



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 11:35 AM JST

PDB ID : 7W4K / pdb_00007w4k
EMDB ID : EMD-32306
Title : Deactive state CI from Q1-NADH dataset, Subclass 2
Authors : Gu, J.; Yang, M.
Deposited on : 2021-11-28
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:

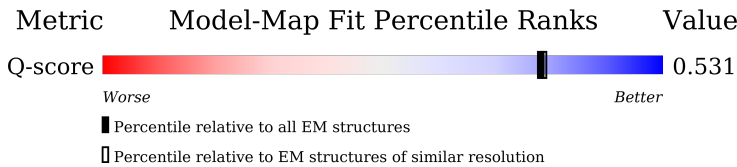
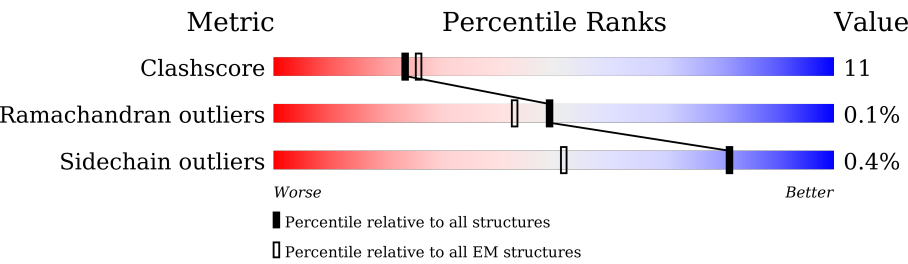
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	433	13% 70% 29% .
2	B	176	77% 23%
3	C	156	81% 19% .
4	E	115	13% 75% 25%

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Mol	Chain	Length	Quality of chain
5	F	86	
6	G	88	
6	X	88	
7	H	112	
8	I	112	
9	J	342	
10	K	43	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	70	
23	Z	84	
24	a	140	
25	b	126	
26	c	156	
27	d	175	
28	e	107	

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Mol	Chain	Length	Quality of chain
29	f	49	
30	g	122	
31	h	105	
32	i	347	
33	j	115	
34	k	98	
35	l	603	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	124	
44	w	320	

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 66374 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3314	2094	590	610	20		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	156	Total	C	N	O	S	0	0
			1248	794	227	213	14		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	115	Total	C	N	O	S	0	0
			971	619	179	168	5		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	86	Total	C	N	O	S	0	0
			672	425	122	123	2		

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			690	446	102	137	5		
6	X	88	Total	C	N	O	S	0	0
			696	449	103	139	5		

- Molecule 7 is a protein called Complex I subunit B13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			906	586	154	163	3		

- Molecule 8 is a protein called Complex I-B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	97	Total	C	N	O	S	0	0
			780	491	147	139	3		

- Molecule 9 is a protein called NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	297	Total	C	N	O	S	0	0
			2355	1512	421	414	8		

- Molecule 10 is a protein called Complex I-9kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	42	Total	C	N	O	S	0	0
			355	219	67	68	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	125	Total	C	N	O	S	0	0
			1016	642	181	190	3		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	690	Total	C	N	O	S	0	0
			5296	3320	923	1014	39		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	144	Total	C	N	O	S	0	0
			1204	770	218	212	4		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	217	Total	C	N	O	S	0	0
			1671	1065	281	315	10		

- Molecule 15 is a protein called Complex I-30kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1738	1124	298	314	2		

- Molecule 16 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	419	Total	C	N	O	S	0	0
			3377	2162	578	613	24		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			567	364	104	94	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	U	83	Total	C	N	O	0	0
			640	415	110	115		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	140	Total	C	N	O	S	0	0
			1015	648	171	190	6		

- Molecule 21 is a protein called Complex I-B16.6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	142	Total	C	N	O	S	0	0
			1173	755	203	206	9		

- Molecule 22 is a protein called Complex I-AGGG.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	70	Total	C	N	O	S	0	0
			597	392	98	106	1		

- Molecule 23 is a protein called Complex I-B12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	84	Total	C	N	O	S	0	0
			674	437	116	120	1		

- Molecule 24 is a protein called Complex I-SGDH.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	140	Total	C	N	O	S	0	0
			1165	762	199	201	3		

- Molecule 25 is a protein called Complex I-B17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	103	Total	C	N	O	S	0	0
			870	569	158	142	1		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	156	Total	C	N	O	S	0	0
			1311	851	213	239	8		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	175	Total	C	N	O	S	0	0
			1461	916	265	272	8		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	107	Total	C	N	O	S	0	0
			890	568	145	173	4		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	42	Total	C	N	O	0	0
			342	225	58	59		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	347	Total	C	N	O	S	0	0
			2706	1780	420	460	46		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	99	Total	C	N	O	S	0	0
			800	545	118	132	5		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	98	Total	C	N	O	S	0	0
			748	493	113	128	14		

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	603	Total	C	N	O	S	0	0
			4782	3172	740	819	51		

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	129	Total	C	N	O	S	0	0
			948	636	138	166	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	56	Total	C	N	O	S	0	0
			466	305	84	76	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	128	Total	C	N	O	S	0	0
			1062	691	182	189			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	178	Total	C	N	O	S	0	0
			1529	979	277	265	8		

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	459	Total	C	N	O	S	0	0
			3631	2412	572	609	38		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	303	Total	C	N	O	S	0	0
			2394	1607	369	397	21		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 43 is a protein called Complex I-B18.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			1028	642	195	182	9		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

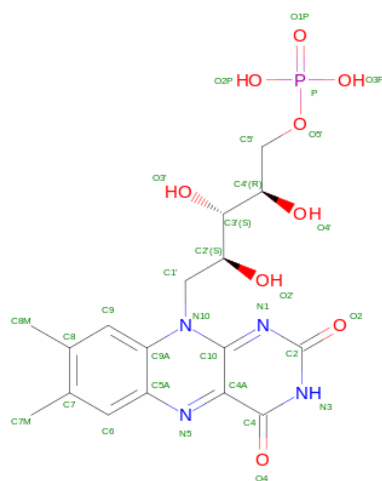
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2579	1642	438	489	10		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



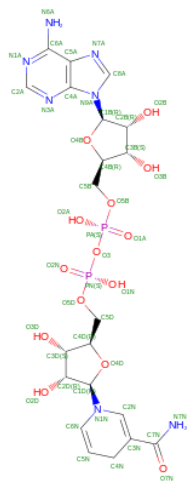
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



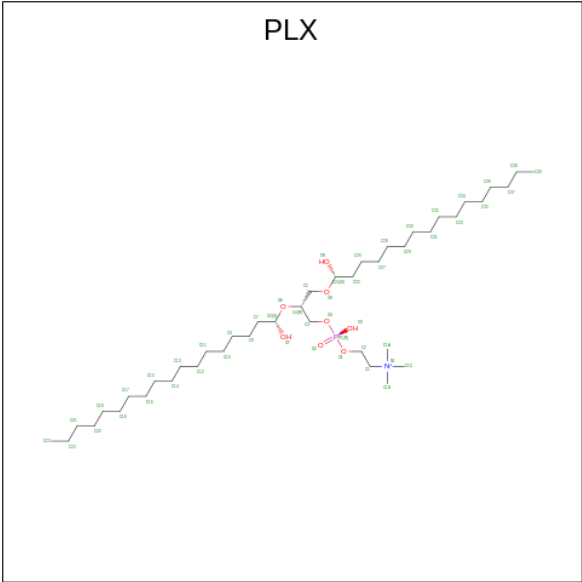
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total 44	C 21	N 7	O 14	P 2	0

- Molecule 48 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



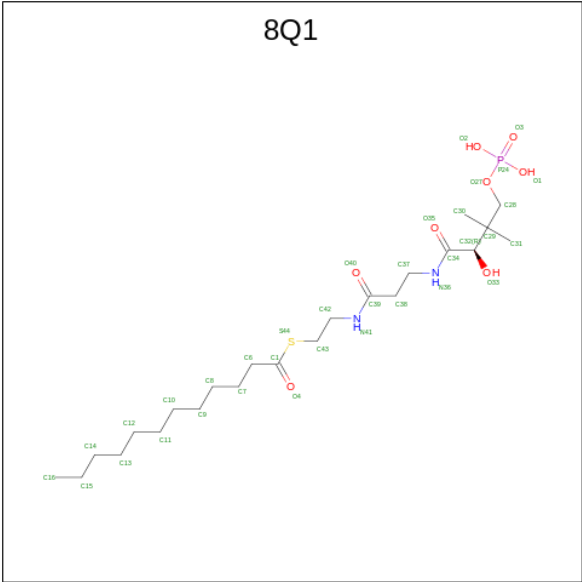
Mol	Chain	Residues	Atoms					AltConf
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	Q	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	Q	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	r	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 49 is (9R,11S)-9-([[(1S)-1-HYDROXYHEXADECYL]OXY]METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



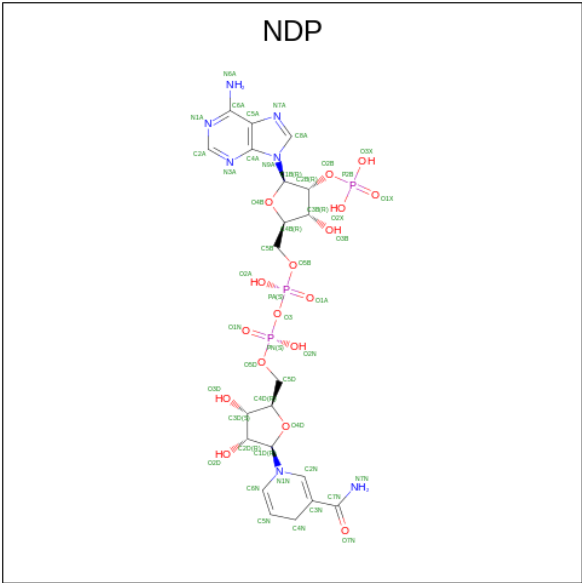
Mol	Chain	Residues	Atoms					AltConf
49	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	i	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 50 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-a
lanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as
"Ligand of Interest" by depositor).

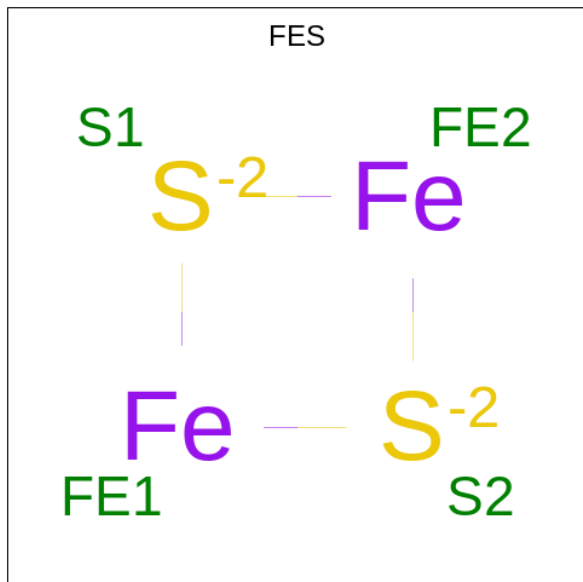


Mol	Chain	Residues	Atoms						AltConf
50	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
50	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 51 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



- Molecule 52 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
52	M	1	Total	Fe	S	0
			4	2	2	
52	O	1	Total	Fe	S	0
			4	2	2	

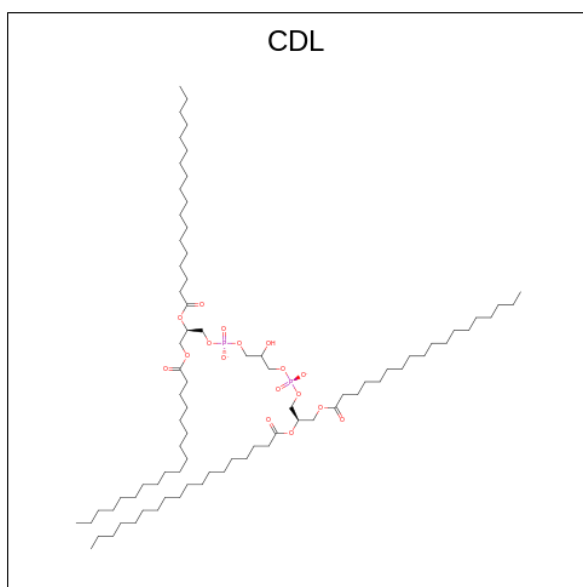
- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
53	M	1	Total	Mg	0
			1	1	

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

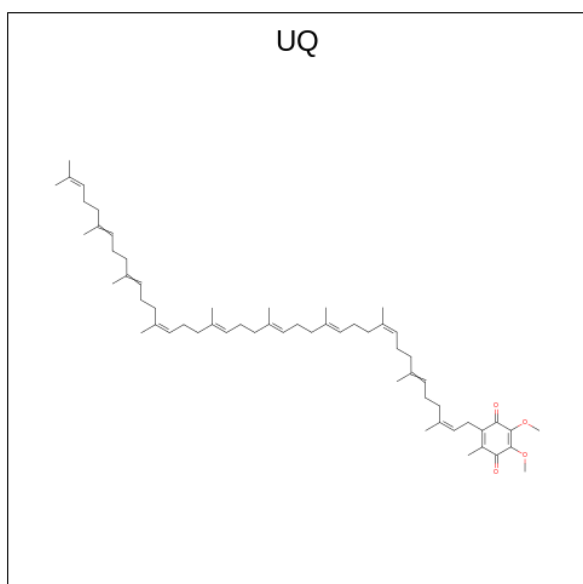
Mol	Chain	Residues	Atoms		AltConf
54	T	1	Total	Zn	0
			1	1	

- Molecule 55 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



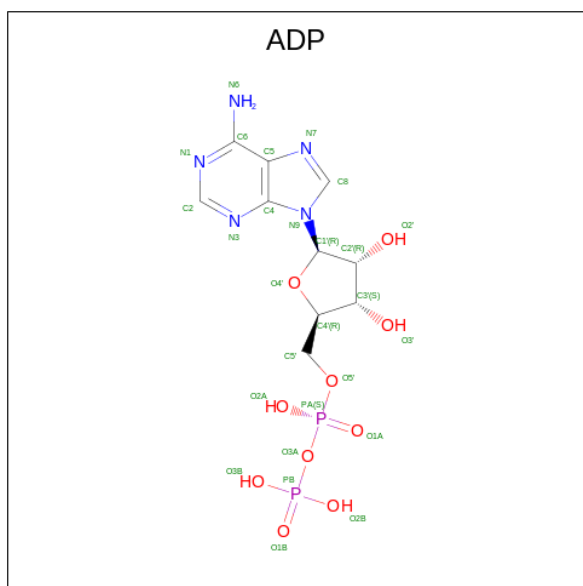
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
55	a	1	91	72	17	2	0
55	i	1	100	81	17	2	0
55	l	1	100	81	17	2	0

- Molecule 56 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
56	s	1	Total	C	O	0
			28	24	4	

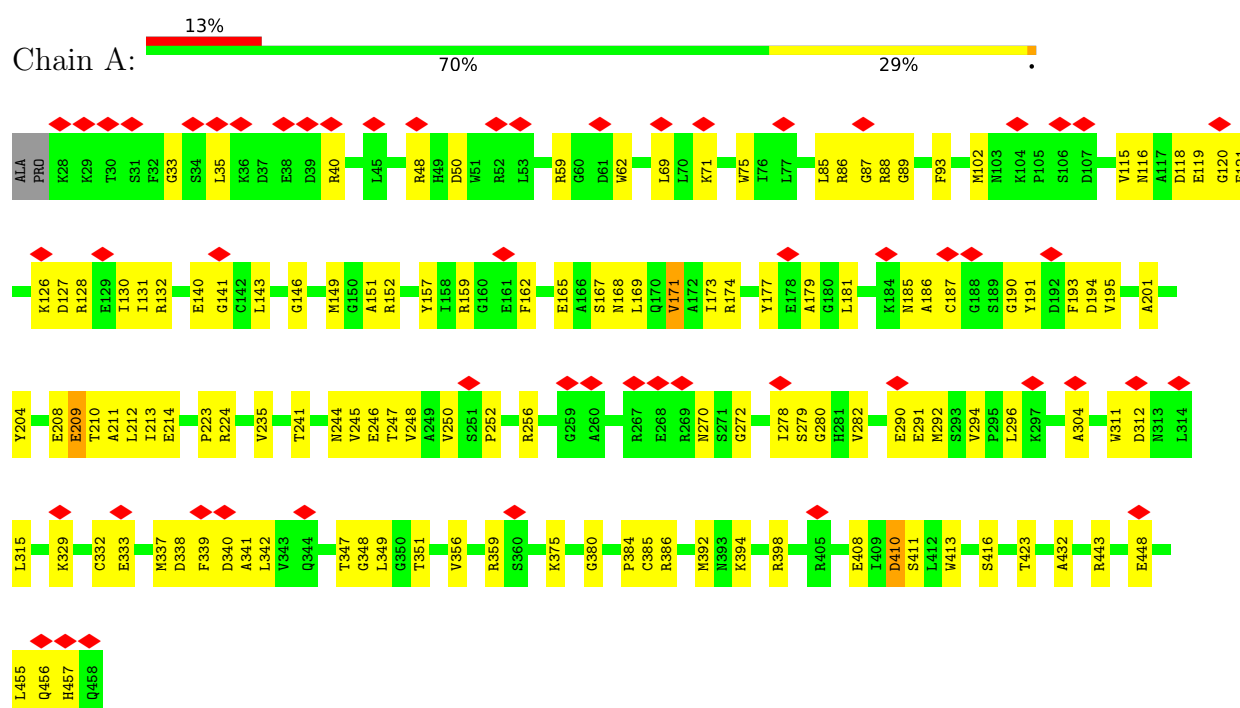
- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



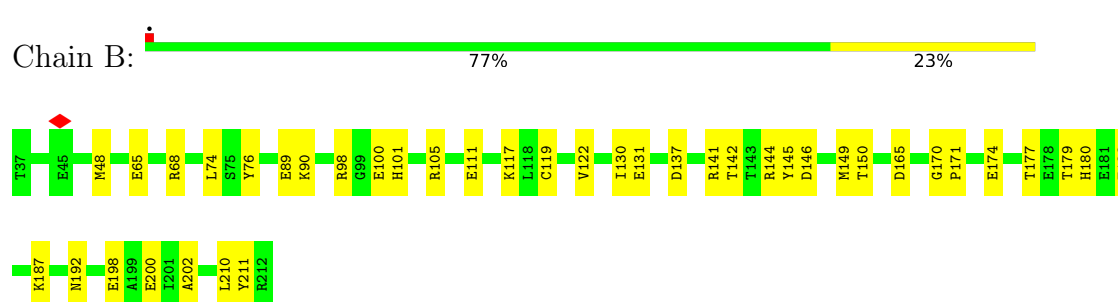
3 Residue-property plots

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.

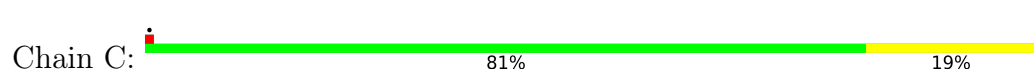
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

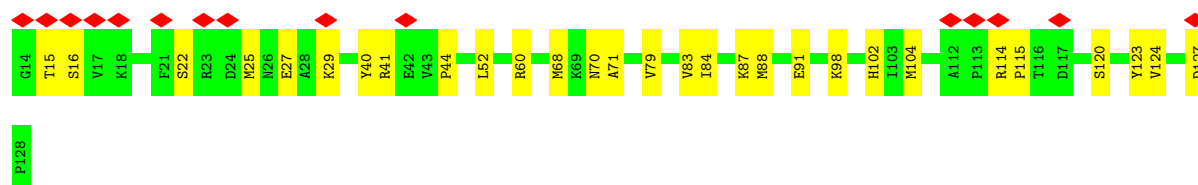
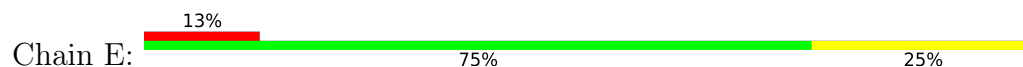


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

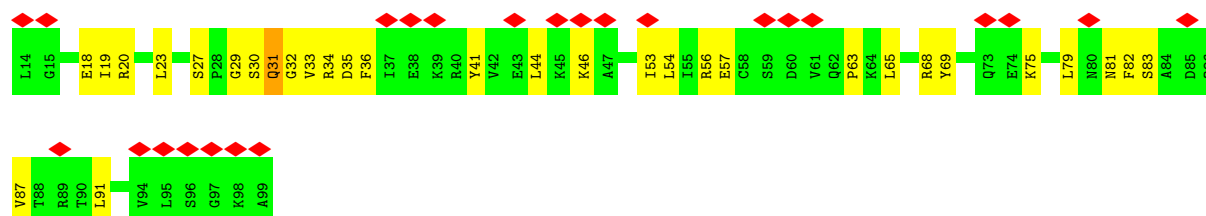




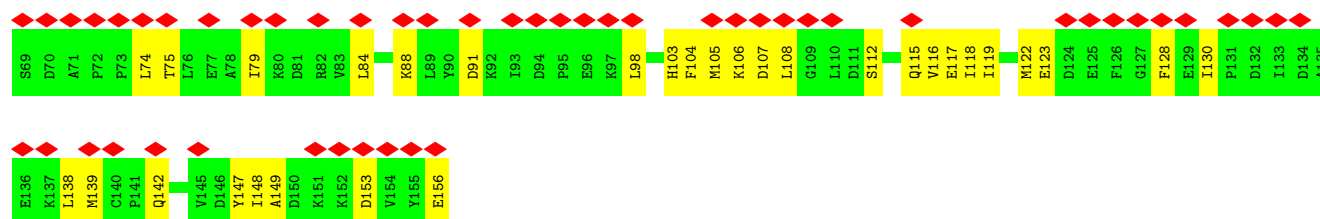
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 6: Acyl carrier protein



- Molecule 6: Acyl carrier protein



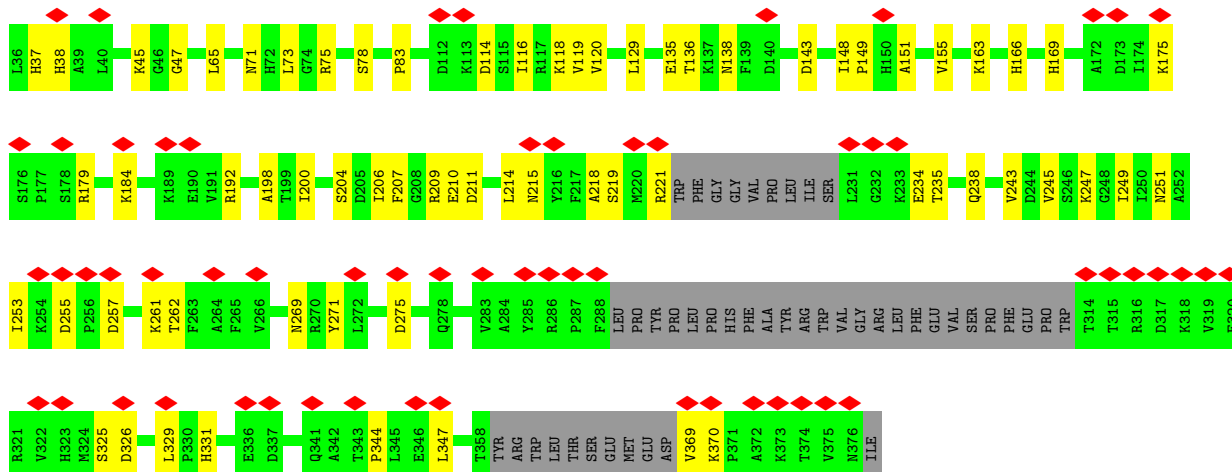
- Molecule 7: Complex I subunit B13



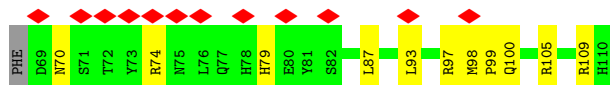
- Molecule 8: Complex I-B14.5a



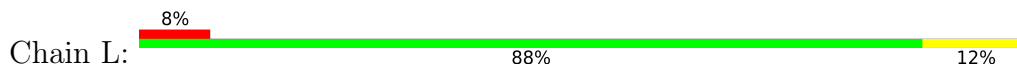
- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial



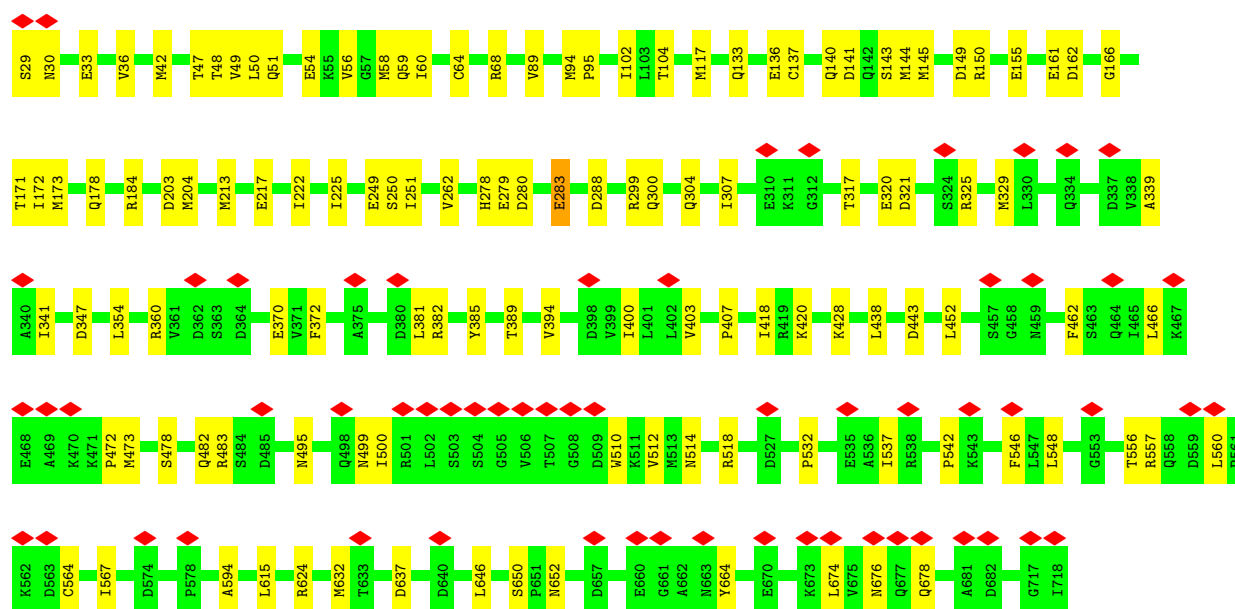
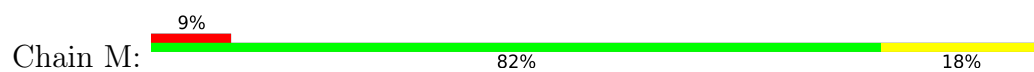
- Molecule 10: Complex I-9kD



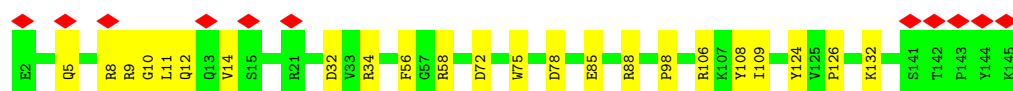
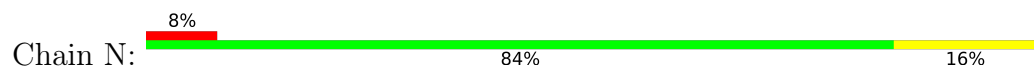
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



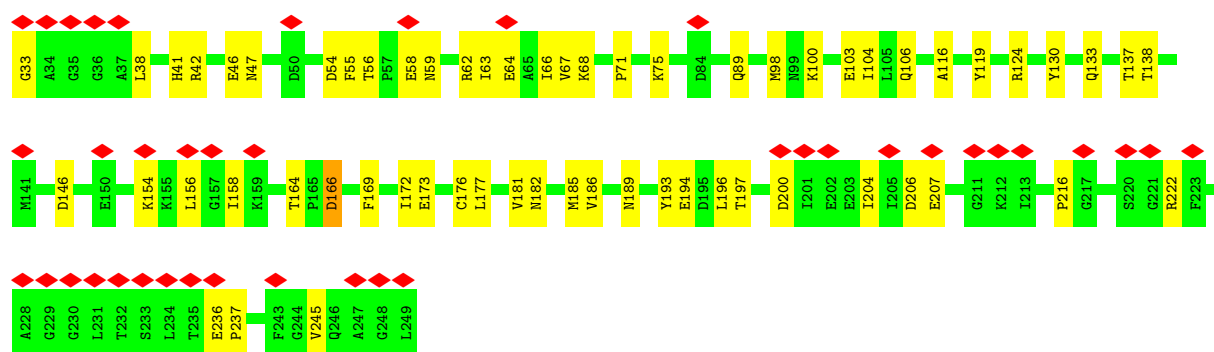
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



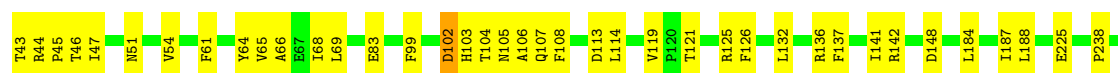
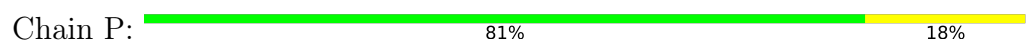
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



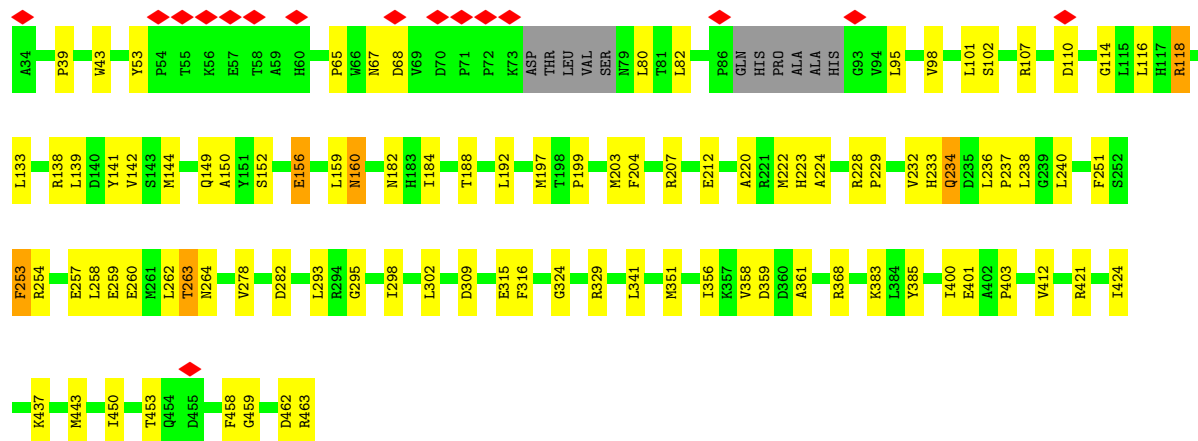
- Molecule 15: Complex I-30kD





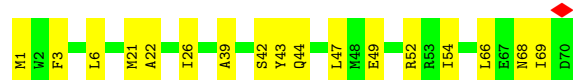
• Molecule 16: Complex I-49kD

Chain Q: 75% 21% ..



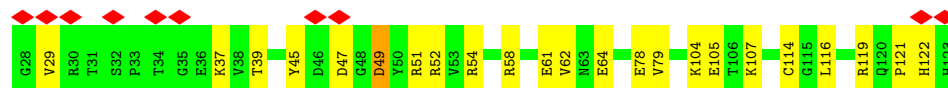
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S: 76% 24%



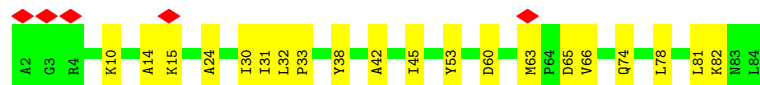
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T: 10% 76% 23%



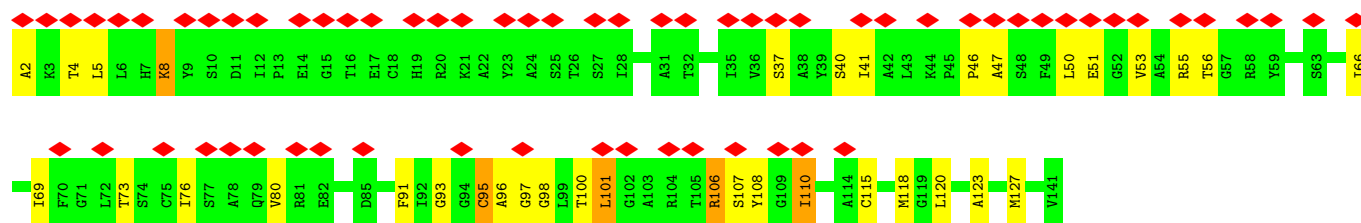
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U: 6% 76% 24%

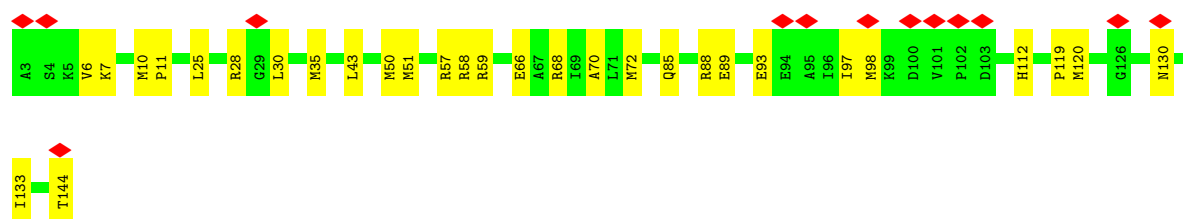
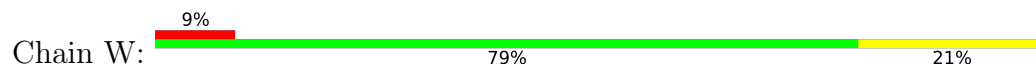


• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

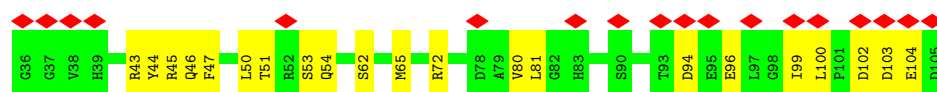
Chain V: 46% 74% 22%



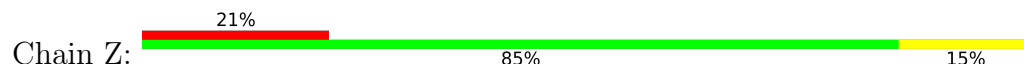
• Molecule 21: Complex I-B16.6



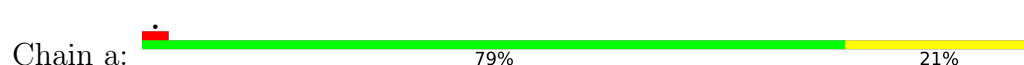
• Molecule 22: Complex I-AGGG



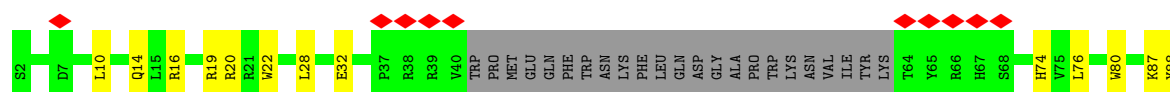
• Molecule 23: Complex I-B12

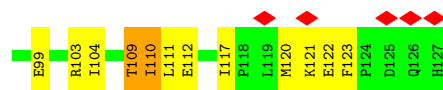


• Molecule 24: Complex I-SGDH

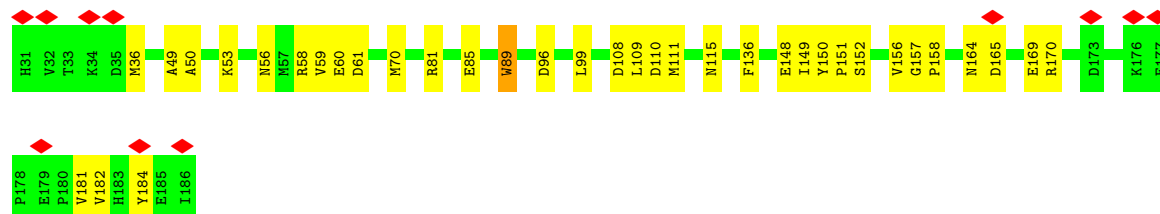
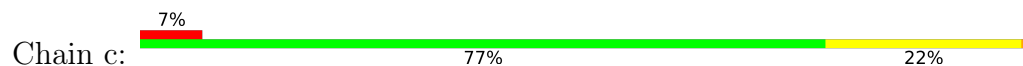


• Molecule 25: Complex I-B17

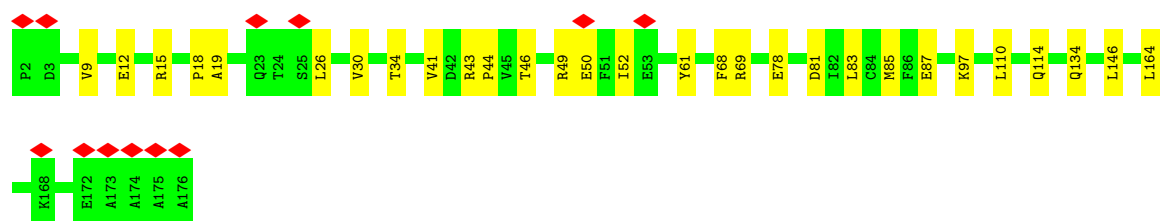
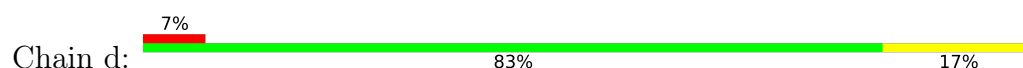




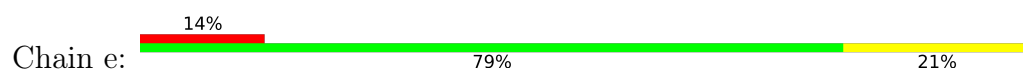
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



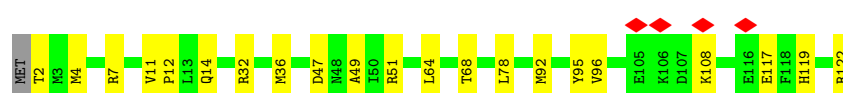
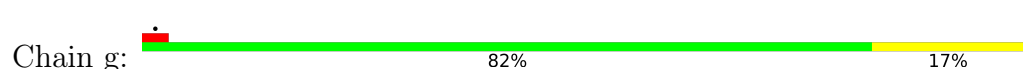
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



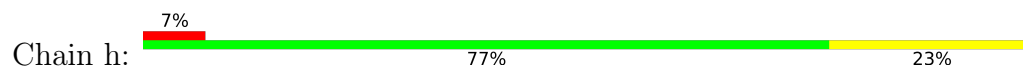
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



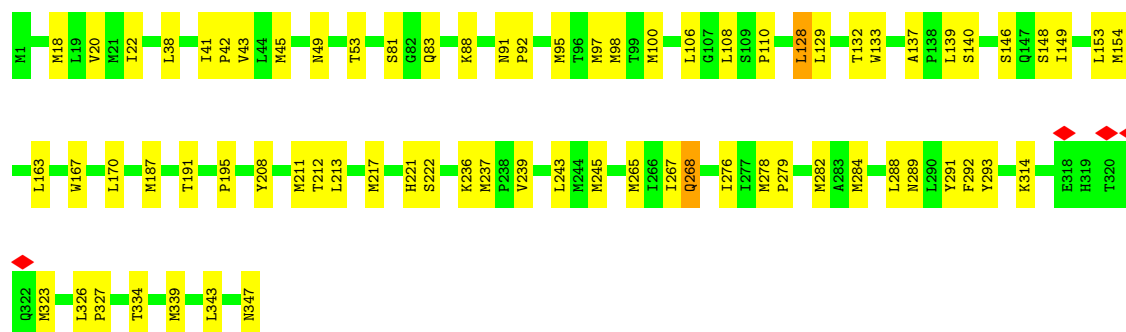
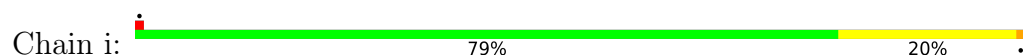
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



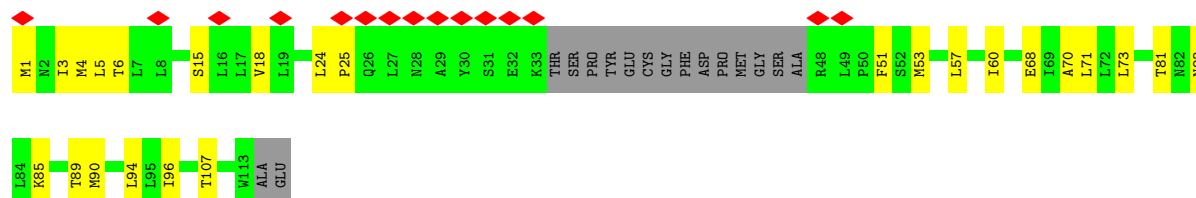
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



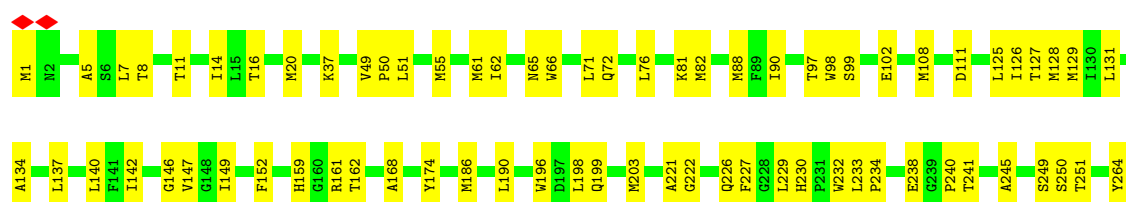
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

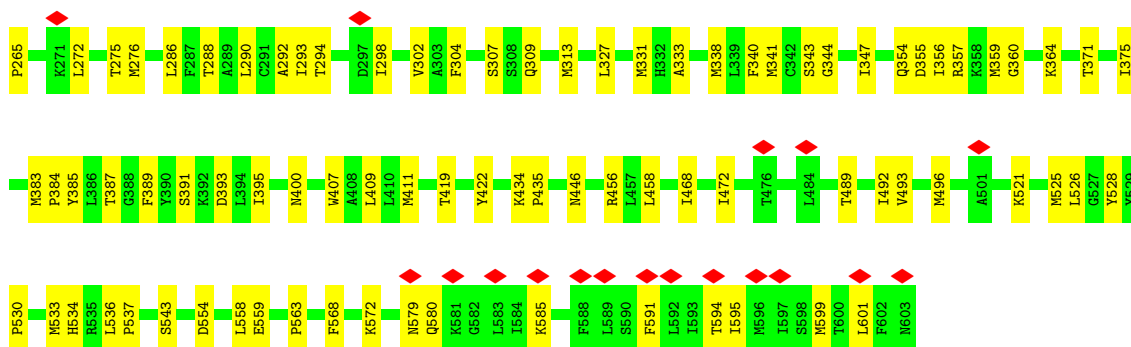


- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

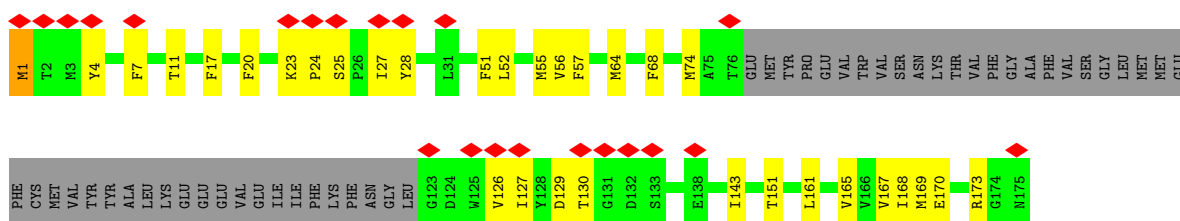


- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

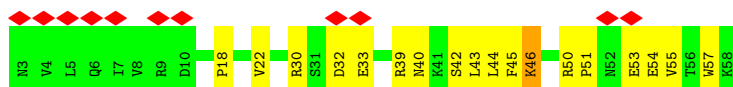




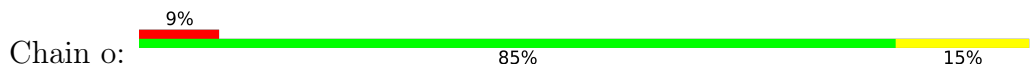
• Molecule 36: NADH-ubiquinone oxidoreductase chain 6



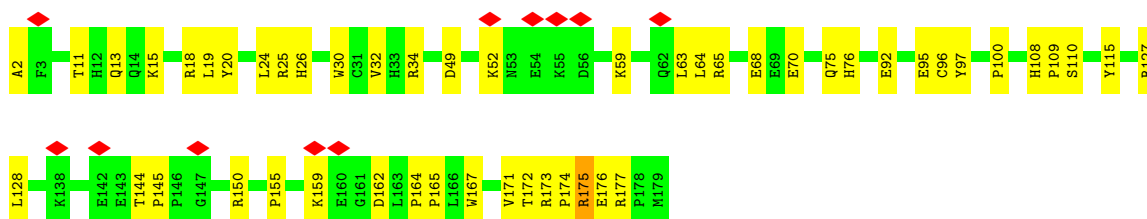
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



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

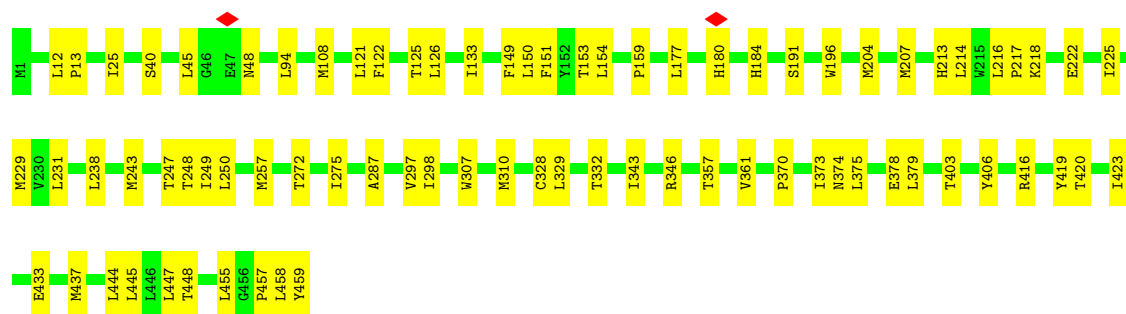


• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



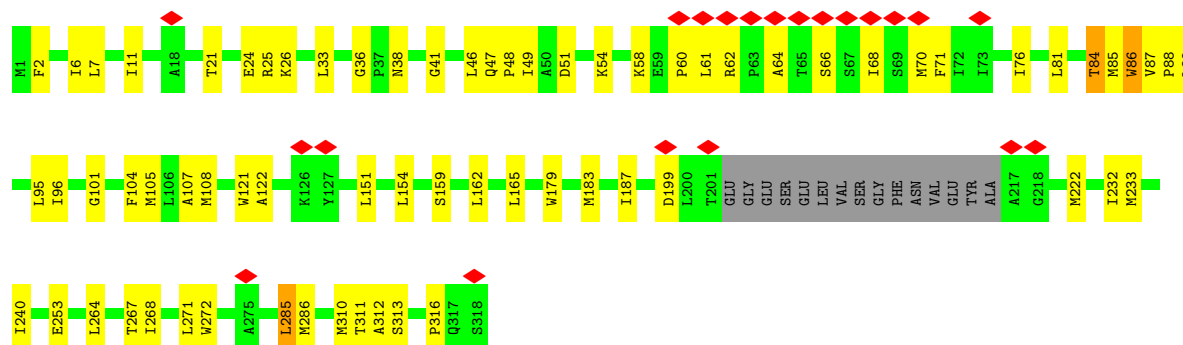
• Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r:  83% 17%



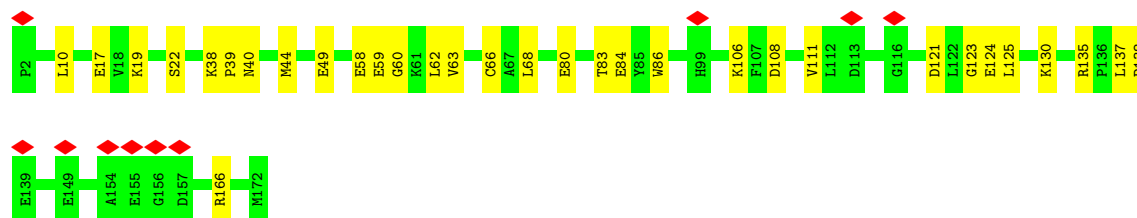
• Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s:  7% 73% 21% 5%



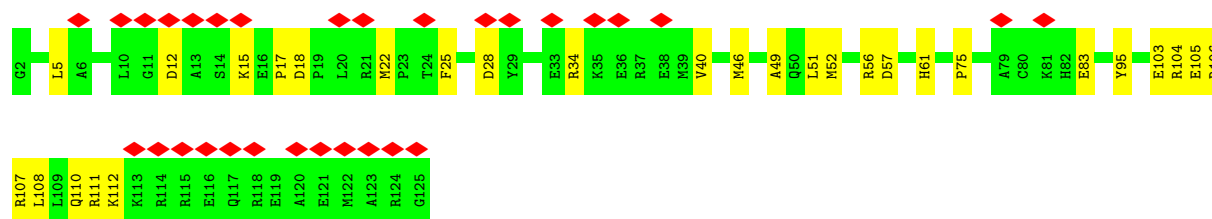
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:  6% 81% 19%

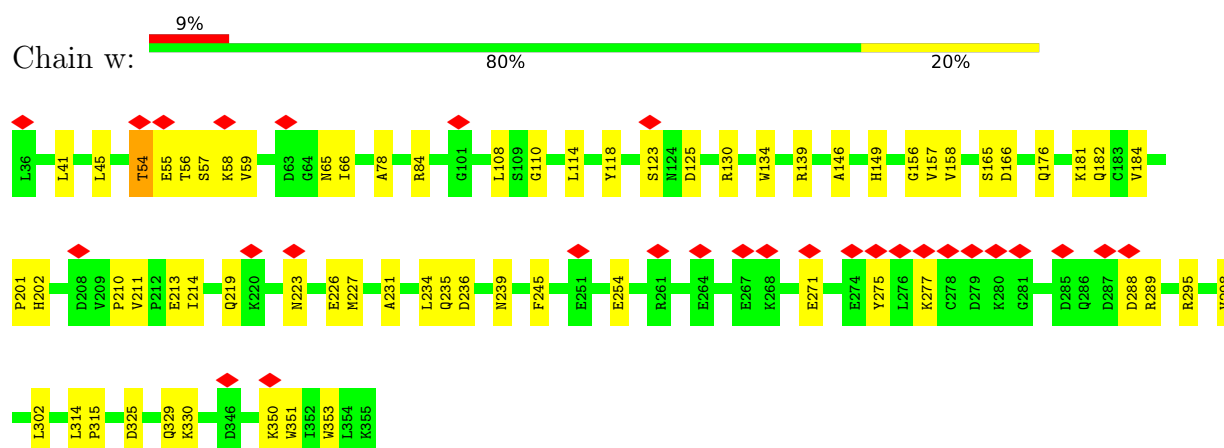


• Molecule 43: Complex I-B18

Chain v:  24% 77% 23%



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23715	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.230	Depositor
Minimum map value	-0.103	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0282	Depositor
Map size ($\text{\AA}$)	333.7616, 333.7616, 333.7616	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, NDP, 8Q1, 2MR, FMN, PLX, UQ, NAI, SF4, MG, FES, PEE, ADP, ZN

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	0.18	0/3389	0.40	2/4579 (0.0%)
2	B	0.16	0/1443	0.29	0/1952
3	C	0.19	0/1279	0.49	2/1730 (0.1%)
4	E	0.13	0/995	0.30	0/1340
5	F	0.18	0/683	0.48	2/922 (0.2%)
6	G	0.17	0/702	0.31	0/952
6	X	0.13	0/708	0.35	0/959
7	H	0.21	0/925	0.45	0/1253
8	I	0.14	0/798	0.35	0/1079
9	J	0.12	0/2407	0.30	0/3249
10	K	0.09	0/365	0.22	0/493
11	L	0.15	0/1039	0.28	0/1403
12	M	0.13	0/5384	0.30	0/7295
13	N	0.12	0/1245	0.30	0/1694
14	O	0.13	0/1711	0.32	0/2328
15	P	0.20	0/1789	0.41	1/2436 (0.0%)
16	Q	0.22	0/3451	0.48	5/4672 (0.1%)
17	S	0.17	0/582	0.38	0/783
18	T	0.12	0/755	0.29	0/1018
19	U	0.17	0/661	0.48	2/909 (0.2%)
20	V	0.28	1/1036 (0.1%)	0.48	0/1404
21	W	0.16	0/1204	0.31	0/1624
22	Y	0.22	0/623	0.49	0/853
23	Z	0.13	0/695	0.28	0/939
24	a	0.16	0/1199	0.35	0/1623
25	b	0.21	0/897	0.56	3/1221 (0.2%)
26	c	0.19	0/1367	0.39	1/1870 (0.1%)
27	d	0.15	0/1494	0.32	0/2015
28	e	0.16	0/916	0.38	0/1246
29	f	0.19	0/350	0.44	0/473
30	g	0.16	0/1031	0.31	0/1394
31	h	0.14	0/889	0.29	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.18	0/2769	0.37	0/3763
33	j	0.19	0/819	0.38	0/1117
34	k	0.19	0/759	0.33	0/1029
35	l	0.17	0/4911	0.38	0/6679
36	m	0.19	0/970	0.40	0/1316
37	n	0.19	0/478	0.49	0/647
38	o	0.15	0/1092	0.37	0/1481
39	p	0.18	0/1584	0.41	0/2147
40	r	0.17	0/3723	0.34	0/5078
41	s	0.20	0/2464	0.45	1/3369 (0.0%)
42	u	0.14	0/1436	0.35	0/1938
43	v	0.15	0/1052	0.35	0/1411
44	w	0.13	0/2639	0.31	0/3576
All	All	0.17	1/66708 (0.0%)	0.37	19/90449 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	V	8	LYS	CE-NZ	-5.03	1.34	1.49

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	233	HIS	N-CA-C	10.07	122.26	111.28
3	C	124	MET	CA-C-N	8.20	128.14	119.85
3	C	124	MET	C-N-CA	8.20	128.14	119.85
15	P	102	ASP	N-CA-C	7.99	120.07	111.36
25	b	111	LEU	N-CA-C	7.81	119.79	111.28
25	b	109	THR	N-CA-C	7.60	119.64	111.36
16	Q	234	GLN	N-CA-C	7.39	124.39	114.12
41	s	86	TRP	N-CA-C	7.01	119.78	111.71
1	A	250	VAL	N-CA-C	6.76	117.54	110.72
26	c	89	TRP	N-CA-C	6.60	119.47	111.82
16	Q	262	LEU	N-CA-C	6.30	121.63	113.88
25	b	112	GLU	N-CA-C	5.72	117.19	111.07
1	A	209	GLU	N-CA-C	5.62	117.08	111.07
19	U	63	MET	CA-C-N	5.47	125.12	119.05
19	U	63	MET	C-N-CA	5.47	125.12	119.05
16	Q	238	LEU	N-CA-C	5.29	117.05	111.28
16	Q	142	VAL	N-CA-C	-5.18	107.78	112.96
5	F	27	SER	CA-C-N	5.10	124.41	118.85
5	F	27	SER	C-N-CA	5.10	124.41	118.85

There are no chirality outliers.

There are no planarity outliers.

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	3314	0	3273	120	0
2	B	1412	0	1363	41	0
3	C	1248	0	1254	29	0
4	E	971	0	975	22	0
5	F	672	0	674	31	0
6	G	690	0	669	33	0
6	X	696	0	680	34	0
7	H	906	0	946	32	0
8	I	780	0	808	15	0
9	J	2355	0	2398	44	0
10	K	355	0	329	12	0
11	L	1016	0	1016	16	0
12	M	5296	0	5326	86	0
13	N	1204	0	1162	20	0
14	O	1671	0	1673	53	0
15	P	1738	0	1693	41	0
16	Q	3377	0	3318	75	0
17	S	567	0	565	15	0
18	T	741	0	702	20	0
19	U	640	0	635	20	0
20	V	1015	0	1018	39	0
21	W	1173	0	1166	39	0
22	Y	597	0	537	21	0
23	Z	674	0	643	14	0
24	a	1165	0	1174	34	0
25	b	870	0	888	30	0
26	c	1311	0	1204	31	0
27	d	1461	0	1429	33	0
28	e	890	0	837	19	0
29	f	342	0	341	14	0
30	g	1000	0	994	21	0
31	h	867	0	871	24	0
32	i	2706	0	2870	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	j	800	0	855	24	0
34	k	748	0	799	26	0
35	l	4782	0	4929	135	0
36	m	948	0	960	41	0
37	n	466	0	467	26	0
38	o	1062	0	1072	14	0
39	p	1529	0	1465	45	0
40	r	3631	0	3839	60	0
41	s	2394	0	2508	77	0
42	u	1398	0	1378	25	0
43	v	1028	0	980	31	0
44	w	2579	0	2529	56	0
45	A	8	0	0	1	0
45	B	16	0	0	0	0
45	C	8	0	0	1	0
45	M	16	0	0	0	0
46	A	31	0	19	6	0
47	A	44	0	27	5	0
48	C	47	0	71	0	0
48	Q	98	0	153	8	0
48	U	51	0	82	3	0
48	l	92	0	138	5	0
48	m	41	0	59	3	0
48	r	51	0	82	6	0
49	C	52	0	88	2	0
49	a	52	0	88	3	0
49	i	52	0	88	3	0
49	j	52	0	88	3	0
49	r	104	0	176	4	0
50	G	35	0	0	8	0
50	X	35	0	0	4	0
51	J	48	0	24	1	0
52	M	4	0	0	0	0
52	O	4	0	0	0	0
53	M	1	0	0	0	0
54	T	1	0	0	0	0
55	a	91	0	132	6	0
55	i	100	0	156	8	0
55	l	100	0	156	4	0
56	s	28	0	31	5	0
57	w	27	0	11	2	0
All	All	66374	0	66881	1459	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 11.

All (1459) 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)
6:G:112:SER:CB	50:G:201:8Q1:O1	1.70	1.38
6:X:112:SER:CB	50:X:201:8Q1:O1	1.70	1.37
20:V:4:THR:HG22	20:V:8:LYS:NZ	1.53	1.22
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.19
24:a:106:VAL:HG13	37:n:50:ARG:NH2	1.56	1.19
51:J:401:NDP:O4D	51:J:401:NDP:C4D	1.68	1.18
41:s:87:VAL:CG2	41:s:88:PRO:HD3	1.75	1.17
20:V:66:ILE:HD11	20:V:101:LEU:CD2	1.77	1.15
20:V:66:ILE:CD1	20:V:101:LEU:HD22	1.81	1.10
1:A:157:TYR:CG	1:A:212:LEU:HD11	1.87	1.10
41:s:87:VAL:HG23	41:s:88:PRO:HD3	1.12	1.07
1:A:456:GLN:OE1	1:A:457:HIS:ND1	1.90	1.04
1:A:278:ILE:HD12	1:A:304:ALA:CB	1.88	1.03
27:d:78:GLU:OE1	30:g:108:LYS:HB3	1.58	1.03
32:i:149:ILE:HD12	32:i:154:MET:HG3	1.41	1.02
1:A:141:GLY:HA2	1:A:252:PRO:HG3	1.38	1.02
1:A:278:ILE:HD12	1:A:304:ALA:HB2	0.98	0.98
30:g:2:THR:HG21	30:g:4:MET:HE2	1.45	0.98
1:A:278:ILE:CD1	1:A:304:ALA:HB2	1.93	0.97
35:l:525:MET:HE2	35:l:528:TYR:HE1	1.27	0.97
24:a:106:VAL:HG13	37:n:50:ARG:HH21	1.12	0.96
7:H:94:MET:HE1	7:H:99:PRO:HG3	1.46	0.96
16:Q:236:LEU:HD22	16:Q:240:LEU:HD23	1.45	0.96
1:A:127:ASP:OD2	1:A:245:VAL:HB	1.64	0.96
6:G:115:GLN:O	6:G:119:ILE:HG12	1.65	0.95
44:w:350:LYS:HB3	44:w:351:TRP:HE3	1.30	0.95
44:w:350:LYS:HB3	44:w:351:TRP:CE3	2.01	0.95
16:Q:282:ASP:OD2	16:Q:437:LYS:HE2	1.68	0.94
44:w:66:ILE:O	44:w:214:ILE:HD11	1.67	0.94
6:G:112:SER:CB	50:G:201:8Q1:P24	2.57	0.92
7:H:31:ILE:HD13	7:H:88:LEU:HA	1.49	0.92
19:U:53:TYR:HB2	21:W:72:MET:HE1	1.52	0.91
12:M:33:GLU:HB2	12:M:42:MET:HE1	1.51	0.91
20:V:98:GLY:HA2	20:V:118:MET:SD	2.10	0.91
20:V:4:THR:HG22	20:V:8:LYS:HZ1	1.25	0.90
21:W:98:MET:HE3	31:h:79:ILE:HG12	1.49	0.90
35:l:90:ILE:HG12	35:l:129:MET:HE2	1.50	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.54	0.90
45:C:301:SF4:S4	16:Q:223:HIS:CD2	2.65	0.89
41:s:87:VAL:HG23	41:s:88:PRO:CD	2.01	0.89
41:s:46:LEU:HA	41:s:49:ILE:HD13	1.54	0.89
25:b:109:THR:CG2	27:d:19:ALA:HB3	2.03	0.89
27:d:164:LEU:HD12	28:e:149:LEU:HD23	1.56	0.88
35:l:331:MET:HB3	35:l:387:THR:HG22	1.56	0.87
22:Y:80:VAL:HG23	35:l:385:TYR:OH	1.75	0.87
32:i:88:LYS:HD2	32:i:148:SER:OG	1.75	0.87
5:F:36:PHE:HD2	5:F:87:VAL:HG23	1.38	0.86
30:g:2:THR:CG2	30:g:4:MET:HE2	2.05	0.86
41:s:285:LEU:HD12	41:s:286:MET:N	1.91	0.86
6:G:112:SER:O	6:G:116:VAL:HG23	1.76	0.86
2:B:130:ILE:HD11	2:B:145:TYR:HE1	1.40	0.85
20:V:66:ILE:HD11	20:V:101:LEU:HD22	0.91	0.85
34:k:10:MET:O	34:k:14:ILE:HG13	1.76	0.85
1:A:168:ASN:O	1:A:171:VAL:HG13	1.77	0.84
7:H:94:MET:HE1	7:H:99:PRO:CG	2.07	0.83
20:V:4:THR:CG2	20:V:8:LYS:NZ	2.38	0.83
5:F:20:ARG:HG2	5:F:54:LEU:HD13	1.60	0.83
20:V:106:ARG:HA	20:V:106:ARG:NE	1.92	0.83
15:P:51:ASN:ND2	15:P:54:VAL:HG23	1.93	0.82
1:A:141:GLY:HA2	1:A:252:PRO:CG	2.10	0.81
1:A:102:MET:HG2	1:A:149:MET:HB3	1.61	0.81
35:l:525:MET:HE2	35:l:528:TYR:CE1	2.15	0.81
41:s:49:ILE:HD12	41:s:49:ILE:H	1.44	0.81
7:H:94:MET:CE	7:H:99:PRO:HG3	2.11	0.81
24:a:87:THR:O	24:a:91:VAL:HG23	1.81	0.81
1:A:181:LEU:O	1:A:186:ALA:HB1	1.80	0.81
20:V:66:ILE:CD1	20:V:101:LEU:CD2	2.49	0.80
32:i:132:THR:CG2	32:i:212:THR:CG2	2.60	0.80
44:w:66:ILE:HD11	44:w:234:LEU:HD23	1.61	0.79
15:P:46:THR:HG23	16:Q:358:VAL:CG2	2.11	0.79
16:Q:282:ASP:OD2	16:Q:437:LYS:CE	2.29	0.79
1:A:169:LEU:O	1:A:173:ILE:HG13	1.82	0.79
37:n:42:SER:OG	37:n:45:PHE:HB2	1.82	0.79
25:b:109:THR:HG21	27:d:19:ALA:HB3	1.65	0.79
12:M:49:VAL:HG13	12:M:102:ILE:HD13	1.65	0.78
1:A:167:SER:O	1:A:171:VAL:HG12	1.82	0.78
15:P:51:ASN:HD22	15:P:54:VAL:CG2	1.97	0.78
21:W:120:MET:CE	36:m:126:VAL:HG13	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:GLU:OE2	1:A:252:PRO:HB3	1.84	0.77
6:X:112:SER:CB	50:X:201:8Q1:P24	2.73	0.77
33:j:73:LEU:HD13	36:m:55:MET:HE1	1.65	0.77
35:l:129:MET:HE3	35:l:129:MET:HA	1.64	0.77
41:s:70:MET:HG3	41:s:121:TRP:HZ3	1.48	0.77
6:X:132:ASP:HB3	39:p:18:ARG:HE	1.50	0.77
36:m:173:ARG:HG2	36:m:173:ARG:HH11	1.50	0.76
5:F:69:TYR:HE2	5:F:75:LYS:HG3	1.51	0.76
34:k:1:MET:HE2	34:k:6:MET:HG2	1.67	0.76
40:r:207:MET:HE3	40:r:298:ILE:HG13	1.66	0.75
32:i:132:THR:CG2	32:i:212:THR:HG21	2.15	0.75
33:j:70:ALA:HA	33:j:73:LEU:HD12	1.68	0.75
30:g:64:LEU:O	30:g:68:THR:HG23	1.86	0.75
44:w:54:THR:HG23	44:w:56:THR:HG22	1.69	0.75
20:V:95:CYS:HB2	20:V:115:CYS:SG	2.27	0.75
20:V:98:GLY:CA	20:V:118:MET:SD	2.75	0.75
36:m:170:GLU:OE1	36:m:173:ARG:NH2	2.20	0.74
40:r:370:PRO:HB3	40:r:375:LEU:HD22	1.66	0.74
6:G:119:ILE:CG2	6:G:130:ILE:HD11	2.17	0.74
34:k:33:LEU:HD23	34:k:36:MET:HE2	1.67	0.74
49:a:202:PLX:H102	40:r:40:SER:HB3	1.69	0.74
39:p:108:HIS:ND1	39:p:110:SER:OG	2.21	0.74
14:O:55:PHE:HA	14:O:89:GLN:HE22	1.52	0.74
26:c:115:ASN:OD1	35:l:162:THR:HG23	1.87	0.74
35:l:383:MET:HG3	35:l:384:PRO:HD2	1.67	0.74
44:w:211:VAL:HA	44:w:214:ILE:HG22	1.70	0.74
32:i:213:LEU:O	32:i:217:MET:HG3	1.88	0.73
29:f:40:ASP:O	29:f:44:VAL:HG23	1.88	0.73
4:E:52:LEU:HG	4:E:104:MET:HE2	1.70	0.73
39:p:174:PRO:O	39:p:175:ARG:HB2	1.88	0.73
6:G:115:GLN:NE2	6:G:119:ILE:HD11	2.03	0.73
3:C:79:MET:HE2	3:C:86:MET:HE2	1.70	0.72
41:s:6:ILE:HD13	41:s:95:LEU:HD21	1.71	0.72
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.21	0.72
6:X:93:ILE:HG22	6:X:110:LEU:HD21	1.70	0.72
35:l:383:MET:CG	35:l:384:PRO:HD2	2.19	0.72
1:A:315:LEU:HB2	1:A:359:ARG:HG3	1.70	0.72
20:V:95:CYS:CB	20:V:115:CYS:SG	2.77	0.72
44:w:325:ASP:O	44:w:329:GLN:HG2	1.89	0.72
5:F:18:GLU:HG2	5:F:68:ARG:HE	1.55	0.71
35:l:591:PHE:O	35:l:595:ILE:HG13	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:36:PHE:CD2	5:F:87:VAL:HG23	2.24	0.71
15:P:105:ASN:O	15:P:137:PHE:CE2	2.43	0.71
39:p:19:LEU:HD13	39:p:68:GLU:OE2	1.91	0.71
1:A:141:GLY:CA	1:A:252:PRO:HG3	2.18	0.71
2:B:171:PRO:HG3	2:B:200:GLU:HG2	1.73	0.71
6:G:112:SER:N	50:G:201:8Q1:O1	2.22	0.71
32:i:132:THR:HG22	32:i:212:THR:HG21	1.70	0.71
25:b:104:ILE:HD12	25:b:110:ILE:HD11	1.72	0.71
35:l:134:ALA:HB3	35:l:140:LEU:HD13	1.72	0.71
6:G:112:SER:CA	50:G:201:8Q1:O1	2.39	0.71
1:A:119:GLU:OE1	1:A:127:ASP:HB2	1.90	0.71
16:Q:152:SER:O	16:Q:156:GLU:CG	2.38	0.71
33:j:18:VAL:HG22	41:s:222:MET:HG3	1.72	0.71
33:j:73:LEU:HD23	41:s:151:LEU:HD21	1.71	0.71
1:A:168:ASN:O	1:A:171:VAL:CG1	2.39	0.71
16:Q:236:LEU:HD22	16:Q:240:LEU:CD2	2.20	0.71
44:w:210:PRO:HD2	44:w:213:GLU:OE1	1.90	0.71
22:Y:100:LEU:HB2	43:v:111:ARG:HH12	1.56	0.70
32:i:139:LEU:HD11	32:i:187:MET:HE1	1.71	0.70
39:p:49:ASP:HB2	39:p:52:LYS:HD2	1.74	0.70
1:A:62:TRP:CE3	1:A:181:LEU:HD12	2.27	0.70
12:M:171:THR:HG23	12:M:173:MET:SD	2.32	0.70
9:J:136:THR:HG22	9:J:138:ASN:H	1.56	0.70
32:i:128:LEU:C	32:i:128:LEU:HD23	2.17	0.70
41:s:87:VAL:HG12	41:s:95:LEU:HD23	1.73	0.70
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.31	0.70
15:P:107:GLN:NE2	15:P:136:ARG:HG2	2.06	0.70
1:A:211:ALA:HB2	1:A:223:PRO:HG3	1.73	0.69
12:M:360:ARG:HH21	12:M:632:MET:HA	1.57	0.69
11:L:109:ASN:ND2	11:L:111:LEU:O	2.24	0.69
15:P:51:ASN:HD22	15:P:54:VAL:HG23	1.55	0.69
18:T:54:ARG:O	18:T:58:ARG:NH2	2.23	0.69
24:a:133:TYR:OH	27:d:87:GLU:HG3	1.92	0.69
33:j:85:LYS:O	33:j:89:THR:HG23	1.92	0.69
7:H:77:ILE:O	7:H:81:ILE:HG13	1.92	0.69
1:A:33:GLY:HA2	1:A:294:VAL:HG12	1.73	0.69
20:V:4:THR:CG2	20:V:8:LYS:HZ1	2.01	0.69
34:k:23:ARG:HG2	36:m:23:LYS:HE2	1.75	0.68
1:A:141:GLY:CA	1:A:252:PRO:CG	2.71	0.68
33:j:25:PRO:HB2	41:s:60:PRO:HD3	1.75	0.68
35:l:159:HIS:HB2	40:r:416:ARG:HG2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:347:ILE:HD13	35:l:354:GLN:HG2	1.75	0.68
1:A:342:LEU:HD22	1:A:347:THR:HG21	1.74	0.68
19:U:66:VAL:CG1	42:u:130:LYS:HD3	2.24	0.68
29:f:62:HIS:O	29:f:66:VAL:HG23	1.94	0.68
12:M:161:GLU:OE1	14:O:42:ARG:NH2	2.27	0.68
41:s:70:MET:HG3	41:s:121:TRP:CZ3	2.28	0.68
9:J:218:ALA:O	9:J:221:ARG:NH1	2.25	0.68
29:f:39:PRO:HG2	44:w:351:TRP:CD1	2.28	0.68
12:M:500:ILE:HD11	12:M:512:VAL:HG11	1.76	0.67
28:e:72:ASP:OD1	39:p:108:HIS:NE2	2.26	0.67
43:v:51:LEU:O	43:v:52:MET:HG2	1.93	0.67
44:w:66:ILE:HD11	44:w:234:LEU:CD2	2.23	0.67
17:S:54:ILE:O	42:u:19:LYS:NZ	2.28	0.67
44:w:146:ALA:HB1	44:w:157:VAL:HG21	1.77	0.67
40:r:374:ASN:O	40:r:378:GLU:HG2	1.94	0.67
5:F:23:LEU:HD12	5:F:34:ARG:HG2	1.76	0.67
5:F:30:SER:O	5:F:33:VAL:N	2.28	0.67
14:O:156:LEU:HD11	14:O:169:PHE:HD2	1.58	0.67
5:F:36:PHE:HD2	5:F:87:VAL:CG2	2.08	0.67
16:Q:152:SER:O	16:Q:156:GLU:HG2	1.94	0.67
21:W:120:MET:HE3	36:m:126:VAL:HG13	1.77	0.67
35:l:161:ARG:NH1	35:l:238:GLU:OE1	2.28	0.67
15:P:51:ASN:ND2	15:P:54:VAL:CG2	2.57	0.66
34:k:32:CYS:O	34:k:36:MET:HG3	1.96	0.66
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.28	0.66
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.77	0.66
2:B:111:GLU:O	2:B:141:ARG:NH1	2.29	0.66
7:H:93:LYS:HA	7:H:96:ARG:NH1	2.11	0.66
18:T:78:GLU:OE2	18:T:119:ARG:NH1	2.26	0.66
32:i:45:MET:HE3	32:i:53:THR:HG22	1.77	0.66
9:J:83:PRO:HG3	9:J:119:VAL:HG11	1.78	0.66
40:r:207:MET:HE3	40:r:298:ILE:CG1	2.26	0.66
43:v:25:PHE:HZ	43:v:112:LYS:HD2	1.59	0.66
18:T:47:ASP:HA	18:T:52:ARG:HH12	1.60	0.66
22:Y:54:GLN:OE1	35:l:446:ASN:ND2	2.29	0.66
29:f:39:PRO:HG3	44:w:351:TRP:HB3	1.78	0.66
2:B:177:THR:HG22	2:B:179:THR:H	1.60	0.66
32:i:88:LYS:HD2	32:i:148:SER:HG	1.61	0.66
19:U:30:ILE:HD11	33:j:96:ILE:HD11	1.78	0.65
21:W:93:GLU:OE2	31:h:95:PRO:HG2	1.96	0.65
35:l:526:LEU:HD12	35:l:530:PRO:HG2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ASP:O	1:A:59:ARG:NH2	2.28	0.65
1:A:157:TYR:CG	1:A:212:LEU:CD1	2.75	0.65
12:M:428:LYS:NZ	12:M:443:ASP:OD2	2.28	0.65
24:a:160:MET:HE2	30:g:95:TYR:CD1	2.31	0.65
20:V:101:LEU:HD12	20:V:101:LEU:O	1.95	0.65
30:g:47:ASP:OD1	30:g:51:ARG:NH1	2.30	0.65
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.79	0.65
34:k:37:MET:HE1	36:m:64:MET:HE1	1.77	0.65
1:A:152:ARG:NH2	10:K:99:PRO:O	2.29	0.65
11:L:88:GLN:NE2	12:M:141:ASP:OD2	2.29	0.65
20:V:47:ALA:HB3	20:V:51:GLU:OE1	1.97	0.65
6:X:134:ASP:OD1	39:p:2:ALA:N	2.30	0.65
35:l:391:SER:O	35:l:395:ILE:HG12	1.97	0.65
1:A:157:TYR:CD2	1:A:212:LEU:HD11	2.31	0.65
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.78	0.65
15:P:44:ARG:HE	15:P:45:PRO:HD3	1.61	0.65
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.29	0.64
32:i:149:ILE:HD11	32:i:195:PRO:HG3	1.79	0.64
35:l:227:PHE:O	35:l:230:HIS:ND1	2.30	0.64
48:r:501:PEE:H71	48:r:501:PEE:H32	1.78	0.64
4:E:71:ALA:HA	50:G:201:8Q1:O40	1.98	0.64
32:i:132:THR:HG21	32:i:212:THR:HG23	1.79	0.64
33:j:4:MET:HE2	48:m:201:PEE:H19	1.78	0.64
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.77	0.64
20:V:4:THR:HG22	20:V:8:LYS:HZ2	1.60	0.64
9:J:169:HIS:H	9:J:184:LYS:HD3	1.61	0.64
8:I:25:GLN:HB3	16:Q:254:ARG:NH1	2.13	0.64
1:A:174:ARG:HD2	1:A:174:ARG:C	2.22	0.64
20:V:106:ARG:HA	20:V:106:ARG:HE	1.63	0.64
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.80	0.64
19:U:53:TYR:HB2	21:W:72:MET:CE	2.26	0.64
1:A:75:TRP:CD1	1:A:75:TRP:C	2.76	0.63
36:m:57:PHE:HD2	41:s:107:ALA:HB1	1.62	0.63
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.79	0.63
44:w:176:GLN:NE2	44:w:236:ASP:OD2	2.30	0.63
2:B:192:ASN:ND2	18:T:61:GLU:OE1	2.31	0.63
7:H:30:LYS:O	7:H:34:VAL:HG23	1.99	0.63
21:W:97:ILE:HG22	21:W:98:MET:HE2	1.80	0.63
6:X:120:MET:HE1	39:p:24:LEU:HD13	1.80	0.63
55:i:402:CDL:H742	55:i:402:CDL:H271	1.79	0.63
16:Q:68:ASP:O	32:i:49:ASN:ND2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:98:CYS:HB2	35:l:580:GLN:HB2	1.80	0.63
43:v:25:PHE:HD2	43:v:108:LEU:HD23	1.62	0.63
44:w:139:ARG:NH1	44:w:166:ASP:OD2	2.31	0.63
14:O:63:ILE:O	14:O:67:VAL:HG23	1.99	0.63
35:l:375:ILE:HD12	35:l:458:LEU:HD11	1.81	0.63
43:v:12:ASP:HB3	43:v:15:LYS:HB2	1.81	0.63
7:H:76:GLN:O	7:H:79:GLU:HG2	1.99	0.63
21:W:85:GLN:OE1	31:h:105:ARG:NH1	2.28	0.63
12:M:178:GLN:HG2	12:M:204:MET:HE2	1.81	0.63
41:s:285:LEU:HD12	41:s:285:LEU:C	2.23	0.63
2:B:177:THR:HG21	2:B:182:GLU:HB2	1.81	0.62
25:b:123:PHE:HB3	43:v:40:VAL:HG21	1.80	0.62
14:O:64:GLU:OE1	14:O:68:LYS:HE3	1.99	0.62
9:J:192:ARG:NH2	9:J:262:THR:OG1	2.32	0.62
5:F:30:SER:O	5:F:32:GLY:N	2.33	0.62
18:T:104:LYS:HD2	18:T:107:LYS:HE2	1.82	0.62
21:W:98:MET:HE1	31:h:79:ILE:HA	1.79	0.62
41:s:87:VAL:CG2	41:s:88:PRO:CD	2.66	0.62
55:a:201:CDL:H322	48:l:703:PEE:H62	1.80	0.62
25:b:22:TRP:CD2	39:p:172:THR:HG22	2.34	0.62
21:W:97:ILE:CG2	21:W:98:MET:HE2	2.29	0.62
27:d:110:LEU:HD11	35:l:203:MET:HE2	1.82	0.62
12:M:347:ASP:HB3	12:M:594:ALA:HB1	1.82	0.62
24:a:120:TRP:O	24:a:124:THR:HG22	2.00	0.62
23:Z:84:ALA:O	23:Z:88:LEU:HG	1.99	0.62
1:A:256:ARG:HG2	14:O:245:VAL:HG12	1.81	0.61
28:e:85:TRP:O	28:e:89:VAL:HG13	2.00	0.61
35:l:108:MET:CE	35:l:240:PRO:HB3	2.30	0.61
3:C:66:THR:HG21	3:C:76:MET:HG3	1.83	0.61
14:O:38:LEU:O	14:O:124:ARG:NH2	2.32	0.61
31:h:97:HIS:HA	31:h:102:GLU:HB3	1.81	0.61
34:k:50:ASN:ND2	36:m:127:ILE:HD12	2.15	0.61
35:l:331:MET:CB	35:l:387:THR:HG22	2.28	0.61
44:w:125:ASP:O	44:w:130:ARG:NH2	2.33	0.61
12:M:68:ARG:NH2	12:M:279:GLU:OE2	2.33	0.61
19:U:81:LEU:O	21:W:59:ARG:NH1	2.33	0.61
15:P:43:THR:HA	15:P:47:ILE:HD12	1.82	0.61
17:S:47:LEU:HD22	42:u:22:SER:HB2	1.81	0.61
7:H:31:ILE:CD1	7:H:88:LEU:HA	2.25	0.61
7:H:96:ARG:HH11	7:H:96:ARG:HB3	1.64	0.61
1:A:71:LYS:HD3	1:A:75:TRP:CZ3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:65:LEU:HD23	9:J:129:LEU:HD22	1.83	0.61
9:J:211:ASP:O	9:J:215:ASN:ND2	2.33	0.61
39:p:64:LEU:O	39:p:68:GLU:HG2	2.00	0.61
14:O:206:ASP:OD1	14:O:207:GLU:N	2.33	0.61
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.32	0.61
16:Q:80:LEU:HD11	16:Q:82:LEU:HD21	1.82	0.61
16:Q:82:LEU:HD12	16:Q:101:LEU:HD13	1.82	0.61
32:i:163:LEU:HD22	32:i:167:TRP:CH2	2.36	0.61
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.30	0.61
4:E:40:TYR:CE2	6:G:117:GLU:HG2	2.36	0.61
16:Q:98:VAL:HG23	16:Q:110:ASP:HB3	1.83	0.61
41:s:46:LEU:HA	41:s:49:ILE:CD1	2.29	0.61
9:J:192:ARG:NH1	9:J:198:ALA:O	2.33	0.61
41:s:24:GLU:OE1	41:s:271:LEU:HD22	2.01	0.60
1:A:375:LYS:NZ	14:O:33:GLY:O	2.35	0.60
32:i:163:LEU:HD22	32:i:167:TRP:CZ3	2.36	0.60
3:C:61:SER:OG	41:s:54:LYS:HD3	2.01	0.60
10:K:105:ARG:NH1	11:L:167:ASN:O	2.34	0.60
27:d:68:PHE:HD1	37:n:44:LEU:HD11	1.65	0.60
25:b:110:ILE:HG22	25:b:110:ILE:O	2.01	0.60
7:H:94:MET:CE	7:H:99:PRO:CG	2.75	0.60
35:l:288:THR:HG21	35:l:307:SER:HB2	1.83	0.60
12:M:472:PRO:O	12:M:510:TRP:NE1	2.30	0.60
14:O:182:ASN:OD1	14:O:222:ARG:NH2	2.35	0.60
24:a:106:VAL:CG1	37:n:50:ARG:NH2	2.48	0.60
35:l:90:ILE:HG12	35:l:129:MET:CE	2.26	0.60
35:l:419:THR:HA	35:l:422:TYR:CE2	2.37	0.60
27:d:69:ARG:NH1	37:n:43:LEU:O	2.35	0.60
36:m:1:MET:HE3	36:m:4:TYR:H	1.67	0.60
5:F:33:VAL:O	5:F:36:PHE:HB3	2.01	0.60
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.83	0.60
36:m:57:PHE:CD2	41:s:107:ALA:HB1	2.37	0.60
1:A:185:ASN:ND2	1:A:187:CYS:O	2.34	0.60
12:M:50:LEU:O	12:M:54:GLU:HG3	2.02	0.60
14:O:156:LEU:HB3	14:O:158:ILE:HG12	1.84	0.60
32:i:132:THR:CG2	32:i:212:THR:HG23	2.32	0.60
9:J:204:SER:OG	9:J:238:GLN:O	2.20	0.59
17:S:39:ALA:HA	17:S:44:GLN:HG3	1.82	0.59
21:W:120:MET:HE1	36:m:126:VAL:HG13	1.84	0.59
15:P:68:ILE:HG21	15:P:99:PHE:CE1	2.37	0.59
18:T:39:THR:HG22	18:T:62:VAL:HG12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:347:ASN:HB3	49:i:401:PLX:H301	1.83	0.59
35:l:579:ASN:O	35:l:579:ASN:OD1	2.19	0.59
1:A:48:ARG:O	10:K:74:ARG:NH1	2.35	0.59
11:L:84:ARG:NH1	11:L:88:GLN:O	2.36	0.59
30:g:11:VAL:HB	30:g:14:GLN:HG3	1.83	0.59
1:A:88:ARG:HG3	1:A:246:GLU:OE2	2.03	0.59
41:s:62:ARG:HD3	41:s:64:ALA:H	1.65	0.59
44:w:84:ARG:HD3	44:w:149:HIS:CD2	2.37	0.59
1:A:282:VAL:HG13	1:A:356:VAL:HG21	1.84	0.59
5:F:30:SER:O	5:F:31:GLN:C	2.46	0.59
6:G:88:LYS:HD3	6:G:98:LEU:HD21	1.85	0.59
25:b:109:THR:HG23	27:d:19:ALA:HB3	1.84	0.59
32:i:110:PRO:HG2	35:l:594:THR:HG21	1.83	0.59
1:A:181:LEU:O	1:A:186:ALA:O	2.21	0.59
4:E:70:ASN:ND2	50:G:201:8Q1:O4	2.35	0.59
1:A:157:TYR:CD1	1:A:212:LEU:HD11	2.36	0.59
1:A:168:ASN:HA	1:A:171:VAL:CG1	2.33	0.59
8:I:9:GLN:O	8:I:13:ASN:ND2	2.32	0.59
24:a:155:GLU:OE1	24:a:158:ARG:NH2	2.33	0.59
15:P:106:ALA:HB1	15:P:108:PHE:CD1	2.38	0.59
6:X:82:ARG:O	6:X:86:VAL:HG23	2.02	0.59
29:f:68:GLU:OE2	29:f:71:ARG:NH2	2.36	0.59
7:H:38:ILE:O	7:H:45:ARG:NH1	2.31	0.59
12:M:58:MET:HE2	12:M:60:ILE:HD13	1.84	0.59
12:M:299:ARG:HG2	12:M:300:GLN:HG2	1.85	0.59
21:W:144:THR:HB	41:s:96:ILE:HG23	1.84	0.59
12:M:495:ASN:O	12:M:499:ASN:OD1	2.21	0.58
16:Q:116:LEU:O	16:Q:116:LEU:HG	2.02	0.58
27:d:114:GLN:HG3	35:l:203:MET:HG2	1.84	0.58
35:l:88:MET:HE1	35:l:468:ILE:HD12	1.83	0.58
40:r:243:MET:O	40:r:247:THR:HG23	2.02	0.58
1:A:456:GLN:OE1	1:A:457:HIS:CE1	2.56	0.58
5:F:30:SER:HB2	5:F:63:PRO:HG3	1.82	0.58
9:J:215:ASN:O	9:J:219:SER:OG	2.20	0.58
20:V:123:ALA:O	20:V:127:MET:HG3	2.03	0.58
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.86	0.58
5:F:33:VAL:HG22	5:F:87:VAL:HG11	1.85	0.58
8:I:18:ARG:HG3	8:I:18:ARG:HH11	1.68	0.58
9:J:234:GLU:OE1	9:J:234:GLU:N	2.35	0.58
32:i:132:THR:HG21	32:i:212:THR:CG2	2.33	0.58
7:H:93:LYS:HA	7:H:96:ARG:HH12	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.36	0.58
27:d:26:LEU:HD22	43:v:75:PRO:HB2	1.84	0.58
2:B:101:HIS:ND1	2:B:149:MET:HE1	2.18	0.58
35:l:8:THR:HB	35:l:82:MET:HE3	1.86	0.58
8:I:70:MET:HG2	15:P:66:ALA:HB1	1.85	0.58
29:f:39:PRO:HG3	44:w:351:TRP:CB	2.34	0.58
12:M:162:ASP:OD1	12:M:172:ILE:HA	2.03	0.58
39:p:59:LYS:HA	39:p:59:LYS:HE2	1.86	0.58
4:E:15:THR:OG1	11:L:55:VAL:O	2.22	0.58
9:J:249:ILE:O	9:J:253:ILE:HG13	2.04	0.58
12:M:546:PHE:CE1	12:M:567:ILE:HD13	2.39	0.58
15:P:51:ASN:HD22	15:P:54:VAL:HG21	1.69	0.58
24:a:152:LYS:HD3	30:g:96:VAL:HG21	1.86	0.58
44:w:114:LEU:HD21	57:w:401:ADP:H1'	1.86	0.58
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.86	0.57
14:O:67:VAL:HG13	14:O:75:LYS:HG3	1.86	0.57
16:Q:152:SER:O	16:Q:156:GLU:HG3	2.03	0.57
32:i:149:ILE:HD12	32:i:154:MET:CG	2.26	0.57
34:k:27:MET:HE1	36:m:68:PHE:HD2	1.69	0.57
44:w:211:VAL:HA	44:w:214:ILE:CG2	2.34	0.57
14:O:100:LYS:O	14:O:104:ILE:HG13	2.03	0.57
39:p:159:LYS:HB2	39:p:162:ASP:OD1	2.04	0.57
3:C:119:LYS:NZ	3:C:123:GLN:HE21	2.03	0.57
18:T:37:LYS:HD3	18:T:62:VAL:HG21	1.87	0.57
35:l:102:GLU:OE1	35:l:456:ARG:NH2	2.32	0.57
12:M:283:GLU:OE2	12:M:420:LYS:NZ	2.34	0.57
15:P:113:ASP:OD1	15:P:114:LEU:N	2.38	0.57
6:X:108:LEU:HB3	6:X:110:LEU:HD23	1.85	0.57
24:a:108:GLU:OE1	24:a:110:TRP:NE1	2.36	0.57
24:a:160:MET:HE2	30:g:95:TYR:CG	2.39	0.57
35:l:186:MET:CE	40:r:379:LEU:HD21	2.35	0.57
15:P:103:HIS:HD2	15:P:105:ASN:HB2	1.69	0.57
20:V:4:THR:HG22	20:V:8:LYS:HZ3	1.62	0.57
22:Y:44:TYR:HB2	23:Z:14:MET:HE1	1.87	0.57
24:a:130:GLU:HB3	37:n:45:PHE:CD1	2.40	0.57
41:s:21:THR:HB	56:s:401:UQ:HM23	1.86	0.57
13:N:85:GLU:HB2	13:N:98:PRO:HB3	1.86	0.57
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.87	0.57
35:l:72:GLN:NE2	40:r:459:TYR:O	2.38	0.57
44:w:231:ALA:HA	44:w:234:LEU:HD12	1.85	0.57
44:w:118:TYR:OH	57:w:401:ADP:O2'	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:89:SER:O	12:M:59:GLN:NE2	2.37	0.57
16:Q:184:ILE:HD11	16:Q:251:PHE:HZ	1.69	0.57
26:c:58:ARG:NH1	26:c:61:ASP:OD2	2.38	0.57
44:w:78:ALA:HB2	44:w:158:VAL:HG11	1.86	0.57
3:C:79:MET:HE1	3:C:177:ILE:HG13	1.87	0.56
37:n:18:PRO:O	37:n:22:VAL:HG23	2.05	0.56
3:C:59:ARG:NH1	49:C:303:PLX:O3	2.30	0.56
50:X:201:8Q1:N36	50:X:201:8Q1:O40	2.38	0.56
24:a:91:VAL:HG13	27:d:52:ILE:HD13	1.86	0.56
25:b:74:HIS:O	35:l:14:ILE:HD12	2.05	0.56
32:i:221:HIS:HB2	32:i:323:MET:HE1	1.86	0.56
4:E:84:ILE:O	4:E:88:MET:HG3	2.05	0.56
7:H:58:MET:HG2	7:H:71:GLN:OE1	2.05	0.56
10:K:109:ARG:NH2	14:O:106:GLN:O	2.38	0.56
18:T:47:ASP:HA	18:T:52:ARG:NH1	2.20	0.56
24:a:91:VAL:HG13	27:d:52:ILE:CD1	2.35	0.56
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.87	0.56
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.88	0.56
35:l:357:ARG:HG3	39:p:32:VAL:HG13	1.86	0.56
35:l:489:THR:O	35:l:493:VAL:HG13	2.05	0.56
8:I:14:TRP:O	21:W:28:ARG:NH2	2.38	0.56
14:O:41:HIS:NE2	14:O:47:ASN:OD1	2.32	0.56
34:k:27:MET:HE1	36:m:68:PHE:CD2	2.40	0.56
2:B:130:ILE:HG12	2:B:145:TYR:CD1	2.41	0.56
44:w:271:GLU:O	44:w:275:TYR:CD1	2.58	0.56
32:i:267:ILE:HG12	32:i:279:PRO:HB3	1.88	0.56
7:H:83:GLN:OE1	7:H:83:GLN:HA	2.06	0.56
12:M:394:VAL:HG22	12:M:473:MET:HE1	1.86	0.56
37:n:42:SER:O	37:n:46:LYS:N	2.38	0.56
6:X:91:ASP:OD2	23:Z:42:ARG:NH2	2.28	0.56
22:Y:65:MET:HE2	35:l:375:ILE:HG12	1.88	0.56
24:a:131:LYS:HE3	37:n:32:ASP:OD2	2.06	0.56
41:s:264:LEU:O	41:s:268:ILE:HG12	2.05	0.56
2:B:68:ARG:NH2	16:Q:260:GLU:OE2	2.39	0.56
21:W:112:HIS:CD2	31:h:58:ILE:CD1	2.89	0.55
1:A:87:GLY:N	1:A:93:PHE:O	2.38	0.55
40:r:328:CYS:O	40:r:332:THR:HG23	2.06	0.55
41:s:89:LEU:HD22	41:s:240:ILE:HD12	1.88	0.55
44:w:350:LYS:CB	44:w:351:TRP:HE3	2.12	0.55
12:M:407:PRO:HD2	12:M:438:LEU:HD21	1.89	0.55
14:O:206:ASP:OD1	14:O:206:ASP:C	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:51:THR:HG22	22:Y:53:SER:H	1.71	0.55
2:B:146:ASP:OD2	11:L:112:MET:CE	2.54	0.55
7:H:83:GLN:NE2	15:P:104:THR:HA	2.22	0.55
11:L:132:GLU:CD	11:L:132:GLU:H	2.14	0.55
16:Q:293:LEU:HD22	16:Q:298:ILE:HD12	1.88	0.55
55:a:201:CDL:H362	25:b:80:TRP:HB3	1.88	0.55
12:M:178:GLN:HG2	12:M:204:MET:CE	2.36	0.55
14:O:193:TYR:CD2	14:O:204:ILE:HD13	2.42	0.55
22:Y:62:SER:HG	35:l:371:THR:HG1	1.54	0.55
1:A:181:LEU:O	1:A:186:ALA:CB	2.54	0.55
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.88	0.55
41:s:86:TRP:CZ2	41:s:232:ILE:HG22	2.41	0.55
3:C:125:PRO:HB2	41:s:58:LYS:HE3	1.88	0.55
9:J:73:LEU:O	9:J:78:SER:OG	2.22	0.55
6:X:69:SER:OG	6:X:70:ASP:N	2.38	0.55
24:a:141:GLN:O	24:a:145:GLU:HG3	2.06	0.55
25:b:123:PHE:HD2	43:v:40:VAL:HG11	1.71	0.55
1:A:290:GLU:HG3	1:A:291:GLU:N	2.22	0.55
12:M:117:MET:HE2	12:M:143:SER:HA	1.89	0.55
19:U:53:TYR:CD1	21:W:72:MET:HE3	2.42	0.55
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.42	0.55
6:X:123:GLU:HG2	6:X:129:GLU:HA	1.89	0.55
31:h:105:ARG:NH2	42:u:17:GLU:OE2	2.40	0.55
33:j:68:GLU:HG2	36:m:161:LEU:HD13	1.88	0.55
35:l:108:MET:HE1	35:l:240:PRO:HB3	1.89	0.55
39:p:59:LYS:O	39:p:59:LYS:HD3	2.07	0.55
41:s:86:TRP:HZ2	41:s:232:ILE:HG22	1.72	0.55
2:B:131:GLU:HG3	2:B:144:ARG:HD2	1.88	0.54
4:E:98:LYS:HB3	4:E:102:HIS:HB2	1.89	0.54
12:M:33:GLU:CB	12:M:42:MET:HE1	2.32	0.54
6:X:130:ILE:HG23	6:X:147:TYR:CZ	2.42	0.54
27:d:46:THR:O	27:d:50:GLU:HG2	2.06	0.54
29:f:44:VAL:O	29:f:48:LEU:HD22	2.07	0.54
1:A:157:TYR:CB	1:A:212:LEU:HD11	2.37	0.54
6:G:103:HIS:ND1	6:G:106:LYS:HG2	2.22	0.54
26:c:158:PRO:HD3	43:v:22:MET:HE2	1.89	0.54
35:l:355:ASP:OD1	35:l:357:ARG:NE	2.34	0.54
40:r:403:THR:HA	40:r:406:TYR:CE2	2.42	0.54
14:O:54:ASP:O	14:O:89:GLN:NE2	2.41	0.54
18:T:45:TYR:HE1	18:T:51:ARG:HH21	1.55	0.54
27:d:26:LEU:C	27:d:26:LEU:HD23	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:62:ARG:HH11	41:s:64:ALA:HA	1.72	0.54
44:w:108:LEU:HD21	44:w:330:LYS:HE3	1.89	0.54
16:Q:182:ASN:ND2	16:Q:403:PRO:HB2	2.22	0.54
25:b:103:ARG:NH1	43:v:49:ALA:O	2.40	0.54
38:o:121:LEU:HD23	38:o:123:GLN:HE21	1.72	0.54
13:N:8:ARG:O	13:N:12:GLN:HG2	2.08	0.54
19:U:65:ASP:O	19:U:74:GLN:HB3	2.08	0.54
1:A:311:TRP:NE1	1:A:333:GLU:OE2	2.37	0.54
9:J:166:HIS:HB3	9:J:200:ILE:HD13	1.90	0.54
10:K:100:GLN:HB3	14:O:71:PRO:HA	1.90	0.54
11:L:92:ASN:HB3	15:P:238:PRO:HA	1.89	0.54
14:O:59:ASN:OD1	14:O:62:ARG:NH1	2.40	0.54
43:v:18:ASP:OD1	43:v:18:ASP:C	2.50	0.54
6:G:130:ILE:HG22	6:G:147:TYR:OH	2.07	0.54
35:l:384:PRO:HA	35:l:389:PHE:CG	2.43	0.54
1:A:185:ASN:OD1	1:A:190:GLY:N	2.20	0.54
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.41	0.54
3:C:188:LYS:HB3	3:C:191:ARG:HD2	1.90	0.54
9:J:206:ILE:HG12	9:J:245:VAL:HG21	1.90	0.54
11:L:111:LEU:HD11	13:N:126:PRO:HG2	1.89	0.54
30:g:36:MET:HE2	32:i:339:MET:HE2	1.88	0.54
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.41	0.54
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.30	0.54
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.42	0.54
33:j:5:LEU:C	33:j:5:LEU:HD23	2.32	0.54
35:l:186:MET:HE1	40:r:379:LEU:HD21	1.90	0.54
41:s:154:LEU:HD12	41:s:159:SER:O	2.07	0.54
25:b:28:LEU:HG	25:b:32:GLU:HG2	1.90	0.53
35:l:407:TRP:CZ2	35:l:411:MET:HE3	2.43	0.53
7:H:21:HIS:O	7:H:25:LYS:HG2	2.08	0.53
25:b:99:GLU:CG	35:l:61:MET:HE2	2.38	0.53
40:r:108:MET:HE3	40:r:121:LEU:HD11	1.91	0.53
5:F:54:LEU:HD12	5:F:54:LEU:H	1.74	0.53
23:Z:43:ASP:OD1	23:Z:43:ASP:O	2.26	0.53
26:c:136:PHE:HD1	55:l:701:CDL:H851	1.74	0.53
34:k:44:SER:HB2	34:k:59:MET:HE1	1.90	0.53
12:M:36:VAL:HB	12:M:56:VAL:HG21	1.90	0.53
34:k:8:ILE:HG21	34:k:43:MET:HB2	1.91	0.53
35:l:288:THR:HG23	35:l:304:PHE:HD1	1.73	0.53
35:l:559:GLU:O	35:l:563:PRO:HD2	2.09	0.53
6:G:104:PHE:HA	6:G:108:LEU:HD12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:142:GLN:C	6:G:142:GLN:OE1	2.51	0.53
16:Q:118:2MR:CD	16:Q:118:2MR:CQ2	2.86	0.53
19:U:60:ASP:OD1	19:U:60:ASP:N	2.39	0.53
1:A:342:LEU:HD22	1:A:347:THR:CG2	2.37	0.53
5:F:36:PHE:HZ	5:F:91:LEU:HD13	1.72	0.53
6:G:119:ILE:HG22	6:G:130:ILE:HD11	1.90	0.53
7:H:96:ARG:NH1	7:H:96:ARG:CB	2.71	0.53
9:J:238:GLN:N	9:J:326:ASP:OD2	2.41	0.53
35:l:558:LEU:HB3	40:r:214:LEU:HD21	1.91	0.53
37:n:50:ARG:HB3	37:n:51:PRO:HD2	1.91	0.53
1:A:120:GLY:HA3	1:A:204:TYR:HD1	1.74	0.53
4:E:68:MET:HE1	50:G:201:8Q1:C30	2.39	0.53
35:l:250:SER:HB2	35:l:333:ALA:HA	1.89	0.53
2:B:142:THR:O	2:B:187:LYS:NZ	2.42	0.53
21:W:98:MET:CE	31:h:79:ILE:HA	2.39	0.53
29:f:44:VAL:O	29:f:48:LEU:CD2	2.57	0.53
30:g:122:ARG:O	38:o:109:ARG:NH2	2.33	0.53
32:i:208:TYR:HA	32:i:211:MET:HE2	1.91	0.53
35:l:111:ASP:OD1	39:p:97:TYR:OH	2.26	0.53
44:w:58:LYS:HA	44:w:202:HIS:ND1	2.24	0.53
1:A:448:GLU:HA	1:A:448:GLU:OE1	2.09	0.53
1:A:456:GLN:CD	1:A:457:HIS:HD1	2.09	0.53
5:F:46:LYS:HE2	12:M:674:LEU:HD21	1.90	0.53
2:B:130:ILE:HD11	2:B:145:TYR:CE1	2.31	0.53
22:Y:94:ASP:OD1	22:Y:99:ILE:HB	2.08	0.53
6:G:115:GLN:NE2	6:G:138:LEU:O	2.41	0.52
48:Q:501:PEE:H27	35:l:563:PRO:HA	1.91	0.52
6:X:83:VAL:HG13	6:X:122:MET:HE3	1.91	0.52
31:h:18:MET:HG3	31:h:18:MET:O	2.08	0.52
35:l:400:ASN:HD22	35:l:409:LEU:HD21	1.74	0.52
41:s:85:MET:CE	41:s:233:MET:HE2	2.39	0.52
1:A:149:MET:HE1	1:A:241:THR:HB	1.92	0.52
12:M:389:THR:HG21	12:M:473:MET:HG3	1.90	0.52
41:s:85:MET:HE2	41:s:233:MET:HE2	1.91	0.52
6:X:90:TYR:HE1	23:Z:44:PRO:HB2	1.74	0.52
38:o:118:GLU:OE1	38:o:120:LYS:NZ	2.31	0.52
15:P:46:THR:HG23	16:Q:358:VAL:HG22	1.88	0.52
16:Q:282:ASP:CG	16:Q:437:LYS:HE2	2.33	0.52
21:W:120:MET:HE1	36:m:126:VAL:CG1	2.40	0.52
34:k:22:TYR:O	35:l:585:LYS:NZ	2.30	0.52
35:l:5:ALA:HB2	35:l:61:MET:SD	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ARG:NH2	14:O:176:CYS:O	2.42	0.52
32:i:43:VAL:HG11	32:i:129:LEU:HD23	1.90	0.52
36:m:1:MET:HE1	36:m:4:TYR:HA	1.90	0.52
26:c:99:LEU:HD11	26:c:109:LEU:HD21	1.91	0.52
3:C:113:MET:HE3	3:C:116:ALA:HB3	1.91	0.52
30:g:32:ARG:HB2	30:g:78:LEU:HD11	1.91	0.52
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.45	0.52
36:m:165:VAL:O	36:m:169:MET:HG2	2.10	0.52
42:u:83:THR:HA	42:u:86:TRP:CD1	2.45	0.52
9:J:116:ILE:CG2	9:J:155:VAL:HG21	2.39	0.52
12:M:462:PHE:O	12:M:466:LEU:HG	2.10	0.52
35:l:272:LEU:O	35:l:276:MET:HG3	2.10	0.52
1:A:69:LEU:HD11	1:A:143:LEU:HD21	1.92	0.52
4:E:25:MET:O	4:E:29:LYS:HG3	2.10	0.52
8:I:18:ARG:HG3	8:I:18:ARG:NH1	2.23	0.52
6:X:103:HIS:HE1	6:X:105:MET:HG2	1.75	0.52
26:c:148:GLU:OE1	35:l:275:THR:HG21	2.10	0.52
26:c:165:ASP:OD2	26:c:170:ARG:NH2	2.43	0.52
27:d:81:ASP:O	27:d:85:MET:HG3	2.10	0.52
27:d:134:GLN:NE2	28:e:135:PRO:O	2.42	0.52
28:e:140:ASN:HD22	28:e:144:PRO:HD3	1.75	0.52
35:l:127:THR:HG22	35:l:147:VAL:HG13	1.92	0.52
41:s:62:ARG:HH21	41:s:68:ILE:HB	1.74	0.52
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.45	0.51
2:B:119:CYS:SG	2:B:145:TYR:OH	2.62	0.51
5:F:29:GLY:HA2	5:F:81:ASN:OD1	2.11	0.51
35:l:343:SER:O	35:l:347:ILE:HG13	2.10	0.51
37:n:46:LYS:NZ	37:n:46:LYS:CB	2.73	0.51
9:J:163:LYS:NZ	9:J:253:ILE:O	2.38	0.51
12:M:339:ALA:HB3	12:M:542:PRO:HG3	1.91	0.51
12:M:400:ILE:HG12	12:M:473:MET:HB3	1.92	0.51
13:N:78:ASP:OD1	13:N:78:ASP:N	2.42	0.51
1:A:71:LYS:HD3	1:A:75:TRP:CE3	2.45	0.51
4:E:114:ARG:HD3	4:E:115:PRO:HD2	1.93	0.51
12:M:372:PHE:H	12:M:532:PRO:HB2	1.75	0.51
14:O:98:MET:HE2	14:O:116:ALA:CB	2.41	0.51
22:Y:47:PHE:HZ	35:l:364:LYS:HG3	1.74	0.51
23:Z:57:PHE:O	35:l:434:LYS:NZ	2.38	0.51
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.91	0.51
3:C:92:VAL:HG12	41:s:25:ARG:HH12	1.74	0.51
4:E:22:SER:HB2	4:E:27:GLU:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:90:LEU:HB2	15:P:102:ASP:HB3	1.92	0.51
20:V:107:SER:HB3	20:V:110:ILE:HB	1.91	0.51
35:l:51:LEU:O	35:l:55:MET:HG3	2.11	0.51
9:J:116:ILE:HG22	9:J:155:VAL:HG21	1.93	0.51
12:M:512:VAL:O	12:M:514:ASN:ND2	2.43	0.51
13:N:124:TYR:HD1	18:T:61:GLU:HG3	1.75	0.51
21:W:85:GLN:O	21:W:89:GLU:HG3	2.10	0.51
32:i:279:PRO:HA	32:i:282:MET:HG3	1.93	0.51
36:m:173:ARG:HH11	36:m:173:ARG:CG	2.23	0.51
7:H:40:LYS:HA	7:H:45:ARG:HD3	1.93	0.51
16:Q:259:GLU:HB3	21:W:25:LEU:HD11	1.92	0.51
24:a:79:GLY:HA3	55:a:201:CDL:H222	1.93	0.51
25:b:117:ILE:HD13	25:b:117:ILE:N	2.25	0.51
2:B:130:ILE:CD1	2:B:145:TYR:HE1	2.18	0.51
48:Q:502:PEE:H20	41:s:183:MET:CE	2.41	0.51
38:o:50:GLN:NE2	38:o:60:ILE:HG23	2.26	0.51
1:A:456:GLN:CD	1:A:457:HIS:ND1	2.65	0.51
2:B:76:TYR:CE1	41:s:33:LEU:HD13	2.46	0.51
43:v:103:GLU:O	43:v:107:ARG:HG2	2.11	0.51
2:B:48:MET:O	19:U:10:LYS:NZ	2.31	0.51
14:O:130:TYR:HA	14:O:189:ASN:HD21	1.76	0.51
21:W:130:ASN:HA	21:W:133:ILE:HD12	1.91	0.51
22:Y:96:GLU:CD	22:Y:96:GLU:H	2.19	0.51
32:i:245:MET:HE1	55:i:402:CDL:H171	1.93	0.51
35:l:245:ALA:O	35:l:249:SER:OG	2.26	0.51
1:A:48:ARG:HD2	10:K:70:ASN:O	2.11	0.50
5:F:36:PHE:CD2	5:F:87:VAL:CG2	2.91	0.50
11:L:90:GLY:HA3	15:P:238:PRO:HB2	1.91	0.50
12:M:403:VAL:HG11	12:M:452:LEU:HD21	1.93	0.50
15:P:148:ASP:N	15:P:148:ASP:OD1	2.43	0.50
20:V:4:THR:CG2	20:V:8:LYS:HZ2	2.19	0.50
26:c:149:ILE:HG22	26:c:150:TYR:CD1	2.46	0.50
33:j:90:MET:SD	36:m:151:THR:HG23	2.51	0.50
35:l:71:LEU:HD23	40:r:310:MET:HE1	1.93	0.50
2:B:146:ASP:CG	11:L:112:MET:HE1	2.36	0.50
25:b:32:GLU:HG3	39:p:115:TYR:HA	1.93	0.50
44:w:65:ASN:OD1	44:w:66:ILE:N	2.45	0.50
16:Q:251:PHE:HB3	16:Q:341:LEU:HD11	1.94	0.50
32:i:132:THR:HG22	32:i:212:THR:CG2	2.34	0.50
34:k:25:HIS:O	34:k:28:SER:N	2.35	0.50
35:l:221:ALA:HA	35:l:226:GLN:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:11:THR:O	39:p:15:LYS:HG3	2.11	0.50
12:M:141:ASP:O	12:M:145:MET:HG2	2.12	0.50
14:O:186:VAL:HG12	14:O:193:TYR:HB2	1.93	0.50
24:a:131:LYS:HD2	37:n:57:TRP:CE3	2.46	0.50
24:a:137:MET:HE1	37:n:42:SER:HB3	1.93	0.50
32:i:239:VAL:O	32:i:243:LEU:HG	2.11	0.50
55:i:402:CDL:H142	40:r:94:LEU:HD13	1.93	0.50
35:l:292:ALA:HB2	35:l:304:PHE:HB3	1.92	0.50
1:A:398:ARG:NH1	12:M:155:GLU:OE1	2.40	0.50
3:C:83:ARG:NH1	16:Q:212:GLU:OE2	2.32	0.50
6:G:103:HIS:CE1	6:G:105:MET:HB2	2.46	0.50
11:L:163:ASN:O	11:L:171:ARG:HA	2.12	0.50
4:E:40:TYR:HE2	6:G:117:GLU:HG2	1.76	0.50
6:G:84:LEU:O	6:G:88:LYS:HG2	2.12	0.50
9:J:38:HIS:NE2	13:N:132:LYS:HD2	2.27	0.50
12:M:676:ASN:O	12:M:678:GLN:NE2	2.44	0.50
14:O:130:TYR:HA	14:O:189:ASN:ND2	2.27	0.50
34:k:57:ASN:HB3	36:m:143:ILE:HG13	1.94	0.50
39:p:164:PRO:O	39:p:167:TRP:HD1	1.94	0.50
40:r:378:GLU:OE2	40:r:378:GLU:HA	2.12	0.50
7:H:96:ARG:HH11	7:H:96:ARG:CB	2.24	0.50
15:P:106:ALA:HB1	15:P:108:PHE:CE1	2.47	0.50
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.47	0.50
6:X:110:LEU:HD12	6:X:114:ASP:HB3	1.92	0.50
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.93	0.50
16:Q:82:LEU:CD1	16:Q:101:LEU:HD13	2.41	0.50
55:i:402:CDL:H662	55:i:402:CDL:H612	1.93	0.50
33:j:15:SER:HA	41:s:76:ILE:HD12	1.94	0.50
35:l:293:ILE:HG23	35:l:294:THR:HG23	1.94	0.50
3:C:71:CYS:HB3	16:Q:141:TYR:CG	2.47	0.50
8:I:94:ALA:HB1	15:P:105:ASN:HD21	1.77	0.50
9:J:37:HIS:CE1	18:T:49:ASP:HA	2.47	0.50
35:l:65:ASN:OD1	35:l:66:TRP:N	2.42	0.50
35:l:521:LYS:HB3	35:l:525:MET:HE1	1.94	0.50
12:M:29:SER:OG	12:M:30:ASN:N	2.45	0.49
15:P:61:PHE:O	15:P:65:VAL:HG22	2.12	0.49
24:a:168:TRP:HB3	30:g:2:THR:O	2.12	0.49
25:b:19:ARG:HD2	39:p:171:VAL:O	2.11	0.49
31:h:69:ARG:O	31:h:73:MET:HG3	2.12	0.49
32:i:347:ASN:N	32:i:347:ASN:OD1	2.45	0.49
35:l:407:TRP:CE2	35:l:411:MET:HE3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.47	0.49
40:r:225:ILE:O	40:r:229:MET:HG3	2.12	0.49
41:s:25:ARG:HD2	56:s:401:UQ:HM21	1.94	0.49
41:s:85:MET:SD	41:s:108:MET:HB2	2.51	0.49
41:s:87:VAL:HG22	41:s:88:PRO:HD3	1.80	0.49
19:U:14:ALA:O	19:U:15:LYS:HG2	2.12	0.49
20:V:4:THR:O	20:V:8:LYS:HG3	2.12	0.49
24:a:106:VAL:CG1	37:n:50:ARG:HH21	2.02	0.49
35:l:525:MET:CE	35:l:528:TYR:HE1	2.12	0.49
42:u:59:GLU:O	42:u:63:VAL:HG13	2.12	0.49
43:v:83:GLU:OE1	43:v:83:GLU:N	2.44	0.49
1:A:270:ASN:HD21	1:A:340:ASP:H	1.59	0.49
4:E:79:VAL:O	4:E:83:VAL:HG23	2.11	0.49
4:E:87:LYS:O	4:E:91:GLU:HG3	2.11	0.49
7:H:83:GLN:HE21	15:P:104:THR:HA	1.77	0.49
24:a:156:VAL:HG13	24:a:160:MET:HE3	1.94	0.49
35:l:131:LEU:O	35:l:140:LEU:CD1	2.61	0.49
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.92	0.49
7:H:7:LYS:HG3	7:H:8:THR:HG23	1.94	0.49
7:H:94:MET:HE1	7:H:99:PRO:HG2	1.93	0.49
32:i:18:MET:HE3	32:i:22:ILE:CG2	2.43	0.49
44:w:84:ARG:HD3	44:w:149:HIS:HD2	1.77	0.49
44:w:288:ASP:OD1	44:w:289:ARG:N	2.45	0.49
9:J:135:GLU:OE1	9:J:179:ARG:NH2	2.46	0.49
16:Q:53:TYR:HE1	48:Q:501:PEE:H2	1.77	0.49
38:o:116:ILE:HG12	38:o:123:GLN:NE2	2.28	0.49
1:A:115:VAL:HG22	1:A:248:VAL:HG21	1.94	0.49
2:B:146:ASP:OD2	11:L:112:MET:HE1	2.13	0.49
22:Y:72:ARG:HA	22:Y:72:ARG:NE	2.28	0.49
26:c:184:TYR:HA	43:v:34:ARG:NH1	2.28	0.49
39:p:100:PRO:HG3	40:r:419:TYR:CE1	2.48	0.49
40:r:357:THR:O	40:r:361:VAL:HG23	2.13	0.49
44:w:110:GLY:HA2	44:w:134:TRP:CD2	2.48	0.49
1:A:131:ILE:HD11	1:A:245:VAL:HG21	1.95	0.49
12:M:483:ARG:HB2	12:M:483:ARG:NH1	2.27	0.49
32:i:100:MET:HE2	32:i:153:LEU:HD21	1.94	0.49
40:r:45:LEU:HD23	40:r:45:LEU:H	1.77	0.49
6:G:91:ASP:OD1	6:G:91:ASP:N	2.42	0.49
12:M:321:ASP:O	12:M:325:ARG:HG3	2.13	0.49
17:S:69:ILE:HD11	42:u:68:LEU:HD23	1.94	0.49
24:a:150:ARG:NH1	42:u:166:ARG:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:159:HIS:NE2	39:p:96:CYS:HB2	2.28	0.49
35:l:568:PHE:CE1	35:l:572:LYS:HE3	2.47	0.49
36:m:1:MET:HE3	36:m:4:TYR:N	2.28	0.49
44:w:165:SER:HB3	44:w:245:PHE:CZ	2.47	0.49
4:E:44:PRO:HD3	4:E:60:ARG:HH12	1.77	0.49
5:F:31:GLN:NE2	5:F:35:ASP:OD1	2.43	0.49
8:I:40:LYS:HB3	21:W:7:LYS:H	1.78	0.49
9:J:47:GLY:HA3	15:P:225:GLU:OE1	2.13	0.49
16:Q:159:LEU:O	16:Q:160:ASN:CB	2.59	0.49
16:Q:182:ASN:HD22	16:Q:403:PRO:HB2	1.78	0.49
17:S:54:ILE:HD11	31:h:106:PRO:HB3	1.94	0.49
20:V:69:ILE:HG21	20:V:100:THR:HG21	1.94	0.49
6:X:132:ASP:HB3	39:p:18:ARG:NE	2.24	0.49
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.48	0.49
20:V:5:LEU:HA	20:V:8:LYS:HG3	1.94	0.49
1:A:151:ALA:O	1:A:191:TYR:OH	2.21	0.48
15:P:44:ARG:HB3	15:P:45:PRO:CD	2.43	0.48
55:a:201:CDL:H541	48:l:703:PEE:H16	1.95	0.48
40:r:12:LEU:HB2	40:r:13:PRO:HD3	1.95	0.48
33:j:3:ILE:HG12	48:m:201:PEE:H50	1.95	0.48
35:l:190:LEU:HD11	40:r:307:TRP:CH2	2.48	0.48
5:F:83:SER:O	5:F:87:VAL:HG22	2.13	0.48
20:V:106:ARG:NE	20:V:106:ARG:CA	2.73	0.48
6:X:117:GLU:OE2	39:p:20:TYR:OH	2.29	0.48
26:c:164:ASN:HA	26:c:181:VAL:HG12	1.95	0.48
32:i:276:ILE:HG21	48:r:501:PEE:H14	1.94	0.48
44:w:350:LYS:HB3	44:w:351:TRP:CZ3	2.48	0.48
1:A:195:VAL:O	10:K:97:ARG:NH1	2.41	0.48
3:C:55:ASN:ND2	3:C:187:GLU:O	2.45	0.48
6:G:103:HIS:HB3	6:G:107:ASP:OD1	2.13	0.48
13:N:32:ASP:OD2	13:N:58:ARG:NH2	2.46	0.48
48:Q:502:PEE:H51	48:Q:502:PEE:H60	1.95	0.48
26:c:152:SER:HA	43:v:5:LEU:HD11	1.96	0.48
43:v:17:PRO:HB3	43:v:105:GLU:OE1	2.13	0.48
44:w:353:TRP:H	44:w:353:TRP:CD1	2.31	0.48
2:B:200:GLU:OE2	13:N:88:ARG:HB2	2.13	0.48
12:M:278:HIS:CE1	12:M:280:ASP:HB2	2.48	0.48
21:W:120:MET:CE	36:m:126:VAL:CG1	2.90	0.48
32:i:106:LEU:HD22	32:i:187:MET:HE2	1.95	0.48
38:o:3:PHE:CZ	39:p:70:GLU:HG3	2.48	0.48
43:v:18:ASP:OD1	43:v:18:ASP:O	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:TYR:CD2	1:A:212:LEU:CD1	2.96	0.48
3:C:61:SER:HG	41:s:54:LYS:HD3	1.77	0.48
48:Q:501:PEE:H37	48:Q:501:PEE:H60	1.95	0.48
35:l:62:ILE:HD13	35:l:81:LYS:HA	1.94	0.48
41:s:51:ASP:HB3	56:s:401:UQ:H8	1.96	0.48
1:A:116:ASN:O	1:A:245:VAL:HG23	2.14	0.48
6:G:75:THR:OG1	6:G:156:GLU:OE1	2.31	0.48
18:T:29:VAL:HG21	18:T:64:GLU:OE1	2.13	0.48
39:p:162:ASP:OD1	39:p:162:ASP:N	2.47	0.48
2:B:130:ILE:HG12	2:B:145:TYR:HD1	1.78	0.48
9:J:257:ASP:O	9:J:261:LYS:NZ	2.45	0.48
15:P:46:THR:HG22	15:P:46:THR:O	2.13	0.48
22:Y:47:PHE:HE2	22:Y:50:LEU:HD11	1.79	0.48
40:r:433:GLU:O	40:r:437:MET:HG2	2.14	0.48
1:A:88:ARG:HB2	1:A:247:THR:OG1	2.14	0.48
1:A:296:LEU:HD13	1:A:337:MET:SD	2.54	0.48
6:G:74:LEU:H	6:G:74:LEU:HD23	1.78	0.48
6:G:74:LEU:HD12	6:G:79:ILE:HD11	1.96	0.48
6:G:128:PHE:HE1	6:G:148:ILE:CD1	2.26	0.48
13:N:5:GLN:O	13:N:9:ARG:HG3	2.14	0.48
14:O:130:TYR:HB2	14:O:169:PHE:HD1	1.79	0.48
21:W:51:MET:HA	41:s:313:SER:HB2	1.95	0.48
26:c:59:VAL:HG12	26:c:60:GLU:OE1	2.14	0.48
35:l:127:THR:HG21	35:l:146:GLY:C	2.39	0.48
14:O:56:THR:HG21	14:O:58:GLU:OE2	2.14	0.47
15:P:64:TYR:HH	15:P:103:HIS:HE2	1.61	0.47
32:i:128:LEU:HD23	32:i:128:LEU:O	2.13	0.47
41:s:7:LEU:O	41:s:11:ILE:HG12	2.14	0.47
12:M:341:ILE:HD11	12:M:537:ILE:HG13	1.95	0.47
15:P:68:ILE:HG22	15:P:69:LEU:HG	1.96	0.47
16:Q:133:LEU:HD22	16:Q:228:ARG:HD3	1.96	0.47
25:b:120:MET:HE1	43:v:61:HIS:HA	1.96	0.47
40:r:150:LEU:O	40:r:153:THR:OG1	2.25	0.47
41:s:101:GLY:O	41:s:105:MET:HG3	2.14	0.47
1:A:338:ASP:OD1	1:A:338:ASP:C	2.58	0.47
2:B:210:LEU:HD12	8:I:38:PRO:HB3	1.96	0.47
9:J:369:VAL:HG12	9:J:370:LYS:HG2	1.96	0.47
14:O:64:GLU:OE1	14:O:64:GLU:O	2.32	0.47
16:Q:192:LEU:HD12	16:Q:197:MET:HB2	1.95	0.47
17:S:1:MET:HB2	17:S:3:PHE:CE2	2.49	0.47
6:X:88:LYS:HG3	6:X:98:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:146:SER:HA	32:i:149:ILE:HG23	1.96	0.47
35:l:1:MET:O	35:l:1:MET:SD	2.72	0.47
1:A:256:ARG:CG	14:O:245:VAL:HG12	2.43	0.47
17:S:66:LEU:O	17:S:69:ILE:HG22	2.15	0.47
24:a:95:GLU:OE2	55:a:201:CDL:O1	2.23	0.47
24:a:156:VAL:CG1	24:a:160:MET:HE3	2.45	0.47
26:c:36:MET:O	26:c:36:MET:HG2	2.14	0.47
32:i:128:LEU:C	32:i:128:LEU:CD2	2.86	0.47
33:j:60:ILE:HG21	36:m:168:ILE:HG21	1.97	0.47
48:r:501:PEE:H79	48:r:501:PEE:H41	1.95	0.47
12:M:178:GLN:HB3	12:M:204:MET:HE2	1.97	0.47
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.94	0.47
32:i:236:LYS:NZ	32:i:314:LYS:O	2.43	0.47
37:n:50:ARG:HB2	37:n:53:GLU:CB	2.44	0.47
39:p:26:HIS:ND1	39:p:75:GLN:O	2.48	0.47
39:p:92:GLU:HB3	39:p:95:GLU:HG3	1.97	0.47
44:w:57:SER:O	44:w:156:GLY:HA3	2.14	0.47
12:M:650:SER:OG	12:M:652:ASN:OD1	2.31	0.47
24:a:106:VAL:O	37:n:50:ARG:NH2	2.48	0.47
24:a:140:LEU:HD21	40:r:177:LEU:HB3	1.97	0.47
35:l:137:LEU:HD13	35:l:186:MET:HG2	1.95	0.47
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.95	0.47
1:A:213:ILE:HG23	1:A:235:VAL:HA	1.96	0.47
2:B:90:LYS:NZ	2:B:174:GLU:OE2	2.48	0.47
3:C:166:CYS:SG	16:Q:138:ARG:NH2	2.76	0.47
10:K:98:MET:SD	10:K:98:MET:N	2.88	0.47
21:W:88:ARG:HG2	42:u:10:LEU:HG	1.97	0.47
6:X:115:GLN:NE2	6:X:138:LEU:O	2.46	0.47
35:l:233:LEU:HB3	35:l:234:PRO:HD3	1.97	0.47
41:s:85:MET:CE	41:s:233:MET:CE	2.93	0.47
1:A:244:ASN:O	1:A:248:VAL:HG23	2.15	0.47
9:J:243:VAL:HG12	9:J:247:LYS:HE2	1.96	0.47
20:V:96:ALA:O	20:V:100:THR:HG23	2.15	0.47
23:Z:43:ASP:OD1	23:Z:43:ASP:C	2.56	0.47
26:c:58:ARG:NH2	26:c:60:GLU:HG3	2.30	0.47
26:c:182:VAL:HG13	43:v:34:ARG:NH2	2.29	0.47
27:d:43:ARG:HB3	27:d:44:PRO:HD3	1.97	0.47
33:j:24:LEU:HB3	33:j:25:PRO:HD3	1.97	0.47
1:A:146:GLY:HA3	1:A:193:PHE:CE1	2.50	0.47
2:B:137:ASP:OD1	2:B:137:ASP:N	2.37	0.47
12:M:478:SER:O	12:M:482:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:560:LEU:HD23	12:M:564:CYS:SG	2.55	0.47
18:T:114:CYS:SG	18:T:116:LEU:HG	2.55	0.47
18:T:119:ARG:HH11	18:T:119:ARG:HG2	1.79	0.47
21:W:50:MET:HE3	21:W:50:MET:HA	1.96	0.47
25:b:10:LEU:HD22	25:b:14:GLN:NE2	2.30	0.47
26:c:50:ALA:HA	26:c:53:LYS:HD3	1.96	0.47
26:c:149:ILE:O	26:c:151:PRO:HD3	2.14	0.47
27:d:68:PHE:CD1	37:n:44:LEU:HD11	2.48	0.47
29:f:40:ASP:O	29:f:44:VAL:CG2	2.62	0.47
7:H:76:GLN:HB2	7:H:79:GLU:OE2	2.15	0.47
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.96	0.47
19:U:24:ALA:HB2	48:U:101:PEE:H72	1.97	0.47
19:U:45:ILE:HD11	19:U:81:LEU:HD13	1.97	0.47
39:p:144:THR:HG22	39:p:145:PRO:O	2.14	0.47
40:r:48:ASN:N	40:r:48:ASN:OD1	2.48	0.47
48:r:501:PEE:H26	48:r:501:PEE:H60	1.97	0.47
1:A:410:ASP:OD1	1:A:443:ARG:NH2	2.32	0.46
7:H:22:GLU:O	7:H:26:ILE:HG13	2.14	0.46
15:P:103:HIS:CD2	15:P:105:ASN:HB2	2.49	0.46
32:i:278:MET:O	32:i:282:MET:HG3	2.15	0.46
39:p:176:GLU:HG3	39:p:177:ARG:HG2	1.97	0.46
41:s:104:PHE:O	41:s:108:MET:HG2	2.15	0.46
12:M:133:GLN:HG3	12:M:136:GLU:HG3	1.96	0.46
12:M:360:ARG:HH21	12:M:632:MET:CA	2.26	0.46
6:X:136:GLU:OE1	39:p:18:ARG:NE	2.48	0.46
27:d:78:GLU:CD	30:g:108:LYS:HB3	2.35	0.46
29:f:39:PRO:HG2	44:w:351:TRP:CG	2.51	0.46
32:i:278:MET:O	32:i:282:MET:CG	2.63	0.46
34:k:22:TYR:HB3	35:l:585:LYS:HG2	1.97	0.46
40:r:343:ILE:O	40:r:346:ARG:NE	2.31	0.46
1:A:157:TYR:CD1	1:A:212:LEU:CD1	2.98	0.46
12:M:307:ILE:HG23	12:M:317:THR:HG21	1.97	0.46
48:U:101:PEE:H35	48:U:101:PEE:H30	1.78	0.46
36:m:23:LYS:N	36:m:24:PRO:HD3	2.30	0.46
40:r:447:LEU:HD11	49:r:503:PLX:H371	1.98	0.46
2:B:198:GLU:OE1	2:B:202:ALA:HB2	2.16	0.46
12:M:381:LEU:HD22	12:M:664:TYR:HD2	1.80	0.46
35:l:534:HIS:CD2	48:l:702:PEE:H13	2.50	0.46
42:u:40:ASN:O	42:u:44:MET:HG2	2.15	0.46
3:C:48:ALA:HB2	3:C:191:ARG:HH12	1.80	0.46
3:C:96:SER:HB3	3:C:99:GLN:NE2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:53:VAL:HA	20:V:56:THR:HG22	1.98	0.46
34:k:23:ARG:HD3	36:m:23:LYS:HB2	1.98	0.46
35:l:407:TRP:O	35:l:411:MET:HG2	2.14	0.46
49:r:503:PLX:H121	49:r:503:PLX:H152	1.47	0.46
44:w:59:VAL:HG13	44:w:201:PRO:HA	1.96	0.46
2:B:98:ARG:NH2	16:Q:224:ALA:O	2.42	0.46
14:O:197:THR:H	14:O:200:ASP:HB2	1.81	0.46
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.50	0.46
19:U:82:LYS:HB3	19:U:82:LYS:HE2	1.74	0.46
21:W:70:ALA:HB2	42:u:125:LEU:HD13	1.97	0.46
40:r:445:LEU:O	40:r:448:THR:HG22	2.16	0.46
9:J:207:PHE:HB2	9:J:214:LEU:HD13	1.97	0.46
12:M:325:ARG:HB3	12:M:325:ARG:CZ	2.46	0.46
18:T:104:LYS:HD2	18:T:107:LYS:CE	2.45	0.46
21:W:119:PRO:O	36:m:130:THR:OG1	2.29	0.46
6:X:91:ASP:OD1	6:X:91:ASP:N	2.48	0.46
26:c:56:ASN:ND2	38:o:43:LEU:HD21	2.31	0.46
35:l:88:MET:CE	35:l:468:ILE:HD12	2.45	0.46
35:l:298:ILE:O	35:l:302:VAL:HG23	2.16	0.46
2:B:74:LEU:HB2	41:s:272:TRP:CZ2	2.49	0.46
14:O:46:GLU:N	14:O:46:GLU:OE2	2.49	0.46
16:Q:443:MET:HE3	16:Q:443:MET:HB3	1.89	0.46
43:v:15:LYS:NZ	43:v:110:GLN:HE22	2.14	0.46
44:w:182:GLN:HB3	44:w:314:LEU:HD21	1.98	0.46
44:w:223:ASN:HB3	44:w:226:GLU:HB3	1.98	0.46
1:A:209:GLU:OE1	47:A:503:NAI:O3B	2.24	0.46
9:J:243:VAL:O	9:J:247:LYS:HG3	2.16	0.46
12:M:178:GLN:HB3	12:M:204:MET:CE	2.46	0.46
12:M:354:LEU:HD22	12:M:548:LEU:HD22	1.97	0.46
12:M:462:PHE:CE2	12:M:466:LEU:HD21	2.51	0.46
32:i:98:MET:HE2	32:i:98:MET:HB2	1.84	0.46
37:n:39:ARG:HG3	37:n:57:TRP:CE2	2.51	0.46
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.97	0.46
5:F:69:TYR:CE2	5:F:75:LYS:HG3	2.40	0.46
19:U:38:TYR:HB2	41:s:310:MET:O	2.16	0.46
21:W:10:MET:HE3	21:W:11:PRO:HD2	1.98	0.46
24:a:96:ALA:HB2	27:d:61:TYR:CE2	2.50	0.46
32:i:334:THR:HG21	55:i:402:CDL:H391	1.98	0.46
35:l:241:THR:HG21	35:l:344:GLY:HA3	1.97	0.46
43:v:46:MET:HE3	43:v:56:ARG:HD3	1.97	0.46
44:w:219:GLN:NE2	44:w:227:MET:SD	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:GLN:CD	1:A:456:GLN:C	2.84	0.45
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.75	0.45
14:O:172:ILE:HD12	14:O:173:GLU:H	1.80	0.45
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.99	0.45
35:l:338:MET:HE2	35:l:338:MET:HB3	1.82	0.45
41:s:61:LEU:HD12	41:s:61:LEU:O	2.17	0.45
1:A:279:SER:OG	1:A:280:GLY:N	2.49	0.45
6:G:139:MET:HE2	6:G:139:MET:HB2	1.85	0.45
9:J:209:ARG:HB3	9:J:210:GLU:OE2	2.17	0.45
20:V:37:SER:O	20:V:41:ILE:HG12	2.16	0.45
30:g:49:ALA:HB2	55:i:402:CDL:H712	1.98	0.45
30:g:117:GLU:OE1	30:g:119:HIS:NE2	2.49	0.45
31:h:2:PRO:HA	32:i:140:SER:HB2	1.98	0.45
32:i:95:MET:HE2	32:i:149:ILE:HA	1.98	0.45
35:l:389:PHE:O	35:l:393:ASP:HB3	2.17	0.45
1:A:85:LEU:HD12	1:A:86:ARG:N	2.31	0.45
2:B:198:GLU:HB3	13:N:109:ILE:HG12	1.98	0.45
9:J:251:ASN:O	9:J:255:ASP:N	2.45	0.45
14:O:154:LYS:HE3	14:O:154:LYS:HB2	1.71	0.45
18:T:64:GLU:OE1	18:T:64:GLU:HA	2.16	0.45
20:V:107:SER:HB3	20:V:110:ILE:CG2	2.46	0.45
21:W:51:MET:HE2	41:s:311:THR:HB	1.98	0.45
22:Y:47:PHE:CZ	35:l:364:LYS:HG3	2.50	0.45
22:Y:100:LEU:O	22:Y:102:ASP:N	2.44	0.45
32:i:265:MET:HE2	32:i:343:LEU:HD21	1.98	0.45
35:l:190:LEU:C	35:l:190:LEU:HD23	2.41	0.45
38:o:59:VAL:HG22	40:r:423:ILE:HG12	1.98	0.45
44:w:254:GLU:OE1	44:w:254:GLU:N	2.49	0.45
3:C:193:TRP:HA	3:C:196:ARG:HG2	1.98	0.45
19:U:66:VAL:HG13	42:u:130:LYS:HD3	1.97	0.45
29:f:61:GLN:O	29:f:65:ASP:OD2	2.34	0.45
55:l:701:CDL:H742	55:l:701:CDL:H711	1.78	0.45
1:A:339:PHE:CE1	1:A:349:LEU:HD23	2.51	0.45
1:A:413:TRP:O	1:A:416:SER:OG	2.23	0.45
12:M:133:GLN:O	12:M:137:CYS:HB2	2.17	0.45
16:Q:232:VAL:HG23	16:Q:356:ILE:HB	1.98	0.45
27:d:26:LEU:HD22	43:v:75:PRO:CB	2.45	0.45
28:e:149:LEU:HD12	28:e:149:LEU:H	1.81	0.45
35:l:152:PHE:CD1	35:l:168:ALA:HB1	2.52	0.45
35:l:533:MET:HE3	48:l:702:PEE:H24	1.97	0.45
36:m:55:MET:HA	36:m:55:MET:HE2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:310:MET:HB3	40:r:455:LEU:HD22	1.97	0.45
44:w:295:ARG:HA	44:w:298:VAL:HG22	1.98	0.45
1:A:272:GLY:O	1:A:292:MET:HB2	2.17	0.45
6:G:128:PHE:CE1	6:G:148:ILE:CD1	3.00	0.45
14:O:172:ILE:HD12	14:O:173:GLU:N	2.32	0.45
16:Q:139:LEU:HD13	16:Q:424:ILE:HG21	1.98	0.45
20:V:40:SER:OG	20:V:55:ARG:NH1	2.50	0.45
32:i:129:LEU:HD12	32:i:133:TRP:HB3	1.98	0.45
43:v:28:ASP:OD1	43:v:28:ASP:N	2.43	0.45
12:M:203:ASP:OD1	12:M:203:ASP:N	2.45	0.45
28:e:53:ILE:O	44:w:315:PRO:HB3	2.17	0.45
30:g:4:MET:HG2	30:g:7:ARG:HD2	1.98	0.45
1:A:89:GLY:O	47:A:503:NAI:H2N	2.17	0.45
2:B:76:TYR:HE1	41:s:33:LEU:HD13	1.81	0.45
16:Q:232:VAL:CG2	16:Q:356:ILE:HB	2.47	0.45
48:U:101:PEE:H59	48:U:101:PEE:H64	1.74	0.45
20:V:2:ALA:HA	35:l:601:LEU:HD12	1.99	0.45
20:V:47:ALA:HB3	20:V:51:GLU:CD	2.42	0.45
25:b:22:TRP:CE2	39:p:172:THR:HG22	2.50	0.45
28:e:121:GLU:O	28:e:124:ARG:HG2	2.17	0.45
29:f:39:PRO:CG	44:w:351:TRP:CB	2.95	0.45
35:l:66:TRP:HZ3	48:l:703:PEE:H38	1.82	0.45
9:J:329:LEU:HD23	9:J:331:HIS:HE1	1.82	0.45
15:P:69:LEU:HD11	15:P:99:PHE:CD2	2.52	0.45
16:Q:152:SER:HB3	16:Q:229:PRO:HA	1.98	0.45
16:Q:156:GLU:OE1	16:Q:229:PRO:O	2.35	0.45
17:S:22:ALA:O	17:S:26:ILE:HG13	2.17	0.45
26:c:108:ASP:HB3	26:c:111:MET:HB3	1.99	0.45
26:c:111:MET:HE1	35:l:543:SER:OG	2.17	0.45
30:g:12:PRO:HG2	31:h:8:LYS:HB3	1.98	0.45
30:g:92:MET:O	30:g:96:VAL:HG23	2.16	0.45
56:s:401:UQ:H101	56:s:401:UQ:H121	1.60	0.45
1:A:181:LEU:HA	1:A:186:ALA:O	2.17	0.45
17:S:21:MET:SD	41:s:253:GLU:HG3	2.56	0.45
17:S:69:ILE:HD11	42:u:68:LEU:CD2	2.46	0.45
26:c:169:GLU:N	26:c:169:GLU:OE2	2.50	0.45
27:d:30:VAL:O	27:d:34:THR:HG22	2.17	0.45
35:l:286:LEU:HD22	35:l:411:MET:SD	2.57	0.45
38:o:8:PRO:HG3	38:o:14:LEU:HD13	1.99	0.45
38:o:81:ARG:HB3	38:o:81:ARG:NH1	2.32	0.45
44:w:54:THR:O	44:w:54:THR:OG1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:42:ALA:HB2	41:s:312:ALA:HA	1.99	0.44
32:i:222:SER:CB	32:i:237:MET:HE3	2.47	0.44
1:A:408:GLU:O	1:A:411:SER:HB3	2.17	0.44
21:W:57:ARG:HB3	41:s:316:PRO:HG3	1.98	0.44
25:b:88:TYR:CE1	27:d:49:ARG:HG2	2.52	0.44
26:c:81:ARG:HD3	26:c:85:GLU:OE2	2.17	0.44
28:e:128:TYR:CD1	28:e:128:TYR:C	2.95	0.44
30:g:12:PRO:HB3	31:h:5:ASP:HB3	1.99	0.44
42:u:121:ASP:N	42:u:124:GLU:OE1	2.43	0.44
1:A:127:ASP:HA	1:A:130:ILE:HG12	1.99	0.44
9:J:235:THR:HG23	9:J:325:SER:HA	1.98	0.44
17:S:69:ILE:HG13	17:S:69:ILE:O	2.18	0.44
18:T:79:VAL:O	18:T:121:PRO:HD3	2.17	0.44
24:a:136:THR:HG21	40:r:48:ASN:HD22	1.81	0.44
55:a:201:CDL:H372	55:a:201:CDL:H341	1.60	0.44
40:r:248:THR:HG23	40:r:249:ILE:HG23	2.00	0.44
12:M:370:GLU:OE2	12:M:518:ARG:NH2	2.40	0.44
32:i:326:LEU:HB3	32:i:327:PRO:HD3	1.99	0.44
33:j:51:PHE:CE2	36:m:74:MET:HB3	2.52	0.44
35:l:174:TYR:CD2	35:l:232:TRP:HB3	2.52	0.44
35:l:327:LEU:O	35:l:331:MET:HG2	2.17	0.44
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.99	0.44
6:G:112:SER:CB	50:G:201:8Q1:O2	2.65	0.44
12:M:495:ASN:O	12:M:499:ASN:CG	2.61	0.44
14:O:133:GLN:HG3	14:O:172:ILE:HG23	1.99	0.44
20:V:50:LEU:O	20:V:53:VAL:HG12	2.18	0.44
21:W:93:GLU:HG3	31:h:98:HIS:NE2	2.32	0.44
34:k:26:LEU:HD23	34:k:78:LEU:HD12	1.98	0.44
55:l:701:CDL:H351	55:l:701:CDL:H382	1.67	0.44
44:w:125:ASP:OD1	44:w:125:ASP:N	2.37	0.44
1:A:185:ASN:C	1:A:187:CYS:H	2.26	0.44
1:A:214:GLU:OE2	1:A:224:ARG:NE	2.39	0.44
12:M:222:ILE:HA	12:M:225:ILE:HG12	2.00	0.44
16:Q:116:LEU:HD23	16:Q:459:GLY:HA2	1.99	0.44
20:V:106:ARG:HE	20:V:106:ARG:CA	2.30	0.44
25:b:32:GLU:HG3	39:p:115:TYR:HD1	1.83	0.44
35:l:37:LYS:HD3	35:l:98:TRP:HE1	1.83	0.44
36:m:25:SER:O	36:m:27:ILE:N	2.49	0.44
36:m:51:PHE:CD2	36:m:143:ILE:HD13	2.52	0.44
40:r:216:LEU:HD23	40:r:287:ALA:HB1	1.99	0.44
3:C:79:MET:CE	3:C:86:MET:HE2	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:55:LYS:HA	7:H:58:MET:HE3	1.99	0.44
12:M:304:GLN:HG2	12:M:615:LEU:HD12	1.99	0.44
28:e:63:ASP:OD1	28:e:63:ASP:C	2.61	0.44
36:m:1:MET:CE	36:m:4:TYR:HA	2.47	0.44
37:n:46:LYS:HZ3	37:n:46:LYS:HB3	1.83	0.44
40:r:207:MET:HE1	40:r:297:VAL:HG12	1.99	0.44
44:w:350:LYS:HA	44:w:350:LYS:HD3	1.82	0.44
1:A:296:LEU:HD12	1:A:296:LEU:HA	1.86	0.44
16:Q:150:ALA:HB2	16:Q:400:ILE:HG12	2.00	0.44
29:f:39:PRO:CG	44:w:351:TRP:HB3	2.47	0.44
31:h:21:GLN:HA	34:k:53:PHE:CE1	2.53	0.44
49:i:401:PLX:H311	49:i:401:PLX:H341	1.73	0.44
35:l:49:VAL:HB	35:l:50:PRO:HD3	2.00	0.44
35:l:292:ALA:HB2	35:l:304:PHE:CB	2.48	0.44
39:p:63:LEU:C	39:p:65:ARG:H	2.25	0.44
42:u:84:GLU:HB2	42:u:106:LYS:NZ	2.33	0.44
44:w:123:SER:OG	44:w:125:ASP:OD1	2.32	0.44
2:B:117:LYS:HE3	2:B:130:ILE:HG22	2.00	0.44
12:M:47:THR:HG23	12:M:51:GLN:HB2	1.99	0.44
16:Q:463:ARG:HE	16:Q:463:ARG:HB2	1.72	0.44
17:S:43:TYR:CZ	21:W:68:ARG:HG3	2.53	0.44
23:Z:13:LYS:HA	23:Z:13:LYS:HD2	1.81	0.44
23:Z:57:PHE:CG	35:l:435:PRO:HG3	2.53	0.44
32:i:38:LEU:HD12	34:k:73:LEU:HD22	2.00	0.44
32:i:97:MET:HG2	35:l:599:MET:HE1	2.00	0.44
35:l:384:PRO:HA	35:l:389:PHE:CD1	2.53	0.44
40:r:191:SER:HB3	48:r:501:PEE:H3	1.99	0.44
41:s:267:THR:O	41:s:271:LEU:HG	2.18	0.44
1:A:88:ARG:CG	1:A:246:GLU:OE2	2.65	0.43
2:B:65:GLU:HG3	16:Q:264:ASN:O	2.18	0.43
6:G:118:ILE:O	6:G:122:MET:HG2	2.19	0.43
9:J:151:ALA:O	9:J:155:VAL:HG22	2.18	0.43
6:X:131:PRO:HB3	26:c:89:TRP:CD2	2.52	0.43
25:b:121:LYS:C	25:b:122:GLU:HG3	2.42	0.43
40:r:218:LYS:O	40:r:222:GLU:HG2	2.17	0.43
1:A:168:ASN:HA	1:A:171:VAL:HG12	1.99	0.43
2:B:198:GLU:HG2	13:N:108:TYR:HE1	1.83	0.43
4:E:120:SER:O	4:E:124:VAL:HG13	2.17	0.43
10:K:87:LEU:HD11	14:O:66:ILE:HD11	2.00	0.43
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.83	0.43
3:C:92:VAL:HG12	41:s:25:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:7:LYS:HA	7:H:16:VAL:HG21	2.00	0.43
14:O:146:ASP:OD1	14:O:146:ASP:N	2.48	0.43
14:O:166:ASP:OD1	14:O:166:ASP:N	2.34	0.43
6:X:80:LYS:HE3	6:X:80:LYS:HB3	1.73	0.43
22:Y:103:ASP:C	22:Y:103:ASP:OD1	2.61	0.43
25:b:109:THR:HG23	27:d:19:ALA:CB	2.47	0.43
32:i:129:LEU:HD12	32:i:129:LEU:O	2.17	0.43
34:k:37:MET:HG3	34:k:67:ALA:CB	2.48	0.43
35:l:492:ILE:O	35:l:496:MET:HG2	2.18	0.43
1:A:312:ASP:HA	1:A:329:LYS:NZ	2.33	0.43
4:E:41:ARG:HG3	4:E:41:ARG:HH11	1.83	0.43
5:F:41:TYR:O	5:F:44:LEU:HB2	2.18	0.43
12:M:217:GLU:C	12:M:288:ASP:OD1	2.61	0.43
14:O:193:TYR:HE1	14:O:216:PRO:HA	1.82	0.43
35:l:290:LEU:HD23	35:l:290:LEU:O	2.18	0.43
5:F:35:ASP:OD1	5:F:35:ASP:N	2.50	0.43
12:M:48:THR:HA	12:M:95:PRO:HA	1.99	0.43
20:V:76:ILE:O	20:V:80:VAL:HG23	2.18	0.43
25:b:99:GLU:HG3	35:l:61:MET:HE2	1.99	0.43
27:d:114:GLN:OE1	35:l:199:GLN:HG3	2.19	0.43
32:i:284:MET:HE1	40:r:159:PRO:HD3	2.00	0.43
40:r:121:LEU:O	40:r:125:THR:HG23	2.18	0.43
1:A:177:TYR:OH	1:A:194:ASP:OD1	2.34	0.43
3:C:98:ARG:HA	3:C:98:ARG:HD3	1.81	0.43
7:H:69:GLU:HG3	7:H:77:ILE:HG12	2.00	0.43
7:H:96:ARG:NH1	7:H:96:ARG:HB2	2.33	0.43
9:J:204:SER:OG	9:J:204:SER:O	2.33	0.43
15:P:61:PHE:HZ	15:P:106:ALA:HB2	1.83	0.43
16:Q:65:PRO:HB2	16:Q:67:ASN:O	2.19	0.43
6:X:113:LEU:O	6:X:117:GLU:HG3	2.19	0.43
25:b:87:LYS:HD3	25:b:88:TYR:CZ	2.54	0.43
26:c:96:ASP:OD1	26:c:96:ASP:N	2.51	0.43
37:n:46:LYS:CB	37:n:46:LYS:HZ3	2.31	0.43
39:p:63:LEU:O	39:p:64:LEU:HB3	2.18	0.43
1:A:126:LYS:NZ	1:A:127:ASP:OD1	2.48	0.43
21:W:30:LEU:HD23	21:W:35:MET:HG2	1.99	0.43
26:c:157:GLY:HA2	43:v:22:MET:CE	2.49	0.43
31:h:32:ARG:NH2	31:h:66:CYS:O	2.51	0.43
33:j:71:LEU:HD23	33:j:71:LEU:HA	1.86	0.43
35:l:468:ILE:O	35:l:472:ILE:HG12	2.19	0.43
40:r:373:ILE:HD11	40:r:444:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:501:PEE:H68	48:r:501:PEE:H62	1.82	0.43
18:T:105:GLU:OE1	18:T:105:GLU:O	2.37	0.43
20:V:91:PHE:HE1	20:V:120:LEU:HD22	1.82	0.43
21:W:66:GLU:OE2	42:u:123:GLY:N	2.41	0.43
22:Y:100:LEU:H	43:v:111:ARG:NH1	2.17	0.43
24:a:134:GLU:OE2	37:n:40:ASN:N	2.50	0.43
25:b:104:ILE:HD13	27:d:18:PRO:HG3	2.00	0.43
26:c:149:ILE:HG22	26:c:150:TYR:HD1	1.83	0.43
27:d:97:LYS:NZ	28:e:114:MET:HE3	2.34	0.43
41:s:26:LYS:HD2	41:s:36:GLY:HA3	2.01	0.43
44:w:181:LYS:O	44:w:184:VAL:HG22	2.18	0.43
1:A:329:LYS:HA	1:A:332:CYS:SG	2.58	0.43
5:F:19:ILE:HG23	5:F:53:ILE:HA	2.00	0.43
5:F:20:ARG:O	5:F:65:LEU:HD12	2.19	0.43
12:M:394:VAL:HG11	12:M:418:ILE:HG12	2.01	0.43
16:Q:159:LEU:O	16:Q:160:ASN:HB3	2.19	0.43
16:Q:351:MET:HE2	16:Q:351:MET:HB2	1.85	0.43
26:c:156:VAL:HG11	43:v:95:TYR:CZ	2.53	0.43
32:i:81:SER:O	32:i:83:GLN:N	2.49	0.43
49:j:201:PLX:H312	49:j:201:PLX:H282	1.74	0.43
35:l:222:GLY:HA2	35:l:229:LEU:HD12	2.00	0.43
48:m:201:PEE:H52	41:s:104:PHE:HE1	1.83	0.43
40:r:420:THR:HB	40:r:423:ILE:HD12	2.01	0.43
41:s:26:LYS:HA	41:s:36:GLY:HA3	2.01	0.43
56:s:401:UQ:HM53	56:s:401:UQ:H72	1.73	0.43
1:A:118:ASP:HB3	46:A:502:FMN:O4	2.18	0.43
12:M:64:CYS:O	12:M:184:ARG:NH2	2.34	0.43
14:O:75:LYS:HB2	14:O:75:LYS:HE3	1.80	0.43
16:Q:220:ALA:HB3	16:Q:224:ALA:HA	2.00	0.43
50:X:201:8Q1:O3	39:p:13:GLN:NE2	2.52	0.43
32:i:170:LEU:HD11	32:i:288:LEU:HD22	1.99	0.43
32:i:268:GLN:HE21	32:i:268:GLN:HB3	1.65	0.43
32:i:292:PHE:CE1	32:i:293:TYR:CE1	3.07	0.43
39:p:173:ARG:O	39:p:174:PRO:C	2.62	0.43
41:s:2:PHE:O	41:s:6:ILE:HG12	2.19	0.43
8:I:33:LYS:N	8:I:33:LYS:HD3	2.34	0.42
12:M:382:ARG:HA	12:M:385:TYR:CE1	2.54	0.42
14:O:164:THR:CG2	14:O:169:PHE:H	2.32	0.42
15:P:44:ARG:NE	15:P:45:PRO:HD3	2.30	0.42
25:b:80:TRP:HE1	27:d:41:VAL:HA	1.84	0.42
35:l:309:GLN:O	35:l:313:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:356:ILE:HA	35:l:359:MET:HE2	2.00	0.42
42:u:39:PRO:HG2	42:u:66:CYS:SG	2.59	0.42
2:B:150:THR:HG21	2:B:180:HIS:CD2	2.54	0.42
8:I:27:ARG:HH21	13:N:56:PHE:HD2	1.65	0.42
9:J:275:ASP:OD1	9:J:275:ASP:N	2.41	0.42
15:P:106:ALA:HB1	15:P:108:PHE:HD1	1.83	0.42
16:Q:450:ILE:O	16:Q:453:THR:HG22	2.19	0.42
23:Z:49:GLU:OE1	39:p:34:ARG:NE	2.46	0.42
55:i:402:CDL:H362	55:i:402:CDL:H392	1.84	0.42
55:l:701:CDL:H511	55:l:701:CDL:H542	1.81	0.42
36:m:25:SER:O	36:m:28:TYR:N	2.50	0.42
1:A:244:ASN:N	46:A:502:FMN:O1P	2.36	0.42
1:A:347:THR:HG23	1:A:348:GLY:N	2.33	0.42
11:L:96:LYS:HA	11:L:96:LYS:HD3	1.94	0.42
14:O:100:LYS:HA	14:O:103:GLU:HG2	2.00	0.42
16:Q:278:VAL:HG12	16:Q:329:ARG:HH21	1.85	0.42
25:b:16:ARG:O	25:b:20:ARG:HG3	2.20	0.42
33:j:53:MET:HG3	33:j:57:LEU:HD23	2.01	0.42
34:k:37:MET:CE	36:m:64:MET:HE1	2.48	0.42
35:l:327:LEU:HD12	35:l:327:LEU:HA	1.85	0.42
4:E:88:MET:HE2	15:P:184:LEU:O	2.19	0.42
5:F:23:LEU:O	5:F:57:GLU:HA	2.19	0.42
9:J:116:ILE:O	9:J:120:VAL:HG22	2.20	0.42
12:M:166:GLY:HA2	12:M:213:MET:SD	2.60	0.42
6:X:119:ILE:HG21	6:X:135:ALA:HB1	2.00	0.42
33:j:94:LEU:HD23	33:j:94:LEU:HA	1.93	0.42
37:n:42:SER:O	37:n:46:LYS:HB2	2.20	0.42
40:r:126:LEU:HD12	40:r:126:LEU:HA	1.89	0.42
1:A:119:GLU:OE2	1:A:128:ARG:HB2	2.20	0.42
3:C:49:LYS:HD2	3:C:49:LYS:HA	1.62	0.42
3:C:167:PRO:HG3	16:Q:222:MET:SD	2.59	0.42
16:Q:263:THR:HG23	16:Q:264:ASN:OD1	2.18	0.42
16:Q:315:GLU:OE1	16:Q:316:PHE:N	2.51	0.42
27:d:12:GLU:HB3	27:d:15:ARG:HH21	1.84	0.42
35:l:7:LEU:O	35:l:11:THR:HG23	2.19	0.42
1:A:380:GLY:O	1:A:386:ARG:NH1	2.52	0.42
46:A:502:FMN:N1	46:A:502:FMN:O3'	2.48	0.42
3:C:124:MET:HA	3:C:125:PRO:HD3	1.64	0.42
5:F:35:ASP:O	5:F:36:PHE:C	2.62	0.42
12:M:250:SER:OG	12:M:251:ILE:N	2.52	0.42
13:N:8:ARG:HE	13:N:8:ARG:HB2	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:72:ASP:C	13:N:72:ASP:OD1	2.62	0.42
14:O:177:LEU:HD12	14:O:185:MET:SD	2.60	0.42
44:w:41:LEU:O	44:w:45:LEU:HD13	2.18	0.42
44:w:54:THR:C	44:w:56:THR:H	2.28	0.42
3:C:119:LYS:HZ2	3:C:123:GLN:HE21	1.68	0.42
5:F:30:SER:HB2	5:F:63:PRO:CG	2.50	0.42
20:V:97:GLY:O	20:V:100:THR:OG1	2.27	0.42
22:Y:45:ARG:HA	23:Z:51:TRP:CE3	2.55	0.42
24:a:168:TRP:CD2	30:g:2:THR:HG23	2.54	0.42
39:p:25:ARG:HD3	39:p:25:ARG:HA	1.93	0.42
40:r:184:HIS:ND1	40:r:184:HIS:N	2.67	0.42
1:A:394:LYS:HD3	12:M:155:GLU:HB3	2.00	0.42
8:I:74:LYS:HD2	8:I:74:LYS:HA	1.76	0.42
6:X:112:SER:O	6:X:116:VAL:HG13	2.19	0.42
22:Y:103:ASP:OD1	22:Y:104:GLU:N	2.52	0.42
32:i:41:ILE:HG13	34:k:73:LEU:HD21	2.02	0.42
33:j:53:MET:HE2	33:j:53:MET:HB2	1.81	0.42
35:l:142:ILE:HG12	40:r:370:PRO:HB2	2.02	0.42
41:s:41:GLY:HA2	41:s:46:LEU:HD12	2.02	0.42
41:s:85:MET:HE3	41:s:233:MET:CE	2.50	0.42
41:s:183:MET:O	41:s:187:ILE:HG12	2.20	0.42
41:s:199:ASP:OD1	41:s:199:ASP:N	2.48	0.42
6:G:115:GLN:O	6:G:118:ILE:HG12	2.20	0.42
9:J:143:ASP:O	9:J:148:ILE:HG12	2.20	0.42
13:N:11:LEU:HD12	13:N:11:LEU:HA	1.76	0.42
14:O:181:VAL:HG12	14:O:222:ARG:HH22	1.85	0.42
32:i:18:MET:HE3	32:i:22:ILE:HG21	2.01	0.42
36:m:7:PHE:O	36:m:11:THR:HG23	2.20	0.42
37:n:46:LYS:NZ	37:n:46:LYS:HB2	2.33	0.42
38:o:121:LEU:HD12	38:o:121:LEU:O	2.19	0.42
40:r:329:LEU:HG	40:r:437:MET:HE2	2.01	0.42
1:A:338:ASP:OD1	1:A:341:ALA:N	2.45	0.42
16:Q:114:GLY:N	16:Q:462:ASP:OD1	2.48	0.42
17:S:42:SER:O	17:S:42:SER:OG	2.35	0.42
19:U:32:LEU:N	19:U:33:PRO:HD2	2.35	0.42
28:e:92:PHE:O	28:e:96:SER:HB3	2.20	0.42
28:e:137:MET:HB2	28:e:137:MET:HE3	1.75	0.42
39:p:150:ARG:HE	39:p:150:ARG:HB3	1.70	0.42
40:r:126:LEU:HD12	40:r:149:PHE:CZ	2.54	0.42
41:s:71:PHE:CD1	41:s:71:PHE:C	2.98	0.42
42:u:83:THR:HA	42:u:86:TRP:NE1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:55:GLU:OE2	44:w:277:LYS:NZ	2.31	0.42
8:I:107:SER:C	8:I:109:ASP:H	2.28	0.41
27:d:83:LEU:O	27:d:87:GLU:OE1	2.37	0.41
32:i:291:TYR:HA	40:r:151:PHE:HZ	1.85	0.41
55:i:402:CDL:H772	55:i:402:CDL:H741	1.74	0.41
34:k:45:THR:HG23	36:m:52:LEU:HD13	2.01	0.41
37:n:54:GLU:HG3	37:n:55:VAL:HG22	2.02	0.41
12:M:249:GLU:HG3	12:M:262:VAL:HG22	2.03	0.41
15:P:125:ARG:HD3	15:P:126:PHE:CZ	2.55	0.41
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	2.02	0.41
16:Q:253:PHE:O	16:Q:257:GLU:HG3	2.20	0.41
6:X:146:ASP:HB3	25:b:16:ARG:CZ	2.51	0.41
24:a:184:LYS:HB3	31:h:30:PRO:HB3	2.02	0.41
28:e:87:MET:HE3	28:e:87:MET:HB3	1.96	0.41
35:l:76:LEU:HD21	35:l:196:TRP:HE3	1.84	0.41
35:l:99:SER:HB3	35:l:341:MET:HE1	2.02	0.41
35:l:108:MET:HE2	35:l:240:PRO:HB3	2.02	0.41
38:o:57:LEU:HD23	38:o:57:LEU:O	2.20	0.41
43:v:106:ARG:O	43:v:110:GLN:HG2	2.20	0.41
3:C:79:MET:HG2	3:C:86:MET:HE3	2.02	0.41
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.56	0.41
14:O:193:TYR:CE1	14:O:216:PRO:HA	2.56	0.41
16:Q:144:MET:HE2	16:Q:144:MET:HB2	1.95	0.41
48:Q:502:PEE:H20	41:s:183:MET:HE2	2.03	0.41
48:Q:502:PEE:H36	48:Q:502:PEE:H41	1.82	0.41
17:S:49:GLU:OE1	17:S:52:ARG:NH2	2.40	0.41
19:U:31:ILE:HD13	19:U:31:ILE:HA	1.89	0.41
27:d:9:VAL:HG11	28:e:123:GLU:HG2	2.02	0.41
35:l:88:MET:HE1	35:l:468:ILE:CD1	2.50	0.41
35:l:198:LEU:HD23	35:l:198:LEU:HA	1.87	0.41
36:m:129:ASP:OD1	36:m:129:ASP:N	2.38	0.41
37:n:30:ARG:O	37:n:33:GLU:HG2	2.20	0.41
38:o:62:ASP:O	38:o:66:ILE:HG12	2.20	0.41
39:p:108:HIS:CD2	39:p:109:PRO:HD2	2.55	0.41
40:r:437:MET:HA	40:r:437:MET:HE3	2.01	0.41
1:A:168:ASN:CA	1:A:171:VAL:HG12	2.51	0.41
1:A:290:GLU:HG2	1:A:294:VAL:HG11	2.02	0.41
6:G:119:ILE:O	6:G:123:GLU:HG2	2.20	0.41
12:M:29:SER:HG	12:M:30:ASN:H	1.68	0.41
12:M:329:MET:HE2	12:M:329:MET:HB3	1.95	0.41
20:V:73:THR:HB	20:V:93:GLY:HA2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:68:GLU:OE2	39:p:68:GLU:HA	2.20	0.41
1:A:118:ASP:O	1:A:159:ARG:HD2	2.20	0.41
3:C:70:ALA:HB1	16:Q:118:2MR:CQ1	2.51	0.41
12:M:144:MET:HG3	16:Q:383:LYS:HG3	2.02	0.41
14:O:137:THR:HG22	14:O:138:THR:H	1.85	0.41
16:Q:199:PRO:HB3	16:Q:258:LEU:HD13	2.02	0.41
16:Q:295:GLY:O	16:Q:324:GLY:HA2	2.21	0.41
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.86	0.41
6:X:147:TYR:CD1	6:X:147:TYR:C	2.99	0.41
32:i:20:VAL:HG11	32:i:137:ALA:HB1	2.03	0.41
49:j:201:PLX:H342	49:j:201:PLX:H372	1.53	0.41
35:l:20:MET:HA	49:r:503:PLX:H211	2.03	0.41
36:m:173:ARG:HG2	36:m:173:ARG:NH1	2.28	0.41
39:p:127:ARG:HG3	39:p:128:LEU:N	2.33	0.41
40:r:272:THR:HA	40:r:275:ILE:HD12	2.02	0.41
42:u:58:GLU:O	42:u:62:LEU:HD23	2.20	0.41
44:w:275:TYR:CD1	44:w:275:TYR:N	2.86	0.41
44:w:302:LEU:HD23	44:w:302:LEU:HA	1.93	0.41
17:S:3:PHE:HA	17:S:6:LEU:HD23	2.02	0.41
22:Y:43:ARG:HD2	22:Y:46:GLN:HB2	2.02	0.41
22:Y:65:MET:HE3	22:Y:65:MET:HB3	1.95	0.41
39:p:24:LEU:HD23	39:p:24:LEU:HA	1.84	0.41
42:u:38:LYS:HB3	42:u:39:PRO:HD3	2.02	0.41
43:v:57:ASP:OD1	43:v:57:ASP:N	2.52	0.41
44:w:235:GLN:NE2	44:w:239:ASN:OD1	2.54	0.41
1:A:35:LEU:HD23	1:A:40:ARG:NH1	2.36	0.41
1:A:337:MET:HE3	1:A:337:MET:HB3	1.84	0.41
5:F:79:LEU:HG	5:F:87:VAL:HG12	2.03	0.41
15:P:119:VAL:HG12	15:P:121:THR:HG22	2.01	0.41
6:X:88:LYS:HB2	6:X:88:LYS:HE3	1.91	0.41
26:c:49:ALA:HA	26:c:59:VAL:HG23	2.02	0.41
32:i:91:ASN:OD1	32:i:92:PRO:HD2	2.21	0.41
35:l:71:LEU:HD23	40:r:310:MET:CE	2.50	0.41
35:l:383:MET:HG2	35:l:384:PRO:HD2	2.01	0.41
49:r:502:PLX:H22	49:r:502:PLX:H1C3	1.74	0.41
41:s:285:LEU:C	41:s:285:LEU:CD1	2.91	0.41
42:u:60:GLY:O	42:u:63:VAL:HG22	2.21	0.41
1:A:456:GLN:C	1:A:456:GLN:NE2	2.78	0.41
3:C:98:ARG:HD2	41:s:61:LEU:HD21	2.02	0.41
4:E:98:LYS:HD3	4:E:102:HIS:HB3	2.03	0.41
26:c:70:MET:H	26:c:70:MET:HG2	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:e:73:SER:C	28:e:75:GLY:H	2.28	0.41
35:l:16:THR:HG22	35:l:126:ILE:HD13	2.02	0.41
35:l:61:MET:HE3	35:l:61:MET:HB2	1.88	0.41
35:l:245:ALA:HB2	35:l:340:PHE:HB3	2.03	0.41
38:o:35:GLU:O	38:o:39:ILE:HG23	2.21	0.41
40:r:122:PHE:HD1	40:r:238:LEU:HD13	1.86	0.41
4:e:16:SER:HA	11:L:54:ALA:HA	2.03	0.41
8:I:42:PRO:HD3	21:W:6:VAL:HG13	2.03	0.41
9:J:344:PRO:HG2	9:J:347:LEU:HG	2.03	0.41
10:K:70:ASN:OD1	10:K:70:ASN:N	2.54	0.41
12:M:58:MET:HE1	12:M:104:THR:HB	2.03	0.41
12:M:483:ARG:HB2	12:M:483:ARG:HH11	1.85	0.41
14:O:68:LYS:HE3	14:O:68:LYS:HB2	1.86	0.41
14:O:193:TYR:HB3	14:O:196:LEU:HD11	2.03	0.41
14:O:236:GLU:HG2	14:O:237:PRO:HD2	2.03	0.41
16:Q:133:LEU:CD2	16:Q:228:ARG:HD3	2.50	0.41
16:Q:188:THR:HG21	16:Q:203:MET:HB2	2.03	0.41
18:T:119:ARG:HD2	18:T:122:HIS:HD2	1.86	0.41
19:U:78:LEU:O	19:U:82:LYS:HG3	2.21	0.41
23:Z:60:ASN:OD1	23:Z:60:ASN:N	2.54	0.41
24:a:117:ILE:HD13	49:a:202:PLX:H211	2.03	0.41
28:e:97:ILE:O	28:e:101:LEU:HB2	2.20	0.41
29:f:73:ASN:HB3	29:f:75:LEU:HD23	2.02	0.41
31:h:65:GLU:OE1	31:h:71:LYS:HB2	2.21	0.41
33:j:107:THR:O	33:j:107:THR:HG22	2.21	0.41
35:l:128:MET:HG2	35:l:251:THR:HG22	2.01	0.41
35:l:149:ILE:HD13	35:l:149:ILE:HA	1.91	0.41
35:l:288:THR:HG21	35:l:307:SER:CB	2.48	0.41
35:l:554:ASP:OD1	40:r:213:HIS:NE2	2.53	0.41
40:r:133:ILE:HD11	40:r:231:LEU:HD11	2.02	0.41
40:r:216:LEU:HB3	40:r:217:PRO:HD3	2.02	0.41
41:s:38:ASN:OD1	41:s:38:ASN:N	2.54	0.41
41:s:162:LEU:HD23	41:s:165:LEU:HD12	2.02	0.41
1:A:179:ALA:HB1	1:A:181:LEU:HD23	2.03	0.41
1:A:392:MET:HE1	1:A:432:ALA:HA	2.01	0.41
46:A:502:FMN:N5	47:A:503:NAI:H4N	2.36	0.41
2:B:68:ARG:NH1	21:W:28:ARG:HG2	2.36	0.41
4:E:127:ASP:OD2	9:J:45:LYS:NZ	2.53	0.41
7:H:31:ILE:HA	7:H:31:ILE:HD12	1.81	0.41
10:K:79:HIS:ND1	14:O:216:PRO:HD2	2.35	0.41
12:M:646:LEU:HD12	12:M:646:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:102:SER:OG	16:Q:107:ARG:NH1	2.54	0.41
19:U:78:LEU:HD23	19:U:78:LEU:HA	1.83	0.41
20:V:69:ILE:HG21	20:V:100:THR:CG2	2.51	0.41
27:d:146:LEU:HD23	27:d:146:LEU:HA	1.92	0.41
32:i:245:MET:HE3	32:i:245:MET:HB3	1.89	0.41
33:j:1:MET:N	33:j:4:MET:HE3	2.36	0.41
40:r:150:LEU:HG	40:r:154:LEU:HD12	2.03	0.41
40:r:457:PRO:HG2	40:r:458:LEU:HD12	2.02	0.41
1:A:185:ASN:O	1:A:187:CYS:N	2.54	0.40
2:B:210:LEU:HD23	2:B:210:LEU:HA	1.88	0.40
5:F:82:PHE:HB3	5:F:87:VAL:HG13	2.03	0.40
9:J:71:ASN:OD1	9:J:75:ARG:NH2	2.50	0.40
9:J:114:ASP:O	9:J:118:LYS:HG2	2.21	0.40
9:J:269:ASN:HB2	9:J:271:TYR:CZ	2.56	0.40
6:X:110:LEU:HD12	6:X:114:ASP:CB	2.51	0.40
6:X:113:LEU:O	6:X:116:VAL:HG22	2.21	0.40
26:c:184:TYR:OH	43:v:104:ARG:NH1	2.54	0.40
31:h:32:ARG:NH1	34:k:50:ASN:OD1	2.53	0.40
31:h:74:LYS:HE3	31:h:74:LYS:HB2	1.94	0.40
2:B:105:ARG:HD2	13:N:108:TYR:CG	2.56	0.40
9:J:148:ILE:HB	9:J:149:PRO:HD3	2.03	0.40
12:M:360:ARG:HE	12:M:632:MET:HB3	1.87	0.40
16:Q:237:PRO:HD2	16:Q:240:LEU:HD22	2.03	0.40
22:Y:99:ILE:HD11	43:v:108:LEU:HD12	2.03	0.40
24:a:127:ASP:OD1	49:a:202:PLX:H12	2.22	0.40
33:j:81:THR:C	33:j:83:ASN:H	2.29	0.40
49:j:201:PLX:H182	49:j:201:PLX:H131	2.02	0.40
34:k:43:MET:HE2	34:k:47:ILE:HD11	2.04	0.40
35:l:140:LEU:HD12	35:l:140:LEU:HA	1.84	0.40
39:p:30:TRP:NE1	39:p:76:HIS:HB2	2.36	0.40
39:p:155:PRO:O	39:p:165:PRO:HD2	2.21	0.40
41:s:81:LEU:HA	41:s:84:THR:HG22	2.03	0.40
43:v:25:PHE:CD2	43:v:108:LEU:HD23	2.50	0.40
1:A:35:LEU:HD23	1:A:40:ARG:HH11	1.86	0.40
2:B:100:GLU:O	2:B:170:GLY:N	2.46	0.40
6:G:119:ILE:HG23	6:G:130:ILE:HD11	2.01	0.40
9:J:175:LYS:HB2	9:J:175:LYS:HE3	1.85	0.40
12:M:217:GLU:O	12:M:288:ASP:OD1	2.39	0.40
12:M:624:ARG:NH2	12:M:637:ASP:OD1	2.40	0.40
13:N:10:GLY:O	13:N:14:VAL:HG23	2.21	0.40
25:b:76:LEU:HD12	25:b:76:LEU:HA	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:e:114:MET:HB3	28:e:117:TRP:HB3	2.04	0.40
31:h:54:LYS:HD3	31:h:54:LYS:HA	1.71	0.40
31:h:76:LEU:HD23	31:h:76:LEU:HA	1.73	0.40
35:l:51:LEU:HG	35:l:55:MET:HE2	2.04	0.40
40:r:196:TRP:CE3	40:r:257:MET:HE3	2.56	0.40
41:s:47:GLN:HB3	41:s:48:PRO:HD3	2.03	0.40
42:u:80:GLU:O	42:u:84:GLU:HG3	2.20	0.40
44:w:211:VAL:CA	44:w:214:ILE:HG22	2.45	0.40
1:A:140:GLU:CD	1:A:252:PRO:HB3	2.46	0.40
49:C:303:PLX:H31	13:N:75:TRP:CD2	2.56	0.40
7:H:28:TYR:O	7:H:31:ILE:HG22	2.22	0.40
12:M:89:VAL:HG11	12:M:94:MET:HE3	2.03	0.40
12:M:556:THR:HG22	12:M:557:ARG:H	1.86	0.40
18:T:119:ARG:HD2	18:T:122:HIS:CD2	2.56	0.40
6:X:93:ILE:O	6:X:93:ILE:HG13	2.20	0.40
26:c:110:ASP:OD1	26:c:110:ASP:N	2.53	0.40
32:i:347:ASN:HB3	49:i:401:PLX:H282	2.04	0.40
1:A:201:ALA:O	14:O:119:TYR:HB3	2.21	0.40
3:C:119:LYS:NZ	3:C:123:GLN:NE2	2.68	0.40
5:F:56:ARG:NH1	12:M:382:ARG:HG3	2.36	0.40
6:G:149:ALA:O	6:G:153:ASP:N	2.52	0.40
14:O:185:MET:SD	14:O:185:MET:C	3.05	0.40
48:Q:502:PEE:H21	48:Q:502:PEE:H16	1.75	0.40
21:W:58:ARG:HA	21:W:58:ARG:HD2	1.87	0.40
23:Z:20:LYS:HE3	23:Z:20:LYS:HB3	1.72	0.40
31:h:17:TRP:CZ3	31:h:18:MET:HB2	2.57	0.40
41:s:66:SER:HB2	41:s:122:ALA:O	2.22	0.40
42:u:108:ASP:O	42:u:111:VAL:HG12	2.22	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	429/433 (99%)	415 (97%)	14 (3%)	0	100	100
2	B	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
3	C	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
4	E	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
5	F	84/86 (98%)	81 (96%)	2 (2%)	1 (1%)	10	42
6	G	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
8	I	93/112 (83%)	82 (88%)	11 (12%)	0	100	100
9	J	289/342 (84%)	276 (96%)	13 (4%)	0	100	100
10	K	40/43 (93%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	669 (97%)	18 (3%)	1 (0%)	48	79
13	N	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
14	O	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
15	P	206/208 (99%)	197 (96%)	9 (4%)	0	100	100
16	Q	412/430 (96%)	398 (97%)	13 (3%)	1 (0%)	43	73
17	S	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
18	T	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
19	U	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
20	V	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	18	52
21	W	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
22	Y	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
23	Z	82/84 (98%)	82 (100%)	0	0	100	100
24	a	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
25	b	99/126 (79%)	93 (94%)	5 (5%)	1 (1%)	12	45
26	c	154/156 (99%)	146 (95%)	8 (5%)	0	100	100
27	d	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
28	e	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
29	f	40/49 (82%)	40 (100%)	0	0	100	100
30	g	119/122 (98%)	114 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	99 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	i	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
33	j	95/115 (83%)	89 (94%)	6 (6%)	0	100	100
34	k	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
35	l	601/603 (100%)	570 (95%)	31 (5%)	0	100	100
36	m	125/175 (71%)	115 (92%)	10 (8%)	0	100	100
37	n	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
38	o	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
39	p	176/178 (99%)	167 (95%)	8 (4%)	1 (1%)	21	56
40	r	457/459 (100%)	440 (96%)	17 (4%)	0	100	100
41	s	299/318 (94%)	282 (94%)	17 (6%)	0	100	100
42	u	169/171 (99%)	161 (95%)	8 (5%)	0	100	100
43	v	122/124 (98%)	115 (94%)	7 (6%)	0	100	100
44	w	318/320 (99%)	303 (95%)	15 (5%)	0	100	100
All	All	8029/8322 (96%)	7702 (96%)	321 (4%)	6 (0%)	49	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	31	GLN
39	p	175	ARG
12	M	283	GLU
16	Q	160	ASN
25	b	110	ILE
20	V	46	PRO

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	343/346 (99%)	337 (98%)	6 (2%)	53	75
2	B	151/151 (100%)	151 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	72/76 (95%)	72 (100%)	0	100	100
6	G	75/81 (93%)	75 (100%)	0	100	100
6	X	77/81 (95%)	77 (100%)	0	100	100
7	H	98/99 (99%)	98 (100%)	0	100	100
8	I	87/97 (90%)	87 (100%)	0	100	100
9	J	254/296 (86%)	254 (100%)	0	100	100
10	K	41/42 (98%)	41 (100%)	0	100	100
11	L	113/113 (100%)	113 (100%)	0	100	100
12	M	580/580 (100%)	580 (100%)	0	100	100
13	N	130/130 (100%)	130 (100%)	0	100	100
14	O	183/183 (100%)	182 (100%)	1 (0%)	81	85
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	361/370 (98%)	357 (99%)	4 (1%)	65	79
17	S	58/58 (100%)	57 (98%)	1 (2%)	53	75
18	T	79/79 (100%)	78 (99%)	1 (1%)	61	78
19	U	68/69 (99%)	68 (100%)	0	100	100
20	V	100/101 (99%)	95 (95%)	5 (5%)	22	55
21	W	123/123 (100%)	123 (100%)	0	100	100
22	Y	62/63 (98%)	61 (98%)	1 (2%)	55	75
23	Z	65/65 (100%)	65 (100%)	0	100	100
24	a	122/122 (100%)	122 (100%)	0	100	100
25	b	95/119 (80%)	95 (100%)	0	100	100
26	c	140/141 (99%)	140 (100%)	0	100	100
27	d	155/155 (100%)	155 (100%)	0	100	100
28	e	99/99 (100%)	99 (100%)	0	100	100
29	f	35/45 (78%)	35 (100%)	0	100	100
30	g	108/109 (99%)	108 (100%)	0	100	100
31	h	93/93 (100%)	93 (100%)	0	100	100
32	i	310/311 (100%)	308 (99%)	2 (1%)	78	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	j	88/100 (88%)	88 (100%)	0	100	100
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	536/537 (100%)	536 (100%)	0	100	100
36	m	98/141 (70%)	96 (98%)	2 (2%)	48	72
37	n	50/53 (94%)	49 (98%)	1 (2%)	48	72
38	o	113/113 (100%)	113 (100%)	0	100	100
39	p	158/159 (99%)	158 (100%)	0	100	100
40	r	410/410 (100%)	408 (100%)	2 (0%)	81	85
41	s	263/275 (96%)	261 (99%)	2 (1%)	73	82
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	104/111 (94%)	104 (100%)	0	100	100
44	w	280/283 (99%)	279 (100%)	1 (0%)	84	86
All	All	7044/7246 (97%)	7015 (100%)	29 (0%)	81	86

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	VAL
1	A	208	GLU
1	A	210	THR
1	A	351	THR
1	A	410	ASP
1	A	455	LEU
14	O	166	ASP
16	Q	156	GLU
16	Q	234	GLN
16	Q	253	PHE
16	Q	263	THR
17	S	68	ASN
18	T	49	ASP
20	V	95	CYS
20	V	101	LEU
20	V	106	ARG
20	V	108	TYR
20	V	110	ILE
22	Y	81	LEU
32	i	128	LEU
32	i	268	GLN

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Mol	Chain	Res	Type
36	m	1	MET
36	m	56	VAL
37	n	46	LYS
40	r	180	HIS
40	r	204	MET
41	s	84	THR
41	s	285	LEU
44	w	54	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	136	HIS
1	A	168	ASN
1	A	422	HIS
1	A	436	GLN
3	C	123	GLN
9	J	376	ASN
11	L	86	ASN
12	M	278	HIS
12	M	304	GLN
12	M	667	GLN
13	N	116	ASN
13	N	123	GLN
14	O	69	ASN
14	O	133	GLN
15	P	51	ASN
15	P	77	GLN
15	P	105	ASN
15	P	107	GLN
15	P	196	HIS
16	Q	60	HIS
16	Q	131	GLN
16	Q	160	ASN
16	Q	234	GLN
16	Q	250	ASN
16	Q	306	GLN
18	T	63	ASN
20	V	134	GLN
24	a	50	HIS
25	b	89	HIS

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Mol	Chain	Res	Type
26	c	83	GLN
29	f	62	HIS
30	g	18	ASN
30	g	48	ASN
30	g	63	GLN
32	i	77	ASN
32	i	134	GLN
32	i	172	GLN
32	i	310	ASN
34	k	57	ASN
35	l	34	ASN
35	l	56	HIS
35	l	192	HIS
35	l	210	ASN
35	l	270	ASN
35	l	309	GLN
35	l	400	ASN
35	l	447	ASN
35	l	470	ASN
37	n	3	ASN
38	o	50	GLN
38	o	123	GLN
39	p	12	HIS
40	r	144	ASN
40	r	415	GLN
41	s	47	GLN
41	s	124	ASN
41	s	235	ASN
41	s	247	HIS
41	s	317	GLN
42	u	35	GLN
42	u	151	ASN
43	v	84	GLN
43	v	110	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
16	2MR	Q	118	16	10,12,13	1.18	1 (10%)	5,13,15	1.18	0

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
16	2MR	Q	118	16	-	5/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NH2	-3.20	1.26	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	Q	118	2MR	NH1-CZ-NE-CD
16	Q	118	2MR	NH2-CZ-NE-CD
16	Q	118	2MR	NE-CD-CG-CB
16	Q	118	2MR	CA-CB-CG-CD
16	Q	118	2MR	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Q	118	2MR	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 2 are monoatomic - leaving 32 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	SF4	C	301	16,3	0,12,12	-	-	-		
45	SF4	M	801	12	0,12,12	-	-	-		
48	PEE	l	703	-	45,45,50	1.22	6 (13%)	48,50,55	0.95	2 (4%)
48	PEE	m	201	-	40,40,50	1.15	5 (12%)	43,45,55	1.01	2 (4%)
55	CDL	l	701	-	99,99,99	1.09	9 (9%)	105,111,111	0.85	4 (3%)
48	PEE	l	702	-	45,45,50	1.21	6 (13%)	48,50,55	0.96	2 (4%)
49	PLX	i	401	-	51,51,51	1.14	3 (5%)	55,59,59	0.61	1 (1%)
55	CDL	i	402	-	99,99,99	1.08	8 (8%)	105,111,111	0.87	4 (3%)
45	SF4	B	301	2	0,12,12	-	-	-		
50	8Q1	X	201	-	31,34,34	1.69	6 (19%)	40,43,43	1.51	6 (15%)
52	FES	M	803	12	0,4,4	-	-	-		
57	ADP	w	401	-	27,29,29	2.96	8 (29%)	42,45,45	2.02	11 (26%)
48	PEE	U	101	-	50,50,50	1.15	6 (12%)	53,55,55	0.95	2 (3%)
49	PLX	r	503	-	51,51,51	1.14	4 (7%)	55,59,59	0.58	1 (1%)
46	FMN	A	502	-	33,33,33	1.09	2 (6%)	48,50,50	1.22	8 (16%)
49	PLX	j	201	-	51,51,51	1.14	4 (7%)	55,59,59	0.60	1 (1%)
45	SF4	B	302	2	0,12,12	-	-	-		
51	NDP	J	401	-	49,52,52	4.40	23 (46%)	66,80,80	2.19	16 (24%)
45	SF4	M	802	12	0,12,12	-	-	-		
50	8Q1	G	201	-	31,34,34	1.69	6 (19%)	40,43,43	1.55	6 (15%)
52	FES	O	301	14	0,4,4	-	-	-		
56	UQ	s	401	-	28,28,63	3.27	7 (25%)	34,37,79	2.74	10 (29%)
48	PEE	C	302	-	46,46,50	1.22	6 (13%)	49,51,55	0.97	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PEE	Q	501	-	46,46,50	1.20	6 (13%)	49,51,55	0.99	2 (4%)
47	NAI	A	503	-	45,48,48	3.91	19 (42%)	60,73,73	1.79	12 (20%)
49	PLX	C	303	-	51,51,51	1.15	3 (5%)	55,59,59	0.62	1 (1%)
45	SF4	A	501	1	0,12,12	-	-	-	-	-
48	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	0.98	2 (3%)
49	PLX	r	502	-	51,51,51	1.14	4 (7%)	55,59,59	0.61	1 (1%)
49	PLX	a	202	-	51,51,51	1.14	4 (7%)	55,59,59	0.61	1 (1%)
55	CDL	a	201	-	90,90,99	1.13	9 (10%)	96,102,111	0.93	4 (4%)
48	PEE	Q	502	-	50,50,50	1.15	6 (12%)	53,55,55	0.96	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	C	301	16,3	-	-	0/6/5/5
45	SF4	M	801	12	-	-	0/6/5/5
48	PEE	l	703	-	-	25/49/49/54	-
48	PEE	m	201	-	-	18/44/44/54	-
55	CDL	l	701	-	-	54/110/110/110	-
48	PEE	l	702	-	-	28/49/49/54	-
49	PLX	i	401	-	-	27/55/55/55	-
55	CDL	i	402	-	-	63/110/110/110	-
50	8Q1	X	201	-	-	21/41/41/41	-
45	SF4	B	301	2	-	-	0/6/5/5
57	ADP	w	401	-	-	4/16/32/32	0/3/3/3
52	FES	M	803	12	-	-	0/1/1/1
48	PEE	U	101	-	-	26/54/54/54	-
49	PLX	r	503	-	-	33/55/55/55	-
46	FMN	A	502	-	-	4/18/18/18	0/3/3/3
49	PLX	j	201	-	-	26/55/55/55	-
45	SF4	B	302	2	-	-	0/6/5/5
51	NDP	J	401	-	-	9/34/77/77	0/4/5/5
45	SF4	M	802	12	-	-	0/6/5/5
50	8Q1	G	201	-	-	20/41/41/41	-
52	FES	O	301	14	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	UQ	s	401	-	-	9/21/45/87	0/1/1/1
48	PEE	C	302	-	-	20/50/50/54	-
48	PEE	Q	501	-	-	25/50/50/54	-
47	NAI	A	503	-	-	6/29/72/72	0/5/5/5
49	PLX	C	303	-	-	25/55/55/55	-
45	SF4	A	501	1	-	-	0/6/5/5
48	PEE	r	501	-	-	25/54/54/54	-
49	PLX	r	502	-	-	33/55/55/55	-
49	PLX	a	202	-	-	20/55/55/55	-
55	CDL	a	201	-	-	41/101/101/110	-
48	PEE	Q	502	-	-	19/54/54/54	-

All (166) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	J	401	NDP	C3B-C2B	-12.71	1.24	1.52
51	J	401	NDP	C6N-C5N	12.47	1.55	1.33
51	J	401	NDP	O4D-C4D	10.66	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.30	1.26	1.53
51	J	401	NDP	C3D-C4D	-9.85	1.27	1.53
56	s	401	UQ	C13-C14	9.34	1.55	1.33
47	A	503	NAI	O4B-C1B	9.17	1.63	1.42
57	w	401	ADP	C3'-C4'	-8.86	1.30	1.53
56	s	401	UQ	C8-C9	8.86	1.54	1.33
47	A	503	NAI	O4B-C4B	-8.34	1.26	1.45
56	s	401	UQ	C18-C19	8.28	1.56	1.32
51	J	401	NDP	O4B-C4B	-8.01	1.27	1.45
57	w	401	ADP	O4'-C4'	7.64	1.62	1.45
51	J	401	NDP	C2N-C3N	7.60	1.56	1.34
47	A	503	NAI	C2D-C1D	-7.56	1.29	1.53
47	A	503	NAI	C2B-C1B	-7.28	1.30	1.53
47	A	503	NAI	O4D-C4D	6.90	1.60	1.45
47	A	503	NAI	C2D-C3D	5.99	1.69	1.53
51	J	401	NDP	C6A-N6A	5.92	1.49	1.34
47	A	503	NAI	C7N-N7N	5.76	1.48	1.33
51	J	401	NDP	P2B-O2B	5.73	1.70	1.59
57	w	401	ADP	C6-N6	5.52	1.48	1.34
47	A	503	NAI	O4D-C1D	5.46	1.54	1.42
51	J	401	NDP	C3B-C4B	5.46	1.66	1.53
50	G	201	8Q1	C34-N36	5.45	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	X	201	8Q1	C34-N36	5.38	1.45	1.33
50	X	201	8Q1	C39-N41	5.35	1.45	1.33
50	G	201	8Q1	C39-N41	5.28	1.45	1.33
47	A	503	NAI	C6A-N6A	5.24	1.47	1.34
47	A	503	NAI	C4N-C3N	-5.06	1.40	1.49
51	J	401	NDP	C6N-N1N	4.96	1.49	1.37
51	J	401	NDP	O4D-C1D	-4.94	1.30	1.42
47	A	503	NAI	O2B-C2B	4.52	1.53	1.43
51	J	401	NDP	C1B-N9A	-4.46	1.33	1.46
51	J	401	NDP	O4B-C1B	4.46	1.52	1.42
57	w	401	ADP	O4'-C1'	-4.44	1.31	1.42
51	J	401	NDP	C7N-N7N	4.20	1.44	1.33
51	J	401	NDP	O2D-C2D	-4.13	1.33	1.43
47	A	503	NAI	C6N-C5N	3.94	1.40	1.33
46	A	502	FMN	C4A-N5	3.89	1.38	1.30
48	C	302	PEE	C18-C19	3.76	1.53	1.31
48	m	201	PEE	C18-C19	3.75	1.53	1.31
48	l	703	PEE	C18-C19	3.74	1.53	1.31
48	r	501	PEE	C18-C19	3.72	1.53	1.31
48	l	702	PEE	C18-C19	3.71	1.53	1.31
48	Q	501	PEE	C18-C19	3.71	1.53	1.31
48	Q	502	PEE	C18-C19	3.71	1.53	1.31
48	U	101	PEE	C18-C19	3.69	1.53	1.31
48	C	302	PEE	C39-C38	3.69	1.53	1.31
48	Q	501	PEE	C39-C38	3.66	1.53	1.31
48	r	501	PEE	C39-C38	3.65	1.52	1.31
48	l	702	PEE	C39-C38	3.64	1.52	1.31
48	U	101	PEE	C39-C38	3.63	1.52	1.31
48	l	703	PEE	C39-C38	3.63	1.52	1.31
48	Q	502	PEE	C39-C38	3.62	1.52	1.31
47	A	503	NAI	C7N-C3N	3.58	1.56	1.48
55	l	701	CDL	OA8-CA7	3.42	1.43	1.33
55	i	402	CDL	OA8-CA7	3.41	1.43	1.33
47	A	503	NAI	C4N-C5N	-3.37	1.40	1.48
57	w	401	ADP	O2'-C2'	-3.37	1.35	1.43
55	a	201	CDL	OA8-CA7	3.36	1.43	1.33
51	J	401	NDP	C7N-C3N	3.21	1.55	1.48
57	w	401	ADP	C8-N9	-3.15	1.31	1.37
57	w	401	ADP	O3'-C3'	3.12	1.50	1.43
51	J	401	NDP	O3D-C3D	3.09	1.50	1.43
55	i	402	CDL	OB6-CB5	3.08	1.43	1.34
55	l	701	CDL	OB6-CB5	3.05	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	a	201	CDL	OB6-CB5	3.04	1.42	1.34
55	l	701	CDL	OA6-CA5	3.04	1.42	1.34
55	a	201	CDL	OB8-CB7	3.03	1.42	1.33
51	J	401	NDP	C8A-N9A	-3.03	1.32	1.37
55	i	402	CDL	OB8-CB7	2.98	1.42	1.33
55	l	701	CDL	OB8-CB7	2.96	1.42	1.33
51	J	401	NDP	C5A-N7A	-2.95	1.33	1.39
55	a	201	CDL	OA6-CA5	2.95	1.42	1.34
55	i	402	CDL	OA6-CA5	2.94	1.42	1.34
49	a	202	PLX	O6-C4	-2.79	1.40	1.44
49	i	401	PLX	O6-C4	-2.78	1.40	1.44
49	C	303	PLX	O6-C4	-2.75	1.40	1.44
49	r	503	PLX	O6-C4	-2.71	1.41	1.44
56	s	401	UQ	C6-C1	2.63	1.54	1.46
48	l	703	PEE	O3-C30	2.55	1.40	1.33
49	j	201	PLX	O6-C4	-2.54	1.41	1.44
48	Q	502	PEE	O2-C2	-2.52	1.40	1.46
47	A	503	NAI	C8A-N9A	-2.51	1.33	1.37
48	Q	501	PEE	O3-C30	2.51	1.40	1.33
48	C	302	PEE	O2-C2	-2.47	1.40	1.46
48	r	501	PEE	O2-C2	-2.47	1.40	1.46
48	Q	502	PEE	O3-C30	2.46	1.40	1.33
48	r	501	PEE	O3-C30	2.46	1.40	1.33
48	C	302	PEE	O3-C30	2.45	1.40	1.33
47	A	503	NAI	PN-O5D	2.45	1.69	1.59
55	i	402	CDL	OA6-CA4	-2.45	1.40	1.46
51	J	401	NDP	O2B-C2B	2.43	1.52	1.44
48	U	101	PEE	O3-C30	2.43	1.40	1.33
48	Q	501	PEE	O2-C2	-2.42	1.40	1.46
47	A	503	NAI	O3B-C3B	-2.41	1.37	1.43
48	l	702	PEE	O3-C30	2.41	1.40	1.33
48	m	201	PEE	O2-C10	2.40	1.41	1.34
49	r	502	PLX	C7-C6	2.40	1.55	1.50
48	m	201	PEE	O3-C30	2.40	1.40	1.33
55	a	201	CDL	OA6-CA4	-2.39	1.40	1.46
46	A	502	FMN	C10-N1	2.39	1.38	1.33
48	l	703	PEE	O2-C2	-2.39	1.40	1.46
50	X	201	8Q1	C1-S44	2.39	1.81	1.76
48	U	101	PEE	O2-C2	-2.38	1.40	1.46
50	G	201	8Q1	C1-S44	2.37	1.81	1.76
51	J	401	NDP	C2D-C3D	2.37	1.59	1.53
48	l	702	PEE	O2-C2	-2.33	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	j	201	PLX	C7-C6	2.33	1.55	1.50
49	r	502	PLX	O6-C4	-2.33	1.41	1.44
48	l	702	PEE	O2-C10	2.32	1.40	1.34
49	C	303	PLX	C7-C6	2.31	1.55	1.50
55	l	701	CDL	OA6-CA4	-2.30	1.40	1.46
50	G	201	8Q1	O40-C39	-2.30	1.18	1.23
49	a	202	PLX	C7-C6	2.29	1.55	1.50
49	r	503	PLX	C7-C6	2.29	1.55	1.50
49	i	401	PLX	C7-C6	2.28	1.55	1.50
48	U	101	PEE	O2-C10	2.27	1.40	1.34
48	Q	501	PEE	O2-C10	2.26	1.40	1.34
48	C	302	PEE	O2-C10	2.25	1.40	1.34
48	l	703	PEE	O2-C10	2.25	1.40	1.34
48	m	201	PEE	O2-C2	-2.24	1.41	1.46
48	Q	502	PEE	O2-C10	2.24	1.40	1.34
57	w	401	ADP	C5-N7	-2.24	1.34	1.39
50	X	201	8Q1	O40-C39	-2.23	1.18	1.23
50	X	201	8Q1	C6-C1	2.22	1.53	1.50
55	l	701	CDL	OB6-CB4	-2.21	1.41	1.46
50	G	201	8Q1	O35-C34	-2.20	1.19	1.23
55	a	201	CDL	PB2-OB2	2.20	1.68	1.59
55	i	402	CDL	PB2-OB2	2.19	1.68	1.59
56	s	401	UQ	O4-C4	-2.19	1.18	1.23
55	l	701	CDL	PB2-OB2	2.19	1.68	1.59
55	i	402	CDL	PB2-OB5	2.18	1.68	1.59
50	X	201	8Q1	O35-C34	-2.17	1.19	1.23
48	r	501	PEE	O2-C10	2.16	1.40	1.34
49	j	201	PLX	P1-O4	2.16	1.68	1.59
47	A	503	NAI	C5B-C4B	2.16	1.58	1.51
50	G	201	8Q1	C6-C1	2.16	1.53	1.50
56	s	401	UQ	C7-C8	2.15	1.53	1.50
55	a	201	CDL	PB2-OB5	2.14	1.68	1.59
48	U	101	PEE	O3-C3	-2.12	1.40	1.45
51	J	401	NDP	PA-O5B	2.12	1.67	1.59
48	l	702	PEE	O3-C3	-2.11	1.40	1.45
48	Q	502	PEE	O3-C3	-2.11	1.40	1.45
49	r	502	PLX	P1-O4	2.10	1.67	1.59
51	J	401	NDP	O7N-C7N	-2.10	1.19	1.24
49	a	202	PLX	P1-O4	2.10	1.67	1.59
49	r	503	PLX	P1-O4	2.09	1.67	1.59
48	m	201	PEE	O3-C3	-2.09	1.40	1.45
49	C	303	PLX	P1-O4	2.09	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	C	302	PEE	O3-C3	-2.08	1.40	1.45
49	i	401	PLX	P1-O4	2.08	1.67	1.59
55	i	402	CDL	OB6-CB4	-2.08	1.41	1.46
55	l	701	CDL	PB2-OB5	2.08	1.67	1.59
48	r	501	PEE	O3-C3	-2.07	1.40	1.45
49	r	502	PLX	P1-O1	2.06	1.67	1.59
49	r	503	PLX	P1-O1	2.06	1.67	1.59
55	a	201	CDL	OB6-CB4	-2.05	1.41	1.46
48	l	703	PEE	O3-C3	-2.05	1.40	1.45
49	j	201	PLX	P1-O1	2.05	1.67	1.59
56	s	401	UQ	O1-C1	-2.04	1.18	1.23
48	Q	501	PEE	O3-C3	-2.02	1.40	1.45
49	a	202	PLX	P1-O1	2.02	1.67	1.59
55	l	701	CDL	C11-CA5	2.00	1.56	1.50
55	a	201	CDL	C11-CA5	2.00	1.56	1.50

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	s	401	UQ	C7-C8-C9	-9.34	111.24	126.79
51	J	401	NDP	C3N-C2N-N1N	-7.60	112.25	123.10
51	J	401	NDP	C1D-N1N-C2N	-6.47	110.34	121.11
50	G	201	8Q1	C6-C1-S44	5.90	120.33	113.46
47	A	503	NAI	C5A-C4A-N3A	-5.90	119.05	126.75
56	s	401	UQ	C12-C13-C14	-5.88	113.50	127.66
51	J	401	NDP	C5A-C4A-N3A	-5.85	119.12	126.75
50	X	201	8Q1	C6-C1-S44	5.83	120.24	113.46
57	w	401	ADP	C5-C4-N3	-5.78	119.21	126.75
51	J	401	NDP	C1D-N1N-C6N	-5.48	109.02	120.83
56	s	401	UQ	C11-C9-C8	-4.64	111.72	121.12
56	s	401	UQ	C10-C9-C8	-4.62	111.82	123.68
57	w	401	ADP	N3-C4-N9	4.46	134.43	127.08
57	w	401	ADP	N3-C2-N1	-4.42	121.69	128.60
47	A	503	NAI	N3A-C2A-N1A	-4.24	121.97	128.60
55	a	201	CDL	OA6-CA5-C11	4.22	120.60	111.50
55	a	201	CDL	OB6-CB5-C51	4.19	120.53	111.50
48	m	201	PEE	O2-C10-C11	4.17	120.49	111.50
55	i	402	CDL	OB6-CB5-C51	4.11	120.37	111.50
51	J	401	NDP	N3A-C4A-N9A	4.11	133.86	127.08
47	A	503	NAI	N3A-C4A-N9A	4.07	133.79	127.08
55	l	701	CDL	OA6-CA5-C11	4.04	120.22	111.50
48	r	501	PEE	O2-C10-C11	4.03	120.18	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	s	401	UQ	C15-C14-C13	-4.02	113.36	123.68
51	J	401	NDP	N3A-C2A-N1A	-4.00	122.35	128.60
48	Q	501	PEE	O2-C10-C11	3.99	120.09	111.50
56	s	401	UQ	C17-C18-C19	-3.98	114.14	127.75
48	C	302	PEE	O2-C10-C11	3.96	120.04	111.50
56	s	401	UQ	C16-C14-C13	-3.95	113.13	121.12
55	i	402	CDL	OA6-CA5-C11	3.94	119.99	111.50
47	A	503	NAI	C2A-N3A-C4A	3.87	120.89	111.75
48	U	101	PEE	O2-C10-C11	3.86	119.82	111.50
48	Q	502	PEE	O2-C10-C11	3.83	119.76	111.50
48	l	703	PEE	O2-C10-C11	3.79	119.67	111.50
47	A	503	NAI	C5A-N7A-C8A	3.76	108.85	103.51
57	w	401	ADP	C2-N3-C4	3.74	120.59	111.75
51	J	401	NDP	C2A-N3A-C4A	3.73	120.56	111.75
48	l	702	PEE	O2-C10-C11	3.71	119.49	111.50
55	l	701	CDL	OB6-CB5-C51	3.66	119.38	111.50
57	w	401	ADP	N9-C8-N7	-3.60	108.99	113.91
50	G	201	8Q1	C37-C38-C39	3.47	118.14	112.36
57	w	401	ADP	C5-N7-C8	3.45	108.41	103.51
50	X	201	8Q1	O4-C1-C6	-3.45	119.92	123.99
47	A	503	NAI	C3D-C2D-C1D	3.42	107.92	101.43
56	s	401	UQ	C21-C19-C18	-3.39	112.84	122.65
47	A	503	NAI	C4A-C5A-N7A	-3.35	106.54	110.62
50	G	201	8Q1	O4-C1-C6	-3.35	120.04	123.99
47	A	503	NAI	N9A-C8A-N7A	-3.34	109.35	113.91
51	J	401	NDP	C5A-N7A-C8A	3.28	108.17	103.51
51	J	401	NDP	N9A-C8A-N7A	-3.23	109.49	113.91
51	J	401	NDP	PN-O3-PA	-3.13	122.08	132.83
46	A	502	FMN	C4-N3-C2	-3.07	119.96	125.64
57	w	401	ADP	C4-N9-C8	3.07	109.05	105.73
51	J	401	NDP	C4A-C5A-N7A	-2.99	106.98	110.62
56	s	401	UQ	C20-C19-C18	-2.97	114.07	122.65
57	w	401	ADP	PA-O3A-PB	-2.94	122.74	132.83
57	w	401	ADP	C4-C5-N7	-2.82	107.19	110.62
56	s	401	UQ	CM5-C5-C6	-2.78	119.86	124.40
48	r	501	PEE	O3-C30-C31	2.73	120.48	111.91
47	A	503	NAI	PN-O3-PA	-2.72	123.49	132.83
47	A	503	NAI	C2D-C3D-C4D	2.72	107.92	102.64
46	A	502	FMN	C4A-C4-N3	2.67	119.98	113.19
48	l	702	PEE	O3-C30-C31	2.67	120.30	111.91
55	a	201	CDL	OB8-CB7-C71	2.65	120.22	111.91
51	J	401	NDP	C2B-C3B-C4B	2.64	107.73	101.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	m	201	PEE	O3-C30-C31	2.62	120.13	111.91
48	C	302	PEE	O3-C30-C31	2.61	120.11	111.91
48	l	703	PEE	O3-C30-C31	2.60	120.07	111.91
48	Q	501	PEE	O3-C30-C31	2.58	120.01	111.91
46	A	502	FMN	O4-C4-C4A	-2.58	119.76	126.60
55	l	701	CDL	OB8-CB7-C71	2.57	119.98	111.91
48	Q	502	PEE	O3-C30-C31	2.56	119.95	111.91
55	i	402	CDL	OA8-CA7-C31	2.55	119.91	111.91
55	i	402	CDL	OB8-CB7-C71	2.49	119.73	111.91
51	J	401	NDP	C4B-O4B-C1B	-2.49	103.97	109.47
47	A	503	NAI	C4D-O4D-C1D	-2.49	103.99	109.47
48	U	101	PEE	O3-C30-C31	2.48	119.68	111.91
55	a	201	CDL	OA8-CA7-C31	2.46	119.61	111.91
55	l	701	CDL	OA8-CA7-C31	2.45	119.60	111.91
49	r	502	PLX	C1A-N1-C1	2.41	119.78	109.92
49	i	401	PLX	C1A-N1-C1	2.41	119.78	109.92
51	J	401	NDP	C4A-N9A-C8A	2.41	108.33	105.73
49	j	201	PLX	C1A-N1-C1	2.38	119.64	109.92
49	a	202	PLX	C1A-N1-C1	2.37	119.61	109.92
46	A	502	FMN	C4A-C10-N10	2.33	119.88	116.48
49	r	503	PLX	C1A-N1-C1	2.31	119.37	109.92
50	X	201	8Q1	C37-C38-C39	2.30	116.19	112.36
50	G	201	8Q1	O4-C1-S44	-2.29	119.63	122.61
50	X	201	8Q1	C38-C39-N41	2.29	120.28	116.42
46	A	502	FMN	C9A-C5A-N5	-2.25	119.99	122.43
50	G	201	8Q1	C38-C39-N41	2.23	120.18	116.42
51	J	401	NDP	C2B-C1B-N9A	-2.20	109.83	113.53
49	C	303	PLX	C1A-N1-C1	2.19	118.89	109.92
47	A	503	NAI	C4A-N9A-C8A	2.19	108.10	105.73
50	X	201	8Q1	C43-S44-C1	2.18	108.65	101.87
46	A	502	FMN	C5A-C9A-N10	2.18	120.20	117.95
57	w	401	ADP	C4'-O4'-C1'	-2.15	104.72	109.47
46	A	502	FMN	C10-C4A-N5	-2.14	120.31	124.86
50	X	201	8Q1	O4-C1-S44	-2.14	119.84	122.61
46	A	502	FMN	C4A-C10-N1	-2.10	119.85	124.73
50	G	201	8Q1	C43-S44-C1	2.05	108.26	101.87
57	w	401	ADP	C2'-C3'-C4'	2.02	106.58	102.64
51	J	401	NDP	O4B-C1B-C2B	-2.01	103.04	106.57

There are no chirality outliers.

All (581) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
47	A	503	NAI	C5B-O5B-PA-O1A
48	C	302	PEE	C1-O3P-P-O2P
48	C	302	PEE	C1-O3P-P-O1P
48	Q	501	PEE	C11-C10-O2-C2
48	Q	501	PEE	C4-O4P-P-O1P
48	Q	502	PEE	C1-O3P-P-O1P
48	U	101	PEE	C17-C18-C19-C20
48	U	101	PEE	C1-O3P-P-O2P
48	U	101	PEE	C1-O3P-P-O1P
48	U	101	PEE	C1-O3P-P-O4P
48	l	702	PEE	C11-C10-O2-C2
48	l	702	PEE	O4-C10-O2-C2
48	l	702	PEE	C4-O4P-P-O3P
48	l	702	PEE	C4-O4P-P-O2P
48	l	702	PEE	C4-O4P-P-O1P
48	l	703	PEE	C37-C38-C39-C40
48	m	201	PEE	C11-C10-O2-C2
48	m	201	PEE	O4-C10-O2-C2
48	m	201	PEE	C4-O4P-P-O3P
48	m	201	PEE	C4-O4P-P-O2P
48	m	201	PEE	C4-O4P-P-O1P
48	m	201	PEE	O4P-C4-C5-N
48	r	501	PEE	C1-O3P-P-O2P
48	r	501	PEE	C1-O3P-P-O1P
48	r	501	PEE	C1-O3P-P-O4P
49	C	303	PLX	C3-C4-O6-C6
49	C	303	PLX	C3-O4-P1-O1
49	C	303	PLX	N1-C1-C2-O1
49	a	202	PLX	O7-C6-C7-C8
49	i	401	PLX	O7-C6-O6-C4
49	j	201	PLX	O7-C6-C7-C8
49	r	502	PLX	O7-C6-O6-C4
49	r	502	PLX	C5-C4-O6-C6
49	r	502	PLX	O9-C24-O8-C5
49	r	502	PLX	O9-C24-C25-C26
49	r	503	PLX	O9-C24-O8-C5
49	r	503	PLX	O9-C24-C25-C26
50	G	201	8Q1	O4-C1-S44-C43
50	G	201	8Q1	C6-C1-S44-C43
50	G	201	8Q1	O27-C28-C29-C31
50	G	201	8Q1	O27-C28-C29-C32

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Mol	Chain	Res	Type	Atoms
50	G	201	8Q1	C28-C29-C32-C34
50	G	201	8Q1	C28-C29-C32-O33
50	G	201	8Q1	N41-C42-C43-S44
50	X	201	8Q1	C1-C6-C7-C8
50	X	201	8Q1	O4-C1-S44-C43
50	X	201	8Q1	C6-C1-S44-C43
50	X	201	8Q1	O27-C28-C29-C31
50	X	201	8Q1	O27-C28-C29-C32
50	X	201	8Q1	C28-C29-C32-C34
50	X	201	8Q1	C28-C29-C32-O33
50	X	201	8Q1	C30-C29-C32-C34
50	X	201	8Q1	C30-C29-C32-O33
50	X	201	8Q1	C31-C29-C32-C34
50	X	201	8Q1	C31-C29-C32-O33
50	X	201	8Q1	N36-C37-C38-C39
50	X	201	8Q1	C42-C43-S44-C1
50	X	201	8Q1	C28-O27-P24-O2
50	X	201	8Q1	C28-O27-P24-O1
51	J	401	NDP	C5B-O5B-PA-O1A
51	J	401	NDP	C5B-O5B-PA-O3
51	J	401	NDP	O4B-C4B-C5B-O5B
51	J	401	NDP	C2B-O2B-P2B-O3X
51	J	401	NDP	C2N-C3N-C7N-N7N
55	a	201	CDL	CA2-OA2-PA1-OA4
55	a	201	CDL	CB3-OB5-PB2-OB2
55	a	201	CDL	CB3-OB5-PB2-OB3
55	i	402	CDL	CA2-OA2-PA1-OA3
55	i	402	CDL	CA2-OA2-PA1-OA4
55	i	402	CDL	CA3-OA5-PA1-OA2
55	i	402	CDL	CA3-OA5-PA1-OA3
55	i	402	CDL	CA3-OA5-PA1-OA4
55	i	402	CDL	CB3-OB5-PB2-OB4
55	l	701	CDL	CA2-OA2-PA1-OA3
55	l	701	CDL	CA2-OA2-PA1-OA4
55	l	701	CDL	CA2-OA2-PA1-OA5
55	l	701	CDL	CB2-OB2-PB2-OB3
55	l	701	CDL	CB2-OB2-PB2-OB4
56	s	401	UQ	C7-C8-C9-C11
56	s	401	UQ	C12-C11-C9-C10
56	s	401	UQ	C12-C13-C14-C16
56	s	401	UQ	C13-C14-C16-C17
56	s	401	UQ	C14-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
56	s	401	UQ	C17-C18-C19-C21
57	w	401	ADP	C5'-O5'-PA-O2A
57	w	401	ADP	C5'-O5'-PA-O3A
48	l	703	PEE	C31-C30-O3-C3
48	Q	502	PEE	C37-C38-C39-C40
48	r	501	PEE	C17-C18-C19-C20
56	s	401	UQ	C7-C8-C9-C10
48	Q	501	PEE	O4-C10-O2-C2
55	l	701	CDL	C59-C60-C61-C62
48	l	702	PEE	C31-C30-O3-C3
48	m	201	PEE	C31-C30-O3-C3
55	i	402	CDL	C71-CB7-OB8-CB6
48	l	703	PEE	O5-C30-O3-C3
51	J	401	NDP	C2D-C1D-N1N-C6N
49	r	502	PLX	C9-C10-C11-C12
49	a	202	PLX	C33-C34-C35-C36
49	i	401	PLX	C7-C8-C9-C10
49	r	503	PLX	C12-C13-C14-C15
49	j	201	PLX	C28-C29-C30-C31
48	l	702	PEE	O5-C30-O3-C3
48	m	201	PEE	O5-C30-O3-C3
55	i	402	CDL	OB9-CB7-OB8-CB6
56	s	401	UQ	C9-C11-C12-C13
48	Q	502	PEE	C12-C13-C14-C15
55	a	201	CDL	C34-C35-C36-C37
55	i	402	CDL	CB2-C1-CA2-OA2
49	r	502	PLX	C30-C31-C32-C33
48	U	101	PEE	C31-C30-O3-C3
55	a	201	CDL	C71-CB7-OB8-CB6
55	l	701	CDL	C71-CB7-OB8-CB6
49	i	401	PLX	C31-C32-C33-C34
55	i	402	CDL	C78-C79-C80-C81
55	l	701	CDL	C35-C36-C37-C38
55	i	402	CDL	OA6-CA4-CA6-OA8
49	j	201	PLX	C34-C35-C36-C37
49	r	502	PLX	C11-C12-C13-C14
49	j	201	PLX	C15-C16-C17-C18
55	i	402	CDL	C74-C75-C76-C77
49	C	303	PLX	C28-C29-C30-C31
48	r	501	PEE	C10-C11-C12-C13
48	U	101	PEE	C34-C35-C36-C37
48	U	101	PEE	O5-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	CA7-C31-C32-C33
55	i	402	CDL	CB7-C71-C72-C73
51	J	401	NDP	C3B-C4B-C5B-O5B
55	l	701	CDL	C11-C12-C13-C14
55	a	201	CDL	OB9-CB7-OB8-CB6
55	l	701	CDL	C39-C40-C41-C42
55	l	701	CDL	OB9-CB7-OB8-CB6
55	i	402	CDL	O1-C1-CA2-OA2
48	C	302	PEE	C1-O3P-P-O4P
49	r	502	PLX	C3-O4-P1-O1
49	r	503	PLX	C3-O4-P1-O1
49	r	503	PLX	C2-O1-P1-O4
55	a	201	CDL	CA2-OA2-PA1-OA5
55	a	201	CDL	CA3-OA5-PA1-OA2
55	i	402	CDL	CA2-OA2-PA1-OA5
55	i	402	CDL	CB2-OB2-PB2-OB5
55	i	402	CDL	CB3-OB5-PB2-OB2
55	l	701	CDL	CA3-OA5-PA1-OA2
55	l	701	CDL	CB2-OB2-PB2-OB5
55	l	701	CDL	CB3-OB5-PB2-OB2
55	i	402	CDL	CB5-C51-C52-C53
49	C	303	PLX	O6-C6-C7-C8
55	l	701	CDL	C51-C52-C53-C54
48	U	101	PEE	C40-C41-C42-C43
55	i	402	CDL	C51-CB5-OB6-CB4
49	a	202	PLX	C28-C29-C30-C31
49	r	503	PLX	C33-C34-C35-C36
55	a	201	CDL	C73-C74-C75-C76
50	G	201	8Q1	O27-C28-C29-C30
50	X	201	8Q1	O27-C28-C29-C30
48	Q	502	PEE	C14-C15-C16-C17
49	C	303	PLX	C17-C18-C19-C20
49	i	401	PLX	C10-C11-C12-C13
49	r	503	PLX	C13-C14-C15-C16
55	l	701	CDL	C75-C76-C77-C78
55	i	402	CDL	OB7-CB5-OB6-CB4
49	i	401	PLX	C11-C10-C9-C8
49	r	502	PLX	C27-C28-C29-C30
55	l	701	CDL	C52-C53-C54-C55
48	Q	501	PEE	C17-C18-C19-C20
48	l	703	PEE	C33-C34-C35-C36
49	a	202	PLX	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
49	i	401	PLX	C27-C28-C29-C30
49	j	201	PLX	C7-C8-C9-C10
55	a	201	CDL	C35-C36-C37-C38
55	i	402	CDL	C17-C18-C19-C20
48	r	501	PEE	C31-C32-C33-C34
49	a	202	PLX	C10-C11-C12-C13
49	i	401	PLX	C25-C26-C27-C28
55	l	701	CDL	C37-C38-C39-C40
55	a	201	CDL	CB5-C51-C52-C53
48	Q	502	PEE	C34-C35-C36-C37
49	r	503	PLX	C14-C15-C16-C17
50	G	201	8Q1	C7-C8-C9-C10
55	i	402	CDL	C73-C74-C75-C76
55	l	701	CDL	C73-C74-C75-C76
55	i	402	CDL	CA7-C31-C32-C33
48	Q	502	PEE	C33-C34-C35-C36
49	C	303	PLX	C14-C15-C16-C17
49	a	202	PLX	C14-C15-C16-C17
49	i	401	PLX	C9-C10-C11-C12
49	i	401	PLX	C32-C33-C34-C35
49	i	401	PLX	C33-C34-C35-C36
49	r	502	PLX	C7-C8-C9-C10
55	a	201	CDL	C17-C18-C19-C20
55	a	201	CDL	C75-C76-C77-C78
55	i	402	CDL	C71-C72-C73-C74
55	i	402	CDL	C75-C76-C77-C78
48	r	501	PEE	C11-C10-O2-C2
48	m	201	PEE	C11-C12-C13-C14
49	i	401	PLX	C30-C31-C32-C33
49	j	201	PLX	C10-C11-C12-C13
49	r	503	PLX	C25-C26-C27-C28
55	i	402	CDL	C55-C56-C57-C58
48	Q	501	PEE	C35-C36-C37-C38
48	C	302	PEE	C42-C43-C44-C45
48	Q	501	PEE	C22-C23-C24-C25
48	l	703	PEE	C12-C13-C14-C15
48	r	501	PEE	C12-C13-C14-C15
49	a	202	PLX	C7-C8-C9-C10
49	a	202	PLX	C29-C30-C31-C32
49	i	401	PLX	C28-C29-C30-C31
49	r	503	PLX	C28-C29-C30-C31
50	X	201	8Q1	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
55	l	701	CDL	C40-C41-C42-C43
48	Q	501	PEE	C21-C22-C23-C24
49	C	303	PLX	C16-C17-C18-C19
55	a	201	CDL	C11-C12-C13-C14
49	j	201	PLX	C27-C28-C29-C30
48	Q	502	PEE	C30-C31-C32-C33
55	l	701	CDL	CB7-C71-C72-C73
48	U	101	PEE	C21-C22-C23-C24
55	i	402	CDL	C56-C57-C58-C59
55	l	701	CDL	CB3-CB4-CB6-OB8
48	r	501	PEE	O4-C10-O2-C2
48	C	302	PEE	C37-C38-C39-C40
49	C	303	PLX	C9-C10-C11-C12
49	i	401	PLX	C14-C15-C16-C17
49	r	503	PLX	C11-C12-C13-C14
55	a	201	CDL	C21-C22-C23-C24
55	a	201	CDL	C37-C38-C39-C40
48	C	302	PEE	C11-C10-O2-C2
48	U	101	PEE	C11-C10-O2-C2
49	C	303	PLX	O7-C6-C7-C8
49	C	303	PLX	C13-C14-C15-C16
49	C	303	PLX	C25-C26-C27-C28
49	r	503	PLX	C27-C28-C29-C30
55	a	201	CDL	C31-C32-C33-C34
55	i	402	CDL	C43-C44-C45-C46
49	j	201	PLX	C25-C26-C27-C28
55	a	201	CDL	C52-C53-C54-C55
49	r	503	PLX	C29-C30-C31-C32
48	C	302	PEE	O4-C10-O2-C2
48	U	101	PEE	O4-C10-O2-C2
49	a	202	PLX	C25-C26-C27-C28
49	r	502	PLX	C28-C29-C30-C31
48	l	702	PEE	C31-C32-C33-C34
48	l	703	PEE	C31-C32-C33-C34
49	r	503	PLX	C2-C1-N1-C1A
48	Q	501	PEE	C10-C11-C12-C13
55	i	402	CDL	C59-C60-C61-C62
49	C	303	PLX	C7-C8-C9-C10
49	C	303	PLX	C33-C34-C35-C36
49	r	503	PLX	C10-C11-C12-C13
48	l	702	PEE	C30-C31-C32-C33
49	j	201	PLX	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
49	r	502	PLX	C16-C17-C18-C19
49	r	503	PLX	C31-C32-C33-C34
55	i	402	CDL	C62-C63-C64-C65
55	l	701	CDL	C58-C59-C60-C61
49	a	202	PLX	C9-C10-C11-C12
49	j	201	PLX	C35-C36-C37-C38
48	r	501	PEE	C20-C21-C22-C23
55	a	201	CDL	C32-C33-C34-C35
55	i	402	CDL	C41-C42-C43-C44
55	l	701	CDL	C32-C33-C34-C35
55	l	701	CDL	C55-C56-C57-C58
48	Q	502	PEE	C42-C43-C44-C45
48	l	702	PEE	C23-C24-C25-C26
49	a	202	PLX	C11-C10-C9-C8
55	l	701	CDL	C51-CB5-OB6-CB4
48	l	702	PEE	O3P-C1-C2-O2
55	l	701	CDL	C60-C61-C62-C63
48	C	302	PEE	C13-C14-C15-C16
49	C	303	PLX	C27-C28-C29-C30
55	a	201	CDL	C33-C34-C35-C36
55	l	701	CDL	OB7-CB5-OB6-CB4
50	G	201	8Q1	C11-C12-C13-C14
48	U	101	PEE	O2-C2-C3-O3
55	l	701	CDL	OA6-CA4-CA6-OA8
55	l	701	CDL	OB6-CB4-CB6-OB8
49	r	503	PLX	C30-C31-C32-C33
49	r	503	PLX	C2-C1-N1-C1C
48	r	501	PEE	C40-C41-C42-C43
49	j	201	PLX	C13-C14-C15-C16
48	Q	501	PEE	C19-C20-C21-C22
48	Q	502	PEE	C19-C20-C21-C22
48	Q	502	PEE	C20-C21-C22-C23
48	U	101	PEE	C36-C37-C38-C39
48	l	702	PEE	C14-C15-C16-C17
49	r	502	PLX	C33-C34-C35-C36
55	i	402	CDL	C14-C15-C16-C17
48	Q	502	PEE	C31-C30-O3-C3
55	i	402	CDL	C60-C61-C62-C63
49	a	202	PLX	C30-C31-C32-C33
49	r	503	PLX	C18-C19-C20-C21
48	r	501	PEE	C36-C37-C38-C39
49	a	202	PLX	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
49	j	201	PLX	C33-C34-C35-C36
55	i	402	CDL	C52-C53-C54-C55
48	C	302	PEE	C11-C12-C13-C14
49	j	201	PLX	C3-C4-C5-O8
49	r	502	PLX	C3-C4-C5-O8
55	i	402	CDL	CA3-CA4-CA6-OA8
55	i	402	CDL	CB3-CB4-CB6-OB8
49	r	502	PLX	C12-C13-C14-C15
55	l	701	CDL	C64-C65-C66-C67
49	r	502	PLX	C18-C19-C20-C21
55	i	402	CDL	C84-C85-C86-C87
50	G	201	8Q1	C12-C13-C14-C15
55	l	701	CDL	C56-C57-C58-C59
48	C	302	PEE	C15-C16-C17-C18
48	Q	501	PEE	C15-C16-C17-C18
49	i	401	PLX	C13-C14-C15-C16
50	G	201	8Q1	C6-C7-C8-C9
55	a	201	CDL	C71-C72-C73-C74
50	G	201	8Q1	C28-O27-P24-O3
50	X	201	8Q1	C28-O27-P24-O3
55	a	201	CDL	OA5-CA3-CA4-OA6
49	r	503	PLX	C2-C1-N1-C1B
55	i	402	CDL	C13-C14-C15-C16
55	i	402	CDL	C23-C24-C25-C26
48	C	302	PEE	O2-C2-C3-O3
55	i	402	CDL	OB6-CB4-CB6-OB8
48	Q	501	PEE	C31-C32-C33-C34
48	Q	502	PEE	C21-C22-C23-C24
48	Q	502	PEE	O5-C30-O3-C3
49	r	502	PLX	C14-C15-C16-C17
55	i	402	CDL	C35-C36-C37-C38
48	Q	502	PEE	C17-C18-C19-C20
48	l	703	PEE	C17-C18-C19-C20
55	l	701	CDL	C77-C78-C79-C80
48	l	702	PEE	O3P-C1-C2-C3
55	l	701	CDL	OA5-CA3-CA4-CA6
49	r	502	PLX	C31-C32-C33-C34
48	r	501	PEE	O4P-C4-C5-N
49	j	201	PLX	C9-C10-C11-C12
49	j	201	PLX	C14-C15-C16-C17
49	j	201	PLX	C31-C32-C33-C34
55	i	402	CDL	C82-C83-C84-C85

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Mol	Chain	Res	Type	Atoms
48	m	201	PEE	C24-C25-C26-C27
55	i	402	CDL	C64-C65-C66-C67
48	l	702	PEE	C11-C12-C13-C14
55	i	402	CDL	C31-CA7-OA8-CA6
48	l	702	PEE	C32-C33-C34-C35
48	C	302	PEE	C1-C2-C3-O3
48	Q	501	PEE	C1-C2-C3-O3
48	U	101	PEE	C1-C2-C3-O3
49	i	401	PLX	C3-C4-C5-O8
55	l	701	CDL	CA3-CA4-CA6-OA8
49	r	502	PLX	C13-C14-C15-C16
50	X	201	8Q1	C10-C11-C12-C13
49	C	303	PLX	C11-C12-C13-C14
49	C	303	PLX	C30-C31-C32-C33
48	Q	501	PEE	C32-C33-C34-C35
49	r	502	PLX	C15-C16-C17-C18
49	i	401	PLX	O9-C24-C25-C26
49	r	503	PLX	C7-C8-C9-C10
55	i	402	CDL	C42-C43-C44-C45
48	C	302	PEE	C39-C40-C41-C42
49	r	502	PLX	C32-C33-C34-C35
49	i	401	PLX	C19-C20-C21-C22
49	j	201	PLX	C30-C31-C32-C33
49	r	503	PLX	C15-C16-C17-C18
48	r	501	PEE	C38-C39-C40-C41
49	j	201	PLX	C18-C19-C20-C21
48	Q	502	PEE	O3P-C1-C2-C3
49	j	201	PLX	O4-C3-C4-C5
55	a	201	CDL	OA5-CA3-CA4-CA6
48	m	201	PEE	O3-C30-C31-C32
49	r	502	PLX	C29-C30-C31-C32
50	G	201	8Q1	C1-C6-C7-C8
49	C	303	PLX	C31-C32-C33-C34
49	i	401	PLX	C12-C13-C14-C15
55	l	701	CDL	C62-C63-C64-C65
50	X	201	8Q1	C7-C8-C9-C10
48	m	201	PEE	C3-C2-O2-C10
55	i	402	CDL	C20-C21-C22-C23
49	r	503	PLX	C26-C27-C28-C29
48	Q	501	PEE	C30-C31-C32-C33
48	r	501	PEE	C1-C2-C3-O3
49	r	503	PLX	C3-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
55	i	402	CDL	CB4-CB3-OB5-PB2
48	Q	502	PEE	O3P-C1-C2-O2
49	j	201	PLX	O4-C3-C4-O6
55	l	701	CDL	OA5-CA3-CA4-OA6
50	G	201	8Q1	C31-C29-C32-C34
55	i	402	CDL	OA9-CA7-OA8-CA6
49	i	401	PLX	C17-C18-C19-C20
48	Q	501	PEE	O2-C2-C3-O3
49	j	201	PLX	O6-C4-C5-O8
49	r	503	PLX	O6-C4-C5-O8
48	U	101	PEE	C23-C24-C25-C26
55	a	201	CDL	C54-C55-C56-C57
55	i	402	CDL	CA5-C11-C12-C13
47	A	503	NAI	C5B-O5B-PA-O3
49	i	401	PLX	C35-C36-C37-C38
48	r	501	PEE	C41-C42-C43-C44
48	Q	501	PEE	C23-C24-C25-C26
49	C	303	PLX	C11-C10-C9-C8
48	U	101	PEE	C41-C42-C43-C44
48	l	702	PEE	C24-C25-C26-C27
48	l	703	PEE	C21-C22-C23-C24
55	l	701	CDL	O1-C1-CB2-OB2
46	A	502	FMN	C3'-C4'-C5'-O5'
48	m	201	PEE	C1-O3P-P-O1P
48	r	501	PEE	C4-O4P-P-O1P
49	C	303	PLX	C3-O4-P1-O3
49	r	502	PLX	C3-O4-P1-O2
49	r	502	PLX	C3-O4-P1-O3
49	r	502	PLX	C2-O1-P1-O3
49	r	503	PLX	C3-O4-P1-O2
49	r	503	PLX	C2-O1-P1-O2
49	r	503	PLX	C2-O1-P1-O3
51	J	401	NDP	C5B-O5B-PA-O2A
55	a	201	CDL	CA2-OA2-PA1-OA3
55	a	201	CDL	CA3-OA5-PA1-OA4
55	a	201	CDL	CB2-OB2-PB2-OB4
55	i	402	CDL	CB2-OB2-PB2-OB3
55	i	402	CDL	CB2-OB2-PB2-OB4
55	i	402	CDL	CB3-OB5-PB2-OB3
55	l	701	CDL	CA3-OA5-PA1-OA4
55	l	701	CDL	CB3-OB5-PB2-OB3
55	l	701	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
57	w	401	ADP	C5'-O5'-PA-O1A
49	i	401	PLX	O4-C3-C4-C5
55	a	201	CDL	C55-C56-C57-C58
50	G	201	8Q1	C11-C10-C9-C8
55	i	402	CDL	C81-C82-C83-C84
48	r	501	PEE	C24-C25-C26-C27
49	j	201	PLX	C25-C24-O8-C5
48	U	101	PEE	C19-C20-C21-C22
55	i	402	CDL	C31-C32-C33-C34
49	i	401	PLX	O4-C3-C4-O6
48	U	101	PEE	C38-C39-C40-C41
55	l	701	CDL	C76-C77-C78-C79
55	l	701	CDL	C14-C15-C16-C17
51	J	401	NDP	C2N-C3N-C7N-O7N
55	a	201	CDL	CB3-CB4-CB6-OB8
48	l	702	PEE	O2-C2-C3-O3
48	r	501	PEE	O2-C2-C3-O3
49	i	401	PLX	O6-C4-C5-O8
55	a	201	CDL	OB6-CB4-CB6-OB8
48	U	101	PEE	C37-C38-C39-C40
49	a	202	PLX	C27-C28-C29-C30
49	j	201	PLX	C26-C27-C28-C29
48	r	501	PEE	C31-C30-O3-C3
48	l	702	PEE	C34-C35-C36-C37
49	C	303	PLX	O8-C24-C25-C26
49	a	202	PLX	O6-C6-C7-C8
49	r	503	PLX	O8-C24-C25-C26
48	l	703	PEE	C18-C19-C20-C21
48	l	703	PEE	C16-C17-C18-C19
49	C	303	PLX	O9-C24-C25-C26
48	l	703	PEE	C14-C15-C16-C17
49	C	303	PLX	C15-C16-C17-C18
48	l	702	PEE	C19-C20-C21-C22
48	Q	501	PEE	C13-C14-C15-C16
48	l	702	PEE	C13-C14-C15-C16
49	r	502	PLX	C20-C21-C22-C23
55	l	701	CDL	C44-C45-C46-C47
49	r	503	PLX	C9-C10-C11-C12
48	r	501	PEE	O5-C30-O3-C3
48	Q	501	PEE	C14-C15-C16-C17
55	l	701	CDL	C72-C73-C74-C75
48	l	703	PEE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
55	l	701	CDL	C33-C34-C35-C36
48	l	703	PEE	C11-C12-C13-C14
55	l	701	CDL	C15-C16-C17-C18
48	C	302	PEE	C41-C42-C43-C44
49	r	502	PLX	O6-C4-C5-O8
49	a	202	PLX	C2-O1-P1-O4
49	i	401	PLX	C3-O4-P1-O1
55	a	201	CDL	CB2-OB2-PB2-OB5
48	Q	502	PEE	C10-C11-C12-C13
49	a	202	PLX	C16-C17-C18-C19
50	G	201	8Q1	C30-C29-C32-O33
50	G	201	8Q1	C31-C29-C32-O33
48	l	702	PEE	C1-C2-C3-O3
48	l	703	PEE	C1-C2-C3-O3
47	A	503	NAI	O4D-C1D-N1N-C2N
55	l	701	CDL	C12-C13-C14-C15
48	Q	501	PEE	C2-C1-O3P-P
49	j	201	PLX	C11-C12-C13-C14
55	i	402	CDL	C39-C40-C41-C42
48	Q	502	PEE	C39-C40-C41-C42
48	r	501	PEE	C39-C40-C41-C42
47	A	503	NAI	C2D-C1D-N1N-C2N
49	C	303	PLX	O4-C3-C4-O6
48	l	703	PEE	C15-C16-C17-C18
48	r	501	PEE	C34-C35-C36-C37
49	a	202	PLX	C19-C20-C21-C22
49	i	401	PLX	O8-C24-C25-C26
49	r	502	PLX	O8-C24-C25-C26
48	Q	501	PEE	C18-C19-C20-C21
48	l	702	PEE	C38-C39-C40-C41
48	l	703	PEE	O4-C10-O2-C2
55	a	201	CDL	C60-C61-C62-C63
55	i	402	CDL	C72-C73-C74-C75
48	l	702	PEE	C1-C2-O2-C10
48	l	702	PEE	C3-C2-O2-C10
48	r	501	PEE	C4-O4P-P-O3P
49	r	502	PLX	C2-O1-P1-O4
55	i	402	CDL	C44-C45-C46-C47
48	Q	501	PEE	C38-C39-C40-C41
48	m	201	PEE	C16-C17-C18-C19
55	a	201	CDL	C59-C60-C61-C62
50	G	201	8Q1	C42-C43-S44-C1

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Mol	Chain	Res	Type	Atoms
48	l	703	PEE	O2-C2-C3-O3
49	r	503	PLX	C16-C17-C18-C19
49	i	401	PLX	C36-C37-C38-C39
55	a	201	CDL	C41-C42-C43-C44
57	w	401	ADP	PB-O3A-PA-O1A
55	l	701	CDL	C31-C32-C33-C34
55	a	201	CDL	C36-C37-C38-C39
49	a	202	PLX	C13-C14-C15-C16
55	a	201	CDL	C76-C77-C78-C79
55	a	201	CDL	C74-C75-C76-C77
55	l	701	CDL	C71-C72-C73-C74
50	X	201	8Q1	C13-C14-C15-C16
48	m	201	PEE	C13-C14-C15-C16
48	l	703	PEE	O4P-C4-C5-N
55	i	402	CDL	C33-C34-C35-C36
48	Q	502	PEE	C15-C16-C17-C18
48	m	201	PEE	C18-C19-C20-C21
48	U	101	PEE	O3-C30-C31-C32
56	s	401	UQ	C12-C11-C9-C8
48	l	702	PEE	C10-C11-C12-C13
48	U	101	PEE	C22-C23-C24-C25
48	l	702	PEE	C20-C21-C22-C23
49	a	202	PLX	C6-C7-C8-C9
55	l	701	CDL	C52-C51-CB5-OB6
48	r	501	PEE	C18-C19-C20-C21
48	m	201	PEE	C10-C11-C12-C13
55	a	201	CDL	C22-C23-C24-C25
48	C	302	PEE	O3-C30-C31-C32
48	l	702	PEE	C35-C36-C37-C38
49	j	201	PLX	C7-C6-O6-C4
55	i	402	CDL	C32-C33-C34-C35
48	C	302	PEE	C18-C19-C20-C21
48	U	101	PEE	C16-C17-C18-C19
55	a	201	CDL	C43-C44-C45-C46
48	l	703	PEE	C11-C10-O2-C2
48	Q	501	PEE	C24-C25-C26-C27
49	r	503	PLX	C36-C37-C38-C39
48	Q	501	PEE	C36-C37-C38-C39
48	l	703	PEE	C38-C39-C40-C41
49	j	201	PLX	C32-C33-C34-C35
48	U	101	PEE	O2-C10-C11-C12
55	i	402	CDL	C83-C84-C85-C86

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Mol	Chain	Res	Type	Atoms
48	l	703	PEE	O3-C30-C31-C32
48	C	302	PEE	C38-C39-C40-C41
48	l	702	PEE	C16-C17-C18-C19
47	A	503	NAI	C3D-C4D-C5D-O5D
48	C	302	PEE	O5-C30-C31-C32
55	i	402	CDL	C37-C38-C39-C40
48	U	101	PEE	O5-C30-C31-C32
50	G	201	8Q1	C9-C10-C11-C12
48	U	101	PEE	C31-C32-C33-C34
48	Q	501	PEE	C4-O4P-P-O3P
49	r	502	PLX	C4-C3-O4-P1
48	l	703	PEE	O5-C30-C31-C32
49	r	502	PLX	C26-C27-C28-C29
48	Q	501	PEE	C1-O3P-P-O1P
48	l	703	PEE	C1-O3P-P-O1P
49	i	401	PLX	C3-O4-P1-O2
55	l	701	CDL	C34-C35-C36-C37
49	C	303	PLX	C24-C25-C26-C27
48	U	101	PEE	O4-C10-C11-C12
48	m	201	PEE	O5-C30-C31-C32
55	i	402	CDL	C76-C77-C78-C79
48	l	703	PEE	C5-C4-O4P-P
49	r	502	PLX	C25-C24-O8-C5
48	C	302	PEE	C43-C44-C45-C46
47	A	503	NAI	C2D-C1D-N1N-C6N
48	l	703	PEE	C39-C40-C41-C42
49	r	502	PLX	C25-C26-C27-C28
55	i	402	CDL	C72-C71-CB7-OB8
55	l	701	CDL	C32-C31-CA7-OA8
46	A	502	FMN	O2'-C2'-C3'-C4'
48	C	302	PEE	C32-C33-C34-C35
49	r	503	PLX	C24-C25-C26-C27
55	l	701	CDL	C32-C31-CA7-OA9
55	a	201	CDL	C12-C11-CA5-OA6

There are no ring outliers.

25 monomers are involved in 88 short contacts:

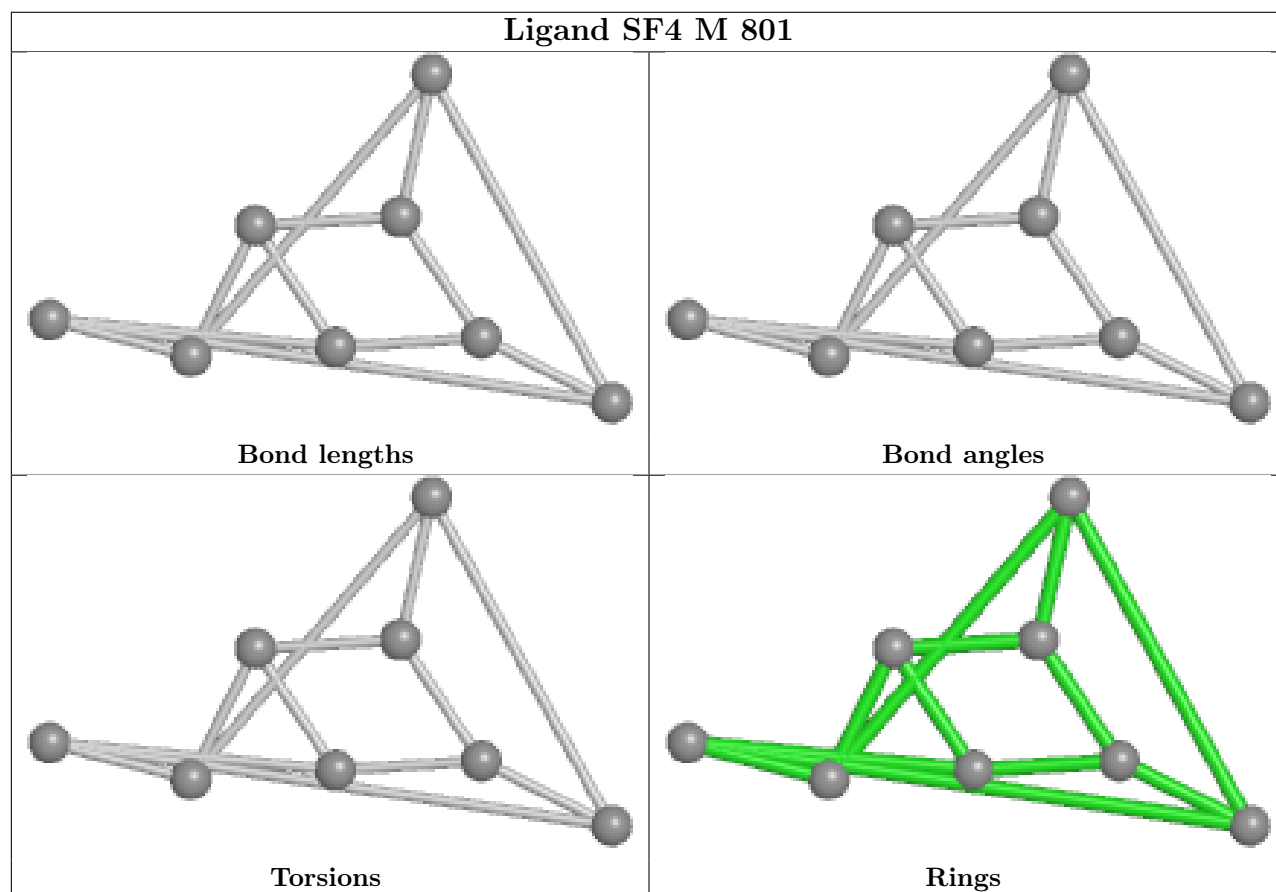
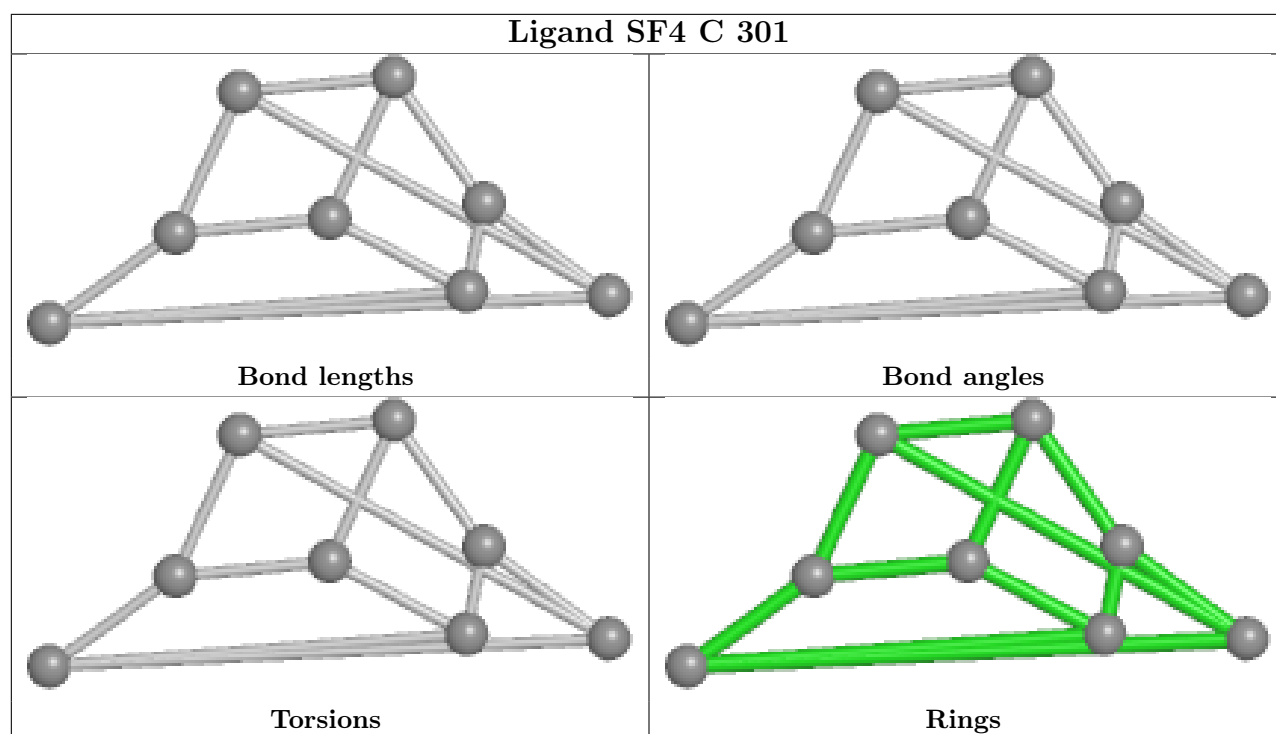
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	C	301	SF4	1	0
48	l	703	PEE	3	0
48	m	201	PEE	3	0

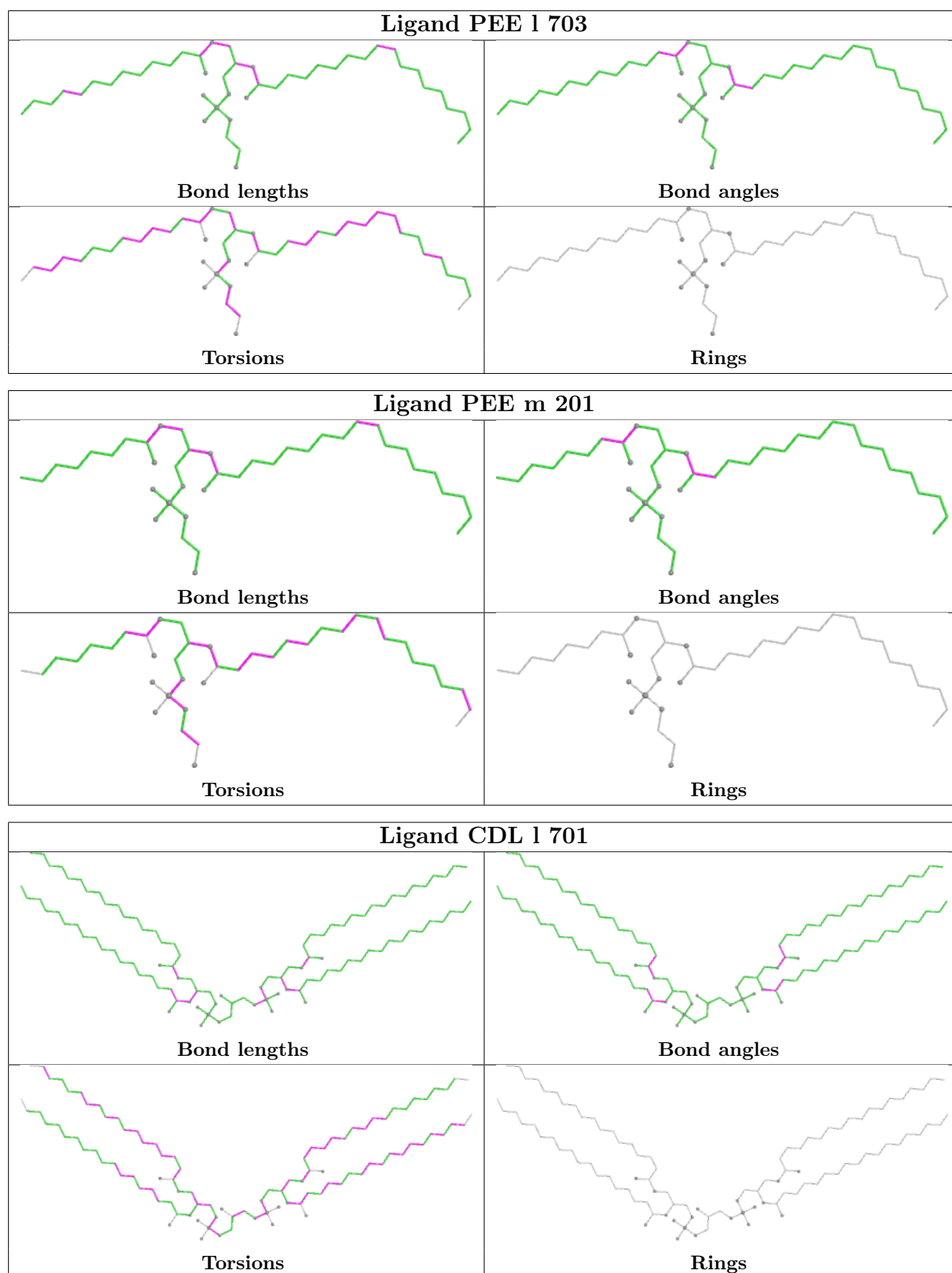
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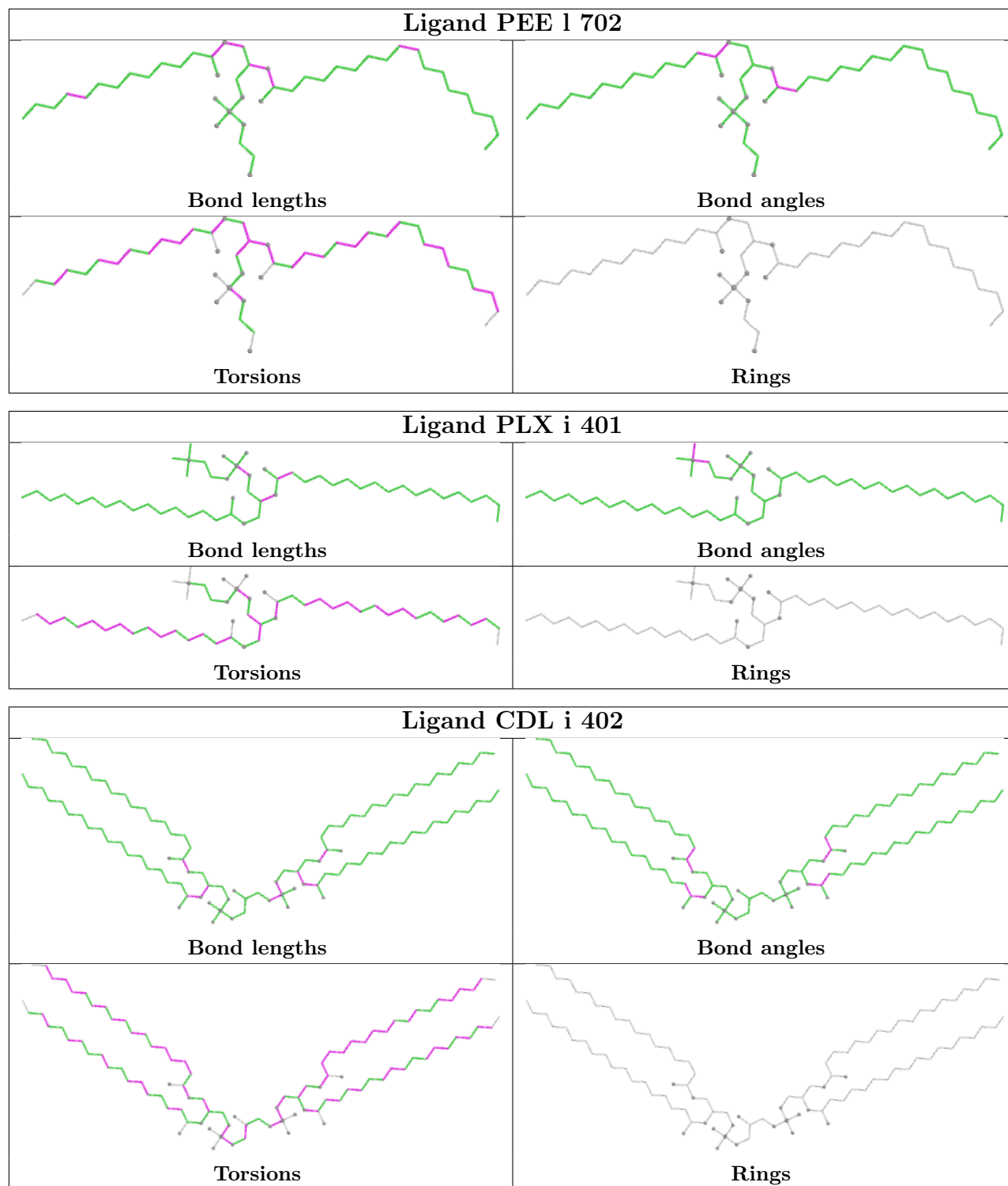
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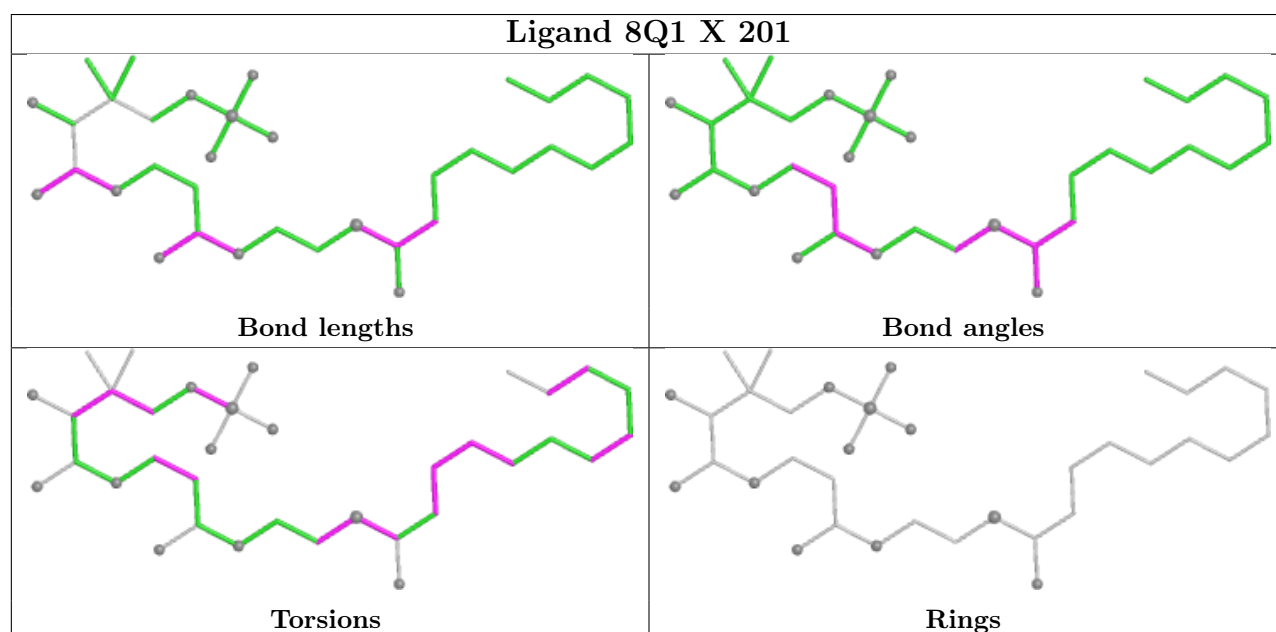
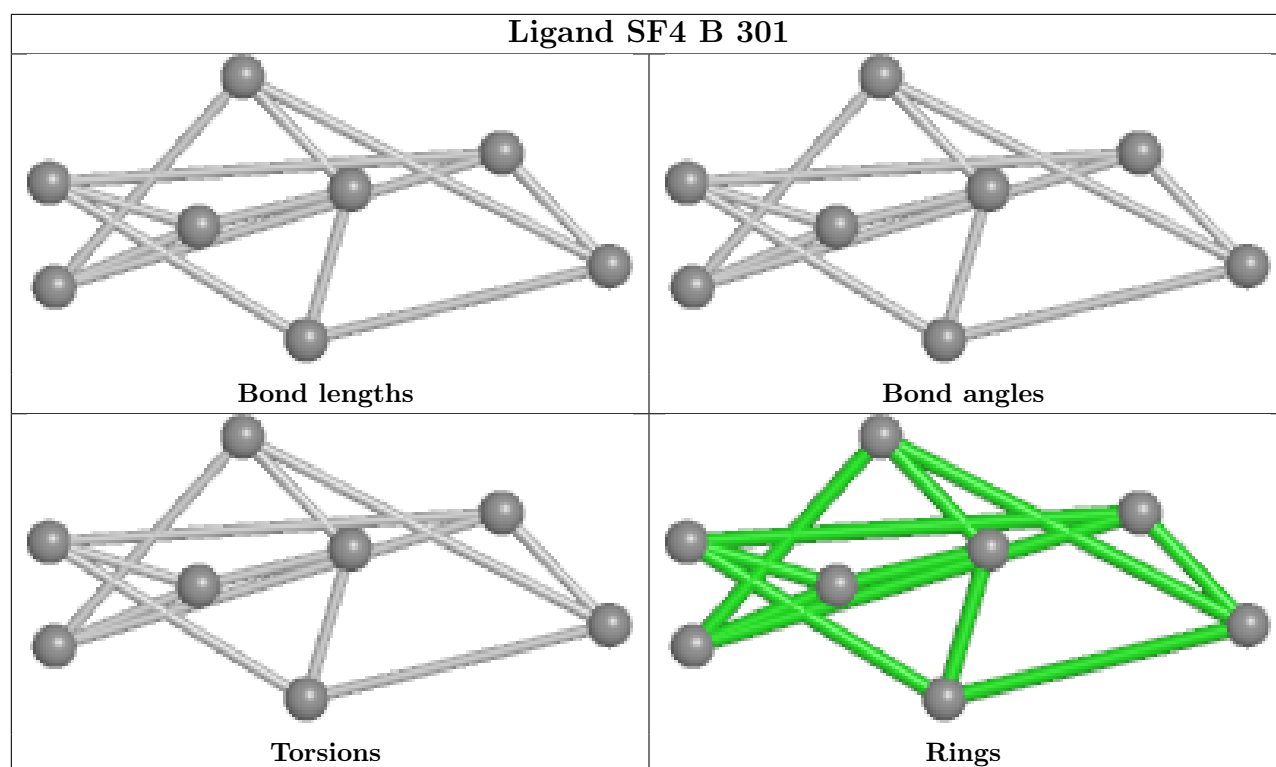
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	l	701	CDL	4	0
48	l	702	PEE	2	0
49	i	401	PLX	3	0
55	i	402	CDL	8	0
50	X	201	8Q1	4	0
57	w	401	ADP	2	0
48	U	101	PEE	3	0
49	r	503	PLX	3	0
46	A	502	FMN	6	0
49	j	201	PLX	3	0
51	J	401	NDP	1	0
50	G	201	8Q1	8	0
56	s	401	UQ	5	0
48	Q	501	PEE	3	0
47	A	503	NAI	5	0
49	C	303	PLX	2	0
45	A	501	SF4	1	0
48	r	501	PEE	6	0
49	r	502	PLX	1	0
49	a	202	PLX	3	0
55	a	201	CDL	6	0
48	Q	502	PEE	5	0

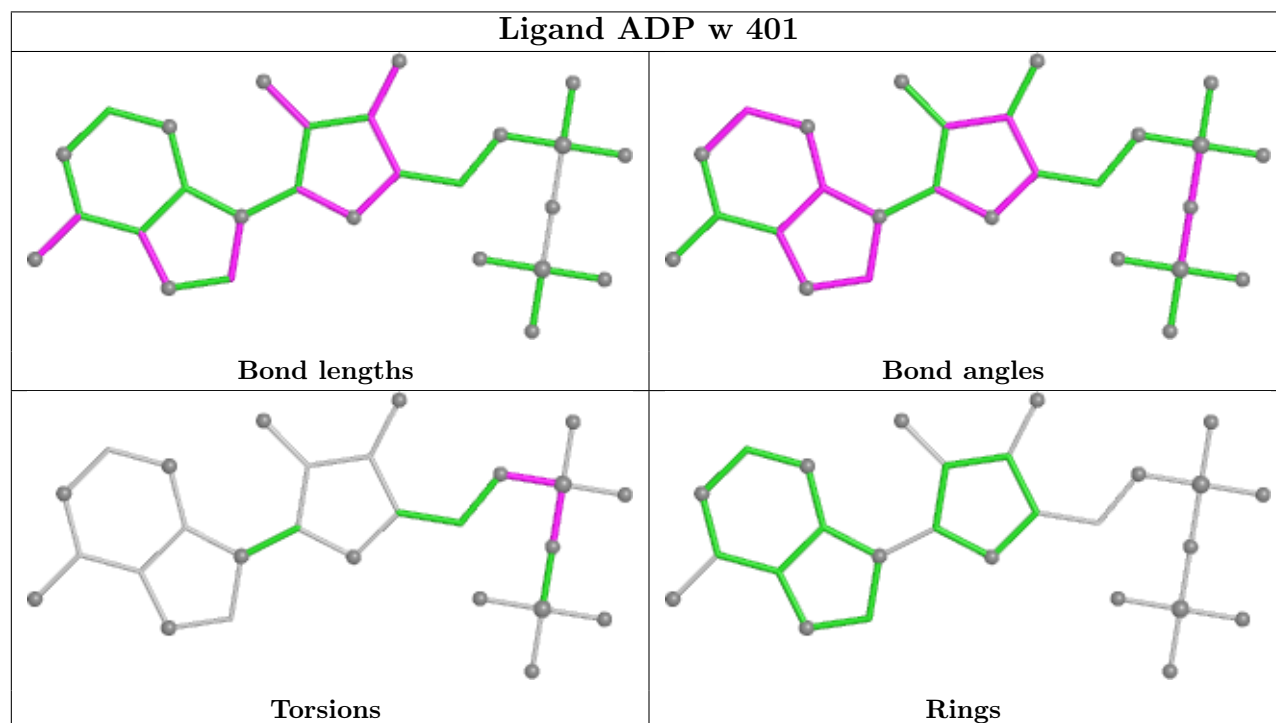
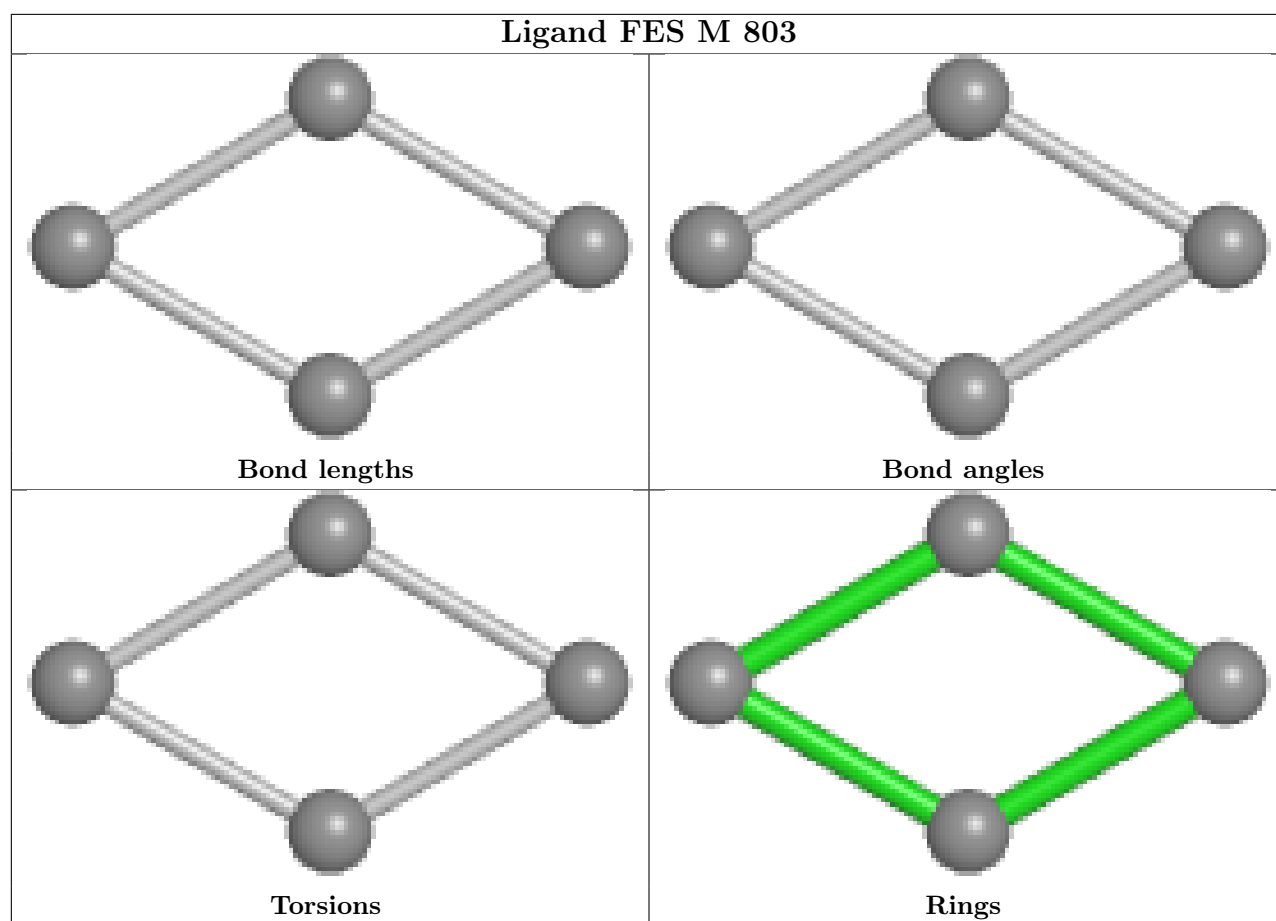
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

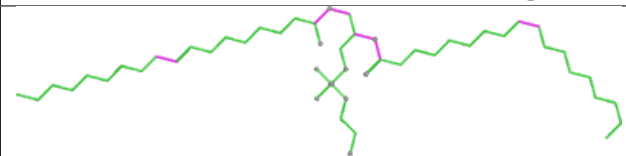
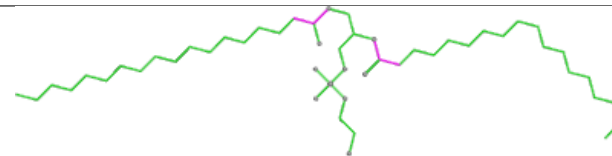
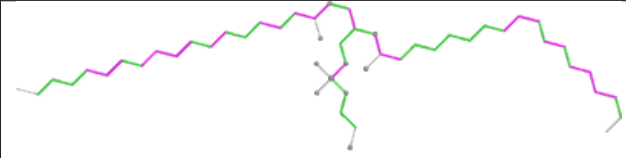
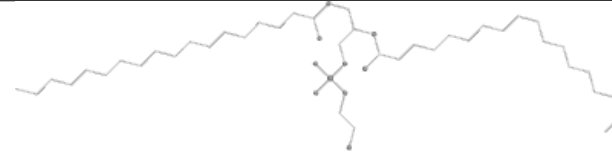
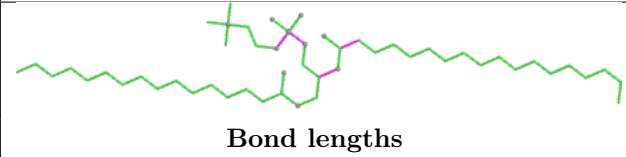
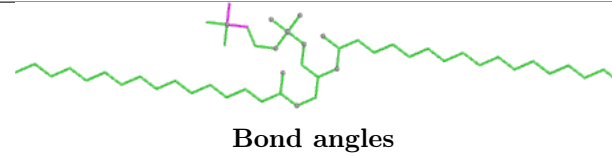
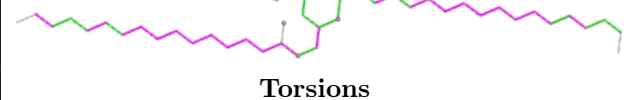
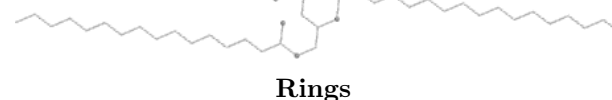


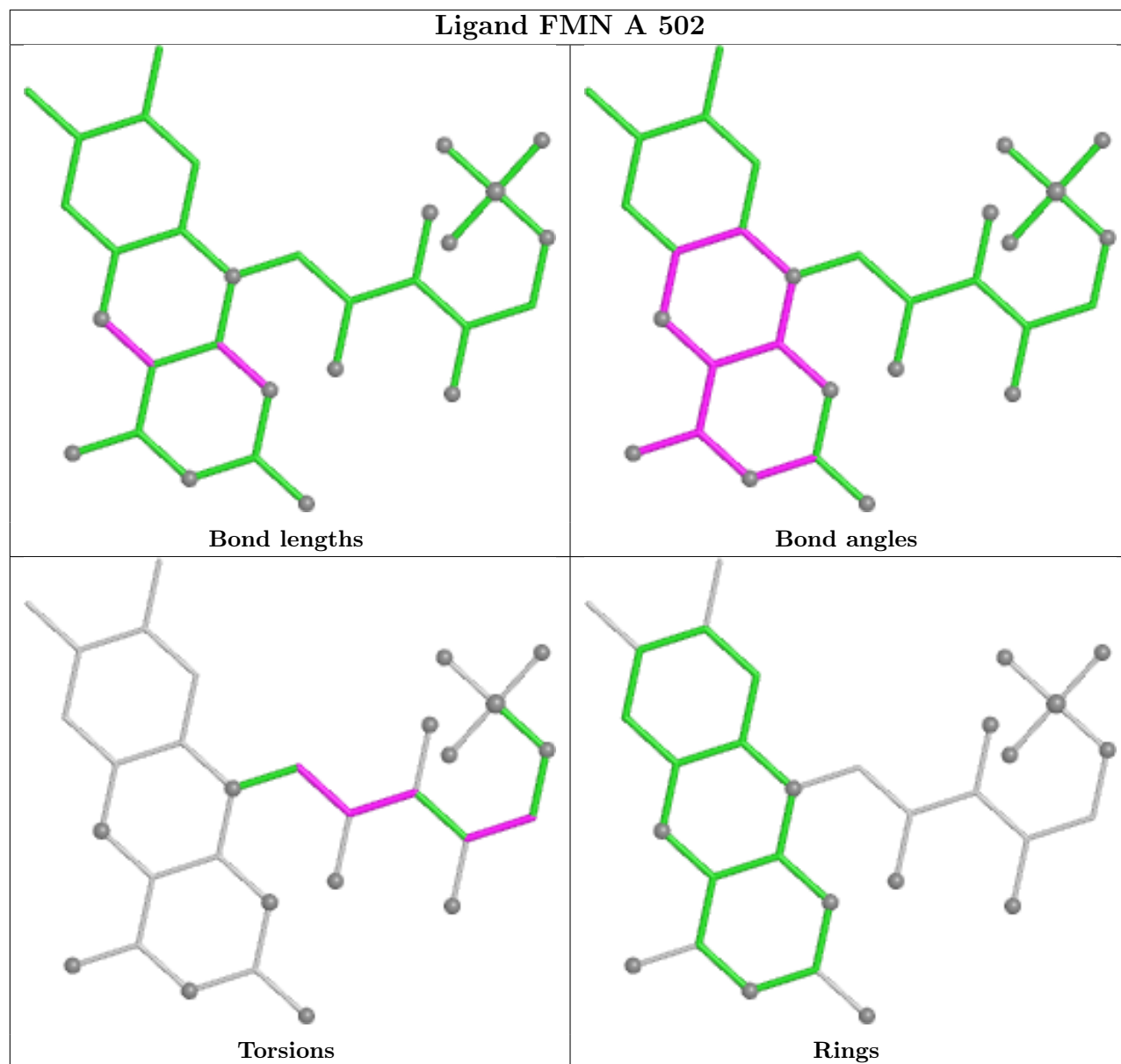




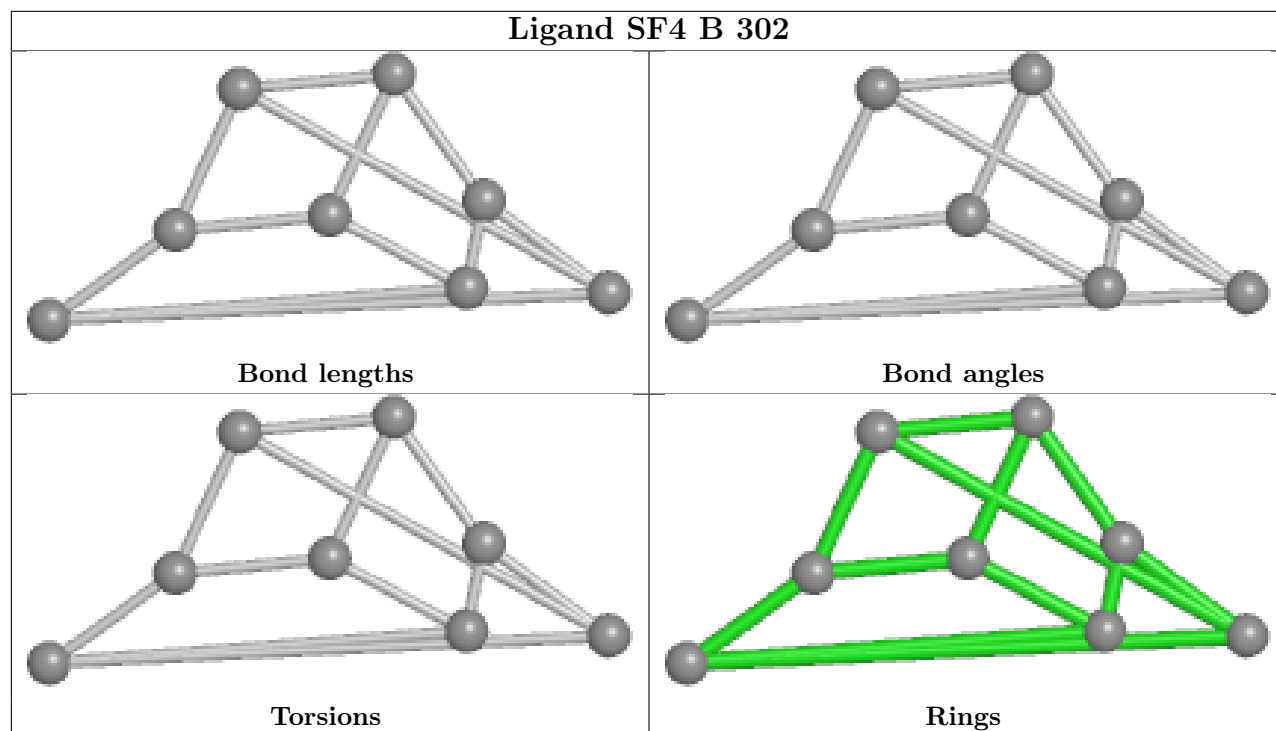




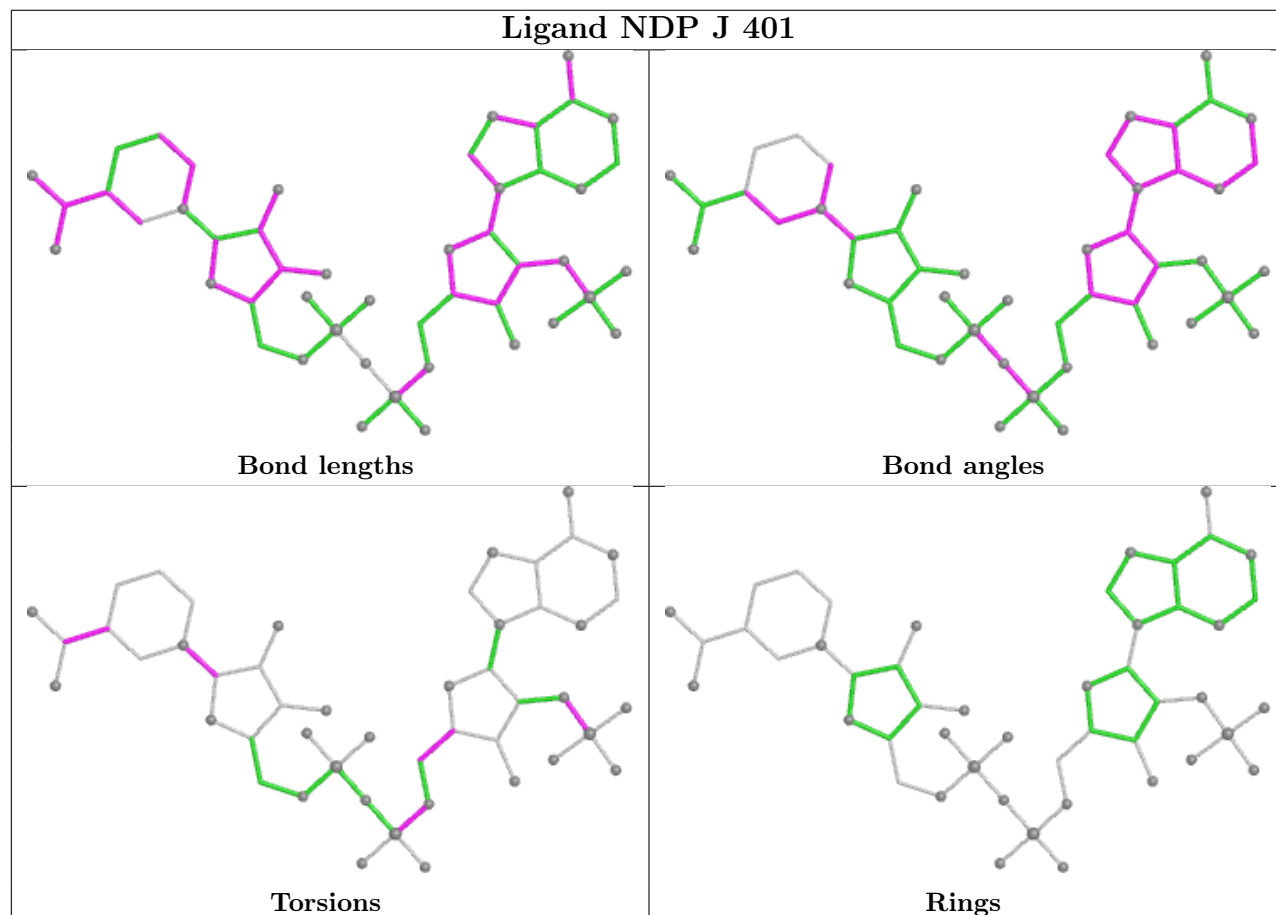
Ligand PEE U 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PLX r 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

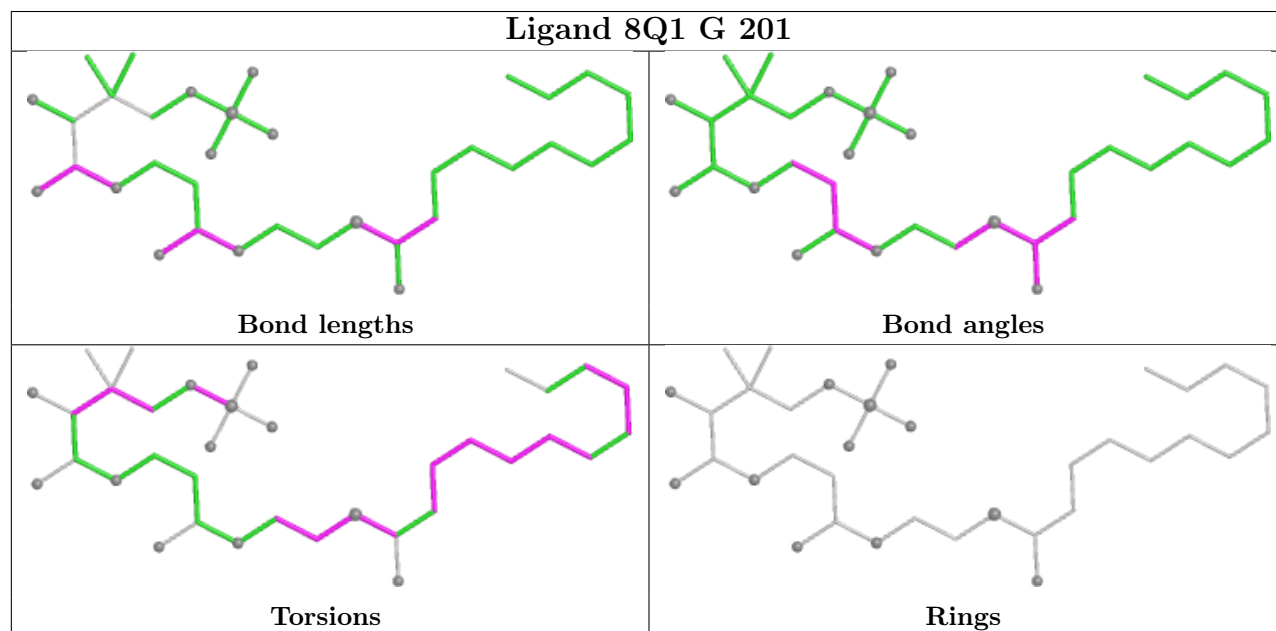
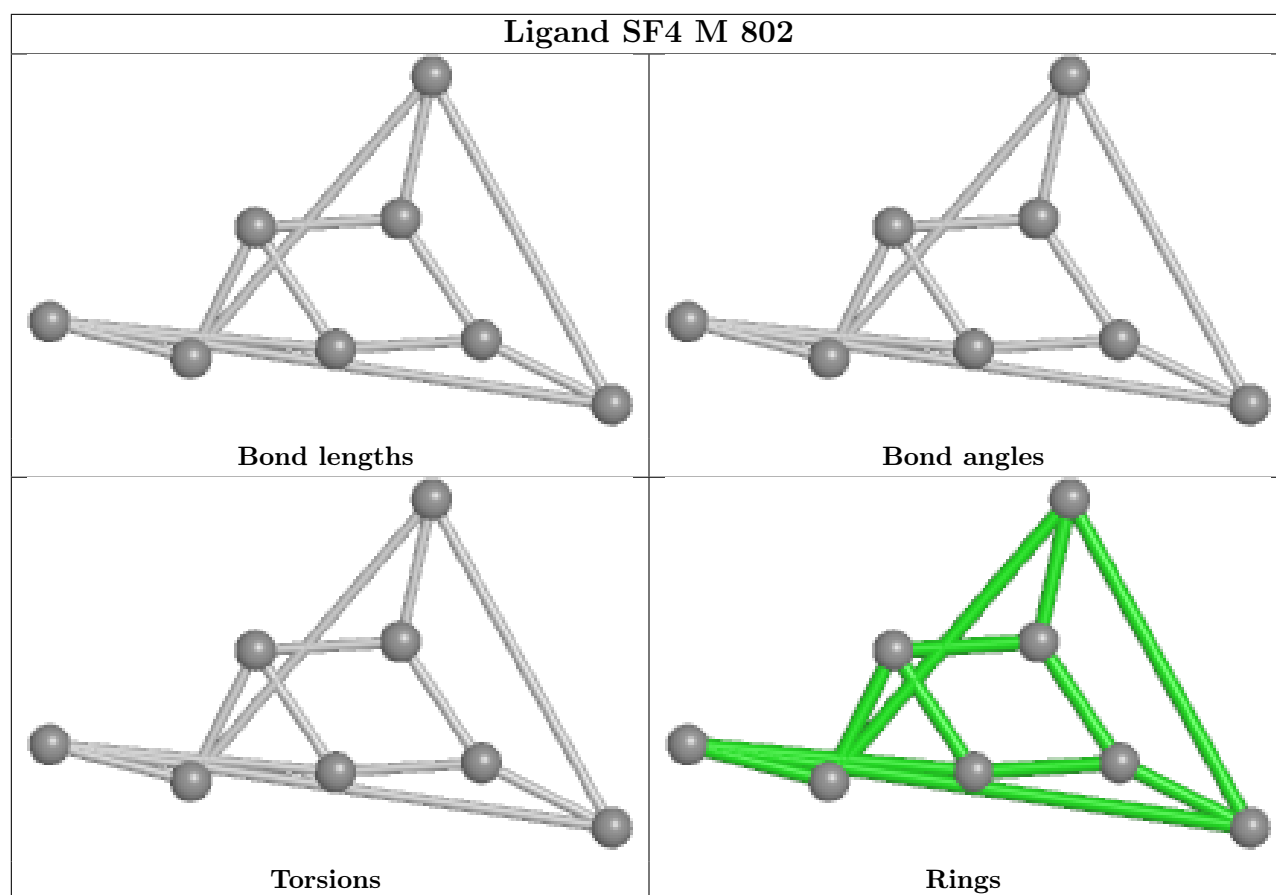


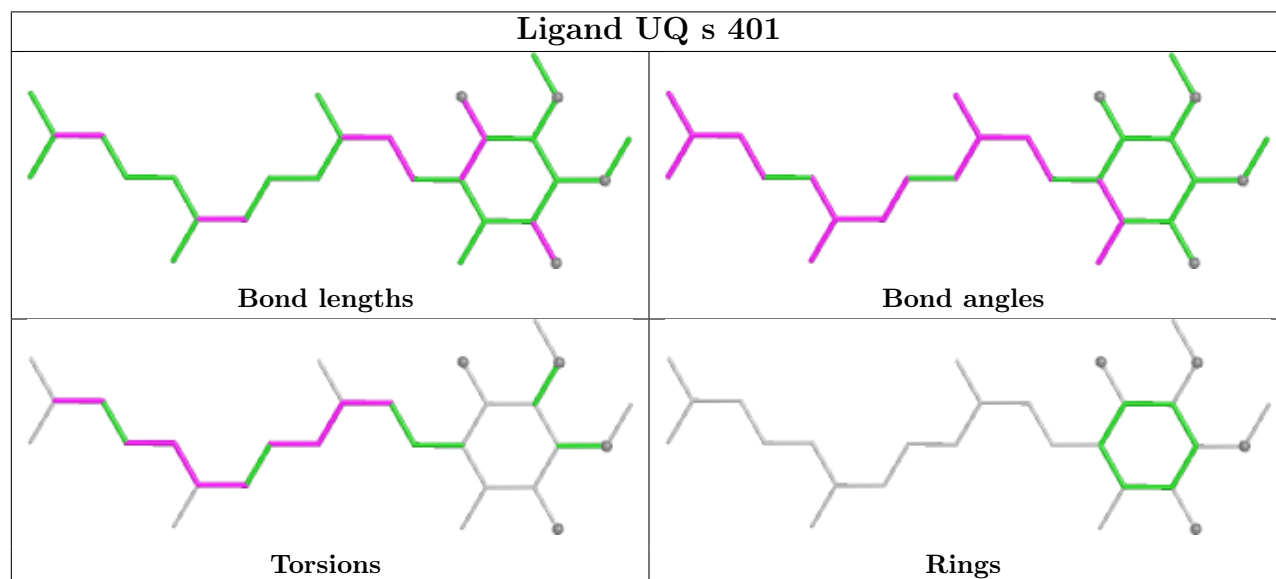
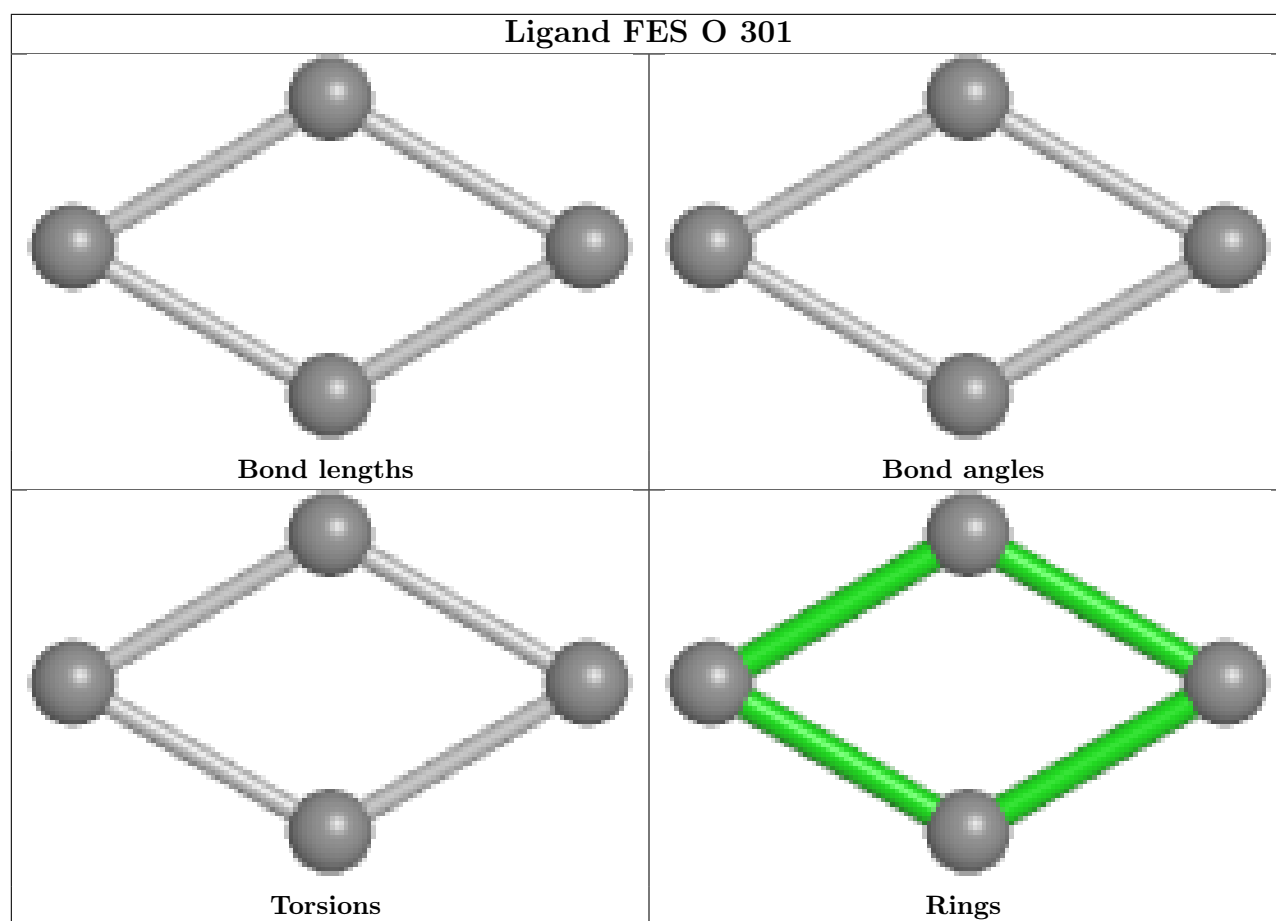
Ligand SF4 B 302

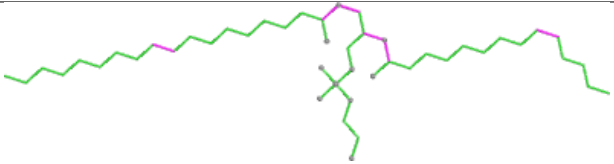
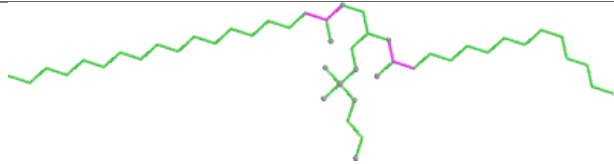
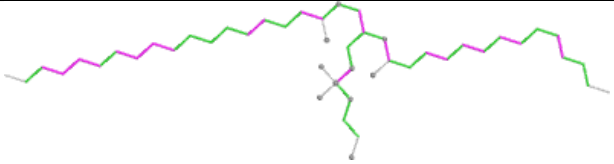
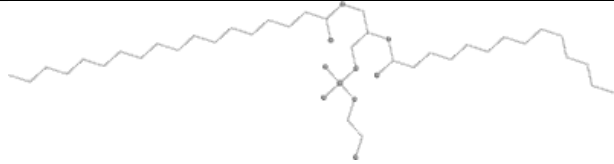
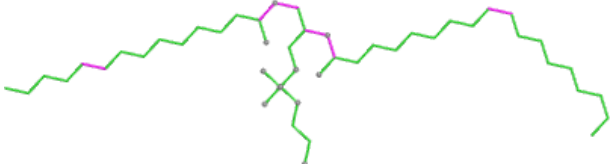
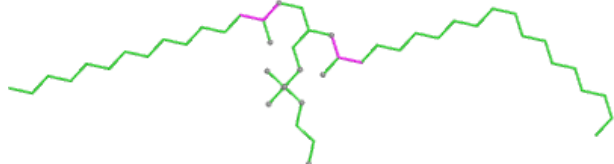
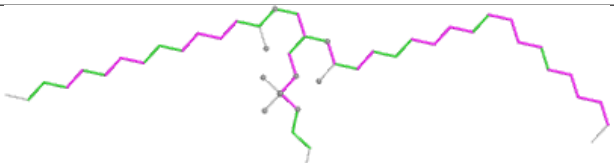
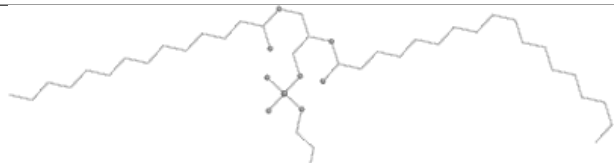


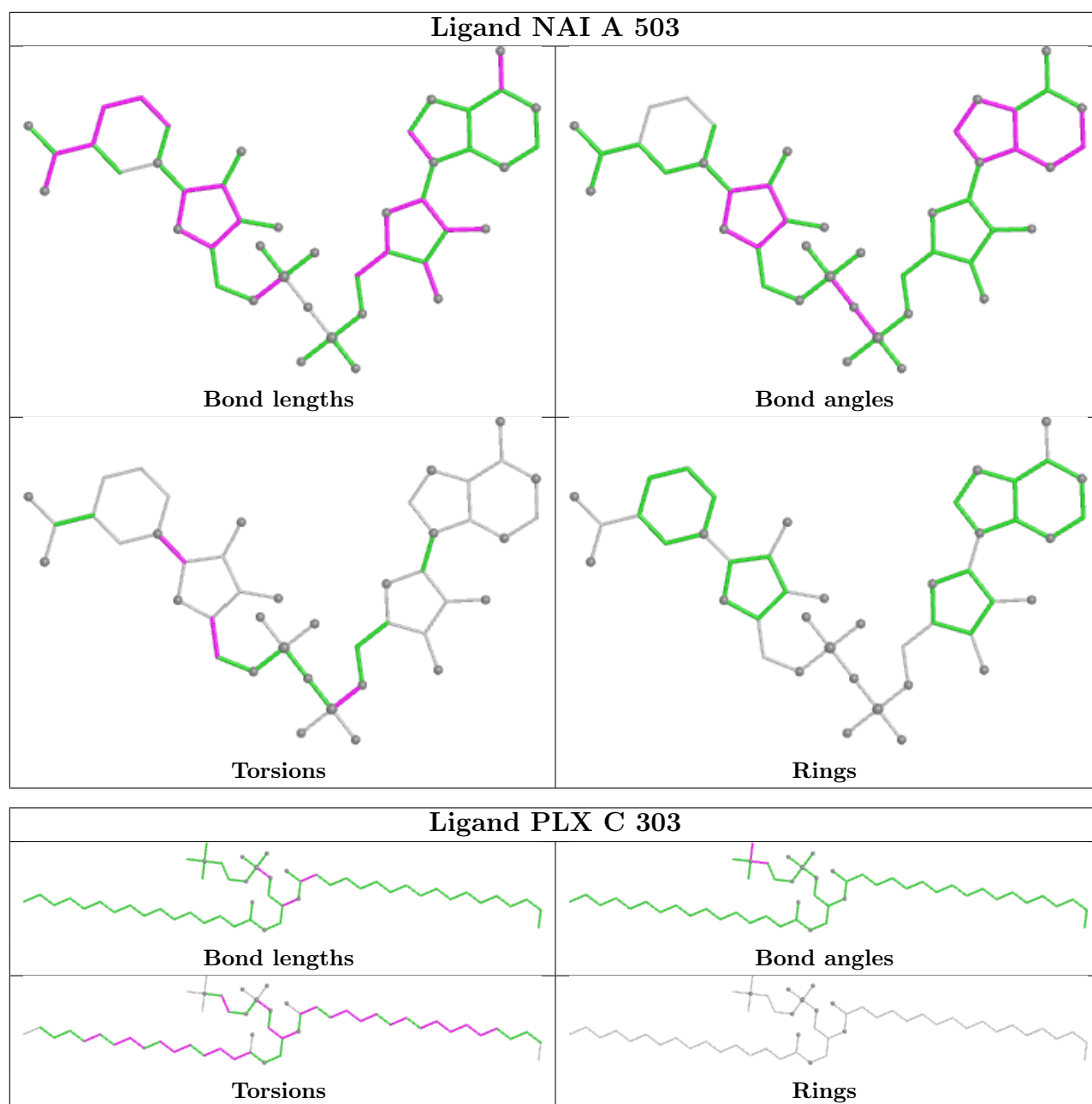
Ligand NDP J 401

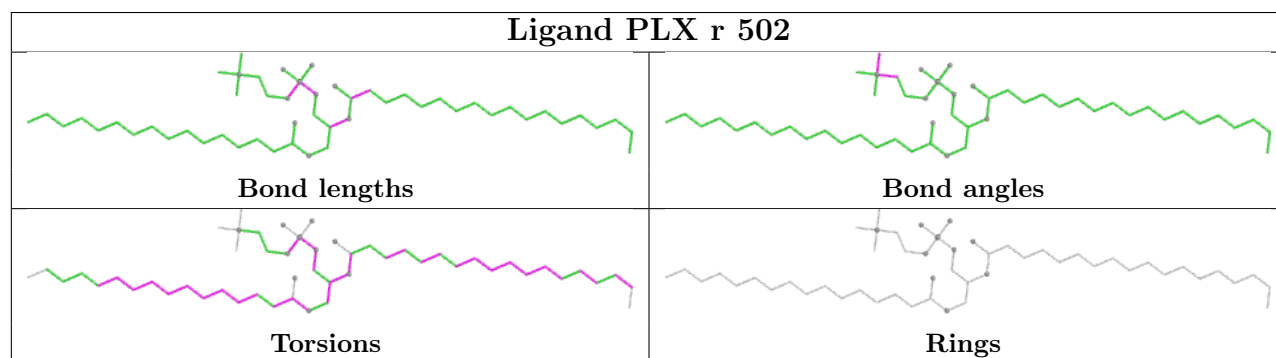
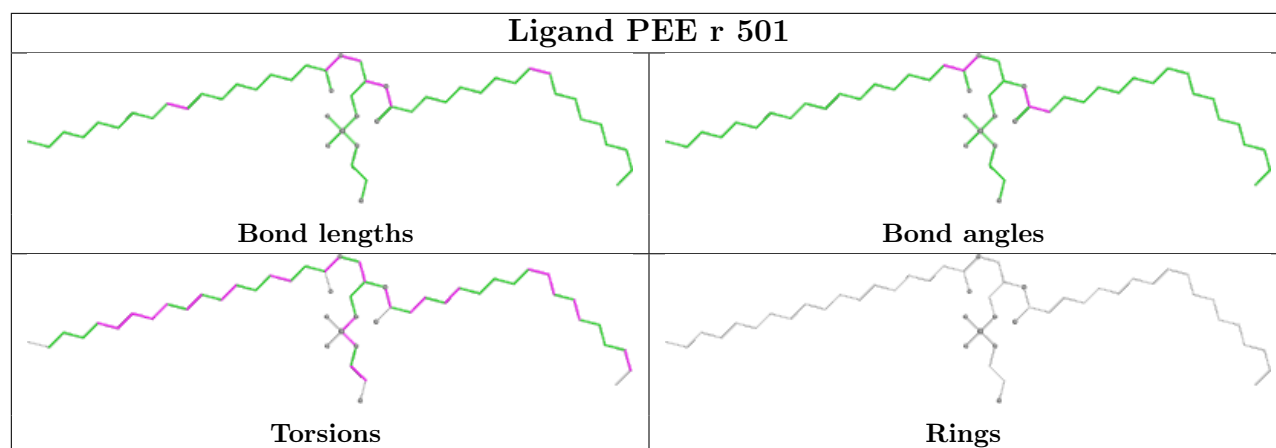
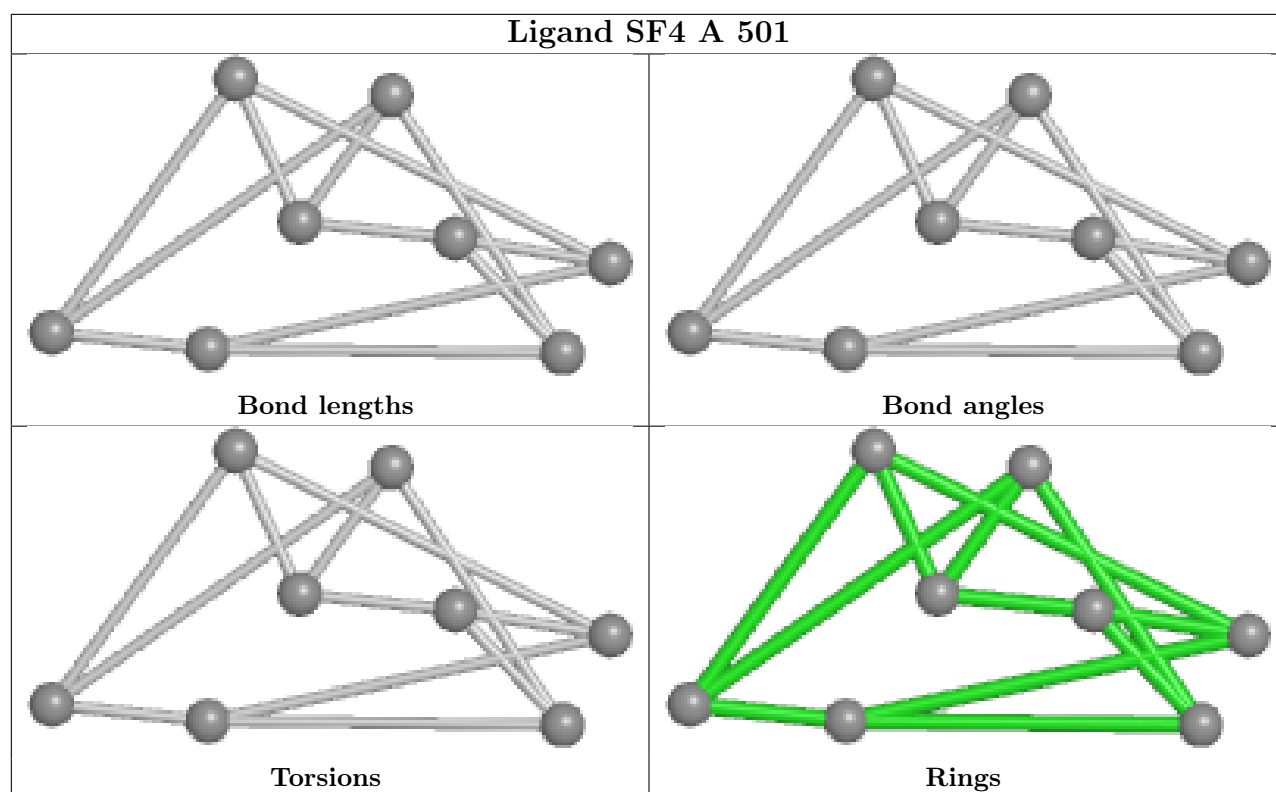


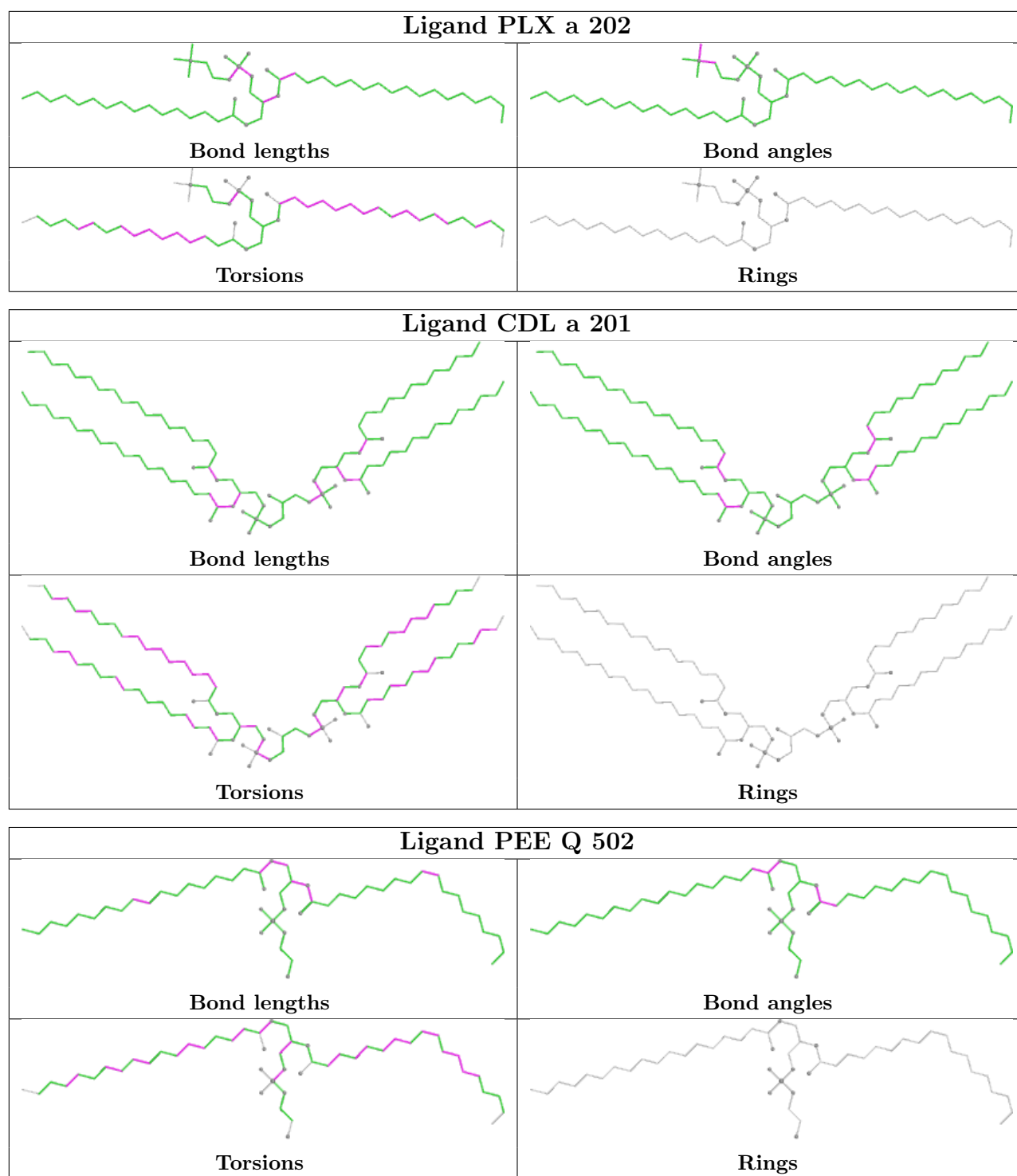




Ligand PEE C 302	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEE Q 501	
 Bond lengths	 Bond angles
 Torsions	 Rings







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

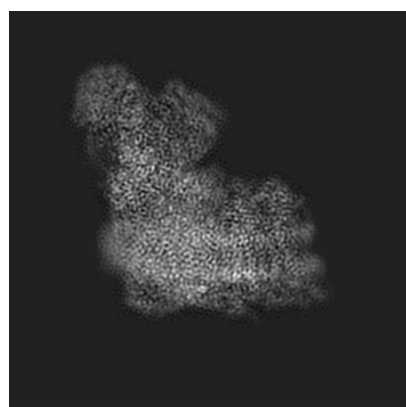
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32306. These allow visual inspection of the internal detail of the map and identification of artifacts.

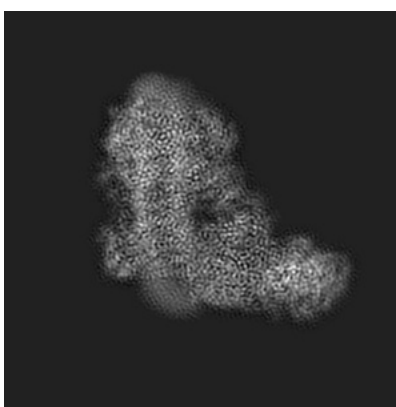
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

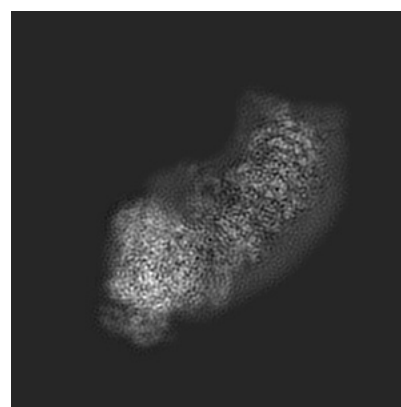
6.1.1 Primary map



X



Y

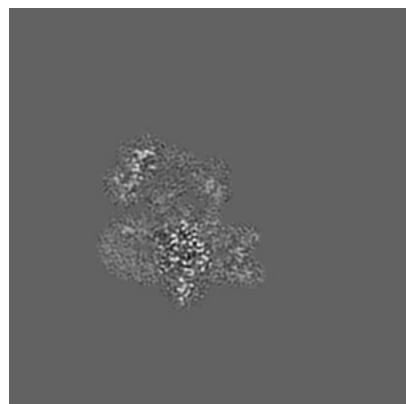


Z

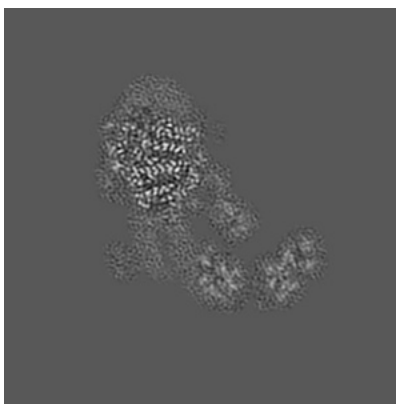
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

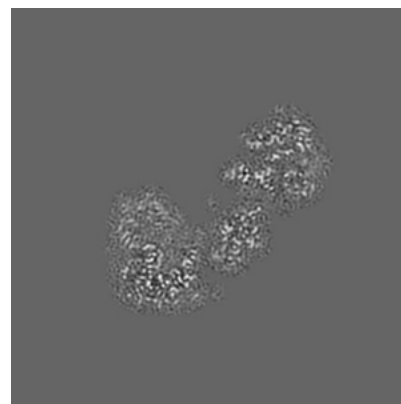
6.2.1 Primary map



X Index: 152



Y Index: 152

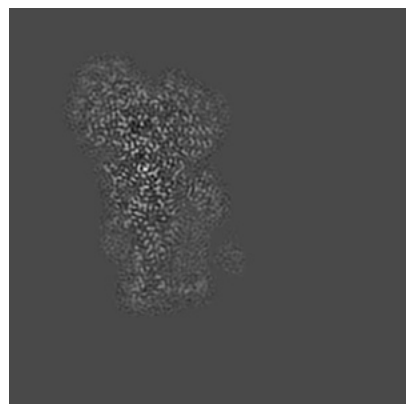


Z Index: 152

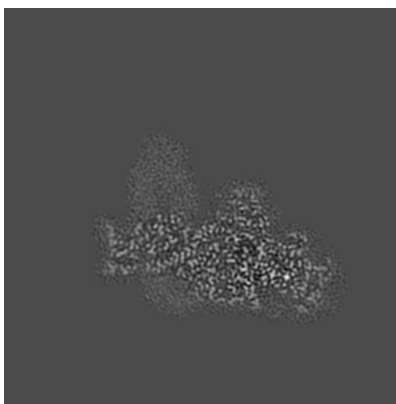
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

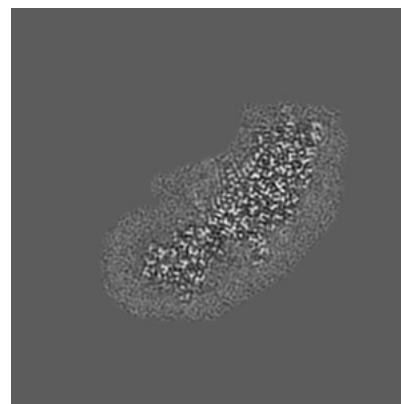
6.3.1 Primary map



X Index: 105



Y Index: 98

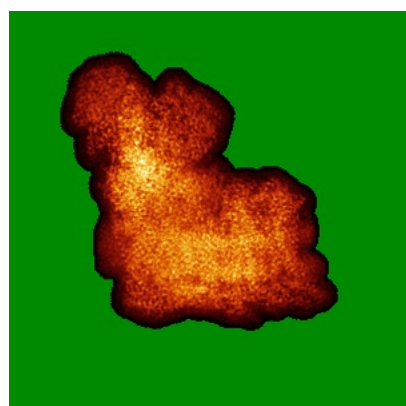


Z Index: 128

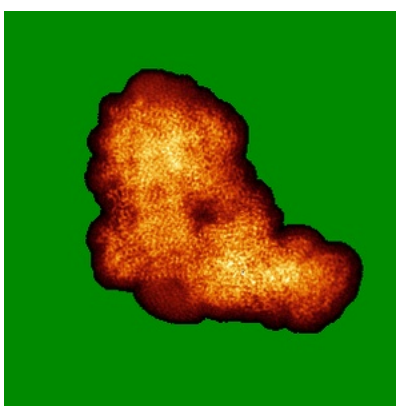
The images above show the largest variance slices of the map in three orthogonal directions.

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

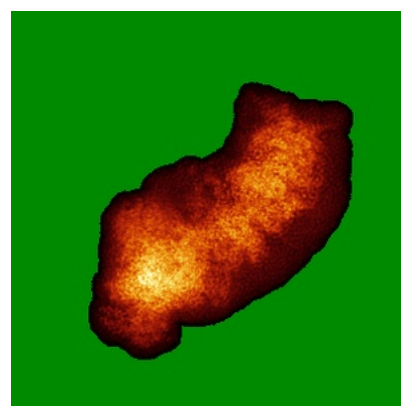
6.4.1 Primary map



X



Y

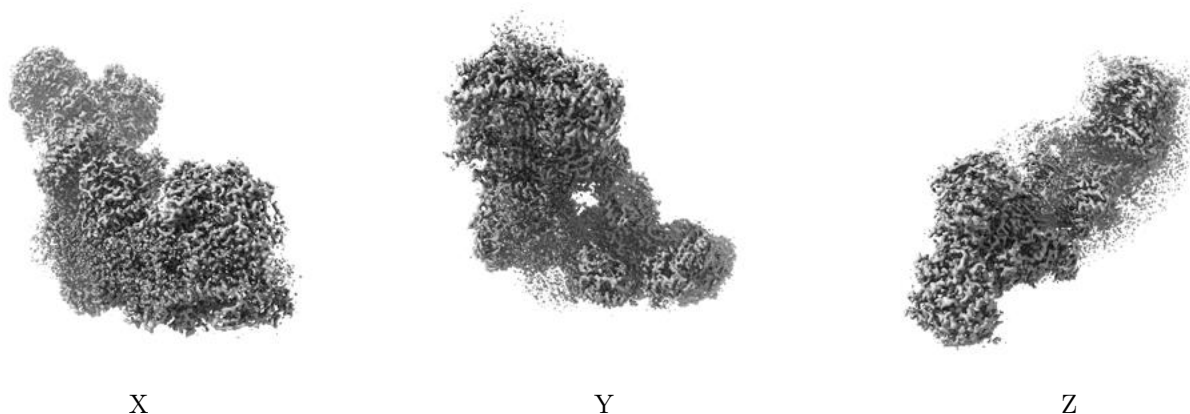


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0282. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

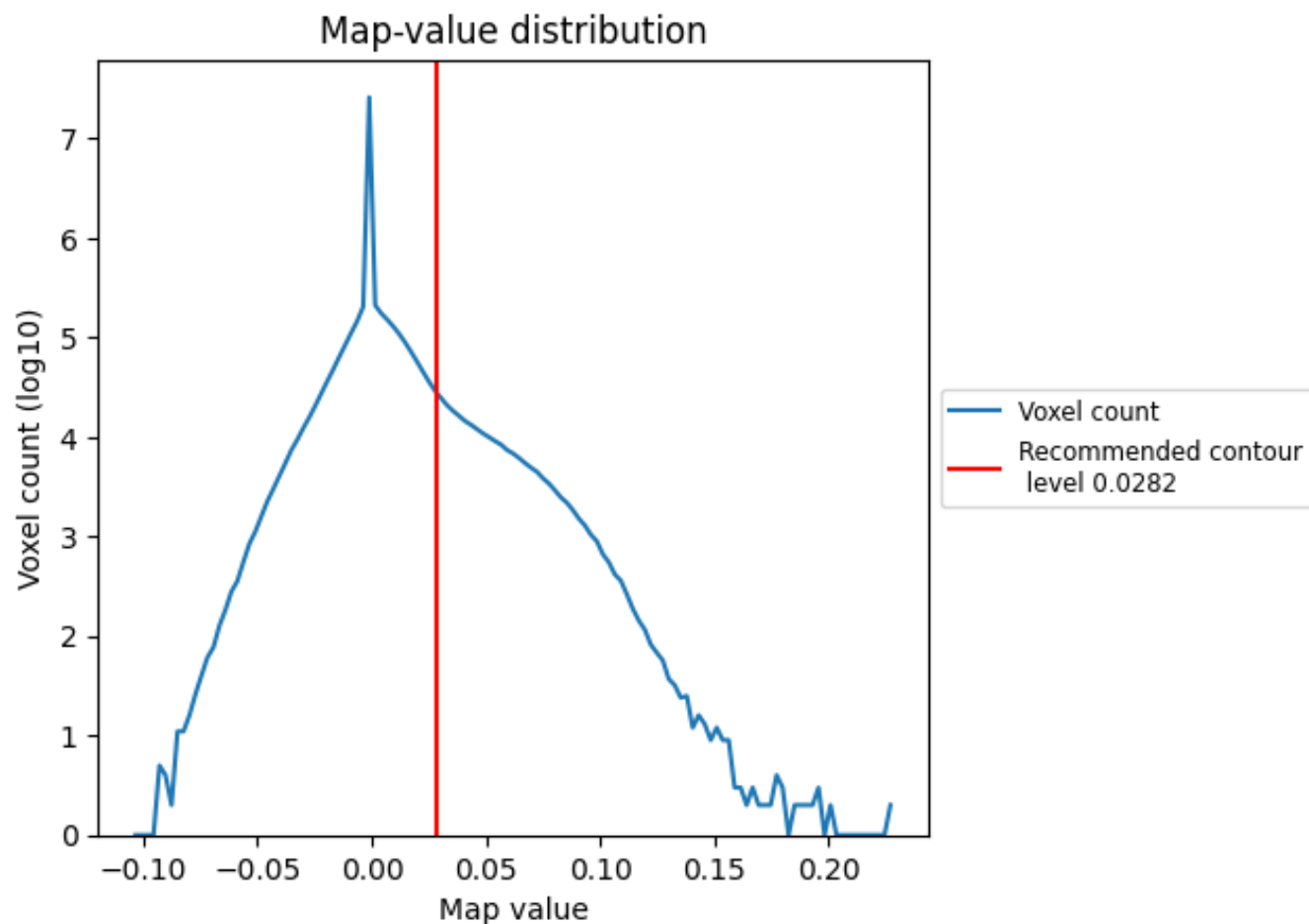
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

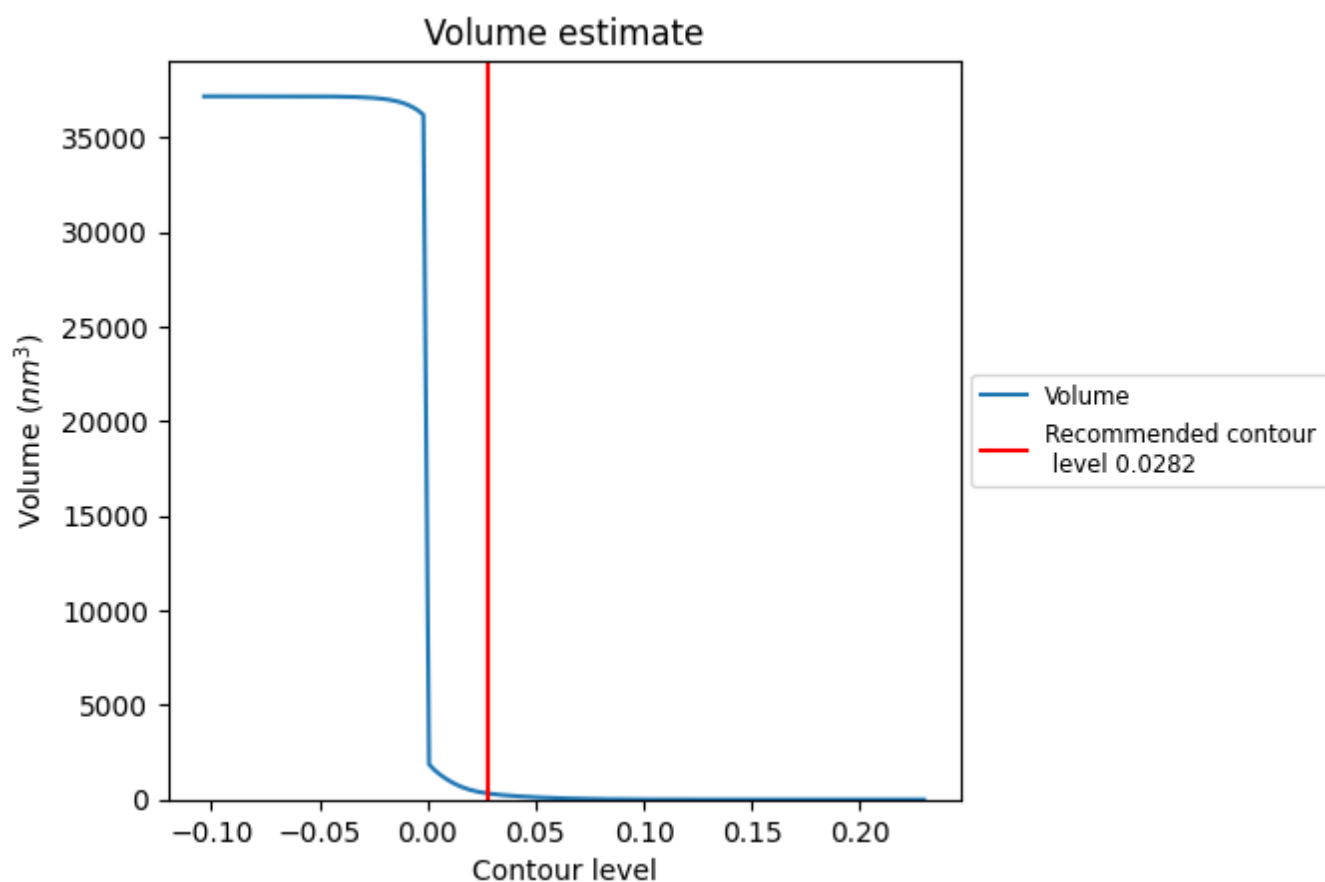
This section contains the results of statistical analysis of the map.

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.

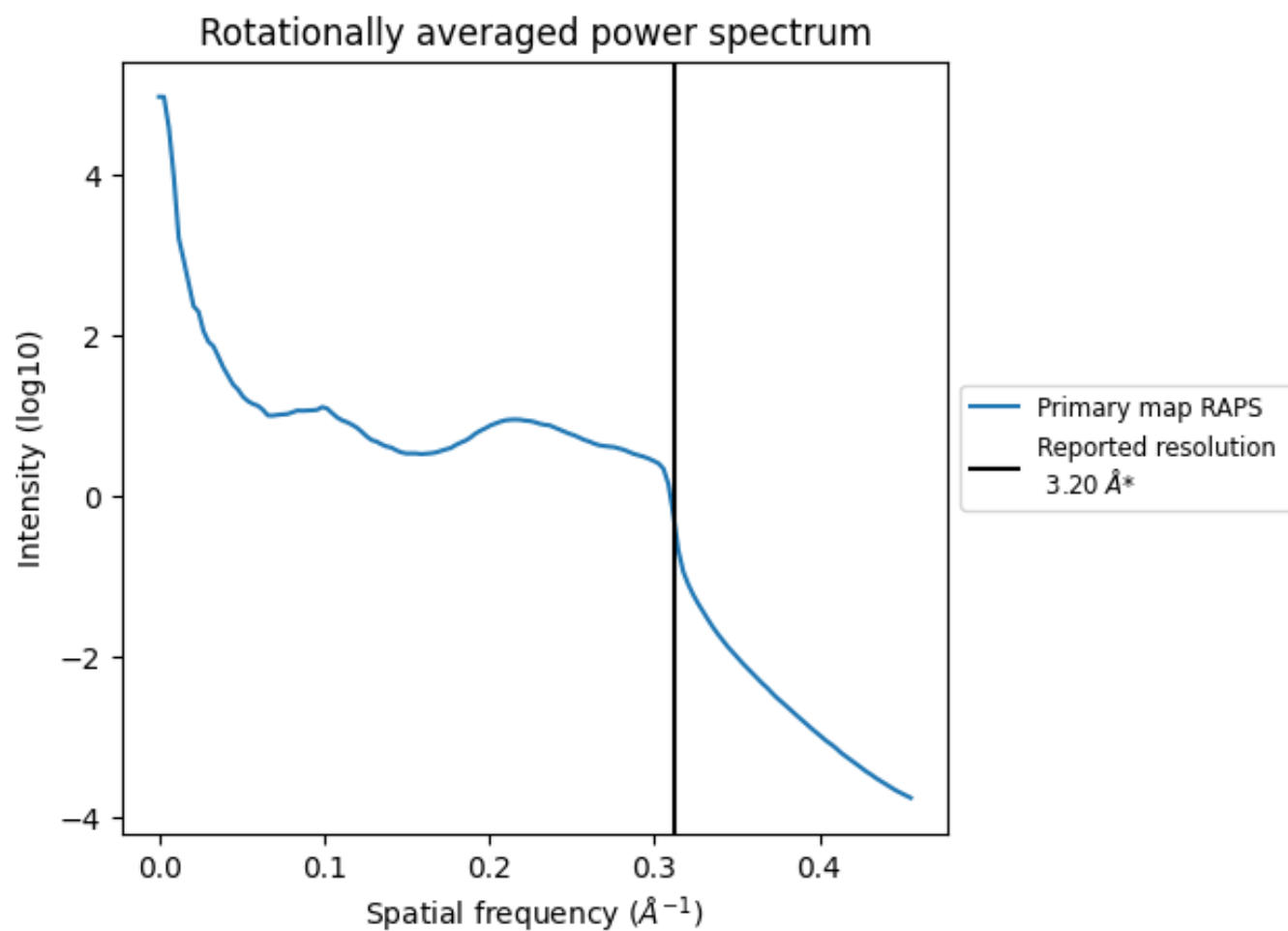
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 321 nm^3 ; this corresponds to an approximate mass of 290 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

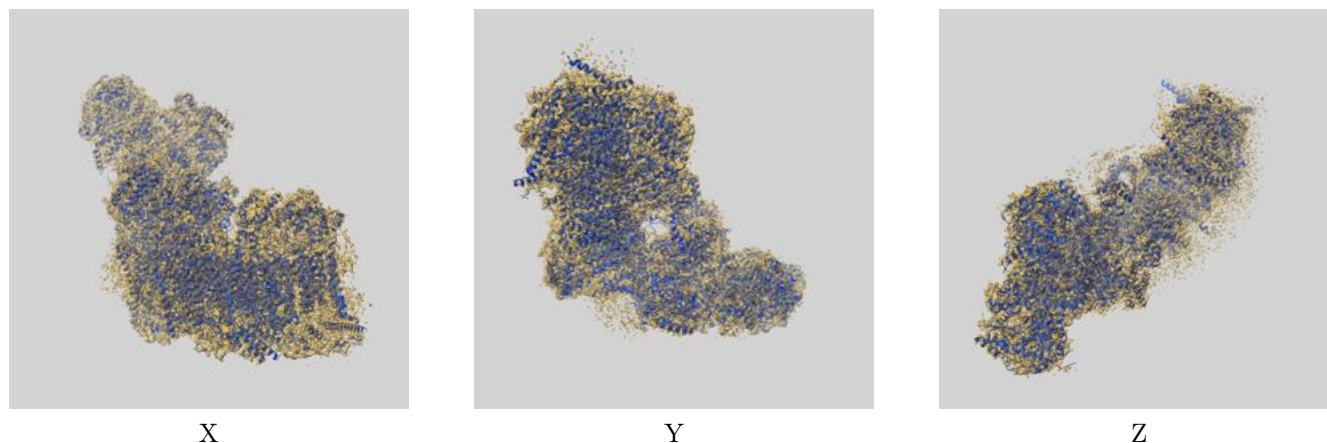
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

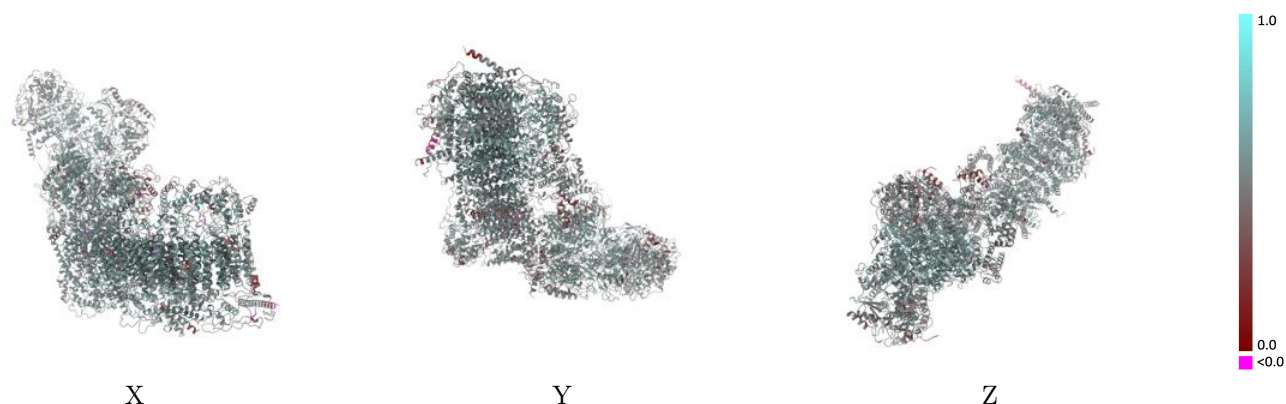
This section contains information regarding the fit between EMDB map EMD-32306 and PDB model 7W4K. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



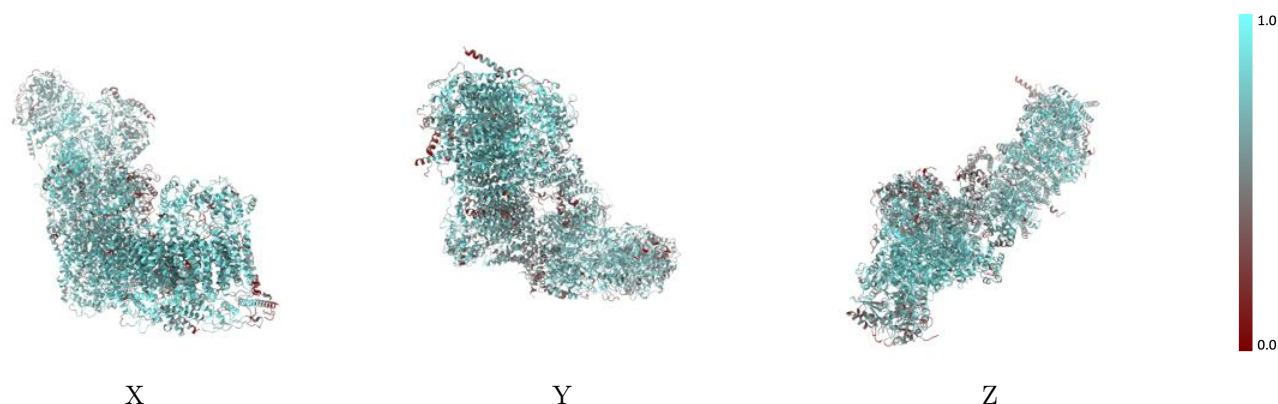
The images above show the 3D surface view of the map at the recommended contour level 0.0282 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



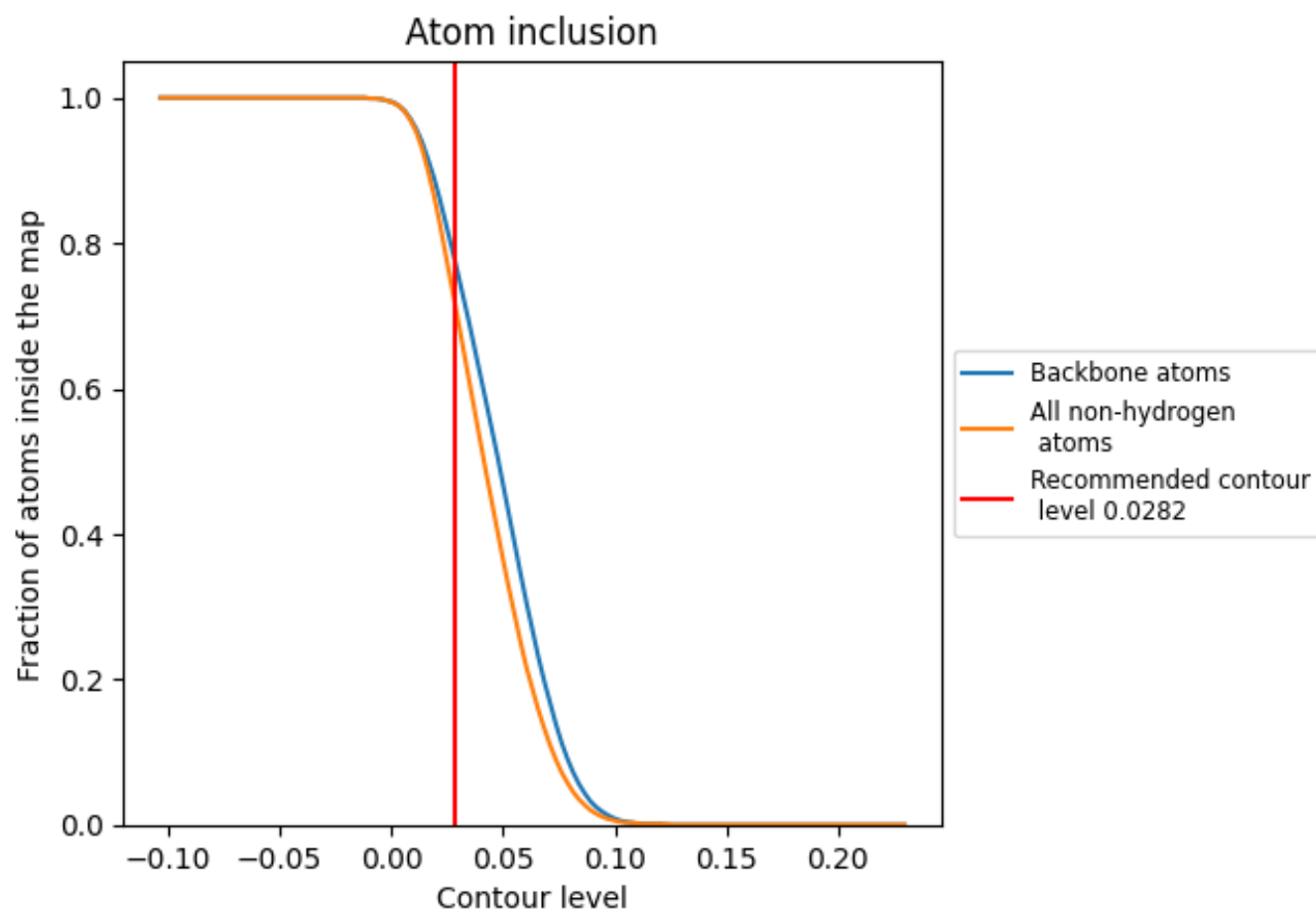
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0282).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0282) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7210	 0.5310
A	 0.6420	 0.5000
B	 0.8720	 0.5840
C	 0.8040	 0.5650
E	 0.6730	 0.5210
F	 0.5170	 0.4330
G	 0.4060	 0.3590
H	 0.6700	 0.5030
I	 0.7390	 0.5420
J	 0.6040	 0.4900
K	 0.5550	 0.4610
L	 0.7440	 0.5530
M	 0.7190	 0.5380
N	 0.7600	 0.5490
O	 0.6180	 0.4960
P	 0.8390	 0.5790
Q	 0.8140	 0.5760
S	 0.7850	 0.5440
T	 0.7180	 0.5400
U	 0.6820	 0.5020
V	 0.4510	 0.4430
W	 0.7250	 0.5310
X	 0.7020	 0.5020
Y	 0.6120	 0.4700
Z	 0.5610	 0.4580
a	 0.7650	 0.5510
b	 0.6800	 0.4870
c	 0.7540	 0.5360
d	 0.7310	 0.5210
e	 0.6750	 0.5140
f	 0.6350	 0.4820
g	 0.8010	 0.5550
h	 0.7420	 0.5310
i	 0.8020	 0.5700
j	 0.6300	 0.5010



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Chain	Atom inclusion	Q-score
k	 0.6760	 0.5330
l	 0.7690	 0.5560
m	 0.6440	 0.5010
n	 0.6510	 0.5010
o	 0.7200	 0.5290
p	 0.7540	 0.5310
r	 0.8250	 0.5740
s	 0.7560	 0.5430
u	 0.7340	 0.5250
v	 0.6180	 0.4730
w	 0.7030	 0.5210