



Full wwPDB EM Validation Report ⓘ

Dec 17, 2024 – 03:54 AM EST

PDB ID : 8E73
EMDB ID : EMD-27934
Title : Vigna radiata supercomplex I+III2 (full bridge)
Authors : Maldonado, M.; Letts, J.A.
Deposited on : 2022-08-23
Resolution : 3.20 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

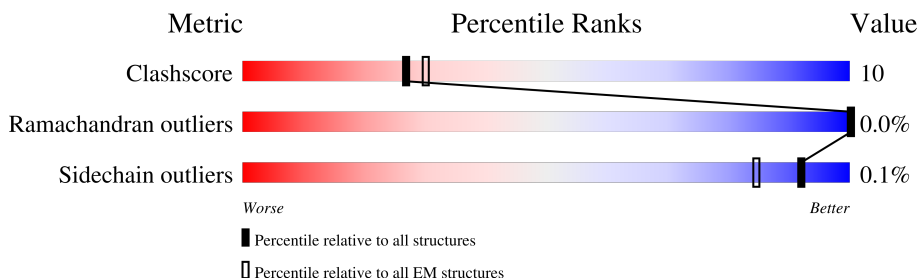
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. 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	527	
1	M	527	
2	B	510	
3	C	394	
3	O	394	
4	D	306	
4	P	306	
5	E	271	




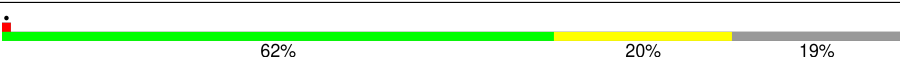
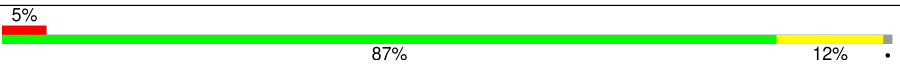

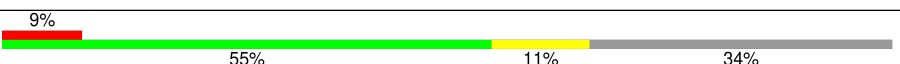
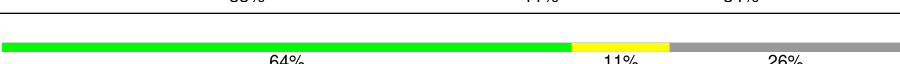
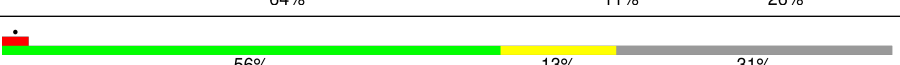
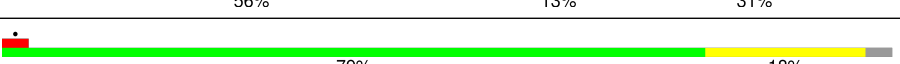
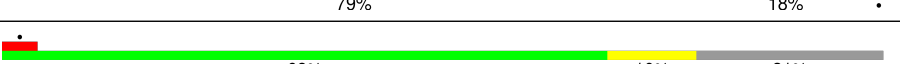
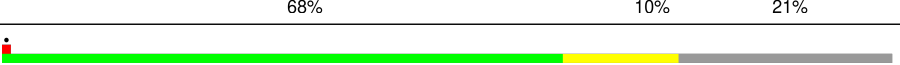

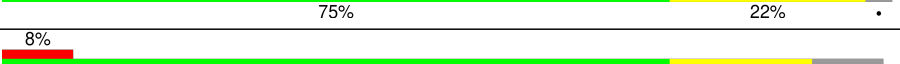



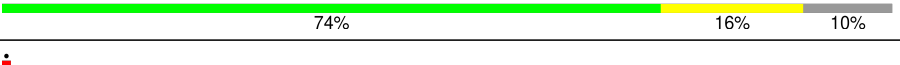

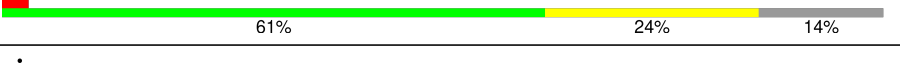
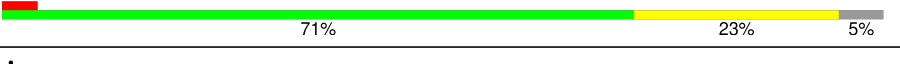


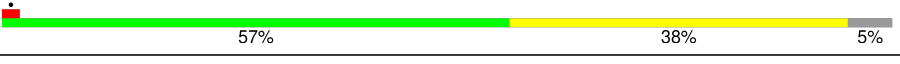

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Mol	Chain	Length	Quality of chain
5	Q	271	
6	F	122	
6	R	122	
7	G	72	
7	S	72	
8	H	69	
8	T	69	
9	J	72	
9	V	72	
10	K	81	
10	W	81	
11	N	506	
12	1M	325	
13	2M	488	
14	3M	118	
15	4M	495	
16	4L	100	
17	5M	673	
18	6M	205	
19	A1	65	
20	A2	98	
21	A3	63	
22	A5	169	
23	A6	132	
24	A7	127	



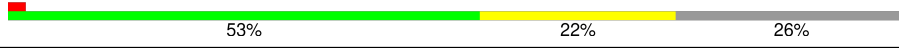



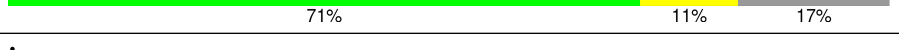
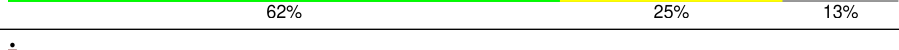
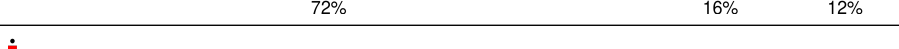
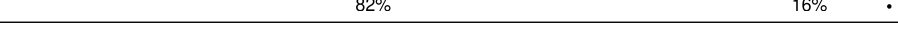
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Mol	Chain	Length	Quality of chain
25	A8	106	
26	A9	396	
27	AK	160	
28	AL	156	
29	AM	143	
30	AC	116	
31	AB	128	
32	B2	66	
33	B3	68	
34	B4	71	
35	B7	98	
36	B8	125	
37	B9	115	
38	BJ	106	
39	BK	118	
40	FD	158	
41	C2	82	
42	P2	115	
43	G1	270	
44	G2	273	
45	L2	256	
46	S1	746	
47	S2	394	
48	S3	190	
49	S4	146	

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Mol	Chain	Length	Quality of chain
50	S5	83	
51	S6	103	
52	S7	213	
53	S8	222	
54	P1	91	
55	P4	61	
56	C1	87	
57	V1	492	
58	V2	251	
59	X1	101	

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
70	SF4	V1	502	-	-	X	-

2 Entry composition [i](#)

There are 72 unique types of molecules in this entry. The entry contains 97737 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 MPP-beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	482	Total	C	N	O	S	0	0
			3800	2387	673	725	15		
1	M	483	Total	C	N	O	S	0	0
			3807	2392	674	726	15		

- Molecule 2 is a protein called MPP-alpha (protomer 1).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	446	Total	C	N	O	S	0	0
			3413	2173	566	662	12		

- Molecule 3 is a protein called COB (cyt b).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	386	Total	C	N	O	S	0	0
			3089	2080	485	510	14		
3	O	384	Total	C	N	O	S	0	0
			3074	2070	483	507	14		

- Molecule 4 is a protein called CYC1 (cyt c1).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	243	Total	C	N	O	S	0	0
			1905	1211	326	357	11		
4	P	243	Total	C	N	O	S	0	0
			1905	1211	326	357	11		

- Molecule 5 is a protein called UCR1 (Rieske iron-sulfur protein subunit).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	74	Total	C	N	O	S	0	0
			574	375	97	101	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	73	Total	C	N	O	S	0	0
			565	370	96	98	1		

- Molecule 6 is a protein called QCR7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	117	Total	C	N	O	S	0	0
			974	621	175	174	4		
6	R	115	Total	C	N	O	S	0	0
			959	613	172	170	4		

- Molecule 7 is a protein called QCR8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	70	Total	C	N	O	S	0	0
			578	382	97	98	1		
7	S	70	Total	C	N	O	S	0	0
			578	382	97	98	1		

- Molecule 8 is a protein called QCR6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	64	Total	C	N	O	S	0	0
			527	339	89	93	6		
8	T	64	Total	C	N	O	S	0	0
			527	339	89	93	6		

- Molecule 9 is a protein called QCR9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	58	Total	C	N	O	S	0	0
			468	305	81	81	1		
9	V	59	Total	C	N	O	S	0	0
			476	311	82	82	1		

- Molecule 10 is a protein called QCR10 (UCRY).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	24	Total	C	N	O	S	0	0
			167	109	27	30	1		
10	W	29	Total	C	N	O	S	0	0
			203	133	33	36	1		

- Molecule 11 is a protein called MPP-alpha (protomer 2).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	445	Total	C	N	O	S	0	0
			3389	2148	573	656	12		

- Molecule 12 is a protein called Nad1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1M	323	Total	C	N	O	S	0	0
			2506	1688	384	419	15		

- Molecule 13 is a protein called Nad2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	2M	488	Total	C	N	O	S	0	0
			3810	2555	578	648	29		

- Molecule 14 is a protein called Nad3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3M	90	Total	C	N	O	S	0	0
			759	537	103	115	4		

- Molecule 15 is a protein called Nad4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	4M	486	Total	C	N	O	S	0	0
			3862	2600	606	634	22		

- Molecule 16 is a protein called Nad4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4L	99	Total	C	N	O	S	0	0
			777	520	120	130	7		

- Molecule 17 is a protein called Nad5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5M	663	Total	C	N	O	S	0	0
			5198	3447	808	903	40		

- Molecule 18 is a protein called Nad6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	6M	192	Total	C	N	O	S	0	0
			1561	1057	245	249	10		

- Molecule 19 is a protein called NDUA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	A1	59	Total	C	N	O	S	0	0
			470	299	89	77	5		

- Molecule 20 is a protein called NDUA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	A2	90	Total	C	N	O	S	0	0
			699	442	123	131	3		

- Molecule 21 is a protein called NDUA3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A3	39	Total	C	N	O	S	0	0
			299	200	46	50	3		

- Molecule 22 is a protein called NDUA5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A5	125	Total	C	N	O	S	0	0
			1004	639	165	196	4		

- Molecule 23 is a protein called NDUA6.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A6	99	Total	C	N	O	S	0	0
			794	507	134	148	5		

- Molecule 24 is a protein called NDUA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	A7	109	Total	C	N	O	S	0	0
			868	549	150	166	3		

- Molecule 25 is a protein called NDUA8.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A8	104	Total	C	N	O	S	0	0
			814	503	144	156	11		

- Molecule 26 is a protein called NDUA9.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A9	330	Total	C	N	O	S	0	0
			2571	1656	441	463	11		

- Molecule 27 is a protein called NDUA11.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AK	149	Total	C	N	O	S	0	0
			1139	731	196	208	4		

- Molecule 28 is a protein called NDUA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AL	127	Total	C	N	O	S	0	0
			1057	674	190	192	1		

- Molecule 29 is a protein called NDUA13.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AM	142	Total	C	N	O	S	0	0
			1134	731	202	197	4		

- Molecule 30 is a protein called NDUAB1-beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AC	82	Total	C	N	O	S	0	0
			650	414	104	129	3		

- Molecule 31 is a protein called NDUAB1-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AB	85	Total	C	N	O	S	0	0
			660	415	111	132	2		

- Molecule 32 is a protein called NDUB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B2	49	Total	C	N	O	S	0	0
			414	275	75	62	2		

- Molecule 33 is a protein called NDUB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	B3	47	Total	C	N	O	S	0	0
			384	248	74	61	1		

- Molecule 34 is a protein called NDUB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B4	69	Total	C	N	O	S	0	0
			576	370	105	98	3		

- Molecule 35 is a protein called NDUB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	B7	77	Total	C	N	O	S	0	0
			648	405	115	119	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B7	81	LYS	GLN	conflict	UNP A0A1S3V2B8

- Molecule 36 is a protein called NDUB8.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B8	95	Total	C	N	O	S	0	0
			737	483	116	134	4		

- Molecule 37 is a protein called NDUB9.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	B9	111	Total	C	N	O	0	0
			927	584	175	168		

- Molecule 38 is a protein called NDUB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BJ	97	Total	C	N	O	S	0	0
			813	517	150	142	4		

- Molecule 39 is a protein called NDUB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BK	77	Total	C	N	O	S	0	0
			631	408	109	113	1		

- Molecule 40 is a protein called NDUFX.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	FD	122	Total	C	N	O	S	0	0
			963	603	176	180	4		

- Molecule 41 is a protein called NDUC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	C2	74	Total	C	N	O	S	0	0
			587	376	104	103	4		

- Molecule 42 is a protein called NDUP2.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	P2	30	Total	C	N	O	0	0
			232	149	42	41		

- Molecule 43 is a protein called NDUCA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	G1	231	Total	C	N	O	S	0	0
			1766	1121	310	329	6		

- Molecule 44 is a protein called NDUCA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	G2	258	Total	C	N	O	S	0	0
			1979	1248	349	376	6		

- Molecule 45 is a protein called NDUCAL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	L2	210	Total	C	N	O	S	0	0
			1622	1038	279	300	5		

- Molecule 46 is a protein called NDUS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	S1	687	Total	C	N	O	S	0	0
			5263	3301	930	999	33		

- Molecule 47 is a protein called NDUS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	S2	376	Total	C	N	O	S	0	0
			3018	1918	530	547	23		

- Molecule 48 is a protein called NDUS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	S3	185	Total	C	N	O	S	0	0
			1579	1021	271	282	5		

- Molecule 49 is a protein called NDUS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	S4	116	Total	C	N	O	S	0	0
			923	592	166	163	2		

- Molecule 50 is a protein called NDUS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	S5	65	Total	C	N	O	S	0	0
			555	342	107	99	7		

- Molecule 51 is a protein called NDUS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	S6	71	Total	C	N	O	S	0	0
			553	349	94	104	6		

- Molecule 52 is a protein called NDUS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	S7	158	Total	C	N	O	S	0	0
			1254	804	221	215	14		

- Molecule 53 is a protein called NDUS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S8	181	Total	C	N	O	S	0	0
			1484	930	251	292	11		

- Molecule 54 is a protein called NDUP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	P1	85	Total	C	N	O	S	0	0
			748	476	135	132	5		

- Molecule 55 is a protein called NDUP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	P4	53	Total	C	N	O	S	0	0
			452	291	81	78	2		

- Molecule 56 is a protein called NDUB6.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	C1	72	Total	C	N	O	S	0	0
			583	376	106	95	6		

- Molecule 57 is a protein called NDUV1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	V1	430	Total	C	N	O	S	0	0
			3327	2099	591	613	24		

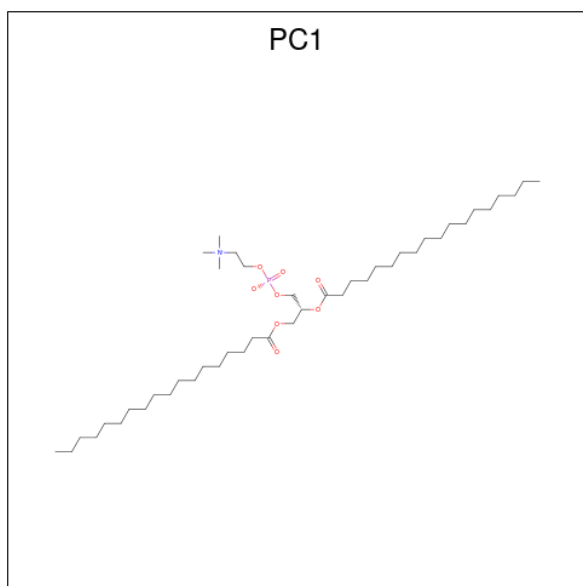
- Molecule 58 is a protein called NDUV2.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	V2	222	Total	C	N	O	S	0	0
			1721	1090	295	324	12		

- Molecule 59 is a protein called NDUX1.

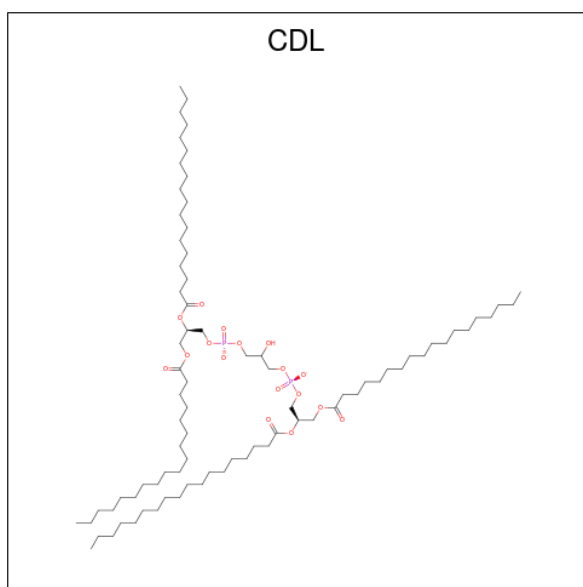
Mol	Chain	Residues	Atoms					AltConf	Trace
59	X1	99	Total	C	N	O	S	0	0
			750	479	126	140	5		

- Molecule 60 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



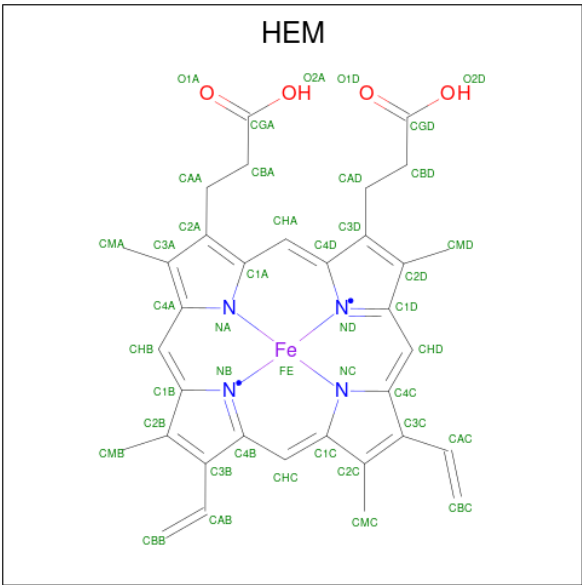
Mol	Chain	Residues	Atoms					AltConf
60	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
60	M	1	Total	C	N	O	P	0
			40	30	1	8	1	
60	S	1	Total	C	N	O	P	0
			38	28	1	8	1	
60	1M	1	Total	C	N	O	P	0
			45	35	1	8	1	
60	G1	1	Total	C	N	O	P	0
			27	17	1	8	1	
60	G1	1	Total	C	N	O	P	0
			37	27	1	8	1	
60	G2	1	Total	C	N	O	P	0
			40	30	1	8	1	
60	P4	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 61 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



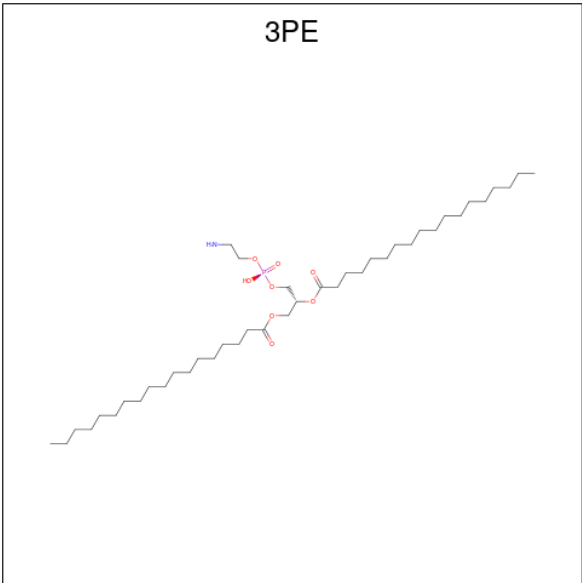
Mol	Chain	Residues	Atoms				AltConf
61	A	1	Total	C	O	P	0
			69	50	17	2	
61	C	1	Total	C	O	P	0
			64	45	17	2	
61	C	1	Total	C	O	P	0
			59	40	17	2	
61	D	1	Total	C	O	P	0
			68	49	17	2	
61	M	1	Total	C	O	P	0
			70	51	17	2	
61	O	1	Total	C	O	P	0
			64	45	17	2	
61	O	1	Total	C	O	P	0
			63	44	17	2	
61	O	1	Total	C	O	P	0
			55	36	17	2	

- Molecule 62 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



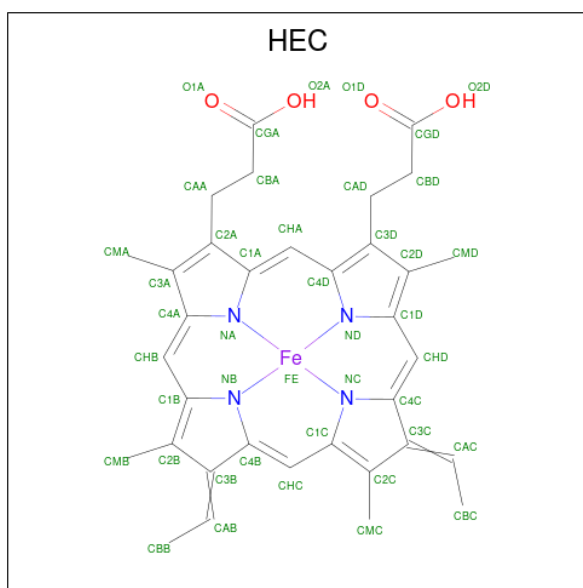
Mol	Chain	Residues	Atoms					AltConf
62	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
62	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
62	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
62	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 63 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P).



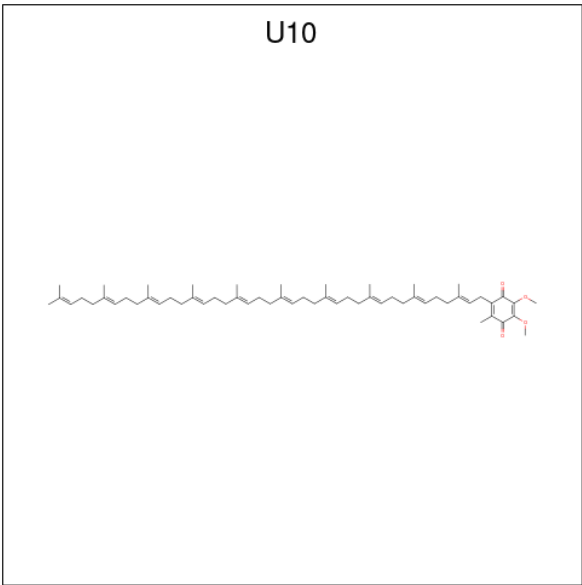
Mol	Chain	Residues	Atoms					AltConf
63	C	1	Total 38	C 28	N 1	O 8	P 1	0
63	C	1	Total 34	C 24	N 1	O 8	P 1	0
63	G	1	Total 37	C 27	N 1	O 8	P 1	0
63	M	1	Total 45	C 35	N 1	O 8	P 1	0
63	O	1	Total 36	C 26	N 1	O 8	P 1	0
63	O	1	Total 39	C 29	N 1	O 8	P 1	0
63	O	1	Total 33	C 23	N 1	O 8	P 1	0
63	R	1	Total 51	C 41	N 1	O 8	P 1	0

- Molecule 64 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



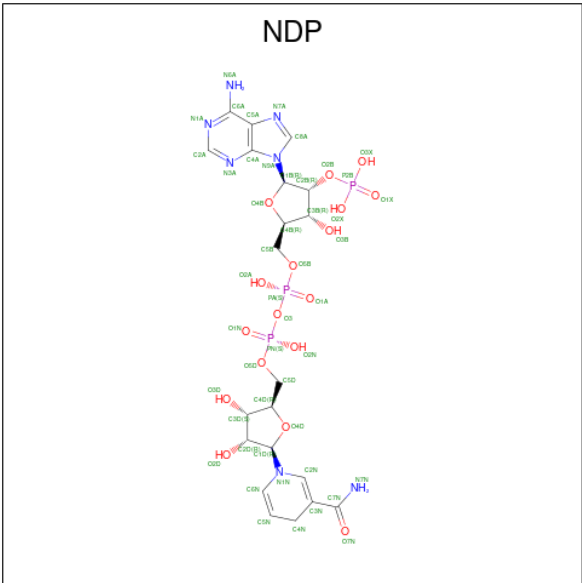
Mol	Chain	Residues	Atoms					AltConf
64	D	1	Total 43	C 34	Fe 1	N 4	O 4	0
64	P	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 65 is UBIQUINONE-10 (three-letter code: U10) (formula: $\text{C}_{59}\text{H}_{90}\text{O}_4$).



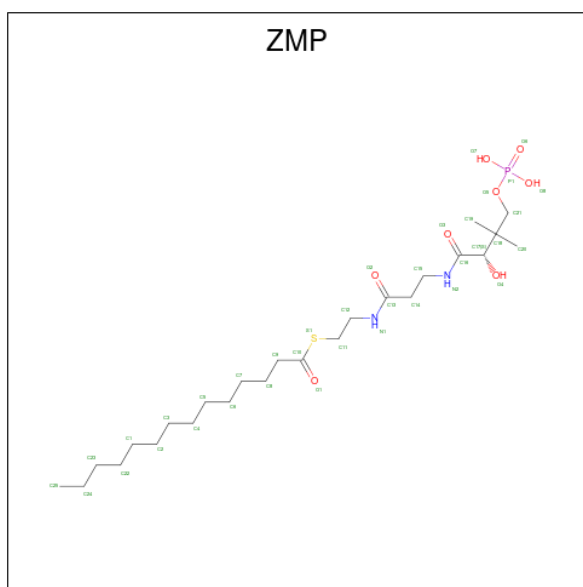
Mol	Chain	Residues	Atoms			AltConf
65	1M	1	Total	C	O	0
			40	36	4	

- Molecule 66 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					AltConf
66	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 67 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



Mol	Chain	Residues	Atoms					AltConf
67	AC	1	Total	C	N	O	P	S
			29	18	2	7	1	1
67	AB	1	Total	C	N	O	P	S
			29	18	2	7	1	1

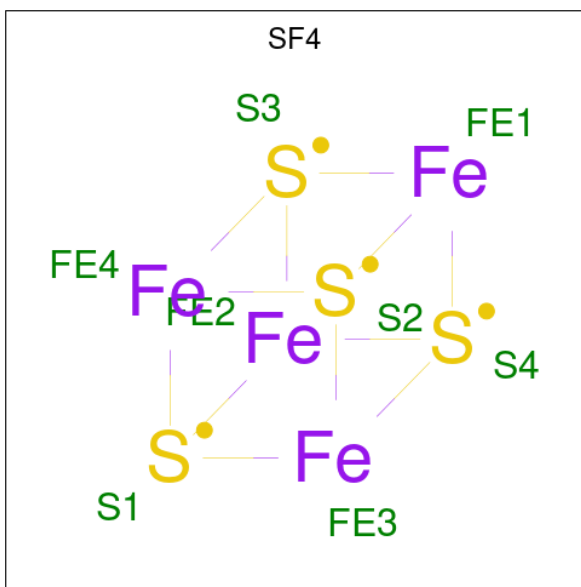
- Molecule 68 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
68	FD	1	Total	Fe	0
			1	1	

- Molecule 69 is ZINC ION (three-letter code: ZN) (formula: Zn).

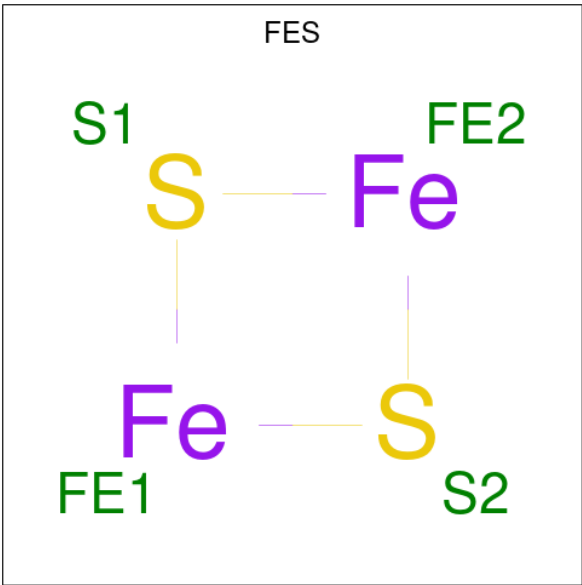
Mol	Chain	Residues	Atoms		AltConf
69	G2	1	Total	Zn	0
			1	1	
69	S6	1	Total	Zn	0
			1	1	

- Molecule 70 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



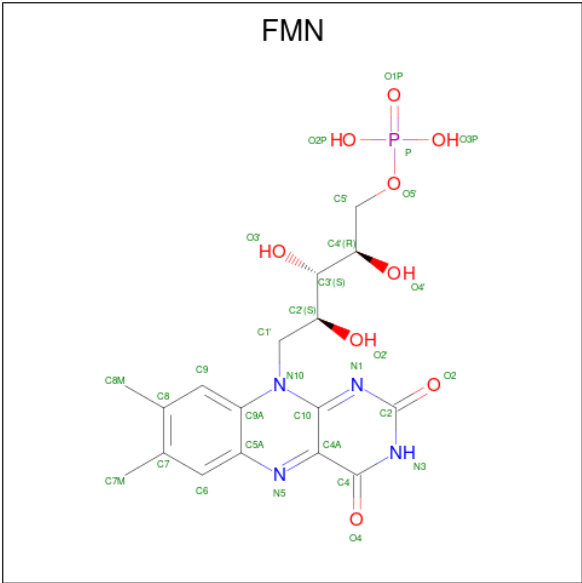
Mol	Chain	Residues	Atoms			AltConf
70	S1	1	Total	Fe	S	0
			8	4	4	
70	S1	1	Total	Fe	S	0
			8	4	4	
70	S7	1	Total	Fe	S	0
			8	4	4	
70	S8	1	Total	Fe	S	0
			8	4	4	
70	S8	1	Total	Fe	S	0
			8	4	4	
70	V1	1	Total	Fe	S	0
			8	4	4	

- Molecule 71 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
71	S1	1	Total	Fe	S	0
			4	2	2	
71	V2	1	Total	Fe	S	0
			4	2	2	

- Molecule 72 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).

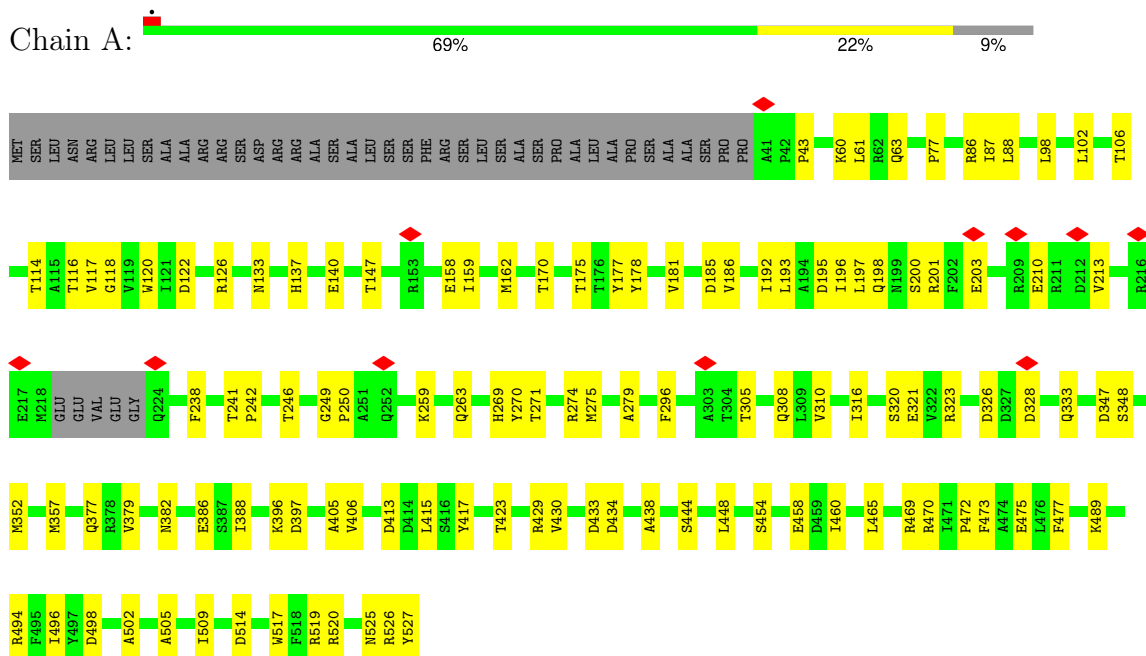


Mol	Chain	Residues	Atoms					AltConf
72	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

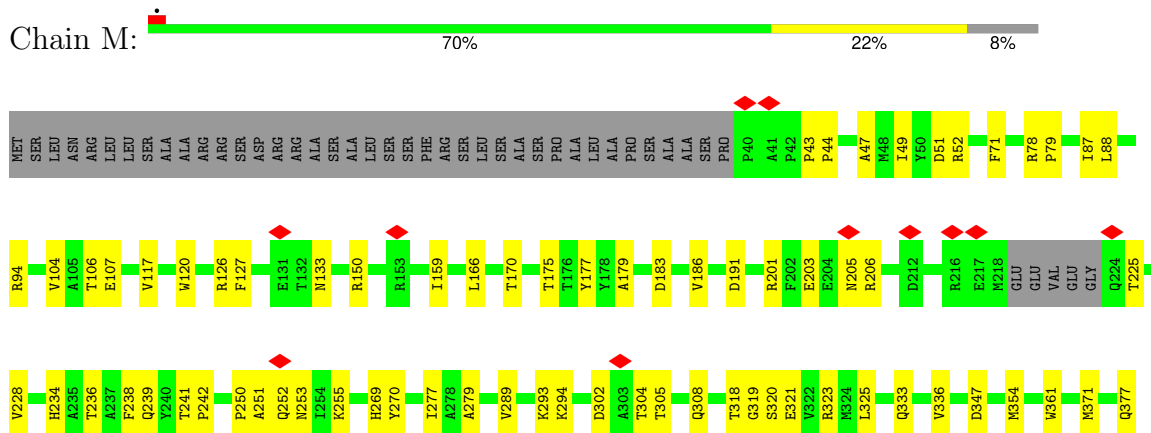
3 Residue-property plots

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.

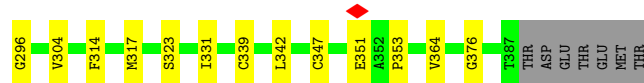
• Molecule 1: MPP-beta



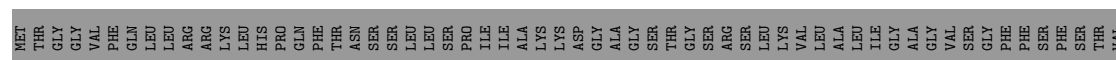
• Molecule 1: MPP-beta



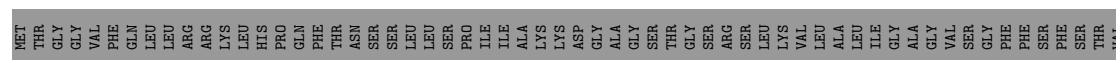




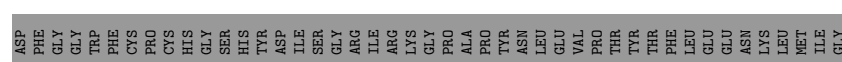
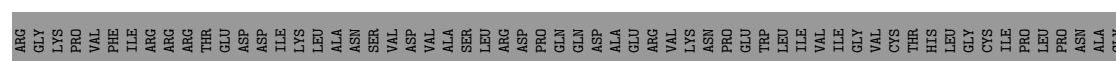
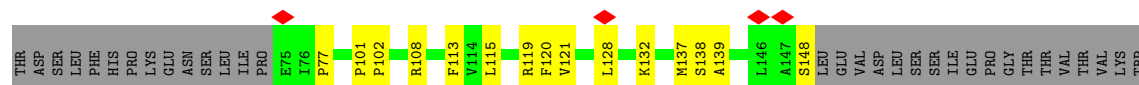
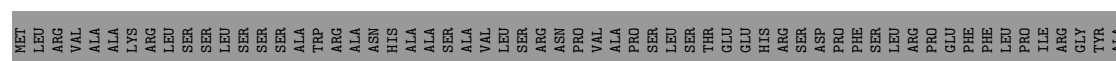
- Molecule 4: CYC1 (cyt c1)



- Molecule 4: CYC1 (cyt c1)

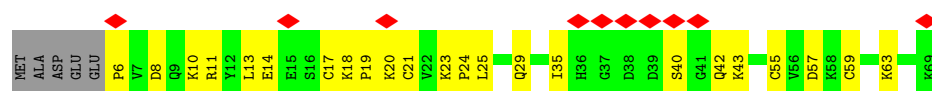


- Molecule 5: UCR1 (Rieske iron-sulfur protein subunit)



- Molecule 5: UCR1 (Rieske iron-sulfur protein subunit)





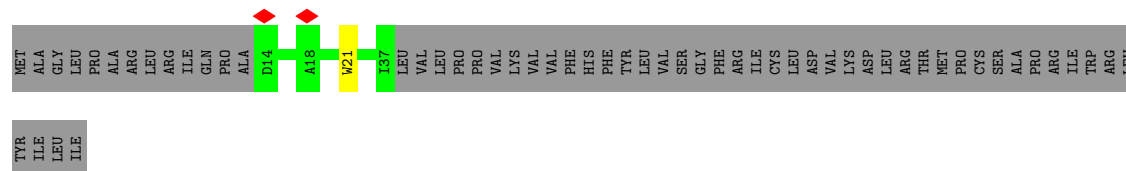
- Molecule 9: QCR9



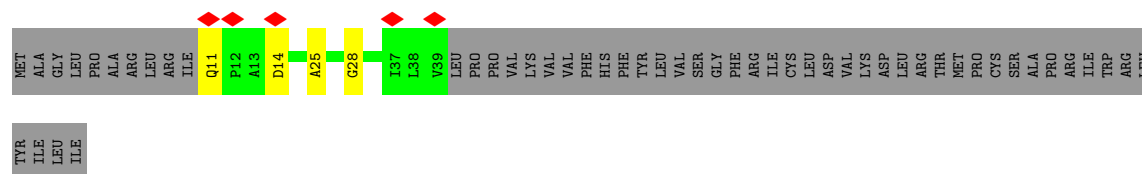
- Molecule 9: QCR9



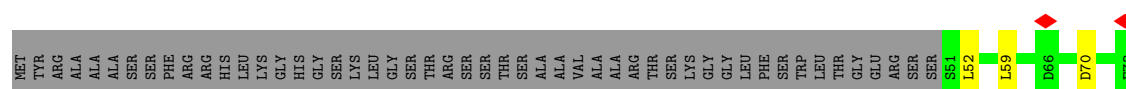
- Molecule 10: QCR10 (UCRY)

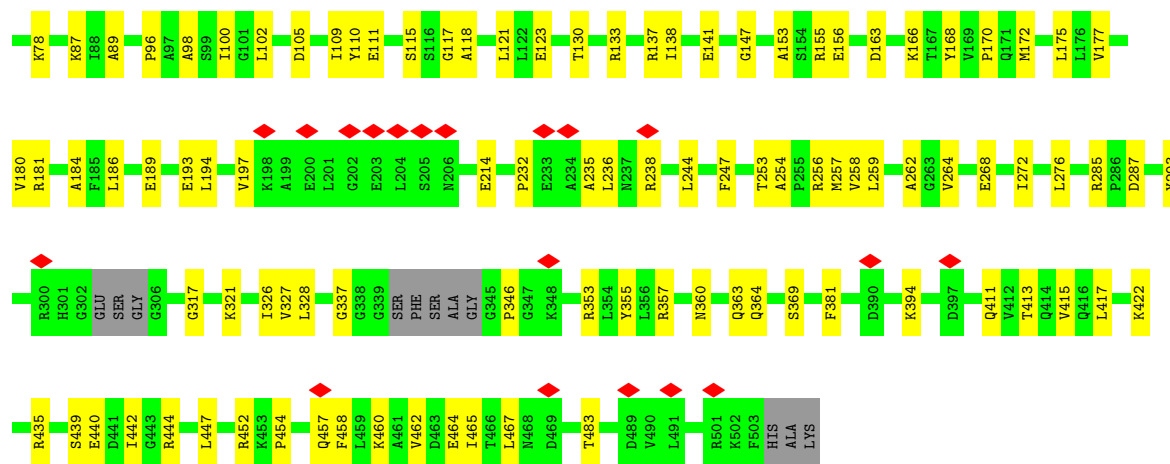


- Molecule 10: QCR10 (UCRY)

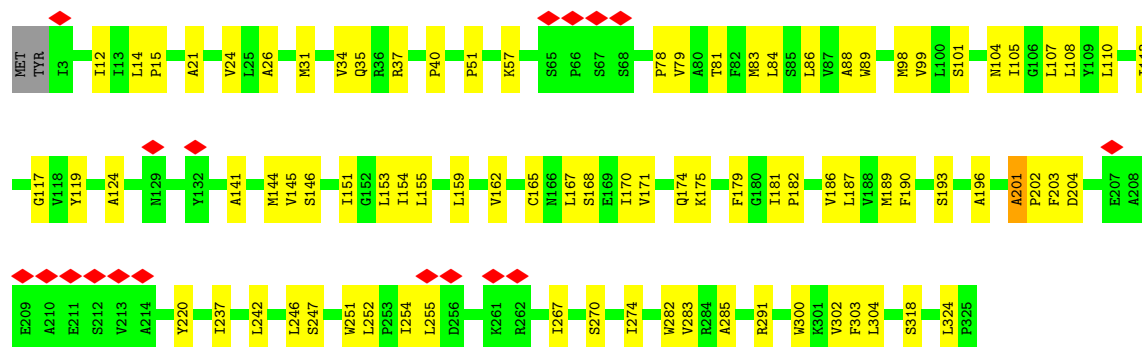
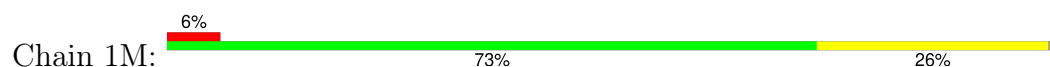


- Molecule 11: MPP-alpha (protomer 2)

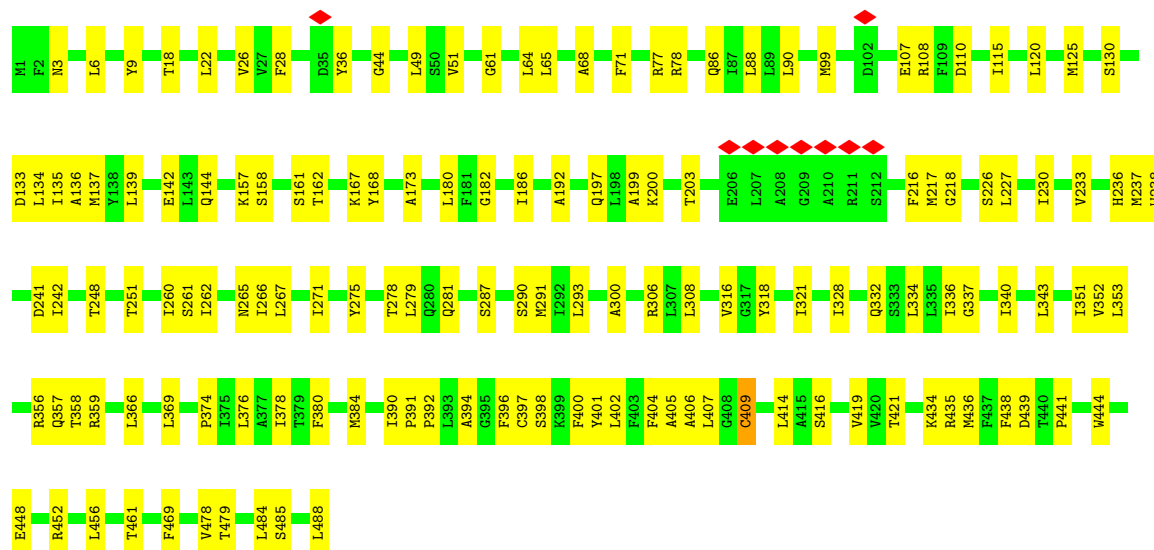




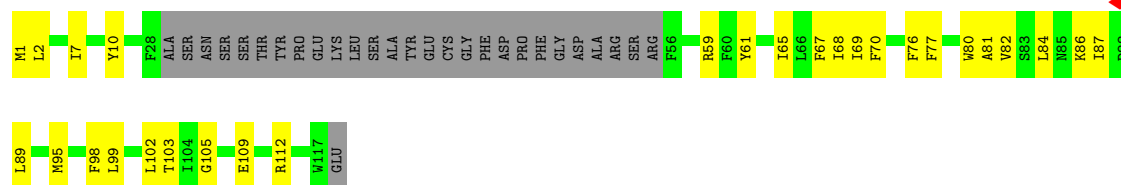
• Molecule 12: Nad1



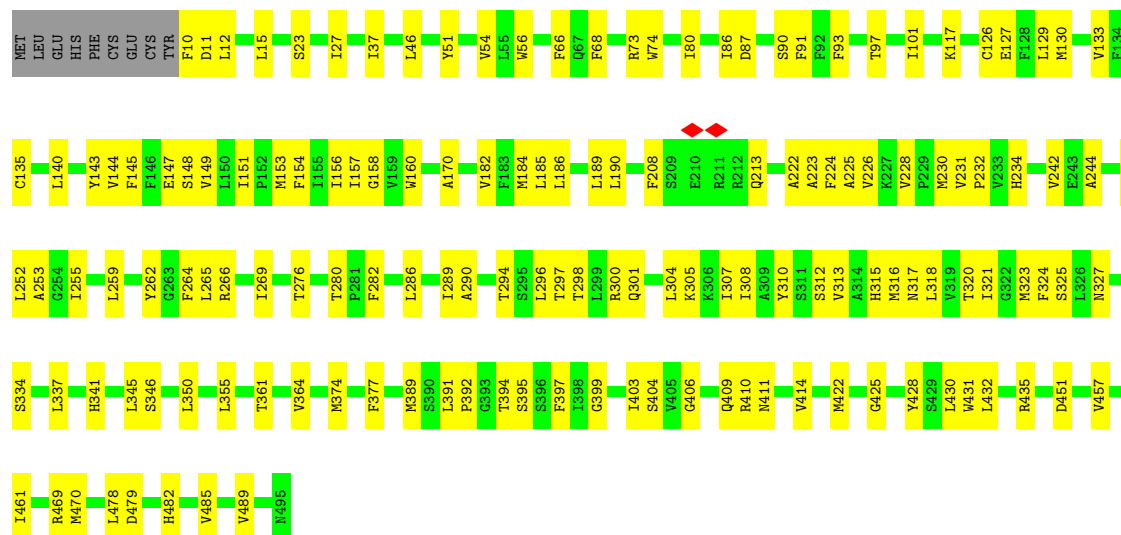
• Molecule 13: Nad2



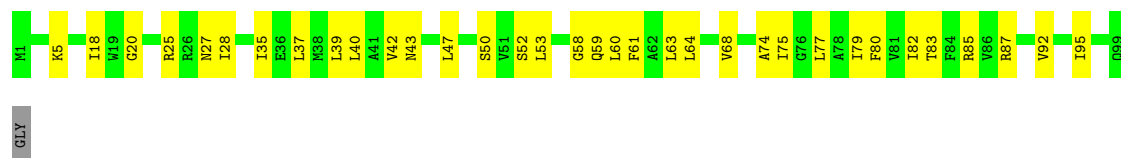
• Molecule 14: Nad3



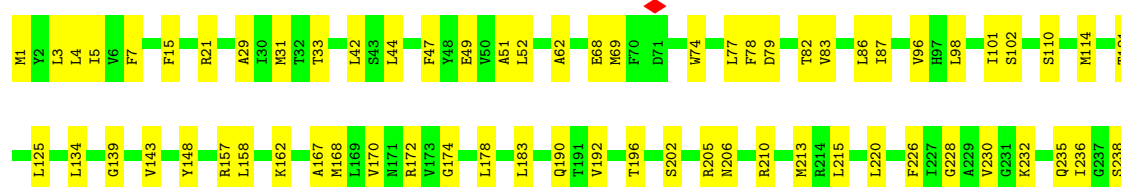
• Molecule 15: Nad4

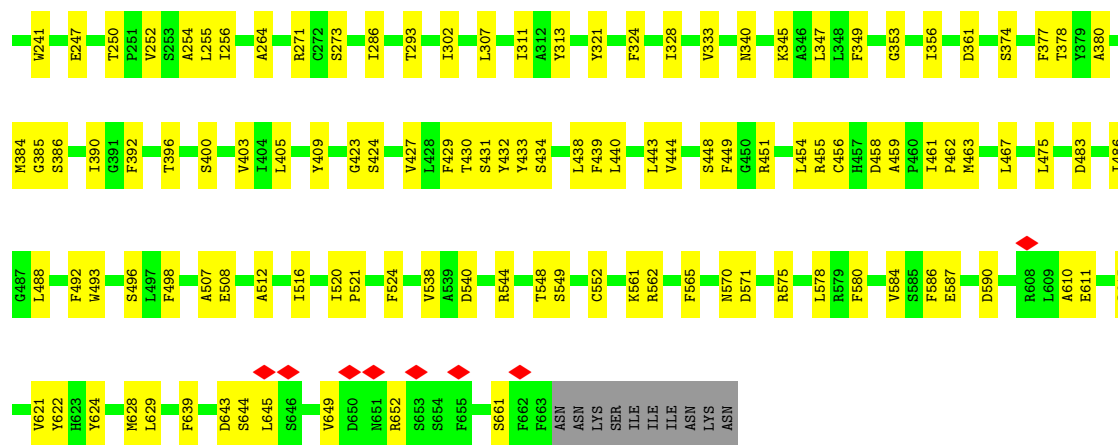


• Molecule 16: Nad4L

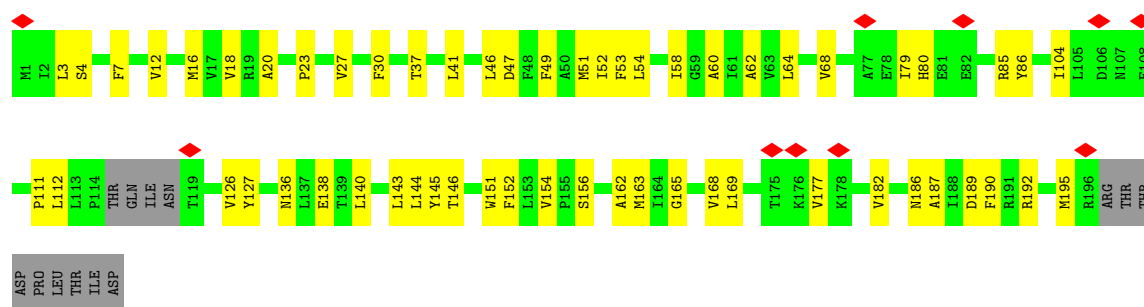


• Molecule 17: Nad5

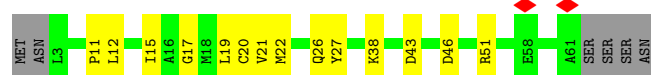




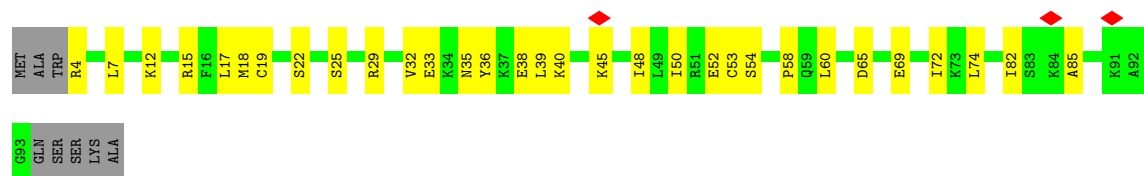
• Molecule 18: Nad6



• Molecule 19: NDUA1

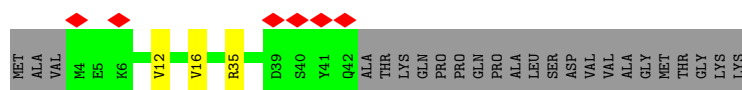


• Molecule 20: NDUA2

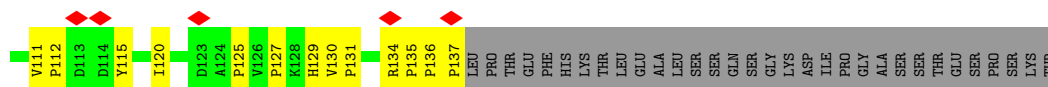


• Molecule 21: NDUA3

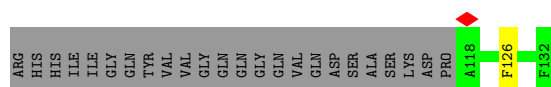
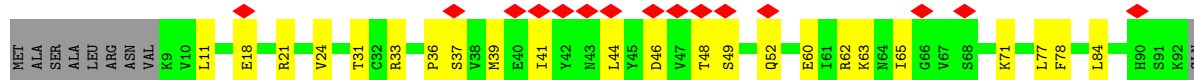




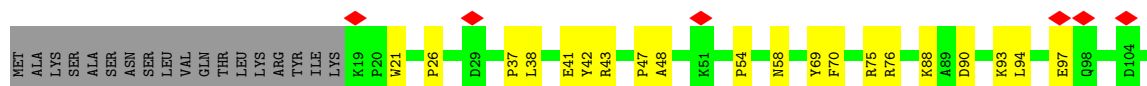
- Molecule 22: NDUA5



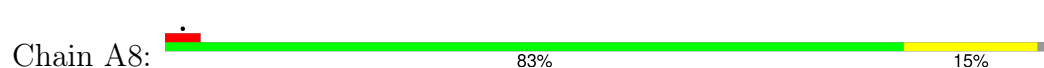
- Molecule 23: NDUA6



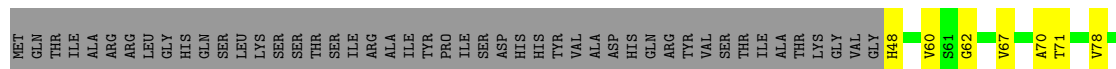
- Molecule 24: NDUA7

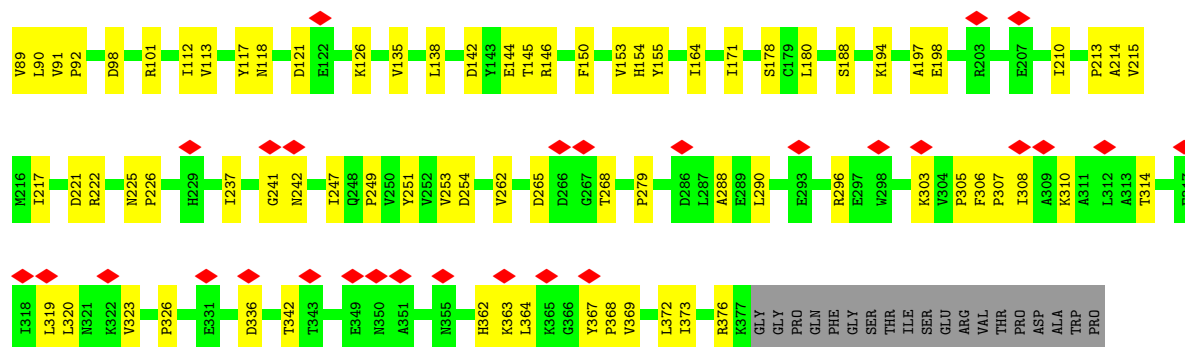


- Molecule 25: NDUA8

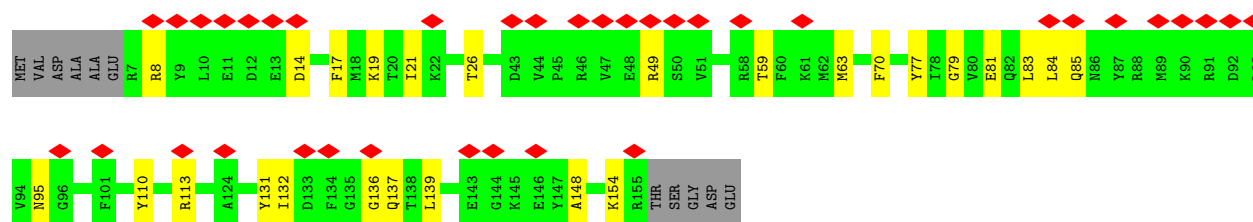


- Molecule 26: NDUA9

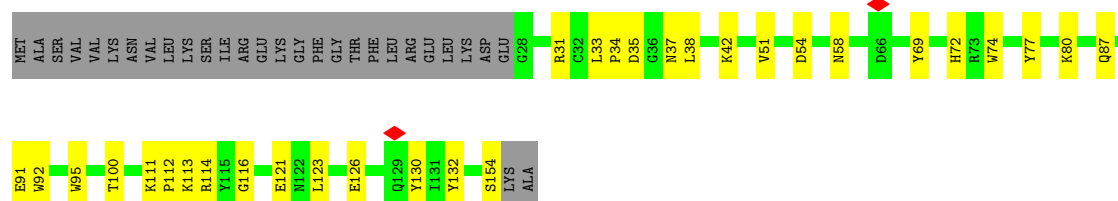




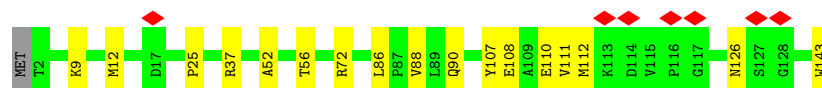
• Molecule 27: NDUA11



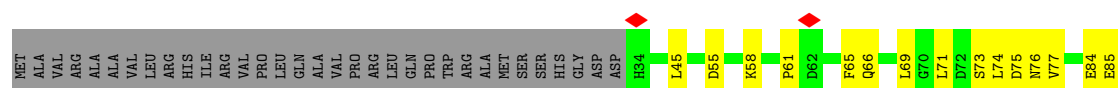
• Molecule 28: NDUA12

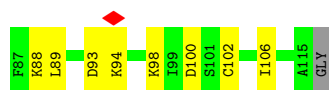


• Molecule 29: NDUA13

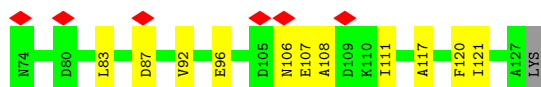
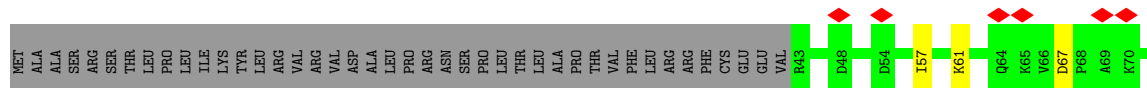


• Molecule 30: NDUAB1-beta





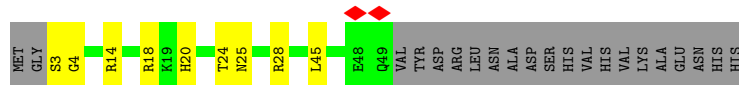
- Molecule 31: NDUAB1-alpha



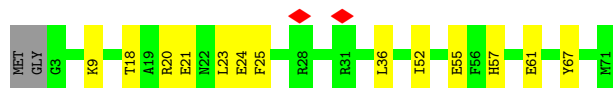
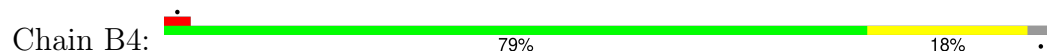
- Molecule 32: NDUB2



- Molecule 33: NDUB3



- Molecule 34: NDUB4

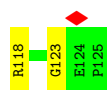


- Molecule 35: NDUB7

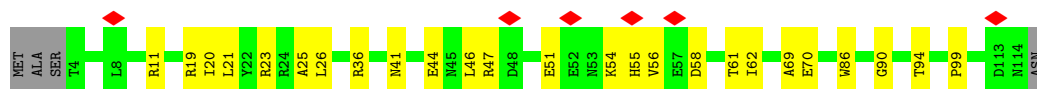
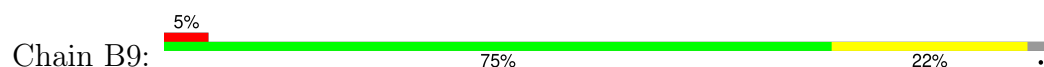


- Molecule 36: NDUB8

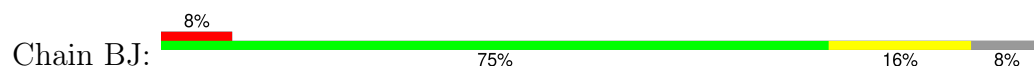




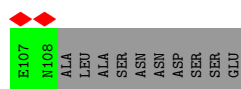
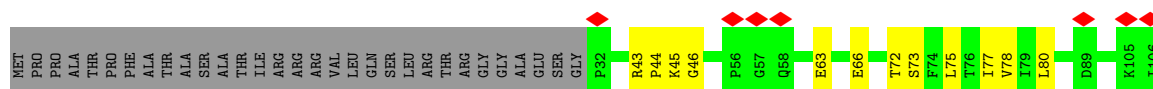
• Molecule 37: NDUB9



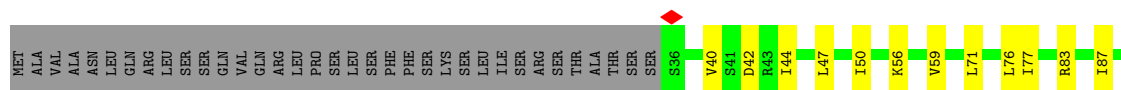
• Molecule 38: NDUB10



• Molecule 39: NDUB11



• Molecule 40: NDUFX

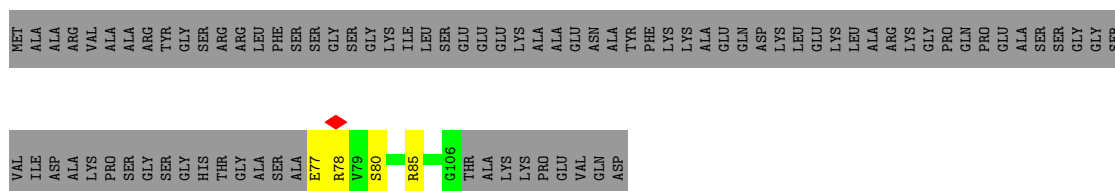


• Molecule 41: NDUC2

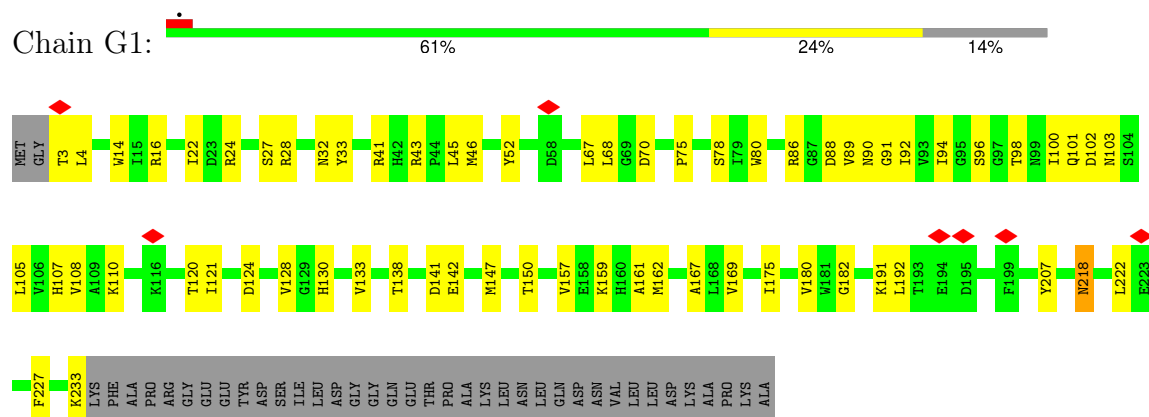


• Molecule 42: NDUP2

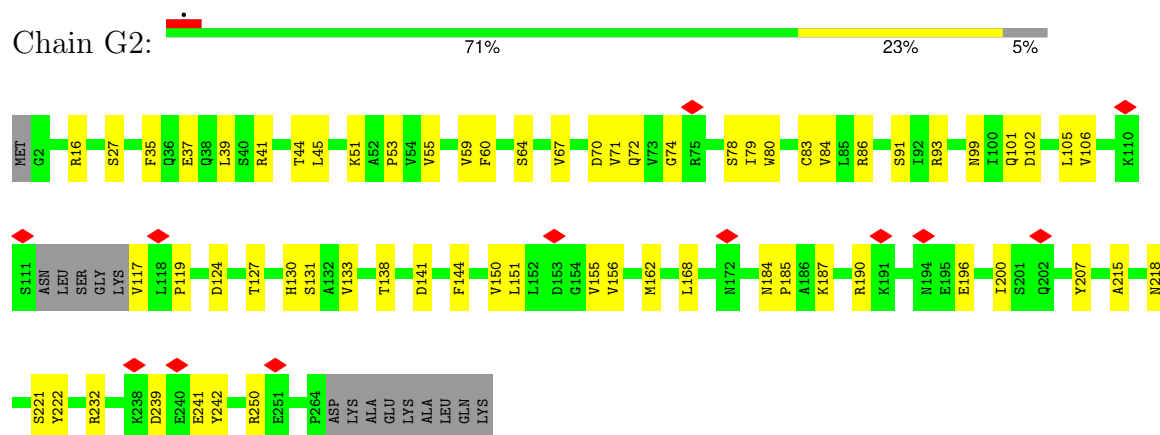




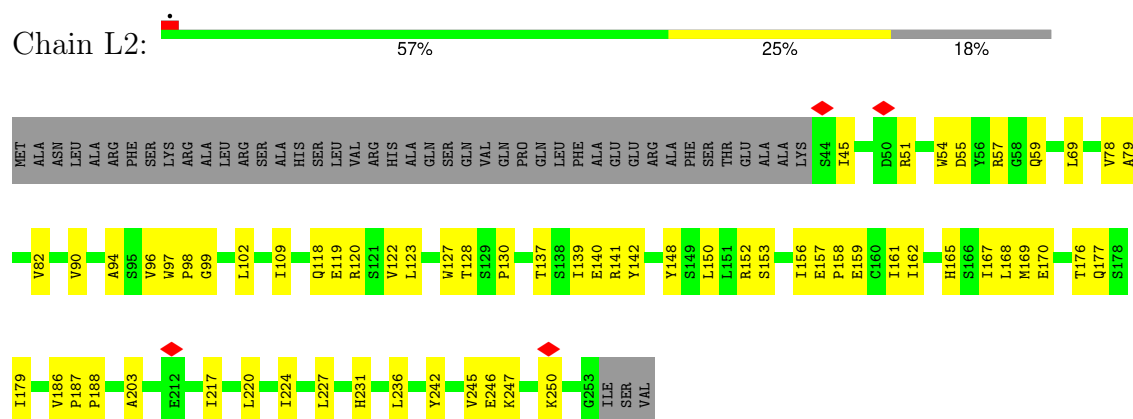
• Molecule 43: NDUCA1



• Molecule 44: NDUCA2



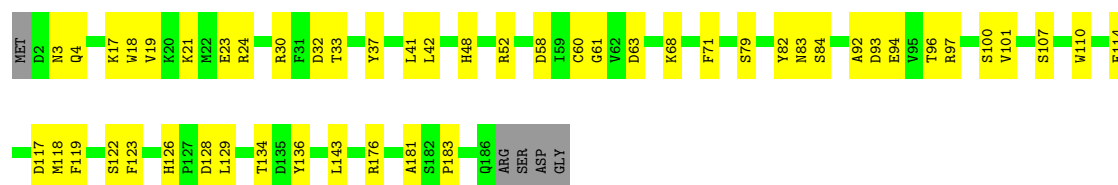
• Molecule 45: NDUCA2



• Molecule 46: NDUS1

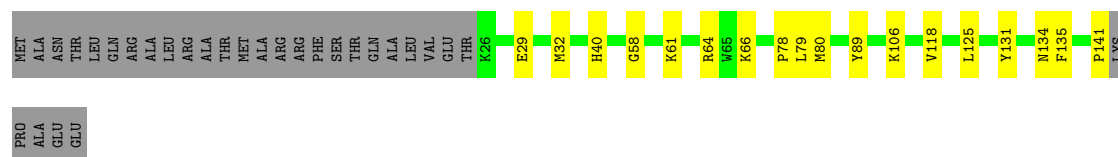


Chain S3:  71% 26% .



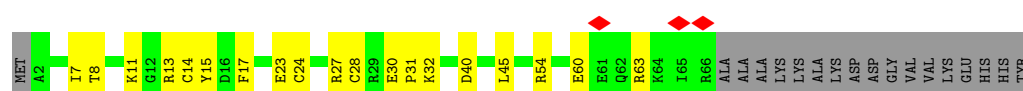
• Molecule 49: NDUS4

Chain S4:  67% 12% 21%



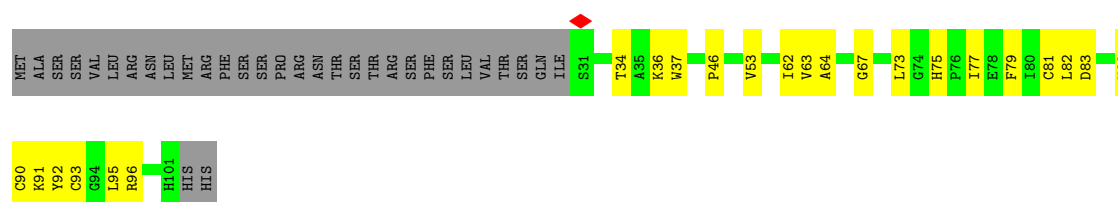
• Molecule 50: NDUS5

Chain S5:  55% 23% 22%



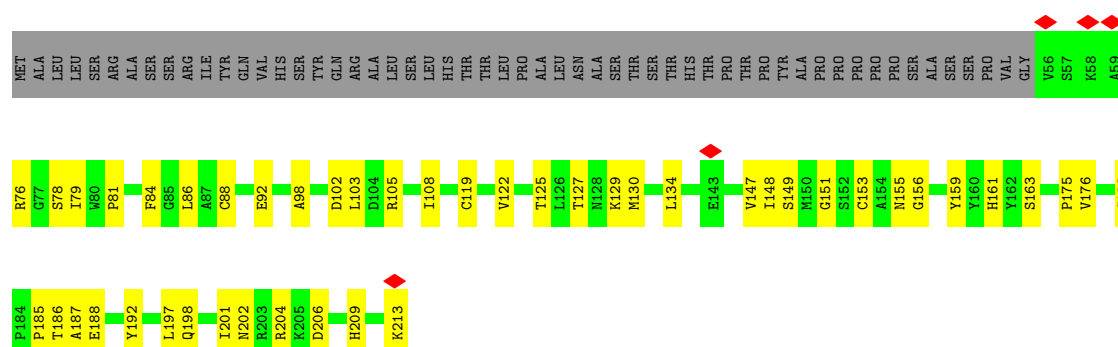
• Molecule 51: NDUS6

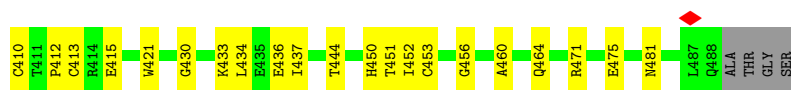
Chain S6:  47% 22% 31%



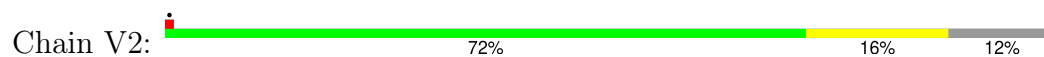
• Molecule 52: NDUS7

Chain S7:  53% 22% 26%

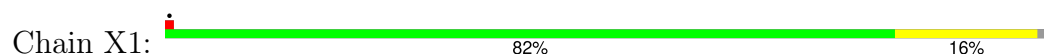




• Molecule 58: NDUV2



• Molecule 59: NDUX1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	123451	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	59.066	Depositor
Minimum map value	-25.094	Depositor
Average map value	0.289	Depositor
Map value standard deviation	2.866	Depositor
Recommended contour level	6.5	Depositor
Map size (\AA)	198.88, 236.72, 330.88	wwPDB
Map dimensions	376, 269, 226	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.88, 0.88, 0.88	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZMP, U10, SF4, FES, FE, FMN, ZN, PC1, CDL, 3PE, HEM, HEC, NDP

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	0.25	0/3875	0.51	0/5255
1	M	0.25	0/3883	0.51	0/5266
2	B	0.25	0/3481	0.46	0/4731
3	C	0.31	0/3205	0.45	0/4392
3	O	0.26	0/3190	0.44	0/4371
4	D	0.26	0/1957	0.46	0/2656
4	P	0.25	0/1957	0.46	0/2656
5	E	0.25	0/588	0.44	0/797
5	Q	0.25	0/579	0.44	0/785
6	F	0.24	0/995	0.47	0/1338
6	R	0.24	0/980	0.48	0/1318
7	G	0.24	0/595	0.40	0/807
7	S	0.23	0/595	0.39	0/807
8	H	0.26	0/541	0.44	0/724
8	T	0.27	0/541	0.47	0/724
9	J	0.25	0/478	0.45	0/644
9	V	0.24	0/486	0.46	0/655
10	K	0.23	0/169	0.38	0/230
10	W	0.23	0/206	0.39	0/282
11	N	0.25	0/3455	0.48	0/4687
12	1M	0.28	0/2578	0.46	0/3514
13	2M	0.27	0/3910	0.48	1/5305 (0.0%)
14	3M	0.28	0/785	0.42	0/1067
15	4M	0.27	0/3966	0.47	0/5388
16	4L	0.26	0/788	0.46	0/1065
17	5M	0.27	0/5344	0.46	0/7256
18	6M	0.26	0/1599	0.50	0/2175
19	A1	0.24	0/481	0.47	0/647
20	A2	0.25	0/707	0.47	0/946
21	A3	0.26	0/305	0.42	0/413
22	A5	0.25	0/1027	0.42	0/1394
23	A6	0.25	0/808	0.49	0/1087

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
24	A7	0.26	0/890	0.52	0/1210
25	A8	0.25	0/827	0.45	0/1106
26	A9	0.25	0/2628	0.49	0/3563
27	AK	0.24	0/1161	0.46	0/1567
28	AL	0.25	0/1092	0.49	0/1480
29	AM	0.25	0/1169	0.46	0/1585
30	AC	0.25	0/661	0.43	0/895
31	AB	0.25	0/672	0.43	0/909
32	B2	0.24	0/432	0.44	0/590
33	B3	0.25	0/396	0.48	0/532
34	B4	0.50	1/590 (0.2%)	0.58	0/791
35	B7	0.25	0/659	0.45	0/880
36	B8	0.26	0/762	0.46	0/1041
37	B9	0.25	0/954	0.49	0/1297
38	BJ	0.24	0/836	0.47	0/1126
39	BK	0.24	0/653	0.45	0/891
40	FD	0.31	1/981 (0.1%)	0.60	2/1329 (0.2%)
41	C2	0.31	0/598	0.45	0/806
42	P2	0.22	0/236	0.44	0/319
43	G1	0.27	0/1803	0.49	0/2445
44	G2	0.26	0/2013	0.52	0/2728
45	L2	0.26	0/1662	0.53	1/2269 (0.0%)
46	S1	0.25	0/5359	0.50	0/7267
47	S2	0.27	0/3086	0.51	0/4171
48	S3	0.25	0/1627	0.52	0/2204
49	S4	0.26	0/952	0.49	0/1286
50	S5	0.25	0/567	0.50	0/753
51	S6	0.27	0/567	0.50	0/771
52	S7	0.27	0/1289	0.51	0/1747
53	S8	0.28	0/1512	0.51	0/2036
54	P1	0.25	0/771	0.49	0/1038
55	P4	0.25	0/461	0.48	0/618
56	C1	0.25	0/603	0.46	0/817
57	V1	0.26	0/3400	0.50	1/4590 (0.0%)
58	V2	0.26	0/1765	0.48	0/2404
59	X1	0.26	0/768	0.47	0/1043
All	All	0.26	2/98456 (0.0%)	0.48	5/133486 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
40	FD	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	FD	156	ASP	C-N	6.04	1.48	1.34
34	B4	67	TYR	C-O	-5.09	1.13	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	FD	156	ASP	O-C-N	-9.43	107.62	122.70
57	V1	453	CYS	CA-CB-SG	6.62	125.91	114.00
45	L2	130	PRO	N-CA-CB	5.67	110.11	103.30
40	FD	156	ASP	CA-C-N	5.38	129.04	117.20
13	2M	409	CYS	CA-CB-SG	5.27	123.49	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
40	FD	156	ASP	Mainchain

5.2 Too-close contacts

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	3800	0	3766	73	0
1	M	3807	0	3774	81	0
2	B	3413	0	3424	53	0
3	C	3089	0	3059	63	0
3	O	3074	0	3041	61	0
4	D	1905	0	1838	33	0
4	P	1905	0	1837	35	0
5	E	574	0	591	17	0
5	Q	565	0	585	15	0
6	F	974	0	990	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	959	0	977	11	0
7	G	578	0	599	7	0
7	S	578	0	599	8	0
8	H	527	0	521	10	0
8	T	527	0	521	14	0
9	J	468	0	472	9	0
9	V	476	0	483	15	0
10	K	167	0	172	1	0
10	W	203	0	212	3	0
11	N	3389	0	3398	65	0
12	1M	2506	0	2596	66	0
13	2M	3810	0	3920	117	0
14	3M	759	0	785	29	0
15	4M	3862	0	4019	109	0
16	4L	777	0	837	36	0
17	5M	5198	0	5201	143	0
18	6M	1561	0	1657	54	0
19	A1	470	0	474	11	0
20	A2	699	0	734	24	0
21	A3	299	0	317	3	0
22	A5	1004	0	993	31	0
23	A6	794	0	798	19	0
24	A7	868	0	860	19	0
25	A8	814	0	807	11	0
26	A9	2571	0	2642	56	0
27	AK	1139	0	1156	20	0
28	AL	1057	0	997	22	0
29	AM	1134	0	1124	15	0
30	AC	650	0	649	19	0
31	AB	660	0	635	11	0
32	B2	414	0	409	6	0
33	B3	384	0	375	7	0
34	B4	576	0	564	9	0
35	B7	648	0	642	9	0
36	B8	737	0	723	18	0
37	B9	927	0	881	20	0
38	BJ	813	0	800	14	0
39	BK	631	0	623	10	0
40	FD	963	0	968	15	0
41	C2	587	0	601	17	0
42	P2	232	0	237	3	0
43	G1	1766	0	1742	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	G2	1979	0	1977	54	0
45	L2	1622	0	1617	44	0
46	S1	5263	0	5267	124	0
47	S2	3018	0	2983	125	0
48	S3	1579	0	1526	42	0
49	S4	923	0	909	15	0
50	S5	555	0	525	12	0
51	S6	553	0	541	16	0
52	S7	1254	0	1247	42	0
53	S8	1484	0	1431	55	0
54	P1	748	0	710	20	0
55	P4	452	0	454	10	0
56	C1	583	0	583	10	0
57	V1	3327	0	3304	80	0
58	V2	1721	0	1691	27	0
59	X1	750	0	743	13	0
60	1M	45	0	64	1	0
60	A	38	0	50	1	0
60	G1	64	0	71	3	0
60	G2	40	0	54	1	0
60	M	40	0	54	2	0
60	P4	54	0	88	1	0
60	S	38	0	50	2	0
61	A	69	0	85	3	0
61	C	123	0	134	3	0
61	D	68	0	83	2	0
61	M	70	0	87	4	0
61	O	182	0	196	7	0
62	C	86	0	60	9	0
62	O	86	0	60	12	0
63	C	72	0	92	2	0
63	G	37	0	48	0	0
63	M	45	0	67	5	0
63	O	108	0	138	4	0
63	R	51	0	82	4	0
64	D	43	0	30	3	0
64	P	43	0	30	3	0
65	1M	40	0	50	2	0
66	A9	48	0	25	4	0
67	AB	29	0	30	3	0
67	AC	29	0	30	1	0
68	FD	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	G2	1	0	0	0	0
69	S6	1	0	0	0	0
70	S1	16	0	0	1	0
70	S7	8	0	0	0	0
70	S8	16	0	0	2	0
70	V1	8	0	0	4	0
71	S1	4	0	0	0	0
71	V2	4	0	0	0	0
72	V1	31	0	19	1	0
All	All	97737	0	97910	1901	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 10.

All (1901) 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)
44:G2:79:ILE:HG23	44:G2:83:CYS:SG	1.75	1.24
44:G2:79:ILE:CG2	44:G2:83:CYS:SG	2.29	1.18
13:2M:168:TYR:HB2	13:2M:242:ILE:HG12	1.53	0.91
1:M:201:ARG:NH1	1:M:203:GLU:OE2	2.06	0.89
4:D:280:ALA:HB2	5:E:121:VAL:HG11	1.52	0.88
44:G2:79:ILE:HG22	44:G2:83:CYS:SG	2.12	0.87
57:V1:413:CYS:HB3	70:V1:502:SF4:S3	2.18	0.83
46:S1:179:GLU:HB3	46:S1:285:ASN:HD22	1.44	0.83
25:A8:28:ARG:HD2	25:A8:63:LEU:HD13	1.59	0.82
27:AK:154:LYS:NZ	41:C2:82:ILE:HG21	1.95	0.82
4:P:280:ALA:HB2	5:Q:121:VAL:HG11	1.61	0.81
53:S8:111:HIS:HE1	70:S8:701:SF4:S1	2.03	0.79
3:C:153:ILE:HA	3:C:156:LEU:HD13	1.64	0.79
17:5M:230:VAL:HG13	17:5M:235:GLN:HB2	1.64	0.79
3:O:35:TRP:HB3	3:O:105:ARG:HG3	1.66	0.78
53:S8:111:HIS:CD2	53:S8:162:CYS:SG	2.73	0.77
12:1M:119:TYR:OH	18:6M:58:ILE:O	2.03	0.76
43:G1:207:TYR:OH	44:G2:86:ARG:NH2	2.18	0.76
17:5M:102:SER:HB2	17:5M:462:PRO:HB2	1.67	0.76
46:S1:193:ARG:NH2	47:S2:290:ASP:OD1	2.18	0.76
12:1M:98:MET:HG2	19:A1:27:TYR:HB2	1.69	0.75
57:V1:451:THR:OG1	70:V1:502:SF4:S4	2.43	0.75
18:6M:54:LEU:O	18:6M:58:ILE:HB	1.87	0.75
14:3M:68:ILE:HG12	18:6M:60:ALA:HB1	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:S2:90:LEU:HD13	47:S2:322:VAL:HG12	1.68	0.74
18:6M:111:PRO:HG2	55:P4:29:ALA:HB2	1.69	0.74
1:A:526:ARG:O	10:K:21:TRP:NE1	2.19	0.74
3:C:105:ARG:HH12	62:C:503:HEM:HBD2	1.52	0.74
1:M:71:PHE:O	11:N:133:ARG:NH2	2.20	0.73
1:A:198:GLN:HE22	1:A:296:PHE:HA	1.54	0.72
13:2M:233:VAL:HG23	13:2M:290:SER:HA	1.71	0.72
57:V1:198:GLU:HG3	57:V1:225:ILE:HD11	1.69	0.72
12:1M:162:VAL:HG11	12:1M:170:ILE:HG12	1.70	0.72
52:S7:147:VAL:HB	52:S7:176:VAL:HA	1.71	0.72
3:O:50:ILE:HA	62:O:402:HEM:HAB	1.71	0.72
3:C:35:TRP:HB3	3:C:105:ARG:HG3	1.72	0.72
46:S1:166:ASN:ND2	57:V1:415:GLU:OE1	2.22	0.72
3:O:351:GLU:HG3	3:O:353:PRO:HD2	1.71	0.72
25:A8:4:ALA:HB2	25:A8:79:VAL:HG11	1.72	0.71
26:A9:364:LEU:HA	26:A9:368:PRO:HG2	1.72	0.71
1:M:170:THR:HG22	1:M:175:THR:HG23	1.71	0.71
57:V1:262:GLY:HA3	57:V1:268:THR:HG22	1.73	0.71
13:2M:419:VAL:HG21	15:4M:186:LEU:HD11	1.71	0.71
5:E:120:PHE:HE1	9:J:31:VAL:HA	1.55	0.71
48:S3:23:GLU:HB3	48:S3:30:ARG:HB3	1.73	0.71
11:N:177:VAL:HG11	11:N:276:LEU:HB3	1.71	0.71
3:O:283:PRO:HG2	61:O:404:CDL:H202	1.72	0.71
45:L2:176:THR:HG22	45:L2:177:GLN:HG3	1.72	0.71
49:S4:80:MET:O	53:S8:154:ARG:NH2	2.23	0.71
17:5M:68:GLU:OE2	38:BJ:88:LYS:NZ	2.22	0.70
43:G1:130:HIS:HB3	43:G1:147:MET:HG3	1.71	0.70
57:V1:451:THR:HG21	57:V1:456:GLY:HA3	1.73	0.70
5:E:137:MET:O	3:O:184:ARG:NH2	2.25	0.70
11:N:442:ILE:HG12	11:N:452:ARG:HD2	1.73	0.70
12:1M:35:GLN:HB3	47:S2:132:LEU:HD12	1.74	0.69
13:2M:180:LEU:HB3	16:4L:42:VAL:HG11	1.73	0.69
44:G2:117:VAL:HG22	44:G2:119:PRO:HD3	1.72	0.69
26:A9:247:ILE:HG13	26:A9:249:PRO:HD3	1.74	0.69
15:4M:269:ILE:HA	15:4M:276:THR:HG21	1.73	0.69
11:N:417:LEU:HD13	11:N:467:LEU:HD22	1.75	0.69
18:6M:16:MET:O	18:6M:20:ALA:HB2	1.92	0.69
17:5M:47:PHE:HA	17:5M:83:VAL:HG11	1.74	0.69
3:C:287:ILE:HG13	3:C:342:LEU:HD21	1.74	0.69
57:V1:191:VAL:HG11	58:V2:191:TYR:HB3	1.75	0.69
16:4L:20:GLY:HA2	18:6M:18:VAL:HG13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2M:397:CYS:HA	13:2M:400:PHE:CE1	2.27	0.68
1:M:336:VAL:HG12	1:M:503:ILE:HG12	1.76	0.68
52:S7:79:ILE:HG22	52:S7:81:PRO:HD3	1.75	0.68
57:V1:63:LEU:HD21	57:V1:319:GLU:HB2	1.76	0.68
2:B:185:ARG:NH2	2:B:283:ASP:OD1	2.25	0.68
47:S2:225:ARG:NH1	47:S2:267:GLU:OE2	2.24	0.68
47:S2:69:ARG:NH2	52:S7:183:CYS:SG	2.64	0.68
13:2M:404:PHE:HB2	15:4M:189:LEU:HD22	1.76	0.68
17:5M:157:ARG:NH1	17:5M:247:GLU:OE1	2.27	0.68
43:G1:68:LEU:HD11	45:L2:98:PRO:HG2	1.76	0.68
48:S3:176:ARG:NH1	53:S8:130:GLU:OE1	2.26	0.68
34:B4:20:ARG:NH1	36:B8:52:GLU:OE1	2.26	0.68
46:S1:565:ASP:OD2	46:S1:632:GLN:NE2	2.25	0.68
46:S1:416:VAL:HG21	46:S1:573:GLU:HG3	1.75	0.68
17:5M:252:VAL:HG13	17:5M:256:ILE:HD12	1.76	0.68
45:L2:142:TYR:O	45:L2:159:GLU:HA	1.94	0.68
44:G2:16:ARG:NH2	45:L2:246:GLU:OE1	2.27	0.67
13:2M:142:GLU:HG3	16:4L:68:VAL:HG11	1.76	0.67
17:5M:77:LEU:HD23	17:5M:271:ARG:HH21	1.57	0.67
13:2M:318:TYR:O	13:2M:321:ILE:HG22	1.93	0.67
27:AK:154:LYS:HZ3	41:C2:82:ILE:HG21	1.57	0.67
47:S2:154:HIS:NE2	52:S7:88:CYS:SG	2.67	0.67
57:V1:310:VAL:HG13	57:V1:384:VAL:HG21	1.77	0.67
27:AK:85:GLN:HB2	27:AK:95:ASN:HD21	1.58	0.67
43:G1:43:ARG:HD2	44:G2:37:GLU:HG2	1.76	0.67
46:S1:339:GLY:O	46:S1:607:HIS:NE2	2.24	0.67
13:2M:3:ASN:ND2	59:X1:19:ASN:OD1	2.28	0.67
58:V2:66:GLN:HG3	58:V2:98:VAL:HG11	1.77	0.67
17:5M:158:LEU:HD22	36:B8:57:ASN:HB2	1.76	0.66
44:G2:102:ASP:OD1	44:G2:130:HIS:ND1	2.23	0.66
3:C:75:MET:HE1	3:C:85:ARG:HH11	1.61	0.66
18:6M:126:VAL:O	29:AM:90:GLN:NE2	2.28	0.66
26:A9:217:ILE:HD11	26:A9:364:LEU:HD22	1.76	0.66
26:A9:373:ILE:O	26:A9:376:ARG:N	2.28	0.66
44:G2:207:TYR:OH	45:L2:152:ARG:NH2	2.27	0.66
49:S4:61:LYS:O	49:S4:64:ARG:NH1	2.29	0.66
3:O:228:TYR:O	3:O:232:TYR:HB3	1.96	0.66
5:Q:120:PHE:HE1	9:V:31:VAL:HA	1.60	0.66
57:V1:182:ALA:HB3	57:V1:223:VAL:HG22	1.77	0.66
3:O:105:ARG:HH12	62:O:403:HEM:HBD2	1.61	0.66
15:4M:327:ASN:HD21	15:4M:406:GLY:HA2	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:4M:73:ARG:NH2	41:C2:53:GLU:OE2	2.29	0.65
36:B8:39:LYS:HA	36:B8:39:LYS:HE3	1.77	0.65
44:G2:67:VAL:HB	44:G2:71:VAL:HG21	1.77	0.65
17:5M:52:LEU:O	56:C1:67:ARG:NH2	2.27	0.65
2:B:106:LEU:HD13	2:B:263:LEU:HD23	1.78	0.65
8:T:35:ILE:HD12	8:T:43:LYS:HB3	1.79	0.65
17:5M:483:ASP:OD2	35:B7:55:ARG:NH1	2.30	0.65
47:S2:190:GLU:OE1	47:S2:269:ARG:NH2	2.27	0.65
57:V1:444:THR:HG23	57:V1:460:ALA:HB1	1.79	0.65
47:S2:209:VAL:HG23	47:S2:227:PRO:HG3	1.79	0.65
57:V1:186:ILE:HD11	57:V1:197:LEU:HD23	1.77	0.65
1:A:259:LYS:NZ	1:A:263:GLN:OE1	2.30	0.65
13:2M:391:PRO:HA	13:2M:396:PHE:CG	2.32	0.65
28:AL:74:TRP:HB3	53:S8:99:GLU:HG2	1.78	0.65
46:S1:416:VAL:HA	46:S1:570:PRO:HG2	1.78	0.65
17:5M:196:THR:HG21	38:BJ:52:ARG:HG3	1.79	0.65
14:3M:76:PHE:O	18:6M:145:TYR:OH	2.12	0.65
46:S1:192:ASP:HB2	47:S2:292:ARG:HB2	1.79	0.65
17:5M:29:ALA:HB1	17:5M:101:ILE:HG12	1.79	0.65
26:A9:118:ASN:HB3	26:A9:121:ASP:HB2	1.78	0.65
26:A9:198:GLU:HB2	26:A9:210:ILE:HD13	1.79	0.65
22:A5:95:ASP:OD2	48:S3:52:ARG:NH2	2.29	0.64
12:1M:302:VAL:HG13	21:A3:16:VAL:HG21	1.79	0.64
17:5M:49:GLU:HG2	56:C1:69:ILE:HB	1.80	0.64
6:F:108:ARG:NH2	1:M:377:GLN:OE1	2.30	0.64
13:2M:391:PRO:HG2	15:4M:147:GLU:HB3	1.78	0.64
46:S1:265:VAL:HG12	46:S1:274:LEU:HD13	1.78	0.64
15:4M:325:SER:HA	15:4M:410:ARG:HG3	1.78	0.64
57:V1:68:ARG:NH1	57:V1:317:GLU:O	2.29	0.64
13:2M:144:GLN:HE22	13:2M:262:ILE:HD11	1.63	0.64
13:2M:275:TYR:HB3	54:P1:49:ARG:NH2	2.12	0.64
1:M:347:ASP:OD2	1:M:494:ARG:NH1	2.30	0.64
3:O:287:ILE:HG13	3:O:342:LEU:HD21	1.80	0.64
13:2M:200:LYS:NZ	54:P1:60:ASN:OD1	2.30	0.64
58:V2:174:ALA:HB3	58:V2:196:ASP:HA	1.79	0.64
12:1M:154:ILE:HG21	12:1M:190:PHE:HB2	1.79	0.64
20:A2:60:LEU:HD23	20:A2:72:ILE:HD11	1.80	0.64
47:S2:80:HIS:NE2	47:S2:240:ASP:OD2	2.30	0.64
15:4M:97:THR:HG22	15:4M:255:ILE:HD12	1.78	0.64
47:S2:108:ILE:HG23	47:S2:141:LEU:HD22	1.79	0.64
1:M:469:ARG:NH2	1:M:475:GLU:OE2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:4M:56:TRP:HA	15:4M:91:PHE:HZ	1.63	0.63
15:4M:391:LEU:O	15:4M:394:THR:OG1	2.14	0.63
3:O:90:ASN:O	3:O:94:MET:HG2	1.97	0.63
13:2M:167:LYS:HG2	17:5M:621:VAL:HG22	1.81	0.63
17:5M:321:TYR:HA	17:5M:324:PHE:CE1	2.33	0.63
50:S5:14:CYS:HB2	50:S5:17:PHE:HB2	1.79	0.63
1:M:150:ARG:NH2	1:M:191:ASP:OD2	2.31	0.63
12:1M:86:LEU:HB3	14:3M:10:TYR:HE1	1.64	0.63
17:5M:643:ASP:OD1	17:5M:644:SER:N	2.32	0.63
48:S3:118:MET:HB3	48:S3:143:LEU:HB2	1.79	0.63
59:X1:33:ASP:OD2	59:X1:84:ARG:NH2	2.31	0.63
5:Q:113:PHE:HZ	9:V:16:LEU:HB3	1.63	0.63
53:S8:129:CYS:SG	53:S8:155:TYR:OH	2.55	0.63
1:M:498:ASP:OD1	1:M:519:ARG:NH1	2.32	0.63
17:5M:652:ARG:NH1	27:AK:77:TYR:OH	2.30	0.63
46:S1:328:TRP:HB2	46:S1:454:MET:HE1	1.81	0.63
1:M:519:ARG:O	1:M:522:THR:OG1	2.16	0.63
17:5M:340:ASN:ND2	17:5M:400:SER:OG	2.32	0.63
57:V1:309:HIS:HD2	57:V1:336:ARG:HH21	1.47	0.63
15:4M:101:ILE:HG13	15:4M:127:GLU:HB2	1.81	0.62
2:B:220:ILE:HD11	2:B:314:ALA:HB3	1.80	0.62
47:S2:209:VAL:HG22	47:S2:260:ARG:HH21	1.63	0.62
54:P1:56:PHE:O	54:P1:60:ASN:ND2	2.32	0.62
22:A5:127:PRO:HD3	47:S2:91:ASN:HA	1.80	0.62
47:S2:109:THR:OG1	47:S2:145:TYR:OH	2.15	0.62
52:S7:148:ILE:HD11	52:S7:197:LEU:HD22	1.81	0.62
13:2M:108:ARG:HB3	44:G2:239:ASP:HB2	1.81	0.62
1:A:177:TYR:HH	1:A:270:TYR:HH	1.47	0.62
16:4L:39:LEU:O	16:4L:43:ASN:ND2	2.29	0.62
23:A6:11:LEU:O	48:S3:97:ARG:NH1	2.32	0.62
4:D:191:TYR:OH	64:D:501:HEC:O2A	2.15	0.62
11:N:102:LEU:HD22	11:N:180:VAL:HG21	1.81	0.62
48:S3:42:LEU:HD12	48:S3:101:VAL:HG11	1.80	0.62
1:M:459:ASP:OD1	1:M:462:ARG:NH2	2.32	0.62
17:5M:403:VAL:HG11	17:5M:486:ILE:HD11	1.81	0.62
23:A6:78:PHE:HZ	48:S3:129:LEU:HB3	1.63	0.62
47:S2:299:ARG:NH2	53:S8:172:CYS:O	2.32	0.62
48:S3:4:GLN:OE1	48:S3:24:ARG:NH2	2.32	0.62
3:C:115:PRO:HA	6:F:119:ARG:HH21	1.64	0.62
15:4M:404:SER:HB3	17:5M:183:LEU:HD21	1.79	0.62
44:G2:72:GLN:HB3	44:G2:93:ARG:HD3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:S1:294:ILE:HD13	46:S1:639:GLN:HG3	1.82	0.62
48:S3:71:PHE:HB2	48:S3:92:ALA:O	1.99	0.62
27:AK:154:LYS:HZ2	41:C2:82:ILE:HG21	1.65	0.62
2:B:331:VAL:HG22	2:B:469:VAL:HG22	1.82	0.62
1:M:106:THR:HG22	1:M:279:ALA:HB3	1.82	0.62
67:AB:201:ZMP:HN2	67:AB:201:ZMP:H19	1.65	0.62
5:E:119:ARG:NH1	9:J:27:TYR:OH	2.33	0.61
8:H:39:ASP:OD1	8:H:40:SER:N	2.31	0.61
23:A6:65:ILE:HA	67:AB:201:ZMP:H15A	1.81	0.61
1:A:170:THR:HG22	1:A:175:THR:HG23	1.82	0.61
11:N:155:ARG:NH2	11:N:214:GLU:OE1	2.33	0.61
49:S4:106:LYS:HE2	49:S4:118:VAL:HG21	1.82	0.61
57:V1:184:ILE:HB	57:V1:225:ILE:HG22	1.82	0.61
13:2M:435:ARG:NH1	13:2M:439:ASP:OD2	2.33	0.61
17:5M:210:ARG:HD3	17:5M:220:LEU:HD21	1.81	0.61
17:5M:390:ILE:HD11	17:5M:434:SER:HB2	1.82	0.61
30:AC:85:GLU:OE2	37:B9:36:ARG:NH1	2.33	0.61
47:S2:74:SER:O	47:S2:78:GLN:NE2	2.33	0.61
47:S2:103:VAL:HG21	47:S2:241:VAL:HG22	1.83	0.61
39:BK:63:GLU:HB2	39:BK:66:GLU:HG3	1.82	0.61
43:G1:52:TYR:HB2	44:G2:35:PHE:HE1	1.65	0.61
47:S2:103:VAL:HG13	47:S2:242:TYR:HE1	1.65	0.61
2:B:136:ASN:ND2	2:B:182:ASP:OD1	2.31	0.61
4:D:273:TRP:HZ2	5:E:128:LEU:HD13	1.66	0.61
11:N:353:ARG:NH2	11:N:411:GLN:O	2.33	0.61
12:1M:88:ALA:HB2	12:1M:113:ILE:HG21	1.81	0.61
18:6M:112:LEU:HD11	50:S5:54:ARG:HD2	1.82	0.61
2:B:167:ASP:OD2	2:B:439:ARG:NH2	2.27	0.61
15:4M:12:LEU:HD21	15:4M:86:ILE:HG23	1.81	0.61
17:5M:390:ILE:HD12	17:5M:431:SER:HA	1.82	0.61
1:M:177:TYR:HH	1:M:270:TYR:HH	1.49	0.60
12:1M:105:ILE:HD11	12:1M:108:LEU:HD23	1.83	0.60
32:B2:46:PRO:HB2	32:B2:52:ARG:HG3	1.83	0.60
47:S2:260:ARG:HH11	47:S2:384:THR:HG21	1.66	0.60
1:A:333:GLN:HG2	1:A:406:VAL:HG22	1.83	0.60
22:A5:135:PRO:HA	48:S3:3:ASN:HD22	1.66	0.60
16:4L:82:ILE:HD13	18:6M:169:LEU:HD22	1.82	0.60
17:5M:62:ALA:HB3	17:5M:74:TRP:HD1	1.64	0.60
37:B9:99:PRO:HG2	56:C1:13:GLY:HA3	1.82	0.60
1:A:430:VAL:HG12	1:A:489:LYS:HE3	1.83	0.60
13:2M:434:LYS:HG2	13:2M:438:PHE:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:G1:86:ARG:NH2	43:G1:108:VAL:O	2.33	0.60
55:P4:15:PHE:O	55:P4:19:GLN:HG2	2.01	0.60
1:A:61:LEU:HD22	6:R:100:LEU:HD13	1.84	0.60
20:A2:15:ARG:NH2	20:A2:69:GLU:OE2	2.32	0.60
47:S2:245:LEU:HD13	47:S2:274:ILE:HG23	1.82	0.60
57:V1:168:GLU:OE2	57:V1:284:ARG:NH1	2.34	0.60
58:V2:245:CYS:SG	58:V2:246:ARG:N	2.74	0.60
59:X1:84:ARG:O	59:X1:91:ASN:ND2	2.34	0.60
13:2M:157:LYS:HG2	44:G2:241:GLU:HG2	1.83	0.60
15:4M:318:LEU:O	15:4M:321:ILE:HG22	2.01	0.60
3:O:156:LEU:HA	3:O:294:LYS:HD2	1.82	0.60
22:A5:71:GLU:HB2	22:A5:77:ILE:HG22	1.83	0.60
27:AK:8:ARG:NH2	27:AK:136:GLY:O	2.34	0.60
46:S1:489:ASP:HB3	46:S1:492:THR:HG23	1.83	0.60
54:P1:66:ASP:HA	54:P1:69:ILE:HG22	1.84	0.60
1:A:86:ARG:HG3	1:A:87:ILE:HG23	1.83	0.60
6:F:119:ARG:HH22	6:F:122:PRO:HG3	1.67	0.60
30:AC:93:ASP:HB3	37:B9:20:ILE:HG12	1.83	0.60
47:S2:369:MET:SD	47:S2:385:GLN:NE2	2.75	0.60
15:4M:46:LEU:HD22	39:BK:72:THR:HG21	1.84	0.60
57:V1:303:LEU:HA	57:V1:317:GLU:HA	1.84	0.60
28:AL:31:ARG:O	28:AL:35:ASP:HB2	2.02	0.59
61:D:502:CDL:H132	7:G:34:ILE:HG12	1.85	0.59
15:4M:126:CYS:O	15:4M:130:MET:HG2	2.01	0.59
15:4M:208:PHE:HB2	15:4M:213:GLN:HG3	1.83	0.59
22:A5:30:ARG:NH1	22:A5:31:GLU:OE2	2.34	0.59
45:L2:97:TRP:HB3	45:L2:119:GLU:HG3	1.84	0.59
46:S1:417:ASN:O	46:S1:527:GLN:NE2	2.35	0.59
47:S2:370:SER:HB2	47:S2:378:VAL:HG22	1.84	0.59
18:6M:3:LEU:HG	18:6M:7:PHE:HE2	1.67	0.59
22:A5:57:VAL:HA	22:A5:60:PHE:CE2	2.37	0.59
46:S1:223:THR:HG22	46:S1:240:MET:HE3	1.84	0.59
46:S1:305:ARG:NH1	46:S1:307:ASP:OD1	2.35	0.59
3:O:77:ASP:OD1	4:P:114:ARG:NH2	2.34	0.59
13:2M:407:LEU:HD12	15:4M:190:LEU:HD13	1.83	0.59
17:5M:3:LEU:HB2	56:C1:55:SER:OG	2.01	0.59
1:M:94:ARG:NH2	11:N:70:ASP:OD2	2.33	0.59
3:O:223:ASP:OD1	4:P:298:ARG:NH2	2.34	0.59
18:6M:127:TYR:HB3	29:AM:86:LEU:HD11	1.85	0.59
28:AL:114:ARG:NH1	53:S8:118:THR:O	2.35	0.59
61:A:602:CDL:H131	61:C:501:CDL:HB4	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:287:ILE:HD13	3:C:304:VAL:HG21	1.84	0.59
13:2M:478:VAL:HG22	41:C2:56:VAL:HG21	1.85	0.59
17:5M:409:TYR:O	36:B8:101:LYS:NZ	2.34	0.59
46:S1:103:ILE:O	46:S1:105:ARG:NH1	2.36	0.59
46:S1:555:LEU:HB2	46:S1:634:THR:HG22	1.84	0.59
13:2M:405:ALA:O	13:2M:409:CYS:HB2	2.01	0.59
26:A9:90:LEU:HD23	26:A9:113:VAL:HB	1.83	0.59
26:A9:92:PRO:HB2	26:A9:117:TYR:CE1	2.37	0.59
46:S1:107:CYS:O	46:S1:227:ARG:NH2	2.34	0.59
46:S1:385:ALA:HA	46:S1:585:MET:HB3	1.85	0.59
6:F:47:VAL:HG13	6:F:94:LEU:HD21	1.83	0.59
13:2M:241:ASP:OD1	13:2M:306:ARG:NH2	2.36	0.59
43:G1:157:VAL:HG22	43:G1:175:ILE:HD13	1.84	0.59
44:G2:168:LEU:HB3	44:G2:184:ASN:O	2.03	0.59
57:V1:245:GLU:OE2	57:V1:252:ARG:NH2	2.36	0.59
19:A1:12:LEU:HA	19:A1:15:ILE:HD12	1.84	0.59
36:B8:37:VAL:HB	36:B8:59:THR:HG22	1.85	0.59
6:R:80:PRO:HD2	6:R:83:LEU:HD12	1.85	0.58
15:4M:307:ILE:HG21	15:4M:432:LEU:HD22	1.85	0.58
18:6M:80:HIS:O	27:AK:49:ARG:NH2	2.36	0.58
2:B:198:LEU:HD22	2:B:240:ILE:HG23	1.86	0.58
13:2M:186:ILE:HG13	13:2M:218:GLY:HA3	1.85	0.58
16:4L:18:ILE:HD12	17:5M:629:LEU:HD21	1.85	0.58
16:4L:83:THR:HG23	16:4L:87:ARG:HH11	1.69	0.58
26:A9:306:PHE:HE2	26:A9:342:THR:HA	1.67	0.58
46:S1:528:ASP:OD1	46:S1:529:ALA:N	2.36	0.58
3:O:18:THR:HG21	63:O:401:3PE:H332	1.85	0.58
8:T:59:CYS:O	8:T:63:LYS:NZ	2.33	0.58
16:4L:75:ILE:O	16:4L:79:ILE:HG12	2.03	0.58
17:5M:440:LEU:HD23	17:5M:444:VAL:HG21	1.86	0.58
11:N:105:ASP:OD2	11:N:285:ARG:NH2	2.36	0.58
11:N:363:GLN:O	11:N:364:GLN:HG3	2.03	0.58
13:2M:49:LEU:HD21	59:X1:44:SER:HA	1.86	0.58
17:5M:374:SER:HG	17:5M:456:CYS:HG	1.51	0.58
30:AC:73:SER:HB3	37:B9:19:ARG:HD3	1.84	0.58
2:B:400:ILE:HD12	2:B:498:PRO:HD2	1.85	0.58
17:5M:273:SER:OG	17:5M:498:PHE:O	2.21	0.58
17:5M:508:GLU:OE2	35:B7:69:ARG:NH2	2.29	0.58
3:C:154:THR:HG22	3:C:168:VAL:HG23	1.86	0.58
17:5M:430:THR:HA	17:5M:433:TYR:CE2	2.39	0.58
41:C2:82:ILE:HG22	41:C2:82:ILE:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:G2:133:VAL:HB	44:G2:150:VAL:HG12	1.86	0.58
11:N:121:LEU:HD23	11:N:244:LEU:HD11	1.85	0.58
15:4M:56:TRP:HA	15:4M:91:PHE:CZ	2.39	0.58
47:S2:72:TYR:CG	52:S7:88:CYS:HB3	2.38	0.58
11:N:111:GLU:OE2	11:N:117:GLY:N	2.27	0.58
8:T:17:CYS:HA	8:T:20:LYS:HD3	1.85	0.58
23:A6:24:VAL:HG22	23:A6:77:LEU:HD21	1.85	0.58
43:G1:86:ARG:NH1	43:G1:88:ASP:OD1	2.37	0.58
47:S2:366:LEU:HD22	47:S2:382:ILE:HD11	1.86	0.58
47:S2:389:PHE:HA	47:S2:392:VAL:HG22	1.86	0.58
44:G2:218:ASN:HD21	45:L2:59:GLN:HE22	1.51	0.58
46:S1:201:ARG:NH2	46:S1:221:GLN:OE1	2.36	0.58
2:B:104:ILE:HD11	2:B:268:VAL:HG21	1.86	0.57
6:R:79:LEU:O	6:R:84:GLN:NE2	2.37	0.57
63:R:201:3PE:H371	63:R:201:3PE:H292	1.85	0.57
12:1M:201:ALA:HB1	12:1M:202:PRO:HD2	1.85	0.57
17:5M:378:THR:OG1	17:5M:458:ASP:OD1	2.21	0.57
46:S1:61:LEU:HB3	46:S1:97:GLU:HG3	1.86	0.57
57:V1:116:ARG:HD2	57:V1:302:LYS:HD3	1.85	0.57
37:B9:55:HIS:ND1	37:B9:55:HIS:O	2.37	0.57
50:S5:30:GLU:OE2	50:S5:32:LYS:NZ	2.28	0.57
52:S7:159:TYR:HE1	53:S8:134:PRO:HB2	1.69	0.57
47:S2:155:ALA:HA	53:S8:108:ARG:HH22	1.68	0.57
52:S7:86:LEU:HD21	52:S7:130:MET:HG2	1.86	0.57
1:A:43:PRO:HG2	4:P:306:ASN:HD21	1.69	0.57
46:S1:171:CYS:HB3	70:S1:903:SF4:S4	2.43	0.57
47:S2:245:LEU:O	47:S2:277:GLN:NE2	2.34	0.57
3:C:85:ARG:NH2	62:C:502:HEM:O2D	2.37	0.57
11:N:111:GLU:OE2	11:N:118:ALA:N	2.31	0.57
18:6M:79:ILE:HG13	18:6M:79:ILE:O	2.05	0.57
45:L2:82:VAL:HG11	45:L2:96:VAL:HG12	1.86	0.57
47:S2:119:THR:HG21	47:S2:134:ALA:HB3	1.86	0.57
52:S7:204:ARG:NH2	52:S7:206:ASP:OD2	2.38	0.57
50:S5:24:CYS:O	50:S5:28:CYS:HB3	2.04	0.57
53:S8:178:VAL:HG11	53:S8:215:LEU:HD11	1.86	0.57
2:B:202:LYS:NZ	2:B:241:ASN:OD1	2.38	0.57
1:M:79:PRO:HG3	1:M:437:ARG:HB2	1.84	0.57
12:1M:324:LEU:O	29:AM:72:ARG:NH2	2.32	0.57
18:6M:49:PHE:HA	18:6M:52:ILE:HG12	1.87	0.57
37:B9:25:ALA:HB1	37:B9:46:LEU:HD11	1.85	0.57
43:G1:133:VAL:HG12	43:G1:150:THR:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:G2:138:THR:HB	44:G2:156:VAL:HG22	1.85	0.57
61:O:407:CDL:HB61	7:S:37:LYS:HE2	1.86	0.57
12:1M:155:LEU:HD23	12:1M:246:LEU:HD21	1.87	0.57
13:2M:18:THR:HG21	13:2M:120:LEU:HG	1.86	0.57
33:B3:25:ASN:O	33:B3:28:ARG:NH1	2.37	0.57
1:M:333:GLN:HG2	1:M:406:VAL:HG22	1.85	0.57
3:O:86:TYR:O	3:O:90:ASN:ND2	2.38	0.57
15:4M:37:ILE:HD13	15:4M:117:LYS:HB3	1.86	0.57
37:B9:21:LEU:HD12	37:B9:70:GLU:HG3	1.86	0.57
45:L2:169:MET:HE2	45:L2:187:PRO:HA	1.87	0.57
11:N:52:LEU:HD22	11:N:59:LEU:HD11	1.86	0.57
31:AB:107:GLU:O	31:AB:111:ILE:HG13	2.05	0.57
46:S1:67:HIS:HB2	49:S4:125:LEU:HD11	1.87	0.57
48:S3:97:ARG:HG2	48:S3:122:SER:HB3	1.85	0.57
53:S8:60:TRP:HA	53:S8:63:VAL:HG12	1.85	0.57
58:V2:53:VAL:HG22	58:V2:72:LEU:HD22	1.85	0.57
11:N:293:TYR:HH	11:N:483:THR:HG1	1.53	0.56
39:BK:45:LYS:NZ	56:C1:26:PRO:O	2.38	0.56
46:S1:261:LEU:HD11	46:S1:457:ALA:HB2	1.87	0.56
12:1M:105:ILE:HG12	12:1M:108:LEU:HB3	1.86	0.56
13:2M:68:ALA:HB1	13:2M:71:PHE:HB3	1.86	0.56
13:2M:173:ALA:HB1	16:4L:35:ILE:HG21	1.87	0.56
22:A5:127:PRO:HG2	22:A5:130:VAL:HG13	1.86	0.56
46:S1:193:ARG:NH2	47:S2:290:ASP:O	2.28	0.56
53:S8:94:ILE:O	53:S8:99:GLU:HB2	2.04	0.56
53:S8:138:ILE:HG12	53:S8:157:ILE:HG12	1.86	0.56
1:A:348:SER:O	1:A:352:MET:HG3	2.06	0.56
17:5M:321:TYR:OH	17:5M:423:GLY:O	2.22	0.56
20:A2:18:MET:HB2	20:A2:25:SER:HB3	1.87	0.56
26:A9:126:LYS:HG3	26:A9:164:ILE:HD12	1.87	0.56
46:S1:614:ARG:O	46:S1:614:ARG:NH1	2.34	0.56
1:A:382:ASN:HD21	3:C:6:GLN:H	1.53	0.56
8:H:35:ILE:HD11	8:H:43:LYS:HB3	1.86	0.56
13:2M:137:MET:HG3	13:2M:265:ASN:HD21	1.69	0.56
15:4M:374:MET:HB3	15:4M:377:PHE:HB3	1.88	0.56
17:5M:380:ALA:O	17:5M:384:MET:HG3	2.04	0.56
43:G1:102:ASP:OD2	44:G2:86:ARG:NE	2.27	0.56
63:M:601:3PE:H2I3	10:W:28:GLY:HA3	1.87	0.56
29:AM:126:ASN:ND2	50:S5:40:ASP:OD1	2.38	0.56
4:D:109:SER:O	4:D:155:ARG:NH1	2.37	0.56
11:N:168:TYR:O	11:N:172:MET:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2M:158:SER:HB3	13:2M:161:SER:HB3	1.88	0.56
14:3M:61:TYR:OH	16:4L:74:ALA:O	2.24	0.56
28:AL:77:TYR:OH	53:S8:97:PRO:O	2.15	0.56
46:S1:203:VAL:H	46:S1:217:THR:HG22	1.70	0.56
46:S1:426:TYR:OH	46:S1:565:ASP:OD1	2.23	0.56
2:B:149:ILE:HD11	2:B:166:PHE:HZ	1.70	0.56
12:1M:79:VAL:O	12:1M:83:MET:HG3	2.06	0.56
13:2M:275:TYR:HB3	54:P1:49:ARG:HH21	1.69	0.56
17:5M:158:LEU:HD11	36:B8:55:TRP:CD1	2.40	0.56
24:A7:21:TRP:CD1	53:S8:85:LYS:HG3	2.41	0.56
46:S1:369:ILE:HD11	46:S1:617:VAL:HG11	1.88	0.56
1:A:114:THR:OG1	2:B:437:GLU:OE2	2.23	0.56
4:P:127:LYS:HG3	4:P:152:LEU:HD13	1.88	0.56
20:A2:4:ARG:NH2	20:A2:38:GLU:OE2	2.36	0.56
47:S2:110:ARG:NH2	47:S2:332:GLU:O	2.36	0.56
48:S3:33:THR:HG21	48:S3:41:LEU:HD22	1.87	0.56
46:S1:283:ALA:HA	53:S8:127:LYS:HE2	1.86	0.56
46:S1:306:ILE:HG12	46:S1:316:ILE:HG12	1.87	0.56
55:P4:42:GLU:O	55:P4:46:ARG:HG3	2.06	0.56
1:A:106:THR:HG22	1:A:279:ALA:HB3	1.87	0.55
9:J:16:LEU:O	9:J:20:VAL:HG22	2.06	0.55
12:1M:159:LEU:HD23	14:3M:81:ALA:HB3	1.88	0.55
17:5M:386:SER:O	17:5M:390:ILE:HG12	2.05	0.55
17:5M:449:PHE:CD2	30:AC:88:LYS:HD3	2.41	0.55
20:A2:35:ASN:O	20:A2:39:LEU:HG	2.06	0.55
45:L2:99:GLY:HA3	45:L2:120:ARG:HD2	1.88	0.55
45:L2:139:ILE:HG12	45:L2:156:ILE:HD12	1.87	0.55
46:S1:238:LEU:HD23	46:S1:250:GLY:HA2	1.88	0.55
57:V1:254:LYS:HE2	57:V1:258:PRO:HD3	1.87	0.55
15:4M:12:LEU:HD23	15:4M:135:CYS:HB3	1.88	0.55
15:4M:264:PHE:HE2	15:4M:324:PHE:HE2	1.53	0.55
22:A5:129:HIS:NE2	47:S2:87:GLU:OE1	2.28	0.55
47:S2:147:ARG:NH2	47:S2:174:ASP:OD2	2.39	0.55
52:S7:127:THR:HG22	52:S7:129:LYS:H	1.70	0.55
57:V1:232:TYR:HB3	57:V1:405:GLU:HB3	1.87	0.55
57:V1:302:LYS:HE2	57:V1:380:ALA:HB3	1.88	0.55
63:C:505:3PE:H222	61:C:506:CDL:HA31	1.89	0.55
1:M:104:VAL:HG21	1:M:289:VAL:HG22	1.89	0.55
15:4M:478:LEU:HB3	15:4M:482:HIS:HE1	1.70	0.55
26:A9:146:ARG:HH22	26:A9:326:PRO:HD3	1.71	0.55
46:S1:229:ALA:HA	46:S1:233:ALA:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:P1:54:TRP:CD1	54:P1:55:THR:HG23	2.41	0.55
24:A7:93:LYS:NZ	24:A7:97:GLU:OE1	2.39	0.55
43:G1:75:PRO:HD2	43:G1:96:SER:HB3	1.89	0.55
47:S2:132:LEU:HD22	52:S7:98:ALA:HA	1.89	0.55
47:S2:162:GLY:HA3	47:S2:288:LYS:HA	1.88	0.55
47:S2:184:SER:OG	47:S2:185:ARG:NH2	2.40	0.55
12:1M:107:LEU:HD22	12:1M:155:LEU:HD22	1.88	0.55
23:A6:62:ARG:NH2	31:AB:87:ASP:OD1	2.38	0.55
2:B:396:ILE:HG12	2:B:497:VAL:HG12	1.88	0.55
3:C:184:ARG:NH2	5:Q:137:MET:O	2.35	0.55
4:P:286:TYR:HD1	7:S:23:MET:HG3	1.72	0.55
13:2M:419:VAL:HB	15:4M:182:VAL:CG1	2.36	0.55
17:5M:454:LEU:HD21	32:B2:13:VAL:HG13	1.89	0.55
17:5M:561:LYS:HG3	36:B8:70:ALA:HB2	1.89	0.55
18:6M:3:LEU:HG	18:6M:7:PHE:CE2	2.41	0.55
46:S1:303:ASN:HD22	46:S1:319:ARG:NH2	2.05	0.55
46:S1:428:MET:HG3	46:S1:552:ASN:HB3	1.88	0.55
47:S2:25:SER:HB3	52:S7:86:LEU:HG	1.88	0.55
50:S5:23:GLU:OE1	50:S5:27:ARG:NH2	2.40	0.55
57:V1:335:VAL:HG21	57:V1:342:LEU:HB2	1.88	0.55
47:S2:298:SER:OG	53:S8:222:ARG:OXT	2.24	0.55
1:M:454:SER:OG	1:M:455:PRO:HD3	2.07	0.55
1:M:526:ARG:HB2	63:M:601:3PE:H241	1.89	0.55
12:1M:186:VAL:HA	12:1M:189:MET:HE3	1.88	0.55
17:5M:52:LEU:HD13	35:B7:45:PHE:HD2	1.72	0.55
22:A5:47:VAL:O	22:A5:54:ARG:NH1	2.34	0.55
46:S1:132:VAL:HB	46:S1:137:MET:HG3	1.89	0.55
1:A:98:LEU:HD22	1:A:102:LEU:HD23	1.89	0.55
11:N:115:SER:HB3	11:N:118:ALA:HB2	1.87	0.55
9:V:20:VAL:HG13	9:V:21:MET:HG3	1.89	0.55
12:1M:159:LEU:HD21	14:3M:82:VAL:HG23	1.89	0.55
13:2M:133:ASP:OD1	13:2M:134:LEU:N	2.40	0.55
17:5M:508:GLU:O	17:5M:512:ALA:HB3	2.06	0.55
26:A9:71:THR:HG1	66:A9:401:NDP:HO3A	1.55	0.55
43:G1:16:ARG:NH1	44:G2:27:SER:OG	2.38	0.55
46:S1:187:MET:HG3	47:S2:314:GLU:HG3	1.88	0.55
1:A:201:ARG:HH21	1:A:203:GLU:HG3	1.73	0.55
1:A:347:ASP:OD2	1:A:494:ARG:NH1	2.39	0.55
1:M:234:HIS:NE2	1:M:395:TYR:OH	2.33	0.55
13:2M:332:GLN:OE1	13:2M:401:TYR:OH	2.19	0.55
13:2M:452:ARG:NH2	41:C2:34:GLU:OE1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:3M:99:LEU:O	14:3M:103:THR:N	2.39	0.55
15:4M:11:ASP:N	15:4M:51:TYR:OH	2.35	0.55
47:S2:242:TYR:HA	47:S2:245:LEU:HD12	1.89	0.55
57:V1:108:MET:HE1	57:V1:282:ILE:HD11	1.89	0.55
26:A9:70:ALA:HB3	26:A9:91:VAL:HG13	1.89	0.54
28:AL:69:TYR:O	28:AL:72:HIS:ND1	2.39	0.54
2:B:185:ARG:NH1	2:B:280:LEU:O	2.40	0.54
1:M:104:VAL:HG12	1:M:277:ILE:HB	1.89	0.54
1:M:417:TYR:HA	1:M:517:TRP:HH2	1.72	0.54
12:1M:291:ARG:NH1	47:S2:377:ASP:OD1	2.41	0.54
26:A9:310:LYS:O	26:A9:314:THR:OG1	2.22	0.54
55:P4:31:HIS:O	55:P4:35:LYS:NZ	2.31	0.54
57:V1:94:LYS:HB2	57:V1:215:CYS:HB3	1.89	0.54
4:D:196:LEU:HB3	4:D:229:LEU:HD12	1.88	0.54
13:2M:390:ILE:HG22	13:2M:392:PRO:HD2	1.88	0.54
15:4M:312:SER:HA	15:4M:341:HIS:NE2	2.22	0.54
15:4M:334:SER:HA	15:4M:403:ILE:HD11	1.89	0.54
17:5M:15:PHE:HB2	17:5M:31:MET:HE1	1.88	0.54
17:5M:157:ARG:NH2	37:B9:90:GLY:O	2.38	0.54
18:6M:23:PRO:O	18:6M:27:VAL:HG23	2.08	0.54
18:6M:187:ALA:HB2	47:S2:204:VAL:HG11	1.89	0.54
23:A6:71:LYS:HE2	48:S3:96:THR:HG22	1.89	0.54
24:A7:76:ARG:NH2	46:S1:188:ALA:O	2.40	0.54
4:D:181:ILE:HG12	64:D:501:HEC:HMA3	1.89	0.54
52:S7:125:THR:HA	52:S7:153:CYS:HB3	1.89	0.54
57:V1:226:HIS:ND1	58:V2:60:TYR:OH	2.29	0.54
17:5M:475:LEU:HD21	32:B2:33:MET:HG3	1.89	0.54
3:C:341:LEU:HD21	7:G:55:THR:HG21	1.89	0.54
3:O:230:TYR:HB3	4:P:292:TRP:CE2	2.43	0.54
53:S8:213:GLU:OE1	53:S8:216:ARG:NH2	2.39	0.54
11:N:100:ILE:HD11	11:N:264:VAL:HG21	1.88	0.54
15:4M:411:ASN:HB3	15:4M:414:VAL:HG12	1.89	0.54
26:A9:60:VAL:HG12	26:A9:62:GLY:H	1.71	0.54
46:S1:92:VAL:HG13	46:S1:145:ILE:HD13	1.90	0.54
48:S3:18:TRP:HB3	48:S3:37:TYR:HD1	1.73	0.54
3:C:90:ASN:O	3:C:94:MET:HG2	2.08	0.54
47:S2:72:TYR:CD2	52:S7:88:CYS:HB3	2.43	0.54
48:S3:181:ALA:HB3	49:S4:61:LYS:HD3	1.90	0.54
1:A:320:SER:O	1:A:502:ALA:HA	2.07	0.54
1:M:525:ASN:O	9:V:24:ASN:ND2	2.32	0.54
13:2M:65:LEU:HB3	13:2M:78:ARG:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2M:374:PRO:O	13:2M:378:ILE:HD12	2.07	0.54
17:5M:458:ASP:OD1	17:5M:459:ALA:N	2.34	0.54
26:A9:48:HIS:NE2	46:S1:361:ASN:OD1	2.31	0.54
57:V1:347:PRO:HA	57:V1:382:VAL:HG12	1.89	0.54
11:N:454:PRO:HG2	11:N:457:GLN:HG3	1.90	0.54
13:2M:359:ARG:O	40:FD:83:ARG:NH2	2.40	0.54
15:4M:304:LEU:HD23	15:4M:432:LEU:HD11	1.89	0.54
17:5M:1:MET:HG3	17:5M:42:LEU:HD22	1.90	0.54
45:L2:150:LEU:HB2	45:L2:167:ILE:HG12	1.90	0.54
51:S6:46:PRO:HB3	53:S8:120:GLU:HA	1.89	0.54
17:5M:302:ILE:HG23	17:5M:432:TYR:HE2	1.73	0.53
47:S2:181:GLN:O	47:S2:185:ARG:HG2	2.07	0.53
4:D:285:ALA:HB2	61:D:502:CDL:HB62	1.90	0.53
1:M:321:GLU:HG2	1:M:515:TYR:HB2	1.90	0.53
13:2M:248:THR:HA	13:2M:251:THR:HG22	1.90	0.53
30:AC:76:ASN:ND2	30:AC:100:ASP:OD1	2.41	0.53
47:S2:112:LEU:HD23	47:S2:138:ARG:HG2	1.90	0.53
47:S2:137:GLU:OE1	47:S2:181:GLN:NE2	2.28	0.53
11:N:327:VAL:HA	11:N:465:ILE:HD12	1.88	0.53
11:N:353:ARG:HG3	11:N:357:ARG:HD2	1.89	0.53
4:P:78:PRO:O	9:V:57:LYS:NZ	2.41	0.53
4:P:85:SER:HB3	9:V:50:TRP:CZ2	2.43	0.53
12:1M:26:ALA:HB2	19:A1:11:PRO:HB2	1.90	0.53
18:6M:189:ASP:OD1	18:6M:190:PHE:N	2.41	0.53
24:A7:37:PRO:HB2	24:A7:42:TYR:HB2	1.89	0.53
35:B7:10:MET:HG2	36:B8:114:TYR:HE1	1.74	0.53
51:S6:83:ASP:HB3	58:V2:27:ALA:HB2	1.90	0.53
57:V1:444:THR:HG21	57:V1:464:GLN:HB2	1.90	0.53
23:A6:39:MET:SD	23:A6:48:THR:HG21	2.49	0.53
23:A6:60:GLU:HA	23:A6:63:LYS:HE3	1.90	0.53
47:S2:70:LEU:O	47:S2:78:GLN:NE2	2.41	0.53
44:G2:144:PHE:HB3	44:G2:162:MET:HG3	1.91	0.53
46:S1:224:ARG:HG2	46:S1:268:ILE:HD12	1.90	0.53
63:O:405:3PE:H112	4:P:80:LYS:HG3	1.91	0.53
23:A6:49:SER:O	23:A6:52:GLN:N	2.41	0.53
45:L2:168:LEU:HA	45:L2:186:VAL:HG22	1.90	0.53
12:1M:89:TRP:HZ2	12:1M:237:ILE:HG22	1.74	0.53
17:5M:167:ALA:HA	17:5M:241:TRP:HB2	1.90	0.53
30:AC:86:GLU:OE1	33:B3:14:ARG:NH2	2.41	0.53
31:AB:111:ILE:HG22	31:AB:111:ILE:O	2.09	0.53
1:M:126:ARG:HG3	1:M:242:PRO:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2M:77:ARG:NH1	13:2M:77:ARG:HB3	2.24	0.53
57:V1:298:ASN:ND2	57:V1:368:ASP:H	2.07	0.53
2:B:218:GLU:OE2	2:B:233:LEU:N	2.42	0.53
46:S1:470:VAL:HG13	46:S1:483:HIS:HA	1.90	0.53
53:S8:159:MET:HB2	53:S8:193:LEU:HD22	1.91	0.53
1:A:505:ALA:HB1	1:A:509:ILE:HG21	1.90	0.53
3:C:172:TRP:O	3:C:181:THR:OG1	2.28	0.53
17:5M:134:LEU:HD23	17:5M:192:VAL:HG21	1.90	0.53
18:6M:4:SER:HA	18:6M:7:PHE:CZ	2.44	0.53
46:S1:497:ALA:HA	46:S1:537:ILE:HG12	1.91	0.53
46:S1:206:LYS:O	46:S1:214:THR:OG1	2.23	0.52
48:S3:52:ARG:HG3	48:S3:82:TYR:HE2	1.74	0.52
4:P:191:TYR:OH	64:P:501:HEC:O2A	2.27	0.52
46:S1:444:VAL:HG21	46:S1:493:LEU:HD22	1.91	0.52
46:S1:557:HIS:HB2	46:S1:560:GLN:HB2	1.91	0.52
48:S3:126:HIS:ND1	48:S3:128:ASP:O	2.42	0.52
6:F:108:ARG:NE	6:F:114:LEU:O	2.28	0.52
15:4M:225:ALA:HB1	15:4M:230:MET:HG3	1.92	0.52
17:5M:544:ARG:HH11	17:5M:548:THR:HG23	1.75	0.52
20:A2:35:ASN:HA	20:A2:38:GLU:HG2	1.91	0.52
40:FD:42:ASP:O	40:FD:140:HIS:NE2	2.33	0.52
46:S1:288:LEU:HB3	46:S1:307:ASP:HB3	1.92	0.52
47:S2:139:GLU:OE1	47:S2:152:ARG:NH1	2.43	0.52
49:S4:29:GLU:HA	49:S4:32:MET:HG2	1.91	0.52
13:2M:291:MET:HB3	13:2M:421:THR:HG21	1.90	0.52
43:G1:78:SER:HG	43:G1:80:TRP:HE1	1.57	0.52
46:S1:490:PRO:HB3	46:S1:530:ILE:HD11	1.91	0.52
1:A:198:GLN:NE2	1:A:296:PHE:HA	2.21	0.52
15:4M:300:ARG:NH1	17:5M:578:LEU:O	2.41	0.52
17:5M:110:SER:O	17:5M:114:MET:HG2	2.09	0.52
46:S1:430:THR:HG22	46:S1:434:GLY:HA3	1.92	0.52
46:S1:725:MET:HB3	46:S1:731:ARG:HG3	1.91	0.52
48:S3:176:ARG:O	53:S8:136:GLN:NE2	2.41	0.52
57:V1:309:HIS:HE1	57:V1:389:THR:HB	1.72	0.52
2:B:358:LEU:HD13	2:B:372:ILE:HG12	1.91	0.52
4:D:73:PRO:HG3	8:H:57:ASP:HB3	1.91	0.52
11:N:137:ARG:NH1	11:N:141:GLU:OE2	2.43	0.52
15:4M:389:MET:HE2	15:4M:430:LEU:HG	1.92	0.52
5:E:120:PHE:CE1	9:J:31:VAL:HA	2.41	0.52
3:O:56:LEU:HD13	62:O:402:HEM:HBA1	1.91	0.52
17:5M:302:ILE:HG23	17:5M:432:TYR:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:G1:169:VAL:HG11	43:G1:175:ILE:HD11	1.90	0.52
47:S2:185:ARG:NH2	47:S2:188:GLU:OE2	2.28	0.52
1:M:305:THR:HG23	1:M:308:GLN:H	1.75	0.52
12:1M:21:ALA:HB1	12:1M:51:PRO:HB3	1.91	0.52
16:4L:59:GLN:NE2	18:6M:136:ASN:OD1	2.37	0.52
26:A9:178:SER:HA	26:A9:194:LYS:HE3	1.91	0.52
46:S1:192:ASP:HA	47:S2:311:HIS:NE2	2.24	0.52
58:V2:46:THR:HG22	58:V2:47:GLU:H	1.75	0.52
3:O:94:MET:HE1	3:O:245:PHE:HD2	1.74	0.52
4:P:302:LEU:HD21	6:R:67:LYS:HD3	1.92	0.52
15:4M:129:LEU:O	15:4M:133:VAL:HG23	2.09	0.52
15:4M:479:ASP:HA	15:4M:482:HIS:HD1	1.74	0.52
17:5M:448:SER:O	33:B3:18:ARG:NH2	2.43	0.52
18:6M:182:VAL:HG21	47:S2:201:GLN:HG2	1.91	0.52
24:A7:26:PRO:HD3	47:S2:191:GLU:HG3	1.91	0.52
26:A9:319:LEU:O	26:A9:323:VAL:HG22	2.10	0.52
50:S5:7:ILE:HG23	50:S5:8:THR:HG23	1.92	0.52
4:D:283:GLN:HE21	5:E:115:LEU:HA	1.73	0.52
1:M:526:ARG:HD3	63:M:601:3PE:H221	1.92	0.52
11:N:355:TYR:O	11:N:360:ASN:ND2	2.37	0.52
7:S:21:LYS:HG2	60:S:101:PC1:H111	1.91	0.52
15:4M:264:PHE:HE2	15:4M:324:PHE:CE2	2.28	0.52
44:G2:99:ASN:OD1	44:G2:127:THR:HA	2.09	0.52
47:S2:133:TRP:CZ2	53:S8:86:TYR:HD2	2.28	0.52
49:S4:131:TYR:CE2	49:S4:135:PHE:HE1	2.27	0.52
49:S4:141:PRO:HB3	58:V2:62:SER:HB2	1.91	0.52
2:B:104:ILE:HD12	2:B:176:MET:HE2	1.91	0.51
2:B:425:LYS:HD3	2:B:467:ASP:HA	1.90	0.51
2:B:444:GLU:OE2	2:B:448:ARG:NH1	2.42	0.51
3:C:62:PRO:HD2	3:O:62:PRO:HD2	1.92	0.51
4:D:136:VAL:HG12	4:D:147:THR:HG22	1.93	0.51
11:N:109:ILE:HG13	11:N:110:TYR:N	2.24	0.51
3:O:103:ILE:HG12	62:O:403:HEM:HAC	1.92	0.51
4:P:283:GLN:HE21	5:Q:115:LEU:HA	1.75	0.51
23:A6:44:LEU:O	23:A6:48:THR:OG1	2.22	0.51
52:S7:92:GLU:OE2	52:S7:187:ALA:N	2.43	0.51
2:B:362:VAL:HG11	2:B:372:ILE:HD13	1.92	0.51
12:1M:31:MET:HG2	12:1M:285:ALA:HB2	1.93	0.51
13:2M:36:TYR:HB2	44:G2:250:ARG:HH21	1.75	0.51
24:A7:38:LEU:HB2	24:A7:41:GLU:HG2	1.91	0.51
31:AB:92:VAL:HG11	31:AB:108:ALA:HB1	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:P2:80:SER:HB2	42:P2:85:ARG:HH12	1.75	0.51
44:G2:55:VAL:HB	44:G2:59:VAL:HG11	1.92	0.51
44:G2:221:SER:OG	44:G2:222:TYR:N	2.43	0.51
52:S7:159:TYR:CD1	53:S8:163:ILE:HG21	2.45	0.51
11:N:328:LEU:HD11	11:N:381:PHE:HB2	1.92	0.51
5:Q:120:PHE:CE1	9:V:31:VAL:HA	2.45	0.51
17:5M:313:TYR:OH	17:5M:562:ARG:HG2	2.10	0.51
22:A5:111:VAL:HG21	24:A7:88:LYS:HG3	1.92	0.51
22:A5:131:PRO:HD3	47:S2:84:LEU:HD13	1.92	0.51
43:G1:46:MET:HB3	43:G1:68:LEU:HD23	1.92	0.51
2:B:216:LEU:HD11	2:B:312:HIS:HB3	1.91	0.51
11:N:147:GLY:HA2	11:N:163:ASP:O	2.11	0.51
4:P:276:VAL:HG12	5:Q:121:VAL:HG13	1.93	0.51
46:S1:209:GLY:HA2	46:S1:256:LEU:HD23	1.92	0.51
46:S1:372:ILE:HG21	46:S1:600:PHE:CG	2.44	0.51
46:S1:538:ALA:HB2	46:S1:551:LEU:HD21	1.92	0.51
57:V1:325:LYS:O	57:V1:329:GLU:HG2	2.10	0.51
3:C:230:TYR:O	4:D:292:TRP:NE1	2.34	0.51
13:2M:369:LEU:HB3	13:2M:436:MET:HG2	1.91	0.51
23:A6:44:LEU:O	23:A6:44:LEU:HD23	2.10	0.51
26:A9:237:ILE:HD11	26:A9:288:ALA:HB1	1.93	0.51
28:AL:38:LEU:O	28:AL:42:LYS:HG2	2.10	0.51
28:AL:154:SER:O	46:S1:356:ARG:NH2	2.43	0.51
59:X1:14:PRO:HG2	59:X1:95:VAL:HG21	1.92	0.51
7:S:29:ASP:HB3	7:S:32:THR:HG22	1.93	0.51
17:5M:405:LEU:HD11	17:5M:427:VAL:HG21	1.93	0.51
35:B7:77:ARG:NH2	36:B8:105:ILE:O	2.31	0.51
3:O:172:TRP:O	3:O:181:THR:OG1	2.27	0.51
43:G1:90:ASN:H	43:G1:108:VAL:HG11	1.76	0.51
43:G1:227:PHE:HB2	45:L2:54:TRP:HZ3	1.76	0.51
44:G2:79:ILE:HG22	44:G2:83:CYS:HG	1.74	0.51
1:A:126:ARG:HG3	1:A:242:PRO:HB2	1.91	0.51
3:C:59:HIS:HB2	3:C:74:VAL:HG22	1.92	0.51
3:C:207:LEU:HD23	62:C:503:HEM:HAA1	1.93	0.51
3:O:331:ILE:HD11	63:R:201:3PE:H2A1	1.92	0.51
13:2M:340:ILE:HD12	13:2M:394:ALA:HB1	1.93	0.51
47:S2:67:PHE:HA	47:S2:70:LEU:HD12	1.93	0.51
57:V1:413:CYS:CB	70:V1:502:SF4:S3	2.91	0.51
3:C:135:PHE:O	3:C:139:VAL:HG23	2.11	0.51
12:1M:171:VAL:HA	12:1M:174:GLN:HG3	1.93	0.51
13:2M:226:SER:HB3	13:2M:266:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:G1:27:SER:OG	43:G1:32:ASN:O	2.24	0.51
2:B:108:VAL:HG12	2:B:110:CYS:H	1.76	0.50
3:O:94:MET:HE1	3:O:245:PHE:CD2	2.46	0.50
13:2M:230:ILE:O	13:2M:316:VAL:HG11	2.11	0.50
13:2M:469:PHE:O	15:4M:74:TRP:NE1	2.26	0.50
43:G1:128:VAL:O	43:G1:128:VAL:HG12	2.11	0.50
46:S1:117:ASN:OD1	46:S1:223:THR:OG1	2.24	0.50
46:S1:174:CYS:O	46:S1:284:ARG:NH1	2.41	0.50
6:F:91:ARG:NH2	1:M:43:PRO:O	2.34	0.50
19:A1:19:LEU:O	19:A1:22:MET:HG2	2.11	0.50
22:A5:134:ARG:HD2	47:S2:238:PRO:HD2	1.92	0.50
25:A8:60:VAL:HG21	29:AM:88:VAL:HB	1.93	0.50
27:AK:132:ILE:HG22	27:AK:137:GLN:HG2	1.94	0.50
47:S2:125:VAL:HG13	47:S2:202:ARG:HE	1.76	0.50
1:A:472:PRO:HG2	1:A:475:GLU:HB3	1.94	0.50
2:B:90:VAL:HG11	2:B:281:LEU:HD13	1.92	0.50
8:H:28:TYR:CZ	8:H:32:ILE:HD11	2.46	0.50
13:2M:135:ILE:HG23	16:4L:61:PHE:HD1	1.76	0.50
13:2M:351:ILE:HG23	13:2M:376:LEU:HD11	1.92	0.50
46:S1:187:MET:SD	47:S2:311:HIS:ND1	2.76	0.50
47:S2:58:LYS:HD2	47:S2:66:TYR:HE2	1.76	0.50
48:S3:18:TRP:HB3	48:S3:37:TYR:CD1	2.47	0.50
58:V2:149:VAL:HG11	58:V2:155:THR:HA	1.92	0.50
2:B:125:LEU:HD11	2:B:198:LEU:HD21	1.93	0.50
20:A2:50:ILE:HG21	46:S1:699:LEU:HD12	1.93	0.50
38:BJ:56:ARG:O	38:BJ:60:ARG:HG3	2.12	0.50
38:BJ:84:ILE:HG13	38:BJ:85:GLY:N	2.26	0.50
45:L2:148:TYR:HD2	45:L2:165:HIS:CE1	2.29	0.50
1:A:525:ASN:O	9:J:24:ASN:ND2	2.38	0.50
3:O:339:CYS:HB3	61:O:404:CDL:H191	1.93	0.50
26:A9:145:THR:HA	26:A9:320:LEU:HD11	1.92	0.50
32:B2:19:LYS:HB2	32:B2:22:HIS:CD2	2.46	0.50
38:BJ:26:ASP:HB3	38:BJ:29:ALA:HB3	1.93	0.50
48:S3:21:LYS:HG3	48:S3:32:ASP:HB3	1.91	0.50
50:S5:31:PRO:HD3	54:P1:54:TRP:CH2	2.45	0.50
15:4M:262:TYR:OH	15:4M:266:ARG:NE	2.44	0.50
16:4L:37:LEU:HG	18:6M:30:PHE:HE1	1.77	0.50
17:5M:424:SER:HB3	17:5M:524:PHE:HE2	1.77	0.50
17:5M:493:TRP:O	17:5M:496:SER:OG	2.28	0.50
22:A5:21:VAL:HG13	47:S2:210:THR:HA	1.93	0.50
25:A8:23:LYS:HE3	25:A8:105:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A9:305:PRO:HB2	26:A9:307:PRO:HD2	1.94	0.50
30:AC:45:LEU:HD11	30:AC:61:PRO:HD3	1.94	0.50
53:S8:103:LEU:HD11	53:S8:183:PHE:HE1	1.76	0.50
53:S8:172:CYS:SG	53:S8:176:ALA:N	2.76	0.50
2:B:92:VAL:HG22	2:B:263:LEU:HD12	1.93	0.50
18:6M:49:PHE:HD2	18:6M:136:ASN:HD21	1.60	0.50
26:A9:180:LEU:HD22	26:A9:214:ALA:HB2	1.93	0.50
57:V1:148:SER:HB3	57:V1:232:TYR:HD1	1.77	0.50
1:A:448:LEU:HD22	2:B:439:ARG:NH2	2.26	0.50
4:P:196:LEU:HD11	64:P:501:HEC:HMB2	1.93	0.50
4:P:225:MET:HB3	64:P:501:HEC:C1D	2.41	0.50
14:3M:61:TYR:O	14:3M:65:ILE:HG12	2.11	0.50
15:4M:228:VAL:HG23	15:4M:316:MET:HB3	1.93	0.50
17:5M:645:LEU:O	17:5M:649:VAL:HG12	2.12	0.50
1:A:397:ASP:OD1	1:A:397:ASP:N	2.43	0.50
3:O:314:PHE:HB3	3:O:317:MET:HE1	1.93	0.50
13:2M:357:GLN:HG2	13:2M:448:GLU:HB2	1.94	0.50
15:4M:143:TYR:CZ	15:4M:185:LEU:HB2	2.47	0.50
17:5M:516:ILE:O	17:5M:520:ILE:HG13	2.12	0.50
26:A9:101:ARG:HG2	52:S7:175:PRO:HB2	1.94	0.50
50:S5:11:LYS:HD2	50:S5:15:TYR:HD2	1.77	0.50
1:A:88:LEU:HD22	1:A:473:PHE:HB3	1.94	0.49
3:C:178:ASP:OD1	3:C:179:ASN:N	2.45	0.49
3:O:85:ARG:HH12	62:O:402:HEM:CGD	2.25	0.49
18:6M:85:ARG:NH2	18:6M:86:TYR:OH	2.45	0.49
38:BJ:79:GLU:OE1	38:BJ:82:ARG:NH2	2.45	0.49
1:A:433:ASP:OD1	1:A:434:ASP:N	2.45	0.49
2:B:94:SER:HA	2:B:265:ALA:HB3	1.94	0.49
4:D:269:MET:HG2	4:D:273:TRP:CD1	2.47	0.49
1:M:225:THR:HA	1:M:228:VAL:HG12	1.93	0.49
1:M:411:CYS:SG	3:O:4:ARG:NH2	2.85	0.49
3:O:204:LEU:HD13	62:O:403:HEM:HMA3	1.94	0.49
38:BJ:61:ILE:O	56:C1:63:HIS:NE2	2.42	0.49
40:FD:76:LEU:HD23	40:FD:76:LEU:H	1.77	0.49
46:S1:596:PRO:HG2	46:S1:599:ALA:HB2	1.94	0.49
2:B:238:SER:O	2:B:242:ARG:HG2	2.13	0.49
3:C:130:MET:HG2	3:C:196:LEU:HD21	1.94	0.49
28:AL:54:ASP:OD1	28:AL:58:ASN:N	2.46	0.49
29:AM:52:ALA:O	29:AM:56:THR:OG1	2.28	0.49
52:S7:192:TYR:HB2	53:S8:96:TYR:OH	2.12	0.49
11:N:262:ALA:HB2	11:N:439:SER:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:25:LEU:O	8:T:29:GLN:HG2	2.11	0.49
18:6M:12:VAL:HG21	55:P4:11:THR:HA	1.94	0.49
46:S1:682:ARG:HE	46:S1:689:VAL:HG21	1.77	0.49
47:S2:161:GLY:O	47:S2:289:ALA:N	2.45	0.49
47:S2:356:ARG:HG3	48:S3:58:ASP:HB3	1.94	0.49
11:N:337:GLY:HA3	11:N:369:SER:HA	1.94	0.49
13:2M:391:PRO:HA	13:2M:396:PHE:CD2	2.46	0.49
15:4M:391:LEU:HD12	15:4M:392:PRO:HD2	1.94	0.49
15:4M:395:SER:HB3	15:4M:470:MET:HB3	1.94	0.49
17:5M:21:ARG:HB2	39:BK:44:PRO:HB3	1.93	0.49
43:G1:218:ASN:O	43:G1:218:ASN:ND2	2.43	0.49
46:S1:346:ASN:HB3	46:S1:648:VAL:HG12	1.95	0.49
47:S2:341:PHE:HB3	47:S2:354:LYS:HB3	1.93	0.49
49:S4:79:LEU:HG	49:S4:80:MET:HG2	1.95	0.49
1:A:88:LEU:HD11	1:A:477:PHE:CD2	2.48	0.49
3:C:101:LEU:HD23	63:C:505:3PE:H382	1.93	0.49
11:N:462:VAL:O	11:N:465:ILE:HG22	2.12	0.49
5:Q:148:SER:O	5:Q:148:SER:OG	2.30	0.49
14:3M:87:ILE:HG22	18:6M:146:THR:HG23	1.94	0.49
17:5M:162:LYS:NZ	36:B8:64:PRO:O	2.41	0.49
24:A7:43:ARG:HD3	28:AL:69:TYR:OH	2.12	0.49
24:A7:69:TYR:CE2	47:S2:293:LYS:HG3	2.47	0.49
44:G2:151:LEU:HB3	44:G2:155:VAL:HG11	1.93	0.49
54:P1:21:GLU:OE2	54:P1:24:ARG:NH2	2.40	0.49
59:X1:57:ILE:O	59:X1:57:ILE:HG13	2.13	0.49
1:A:417:TYR:HA	1:A:517:TRP:HH2	1.77	0.49
1:A:498:ASP:OD1	1:A:519:ARG:NH1	2.36	0.49
3:C:329:GLN:NE2	6:F:27:ARG:HH12	2.11	0.49
3:O:364:VAL:HG13	63:R:201:3PE:H2I3	1.94	0.49
16:4L:50:SER:HB2	16:4L:58:GLY:HA3	1.94	0.49
20:A2:40:LYS:HG2	20:A2:48:ILE:HD12	1.95	0.49
22:A5:20:ILE:HG22	22:A5:23:LEU:H	1.77	0.49
44:G2:70:ASP:HB3	44:G2:91:SER:HA	1.95	0.49
53:S8:89:GLU:O	53:S8:91:LYS:NZ	2.30	0.49
15:4M:184:MET:HB2	15:4M:223:ALA:CB	2.43	0.49
17:5M:586:PHE:HA	17:5M:590:ASP:HB2	1.95	0.49
25:A8:51:ASP:N	25:A8:51:ASP:OD1	2.45	0.49
52:S7:92:GLU:HG2	52:S7:185:PRO:O	2.12	0.49
58:V2:138:GLY:O	58:V2:141:GLU:HG3	2.12	0.49
2:B:202:LYS:HG3	2:B:240:ILE:HG21	1.94	0.49
3:C:123:GLY:HA3	62:C:503:HEM:HBC2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:276:VAL:HG12	5:E:121:VAL:HG13	1.94	0.49
1:M:87:ILE:HG22	11:N:96:PRO:HB3	1.95	0.49
3:O:135:PHE:O	3:O:139:VAL:HG23	2.13	0.49
15:4M:253:ALA:HB1	15:4M:345:LEU:HD13	1.93	0.49
47:S2:373:HIS:HB3	47:S2:377:ASP:HB2	1.94	0.49
48:S3:183:PRO:HB2	49:S4:58:GLY:HA3	1.94	0.49
4:P:73:PRO:HG3	8:T:57:ASP:HB3	1.94	0.49
13:2M:438:PHE:CZ	15:4M:158:GLY:HA3	2.48	0.49
15:4M:327:ASN:ND2	15:4M:409:GLN:OE1	2.46	0.49
15:4M:485:VAL:O	15:4M:489:VAL:HG23	2.13	0.49
38:BJ:75:ASN:O	38:BJ:79:GLU:HG2	2.12	0.49
46:S1:423:ARG:O	46:S1:427:ILE:HG12	2.12	0.49
47:S2:118:LEU:HD22	47:S2:261:TYR:HD1	1.77	0.49
1:A:117:VAL:HG21	1:A:186:VAL:HG13	1.95	0.48
1:M:183:ASP:N	1:M:183:ASP:OD1	2.45	0.48
15:4M:276:THR:O	15:4M:280:THR:OG1	2.22	0.48
15:4M:411:ASN:ND2	34:B4:52:ILE:HG23	2.28	0.48
15:4M:411:ASN:OD1	34:B4:55:GLU:HG2	2.12	0.48
29:AM:25:PRO:HG3	47:S2:279:LEU:O	2.12	0.48
30:AC:94:LYS:O	30:AC:98:LYS:HG2	2.13	0.48
36:B8:118:ARG:HG2	36:B8:123:GLY:HA3	1.95	0.48
46:S1:659:ARG:NH1	46:S1:663:GLU:OE1	2.25	0.48
48:S3:60:CYS:SG	48:S3:61:GLY:N	2.86	0.48
49:S4:80:MET:HG3	53:S8:194:LEU:HD23	1.94	0.48
2:B:339:LEU:HD21	2:B:410:VAL:HG21	1.94	0.48
12:1M:141:ALA:HA	12:1M:144:MET:HE3	1.95	0.48
12:1M:168:SER:HA	12:1M:251:TRP:HH2	1.78	0.48
15:4M:184:MET:HB2	15:4M:223:ALA:HB2	1.94	0.48
29:AM:37:ARG:HB3	47:S2:269:ARG:CZ	2.43	0.48
43:G1:121:ILE:HB	43:G1:138:THR:HG23	1.94	0.48
47:S2:363:LEU:HD13	47:S2:387:ILE:HG13	1.96	0.48
51:S6:63:VAL:HG13	51:S6:82:LEU:HD11	1.95	0.48
6:F:91:ARG:NH1	1:M:51:ASP:OD2	2.47	0.48
12:1M:34:VAL:HG13	53:S8:83:THR:HG23	1.94	0.48
20:A2:22:SER:O	20:A2:29:ARG:NH2	2.47	0.48
37:B9:58:ASP:HB3	37:B9:61:THR:HG22	1.95	0.48
46:S1:179:GLU:HB3	46:S1:285:ASN:ND2	2.21	0.48
51:S6:75:HIS:CD2	51:S6:92:TYR:HB3	2.49	0.48
3:C:159:ALA:HB1	3:C:295:SER:HA	1.95	0.48
4:D:305:VAL:O	6:F:87:GLN:NE2	2.46	0.48
63:M:601:3PE:H271	61:M:602:CDL:H511	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:123:GLY:HA3	62:O:403:HEM:HBC2	1.95	0.48
12:1M:282:TRP:CZ2	53:S8:84:LEU:HB2	2.49	0.48
17:5M:661:SER:HB2	27:AK:70:PHE:HZ	1.78	0.48
30:AC:69:LEU:HD23	30:AC:69:LEU:H	1.77	0.48
47:S2:200:LYS:O	47:S2:204:VAL:HG22	2.13	0.48
2:B:190:LEU:HD13	2:B:192:TRP:CZ2	2.49	0.48
12:1M:40:PRO:HA	52:S7:105:ARG:HA	1.95	0.48
17:5M:51:ALA:HB1	17:5M:492:PHE:CE1	2.49	0.48
20:A2:53:CYS:SG	20:A2:54:SER:N	2.86	0.48
21:A3:12:VAL:HG21	53:S8:57:SER:HB3	1.94	0.48
26:A9:265:ASP:HB3	26:A9:268:THR:HG22	1.95	0.48
26:A9:369:VAL:HB	26:A9:372:LEU:HD12	1.96	0.48
27:AK:148:ALA:HA	54:P1:49:ARG:HB3	1.96	0.48
28:AL:123:LEU:HD22	28:AL:130:TYR:HB3	1.95	0.48
30:AC:71:LEU:HB3	30:AC:75:ASP:HB2	1.96	0.48
46:S1:366:LEU:HD22	46:S1:661:LEU:HB2	1.96	0.48
1:M:120:TRP:CZ2	1:M:458:GLU:HA	2.48	0.48
11:N:194:LEU:HD22	11:N:236:LEU:HG	1.94	0.48
4:P:126:VAL:HA	4:P:129:MET:HG2	1.94	0.48
13:2M:136:ALA:HB2	18:6M:151:TRP:HE1	1.78	0.48
15:4M:425:GLY:HA2	15:4M:428:TYR:CE2	2.48	0.48
17:5M:190:GLN:O	38:BJ:52:ARG:NH1	2.47	0.48
26:A9:144:GLU:HG3	26:A9:150:PHE:CE2	2.48	0.48
43:G1:94:ILE:HG23	43:G1:98:THR:HG21	1.94	0.48
47:S2:87:GLU:HG2	47:S2:92:CYS:SG	2.54	0.48
58:V2:74:ASP:O	58:V2:78:GLN:HG3	2.13	0.48
58:V2:151:ARG:NH1	58:V2:164:GLU:HG2	2.27	0.48
2:B:470:THR:HG23	2:B:473:ASP:H	1.78	0.48
1:M:450:ILE:O	1:M:455:PRO:HB2	2.14	0.48
17:5M:356:ILE:HG23	17:5M:361:ASP:HA	1.95	0.48
35:B7:42:GLN:NE2	35:B7:46:TYR:OH	2.43	0.48
44:G2:59:VAL:O	45:L2:51:ARG:NH2	2.46	0.48
44:G2:144:PHE:HD2	44:G2:200:ILE:HG12	1.78	0.48
54:P1:81:ASP:OD1	54:P1:84:GLN:NE2	2.38	0.48
11:N:138:ILE:HD13	11:N:175:LEU:HD11	1.96	0.48
17:5M:96:VAL:HG21	17:5M:255:LEU:HB2	1.96	0.48
26:A9:305:PRO:HG2	26:A9:308:ILE:HG12	1.95	0.48
28:AL:91:GLU:HG3	28:AL:92:TRP:CD1	2.49	0.48
46:S1:441:PHE:HB2	46:S1:470:VAL:HG23	1.96	0.48
47:S2:182:PHE:CE2	47:S2:186:ILE:HD11	2.49	0.48
53:S8:139:THR:HB	53:S8:156:ASP:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:V1:82:LYS:HD3	57:V1:82:LYS:HA	1.71	0.48
1:A:305:THR:HG23	1:A:308:GLN:H	1.79	0.48
61:A:602:CDL:H141	3:C:24:ILE:HD11	1.95	0.48
13:2M:135:ILE:HD12	18:6M:151:TRP:CZ3	2.49	0.48
15:4M:130:MET:CE	15:4M:259:LEU:HD12	2.44	0.48
17:5M:232:LYS:HG2	17:5M:264:ALA:HB3	1.96	0.48
35:B7:74:GLN:O	35:B7:78:GLU:HG2	2.14	0.48
1:A:271:THR:O	1:A:275:MET:HG3	2.14	0.48
3:C:138:TYR:O	3:C:141:PRO:HD2	2.14	0.48
3:C:350:VAL:O	3:C:350:VAL:HG12	2.13	0.48
6:F:88:THR:HG23	6:F:88:THR:O	2.14	0.48
9:V:21:MET:HB3	9:V:21:MET:HE2	1.70	0.48
13:2M:28:PHE:CZ	59:X1:60:PRO:HB3	2.48	0.48
43:G1:101:GLN:HB2	43:G1:130:HIS:HA	1.95	0.48
44:G2:80:TRP:CD1	44:G2:101:GLN:HA	2.49	0.48
45:L2:140:GLU:HG3	45:L2:141:ARG:H	1.78	0.48
47:S2:62:GLN:O	52:S7:159:TYR:OH	2.32	0.48
52:S7:84:PHE:CE2	52:S7:134:LEU:HD12	2.49	0.48
52:S7:105:ARG:HD2	53:S8:93:THR:HG21	1.96	0.48
57:V1:255:PRO:HB2	57:V1:256:PRO:HD3	1.96	0.48
59:X1:93:ASP:OD1	59:X1:93:ASP:N	2.44	0.48
1:A:133:ASN:HB3	1:A:250:PRO:HD2	1.96	0.47
12:1M:124:ALA:HB1	12:1M:220:TYR:HE2	1.79	0.47
17:5M:250:THR:HG21	17:5M:353:GLY:HA3	1.95	0.47
17:5M:459:ALA:O	32:B2:22:HIS:HE1	1.97	0.47
51:S6:34:THR:HA	51:S6:37:TRP:NE1	2.29	0.47
52:S7:151:GLY:O	52:S7:155:ASN:ND2	2.46	0.47
60:A:601:PC1:H221	61:C:501:CDL:HB32	1.96	0.47
2:B:88:ASN:HD21	2:B:282:SER:HA	1.79	0.47
1:M:117:VAL:HG21	1:M:186:VAL:HG13	1.96	0.47
1:M:252:GLN:HA	1:M:255:LYS:NZ	2.28	0.47
3:O:75:MET:SD	3:O:85:ARG:HD2	2.55	0.47
13:2M:44:GLY:HA2	13:2M:115:ILE:HG21	1.96	0.47
15:4M:145:PHE:O	15:4M:149:VAL:HG23	2.15	0.47
16:4L:27:ASN:ND2	18:6M:79:ILE:HD12	2.29	0.47
17:5M:226:PHE:O	17:5M:230:VAL:HG23	2.15	0.47
1:M:319:GLY:HA3	1:M:500:ASP:HB3	1.95	0.47
63:M:601:3PE:H2G1	10:W:25:ALA:HA	1.95	0.47
3:O:317:MET:SD	3:O:376:GLY:HA3	2.54	0.47
5:Q:114:VAL:HG22	60:S:101:PC1:H252	1.96	0.47
12:1M:270:SER:O	12:1M:274:ILE:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1M:318:SER:HB3	12:1M:324:LEU:HD13	1.96	0.47
28:AL:116:GLY:HA2	53:S8:205:ASP:HB3	1.95	0.47
49:S4:40:HIS:HB3	49:S4:89:TYR:HE2	1.80	0.47
6:F:110:ALA:O	1:M:78:ARG:NH2	2.46	0.47
13:2M:139:LEU:HB3	18:6M:154:VAL:HG11	1.96	0.47
14:3M:61:TYR:CE1	18:6M:64:LEU:HD11	2.50	0.47
25:A8:41:LYS:HB3	25:A8:41:LYS:HE2	1.63	0.47
26:A9:142:ASP:OD2	26:A9:222:ARG:NH1	2.47	0.47
41:C2:82:ILE:HD13	41:C2:82:ILE:N	2.29	0.47
45:L2:78:VAL:HG12	45:L2:96:VAL:HB	1.94	0.47
51:S6:95:LEU:HD21	53:S8:118:THR:HG21	1.96	0.47
4:D:276:VAL:HG13	5:E:121:VAL:HG22	1.96	0.47
1:M:526:ARG:HH21	61:M:602:CDL:HB21	1.80	0.47
12:1M:175:LYS:HA	12:1M:252:LEU:HD13	1.96	0.47
16:4L:28:ILE:HG22	16:4L:80:PHE:HZ	1.80	0.47
52:S7:186:THR:HG22	52:S7:188:GLU:H	1.79	0.47
57:V1:97:VAL:HG22	57:V1:175:VAL:HG21	1.96	0.47
3:C:144:GLN:HE21	3:C:148:TRP:HD1	1.61	0.47
5:E:108:ARG:NH1	9:J:17:TYR:OH	2.47	0.47
4:P:107:SER:HB3	4:P:159:PRO:HD2	1.97	0.47
15:4M:93:PHE:O	15:4M:97:THR:HG23	2.15	0.47
17:5M:333:VAL:HG22	17:5M:486:ILE:HG13	1.97	0.47
18:6M:58:ILE:O	18:6M:62:ALA:HB3	2.14	0.47
19:A1:43:ASP:H	19:A1:46:ASP:HB2	1.80	0.47
43:G1:141:ASP:HB3	43:G1:142:GLU:OE2	2.14	0.47
44:G2:102:ASP:OD1	44:G2:102:ASP:N	2.46	0.47
46:S1:346:ASN:HB2	46:S1:649:GLY:HA3	1.97	0.47
46:S1:436:GLU:HG3	46:S1:458:ARG:HH11	1.80	0.47
51:S6:53:VAL:O	51:S6:96:ARG:NH2	2.42	0.47
57:V1:166:LEU:HD13	57:V1:273:VAL:HG13	1.97	0.47
1:A:238:PHE:O	1:A:241:THR:OG1	2.33	0.47
2:B:140:PHE:HE2	6:R:111:LEU:HD12	1.79	0.47
2:B:494:VAL:O	2:B:497:VAL:HG22	2.14	0.47
13:2M:300:ALA:HB2	17:5M:610:ALA:HB1	1.97	0.47
23:A6:31:THR:HG22	23:A6:84:LEU:HD12	1.96	0.47
26:A9:98:ASP:HB2	26:A9:101:ARG:HE	1.79	0.47
26:A9:188:SER:OG	26:A9:336:ASP:OD1	2.32	0.47
30:AC:102:CYS:O	30:AC:106:ILE:HD12	2.15	0.47
37:B9:41:ASN:O	37:B9:44:GLU:HG2	2.13	0.47
43:G1:161:ALA:HB1	43:G1:175:ILE:HG22	1.95	0.47
44:G2:53:PRO:HB3	44:G2:71:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:L2:153:SER:HB2	45:L2:170:GLU:HA	1.97	0.47
47:S2:277:GLN:O	47:S2:281:LYS:HG2	2.14	0.47
48:S3:100:SER:HB2	48:S3:123:PHE:HB3	1.96	0.47
51:S6:62:ILE:HD11	51:S6:79:PHE:HB3	1.97	0.47
2:B:444:GLU:HG3	2:B:448:ARG:HD3	1.97	0.47
11:N:102:LEU:HD12	11:N:259:LEU:HD13	1.97	0.47
4:P:124:GLU:HB3	9:V:69:LEU:HD21	1.97	0.47
12:1M:304:LEU:HD21	14:3M:70:PHE:CZ	2.50	0.47
36:B8:59:THR:HG21	37:B9:94:THR:HG21	1.96	0.47
43:G1:88:ASP:OD2	45:L2:231:HIS:NE2	2.33	0.47
48:S3:79:SER:O	48:S3:83:ASN:N	2.48	0.47
57:V1:160:ARG:O	57:V1:196:ASN:ND2	2.48	0.47
2:B:112:SER:HB3	2:B:159:ARG:HA	1.97	0.47
3:C:102:HIS:HD2	62:C:503:HEM:C1C	2.33	0.47
3:C:142:TRP:HH2	3:C:177:VAL:HG12	1.80	0.47
6:F:32:GLY:HA2	6:F:87:GLN:HG3	1.96	0.47
23:A6:46:ASP:N	23:A6:46:ASP:OD1	2.46	0.47
24:A7:54:PRO:HG3	53:S8:221:TYR:CE1	2.50	0.47
26:A9:364:LEU:HD23	26:A9:368:PRO:HG2	1.96	0.47
38:BJ:5:LYS:HA	38:BJ:5:LYS:HD2	1.74	0.47
50:S5:60:GLU:HA	50:S5:63:ARG:HG2	1.97	0.47
1:M:444:SER:O	1:M:448:LEU:HG	2.15	0.47
1:M:484:ASP:N	1:M:484:ASP:OD1	2.49	0.47
3:O:331:ILE:HG23	63:R:201:3PE:H2H2	1.96	0.47
16:4L:83:THR:O	16:4L:87:ARG:HG2	2.15	0.47
17:5M:33:THR:OG1	17:5M:101:ILE:HD11	2.14	0.47
17:5M:347:LEU:HD22	17:5M:385:GLY:HA3	1.96	0.47
29:AM:9:LYS:HB3	29:AM:12:MET:HB3	1.97	0.47
45:L2:161:ILE:HG13	45:L2:217:ILE:HG23	1.97	0.47
45:L2:247:LYS:HA	45:L2:250:LYS:HE3	1.97	0.47
46:S1:234:GLY:HA2	46:S1:460:ARG:HH21	1.80	0.47
47:S2:54:LEU:HD11	52:S7:163:SER:HB2	1.96	0.47
47:S2:166:ASP:OD1	47:S2:167:LEU:N	2.47	0.47
1:M:397:ASP:OD1	1:M:397:ASP:N	2.47	0.46
13:2M:233:VAL:HA	13:2M:236:HIS:ND1	2.31	0.46
15:4M:90:SER:HB3	15:4M:262:TYR:OH	2.15	0.46
15:4M:457:VAL:O	15:4M:461:ILE:HG12	2.15	0.46
47:S2:183:ALA:HA	47:S2:272:MET:HE1	1.97	0.46
54:P1:53:PHE:HA	54:P1:56:PHE:CD2	2.50	0.46
57:V1:471:ARG:O	57:V1:475:GLU:HG2	2.15	0.46
1:A:210:GLU:HA	1:A:213:VAL:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:VAL:HG21	1:A:388:ILE:HD13	1.97	0.46
3:C:10:LEU:HA	3:C:13:GLU:HG2	1.97	0.46
1:M:514:ASP:OD2	3:O:230:TYR:OH	2.20	0.46
11:N:235:ALA:HA	11:N:238:ARG:HH11	1.81	0.46
12:1M:14:LEU:HB2	12:1M:15:PRO:HD3	1.97	0.46
12:1M:267:ILE:HD13	19:A1:20:CYS:SG	2.56	0.46
13:2M:36:TYR:O	44:G2:250:ARG:NH2	2.48	0.46
15:4M:153:MET:HE2	15:4M:252:LEU:HD13	1.96	0.46
22:A5:78:GLU:HG3	22:A5:86:VAL:HG13	1.97	0.46
27:AK:110:TYR:O	27:AK:113:ARG:NH1	2.38	0.46
29:AM:37:ARG:HB2	47:S2:187:ASP:OD1	2.15	0.46
57:V1:80:PHE:CZ	57:V1:199:LYS:HD3	2.51	0.46
11:N:123:GLU:HB2	11:N:153:ALA:HB2	1.97	0.46
6:R:79:LEU:HD13	6:R:83:LEU:HB3	1.96	0.46
16:4L:47:LEU:HD22	18:6M:46:LEU:HD13	1.98	0.46
17:5M:47:PHE:CG	17:5M:87:ILE:HD11	2.50	0.46
17:5M:139:GLY:O	17:5M:143:VAL:HG23	2.14	0.46
23:A6:24:VAL:HG21	67:AB:201:ZMP:HN1	1.80	0.46
43:G1:89:VAL:HG21	43:G1:110:LYS:HA	1.98	0.46
43:G1:167:ALA:HB2	43:G1:182:GLY:HA2	1.98	0.46
46:S1:276:SER:OG	46:S1:279:PHE:HB3	2.15	0.46
46:S1:519:ALA:HB2	46:S1:555:LEU:HA	1.98	0.46
46:S1:522:PHE:HA	46:S1:527:GLN:OE1	2.15	0.46
47:S2:95:PRO:HG3	47:S2:286:MET:HG3	1.97	0.46
48:S3:68:LYS:HE2	48:S3:68:LYS:HB2	1.69	0.46
57:V1:159:MET:HE1	57:V1:186:ILE:HG23	1.98	0.46
1:A:158:GLU:HG2	1:A:192:ILE:HD11	1.96	0.46
2:B:339:LEU:HD12	2:B:385:PHE:HZ	1.80	0.46
2:B:385:PHE:HB3	2:B:481:LEU:HD21	1.97	0.46
1:M:236:THR:O	1:M:320:SER:OG	2.31	0.46
1:M:405:ALA:HB1	1:M:415:LEU:HD21	1.97	0.46
3:O:272:PRO:HG2	3:O:275:ILE:HG12	1.96	0.46
12:1M:201:ALA:O	12:1M:204:ASP:HB2	2.15	0.46
20:A2:69:GLU:OE1	46:S1:680:ARG:NH1	2.49	0.46
24:A7:54:PRO:HG3	53:S8:221:TYR:CD1	2.50	0.46
26:A9:71:THR:OG1	66:A9:401:NDP:O2X	2.34	0.46
34:B4:57:HIS:O	34:B4:61:GLU:HG3	2.15	0.46
12:1M:202:PRO:HD2	12:1M:283:VAL:HG12	1.97	0.46
14:3M:98:PHE:CD1	18:6M:156:SER:HB3	2.51	0.46
17:5M:611:GLU:O	17:5M:615:GLN:HG2	2.15	0.46
35:B7:10:MET:HG2	36:B8:114:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:S1:329:ILE:HD11	46:S1:333:THR:HG22	1.96	0.46
47:S2:217:TRP:HA	48:S3:107:SER:HB3	1.97	0.46
1:A:326:ASP:OD1	7:G:9:LYS:HG3	2.15	0.46
4:D:95:HIS:O	4:D:99:THR:HG23	2.15	0.46
1:M:354:MET:HE2	1:M:354:MET:HB3	1.70	0.46
12:1M:84:LEU:HD13	12:1M:117:GLY:HA2	1.98	0.46
13:2M:88:LEU:HD23	13:2M:260:ILE:HD12	1.98	0.46
13:2M:337:GLY:HA2	13:2M:398:SER:HB2	1.98	0.46
17:5M:449:PHE:HD2	30:AC:88:LYS:HD3	1.77	0.46
22:A5:115:TYR:OH	48:S3:19:VAL:O	2.30	0.46
52:S7:156:GLY:O	52:S7:161:HIS:ND1	2.38	0.46
1:A:269:HIS:HD2	1:A:274:ARG:HH22	1.63	0.46
1:A:413:ASP:OD1	1:A:413:ASP:N	2.48	0.46
13:2M:86:GLN:NE2	13:2M:130:SER:OG	2.48	0.46
26:A9:60:VAL:HG22	49:S4:78:PRO:HG3	1.97	0.46
40:FD:94:CYS:SG	40:FD:133:GLY:N	2.87	0.46
40:FD:109:ARG:HH21	40:FD:126:LEU:HD21	1.81	0.46
44:G2:84:VAL:HB	44:G2:105:LEU:HD13	1.97	0.46
46:S1:173:ILE:O	53:S8:150:ARG:NH1	2.48	0.46
46:S1:295:ASP:OD2	46:S1:333:THR:HG23	2.15	0.46
47:S2:142:LEU:HB3	47:S2:152:ARG:HB3	1.98	0.46
47:S2:202:ARG:HH12	47:S2:376:ALA:HB1	1.81	0.46
48:S3:21:LYS:CG	48:S3:32:ASP:HB3	2.45	0.46
58:V2:46:THR:HB	58:V2:49:ASN:HD22	1.81	0.46
58:V2:139:ILE:HD12	58:V2:175:PRO:HB2	1.97	0.46
58:V2:177:ILE:HD13	58:V2:202:VAL:HG13	1.97	0.46
3:O:287:ILE:HD13	3:O:304:VAL:HG21	1.98	0.46
13:2M:287:SER:O	13:2M:291:MET:HG3	2.16	0.46
15:4M:80:ILE:HG21	15:4M:140:LEU:HD23	1.96	0.46
17:5M:377:PHE:HB3	17:5M:458:ASP:OD2	2.16	0.46
18:6M:186:ASN:O	18:6M:190:PHE:HB2	2.16	0.46
40:FD:40:VAL:O	40:FD:44:ILE:HG12	2.16	0.46
41:C2:37:VAL:HG21	60:G1:702:PC1:H282	1.98	0.46
46:S1:436:GLU:HG2	46:S1:458:ARG:HD2	1.98	0.46
57:V1:81:LEU:HD13	57:V1:164:HIS:CE1	2.51	0.46
1:A:181:VAL:HB	1:A:185:ASP:HB2	1.97	0.46
3:C:41:LEU:HD11	3:C:242:PHE:CG	2.51	0.46
8:H:57:ASP:HA	8:H:60:VAL:HG12	1.98	0.46
1:M:127:PHE:O	1:M:269:HIS:NE2	2.42	0.46
11:N:317:GLY:HA3	11:N:321:LYS:HD3	1.97	0.46
13:2M:199:ALA:O	13:2M:203:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:4M:364:VAL:HG21	15:4M:435:ARG:NH1	2.31	0.46
17:5M:47:PHE:HB2	17:5M:87:ILE:HD11	1.98	0.46
17:5M:68:GLU:HB2	38:BJ:45:ILE:HD13	1.98	0.46
17:5M:451:ARG:HD3	30:AC:88:LYS:HB3	1.96	0.46
17:5M:565:PHE:HA	36:B8:82:LEU:HD22	1.98	0.46
25:A8:6:ASP:HB3	25:A8:10:ASN:HB2	1.97	0.46
47:S2:27:ARG:NH1	48:S3:136:TYR:OH	2.49	0.46
52:S7:103:LEU:HB3	52:S7:108:ILE:HB	1.97	0.46
1:A:137:HIS:O	1:A:140:GLU:HG3	2.16	0.46
1:M:361:TRP:HD1	1:M:371:MET:SD	2.39	0.46
13:2M:125:MET:HG2	13:2M:261:SER:OG	2.16	0.46
14:3M:69:ILE:HG13	18:6M:163:MET:HG3	1.97	0.46
15:4M:231:VAL:HG22	15:4M:290:ALA:HB2	1.97	0.46
18:6M:144:LEU:HD11	18:6M:152:PHE:HB2	1.97	0.46
24:A7:90:ASP:O	24:A7:94:LEU:HG	2.16	0.46
26:A9:221:ASP:OD2	26:A9:225:ASN:ND2	2.49	0.46
33:B3:20:HIS:O	33:B3:24:THR:HG23	2.15	0.46
46:S1:228:PHE:CZ	46:S1:264:ASN:HB2	2.51	0.46
1:A:460:ILE:HG12	1:A:470:ARG:HD2	1.98	0.45
3:C:290:SER:OG	3:C:291:ILE:N	2.49	0.45
1:M:517:TRP:O	1:M:521:ARG:HG2	2.15	0.45
11:N:326:ILE:HD11	11:N:458:PHE:HD2	1.81	0.45
3:O:20:ASN:HA	3:O:24:ILE:HD12	1.97	0.45
13:2M:110:ASP:OD2	13:2M:110:ASP:N	2.49	0.45
15:4M:294:THR:HA	15:4M:297:THR:HG22	1.98	0.45
17:5M:1:MET:HE2	56:C1:74:TRP:HZ2	1.81	0.45
26:A9:71:THR:OG1	66:A9:401:NDP:O3B	2.29	0.45
41:C2:4:SER:HB3	41:C2:7:THR:HG22	1.98	0.45
46:S1:243:ARG:NH2	58:V2:111:SER:OG	2.49	0.45
47:S2:185:ARG:HE	47:S2:188:GLU:CD	2.19	0.45
57:V1:412:PRO:HG2	57:V1:450:HIS:O	2.15	0.45
13:2M:233:VAL:HG21	13:2M:293:LEU:HB3	1.97	0.45
20:A2:17:LEU:O	20:A2:58:PRO:HA	2.16	0.45
28:AL:51:VAL:HG11	28:AL:95:TRP:CZ2	2.51	0.45
43:G1:96:SER:N	43:G1:124:ASP:OD1	2.37	0.45
46:S1:231:GLU:HG2	46:S1:464:ARG:CZ	2.46	0.45
46:S1:332:LYS:O	46:S1:336:CYS:HB3	2.16	0.45
47:S2:355:ILE:HB	47:S2:394:ARG:HG3	1.98	0.45
54:P1:49:ARG:HD3	54:P1:53:PHE:CE1	2.50	0.45
57:V1:115:GLY:O	57:V1:367:TYR:OH	2.28	0.45
1:A:357:MET:HB3	1:A:438:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:ALA:HB2	2:B:293:PRO:HB2	1.97	0.45
2:B:439:ARG:HG3	2:B:440:MET:N	2.31	0.45
3:O:35:TRP:HZ2	61:O:408:CDL:H522	1.81	0.45
3:O:85:ARG:NH1	62:O:402:HEM:O2D	2.45	0.45
12:1M:154:ILE:HG23	12:1M:186:VAL:HG12	1.99	0.45
12:1M:179:PHE:C	12:1M:182:PRO:HD2	2.37	0.45
13:2M:267:LEU:HD11	13:2M:334:LEU:HD22	1.97	0.45
13:2M:328:ILE:HG12	54:P1:48:MET:HA	1.98	0.45
33:B3:3:SER:OG	33:B3:4:GLY:N	2.49	0.45
51:S6:92:TYR:CE1	53:S8:124:ILE:HD13	2.51	0.45
2:B:303:ARG:HB3	2:B:494:VAL:HG11	1.99	0.45
13:2M:391:PRO:HB3	15:4M:144:VAL:HG13	1.99	0.45
16:4L:83:THR:HG23	16:4L:87:ARG:NH1	2.32	0.45
17:5M:102:SER:HB3	17:5M:463:MET:HG3	1.97	0.45
17:5M:540:ASP:N	17:5M:540:ASP:OD1	2.48	0.45
17:5M:571:ASP:O	17:5M:575:ARG:HB2	2.16	0.45
22:A5:125:PRO:HG2	47:S2:91:ASN:ND2	2.31	0.45
22:A5:131:PRO:HB3	47:S2:239:TYR:HB3	1.99	0.45
38:BJ:53:GLU:O	38:BJ:56:ARG:HG2	2.15	0.45
40:FD:59:VAL:HG21	40:FD:71:LEU:HD23	1.99	0.45
45:L2:122:VAL:HB	45:L2:150:LEU:HD13	1.98	0.45
46:S1:301:GLY:O	46:S1:639:GLN:NE2	2.48	0.45
47:S2:299:ARG:O	47:S2:302:MET:HG3	2.16	0.45
53:S8:97:PRO:HG2	53:S8:98:PHE:CD1	2.51	0.45
54:P1:39:LYS:O	54:P1:42:GLU:HG2	2.16	0.45
6:F:40:ASP:HB3	6:F:43:TYR:HB2	1.98	0.45
8:H:26:LEU:HD21	55:P4:48:VAL:HG21	1.98	0.45
20:A2:45:LYS:HA	20:A2:45:LYS:HE3	1.98	0.45
22:A5:106:TRP:O	22:A5:108:PRO:HD3	2.15	0.45
28:AL:54:ASP:OD2	28:AL:58:ASN:ND2	2.46	0.45
46:S1:635:GLU:HG2	46:S1:694:ARG:HD2	1.99	0.45
46:S1:653:ASP:HB2	46:S1:656:LYS:HD2	1.99	0.45
53:S8:163:ILE:HG13	53:S8:165:CYS:HB3	1.99	0.45
56:C1:82:ASP:OD1	56:C1:82:ASP:N	2.49	0.45
3:C:189:HIS:HE1	62:C:502:HEM:C4C	2.35	0.45
4:D:273:TRP:CZ2	5:E:128:LEU:HD13	2.48	0.45
1:M:238:PHE:O	1:M:241:THR:HB	2.16	0.45
17:5M:68:GLU:HG3	17:5M:69:MET:H	1.82	0.45
26:A9:78:VAL:HG11	26:A9:138:LEU:HD11	1.98	0.45
43:G1:162:MET:O	43:G1:180:VAL:HA	2.17	0.45
47:S2:70:LEU:HD11	47:S2:355:ILE:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:S2:292:ARG:HA	47:S2:292:ARG:HD3	1.75	0.45
52:S7:197:LEU:O	52:S7:201:ILE:HG12	2.16	0.45
56:C1:23:THR:O	56:C1:23:THR:HG22	2.15	0.45
57:V1:309:HIS:ND1	57:V1:386:ASP:OD1	2.50	0.45
57:V1:433:LYS:H	57:V1:436:GLU:HB2	1.82	0.45
2:B:149:ILE:HD11	2:B:166:PHE:CZ	2.50	0.45
1:M:177:TYR:OH	1:M:270:TYR:OH	2.22	0.45
11:N:147:GLY:CA	11:N:163:ASP:O	2.64	0.45
12:1M:141:ALA:O	12:1M:145:VAL:HG23	2.16	0.45
16:4L:40:LEU:HD11	18:6M:37:THR:HG21	1.98	0.45
28:AL:87:GLN:HG2	28:AL:121:GLU:HG2	1.97	0.45
43:G1:22:ILE:HD11	60:G1:702:PC1:H362	1.97	0.45
52:S7:76:ARG:NH1	52:S7:202:ASN:OD1	2.50	0.45
52:S7:81:PRO:HB3	52:S7:119:CYS:SG	2.57	0.45
3:O:189:HIS:HE1	62:O:402:HEM:C4C	2.35	0.45
8:T:13:LEU:HD21	8:T:63:LYS:HB2	1.98	0.45
15:4M:15:LEU:HB2	15:4M:51:TYR:HE2	1.82	0.45
15:4M:294:THR:HG21	15:4M:313:VAL:HB	1.99	0.45
15:4M:320:THR:HA	15:4M:323:MET:HE2	1.98	0.45
15:4M:337:LEU:HB2	15:4M:399:GLY:HA3	1.97	0.45
15:4M:430:LEU:HD11	17:5M:168:MET:SD	2.57	0.45
19:A1:51:ARG:NH2	29:AM:143:TRP:O	2.48	0.45
31:AB:107:GLU:HG2	31:AB:120:PHE:CE1	2.52	0.45
45:L2:102:LEU:HG	45:L2:123:LEU:HB2	1.99	0.45
46:S1:240:MET:HE2	46:S1:249:ILE:HD12	1.98	0.45
52:S7:81:PRO:CG	52:S7:108:ILE:HG23	2.47	0.45
53:S8:172:CYS:HA	70:S8:702:SF4:S1	2.57	0.45
57:V1:434:LEU:O	57:V1:437:ILE:HG12	2.16	0.45
58:V2:173:ASN:HB3	58:V2:195:GLU:HB3	1.99	0.45
1:A:405:ALA:HB1	1:A:415:LEU:HD21	1.98	0.45
6:F:82:ASP:OD1	6:F:82:ASP:N	2.50	0.45
1:M:526:ARG:HB3	61:M:602:CDL:HB32	1.99	0.45
11:N:102:LEU:HD21	11:N:257:MET:HG2	1.98	0.45
3:O:291:ILE:HG21	3:O:296:GLY:HA3	1.99	0.45
26:A9:89:VAL:HB	26:A9:112:ILE:HD13	1.98	0.45
34:B4:18:THR:HA	34:B4:21:GLU:HG2	1.99	0.45
44:G2:64:SER:HB2	45:L2:59:GLN:HB2	1.99	0.45
45:L2:242:TYR:HA	45:L2:245:VAL:HG22	1.97	0.45
48:S3:93:ASP:OD1	48:S3:93:ASP:N	2.48	0.45
53:S8:109:GLY:N	53:S8:179:GLU:HG2	2.32	0.45
58:V2:31:HIS:HE1	58:V2:38:ASN:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:27:PRO:HG2	7:G:3:LYS:HE3	1.99	0.45
3:C:177:VAL:HG13	3:C:181:THR:HG21	1.99	0.45
4:D:294:VAL:HG13	7:G:17:PRO:HG3	1.98	0.45
3:O:145:MET:HE2	3:O:276:VAL:H	1.82	0.45
63:O:406:3PE:H231	61:O:408:CDL:H521	1.98	0.45
12:1M:162:VAL:HG21	12:1M:170:ILE:HA	1.99	0.45
13:2M:380:PHE:O	13:2M:384:MET:HG2	2.16	0.45
14:3M:105:GLY:O	14:3M:109:GLU:HG2	2.17	0.45
15:4M:242:VAL:HG22	15:4M:305:LYS:HB2	1.98	0.45
15:4M:265:LEU:HD12	15:4M:269:ILE:HD12	1.99	0.45
15:4M:431:TRP:O	15:4M:435:ARG:HG3	2.17	0.45
26:A9:367:TYR:HB2	26:A9:368:PRO:HD3	1.99	0.45
43:G1:45:LEU:HD23	43:G1:67:LEU:HB2	1.98	0.45
45:L2:55:ASP:O	45:L2:57:ARG:HG2	2.18	0.45
47:S2:110:ARG:HA	47:S2:334:PRO:HG3	1.98	0.45
1:A:241:THR:HG21	1:A:316:ILE:H	1.82	0.44
3:C:228:TYR:O	3:C:232:TYR:HB3	2.17	0.44
1:M:289:VAL:HG12	1:M:293:LYS:HE2	1.99	0.44
11:N:440:GLU:O	11:N:444:ARG:HG2	2.16	0.44
3:O:282:LEU:HD13	3:O:347:CYS:HB2	1.98	0.44
12:1M:174:GLN:HE22	12:1M:246:LEU:C	2.19	0.44
17:5M:236:ILE:N	17:5M:293:THR:OG1	2.50	0.44
23:A6:126:PHE:CE1	46:S1:657:ILE:HG22	2.51	0.44
26:A9:251:TYR:CD1	26:A9:368:PRO:HB3	2.52	0.44
34:B4:24:GLU:HG3	34:B4:25:PHE:CD2	2.52	0.44
39:BK:43:ARG:NH1	39:BK:46:GLY:O	2.50	0.44
45:L2:97:TRP:CD1	45:L2:118:GLN:HA	2.52	0.44
47:S2:168:PRO:HD2	47:S2:171:LEU:HD22	1.98	0.44
51:S6:89:VAL:HG12	51:S6:91:LYS:H	1.82	0.44
57:V1:103:TRP:O	57:V1:107:GLU:HG2	2.17	0.44
57:V1:130:MET:SD	57:V1:269:THR:OG1	2.72	0.44
3:C:190:TYR:CD1	62:C:502:HEM:HMB3	2.52	0.44
13:2M:281:GLN:HG2	27:AK:139:LEU:HD12	1.99	0.44
13:2M:321:ILE:CD1	13:2M:414:LEU:HG	2.47	0.44
15:4M:374:MET:HG2	15:4M:451:ASP:HA	1.98	0.44
17:5M:652:ARG:NH1	27:AK:81:GLU:OE1	2.48	0.44
22:A5:52:GLY:HA2	22:A5:55:LYS:HE3	1.99	0.44
26:A9:242:ASN:HA	26:A9:303:LYS:HG2	1.99	0.44
44:G2:51:LYS:HZ1	44:G2:70:ASP:HB2	1.82	0.44
44:G2:51:LYS:NZ	44:G2:70:ASP:HB2	2.32	0.44
44:G2:60:PHE:HB2	44:G2:215:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:S2:224:LEU:HG	47:S2:229:VAL:HG21	1.99	0.44
47:S2:241:VAL:HG23	47:S2:245:LEU:HD11	1.99	0.44
51:S6:67:GLY:HA2	51:S6:93:CYS:SG	2.58	0.44
52:S7:159:TYR:CE1	53:S8:134:PRO:HB2	2.50	0.44
57:V1:400:TYR:HB2	57:V1:421:TRP:CD1	2.52	0.44
1:A:122:ASP:HB2	1:A:465:LEU:HD22	1.99	0.44
3:C:75:MET:HE1	3:C:85:ARG:NH1	2.29	0.44
8:H:22:VAL:HG22	55:P4:52:LEU:HD12	2.00	0.44
9:V:21:MET:HG2	9:V:27:TYR:HD1	1.81	0.44
17:5M:79:ASP:N	17:5M:82:THR:OG1	2.50	0.44
17:5M:213:MET:HE3	17:5M:215:LEU:HD11	1.99	0.44
17:5M:538:VAL:HG23	17:5M:538:VAL:O	2.18	0.44
48:S3:143:LEU:HD23	48:S3:143:LEU:HA	1.84	0.44
1:A:321:GLU:OE1	1:A:323:ARG:NE	2.47	0.44
11:N:193:GLU:O	11:N:197:VAL:HG23	2.17	0.44
3:O:148:TRP:HA	3:O:151:THR:HG22	1.99	0.44
3:O:159:ALA:HB2	3:O:294:LYS:HG2	1.99	0.44
3:O:207:LEU:HD22	62:O:403:HEM:HAA1	1.98	0.44
14:3M:1:MET:HB3	14:3M:1:MET:HE2	1.77	0.44
15:4M:231:VAL:HB	15:4M:232:PRO:HD3	2.00	0.44
17:5M:202:SER:O	17:5M:205:ARG:NH1	2.51	0.44
17:5M:488:LEU:HD11	17:5M:507:ALA:HB2	2.00	0.44
24:A7:58:ASN:OD1	47:S2:301:ARG:NH1	2.51	0.44
30:AC:89:LEU:HA	37:B9:86:TRP:CZ2	2.52	0.44
43:G1:92:ILE:HG12	43:G1:120:THR:HB	1.99	0.44
46:S1:111:ARG:HD2	46:S1:326:GLU:OE1	2.18	0.44
47:S2:360:PHE:O	47:S2:364:GLN:HG3	2.18	0.44
53:S8:113:LEU:O	53:S8:204:GLY:HA3	2.18	0.44
58:V2:124:LEU:HB2	58:V2:178:THR:OG1	2.18	0.44
58:V2:151:ARG:HG2	58:V2:152:ASN:OD1	2.17	0.44
1:M:472:PRO:HG2	1:M:475:GLU:HB3	1.99	0.44
60:M:603:PC1:H3B1	5:Q:126:ILE:HG12	1.98	0.44
11:N:109:ILE:HD13	11:N:156:GLU:OE1	2.18	0.44
12:1M:78:PRO:HA	12:1M:81:THR:HG22	1.99	0.44
12:1M:145:VAL:HG13	14:3M:67:PHE:CG	2.51	0.44
15:4M:23:SER:O	15:4M:27:ILE:HG13	2.17	0.44
16:4L:77:LEU:HD12	18:6M:68:VAL:HG11	1.99	0.44
26:A9:290:LEU:HD21	26:A9:369:VAL:HG11	1.98	0.44
44:G2:232:ARG:HD3	45:L2:69:LEU:HB2	2.00	0.44
48:S3:48:HIS:O	48:S3:52:ARG:HG2	2.18	0.44
57:V1:309:HIS:CD2	57:V1:336:ARG:HH21	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:GLN:HE21	2:B:388:GLN:HE22	1.64	0.44
4:D:85:SER:HB3	9:J:50:TRP:CZ2	2.52	0.44
4:P:286:TYR:CD1	7:S:23:MET:HG3	2.51	0.44
8:T:40:SER:O	8:T:42:GLN:NE2	2.50	0.44
13:2M:182:GLY:HA2	13:2M:218:GLY:HA2	2.00	0.44
13:2M:488:LEU:HD12	41:C:66:LYS:HG2	1.98	0.44
17:5M:174:GLY:O	17:5M:228:GLY:HA2	2.18	0.44
27:AK:79:GLY:O	27:AK:83:LEU:HG	2.17	0.44
28:AL:132:TYR:OH	53:S8:196:ASP:OD2	2.31	0.44
38:BJ:73:LEU:HD23	38:BJ:73:LEU:HA	1.86	0.44
43:G1:222:LEU:HD13	44:G2:39:LEU:HD23	2.00	0.44
44:G2:144:PHE:CD2	44:G2:200:ILE:HG12	2.52	0.44
46:S1:288:LEU:HD23	46:S1:309:ARG:HB2	1.98	0.44
51:S6:90:CYS:C	51:S6:92:TYR:H	2.20	0.44
54:P1:72:VAL:HG12	54:P1:74:GLY:H	1.82	0.44
5:E:138:SER:OG	5:E:139:ALA:N	2.51	0.44
1:M:385:ALA:HB2	1:M:415:LEU:HD13	1.98	0.44
4:P:227:LYS:NZ	4:P:244:GLU:OE2	2.43	0.44
14:3M:65:ILE:HD12	16:4L:74:ALA:HB1	2.00	0.44
43:G1:90:ASN:HB3	43:G1:108:VAL:HG21	2.00	0.44
43:G1:110:LYS:HD3	45:L2:227:LEU:HD23	1.98	0.44
43:G1:233:LYS:HA	43:G1:233:LYS:HD3	1.69	0.44
46:S1:318:PRO:HB3	46:S1:329:ILE:HB	1.98	0.44
46:S1:436:GLU:CG	46:S1:458:ARG:HD2	2.48	0.44
47:S2:152:ARG:HH21	52:S7:92:GLU:CD	2.21	0.44
57:V1:342:LEU:HD11	57:V1:345:VAL:HG23	1.99	0.44
57:V1:430:GLY:C	57:V1:481:ASN:HD22	2.21	0.44
4:D:97:VAL:HG23	4:D:234:VAL:HG21	2.00	0.44
1:M:333:GLN:HG2	1:M:406:VAL:HG13	2.00	0.44
61:M:602:CDL:H202	3:O:239:TRP:HH2	1.82	0.44
9:V:21:MET:HG2	9:V:27:TYR:CD1	2.53	0.44
13:2M:233:VAL:CG2	13:2M:290:SER:HA	2.44	0.44
15:4M:392:PRO:HA	15:4M:397:PHE:CD2	2.52	0.44
17:5M:178:LEU:HB2	17:5M:228:GLY:HA3	1.99	0.44
18:6M:143:LEU:HD12	18:6M:143:LEU:HA	1.78	0.44
18:6M:192:ARG:O	24:A7:115:GLU:HA	2.18	0.44
20:A2:72:ILE:HD12	20:A2:85:ALA:HB1	2.00	0.44
20:A2:74:LEU:HD22	20:A2:82:ILE:HG12	1.99	0.44
26:A9:135:VAL:HG23	26:A9:171:ILE:HD12	2.00	0.44
33:B3:14:ARG:HD2	33:B3:14:ARG:HA	1.86	0.44
37:B9:11:ARG:HD2	37:B9:11:ARG:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:FD:127:ASN:O	40:FD:128:LYS:HG2	2.18	0.44
43:G1:105:LEU:HD11	43:G1:107:HIS:HB3	2.00	0.44
45:L2:127:TRP:O	45:L2:128:THR:OG1	2.32	0.44
1:A:444:SER:O	1:A:448:LEU:HG	2.18	0.44
3:C:99:VAL:HG21	3:C:130:MET:SD	2.57	0.44
6:R:26:LYS:O	6:R:30:LYS:HG3	2.17	0.44
13:2M:192:ALA:HB1	13:2M:197:GLN:HB2	2.00	0.44
15:4M:10:PHE:CZ	15:4M:54:VAL:HG11	2.53	0.44
15:4M:469:ARG:HH22	39:BK:80:LEU:HD13	1.83	0.44
22:A5:112:PRO:HG3	48:S3:17:LYS:HG3	1.99	0.44
27:AK:14:ASP:HB3	27:AK:19:LYS:HE3	1.99	0.44
41:C2:66:LYS:HB2	41:C2:66:LYS:HE3	1.70	0.44
2:B:479:GLN:HA	2:B:482:ILE:HG12	2.00	0.43
3:C:386:TYR:CD2	6:F:21:MET:HG3	2.53	0.43
1:M:205:ASN:OD1	1:M:206:ARG:N	2.50	0.43
12:1M:145:VAL:HG13	14:3M:67:PHE:CD1	2.53	0.43
12:1M:151:ILE:HG13	12:1M:193:SER:HB3	2.00	0.43
16:4L:52:SER:O	50:S5:13:ARG:NH2	2.44	0.43
30:AC:84:GLU:OE2	37:B9:23:ARG:NH2	2.45	0.43
44:G2:41:ARG:HG3	44:G2:41:ARG:O	2.18	0.43
57:V1:293:PHE:HB3	57:V1:319:GLU:HG3	1.99	0.43
1:M:448:LEU:HD22	11:N:435:ARG:NH2	2.32	0.43
11:N:186:LEU:HB2	11:N:189:GLU:HG3	2.00	0.43
9:V:42:VAL:O	9:V:46:ILE:HG12	2.18	0.43
13:2M:99:MET:HG3	13:2M:353:LEU:HD12	1.99	0.43
13:2M:107:GLU:OE2	13:2M:356:ARG:NE	2.44	0.43
17:5M:307:LEU:O	17:5M:311:ILE:HG13	2.18	0.43
17:5M:392:PHE:HE2	32:B2:37:VAL:HG11	1.83	0.43
17:5M:549:SER:HB3	17:5M:552:CYS:HB2	2.01	0.43
26:A9:155:TYR:HA	26:A9:197:ALA:HB2	2.00	0.43
28:AL:113:LYS:HE2	28:AL:113:LYS:HB2	1.86	0.43
30:AC:55:ASP:HB3	30:AC:58:LYS:HG2	2.00	0.43
57:V1:307:SER:HA	57:V1:313:PRO:HB3	1.99	0.43
1:A:509:ILE:O	1:A:509:ILE:HG13	2.18	0.43
2:B:458:PRO:HG2	2:B:461:GLU:HG3	2.01	0.43
4:D:75:TYR:HB3	8:H:65:PHE:CE2	2.53	0.43
6:F:119:ARG:HH12	6:F:122:PRO:HD3	1.83	0.43
1:M:452:GLY:O	1:M:456:VAL:HG23	2.18	0.43
11:N:287:ASP:N	11:N:287:ASP:OD1	2.50	0.43
3:O:323:SER:O	6:R:27:ARG:NH1	2.38	0.43
12:1M:12:ILE:HD11	19:A1:26:GLN:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1M:110:LEU:HD11	12:1M:167:LEU:HD11	2.01	0.43
15:4M:478:LEU:HB3	15:4M:482:HIS:CE1	2.51	0.43
22:A5:135:PRO:HA	48:S3:3:ASN:ND2	2.33	0.43
24:A7:111:ASN:HB3	47:S2:230:CYS:SG	2.58	0.43
29:AM:108:GLU:O	29:AM:112:MET:HB2	2.18	0.43
67:AC:201:ZMP:H8A	37:B9:69:ALA:HB1	2.01	0.43
40:FD:131:ARG:NH1	40:FD:131:ARG:HB3	2.33	0.43
45:L2:109:ILE:HG12	45:L2:137:THR:HB	2.00	0.43
46:S1:208:LEU:HD13	46:S1:257:LEU:HD23	2.00	0.43
54:P1:76:ARG:HH22	54:P1:84:GLN:HG2	1.83	0.43
60:P4:101:PC1:H3B2	60:P4:101:PC1:H372	1.99	0.43
57:V1:90:TRP:CD2	57:V1:209:LEU:HD13	2.52	0.43
57:V1:313:PRO:O	58:V2:224:ARG:NH2	2.51	0.43
1:A:423:THR:HG22	1:A:496:ILE:HG21	2.00	0.43
2:B:301:ASP:OD2	2:B:500:TYR:HB2	2.18	0.43
3:C:207:LEU:CD2	62:C:503:HEM:HAA1	2.48	0.43
3:C:244:ILE:HG12	4:D:277:LEU:HB3	2.00	0.43
1:M:239:GLN:HE21	1:M:318:THR:HG21	1.82	0.43
15:4M:66:PHE:CD1	15:4M:87:ASP:HB3	2.53	0.43
15:4M:422:MET:HB3	17:5M:172:ARG:HH11	1.83	0.43
19:A1:12:LEU:HD23	19:A1:15:ILE:HD12	2.01	0.43
26:A9:215:VAL:HG11	26:A9:247:ILE:HD12	2.00	0.43
44:G2:106:VAL:O	44:G2:106:VAL:HG12	2.17	0.43
1:A:193:LEU:O	1:A:197:LEU:HD23	2.18	0.43
6:R:83:LEU:O	6:R:87:GLN:HG2	2.19	0.43
12:1M:254:ILE:HG22	12:1M:255:LEU:HG	1.99	0.43
13:2M:6:LEU:HD13	13:2M:9:TYR:CE2	2.53	0.43
15:4M:157:ILE:HG12	15:4M:244:ALA:HB2	2.00	0.43
18:6M:47:ASP:N	18:6M:47:ASP:OD1	2.49	0.43
28:AL:111:LYS:HG3	28:AL:112:PRO:HD2	1.99	0.43
44:G2:185:PRO:HD2	44:G2:187:LYS:HZ3	1.84	0.43
46:S1:385:ALA:HB3	46:S1:411:GLY:HA2	2.00	0.43
46:S1:604:GLN:HG3	46:S1:657:ILE:HD11	1.99	0.43
57:V1:368:ASP:O	57:V1:372:ALA:N	2.42	0.43
3:C:186:PHE:HE2	3:O:186:PHE:HE2	1.65	0.43
10:W:11:GLN:HB3	10:W:14:ASP:HB2	1.99	0.43
13:2M:271:ILE:O	13:2M:275:TYR:HB2	2.18	0.43
16:4L:53:LEU:HG	50:S5:45:LEU:HD22	2.01	0.43
17:5M:79:ASP:HB3	17:5M:496:SER:HB3	1.99	0.43
26:A9:153:VAL:HG13	26:A9:154:HIS:CD2	2.54	0.43
30:AC:66:GLN:OE1	30:AC:76:ASN:ND2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:S1:117:ASN:O	57:V1:410:CYS:HA	2.18	0.43
57:V1:346:ILE:HG12	57:V1:354:LEU:HB3	2.00	0.43
3:C:156:LEU:HD21	3:C:288:LEU:HD22	2.01	0.43
1:M:49:ILE:HD13	1:M:52:ARG:HH21	1.82	0.43
1:M:166:LEU:HD13	1:M:179:ALA:HB2	2.00	0.43
12:1M:99:VAL:HG23	19:A1:38:LYS:HE2	2.00	0.43
12:1M:181:ILE:HB	12:1M:182:PRO:HD3	2.01	0.43
14:3M:112:ARG:NH2	44:G2:242:TYR:OH	2.51	0.43
26:A9:251:TYR:CE2	26:A9:253:VAL:HB	2.54	0.43
26:A9:262:VAL:HA	26:A9:265:ASP:OD2	2.19	0.43
41:C2:29:MET:HG2	43:G1:14:TRP:CE2	2.54	0.43
47:S2:59:THR:HG22	47:S2:60:TYR:N	2.34	0.43
47:S2:316:TYR:HD1	53:S8:132:ILE:HG12	1.84	0.43
57:V1:138:PRO:HD2	57:V1:266:CYS:SG	2.58	0.43
57:V1:322:ILE:HD11	57:V1:326:GLU:HG2	2.00	0.43
3:O:102:HIS:HD2	62:O:403:HEM:C1C	2.36	0.43
5:Q:146:LEU:HD23	5:Q:146:LEU:HA	1.88	0.43
12:1M:151:ILE:HG23	12:1M:190:PHE:HE1	1.84	0.43
12:1M:153:LEU:HD23	12:1M:153:LEU:HA	1.89	0.43
13:2M:137:MET:CG	13:2M:265:ASN:HD21	2.31	0.43
15:4M:315:HIS:HB2	15:4M:341:HIS:NE2	2.34	0.43
16:4L:28:ILE:HD11	16:4L:92:VAL:HG22	2.00	0.43
17:5M:148:TYR:HB2	17:5M:168:MET:HB2	1.99	0.43
22:A5:127:PRO:O	22:A5:130:VAL:HG22	2.18	0.43
43:G1:105:LEU:HD23	43:G1:133:VAL:HG23	2.00	0.43
43:G1:191:LYS:HE3	43:G1:191:LYS:HB3	1.76	0.43
47:S2:318:GLU:HG2	47:S2:319:GLY:H	1.81	0.43
1:A:429:ARG:HG3	1:A:429:ARG:O	2.18	0.43
1:A:469:ARG:NH2	1:A:475:GLU:OE2	2.27	0.43
2:B:313:PHE:CE2	2:B:400:ILE:HG12	2.54	0.43
1:M:107:GLU:HB2	1:M:460:ILE:HD11	2.01	0.43
11:N:78:LYS:HE3	11:N:78:LYS:HB3	1.84	0.43
11:N:98:ALA:HB2	11:N:166:LYS:HG2	2.00	0.43
4:P:72:CYS:SG	4:P:191:TYR:HA	2.58	0.43
4:P:289:ARG:HD2	7:S:26:LEU:HD21	2.01	0.43
13:2M:406:ALA:O	13:2M:409:CYS:HB3	2.19	0.43
14:3M:86:LYS:NZ	18:6M:138:GLU:HG3	2.33	0.43
14:3M:89:LEU:HD11	21:A3:35:ARG:HG2	2.01	0.43
17:5M:424:SER:HB3	17:5M:524:PHE:CE2	2.54	0.43
23:A6:18:GLU:HG2	23:A6:21:ARG:HH21	1.83	0.43
39:BK:73:SER:O	39:BK:77:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:FD:47:LEU:HB2	40:FD:145:MET:O	2.18	0.43
46:S1:533:ALA:O	46:S1:537:ILE:HG13	2.18	0.43
47:S2:65:PRO:HA	47:S2:68:ASP:HB2	2.01	0.43
47:S2:198:ILE:O	47:S2:202:ARG:HG2	2.19	0.43
1:A:386:GLU:N	1:A:406:VAL:O	2.52	0.43
3:C:190:TYR:CD2	3:O:190:TYR:CD2	3.07	0.43
1:M:423:THR:HG22	1:M:496:ILE:HG21	2.00	0.43
11:N:254:ALA:HA	11:N:257:MET:HE3	2.00	0.43
22:A5:100:ILE:O	22:A5:104:ILE:HG12	2.17	0.43
45:L2:169:MET:HE2	45:L2:188:PRO:HD3	2.01	0.43
47:S2:345:ASN:N	47:S2:345:ASN:OD1	2.52	0.43
57:V1:61:GLY:HA2	57:V1:319:GLU:HB3	2.00	0.43
2:B:213:GLN:O	2:B:217:LEU:HD23	2.19	0.42
4:D:107:SER:HB3	4:D:159:PRO:HD2	2.00	0.42
1:M:252:GLN:HA	1:M:255:LYS:HZ2	1.84	0.42
3:O:246:PHE:CZ	3:O:250:ILE:HD11	2.54	0.42
4:P:273:TRP:CZ2	5:Q:128:LEU:HD13	2.54	0.42
13:2M:216:PHE:HZ	17:5M:639:PHE:HB3	1.84	0.42
13:2M:217:MET:HG3	18:6M:104:ILE:HD11	2.01	0.42
13:2M:238:TRP:HB2	13:2M:242:ILE:HD13	2.00	0.42
19:A1:17:GLY:O	19:A1:21:VAL:HG23	2.18	0.42
22:A5:74:TRP:HA	22:A5:77:ILE:HG12	2.01	0.42
28:AL:33:LEU:HB2	28:AL:34:PRO:HD3	2.01	0.42
29:AM:111:VAL:HG13	29:AM:112:MET:HG2	2.01	0.42
31:AB:117:ALA:O	31:AB:121:ILE:HG12	2.19	0.42
41:C2:53:GLU:HA	41:C2:56:VAL:HG12	2.01	0.42
42:P2:77:GLU:HG2	42:P2:78:ARG:HG3	2.01	0.42
45:L2:186:VAL:HG12	45:L2:203:ALA:HB2	2.01	0.42
46:S1:652:ARG:HB2	46:S1:657:ILE:CG2	2.49	0.42
47:S2:119:THR:HB	47:S2:131:PHE:HD1	1.84	0.42
57:V1:143:VAL:HG21	57:V1:170:CYS:SG	2.59	0.42
3:C:126:ILE:HG22	3:C:130:MET:HE2	2.02	0.42
3:O:59:HIS:HB2	3:O:74:VAL:HG22	2.01	0.42
4:P:83:LEU:HD23	4:P:83:LEU:HA	1.85	0.42
4:P:87:ASP:HB3	4:P:90:SER:HB3	2.00	0.42
15:4M:130:MET:HE1	15:4M:259:LEU:HD12	2.01	0.42
15:4M:321:ILE:HD11	15:4M:414:VAL:HG22	2.00	0.42
16:4L:27:ASN:HD21	18:6M:79:ILE:HD12	1.84	0.42
17:5M:226:PHE:CD1	17:5M:286:ILE:HG12	2.54	0.42
20:A2:7:LEU:HD11	20:A2:39:LEU:HD13	2.01	0.42
43:G1:28:ARG:HG2	43:G1:33:TYR:HE2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:S1:107:CYS:HB3	46:S1:222:CYS:HB2	2.01	0.42
47:S2:119:THR:HG21	47:S2:134:ALA:CB	2.48	0.42
1:A:60:LYS:O	1:A:63:GLN:HG2	2.20	0.42
1:A:520:ARG:NH2	61:A:602:CDL:OB4	2.40	0.42
2:B:109:ASP:OD2	2:B:289:ARG:NH2	2.52	0.42
3:C:372:THR:HB	3:C:373:PRO:HD3	2.01	0.42
11:N:321:LYS:HE3	11:N:321:LYS:HB3	1.91	0.42
3:O:104:PHE:HE2	61:O:404:CDL:H192	1.84	0.42
6:R:33:LEU:HD21	6:R:66:LEU:HD23	2.02	0.42
12:1M:57:LYS:HE2	52:S7:78:SER:O	2.19	0.42
13:2M:51:VAL:HG13	13:2M:90:LEU:HD12	2.00	0.42
13:2M:227:LEU:HA	13:2M:230:ILE:HG12	2.01	0.42
13:2M:318:TYR:HB3	13:2M:402:LEU:HD13	2.00	0.42
13:2M:343:LEU:HG	13:2M:461:THR:HG23	2.00	0.42
13:2M:456:LEU:HD23	13:2M:456:LEU:HA	1.88	0.42
14:3M:77:PHE:CZ	14:3M:99:LEU:HD21	2.55	0.42
15:4M:304:LEU:O	15:4M:308:ILE:HD12	2.19	0.42
15:4M:325:SER:O	15:4M:327:ASN:N	2.53	0.42
17:5M:439:PHE:CD1	17:5M:443:LEU:HD12	2.54	0.42
17:5M:649:VAL:HG23	27:AK:26:THR:HG21	2.00	0.42
24:A7:48:ALA:HB3	28:AL:100:THR:HG22	2.01	0.42
29:AM:107:TYR:O	29:AM:110:GLU:HG3	2.18	0.42
31:AB:57:ILE:O	31:AB:61:LYS:HG2	2.19	0.42
44:G2:44:THR:HG22	44:G2:45:LEU:HD12	2.01	0.42
47:S2:70:LEU:CD1	47:S2:355:ILE:HD13	2.49	0.42
53:S8:193:LEU:HD23	53:S8:193:LEU:HA	1.84	0.42
54:P1:72:VAL:O	54:P1:76:ARG:HG3	2.19	0.42
3:C:94:MET:HG3	3:C:246:PHE:HD1	1.84	0.42
4:D:98:TYR:HA	4:D:102:CYS:HB2	2.01	0.42
4:D:129:MET:O	4:D:132:GLU:HG3	2.19	0.42
5:E:113:PHE:CZ	9:J:16:LEU:HB3	2.54	0.42
3:O:222:MET:HG3	7:S:6:VAL:HG23	2.01	0.42
12:1M:187:LEU:HD13	12:1M:247:SER:HB2	2.01	0.42
13:2M:441:PRO:HG2	13:2M:444:TRP:CD1	2.55	0.42
14:3M:59:ARG:HD3	14:3M:59:ARG:HA	1.94	0.42
15:4M:222:ALA:O	15:4M:226:VAL:HG23	2.19	0.42
25:A8:96:GLN:O	25:A8:100:GLU:HG2	2.19	0.42
57:V1:84:ALA:HB1	57:V1:89:ASP:HB2	2.01	0.42
57:V1:304:PHE:CD2	57:V1:380:ALA:HB1	2.55	0.42
4:D:208:ILE:HD13	4:D:214:TYR:HB2	2.01	0.42
4:D:303:ASP:OD2	5:E:77:PRO:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:32:ILE:HA	8:H:35:ILE:HG22	2.01	0.42
4:P:245:ALA:HB2	8:T:10:LYS:HB2	2.00	0.42
8:T:23:LYS:HB3	8:T:24:PRO:HD3	2.01	0.42
13:2M:484:LEU:HB3	41:C2:63:MET:HG2	2.01	0.42
15:4M:154:PHE:CD1	15:4M:170:ALA:HB1	2.54	0.42
18:6M:165:GLY:HA2	18:6M:168:VAL:HG12	2.01	0.42
46:S1:474:GLY:O	46:S1:488:THR:HG22	2.19	0.42
47:S2:87:GLU:O	47:S2:91:ASN:N	2.46	0.42
47:S2:203:LEU:HD22	47:S2:257:CYS:HB3	2.01	0.42
51:S6:73:LEU:HD11	53:S8:216:ARG:HG2	2.02	0.42
52:S7:76:ARG:HG3	52:S7:198:GLN:HB3	2.00	0.42
3:C:219:HIS:NE2	3:C:221:GLU:HG3	2.34	0.42
3:C:314:PHE:CD2	3:C:373:PRO:HG3	2.55	0.42
11:N:422:LYS:HD2	11:N:422:LYS:HA	1.92	0.42
15:4M:361:THR:HB	34:B4:9:LYS:HE2	2.00	0.42
15:4M:478:LEU:O	15:4M:482:HIS:ND1	2.53	0.42
16:4L:25:ARG:HG3	17:5M:622:TYR:CD2	2.54	0.42
20:A2:33:GLU:HG2	46:S1:703:LEU:HD11	2.01	0.42
20:A2:40:LYS:HA	20:A2:40:LYS:HD2	1.87	0.42
46:S1:392:GLU:HA	46:S1:681:ILE:HD11	2.02	0.42
46:S1:699:LEU:HD23	46:S1:699:LEU:HA	1.83	0.42
47:S2:219:PHE:HZ	47:S2:365:GLY:HA3	1.85	0.42
47:S2:364:GLN:CD	48:S3:110:TRP:HB2	2.39	0.42
1:A:116:THR:HG21	1:A:454:SER:HA	2.01	0.42
3:C:139:VAL:HG22	3:C:150:ALA:HB2	2.02	0.42
3:C:370:ALA:O	3:C:374:ILE:HG12	2.19	0.42
1:M:251:ALA:O	1:M:255:LYS:HG3	2.19	0.42
13:2M:237:MET:HB3	17:5M:624:TYR:CD1	2.54	0.42
14:3M:102:LEU:HD23	14:3M:102:LEU:HA	1.91	0.42
15:4M:317:ASN:HA	15:4M:320:THR:HG22	2.01	0.42
16:4L:95:ILE:O	16:4L:95:ILE:HG22	2.19	0.42
18:6M:177:VAL:HG11	47:S2:36:VAL:HG21	2.02	0.42
44:G2:78:SER:HG	44:G2:80:TRP:HE1	1.66	0.42
46:S1:120:MET:HB2	46:S1:159:VAL:HG11	2.02	0.42
46:S1:295:ASP:OD1	46:S1:297:THR:N	2.48	0.42
46:S1:381:ILE:HG23	46:S1:581:PHE:HD2	1.85	0.42
52:S7:76:ARG:HA	52:S7:201:ILE:HD11	2.02	0.42
52:S7:149:SER:HB2	52:S7:176:VAL:HG21	2.02	0.42
57:V1:144:ASN:ND2	72:V1:501:FMN:O4'	2.53	0.42
1:A:377:GLN:OE1	6:R:108:ARG:NH2	2.53	0.42
3:C:32:LEU:HB2	3:C:231:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:159:ILE:HG21	11:N:346:PRO:HB2	2.02	0.42
1:M:325:LEU:O	7:S:9:LYS:HA	2.20	0.42
11:N:170:PRO:HA	11:N:272:ILE:HG21	2.00	0.42
11:N:413:THR:HG22	11:N:415:VAL:H	1.84	0.42
3:O:259:HIS:HE1	3:O:278:GLU:HA	1.84	0.42
12:1M:101:SER:OG	14:3M:7:ILE:HG13	2.20	0.42
13:2M:108:ARG:HD2	13:2M:108:ARG:HA	1.77	0.42
13:2M:144:GLN:NE2	13:2M:262:ILE:HD11	2.31	0.42
13:2M:336:ILE:HG13	13:2M:479:THR:HG21	2.01	0.42
15:4M:145:PHE:HA	15:4M:148:SER:OG	2.20	0.42
15:4M:355:LEU:HD23	15:4M:355:LEU:HA	1.90	0.42
16:4L:63:LEU:HD22	18:6M:140:LEU:HD21	2.02	0.42
17:5M:206:ASN:HD22	38:BJ:94:SER:HB2	1.85	0.42
20:A2:19:CYS:HB3	20:A2:22:SER:HB2	2.01	0.42
39:BK:45:LYS:HE2	39:BK:45:LYS:HB3	1.89	0.42
46:S1:300:VAL:HG11	46:S1:454:MET:HB2	2.00	0.42
47:S2:193:LEU:HD23	47:S2:193:LEU:HA	1.92	0.42
60:M:603:PC1:H151	9:V:21:MET:HB3	2.01	0.42
11:N:268:GLU:O	11:N:272:ILE:HG12	2.20	0.42
12:1M:201:ALA:HB1	12:1M:283:VAL:HG12	2.02	0.42
14:3M:77:PHE:HZ	14:3M:99:LEU:HD21	1.84	0.42
15:4M:56:TRP:CA	15:4M:91:PHE:HZ	2.32	0.42
17:5M:250:THR:HG21	17:5M:353:GLY:CA	2.50	0.42
17:5M:438:LEU:HD23	17:5M:438:LEU:HA	1.91	0.42
25:A8:37:LEU:HD13	54:P1:82:LEU:HB3	2.02	0.42
31:AB:83:LEU:HB3	31:AB:87:ASP:HB2	2.02	0.42
45:L2:79:ALA:O	45:L2:82:VAL:HG22	2.20	0.42
1:A:88:LEU:O	2:B:69:SER:OG	2.31	0.42
2:B:174:PRO:HA	2:B:276:VAL:HG11	2.01	0.42
7:G:67:LYS:O	7:G:71:ARG:HG2	2.19	0.42
11:N:130:THR:HA	11:N:184:ALA:H	1.84	0.42
3:O:99:VAL:HG21	3:O:130:MET:SD	2.59	0.42
17:5M:1:MET:O	17:5M:5:ILE:HG13	2.19	0.42
17:5M:254:ALA:HB2	17:5M:349:PHE:HB3	2.02	0.42
17:5M:461:ILE:H	17:5M:461:ILE:HD12	1.85	0.42
18:6M:186:ASN:OD1	18:6M:186:ASN:N	2.53	0.42
22:A5:43:GLU:HB3	22:A5:100:ILE:HG21	2.02	0.42
26:A9:222:ARG:NH2	66:A9:401:NDP:O2N	2.52	0.42
26:A9:296:ARG:HD2	26:A9:376:ARG:HD3	2.02	0.42
37:B9:54:LYS:HG2	37:B9:55:HIS:N	2.35	0.42
43:G1:80:TRP:HB3	43:G1:102:ASP:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:L2:90:VAL:HG13	45:L2:94:ALA:HB3	2.02	0.42
46:S1:652:ARG:HB2	46:S1:657:ILE:HG23	2.02	0.42
53:S8:91:LYS:HA	53:S8:91:LYS:HD3	1.90	0.42
55:P4:24:VAL:O	55:P4:28:ILE:HG12	2.20	0.42
57:V1:81:LEU:O	57:V1:85:MET:HG2	2.20	0.42
1:A:77:PRO:HG3	2:B:141:ARG:HG3	2.02	0.41
3:C:178:ASP:CG	3:C:179:ASN:H	2.22	0.41
3:C:246:PHE:CZ	3:C:250:ILE:HD11	2.56	0.41
5:E:148:SER:O	5:E:148:SER:OG	2.30	0.41
11:N:232:PRO:HD2	11:N:235:ALA:HB3	2.01	0.41
3:O:143:GLY:N	3:O:146:SER:OG	2.53	0.41
17:5M:340:ASN:ND2	17:5M:396:THR:O	2.53	0.41
23:A6:36:PRO:O	23:A6:39:MET:HB2	2.20	0.41
43:G1:24:ARG:HH12	60:G1:702:PC1:H142	1.60	0.41
43:G1:141:ASP:O	43:G1:159:LYS:HG3	2.20	0.41
46:S1:146:LYS:HB3	46:S1:149:THR:HG23	2.02	0.41
46:S1:257:LEU:HD13	46:S1:262:SER:HB2	2.02	0.41
58:V2:28:LEU:O	58:V2:115:ARG:NH2	2.46	0.41
1:M:225:THR:HB	1:M:333:GLN:HE22	1.85	0.41
1:M:409:PRO:HB3	1:M:508:PRO:HB2	2.01	0.41
5:Q:132:LYS:HA	5:Q:132:LYS:HD2	1.90	0.41
13:2M:390:ILE:HG21	15:4M:151:ILE:HD11	2.02	0.41
15:4M:230:MET:O	15:4M:234:HIS:HB3	2.20	0.41
17:5M:508:GLU:O	17:5M:512:ALA:CB	2.68	0.41
40:FD:77:ILE:HD11	40:FD:149:LEU:HD11	2.02	0.41
46:S1:263:GLY:O	46:S1:266:ILE:HG12	2.20	0.41
46:S1:380:GLU:HB2	46:S1:579:ALA:HA	2.01	0.41
47:S2:72:TYR:CZ	47:S2:388:VAL:HG13	2.54	0.41
47:S2:232:ASP:HB2	47:S2:249:VAL:HG11	2.02	0.41
49:S4:64:ARG:HE	49:S4:66:LYS:HZ1	1.68	0.41
52:S7:81:PRO:HA	52:S7:119:CYS:O	2.20	0.41
57:V1:174:GLY:HA3	57:V1:221:PHE:CE1	2.55	0.41
1:A:514:ASP:OD2	3:C:230:TYR:OH	2.29	0.41
1:M:44:PRO:HG2	1:M:47:ALA:HB2	2.01	0.41
11:N:121:LEU:HD12	11:N:121:LEU:HA	1.94	0.41
63:O:405:3PE:H262	4:P:274:ILE:HG21	2.02	0.41
13:2M:139:LEU:HD11	16:4L:64:LEU:HD13	2.02	0.41
13:2M:358:THR:HG22	40:FD:83:ARG:HH12	1.85	0.41
16:4L:5:LYS:NZ	55:P4:22:ASP:OD1	2.51	0.41
17:5M:3:LEU:HD22	17:5M:7:PHE:HE2	1.85	0.41
17:5M:170:VAL:HG13	17:5M:238:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:5M:302:ILE:HD11	17:5M:429:PHE:CD1	2.55	0.41
17:5M:324:PHE:O	17:5M:328:ILE:HG12	2.20	0.41
22:A5:72:GLU:OE1	22:A5:72:GLU:HA	2.20	0.41
37:B9:26:LEU:HD12	37:B9:26:LEU:HA	1.93	0.41
39:BK:43:ARG:HG2	39:BK:44:PRO:HD2	2.01	0.41
43:G1:192:LEU:HD23	43:G1:192:LEU:HA	1.86	0.41
48:S3:114:GLU:OE2	48:S3:118:MET:HG3	2.21	0.41
51:S6:64:ALA:HB1	51:S6:77:ILE:HD11	2.03	0.41
57:V1:250:LYS:HD3	57:V1:409:GLN:HB3	2.03	0.41
57:V1:401:PHE:CE1	57:V1:405:GLU:HG3	2.55	0.41
58:V2:99:PRO:HA	58:V2:100:PRO:HD3	1.96	0.41
3:C:114:SER:HB3	3:C:115:PRO:HD3	2.03	0.41
11:N:78:LYS:O	11:N:89:ALA:HA	2.20	0.41
4:P:116:LEU:HD11	4:P:156:PHE:HZ	1.85	0.41
4:P:192:VAL:HG12	4:P:252:VAL:HG22	2.02	0.41
12:1M:104:ASN:O	12:1M:165:CYS:HB3	2.21	0.41
12:1M:146:SER:OG	12:1M:300:TRP:NE1	2.42	0.41
15:4M:389:MET:HG2	17:5M:172:ARG:HH22	1.85	0.41
17:5M:570:ASN:OD1	36:B8:66:ILE:HG23	2.20	0.41
20:A2:18:MET:HG2	20:A2:52:GLU:HG2	2.02	0.41
24:A7:75:ARG:HD3	47:S2:90:LEU:HD11	2.02	0.41
30:AC:74:LEU:HA	30:AC:77:VAL:HG12	2.01	0.41
40:FD:87:ILE:HB	40:FD:135:GLN:HE22	1.86	0.41
46:S1:722:ASN:O	46:S1:723:PHE:HB3	2.19	0.41
52:S7:209:HIS:O	52:S7:213:LYS:HG3	2.20	0.41
53:S8:160:THR:HG21	53:S8:190:HIS:CD2	2.55	0.41
3:C:329:GLN:HE22	6:F:27:ARG:HH12	1.67	0.41
1:M:323:ARG:HB3	1:M:509:ILE:CD1	2.51	0.41
4:P:243:THR:HG22	8:T:6:PRO:HB2	2.03	0.41
8:T:21:CYS:HB3	8:T:55:CYS:HB3	1.79	0.41
13:2M:216:PHE:CZ	13:2M:278:THR:HG21	2.55	0.41
13:2M:328:ILE:HD12	13:2M:484:LEU:HD23	2.03	0.41
14:3M:80:TRP:CD2	14:3M:95:MET:HG2	2.55	0.41
15:4M:297:THR:O	15:4M:301:GLN:HG2	2.20	0.41
15:4M:298:THR:OG1	15:4M:310:TYR:HB3	2.21	0.41
17:5M:78:PHE:HE1	17:5M:86:LEU:HD11	1.85	0.41
22:A5:26:VAL:HG23	22:A5:29:ALA:HB2	2.03	0.41
24:A7:43:ARG:HH21	24:A7:47:PRO:HG3	1.85	0.41
24:A7:70:PHE:HB2	46:S1:153:LYS:HD3	2.03	0.41
28:AL:123:LEU:HD23	28:AL:126:GLU:HB2	2.02	0.41
30:AC:65:PHE:HA	30:AC:69:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:L2:162:ILE:HD13	45:L2:168:LEU:HD11	2.01	0.41
46:S1:307:ASP:HB2	46:S1:315:ARG:HG2	2.02	0.41
47:S2:103:VAL:HG13	47:S2:242:TYR:CE1	2.51	0.41
48:S3:3:ASN:OD1	48:S3:84:SER:HB3	2.20	0.41
48:S3:63:ASP:HB2	48:S3:119:PHE:HE1	1.86	0.41
48:S3:117:ASP:OD2	48:S3:134:THR:HG23	2.21	0.41
52:S7:84:PHE:HB3	52:S7:122:VAL:HA	2.02	0.41
1:A:527:TYR:OXT	9:J:24:ASN:N	2.40	0.41
3:C:190:TYR:HA	62:C:502:HEM:HBB2	2.01	0.41
4:D:195:LEU:HG	4:D:215:ASN:ND2	2.36	0.41
1:M:71:PHE:HE1	11:N:177:VAL:HG12	1.85	0.41
13:2M:64:LEU:HD21	59:X1:83:GLY:HA2	2.01	0.41
13:2M:125:MET:HG2	13:2M:261:SER:CB	2.50	0.41
13:2M:416:SER:OG	27:AK:131:TYR:OH	2.25	0.41
14:3M:80:TRP:CE2	14:3M:84:LEU:HD21	2.55	0.41
17:5M:587:GLU:HG3	34:B4:23:LEU:HD22	2.03	0.41
20:A2:12:LYS:NZ	20:A2:65:ASP:HB3	2.36	0.41
20:A2:32:VAL:O	20:A2:36:TYR:HB3	2.19	0.41
22:A5:54:ARG:NE	22:A5:58:GLU:OE2	2.52	0.41
22:A5:120:ILE:HG13	48:S3:21:LYS:NZ	2.36	0.41
22:A5:136:PRO:HA	22:A5:137:PRO:HD3	1.93	0.41
25:A8:37:LEU:HD23	25:A8:37:LEU:HA	1.86	0.41
27:AK:84:LEU:HD23	27:AK:84:LEU:HA	1.88	0.41
37:B9:56:VAL:O	37:B9:62:ILE:HD11	2.21	0.41
43:G1:70:ASP:HB3	43:G1:91:GLY:HA2	2.03	0.41
43:G1:130:HIS:CE1	44:G2:105:LEU:HD21	2.55	0.41
45:L2:157:GLU:HB3	45:L2:158:PRO:HD2	2.02	0.41
53:S8:85:LYS:HD3	53:S8:86:TYR:CE1	2.56	0.41
57:V1:140:TYR:O	57:V1:268:THR:HA	2.20	0.41
59:X1:85:LEU:HD12	59:X1:85:LEU:HA	1.92	0.41
4:D:72:CYS:SG	4:D:191:TYR:HA	2.60	0.41
4:D:294:VAL:HG12	7:G:15:LEU:O	2.21	0.41
1:M:452:GLY:C	1:M:455:PRO:HD2	2.41	0.41
3:O:41:LEU:HD21	3:O:242:PHE:HB2	2.03	0.41
5:Q:115:LEU:HB3	5:Q:119:ARG:NH1	2.36	0.41
12:1M:37:ARG:HD2	52:S7:102:ASP:OD2	2.21	0.41
65:1M:402:U10:H121	65:1M:402:U10:H162	1.92	0.41
13:2M:180:LEU:HD23	13:2M:180:LEU:HA	1.86	0.41
13:2M:233:VAL:CG1	13:2M:293:LEU:HD13	2.51	0.41
13:2M:308:LEU:HD11	13:2M:352:VAL:HG21	2.01	0.41
15:4M:12:LEU:HD13	15:4M:68:PHE:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:4L:28:ILE:HG22	16:4L:80:PHE:CZ	2.55	0.41
29:AM:86:LEU:HD23	54:P1:82:LEU:HD11	2.02	0.41
43:G1:100:ILE:HD13	43:G1:128:VAL:HB	2.02	0.41
44:G2:124:ASP:N	44:G2:141:ASP:OD1	2.45	0.41
44:G2:190:ARG:NH1	44:G2:196:GLU:OE2	2.44	0.41
55:P4:21:MET:HA	55:P4:24:VAL:HG12	2.03	0.41
57:V1:359:ILE:HD13	57:V1:373:VAL:HG21	2.02	0.41
1:A:118:GLY:HA2	1:A:178:TYR:HA	2.02	0.41
13:2M:366:LEU:HD13	13:2M:436:MET:HG3	2.03	0.41
14:3M:1:MET:HB2	14:3M:2:LEU:H	1.66	0.41
15:4M:156:ILE:HA	15:4M:160:TRP:CE3	2.56	0.41
15:4M:289:ILE:HD13	15:4M:289:ILE:HA	1.92	0.41
15:4M:296:LEU:HD13	17:5M:580:PHE:CD2	2.56	0.41
17:5M:451:ARG:HE	17:5M:455:ARG:NH2	2.19	0.41
18:6M:41:LEU:HD11	18:6M:53:PHE:CE2	2.55	0.41
23:A6:37:SER:O	23:A6:41:ILE:HG12	2.20	0.41
25:A8:32:GLU:HA	25:A8:35:ASP:HB2	2.03	0.41
27:AK:17:PHE:O	27:AK:21:ILE:HG12	2.20	0.41
47:S2:42:PRO:HG3	47:S2:366:LEU:HD23	2.03	0.41
58:V2:226:ARG:H	58:V2:226:ARG:HG2	1.70	0.41
1:A:120:TRP:CZ2	1:A:458:GLU:HA	2.56	0.41
1:A:196:ILE:O	1:A:200:SER:HB2	2.21	0.41
1:A:382:ASN:ND2	3:C:6:GLN:H	2.18	0.41
4:D:185:ARG:NH2	64:D:501:HEC:O1A	2.48	0.41
1:M:464:LEU:HD23	1:M:464:LEU:HA	1.87	0.41
11:N:253:THR:OG1	11:N:256:ARG:HD3	2.21	0.41
11:N:447:LEU:HD23	11:N:447:LEU:HA	1.89	0.41
5:Q:77:PRO:HB2	5:Q:80:VAL:HG22	2.03	0.41
8:T:8:ASP:HB3	8:T:11:ARG:HG3	2.03	0.41
13:2M:61:GLY:O	13:2M:65:LEU:HG	2.21	0.41
13:2M:279:LEU:HA	13:2M:279:LEU:HD23	1.81	0.41
13:2M:358:THR:HG22	40:FD:83:ARG:NH1	2.36	0.41
13:2M:485:SER:HA	13:2M:488:LEU:OXT	2.21	0.41
15:4M:282:PHE:CZ	15:4M:286:LEU:HD11	2.56	0.41
17:5M:584:VAL:HG22	34:B4:36:LEU:HD13	2.01	0.41
23:A6:33:ARG:NH1	31:AB:96:GLU:OE2	2.54	0.41
28:AL:80:LYS:H	28:AL:80:LYS:HG2	1.68	0.41
33:B3:45:LEU:HD23	33:B3:45:LEU:HA	1.90	0.41
37:B9:47:ARG:NH2	37:B9:51:GLU:OE2	2.49	0.41
44:G2:131:SER:HB2	45:L2:150:LEU:HD11	2.02	0.41
60:G2:801:PC1:H362	59:X1:50:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:S1:79:VAL:HG22	46:S1:145:ILE:HD12	2.02	0.41
46:S1:221:GLN:HE21	46:S1:247:GLU:HG3	1.85	0.41
46:S1:351:ARG:NH1	46:S1:355:GLY:O	2.54	0.41
47:S2:71:ASP:OD2	47:S2:335:LYS:NZ	2.37	0.41
53:S8:89:GLU:HG2	53:S8:90:THR:H	1.85	0.41
54:P1:81:ASP:HA	54:P1:84:GLN:HG3	2.03	0.41
57:V1:60:PHE:CZ	57:V1:295:ARG:HB3	2.56	0.41
57:V1:360:CYS:HA	57:V1:363:VAL:HG12	2.02	0.41
59:X1:54:LYS:HB3	59:X1:55:PRO:HD3	2.03	0.41
1:A:147:THR:HG21	1:A:195:ASP:OD2	2.21	0.41
1:A:310:VAL:HG21	1:A:396:LYS:HD2	2.02	0.41
4:D:163:GLU:O	4:D:167:ARG:HG3	2.20	0.41
1:M:294:LYS:HB3	1:M:294:LYS:HE2	1.86	0.41
1:M:302:ASP:HB3	1:M:304:THR:HG22	2.03	0.41
11:N:460:LYS:HG3	11:N:464:GLU:OE2	2.21	0.41
4:P:137:ASP:HB3	4:P:146:PHE:CE1	2.56	0.41
8:T:10:LYS:NZ	8:T:14:GLU:OE2	2.51	0.41
8:T:18:LYS:HB3	8:T:19:PRO:HD3	2.03	0.41
13:2M:22:LEU:O	13:2M:26:VAL:HG23	2.21	0.41
16:4L:60:LEU:O	16:4L:64:LEU:HG	2.21	0.41
16:4L:85:ARG:HH11	16:4L:85:ARG:HG3	1.85	0.41
18:6M:47:ASP:O	18:6M:51:MET:HG2	2.22	0.41
20:A2:32:VAL:O	20:A2:36:TYR:CB	2.69	0.41
27:AK:59:THR:O	27:AK:63:MET:HG3	2.21	0.41
47:S2:141:LEU:HD21	47:S2:178:PHE:CE2	2.56	0.41
53:S8:52:LEU:O	53:S8:56:ILE:HG12	2.21	0.41
4:D:244:GLU:OE1	8:H:11:ARG:NH2	2.54	0.40
11:N:111:GLU:HA	11:N:247:PHE:HE1	1.86	0.40
11:N:177:VAL:O	11:N:181:ARG:HB2	2.21	0.40
4:P:291:ARG:HD3	4:P:291:ARG:HA	1.78	0.40
12:1M:21:ALA:O	12:1M:24:VAL:HG12	2.21	0.40
12:1M:196:ALA:HB2	12:1M:203:PHE:CD2	2.56	0.40
12:1M:303:PHE:HE1	60:1M:401:PC1:H32	1.86	0.40
13:2M:162:THR:HG22	16:4L:82:ILE:HD12	2.02	0.40
16:4L:75:ILE:HD11	18:6M:162:ALA:HA	2.03	0.40
35:B7:75:LYS:HB2	35:B7:75:LYS:HE3	1.74	0.40
43:G1:41:ARG:NH2	45:L2:236:LEU:O	2.43	0.40
43:G1:103:ASN:HD22	44:G2:105:LEU:HB2	1.86	0.40
45:L2:220:LEU:O	45:L2:224:ILE:HD12	2.20	0.40
47:S2:38:GLU:HA	47:S2:38:GLU:OE2	2.21	0.40
47:S2:112:LEU:HD21	47:S2:141:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:S2:246:ASP:O	47:S2:273:ARG:NH2	2.54	0.40
48:S3:94:GLU:OE1	48:S3:94:GLU:N	2.45	0.40
57:V1:452:ILE:HB	70:V1:502:SF4:S2	2.60	0.40
61:O:407:CDL:H722	61:O:408:CDL:H121	2.03	0.40
9:V:40:ARG:HA	9:V:40:ARG:HD2	1.88	0.40
65:1M:402:U10:H71	65:1M:402:U10:H1M1	1.84	0.40
17:5M:98:LEU:HD12	17:5M:101:ILE:HD12	2.03	0.40
17:5M:121:THR:O	17:5M:125:LEU:HG	2.21	0.40
17:5M:345:LYS:HD3	17:5M:345:LYS:HA	1.91	0.40
17:5M:467:LEU:HD23	17:5M:467:LEU:HA	1.95	0.40
17:5M:628:MET:HE2	17:5M:628:MET:HB3	1.87	0.40
18:6M:195:MET:HB2	47:S2:249:VAL:HB	2.04	0.40
26:A9:241:GLY:O	26:A9:242:ASN:OD1	2.38	0.40
26:A9:279:PRO:HG2	26:A9:363:LYS:HA	2.03	0.40
31:AB:67:ASP:OD1	31:AB:67:ASP:N	2.53	0.40
31:AB:106:ASN:OD1	31:AB:106:ASN:N	2.54	0.40
41:C2:41:LEU:HD23	41:C2:41:LEU:HA	1.90	0.40
46:S1:237:ASP:OD1	46:S1:237:ASP:N	2.49	0.40
49:S4:131:TYR:O	49:S4:134:ASN:HB3	2.22	0.40
51:S6:36:LYS:HB2	51:S6:36:LYS:HE3	1.69	0.40
58:V2:134:ARG:HB3	58:V2:175:PRO:HD3	2.03	0.40
1:A:326:ASP:C	1:A:328:ASP:H	2.24	0.40
11:N:87:LYS:HB2	11:N:258:VAL:HG22	2.03	0.40
12:1M:242:LEU:HD12	12:1M:242:LEU:HA	1.90	0.40
15:4M:224:PHE:O	15:4M:228:VAL:HG12	2.22	0.40
15:4M:389:MET:HG2	17:5M:172:ARG:NH2	2.37	0.40
26:A9:178:SER:O	26:A9:213:PRO:HD2	2.21	0.40
26:A9:225:ASN:HB2	26:A9:226:PRO:HD3	2.03	0.40
39:BK:75:LEU:HA	39:BK:78:VAL:HG12	2.03	0.40
42:P2:80:SER:HB2	42:P2:85:ARG:NH1	2.36	0.40
45:L2:161:ILE:HB	45:L2:179:ILE:HG12	2.04	0.40
46:S1:472:TYR:HB3	46:S1:483:HIS:HD2	1.87	0.40
47:S2:233:LEU:HB2	47:S2:332:GLU:HB2	2.03	0.40
47:S2:266:GLU:O	47:S2:270:GLN:HG2	2.22	0.40
58:V2:46:THR:HG22	58:V2:47:GLU:N	2.36	0.40
1:A:159:ILE:HD13	1:A:162:MET:HE1	2.02	0.40
5:E:101:PRO:HA	5:E:102:PRO:HD3	1.96	0.40
1:M:133:ASN:HB3	1:M:250:PRO:HD2	2.04	0.40
1:M:336:VAL:O	1:M:402:GLY:HA3	2.22	0.40
3:O:10:LEU:HA	3:O:13:GLU:HG2	2.03	0.40
3:O:207:LEU:HD13	62:O:403:HEM:HAD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:112:SER:O	4:P:115:ASP:HB2	2.22	0.40
9:V:50:TRP:O	9:V:54:ASN:ND2	2.53	0.40
15:4M:346:SER:O	15:4M:350:LEU:HG	2.22	0.40
17:5M:520:ILE:N	17:5M:521:PRO:HD2	2.37	0.40
17:5M:570:ASN:OD1	36:B8:66:ILE:HD12	2.22	0.40
20:A2:29:ARG:HA	20:A2:32:VAL:HG22	2.03	0.40
26:A9:67:VAL:O	26:A9:92:PRO:HD2	2.22	0.40
26:A9:92:PRO:HB2	26:A9:117:TYR:CD1	2.56	0.40
36:B8:37:VAL:HG12	37:B9:94:THR:HG22	2.03	0.40
44:G2:74:GLY:HA2	45:L2:45:ILE:HG21	2.03	0.40
45:L2:140:GLU:HG2	45:L2:158:PRO:HD3	2.04	0.40
57:V1:156:ARG:HB2	57:V1:190:TYR:CZ	2.57	0.40
57:V1:279:SER:HB2	57:V1:280:PRO:HD3	2.04	0.40
57:V1:309:HIS:CE1	57:V1:389:THR:HB	2.55	0.40
59:X1:84:ARG:HB3	59:X1:94:GLU:OE2	2.21	0.40
1:A:246:THR:HG23	1:A:249:GLY:H	1.87	0.40
3:C:370:ALA:O	3:C:373:PRO:HD2	2.21	0.40
5:E:132:LYS:HD3	5:E:132:LYS:HA	1.96	0.40
1:M:88:LEU:HD11	1:M:477:PHE:CD2	2.56	0.40
15:4M:251:ILE:O	15:4M:255:ILE:HB	2.21	0.40
17:5M:4:LEU:HD11	56:C1:52:ALA:HB2	2.02	0.40
17:5M:44:LEU:HD23	17:5M:44:LEU:HA	1.97	0.40
26:A9:254:ASP:OD2	26:A9:362:HIS:N	2.54	0.40
36:B8:47:LEU:HD23	36:B8:47:LEU:HA	1.92	0.40
40:FD:50:ILE:HG13	40:FD:56:LYS:HD3	2.03	0.40
41:C2:14:LEU:HB2	41:C2:39:MET:HG2	2.03	0.40
43:G1:3:THR:OG1	43:G1:4:LEU:N	2.54	0.40
46:S1:202:SER:OG	51:S6:81:CYS:N	2.54	0.40
46:S1:388:LEU:HD23	46:S1:727:ASP:OD1	2.21	0.40
46:S1:642:LEU:HD23	46:S1:642:LEU:HA	1.95	0.40
46:S1:671:TYR:CD1	46:S1:677:VAL:HG22	2.57	0.40
57:V1:298:ASN:HD22	57:V1:367:TYR:N	2.20	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	478/527 (91%)	462 (97%)	16 (3%)	0	100	100
1	M	479/527 (91%)	468 (98%)	11 (2%)	0	100	100
2	B	440/510 (86%)	427 (97%)	13 (3%)	0	100	100
3	C	384/394 (98%)	365 (95%)	19 (5%)	0	100	100
3	O	382/394 (97%)	367 (96%)	15 (4%)	0	100	100
4	D	241/306 (79%)	235 (98%)	6 (2%)	0	100	100
4	P	241/306 (79%)	234 (97%)	7 (3%)	0	100	100
5	E	72/271 (27%)	71 (99%)	1 (1%)	0	100	100
5	Q	71/271 (26%)	67 (94%)	4 (6%)	0	100	100
6	F	115/122 (94%)	113 (98%)	2 (2%)	0	100	100
6	R	113/122 (93%)	109 (96%)	4 (4%)	0	100	100
7	G	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
7	S	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
8	H	62/69 (90%)	60 (97%)	2 (3%)	0	100	100
8	T	62/69 (90%)	61 (98%)	1 (2%)	0	100	100
9	J	56/72 (78%)	55 (98%)	1 (2%)	0	100	100
9	V	57/72 (79%)	55 (96%)	2 (4%)	0	100	100
10	K	22/81 (27%)	20 (91%)	2 (9%)	0	100	100
10	W	27/81 (33%)	25 (93%)	2 (7%)	0	100	100
11	N	439/506 (87%)	424 (97%)	15 (3%)	0	100	100
12	1M	321/325 (99%)	302 (94%)	18 (6%)	1 (0%)	37	69
13	2M	486/488 (100%)	472 (97%)	14 (3%)	0	100	100
14	3M	86/118 (73%)	85 (99%)	1 (1%)	0	100	100
15	4M	484/495 (98%)	466 (96%)	18 (4%)	0	100	100
16	4L	97/100 (97%)	96 (99%)	1 (1%)	0	100	100
17	5M	661/673 (98%)	637 (96%)	24 (4%)	0	100	100
18	6M	188/205 (92%)	177 (94%)	11 (6%)	0	100	100
19	A1	57/65 (88%)	56 (98%)	1 (2%)	0	100	100
20	A2	88/98 (90%)	81 (92%)	7 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	A3	37/63 (59%)	37 (100%)	0	0	100	100
22	A5	123/169 (73%)	116 (94%)	7 (6%)	0	100	100
23	A6	95/132 (72%)	86 (90%)	9 (10%)	0	100	100
24	A7	107/127 (84%)	101 (94%)	6 (6%)	0	100	100
25	A8	102/106 (96%)	95 (93%)	7 (7%)	0	100	100
26	A9	326/396 (82%)	307 (94%)	19 (6%)	0	100	100
27	AK	147/160 (92%)	143 (97%)	4 (3%)	0	100	100
28	AL	125/156 (80%)	118 (94%)	7 (6%)	0	100	100
29	AM	140/143 (98%)	133 (95%)	7 (5%)	0	100	100
30	AC	80/116 (69%)	74 (92%)	6 (8%)	0	100	100
31	AB	83/128 (65%)	78 (94%)	5 (6%)	0	100	100
32	B2	47/66 (71%)	45 (96%)	2 (4%)	0	100	100
33	B3	45/68 (66%)	43 (96%)	2 (4%)	0	100	100
34	B4	67/71 (94%)	66 (98%)	1 (2%)	0	100	100
35	B7	75/98 (76%)	73 (97%)	2 (3%)	0	100	100
36	B8	93/125 (74%)	90 (97%)	3 (3%)	0	100	100
37	B9	109/115 (95%)	106 (97%)	3 (3%)	0	100	100
38	BJ	95/106 (90%)	91 (96%)	4 (4%)	0	100	100
39	BK	75/118 (64%)	75 (100%)	0	0	100	100
40	FD	120/158 (76%)	115 (96%)	5 (4%)	0	100	100
41	C2	72/82 (88%)	71 (99%)	1 (1%)	0	100	100
42	P2	28/115 (24%)	28 (100%)	0	0	100	100
43	G1	229/270 (85%)	221 (96%)	8 (4%)	0	100	100
44	G2	254/273 (93%)	242 (95%)	12 (5%)	0	100	100
45	L2	208/256 (81%)	200 (96%)	8 (4%)	0	100	100
46	S1	685/746 (92%)	663 (97%)	22 (3%)	0	100	100
47	S2	372/394 (94%)	352 (95%)	20 (5%)	0	100	100
48	S3	183/190 (96%)	175 (96%)	8 (4%)	0	100	100
49	S4	114/146 (78%)	109 (96%)	5 (4%)	0	100	100
50	S5	63/83 (76%)	63 (100%)	0	0	100	100
51	S6	69/103 (67%)	65 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	S7	156/213 (73%)	149 (96%)	7 (4%)	0	100	100
53	S8	179/222 (81%)	174 (97%)	5 (3%)	0	100	100
54	P1	83/91 (91%)	81 (98%)	2 (2%)	0	100	100
55	P4	51/61 (84%)	51 (100%)	0	0	100	100
56	C1	70/87 (80%)	65 (93%)	5 (7%)	0	100	100
57	V1	428/492 (87%)	412 (96%)	16 (4%)	0	100	100
58	V2	218/251 (87%)	209 (96%)	8 (4%)	1 (0%)	25	60
59	X1	97/101 (96%)	94 (97%)	3 (3%)	0	100	100
All	All	11995/14208 (84%)	11540 (96%)	453 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	1M	201	ALA
58	V2	174	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	403/438 (92%)	403 (100%)	0	100	100
1	M	404/438 (92%)	402 (100%)	2 (0%)	86	93
2	B	377/428 (88%)	376 (100%)	1 (0%)	91	96
3	C	331/339 (98%)	327 (99%)	4 (1%)	67	85
3	O	329/339 (97%)	328 (100%)	1 (0%)	91	96
4	D	198/247 (80%)	198 (100%)	0	100	100
4	P	198/247 (80%)	198 (100%)	0	100	100
5	E	62/233 (27%)	62 (100%)	0	100	100
5	Q	61/233 (26%)	61 (100%)	0	100	100
6	F	103/107 (96%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	R	101/107 (94%)	101 (100%)	0	100	100
7	G	64/65 (98%)	64 (100%)	0	100	100
7	S	64/65 (98%)	64 (100%)	0	100	100
8	H	59/63 (94%)	59 (100%)	0	100	100
8	T	59/63 (94%)	59 (100%)	0	100	100
9	J	48/59 (81%)	48 (100%)	0	100	100
9	V	49/59 (83%)	49 (100%)	0	100	100
10	K	15/66 (23%)	15 (100%)	0	100	100
10	W	19/66 (29%)	19 (100%)	0	100	100
11	N	370/414 (89%)	369 (100%)	1 (0%)	91	96
12	1M	269/271 (99%)	269 (100%)	0	100	100
13	2M	408/408 (100%)	408 (100%)	0	100	100
14	3M	82/105 (78%)	82 (100%)	0	100	100
15	4M	422/431 (98%)	422 (100%)	0	100	100
16	4L	86/86 (100%)	86 (100%)	0	100	100
17	5M	561/571 (98%)	561 (100%)	0	100	100
18	6M	173/186 (93%)	173 (100%)	0	100	100
19	A1	46/52 (88%)	46 (100%)	0	100	100
20	A2	75/81 (93%)	75 (100%)	0	100	100
21	A3	33/51 (65%)	33 (100%)	0	100	100
22	A5	112/149 (75%)	112 (100%)	0	100	100
23	A6	91/118 (77%)	91 (100%)	0	100	100
24	A7	95/111 (86%)	95 (100%)	0	100	100
25	A8	94/96 (98%)	94 (100%)	0	100	100
26	A9	279/334 (84%)	279 (100%)	0	100	100
27	AK	113/121 (93%)	113 (100%)	0	100	100
28	AL	109/134 (81%)	108 (99%)	1 (1%)	75	89
29	AM	115/116 (99%)	115 (100%)	0	100	100
30	AC	75/102 (74%)	75 (100%)	0	100	100
31	AB	73/112 (65%)	73 (100%)	0	100	100
32	B2	42/52 (81%)	42 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	B3	37/55 (67%)	37 (100%)	0	100	100
34	B4	58/59 (98%)	58 (100%)	0	100	100
35	B7	71/88 (81%)	71 (100%)	0	100	100
36	B8	79/101 (78%)	79 (100%)	0	100	100
37	B9	93/97 (96%)	93 (100%)	0	100	100
38	BJ	86/95 (90%)	86 (100%)	0	100	100
39	BK	69/100 (69%)	69 (100%)	0	100	100
40	FD	108/141 (77%)	108 (100%)	0	100	100
41	C2	60/67 (90%)	60 (100%)	0	100	100
42	P2	23/85 (27%)	23 (100%)	0	100	100
43	G1	184/216 (85%)	183 (100%)	1 (0%)	86	93
44	G2	214/226 (95%)	214 (100%)	0	100	100
45	L2	176/217 (81%)	176 (100%)	0	100	100
46	S1	571/622 (92%)	570 (100%)	1 (0%)	92	97
47	S2	325/340 (96%)	323 (99%)	2 (1%)	84	92
48	S3	174/179 (97%)	174 (100%)	0	100	100
49	S4	95/119 (80%)	95 (100%)	0	100	100
50	S5	59/72 (82%)	59 (100%)	0	100	100
51	S6	63/94 (67%)	63 (100%)	0	100	100
52	S7	133/180 (74%)	133 (100%)	0	100	100
53	S8	162/193 (84%)	162 (100%)	0	100	100
54	P1	80/85 (94%)	80 (100%)	0	100	100
55	P4	47/53 (89%)	47 (100%)	0	100	100
56	C1	63/71 (89%)	63 (100%)	0	100	100
57	V1	348/401 (87%)	348 (100%)	0	100	100
58	V2	191/216 (88%)	191 (100%)	0	100	100
59	X1	82/84 (98%)	82 (100%)	0	100	100
All	All	10318/12019 (86%)	10304 (100%)	14 (0%)	92	98

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	448	ARG

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Mol	Chain	Res	Type
3	C	179	ASN
3	C	222	MET
3	C	387	THR
3	C	394	THR
1	M	253	ASN
1	M	520	ARG
11	N	394	LYS
3	O	85	ARG
28	AL	37	ASN
43	G1	218	ASN
46	S1	460	ARG
47	S2	113	ASN
47	S2	394	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	GLN
2	B	388	GLN
15	4M	327	ASN
15	4M	409	GLN
16	4L	27	ASN
17	5M	340	ASN
26	A9	154	HIS
27	AK	95	ASN
32	B2	22	HIS
43	G1	130	HIS
43	G1	202	GLN
44	G2	218	ASN
46	S1	285	ASN
48	S3	3	ASN
57	V1	481	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 46 ligands modelled in this entry, 3 are monoatomic - leaving 43 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
63	3PE	O	401	-	35,35,50	0.35	0	38,40,55	0.34	0
63	3PE	O	405	-	38,38,50	0.34	0	41,43,55	0.30	0
61	CDL	C	501	-	63,63,99	0.36	0	69,75,111	0.32	0
63	3PE	C	505	-	33,33,50	0.37	0	36,38,55	0.32	0
70	SF4	S8	702	53	0,12,12	-	-	-	-	-
61	CDL	D	502	-	67,67,99	0.35	0	73,79,111	0.30	0
71	FES	S1	902	46	0,4,4	-	-	-	-	-
63	3PE	C	504	-	37,37,50	0.35	0	40,42,55	0.33	0
61	CDL	O	408	-	54,54,99	0.39	0	60,66,111	0.39	0
70	SF4	S7	301	52	0,12,12	-	-	-	-	-
60	PC1	G1	701	-	26,26,53	0.39	0	32,34,61	0.36	0
60	PC1	A	601	-	37,37,53	0.34	0	43,45,61	0.30	0
62	HEM	O	403	3	42,50,50	1.24	5 (11%)	46,82,82	1.66	7 (15%)
63	3PE	M	601	-	44,44,50	0.32	0	47,49,55	0.30	0
64	HEC	D	501	4	32,50,50	1.95	4 (12%)	30,82,82	2.76	17 (56%)
60	PC1	G1	702	-	36,36,53	0.34	0	42,44,61	0.36	0
63	3PE	O	406	-	32,32,50	0.36	0	35,37,55	0.36	0
70	SF4	V1	502	57	0,12,12	-	-	-	-	-
62	HEM	C	503	3	42,50,50	1.24	5 (11%)	46,82,82	1.66	7 (15%)
70	SF4	S1	903	46	0,12,12	-	-	-	-	-
66	NDP	A9	401	-	47,52,52	0.58	1 (2%)	61,80,80	0.59	1 (1%)
61	CDL	A	602	-	68,68,99	0.35	0	74,80,111	0.30	0
63	3PE	R	201	-	50,50,50	0.30	0	53,55,55	0.29	0
60	PC1	M	603	-	39,39,53	0.33	0	45,47,61	0.30	0
61	CDL	M	602	-	69,69,99	0.35	0	75,81,111	0.35	0
70	SF4	S8	701	53	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	PC1	1M	401	-	44,44,53	0.32	0	50,52,61	0.30	0
61	CDL	O	404	-	63,63,99	0.36	0	69,75,111	0.38	0
65	U10	1M	402	-	40,40,63	2.49	18 (45%)	49,51,79	1.66	13 (26%)
61	CDL	O	407	-	62,62,99	0.37	0	68,74,111	0.38	0
67	ZMP	AB	201	31	23,28,36	0.77	1 (4%)	27,35,45	1.04	1 (3%)
60	PC1	P4	101	-	53,53,53	0.29	0	59,61,61	0.29	0
64	HEC	P	501	4	32,50,50	1.93	4 (12%)	30,82,82	2.76	17 (56%)
61	CDL	C	506	-	58,58,99	0.37	0	64,70,111	0.31	0
60	PC1	G2	801	-	39,39,53	0.32	0	45,47,61	0.32	0
62	HEM	C	502	3	42,50,50	1.24	4 (9%)	46,82,82	1.72	10 (21%)
62	HEM	O	402	3	42,50,50	1.23	4 (9%)	46,82,82	1.68	8 (17%)
72	FMN	V1	501	-	33,33,33	0.20	0	48,50,50	0.34	0
63	3PE	G	101	-	36,36,50	0.35	0	39,41,55	0.30	0
67	ZMP	AC	201	30	23,28,36	0.82	1 (4%)	27,35,45	1.37	3 (11%)
71	FES	V2	300	58	0,4,4	-	-	-	-	-
60	PC1	S	101	-	37,37,53	0.34	0	43,45,61	0.32	0
70	SF4	S1	901	46	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
63	3PE	O	401	-	-	11/39/39/54	-
63	3PE	O	405	-	-	9/42/42/54	-
61	CDL	C	501	-	-	14/74/74/110	-
63	3PE	C	505	-	-	2/37/37/54	-
70	SF4	S8	702	53	-	-	0/6/5/5
61	CDL	D	502	-	-	11/78/78/110	-
71	FES	S1	902	46	-	-	0/1/1/1
63	3PE	C	504	-	-	9/41/41/54	-
61	CDL	O	408	-	-	13/65/65/110	-
70	SF4	S7	301	52	-	-	0/6/5/5
60	PC1	G1	701	-	-	4/30/30/57	-
60	PC1	A	601	-	-	2/41/41/57	-
62	HEM	O	403	3	-	6/12/54/54	-
63	3PE	M	601	-	-	11/48/48/54	-
64	HEC	D	501	4	-	2/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PC1	G1	702	-	-	8/40/40/57	-
63	3PE	O	406	-	-	7/36/36/54	-
70	SF4	V1	502	57	-	-	0/6/5/5
62	HEM	C	503	3	-	6/12/54/54	-
70	SF4	S1	903	46	-	-	0/6/5/5
66	NDP	A9	401	-	-	14/30/77/77	0/5/5/5
61	CDL	A	602	-	-	15/79/79/110	-
63	3PE	R	201	-	-	5/54/54/54	-
60	PC1	M	603	-	-	3/43/43/57	-
61	CDL	M	602	-	-	12/80/80/110	-
70	SF4	S8	701	53	-	-	0/6/5/5
60	PC1	1M	401	-	-	10/48/48/57	-
61	CDL	O	404	-	-	14/74/74/110	-
65	U10	1M	402	-	-	10/36/60/87	0/1/1/1
61	CDL	O	407	-	-	18/73/73/110	-
67	ZMP	AB	201	31	-	12/33/35/43	-
60	PC1	P4	101	-	-	14/57/57/57	-
64	HEC	P	501	4	-	4/10/54/54	-
61	CDL	C	506	-	-	13/69/69/110	-
60	PC1	G2	801	-	-	9/43/43/57	-
62	HEM	C	502	3	-	5/12/54/54	-
62	HEM	O	402	3	-	5/12/54/54	-
72	FMN	V1	501	-	-	5/18/18/18	0/3/3/3
63	3PE	G	101	-	-	5/40/40/54	-
67	ZMP	AC	201	30	-	9/33/35/43	-
71	FES	V2	300	58	-	-	0/1/1/1
60	PC1	S	101	-	-	10/41/41/57	-
70	SF4	S1	901	46	-	-	0/6/5/5

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	1M	402	U10	C6-C1	10.26	1.53	1.35
64	P	501	HEC	C3C-C2C	-6.01	1.34	1.40
64	D	501	HEC	C3C-C2C	-5.98	1.34	1.40
64	D	501	HEC	C2B-C3B	-5.85	1.34	1.40
64	P	501	HEC	C2B-C3B	-5.68	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	1M	402	U10	C4-C3	4.81	1.53	1.36
62	O	402	HEM	C4D-ND	-3.64	1.33	1.40
62	C	502	HEM	C4D-ND	-3.56	1.34	1.40
62	C	503	HEM	C4D-ND	-3.54	1.34	1.40
62	O	403	HEM	C4D-ND	-3.51	1.34	1.40
64	D	501	HEC	CBC-CAC	-3.43	1.36	1.49
64	P	501	HEC	CBC-CAC	-3.42	1.36	1.49
62	C	502	HEM	C1B-NB	-3.21	1.34	1.40
62	O	402	HEM	C1B-NB	-3.11	1.34	1.40
62	O	403	HEM	C1B-NB	-3.10	1.34	1.40
62	C	503	HEM	C1B-NB	-3.09	1.34	1.40
65	1M	402	U10	C26-C24	2.78	1.57	1.51
65	1M	402	U10	C31-C29	2.74	1.56	1.51
62	O	403	HEM	C1D-ND	-2.69	1.33	1.38
62	C	503	HEM	C1D-ND	-2.69	1.33	1.38
62	O	402	HEM	C1D-ND	-2.68	1.33	1.38
62	C	502	HEM	C1D-ND	-2.67	1.33	1.38
65	1M	402	U10	C7-C8	2.66	1.54	1.50
65	1M	402	U10	C21-C19	2.64	1.56	1.51
67	AC	201	ZMP	C9-C10	2.59	1.53	1.50
67	AB	201	ZMP	C9-C10	2.47	1.53	1.50
62	C	502	HEM	CHB-C1B	2.39	1.40	1.34
65	1M	402	U10	O5-C5	-2.36	1.18	1.23
62	O	402	HEM	CHB-C1B	2.36	1.40	1.34
65	1M	402	U10	C11-C9	2.36	1.56	1.51
65	1M	402	U10	C27-C28	2.35	1.57	1.50
64	D	501	HEC	CBB-CAB	-2.32	1.40	1.49
64	P	501	HEC	CBB-CAB	-2.32	1.40	1.49
65	1M	402	U10	C7-C6	2.28	1.55	1.51
65	1M	402	U10	C6-C5	2.28	1.52	1.46
65	1M	402	U10	C22-C23	2.24	1.57	1.50
65	1M	402	U10	O2-C2	-2.23	1.18	1.23
65	1M	402	U10	C16-C14	2.20	1.55	1.51
65	1M	402	U10	O3-C3M	-2.19	1.40	1.45
62	O	403	HEM	CHB-C1B	2.19	1.39	1.34
62	O	403	HEM	CHA-C4D	2.13	1.39	1.34
65	1M	402	U10	O4-C4M	-2.13	1.40	1.45
62	C	503	HEM	CHB-C1B	2.12	1.39	1.34
65	1M	402	U10	C12-C13	2.11	1.56	1.50
65	1M	402	U10	C17-C18	2.10	1.56	1.50
62	C	503	HEM	CHA-C4D	2.07	1.39	1.34
66	A9	401	NDP	P2B-O2B	2.01	1.63	1.59

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	D	501	HEC	CBB-CAB-C3B	-7.56	109.81	127.49
64	P	501	HEC	CBB-CAB-C3B	-7.42	110.13	127.49
64	P	501	HEC	CBC-CAC-C3C	-5.85	113.79	127.49
64	D	501	HEC	CBC-CAC-C3C	-5.80	113.93	127.49
62	C	502	HEM	CHC-C4B-NB	4.75	129.54	124.44
62	O	402	HEM	CHC-C4B-NB	4.68	129.47	124.44
62	O	403	HEM	CHC-C4B-NB	4.52	129.29	124.44
64	P	501	HEC	CMD-C2D-C1D	-4.44	121.94	128.46
62	C	503	HEM	CHC-C4B-NB	4.44	129.21	124.44
62	C	502	HEM	CHB-C1B-NB	4.38	129.79	124.37
64	D	501	HEC	CMD-C2D-C1D	-4.37	122.06	128.46
62	C	503	HEM	CHB-C1B-NB	4.08	129.43	124.37
62	O	402	HEM	CHB-C1B-NB	4.01	129.34	124.37
62	O	403	HEM	CHB-C1B-NB	4.00	129.33	124.37
64	D	501	HEC	CMB-C2B-C1B	-3.70	123.03	128.46
67	AC	201	ZMP	C15-N2-C16	3.65	129.11	122.55
64	P	501	HEC	CBD-CAD-C3D	3.58	118.55	112.54
64	D	501	HEC	CMB-C2B-C3B	3.48	129.91	125.82
64	P	501	HEC	CMB-C2B-C1B	-3.43	123.43	128.46
62	O	403	HEM	C4D-ND-C1D	3.36	109.19	105.21
65	1M	402	U10	C17-C18-C19	-3.31	120.04	127.62
62	C	503	HEM	C4D-ND-C1D	3.30	109.11	105.21
64	P	501	HEC	CMC-C2C-C3C	3.19	129.57	125.82
64	D	501	HEC	CMC-C2C-C3C	3.18	129.56	125.82
65	1M	402	U10	C27-C28-C29	-3.17	120.38	127.62
64	P	501	HEC	CMB-C2B-C3B	3.16	129.53	125.82
64	D	501	HEC	CBD-CAD-C3D	3.14	117.82	112.54
65	1M	402	U10	C12-C13-C14	-3.14	120.43	127.62
65	1M	402	U10	C22-C23-C24	-3.13	120.47	127.62
62	C	502	HEM	C1B-NB-C4B	3.11	108.89	105.21
62	O	402	HEM	C4D-ND-C1D	3.07	108.84	105.21
62	C	502	HEM	CHA-C4D-ND	2.99	128.08	124.37
62	C	502	HEM	C4D-ND-C1D	2.99	108.75	105.21
62	O	403	HEM	CHD-C1D-ND	2.98	127.64	124.44
62	O	402	HEM	CHA-C4D-ND	2.94	128.01	124.37
65	1M	402	U10	C1M-C1-C6	-2.89	119.69	124.45
67	AB	201	ZMP	O1-C10-C9	-2.88	120.65	123.98
64	P	501	HEC	C4C-C3C-C2C	2.88	109.46	106.35
65	1M	402	U10	C10-C9-C11	2.87	120.21	115.23
64	D	501	HEC	C4C-C3C-C2C	2.87	109.45	106.35
62	C	503	HEM	CHA-C4D-ND	2.86	127.92	124.37
62	O	402	HEM	CHD-C1D-ND	2.83	127.48	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	1M	402	U10	C15-C14-C16	2.83	120.13	115.23
64	D	501	HEC	O1D-CGD-CBD	-2.82	114.14	123.09
62	C	503	HEM	CHD-C1D-ND	2.82	127.47	124.44
62	O	402	HEM	C1B-NB-C4B	2.80	108.52	105.21
65	1M	402	U10	C7-C8-C9	-2.78	122.04	126.83
64	P	501	HEC	O1D-CGD-CBD	-2.77	114.30	123.09
62	O	403	HEM	CHA-C4D-ND	2.75	127.78	124.37
65	1M	402	U10	C25-C24-C26	2.75	120.00	115.23
64	P	501	HEC	CMC-C2C-C1C	-2.72	124.47	128.46
67	AC	201	ZMP	C17-C16-N2	2.72	121.64	116.48
65	1M	402	U10	C30-C29-C31	2.71	119.93	115.23
64	D	501	HEC	CMC-C2C-C1C	-2.68	124.53	128.46
62	C	502	HEM	CHD-C1D-ND	2.67	127.31	124.44
65	1M	402	U10	C20-C19-C21	2.65	119.82	115.23
62	C	503	HEM	CHB-C1B-C2B	-2.60	119.56	126.94
65	1M	402	U10	C7-C6-C1	-2.58	120.46	124.89
62	O	403	HEM	CHB-C1B-C2B	-2.52	119.81	126.94
64	P	501	HEC	CBA-CAA-C2A	2.52	116.70	112.55
67	AC	201	ZMP	O1-C10-C9	-2.50	121.10	123.98
64	P	501	HEC	CMA-C3A-C2A	2.49	129.64	124.94
64	P	501	HEC	CMD-C2D-C3D	2.42	129.50	124.94
64	D	501	HEC	O1A-CGA-CBA	-2.40	115.47	123.09
64	D	501	HEC	CMD-C2D-C3D	2.39	129.46	124.94
64	P	501	HEC	O1A-CGA-CBA	-2.36	115.61	123.09
62	O	403	HEM	C1B-NB-C4B	2.36	108.00	105.21
64	D	501	HEC	CBA-CAA-C2A	2.32	116.38	112.55
64	D	501	HEC	CMA-C3A-C2A	2.31	129.29	124.94
62	C	502	HEM	CHB-C1B-C2B	-2.29	120.45	126.94
66	A9	401	NDP	C5A-C6A-N6A	2.28	123.78	120.31
64	P	501	HEC	C1D-C2D-C3D	2.24	108.55	107.00
62	C	503	HEM	C1B-NB-C4B	2.23	107.85	105.21
62	O	402	HEM	CHB-C1B-C2B	-2.22	120.66	126.94
64	D	501	HEC	C2B-C3B-C4B	2.17	108.69	106.35
62	C	502	HEM	O2A-CGA-CBA	2.16	120.81	114.00
64	D	501	HEC	C1D-C2D-C3D	2.14	108.48	107.00
64	P	501	HEC	O2A-CGA-O1A	2.09	128.71	123.33
62	O	402	HEM	C4B-C3B-C2B	-2.09	105.36	107.28
62	C	502	HEM	C4B-C3B-C2B	-2.09	105.36	107.28
64	D	501	HEC	O2A-CGA-O1A	2.05	128.61	123.33
65	1M	402	U10	C8-C7-C6	-2.05	107.03	112.08
64	P	501	HEC	C2B-C3B-C4B	2.05	108.56	106.35
62	C	502	HEM	C3B-C2B-C1B	2.03	107.93	106.41

There are no chirality outliers.

All (307) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	S	101	PC1	C11-O13-P-O12
60	S	101	PC1	C11-O13-P-O14
60	S	101	PC1	C11-O13-P-O11
60	S	101	PC1	C1-O11-P-O13
60	1M	401	PC1	C1-O11-P-O12
60	1M	401	PC1	C1-O11-P-O13
60	1M	401	PC1	C2-C1-O11-P
60	G2	801	PC1	C11-O13-P-O11
60	G2	801	PC1	C1-O11-P-O12
60	P4	101	PC1	C11-O13-P-O12
60	P4	101	PC1	C11-O13-P-O14
60	P4	101	PC1	C11-O13-P-O11
60	P4	101	PC1	C1-O11-P-O14
60	P4	101	PC1	C1-O11-P-O13
61	A	602	CDL	CB2-OB2-PB2-OB3
61	A	602	CDL	CB2-OB2-PB2-OB5
61	A	602	CDL	CB3-OB5-PB2-OB3
61	A	602	CDL	CB3-OB5-PB2-OB4
61	C	501	CDL	CA2-OA2-PA1-OA4
61	C	501	CDL	CA2-OA2-PA1-OA5
61	C	501	CDL	CA3-OA5-PA1-OA2
61	C	501	CDL	CB2-OB2-PB2-OB3
61	C	506	CDL	CA3-OA5-PA1-OA3
61	C	506	CDL	CB2-OB2-PB2-OB3
61	C	506	CDL	CB2-OB2-PB2-OB4
61	C	506	CDL	CB2-OB2-PB2-OB5
61	C	506	CDL	OB5-CB3-CB4-OB6
61	D	502	CDL	CB2-OB2-PB2-OB3
61	M	602	CDL	CB2-OB2-PB2-OB3
61	M	602	CDL	CB3-OB5-PB2-OB2
61	M	602	CDL	CB3-OB5-PB2-OB3
61	M	602	CDL	CB3-OB5-PB2-OB4
61	O	404	CDL	CA2-OA2-PA1-OA5
61	O	404	CDL	CB3-OB5-PB2-OB2
61	O	404	CDL	CB3-OB5-PB2-OB3
61	O	407	CDL	CA2-OA2-PA1-OA4
61	O	407	CDL	CA2-OA2-PA1-OA5
61	O	407	CDL	CA3-OA5-PA1-OA2
61	O	407	CDL	CA3-OA5-PA1-OA4
61	O	407	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
61	O	407	CDL	CB2-OB2-PB2-OB4
61	O	407	CDL	CB2-OB2-PB2-OB5
61	O	408	CDL	CA3-OA5-PA1-OA4
61	O	408	CDL	CB3-OB5-PB2-OB2
61	O	408	CDL	CB3-OB5-PB2-OB3
61	O	408	CDL	CB3-OB5-PB2-OB4
62	C	502	HEM	C2B-C3B-CAB-CBB
63	C	504	3PE	C11-O13-P-O11
63	C	504	3PE	C11-O13-P-O12
63	C	504	3PE	C11-O13-P-O14
63	C	505	3PE	C1-O11-P-O12
63	C	505	3PE	C1-O11-P-O13
63	G	101	3PE	C1-O11-P-O12
63	G	101	3PE	C1-O11-P-O13
63	G	101	3PE	C1-O11-P-O14
63	M	601	3PE	C1-O11-P-O12
63	M	601	3PE	C1-O11-P-O13
63	M	601	3PE	C1-O11-P-O14
63	M	601	3PE	C11-O13-P-O11
63	M	601	3PE	C11-O13-P-O14
63	M	601	3PE	O13-C11-C12-N
63	O	401	3PE	C1-O11-P-O12
63	O	401	3PE	C11-O13-P-O11
63	O	405	3PE	C11-O13-P-O11
63	O	405	3PE	C11-O13-P-O12
63	O	405	3PE	C11-O13-P-O14
63	O	405	3PE	O13-C11-C12-N
63	O	406	3PE	C11-O13-P-O14
63	O	406	3PE	O13-C11-C12-N
63	R	201	3PE	C11-O13-P-O11
63	R	201	3PE	C11-O13-P-O14
65	1M	402	U10	C12-C11-C9-C10
66	A9	401	NDP	C5B-O5B-PA-O1A
66	A9	401	NDP	C5B-O5B-PA-O2A
66	A9	401	NDP	C5B-O5B-PA-O3
66	A9	401	NDP	C1B-C2B-O2B-P2B
66	A9	401	NDP	C2N-C3N-C7N-N7N
67	AC	201	ZMP	C17-C16-N2-C15
67	AC	201	ZMP	S1-C11-C12-N1
67	AB	201	ZMP	O3-C16-C17-C18
67	AB	201	ZMP	N2-C16-C17-C18
67	AB	201	ZMP	C12-C11-S1-C10

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Mol	Chain	Res	Type	Atoms
67	AB	201	ZMP	O1-C10-S1-C11
67	AB	201	ZMP	C9-C10-S1-C11
72	V1	501	FMN	N10-C1'-C2'-O2'
72	V1	501	FMN	C5'-O5'-P-O1P
72	V1	501	FMN	C5'-O5'-P-O2P
72	V1	501	FMN	C5'-O5'-P-O3P
65	1M	402	U10	C12-C11-C9-C8
67	AB	201	ZMP	C14-C13-N1-C12
67	AC	201	ZMP	O3-C16-N2-C15
65	1M	402	U10	C14-C16-C17-C18
65	1M	402	U10	C19-C21-C22-C23
61	C	501	CDL	C1-CB2-OB2-PB2
67	AB	201	ZMP	O2-C13-N1-C12
60	G1	702	PC1	C11-C12-N-C15
62	C	502	HEM	C2A-CAA-CBA-CGA
62	O	402	HEM	C2A-CAA-CBA-CGA
60	S	101	PC1	C11-C12-N-C15
60	G1	701	PC1	C11-C12-N-C13
60	G1	702	PC1	C11-C12-N-C13
65	1M	402	U10	C9-C11-C12-C13
60	1M	401	PC1	C11-C12-N-C15
60	G1	701	PC1	C11-C12-N-C14
60	G1	702	PC1	C11-C12-N-C14
60	S	101	PC1	C11-C12-N-C13
60	S	101	PC1	C11-C12-N-C14
60	1M	401	PC1	C11-C12-N-C13
60	1M	401	PC1	C11-C12-N-C14
60	G1	701	PC1	C11-C12-N-C15
62	C	502	HEM	C4B-C3B-CAB-CBB
60	M	603	PC1	C11-C12-N-C15
60	1M	401	PC1	O11-C1-C2-C3
61	C	501	CDL	OB5-CB3-CB4-CB6
61	C	506	CDL	OB5-CB3-CB4-CB6
61	M	602	CDL	OB5-CB3-CB4-CB6
61	D	502	CDL	CB3-CB4-CB6-OB8
63	C	504	3PE	C2-C1-O11-P
61	O	404	CDL	OB5-CB3-CB4-OB6
61	O	407	CDL	OB5-CB3-CB4-OB6
61	D	502	CDL	OB6-CB4-CB6-OB8
67	AC	201	ZMP	C4-C5-C6-C7
63	O	401	3PE	C2-C1-O11-P
60	M	603	PC1	C11-C12-N-C13

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Mol	Chain	Res	Type	Atoms
60	1M	401	PC1	O11-C1-C2-O21
61	M	602	CDL	OB5-CB3-CB4-OB6
61	M	602	CDL	CA4-CA3-OA5-PA1
67	AC	201	ZMP	O1-C10-S1-C11
63	O	405	3PE	O31-C31-C32-C33
66	A9	401	NDP	PN-O3-PA-O5B
65	1M	402	U10	C25-C24-C26-C27
67	AC	201	ZMP	C9-C10-S1-C11
61	O	404	CDL	C11-C12-C13-C14
62	C	503	HEM	C2B-C3B-CAB-CBB
62	O	402	HEM	C2B-C3B-CAB-CBB
62	O	403	HEM	C2B-C3B-CAB-CBB
61	A	602	CDL	C17-C18-C19-C20
64	P	501	HEC	C1A-C2A-CAA-CBA
61	O	407	CDL	C53-C54-C55-C56
61	A	602	CDL	OB5-CB3-CB4-OB6
60	G2	801	PC1	C12-C11-O13-P
67	AB	201	ZMP	C14-C15-N2-C16
61	C	501	CDL	C1-CA2-OA2-PA1
60	G1	702	PC1	C26-C27-C28-C29
60	G1	702	PC1	O13-C11-C12-N
60	G2	801	PC1	O13-C11-C12-N
60	P4	101	PC1	O13-C11-C12-N
66	A9	401	NDP	PA-O3-PN-O1N
61	A	602	CDL	C16-C17-C18-C19
61	O	407	CDL	OB5-CB3-CB4-CB6
67	AC	201	ZMP	C19-C18-C21-O5
67	AB	201	ZMP	C19-C18-C21-O5
67	AB	201	ZMP	C20-C18-C21-O5
60	P4	101	PC1	C2-C1-O11-P
61	A	602	CDL	CA4-CA3-OA5-PA1
61	C	501	CDL	OB5-CB3-CB4-OB6
61	O	407	CDL	OA5-CA3-CA4-OA6
63	O	401	3PE	O11-C1-C2-O21
60	M	603	PC1	C11-C12-N-C14
60	S	101	PC1	C1-O11-P-O14
60	1M	401	PC1	C11-O13-P-O14
60	G1	701	PC1	C1-O11-P-O12
60	G2	801	PC1	C11-O13-P-O14
60	P4	101	PC1	C1-O11-P-O12
61	A	602	CDL	CB2-OB2-PB2-OB4
61	A	602	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
61	C	501	CDL	CA2-OA2-PA1-OA3
61	C	501	CDL	CA3-OA5-PA1-OA3
61	C	501	CDL	CB2-OB2-PB2-OB5
61	C	506	CDL	CA3-OA5-PA1-OA2
61	C	506	CDL	CA3-OA5-PA1-OA4
61	D	502	CDL	CB2-OB2-PB2-OB4
61	D	502	CDL	CB2-OB2-PB2-OB5
61	O	404	CDL	CA2-OA2-PA1-OA3
61	O	404	CDL	CA3-OA5-PA1-OA2
61	O	404	CDL	CA3-OA5-PA1-OA3
61	O	404	CDL	CA3-OA5-PA1-OA4
61	O	404	CDL	CB3-OB5-PB2-OB4
61	O	407	CDL	CA3-OA5-PA1-OA3
61	O	408	CDL	CA2-OA2-PA1-OA3
61	O	408	CDL	CA2-OA2-PA1-OA4
61	O	408	CDL	CA2-OA2-PA1-OA5
61	O	408	CDL	CA3-OA5-PA1-OA2
61	O	408	CDL	CA3-OA5-PA1-OA3
63	C	504	3PE	C1-O11-P-O12
63	C	504	3PE	C1-O11-P-O13
63	C	504	3PE	C1-O11-P-O14
63	O	401	3PE	C1-O11-P-O13
63	O	401	3PE	C1-O11-P-O14
63	O	401	3PE	C11-O13-P-O14
63	O	405	3PE	C1-O11-P-O12
63	O	405	3PE	C1-O11-P-O13
63	O	405	3PE	C1-O11-P-O14
63	R	201	3PE	C11-O13-P-O12
63	R	201	3PE	O13-C11-C12-N
65	1M	402	U10	C30-C29-C31-C32
61	C	506	CDL	C1-CA2-OA2-PA1
61	O	407	CDL	C1-CB2-OB2-PB2
61	A	602	CDL	C15-C16-C17-C18
65	1M	402	U10	C24-C26-C27-C28
61	O	404	CDL	OB5-CB3-CB4-CB6
63	O	401	3PE	O11-C1-C2-C3
61	A	602	CDL	OA5-CA3-CA4-OA6
66	A9	401	NDP	C2B-O2B-P2B-O3X
65	1M	402	U10	C28-C29-C31-C32
62	O	402	HEM	C4B-C3B-CAB-CBB
62	O	403	HEM	C4B-C3B-CAB-CBB
63	M	601	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
61	O	404	CDL	CB6-CB4-OB6-CB5
61	O	408	CDL	CA3-CA4-OA6-CA5
62	O	402	HEM	CAD-CBD-CGD-O2D
66	A9	401	NDP	O4D-C1D-N1N-C6N
62	O	402	HEM	CAD-CBD-CGD-O1D
64	P	501	HEC	CAD-CBD-CGD-O2D
72	V1	501	FMN	C4'-C5'-O5'-P
62	O	403	HEM	CAD-CBD-CGD-O1D
61	A	602	CDL	OA5-CA3-CA4-CA6
61	O	407	CDL	OA5-CA3-CA4-CA6
63	C	504	3PE	O21-C2-C3-O31
66	A9	401	NDP	C2B-O2B-P2B-O1X
61	A	602	CDL	C32-C31-CA7-OA8
65	1M	402	U10	C23-C24-C26-C27
64	P	501	HEC	CAD-CBD-CGD-O1D
62	C	502	HEM	CAD-CBD-CGD-O2D
63	O	406	3PE	O21-C21-C22-C23
63	C	504	3PE	C1-C2-C3-O31
62	O	403	HEM	CAA-CBA-CGA-O2A
62	O	403	HEM	CAA-CBA-CGA-O1A
63	O	406	3PE	O11-C1-C2-O21
63	O	406	3PE	O11-C1-C2-C3
62	C	502	HEM	CAD-CBD-CGD-O1D
62	O	403	HEM	CAD-CBD-CGD-O2D
64	P	501	HEC	C3A-C2A-CAA-CBA
60	P4	101	PC1	C2A-C2B-C2C-C2D
62	C	503	HEM	CAA-CBA-CGA-O2A
60	G1	702	PC1	O21-C21-C22-C23
61	M	602	CDL	CA6-CA4-OA6-CA5
63	O	405	3PE	O32-C31-C32-C33
60	P4	101	PC1	C38-C39-C3A-C3B
62	C	503	HEM	CAA-CBA-CGA-O1A
61	O	404	CDL	C1-CB2-OB2-PB2
62	C	503	HEM	C4B-C3B-CAB-CBB
63	O	406	3PE	C24-C25-C26-C27
60	1M	401	PC1	C36-C37-C38-C39
61	C	501	CDL	C72-C71-CB7-OB8
60	S	101	PC1	O31-C31-C32-C33
61	C	501	CDL	C32-C31-CA7-OA8
62	C	503	HEM	CAD-CBD-CGD-O1D
60	P4	101	PC1	O21-C21-C22-C23
60	P4	101	PC1	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
61	C	506	CDL	C52-C51-CB5-OB6
61	O	407	CDL	C52-C51-CB5-OB6
61	D	502	CDL	C32-C31-CA7-OA8
63	M	601	3PE	O21-C21-C22-C23
63	O	401	3PE	O31-C31-C32-C33
67	AB	201	ZMP	C6-C7-C8-C9
63	G	101	3PE	O31-C31-C32-C33
63	O	406	3PE	C23-C24-C25-C26
66	A9	401	NDP	O4B-C4B-C5B-O5B
66	A9	401	NDP	C2B-O2B-P2B-O2X
64	D	501	HEC	CAD-CBD-CGD-O2D
61	C	506	CDL	C72-C71-CB7-OB8
61	O	408	CDL	C12-C11-CA5-OA6
63	O	401	3PE	O21-C2-C3-O31
64	D	501	HEC	CAD-CBD-CGD-O1D
60	G2	801	PC1	O31-C31-C32-C33
61	D	502	CDL	C52-C51-CB5-OB6
61	D	502	CDL	C72-C71-CB7-OB8
61	M	602	CDL	C52-C51-CB5-OB6
63	M	601	3PE	C28-C29-C2A-C2B
63	M	601	3PE	C26-C27-C28-C29
61	A	602	CDL	C72-C71-CB7-OB8
67	AC	201	ZMP	C20-C18-C21-O5
60	G1	702	PC1	O31-C31-C32-C33
61	M	602	CDL	CA3-CA4-OA6-CA5
61	O	404	CDL	CB3-CB4-OB6-CB5
61	O	407	CDL	CA3-CA4-OA6-CA5
61	O	407	CDL	CA6-CA4-OA6-CA5
61	O	408	CDL	CA6-CA4-OA6-CA5
60	P4	101	PC1	O22-C21-C22-C23
60	A	601	PC1	C11-C12-N-C15
60	P4	101	PC1	O32-C31-C32-C33
60	S	101	PC1	O32-C31-C32-C33
61	C	506	CDL	C72-C71-CB7-OB9
61	O	407	CDL	C52-C51-CB5-OB7
66	A9	401	NDP	C2N-C3N-C7N-O7N
62	C	503	HEM	CAD-CBD-CGD-O2D
61	O	408	CDL	C12-C11-CA5-OA7
63	M	601	3PE	O22-C21-C22-C23
60	G2	801	PC1	O21-C21-C22-C23
60	G2	801	PC1	O32-C31-C32-C33
61	D	502	CDL	C72-C71-CB7-OB9

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Mol	Chain	Res	Type	Atoms
63	O	401	3PE	O32-C31-C32-C33
61	C	501	CDL	C72-C71-CB7-OB9
61	C	506	CDL	C52-C51-CB5-OB7
63	G	101	3PE	O32-C31-C32-C33
67	AB	201	ZMP	N2-C16-C17-O4
60	A	601	PC1	C22-C23-C24-C25
60	G1	702	PC1	O32-C31-C32-C33
61	D	502	CDL	C32-C31-CA7-OA9
61	D	502	CDL	C52-C51-CB5-OB7
67	AC	201	ZMP	C17-C18-C21-O5
61	M	602	CDL	C52-C51-CB5-OB7
60	G2	801	PC1	O22-C21-C22-C23
66	A9	401	NDP	PA-O3-PN-O2N
61	M	602	CDL	C32-C31-CA7-OA8
63	R	201	3PE	O31-C31-C32-C33

There are no ring outliers.

36 monomers are involved in 85 short contacts:

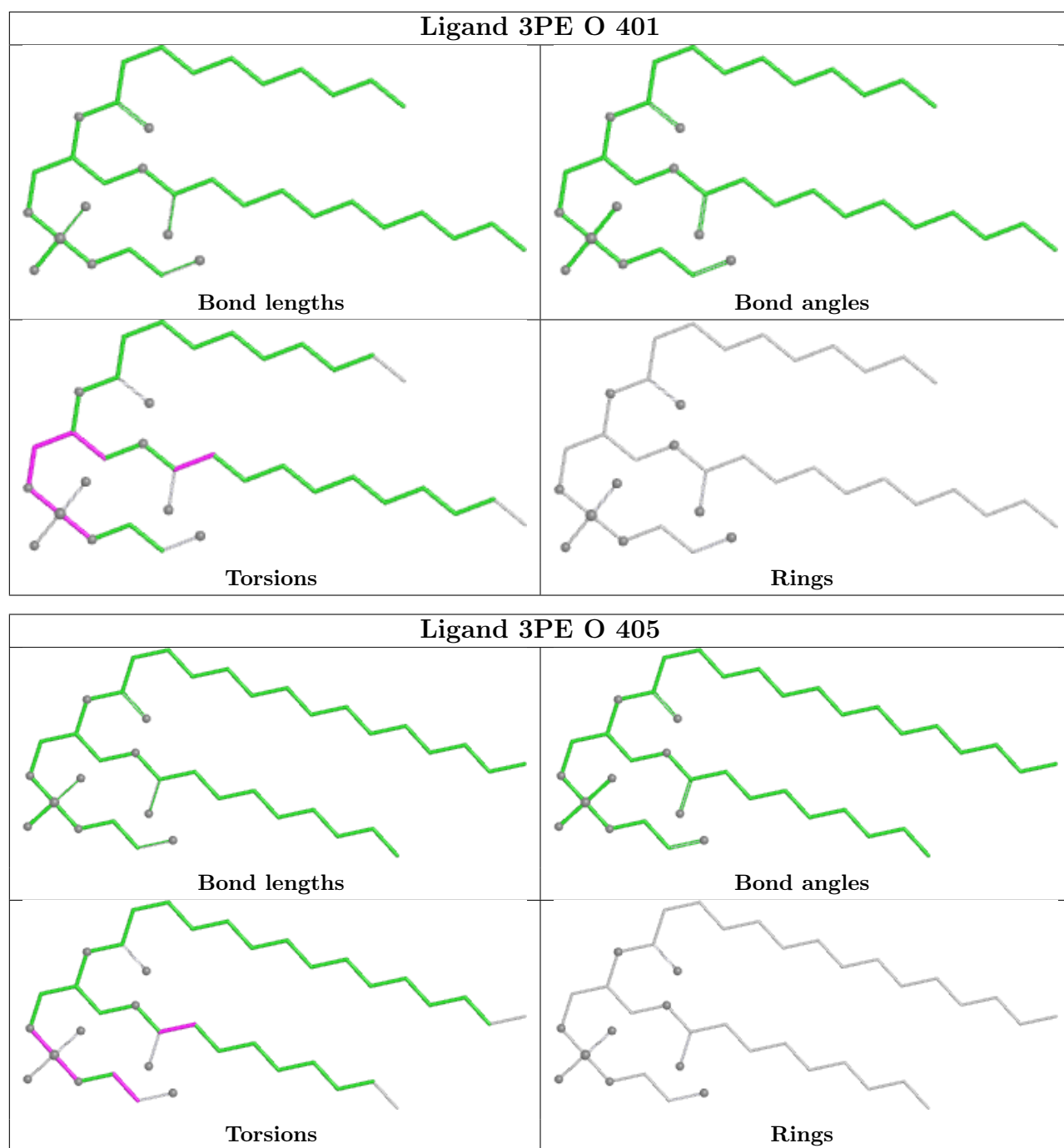
Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	O	401	3PE	1	0
63	O	405	3PE	2	0
61	C	501	CDL	2	0
63	C	505	3PE	2	0
70	S8	702	SF4	1	0
61	D	502	CDL	2	0
61	O	408	CDL	3	0
60	A	601	PC1	1	0
62	O	403	HEM	7	0
63	M	601	3PE	5	0
64	D	501	HEC	3	0
60	G1	702	PC1	3	0
63	O	406	3PE	1	0
70	V1	502	SF4	4	0
62	C	503	HEM	5	0
70	S1	903	SF4	1	0
66	A9	401	NDP	4	0
61	A	602	CDL	3	0
63	R	201	3PE	4	0
60	M	603	PC1	2	0
61	M	602	CDL	4	0
70	S8	701	SF4	1	0

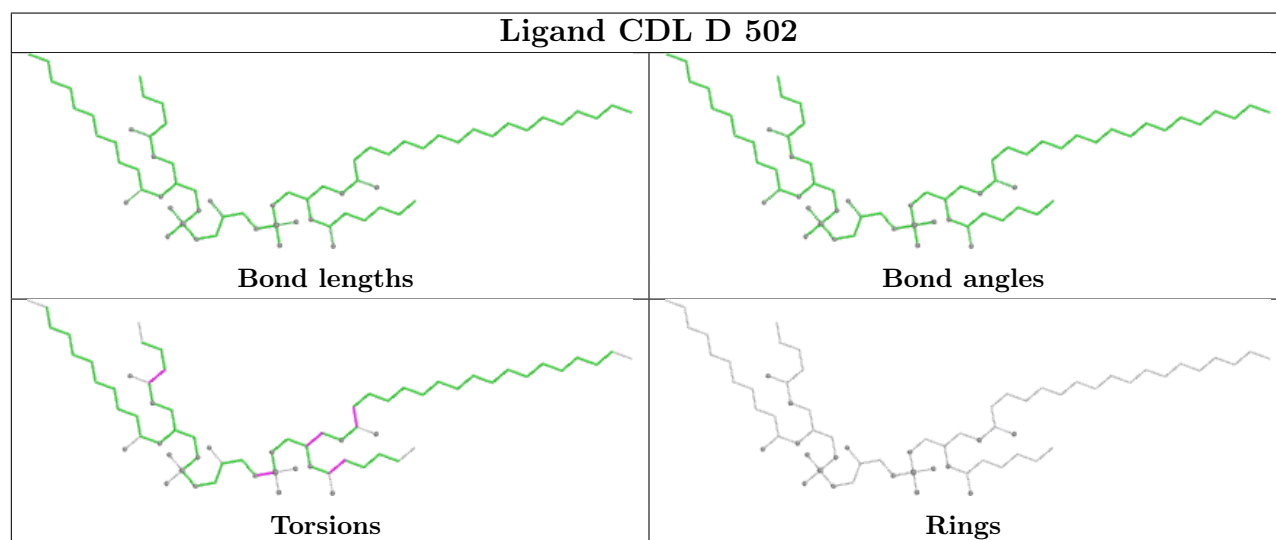
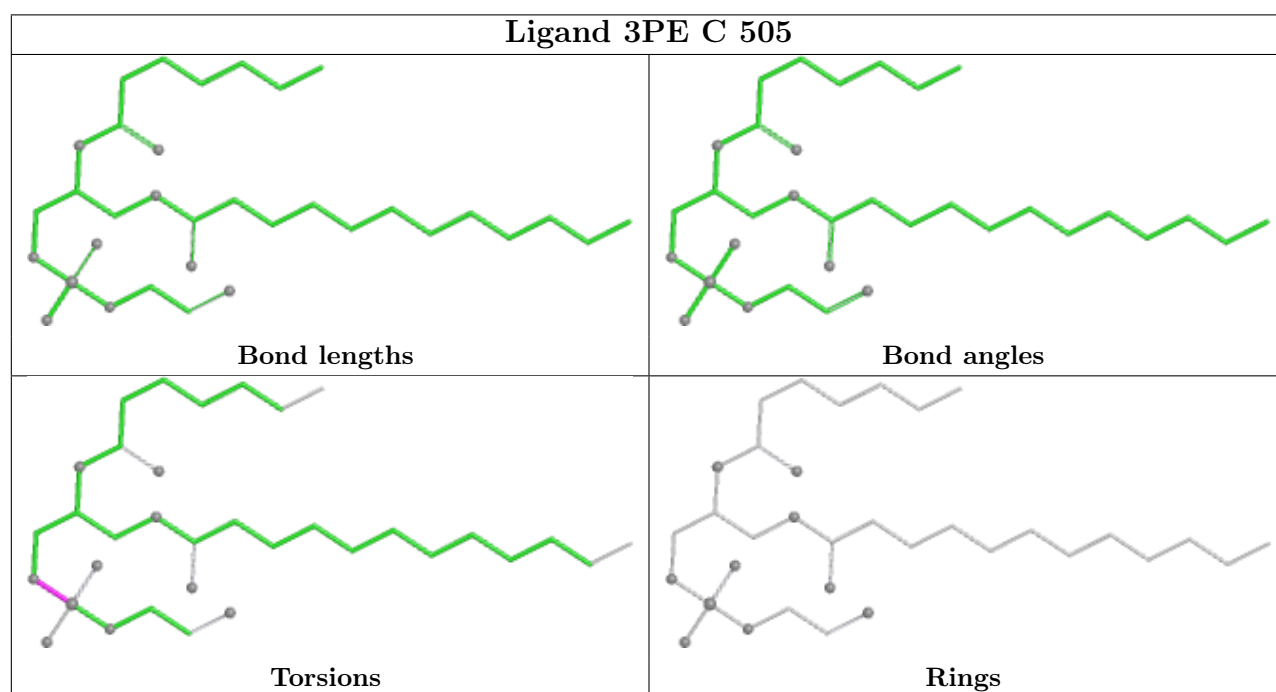
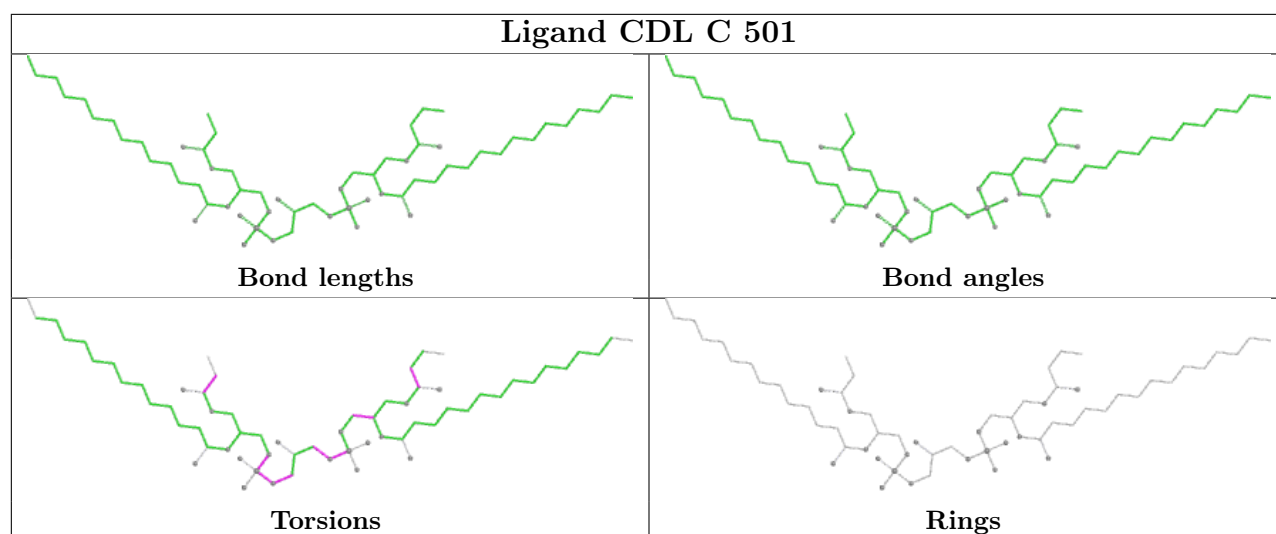
Continued on next page...

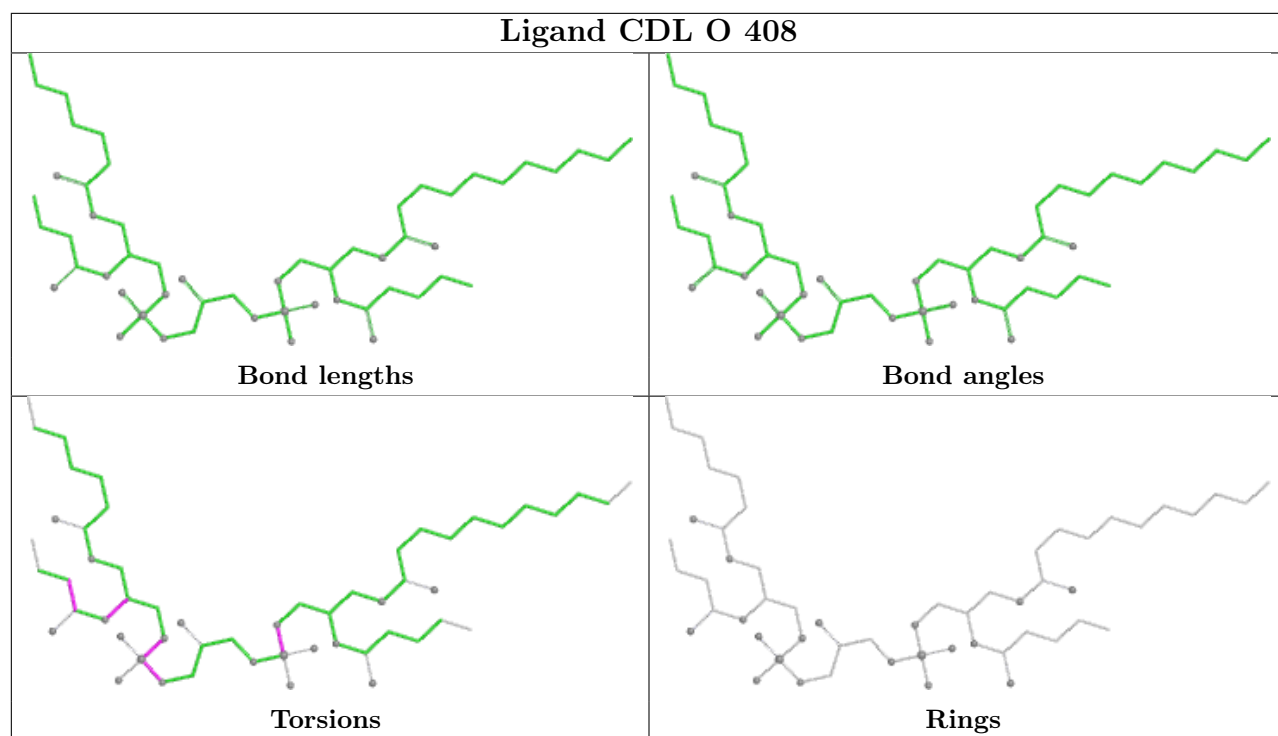
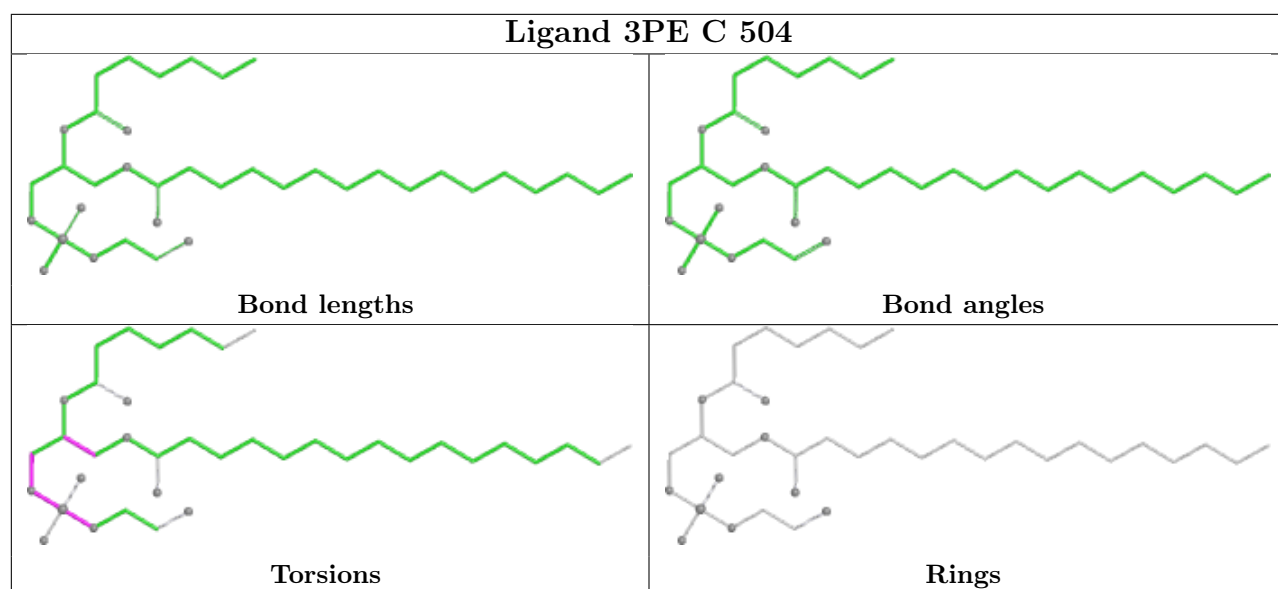
Continued from previous page...

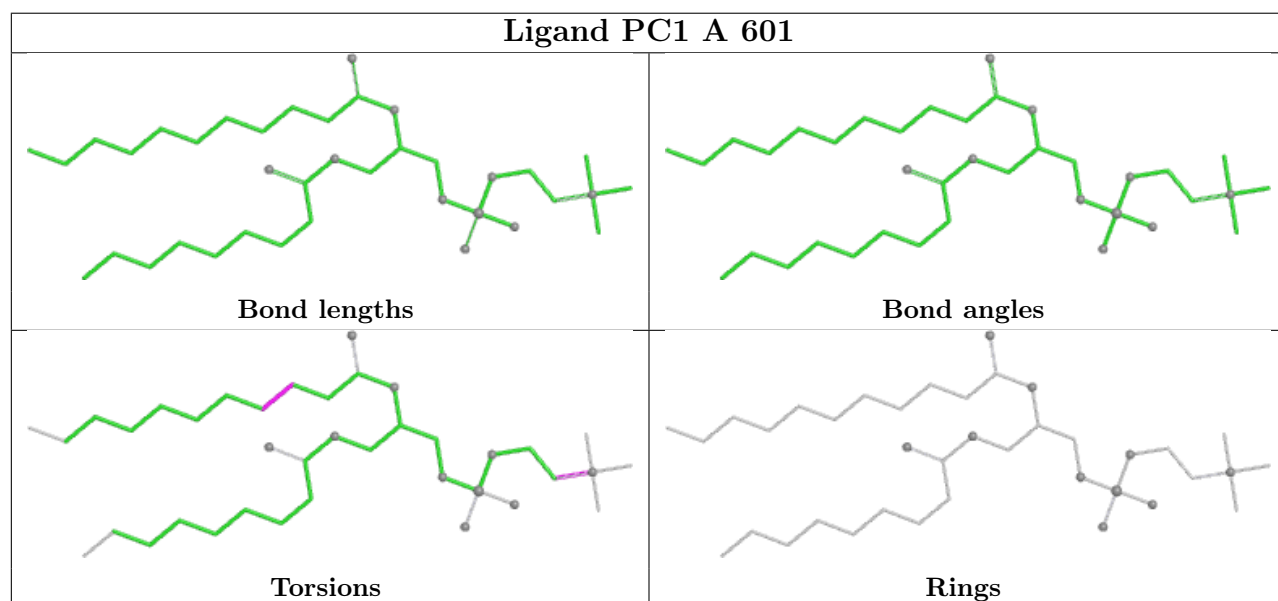
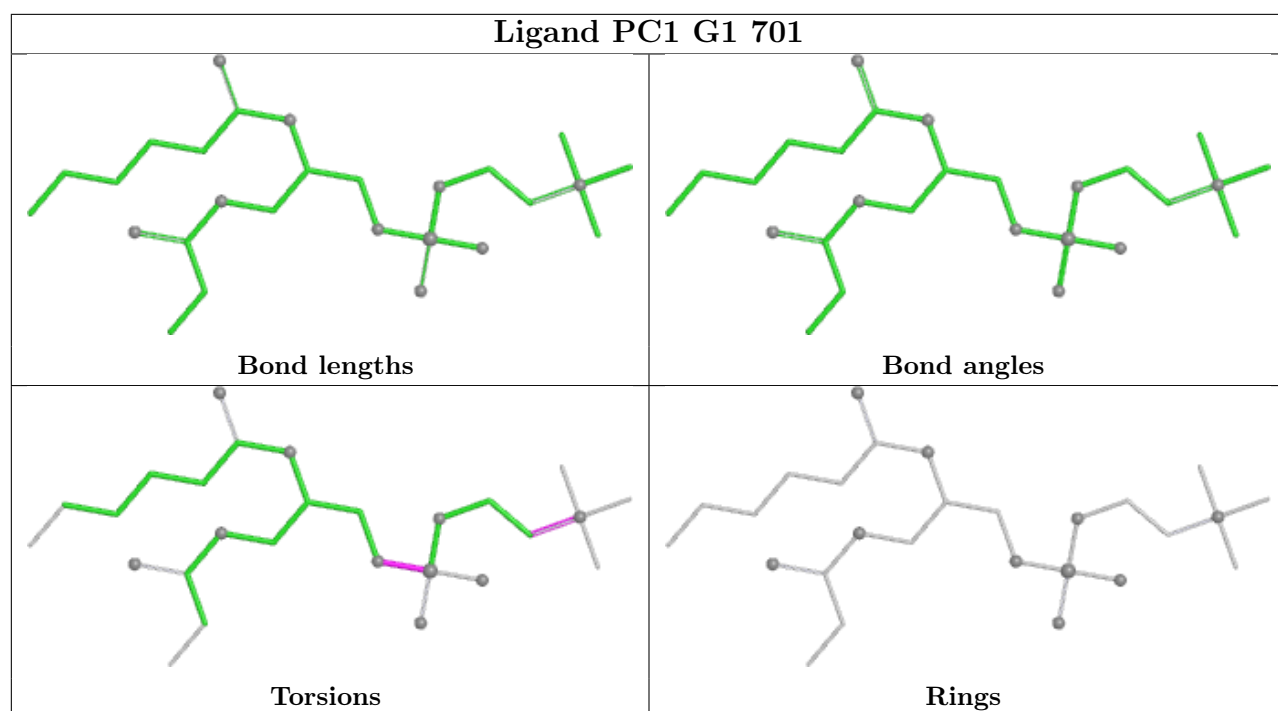
Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	1M	401	PC1	1	0
61	O	404	CDL	3	0
65	1M	402	U10	2	0
61	O	407	CDL	2	0
67	AB	201	ZMP	3	0
60	P4	101	PC1	1	0
64	P	501	HEC	3	0
61	C	506	CDL	1	0
60	G2	801	PC1	1	0
62	C	502	HEM	4	0
62	O	402	HEM	5	0
72	V1	501	FMN	1	0
67	AC	201	ZMP	1	0
60	S	101	PC1	2	0

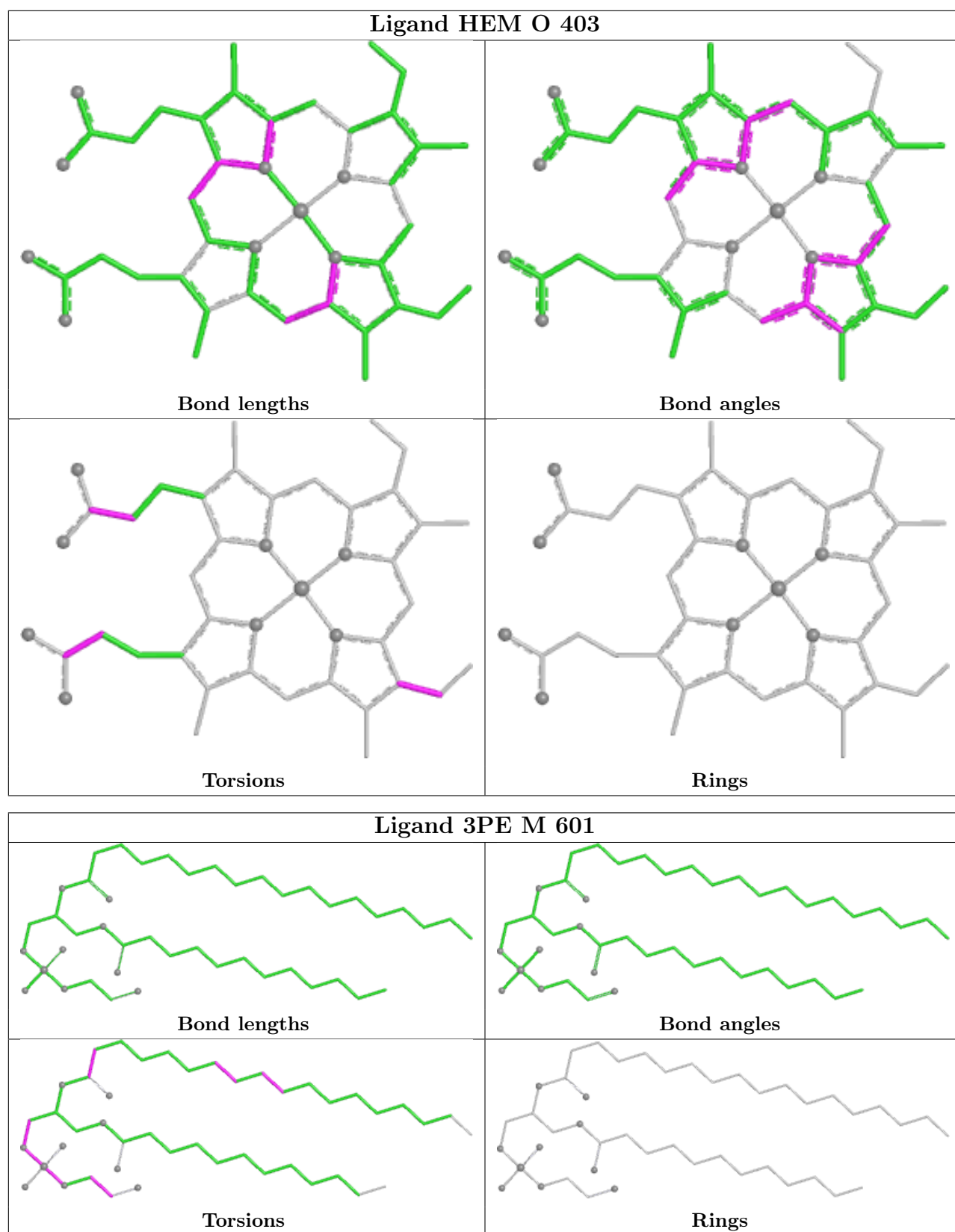
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

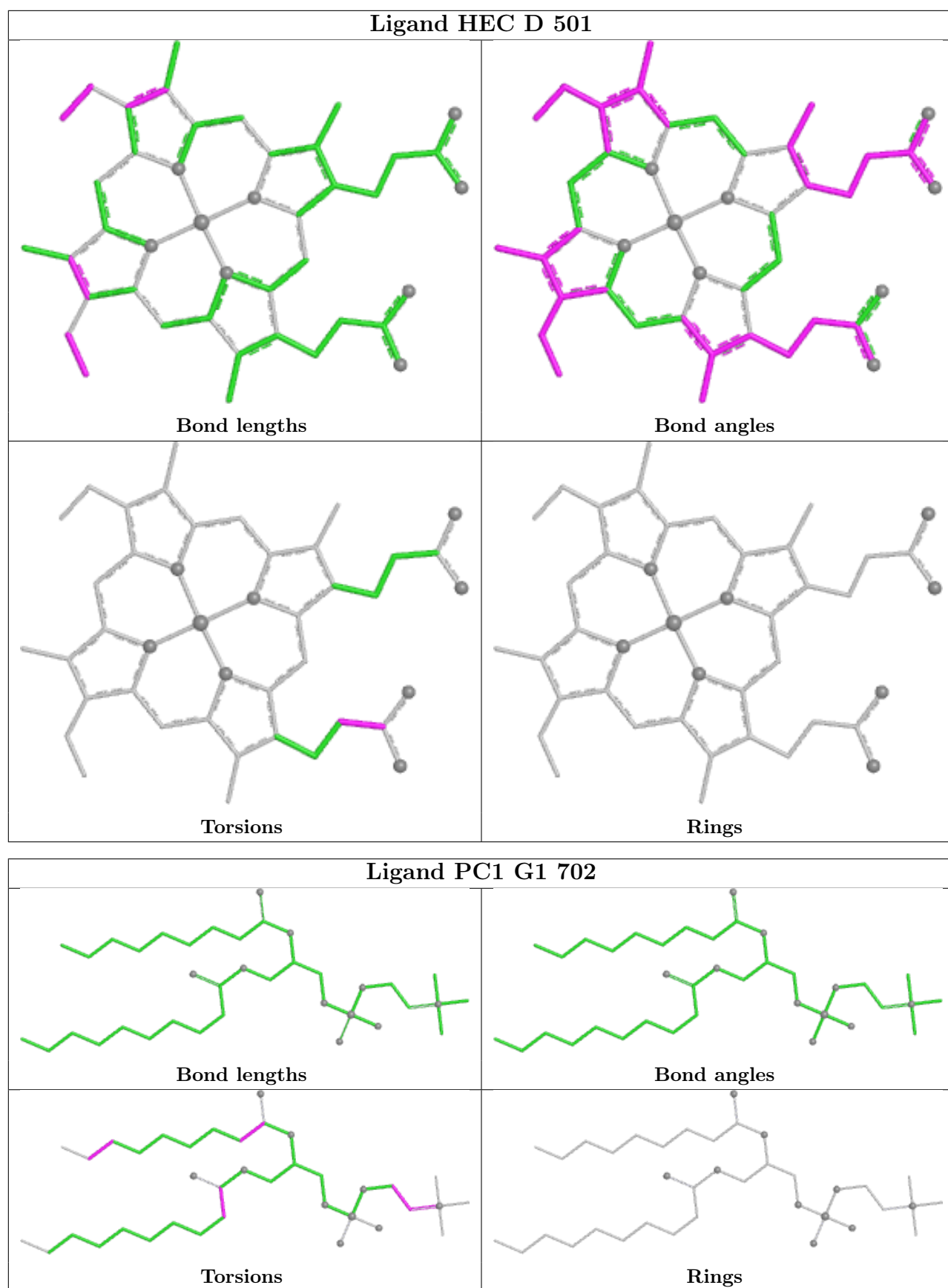


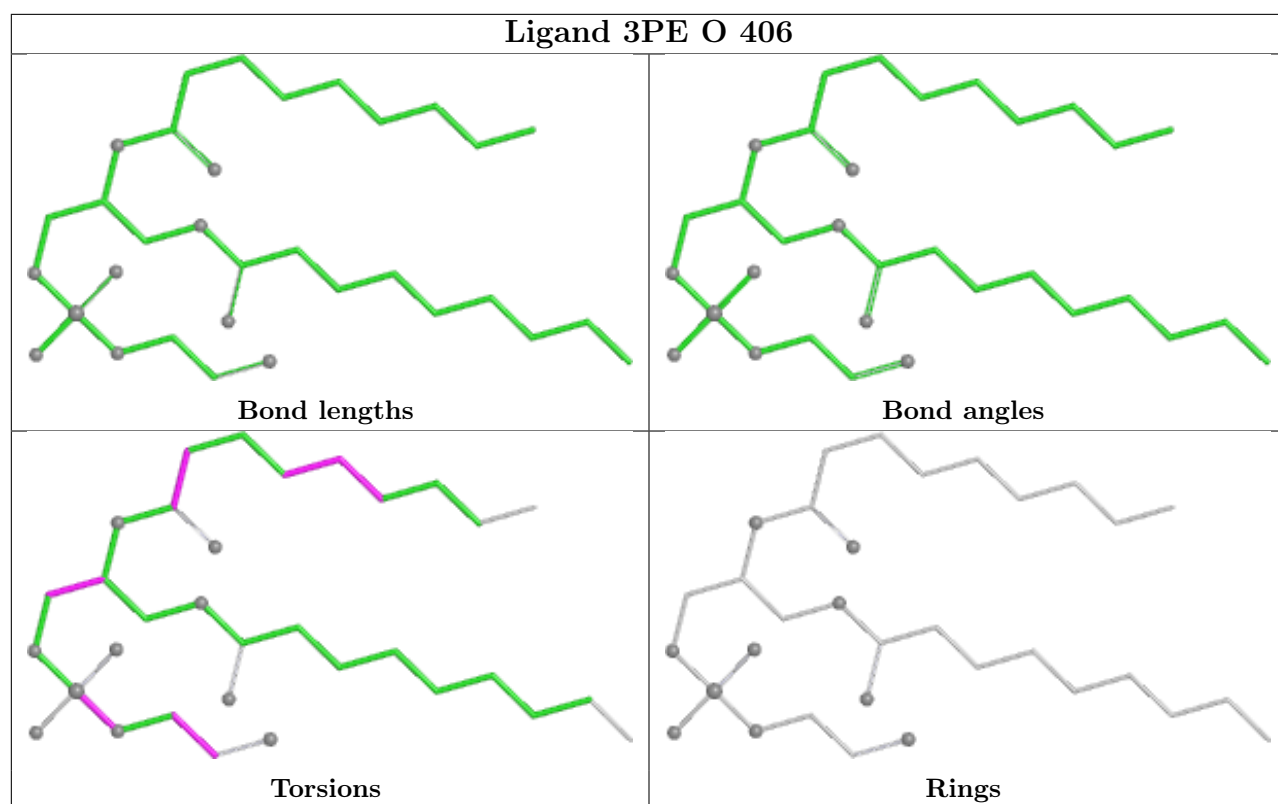


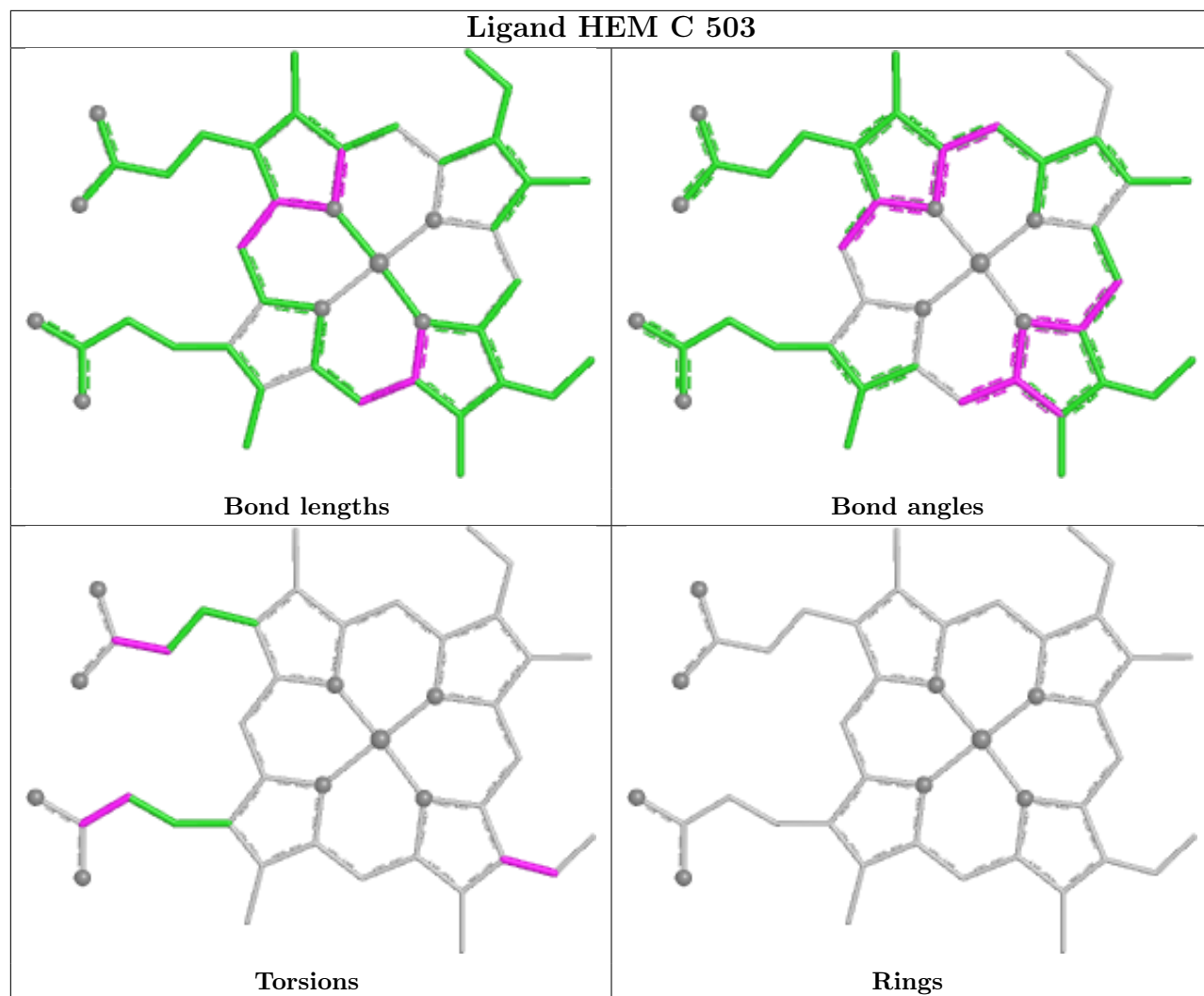




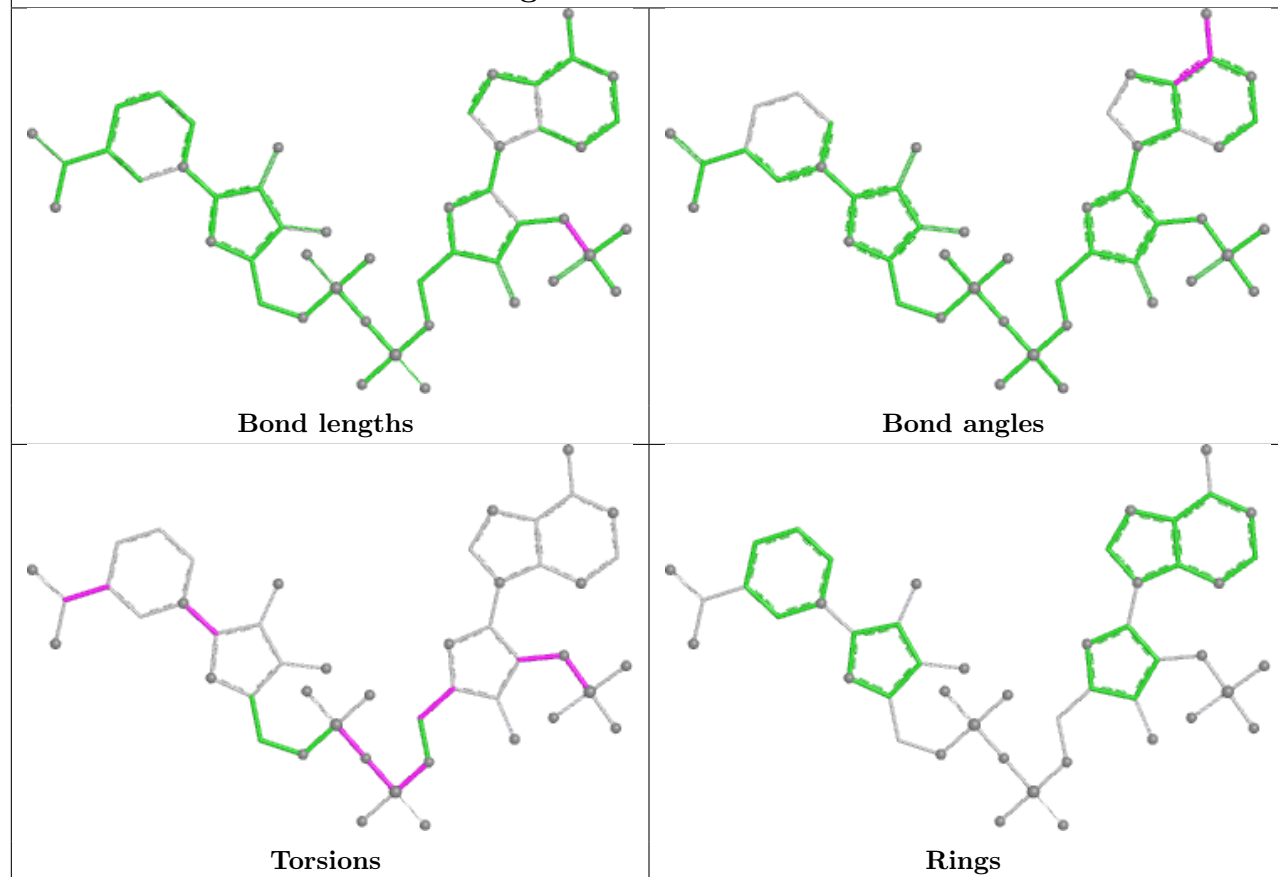




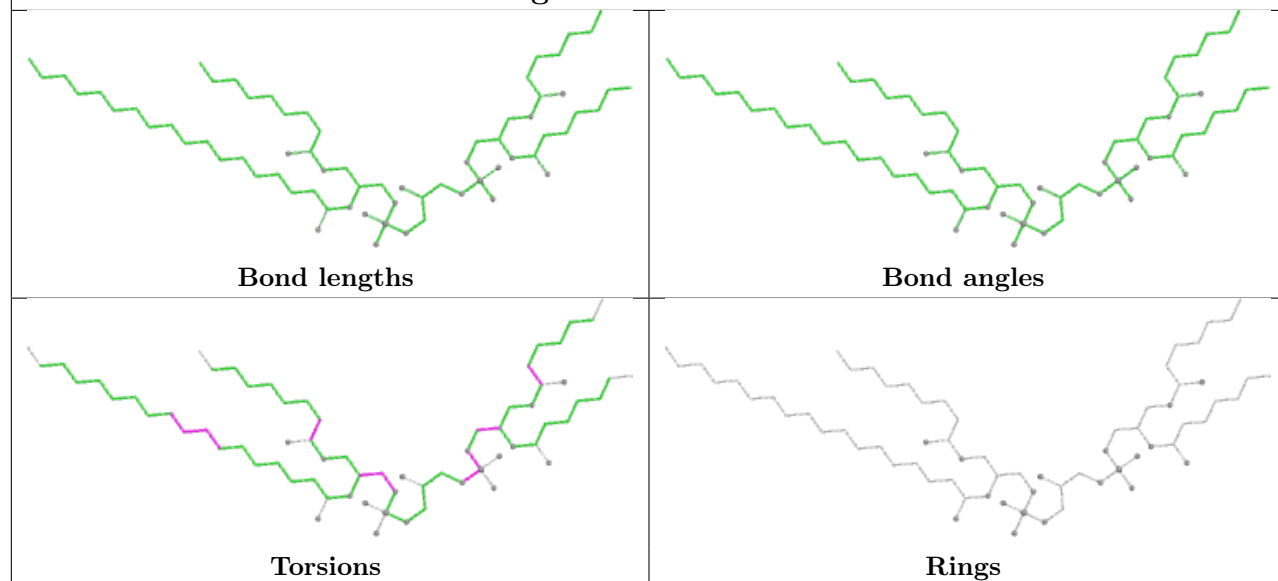


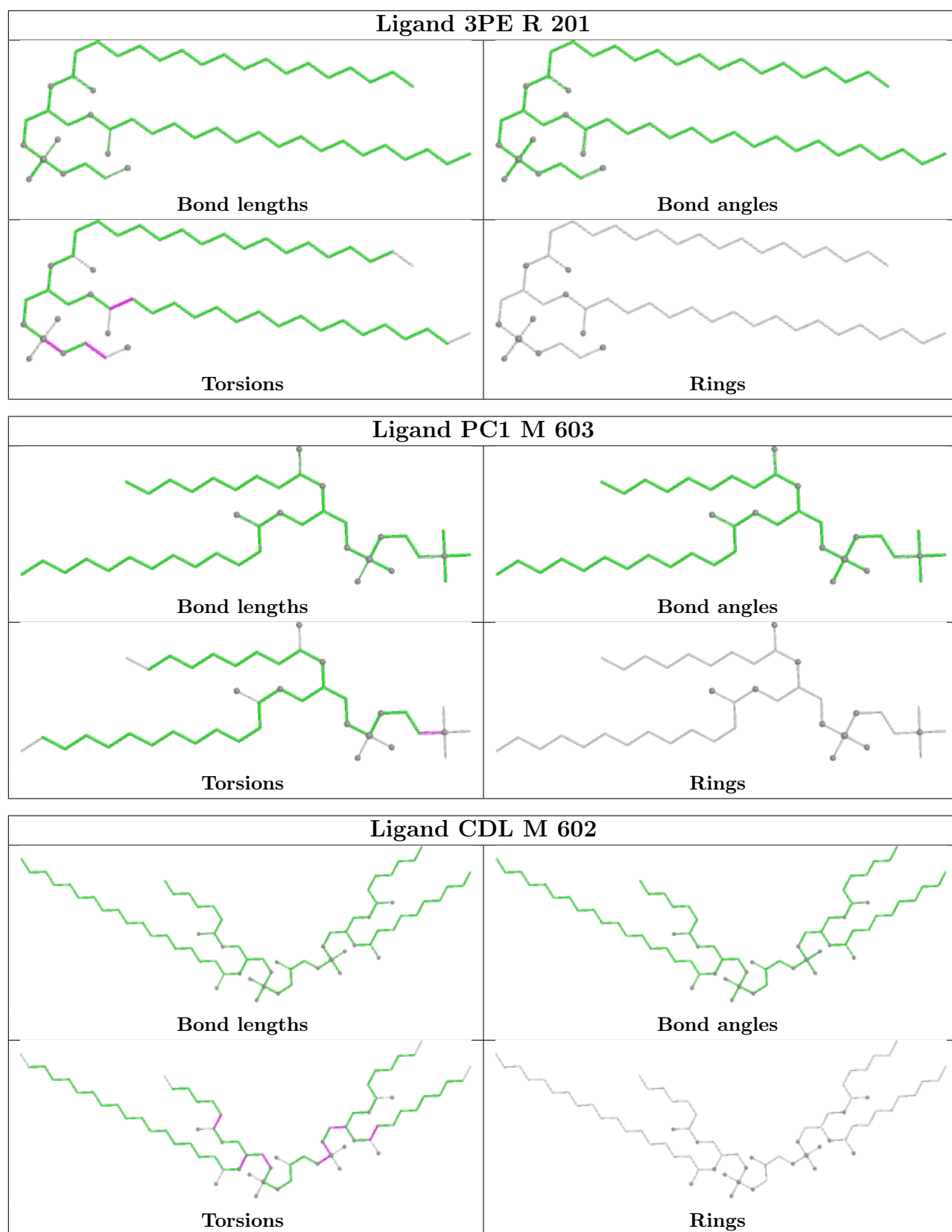


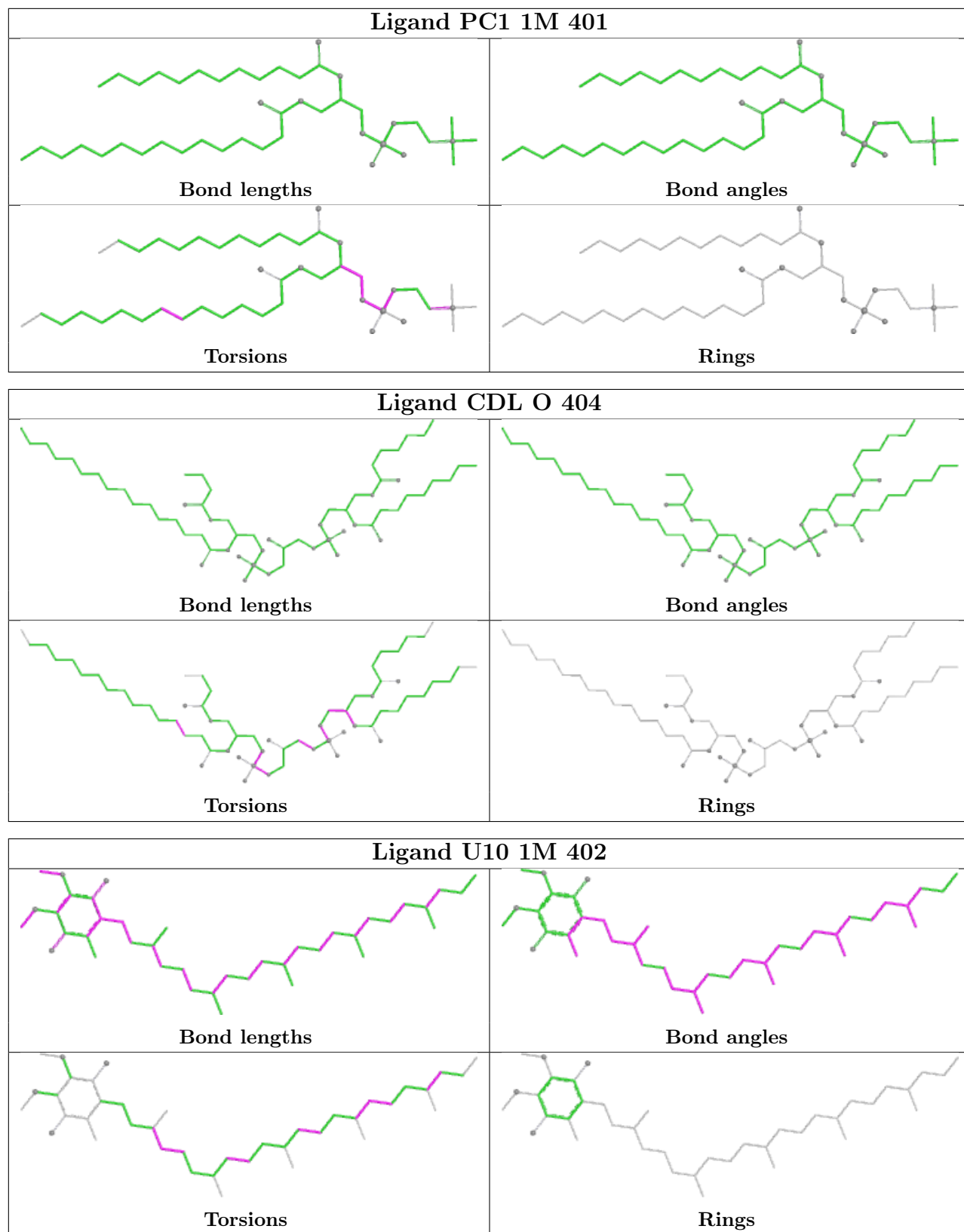
Ligand NDP A9 401

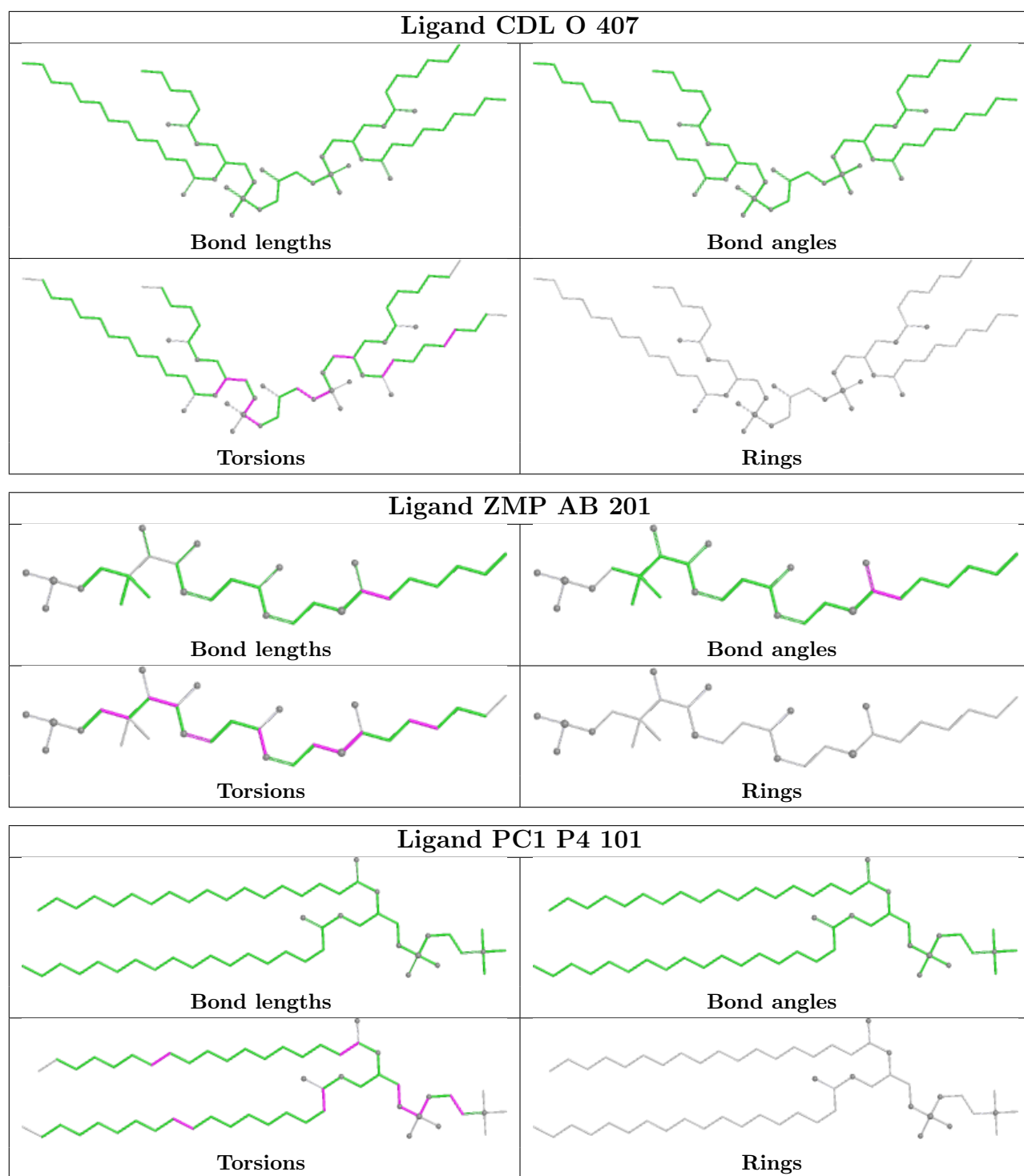


Ligand CDL A 602

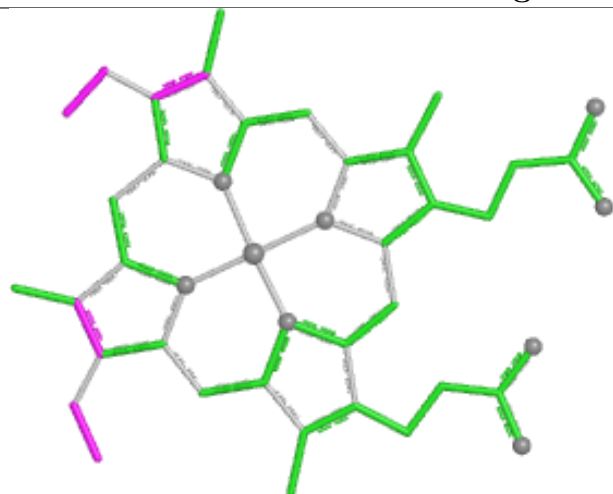




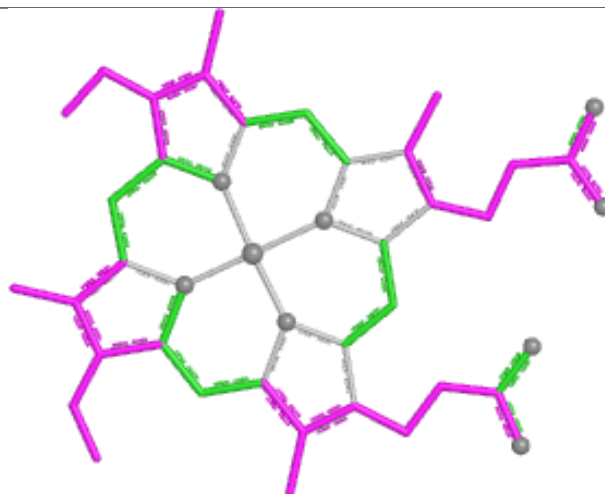




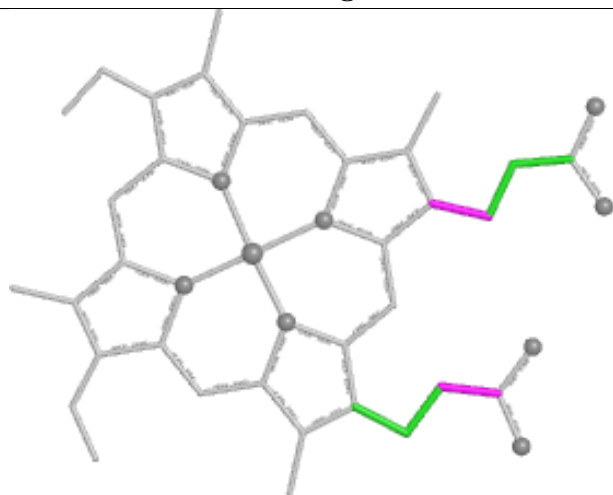
Ligand HEC P 501



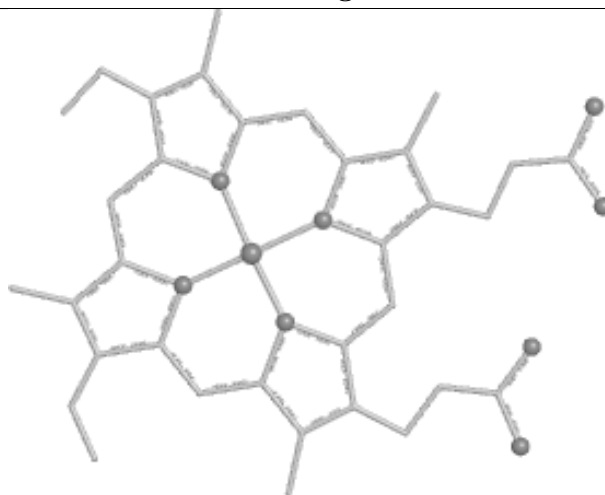
Bond lengths



Bond angles

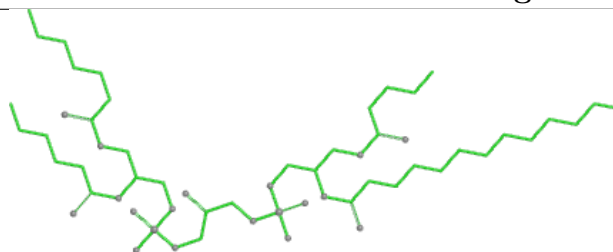


Torsions

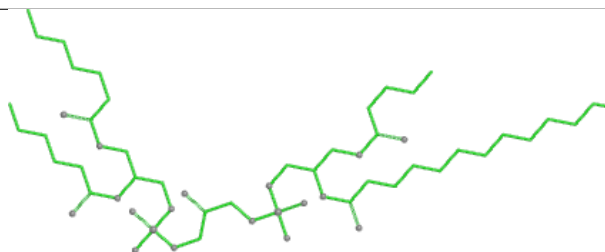


Rings

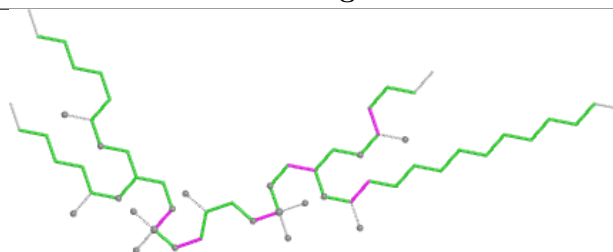
Ligand CDL C 506



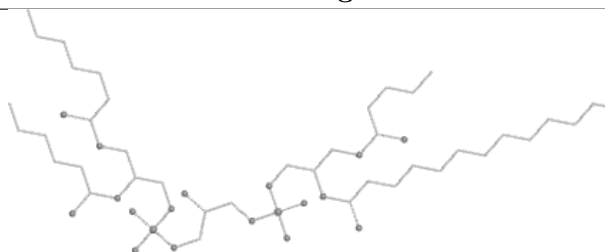
Bond lengths



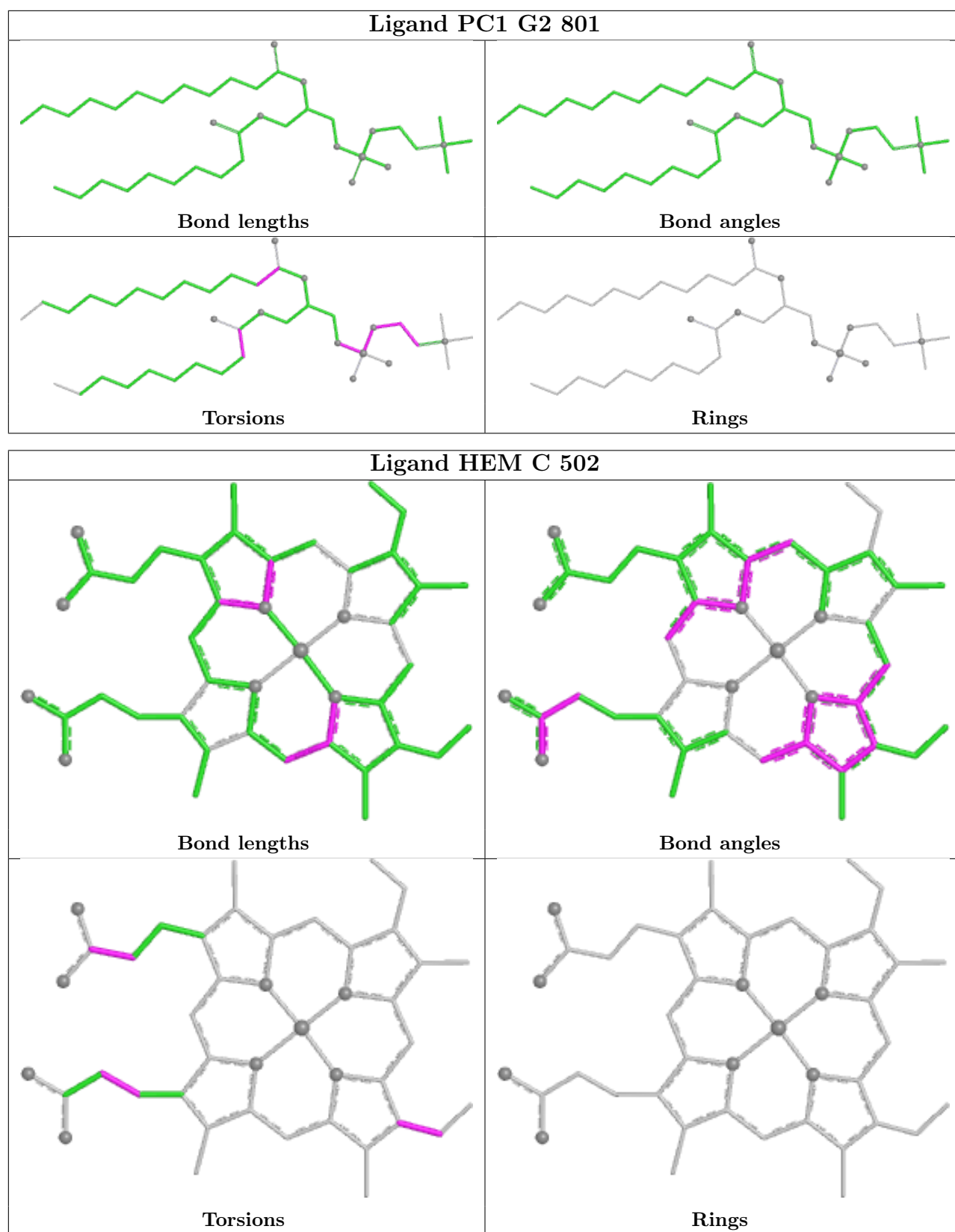
Bond angles

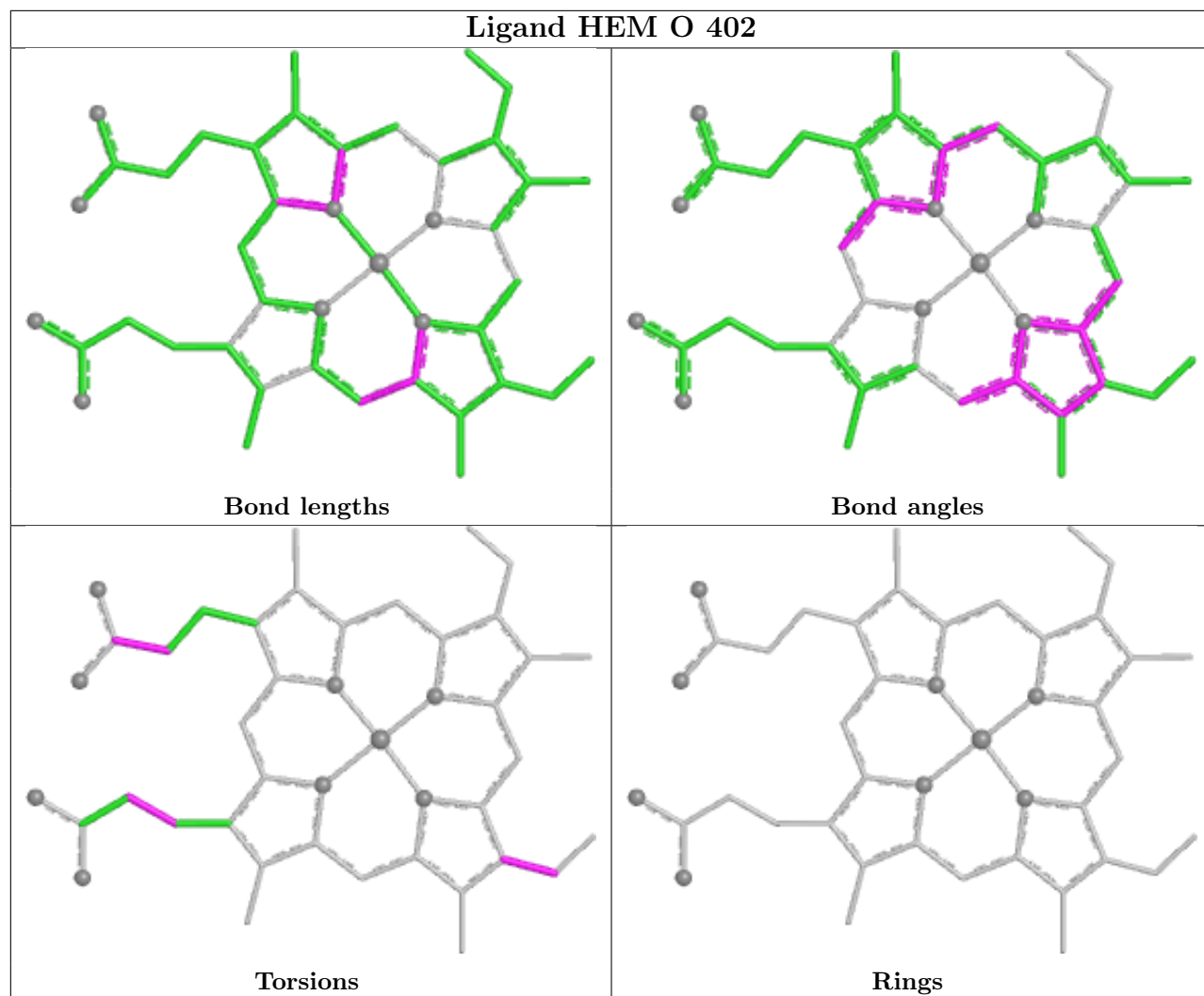


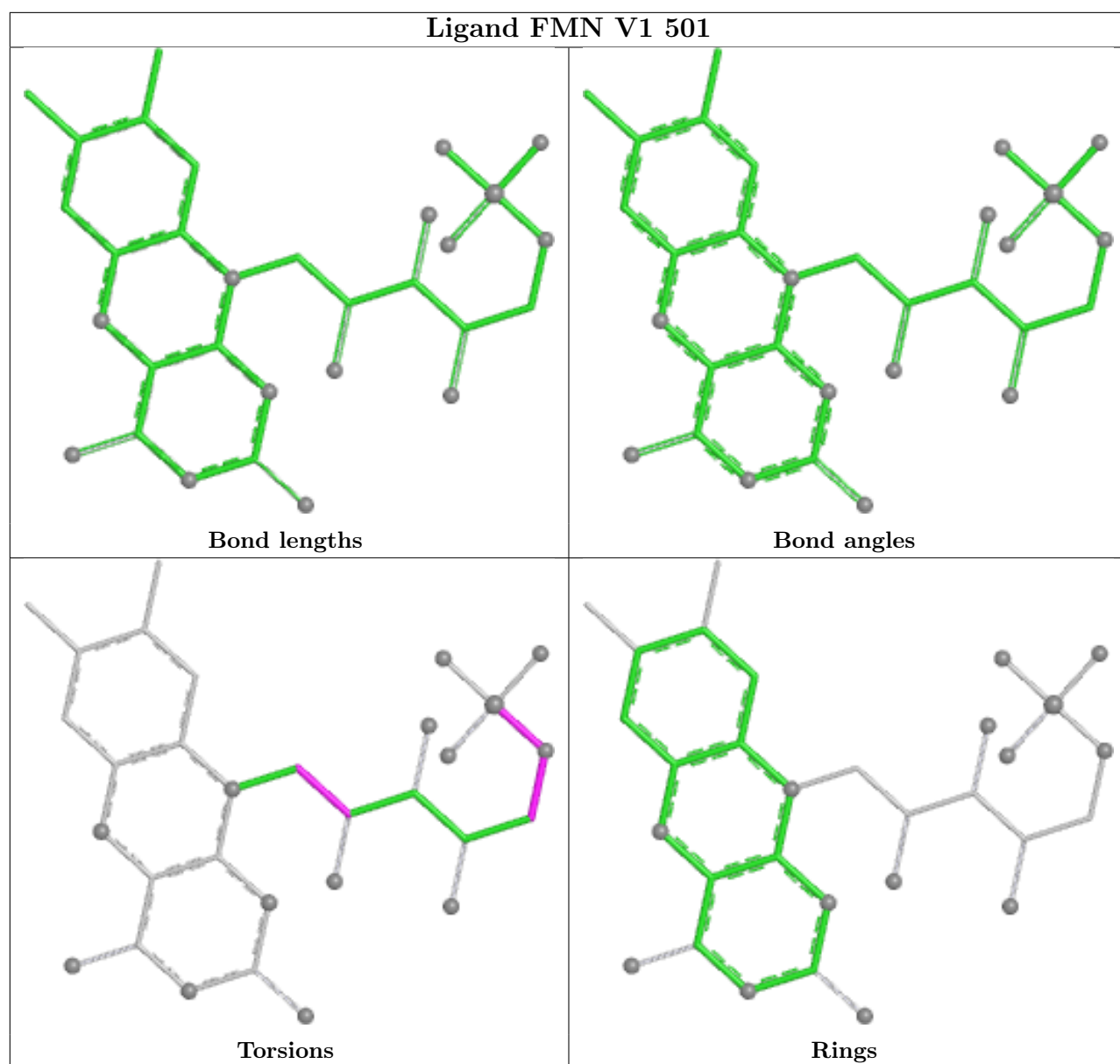
Torsions

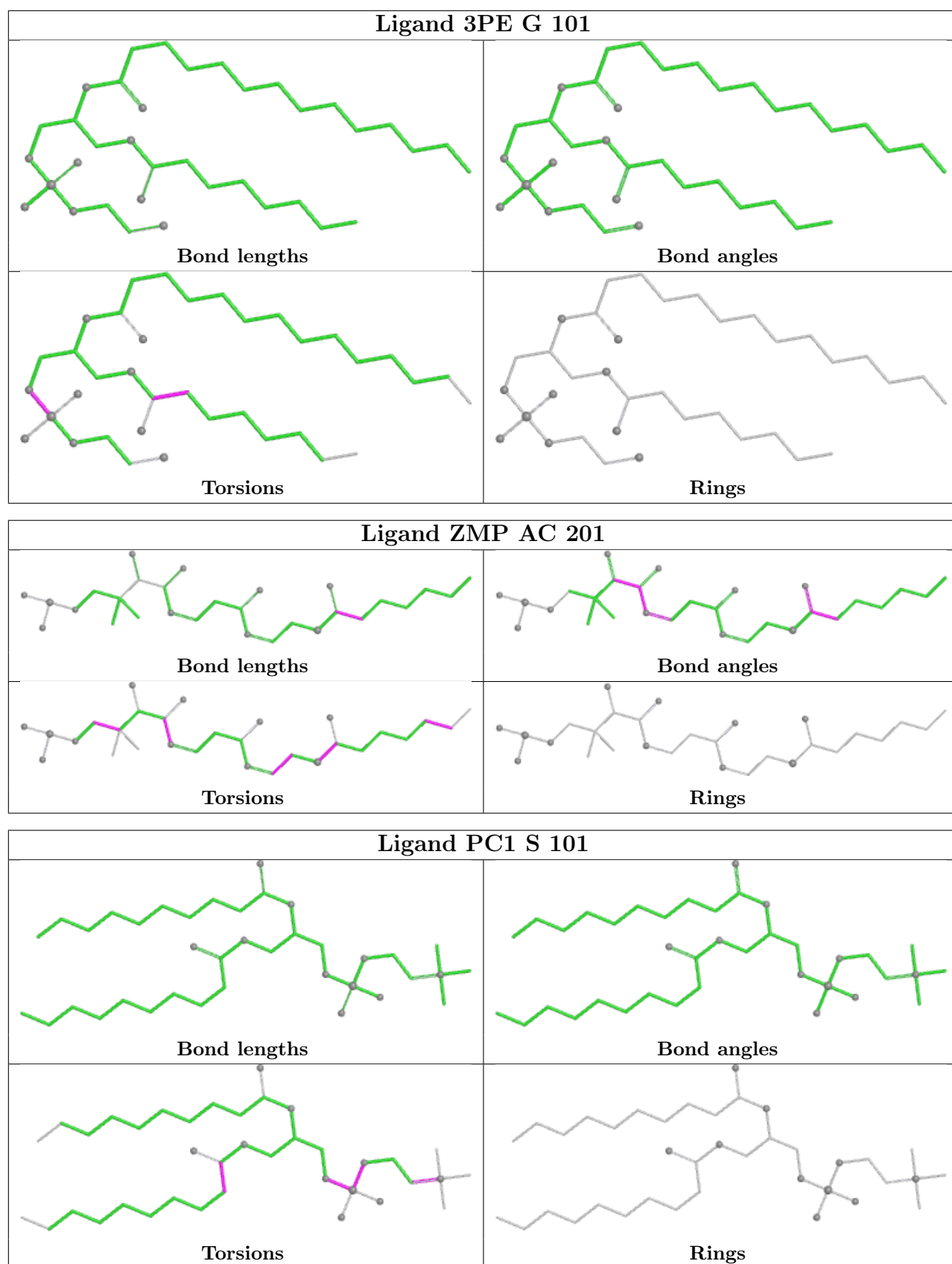


Rings









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
58	V2	1
26	A9	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	V2	246:ARG	C	247:ASP	N	3.88
1	A9	375:TYR	C	376:ARG	N	3.06

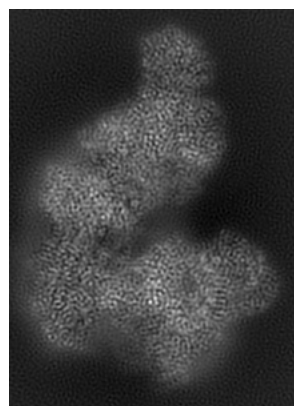
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27934. These allow visual inspection of the internal detail of the map and identification of artifacts.

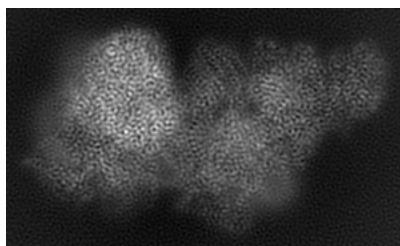
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

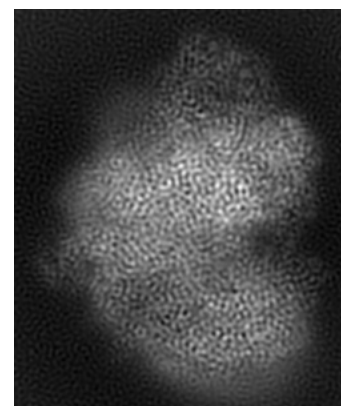
6.1.1 Primary map



X

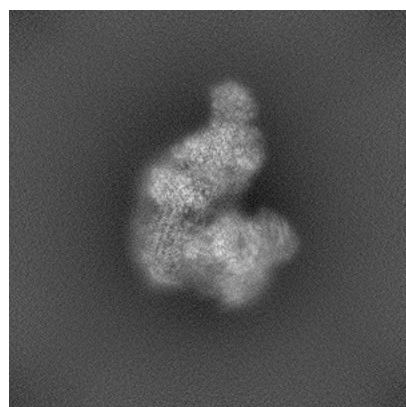


Y

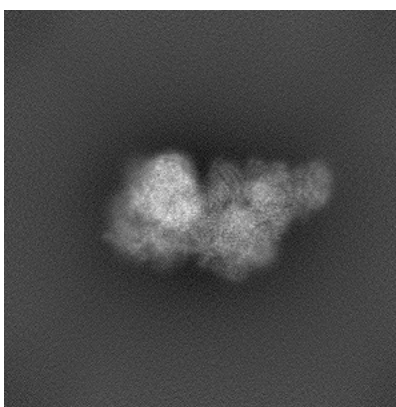


Z

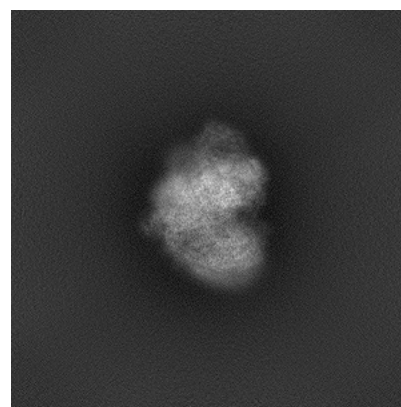
6.1.2 Raw map



X



Y

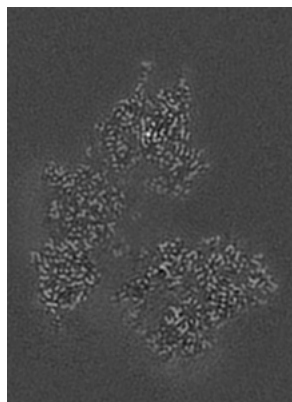


Z

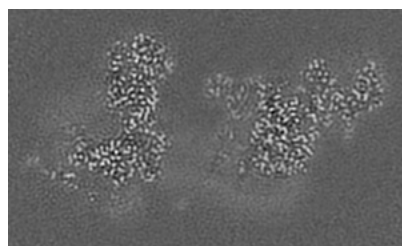
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

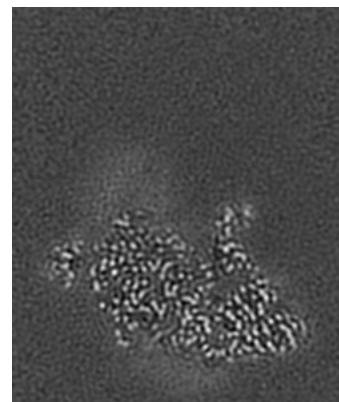
6.2.1 Primary map



X Index: 113

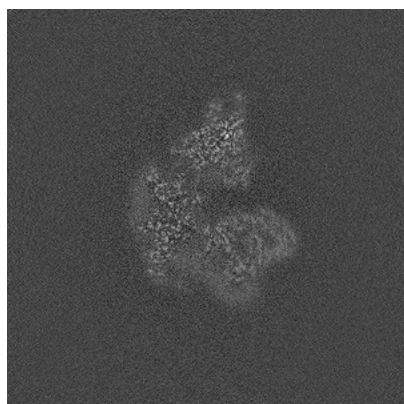


Y Index: 134

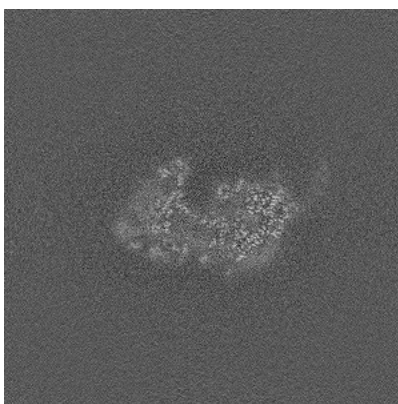


Z Index: 188

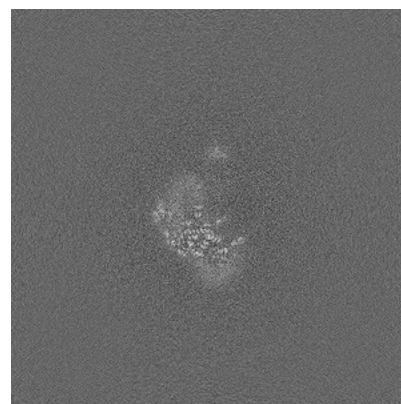
6.2.2 Raw map



X Index: 300



Y Index: 300

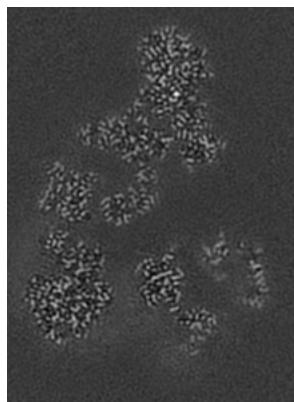


Z Index: 300

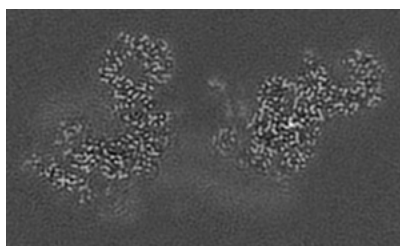
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

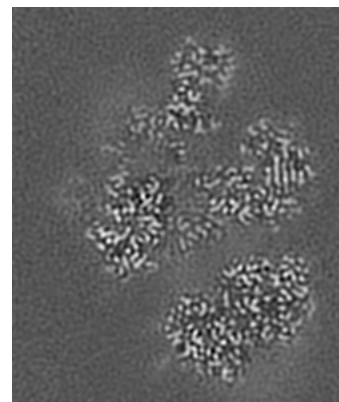
6.3.1 Primary map



X Index: 146

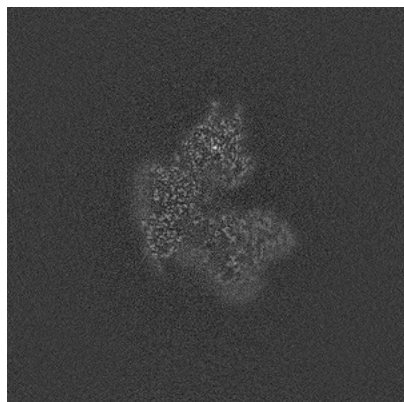


Y Index: 142

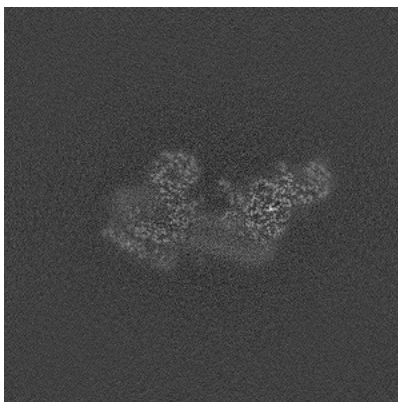


Z Index: 100

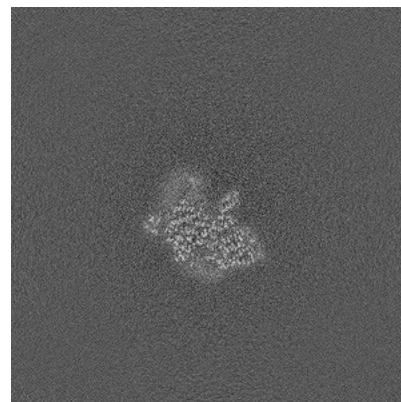
6.3.2 Raw map



X Index: 292



Y Index: 322

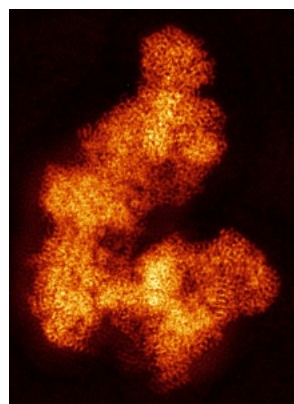


Z Index: 324

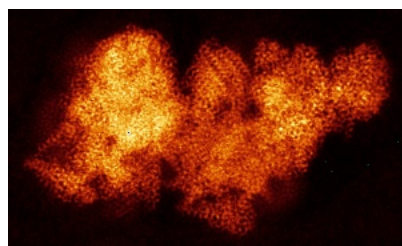
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

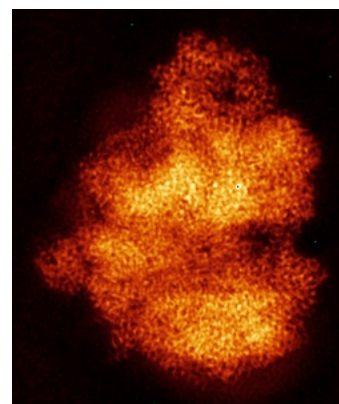
6.4.1 Primary map



X

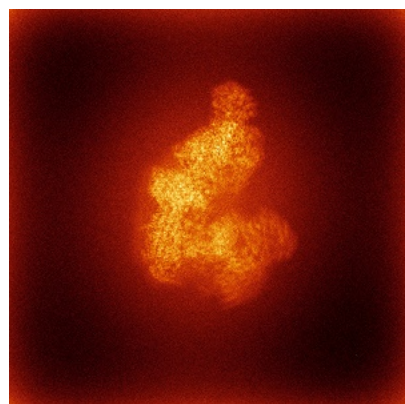


Y

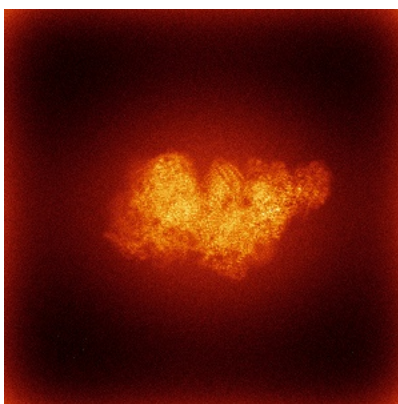


Z

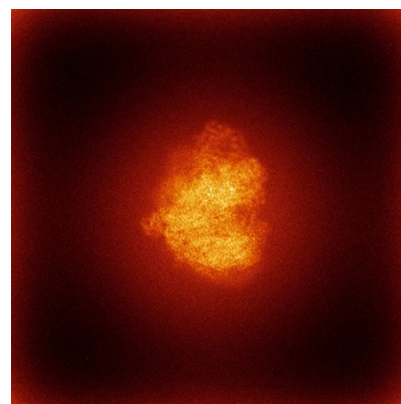
6.4.2 Raw map



X



Y

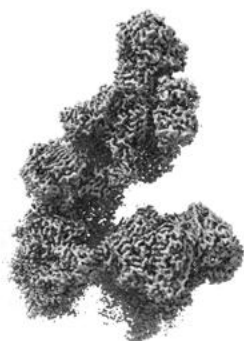


Z

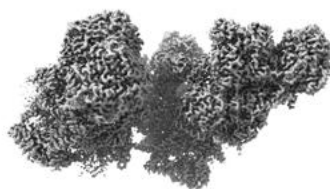
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

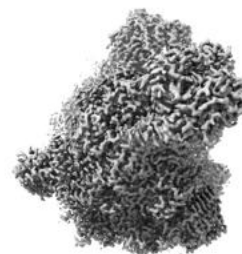
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

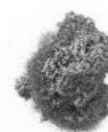
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

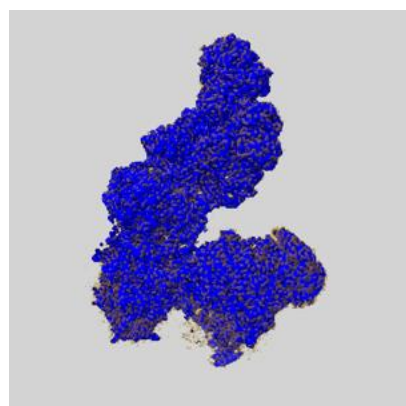
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

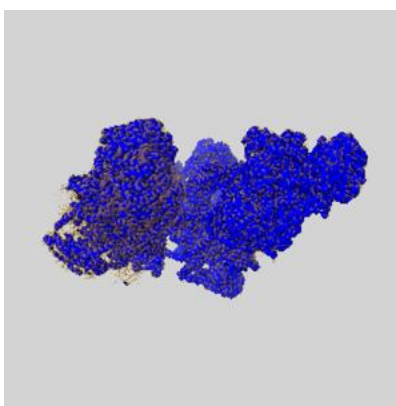
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

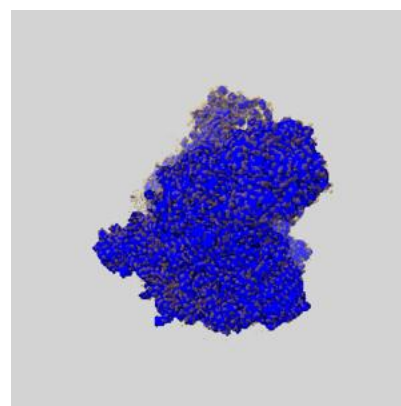
6.6.1 emd_27934_msk_1.map [i](#)



X



Y

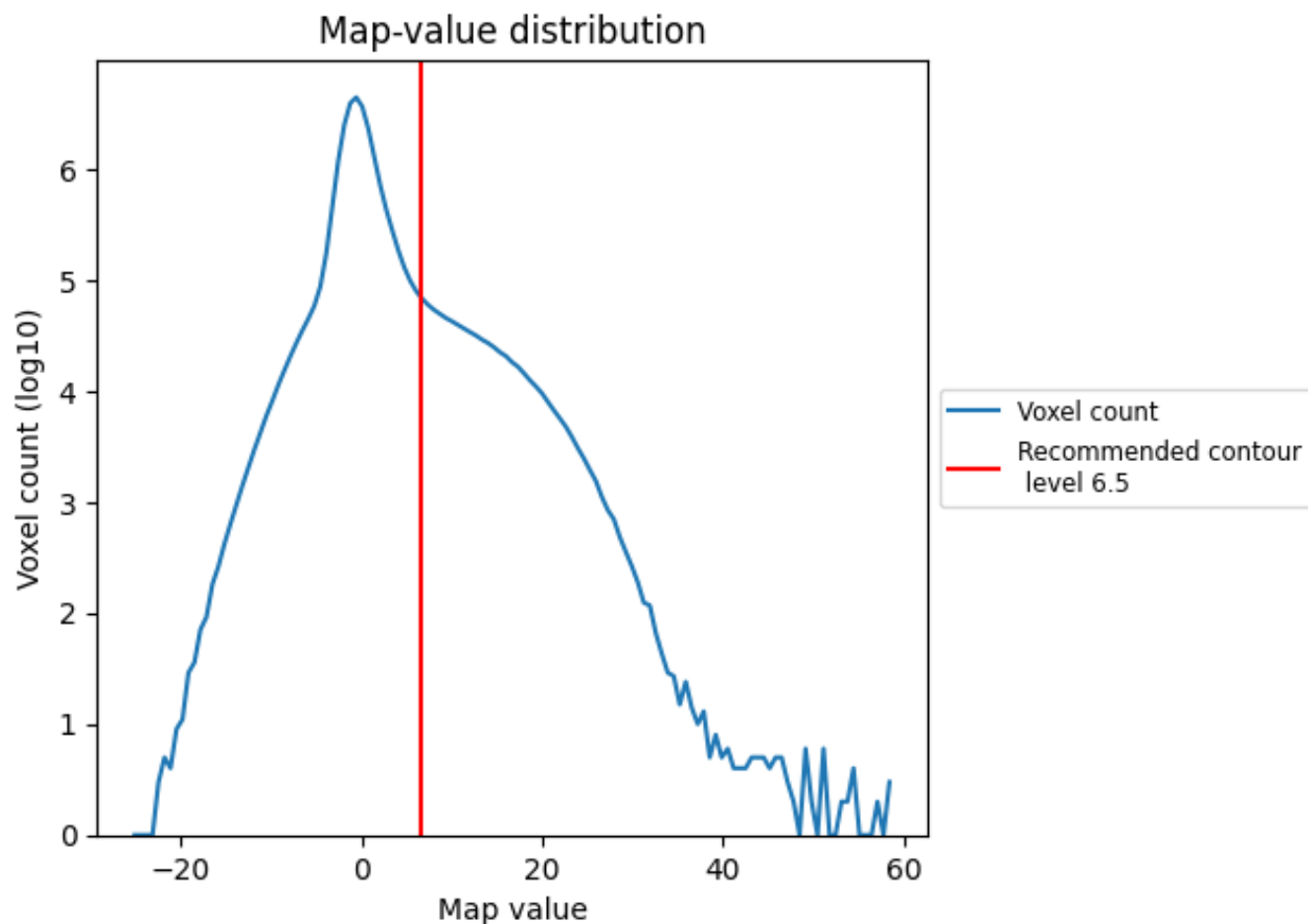


Z

7 Map analysis [i](#)

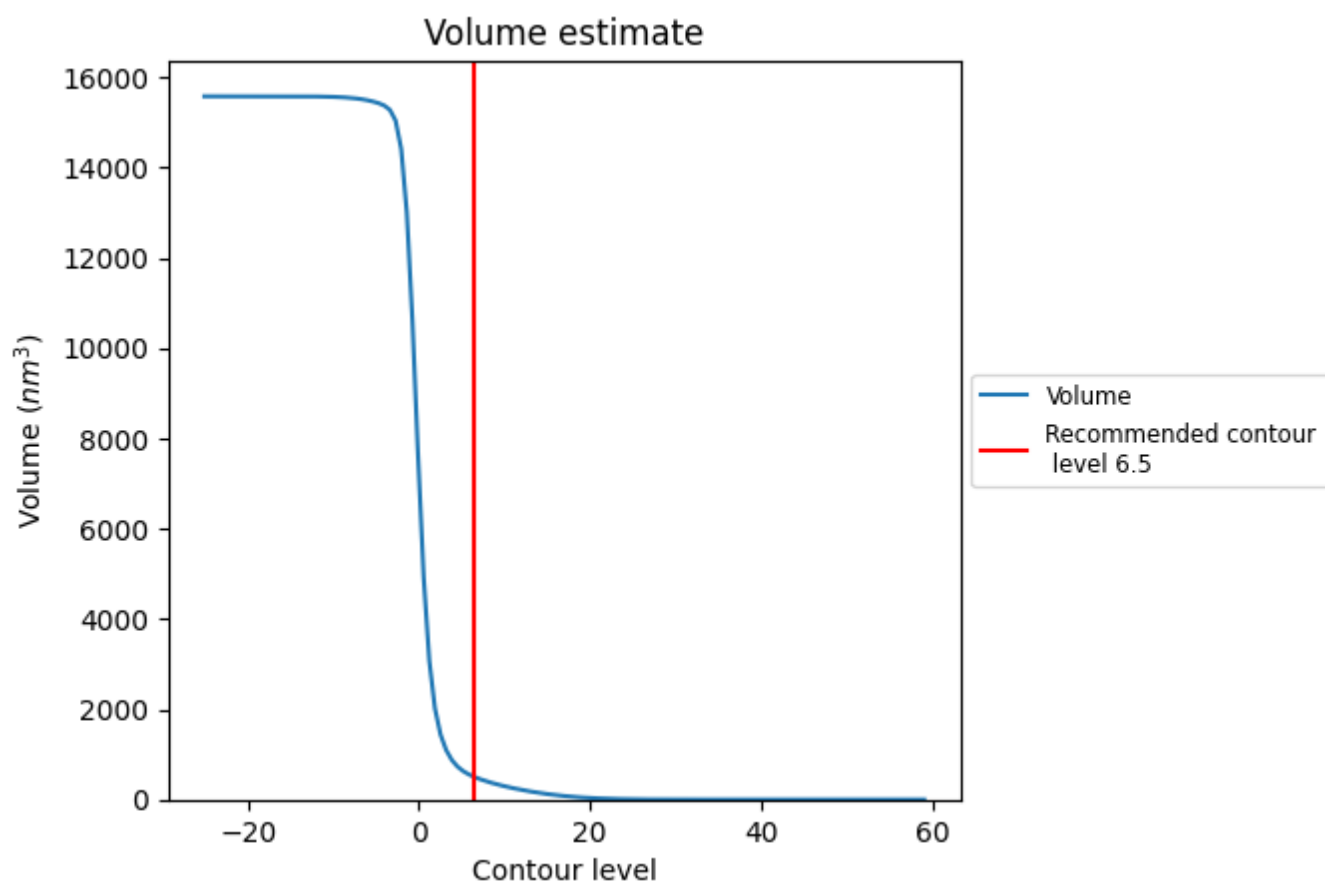
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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 [i](#)



The volume at the recommended contour level is 499 nm³; this corresponds to an approximate mass of 451 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

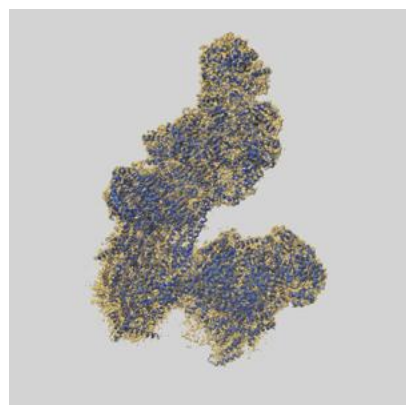
8 Fourier-Shell correlation

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

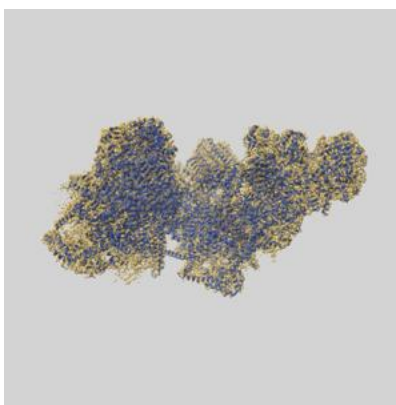
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27934 and PDB model 8E73. Per-residue inclusion information can be found in section [3](#) on page [23](#).

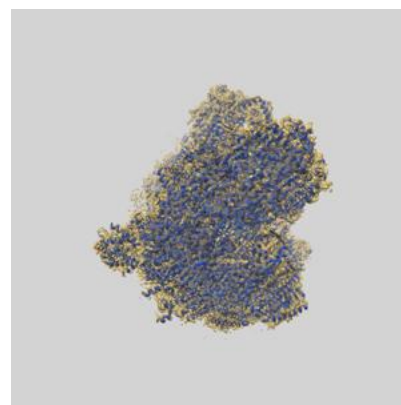
9.1 Map-model overlay [i](#)



X



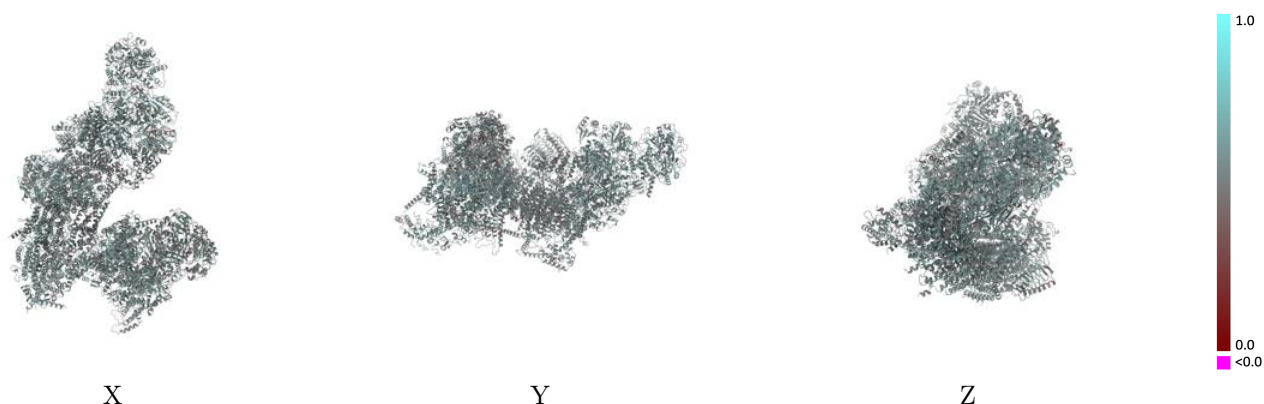
Y



Z

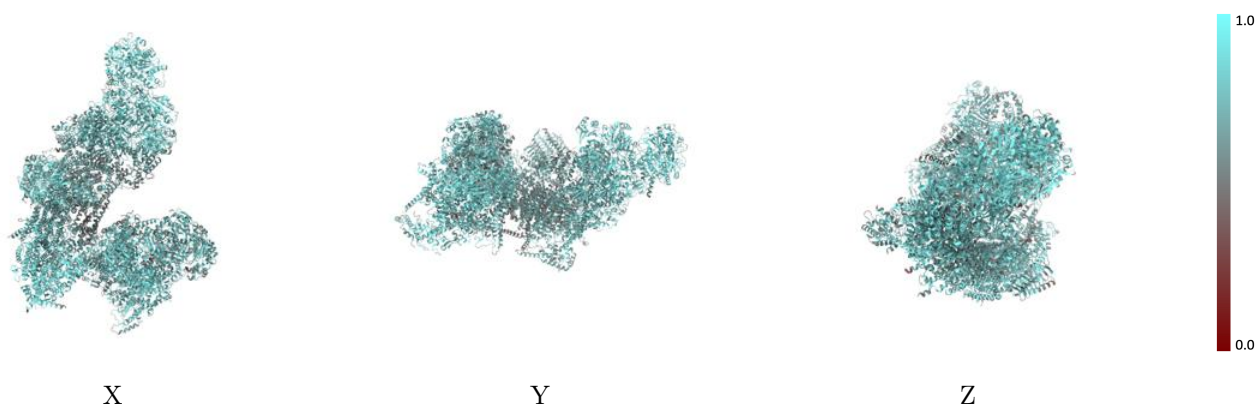
The images above show the 3D surface view of the map at the recommended contour level 6.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



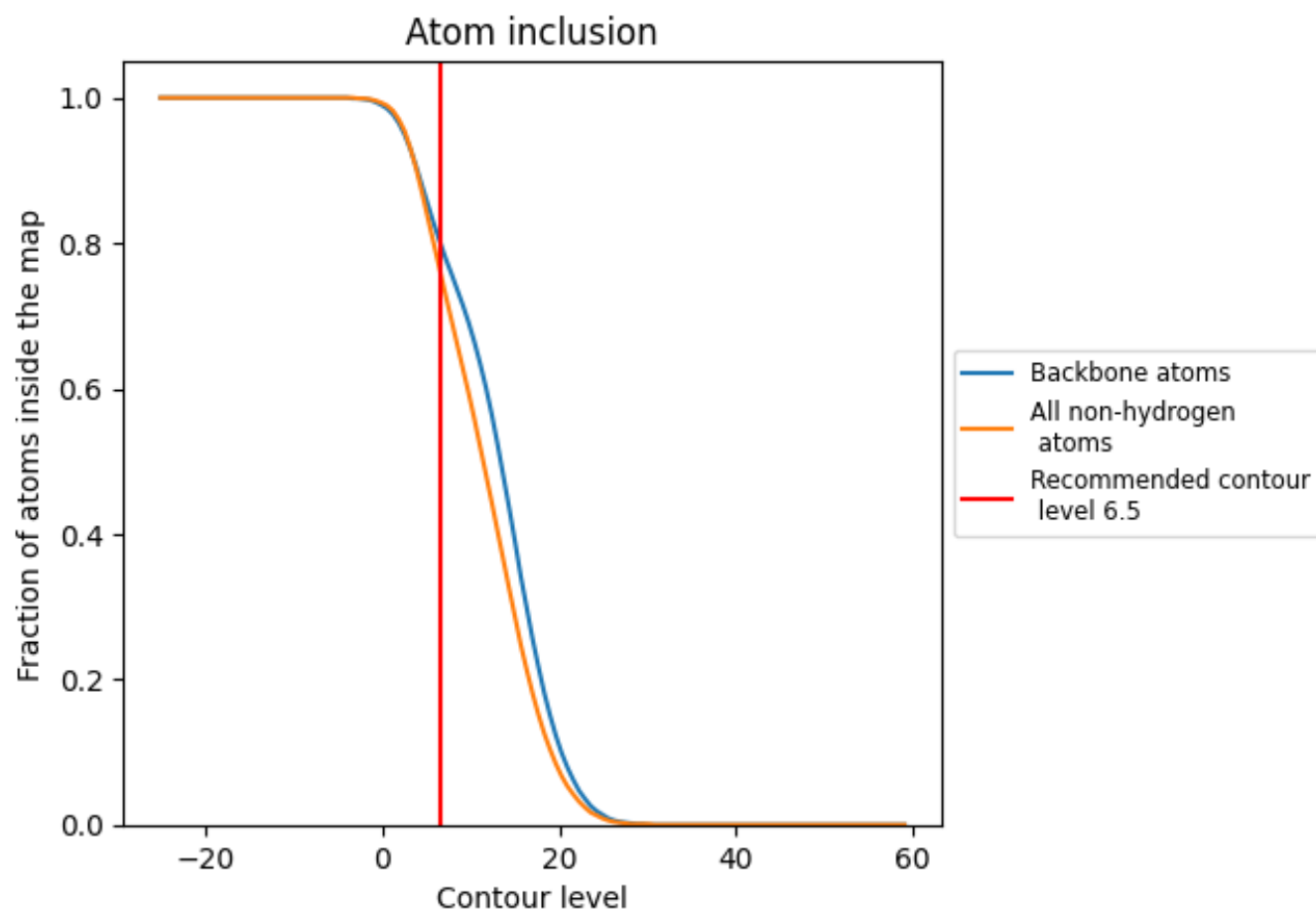
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [i](#)



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 (6.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 76% 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 (6.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7630	 0.5360
1M	 0.7490	 0.5360
2M	 0.7720	 0.5440
3M	 0.7540	 0.5410
4L	 0.7380	 0.5480
4M	 0.7950	 0.5390
5M	 0.8190	 0.5430
6M	 0.7180	 0.5300
A	 0.7690	 0.5450
A1	 0.7620	 0.5260
A2	 0.7550	 0.5050
A3	 0.6690	 0.5170
A5	 0.6670	 0.5220
A6	 0.6320	 0.4870
A7	 0.6980	 0.5330
A8	 0.6850	 0.5110
A9	 0.6750	 0.5190
AB	 0.6390	 0.4960
AC	 0.7560	 0.5160
AK	 0.5110	 0.4930
AL	 0.7840	 0.5500
AM	 0.7400	 0.5270
B	 0.7410	 0.5210
B2	 0.8450	 0.5450
B3	 0.7820	 0.5270
B4	 0.7540	 0.5440
B7	 0.7960	 0.5480
B8	 0.7970	 0.5270
B9	 0.7860	 0.5280
BJ	 0.7970	 0.5410
BK	 0.7420	 0.5330
C	 0.8060	 0.5530
C1	 0.8290	 0.5560
C2	 0.7770	 0.5500
D	 0.7960	 0.5550



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
E	 0.7280	 0.5270
F	 0.7760	 0.5510
FD	 0.7510	 0.5460
G	 0.7180	 0.5330
G1	 0.7500	 0.5310
G2	 0.7290	 0.5320
H	 0.6850	 0.5070
J	 0.7340	 0.5230
K	 0.6480	 0.5190
L2	 0.7740	 0.5440
M	 0.7580	 0.5340
N	 0.7150	 0.5080
O	 0.7900	 0.5470
P	 0.8210	 0.5570
P1	 0.7420	 0.5240
P2	 0.7200	 0.5430
P4	 0.5250	 0.4930
Q	 0.7240	 0.5270
R	 0.7820	 0.5490
S	 0.7150	 0.5280
S1	 0.7980	 0.5490
S2	 0.8060	 0.5460
S3	 0.8100	 0.5630
S4	 0.8330	 0.5550
S5	 0.7330	 0.5330
S6	 0.7600	 0.5440
S7	 0.8110	 0.5490
S8	 0.8210	 0.5450
T	 0.6600	 0.4840
V	 0.6690	 0.5150
V1	 0.8020	 0.5360
V2	 0.8070	 0.5370
W	 0.5570	 0.4830
X1	 0.7730	 0.5460