0.7080	0.4270
G	0.7300	0.4520
H	0.5850	0.3950
I	0.5690	0.3810
J	0.4370	0.3530
K	0.5780	0.3770
M	0.4620	0.3120
N	0.4910	0.3570
O	0.7180	0.4410
P	0.7020	0.4350
Q	0.6090	0.3270
R	0.6310	0.3710
S	0.6060	0.3930
T	0.6050	0.3630
U	0.6830	0.4150
V	0.6490	0.3530
W	0.6540	0.4230
X	0.4210	0.2880
Y	0.5930	0.3280
Z	0.6220	0.3560
a	0.1390	0.1650
b	0.1360	0.1300
c	0.6500	0.4030
d	0.0090	0.0930
e	0.0020	0.1210
f	0.4360	0.2460
g	0.3580	0.2190
h	0.0660	0.1130
i	0.6290	0.3360



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Chain	Atom inclusion	Q-score
j	0.5940	0.3200
k	0.1080	0.1130
l	0.5980	0.2820
m	0.6050	0.2770
n	0.5100	0.3030
o	0.5260	0.3010
p	0.4400	0.2200
q	0.4600	0.2210
r	0.6500	0.4050
s	0.3200	0.2040
t	0.0090	0.0990