



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 10:23 PM UTC

PDB ID : 7V3M / pdb_00007v3m
EMDB ID : EMD-31652
Title : Deactive state complex I from rotenone-NADH dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-08-10
Resolution : 2.90 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:

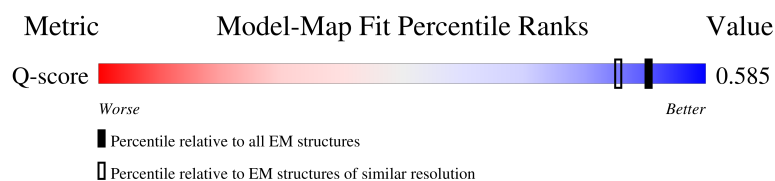
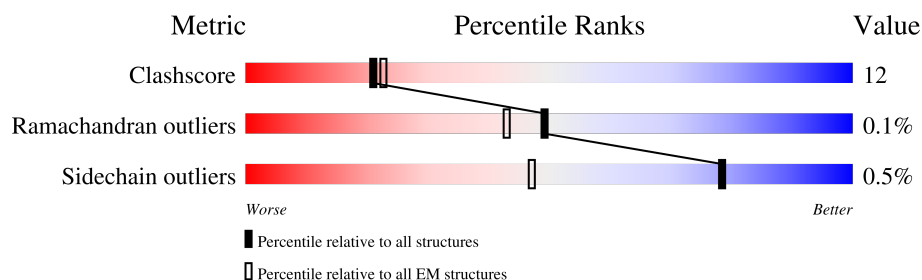
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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	11806 (2.30 - 3.30)

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	431	 71% 28% .
2	B	176	 78% 22%
3	C	156	 78% 21% .
4	E	115	 5% 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	341	
10	K	42	
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	42	
30	g	121	
31	h	105	
32	i	347	
33	j	113	
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	131	
44	w	320	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	A	501	-	-	X	-
48	PEE	Q	501	-	-	X	-
48	PEE	l	704	-	-	X	-
51	CDL	a	201	-	-	X	-
51	CDL	l	701	-	-	X	-

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 66644 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
			3318	2095	591	612	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
			691	434	129	126	2		

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			693	447	102	139	5		
6	X	88	Total	C	N	O	S	0	0
			696	449	103	139	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	97	Total	C	N	O	S	0	0
			762	479	144	136	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
			2359	1514	421	416	8		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

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 NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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 NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

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	S	0	0
			643	417	110	115	1		

- 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
			1021	651	174	190	6		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	142	Total	C	N	O	S	0	0
			1161	749	197	206	9		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	70	Total	C	N	O	S	0	0
			583	386	98	98	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

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 NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	140	Total	C	N	O	S	0	0
			1152	754	196	199	3		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	103	Total	C	N	O	S	0	0
			875	571	158	145	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
			1315	853	213	241	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	1779	419	462	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
			4785	3173	741	820	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
			456	295	83	77	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	0	0
			1058	688	181	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
			1534	982	279	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 NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			1020	637	189	185	9		

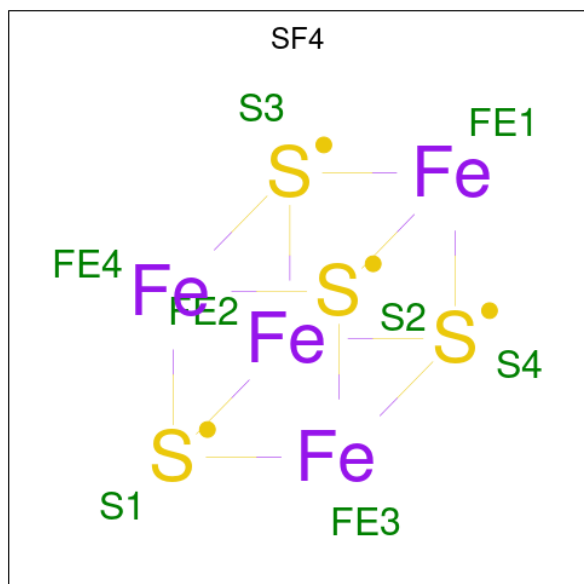
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	1	MYR	-	acetylation	UNP F1SCH1

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

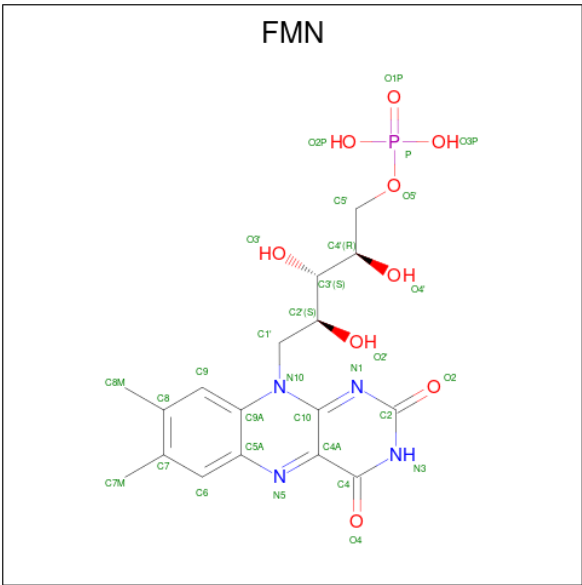
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2574	1638	437	489	10		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



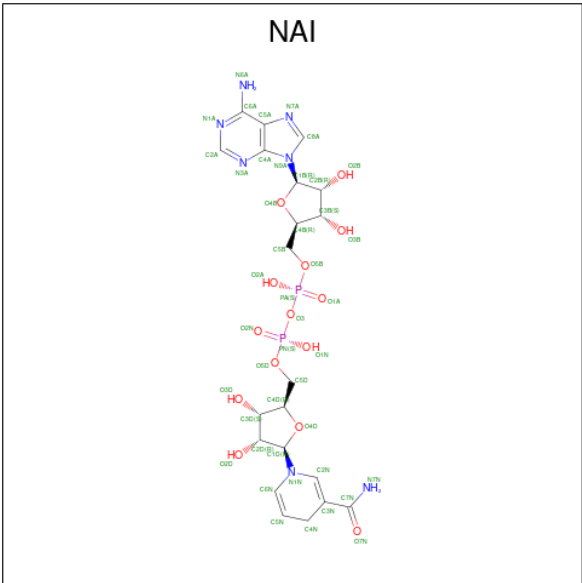
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



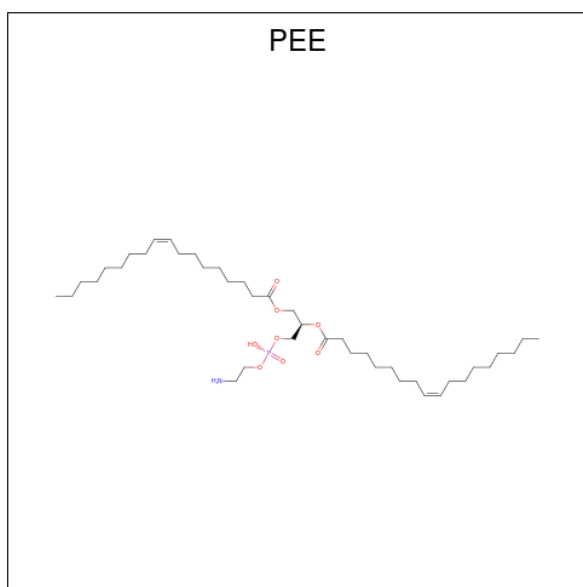
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

- 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).



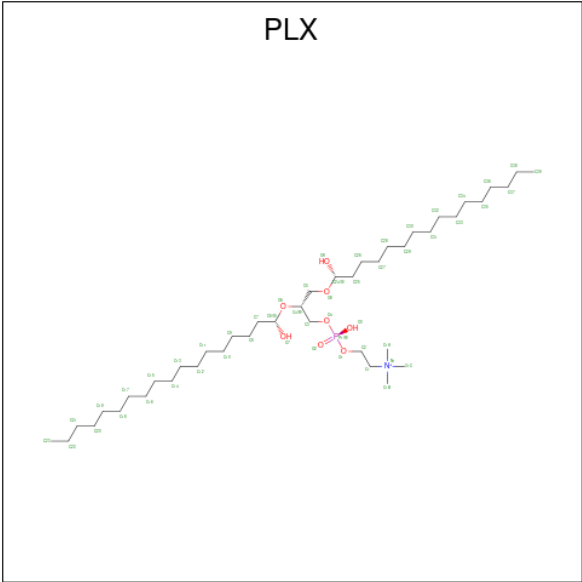
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

- 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).



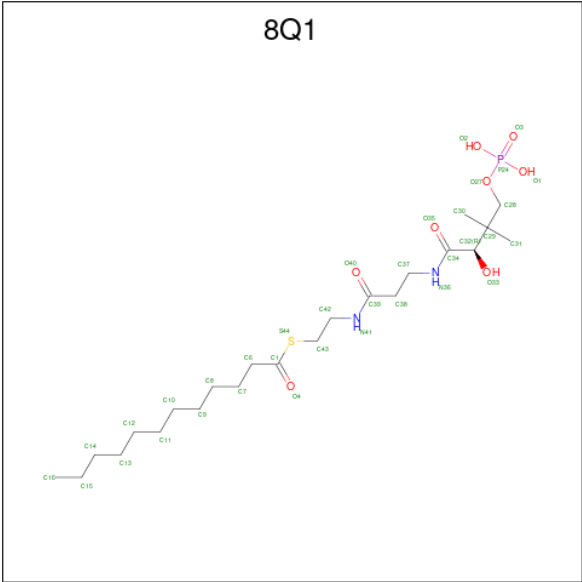
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	Q	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	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).



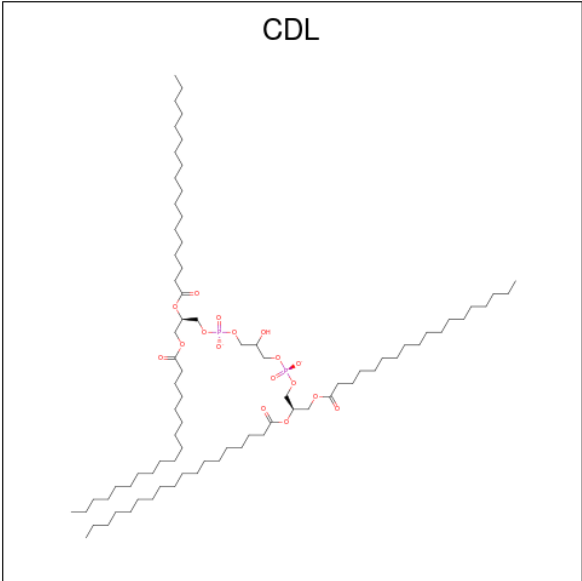
Mol	Chain	Residues	Atoms					AltConf
49	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 50 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}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 CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



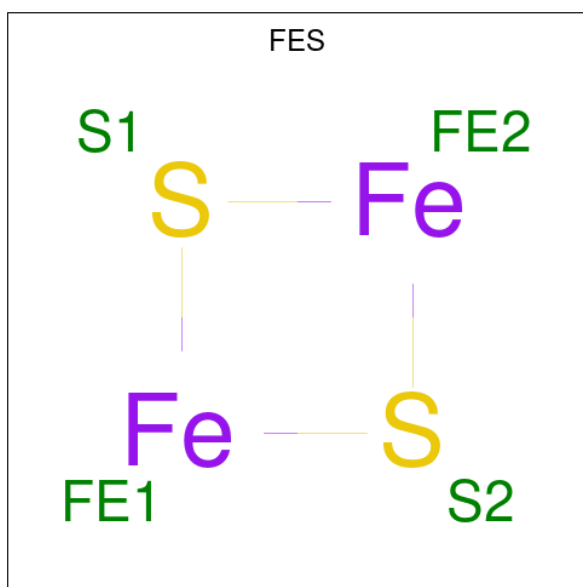
Mol	Chain	Residues	Atoms				AltConf
51	I	1	Total	C	O	P	0
			51	32	17	2	

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Mol	Chain	Residues	Atoms				AltConf
51	a	1	Total 91	C 72	O 17	P 2	0
51	i	1	Total 66	C 47	O 17	P 2	0
51	l	1	Total 99	C 80	O 17	P 2	0
51	l	1	Total 100	C 81	O 17	P 2	0
51	r	1	Total 100	C 81	O 17	P 2	0
51	u	1	Total 78	C 59	O 17	P 2	0

- [illegible]

- Molecule 53 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



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

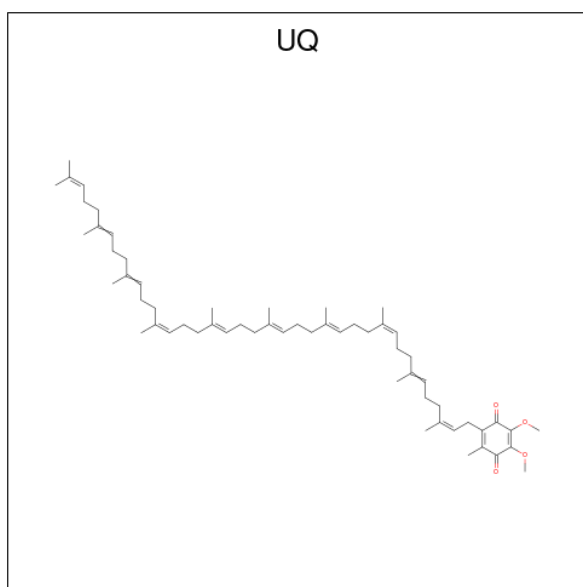
- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

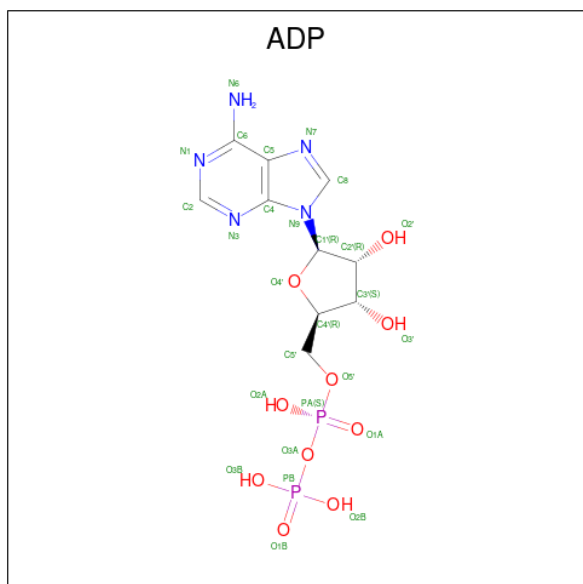
Mol	Chain	Residues	Atoms		AltConf
55	T	1	Total	Zn	0
			1	1	

- 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).

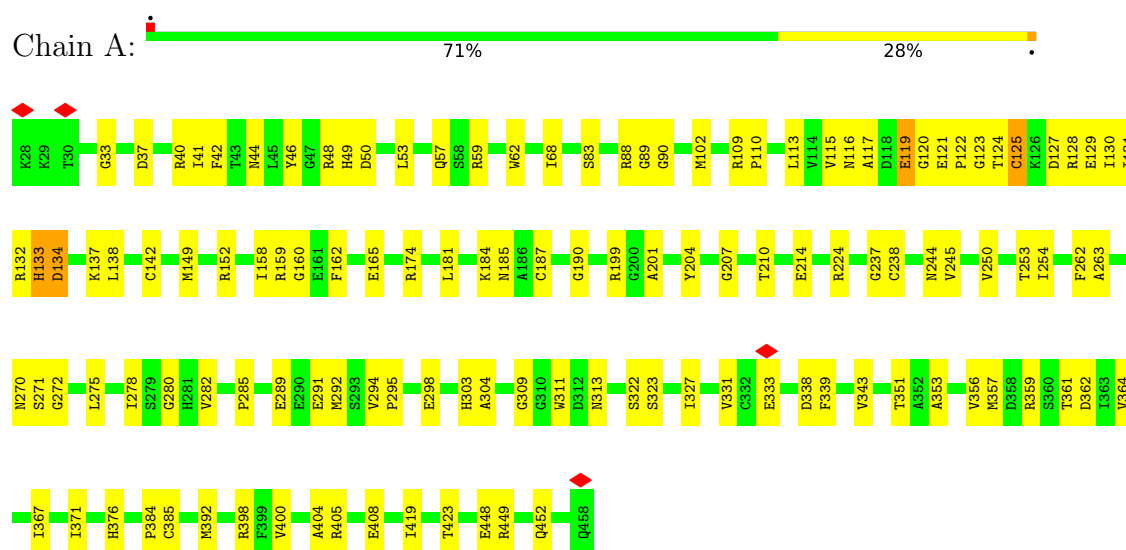


Mol	Chain	Residues	Atoms					AltConf
57	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

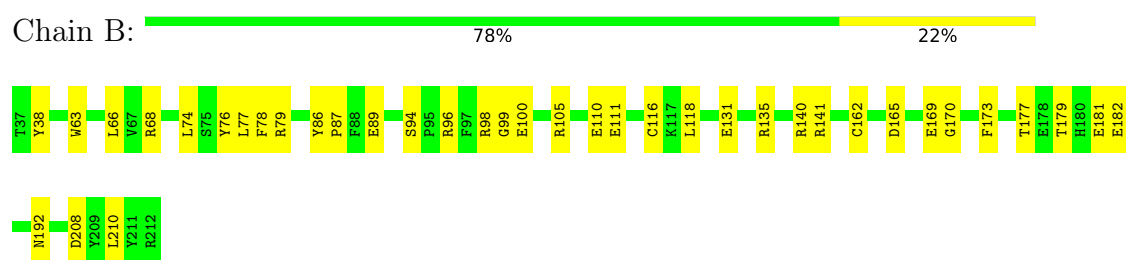
3 Residue-property plots

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.

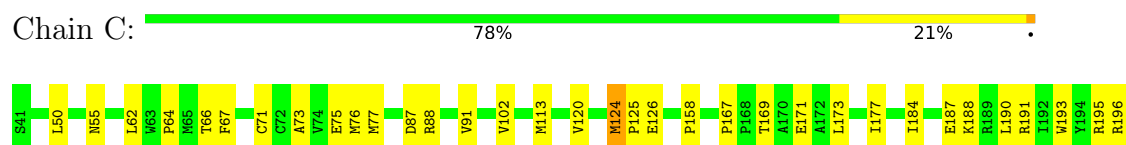
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



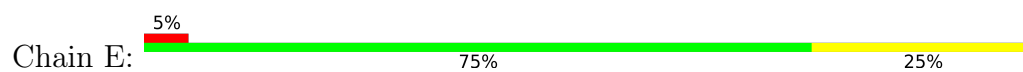
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



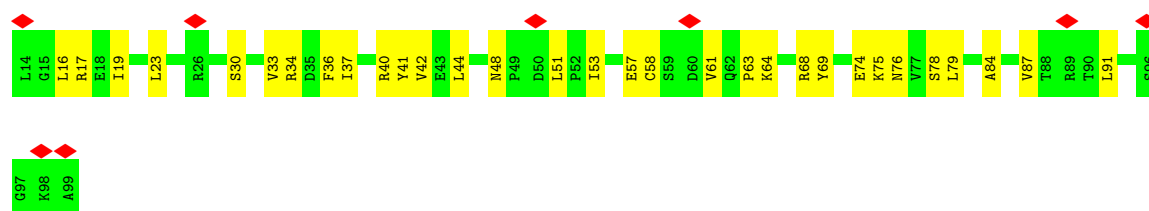
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



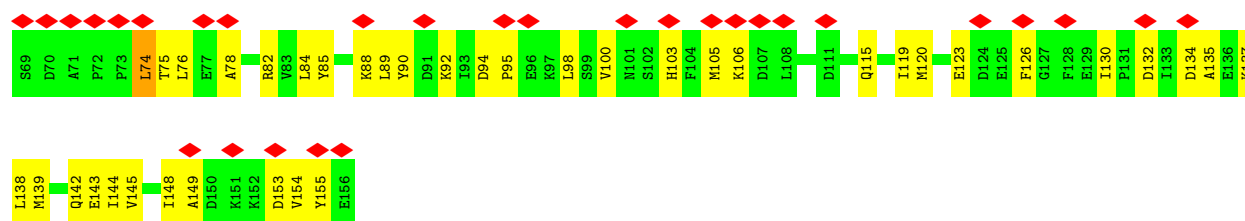
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



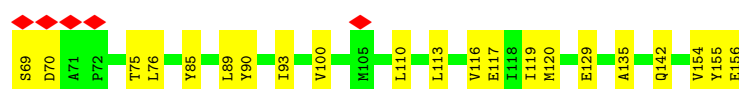
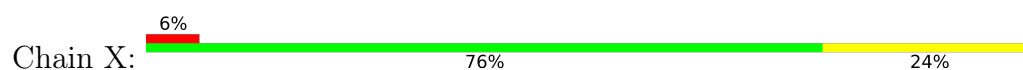
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



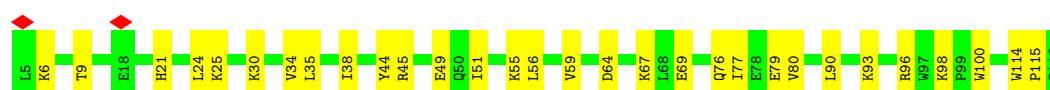
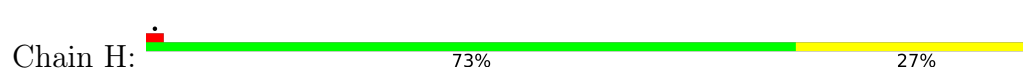
- Molecule 6: Acyl carrier protein, mitochondrial



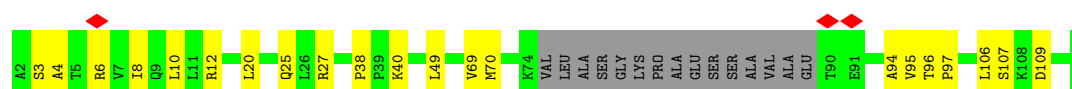
- Molecule 6: Acyl carrier protein, mitochondrial



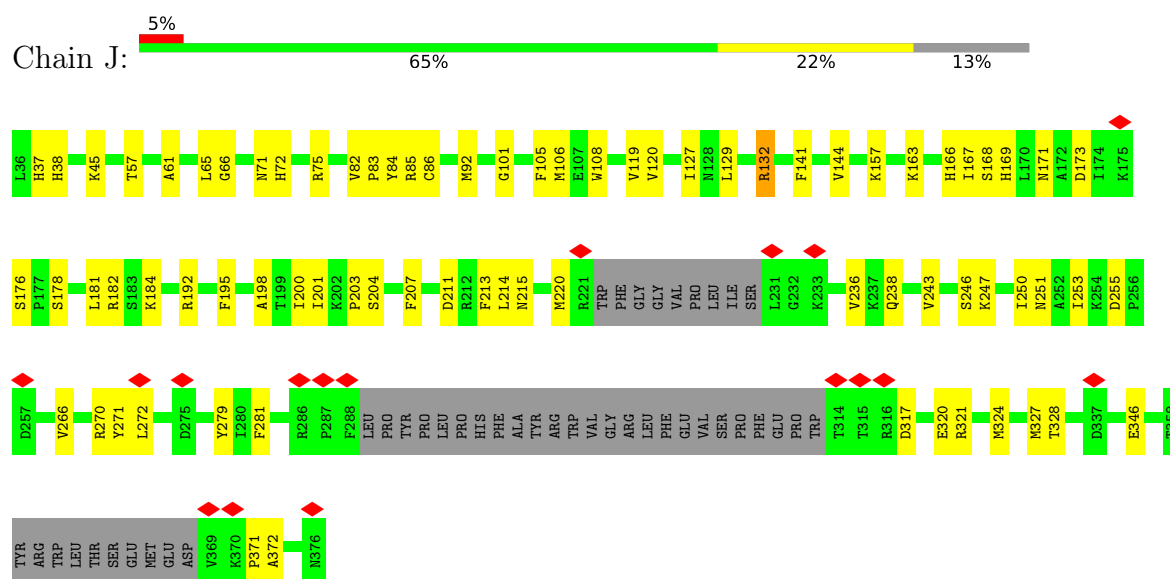
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



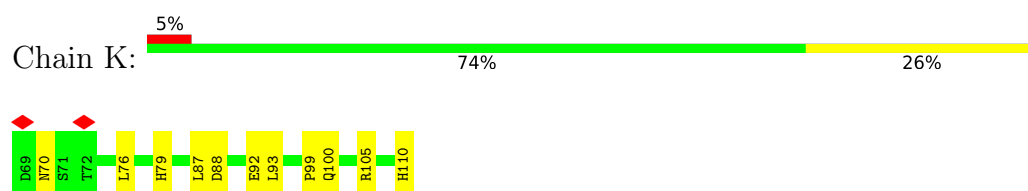
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



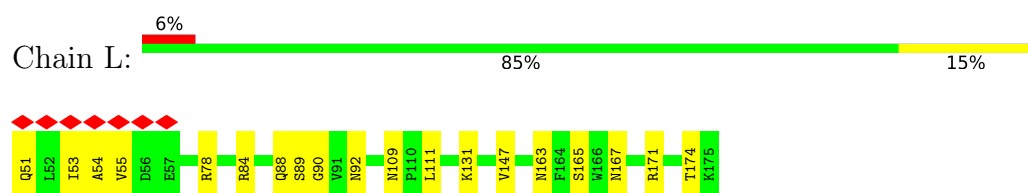
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



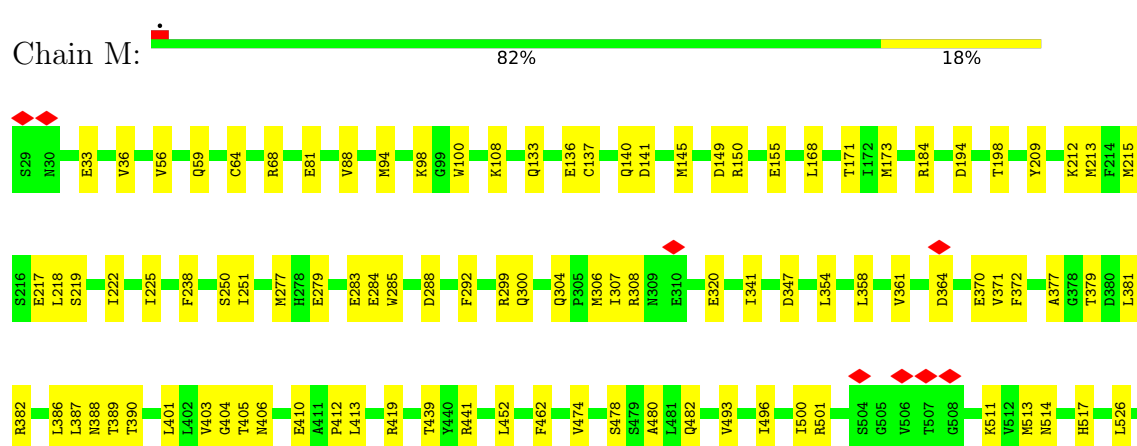
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



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

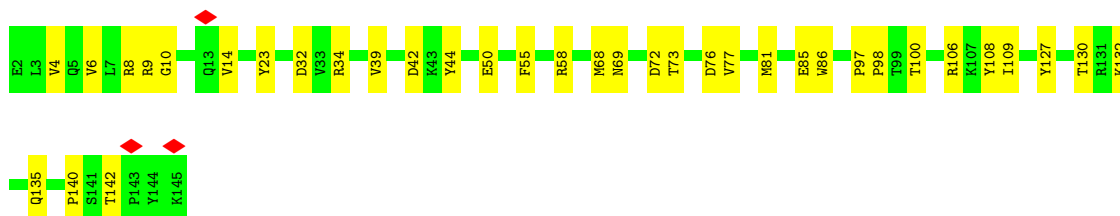
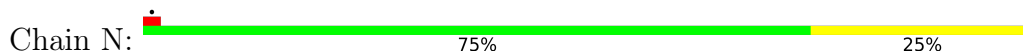


- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

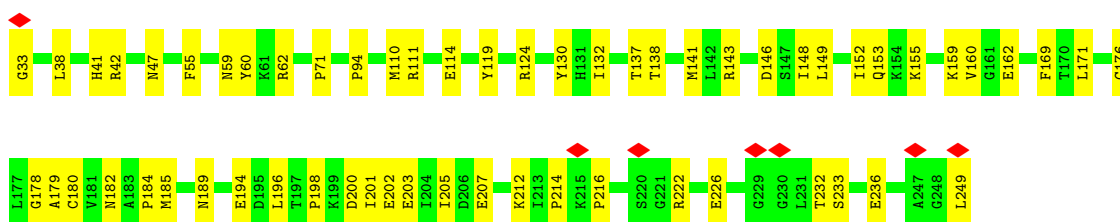




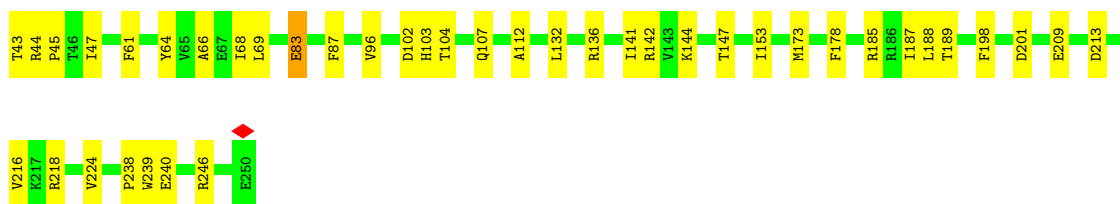
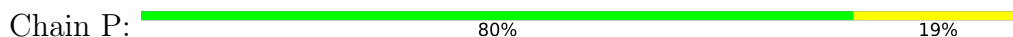
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



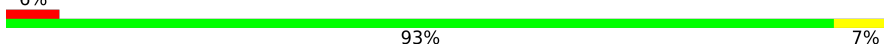
R463

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

Chain S:  89% 11%



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

Chain T:  6% 93% 7%



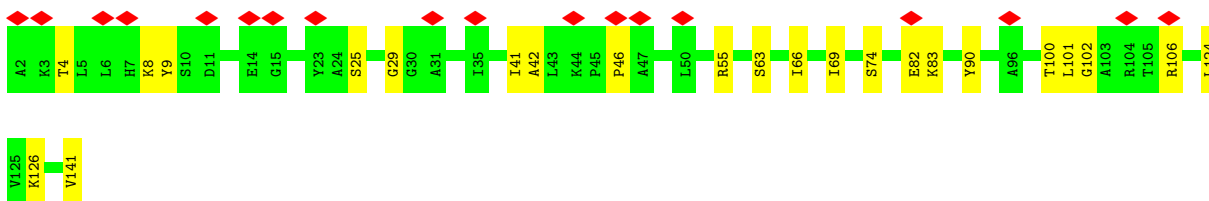
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:  89% 11%



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

Chain V:  13% 84% 16%



- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:  80% 20%

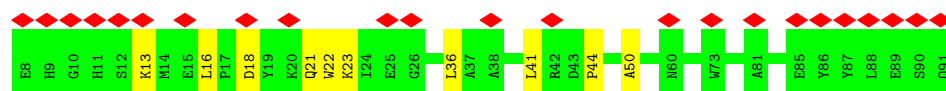
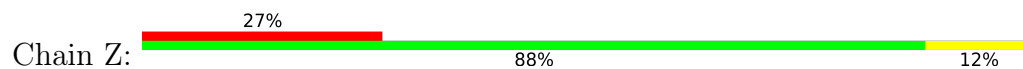


- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

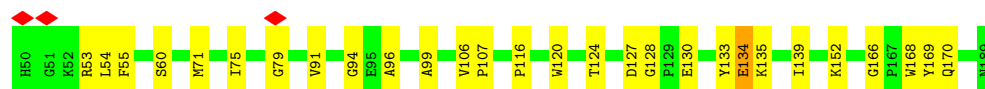
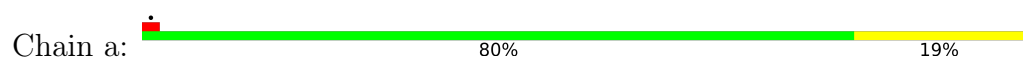
Chain Y:  17% 71% 26%



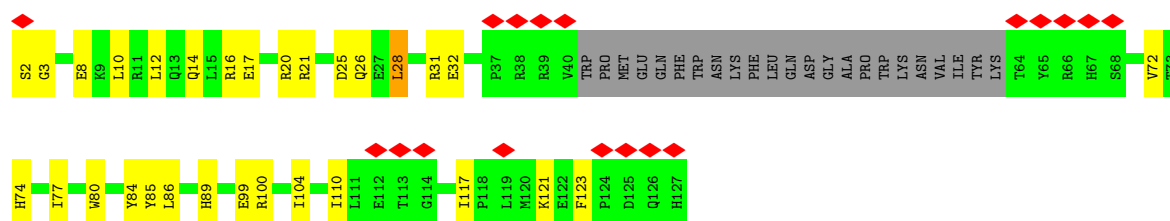
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



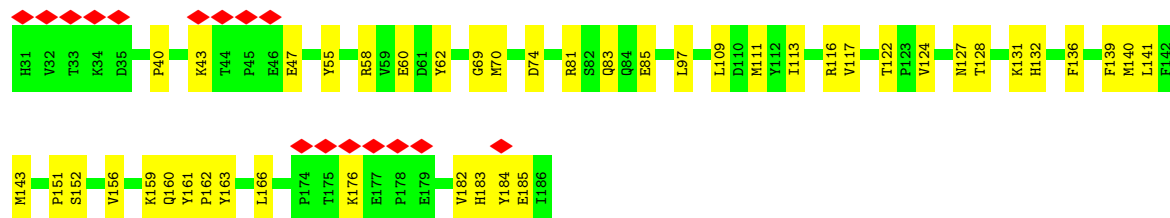
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



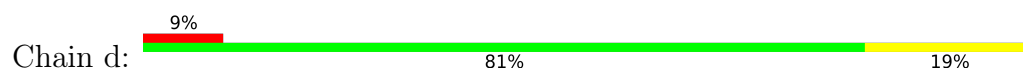
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

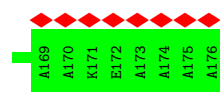


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

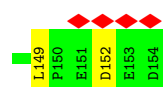
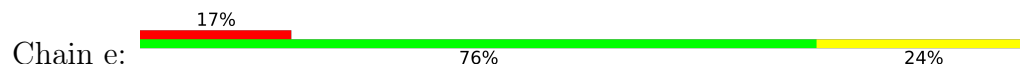


- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

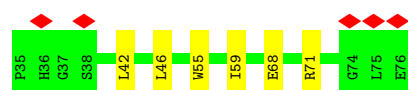
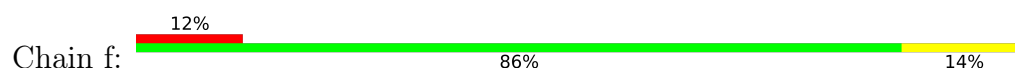




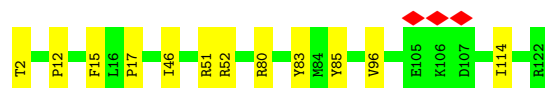
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



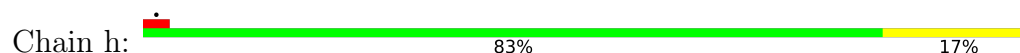
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



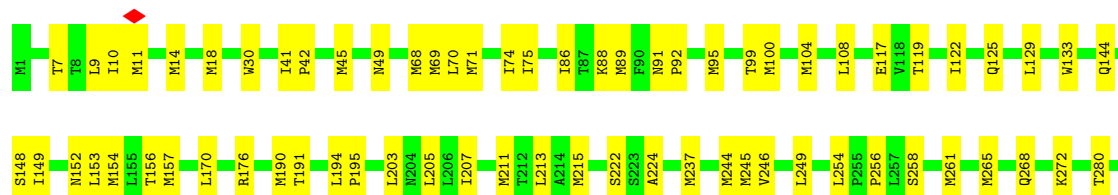
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



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

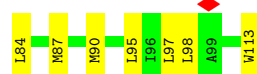
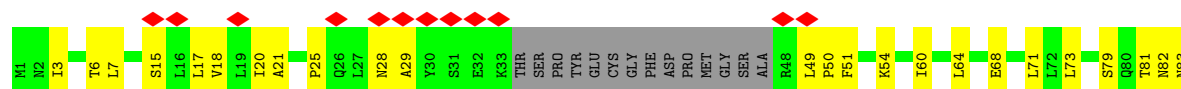


- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

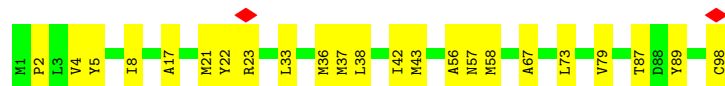
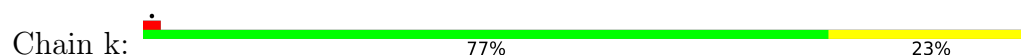




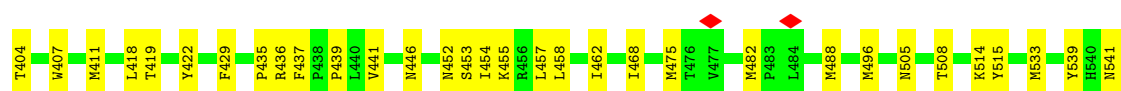
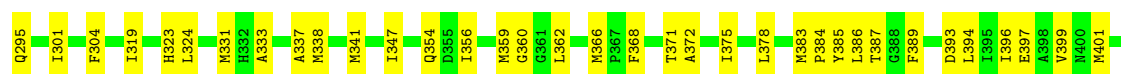
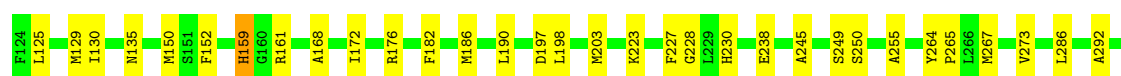
• Molecule 33: NADH-ubiquinone oxidoreductase chain 3



• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

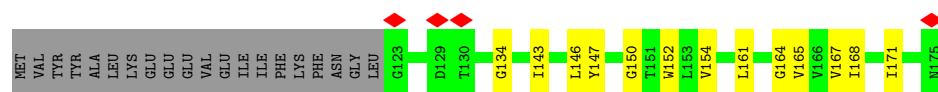


• Molecule 35: NADH-ubiquinone oxidoreductase chain 5

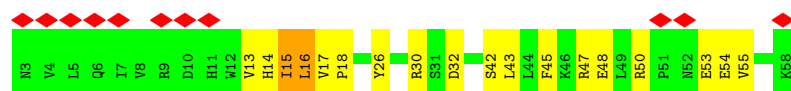


• Molecule 36: NADH-ubiquinone oxidoreductase chain 6





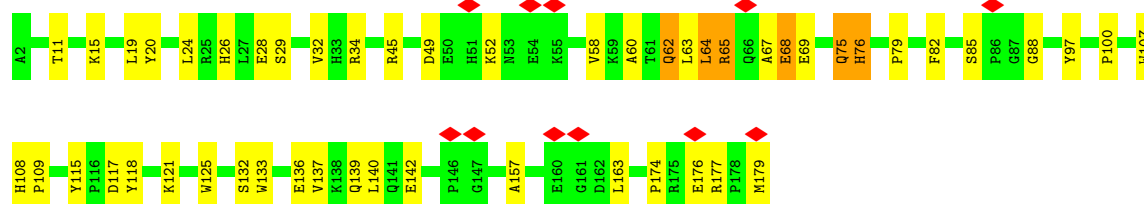
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



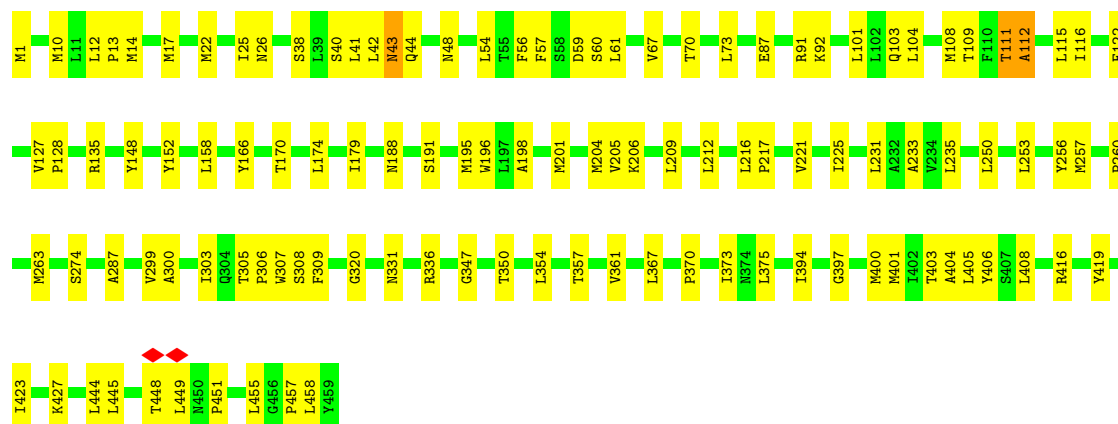
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



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

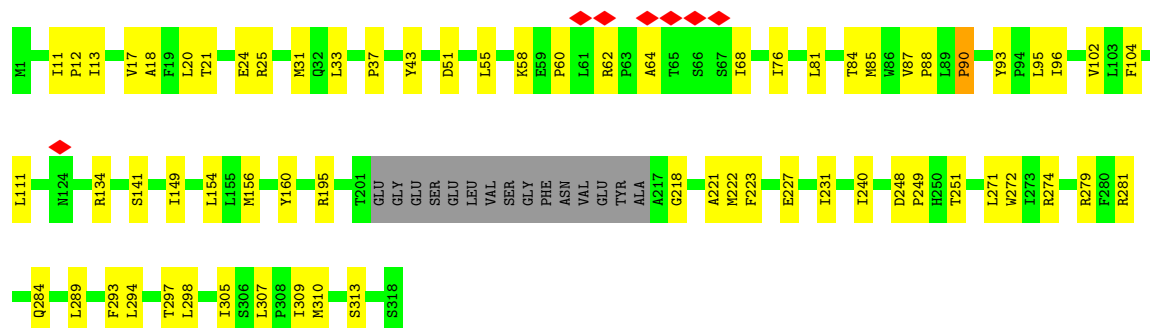


- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

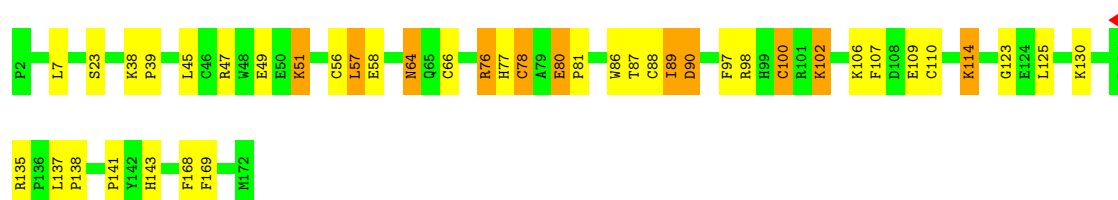
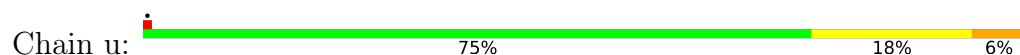


- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

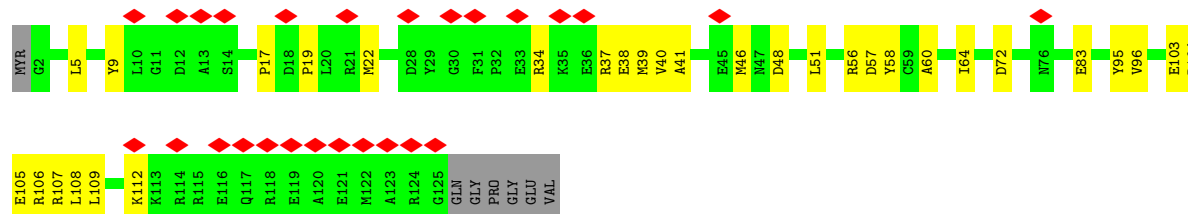




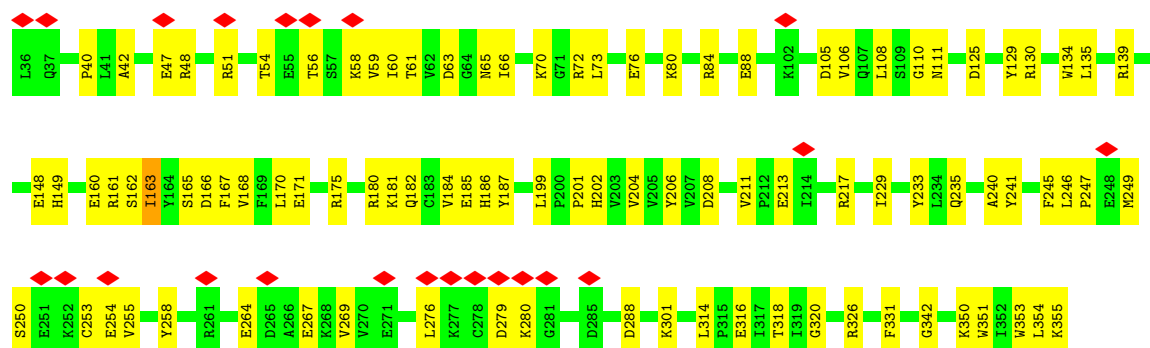
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- 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	169835	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	0.209	Depositor
Minimum map value	-0.127	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0243	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.23	0/3393	0.48	5/4584 (0.1%)
2	B	0.27	0/1443	0.41	0/1952
3	C	0.26	0/1279	0.51	2/1730 (0.1%)
4	E	0.18	0/995	0.34	0/1340
5	F	0.19	0/702	0.46	0/945
6	G	0.19	0/705	0.47	0/956
6	X	0.18	0/708	0.42	0/959
7	H	0.19	0/929	0.34	0/1258
8	I	0.29	0/780	0.54	0/1059
9	J	0.21	0/2411	0.45	1/3254 (0.0%)
10	K	0.17	0/365	0.44	0/493
11	L	0.22	0/1039	0.36	0/1403
12	M	0.22	0/5384	0.38	0/7295
13	N	0.19	0/1245	0.38	0/1694
14	O	0.20	0/1711	0.41	0/2328
15	P	0.24	0/1789	0.43	0/2436
16	Q	0.27	0/3451	0.48	3/4672 (0.1%)
17	S	0.25	0/582	0.46	0/783
18	T	0.17	0/755	0.32	0/1018
19	U	0.17	0/664	0.33	0/912
20	V	0.17	0/1042	0.37	0/1411
21	W	0.20	0/1192	0.31	0/1610
22	Y	0.21	0/609	0.56	2/835 (0.2%)
23	Z	0.13	0/695	0.30	0/939
24	a	0.24	0/1185	0.47	2/1606 (0.1%)
25	b	0.22	0/902	0.47	0/1227
26	c	0.20	0/1371	0.37	0/1875
27	d	0.18	0/1494	0.37	0/2015
28	e	0.18	0/916	0.37	0/1246
29	f	0.15	0/350	0.27	0/473
30	g	0.18	0/1031	0.33	0/1394
31	h	0.19	0/889	0.35	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.26	0/2769	0.47	0/3764
33	j	0.26	0/819	0.47	0/1117
34	k	0.23	0/759	0.41	0/1029
35	l	0.23	0/4914	0.46	2/6683 (0.0%)
36	m	0.23	0/970	0.43	0/1316
37	n	0.25	0/468	0.65	1/633 (0.2%)
38	o	0.17	0/1088	0.33	0/1477
39	p	0.22	0/1590	0.55	3/2155 (0.1%)
40	r	0.26	0/3723	0.47	0/5078
41	s	0.25	0/2464	0.49	2/3369 (0.1%)
42	u	0.27	0/1436	0.53	2/1938 (0.1%)
43	v	0.20	0/1044	0.45	0/1403
44	w	0.21	0/2634	0.48	1/3571 (0.0%)
All	All	0.22	0/66684	0.44	26/90425 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	p	75	GLN	N-CA-C	9.47	121.60	111.28
39	p	62	GLN	N-CA-C	-9.05	101.41	111.28
1	A	120	GLY	N-CA-C	8.29	122.68	112.73
39	p	65	ARG	N-CA-C	-7.66	103.55	113.12
35	l	600	THR	N-CA-C	7.55	119.30	111.14
1	A	133	HIS	N-CA-C	6.66	118.62	111.36
9	J	86	CYS	N-CA-C	6.11	118.41	110.53
3	C	124	MET	CA-C-N	6.10	126.01	119.85
3	C	124	MET	C-N-CA	6.10	126.01	119.85
41	s	93	TYR	CA-C-N	5.77	125.68	119.85
41	s	93	TYR	C-N-CA	5.77	125.68	119.85
35	l	601	LEU	N-CA-C	5.73	117.33	111.14
16	Q	217	VAL	N-CA-C	5.66	116.44	110.72
24	a	128	GLY	CA-C-N	5.66	125.34	119.05
24	a	128	GLY	C-N-CA	5.66	125.34	119.05

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	ARG	N-CA-C	5.53	117.11	111.14
44	w	163	ILE	N-CA-C	-5.52	104.99	110.62
22	Y	88	ASP	CA-C-N	5.43	125.08	119.05
22	Y	88	ASP	C-N-CA	5.43	125.08	119.05
37	n	16	LEU	N-CA-C	5.37	117.13	111.28
16	Q	224	ALA	N-CA-C	5.29	117.05	111.28
16	Q	142	VAL	N-CA-C	-5.15	107.40	113.42
1	A	134	ASP	CA-C-N	5.04	124.34	118.85
1	A	134	ASP	C-N-CA	5.04	124.34	118.85
42	u	80	GLU	CA-C-N	5.04	125.06	119.32
42	u	80	GLU	C-N-CA	5.04	125.06	119.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	126	GLU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3318	0	3280	100	0
2	B	1412	0	1363	41	0
3	C	1248	0	1254	39	0
4	E	971	0	975	21	0
5	F	691	0	704	21	0
6	G	693	0	671	35	0
6	X	696	0	680	18	0
7	H	910	0	950	20	0
8	I	762	0	766	21	0
9	J	2359	0	2402	56	0
10	K	355	0	329	11	0
11	L	1016	0	1016	16	0
12	M	5296	0	5326	81	0
13	N	1204	0	1162	27	0
14	O	1671	0	1673	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	P	1738	0	1693	32	0
16	Q	3377	0	3320	76	0
17	S	567	0	565	7	0
18	T	741	0	702	7	0
19	U	643	0	642	8	0
20	V	1021	0	1027	16	0
21	W	1161	0	1144	33	0
22	Y	583	0	525	57	0
23	Z	674	0	643	7	0
24	a	1152	0	1154	29	0
25	b	875	0	895	45	0
26	c	1315	0	1208	40	0
27	d	1461	0	1429	34	0
28	e	890	0	837	26	0
29	f	342	0	341	3	0
30	g	1000	0	994	10	0
31	h	867	0	871	14	0
32	i	2706	0	2863	84	0
33	j	800	0	855	44	0
34	k	748	0	799	24	0
35	l	4785	0	4933	145	0
36	m	948	0	960	33	0
37	n	456	0	433	22	0
38	o	1058	0	1061	13	0
39	p	1534	0	1470	51	0
40	r	3631	0	3839	104	0
41	s	2394	0	2508	61	0
42	u	1398	0	1380	42	0
43	v	1020	0	957	71	0
44	w	2574	0	2516	71	0
45	A	8	0	0	2	0
45	B	16	0	0	0	0
45	C	8	0	0	0	0
45	M	16	0	0	0	0
46	A	31	0	19	2	0
47	A	44	0	27	7	0
48	B	51	0	82	1	0
48	C	47	0	71	16	0
48	Q	47	0	71	22	0
48	W	41	0	59	16	0
48	j	51	0	82	5	0
48	l	92	0	138	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	r	51	0	82	12	0
49	C	52	0	88	2	0
49	a	52	0	88	6	0
49	g	52	0	88	5	0
49	j	52	0	88	4	0
49	r	104	0	176	10	0
50	G	35	0	0	0	0
50	X	35	0	0	0	0
51	I	51	0	46	12	0
51	a	91	0	132	44	0
51	i	66	0	76	18	0
51	l	199	0	307	65	0
51	r	100	0	156	11	0
51	u	78	0	103	18	0
52	J	48	0	23	6	0
53	M	4	0	0	0	0
53	O	4	0	0	0	0
54	M	1	0	0	0	0
55	T	1	0	0	0	0
56	s	28	0	31	6	0
57	w	27	0	11	1	0
All	All	66644	0	67159	1596	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 12.

All (1596) 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)
22:Y:99:ILE:CD1	43:v:108:LEU:HD23	1.15	1.54
22:Y:99:ILE:HD13	43:v:108:LEU:CD2	1.36	1.52
22:Y:97:LEU:HD12	43:v:104:ARG:CA	1.50	1.40
33:j:68:GLU:OE2	33:j:98:LEU:CD1	1.78	1.30
1:A:119:GLU:OE2	1:A:127:ASP:CB	1.83	1.24
1:A:119:GLU:OE2	1:A:127:ASP:HB2	1.05	1.22
42:u:78:CYS:HB3	42:u:110:CYS:SG	1.79	1.21
22:Y:97:LEU:CG	43:v:107:ARG:HH21	1.53	1.20
42:u:80:GLU:HB2	42:u:81:PRO:HD3	1.21	1.18
52:J:401:NDP:O4D	52:J:401:NDP:C4D	1.69	1.16
26:c:128:THR:O	26:c:132:HIS:HD2	1.27	1.14
51:a:201:CDL:H772	51:a:201:CDL:H201	1.25	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:99:ILE:CD1	43:v:108:LEU:CD2	2.05	1.13
1:A:119:GLU:CD	1:A:127:ASP:HB2	1.73	1.11
22:Y:97:LEU:HG	43:v:107:ARG:HH21	0.98	1.10
22:Y:99:ILE:HG13	43:v:107:ARG:HB3	1.35	1.08
48:W:201:PEE:H13	33:j:3:ILE:HG21	1.23	1.07
22:Y:97:LEU:HD12	43:v:104:ARG:HA	1.31	1.07
51:u:201:CDL:H581	51:u:201:CDL:H542	1.33	1.05
39:p:19:LEU:HD13	39:p:68:GLU:OE2	1.56	1.05
51:a:201:CDL:H521	48:l:704:PEE:H14	1.36	1.04
40:r:1:MET:SD	40:r:111:THR:HG21	1.97	1.04
51:l:701:CDL:H312	51:l:701:CDL:H742	1.04	1.04
22:Y:99:ILE:HD11	43:v:108:LEU:HD23	1.37	1.03
22:Y:97:LEU:HD12	43:v:104:ARG:N	1.74	1.03
51:a:201:CDL:H251	51:a:201:CDL:H211	1.37	1.02
51:l:701:CDL:C65	51:l:701:CDL:H862	1.89	1.02
51:a:201:CDL:H761	51:a:201:CDL:H192	1.40	1.02
3:C:50:LEU:CD2	48:C:302:PEE:H27	1.89	1.02
22:Y:97:LEU:HG	43:v:107:ARG:NH2	1.74	1.01
48:l:703:PEE:H55	40:r:405:LEU:HD21	1.42	1.01
44:w:165:SER:HB3	44:w:245:PHE:CE1	1.95	1.01
51:a:201:CDL:H521	48:l:704:PEE:C11	1.90	1.00
51:a:201:CDL:H761	51:a:201:CDL:C19	1.92	1.00
32:i:100:MET:HE1	35:l:599:MET:HE2	1.42	1.00
1:A:134:ASP:OD2	1:A:137:LYS:HD2	1.61	1.00
25:b:99:GLU:HG2	35:l:61:MET:HG2	1.42	0.99
51:i:401:CDL:HB31	44:w:40:PRO:CG	1.92	0.99
51:l:701:CDL:H271	51:l:701:CDL:H232	1.44	0.99
22:Y:97:LEU:HD12	43:v:104:ARG:CB	1.93	0.98
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.43	0.98
33:j:68:GLU:OE2	33:j:98:LEU:HD13	1.61	0.98
51:l:701:CDL:H312	51:l:701:CDL:C74	1.92	0.98
3:C:50:LEU:HD21	48:C:302:PEE:H27	1.45	0.97
33:j:68:GLU:OE2	33:j:98:LEU:HD12	1.61	0.97
26:c:128:THR:O	26:c:132:HIS:CD2	2.18	0.97
48:W:201:PEE:H13	33:j:3:ILE:CG2	1.94	0.96
51:l:701:CDL:H432	51:l:701:CDL:H602	1.47	0.96
22:Y:97:LEU:CD2	43:v:107:ARG:HH21	1.77	0.96
40:r:191:SER:HB3	48:r:501:PEE:H2	1.47	0.96
51:a:201:CDL:H201	51:a:201:CDL:C77	1.96	0.96
51:a:201:CDL:H431	27:d:44:PRO:HB3	1.45	0.95
51:i:401:CDL:HB31	44:w:40:PRO:HG3	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:97:LEU:CD1	43:v:104:ARG:HB2	1.96	0.95
25:b:25:ASP:OD2	39:p:125:TRP:NE1	1.98	0.95
51:I:201:CDL:H532	51:I:201:CDL:CA7	1.97	0.94
6:G:74:LEU:H	6:G:74:LEU:HD23	1.31	0.94
22:Y:97:LEU:CD1	43:v:104:ARG:CA	2.45	0.93
24:a:79:GLY:HA3	51:a:201:CDL:H222	1.50	0.93
48:W:201:PEE:H10	48:W:201:PEE:H2	1.50	0.92
48:Q:501:PEE:H37	48:Q:501:PEE:H60	1.51	0.92
26:c:116:ARG:HG2	48:l:703:PEE:H49	1.52	0.91
41:s:87:VAL:HG23	41:s:88:PRO:HD3	1.48	0.91
22:Y:97:LEU:CD2	43:v:107:ARG:NH2	2.32	0.91
22:Y:97:LEU:CG	43:v:107:ARG:NH2	2.31	0.91
51:I:201:CDL:H532	51:I:201:CDL:C31	2.02	0.89
22:Y:97:LEU:HD23	43:v:107:ARG:NH2	1.88	0.89
39:p:19:LEU:CD1	39:p:68:GLU:OE2	2.20	0.88
51:l:701:CDL:H862	51:l:701:CDL:H651	1.54	0.88
22:Y:97:LEU:CD1	43:v:104:ARG:N	2.37	0.88
51:l:701:CDL:H601	51:l:701:CDL:H791	1.56	0.87
22:Y:97:LEU:HD13	43:v:104:ARG:HB2	1.55	0.87
51:l:701:CDL:H472	40:r:445:LEU:HB2	1.57	0.87
32:i:256:PRO:HB2	51:u:201:CDL:H612	1.55	0.87
51:l:701:CDL:H452	40:r:445:LEU:HB3	1.55	0.87
22:Y:99:ILE:HD12	43:v:108:LEU:HD23	1.54	0.86
42:u:80:GLU:CB	42:u:81:PRO:HD3	2.05	0.86
8:I:3:SER:O	51:I:201:CDL:HA22	1.74	0.86
6:G:75:THR:HG23	6:G:78:ALA:H	1.40	0.86
51:i:401:CDL:HB31	44:w:40:PRO:CB	2.05	0.86
22:Y:99:ILE:HG13	43:v:107:ARG:CB	2.06	0.85
9:J:83:PRO:HA	9:J:106:MET:O	1.77	0.85
32:i:95:MET:CE	32:i:149:ILE:HG22	2.07	0.85
51:a:201:CDL:H422	51:a:201:CDL:H381	1.59	0.85
48:Q:501:PEE:H7	35:l:567:SER:OG	1.77	0.84
51:l:701:CDL:H541	51:l:701:CDL:HA62	1.57	0.84
16:Q:46:GLN:HB3	48:Q:501:PEE:N	1.92	0.84
42:u:80:GLU:HB2	42:u:81:PRO:CD	2.06	0.84
39:p:60:ALA:O	39:p:63:LEU:O	1.95	0.83
43:v:104:ARG:O	43:v:108:LEU:HG	1.78	0.83
51:l:701:CDL:H862	51:l:701:CDL:H652	1.59	0.83
40:r:1:MET:SD	40:r:111:THR:CG2	2.66	0.83
35:l:78:LEU:HD11	51:l:701:CDL:H251	1.61	0.83
44:w:139:ARG:NH1	44:w:166:ASP:OD2	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:97:LEU:CD1	43:v:104:ARG:CB	2.55	0.82
24:a:127:ASP:OD1	49:a:202:PLX:H12	1.79	0.82
48:W:201:PEE:H15	48:W:201:PEE:H24	1.61	0.82
35:l:541:ASN:HD22	48:l:703:PEE:H61	1.40	0.82
41:s:51:ASP:HB3	56:s:401:UQ:H8	1.62	0.81
22:Y:99:ILE:HD13	43:v:108:LEU:HD21	1.57	0.81
22:Y:99:ILE:CG1	43:v:107:ARG:HB3	2.10	0.81
51:l:701:CDL:H601	51:l:701:CDL:H772	1.62	0.81
3:C:50:LEU:HD11	48:C:302:PEE:H59	1.60	0.81
51:l:701:CDL:H742	51:l:701:CDL:C31	2.00	0.81
37:n:13:VAL:CG1	40:r:14:MET:HG2	2.09	0.81
35:l:103:PHE:HB2	35:l:341:MET:HE1	1.62	0.81
27:d:26:LEU:HD12	27:d:27:PRO:HD2	1.63	0.80
48:W:201:PEE:H24	48:W:201:PEE:C12	2.11	0.80
51:u:201:CDL:H542	51:u:201:CDL:C58	2.10	0.80
1:A:204:TYR:OH	47:A:503:NAI:H5N	1.81	0.80
38:o:121:LEU:HD23	38:o:123:GLN:HE21	1.44	0.80
44:w:165:SER:HB3	44:w:245:PHE:CD1	2.16	0.80
32:i:88:LYS:HA	32:i:148:SER:OG	1.82	0.79
41:s:84:THR:O	41:s:87:VAL:HG22	1.82	0.79
25:b:104:ILE:HB	43:v:48:ASP:HB3	1.65	0.79
25:b:100:ARG:HB3	35:l:60:GLU:HB2	1.65	0.79
22:Y:99:ILE:HD13	43:v:108:LEU:HD23	0.79	0.79
20:V:69:ILE:HG13	20:V:100:THR:HG21	1.65	0.78
25:b:14:GLN:HE22	39:p:157:ALA:HB3	1.46	0.78
48:l:704:PEE:H31	40:r:449:LEU:CD2	2.13	0.78
41:s:307:LEU:HA	41:s:310:MET:HE2	1.65	0.78
3:C:50:LEU:HD22	48:C:302:PEE:H27	1.65	0.78
24:a:130:GLU:HG3	37:n:45:PHE:CD1	2.19	0.78
1:A:33:GLY:HA2	1:A:294:VAL:HG12	1.65	0.78
5:F:16:LEU:HD21	5:F:19:ILE:HD11	1.63	0.78
42:u:169:PHE:CE1	51:u:201:CDL:H561	2.19	0.78
48:Q:501:PEE:C22	48:Q:501:PEE:H28	2.14	0.77
17:S:31:ASN:OD1	17:S:60:TYR:OH	2.01	0.77
51:a:201:CDL:H712	51:a:201:CDL:H172	1.67	0.77
44:w:72:ARG:HH12	44:w:264:GLU:HA	1.49	0.77
44:w:168:VAL:HG12	44:w:240:ALA:HB1	1.66	0.77
51:l:701:CDL:H791	51:l:701:CDL:C60	2.15	0.77
1:A:119:GLU:OE2	1:A:127:ASP:CA	2.32	0.76
8:I:4:ALA:HA	51:I:201:CDL:OA2	1.84	0.76
24:a:133:TYR:OH	27:d:87:GLU:HG2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:71:CYS:HB3	16:Q:141:TYR:CG	2.21	0.76
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.19	0.76
8:I:6:ARG:O	8:I:10:LEU:HD23	1.83	0.76
43:v:109:LEU:O	43:v:109:LEU:HD23	1.86	0.76
51:a:201:CDL:C43	27:d:44:PRO:HB3	2.16	0.76
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.19	0.76
26:c:136:PHE:O	26:c:140:MET:HG2	1.86	0.76
40:r:56:PHE:HB3	40:r:111:THR:HB	1.68	0.76
32:i:88:LYS:CA	32:i:148:SER:OG	2.33	0.75
51:l:701:CDL:HA62	51:l:701:CDL:C54	2.16	0.75
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.19	0.75
2:B:68:ARG:NH2	21:W:26:PRO:O	2.19	0.74
8:I:70:MET:HG2	15:P:66:ALA:HB1	1.68	0.74
51:a:201:CDL:H192	51:a:201:CDL:H732	1.67	0.74
32:i:125:GLN:CG	51:i:401:CDL:OA3	2.34	0.74
43:v:19:PRO:HA	43:v:22:MET:HE2	1.69	0.74
24:a:130:GLU:HG3	37:n:45:PHE:CE1	2.22	0.74
51:l:701:CDL:C57	51:l:701:CDL:H871	2.18	0.74
51:l:701:CDL:H351	40:r:361:VAL:HG13	1.70	0.74
33:j:79:SER:HA	33:j:87:MET:HE2	1.70	0.74
51:u:201:CDL:H581	51:u:201:CDL:C54	2.07	0.74
16:Q:81:THR:HG22	16:Q:100:GLU:HG2	1.70	0.74
1:A:102:MET:HG2	1:A:149:MET:HB3	1.69	0.74
48:l:704:PEE:O2P	49:r:503:PLX:C1C	2.36	0.74
1:A:134:ASP:OD2	1:A:137:LYS:CD	2.35	0.74
48:Q:501:PEE:C25	48:Q:501:PEE:H34	2.17	0.74
32:i:125:GLN:HG2	51:i:401:CDL:OA3	1.87	0.74
32:i:213:LEU:HD13	51:i:401:CDL:H141	1.68	0.73
35:l:419:THR:HA	35:l:422:TYR:CE2	2.23	0.73
1:A:41:ILE:O	1:A:137:LYS:NZ	2.21	0.73
51:l:701:CDL:H581	51:l:701:CDL:H622	1.70	0.73
48:Q:501:PEE:H28	48:Q:501:PEE:H36	1.70	0.73
40:r:370:PRO:HB3	40:r:375:LEU:HD22	1.71	0.73
1:A:282:VAL:HG13	1:A:356:VAL:HG21	1.69	0.73
16:Q:68:ASP:O	32:i:49:ASN:ND2	2.21	0.73
32:i:213:LEU:CD1	51:i:401:CDL:H141	2.19	0.73
16:Q:139:LEU:HD11	16:Q:424:ILE:HD13	1.70	0.73
51:l:701:CDL:H792	51:l:701:CDL:H552	1.68	0.73
1:A:121:GLU:OE2	1:A:323:SER:HB2	1.89	0.72
51:a:201:CDL:H211	51:a:201:CDL:C25	2.19	0.72
51:l:701:CDL:H541	51:l:701:CDL:CA6	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:60:ILE:HG21	36:m:168:ILE:HG21	1.71	0.72
40:r:42:LEU:O	40:r:44:GLN:N	2.23	0.72
51:a:201:CDL:H422	51:a:201:CDL:C38	2.17	0.71
48:C:302:PEE:H9	33:j:29:ALA:HB3	1.73	0.71
6:G:82:ARG:HE	6:G:126:PHE:HE1	1.38	0.71
32:i:100:MET:CE	35:l:599:MET:HE2	2.19	0.71
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.71	0.71
12:M:299:ARG:HG2	13:N:135:GLN:HE21	1.55	0.71
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.22	0.71
51:l:701:CDL:H572	51:l:701:CDL:C87	2.21	0.71
1:A:362:ASP:OD1	1:A:449:ARG:NH2	2.23	0.71
25:b:123:PHE:HB3	43:v:40:VAL:HG21	1.70	0.71
32:i:95:MET:HE2	32:i:149:ILE:HG22	1.70	0.71
51:l:701:CDL:H851	51:l:701:CDL:H811	1.73	0.71
12:M:81:GLU:HB3	12:M:88:VAL:HG12	1.73	0.71
6:G:74:LEU:HD23	6:G:74:LEU:N	2.06	0.70
34:k:98:CYS:HB2	35:l:580:GLN:HB2	1.73	0.70
44:w:139:ARG:HD2	44:w:166:ASP:OD2	1.90	0.70
3:C:50:LEU:CD2	48:C:302:PEE:C18	2.68	0.70
32:i:71:MET:HE3	32:i:71:MET:HA	1.73	0.70
3:C:50:LEU:HD21	48:C:302:PEE:C18	2.21	0.70
44:w:246:LEU:HD12	44:w:255:VAL:HG11	1.73	0.70
6:G:76:LEU:HD21	6:G:154:VAL:HG23	1.72	0.70
18:T:28:GLY:N	18:T:69:ASP:OD2	2.24	0.70
25:b:28:LEU:HD12	25:b:28:LEU:N	2.05	0.70
41:s:62:ARG:HE	41:s:68:ILE:HD13	1.55	0.70
16:Q:46:GLN:HB3	48:Q:501:PEE:H4	1.56	0.70
8:I:70:MET:HG2	15:P:66:ALA:CB	2.21	0.70
44:w:88:GLU:OE2	44:w:161:ARG:NH1	2.25	0.70
48:Q:501:PEE:H34	48:Q:501:PEE:H41	1.72	0.69
4:E:127:ASP:OD2	9:J:45:LYS:NZ	2.25	0.69
32:i:88:LYS:CB	32:i:148:SER:OG	2.40	0.69
32:i:11:MET:HE1	51:i:401:CDL:H771	1.72	0.69
1:A:121:GLU:OE2	1:A:323:SER:CB	2.40	0.69
51:l:701:CDL:H273	51:l:701:CDL:C66	2.23	0.69
27:d:24:THR:HG22	27:d:26:LEU:H	1.56	0.69
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.74	0.69
42:u:77:HIS:CD2	42:u:114:LYS:HG2	2.27	0.69
2:B:177:THR:HG21	2:B:182:GLU:HB2	1.74	0.69
6:G:145:VAL:HA	6:G:148:ILE:HD12	1.75	0.69
24:a:54:LEU:C	25:b:28:LEU:HD11	2.18	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:182:VAL:HG13	43:v:34:ARG:HH22	1.58	0.69
35:l:593:ILE:HA	35:l:596:MET:HE2	1.73	0.69
1:A:119:GLU:OE1	1:A:124:THR:HG22	1.93	0.68
51:a:201:CDL:H761	51:a:201:CDL:C20	2.23	0.68
51:a:201:CDL:H201	51:a:201:CDL:C76	2.23	0.68
35:l:590:SER:O	35:l:594:THR:HG22	1.93	0.68
48:W:201:PEE:H10	48:W:201:PEE:C1	2.22	0.68
25:b:89:HIS:CE1	48:l:704:PEE:H50	2.29	0.68
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.76	0.68
22:Y:97:LEU:HD23	43:v:107:ARG:HH22	1.57	0.68
51:a:201:CDL:H751	28:e:103:SER:HB2	1.76	0.68
35:l:123:LEU:HB2	35:l:150:MET:HE2	1.74	0.68
48:l:704:PEE:O2P	49:r:503:PLX:H1C3	1.93	0.68
32:i:207:ILE:HG22	32:i:211:MET:HE2	1.74	0.68
35:l:372:ALA:HA	35:l:458:LEU:HD21	1.76	0.67
40:r:260:PRO:HG2	49:r:502:PLX:H132	1.75	0.67
51:a:201:CDL:H521	48:l:704:PEE:H13	1.74	0.67
34:k:58:MET:HE1	36:m:150:GLY:HA3	1.75	0.67
51:l:201:CDL:C55	51:l:201:CDL:H322	2.24	0.67
1:A:159:ARG:NH2	14:O:176:CYS:O	2.27	0.67
6:G:139:MET:N	6:G:143:GLU:OE2	2.25	0.67
30:g:51:ARG:NH1	32:i:322:GLN:OE1	2.27	0.67
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.76	0.67
51:a:201:CDL:H751	28:e:103:SER:CB	2.25	0.67
39:p:68:GLU:OE2	39:p:68:GLU:HA	1.93	0.67
32:i:91:ASN:ND2	32:i:92:PRO:HD2	2.09	0.67
22:Y:51:THR:HG22	22:Y:53:SER:H	1.60	0.67
5:F:64:LYS:HZ3	5:F:76:ASN:HB2	1.60	0.67
39:p:29:SER:HB3	39:p:76:HIS:HD2	1.60	0.67
4:E:114:ARG:HD3	4:E:115:PRO:HD2	1.77	0.66
32:i:95:MET:HE2	32:i:149:ILE:HA	1.76	0.66
32:i:89:MET:HG3	32:i:95:MET:SD	2.35	0.66
21:W:66:GLU:OE2	42:u:123:GLY:N	2.28	0.66
14:O:38:LEU:O	14:O:124:ARG:NH2	2.26	0.66
6:X:120:MET:HE1	39:p:24:LEU:HB2	1.77	0.66
37:n:14:HIS:CE1	40:r:26:ASN:OD1	2.49	0.66
13:N:32:ASP:OD2	13:N:58:ARG:NH2	2.28	0.66
15:P:44:ARG:HB3	15:P:45:PRO:HD3	1.78	0.66
38:o:27:PRO:HB2	38:o:31:LYS:HZ1	1.61	0.66
40:r:87:GLU:O	40:r:92:LYS:NZ	2.28	0.66
9:J:238:GLN:HG2	9:J:266:VAL:HB	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:63:MET:O	42:u:130:LYS:NZ	2.27	0.65
26:c:160:GLN:OE1	43:v:37:ARG:NH1	2.30	0.65
48:j:201:PEE:H72	48:j:201:PEE:H81	1.79	0.65
39:p:58:VAL:O	39:p:62:GLN:HG2	1.97	0.65
41:s:87:VAL:CG2	41:s:88:PRO:HD3	2.23	0.65
42:u:23:SER:CB	42:u:90:ASP:HB2	2.26	0.65
42:u:78:CYS:CB	42:u:110:CYS:SG	2.72	0.65
35:l:119:LYS:NZ	51:l:701:CDL:H512	2.12	0.65
40:r:1:MET:CG	40:r:111:THR:HG21	2.25	0.65
11:L:109:ASN:ND2	11:L:111:LEU:O	2.30	0.65
41:s:87:VAL:HG23	41:s:88:PRO:CD	2.24	0.65
22:Y:72:ARG:NH1	22:Y:76:ASP:OD2	2.29	0.65
51:l:701:CDL:H581	51:l:701:CDL:H851	1.79	0.65
12:M:308:ARG:NH2	12:M:578:PRO:O	2.30	0.65
16:Q:140:ASP:OD2	16:Q:143:SER:OG	2.15	0.65
51:I:201:CDL:H711	41:s:43:TYR:OH	1.97	0.65
33:j:90:MET:HE3	36:m:154:VAL:HG11	1.79	0.65
41:s:62:ARG:HD3	41:s:64:ALA:H	1.61	0.65
44:w:167:PHE:O	44:w:170:LEU:HB3	1.97	0.65
5:F:40:ARG:HH12	5:F:84:ALA:HB1	1.61	0.64
51:a:201:CDL:H771	28:e:100:VAL:HG13	1.77	0.64
1:A:50:ASP:O	1:A:59:ARG:NH2	2.28	0.64
23:Z:21:GLN:O	23:Z:23:LYS:NZ	2.30	0.64
44:w:246:LEU:CD1	44:w:255:VAL:HG11	2.26	0.64
16:Q:259:GLU:OE1	16:Q:338:ARG:NH2	2.29	0.64
33:j:68:GLU:OE2	33:j:98:LEU:HD11	1.94	0.64
1:A:116:ASN:ND2	1:A:207:GLY:O	2.29	0.64
1:A:123:GLY:N	14:O:180:CYS:SG	2.68	0.64
24:a:135:LYS:NZ	37:n:32:ASP:OD1	2.21	0.64
37:n:13:VAL:HG12	40:r:14:MET:HG2	1.76	0.64
51:a:201:CDL:H381	51:a:201:CDL:C42	2.25	0.64
35:l:591:PHE:O	35:l:595:ILE:HG13	1.97	0.64
32:i:7:THR:HG22	32:i:11:MET:HE2	1.79	0.64
42:u:77:HIS:HD2	42:u:114:LYS:HG2	1.63	0.64
29:f:68:GLU:OE2	29:f:71:ARG:NH2	2.30	0.64
32:i:41:ILE:HG13	34:k:73:LEU:HD21	1.79	0.64
33:j:17:LEU:HD23	41:s:222:MET:HE1	1.78	0.64
22:Y:99:ILE:HD12	43:v:107:ARG:C	2.22	0.64
32:i:45:MET:HE2	36:m:171:ILE:HD12	1.80	0.64
23:Z:22:TRP:HB3	23:Z:50:ALA:HB3	1.80	0.64
25:b:100:ARG:HD3	35:l:60:GLU:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:191:SER:HB3	48:r:501:PEE:C1	2.25	0.64
14:O:152:ILE:HG21	14:O:171:LEU:HD13	1.79	0.63
41:s:87:VAL:N	41:s:88:PRO:HD2	2.13	0.63
34:k:58:MET:HE3	36:m:146:LEU:HA	1.80	0.63
35:l:603:ASN:C	35:l:603:ASN:HD22	2.05	0.63
42:u:76:ARG:O	42:u:76:ARG:HG3	1.97	0.63
16:Q:83:ASN:HD22	16:Q:83:ASN:C	2.06	0.63
25:b:121:LYS:NZ	43:v:38:GLU:OE1	2.29	0.63
35:l:51:LEU:HG	35:l:55:MET:HE3	1.78	0.63
16:Q:46:GLN:HB3	48:Q:501:PEE:H6	1.61	0.63
35:l:383:MET:HB3	35:l:386:LEU:HD12	1.80	0.63
48:Q:501:PEE:H36	48:Q:501:PEE:C18	2.27	0.63
51:l:701:CDL:H271	51:l:701:CDL:C23	2.19	0.63
48:l:704:PEE:H31	40:r:449:LEU:HD23	1.80	0.63
3:C:125:PRO:HB2	41:s:58:LYS:HE3	1.81	0.63
24:a:53:ARG:O	25:b:28:LEU:HD13	1.99	0.63
48:l:703:PEE:H68	40:r:401:MET:HE1	1.81	0.63
4:E:15:THR:OG1	11:L:55:VAL:O	2.15	0.62
11:L:88:GLN:NE2	12:M:141:ASP:OD2	2.30	0.62
16:Q:182:ASN:HD22	16:Q:403:PRO:HB2	1.61	0.62
19:U:26:GLY:HA3	48:j:201:PEE:H37	1.81	0.62
6:X:69:SER:OG	6:X:70:ASP:N	2.32	0.62
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.80	0.62
35:l:227:PHE:O	35:l:230:HIS:ND1	2.30	0.62
1:A:62:TRP:CD2	1:A:181:LEU:HD23	2.34	0.62
14:O:41:HIS:NE2	14:O:47:ASN:OD1	2.31	0.62
7:H:76:GLN:O	7:H:79:GLU:HG2	1.99	0.62
26:c:152:SER:HA	43:v:5:LEU:HD21	1.80	0.62
48:W:201:PEE:C11	33:j:3:ILE:CG2	2.76	0.62
32:i:75:ILE:CG2	34:k:43:MET:HE3	2.30	0.62
41:s:62:ARG:HH21	41:s:68:ILE:HB	1.64	0.62
51:l:701:CDL:H232	51:l:701:CDL:C27	2.16	0.62
48:l:704:PEE:O1P	48:l:704:PEE:H8	1.99	0.62
16:Q:182:ASN:ND2	16:Q:403:PRO:HB2	2.14	0.62
20:V:124:LEU:HD11	48:r:501:PEE:H64	1.81	0.62
12:M:517:HIS:HB2	12:M:599:THR:HG22	1.80	0.62
32:i:99:THR:HG22	32:i:157:MET:HE1	1.82	0.62
35:l:359:MET:O	35:l:436:ARG:NH2	2.33	0.62
2:B:192:ASN:ND2	18:T:61:GLU:OE2	2.32	0.62
51:I:201:CDL:H532	51:I:201:CDL:H312	1.79	0.62
14:O:148:ILE:HG23	14:O:201:ILE:HG13	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:a:201:CDL:H782	28:e:100:VAL:HG22	1.80	0.62
41:s:90:PRO:HD2	41:s:240:ILE:HD13	1.82	0.62
44:w:76:GLU:OE1	44:w:76:GLU:HA	1.98	0.62
3:C:73:ALA:O	3:C:77:MET:HG3	2.00	0.62
43:v:109:LEU:HD23	43:v:109:LEU:C	2.25	0.62
9:J:271:TYR:OH	9:J:346:GLU:OE2	2.18	0.61
9:J:192:ARG:NH1	9:J:198:ALA:O	2.33	0.61
12:M:388:ASN:ND2	12:M:513:MET:O	2.29	0.61
14:O:207:GLU:HB2	14:O:212:LYS:HE3	1.81	0.61
44:w:61:THR:CG2	44:w:204:VAL:HG12	2.30	0.61
1:A:309:GLY:HA3	1:A:313:ASN:HD22	1.64	0.61
13:N:127:TYR:OH	18:T:61:GLU:O	2.15	0.61
13:N:73:THR:HG22	13:N:77:VAL:HG12	1.82	0.61
26:c:128:THR:HG23	26:c:132:HIS:NE2	2.15	0.61
51:l:701:CDL:H762	51:l:701:CDL:H311	1.83	0.61
8:I:27:ARG:NH1	16:Q:212:GLU:OE2	2.29	0.61
43:v:39:MET:HE1	43:v:58:TYR:HA	1.81	0.61
1:A:109:ARG:NH1	1:A:237:GLY:O	2.33	0.61
32:i:268:GLN:HE22	32:i:272:LYS:HE2	1.65	0.61
25:b:74:HIS:NE2	35:l:35:TYR:OH	2.26	0.61
32:i:125:GLN:HG3	51:i:401:CDL:OA3	2.00	0.61
41:s:102:VAL:HG11	41:s:154:LEU:HD11	1.81	0.61
8:I:8:ILE:HG21	51:I:201:CDL:OA4	2.01	0.61
21:W:85:GLN:OE1	31:h:105:ARG:NH1	2.34	0.61
6:X:154:VAL:HG23	6:X:154:VAL:O	2.01	0.61
16:Q:79:ASN:HA	16:Q:101:LEU:O	2.01	0.60
2:B:76:TYR:HE1	8:I:25:GLN:HE22	1.49	0.60
44:w:245:PHE:HD2	44:w:246:LEU:HD22	1.66	0.60
48:W:201:PEE:H57	48:W:201:PEE:H25	1.82	0.60
51:l:701:CDL:H422	40:r:448:THR:HG21	1.83	0.60
39:p:19:LEU:HD22	39:p:64:LEU:HD12	1.84	0.60
21:W:130:ASN:HA	21:W:133:ILE:HD12	1.83	0.60
51:a:201:CDL:H251	51:a:201:CDL:C21	2.21	0.60
35:l:172:ILE:O	35:l:176:ARG:HG2	2.02	0.60
51:u:201:CDL:H161	51:u:201:CDL:HB31	1.83	0.60
16:Q:302:LEU:HD11	16:Q:406:GLU:HG3	1.84	0.60
24:a:134:GLU:OE2	37:n:42:SER:OG	2.14	0.60
26:c:162:PRO:HG3	43:v:39:MET:HE3	1.83	0.60
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.34	0.60
49:a:202:PLX:H82	40:r:40:SER:HB3	1.84	0.60
48:C:302:PEE:H1	33:j:28:ASN:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:163:LYS:NZ	9:J:253:ILE:O	2.33	0.60
12:M:372:PHE:H	12:M:532:PRO:HB2	1.66	0.60
16:Q:102:SER:OG	16:Q:107:ARG:NH1	2.34	0.60
32:i:69:MET:SD	32:i:104:MET:HE1	2.41	0.60
35:l:429:PHE:CZ	39:p:32:VAL:HG11	2.37	0.60
40:r:1:MET:HG2	40:r:111:THR:HG21	1.84	0.60
1:A:90:GLY:HA3	47:A:503:NAI:H1D	1.84	0.60
6:G:76:LEU:CD2	6:G:154:VAL:HG23	2.31	0.60
51:l:701:CDL:H871	51:l:701:CDL:H572	1.81	0.60
16:Q:104:GLU:OE2	41:s:134:ARG:NH2	2.29	0.60
33:j:64:LEU:HD13	36:m:165:VAL:HG22	1.84	0.60
24:a:152:LYS:HD3	30:g:96:VAL:HG21	1.83	0.59
15:P:240:GLU:OE2	15:P:246:ARG:NH1	2.35	0.59
35:l:401:MET:HG3	35:l:482:MET:HE2	1.85	0.59
1:A:116:ASN:O	1:A:245:VAL:HG23	2.03	0.59
2:B:111:GLU:O	2:B:141:ARG:NH1	2.36	0.59
24:a:130:GLU:CG	37:n:45:PHE:CD1	2.84	0.59
35:l:383:MET:HE3	35:l:384:PRO:HD2	1.83	0.59
51:r:504:CDL:H332	51:r:504:CDL:H202	1.85	0.59
26:c:55:TYR:OH	26:c:74:ASP:O	2.19	0.59
41:s:281:ARG:HB2	41:s:284:GLN:HG3	1.85	0.59
5:F:19:ILE:HD13	5:F:51:LEU:HD21	1.83	0.59
9:J:85:ARG:HD3	52:J:401:NDP:C2A	2.33	0.59
21:W:90:ASN:ND2	21:W:123:GLU:O	2.36	0.59
27:d:33:LEU:HD23	27:d:36:ILE:HD11	1.82	0.59
34:k:23:ARG:HG2	36:m:23:LYS:HE2	1.84	0.59
22:Y:99:ILE:CD1	43:v:108:LEU:N	2.66	0.59
34:k:22:TYR:O	35:l:585:LYS:NZ	2.27	0.59
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.85	0.59
25:b:31:ARG:NH2	39:p:117:ASP:OD1	2.36	0.59
1:A:41:ILE:HG23	1:A:42:PHE:CD2	2.38	0.59
24:a:106:VAL:HG13	37:n:50:ARG:HH21	1.68	0.59
26:c:58:ARG:NH2	26:c:60:GLU:OE1	2.35	0.59
44:w:58:LYS:HA	44:w:202:HIS:ND1	2.18	0.59
32:i:154:MET:HE3	32:i:191:THR:HB	1.84	0.58
39:p:75:GLN:O	39:p:76:HIS:CB	2.49	0.58
15:P:147:THR:HB	15:P:153:ILE:HD11	1.85	0.58
26:c:122:THR:OG1	26:c:124:VAL:O	2.20	0.58
26:c:185:GLU:HB2	43:v:37:ARG:HG2	1.85	0.58
38:o:27:PRO:HB2	38:o:31:LYS:NZ	2.18	0.58
40:r:403:THR:HA	40:r:406:TYR:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:83:PRO:HB2	9:J:108:TRP:CD1	2.38	0.58
17:S:35:GLU:OE1	41:s:249:PRO:HB3	2.04	0.58
12:M:501:ARG:HH11	12:M:665:PHE:HD2	1.49	0.58
17:S:27:HIS:O	17:S:31:ASN:HB2	2.03	0.58
35:l:362:LEU:HD22	35:l:366:MET:HE2	1.85	0.58
12:M:406:ASN:ND2	12:M:688:GLN:O	2.27	0.58
6:G:103:HIS:CE1	6:G:105:MET:HE2	2.39	0.58
51:a:201:CDL:H201	51:a:201:CDL:H761	1.85	0.58
1:A:263:ALA:HA	1:A:271:SER:HB3	1.86	0.58
48:C:302:PEE:H82	56:s:401:UQ:H172	1.86	0.58
48:W:201:PEE:H2	48:W:201:PEE:C4	2.29	0.58
35:l:389:PHE:O	35:l:393:ASP:HB3	2.04	0.58
8:I:96:THR:HB	8:I:97:PRO:HD2	1.85	0.58
12:M:300:GLN:H	13:N:135:GLN:NE2	2.02	0.58
20:V:66:ILE:HD11	20:V:101:LEU:HD13	1.86	0.58
4:E:47:VAL:HA	4:E:52:LEU:HD12	1.86	0.57
12:M:388:ASN:HB3	12:M:511:LYS:HE2	1.86	0.57
15:P:44:ARG:HB3	15:P:45:PRO:CD	2.34	0.57
34:k:8:ILE:HG21	34:k:43:MET:HB2	1.86	0.57
27:d:159:GLN:O	27:d:163:MET:HG2	2.03	0.57
35:l:429:PHE:HZ	39:p:32:VAL:HG11	1.69	0.57
21:W:80:ASP:OD2	42:u:47:ARG:NE	2.26	0.57
41:s:24:GLU:HG3	41:s:271:LEU:HD22	1.84	0.57
35:l:62:ILE:HD11	35:l:81:LYS:HG3	1.87	0.57
40:r:56:PHE:CB	40:r:111:THR:HB	2.34	0.57
44:w:73:LEU:HD12	44:w:73:LEU:O	2.05	0.57
40:r:1:MET:HE1	40:r:41:LEU:HD11	1.87	0.57
40:r:17:MET:HG3	51:r:504:CDL:H582	1.86	0.57
1:A:357:MET:HB2	1:A:361:THR:HG21	1.86	0.57
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.86	0.57
21:W:88:ARG:NH2	42:u:7:LEU:O	2.37	0.57
6:X:76:LEU:HD11	25:b:20:ARG:HH12	1.69	0.57
22:Y:97:LEU:O	43:v:104:ARG:HG3	2.05	0.57
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.86	0.57
40:r:198:ALA:HB2	48:r:501:PEE:H22	1.87	0.57
12:M:36:VAL:HB	12:M:56:VAL:HG21	1.85	0.57
49:a:202:PLX:H102	40:r:40:SER:HB3	1.86	0.57
6:X:93:ILE:HD11	6:X:110:LEU:HD11	1.85	0.57
28:e:57:GLU:OE1	44:w:320:GLY:HA3	2.05	0.57
1:A:303:HIS:HA	14:O:232:THR:HG21	1.87	0.57
48:C:302:PEE:H1	33:j:28:ASN:CB	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:74:LEU:O	21:W:78:GLU:HG3	2.05	0.57
1:A:152:ARG:NH2	10:K:99:PRO:O	2.36	0.56
1:A:244:ASN:N	46:A:502:FMN:O1P	2.34	0.56
44:w:111:ASN:O	44:w:130:ARG:NH1	2.36	0.56
1:A:113:LEU:HD13	1:A:149:MET:HE1	1.86	0.56
22:Y:54:GLN:NE2	35:l:446:ASN:OD1	2.38	0.56
24:a:91:VAL:HA	27:d:52:ILE:HD11	1.87	0.56
1:A:174:ARG:HB2	10:K:93:LEU:HD11	1.86	0.56
6:G:138:LEU:HB3	6:G:144:ILE:HG12	1.88	0.56
9:J:204:SER:OG	9:J:238:GLN:O	2.22	0.56
16:Q:41:VAL:O	16:Q:45:GLU:HG2	2.05	0.56
20:V:29:GLY:O	20:V:63:SER:OG	2.20	0.56
51:a:201:CDL:OA7	51:a:201:CDL:HA61	2.05	0.56
26:c:83:GLN:NE2	26:c:97:LEU:O	2.39	0.56
32:i:211:MET:HG2	32:i:333:SER:HB2	1.86	0.56
35:l:228:GLY:HA3	48:l:703:PEE:H38	1.87	0.56
35:l:407:TRP:CE2	35:l:411:MET:HE3	2.39	0.56
39:p:28:GLU:OE2	39:p:34:ARG:NH1	2.32	0.56
21:W:98:MET:HE1	31:h:82:GLN:HB3	1.87	0.56
27:d:104:ASN:O	27:d:108:GLU:HG3	2.06	0.56
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.41	0.56
11:L:90:GLY:HA3	15:P:238:PRO:HB2	1.85	0.56
51:a:201:CDL:H111	48:l:704:PEE:H60	1.88	0.56
25:b:28:LEU:CD2	39:p:115:TYR:HE1	2.19	0.56
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.40	0.56
12:M:390:THR:HA	12:M:600:GLU:HG2	1.87	0.56
21:W:66:GLU:HG2	42:u:125:LEU:HB2	1.87	0.56
6:X:90:TYR:HE1	23:Z:44:PRO:HB2	1.70	0.56
35:l:15:LEU:HD21	35:l:125:LEU:HG	1.88	0.56
35:l:250:SER:HB2	35:l:333:ALA:HA	1.88	0.56
35:l:559:GLU:O	35:l:563:PRO:HD2	2.06	0.56
35:l:591:PHE:HA	35:l:594:THR:CG2	2.34	0.56
42:u:89:ILE:HG12	42:u:100:CYS:SG	2.45	0.56
6:G:103:HIS:ND1	6:G:106:LYS:HG2	2.21	0.56
7:H:55:LYS:HE3	15:P:104:THR:HG21	1.88	0.56
38:o:25:ILE:HD12	38:o:30:ARG:HH12	1.71	0.56
2:B:177:THR:HG22	2:B:179:THR:H	1.70	0.56
12:M:419:ARG:NH1	12:M:439:THR:O	2.37	0.56
10:K:105:ARG:NH1	11:L:167:ASN:O	2.39	0.56
35:l:267:MET:HE1	35:l:273:VAL:HG12	1.88	0.56
35:l:407:TRP:CZ2	35:l:411:MET:HE3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:l:701:CDL:H572	51:l:701:CDL:H872	1.88	0.56
2:B:110:GLU:HG3	18:T:71:ILE:HB	1.87	0.56
31:h:18:MET:HE3	34:k:56:ALA:HA	1.87	0.56
33:j:90:MET:CE	36:m:154:VAL:CG1	2.84	0.56
9:J:236:VAL:HG12	9:J:272:LEU:HD23	1.88	0.55
12:M:474:VAL:HG11	12:M:493:VAL:HG13	1.89	0.55
22:Y:99:ILE:HD12	43:v:108:LEU:N	2.21	0.55
24:a:130:GLU:H	24:a:130:GLU:CD	2.12	0.55
3:C:190:LEU:HD21	48:C:302:PEE:H14	1.88	0.55
6:G:154:VAL:HG23	6:G:154:VAL:O	2.05	0.55
21:W:93:GLU:OE1	31:h:92:TYR:OH	2.19	0.55
38:o:17:THR:O	38:o:23:TYR:OH	2.19	0.55
43:v:51:LEU:HD21	43:v:64:ILE:HD13	1.88	0.55
12:M:68:ARG:NH1	12:M:284:GLU:OE1	2.38	0.55
21:W:130:ASN:HB3	36:m:1:MET:N	2.22	0.55
24:a:55:PHE:N	25:b:28:LEU:HD11	2.22	0.55
51:a:201:CDL:OB7	48:l:704:PEE:H14	2.05	0.55
32:i:170:LEU:HD11	32:i:288:LEU:HD22	1.87	0.55
2:B:38:TYR:CZ	8:I:106:LEU:HD13	2.42	0.55
7:H:69:GLU:HG3	7:H:77:ILE:HG12	1.88	0.55
14:O:149:LEU:O	14:O:153:GLN:HG2	2.05	0.55
21:W:50:MET:HB3	41:s:156:MET:HE2	1.88	0.55
25:b:17:GLU:OE2	25:b:21:ARG:NE	2.35	0.55
28:e:92:PHE:O	28:e:96:SER:HB2	2.05	0.55
35:l:51:LEU:HD22	35:l:91:PRO:HG3	1.89	0.55
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.89	0.55
32:i:95:MET:HE2	32:i:149:ILE:CA	2.36	0.55
48:C:302:PEE:H32	48:C:302:PEE:H58	1.89	0.55
20:V:9:TYR:HE1	20:V:25:SER:HG	1.53	0.55
35:l:514:LYS:HD3	35:l:515:TYR:O	2.06	0.55
39:p:29:SER:HB3	39:p:76:HIS:CD2	2.40	0.55
5:F:23:LEU:O	5:F:57:GLU:HA	2.07	0.55
35:l:545:SER:OG	40:r:274:SER:O	2.24	0.55
44:w:129:TYR:OH	44:w:186:HIS:ND1	2.28	0.55
22:Y:97:LEU:HD11	43:v:104:ARG:N	2.22	0.55
1:A:48:ARG:NH1	10:K:70:ASN:O	2.39	0.55
49:a:202:PLX:H82	40:r:40:SER:CB	2.37	0.55
32:i:86:ILE:O	32:i:86:ILE:HG23	2.07	0.55
12:M:194:ASP:OD2	12:M:212:LYS:NZ	2.30	0.55
37:n:26:TYR:CE2	37:n:30:ARG:HD2	2.42	0.55
43:v:112:LYS:HD2	43:v:112:LYS:C	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:73:ALA:HA	3:C:76:MET:HG3	1.89	0.54
8:I:40:LYS:HB3	21:W:7:LYS:H	1.72	0.54
22:Y:100:LEU:N	22:Y:100:LEU:HD22	2.22	0.54
32:i:268:GLN:NE2	32:i:272:LYS:HE2	2.21	0.54
26:c:159:LYS:NZ	43:v:57:ASP:OD2	2.39	0.54
37:n:14:HIS:HE1	40:r:26:ASN:OD1	1.90	0.54
44:w:171:GLU:O	44:w:175:ARG:HG2	2.07	0.54
48:W:201:PEE:C1	48:W:201:PEE:C4	2.86	0.54
51:l:701:CDL:H311	51:l:701:CDL:C76	2.38	0.54
40:r:188:ASN:OD1	40:r:256:TYR:OH	2.26	0.54
13:N:6:VAL:HG12	13:N:9:ARG:NH2	2.23	0.54
25:b:89:HIS:CE1	48:l:704:PEE:H54	2.43	0.54
26:c:111:MET:HE3	35:l:542:LEU:HB2	1.90	0.54
51:u:201:CDL:H1	51:u:201:CDL:H151	1.89	0.54
3:C:158:PRO:HB2	9:J:92:MET:HE3	1.89	0.54
24:a:96:ALA:HB2	27:d:61:TYR:CE2	2.43	0.54
27:d:71:VAL:HG11	27:d:87:GLU:HB3	1.90	0.54
51:l:701:CDL:H472	40:r:445:LEU:CB	2.35	0.54
51:l:701:CDL:H811	51:l:701:CDL:H611	1.89	0.54
9:J:220:MET:HB2	9:J:281:PHE:HZ	1.72	0.54
51:a:201:CDL:H772	51:a:201:CDL:C20	2.17	0.54
24:a:166:GLY:O	24:a:170:GLN:NE2	2.41	0.54
35:l:393:ASP:O	35:l:397:GLU:HG2	2.08	0.54
38:o:23:TYR:CE2	39:p:65:ARG:HG3	2.43	0.54
1:A:160:GLY:O	1:A:199:ARG:NH2	2.40	0.54
12:M:377:ALA:HB1	12:M:381:LEU:HD23	1.89	0.54
21:W:68:ARG:O	21:W:72:MET:HG3	2.08	0.54
22:Y:99:ILE:HD11	43:v:108:LEU:CD2	2.10	0.54
35:l:6:SER:O	35:l:10:THR:OG1	2.18	0.54
35:l:337:ALA:O	35:l:341:MET:HG2	2.08	0.54
35:l:562:LEU:HB3	35:l:563:PRO:HD3	1.88	0.54
37:n:16:LEU:CD2	51:r:504:CDL:H661	2.38	0.54
1:A:250:VAL:O	1:A:254:ILE:HG12	2.07	0.54
9:J:157:LYS:HE2	9:J:195:PHE:CD1	2.43	0.54
28:e:125:LEU:O	28:e:129:ARG:HG3	2.07	0.54
51:l:701:CDL:C66	51:l:701:CDL:C27	2.86	0.54
37:n:17:VAL:HB	37:n:18:PRO:HD3	1.89	0.54
44:w:125:ASP:O	44:w:130:ARG:NH2	2.41	0.54
2:B:77:LEU:HD12	41:s:31:MET:HG3	1.91	0.54
14:O:59:ASN:OD1	14:O:62:ARG:NH2	2.40	0.54
48:Q:501:PEE:C25	48:Q:501:PEE:C21	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:72:ARG:HB3	35:l:385:TYR:CD2	2.43	0.54
1:A:134:ASP:OD2	1:A:137:LYS:CG	2.56	0.53
51:I:201:CDL:H312	51:I:201:CDL:C53	2.38	0.53
35:l:161:ARG:NH1	35:l:238:GLU:OE1	2.41	0.53
51:l:701:CDL:C31	51:l:701:CDL:C76	2.86	0.53
15:P:107:GLN:NE2	15:P:136:ARG:HG2	2.22	0.53
51:a:201:CDL:H362	25:b:80:TRP:HB3	1.90	0.53
32:i:18:MET:HE2	32:i:18:MET:HA	1.89	0.53
33:j:90:MET:HE3	36:m:154:VAL:CG1	2.37	0.53
51:l:701:CDL:H811	51:l:701:CDL:H582	1.90	0.53
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.41	0.53
1:A:210:THR:HB	1:A:224:ARG:HG2	1.90	0.53
20:V:90:TYR:CE2	20:V:126:LYS:HD3	2.43	0.53
26:c:117:VAL:HG21	35:l:539:TYR:HB2	1.91	0.53
34:k:37:MET:HG3	34:k:67:ALA:CB	2.38	0.53
5:F:33:VAL:O	5:F:36:PHE:HB3	2.08	0.53
12:M:94:MET:HE2	12:M:100:TRP:HH2	1.74	0.53
48:Q:501:PEE:H34	48:Q:501:PEE:H42	1.90	0.53
22:Y:89:PRO:HA	22:Y:92:TRP:CE3	2.44	0.53
25:b:121:LYS:HB3	43:v:40:VAL:HG13	1.90	0.53
51:i:401:CDL:OA7	51:i:401:CDL:HA62	2.04	0.53
40:r:109:THR:O	40:r:112:ALA:HB3	2.08	0.53
1:A:285:PRO:O	14:O:222:ARG:NH2	2.42	0.53
3:C:191:ARG:O	3:C:195:ARG:HG3	2.09	0.53
48:l:704:PEE:H31	40:r:449:LEU:HD21	1.89	0.53
42:u:169:PHE:CZ	51:u:201:CDL:H561	2.43	0.53
51:a:201:CDL:C52	48:l:704:PEE:H14	2.25	0.53
32:i:95:MET:HE2	32:i:149:ILE:CG2	2.39	0.53
44:w:65:ASN:OD1	44:w:66:ILE:N	2.42	0.53
6:G:74:LEU:H	6:G:74:LEU:CD2	2.14	0.53
14:O:132:ILE:HD11	14:O:169:PHE:HD2	1.72	0.53
21:W:97:ILE:HG23	31:h:86:LEU:HD12	1.90	0.53
35:l:119:LYS:HZ3	51:l:701:CDL:H512	1.72	0.53
5:F:23:LEU:HD12	5:F:34:ARG:HG2	1.90	0.53
51:I:201:CDL:C55	51:I:201:CDL:C32	2.86	0.53
9:J:141:PHE:HA	9:J:144:VAL:HG12	1.91	0.53
16:Q:137:ASP:OD1	16:Q:144:MET:HB3	2.09	0.53
17:S:12:MET:HE1	41:s:20:LEU:HD13	1.90	0.53
20:V:102:GLY:O	20:V:106:ARG:N	2.41	0.53
40:r:10:MET:HE1	51:r:504:CDL:H632	1.90	0.53
21:W:68:ARG:CZ	21:W:72:MET:HE2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:18:ASP:HB3	23:Z:21:GLN:HG3	1.90	0.53
51:a:201:CDL:C42	27:d:44:PRO:HB3	2.38	0.53
26:c:62:TYR:OH	26:c:74:ASP:OD1	2.26	0.53
27:d:31:THR:HG22	27:d:35:LYS:NZ	2.23	0.53
44:w:213:GLU:OE1	44:w:217:ARG:NE	2.38	0.53
25:b:99:GLU:OE2	35:l:2:ASN:ND2	2.42	0.53
26:c:127:ASN:O	26:c:131:LYS:HG3	2.09	0.53
32:i:280:THR:O	32:i:284:MET:HG2	2.09	0.53
14:O:111:ARG:NH1	14:O:114:GLU:OE2	2.41	0.52
15:P:209:GLU:HG2	15:P:224:VAL:HA	1.89	0.52
16:Q:35:ARG:HD3	28:e:61:PRO:HD2	1.90	0.52
19:U:47:ARG:HG2	33:j:82:ASN:ND2	2.24	0.52
1:A:398:ARG:HE	1:A:404:ALA:HB2	1.74	0.52
28:e:114:MET:HB3	28:e:117:TRP:HB3	1.92	0.52
39:p:75:GLN:O	39:p:76:HIS:HB3	2.10	0.52
42:u:86:TRP:HE3	42:u:86:TRP:O	1.92	0.52
25:b:26:GLN:OE1	39:p:118:TYR:HE1	1.92	0.52
35:l:7:LEU:HD22	35:l:46:LEU:HD11	1.90	0.52
3:C:55:ASN:ND2	3:C:187:GLU:O	2.40	0.52
51:a:201:CDL:OB7	48:l:704:PEE:C11	2.57	0.52
25:b:28:LEU:HD23	39:p:115:TYR:HE1	1.75	0.52
32:i:154:MET:HE2	32:i:194:LEU:HD12	1.91	0.52
32:i:245:MET:HE1	51:r:504:CDL:H171	1.91	0.52
44:w:241:TYR:HA	44:w:245:PHE:HB3	1.90	0.52
9:J:85:ARG:NE	52:J:401:NDP:O1X	2.43	0.52
10:K:79:HIS:CD2	14:O:216:PRO:HD2	2.44	0.52
48:Q:501:PEE:H7	35:l:567:SER:HG	1.73	0.52
27:d:37:PHE:CE1	35:l:3:PRO:HB3	2.44	0.52
31:h:7:GLN:NE2	31:h:15:ASP:OD1	2.37	0.52
4:E:39:TRP:O	4:E:43:VAL:HG23	2.10	0.52
10:K:100:GLN:HB3	14:O:71:PRO:HA	1.92	0.52
16:Q:274:ASP:OD1	16:Q:323:ARG:NH2	2.43	0.52
6:X:75:THR:OG1	6:X:156:GLU:O	2.27	0.52
37:n:15:ILE:O	37:n:15:ILE:HG12	2.09	0.52
13:N:72:ASP:OD1	13:N:72:ASP:N	2.43	0.52
21:W:68:ARG:NH2	36:m:134:GLY:HA2	2.25	0.52
33:j:68:GLU:HG2	36:m:161:LEU:HD13	1.91	0.52
35:l:292:ALA:HB2	35:l:304:PHE:HB3	1.92	0.52
36:m:57:PHE:CZ	41:s:111:LEU:HD11	2.44	0.52
44:w:110:GLY:HA2	44:w:134:TRP:CD2	2.44	0.52
7:H:77:ILE:HA	7:H:80:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:110:MET:O	14:O:114:GLU:HG3	2.10	0.52
14:O:138:THR:HA	14:O:141:MET:HG3	1.91	0.52
17:S:43:TYR:CZ	21:W:68:ARG:HG3	2.45	0.52
27:d:81:ASP:O	27:d:85:MET:HG3	2.10	0.52
27:d:99:ASP:OD2	27:d:142:ARG:NH1	2.43	0.52
49:g:201:PLX:H292	49:g:201:PLX:H192	1.92	0.52
16:Q:101:LEU:HD23	16:Q:106:VAL:HA	1.92	0.51
21:W:86:MET:HE2	21:W:124:LEU:HB3	1.92	0.51
25:b:123:PHE:HD2	43:v:40:VAL:HG11	1.75	0.51
26:c:128:THR:HG22	26:c:132:HIS:CD2	2.45	0.51
1:A:185:ASN:C	1:A:187:CYS:H	2.19	0.51
4:E:16:SER:HA	11:L:54:ALA:HA	1.92	0.51
7:H:93:LYS:HG2	7:H:96:ARG:HH21	1.76	0.51
35:l:331:MET:HE1	35:l:468:ILE:HD12	1.93	0.51
39:p:176:GLU:HG2	39:p:177:ARG:N	2.24	0.51
9:J:132:ARG:NH2	52:J:401:NDP:O2X	2.42	0.51
13:N:4:VAL:O	13:N:8:ARG:HG2	2.10	0.51
32:i:256:PRO:CB	51:u:201:CDL:H612	2.36	0.51
40:r:41:LEU:O	40:r:44:GLN:NE2	2.44	0.51
40:r:59:ASP:OD1	40:r:60:SER:N	2.43	0.51
43:v:60:ALA:O	43:v:64:ILE:HG12	2.09	0.51
1:A:130:ILE:CD1	1:A:245:VAL:HG12	2.40	0.51
6:G:74:LEU:N	6:G:74:LEU:CD2	2.73	0.51
44:w:170:LEU:HD22	44:w:187:TYR:CD1	2.44	0.51
33:j:83:ASN:HD21	49:j:202:PLX:H1A2	1.75	0.51
36:m:25:SER:O	36:m:27:ILE:N	2.43	0.51
8:I:12:ARG:HD3	8:I:20:LEU:HD22	1.92	0.51
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.93	0.51
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.93	0.51
48:Q:501:PEE:H28	48:Q:501:PEE:H35	1.93	0.51
28:e:58:ASP:OD2	44:w:326:ARG:NE	2.40	0.51
48:l:704:PEE:O3P	49:r:503:PLX:O2	2.28	0.51
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.93	0.51
9:J:211:ASP:O	9:J:215:ASN:ND2	2.42	0.51
48:Q:501:PEE:H47	48:r:501:PEE:H40	1.92	0.51
51:a:201:CDL:H192	51:a:201:CDL:C73	2.39	0.51
26:c:139:PHE:O	26:c:143:MET:HG2	2.11	0.51
27:d:163:MET:HE2	28:e:149:LEU:HD11	1.93	0.51
30:g:46:ILE:HD13	51:r:504:CDL:H732	1.92	0.51
35:l:591:PHE:HA	35:l:594:THR:HG22	1.93	0.51
16:Q:83:ASN:C	16:Q:83:ASN:ND2	2.67	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:129:LEU:CD1	51:i:401:CDL:H341	2.41	0.51
41:s:18:ALA:HB2	56:s:401:UQ:H152	1.92	0.51
4:E:98:LYS:HB3	4:E:102:HIS:HB2	1.92	0.51
15:P:173:MET:HE1	15:P:189:THR:HG23	1.92	0.51
6:X:113:LEU:O	6:X:117:GLU:HG3	2.11	0.51
22:Y:80:VAL:HG12	35:l:488:MET:HE1	1.91	0.51
26:c:128:THR:CG2	26:c:132:HIS:NE2	2.74	0.51
51:l:701:CDL:C54	51:l:701:CDL:CA6	2.85	0.51
51:l:701:CDL:H851	51:l:701:CDL:C58	2.41	0.51
2:B:74:LEU:HB2	41:s:272:TRP:CZ2	2.45	0.51
33:j:97:LEU:C	33:j:97:LEU:HD13	2.35	0.51
35:l:338:MET:O	35:l:341:MET:HB2	2.12	0.51
41:s:223:PHE:O	41:s:227:GLU:HG2	2.11	0.51
1:A:278:ILE:HG21	1:A:304:ALA:HB2	1.93	0.50
9:J:129:LEU:HD23	9:J:167:ILE:HG13	1.92	0.50
9:J:204:SER:OG	9:J:204:SER:O	2.28	0.50
12:M:379:THR:HG21	12:M:526:LEU:HD22	1.93	0.50
26:c:40:PRO:O	26:c:74:ASP:HB2	2.11	0.50
37:n:16:LEU:HD22	40:r:10:MET:CE	2.42	0.50
43:v:17:PRO:HB3	43:v:105:GLU:OE1	2.10	0.50
7:H:30:LYS:O	7:H:34:VAL:HG23	2.11	0.50
25:b:28:LEU:N	25:b:28:LEU:CD1	2.73	0.50
26:c:81:ARG:HB3	26:c:85:GLU:OE2	2.11	0.50
11:L:174:THR:HG23	14:O:111:ARG:HD2	1.92	0.50
22:Y:99:ILE:CD1	43:v:107:ARG:HB3	2.41	0.50
40:r:231:LEU:HD23	40:r:235:LEU:HD12	1.94	0.50
1:A:214:GLU:OE2	1:A:224:ARG:NE	2.45	0.50
12:M:299:ARG:CG	13:N:135:GLN:HE21	2.23	0.50
26:c:161:TYR:HB3	26:c:166:LEU:HG	1.92	0.50
39:p:100:PRO:HG3	40:r:419:TYR:CE1	2.47	0.50
40:r:174:LEU:HA	40:r:179:ILE:HD11	1.93	0.50
1:A:83:SER:HB2	1:A:262:PHE:HD2	1.77	0.50
1:A:130:ILE:HD11	1:A:245:VAL:HG12	1.94	0.50
48:Q:501:PEE:H19	40:r:148:TYR:CE1	2.46	0.50
32:i:88:LYS:CB	32:i:148:SER:HG	2.25	0.50
32:i:283:ALA:HB1	40:r:158:LEU:HD13	1.93	0.50
33:j:15:SER:HA	41:s:76:ILE:HD12	1.93	0.50
35:l:66:TRP:HB2	48:l:704:PEE:H19	1.94	0.50
51:l:701:CDL:H331	51:l:701:CDL:OA9	2.10	0.50
39:p:97:TYR:HB3	39:p:179:MET:HE2	1.94	0.50
40:r:309:PHE:HB2	40:r:458:LEU:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:545:LEU:HD22	12:M:560:LEU:HD21	1.94	0.50
25:b:86:LEU:HD11	35:l:9:LEU:HD12	1.94	0.50
27:d:69:ARG:NH1	37:n:43:LEU:O	2.45	0.50
35:l:66:TRP:HZ3	48:l:704:PEE:H38	1.76	0.50
40:r:367:LEU:HD12	40:r:404:ALA:HA	1.94	0.50
42:u:169:PHE:CE1	51:u:201:CDL:C56	2.92	0.50
5:F:68:ARG:HG3	5:F:74:GLU:HG2	1.94	0.50
15:P:64:TYR:HH	15:P:103:HIS:HE2	1.57	0.50
16:Q:196:ALA:O	16:Q:197:MET:HG2	2.12	0.50
48:W:201:PEE:H25	48:W:201:PEE:C35	2.42	0.50
32:i:75:ILE:HG22	34:k:43:MET:HE3	1.92	0.50
51:l:701:CDL:H791	51:l:701:CDL:H582	1.93	0.50
37:n:13:VAL:HG12	40:r:14:MET:CG	2.42	0.50
42:u:169:PHE:HE1	51:u:201:CDL:H561	1.75	0.50
44:w:254:GLU:HG3	44:w:276:LEU:HD13	1.93	0.50
3:C:66:THR:HG21	3:C:76:MET:HE3	1.94	0.50
6:G:155:TYR:HD1	6:G:155:TYR:H	1.58	0.50
9:J:270:ARG:NH2	9:J:327:MET:O	2.44	0.50
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.94	0.50
32:i:213:LEU:HD13	51:i:401:CDL:C14	2.39	0.50
40:r:225:ILE:HD13	40:r:331:ASN:HB2	1.93	0.50
44:w:168:VAL:HG12	44:w:240:ALA:CB	2.39	0.50
9:J:207:PHE:HB2	9:J:214:LEU:HD13	1.94	0.50
28:e:109:LEU:HD22	40:r:43:ASN:HB2	1.94	0.50
31:h:3:PHE:HB2	32:i:144:GLN:CD	2.37	0.50
41:s:87:VAL:CG2	41:s:88:PRO:CD	2.87	0.50
1:A:311:TRP:NE1	1:A:333:GLU:OE2	2.44	0.49
6:G:84:LEU:O	6:G:88:LYS:HG2	2.11	0.49
1:A:295:PRO:HD2	1:A:298:GLU:OE2	2.11	0.49
1:A:405:ARG:NH2	8:I:49:LEU:HD11	2.27	0.49
20:V:90:TYR:HD2	20:V:126:LYS:HB2	1.76	0.49
26:c:156:VAL:HG11	43:v:95:TYR:CZ	2.47	0.49
32:i:71:MET:HE3	32:i:74:ILE:HB	1.94	0.49
51:i:401:CDL:CB3	44:w:40:PRO:CB	2.86	0.49
39:p:132:SER:O	39:p:136:GLU:HG3	2.12	0.49
48:r:501:PEE:H71	48:r:501:PEE:H62	1.94	0.49
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.93	0.49
3:C:193:TRP:HA	3:C:196:ARG:HG2	1.94	0.49
5:F:41:TYR:CE2	12:M:381:LEU:HD21	2.46	0.49
12:M:496:ILE:O	12:M:500:ILE:HG12	2.12	0.49
14:O:55:PHE:HB2	14:O:60:TYR:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Q:501:PEE:H67	32:i:284:MET:O	2.12	0.49
51:a:201:CDL:C25	51:a:201:CDL:C21	2.86	0.49
51:a:201:CDL:HB21	48:l:704:PEE:C32	2.42	0.49
28:e:129:ARG:NH1	28:e:138:GLU:OE2	2.38	0.49
35:l:356:ILE:HG13	35:l:429:PHE:CE2	2.47	0.49
6:G:115:GLN:O	6:G:119:ILE:HG12	2.13	0.49
9:J:83:PRO:HG3	9:J:119:VAL:HG11	1.93	0.49
12:M:81:GLU:HG2	12:M:108:LYS:HB3	1.94	0.49
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.93	0.49
19:U:14:ALA:O	19:U:15:LYS:HG2	2.12	0.49
6:X:119:ILE:HG21	6:X:135:ALA:HB1	1.94	0.49
22:Y:87:PRO:HG3	43:v:96:VAL:HG22	1.94	0.49
36:m:45:LEU:HD23	36:m:50:SER:HA	1.94	0.49
40:r:87:GLU:OE2	40:r:91:ARG:HD2	2.11	0.49
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.92	0.49
15:P:216:VAL:HG23	15:P:218:ARG:HG2	1.94	0.49
16:Q:181:LEU:HD21	16:Q:210:MET:HB2	1.94	0.49
25:b:32:GLU:HG3	39:p:115:TYR:HA	1.94	0.49
33:j:71:LEU:O	36:m:147:TYR:OH	2.27	0.49
35:l:533:MET:HE3	48:l:703:PEE:H24	1.95	0.49
40:r:306:PRO:HA	40:r:458:LEU:HD13	1.93	0.49
32:i:203:LEU:HB2	32:i:347:ASN:HD21	1.77	0.49
40:r:38:SER:OG	40:r:70:THR:HG21	2.12	0.49
1:A:37:ASP:HB3	14:O:236:GLU:HG2	1.93	0.49
1:A:40:ARG:HH12	14:O:233:SER:HA	1.77	0.49
1:A:41:ILE:HG22	1:A:289:GLU:CD	2.38	0.49
1:A:89:GLY:O	47:A:503:NAI:H2N	2.12	0.49
8:I:70:MET:SD	8:I:70:MET:C	2.96	0.49
9:J:166:HIS:HB3	9:J:200:ILE:HD13	1.94	0.49
25:b:14:GLN:NE2	39:p:157:ALA:HB3	2.22	0.49
28:e:70:ASN:O	28:e:73:SER:HB2	2.13	0.49
9:J:320:GLU:O	9:J:324:MET:HG3	2.12	0.49
35:l:190:LEU:HD11	40:r:307:TRP:CH2	2.46	0.49
44:w:182:GLN:HA	44:w:185:GLU:OE2	2.13	0.49
9:J:195:PHE:HD2	9:J:198:ALA:HB2	1.78	0.49
12:M:292:PHE:HB3	12:M:706:THR:HG21	1.94	0.49
12:M:478:SER:O	12:M:482:GLN:HG2	2.12	0.49
20:V:74:SER:HB2	20:V:90:TYR:CD1	2.48	0.49
51:i:401:CDL:CA7	51:i:401:CDL:H342	2.42	0.49
44:w:70:LYS:NZ	44:w:160:GLU:HG2	2.27	0.49
1:A:119:GLU:OE2	1:A:127:ASP:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LEU:HD13	1:A:245:VAL:HG13	1.94	0.49
3:C:67:PHE:HZ	3:C:120:VAL:HG21	1.77	0.49
10:K:79:HIS:HD2	14:O:216:PRO:HD2	1.78	0.49
6:X:76:LEU:HD11	25:b:20:ARG:NH1	2.28	0.49
22:Y:45:ARG:HG2	35:l:439:PRO:HB3	1.95	0.49
1:A:44:ASN:ND2	1:A:49:HIS:HB2	2.28	0.48
1:A:46:TYR:CD1	14:O:226:GLU:HB3	2.48	0.48
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.95	0.48
3:C:169:THR:HG22	16:Q:221:ARG:HD3	1.95	0.48
12:M:217:GLU:HG2	12:M:218:LEU:HG	1.95	0.48
16:Q:145:MET:HG3	16:Q:214:TYR:CZ	2.48	0.48
22:Y:97:LEU:HG	43:v:107:ARG:CZ	2.40	0.48
32:i:152:ASN:O	32:i:156:THR:OG1	2.22	0.48
2:B:98:ARG:NH2	16:Q:224:ALA:O	2.45	0.48
5:F:42:VAL:HG23	12:M:671:LEU:HG	1.93	0.48
13:N:132:LYS:HE3	13:N:135:GLN:HA	1.95	0.48
22:Y:88:ASP:OD1	22:Y:89:PRO:HD2	2.12	0.48
49:a:202:PLX:H351	49:a:202:PLX:H381	1.61	0.48
26:c:81:ARG:NE	26:c:85:GLU:OE2	2.45	0.48
26:c:160:GLN:HG2	26:c:183:HIS:ND1	2.29	0.48
33:j:18:VAL:HG22	41:s:222:MET:HG3	1.94	0.48
35:l:591:PHE:O	35:l:594:THR:HG23	2.13	0.48
41:s:62:ARG:HH11	41:s:64:ALA:HA	1.78	0.48
1:A:313:ASN:O	1:A:359:ARG:HG3	2.13	0.48
3:C:184:ILE:O	3:C:187:GLU:HG2	2.14	0.48
4:E:56:VAL:HG12	4:E:60:ARG:HD2	1.96	0.48
7:H:51:ILE:HD11	8:I:94:ALA:HB3	1.94	0.48
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.95	0.48
19:U:56:PRO:HG2	42:u:45:LEU:HB2	1.94	0.48
21:W:114:THR:OG1	42:u:143:HIS:ND1	2.37	0.48
34:k:38:LEU:O	34:k:42:ILE:HG12	2.13	0.48
35:l:245:ALA:O	35:l:249:SER:OG	2.18	0.48
40:r:116:ILE:HG13	42:u:168:PHE:CD1	2.49	0.48
43:v:109:LEU:C	43:v:109:LEU:CD2	2.85	0.48
44:w:180:ARG:NH1	44:w:316:GLU:OE2	2.45	0.48
25:b:16:ARG:HG2	25:b:20:ARG:HE	1.79	0.48
31:h:97:HIS:HA	31:h:102:GLU:HB3	1.96	0.48
33:j:95:LEU:CD1	41:s:305:ILE:HD12	2.43	0.48
35:l:62:ILE:HD12	35:l:135:ASN:ND2	2.28	0.48
40:r:104:LEU:HG	40:r:108:MET:HE2	1.94	0.48
11:L:92:ASN:HB3	15:P:238:PRO:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.42	0.48
27:d:31:THR:HG22	27:d:35:LYS:HZ2	1.78	0.48
41:s:294:LEU:O	41:s:298:LEU:HG	2.14	0.48
1:A:123:GLY:O	1:A:353:ALA:HB1	2.14	0.48
12:M:354:LEU:HD22	12:M:548:LEU:HD22	1.95	0.48
12:M:358:LEU:HA	12:M:361:VAL:HG12	1.96	0.48
13:N:85:GLU:HB2	13:N:98:PRO:HB3	1.94	0.48
26:c:43:LYS:N	26:c:47:GLU:OE2	2.38	0.48
32:i:119:THR:HG22	32:i:176:ARG:HB3	1.96	0.48
32:i:246:VAL:HG11	51:r:504:CDL:H392	1.95	0.48
33:j:3:ILE:O	33:j:7:LEU:HG	2.13	0.48
36:m:51:PHE:O	36:m:55:MET:HG2	2.14	0.48
1:A:115:VAL:HG21	1:A:142:CYS:SG	2.53	0.48
1:A:275:LEU:HD23	1:A:289:GLU:HB2	1.95	0.48
4:E:37:ARG:HG2	6:G:120:MET:SD	2.54	0.48
6:G:85:TYR:CE1	6:G:89:LEU:HD11	2.49	0.48
51:I:201:CDL:H532	51:I:201:CDL:C32	2.43	0.48
14:O:146:ASP:O	14:O:149:LEU:N	2.47	0.48
27:d:32:TYR:HD1	27:d:35:LYS:HZ1	1.59	0.48
35:l:27:TYR:O	35:l:115:ASN:ND2	2.39	0.48
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.96	0.48
35:l:437:PHE:HE1	35:l:441:VAL:HG22	1.79	0.48
51:l:701:CDL:H791	51:l:701:CDL:C61	2.44	0.48
41:s:195:ARG:HD3	41:s:231:ILE:HD11	1.95	0.48
5:F:58:CYS:HB2	5:F:61:VAL:HB	1.95	0.48
22:Y:65:MET:HE1	35:l:378:LEU:HD12	1.95	0.48
26:c:163:TYR:OH	43:v:41:ALA:O	2.31	0.48
28:e:65:ASN:ND2	40:r:427:LYS:HE2	2.29	0.48
40:r:204:MET:HG3	40:r:209:LEU:HB2	1.95	0.48
42:u:86:TRP:CE3	42:u:86:TRP:C	2.92	0.48
4:E:23:ARG:HH12	11:L:51:GLN:HA	1.79	0.48
20:V:42:ALA:HB2	35:l:593:ILE:HD11	1.96	0.48
48:W:201:PEE:H23	36:m:42:GLY:HA2	1.96	0.48
22:Y:60:PHE:O	22:Y:64:THR:HG23	2.14	0.48
32:i:75:ILE:HG21	34:k:43:MET:HE3	1.95	0.48
35:l:56:HIS:ND1	35:l:57:THR:HG23	2.29	0.48
40:r:205:VAL:HG22	40:r:212:LEU:HD13	1.96	0.48
40:r:205:VAL:HG21	48:r:501:PEE:H47	1.96	0.48
51:r:504:CDL:H772	51:r:504:CDL:H741	1.61	0.48
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.96	0.48
1:A:280:GLY:O	14:O:143:ARG:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:173:ASP:OD1	9:J:176:SER:HB2	2.13	0.47
51:a:201:CDL:H111	48:l:704:PEE:C37	2.44	0.47
32:i:213:LEU:CD1	51:i:401:CDL:C14	2.89	0.47
35:l:452:ASN:HA	35:l:455:LYS:HG2	1.95	0.47
39:p:62:GLN:OE1	39:p:62:GLN:HA	2.14	0.47
5:F:48:ASN:HB3	5:F:51:LEU:HB3	1.95	0.47
9:J:127:ILE:HD11	9:J:253:ILE:HD11	1.96	0.47
16:Q:179:ARG:NH2	16:Q:401:GLU:O	2.37	0.47
48:W:201:PEE:H36	36:m:38:GLY:HA3	1.96	0.47
24:a:94:GLY:HA2	24:a:116:PRO:HG3	1.95	0.47
32:i:149:ILE:HD11	32:i:195:PRO:HG3	1.97	0.47
34:k:87:THR:HG1	34:k:89:TYR:HD1	1.60	0.47
37:n:50:ARG:HB2	37:n:53:GLU:HB2	1.95	0.47
48:r:501:PEE:H81	49:r:502:PLX:H393	1.96	0.47
1:A:44:ASN:O	1:A:133:HIS:HB3	2.13	0.47
1:A:376:HIS:HE2	14:O:33:GLY:N	2.11	0.47
6:G:94:ASP:OD1	6:G:94:ASP:N	2.46	0.47
51:I:201:CDL:C31	51:I:201:CDL:C53	2.85	0.47
11:L:78:ARG:HD2	12:M:607:LYS:HE3	1.97	0.47
16:Q:65:PRO:HB2	16:Q:67:ASN:O	2.14	0.47
51:l:701:CDL:C31	51:l:701:CDL:H761	2.44	0.47
41:s:24:GLU:OE1	41:s:274:ARG:NH1	2.47	0.47
44:w:182:GLN:HB3	44:w:314:LEU:HD21	1.95	0.47
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.49	0.47
16:Q:47:PHE:CD1	16:Q:52:MET:HE1	2.49	0.47
16:Q:137:ASP:OD1	16:Q:148:GLU:OE2	2.32	0.47
22:Y:99:ILE:HD11	43:v:108:LEU:N	2.30	0.47
36:m:167:VAL:O	36:m:171:ILE:HG12	2.14	0.47
39:p:117:ASP:O	39:p:121:LYS:HG3	2.14	0.47
39:p:133:TRP:O	39:p:137:VAL:HG23	2.14	0.47
1:A:68:ILE:HD11	14:O:249:LEU:HD11	1.97	0.47
1:A:102:MET:CG	1:A:149:MET:HB3	2.42	0.47
3:C:87:ASP:OD1	41:s:25:ARG:NH2	2.48	0.47
4:E:28:ALA:HB1	4:E:79:VAL:HG11	1.96	0.47
9:J:168:SER:O	9:J:203:PRO:HD2	2.14	0.47
12:M:347:ASP:HB3	12:M:594:ALA:HB1	1.97	0.47
14:O:198:PRO:O	14:O:201:ILE:N	2.48	0.47
6:X:85:TYR:O	6:X:89:LEU:HD23	2.15	0.47
24:a:120:TRP:O	24:a:124:THR:HG22	2.14	0.47
26:c:128:THR:CG2	26:c:132:HIS:CD2	2.98	0.47
51:i:401:CDL:H331	51:i:401:CDL:OA9	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:233:ALA:HA	40:r:320:GLY:HA2	1.96	0.47
44:w:246:LEU:N	44:w:247:PRO:HD2	2.29	0.47
6:G:100:VAL:HG12	6:G:142:GLN:HB2	1.95	0.47
48:W:201:PEE:C11	33:j:3:ILE:HG21	2.17	0.47
51:a:201:CDL:H751	28:e:103:SER:HB3	1.93	0.47
26:c:69:GLY:HA3	38:o:86:THR:HG21	1.97	0.47
4:E:62:LYS:O	4:E:66:MET:HG2	2.15	0.47
6:G:130:ILE:HG22	6:G:135:ALA:HB2	1.97	0.47
6:G:155:TYR:CD1	6:G:155:TYR:N	2.83	0.47
12:M:133:GLN:HG3	12:M:136:GLU:HG3	1.95	0.47
12:M:389:THR:O	12:M:390:THR:OG1	2.26	0.47
27:d:160:LYS:NZ	30:g:114:ILE:O	2.47	0.47
35:l:159:HIS:HB3	40:r:416:ARG:HG2	1.97	0.47
39:p:139:GLN:O	39:p:142:GLU:HG2	2.13	0.47
40:r:12:LEU:HB2	40:r:13:PRO:HD3	1.96	0.47
5:F:51:LEU:HD23	5:F:53:ILE:HD11	1.97	0.47
13:N:68:MET:HG2	13:N:69:ASN:H	1.80	0.47
21:W:144:THR:HB	41:s:96:ILE:HG23	1.97	0.47
35:l:496:MET:HE1	51:l:702:CDL:H622	1.97	0.47
9:J:270:ARG:NH2	9:J:328:THR:OG1	2.44	0.47
13:N:14:VAL:HA	13:N:23:TYR:CD1	2.50	0.47
15:P:173:MET:HE3	15:P:188:LEU:HB2	1.97	0.47
16:Q:86:PRO:HB3	16:Q:94:VAL:HG23	1.96	0.47
49:g:201:PLX:H232	32:i:332:LEU:HD13	1.96	0.47
33:j:68:GLU:CB	33:j:98:LEU:HD13	2.44	0.47
37:n:17:VAL:N	37:n:18:PRO:CD	2.78	0.47
40:r:299:VAL:O	40:r:303:ILE:HG12	2.15	0.47
8:I:97:PRO:HD3	15:P:61:PHE:CE1	2.50	0.47
11:L:165:SER:O	11:L:171:ARG:NE	2.46	0.47
22:Y:95:GLU:HA	22:Y:95:GLU:OE1	2.15	0.47
27:d:33:LEU:HD13	35:l:49:VAL:HG13	1.97	0.47
34:k:4:VAL:O	34:k:8:ILE:HG12	2.14	0.47
35:l:356:ILE:HG13	35:l:429:PHE:HE2	1.79	0.47
40:r:195:MET:HB2	48:r:501:PEE:O4	2.15	0.47
42:u:80:GLU:CD	42:u:80:GLU:N	2.73	0.47
35:l:176:ARG:NH2	40:r:400:MET:HB3	2.30	0.46
35:l:401:MET:CG	35:l:482:MET:HE2	2.44	0.46
1:A:184:LYS:HD2	1:A:184:LYS:HA	1.79	0.46
21:W:130:ASN:HB3	36:m:1:MET:H1	1.78	0.46
35:l:130:ILE:CD1	51:l:701:CDL:H262	2.46	0.46
44:w:58:LYS:O	44:w:60:ILE:HD12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:249:MET:HE3	44:w:253:CYS:SG	2.55	0.46
49:C:303:PLX:H21	49:C:303:PLX:H1C3	1.63	0.46
12:M:299:ARG:HG2	13:N:135:GLN:NE2	2.26	0.46
51:a:201:CDL:H331	25:b:84:TYR:CG	2.50	0.46
32:i:222:SER:O	32:i:224:ALA:N	2.49	0.46
35:l:80:PHE:HB3	35:l:82:MET:HE2	1.97	0.46
35:l:102:GLU:HG2	35:l:453:SER:HB3	1.97	0.46
51:l:701:CDL:H432	51:l:701:CDL:C60	2.32	0.46
44:w:48:ARG:HD2	44:w:288:ASP:OD2	2.15	0.46
44:w:80:LYS:NZ	44:w:267:GLU:OE2	2.39	0.46
4:E:121:LYS:HA	4:E:124:VAL:HG22	1.98	0.46
27:d:105:ILE:HG13	28:e:119:ARG:HH11	1.80	0.46
28:e:74:HIS:HB2	28:e:83:ASP:OD1	2.16	0.46
40:r:115:LEU:HD12	40:r:174:LEU:HD22	1.97	0.46
51:u:201:CDL:H781	51:u:201:CDL:H812	1.73	0.46
1:A:127:ASP:O	1:A:131:ILE:HG13	2.16	0.46
2:B:96:ARG:HG2	2:B:208:ASP:OD2	2.14	0.46
7:H:21:HIS:O	7:H:25:LYS:HG3	2.16	0.46
13:N:140:PRO:HB2	13:N:142:THR:HG22	1.97	0.46
14:O:196:LEU:HD13	14:O:201:ILE:HD11	1.97	0.46
15:P:173:MET:HB3	15:P:198:PHE:HB2	1.98	0.46
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	1.96	0.46
48:Q:501:PEE:H47	48:r:501:PEE:C24	2.46	0.46
33:j:81:THR:C	33:j:83:ASN:H	2.24	0.46
43:v:46:MET:HE2	43:v:56:ARG:HG2	1.96	0.46
9:J:82:VAL:O	9:J:105:PHE:HA	2.15	0.46
12:M:370:GLU:OE2	12:M:482:GLN:NE2	2.49	0.46
14:O:155:LYS:HD2	14:O:202:GLU:HG3	1.96	0.46
20:V:74:SER:HB2	20:V:90:TYR:HD1	1.81	0.46
48:j:201:PEE:H49	48:j:201:PEE:H14	1.97	0.46
44:w:229:ILE:HG23	44:w:233:TYR:HD2	1.80	0.46
1:A:121:GLU:HG3	1:A:122:PRO:HD2	1.98	0.46
21:W:131:GLU:N	21:W:131:GLU:OE2	2.49	0.46
26:c:184:TYR:CD1	43:v:34:ARG:HG3	2.51	0.46
32:i:9:LEU:HD13	32:i:42:PRO:HB2	1.98	0.46
34:k:57:ASN:HB3	36:m:143:ILE:HG13	1.96	0.46
40:r:253:LEU:HG	40:r:257:MET:HG3	1.97	0.46
41:s:141:SER:HB3	41:s:289:LEU:HD22	1.98	0.46
41:s:248:ASP:OD2	41:s:251:THR:HG22	2.15	0.46
1:A:53:LEU:O	1:A:57:GLN:HG2	2.16	0.46
1:A:185:ASN:HB3	1:A:190:GLY:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:75:GLU:HG3	3:C:167:PRO:HB2	1.98	0.46
6:G:149:ALA:O	6:G:153:ASP:N	2.46	0.46
9:J:317:ASP:O	9:J:321:ARG:HG3	2.16	0.46
15:P:112:ALA:O	16:Q:425:LYS:HE3	2.16	0.46
16:Q:53:TYR:CD1	35:l:571:MET:HE2	2.51	0.46
20:V:9:TYR:HE1	20:V:25:SER:OG	1.99	0.46
51:a:201:CDL:HB21	48:l:704:PEE:H51	1.97	0.46
34:k:2:PRO:HD2	34:k:5:TYR:CD2	2.51	0.46
51:l:701:CDL:C23	51:l:701:CDL:C27	2.86	0.46
37:n:54:GLU:HG2	37:n:55:VAL:HG22	1.98	0.46
44:w:250:SER:O	44:w:280:LYS:NZ	2.43	0.46
2:B:76:TYR:OH	41:s:33:LEU:HB2	2.15	0.46
4:E:19:PRO:HG2	4:E:23:ARG:NH1	2.31	0.46
7:H:56:LEU:HA	7:H:59:VAL:HG12	1.97	0.46
12:M:382:ARG:HG2	12:M:386:LEU:HD11	1.98	0.46
48:Q:501:PEE:C22	48:Q:501:PEE:C18	2.86	0.46
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.51	0.46
35:l:324:LEU:HD11	35:l:394:LEU:HB2	1.98	0.46
35:l:396:ILE:HA	35:l:399:VAL:HG12	1.97	0.46
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.51	0.46
3:C:188:LYS:HD3	3:C:191:ARG:HH11	1.80	0.46
33:j:95:LEU:HD11	41:s:305:ILE:HD12	1.97	0.46
35:l:557:TRP:O	35:l:561:ILE:HG12	2.16	0.46
40:r:101:LEU:HD13	51:r:504:CDL:H441	1.96	0.46
13:N:42:ASP:OD2	13:N:44:TYR:HD1	1.99	0.45
21:W:51:MET:HA	41:s:313:SER:HB2	1.98	0.45
27:d:105:ILE:HG13	28:e:119:ARG:NH1	2.31	0.45
49:j:202:PLX:H372	49:j:202:PLX:H342	1.71	0.45
41:s:87:VAL:HG12	41:s:95:LEU:HD23	1.99	0.45
1:A:41:ILE:HD11	1:A:253:THR:HB	1.98	0.45
14:O:201:ILE:O	14:O:205:ILE:HG12	2.16	0.45
16:Q:278:VAL:HG12	16:Q:329:ARG:HH21	1.81	0.45
32:i:215:MET:HE1	32:i:244:MET:HG3	1.98	0.45
35:l:10:THR:O	35:l:14:ILE:HG12	2.16	0.45
35:l:338:MET:HB2	35:l:457:LEU:HB3	1.97	0.45
5:F:78:SER:C	5:F:79:LEU:HD12	2.42	0.45
7:H:64:ASP:OD2	7:H:67:LYS:NZ	2.32	0.45
9:J:84:TYR:CE1	9:J:105:PHE:HB3	2.51	0.45
6:X:155:TYR:H	6:X:155:TYR:HD1	1.60	0.45
51:l:701:CDL:H871	51:l:701:CDL:C58	2.46	0.45
51:u:201:CDL:H601	51:u:201:CDL:H572	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:ARG:HD2	13:N:108:TYR:CG	2.51	0.45
3:C:113:MET:HE1	16:Q:86:PRO:HB2	1.99	0.45
4:E:37:ARG:NH2	6:G:132:ASP:OD2	2.41	0.45
9:J:201:ILE:HG22	9:J:203:PRO:HD3	1.97	0.45
12:M:198:THR:HG21	12:M:209:TYR:HB2	1.98	0.45
24:a:168:TRP:HB3	30:g:2:THR:O	2.17	0.45
34:k:33:LEU:HD23	34:k:36:MET:HE3	1.99	0.45
51:l:701:CDL:H871	51:l:701:CDL:H581	1.98	0.45
51:u:201:CDL:H781	51:u:201:CDL:H752	1.40	0.45
44:w:181:LYS:O	44:w:184:VAL:HG22	2.16	0.45
1:A:201:ALA:O	14:O:119:TYR:HB3	2.16	0.45
49:C:303:PLX:H311	49:C:303:PLX:H281	1.67	0.45
9:J:37:HIS:CE1	18:T:49:ASP:HA	2.51	0.45
12:M:133:GLN:O	12:M:137:CYS:HB2	2.17	0.45
25:b:2:SER:OG	25:b:3:GLY:N	2.48	0.45
26:c:176:LYS:HD2	26:c:176:LYS:HA	1.74	0.45
38:o:45:ARG:NH1	39:p:140:LEU:HD11	2.31	0.45
40:r:57:PHE:O	40:r:111:THR:HA	2.16	0.45
1:A:385:CYS:HB3	45:A:501:SF4:S2	2.56	0.45
2:B:76:TYR:CE2	41:s:33:LEU:HB2	2.51	0.45
7:H:6:LYS:HE3	7:H:9:THR:HG22	1.99	0.45
39:p:132:SER:OG	39:p:163:LEU:HB2	2.17	0.45
40:r:61:LEU:HB2	40:r:457:PRO:HD3	1.99	0.45
1:A:117:ALA:HB3	1:A:158:ILE:HA	1.98	0.45
3:C:64:PRO:HB3	3:C:102:VAL:HG13	1.99	0.45
9:J:171:ASN:HA	9:J:327:MET:SD	2.57	0.45
15:P:87:PHE:CE2	15:P:144:LYS:HD2	2.51	0.45
25:b:72:VAL:O	25:b:77:ILE:HG12	2.17	0.45
31:h:44:ALA:O	31:h:47:ILE:HG22	2.17	0.45
32:i:261:MET:O	32:i:265:MET:HG2	2.17	0.45
2:B:181:GLU:OE2	9:J:101:GLY:N	2.49	0.45
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.51	0.45
12:M:401:LEU:HD12	12:M:462:PHE:CE2	2.52	0.45
48:Q:501:PEE:H52	32:i:291:TYR:CD1	2.52	0.45
25:b:10:LEU:O	25:b:14:GLN:HG3	2.16	0.45
35:l:66:TRP:CZ3	48:l:704:PEE:H32	2.51	0.45
35:l:90:ILE:HG12	35:l:129:MET:SD	2.57	0.45
1:A:40:ARG:NH1	14:O:233:SER:OG	2.50	0.45
1:A:392:MET:HE2	1:A:419:ILE:HD12	1.98	0.45
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.99	0.45
51:a:201:CDL:H422	27:d:44:PRO:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:56:PHE:HB3	40:r:111:THR:CB	2.44	0.45
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.98	0.45
15:P:43:THR:HA	15:P:47:ILE:HD12	1.99	0.45
20:V:82:GLU:C	20:V:83:LYS:HD2	2.41	0.45
32:i:30:TRP:HD1	32:i:70:LEU:HD23	1.82	0.45
35:l:319:ILE:HG22	35:l:404:THR:HG21	1.99	0.45
35:l:384:PRO:HA	35:l:389:PHE:CD1	2.52	0.45
35:l:560:THR:O	35:l:565:THR:OG1	2.28	0.45
36:m:23:LYS:N	36:m:24:PRO:HD3	2.32	0.45
39:p:19:LEU:HD22	39:p:64:LEU:CD1	2.47	0.45
39:p:26:HIS:CD2	39:p:79:PRO:HB3	2.52	0.45
39:p:64:LEU:O	39:p:64:LEU:HG	2.16	0.45
40:r:354:LEU:HA	40:r:357:THR:HG22	1.99	0.45
42:u:88:CYS:SG	42:u:100:CYS:HB3	2.57	0.45
11:L:163:ASN:O	11:L:171:ARG:HA	2.16	0.44
12:M:171:THR:HG23	12:M:173:MET:SD	2.57	0.44
12:M:638:THR:O	12:M:642:VAL:HG23	2.17	0.44
16:Q:36:GLN:NE2	40:r:135:ARG:O	2.48	0.44
26:c:70:MET:HE2	38:o:86:THR:HG22	1.99	0.44
33:j:49:LEU:N	33:j:50:PRO:HD2	2.32	0.44
38:o:17:THR:HB	39:p:68:GLU:CG	2.47	0.44
40:r:408:LEU:HD23	40:r:408:LEU:HA	1.85	0.44
1:A:339:PHE:O	1:A:343:VAL:HG23	2.17	0.44
2:B:135:ARG:HD3	2:B:141:ARG:HG3	1.99	0.44
9:J:169:HIS:HB2	9:J:184:LYS:HE3	1.98	0.44
32:i:42:PRO:HG3	36:m:167:VAL:HG13	2.00	0.44
32:i:245:MET:HB2	32:i:301:SER:OG	2.18	0.44
35:l:62:ILE:HD13	35:l:81:LYS:HA	1.99	0.44
35:l:505:ASN:O	35:l:508:THR:HG22	2.17	0.44
35:l:603:ASN:C	35:l:603:ASN:ND2	2.73	0.44
38:o:59:VAL:HG22	40:r:423:ILE:HG12	1.99	0.44
42:u:107:PHE:O	42:u:107:PHE:CG	2.70	0.44
44:w:143:TYR:OH	44:w:199:LEU:O	2.29	0.44
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.72	0.44
2:B:99:GLY:CA	2:B:170:GLY:O	2.65	0.44
4:E:88:MET:HE2	15:P:185:ARG:HA	1.99	0.44
9:J:84:TYR:CD2	9:J:84:TYR:O	2.70	0.44
10:K:87:LEU:HB3	14:O:62:ARG:HG2	1.99	0.44
12:M:250:SER:OG	12:M:251:ILE:N	2.44	0.44
12:M:285:TRP:HB2	12:M:413:LEU:HD11	1.99	0.44
16:Q:80:LEU:HD13	33:j:50:PRO:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:33:PRO:HA	41:s:310:MET:HG2	2.00	0.44
32:i:10:ILE:O	32:i:14:MET:HG2	2.16	0.44
49:r:502:PLX:H1C3	49:r:502:PLX:H22	1.72	0.44
56:s:401:UQ:HM53	56:s:401:UQ:H72	1.69	0.44
7:H:38:ILE:HB	7:H:45:ARG:HD2	1.99	0.44
9:J:61:ALA:HA	9:J:66:GLY:HA3	1.98	0.44
12:M:347:ASP:OD1	12:M:347:ASP:N	2.49	0.44
15:P:153:ILE:O	15:P:178:PHE:HA	2.18	0.44
25:b:121:LYS:HE2	43:v:40:VAL:HA	2.00	0.44
48:j:201:PEE:H72	48:j:201:PEE:C47	2.47	0.44
51:l:702:CDL:H581	51:l:702:CDL:H352	1.98	0.44
40:r:347:GLY:O	40:r:350:THR:OG1	2.35	0.44
42:u:169:PHE:HE1	51:u:201:CDL:C56	2.30	0.44
43:v:103:GLU:OE2	43:v:106:ARG:NH2	2.42	0.44
30:g:12:PRO:HG3	31:h:8:LYS:HE2	2.00	0.44
31:h:38:LYS:HE2	31:h:42:GLU:OE2	2.18	0.44
32:i:117:GLU:OE2	35:l:587:TYR:OH	2.30	0.44
49:j:202:PLX:H132	36:m:152:TRP:HZ3	1.82	0.44
35:l:49:VAL:HB	35:l:50:PRO:HD3	1.99	0.44
35:l:292:ALA:HB2	35:l:304:PHE:CB	2.47	0.44
35:l:418:LEU:HD23	51:l:702:CDL:H562	2.00	0.44
12:M:304:GLN:HG2	12:M:615:LEU:HD12	2.00	0.44
14:O:148:ILE:HD12	14:O:184:PRO:HB2	1.99	0.44
6:X:155:TYR:CD2	6:X:156:GLU:HG3	2.53	0.44
39:p:108:HIS:CD2	39:p:109:PRO:HD2	2.53	0.44
44:w:279:ASP:OD1	44:w:279:ASP:N	2.50	0.44
1:A:89:GLY:HA2	1:A:244:ASN:ND2	2.32	0.44
3:C:190:LEU:CD2	48:C:302:PEE:H14	2.48	0.44
7:H:90:LEU:HB2	15:P:102:ASP:HB3	2.00	0.44
12:M:405:THR:OG1	12:M:410:GLU:OE2	2.32	0.44
21:W:98:MET:HG3	21:W:104:TRP:NE1	2.33	0.44
22:Y:88:ASP:HA	22:Y:89:PRO:HD3	1.83	0.44
27:d:144:SER:O	27:d:158:LYS:NZ	2.46	0.44
49:g:201:PLX:H332	32:i:342:ALA:HB3	2.00	0.44
40:r:357:THR:O	40:r:361:VAL:HG23	2.17	0.44
40:r:397:GLY:HA2	40:r:400:MET:HE2	2.00	0.44
1:A:128:ARG:HD2	1:A:165:GLU:OE2	2.18	0.44
4:E:90:LEU:HA	4:E:93:THR:HG22	2.00	0.44
28:e:65:ASN:OD1	28:e:67:TYR:N	2.37	0.44
35:l:323:HIS:ND1	35:l:475:MET:SD	2.91	0.44
40:r:373:ILE:HD11	40:r:444:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:38:LYS:HB3	42:u:39:PRO:HD3	2.00	0.44
44:w:139:ARG:HH12	57:w:401:ADP:HN61	1.66	0.44
1:A:83:SER:HB2	1:A:262:PHE:CD2	2.53	0.44
1:A:125:CYS:HB3	14:O:178:GLY:O	2.18	0.44
5:F:30:SER:OG	5:F:63:PRO:HG3	2.17	0.44
5:F:68:ARG:HH11	5:F:68:ARG:HG2	1.83	0.44
12:M:306:MET:HB2	12:M:583:ILE:HB	2.00	0.44
12:M:560:LEU:HD23	12:M:564:CYS:SG	2.58	0.44
24:a:60:SER:HB3	39:p:107:TRP:HA	2.00	0.44
35:l:96:VAL:O	35:l:100:ILE:HG12	2.17	0.44
36:m:25:SER:O	36:m:28:TYR:N	2.44	0.44
40:r:196:TRP:HB2	40:r:253:LEU:HD23	2.00	0.44
40:r:300:ALA:O	40:r:308:SER:HB3	2.17	0.44
41:s:81:LEU:O	41:s:85:MET:HG3	2.17	0.44
51:u:201:CDL:H252	51:u:201:CDL:H221	1.70	0.44
1:A:448:GLU:O	1:A:452:GLN:HG2	2.18	0.43
2:B:99:GLY:O	2:B:169:GLU:CG	2.66	0.43
9:J:85:ARG:HE	52:J:401:NDP:P2B	2.41	0.43
51:a:201:CDL:H532	48:l:704:PEE:H56	1.99	0.43
25:b:28:LEU:HD23	39:p:115:TYR:CE1	2.53	0.43
27:d:30:VAL:O	27:d:34:THR:HG23	2.18	0.43
27:d:114:GLN:HG3	35:l:203:MET:HG2	2.00	0.43
39:p:64:LEU:HA	39:p:67:ALA:HB3	2.00	0.43
40:r:303:ILE:HG22	40:r:305:THR:HG23	1.99	0.43
44:w:353:TRP:CE3	44:w:354:LEU:HG	2.53	0.43
3:C:71:CYS:HB2	16:Q:222:MET:HE1	1.99	0.43
6:G:88:LYS:HD3	6:G:98:LEU:HD21	1.99	0.43
14:O:42:ARG:NH2	18:T:104:LYS:HG2	2.32	0.43
14:O:160:VAL:HA	14:O:171:LEU:HD23	2.00	0.43
15:P:213:ASP:HB3	15:P:216:VAL:HG22	2.00	0.43
22:Y:99:ILE:CD1	43:v:107:ARG:C	2.91	0.43
27:d:23:GLN:HB2	43:v:72:ASP:HB3	2.00	0.43
38:o:26:SER:OG	38:o:27:PRO:HD2	2.18	0.43
40:r:122:PHE:CZ	40:r:206:LYS:HD2	2.52	0.43
49:r:503:PLX:H121	49:r:503:PLX:H152	1.45	0.43
42:u:86:TRP:O	42:u:86:TRP:CE3	2.70	0.43
51:u:201:CDL:H171	51:u:201:CDL:H201	1.76	0.43
44:w:63:ASP:O	44:w:206:TYR:HA	2.18	0.43
2:B:131:GLU:OE1	13:N:130:THR:HG21	2.18	0.43
3:C:88:ARG:HA	41:s:37:PRO:HA	2.01	0.43
12:M:33:GLU:HB3	12:M:98:LYS:HZ2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:155:VAL:HB	16:Q:229:PRO:HB3	2.01	0.43
21:W:70:ALA:HB2	42:u:125:LEU:HD13	2.00	0.43
21:W:84:LEU:HD12	42:u:57:LEU:HD21	2.00	0.43
51:a:201:CDL:C19	51:a:201:CDL:H732	2.41	0.43
25:b:8:GLU:O	25:b:12:LEU:HG	2.17	0.43
51:l:701:CDL:H791	51:l:701:CDL:H611	2.00	0.43
51:l:701:CDL:H461	40:r:445:LEU:O	2.17	0.43
39:p:20:TYR:CZ	39:p:24:LEU:HD11	2.53	0.43
51:r:504:CDL:H271	51:r:504:CDL:H742	2.00	0.43
2:B:79:ARG:NH2	8:I:20:LEU:HD21	2.33	0.43
3:C:167:PRO:HG3	16:Q:222:MET:HE2	2.00	0.43
3:C:188:LYS:HG3	3:C:188:LYS:O	2.18	0.43
5:F:17:ARG:HD2	12:M:364:ASP:OD2	2.18	0.43
7:H:98:LYS:HG3	7:H:100:TRP:CZ2	2.54	0.43
9:J:57:THR:HG21	9:J:120:VAL:HG12	1.99	0.43
25:b:17:GLU:CD	25:b:21:ARG:HH21	2.25	0.43
28:e:103:SER:HA	49:r:503:PLX:H271	2.00	0.43
33:j:87:MET:HE1	41:s:309:ILE:HD11	2.00	0.43
35:l:161:ARG:NH2	39:p:88:GLY:O	2.51	0.43
37:n:47:ARG:CG	37:n:48:GLU:N	2.81	0.43
42:u:89:ILE:HD11	42:u:97:PHE:HD1	1.83	0.43
44:w:58:LYS:HD3	44:w:202:HIS:ND1	2.33	0.43
2:B:173:PHE:HE2	3:C:171:GLU:HG2	1.83	0.43
3:C:73:ALA:O	3:C:76:MET:HG3	2.18	0.43
9:J:71:ASN:O	9:J:75:ARG:HG3	2.18	0.43
11:L:89:SER:O	12:M:59:GLN:NE2	2.48	0.43
15:P:69:LEU:HD22	15:P:96:VAL:HG22	2.00	0.43
17:S:1:MET:HE3	17:S:1:MET:HB3	1.90	0.43
38:o:105:PHE:CD2	40:r:263:MET:HE1	2.53	0.43
40:r:455:LEU:HD23	40:r:455:LEU:HA	1.91	0.43
3:C:71:CYS:HB3	16:Q:141:TYR:CB	2.48	0.43
12:M:145:MET:HE3	15:P:239:TRP:O	2.17	0.43
12:M:307:ILE:HG22	12:M:582:VAL:HG22	2.01	0.43
48:Q:501:PEE:H30	40:r:152:TYR:CD1	2.54	0.43
6:X:100:VAL:HG12	6:X:142:GLN:HB2	2.01	0.43
27:d:102:ILE:HG13	28:e:122:ALA:HB1	2.00	0.43
35:l:375:ILE:HD12	35:l:458:LEU:HD22	2.01	0.43
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.53	0.43
12:M:68:ARG:NH1	12:M:284:GLU:HB2	2.34	0.43
16:Q:145:MET:HG3	16:Q:214:TYR:CE2	2.54	0.43
16:Q:182:ASN:HD21	16:Q:404:LYS:HG3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:397:TYR:OH	16:Q:406:GLU:OE1	2.34	0.43
22:Y:97:LEU:CD1	43:v:104:ARG:HA	2.23	0.43
33:j:54:LYS:HD3	33:j:113:TRP:HA	2.01	0.43
35:l:347:ILE:HD13	35:l:354:GLN:HG2	2.01	0.43
35:l:592:LEU:O	35:l:596:MET:HG3	2.18	0.43
42:u:23:SER:HB2	42:u:90:ASP:HB2	1.97	0.43
51:u:201:CDL:H1	51:u:201:CDL:C15	2.48	0.43
1:A:122:PRO:HD2	1:A:322:SER:OG	2.19	0.43
1:A:270:ASN:O	1:A:292:MET:HG2	2.19	0.43
1:A:367:ILE:O	1:A:371:ILE:HG12	2.18	0.43
2:B:76:TYR:HA	2:B:79:ARG:HE	1.84	0.43
3:C:50:LEU:CD2	48:C:302:PEE:H26	2.48	0.43
13:N:73:THR:HG21	13:N:81:MET:HE1	2.01	0.43
14:O:207:GLU:OE2	14:O:214:PRO:HB3	2.19	0.43
6:X:129:GLU:HB2	39:p:82:PHE:CD1	2.54	0.43
24:a:127:ASP:OD1	49:a:202:PLX:C1	2.58	0.43
32:i:95:MET:HE1	32:i:149:ILE:HG22	1.94	0.43
32:i:153:LEU:HG	32:i:157:MET:HE2	2.01	0.43
35:l:368:PHE:HA	35:l:371:THR:HG22	2.00	0.43
44:w:70:LYS:HZ3	44:w:160:GLU:HG2	1.83	0.43
1:A:364:VAL:HG12	1:A:400:VAL:HG22	2.00	0.43
13:N:73:THR:HG23	13:N:76:ASP:O	2.19	0.43
13:N:97:PRO:HG2	13:N:100:THR:HG23	2.00	0.43
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.54	0.43
16:Q:238:LEU:HA	16:Q:238:LEU:HD23	1.77	0.43
23:Z:13:LYS:HA	23:Z:13:LYS:HD2	1.76	0.43
33:j:84:LEU:HD23	33:j:84:LEU:HA	1.81	0.43
48:j:201:PEE:H35	48:j:201:PEE:H30	1.43	0.43
35:l:7:LEU:O	35:l:11:THR:HG23	2.19	0.43
1:A:62:TRP:CE3	1:A:181:LEU:HD23	2.54	0.43
2:B:94:SER:OG	16:Q:215:GLU:OE2	2.33	0.43
4:E:114:ARG:NH2	9:J:45:LYS:HG2	2.33	0.43
6:G:119:ILE:HG21	6:G:135:ALA:HB1	1.99	0.43
7:H:35:LEU:HD13	7:H:49:GLU:HG3	2.00	0.43
10:K:110:HIS:HA	12:M:441:ARG:HH11	1.83	0.43
11:L:131:LYS:HD2	11:L:147:VAL:HG11	2.00	0.43
14:O:137:THR:HG22	14:O:138:THR:H	1.83	0.43
24:a:99:ALA:HB2	27:d:62:TYR:HD2	1.84	0.43
33:j:73:LEU:O	41:s:160:TYR:OH	2.36	0.43
35:l:130:ILE:HD13	51:l:701:CDL:H262	2.00	0.43
35:l:407:TRP:O	35:l:411:MET:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:19:LEU:HD13	39:p:68:GLU:CD	2.36	0.43
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.53	0.43
3:C:124:MET:HA	3:C:125:PRO:HD3	1.74	0.42
3:C:173:LEU:O	3:C:177:ILE:HG12	2.19	0.42
9:J:72:HIS:HB3	9:J:250:ILE:HG13	2.00	0.42
10:K:88:ASP:O	10:K:92:GLU:OE1	2.37	0.42
16:Q:80:LEU:HD23	16:Q:80:LEU:H	1.84	0.42
19:U:53:TYR:HB2	21:W:72:MET:SD	2.58	0.42
28:e:129:ARG:HB3	28:e:134:LEU:HB2	2.01	0.42
29:f:55:TRP:O	29:f:59:ILE:HG12	2.18	0.42
49:j:202:PLX:H152	49:j:202:PLX:H182	1.86	0.42
41:s:13:ILE:O	41:s:17:VAL:HG13	2.19	0.42
44:w:59:VAL:HG13	44:w:201:PRO:HA	2.00	0.42
44:w:241:TYR:HB3	44:w:246:LEU:HD23	2.00	0.42
44:w:258:TYR:CE2	44:w:269:VAL:HG22	2.54	0.42
44:w:342:GLY:O	44:w:355:LYS:NZ	2.34	0.42
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.59	0.42
3:C:188:LYS:HD3	3:C:191:ARG:HD3	2.01	0.42
5:F:44:LEU:HD22	5:F:91:LEU:HD21	2.01	0.42
9:J:238:GLN:NE2	9:J:270:ARG:HG3	2.34	0.42
9:J:251:ASN:O	9:J:255:ASP:N	2.53	0.42
14:O:130:TYR:HA	14:O:189:ASN:OD1	2.19	0.42
16:Q:150:ALA:HB2	16:Q:400:ILE:HG12	2.01	0.42
21:W:97:ILE:HD13	31:h:83:ARG:HB2	2.00	0.42
23:Z:36:LEU:HG	23:Z:41:LEU:HB2	2.00	0.42
51:l:701:CDL:H761	51:l:701:CDL:H321	2.01	0.42
39:p:19:LEU:HD11	39:p:68:GLU:OE2	2.12	0.42
1:A:204:TYR:HH	47:A:503:NAI:H5N	1.82	0.42
12:M:341:ILE:HD12	12:M:545:LEU:HD11	2.01	0.42
48:W:201:PEE:H48	36:m:45:LEU:HD13	2.01	0.42
24:a:53:ARG:C	25:b:28:LEU:HD13	2.44	0.42
27:d:37:PHE:CD1	35:l:3:PRO:HB3	2.53	0.42
27:d:49:ARG:O	27:d:52:ILE:HG22	2.19	0.42
32:i:122:ILE:O	32:i:176:ARG:NH1	2.51	0.42
51:l:701:CDL:H851	51:l:701:CDL:C81	2.46	0.42
39:p:26:HIS:HB3	39:p:75:GLN:O	2.18	0.42
47:A:503:NAI:H6N	47:A:503:NAI:H2D	1.69	0.42
2:B:76:TYR:O	2:B:79:ARG:HG2	2.19	0.42
2:B:100:GLU:O	2:B:170:GLY:N	2.46	0.42
12:M:371:VAL:HG22	12:M:533:GLY:HA2	2.02	0.42
22:Y:65:MET:SD	35:l:375:ILE:HG12	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:42:LEU:O	29:f:46:LEU:HG	2.19	0.42
30:g:17:PRO:HG2	30:g:83:TYR:CZ	2.55	0.42
35:l:295:GLN:HB2	35:l:301:ILE:HG12	2.02	0.42
39:p:45:ARG:O	39:p:49:ASP:HB2	2.19	0.42
40:r:336:ARG:HG3	40:r:336:ARG:HH11	1.84	0.42
40:r:394:ILE:H	40:r:394:ILE:HD12	1.83	0.42
12:M:624:ARG:NH2	12:M:637:ASP:OD1	2.32	0.42
13:N:39:VAL:CG2	13:N:50:GLU:HG2	2.50	0.42
14:O:200:ASP:O	14:O:203:GLU:HG2	2.19	0.42
24:a:99:ALA:HB2	27:d:62:TYR:CD2	2.55	0.42
32:i:258:SER:OG	32:i:336:VAL:HG22	2.20	0.42
40:r:73:LEU:HD22	40:r:103:GLN:OE1	2.19	0.42
42:u:51:LYS:HD2	42:u:141:PRO:HB2	2.01	0.42
44:w:245:PHE:CD2	44:w:246:LEU:HD22	2.51	0.42
2:B:162:CYS:O	16:Q:368:ARG:NH1	2.45	0.42
9:J:178:SER:O	9:J:182:ARG:HG3	2.19	0.42
11:L:53:ILE:HD12	11:L:53:ILE:H	1.83	0.42
12:M:404:GLY:HA3	12:M:480:ALA:HB2	2.01	0.42
48:Q:501:PEE:H32	35:l:562:LEU:HG	2.01	0.42
49:g:201:PLX:H22	49:g:201:PLX:H1C3	1.82	0.42
33:j:25:PRO:HB2	41:s:60:PRO:HD3	2.01	0.42
35:l:341:MET:HB3	35:l:454:ILE:HD13	2.01	0.42
48:r:501:PEE:H69	49:r:502:PLX:H381	2.02	0.42
44:w:108:LEU:HD22	44:w:331:PHE:HB2	2.00	0.42
12:M:141:ASP:O	12:M:145:MET:HG2	2.19	0.42
12:M:650:SER:OG	12:M:652:ASN:OD1	2.29	0.42
16:Q:198:THR:HB	16:Q:199:PRO:HD3	2.01	0.42
6:X:85:TYR:CD2	23:Z:16:LEU:HD23	2.55	0.42
22:Y:92:TRP:HE3	43:v:103:GLU:HG2	1.84	0.42
33:j:73:LEU:HD13	36:m:55:MET:HE1	2.02	0.42
35:l:331:MET:SD	35:l:387:THR:HG23	2.60	0.42
40:r:48:ASN:N	40:r:48:ASN:OD1	2.52	0.42
5:F:69:TYR:OH	5:F:75:LYS:HE2	2.19	0.42
6:G:76:LEU:N	6:G:76:LEU:HD23	2.34	0.42
6:G:88:LYS:HE3	6:G:95:PRO:HB3	2.02	0.42
16:Q:47:PHE:HD1	16:Q:52:MET:HE1	1.83	0.42
35:l:66:TRP:CB	48:l:704:PEE:H19	2.49	0.42
35:l:69:MET:SD	40:r:451:PRO:HG2	2.60	0.42
35:l:286:LEU:HD22	35:l:411:MET:SD	2.60	0.42
51:l:701:CDL:H582	51:l:701:CDL:C79	2.50	0.42
51:l:702:CDL:H391	51:l:702:CDL:H421	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:l:702:CDL:H572	51:l:702:CDL:H541	1.58	0.42
44:w:42:ALA:HB1	44:w:47:GLU:HG3	2.01	0.42
5:F:37:ILE:HA	5:F:41:TYR:HB2	2.01	0.42
9:J:213:PHE:HD2	9:J:214:LEU:HD12	1.85	0.42
16:Q:432:LEU:HD12	16:Q:432:LEU:HA	1.91	0.42
35:l:123:LEU:CB	35:l:150:MET:HE2	2.44	0.42
40:r:127:VAL:HB	40:r:128:PRO:HD3	2.01	0.42
41:s:11:ILE:HB	41:s:12:PRO:HD3	2.01	0.42
44:w:211:VAL:HG21	44:w:235:GLN:OE1	2.20	0.42
3:C:50:LEU:HD11	48:C:302:PEE:C36	2.41	0.42
6:G:88:LYS:NZ	6:G:98:LEU:HD11	2.35	0.42
14:O:47:ASN:HD21	14:O:94:PRO:HA	1.83	0.42
16:Q:392:PRO:HA	16:Q:393:PRO:HD3	1.97	0.42
32:i:129:LEU:HD12	51:i:401:CDL:H341	2.02	0.42
33:j:51:PHE:CE1	34:k:79:VAL:HG13	2.55	0.42
37:n:54:GLU:HG2	37:n:55:VAL:N	2.35	0.42
44:w:51:ARG:HH11	44:w:51:ARG:HG2	1.83	0.42
3:C:62:LEU:O	3:C:91:VAL:HA	2.20	0.41
5:F:33:VAL:HG22	5:F:87:VAL:HG11	2.01	0.41
6:G:82:ARG:NE	6:G:126:PHE:HE1	2.11	0.41
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.53	0.41
12:M:213:MET:HB3	12:M:215:MET:HG2	2.02	0.41
12:M:647:GLU:HB2	12:M:654:VAL:HG21	2.01	0.41
20:V:41:ILE:HD11	20:V:55:ARG:HD2	2.02	0.41
21:W:60:LEU:HD13	42:u:98:ARG:HD3	2.02	0.41
35:l:223:LYS:HG2	35:l:255:ALA:HB3	2.02	0.41
40:r:13:PRO:HB3	51:r:504:CDL:H581	2.02	0.41
40:r:22:MET:HE3	40:r:22:MET:HB3	1.91	0.41
40:r:67:VAL:HG12	49:r:503:PLX:H382	2.02	0.41
2:B:177:THR:CG2	2:B:182:GLU:HB2	2.45	0.41
10:K:76:LEU:HG	10:K:79:HIS:CE1	2.54	0.41
6:X:113:LEU:HA	6:X:116:VAL:HG12	2.01	0.41
6:X:155:TYR:CD1	6:X:155:TYR:N	2.87	0.41
28:e:152:ASP:OD1	28:e:152:ASP:N	2.49	0.41
35:l:341:MET:HB3	35:l:454:ILE:CD1	2.50	0.41
42:u:102:LYS:HD3	42:u:102:LYS:N	2.35	0.41
1:A:110:PRO:O	1:A:238:CYS:HB3	2.19	0.41
6:G:134:ASP:O	6:G:137:LYS:HG2	2.20	0.41
14:O:137:THR:HG22	14:O:138:THR:N	2.36	0.41
14:O:159:LYS:HB2	14:O:162:GLU:HG3	2.02	0.41
16:Q:194:ILE:O	41:s:279:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:g:201:PLX:H232	49:g:201:PLX:H202	1.92	0.41
35:l:78:LEU:CD1	51:l:701:CDL:H251	2.41	0.41
35:l:593:ILE:HA	35:l:596:MET:CE	2.46	0.41
6:G:90:TYR:CE2	6:G:92:LYS:HB2	2.56	0.41
9:J:246:SER:O	9:J:250:ILE:HG12	2.21	0.41
16:Q:209:LYS:O	16:Q:212:GLU:HB2	2.19	0.41
25:b:89:HIS:CE1	48:l:704:PEE:C32	3.02	0.41
35:l:9:LEU:HD11	35:l:63:ILE:HG21	2.02	0.41
42:u:39:PRO:HG2	42:u:66:CYS:SG	2.60	0.41
44:w:105:ASP:OD1	44:w:106:VAL:N	2.52	0.41
6:G:123:GLU:HG2	6:G:130:ILE:HG13	2.01	0.41
7:H:76:GLN:O	7:H:79:GLU:N	2.48	0.41
9:J:65:LEU:HD23	9:J:129:LEU:HD22	2.02	0.41
9:J:171:ASN:C	9:J:181:LEU:HD12	2.46	0.41
13:N:55:PHE:CZ	13:N:58:ARG:HG3	2.56	0.41
15:P:83:GLU:HG2	15:P:142:ARG:HH22	1.85	0.41
24:a:71:MET:O	24:a:75:ILE:HG12	2.20	0.41
30:g:52:ARG:NH1	32:i:318:GLU:OE2	2.53	0.41
2:B:78:PHE:O	8:I:12:ARG:NH2	2.50	0.41
2:B:99:GLY:N	2:B:170:GLY:O	2.53	0.41
48:B:303:PEE:H21	48:B:303:PEE:H16	1.53	0.41
7:H:24:LEU:HD23	7:H:24:LEU:HA	1.88	0.41
9:J:203:PRO:HG2	52:J:401:NDP:C6N	2.51	0.41
16:Q:153:LEU:HD11	16:Q:308:TYR:CD1	2.55	0.41
28:e:85:TRP:O	28:e:89:VAL:HG22	2.21	0.41
31:h:17:TRP:CD1	31:h:17:TRP:H	2.38	0.41
32:i:133:TRP:HE3	51:i:401:CDL:H391	1.85	0.41
34:k:17:ALA:O	34:k:21:MET:HG2	2.20	0.41
40:r:217:PRO:O	40:r:221:VAL:HG23	2.21	0.41
56:s:401:UQ:H203	56:s:401:UQ:H171	1.82	0.41
2:B:99:GLY:HA3	2:B:170:GLY:O	2.20	0.41
2:B:118:LEU:HD11	16:Q:382:PHE:CE2	2.56	0.41
16:Q:226:TYR:OH	16:Q:234:GLN:O	2.30	0.41
18:T:46:ASP:OD1	18:T:49:ASP:HB2	2.20	0.41
31:h:12:LEU:HD23	31:h:12:LEU:HA	1.91	0.41
41:s:55:LEU:HD13	41:s:221:ALA:HB2	2.01	0.41
1:A:272:GLY:O	1:A:292:MET:HB2	2.21	0.41
1:A:338:ASP:OD1	1:A:338:ASP:N	2.53	0.41
2:B:116:CYS:SG	2:B:118:LEU:HD13	2.61	0.41
9:J:346:GLU:HG2	9:J:371:PRO:HB3	2.02	0.41
12:M:219:SER:HB3	12:M:288:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:277:MET:SD	12:M:279:GLU:HG2	2.61	0.41
20:V:4:THR:O	20:V:8:LYS:HD3	2.21	0.41
48:W:201:PEE:H52	41:s:104:PHE:CE1	2.55	0.41
22:Y:89:PRO:HA	22:Y:92:TRP:CZ3	2.55	0.41
26:c:111:MET:HE1	35:l:539:TYR:CD1	2.55	0.41
30:g:15:PHE:O	30:g:80:ARG:HD2	2.20	0.41
32:i:99:THR:CG2	32:i:157:MET:HE1	2.47	0.41
32:i:190:MET:HE2	32:i:205:LEU:HA	2.02	0.41
34:k:37:MET:HG3	34:k:67:ALA:HB1	2.02	0.41
35:l:182:PHE:CE1	35:l:186:MET:HE3	2.55	0.41
35:l:371:THR:O	35:l:375:ILE:HG13	2.20	0.41
40:r:166:TYR:O	40:r:170:THR:HG23	2.21	0.41
41:s:18:ALA:HB2	56:s:401:UQ:C15	2.51	0.41
41:s:293:PHE:O	41:s:297:THR:OG1	2.33	0.41
43:v:112:LYS:HD2	43:v:112:LYS:O	2.19	0.41
44:w:84:ARG:HD3	44:w:149:HIS:NE2	2.35	0.41
44:w:139:ARG:HD3	44:w:162:SER:O	2.21	0.41
44:w:314:LEU:O	44:w:318:THR:HG22	2.21	0.41
44:w:350:LYS:HG3	44:w:351:TRP:N	2.36	0.41
1:A:351:THR:HG21	47:A:503:NAI:N7N	2.36	0.41
2:B:210:LEU:HD12	8:I:38:PRO:HB3	2.02	0.41
4:E:115:PRO:HB2	4:E:120:SER:OG	2.20	0.41
12:M:403:VAL:HG21	12:M:452:LEU:HD21	2.02	0.41
13:N:10:GLY:O	13:N:14:VAL:HG23	2.21	0.41
13:N:85:GLU:HG2	13:N:86:TRP:N	2.36	0.41
15:P:83:GLU:HG2	15:P:142:ARG:NH2	2.36	0.41
15:P:201:ASP:OD1	15:P:201:ASP:N	2.45	0.41
21:W:30:LEU:HD12	21:W:30:LEU:HA	1.79	0.41
24:a:139:ILE:HG23	40:r:54:LEU:HD23	2.03	0.41
26:c:151:PRO:HD2	43:v:9:TYR:OH	2.21	0.41
33:j:17:LEU:HD12	33:j:20:ILE:HD11	2.02	0.41
33:j:21:ALA:HB1	41:s:218:GLY:HA3	2.03	0.41
35:l:60:GLU:OE1	35:l:83:ASP:HA	2.20	0.41
35:l:573:MET:HE3	35:l:573:MET:HA	2.01	0.41
36:m:164:GLY:O	36:m:168:ILE:HG12	2.21	0.41
39:p:11:THR:O	39:p:15:LYS:HG3	2.20	0.41
39:p:82:PHE:HB2	39:p:85:SER:OG	2.20	0.41
42:u:23:SER:OG	42:u:90:ASP:HB2	2.21	0.41
44:w:63:ASP:O	44:w:206:TYR:HD1	2.04	0.41
44:w:135:LEU:HD23	44:w:135:LEU:HA	1.88	0.41
2:B:76:TYR:CE2	16:Q:202:TRP:NE1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:63:PRO:HA	16:Q:64:PRO:HD3	1.95	0.41
19:U:15:LYS:HG3	19:U:16:GLU:HG2	2.02	0.41
25:b:110:ILE:HD11	25:b:117:ILE:HD11	2.03	0.41
25:b:117:ILE:H	25:b:117:ILE:HG12	1.71	0.41
26:c:109:LEU:O	26:c:113:ILE:HG23	2.21	0.41
30:g:85:TYR:CZ	32:i:344:SER:HB3	2.55	0.41
32:i:237:MET:HG3	32:i:237:MET:O	2.21	0.41
51:l:702:CDL:H382	51:l:702:CDL:H351	1.80	0.41
43:v:83:GLU:OE1	43:v:83:GLU:N	2.51	0.41
44:w:208:ASP:N	44:w:258:TYR:O	2.37	0.41
1:A:327:ILE:HB	1:A:331:VAL:HG11	2.04	0.40
3:C:50:LEU:HD22	48:C:302:PEE:C18	2.39	0.40
4:E:22:SER:HB3	4:E:27:GLU:HB2	2.02	0.40
7:H:44:TYR:HB2	15:P:68:ILE:HG23	2.03	0.40
8:I:107:SER:C	8:I:109:ASP:H	2.29	0.40
11:L:84:ARG:NH1	11:L:88:GLN:O	2.54	0.40
16:Q:145:MET:HE2	16:Q:224:ALA:HB3	2.03	0.40
16:Q:251:PHE:O	16:Q:255:ILE:HG13	2.21	0.40
22:Y:51:THR:O	22:Y:54:GLN:HG2	2.21	0.40
51:a:201:CDL:H571	25:b:85:TYR:CE2	2.56	0.40
26:c:162:PRO:HB2	26:c:163:TYR:CD1	2.56	0.40
32:i:68:MET:CE	34:k:37:MET:HB2	2.51	0.40
35:l:197:ASP:OD1	35:l:198:LEU:N	2.54	0.40
35:l:375:ILE:HD13	35:l:462:ILE:HD11	2.02	0.40
36:m:34:ILE:HG13	36:m:65:LEU:HD23	2.03	0.40
40:r:201:MET:O	40:r:205:VAL:HG23	2.21	0.40
41:s:149:ILE:HG13	41:s:297:THR:HG23	2.03	0.40
44:w:148:GLU:OE1	44:w:301:LYS:NZ	2.33	0.40
1:A:291:GLU:HG2	1:A:292:MET:H	1.86	0.40
2:B:79:ARG:HA	8:I:12:ARG:NH2	2.35	0.40
7:H:38:ILE:O	7:H:45:ARG:NH1	2.55	0.40
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.57	0.40
17:S:34:LYS:HE3	17:S:34:LYS:HB2	1.79	0.40
24:a:106:VAL:HA	24:a:107:PRO:HD3	1.93	0.40
26:c:141:LEU:HD23	26:c:141:LEU:HA	1.92	0.40
35:l:198:LEU:HD23	35:l:198:LEU:HA	1.87	0.40
51:l:702:CDL:H521	51:l:702:CDL:H711	2.03	0.40
39:p:49:ASP:OD1	39:p:52:LYS:HE3	2.21	0.40
48:r:501:PEE:H71	48:r:501:PEE:C38	2.51	0.40
42:u:64:ASN:HD22	42:u:64:ASN:HA	1.56	0.40
44:w:54:THR:C	44:w:56:THR:H	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:173:ASP:OD1	9:J:173:ASP:N	2.53	0.40
12:M:168:LEU:HD23	12:M:168:LEU:HA	1.90	0.40
16:Q:158:LEU:HD23	16:Q:158:LEU:HA	1.93	0.40
16:Q:168:GLN:HB3	16:Q:310:VAL:HG13	2.02	0.40
22:Y:43:ARG:HG3	22:Y:48:PRO:HA	2.03	0.40
33:j:68:GLU:CD	33:j:98:LEU:HD13	2.40	0.40
41:s:21:THR:O	41:s:25:ARG:HG3	2.21	0.40
6:G:137:LYS:HB3	6:G:137:LYS:HE2	1.79	0.40
12:M:64:CYS:O	12:M:184:ARG:NH2	2.35	0.40
16:Q:40:ASP:OD1	16:Q:40:ASP:N	2.40	0.40
20:V:141:VAL:O	24:a:169:TYR:OH	2.30	0.40
21:W:97:ILE:HG22	21:W:98:MET:HE2	2.04	0.40
25:b:16:ARG:CG	25:b:20:ARG:HE	2.34	0.40
32:i:249:LEU:HD22	32:i:254:LEU:HD12	2.01	0.40
33:j:90:MET:HE2	36:m:154:VAL:HB	2.04	0.40
35:l:152:PHE:CD1	35:l:168:ALA:HB1	2.56	0.40
35:l:589:LEU:HD12	35:l:589:LEU:HA	1.89	0.40
40:r:216:LEU:HD23	40:r:287:ALA:HB1	2.03	0.40
44:w:204:VAL:HG23	44:w:255:VAL:HG13	2.04	0.40
1:A:384:PRO:HB2	1:A:423:THR:HG22	2.04	0.40
9:J:243:VAL:O	9:J:247:LYS:HG3	2.21	0.40
12:M:501:ARG:NH1	12:M:666:GLN:OE1	2.55	0.40
14:O:179:ALA:HB3	14:O:185:MET:HE3	2.03	0.40
32:i:68:MET:HE1	34:k:37:MET:HB2	2.03	0.40
34:k:22:TYR:O	35:l:585:LYS:HG2	2.21	0.40
51:l:701:CDL:OA7	51:l:701:CDL:HA61	2.15	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	429/431 (100%)	417 (97%)	12 (3%)	0	100	100
2	B	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
3	C	154/156 (99%)	146 (95%)	8 (5%)	0	100	100
4	E	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
5	F	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
6	G	86/88 (98%)	86 (100%)	0	0	100	100
6	X	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
7	H	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
8	I	93/112 (83%)	80 (86%)	12 (13%)	1 (1%)	11	36
9	J	289/341 (85%)	277 (96%)	11 (4%)	1 (0%)	36	65
10	K	40/42 (95%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	665 (97%)	22 (3%)	1 (0%)	48	77
13	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
14	O	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
15	P	206/208 (99%)	196 (95%)	10 (5%)	0	100	100
16	Q	412/430 (96%)	398 (97%)	13 (3%)	1 (0%)	43	72
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%)	133 (96%)	4 (3%)	1 (1%)	18	48
21	W	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
22	Y	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
23	Z	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
24	a	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
25	b	99/126 (79%)	94 (95%)	5 (5%)	0	100	100
26	c	154/156 (99%)	146 (95%)	8 (5%)	0	100	100
27	d	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
28	e	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
29	f	40/42 (95%)	40 (100%)	0	0	100	100
30	g	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	100 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	i	345/347 (99%)	337 (98%)	8 (2%)	0	100	100
33	j	95/113 (84%)	88 (93%)	7 (7%)	0	100	100
34	k	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
35	l	601/603 (100%)	576 (96%)	25 (4%)	0	100	100
36	m	125/175 (71%)	112 (90%)	12 (10%)	1 (1%)	16	44
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
39	p	176/178 (99%)	165 (94%)	9 (5%)	2 (1%)	11	36
40	r	457/459 (100%)	441 (96%)	14 (3%)	2 (0%)	30	59
41	s	299/318 (94%)	284 (95%)	14 (5%)	1 (0%)	36	65
42	u	169/171 (99%)	160 (95%)	9 (5%)	0	100	100
43	v	122/131 (93%)	112 (92%)	10 (8%)	0	100	100
44	w	318/320 (99%)	300 (94%)	18 (6%)	0	100	100
All	All	8029/8315 (97%)	7699 (96%)	319 (4%)	11 (0%)	49	77

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
40	r	112	ALA
8	I	69	VAL
40	r	43	ASN
12	M	283	GLU
39	p	76	HIS
9	J	38	HIS
20	V	46	PRO
39	p	174	PRO
36	m	26	PRO
41	s	90	PRO
16	Q	229	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	345/345 (100%)	341 (99%)	4 (1%)	63	86
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	76/76 (100%)	76 (100%)	0	100	100
6	G	76/81 (94%)	75 (99%)	1 (1%)	61	86
6	X	77/81 (95%)	77 (100%)	0	100	100
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	82/97 (84%)	81 (99%)	1 (1%)	63	86
9	J	255/295 (86%)	254 (100%)	1 (0%)	84	94
10	K	41/41 (100%)	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%)	183 (100%)	0	100	100
15	P	190/190 (100%)	189 (100%)	1 (0%)	81	93
16	Q	361/370 (98%)	359 (99%)	2 (1%)	78	93
17	S	58/58 (100%)	58 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	101 (100%)	0	100	100
21	W	121/123 (98%)	121 (100%)	0	100	100
22	Y	58/63 (92%)	57 (98%)	1 (2%)	53	82
23	Z	65/65 (100%)	65 (100%)	0	100	100
24	a	119/122 (98%)	118 (99%)	1 (1%)	73	90
25	b	97/119 (82%)	96 (99%)	1 (1%)	68	89
26	c	141/141 (100%)	141 (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	35/38 (92%)	35 (100%)	0	100	100
30	g	108/108 (100%)	108 (100%)	0	100	100
31	h	93/93 (100%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	i	310/311 (100%)	310 (100%)	0	100	100
33	j	88/99 (89%)	88 (100%)	0	100	100
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	537/537 (100%)	535 (100%)	2 (0%)	84	94
36	m	98/141 (70%)	98 (100%)	0	100	100
37	n	46/53 (87%)	45 (98%)	1 (2%)	45	77
38	o	112/113 (99%)	112 (100%)	0	100	100
39	p	159/159 (100%)	156 (98%)	3 (2%)	50	79
40	r	410/410 (100%)	409 (100%)	1 (0%)	87	96
41	s	263/275 (96%)	263 (100%)	0	100	100
42	u	153/153 (100%)	138 (90%)	15 (10%)	7	25
43	v	103/115 (90%)	103 (100%)	0	100	100
44	w	279/283 (99%)	278 (100%)	1 (0%)	84	94
All	All	7039/7238 (97%)	7003 (100%)	36 (0%)	78	93

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ARG
1	A	119	GLU
1	A	125	CYS
1	A	129	GLU
6	G	74	LEU
8	I	95	VAL
9	J	132	ARG
15	P	83	GLU
16	Q	83	ASN
16	Q	217	VAL
22	Y	100	LEU
24	a	134	GLU
25	b	28	LEU
35	l	159	HIS
35	l	603	ASN
37	n	15	ILE
39	p	64	LEU
39	p	68	GLU
39	p	69	GLU

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Mol	Chain	Res	Type
40	r	111	THR
42	u	51	LYS
42	u	56	CYS
42	u	57	LEU
42	u	58	GLU
42	u	64	ASN
42	u	76	ARG
42	u	78	CYS
42	u	87	THR
42	u	89	ILE
42	u	90	ASP
42	u	100	CYS
42	u	102	LYS
42	u	106	LYS
42	u	109	GLU
42	u	114	LYS
44	w	163	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	HIS
1	A	244	ASN
1	A	270	ASN
1	A	284	HIS
1	A	313	ASN
1	A	418	GLN
1	A	436	GLN
1	A	457	HIS
4	E	126	HIS
7	H	53	ASN
7	H	83	GLN
8	I	25	GLN
9	J	122	HIS
9	J	128	ASN
9	J	238	GLN
10	K	79	HIS
12	M	205	GLN
12	M	300	GLN
12	M	460	HIS
12	M	569	GLN
13	N	135	GLN

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Mol	Chain	Res	Type
14	O	133	GLN
15	P	55	HIS
15	P	77	GLN
15	P	196	HIS
16	Q	183	HIS
16	Q	190	HIS
16	Q	234	GLN
17	S	46	ASN
21	W	76	GLN
22	Y	54	GLN
25	b	14	GLN
25	b	89	HIS
26	c	83	GLN
26	c	132	HIS
27	d	23	GLN
27	d	124	ASN
28	e	148	GLN
31	h	97	HIS
32	i	91	ASN
32	i	268	GLN
33	j	83	ASN
34	k	57	ASN
35	l	23	ASN
35	l	34	ASN
35	l	135	ASN
35	l	159	HIS
35	l	194	ASN
35	l	199	GLN
35	l	309	GLN
35	l	446	ASN
35	l	447	ASN
35	l	471	ASN
35	l	541	ASN
35	l	603	ASN
36	m	46	ASN
37	n	11	HIS
37	n	14	HIS
38	o	123	GLN
39	p	12	HIS
39	p	51	HIS
40	r	51	ASN
40	r	175	ASN

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Mol	Chain	Res	Type
40	r	399	ASN
41	s	171	HIS
41	s	284	GLN
41	s	287	HIS
42	u	64	ASN
42	u	77	HIS
43	v	47	ASN
43	v	55	GLN
43	v	76	ASN
43	v	110	GLN
44	w	92	HIS

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	2.02	2 (20%)	5,13,15	6.48	3 (60%)

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	-	3/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.44	1.45	1.34
16	Q	118	2MR	CQ2-NH2	-2.21	1.41	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	13.33	131.70	119.48
16	Q	118	2MR	CD-NE-CZ	4.61	132.01	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.05	130.20	123.65

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 2 are monoatomic - leaving 36 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
50	8Q1	G	201	-	32,34,34	2.19	7 (21%)	39,43,43	1.61	10 (25%)
51	CDL	r	504	-	99,99,99	1.10	8 (8%)	105,111,111	0.86	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PEE	C	302	-	46,46,50	1.25	6 (13%)	49,51,55	1.02	2 (4%)
49	PLX	C	303	-	51,51,51	1.18	4 (7%)	53,59,59	0.64	1 (1%)
48	PEE	W	201	-	40,40,50	1.16	5 (12%)	43,45,55	1.03	2 (4%)
52	NDP	J	401	-	51,52,52	4.23	25 (49%)	71,80,80	2.29	12 (16%)
45	SF4	A	501	1	0,12,12	-	-	-		
53	FES	O	301	14	0,4,4	-	-	-		
49	PLX	a	202	-	51,51,51	0.59	0	53,59,59	0.74	0
45	SF4	M	802	12	0,12,12	-	-	-		
49	PLX	r	503	-	51,51,51	1.19	4 (7%)	53,59,59	0.62	1 (1%)
48	PEE	j	201	-	50,50,50	1.17	6 (12%)	53,55,55	1.01	2 (3%)
51	CDL	u	201	-	77,77,99	1.03	4 (5%)	83,89,111	1.15	4 (4%)
48	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	0.97	2 (3%)
48	PEE	l	703	-	45,45,50	1.25	6 (13%)	48,50,55	1.01	2 (4%)
49	PLX	r	502	-	51,51,51	1.18	4 (7%)	53,59,59	0.61	1 (1%)
48	PEE	B	303	-	50,50,50	1.17	6 (12%)	53,55,55	0.99	2 (3%)
45	SF4	B	301	2	0,12,12	-	-	-		
51	CDL	i	401	-	65,65,99	1.13	4 (6%)	71,77,111	1.24	8 (11%)
56	UQ	s	401	-	28,28,63	3.30	7 (25%)	36,37,79	2.77	12 (33%)
49	PLX	g	201	-	51,51,51	1.20	4 (7%)	53,59,59	0.64	1 (1%)
51	CDL	a	201	-	90,90,99	0.96	4 (4%)	96,102,111	1.08	6 (6%)
57	ADP	w	401	-	28,29,29	3.17	9 (32%)	43,45,45	1.86	8 (18%)
53	FES	M	803	12	0,4,4	-	-	-		
51	CDL	I	201	-	50,50,99	1.29	4 (8%)	56,62,111	1.34	7 (12%)
47	NAI	A	503	-	47,48,48	4.01	22 (46%)	64,73,73	1.65	11 (17%)
48	PEE	Q	501	-	46,46,50	1.22	6 (13%)	49,51,55	1.03	2 (4%)
45	SF4	C	301	3	0,12,12	-	-	-		
50	8Q1	X	201	-	32,34,34	2.19	7 (21%)	39,43,43	1.80	9 (23%)
48	PEE	l	704	-	45,45,50	1.24	6 (13%)	48,50,55	1.00	2 (4%)
46	FMN	A	502	-	33,33,33	1.09	2 (6%)	48,50,50	1.30	8 (16%)
49	PLX	j	202	-	51,51,51	1.20	4 (7%)	53,59,59	0.62	1 (1%)
51	CDL	l	701	-	98,98,99	0.92	4 (4%)	104,110,111	1.19	9 (8%)
45	SF4	B	302	2	0,12,12	-	-	-		
45	SF4	M	801	12	0,12,12	-	-	-		
51	CDL	l	702	-	99,99,99	1.11	8 (8%)	105,111,111	0.89	4 (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
50	8Q1	G	201	-	-	19/41/41/41	-
51	CDL	r	504	-	-	75/110/110/110	-
48	PEE	C	302	-	-	27/50/50/54	-
49	PLX	C	303	-	-	29/55/55/55	-
48	PEE	W	201	-	-	23/44/44/54	-
52	NDP	J	401	-	-	5/34/77/77	0/5/5/5
45	SF4	A	501	1	-	-	0/6/5/5
53	FES	O	301	14	-	-	0/1/1/1
49	PLX	a	202	-	-	20/55/55/55	-
45	SF4	M	802	12	-	-	0/6/5/5
49	PLX	r	503	-	-	33/55/55/55	-
48	PEE	j	201	-	-	23/54/54/54	-
51	CDL	u	201	-	-	20/88/88/110	-
48	PEE	r	501	-	-	28/54/54/54	-
48	PEE	l	703	-	-	21/49/49/54	-
49	PLX	r	502	-	-	25/55/55/55	-
48	PEE	B	303	-	-	24/54/54/54	-
45	SF4	B	301	2	-	-	0/6/5/5
51	CDL	i	401	-	-	29/76/76/110	-
56	UQ	s	401	-	-	8/21/45/87	0/1/1/1
49	PLX	g	201	-	-	30/55/55/55	-
51	CDL	a	201	-	-	28/101/101/110	-
57	ADP	w	401	-	-	4/16/32/32	0/3/3/3
53	FES	M	803	12	-	-	0/1/1/1
51	CDL	I	201	-	-	24/61/61/110	-
47	NAI	A	503	-	-	9/29/72/72	0/5/5/5
48	PEE	Q	501	-	-	19/50/50/54	-
45	SF4	C	301	3	-	-	0/6/5/5
50	8Q1	X	201	-	-	22/41/41/41	-
48	PEE	l	704	-	-	24/49/49/54	-
46	FMN	A	502	-	-	9/18/18/18	0/3/3/3
49	PLX	j	202	-	-	29/55/55/55	-
51	CDL	l	701	-	-	40/109/109/110	-
45	SF4	B	302	2	-	-	0/6/5/5
45	SF4	M	801	12	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	CDL	1	702	-	-	54/110/110/110	-

All (182) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	J	401	NDP	C3B-C2B	-12.70	1.25	1.53
52	J	401	NDP	O4D-C4D	10.78	1.69	1.45
47	A	503	NAI	C3D-C4D	-10.29	1.26	1.53
52	J	401	NDP	C3D-C4D	-10.13	1.27	1.53
56	s	401	UQ	C13-C14	9.53	1.55	1.33
56	s	401	UQ	C8-C9	9.28	1.54	1.33
47	A	503	NAI	O4B-C1B	9.27	1.63	1.42
57	w	401	ADP	C3'-C4'	-9.02	1.30	1.53
47	A	503	NAI	O4B-C4B	-8.45	1.26	1.45
52	J	401	NDP	O4B-C4B	-8.18	1.26	1.45
47	A	503	NAI	C2D-C1D	-7.94	1.28	1.53
56	s	401	UQ	C18-C19	7.92	1.56	1.32
57	w	401	ADP	O4'-C4'	7.81	1.62	1.45
50	G	201	8Q1	P24-O27	7.54	1.84	1.60
47	A	503	NAI	C2B-C1B	-7.40	1.30	1.53
50	X	201	8Q1	P24-O27	7.39	1.83	1.60
52	J	401	NDP	C2N-C3N	7.34	1.55	1.35
52	J	401	NDP	C6N-C5N	7.26	1.55	1.33
47	A	503	NAI	O4D-C4D	7.13	1.60	1.45
57	w	401	ADP	PA-O3A	6.43	1.66	1.59
47	A	503	NAI	PA-O3	6.15	1.66	1.59
52	J	401	NDP	PN-O3	6.12	1.66	1.59
47	A	503	NAI	C2D-C3D	5.79	1.69	1.53
52	J	401	NDP	C6A-N6A	5.70	1.48	1.34
47	A	503	NAI	O4D-C1D	5.56	1.54	1.42
52	J	401	NDP	P2B-O2B	5.54	1.69	1.59
57	w	401	ADP	C6-N6	5.45	1.48	1.34
47	A	503	NAI	PN-O3	5.40	1.65	1.59
50	G	201	8Q1	C28-C29	5.30	1.61	1.52
47	A	503	NAI	C4N-C3N	-5.29	1.40	1.50
52	J	401	NDP	C3B-C4B	5.27	1.66	1.53
47	A	503	NAI	C7N-N7N	5.25	1.48	1.33
52	J	401	NDP	PA-O3	5.23	1.65	1.59
47	A	503	NAI	C6A-N6A	5.08	1.47	1.34
52	J	401	NDP	O4D-C1D	-5.07	1.30	1.42
52	J	401	NDP	C6N-N1N	4.92	1.49	1.37
52	J	401	NDP	C1B-N9A	-4.61	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	J	401	NDP	O4B-C1B	4.50	1.52	1.42
50	X	201	8Q1	C28-C29	4.50	1.59	1.52
57	w	401	ADP	O4'-C1'	-4.43	1.31	1.42
51	i	401	CDL	OB8-CB7	4.32	1.45	1.33
47	A	503	NAI	O2B-C2B	4.29	1.53	1.43
51	I	201	CDL	OB8-CB7	4.28	1.45	1.33
51	l	701	CDL	OA8-CA7	4.28	1.45	1.33
51	u	201	CDL	OA8-CA7	4.24	1.45	1.33
51	a	201	CDL	OB6-CB5	4.22	1.46	1.34
51	i	401	CDL	OA8-CA7	4.22	1.45	1.33
51	a	201	CDL	OB8-CB7	4.21	1.45	1.33
51	I	201	CDL	OA6-CA5	4.20	1.46	1.34
51	a	201	CDL	OA8-CA7	4.18	1.45	1.33
51	I	201	CDL	OA8-CA7	4.17	1.45	1.33
51	l	701	CDL	OA6-CA5	4.15	1.46	1.34
51	l	701	CDL	OB6-CB5	4.14	1.46	1.34
51	I	201	CDL	OB6-CB5	4.14	1.46	1.34
51	i	401	CDL	OB6-CB5	4.13	1.45	1.34
51	u	201	CDL	OB8-CB7	4.13	1.45	1.33
51	u	201	CDL	OA6-CA5	4.12	1.45	1.34
51	l	701	CDL	OB8-CB7	4.12	1.45	1.33
51	i	401	CDL	OA6-CA5	4.04	1.45	1.34
51	a	201	CDL	OA6-CA5	4.03	1.45	1.34
52	J	401	NDP	O2D-C2D	-3.96	1.33	1.43
51	u	201	CDL	OB6-CB5	3.94	1.45	1.34
50	G	201	8Q1	C1-S44	3.90	1.85	1.76
52	J	401	NDP	C7N-N7N	3.89	1.44	1.33
48	C	302	PEE	C18-C19	3.86	1.53	1.31
48	l	703	PEE	C18-C19	3.84	1.53	1.31
48	W	201	PEE	C18-C19	3.83	1.53	1.31
48	l	704	PEE	C18-C19	3.81	1.53	1.31
48	j	201	PEE	C18-C19	3.80	1.53	1.31
48	r	501	PEE	C18-C19	3.79	1.53	1.31
48	B	303	PEE	C18-C19	3.79	1.53	1.31
48	Q	501	PEE	C18-C19	3.77	1.53	1.31
48	C	302	PEE	C39-C38	3.75	1.53	1.31
48	l	703	PEE	C39-C38	3.74	1.52	1.31
48	r	501	PEE	C39-C38	3.73	1.52	1.31
48	l	704	PEE	C39-C38	3.72	1.52	1.31
48	Q	501	PEE	C39-C38	3.71	1.52	1.31
48	j	201	PEE	C39-C38	3.69	1.52	1.31
48	B	303	PEE	C39-C38	3.66	1.52	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	X	201	8Q1	C1-S44	3.51	1.84	1.76
46	A	502	FMN	C4A-N5	3.44	1.38	1.30
47	A	503	NAI	C7N-C3N	3.42	1.56	1.48
47	A	503	NAI	C4N-C5N	-3.41	1.40	1.49
50	G	201	8Q1	O27-C28	-3.39	1.33	1.43
50	X	201	8Q1	O27-C28	-3.38	1.33	1.43
51	l	702	CDL	OA8-CA7	3.36	1.43	1.33
51	r	504	CDL	OA8-CA7	3.35	1.43	1.33
50	X	201	8Q1	C39-N41	3.32	1.41	1.33
50	G	201	8Q1	C34-N36	3.31	1.41	1.33
57	w	401	ADP	C8-N9	-3.30	1.31	1.37
52	J	401	NDP	C8A-N9A	-3.29	1.31	1.37
50	X	201	8Q1	C6-C1	3.22	1.54	1.50
52	J	401	NDP	C5A-N7A	-3.17	1.33	1.39
50	X	201	8Q1	C34-N36	3.11	1.40	1.33
51	l	702	CDL	OB6-CB5	3.11	1.43	1.34
57	w	401	ADP	O2'-C2'	-3.10	1.35	1.43
51	r	504	CDL	OB6-CB5	3.01	1.42	1.34
57	w	401	ADP	O3'-C3'	2.99	1.50	1.43
49	C	303	PLX	O6-C4	-2.99	1.40	1.44
51	l	702	CDL	OA6-CA5	2.97	1.42	1.34
51	r	504	CDL	OB8-CB7	2.96	1.42	1.33
51	l	702	CDL	OB8-CB7	2.93	1.41	1.33
49	g	201	PLX	O6-C4	-2.89	1.40	1.44
52	J	401	NDP	C7N-C3N	2.86	1.54	1.48
49	r	503	PLX	O6-C4	-2.85	1.41	1.44
50	G	201	8Q1	C39-N41	2.84	1.40	1.33
52	J	401	NDP	O3D-C3D	2.82	1.49	1.43
51	r	504	CDL	OA6-CA5	2.81	1.42	1.34
48	B	303	PEE	O2-C2	-2.73	1.40	1.46
47	A	503	NAI	C8A-N9A	-2.73	1.32	1.37
48	l	703	PEE	O2-C2	-2.71	1.40	1.46
51	r	504	CDL	OA6-CA4	-2.68	1.40	1.46
52	J	401	NDP	O2B-C2B	2.67	1.53	1.44
56	s	401	UQ	C6-C1	2.65	1.54	1.46
49	j	202	PLX	O6-C4	-2.60	1.41	1.44
48	Q	501	PEE	O2-C2	-2.57	1.40	1.46
51	l	702	CDL	OA6-CA4	-2.53	1.40	1.46
48	W	201	PEE	O2-C2	-2.53	1.40	1.46
48	l	704	PEE	O2-C2	-2.53	1.40	1.46
48	C	302	PEE	O2-C2	-2.52	1.40	1.46
50	G	201	8Q1	C6-C1	2.49	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	Q	501	PEE	O3-C30	2.49	1.40	1.33
48	j	201	PEE	O2-C2	-2.48	1.40	1.46
48	C	302	PEE	O2-C10	2.48	1.41	1.34
48	C	302	PEE	O3-C30	2.47	1.40	1.33
49	r	502	PLX	C7-C6	2.46	1.55	1.50
47	A	503	NAI	C6N-C5N	2.44	1.40	1.33
47	A	503	NAI	PN-O5D	2.43	1.68	1.59
48	l	704	PEE	O3-C30	2.43	1.40	1.33
57	w	401	ADP	C5-N7	-2.42	1.34	1.39
48	r	501	PEE	O3-C30	2.42	1.40	1.33
49	j	202	PLX	C7-C6	2.41	1.55	1.50
48	j	201	PEE	O3-C30	2.41	1.40	1.33
48	l	703	PEE	O3-C30	2.40	1.40	1.33
48	r	501	PEE	O2-C2	-2.40	1.41	1.46
47	A	503	NAI	C5B-C4B	2.37	1.58	1.51
47	A	503	NAI	O3B-C3B	-2.34	1.37	1.43
56	s	401	UQ	O4-C4	-2.34	1.18	1.23
48	j	201	PEE	O2-C10	2.33	1.40	1.34
49	r	503	PLX	C7-C6	2.32	1.55	1.50
49	g	201	PLX	C7-C6	2.32	1.55	1.50
48	W	201	PEE	O3-C30	2.32	1.40	1.33
48	B	303	PEE	O3-C30	2.31	1.40	1.33
48	l	704	PEE	O2-C10	2.29	1.40	1.34
51	r	504	CDL	OB6-CB4	-2.28	1.41	1.46
48	Q	501	PEE	O2-C10	2.26	1.40	1.34
48	l	703	PEE	O2-C10	2.25	1.40	1.34
51	l	702	CDL	PB2-OB5	2.25	1.68	1.59
51	r	504	CDL	PB2-OB5	2.25	1.68	1.59
49	r	502	PLX	O6-C4	-2.24	1.41	1.44
52	J	401	NDP	O7N-C7N	-2.22	1.19	1.24
48	l	703	PEE	O3-C3	-2.22	1.40	1.45
46	A	502	FMN	C10-N1	2.22	1.37	1.33
51	r	504	CDL	PB2-OB2	2.21	1.68	1.59
52	J	401	NDP	C2D-C3D	2.21	1.59	1.53
49	C	303	PLX	C7-C6	2.21	1.55	1.50
48	W	201	PEE	O2-C10	2.20	1.40	1.34
48	l	704	PEE	O3-C3	-2.20	1.40	1.45
49	j	202	PLX	P1-O4	2.20	1.68	1.59
48	B	303	PEE	O2-C10	2.19	1.40	1.34
51	l	702	CDL	PB2-OB2	2.19	1.68	1.59
48	B	303	PEE	O3-C3	-2.18	1.40	1.45
48	W	201	PEE	O3-C3	-2.18	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	g	201	PLX	P1-O4	2.17	1.67	1.59
51	l	702	CDL	OB6-CB4	-2.17	1.41	1.46
48	Q	501	PEE	O3-C3	-2.15	1.40	1.45
48	C	302	PEE	O3-C3	-2.15	1.40	1.45
48	r	501	PEE	O3-C3	-2.14	1.40	1.45
49	r	502	PLX	P1-O4	2.14	1.67	1.59
47	A	503	NAI	C5A-N7A	-2.13	1.35	1.39
49	j	202	PLX	P1-O1	2.11	1.67	1.59
56	s	401	UQ	O1-C1	-2.10	1.18	1.23
48	r	501	PEE	O2-C10	2.09	1.40	1.34
49	C	303	PLX	P1-O4	2.09	1.67	1.59
49	r	502	PLX	P1-O1	2.08	1.67	1.59
49	r	503	PLX	P1-O4	2.06	1.67	1.59
49	r	503	PLX	P1-O1	2.04	1.67	1.59
49	g	201	PLX	C25-C24	2.03	1.55	1.50
49	C	303	PLX	P1-O1	2.02	1.67	1.59
48	j	201	PEE	O3-C3	-2.02	1.40	1.45
56	s	401	UQ	O3-CM3	-2.01	1.40	1.45
52	J	401	NDP	PA-O5B	2.00	1.67	1.59

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	s	401	UQ	C7-C8-C9	-9.22	110.95	126.83
52	J	401	NDP	C3N-C2N-N1N	-9.08	109.86	123.20
52	J	401	NDP	C6N-N1N-C2N	-7.41	111.39	119.32
56	s	401	UQ	C12-C13-C14	-6.56	112.61	127.62
52	J	401	NDP	C1D-N1N-C2N	-6.19	110.95	121.14
52	J	401	NDP	C5A-C4A-N3A	-5.57	119.05	126.72
47	A	503	NAI	C5A-C4A-N3A	-5.49	119.16	126.72
57	w	401	ADP	C5-C4-N3	-5.47	119.19	126.72
51	l	701	CDL	OA6-CA5-C11	5.10	122.52	111.48
50	X	201	8Q1	C6-C1-S44	5.08	119.45	113.40
52	J	401	NDP	C1D-N1N-C6N	-4.93	110.36	120.77
51	u	201	CDL	OA6-CA5-C11	4.56	121.33	111.48
51	i	401	CDL	OA6-CA5-C11	4.51	121.24	111.48
57	w	401	ADP	N3-C2-N1	-4.51	121.76	128.58
47	A	503	NAI	N3A-C2A-N1A	-4.38	121.96	128.58
57	w	401	ADP	N3-C4-N9	4.31	134.50	127.17
56	s	401	UQ	C15-C14-C13	-4.27	112.67	123.63
56	s	401	UQ	C10-C9-C8	-4.25	112.71	123.63
51	l	702	CDL	OB6-CB5-C51	4.23	120.62	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	s	401	UQ	C17-C18-C19	-4.22	113.57	127.64
51	l	702	CDL	OA6-CA5-C11	4.22	120.60	111.48
56	s	401	UQ	C11-C9-C8	-4.20	111.74	121.17
51	a	201	CDL	OB6-CB5-C51	4.15	120.47	111.48
48	Q	501	PEE	O2-C10-C11	4.11	120.38	111.48
52	J	401	NDP	N3A-C2A-N1A	-4.10	122.38	128.58
51	I	201	CDL	OB6-CB5-C51	4.06	120.27	111.48
48	l	703	PEE	O2-C10-C11	4.06	120.26	111.48
48	W	201	PEE	O2-C10-C11	4.05	120.25	111.48
48	C	302	PEE	O2-C10-C11	4.04	120.22	111.48
50	G	201	8Q1	C6-C1-S44	4.04	118.21	113.40
48	j	201	PEE	O2-C10-C11	4.04	120.21	111.48
51	I	201	CDL	OA6-CA5-C11	3.99	120.11	111.48
56	s	401	UQ	C16-C14-C13	-3.97	112.25	121.17
52	J	401	NDP	N3A-C4A-N9A	3.95	133.89	127.17
51	r	504	CDL	OB6-CB5-C51	3.95	120.02	111.48
51	i	401	CDL	OB6-CB5-C51	3.93	119.99	111.48
47	A	503	NAI	N3A-C4A-N9A	3.92	133.83	127.17
51	r	504	CDL	OA6-CA5-C11	3.91	119.93	111.48
48	B	303	PEE	O2-C10-C11	3.89	119.90	111.48
51	u	201	CDL	OB6-CB5-C51	3.86	119.83	111.48
51	l	701	CDL	OB6-CB5-C51	3.85	119.82	111.48
48	r	501	PEE	O2-C10-C11	3.84	119.78	111.48
51	a	201	CDL	OA6-CA5-C11	3.82	119.74	111.48
48	l	704	PEE	O2-C10-C11	3.80	119.70	111.48
50	X	201	8Q1	C43-S44-C1	3.71	112.80	101.84
47	A	503	NAI	C2A-N3A-C4A	3.67	120.80	111.83
52	J	401	NDP	C2A-N3A-C4A	3.59	120.60	111.83
57	w	401	ADP	C2-N3-C4	3.53	120.45	111.83
57	w	401	ADP	N9-C8-N7	-3.48	109.00	113.94
51	l	701	CDL	CA4-OA6-CA5	-3.41	109.65	117.80
46	A	502	FMN	C4-N3-C2	-3.39	119.63	125.64
56	s	401	UQ	C7-C6-C5	-3.38	119.09	124.89
47	A	503	NAI	C5A-N7A-C8A	3.35	108.71	103.45
47	A	503	NAI	C4A-C5A-N7A	-3.34	106.77	110.58
50	G	201	8Q1	C43-S44-C1	3.32	111.64	101.84
56	s	401	UQ	C21-C19-C18	-3.31	112.71	122.66
50	X	201	8Q1	O35-C34-N36	-3.31	115.97	122.98
47	A	503	NAI	N9A-C8A-N7A	-3.30	109.25	113.94
52	J	401	NDP	C4A-C5A-N7A	-3.28	106.83	110.58
52	J	401	NDP	N9A-C8A-N7A	-3.19	109.41	113.94
57	w	401	ADP	C5-N7-C8	3.18	108.44	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	G	201	8Q1	O35-C34-N36	-3.16	116.28	122.98
52	J	401	NDP	C5A-N7A-C8A	3.14	108.39	103.45
57	w	401	ADP	C4-N9-C8	3.13	109.03	105.74
51	a	201	CDL	OB8-CB7-C71	3.11	121.33	111.83
51	l	701	CDL	OB8-CB7-C71	3.10	121.28	111.83
56	s	401	UQ	C20-C19-C18	-3.00	113.66	122.66
50	X	201	8Q1	O4-C1-S44	-2.99	118.88	122.68
48	B	303	PEE	O3-C30-C31	2.97	120.89	111.83
51	I	201	CDL	OA8-CA7-C31	2.95	120.83	111.83
57	w	401	ADP	C4-C5-N7	-2.94	107.22	110.58
51	i	401	CDL	CA4-OA6-CA5	-2.93	110.78	117.80
50	X	201	8Q1	O2-P24-O27	-2.91	99.08	106.67
48	l	703	PEE	O3-C30-C31	2.89	120.65	111.83
48	W	201	PEE	O3-C30-C31	2.89	120.65	111.83
51	l	701	CDL	OA8-CA7-C31	2.88	120.62	111.83
51	u	201	CDL	OA8-CA7-C31	2.87	120.59	111.83
50	G	201	8Q1	O2-P24-O27	-2.87	99.20	106.67
56	s	401	UQ	CM5-C5-C6	-2.86	119.75	124.45
48	r	501	PEE	O3-C30-C31	2.85	120.52	111.83
47	A	503	NAI	C4D-O4D-C1D	-2.84	103.19	109.47
51	i	401	CDL	OA8-CA7-C31	2.82	120.44	111.83
51	I	201	CDL	CB4-OB6-CB5	-2.80	111.11	117.80
46	A	502	FMN	C4A-C4-N3	2.78	120.33	113.25
48	C	302	PEE	O3-C30-C31	2.76	120.25	111.83
51	I	201	CDL	OB8-CB7-C71	2.76	120.24	111.83
49	g	201	PLX	C1A-N1-C1	2.69	120.59	109.91
48	l	704	PEE	O3-C30-C31	2.67	119.98	111.83
49	r	503	PLX	C1A-N1-C1	2.67	120.52	109.91
51	r	504	CDL	OA8-CA7-C31	2.66	119.94	111.83
51	u	201	CDL	OB8-CB7-C71	2.65	119.91	111.83
48	j	201	PEE	O3-C30-C31	2.63	119.85	111.83
48	Q	501	PEE	O3-C30-C31	2.62	119.82	111.83
51	l	702	CDL	OA8-CA7-C31	2.60	119.75	111.83
51	I	201	CDL	CA6-CA4-CA3	-2.58	105.76	111.78
50	X	201	8Q1	C32-C34-N36	2.58	121.38	116.48
46	A	502	FMN	O4-C4-C4A	-2.58	119.72	126.53
46	A	502	FMN	C9A-C5A-N5	-2.57	119.72	122.45
51	l	701	CDL	CB6-CB4-CB3	-2.57	105.79	111.78
46	A	502	FMN	C5A-C9A-N10	2.57	120.29	117.97
51	a	201	CDL	OA8-CA7-C31	2.56	119.63	111.83
51	l	702	CDL	OB8-CB7-C71	2.55	119.61	111.83
51	r	504	CDL	OB8-CB7-C71	2.54	119.59	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	i	401	CDL	OB8-CB7-C71	2.53	119.55	111.83
50	G	201	8Q1	O40-C39-N41	-2.46	118.19	123.03
52	J	401	NDP	C4A-N9A-C8A	2.44	108.30	105.74
50	G	201	8Q1	O1-P24-O2	2.42	116.89	107.80
49	j	202	PLX	C1A-N1-C1	2.42	119.52	109.91
50	X	201	8Q1	O1-P24-O2	2.41	116.84	107.80
47	A	503	NAI	C4A-N9A-C8A	2.41	108.27	105.74
56	s	401	UQ	C7-C6-C1	2.40	121.31	118.52
46	A	502	FMN	C4A-C10-N10	2.39	119.91	116.48
51	l	701	CDL	OB8-CB7-OB9	-2.37	117.70	123.63
50	X	201	8Q1	C37-C38-C39	2.37	116.33	112.39
49	r	502	PLX	C1A-N1-C1	2.33	119.15	109.91
51	l	701	CDL	OA6-CA5-OA7	-2.30	118.34	123.70
46	A	502	FMN	C10-C4A-N5	-2.25	120.21	124.81
49	C	303	PLX	C1A-N1-C1	2.23	118.77	109.91
47	A	503	NAI	C6N-N1N-C2N	2.19	121.67	119.32
47	A	503	NAI	C2D-C3D-C4D	2.19	106.84	102.61
51	i	401	CDL	OA6-CA5-OA7	-2.17	118.63	123.70
51	a	201	CDL	OB8-CB7-OB9	-2.16	118.23	123.63
51	I	201	CDL	OA8-CA7-OA9	-2.13	118.29	123.63
50	G	201	8Q1	C32-C34-N36	2.13	120.52	116.48
50	G	201	8Q1	C38-C39-N41	2.12	120.21	116.34
51	i	401	CDL	CB4-OB6-CB5	-2.12	112.72	117.80
51	a	201	CDL	CB4-OB6-CB5	-2.12	112.72	117.80
50	G	201	8Q1	O27-P24-O3	-2.10	100.76	106.44
51	l	701	CDL	CB4-OB6-CB5	-2.07	112.84	117.80
46	A	502	FMN	C4A-C10-N1	-2.05	119.56	124.59
50	G	201	8Q1	O4-C1-C6	-2.03	121.63	123.98
51	i	401	CDL	OA8-CA7-OA9	-2.02	118.58	123.63
50	X	201	8Q1	O4-C1-C6	-2.01	121.66	123.98

There are no chirality outliers.

All (701) 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'
46	A	502	FMN	C1'-C2'-C3'-O3'
46	A	502	FMN	C1'-C2'-C3'-C4'
46	A	502	FMN	C3'-C4'-C5'-O5'
48	B	303	PEE	C4-O4P-P-O2P
48	B	303	PEE	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
48	C	302	PEE	C1-O3P-P-O1P
48	C	302	PEE	C1-O3P-P-O4P
48	C	302	PEE	C4-O4P-P-O3P
48	C	302	PEE	O4P-C4-C5-N
48	Q	501	PEE	C11-C10-O2-C2
48	W	201	PEE	C11-C10-O2-C2
48	W	201	PEE	C1-O3P-P-O2P
48	W	201	PEE	C1-O3P-P-O1P
48	W	201	PEE	C4-O4P-P-O1P
48	W	201	PEE	O4P-C4-C5-N
48	l	703	PEE	C11-C10-O2-C2
48	l	703	PEE	C4-O4P-P-O3P
48	l	703	PEE	C4-O4P-P-O2P
48	l	703	PEE	C4-O4P-P-O1P
48	r	501	PEE	C4-O4P-P-O3P
48	r	501	PEE	C4-O4P-P-O2P
48	r	501	PEE	C4-O4P-P-O1P
49	C	303	PLX	C3-O4-P1-O1
49	C	303	PLX	C3-O4-P1-O3
49	C	303	PLX	C2-O1-P1-O2
49	a	202	PLX	C3-O4-P1-O1
49	a	202	PLX	C3-O4-P1-O2
49	a	202	PLX	C3-O4-P1-O3
49	a	202	PLX	C2-O1-P1-O2
49	g	201	PLX	O7-C6-C7-C8
49	g	201	PLX	O7-C6-O6-C4
49	g	201	PLX	C3-O4-P1-O2
49	g	201	PLX	O9-C24-O8-C5
49	g	201	PLX	O9-C24-C25-C26
49	j	202	PLX	O7-C6-C7-C8
49	j	202	PLX	C3-O4-P1-O3
49	r	502	PLX	O7-C6-O6-C4
49	r	502	PLX	C5-C4-O6-C6
49	r	502	PLX	O9-C24-C25-C26
49	r	503	PLX	O7-C6-O6-C4
49	r	503	PLX	C5-C4-O6-C6
49	r	503	PLX	C3-O4-P1-O1
49	r	503	PLX	C3-O4-P1-O2
49	r	503	PLX	C3-O4-P1-O3
49	r	503	PLX	O9-C24-O8-C5
50	G	201	8Q1	N36-C37-C38-C39
50	G	201	8Q1	N41-C42-C43-S44

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Mol	Chain	Res	Type	Atoms
50	G	201	8Q1	C42-C43-S44-C1
50	G	201	8Q1	C28-O27-P24-O3
50	G	201	8Q1	C28-O27-P24-O2
50	G	201	8Q1	C28-O27-P24-O1
50	X	201	8Q1	O4-C1-S44-C43
50	X	201	8Q1	C6-C1-S44-C43
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	I	201	CDL	CA2-OA2-PA1-OA3
51	I	201	CDL	CA3-OA5-PA1-OA2
51	I	201	CDL	CA3-OA5-PA1-OA3
51	I	201	CDL	CA3-OA5-PA1-OA4
51	I	201	CDL	CB2-OB2-PB2-OB4
51	I	201	CDL	CB2-OB2-PB2-OB5
51	I	201	CDL	CB3-OB5-PB2-OB2
51	I	201	CDL	CB3-OB5-PB2-OB4
51	a	201	CDL	CA2-OA2-PA1-OA4
51	a	201	CDL	CA2-OA2-PA1-OA5
51	a	201	CDL	CA3-OA5-PA1-OA2
51	a	201	CDL	CA3-OA5-PA1-OA4
51	a	201	CDL	CB2-OB2-PB2-OB3
51	a	201	CDL	CB3-OB5-PB2-OB3
51	i	401	CDL	CA3-OA5-PA1-OA2
51	i	401	CDL	CA3-OA5-PA1-OA4
51	i	401	CDL	CB2-OB2-PB2-OB4
51	i	401	CDL	CB2-OB2-PB2-OB5
51	i	401	CDL	CB3-OB5-PB2-OB2
51	i	401	CDL	CB3-OB5-PB2-OB4
51	l	701	CDL	O1-C1-CB2-OB2
51	l	701	CDL	CA2-OA2-PA1-OA5
51	l	701	CDL	CB2-OB2-PB2-OB4
51	l	702	CDL	O1-C1-CA2-OA2
51	l	702	CDL	CA2-OA2-PA1-OA3
51	l	702	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
51	l	702	CDL	CA3-OA5-PA1-OA2
51	l	702	CDL	CB2-OB2-PB2-OB4
51	l	702	CDL	CB2-OB2-PB2-OB5
51	l	702	CDL	CB3-OB5-PB2-OB2
51	l	702	CDL	CB3-OB5-PB2-OB3
51	l	702	CDL	OB6-CB4-CB6-OB8
51	r	504	CDL	CA2-OA2-PA1-OA4
51	r	504	CDL	CA3-OA5-PA1-OA2
51	r	504	CDL	CA3-OA5-PA1-OA3
51	r	504	CDL	CA3-OA5-PA1-OA4
51	r	504	CDL	CB2-OB2-PB2-OB3
51	r	504	CDL	CB3-OB5-PB2-OB2
51	r	504	CDL	CB3-OB5-PB2-OB4
51	u	201	CDL	CB2-C1-CA2-OA2
51	u	201	CDL	CA3-OA5-PA1-OA2
51	u	201	CDL	CA3-OA5-PA1-OA3
51	u	201	CDL	CA3-OA5-PA1-OA4
51	u	201	CDL	CB2-OB2-PB2-OB4
51	u	201	CDL	CB2-OB2-PB2-OB5
56	s	401	UQ	C7-C8-C9-C11
56	s	401	UQ	C12-C13-C14-C15
57	w	401	ADP	C5'-O5'-PA-O1A
57	w	401	ADP	C5'-O5'-PA-O2A
57	w	401	ADP	C5'-O5'-PA-O3A
48	W	201	PEE	O5-C30-O3-C3
56	s	401	UQ	C17-C18-C19-C21
48	W	201	PEE	C31-C30-O3-C3
48	Q	501	PEE	O4-C10-O2-C2
48	W	201	PEE	O4-C10-O2-C2
48	l	703	PEE	O4-C10-O2-C2
51	r	504	CDL	OB7-CB5-OB6-CB4
51	r	504	CDL	C51-CB5-OB6-CB4
48	j	201	PEE	C31-C30-O3-C3
51	l	701	CDL	C31-CA7-OA8-CA6
51	r	504	CDL	C71-CB7-OB8-CB6
56	s	401	UQ	C7-C8-C9-C10
48	j	201	PEE	C17-C18-C19-C20
51	l	702	CDL	OB9-CB7-OB8-CB6
51	r	504	CDL	OB9-CB7-OB8-CB6
51	i	401	CDL	O1-C1-CA2-OA2
51	l	702	CDL	O1-C1-CB2-OB2
51	r	504	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
51	u	201	CDL	O1-C1-CA2-OA2
48	C	302	PEE	C31-C30-O3-C3
51	l	702	CDL	C71-CB7-OB8-CB6
51	l	701	CDL	OA9-CA7-OA8-CA6
48	j	201	PEE	C11-C10-O2-C2
52	J	401	NDP	C2D-C1D-N1N-C6N
48	j	201	PEE	O5-C30-O3-C3
49	j	202	PLX	C28-C29-C30-C31
48	C	302	PEE	O5-C30-O3-C3
48	l	704	PEE	C31-C30-O3-C3
49	C	303	PLX	C28-C29-C30-C31
48	B	303	PEE	C37-C38-C39-C40
48	l	704	PEE	C37-C38-C39-C40
49	r	502	PLX	C9-C10-C11-C12
51	I	201	CDL	C11-CA5-OA6-CA4
49	r	503	PLX	C12-C13-C14-C15
48	l	704	PEE	O5-C30-O3-C3
48	j	201	PEE	O4-C10-O2-C2
51	i	401	CDL	CB2-C1-CA2-OA2
51	l	701	CDL	CA2-C1-CB2-OB2
51	l	702	CDL	CA2-C1-CB2-OB2
51	i	401	CDL	C31-CA7-OA8-CA6
51	l	702	CDL	C11-C12-C13-C14
51	l	702	CDL	C75-C76-C77-C78
56	s	401	UQ	C12-C11-C9-C10
49	g	201	PLX	C7-C8-C9-C10
48	l	704	PEE	C10-C11-C12-C13
51	r	504	CDL	CB5-C51-C52-C53
48	W	201	PEE	C13-C14-C15-C16
48	j	201	PEE	C40-C41-C42-C43
48	r	501	PEE	C17-C18-C19-C20
48	Q	501	PEE	C10-C11-C12-C13
48	B	303	PEE	C31-C30-O3-C3
51	i	401	CDL	C71-CB7-OB8-CB6
49	r	502	PLX	C11-C12-C13-C14
51	r	504	CDL	C74-C75-C76-C77
56	s	401	UQ	C9-C11-C12-C13
48	r	501	PEE	C41-C42-C43-C44
51	l	702	CDL	C35-C36-C37-C38
51	l	702	CDL	C54-C55-C56-C57
51	l	702	CDL	CB5-C51-C52-C53
51	r	504	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
48	B	303	PEE	C10-C11-C12-C13
48	r	501	PEE	C10-C11-C12-C13
51	l	702	CDL	CB7-C71-C72-C73
51	i	401	CDL	OA9-CA7-OA8-CA6
48	j	201	PEE	C34-C35-C36-C37
49	r	502	PLX	C30-C31-C32-C33
51	I	201	CDL	OA7-CA5-OA6-CA4
48	j	201	PEE	C19-C20-C21-C22
51	a	201	CDL	CB5-C51-C52-C53
51	l	701	CDL	CB5-C51-C52-C53
49	g	201	PLX	C12-C13-C14-C15
48	l	703	PEE	C31-C30-O3-C3
46	A	502	FMN	O2'-C2'-C3'-C4'
49	g	201	PLX	C15-C16-C17-C18
51	a	201	CDL	C39-C40-C41-C42
49	j	202	PLX	C34-C35-C36-C37
51	u	201	CDL	C75-C76-C77-C78
51	l	701	CDL	C23-C24-C25-C26
48	B	303	PEE	C12-C13-C14-C15
49	r	503	PLX	C2-C1-N1-C1C
49	r	503	PLX	C2-C1-N1-C1A
49	C	303	PLX	O6-C6-C7-C8
48	C	302	PEE	C11-C10-O2-C2
49	j	202	PLX	C15-C16-C17-C18
48	C	302	PEE	O4-C10-O2-C2
48	Q	501	PEE	C22-C23-C24-C25
51	l	702	CDL	C39-C40-C41-C42
51	i	401	CDL	OB9-CB7-OB8-CB6
48	r	501	PEE	C30-C31-C32-C33
51	I	201	CDL	CA6-CA4-OA6-CA5
48	B	303	PEE	O5-C30-O3-C3
51	u	201	CDL	C11-CA5-OA6-CA4
51	l	701	CDL	C58-C59-C60-C61
48	B	303	PEE	C23-C24-C25-C26
48	r	501	PEE	C12-C13-C14-C15
48	l	704	PEE	C31-C32-C33-C34
49	C	303	PLX	C33-C34-C35-C36
49	j	202	PLX	C25-C26-C27-C28
49	r	503	PLX	C28-C29-C30-C31
51	l	702	CDL	C55-C56-C57-C58
48	l	704	PEE	C17-C18-C19-C20
51	r	504	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
48	l	703	PEE	O5-C30-O3-C3
49	C	303	PLX	O7-C6-C7-C8
49	r	503	PLX	O9-C24-C25-C26
49	g	201	PLX	C35-C36-C37-C38
49	j	202	PLX	C13-C14-C15-C16
49	j	202	PLX	C12-C13-C14-C15
49	r	502	PLX	C15-C16-C17-C18
51	l	702	CDL	C60-C61-C62-C63
51	r	504	CDL	C73-C74-C75-C76
48	l	703	PEE	C31-C32-C33-C34
51	r	504	CDL	C15-C16-C17-C18
49	C	303	PLX	C7-C8-C9-C10
48	W	201	PEE	C19-C20-C21-C22
50	G	201	8Q1	C10-C11-C12-C13
48	r	501	PEE	C11-C10-O2-C2
51	l	702	CDL	C56-C57-C58-C59
51	I	201	CDL	O1-C1-CB2-OB2
51	r	504	CDL	C17-C18-C19-C20
49	a	202	PLX	C7-C8-C9-C10
49	r	503	PLX	C25-C26-C27-C28
51	l	702	CDL	C72-C73-C74-C75
51	r	504	CDL	CB7-C71-C72-C73
51	u	201	CDL	OA7-CA5-OA6-CA4
51	l	702	CDL	CB2-C1-CA2-OA2
51	l	701	CDL	C71-CB7-OB8-CB6
48	l	703	PEE	C22-C23-C24-C25
49	r	503	PLX	C33-C34-C35-C36
51	l	702	CDL	C62-C63-C64-C65
46	A	502	FMN	O2'-C2'-C3'-O3'
49	C	303	PLX	C16-C17-C18-C19
49	g	201	PLX	C9-C10-C11-C12
49	r	502	PLX	C27-C28-C29-C30
49	r	503	PLX	C14-C15-C16-C17
49	g	201	PLX	C10-C11-C12-C13
49	r	503	PLX	C29-C30-C31-C32
51	r	504	CDL	C12-C13-C14-C15
49	j	202	PLX	C19-C20-C21-C22
49	r	503	PLX	C2-C1-N1-C1B
48	r	501	PEE	C20-C21-C22-C23
49	a	202	PLX	C14-C15-C16-C17
51	r	504	CDL	C35-C36-C37-C38
51	a	201	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
49	r	502	PLX	C12-C13-C14-C15
49	j	202	PLX	C9-C10-C11-C12
51	r	504	CDL	C55-C56-C57-C58
48	B	303	PEE	C30-C31-C32-C33
48	r	501	PEE	C13-C14-C15-C16
50	X	201	8Q1	C11-C12-C13-C14
51	r	504	CDL	C37-C38-C39-C40
51	r	504	CDL	C41-C42-C43-C44
51	r	504	CDL	C75-C76-C77-C78
48	B	303	PEE	C33-C34-C35-C36
48	C	302	PEE	C32-C33-C34-C35
48	C	302	PEE	C42-C43-C44-C45
51	i	401	CDL	C36-C37-C38-C39
51	l	702	CDL	C37-C38-C39-C40
49	r	502	PLX	C13-C14-C15-C16
50	G	201	8Q1	C9-C10-C11-C12
51	l	702	CDL	C73-C74-C75-C76
51	l	701	CDL	C52-C53-C54-C55
51	r	504	CDL	C76-C77-C78-C79
49	r	503	PLX	C13-C14-C15-C16
48	l	704	PEE	C33-C34-C35-C36
49	a	202	PLX	C28-C29-C30-C31
50	G	201	8Q1	C12-C13-C14-C15
51	r	504	CDL	C34-C35-C36-C37
49	g	201	PLX	C11-C10-C9-C8
51	r	504	CDL	C31-CA7-OA8-CA6
51	a	201	CDL	C31-C32-C33-C34
51	l	702	CDL	C59-C60-C61-C62
51	I	201	CDL	C51-CB5-OB6-CB4
51	i	401	CDL	C11-CA5-OA6-CA4
51	l	701	CDL	C11-CA5-OA6-CA4
49	r	502	PLX	C28-C29-C30-C31
51	r	504	CDL	C23-C24-C25-C26
48	r	501	PEE	O4-C10-O2-C2
49	g	201	PLX	C27-C28-C29-C30
50	X	201	8Q1	C7-C8-C9-C10
51	i	401	CDL	C11-C12-C13-C14
48	B	303	PEE	C15-C16-C17-C18
48	C	302	PEE	C15-C16-C17-C18
48	j	201	PEE	C21-C22-C23-C24
49	j	202	PLX	C27-C28-C29-C30
49	r	503	PLX	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
49	g	201	PLX	C28-C29-C30-C31
51	r	504	CDL	C62-C63-C64-C65
49	C	303	PLX	C36-C37-C38-C39
51	r	504	CDL	C11-C12-C13-C14
50	G	201	8Q1	C11-C12-C13-C14
48	j	201	PEE	O2-C2-C3-O3
51	i	401	CDL	OB6-CB4-CB6-OB8
51	r	504	CDL	OA6-CA4-CA6-OA8
51	r	504	CDL	OB6-CB4-CB6-OB8
49	j	202	PLX	C7-C8-C9-C10
49	r	502	PLX	C7-C8-C9-C10
49	g	201	PLX	C33-C34-C35-C36
51	l	701	CDL	OB9-CB7-OB8-CB6
49	C	303	PLX	C31-C32-C33-C34
49	r	503	PLX	C16-C17-C18-C19
51	r	504	CDL	C42-C43-C44-C45
49	r	502	PLX	C31-C32-C33-C34
51	r	504	CDL	C52-C53-C54-C55
48	Q	501	PEE	C35-C36-C37-C38
51	r	504	CDL	C14-C15-C16-C17
51	I	201	CDL	OB7-CB5-OB6-CB4
51	i	401	CDL	OA7-CA5-OA6-CA4
51	l	702	CDL	C57-C58-C59-C60
51	r	504	CDL	C33-C34-C35-C36
48	B	303	PEE	C14-C15-C16-C17
48	l	704	PEE	C11-C10-O2-C2
49	C	303	PLX	C11-C12-C13-C14
48	W	201	PEE	C11-C12-C13-C14
51	l	701	CDL	OA7-CA5-OA6-CA4
48	B	303	PEE	C17-C18-C19-C20
50	X	201	8Q1	C10-C11-C12-C13
48	j	201	PEE	C1-C2-C3-O3
51	l	701	CDL	CB3-CB4-CB6-OB8
51	l	702	CDL	CB3-CB4-CB6-OB8
51	u	201	CDL	CA3-CA4-CA6-OA8
51	l	702	CDL	C52-C53-C54-C55
51	r	504	CDL	C63-C64-C65-C66
48	C	302	PEE	C43-C44-C45-C46
49	a	202	PLX	C34-C35-C36-C37
51	r	504	CDL	OA9-CA7-OA8-CA6
51	r	504	CDL	C32-C33-C34-C35
48	l	703	PEE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
51	l	701	CDL	C20-C21-C22-C23
51	l	702	CDL	C40-C41-C42-C43
48	r	501	PEE	C22-C23-C24-C25
51	i	401	CDL	C31-C32-C33-C34
51	i	401	CDL	C33-C34-C35-C36
50	X	201	8Q1	C28-O27-P24-O3
48	B	303	PEE	C13-C14-C15-C16
49	C	303	PLX	C14-C15-C16-C17
49	r	502	PLX	C14-C15-C16-C17
51	r	504	CDL	C43-C44-C45-C46
48	C	302	PEE	C14-C15-C16-C17
49	r	503	PLX	C10-C11-C12-C13
48	W	201	PEE	C3-C2-O2-C10
51	u	201	CDL	CA6-CA4-OA6-CA5
51	l	702	CDL	C17-C18-C19-C20
48	C	302	PEE	C39-C40-C41-C42
48	Q	501	PEE	C14-C15-C16-C17
48	j	201	PEE	C22-C23-C24-C25
51	l	702	CDL	C76-C77-C78-C79
51	r	504	CDL	C56-C57-C58-C59
48	C	302	PEE	C20-C21-C22-C23
49	g	201	PLX	C25-C26-C27-C28
49	j	202	PLX	C14-C15-C16-C17
49	C	303	PLX	C17-C18-C19-C20
48	r	501	PEE	C36-C37-C38-C39
48	r	501	PEE	O3P-C1-C2-O2
51	l	702	CDL	C64-C65-C66-C67
48	j	201	PEE	C11-C12-C13-C14
50	X	201	8Q1	C6-C7-C8-C9
48	j	201	PEE	C12-C13-C14-C15
49	j	202	PLX	C26-C27-C28-C29
51	r	504	CDL	O1-C1-CA2-OA2
51	l	702	CDL	C14-C15-C16-C17
49	r	503	PLX	C7-C8-C9-C10
51	l	701	CDL	C51-C52-C53-C54
49	g	201	PLX	C14-C15-C16-C17
48	j	201	PEE	C36-C37-C38-C39
48	l	703	PEE	C32-C33-C34-C35
51	r	504	CDL	CA5-C11-C12-C13
56	s	401	UQ	C17-C18-C19-C20
51	i	401	CDL	OA5-CA3-CA4-CA6
51	l	702	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
51	r	504	CDL	OB5-CB3-CB4-CB6
48	W	201	PEE	C21-C22-C23-C24
51	r	504	CDL	C44-C45-C46-C47
51	a	201	CDL	C32-C33-C34-C35
50	G	201	8Q1	C29-C32-C34-N36
51	i	401	CDL	C35-C36-C37-C38
51	r	504	CDL	C60-C61-C62-C63
48	r	501	PEE	C38-C39-C40-C41
48	j	201	PEE	C30-C31-C32-C33
48	C	302	PEE	C11-C12-C13-C14
50	G	201	8Q1	C7-C8-C9-C10
51	i	401	CDL	CA7-C31-C32-C33
51	r	504	CDL	CA2-C1-CB2-OB2
48	l	704	PEE	C1-C2-C3-O3
48	r	501	PEE	C1-C2-C3-O3
49	g	201	PLX	C3-C4-C5-O8
49	j	202	PLX	C3-C4-C5-O8
50	X	201	8Q1	C43-C42-N41-C39
51	l	702	CDL	CA3-CA4-CA6-OA8
51	r	504	CDL	CA3-CA4-CA6-OA8
51	r	504	CDL	CB3-CB4-CB6-OB8
51	u	201	CDL	C57-C58-C59-C60
49	r	503	PLX	C9-C10-C11-C12
50	G	201	8Q1	C11-C10-C9-C8
49	r	503	PLX	C27-C28-C29-C30
48	C	302	PEE	O3P-C1-C2-O2
48	W	201	PEE	O3P-C1-C2-O2
51	l	702	CDL	OA5-CA3-CA4-OA6
51	r	504	CDL	OB5-CB3-CB4-OB6
50	G	201	8Q1	O4-C1-S44-C43
51	l	701	CDL	OB6-CB4-CB6-OB8
51	l	702	CDL	OA6-CA4-CA6-OA8
48	l	704	PEE	O4-C10-O2-C2
49	g	201	PLX	C18-C19-C20-C21
48	B	303	PEE	C21-C22-C23-C24
49	a	202	PLX	C27-C28-C29-C30
51	l	701	CDL	C35-C36-C37-C38
49	g	201	PLX	O8-C24-C25-C26
48	W	201	PEE	C12-C13-C14-C15
49	r	503	PLX	C31-C32-C33-C34
50	X	201	8Q1	C11-C10-C9-C8
51	u	201	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
50	X	201	8Q1	C1-C6-C7-C8
49	a	202	PLX	C33-C34-C35-C36
49	j	202	PLX	C18-C19-C20-C21
51	l	701	CDL	C24-C25-C26-C27
48	B	303	PEE	C20-C21-C22-C23
51	u	201	CDL	C53-C54-C55-C56
51	r	504	CDL	C64-C65-C66-C67
50	G	201	8Q1	C6-C1-S44-C43
48	C	302	PEE	C13-C14-C15-C16
49	g	201	PLX	C32-C33-C34-C35
51	l	701	CDL	C37-C38-C39-C40
48	l	703	PEE	C15-C16-C17-C18
49	r	502	PLX	C16-C17-C18-C19
51	r	504	CDL	C61-C62-C63-C64
48	Q	501	PEE	C24-C25-C26-C27
49	j	202	PLX	O4-C3-C4-C5
48	j	201	PEE	C38-C39-C40-C41
47	A	503	NAI	C2D-C1D-N1N-C6N
49	r	503	PLX	C24-C25-C26-C27
51	i	401	CDL	C71-C72-C73-C74
51	a	201	CDL	C54-C55-C56-C57
49	r	502	PLX	C25-C26-C27-C28
51	l	701	CDL	CA6-CA4-OA6-CA5
49	C	303	PLX	C30-C31-C32-C33
48	Q	501	PEE	C39-C40-C41-C42
49	a	202	PLX	C35-C36-C37-C38
51	a	201	CDL	OA5-CA3-CA4-OA6
51	i	401	CDL	OA5-CA3-CA4-OA6
51	l	701	CDL	OA5-CA3-CA4-OA6
51	l	702	CDL	C32-C33-C34-C35
49	r	503	PLX	C3-C4-C5-O8
51	i	401	CDL	CB3-CB4-CB6-OB8
49	C	303	PLX	C13-C14-C15-C16
48	r	501	PEE	C15-C16-C17-C18
49	g	201	PLX	O6-C4-C5-O8
49	j	202	PLX	O6-C4-C5-O8
49	r	503	PLX	O6-C4-C5-O8
48	B	303	PEE	C34-C35-C36-C37
49	g	201	PLX	C19-C20-C21-C22
49	C	303	PLX	C2-C1-N1-C1B
47	A	503	NAI	C2D-C1D-N1N-C2N
47	A	503	NAI	C3D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
49	C	303	PLX	N1-C1-C2-O1
51	I	201	CDL	O1-C1-CA2-OA2
51	l	702	CDL	C22-C23-C24-C25
49	a	202	PLX	C25-C24-O8-C5
49	j	202	PLX	C25-C24-O8-C5
48	B	303	PEE	C38-C39-C40-C41
48	l	703	PEE	C38-C39-C40-C41
51	l	702	CDL	C31-C32-C33-C34
49	a	202	PLX	C12-C13-C14-C15
46	A	502	FMN	O4'-C4'-C5'-O5'
50	G	201	8Q1	C13-C14-C15-C16
48	B	303	PEE	O3P-C1-C2-C3
48	C	302	PEE	O3P-C1-C2-C3
48	W	201	PEE	O3P-C1-C2-C3
48	r	501	PEE	O3P-C1-C2-C3
49	g	201	PLX	O4-C3-C4-C5
51	r	504	CDL	C36-C37-C38-C39
50	X	201	8Q1	C13-C14-C15-C16
48	l	704	PEE	C13-C14-C15-C16
50	G	201	8Q1	O27-C28-C29-C30
51	r	504	CDL	C16-C17-C18-C19
49	a	202	PLX	C26-C27-C28-C29
49	r	502	PLX	C35-C36-C37-C38
49	C	303	PLX	C25-C26-C27-C28
48	C	302	PEE	C44-C45-C46-C47
52	J	401	NDP	C2B-O2B-P2B-O1X
49	r	502	PLX	O8-C24-C25-C26
48	B	303	PEE	O3P-C1-C2-O2
49	g	201	PLX	O4-C3-C4-O6
49	j	202	PLX	O4-C3-C4-O6
51	a	201	CDL	C38-C39-C40-C41
49	C	303	PLX	C2-C1-N1-C1C
48	r	501	PEE	C34-C35-C36-C37
51	l	702	CDL	C83-C84-C85-C86
48	l	703	PEE	O2-C2-C3-O3
48	l	704	PEE	O2-C2-C3-O3
48	r	501	PEE	O2-C2-C3-O3
51	u	201	CDL	OA6-CA4-CA6-OA8
49	C	303	PLX	C11-C10-C9-C8
51	r	504	CDL	C84-C85-C86-C87
51	r	504	CDL	C78-C79-C80-C81
51	l	701	CDL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
51	l	701	CDL	O1-C1-CA2-OA2
51	l	701	CDL	C74-C75-C76-C77
51	l	702	CDL	C12-C13-C14-C15
49	r	503	PLX	C36-C37-C38-C39
51	r	504	CDL	C31-C32-C33-C34
51	a	201	CDL	C42-C43-C44-C45
47	A	503	NAI	C5D-O5D-PN-O3
48	B	303	PEE	C4-O4P-P-O3P
48	C	302	PEE	C4-O4P-P-O1P
48	Q	501	PEE	C1-O3P-P-O1P
48	Q	501	PEE	C1-O3P-P-O4P
48	W	201	PEE	C1-O3P-P-O4P
48	l	703	PEE	C1-O3P-P-O2P
48	l	704	PEE	C4-O4P-P-O3P
49	C	303	PLX	C2-O1-P1-O4
49	C	303	PLX	C2-O1-P1-O3
49	j	202	PLX	C3-O4-P1-O1
49	j	202	PLX	C3-O4-P1-O2
49	r	503	PLX	C2-O1-P1-O4
49	r	503	PLX	C2-O1-P1-O2
49	r	503	PLX	C2-O1-P1-O3
51	I	201	CDL	CA2-OA2-PA1-OA4
51	I	201	CDL	CA2-OA2-PA1-OA5
51	a	201	CDL	CB2-OB2-PB2-OB4
51	a	201	CDL	CB2-OB2-PB2-OB5
51	i	401	CDL	CA2-OA2-PA1-OA3
51	i	401	CDL	CB2-OB2-PB2-OB3
51	l	701	CDL	CA2-OA2-PA1-OA3
51	l	701	CDL	CB2-OB2-PB2-OB5
51	l	702	CDL	CB2-OB2-PB2-OB3
51	r	504	CDL	CA2-OA2-PA1-OA3
51	r	504	CDL	CA2-OA2-PA1-OA5
51	r	504	CDL	CB3-OB5-PB2-OB3
52	J	401	NDP	C5B-O5B-PA-O1A
52	J	401	NDP	C5D-O5D-PN-O2N
48	B	303	PEE	C40-C41-C42-C43
48	l	704	PEE	C39-C40-C41-C42
46	A	502	FMN	C5'-O5'-P-O1P
49	j	202	PLX	C31-C32-C33-C34
51	r	504	CDL	C54-C55-C56-C57
51	r	504	CDL	C20-C21-C22-C23
48	l	704	PEE	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
51	i	401	CDL	CA6-CA4-OA6-CA5
49	g	201	PLX	C34-C35-C36-C37
51	a	201	CDL	C75-C76-C77-C78
51	u	201	CDL	C76-C77-C78-C79
51	a	201	CDL	OA5-CA3-CA4-CA6
48	Q	501	PEE	C38-C39-C40-C41
51	r	504	CDL	C80-C81-C82-C83
51	u	201	CDL	C22-C23-C24-C25
48	C	302	PEE	C10-C11-C12-C13
51	I	201	CDL	CA3-CA4-CA6-OA8
51	l	701	CDL	C59-C60-C61-C62
51	r	504	CDL	C79-C80-C81-C82
52	J	401	NDP	O4B-C4B-C5B-O5B
49	a	202	PLX	C30-C31-C32-C33
49	j	202	PLX	C10-C11-C12-C13
50	G	201	8Q1	C29-C32-C34-O35
48	r	501	PEE	C23-C24-C25-C26
51	l	701	CDL	C54-C55-C56-C57
51	i	401	CDL	C37-C38-C39-C40
49	a	202	PLX	O7-C6-C7-C8
49	j	202	PLX	O6-C6-C7-C8
51	I	201	CDL	C1-CA2-OA2-PA1
48	Q	501	PEE	C31-C32-C33-C34
49	j	202	PLX	C16-C17-C18-C19
47	A	503	NAI	O4D-C1D-N1N-C2N
48	j	201	PEE	C43-C44-C45-C46
51	l	701	CDL	C36-C37-C38-C39
49	a	202	PLX	O4-C3-C4-O6
48	W	201	PEE	C16-C17-C18-C19
49	r	502	PLX	C20-C21-C22-C23
49	C	303	PLX	C2-C1-N1-C1A
51	l	701	CDL	C12-C13-C14-C15
48	W	201	PEE	C18-C19-C20-C21
49	r	502	PLX	C26-C27-C28-C29
49	r	502	PLX	O6-C4-C5-O8
51	a	201	CDL	C17-C18-C19-C20
51	u	201	CDL	C21-C22-C23-C24
49	a	202	PLX	C25-C26-C27-C28
51	a	201	CDL	C36-C37-C38-C39
48	l	704	PEE	C2-C1-O3P-P
51	a	201	CDL	CA4-CA3-OA5-PA1
51	r	504	CDL	CB4-CB3-OB5-PB2

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Mol	Chain	Res	Type	Atoms
49	j	202	PLX	C33-C34-C35-C36
49	r	502	PLX	C18-C19-C20-C21
49	C	303	PLX	C26-C27-C28-C29
51	r	504	CDL	CB2-C1-CA2-OA2
48	r	501	PEE	C31-C32-C33-C34
48	l	703	PEE	C1-C2-C3-O3
48	l	704	PEE	C16-C17-C18-C19
56	s	401	UQ	C14-C16-C17-C18
51	r	504	CDL	C59-C60-C61-C62
48	W	201	PEE	C24-C25-C26-C27
51	I	201	CDL	CB6-CB4-OB6-CB5
51	a	201	CDL	CA6-CA4-OA6-CA5
48	l	704	PEE	C15-C16-C17-C18
49	r	503	PLX	C30-C31-C32-C33
48	j	201	PEE	C41-C42-C43-C44
51	l	701	CDL	OA5-CA3-CA4-CA6
51	I	201	CDL	OA6-CA4-CA6-OA8
47	A	503	NAI	C3B-C4B-C5B-O5B
48	l	703	PEE	C14-C15-C16-C17
51	l	702	CDL	C80-C81-C82-C83
49	r	503	PLX	O8-C24-C25-C26
48	W	201	PEE	C23-C24-C25-C26
51	l	702	CDL	C43-C44-C45-C46
48	r	501	PEE	C39-C40-C41-C42
49	g	201	PLX	C36-C37-C38-C39
48	r	501	PEE	O5-C30-O3-C3
48	r	501	PEE	C31-C30-O3-C3
49	C	303	PLX	C32-C33-C34-C35
49	g	201	PLX	C20-C21-C22-C23
48	l	704	PEE	C30-C31-C32-C33
51	a	201	CDL	C32-C31-CA7-OA8
48	Q	501	PEE	C32-C33-C34-C35
48	l	703	PEE	C37-C38-C39-C40
47	A	503	NAI	O4D-C1D-N1N-C6N
51	a	201	CDL	OB5-CB3-CB4-CB6
51	l	701	CDL	C76-C77-C78-C79
48	j	201	PEE	C16-C17-C18-C19
51	l	701	CDL	CA4-CA3-OA5-PA1
49	C	303	PLX	C18-C19-C20-C21
48	r	501	PEE	C43-C44-C45-C46
48	r	501	PEE	C24-C25-C26-C27
48	C	302	PEE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
47	A	503	NAI	O4D-C4D-C5D-O5D
48	W	201	PEE	C33-C34-C35-C36
51	u	201	CDL	C77-C78-C79-C80
51	r	504	CDL	C82-C83-C84-C85
48	l	704	PEE	C12-C13-C14-C15
51	I	201	CDL	C51-C52-C53-C54
48	l	703	PEE	C36-C37-C38-C39
48	l	703	PEE	O3P-C1-C2-O2
51	I	201	CDL	OA5-CA3-CA4-OA6
51	l	701	CDL	C39-C40-C41-C42
48	j	201	PEE	C13-C14-C15-C16
48	Q	501	PEE	C1-C2-C3-O3
49	r	502	PLX	C3-C4-C5-O8
48	j	201	PEE	C20-C21-C22-C23
51	a	201	CDL	C33-C34-C35-C36
48	Q	501	PEE	C36-C37-C38-C39
48	l	704	PEE	C38-C39-C40-C41
48	B	303	PEE	C32-C33-C34-C35
49	a	202	PLX	C13-C14-C15-C16
48	C	302	PEE	C41-C42-C43-C44
48	W	201	PEE	C20-C21-C22-C23
49	C	303	PLX	C27-C28-C29-C30
48	Q	501	PEE	O2-C2-C3-O3
48	C	302	PEE	C38-C39-C40-C41
48	l	704	PEE	C23-C24-C25-C26
51	r	504	CDL	C72-C73-C74-C75
49	g	201	PLX	C7-C6-O6-C4
49	j	202	PLX	C7-C6-O6-C4
48	B	303	PEE	C44-C45-C46-C47
48	l	703	PEE	C16-C17-C18-C19
51	r	504	CDL	C39-C40-C41-C42
51	r	504	CDL	C52-C51-CB5-OB6
51	l	701	CDL	C33-C34-C35-C36
48	Q	501	PEE	C17-C18-C19-C20
48	j	201	PEE	O3P-C1-C2-O2
48	Q	501	PEE	C2-C1-O3P-P
49	r	502	PLX	C25-C24-O8-C5
48	C	302	PEE	O3-C30-C31-C32
48	Q	501	PEE	C18-C19-C20-C21
51	r	504	CDL	C40-C41-C42-C43
51	l	701	CDL	C56-C57-C58-C59
50	G	201	8Q1	O27-C28-C29-C31

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Mol	Chain	Res	Type	Atoms
48	l	704	PEE	O2-C10-C11-C12
49	g	201	PLX	C29-C30-C31-C32
49	C	303	PLX	C6-C7-C8-C9
49	a	202	PLX	C24-C25-C26-C27
51	r	504	CDL	C52-C51-CB5-OB7
51	l	702	CDL	C12-C11-CA5-OA6
51	a	201	CDL	C77-C78-C79-C80
48	C	302	PEE	O5-C30-C31-C32
49	r	502	PLX	O9-C24-O8-C5
51	l	702	CDL	C58-C59-C60-C61
49	j	202	PLX	C4-C5-O8-C24
51	l	702	CDL	OA7-CA5-OA6-CA4
51	l	701	CDL	OA6-CA4-CA6-OA8
51	a	201	CDL	C34-C35-C36-C37
50	X	201	8Q1	O33-C32-C34-N36
51	I	201	CDL	C52-C51-CB5-OB6
48	l	704	PEE	C2-C3-O3-C30
51	l	702	CDL	C32-C31-CA7-OA8
51	l	701	CDL	C14-C15-C16-C17
51	l	702	CDL	C11-CA5-OA6-CA4
57	w	401	ADP	PB-O3A-PA-O2A
47	A	503	NAI	O4B-C4B-C5B-O5B

There are no ring outliers.

27 monomers are involved in 303 short contacts:

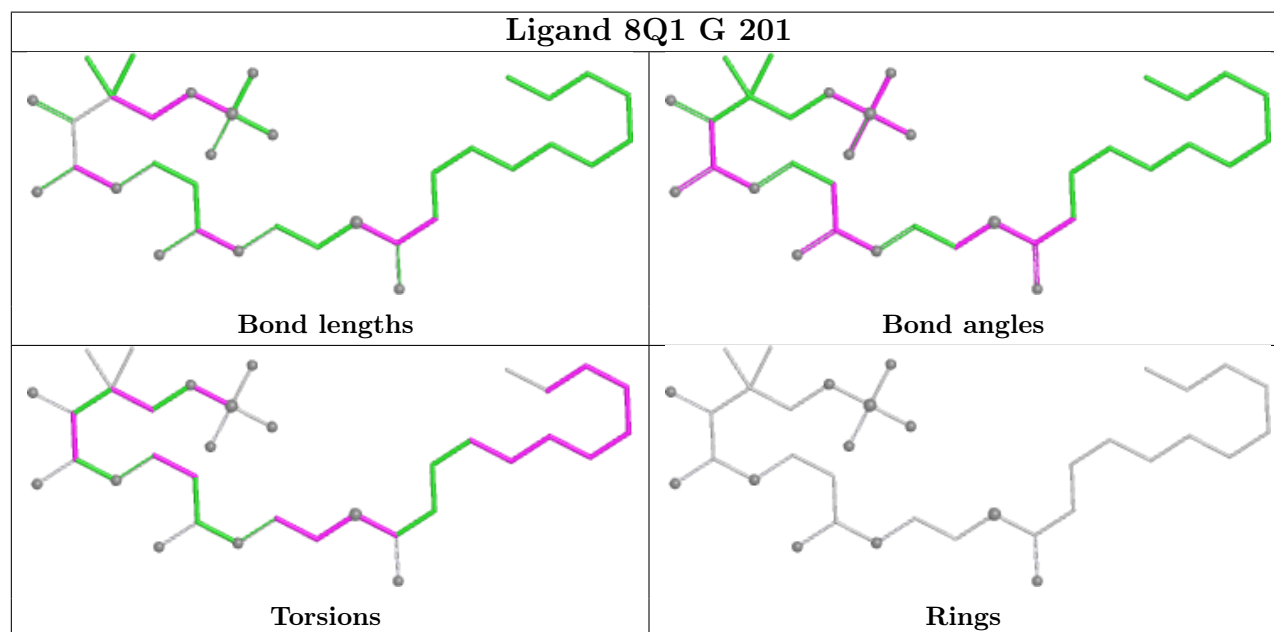
Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	r	504	CDL	11	0
48	C	302	PEE	16	0
49	C	303	PLX	2	0
48	W	201	PEE	16	0
52	J	401	NDP	6	0
45	A	501	SF4	2	0
49	a	202	PLX	6	0
49	r	503	PLX	6	0
48	j	201	PEE	5	0
51	u	201	CDL	18	0
48	r	501	PEE	12	0
48	l	703	PEE	6	0
49	r	502	PLX	4	0
48	B	303	PEE	1	0
51	i	401	CDL	18	0

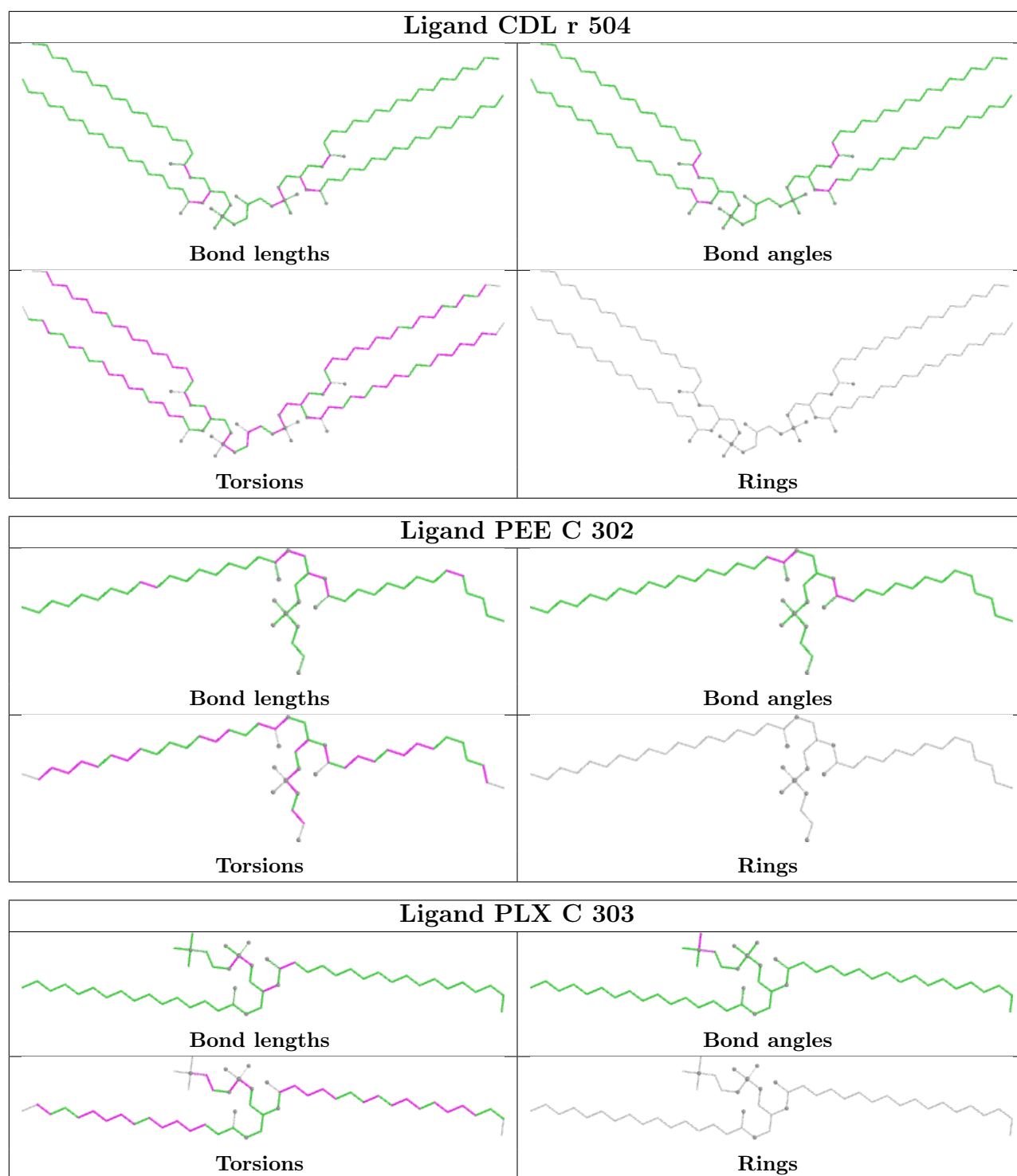
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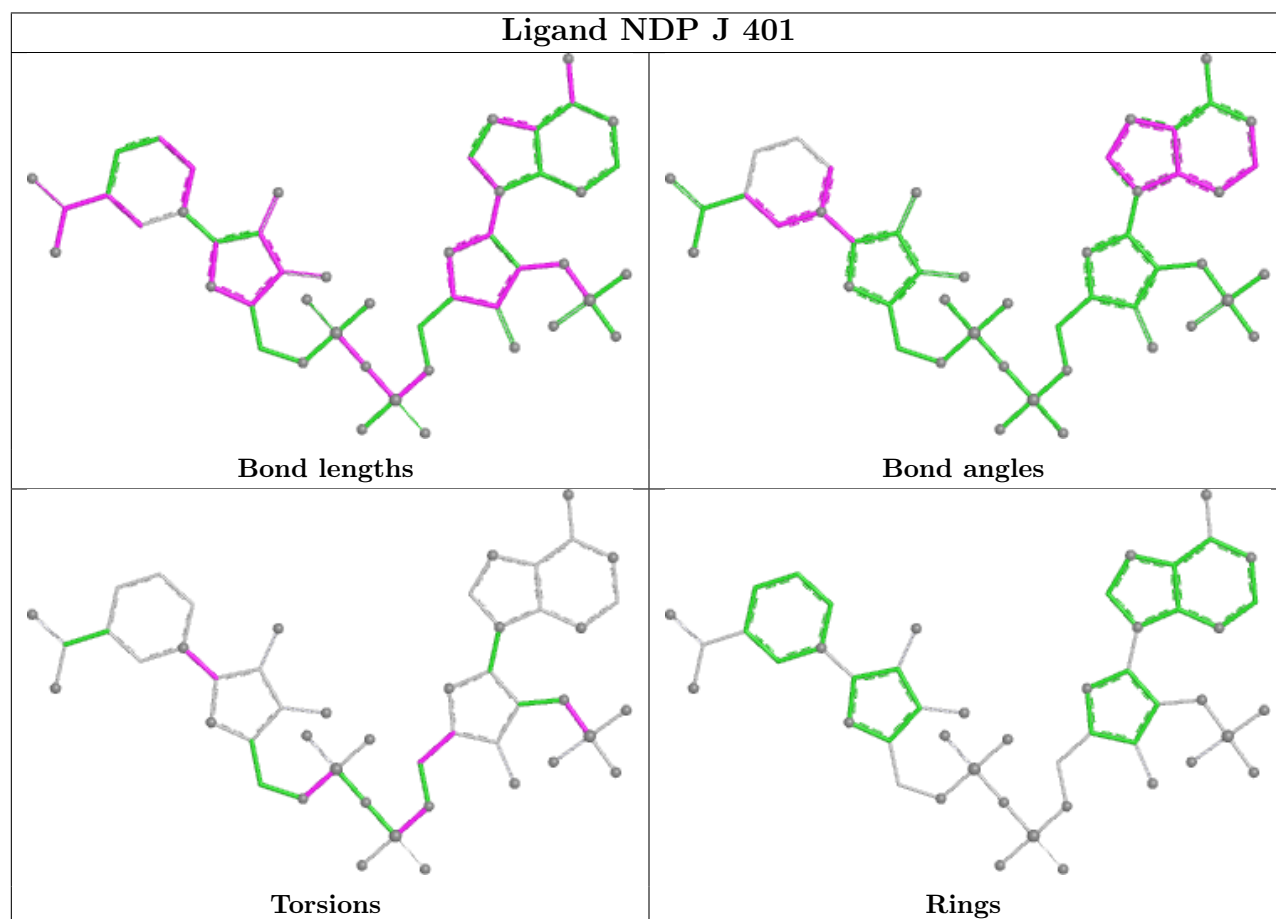
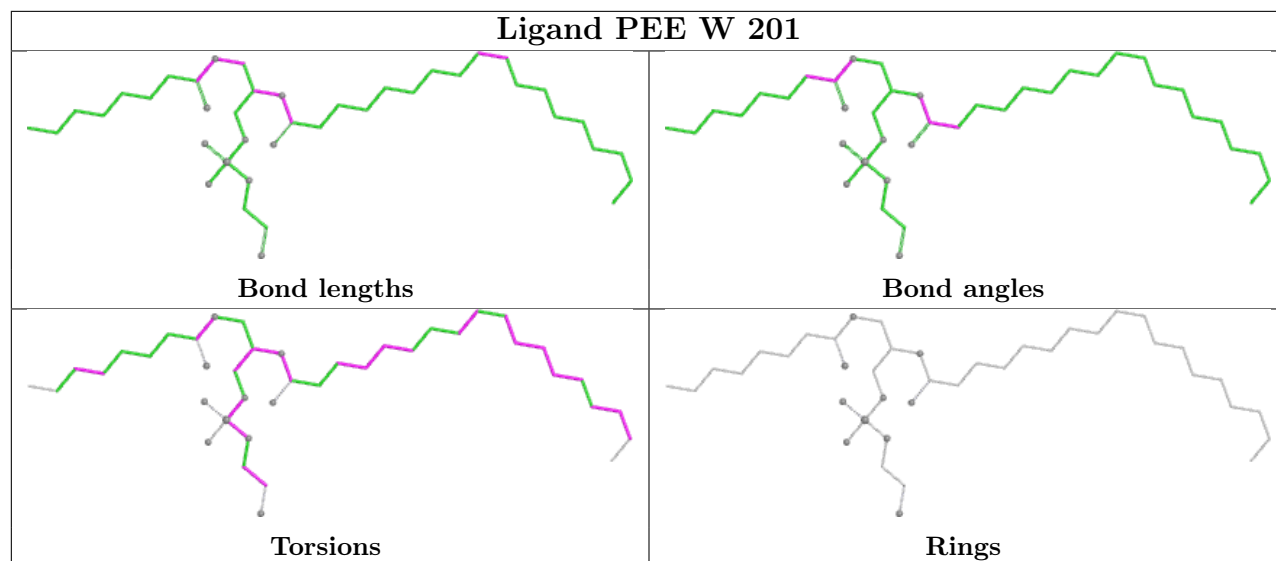
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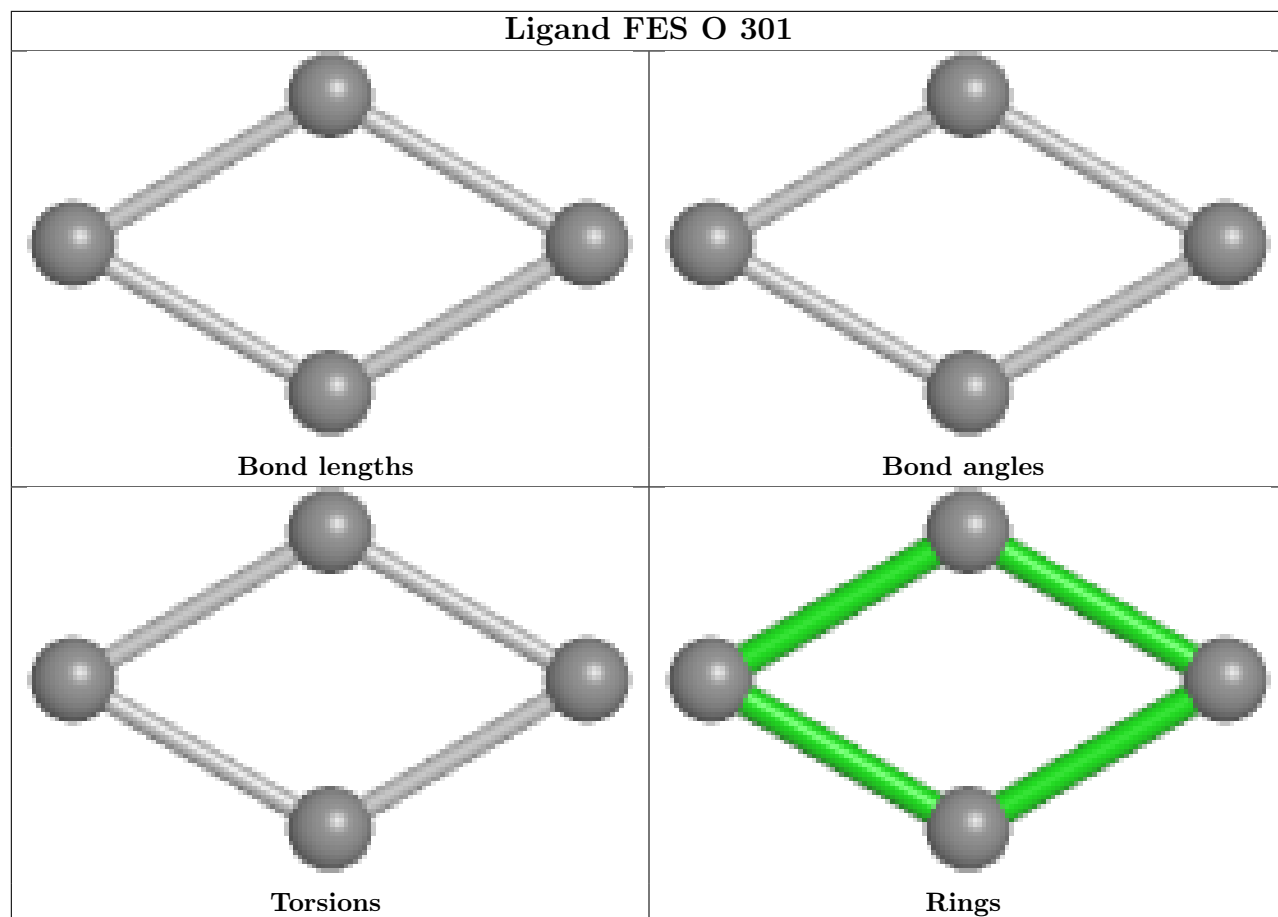
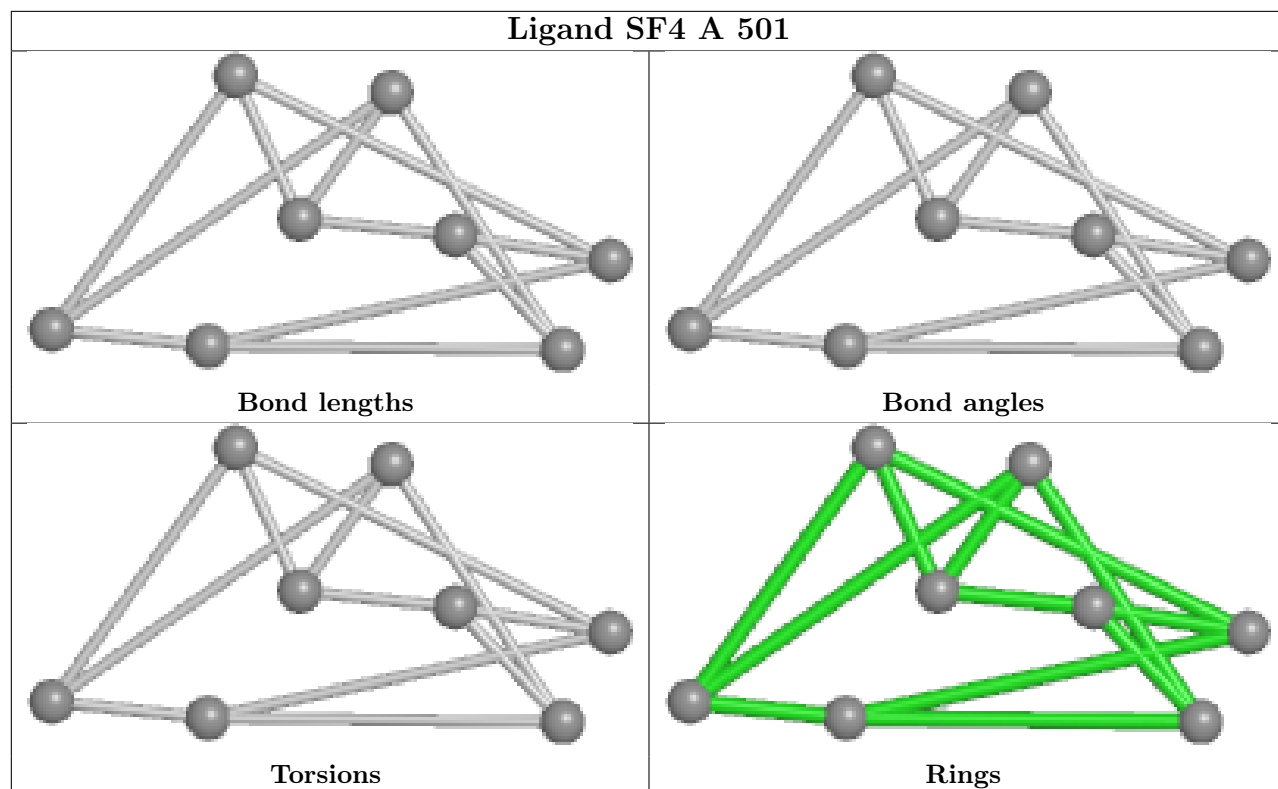
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	s	401	UQ	6	0
49	g	201	PLX	5	0
51	a	201	CDL	44	0
57	w	401	ADP	1	0
51	I	201	CDL	12	0
47	A	503	NAI	7	0
48	Q	501	PEE	22	0
48	l	704	PEE	25	0
46	A	502	FMN	2	0
49	j	202	PLX	4	0
51	l	701	CDL	58	0
51	l	702	CDL	7	0

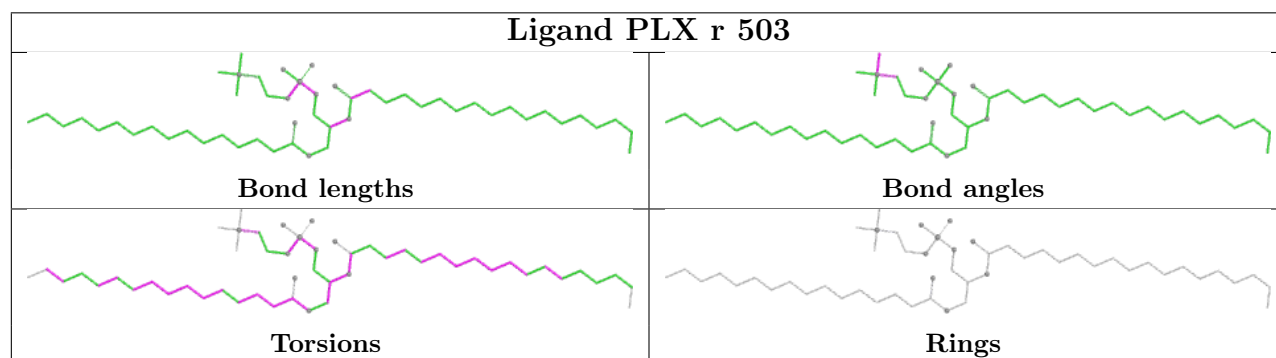
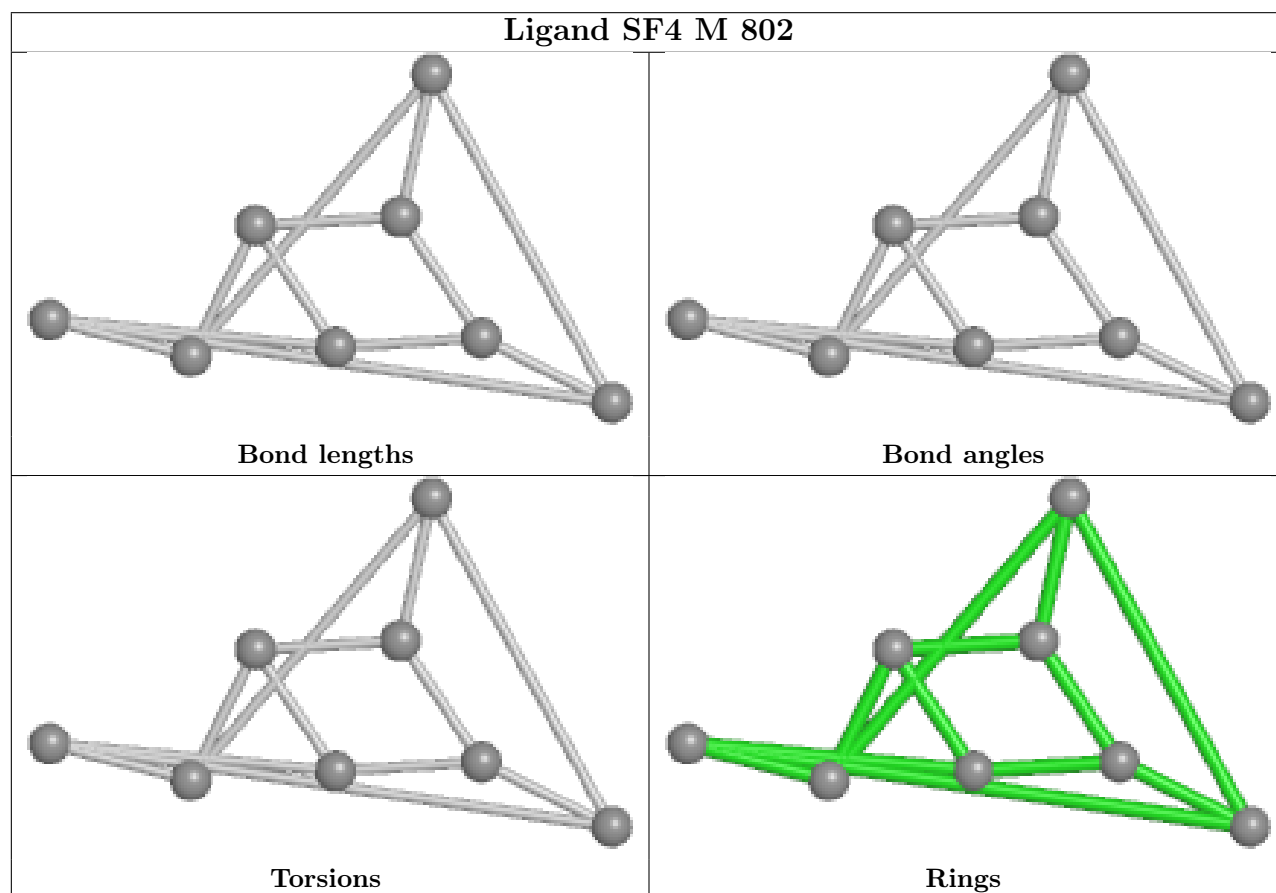
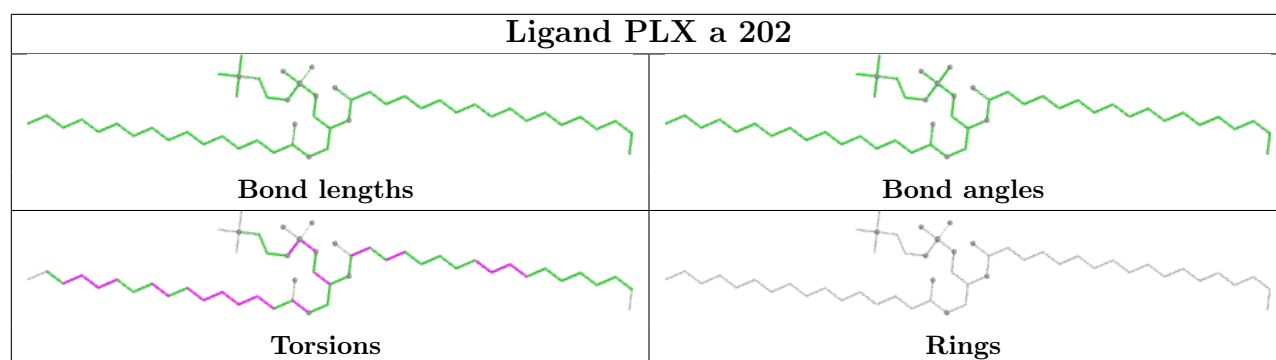
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

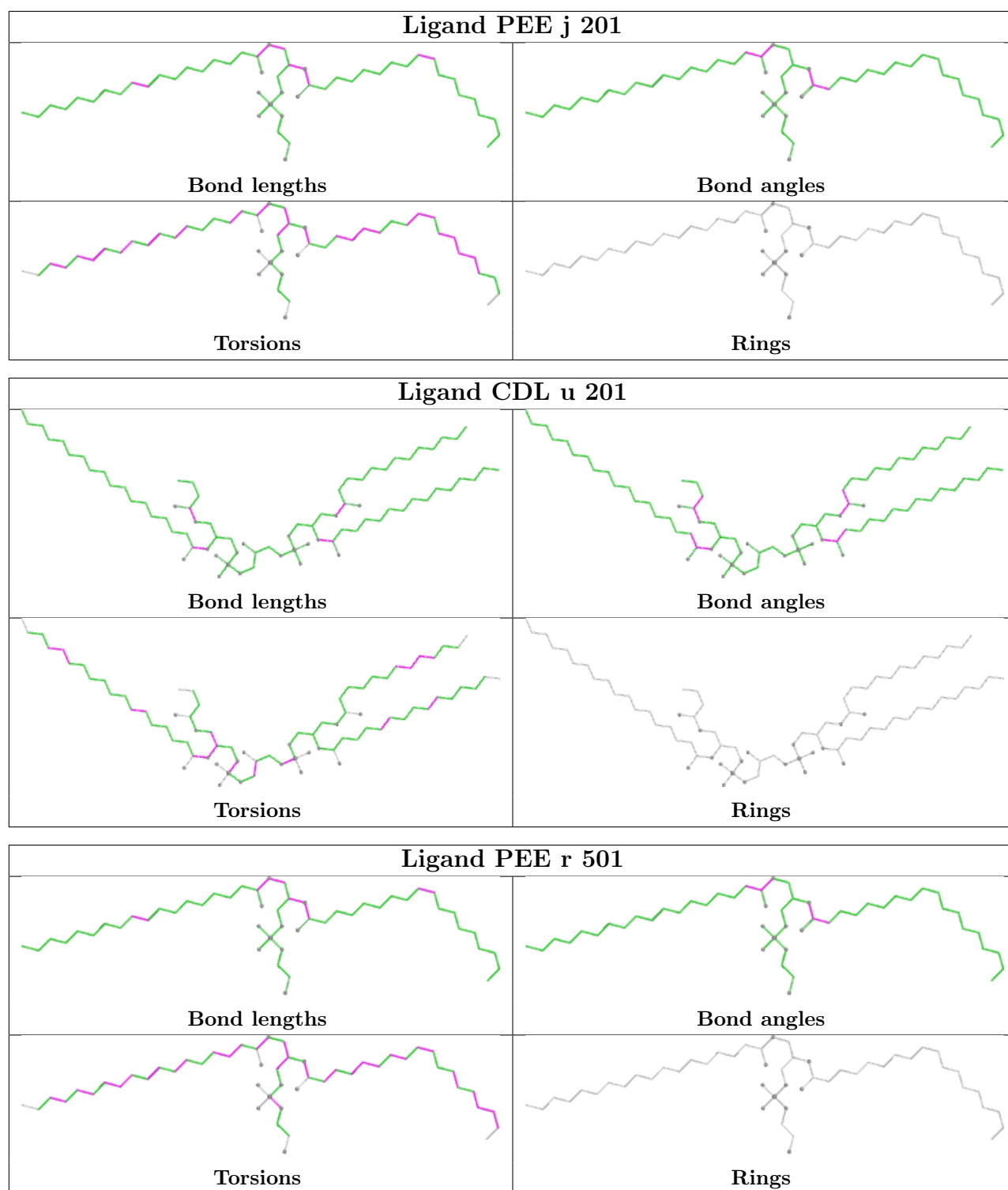


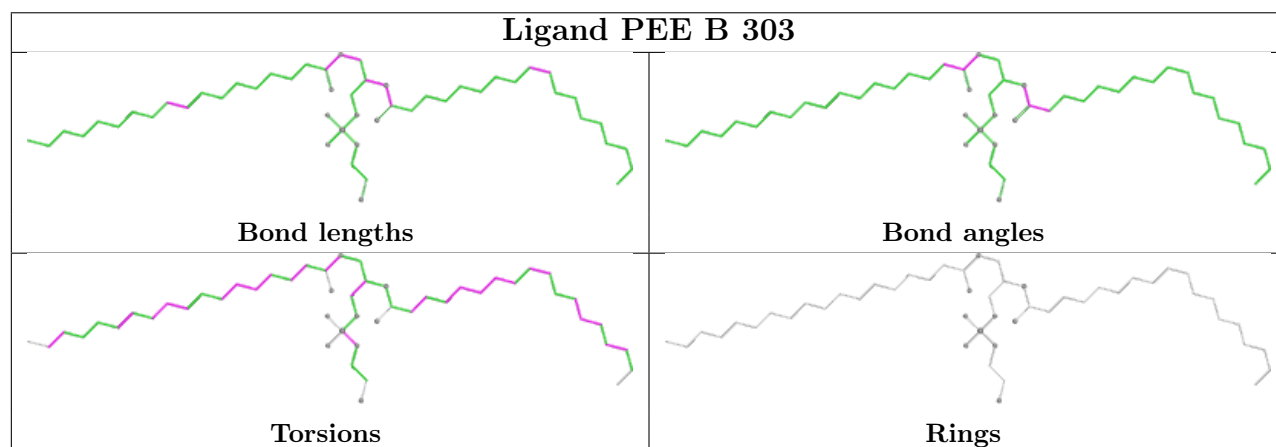
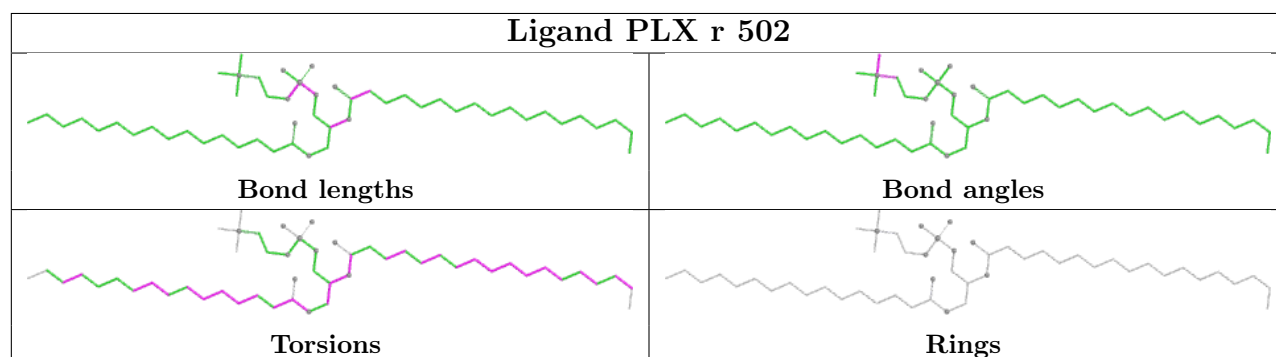
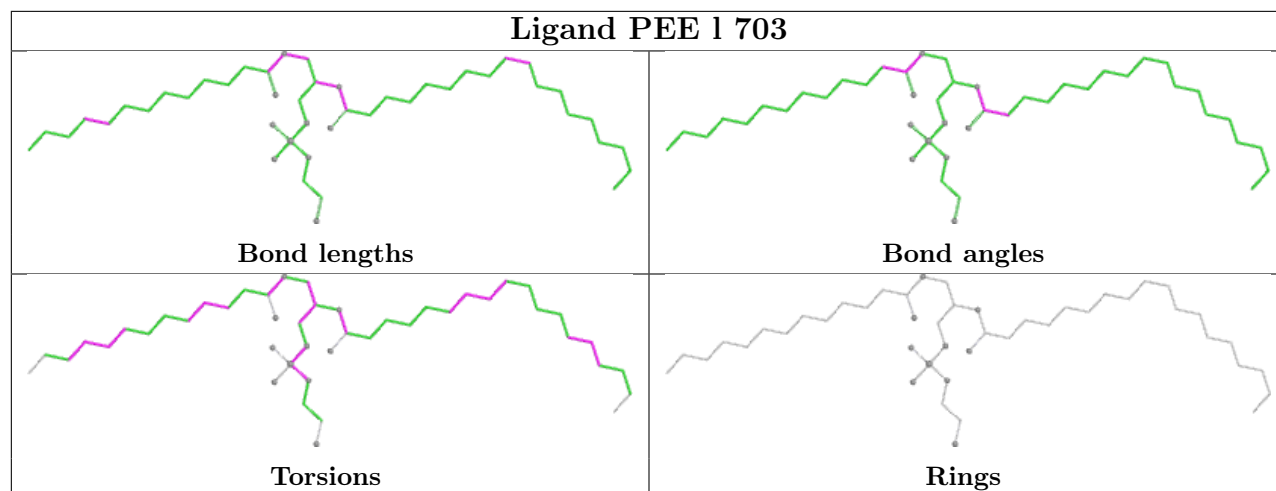


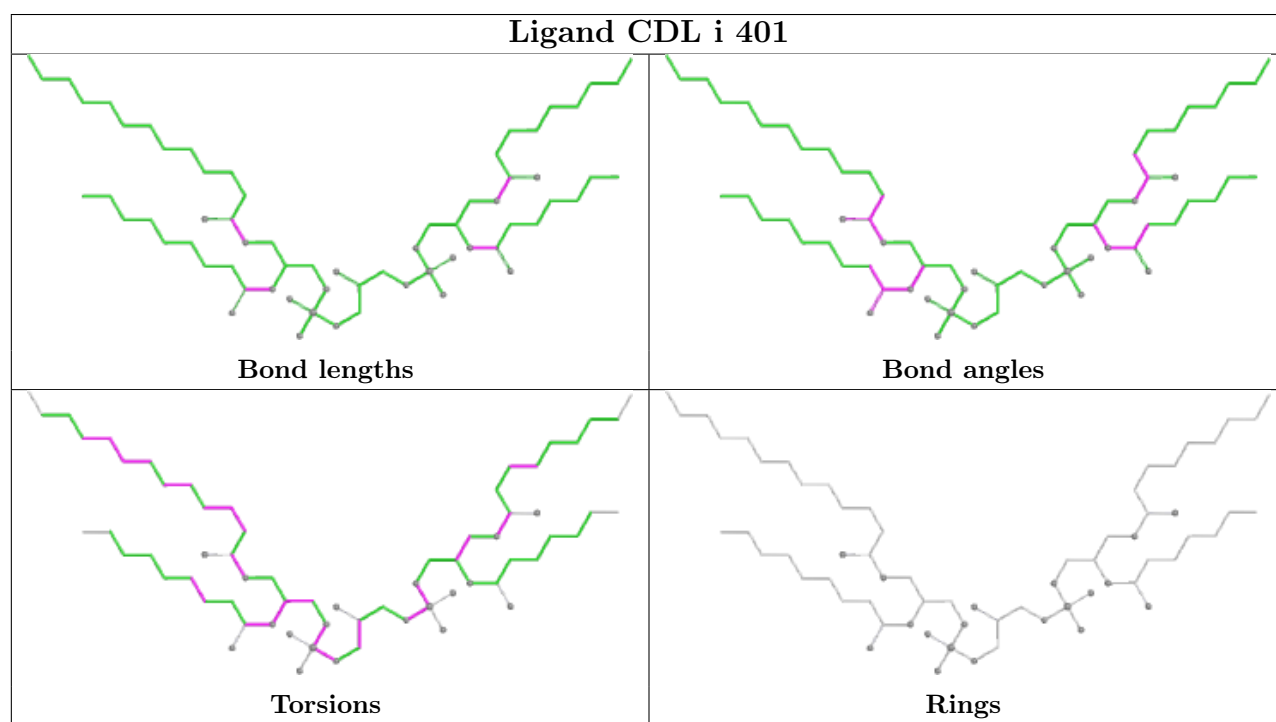
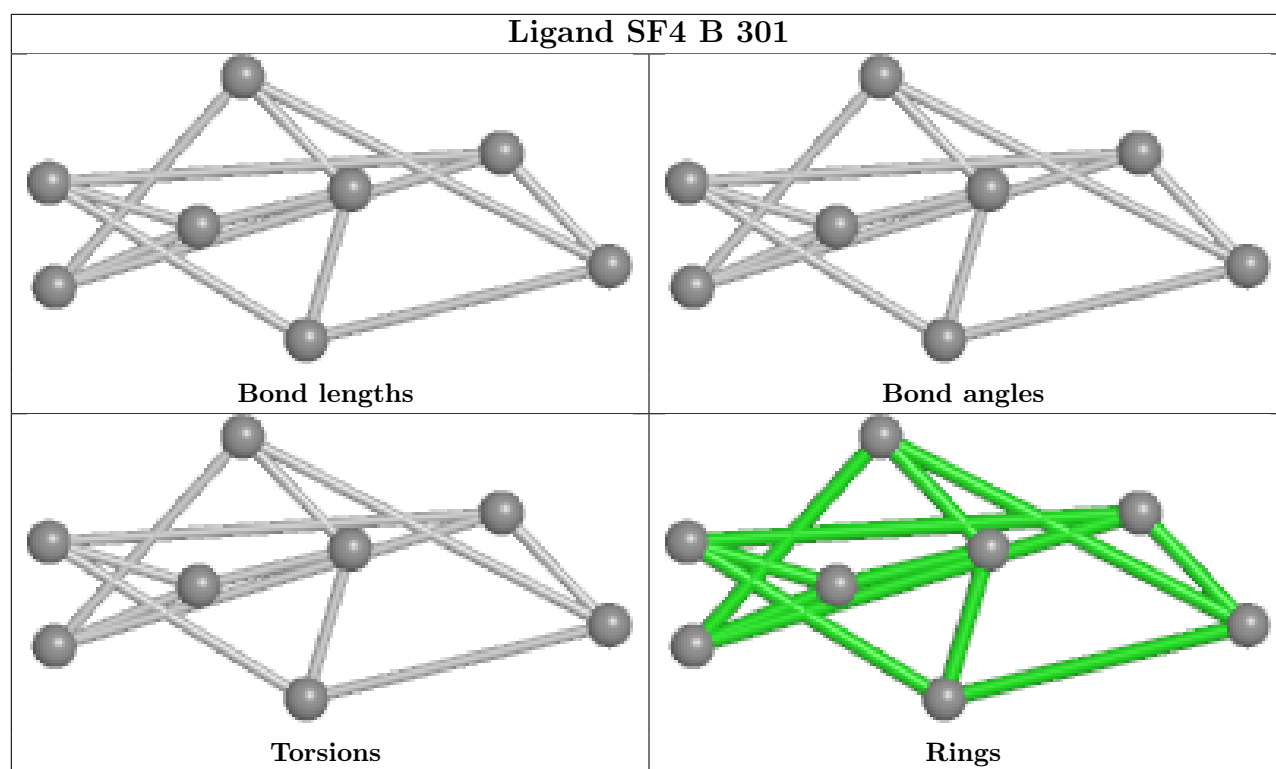


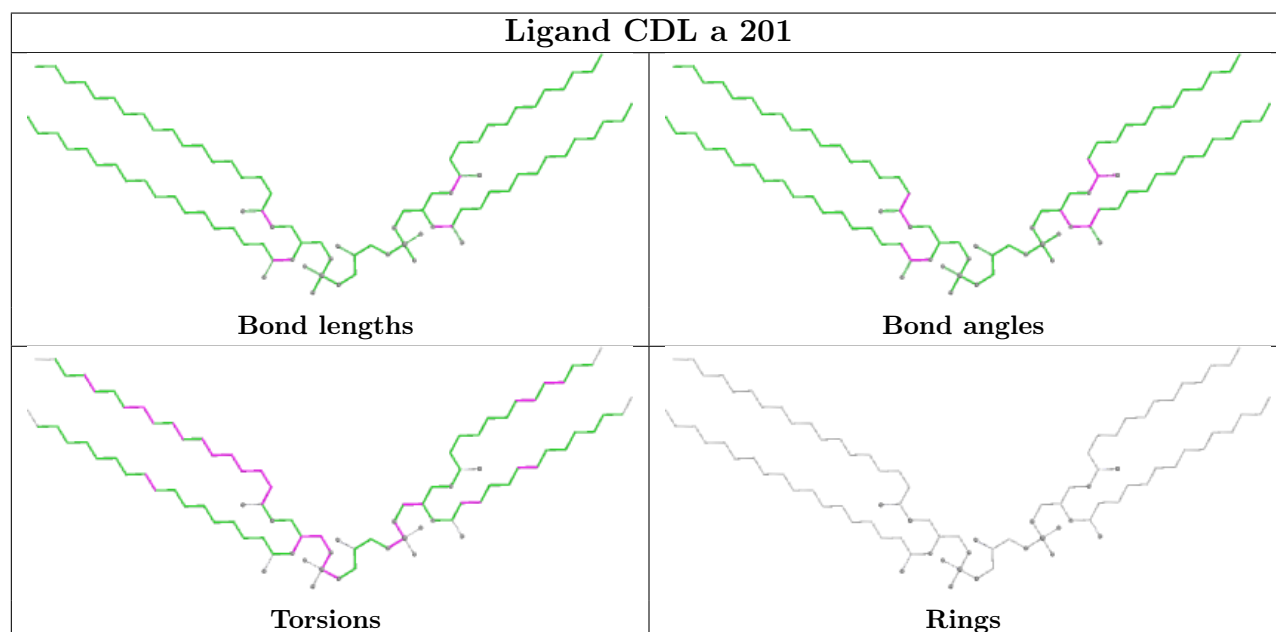
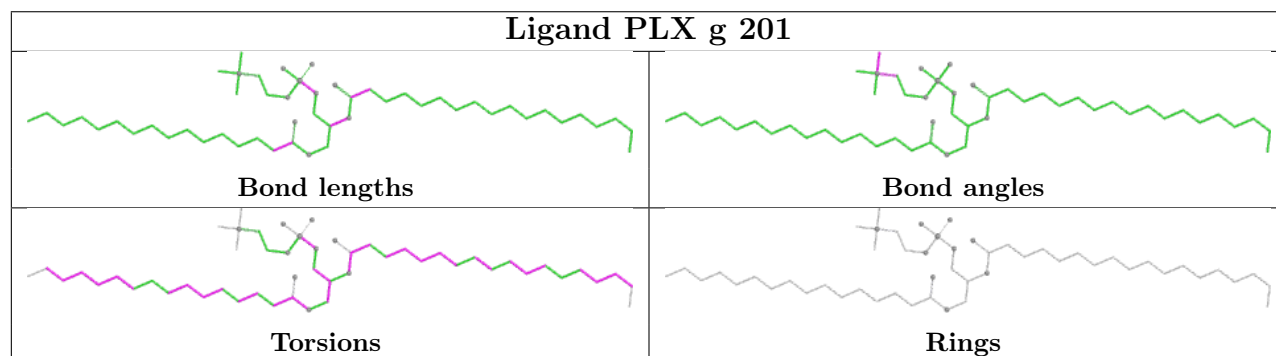
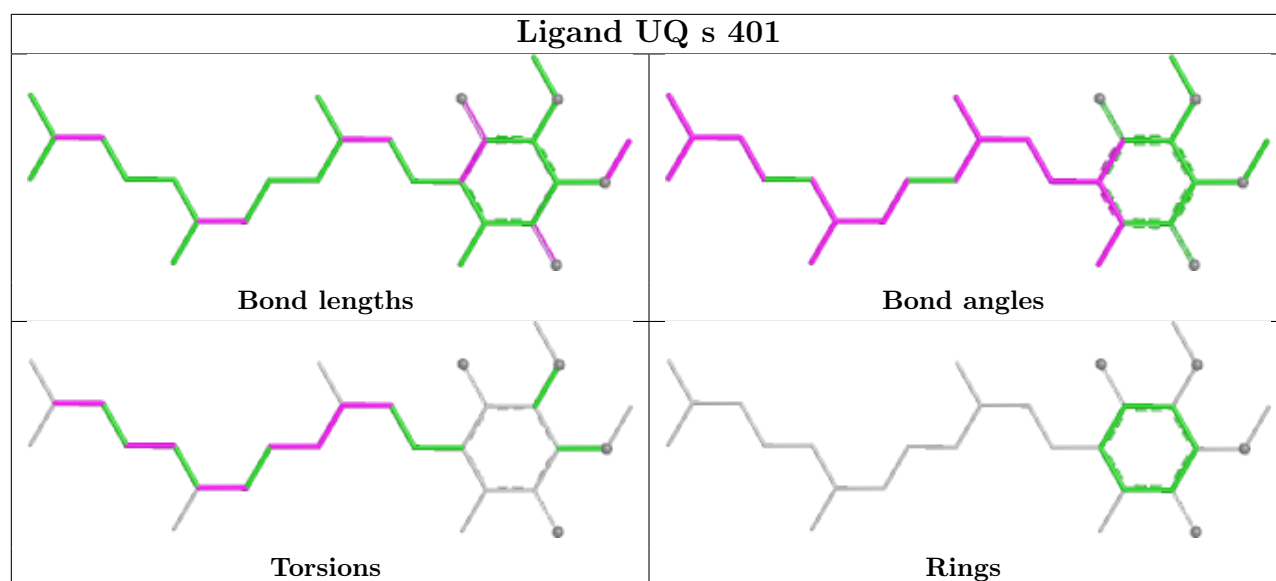


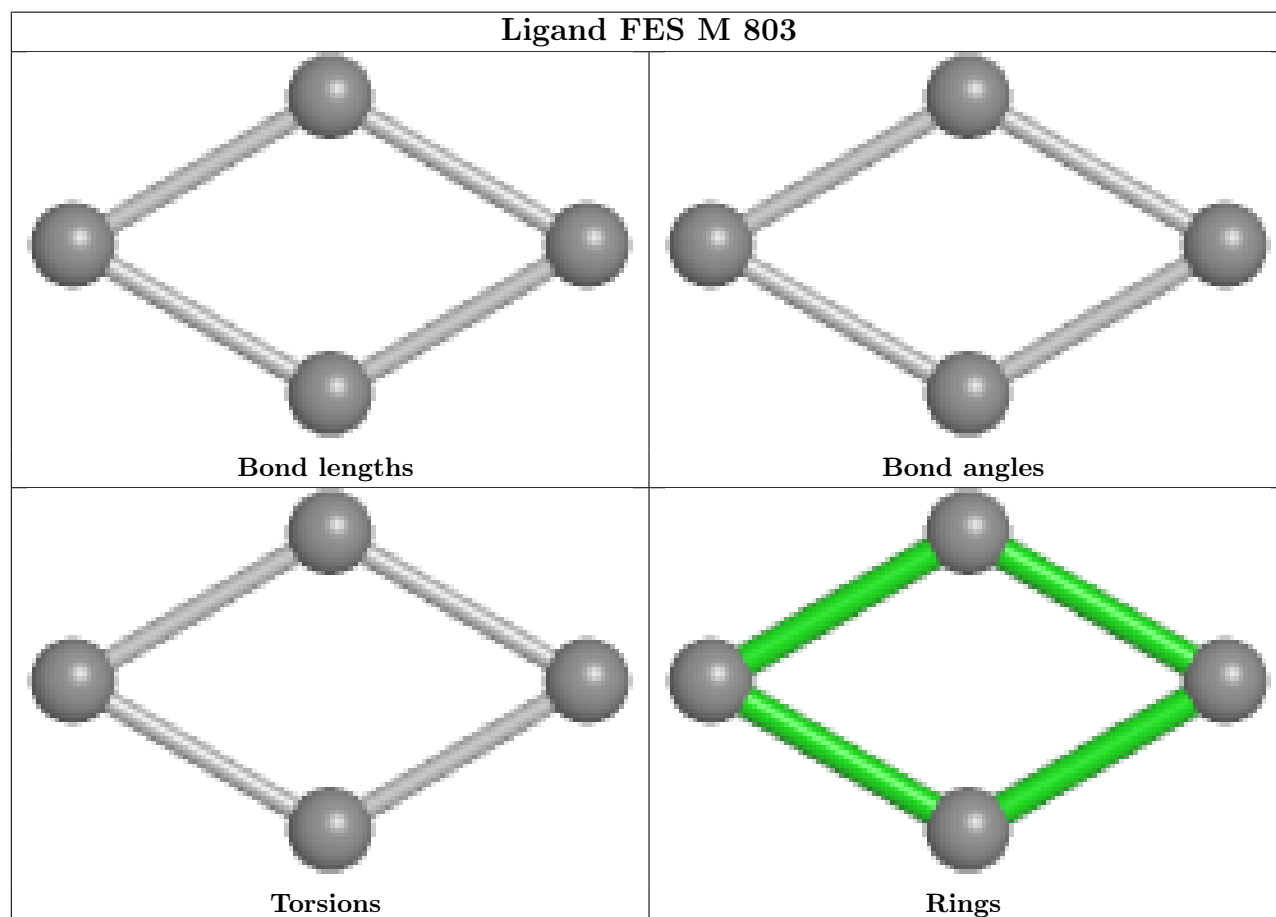
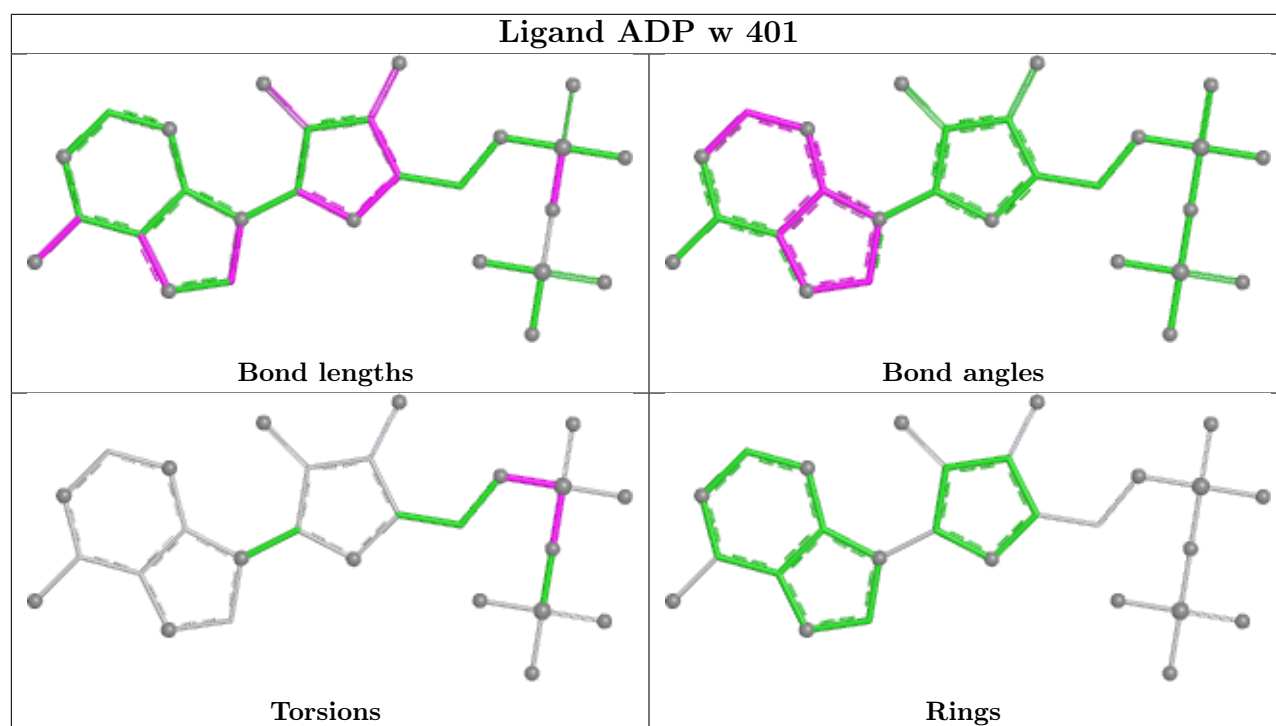


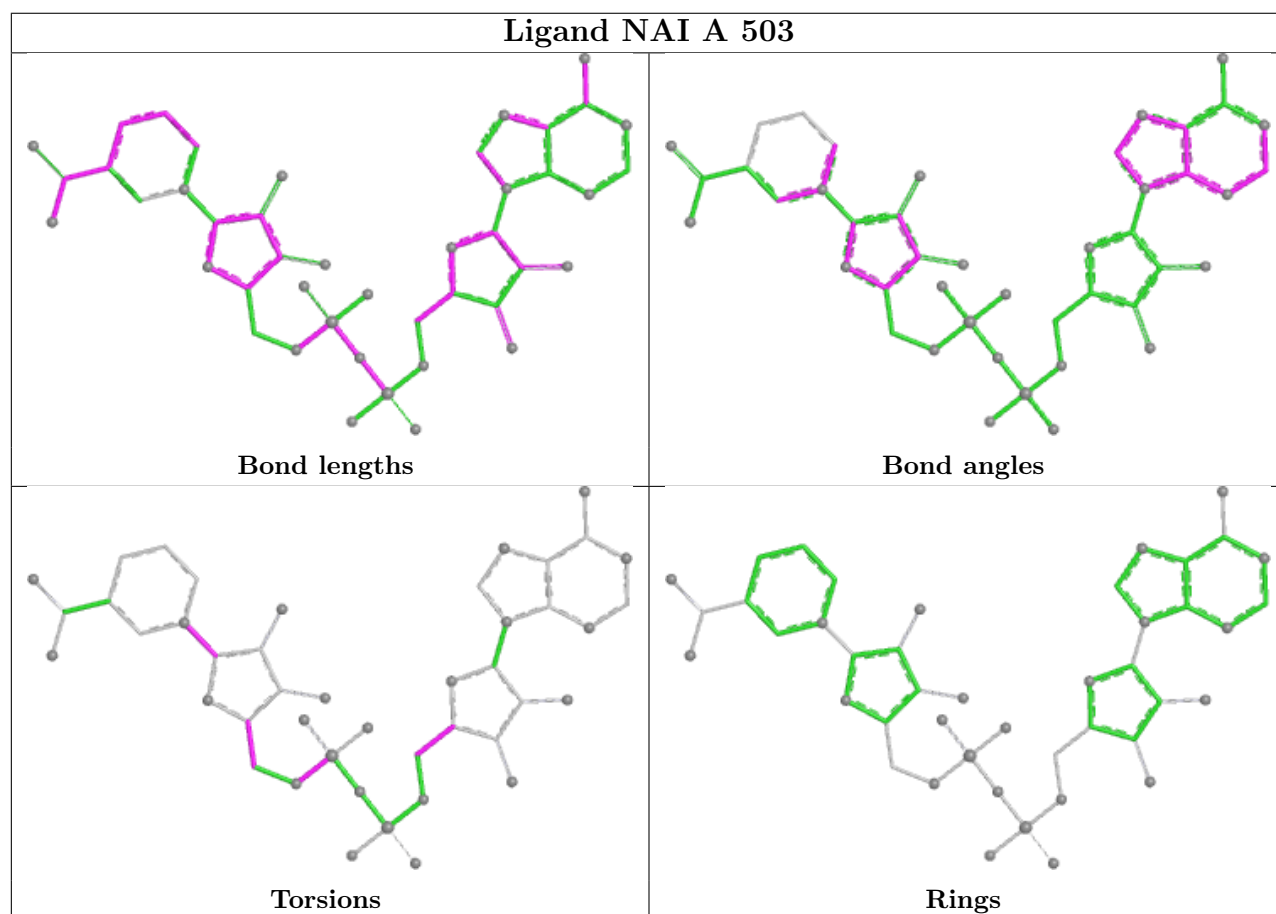
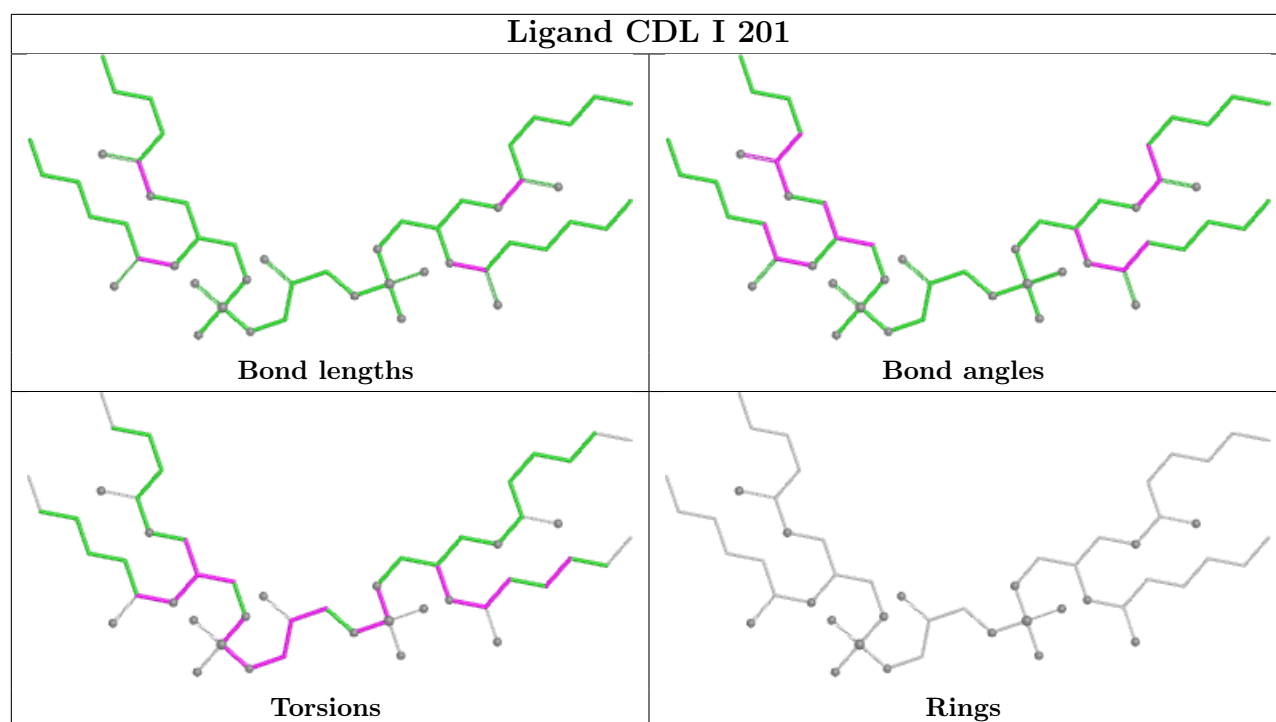


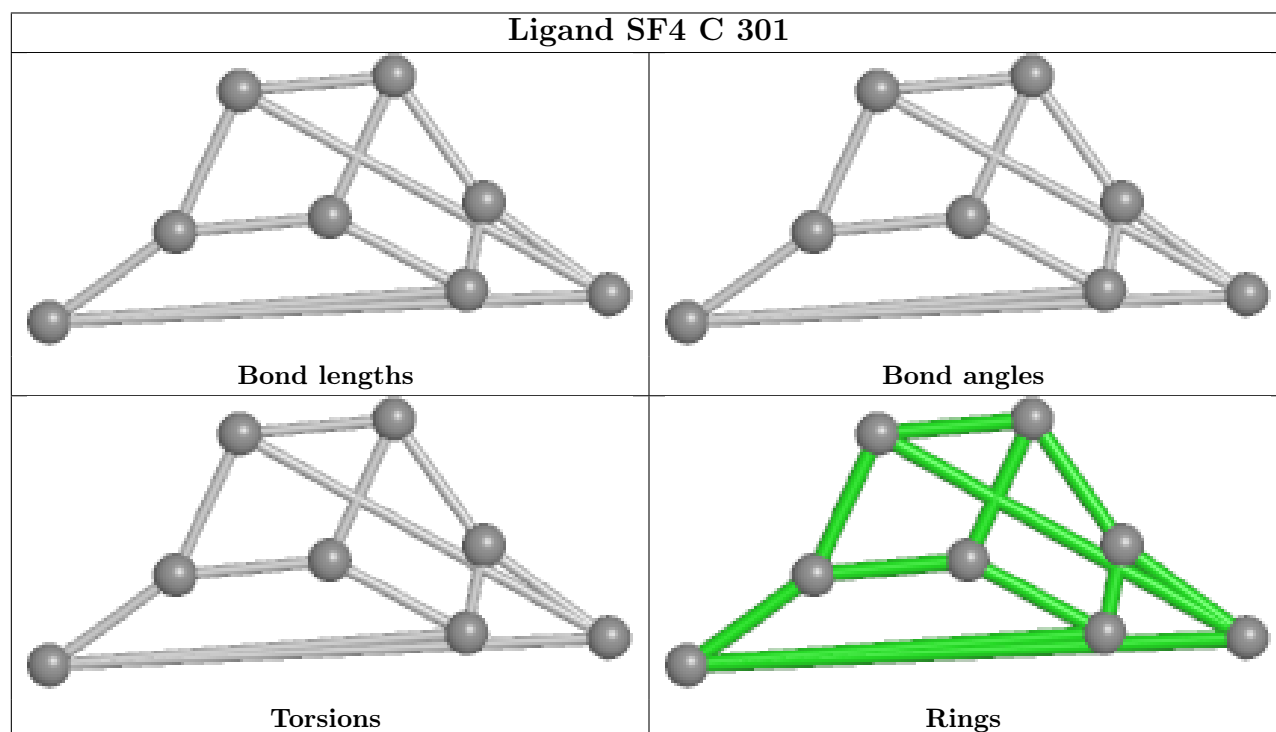
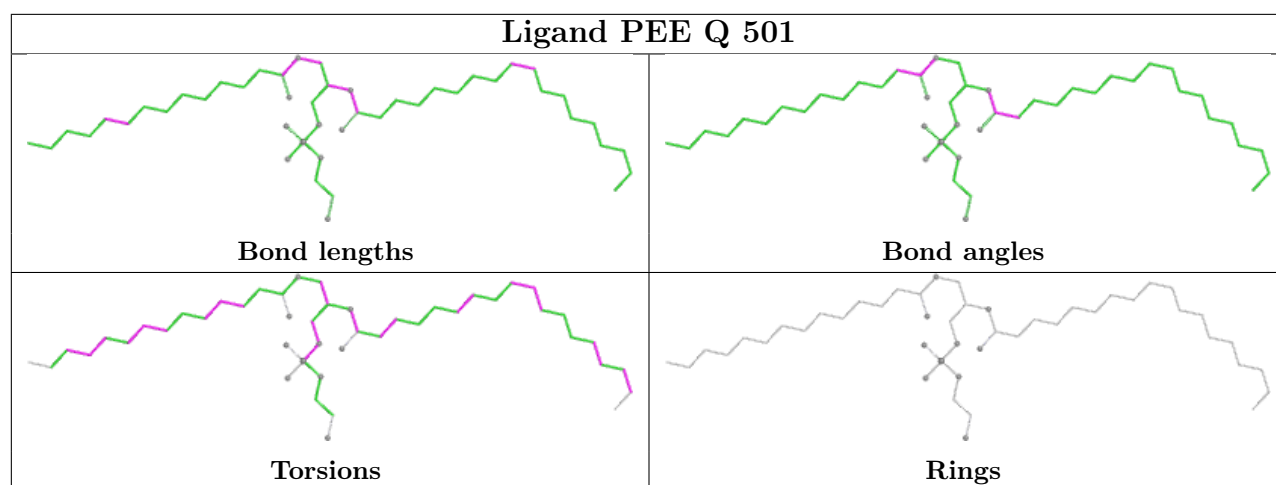


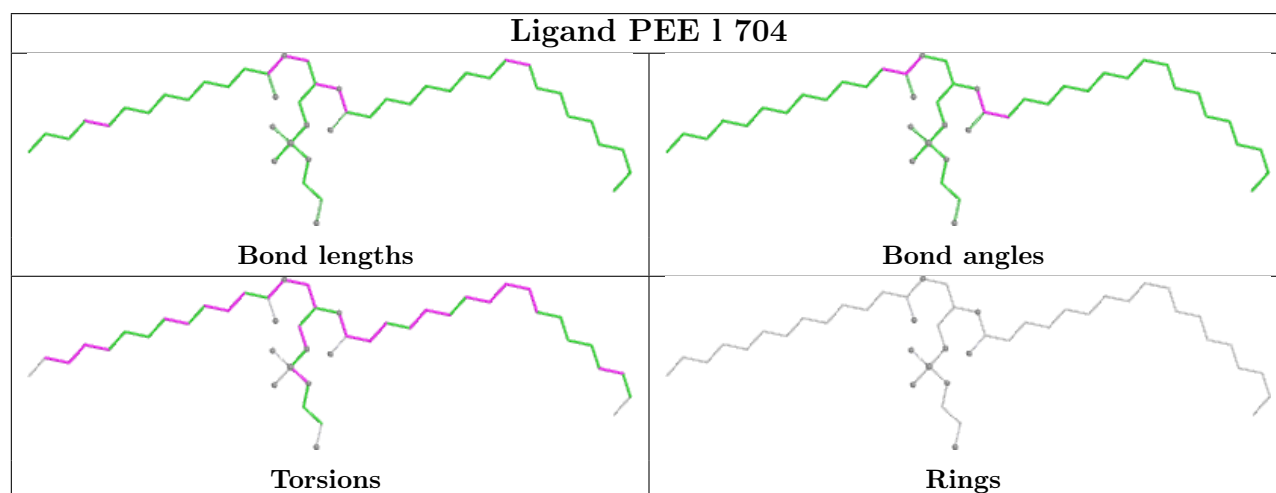
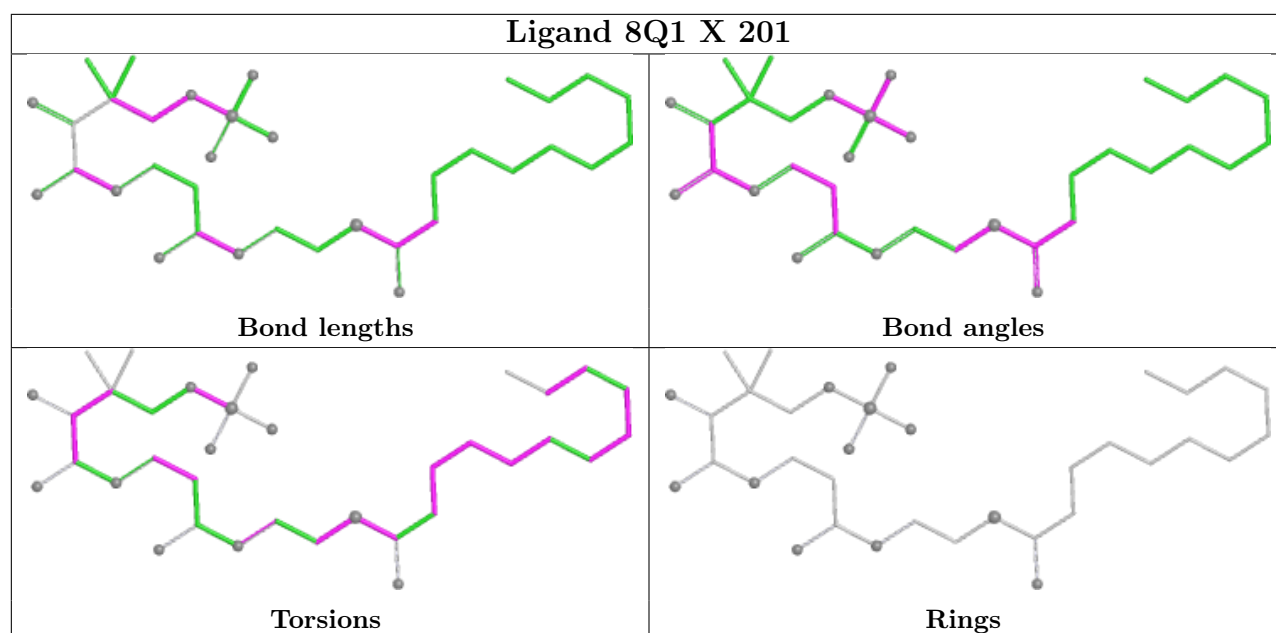


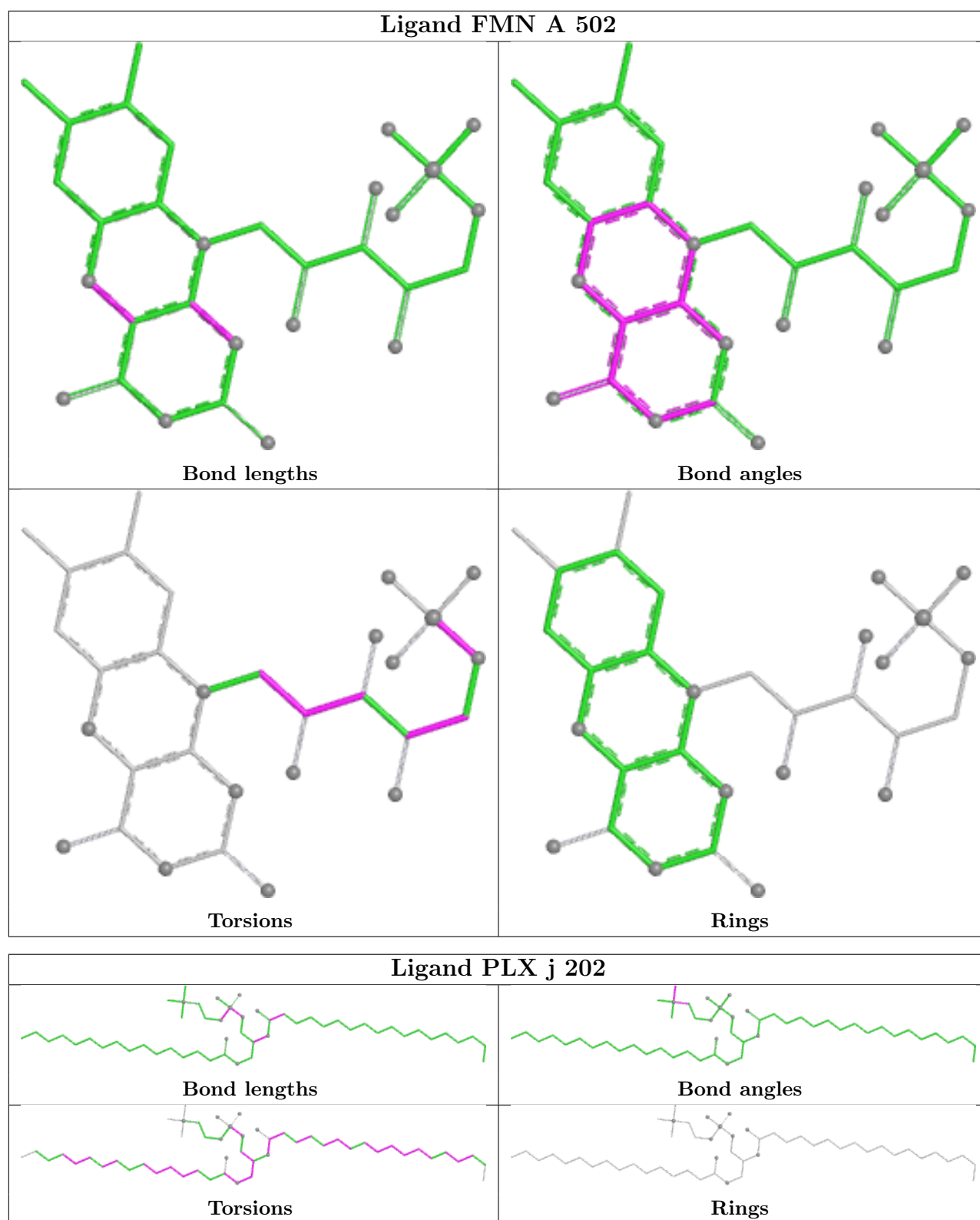


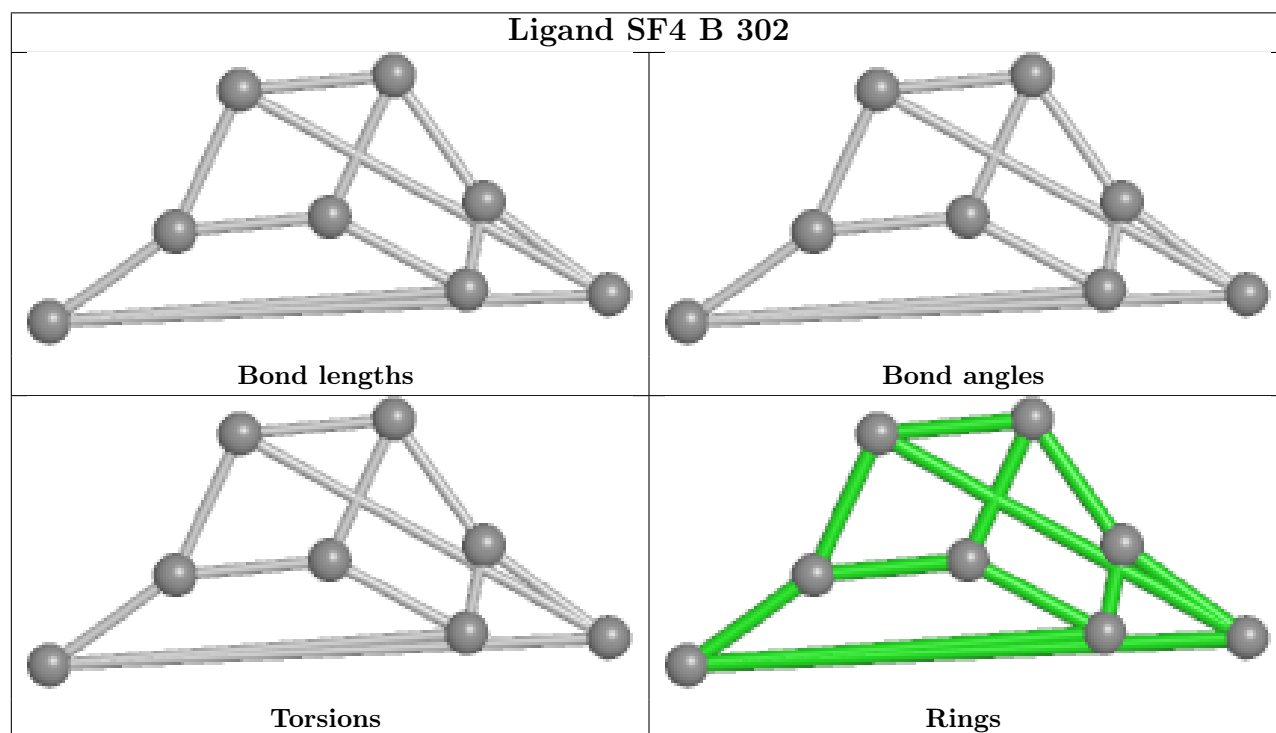
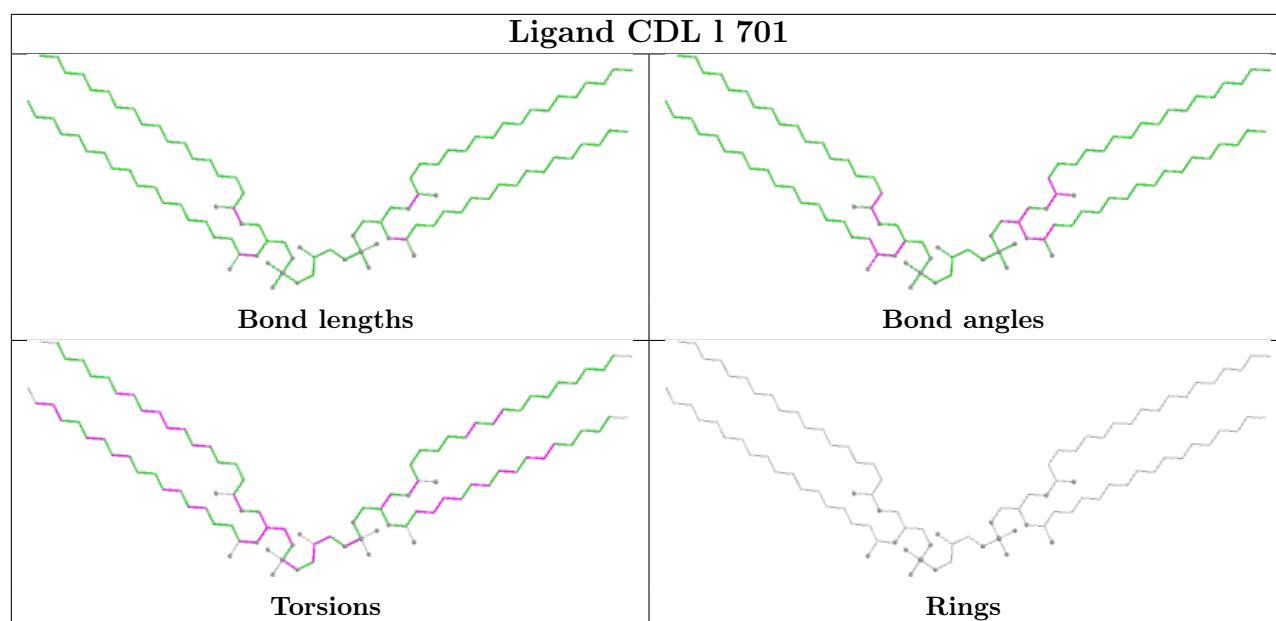


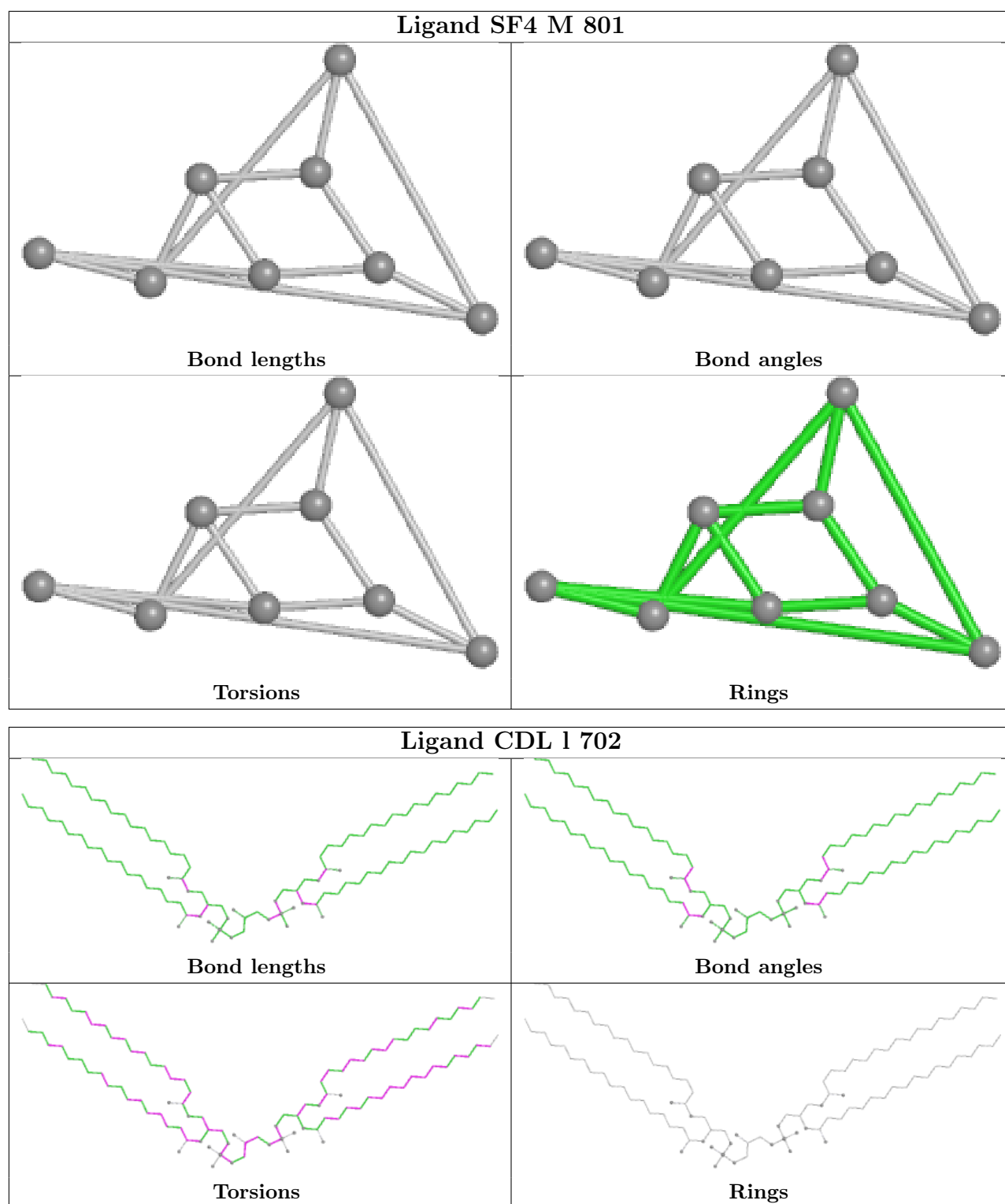












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

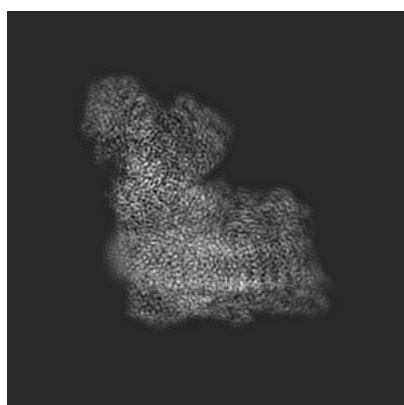
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31652. These allow visual inspection of the internal detail of the map and identification of artifacts.

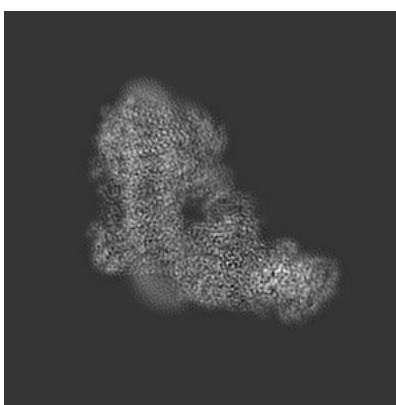
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

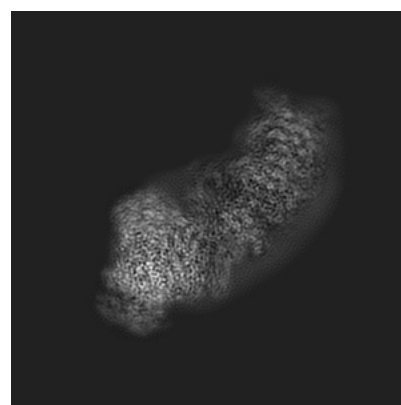
6.1.1 Primary map



X



Y

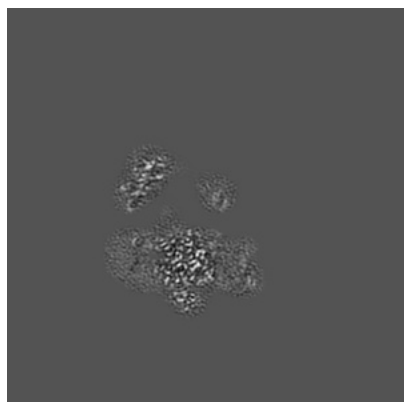


Z

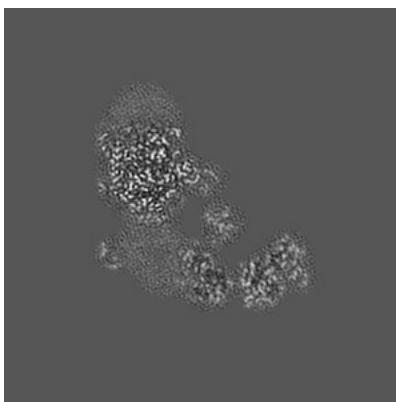
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

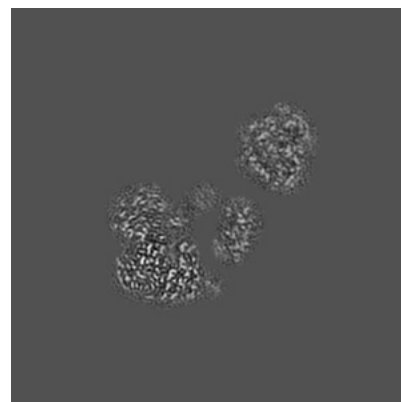
6.2.1 Primary map



X Index: 155



Y Index: 155



Z Index: 155

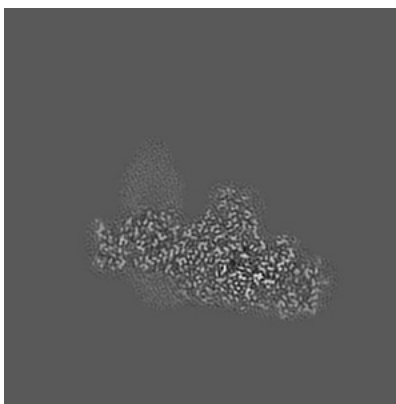
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

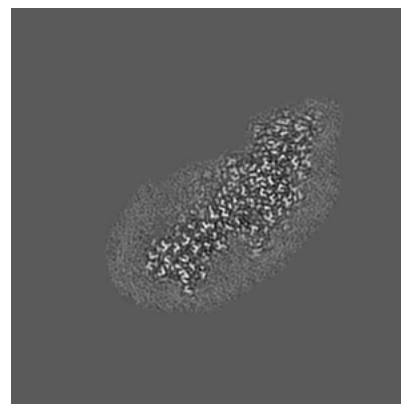
6.3.1 Primary map



X Index: 107



Y Index: 105

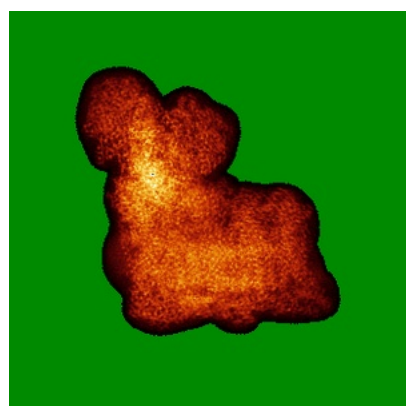


Z Index: 121

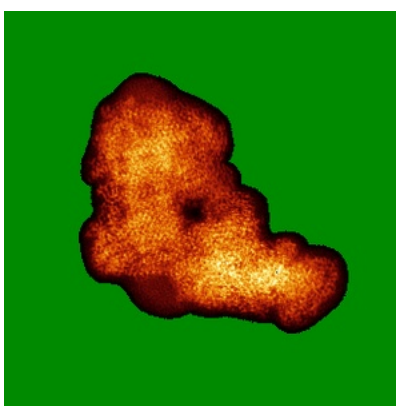
The images above show the largest variance slices of the map in three orthogonal directions.

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

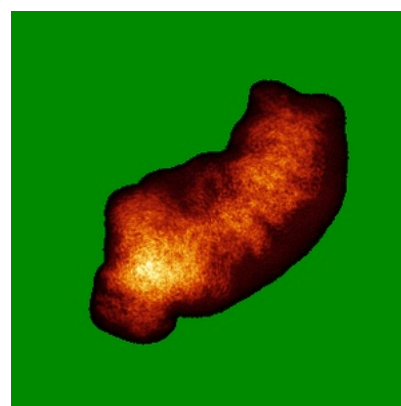
6.4.1 Primary map



X



Y

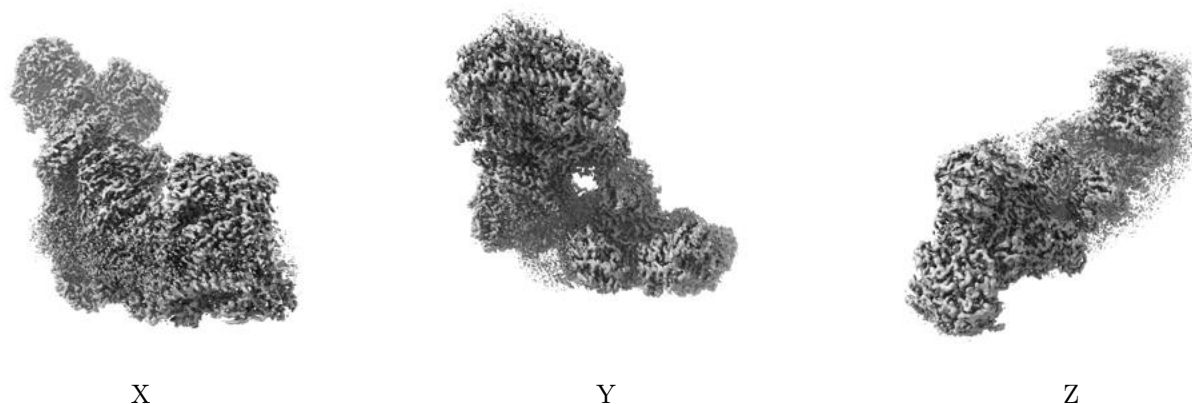


Z

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 0.0243. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

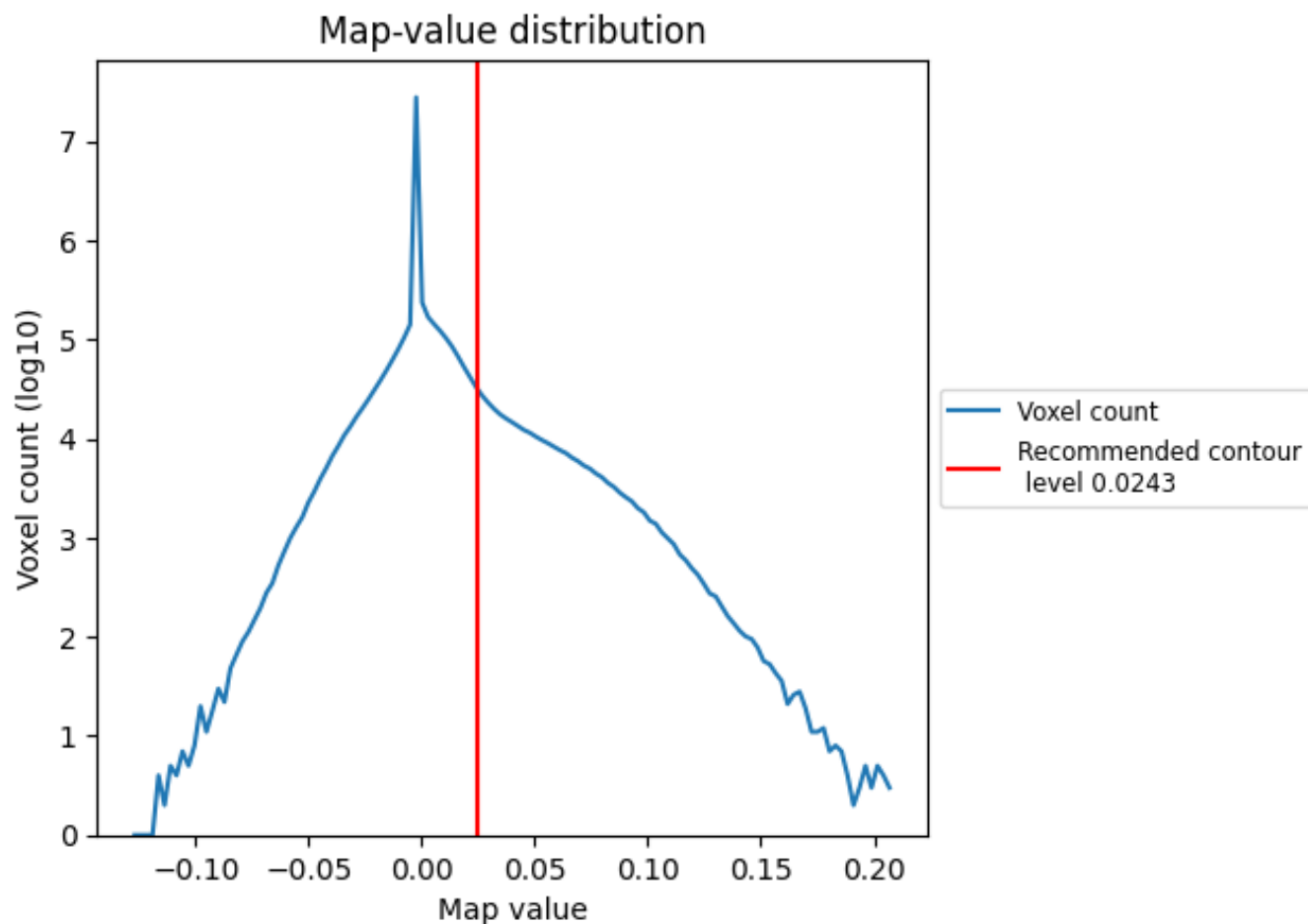
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

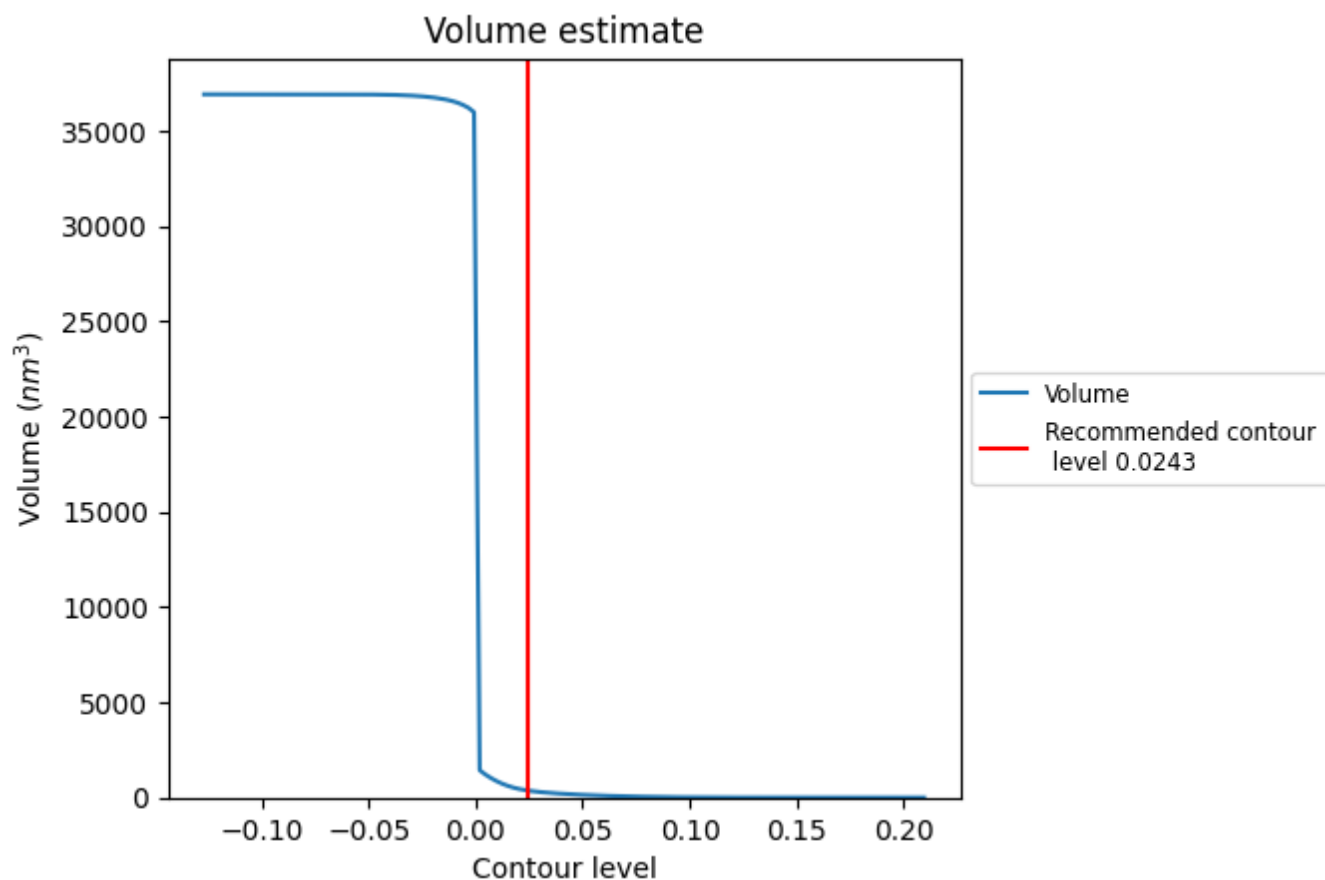
This section contains the results of statistical analysis of the map.

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.

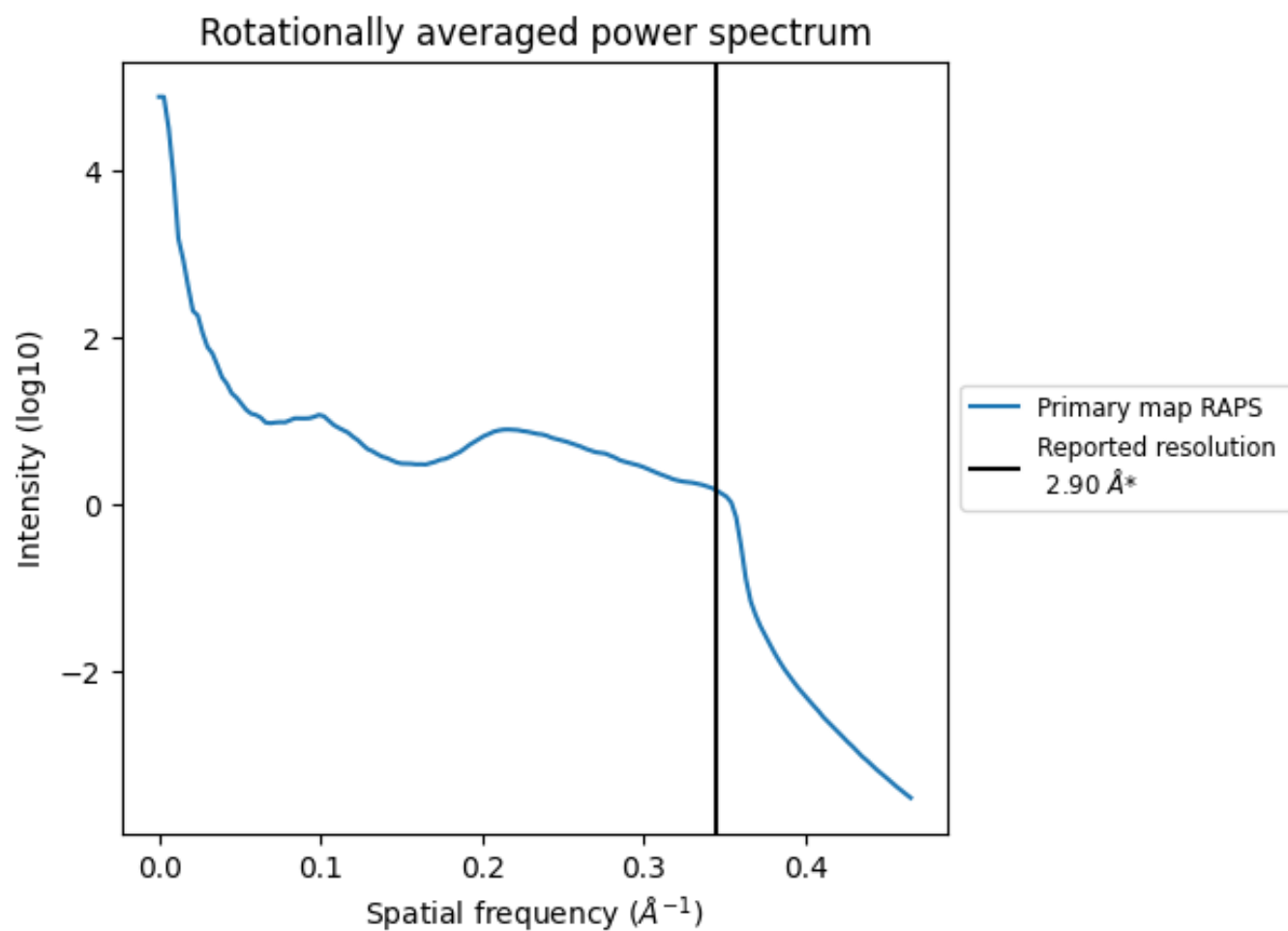
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 370 nm^3 ; this corresponds to an approximate mass of 335 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 0.345 Å⁻¹

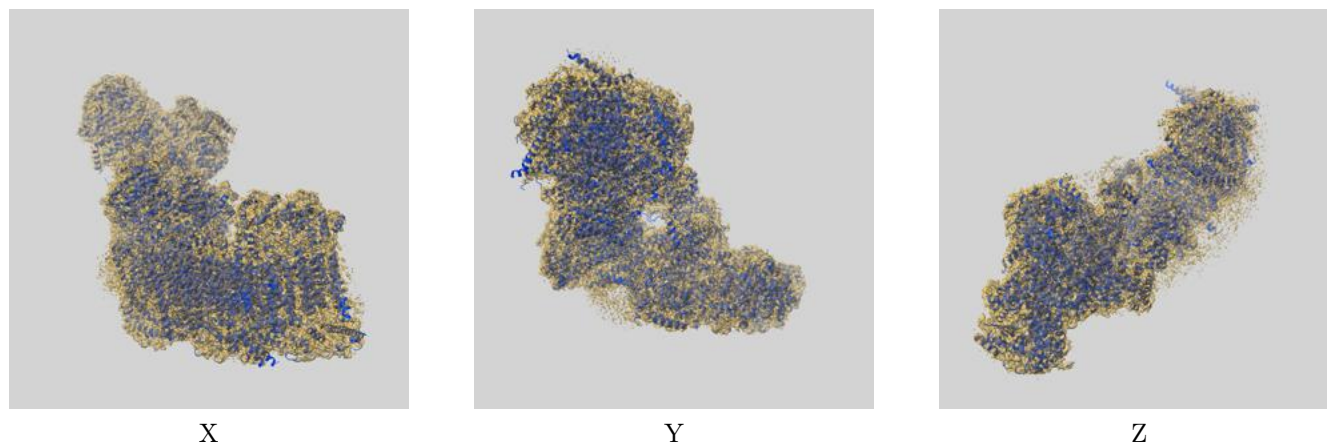
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

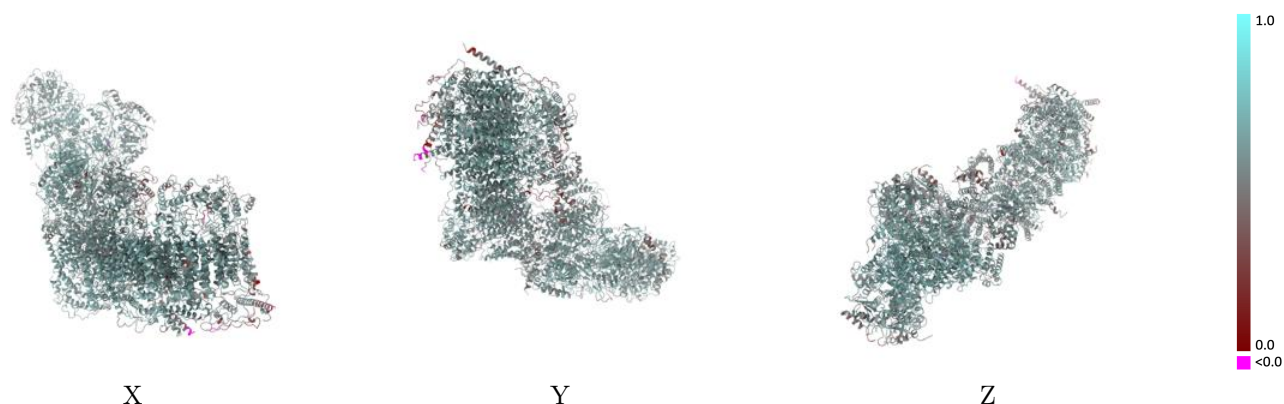
This section contains information regarding the fit between EMDB map EMD-31652 and PDB model 7V3M. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



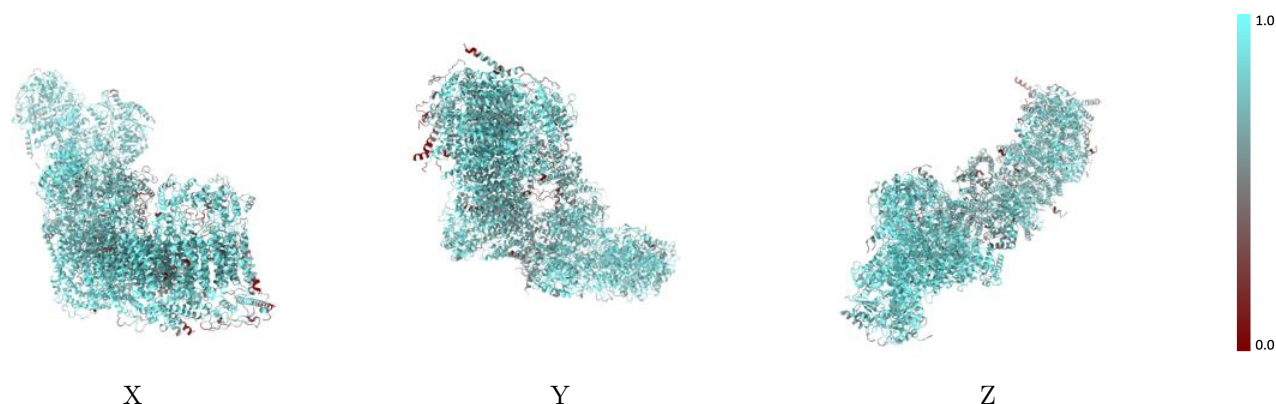
The images above show the 3D surface view of the map at the recommended contour level 0.0243 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



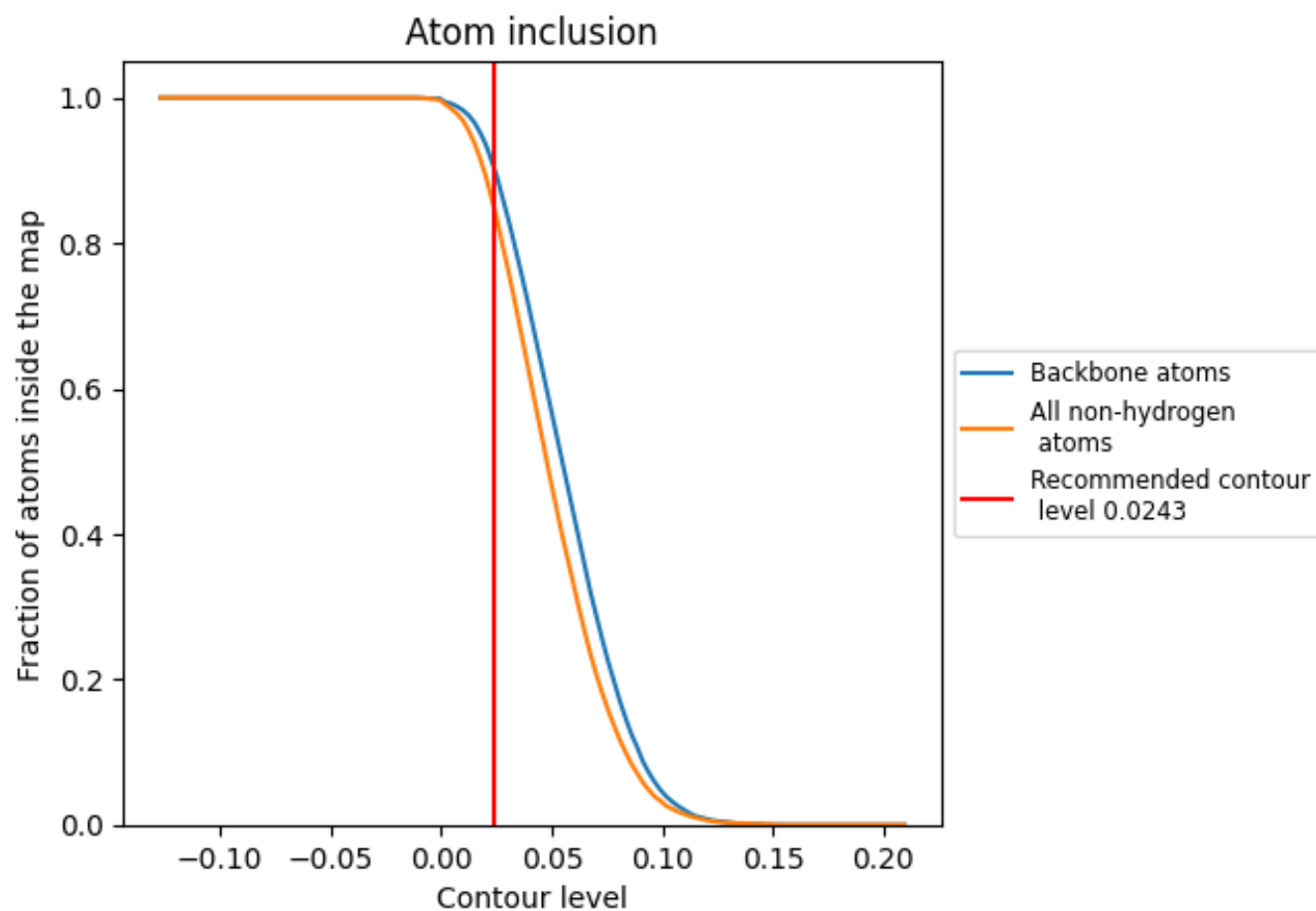
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0243).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 84% 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 (0.0243) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8440	 0.5850
A	 0.8610	 0.5810
B	 0.9650	 0.6460
C	 0.9000	 0.6260
E	 0.8220	 0.5680
F	 0.7340	 0.5050
G	 0.5550	 0.4150
H	 0.8450	 0.5660
I	 0.8190	 0.5940
J	 0.8210	 0.5660
K	 0.7990	 0.5470
L	 0.8910	 0.6180
M	 0.8940	 0.6040
N	 0.8670	 0.6080
O	 0.8180	 0.5520
P	 0.9390	 0.6330
Q	 0.9190	 0.6290
S	 0.9370	 0.6250
T	 0.8680	 0.6060
U	 0.8540	 0.5850
V	 0.6450	 0.5180
W	 0.8720	 0.5970
X	 0.7480	 0.5260
Y	 0.7080	 0.5110
Z	 0.6110	 0.4640
a	 0.8560	 0.6060
b	 0.7020	 0.5040
c	 0.7650	 0.5460
d	 0.7940	 0.5580
e	 0.7310	 0.5330
f	 0.7510	 0.5530
g	 0.8850	 0.6110
h	 0.8910	 0.6050
i	 0.9270	 0.6320
j	 0.7490	 0.5680



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Chain	Atom inclusion	Q-score
k	 0.8520	 0.5960
l	 0.8490	 0.5990
m	 0.8070	 0.5700
n	 0.7200	 0.5490
o	 0.7840	 0.5660
p	 0.8080	 0.5530
r	 0.9120	 0.6240
s	 0.9130	 0.6190
u	 0.8780	 0.6110
v	 0.6610	 0.4690
w	 0.7830	 0.5470