



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 01:15 PM JST

PDB ID : 7W4L / pdb_00007w4l
EMDB ID : EMD-32307
Title : Deactive state CI from Q1-NADH dataset, Subclass 3
Authors : Gu, J.; Yang, M.
Deposited on : 2021-11-28
Resolution : 3.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

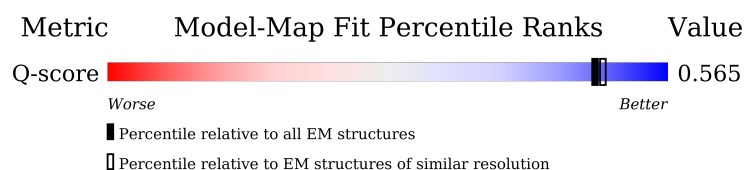
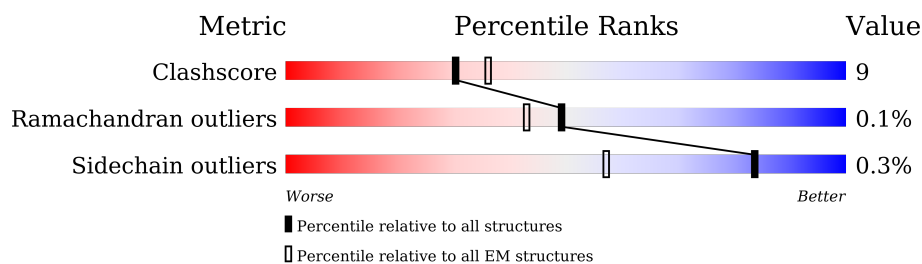
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	176	
3	C	156	
4	E	115	

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

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

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 66469 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
			3300	2085	590	605	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.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			686	441	102	138	5		
6	X	88	Total	C	N	O	S	0	0
			696	449	103	139	5		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	297	Total	C	N	O	S	0	0
			2352	1510	420	414	8		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	690	Total	C	N	O	S	0	0
			5295	3320	923	1013	39		

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	83	Total	C	N	O	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
			1014	648	171	189	6		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	70	Total	C	N	O	S	0	0
			587	386	98	102	1		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	103	Total	C	N	O	S	0	0
			867	567	152	147	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
			1307	849	213	237	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
			1457	914	265	270	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
			996	647	172	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
			2707	1780	420	462	45		

- 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
			799	545	118	131	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
			4781	3172	740	818	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
			473	308	85	79	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	128	Total	C	N	O	S	0	0
			1058	689	182	187			

- 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
			1528	979	279	262	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
			1386	881	250	245	10		

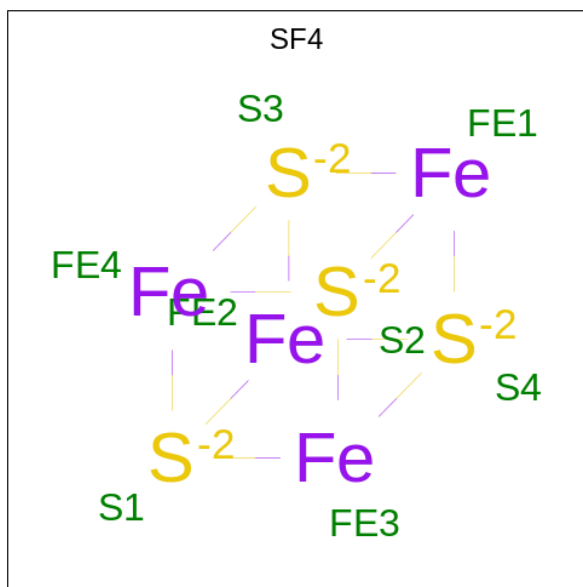
- Molecule 43 is a protein called Complex I-B18.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			1016	636	189	182	9		

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

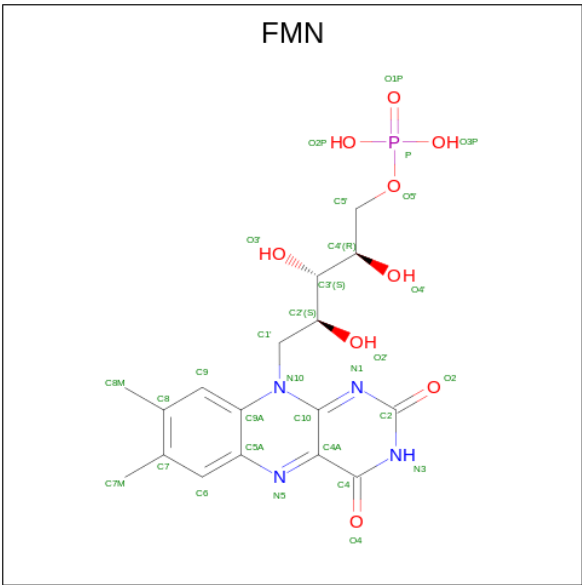
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2582	1643	438	491	10		

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



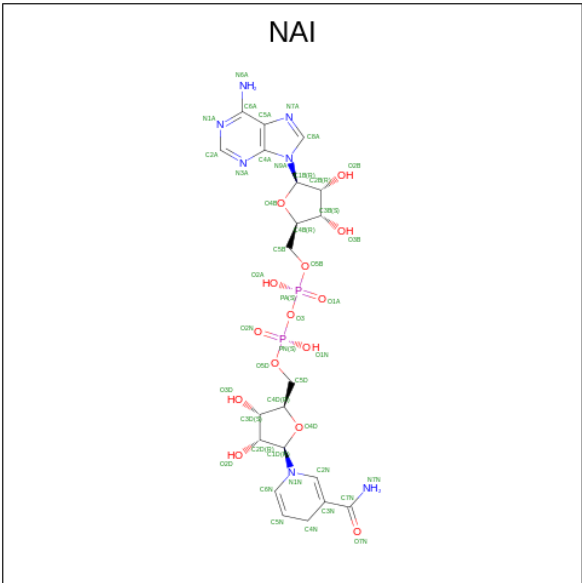
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

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



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

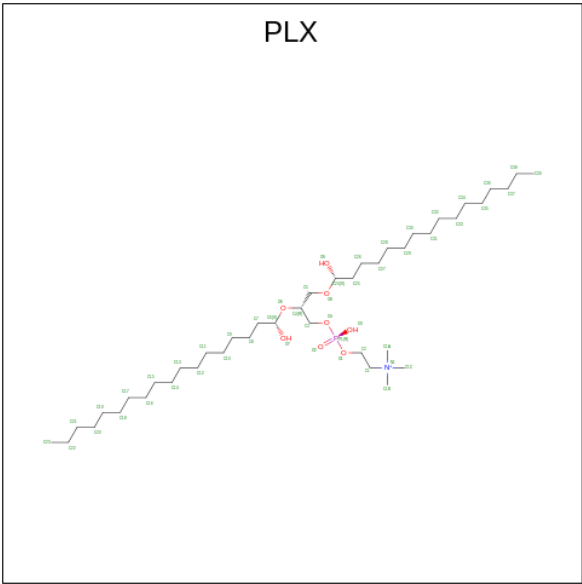
- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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

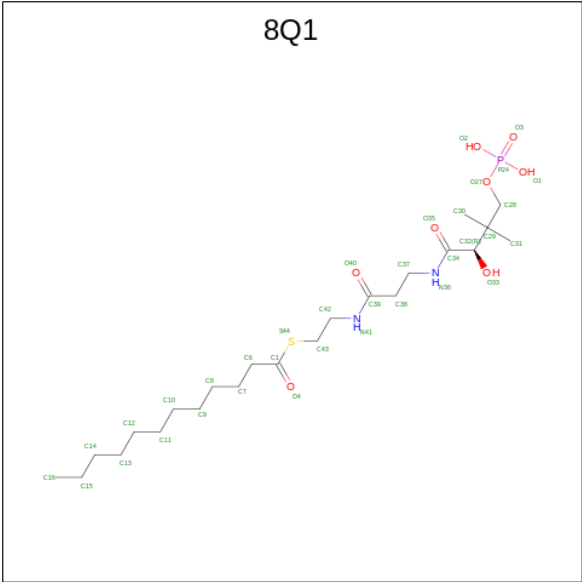
- Molecule 48 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-

6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



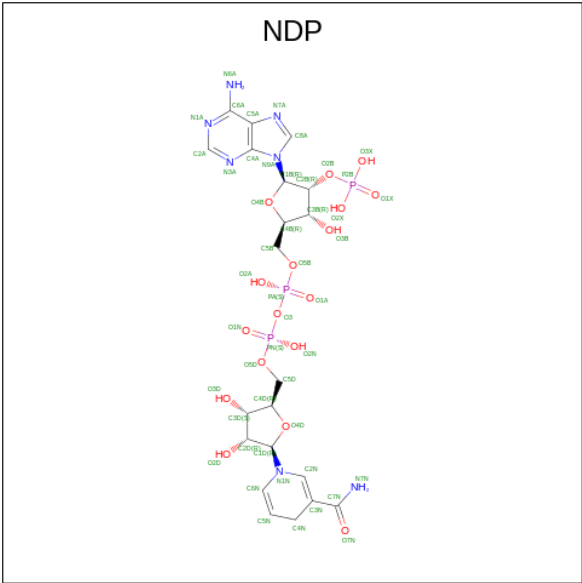
Mol	Chain	Residues	Atoms					AltConf
48	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 49 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS).



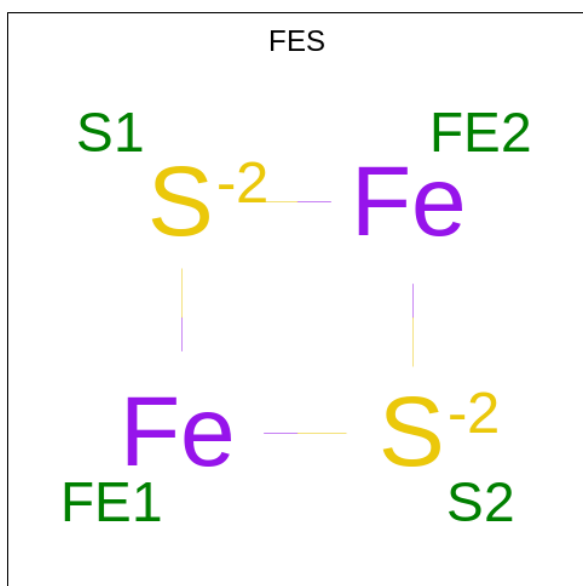
Mol	Chain	Residues	Atoms						AltConf
49	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
49	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 50 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



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

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

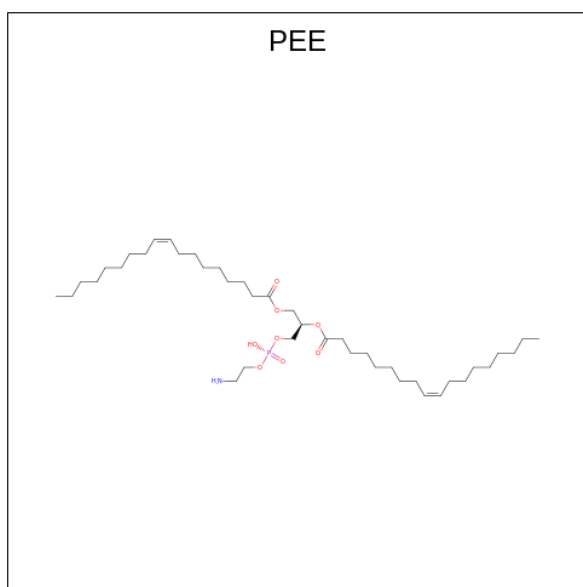


Mol	Chain	Residues	Atoms			AltConf
51	M	1	Total	Fe	S	0
			4	2	2	
51	O	1	Total	Fe	S	0
			4	2	2	

- Molecule 52 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 53 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $\text{C}_{41}\text{H}_{78}\text{NO}_8\text{P}$) (labeled as "Ligand of Interest" by depositor).

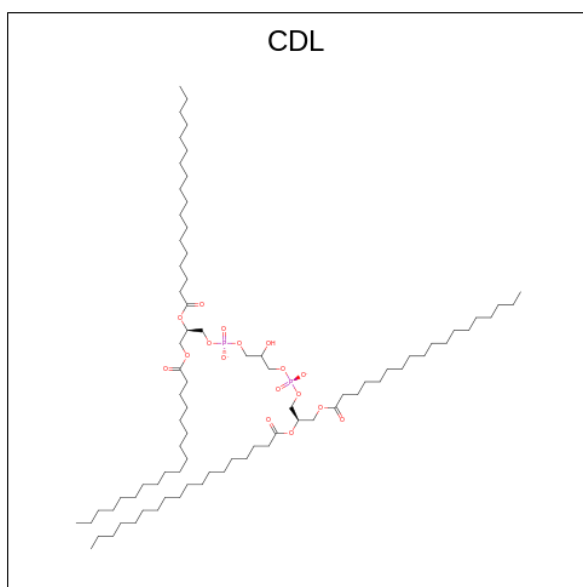


Mol	Chain	Residues	Atoms					AltConf
53	Q	1	Total	C	N	O	P	0
			47	37	1	8	1	
53	Q	1	Total	C	N	O	P	0
			51	41	1	8	1	
53	j	1	Total	C	N	O	P	0
			47	37	1	8	1	
53	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
53	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
53	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
53	m	1	Total	C	N	O	P	0
			41	31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

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

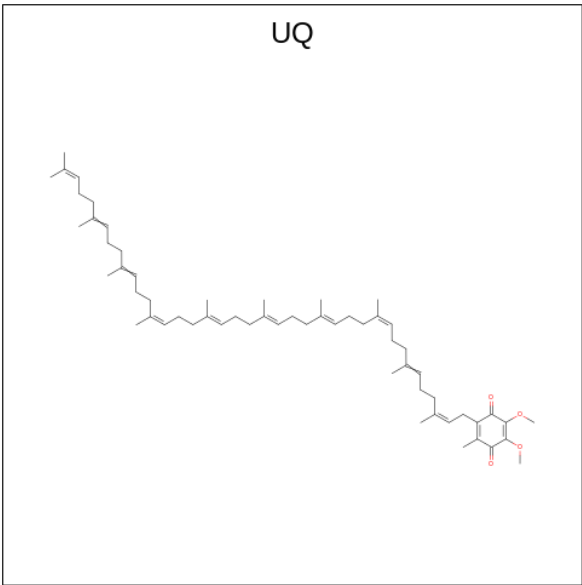
Mol	Chain	Residues	Atoms		AltConf
54	T	1	Total	Zn	0
			1	1	

- Molecule 55 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



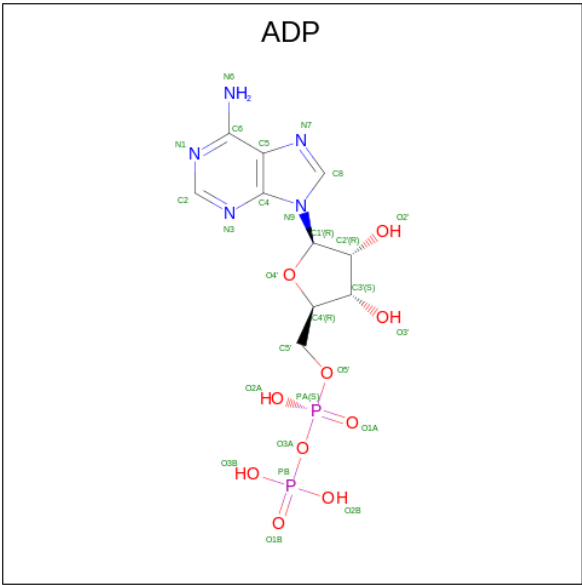
Mol	Chain	Residues	Atoms				AltConf
55	V	1	Total	C	O	P	0
			71	52	17	2	
55	a	1	Total	C	O	P	0
			91	72	17	2	
55	g	1	Total	C	O	P	0
			100	81	17	2	
55	i	1	Total	C	O	P	0
			66	47	17	2	
55	l	1	Total	C	O	P	0
			100	81	17	2	

- 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: $C_{10}H_{15}N_5O_{10}P_2$).



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

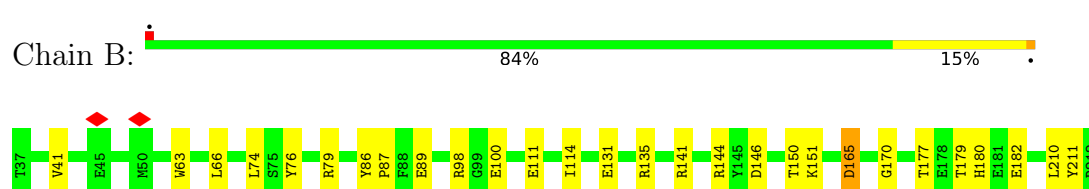
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

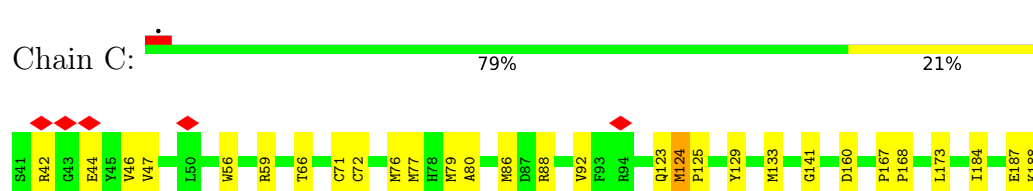
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



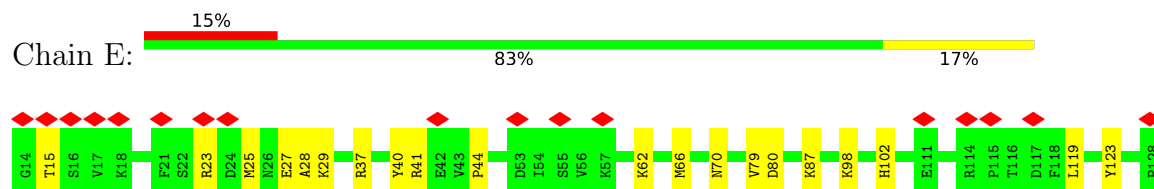
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



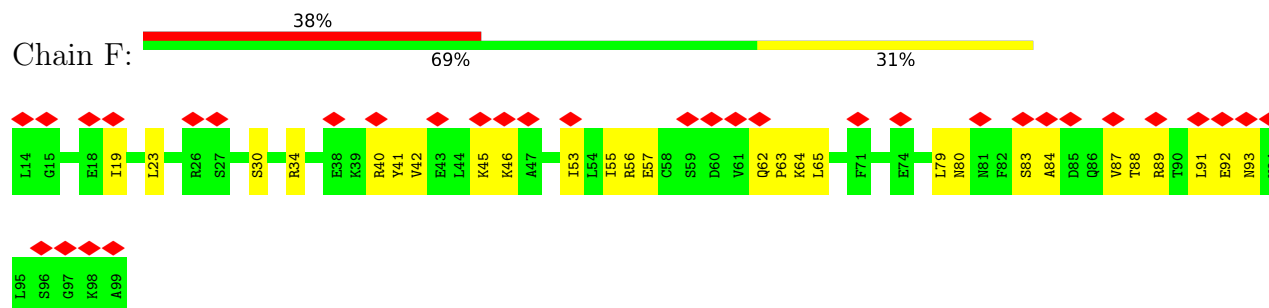
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



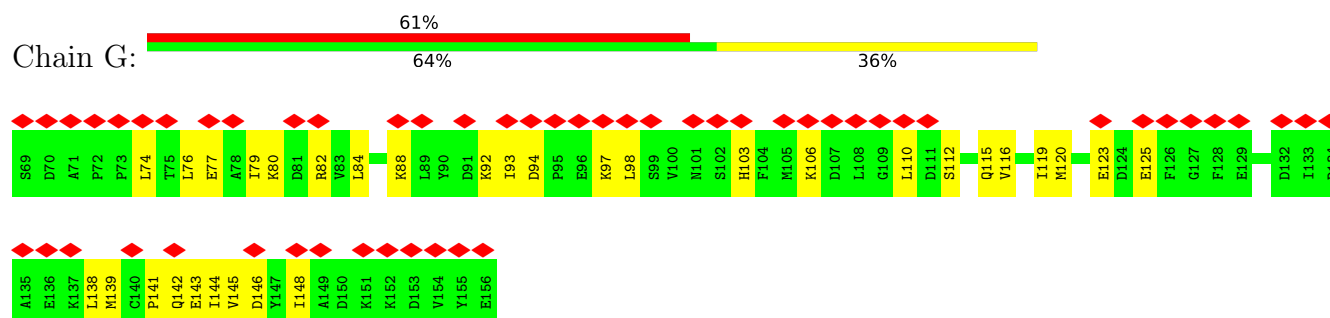
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



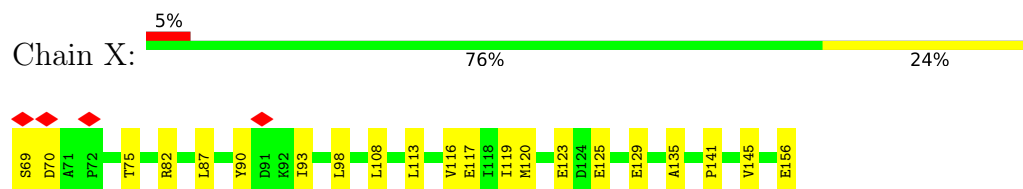
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



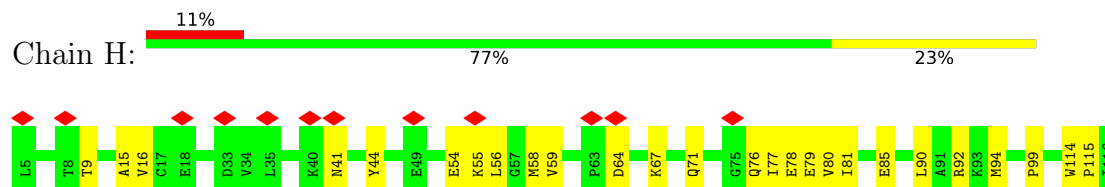
- Molecule 6: Acyl carrier protein



- Molecule 6: Acyl carrier protein



- Molecule 7: Complex I subunit B13

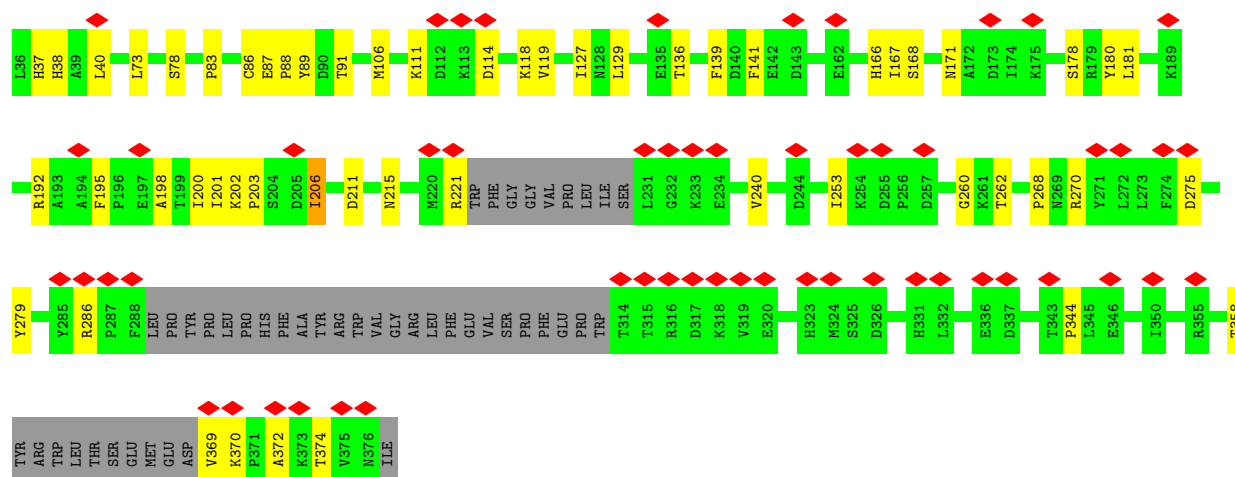
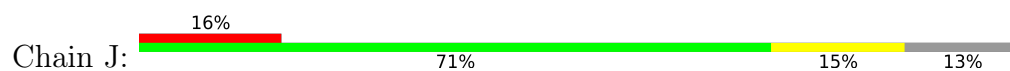


- Molecule 8: Complex I-B14.5a

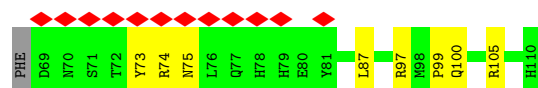
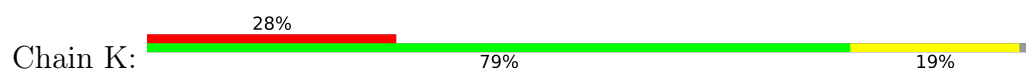




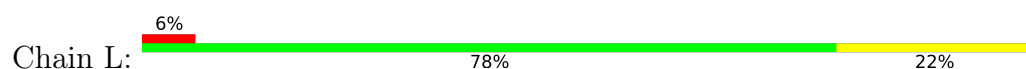
- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial



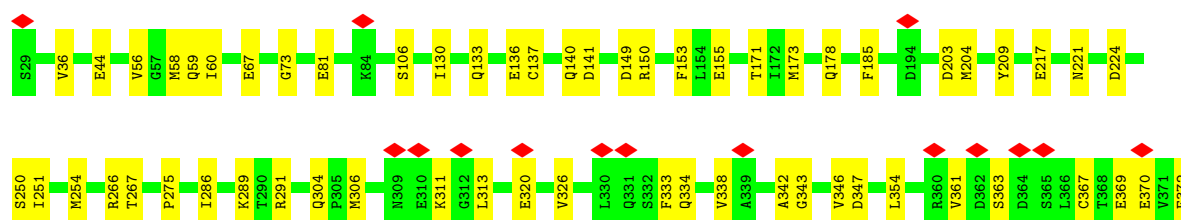
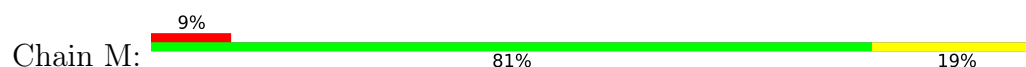
- Molecule 10: Complex I-9kD

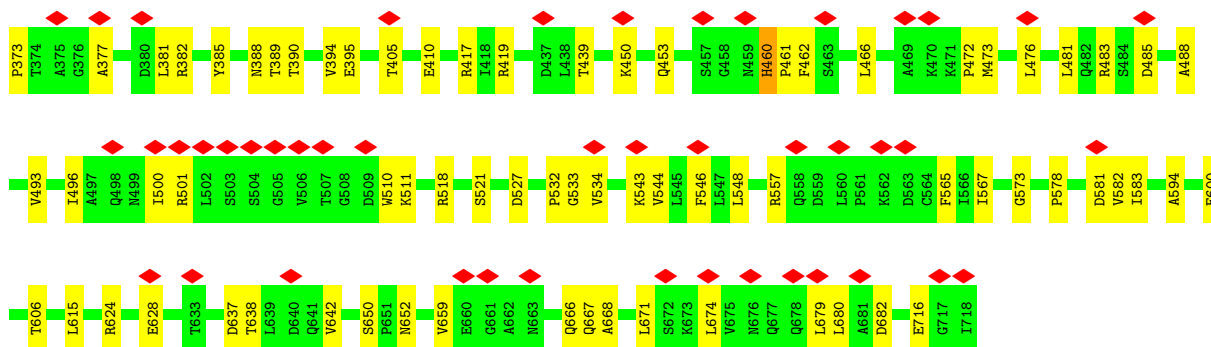


- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

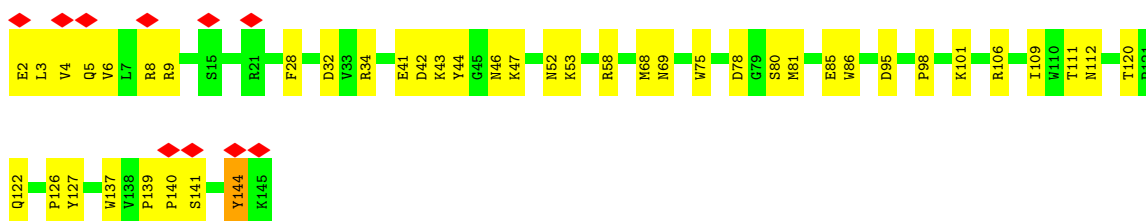


- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

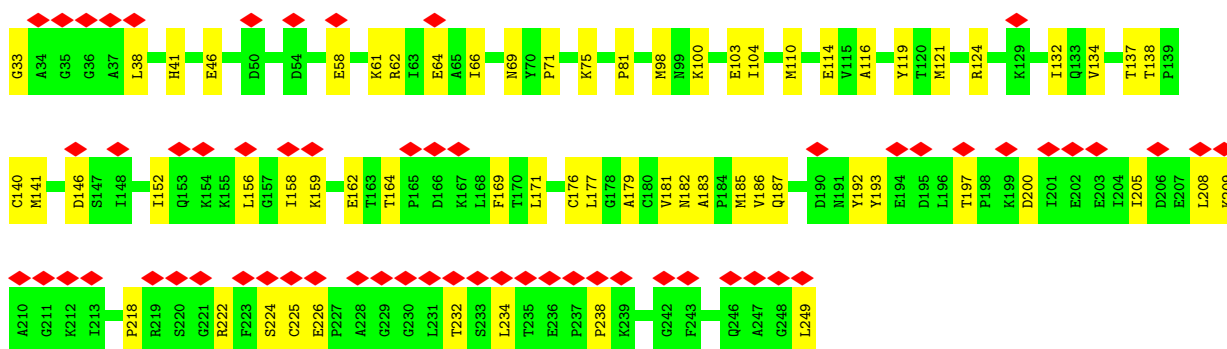
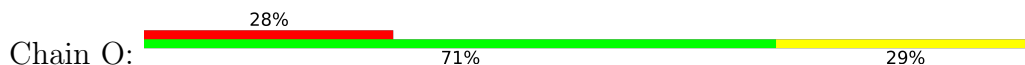




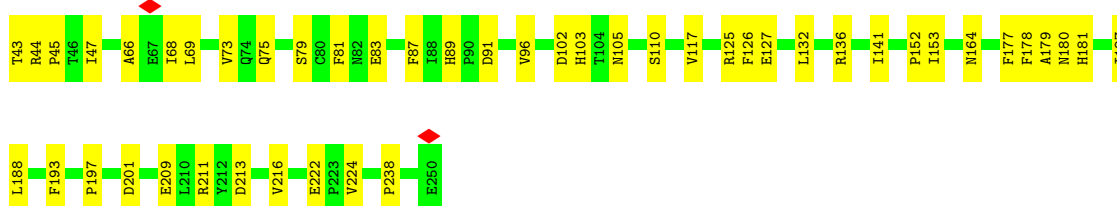
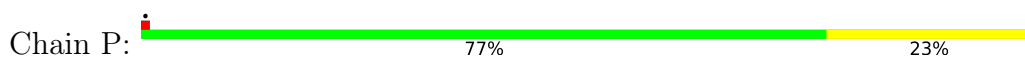
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



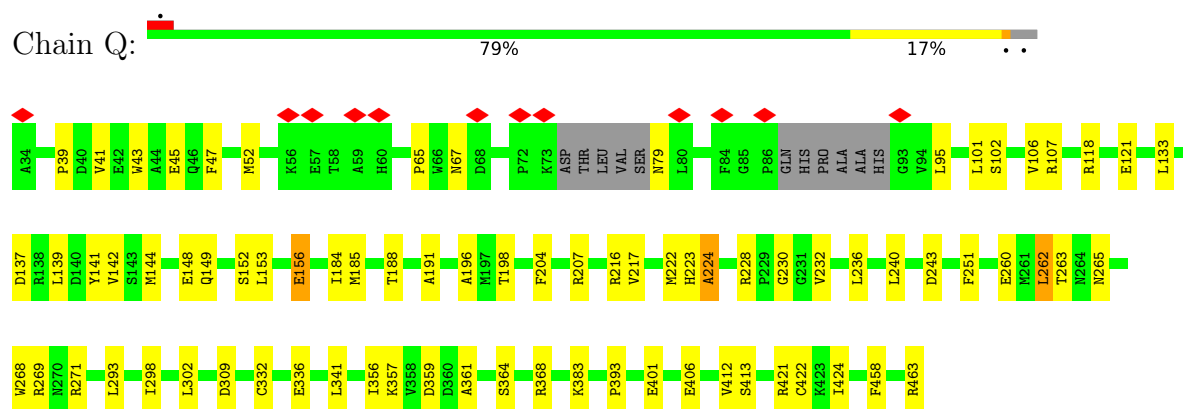
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



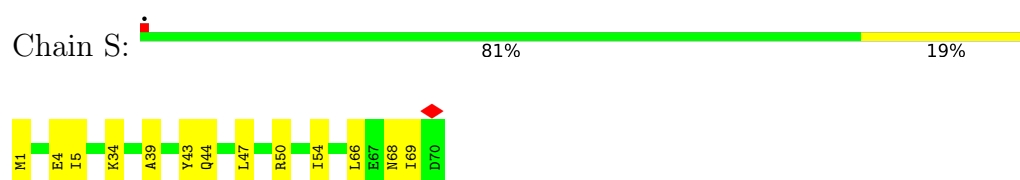
- Molecule 15: Complex I-30kD



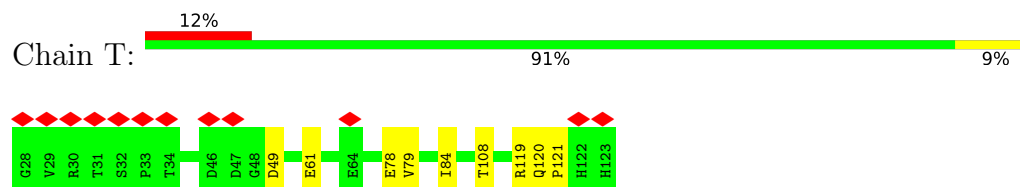
- Molecule 16: Complex I-49kD



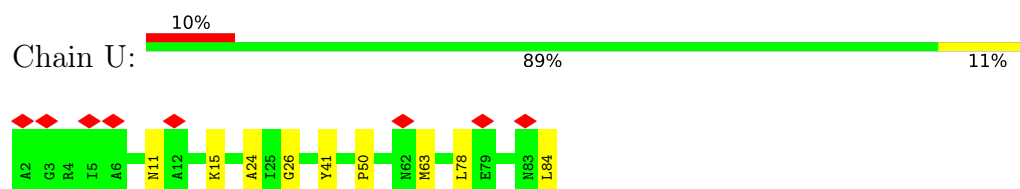
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



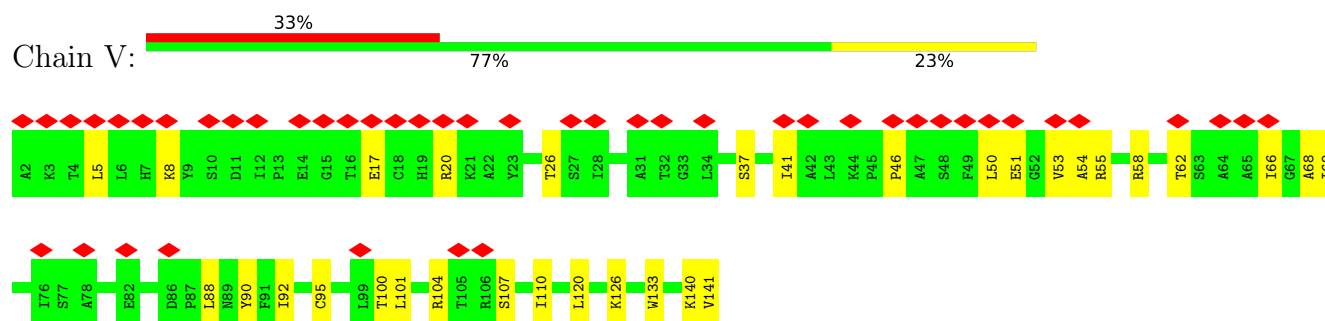
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



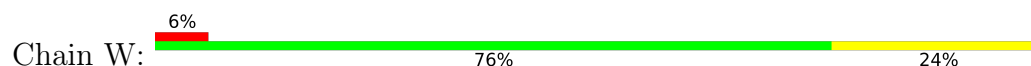
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

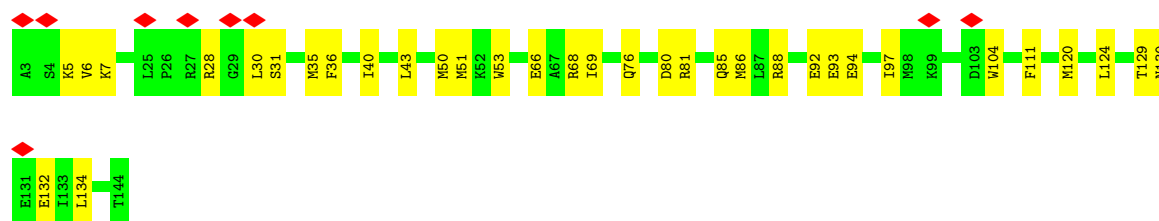


- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

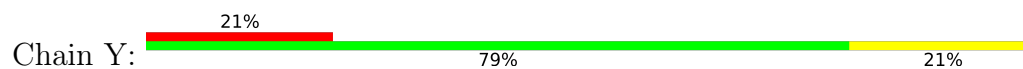


- Molecule 21: Complex I-B16.6

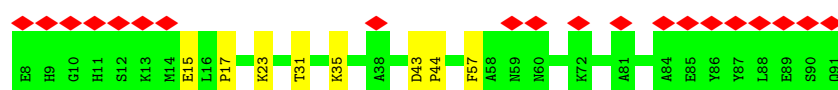
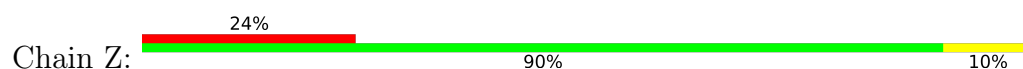




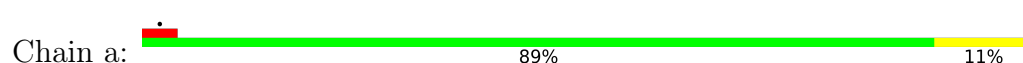
• Molecule 22: Complex I-AGGG



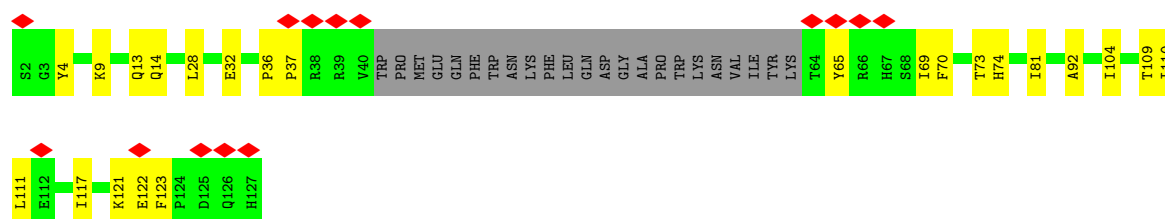
• Molecule 23: Complex I-B12



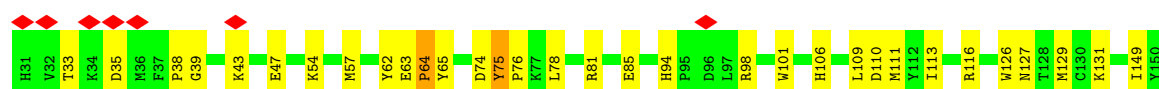
• Molecule 24: Complex I-SGDH

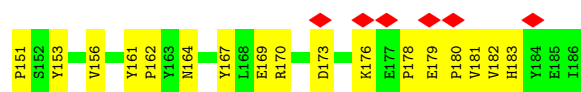


• Molecule 25: Complex I-B17

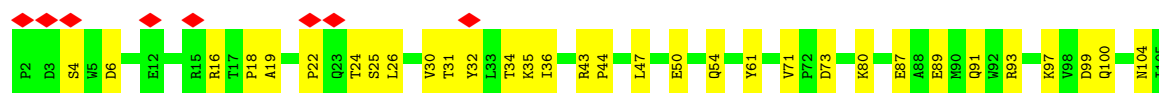


• Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

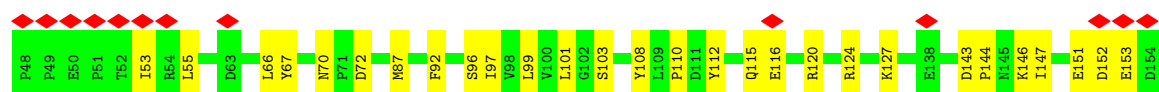




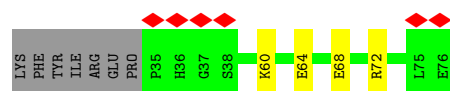
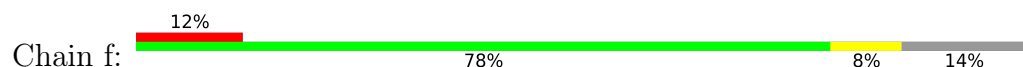
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



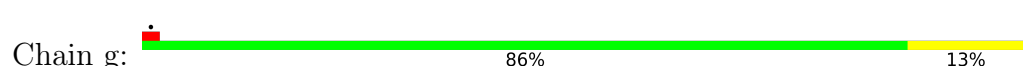
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



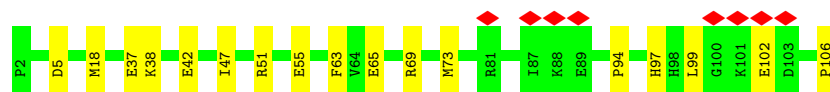
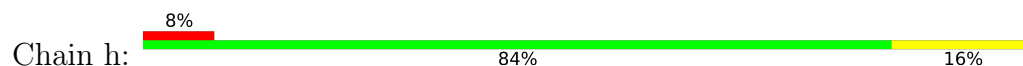
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



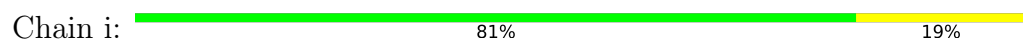
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

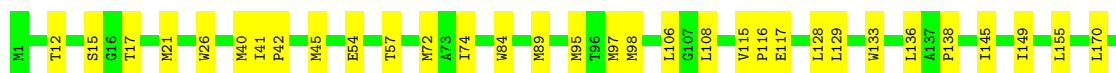


- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

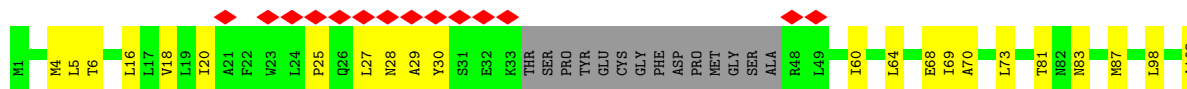


- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

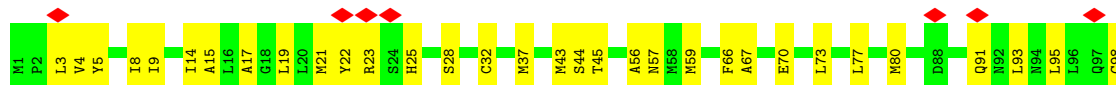




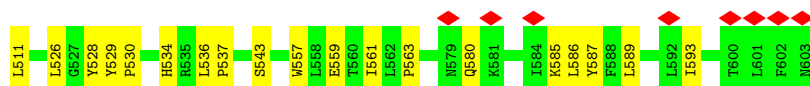
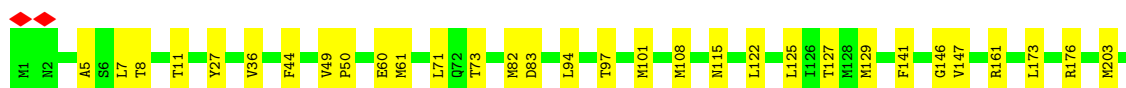
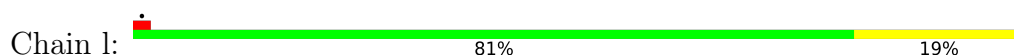
• Molecule 33: NADH-ubiquinone oxidoreductase chain 3



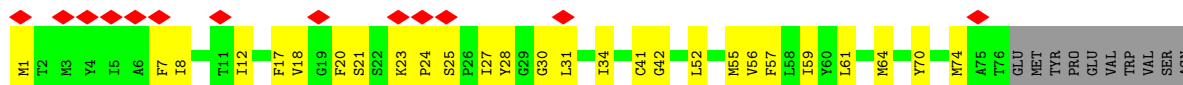
• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

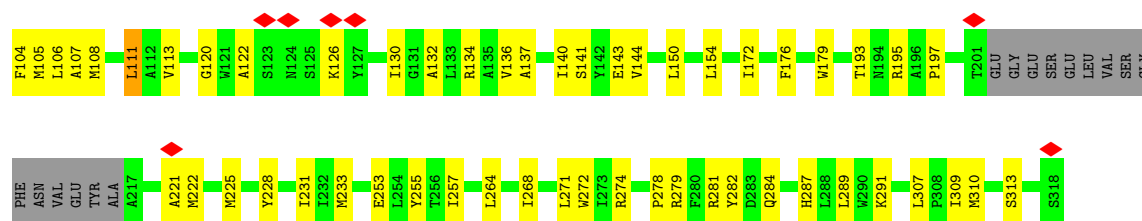


• Molecule 35: NADH-ubiquinone oxidoreductase chain 5

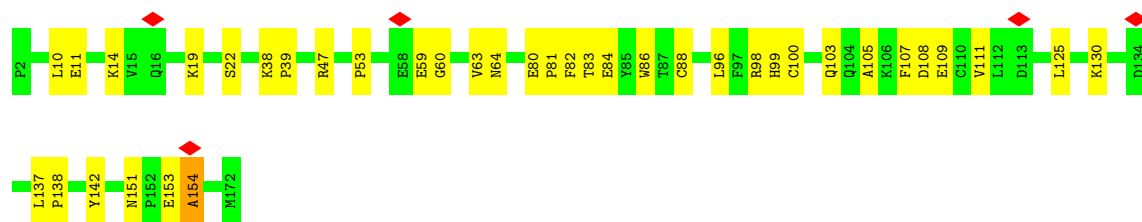
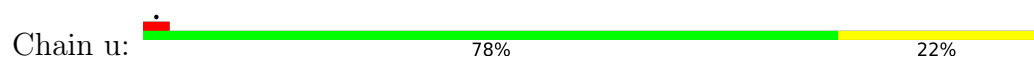


• Molecule 36: NADH-ubiquinone oxidoreductase chain 6

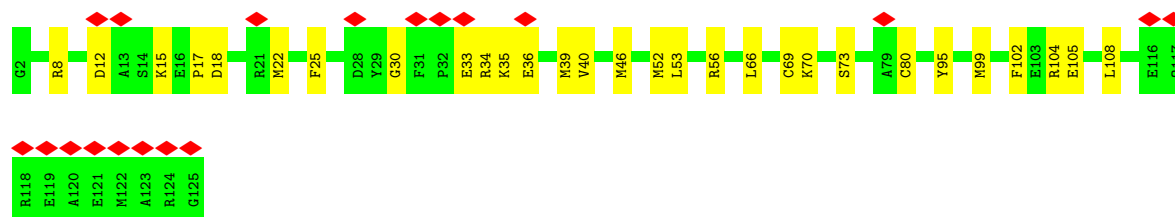
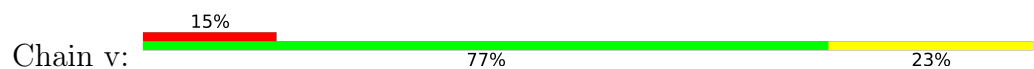




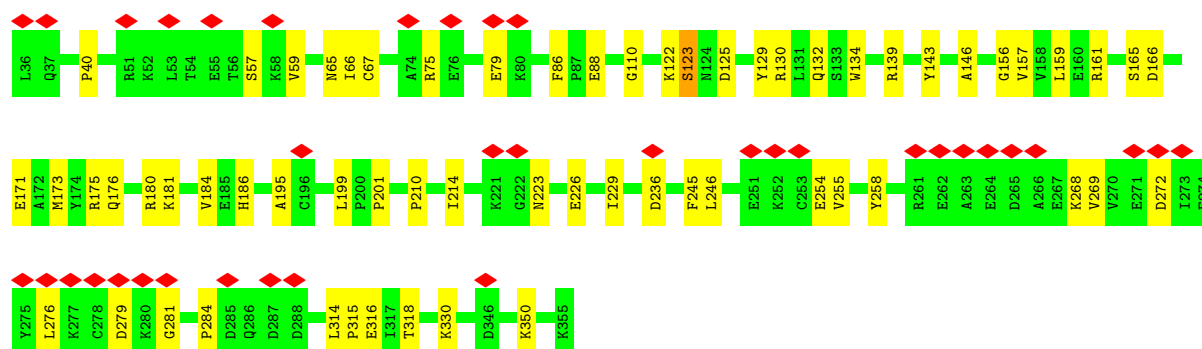
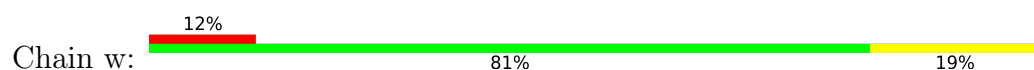
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 43: Complex I-B18



- 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	42665	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	0.219	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0296	Depositor
Map size ($\text{\AA}$)	333.7616, 333.7616, 333.7616	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.16	0/3374	0.41	0/4559
2	B	0.14	0/1443	0.33	0/1952
3	C	0.16	0/1279	0.45	2/1730 (0.1%)
4	E	0.15	0/995	0.34	0/1340
5	F	0.14	0/702	0.38	0/945
6	G	0.17	0/697	0.42	0/945
6	X	0.12	0/708	0.35	0/959
7	H	0.14	0/929	0.32	0/1258
8	I	0.17	0/798	0.37	0/1079
9	J	0.13	0/2404	0.37	0/3246
10	K	0.10	0/365	0.28	0/493
11	L	0.12	0/1039	0.32	0/1403
12	M	0.13	0/5383	0.37	4/7294 (0.1%)
13	N	0.14	0/1245	0.42	0/1694
14	O	0.15	0/1711	0.38	0/2328
15	P	0.18	0/1789	0.47	0/2436
16	Q	0.20	0/3451	0.48	4/4672 (0.1%)
17	S	0.18	0/582	0.45	0/783
18	T	0.12	0/755	0.32	0/1018
19	U	0.13	0/664	0.31	0/912
20	V	0.20	0/1035	0.41	0/1403
21	W	0.18	0/1204	0.36	0/1624
22	Y	0.18	0/613	0.40	0/840
23	Z	0.11	0/695	0.29	0/939
24	a	0.15	0/1199	0.35	0/1623
25	b	0.16	0/894	0.40	0/1218
26	c	0.20	0/1363	0.62	4/1865 (0.2%)
27	d	0.21	0/1490	0.48	1/2010 (0.0%)
28	e	0.22	0/916	0.53	0/1246
29	f	0.23	0/350	0.48	0/473
30	g	0.16	0/1027	0.33	0/1390
31	h	0.13	0/889	0.31	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.18	0/2770	0.38	0/3765
33	j	0.22	0/818	0.46	0/1116
34	k	0.18	0/759	0.37	0/1029
35	l	0.18	0/4910	0.41	2/6678 (0.0%)
36	m	0.20	0/970	0.42	0/1316
37	n	0.14	0/485	0.37	0/656
38	o	0.14	0/1088	0.40	1/1476 (0.1%)
39	p	0.15	0/1584	0.35	0/2147
40	r	0.17	0/3723	0.38	0/5078
41	s	0.20	0/2464	0.44	1/3369 (0.0%)
42	u	0.19	0/1424	0.56	3/1923 (0.2%)
43	v	0.19	0/1040	0.45	0/1397
44	w	0.15	0/2642	0.38	2/3580 (0.1%)
All	All	0.17	0/66665	0.41	24/90397 (0.0%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	224	ALA	N-CA-C	9.13	120.84	111.07
26	c	75	TYR	CA-C-N	8.88	128.82	119.85
26	c	75	TYR	C-N-CA	8.88	128.82	119.85
42	u	151	ASN	CA-C-N	7.21	127.21	119.28
42	u	151	ASN	C-N-CA	7.21	127.21	119.28
3	C	124	MET	CA-C-N	6.85	126.81	120.03
3	C	124	MET	C-N-CA	6.85	126.81	120.03
27	d	124	ASN	N-CA-C	6.42	118.36	111.36
35	l	366	MET	CA-C-N	6.12	125.52	118.85
35	l	366	MET	C-N-CA	6.12	125.52	118.85
42	u	98	ARG	N-CA-C	6.02	117.93	111.36
38	o	59	VAL	N-CA-C	5.88	116.40	108.17
26	c	179	GLU	CA-C-N	5.78	125.54	119.76
26	c	179	GLU	C-N-CA	5.78	125.54	119.76
41	s	60	PRO	CA-N-CD	-5.68	104.04	112.00
12	M	534	VAL	N-CA-C	-5.65	107.62	113.10
16	Q	262	LEU	N-CA-C	5.46	121.35	114.31
44	w	195	ALA	CA-C-N	-5.24	111.84	122.31
44	w	195	ALA	C-N-CA	-5.24	111.84	122.31
12	M	460	HIS	CA-C-N	5.11	124.72	119.05
12	M	460	HIS	C-N-CA	5.11	124.72	119.05
16	Q	142	VAL	N-CA-C	-5.11	107.45	113.42
16	Q	263	THR	N-CA-C	5.07	116.80	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	659	VAL	N-CA-C	-5.03	108.93	113.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3300	0	3260	94	0
2	B	1412	0	1363	22	0
3	C	1248	0	1254	28	0
4	E	971	0	975	20	0
5	F	691	0	704	22	0
6	G	686	0	664	29	0
6	X	696	0	680	15	0
7	H	910	0	950	20	0
8	I	780	0	808	19	0
9	J	2352	0	2389	34	0
10	K	355	0	329	7	0
11	L	1016	0	1016	21	0
12	M	5295	0	5323	88	0
13	N	1204	0	1162	35	0
14	O	1671	0	1673	53	0
15	P	1738	0	1693	31	0
16	Q	3377	0	3319	53	0
17	S	567	0	565	11	0
18	T	741	0	702	7	0
19	U	643	0	642	7	0
20	V	1014	0	1013	22	0
21	W	1173	0	1166	27	0
22	Y	587	0	522	10	0
23	Z	674	0	643	7	0
24	a	1165	0	1174	19	0
25	b	867	0	877	23	0
26	c	1307	0	1200	46	0
27	d	1457	0	1427	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	e	890	0	837	25	0
29	f	342	0	341	2	0
30	g	996	0	983	12	0
31	h	867	0	871	13	0
32	i	2707	0	2867	53	0
33	j	799	0	852	23	0
34	k	748	0	799	28	0
35	l	4781	0	4926	94	0
36	m	948	0	960	35	0
37	n	473	0	475	7	0
38	o	1058	0	1068	13	0
39	p	1528	0	1461	24	0
40	r	3631	0	3839	54	0
41	s	2394	0	2508	67	0
42	u	1386	0	1368	28	0
43	v	1016	0	958	44	0
44	w	2582	0	2531	41	0
45	A	8	0	0	1	0
45	B	16	0	0	0	0
45	C	8	0	0	1	0
45	M	16	0	0	0	0
46	A	31	0	19	4	0
47	A	44	0	27	7	0
48	C	52	0	88	6	0
48	a	52	0	88	0	0
48	g	52	0	88	3	0
48	j	52	0	88	2	0
48	r	104	0	176	9	0
49	G	35	0	0	5	0
49	X	35	0	0	3	0
50	J	48	0	24	3	0
51	M	4	0	0	1	0
51	O	4	0	0	0	0
52	M	1	0	0	0	0
53	Q	98	0	153	3	0
53	j	98	0	153	4	0
53	l	92	0	138	5	0
53	m	41	0	59	3	0
53	r	51	0	82	2	0
54	T	1	0	0	0	0
55	V	71	0	92	4	0
55	a	91	0	132	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	g	100	0	156	10	0
55	i	66	0	76	5	0
55	l	100	0	156	5	0
56	s	28	0	31	4	0
57	w	27	0	11	0	0
All	All	66469	0	66974	1199	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 9.

All (1199) 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)
50:J:401:NDP:O4D	50:J:401:NDP:C4D	1.68	1.17
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.16
24:a:70:LEU:HD13	28:e:87:MET:HE3	1.12	1.09
26:c:182:VAL:HG13	43:v:34:ARG:HH22	0.92	1.09
26:c:182:VAL:HG13	43:v:34:ARG:NH2	1.67	1.08
42:u:80:GLU:HG2	42:u:81:PRO:HD3	1.29	1.07
25:b:104:ILE:HD13	27:d:18:PRO:HG3	1.37	1.06
24:a:70:LEU:CD1	28:e:87:MET:HE3	1.94	0.97
24:a:70:LEU:HD13	28:e:87:MET:CE	1.98	0.93
26:c:182:VAL:HG21	43:v:36:GLU:OE2	1.69	0.93
35:l:331:MET:HE1	35:l:465:GLY:HA2	1.50	0.92
25:b:123:PHE:HB3	43:v:40:VAL:HG21	1.52	0.92
26:c:182:VAL:CG1	43:v:34:ARG:HH22	1.83	0.87
41:s:281:ARG:HB2	41:s:284:GLN:HG3	1.57	0.87
20:V:69:ILE:HG13	20:V:100:THR:HG21	1.55	0.86
1:A:157:TYR:CB	1:A:212:LEU:HD11	2.06	0.84
27:d:110:LEU:HD11	35:l:203:MET:HE3	1.58	0.84
32:i:149:ILE:HD11	32:i:195:PRO:HG3	1.60	0.83
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.59	0.82
1:A:210:THR:OG1	1:A:224:ARG:HG2	1.80	0.82
27:d:24:THR:HG23	43:v:73:SER:HA	1.62	0.81
1:A:113:LEU:HD13	1:A:149:MET:HE1	1.61	0.81
6:G:88:LYS:HD3	6:G:98:LEU:HD21	1.62	0.81
32:i:155:LEU:HD22	32:i:278:MET:HE1	1.62	0.80
42:u:80:GLU:CG	42:u:81:PRO:HD3	2.12	0.78
9:J:127:ILE:HD11	9:J:253:ILE:HD11	1.65	0.78
24:a:169:TYR:HH	30:g:2:THR:N	1.80	0.78
27:d:24:THR:CG2	43:v:73:SER:CB	2.62	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:62:ARG:HH21	41:s:68:ILE:HB	1.50	0.76
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.25	0.75
25:b:14:GLN:HE22	39:p:157:ALA:HB3	1.49	0.75
26:c:182:VAL:CG1	43:v:34:ARG:NH2	2.45	0.75
12:M:544:VAL:HG23	12:M:565:PHE:HB3	1.67	0.75
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.20	0.75
16:Q:79:ASN:HA	16:Q:101:LEU:O	1.87	0.74
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.21	0.74
55:g:202:CDL:H742	55:g:202:CDL:H271	1.69	0.73
17:S:54:ILE:HG23	42:u:19:LYS:HD2	1.70	0.73
13:N:144:TYR:HD1	13:N:144:TYR:H	1.37	0.73
25:b:104:ILE:CD1	27:d:18:PRO:HG3	2.18	0.73
44:w:258:TYR:HE2	44:w:269:VAL:HG13	1.53	0.73
12:M:171:THR:HG23	12:M:173:MET:HE3	1.70	0.73
26:c:161:TYR:O	26:c:183:HIS:HE1	1.72	0.73
44:w:268:LYS:NZ	44:w:272:ASP:OD2	2.20	0.73
1:A:401:LYS:HB2	1:A:403:ASP:OD1	1.89	0.73
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.20	0.73
1:A:157:TYR:HB3	1:A:212:LEU:HD11	1.71	0.73
24:a:70:LEU:HD22	28:e:87:MET:HE1	1.71	0.72
5:F:40:ARG:HH12	5:F:84:ALA:HB1	1.52	0.72
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.71	0.72
20:V:140:LYS:HG2	20:V:141:VAL:HG23	1.71	0.72
12:M:313:LEU:CD2	13:N:141:SER:O	2.38	0.72
1:A:157:TYR:CG	1:A:212:LEU:HD11	2.24	0.72
17:S:5:ILE:HG12	41:s:26:LYS:HB3	1.69	0.72
34:k:98:CYS:HB2	35:l:580:GLN:HB2	1.70	0.72
17:S:39:ALA:HA	17:S:44:GLN:HG3	1.72	0.71
6:X:123:GLU:HG2	6:X:129:GLU:HA	1.71	0.71
37:n:47:ARG:HH21	37:n:56:THR:HG23	1.55	0.71
3:C:71:CYS:HB3	16:Q:141:TYR:CG	2.25	0.71
1:A:41:ILE:O	1:A:137:LYS:NZ	2.23	0.71
27:d:104:ASN:O	27:d:108:GLU:HG3	1.91	0.71
2:B:177:THR:HG22	2:B:179:THR:H	1.55	0.71
18:T:108:THR:HG22	18:T:119:ARG:HB2	1.71	0.71
27:d:130:GLU:OE2	27:d:134:GLN:NE2	2.24	0.70
33:j:60:ILE:HG21	36:m:168:ILE:HG21	1.71	0.70
45:C:301:SF4:S4	16:Q:223:HIS:CD2	2.83	0.70
1:A:364:VAL:HG12	1:A:400:VAL:HG22	1.74	0.70
16:Q:102:SER:OG	16:Q:107:ARG:NH1	2.24	0.70
35:l:60:GLU:HG2	35:l:83:ASP:HA	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:159:LYS:HE3	14:O:159:LYS:HA	1.72	0.70
27:d:97:LYS:NZ	28:e:115:GLN:OE1	2.25	0.70
42:u:80:GLU:HG2	42:u:81:PRO:CD	2.15	0.70
35:l:227:PHE:O	35:l:230:HIS:ND1	2.24	0.69
35:l:327:LEU:O	35:l:331:MET:HG2	1.91	0.69
35:l:338:MET:HA	35:l:341:MET:HG3	1.75	0.69
2:B:76:TYR:HE1	41:s:33:LEU:HD13	1.58	0.69
5:F:89:ARG:O	5:F:93:ASN:ND2	2.25	0.69
26:c:156:VAL:HG12	43:v:99:MET:HG3	1.75	0.69
44:w:139:ARG:NH1	44:w:166:ASP:OD1	2.25	0.69
1:A:210:THR:HG23	1:A:223:PRO:HA	1.75	0.68
32:i:40:MET:HE1	32:i:129:LEU:HD23	1.74	0.68
1:A:311:TRP:NE1	1:A:333:GLU:OE2	2.25	0.68
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.27	0.68
44:w:67:CYS:HB3	44:w:214:ILE:HD11	1.75	0.68
8:I:18:ARG:NH2	16:Q:260:GLU:OE2	2.27	0.68
1:A:328:PRO:HD3	1:A:441:HIS:CD2	2.29	0.68
5:F:45:LYS:HG2	12:M:671:LEU:HD21	1.75	0.68
10:K:105:ARG:NH1	11:L:167:ASN:O	2.27	0.68
17:S:50:ARG:O	17:S:54:ILE:HG12	1.94	0.68
20:V:69:ILE:CG1	20:V:100:THR:HG21	2.24	0.68
24:a:152:LYS:HD3	30:g:96:VAL:HG21	1.76	0.68
12:M:224:ASP:OD2	12:M:291:ARG:NH2	2.27	0.67
16:Q:332:CYS:O	16:Q:336:GLU:HG3	1.95	0.67
5:F:23:LEU:HD12	5:F:34:ARG:HG2	1.76	0.67
6:G:77:GLU:HA	6:G:80:LYS:HE2	1.76	0.67
1:A:50:ASP:O	1:A:59:ARG:NH2	2.28	0.67
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.76	0.67
39:p:92:GLU:HB3	39:p:95:GLU:HG3	1.75	0.67
35:l:161:ARG:NH1	35:l:238:GLU:OE1	2.28	0.67
4:E:62:LYS:HD2	4:E:66:MET:HE2	1.75	0.67
10:K:100:GLN:HB3	14:O:71:PRO:HA	1.77	0.67
12:M:306:MET:HE3	12:M:583:ILE:HD12	1.77	0.67
14:O:38:LEU:O	14:O:124:ARG:NH2	2.28	0.67
49:X:201:8Q1:N36	49:X:201:8Q1:O40	2.28	0.67
26:c:167:TYR:CE2	26:c:178:PRO:HG3	2.29	0.66
6:X:93:ILE:HD11	6:X:98:LEU:HB2	1.77	0.66
21:W:36:PHE:O	21:W:40:ILE:HG12	1.96	0.66
33:j:27:LEU:HD13	53:j:201:PEE:H15	1.77	0.66
27:d:24:THR:CG2	43:v:73:SER:HB2	2.24	0.66
27:d:24:THR:HG23	43:v:73:SER:CB	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:391:SER:O	35:l:395:ILE:HG12	1.95	0.66
55:V:201:CDL:HB61	38:o:82:PRO:HB2	1.76	0.66
27:d:24:THR:CG2	43:v:73:SER:HA	2.25	0.66
27:d:24:THR:HG21	43:v:73:SER:HB2	1.77	0.65
9:J:192:ARG:NH2	9:J:262:THR:OG1	2.30	0.65
43:v:12:ASP:HB3	43:v:15:LYS:HB2	1.78	0.65
26:c:129:MET:HG2	35:l:528:TYR:CG	2.32	0.65
35:l:250:SER:HB2	35:l:333:ALA:HA	1.79	0.65
27:d:117:GLU:HA	27:d:117:GLU:OE1	1.97	0.65
27:d:24:THR:HG23	43:v:73:SER:CA	2.27	0.65
44:w:88:GLU:OE2	44:w:161:ARG:NH1	2.30	0.65
30:g:7:ARG:NH1	30:g:91:ASP:OD1	2.30	0.65
2:B:111:GLU:O	2:B:141:ARG:NH1	2.30	0.65
26:c:170:ARG:HG2	43:v:53:LEU:HD13	1.79	0.65
27:d:114:GLN:HG3	35:l:203:MET:HG2	1.78	0.64
22:Y:60:PHE:O	22:Y:64:THR:HG23	1.97	0.64
12:M:44:GLU:N	12:M:44:GLU:OE2	2.30	0.64
27:d:124:ASN:N	27:d:124:ASN:HD22	1.95	0.64
9:J:203:PRO:O	50:J:401:NDP:H5N	1.97	0.64
12:M:313:LEU:HD22	13:N:141:SER:O	1.98	0.64
21:W:93:GLU:O	21:W:97:ILE:HG13	1.97	0.64
27:d:125:CYS:HB3	35:l:203:MET:CE	2.28	0.64
11:L:79:ILE:HG12	11:L:99:MET:HG3	1.80	0.64
2:B:177:THR:HG21	2:B:182:GLU:HB2	1.80	0.64
3:C:123:GLN:O	41:s:61:LEU:HD11	1.98	0.64
35:l:399:VAL:HG12	35:l:409:LEU:HD12	1.80	0.64
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.80	0.63
21:W:68:ARG:HD2	36:m:135:PHE:CD2	2.33	0.63
24:a:106:VAL:HG23	37:n:50:ARG:HH21	1.61	0.63
27:d:32:TYR:O	27:d:36:ILE:HG13	1.98	0.63
35:l:5:ALA:HB2	35:l:61:MET:HE1	1.78	0.63
40:r:207:MET:HG2	40:r:298:ILE:CG1	2.28	0.63
1:A:185:ASN:ND2	1:A:187:CYS:O	2.31	0.63
20:V:66:ILE:HD11	20:V:101:LEU:HB2	1.80	0.63
16:Q:133:LEU:CD2	16:Q:228:ARG:HD3	2.29	0.63
12:M:460:HIS:CG	12:M:461:PRO:HD2	2.34	0.63
15:P:209:GLU:HG2	15:P:224:VAL:HA	1.79	0.63
32:i:278:MET:O	32:i:282:MET:HG3	1.99	0.63
1:A:33:GLY:HA2	1:A:294:VAL:HG22	1.79	0.63
17:S:66:LEU:O	17:S:69:ILE:HG22	1.99	0.63
26:c:167:TYR:CD2	26:c:178:PRO:HG3	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:42:VAL:HG23	12:M:671:LEU:HD13	1.79	0.63
44:w:223:ASN:OD1	44:w:226:GLU:N	2.31	0.63
25:b:9:LYS:O	25:b:13:GLN:HG3	1.99	0.63
24:a:166:GLY:O	24:a:170:GLN:NE2	2.32	0.63
6:X:69:SER:OG	6:X:70:ASP:N	2.31	0.62
12:M:388:ASN:HB3	12:M:511:LYS:HE2	1.80	0.62
13:N:120:THR:HG22	13:N:122:GLN:H	1.64	0.62
40:r:14:MET:SD	40:r:30:HIS:ND1	2.71	0.62
42:u:103:GLN:N	42:u:103:GLN:OE1	2.33	0.62
3:C:59:ARG:NH1	48:C:302:PLX:O3	2.25	0.62
22:Y:54:GLN:OE1	35:l:446:ASN:ND2	2.32	0.62
27:d:128:GLU:N	27:d:128:GLU:OE1	2.31	0.62
32:i:283:ALA:HB1	40:r:158:LEU:HD13	1.80	0.62
15:P:164:ASN:OD1	15:P:181:HIS:HE1	1.83	0.62
20:V:120:LEU:HD21	48:r:502:PLX:H332	1.80	0.62
35:l:127:THR:HG22	35:l:147:VAL:HG13	1.81	0.62
1:A:208:GLU:OE1	1:A:210:THR:N	2.33	0.62
3:C:66:THR:HG21	3:C:76:MET:HG2	1.82	0.62
12:M:313:LEU:HD21	13:N:141:SER:O	1.99	0.61
41:s:24:GLU:OE2	41:s:274:ARG:NH1	2.33	0.61
5:F:65:LEU:HD11	5:F:91:LEU:HD13	1.82	0.61
7:H:76:GLN:HB3	7:H:79:GLU:HG2	1.81	0.61
9:J:221:ARG:NE	9:J:286:ARG:HD2	2.15	0.61
24:a:179:ILE:HG21	31:h:38:LYS:HG3	1.81	0.61
33:j:73:LEU:HD13	36:m:55:MET:HE1	1.82	0.61
27:d:125:CYS:CB	35:l:203:MET:HE1	2.31	0.61
13:N:4:VAL:O	13:N:8:ARG:HG3	2.01	0.61
30:g:12:PRO:HB3	31:h:5:ASP:HB3	1.82	0.61
12:M:496:ILE:O	12:M:500:ILE:HG12	2.00	0.61
12:M:624:ARG:NH2	12:M:637:ASP:OD1	2.30	0.61
27:d:110:LEU:HD11	35:l:203:MET:CE	2.29	0.61
42:u:96:LEU:HD12	42:u:99:HIS:CD2	2.36	0.61
9:J:88:PRO:HA	9:J:91:THR:HG22	1.83	0.61
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.82	0.61
40:r:328:CYS:HB3	40:r:437:MET:HE1	1.83	0.61
4:E:37:ARG:HG2	6:G:120:MET:HE2	1.82	0.60
32:i:211:MET:HG3	32:i:333:SER:HB2	1.83	0.60
5:F:41:TYR:CE2	5:F:55:ILE:HD11	2.36	0.60
35:l:71:LEU:HD21	40:r:380:PHE:CZ	2.36	0.60
1:A:185:ASN:OD1	1:A:190:GLY:N	2.24	0.60
13:N:41:GLU:OE1	13:N:47:LYS:HD3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:HG12	14:O:249:LEU:HD11	1.82	0.60
1:A:447:GLU:HA	1:A:450:MET:HE2	1.83	0.60
20:V:54:ALA:O	20:V:58:ARG:HG2	2.01	0.60
27:d:110:LEU:CD1	35:l:203:MET:HE3	2.30	0.60
43:v:17:PRO:HB2	43:v:22:MET:HE2	1.83	0.60
33:j:68:GLU:HG2	36:m:161:LEU:HD13	1.83	0.60
1:A:41:ILE:HG21	1:A:250:VAL:HG12	1.83	0.60
8:I:40:LYS:HB3	21:W:7:LYS:H	1.66	0.60
20:V:62:THR:HG23	20:V:104:ARG:HG2	1.83	0.60
21:W:66:GLU:HG2	42:u:125:LEU:HB2	1.83	0.60
49:X:201:8Q1:O3	39:p:13:GLN:NE2	2.33	0.60
12:M:133:GLN:HG3	12:M:136:GLU:HG3	1.84	0.60
40:r:227:GLY:O	40:r:231:LEU:HG	2.02	0.59
1:A:282:VAL:HG13	1:A:356:VAL:HG21	1.83	0.59
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.35	0.59
15:P:44:ARG:HE	15:P:45:PRO:HD3	1.66	0.59
27:d:125:CYS:HB3	35:l:203:MET:HE1	1.84	0.59
55:g:202:CDL:H332	55:g:202:CDL:H202	1.84	0.59
22:Y:46:GLN:HE22	23:Z:17:PRO:HG3	1.67	0.59
11:L:131:LYS:NZ	11:L:149:GLU:OE2	2.35	0.59
36:m:57:PHE:CD2	41:s:107:ALA:HB1	2.37	0.59
6:G:115:GLN:O	6:G:119:ILE:HD12	2.01	0.59
35:l:559:GLU:O	35:l:563:PRO:HD2	2.02	0.59
1:A:152:ARG:NH2	10:K:99:PRO:O	2.35	0.59
55:g:202:CDL:H402	32:i:335:LEU:HD21	1.83	0.59
1:A:266:GLY:N	1:A:291:GLU:OE2	2.36	0.59
1:A:383:THR:HG23	1:A:384:PRO:HD3	1.84	0.59
1:A:60:GLY:O	1:A:256:ARG:NH1	2.36	0.59
44:w:125:ASP:O	44:w:130:ARG:NH2	2.36	0.59
3:C:129:TYR:HD2	3:C:160:ASP:OD2	1.85	0.59
1:A:210:THR:CG2	1:A:223:PRO:HB3	2.33	0.58
3:C:79:MET:HE3	3:C:86:MET:HE3	1.85	0.58
6:G:144:ILE:O	6:G:148:ILE:HG12	2.03	0.58
55:g:202:CDL:H632	40:r:10:MET:HE1	1.84	0.58
40:r:342:MET:HE3	40:r:413:THR:HG21	1.85	0.58
44:w:129:TYR:OH	44:w:186:HIS:ND1	2.28	0.58
44:w:146:ALA:HB1	44:w:157:VAL:HG21	1.85	0.58
26:c:161:TYR:O	26:c:183:HIS:CE1	2.54	0.58
1:A:117:ALA:HB3	1:A:158:ILE:HA	1.84	0.58
25:b:4:TYR:HB2	25:b:9:LYS:HG2	1.86	0.58
6:G:141:PRO:O	6:G:145:VAL:HG23	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:37:SER:O	20:V:41:ILE:HG12	2.04	0.58
35:l:293:ILE:HG21	35:l:418:LEU:HD22	1.85	0.58
1:A:210:THR:HG23	1:A:223:PRO:CA	2.33	0.58
35:l:286:LEU:HD22	35:l:411:MET:SD	2.44	0.58
40:r:370:PRO:HB3	40:r:375:LEU:HD22	1.86	0.57
7:H:67:LYS:O	7:H:71:GLN:HG2	2.05	0.57
7:H:79:GLU:OE2	15:P:136:ARG:NH2	2.37	0.57
12:M:333:PHE:HE2	12:M:543:LYS:HD2	1.68	0.57
33:j:64:LEU:HD13	36:m:165:VAL:HG22	1.86	0.57
14:O:100:LYS:O	14:O:104:ILE:HG12	2.04	0.57
4:E:29:LYS:NZ	49:G:201:8Q1:O2	2.37	0.57
9:J:87:GLU:HG3	9:J:89:TYR:H	1.68	0.57
16:Q:251:PHE:HB3	16:Q:341:LEU:HD11	1.87	0.57
27:d:71:VAL:HG11	27:d:87:GLU:HB3	1.87	0.57
39:p:120:ALA:O	39:p:124:GLN:HG3	2.04	0.57
2:B:74:LEU:HB2	41:s:272:TRP:CZ2	2.39	0.57
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.87	0.57
16:Q:133:LEU:HD22	16:Q:228:ARG:HD3	1.85	0.57
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.87	0.57
32:i:237:MET:HE1	32:i:319:HIS:NE2	2.19	0.57
55:g:202:CDL:H812	55:g:202:CDL:H241	1.87	0.57
35:l:489:THR:O	35:l:493:VAL:HG22	2.05	0.57
1:A:157:TYR:CG	1:A:212:LEU:CD1	2.87	0.57
1:A:290:GLU:HG3	1:A:294:VAL:HG21	1.86	0.57
16:Q:184:ILE:O	16:Q:188:THR:OG1	2.21	0.57
37:n:54:GLU:OE2	37:n:54:GLU:N	2.30	0.57
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.86	0.56
11:L:88:GLN:NE2	12:M:141:ASP:OD2	2.32	0.56
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.86	0.56
1:A:303:HIS:ND1	14:O:232:THR:OG1	2.36	0.56
4:E:37:ARG:O	4:E:41:ARG:HG2	2.05	0.56
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.87	0.56
26:c:153:TYR:OH	43:v:8:ARG:NH1	2.32	0.56
28:e:152:ASP:OD1	28:e:153:GLU:N	2.36	0.56
29:f:68:GLU:OE1	29:f:72:ARG:HG3	2.05	0.56
30:g:32:ARG:O	30:g:36:MET:HG2	2.05	0.56
41:s:140:ILE:HA	41:s:143:GLU:HG2	1.88	0.56
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.88	0.56
12:M:419:ARG:NH1	12:M:439:THR:O	2.38	0.56
15:P:43:THR:HA	15:P:47:ILE:HD12	1.86	0.56
26:c:39:GLY:H	26:c:74:ASP:HB2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:127:LYS:HA	27:d:127:LYS:HE3	1.86	0.56
3:C:42:ARG:O	3:C:46:VAL:HG23	2.05	0.56
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.86	0.56
25:b:28:LEU:HG	25:b:32:GLU:HG2	1.86	0.56
26:c:156:VAL:HG11	43:v:95:TYR:CZ	2.40	0.56
1:A:102:MET:HG2	1:A:149:MET:HB3	1.87	0.56
22:Y:65:MET:SD	35:l:375:ILE:HG12	2.45	0.56
31:h:18:MET:HE3	34:k:56:ALA:HA	1.87	0.56
13:N:28:PHE:HE1	41:s:42:PRO:HG3	1.70	0.56
31:h:51:ARG:O	31:h:55:GLU:HG3	2.06	0.56
32:i:54:GLU:HG3	34:k:93:LEU:HD22	1.88	0.56
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.88	0.56
7:H:76:GLN:O	7:H:79:GLU:HG2	2.06	0.56
33:j:18:VAL:HG23	41:s:222:MET:HE1	1.88	0.56
39:p:54:GLU:OE2	39:p:59:LYS:HD2	2.06	0.56
41:s:62:ARG:HH11	41:s:64:ALA:HA	1.70	0.56
1:A:211:ALA:HB2	1:A:223:PRO:HG3	1.88	0.55
14:O:61:LYS:O	14:O:64:GLU:HG3	2.06	0.55
27:d:73:ASP:OD1	27:d:73:ASP:N	2.37	0.55
9:J:83:PRO:HG3	9:J:119:VAL:HG11	1.87	0.55
21:W:50:MET:HE1	21:W:53:TRP:HD1	1.72	0.55
32:i:211:MET:HE3	32:i:251:MET:HA	1.88	0.55
16:Q:236:LEU:HD22	16:Q:240:LEU:HD23	1.87	0.55
16:Q:302:LEU:HD11	16:Q:406:GLU:HG3	1.88	0.55
33:j:87:MET:HE1	41:s:309:ILE:HD11	1.88	0.55
35:l:289:ALA:O	35:l:293:ILE:HG23	2.06	0.55
1:A:210:THR:OG1	1:A:224:ARG:CG	2.51	0.55
13:N:144:TYR:HD1	13:N:144:TYR:N	2.05	0.55
20:V:88:LEU:O	20:V:92:ILE:HG13	2.05	0.55
55:a:201:CDL:H541	53:l:703:PEE:H16	1.89	0.55
35:l:173:LEU:HD12	40:r:405:LEU:HD21	1.89	0.55
12:M:462:PHE:CE2	12:M:466:LEU:HD11	2.42	0.55
16:Q:121:GLU:HG2	16:Q:422:CYS:O	2.07	0.55
25:b:110:ILE:HG12	27:d:16:ARG:HB2	1.87	0.55
28:e:151:GLU:HG3	28:e:153:GLU:HG3	1.89	0.55
33:j:16:LEU:O	33:j:20:ILE:HG23	2.06	0.55
40:r:373:ILE:HD11	40:r:444:LEU:HD23	1.89	0.55
44:w:258:TYR:OH	44:w:272:ASP:OD2	2.24	0.55
11:L:89:SER:O	12:M:59:GLN:NE2	2.38	0.55
13:N:78:ASP:OD2	13:N:80:SER:OG	2.20	0.55
15:P:44:ARG:HB3	15:P:45:PRO:CD	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:66:SER:HB2	41:s:122:ALA:O	2.06	0.55
6:G:76:LEU:HB3	6:G:80:LYS:NZ	2.22	0.55
12:M:36:VAL:HB	12:M:56:VAL:HG21	1.87	0.55
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.88	0.55
3:C:88:ARG:HA	41:s:37:PRO:HA	1.88	0.55
14:O:137:THR:HG22	14:O:138:THR:H	1.72	0.55
2:B:100:GLU:O	2:B:170:GLY:N	2.35	0.55
26:c:162:PRO:HB3	43:v:39:MET:SD	2.47	0.55
15:P:81:PHE:CE1	15:P:83:GLU:OE2	2.60	0.54
41:s:81:LEU:O	41:s:85:MET:HG2	2.07	0.54
6:G:93:ILE:HA	6:G:97:LYS:NZ	2.21	0.54
8:I:35:THR:HG23	13:N:95:ASP:H	1.72	0.54
12:M:472:PRO:O	12:M:510:TRP:NE1	2.36	0.54
16:Q:293:LEU:HD22	16:Q:298:ILE:HD12	1.89	0.54
34:k:5:TYR:O	34:k:9:ILE:HG13	2.08	0.54
2:B:98:ARG:NH2	16:Q:224:ALA:O	2.41	0.54
41:s:106:LEU:HD13	41:s:150:LEU:HD23	1.88	0.54
12:M:370:GLU:OE2	12:M:518:ARG:NH2	2.39	0.54
32:i:89:MET:HE1	32:i:98:MET:HE2	1.90	0.54
11:L:84:ARG:HD3	11:L:91:VAL:HG12	1.89	0.54
27:d:110:LEU:CD1	35:l:203:MET:CE	2.86	0.54
35:l:71:LEU:HG	40:r:310:MET:HE1	1.90	0.54
1:A:118:ASP:CB	1:A:207:GLY:HA2	2.38	0.54
29:f:60:LYS:O	29:f:64:GLU:HG2	2.07	0.54
26:c:54:LYS:NZ	26:c:74:ASP:OD2	2.30	0.54
36:m:25:SER:O	36:m:28:TYR:N	2.38	0.54
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.90	0.54
21:W:76:GLN:NE2	21:W:80:ASP:OD1	2.41	0.54
32:i:72:MET:HE1	34:k:43:MET:HE1	1.90	0.54
16:Q:265:ASN:O	16:Q:269:ARG:HG3	2.07	0.54
27:d:6:ASP:OD2	28:e:127:LYS:NZ	2.37	0.54
9:J:206:ILE:HG22	9:J:240:VAL:HG13	1.90	0.53
14:O:156:LEU:HB2	14:O:158:ILE:HG12	1.90	0.53
44:w:75:ARG:O	44:w:79:GLU:HG3	2.08	0.53
14:O:138:THR:HA	14:O:141:MET:HE3	1.90	0.53
34:k:44:SER:HB2	34:k:59:MET:HE1	1.90	0.53
9:J:211:ASP:O	9:J:215:ASN:ND2	2.41	0.53
13:N:127:TYR:OH	18:T:61:GLU:O	2.20	0.53
14:O:179:ALA:HB3	14:O:185:MET:HE3	1.90	0.53
26:c:63:GLU:O	26:c:76:PRO:HA	2.08	0.53
6:G:74:LEU:H	6:G:74:LEU:HD23	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:501:ARG:HH21	12:M:666:GLN:HE21	1.57	0.53
14:O:186:VAL:HG12	14:O:193:TYR:HB2	1.89	0.53
6:X:113:LEU:O	6:X:117:GLU:HG3	2.09	0.53
1:A:201:ALA:C	14:O:121:MET:HG3	2.33	0.53
12:M:343:GLY:HA2	12:M:369:GLU:OE1	2.08	0.53
13:N:2:GLU:HG3	13:N:4:VAL:HG22	1.90	0.53
14:O:103:GLU:HG3	14:O:104:ILE:HD13	1.89	0.53
40:r:129:THR:HG21	40:r:235:LEU:HD11	1.90	0.53
41:s:62:ARG:HD3	41:s:64:ALA:H	1.74	0.53
44:w:122:LYS:O	44:w:123:SER:C	2.50	0.53
11:L:109:ASN:HB2	11:L:116:SER:OG	2.08	0.53
40:r:3:LYS:HG3	40:r:4:ILE:HD12	1.91	0.53
44:w:65:ASN:OD1	44:w:66:ILE:N	2.36	0.53
25:b:121:LYS:HG2	43:v:40:VAL:HG13	1.88	0.53
27:d:99:ASP:OD2	27:d:143:TYR:OH	2.24	0.53
41:s:102:VAL:HG11	41:s:154:LEU:HD11	1.90	0.53
41:s:104:PHE:CE1	41:s:108:MET:HE3	2.44	0.53
44:w:59:VAL:HG13	44:w:201:PRO:HA	1.91	0.53
16:Q:156:GLU:CD	16:Q:230:GLY:H	2.16	0.53
44:w:246:LEU:HD12	44:w:255:VAL:HG11	1.91	0.53
1:A:446:LEU:O	1:A:450:MET:HG3	2.09	0.53
6:G:82:ARG:NH2	6:G:125:GLU:OE2	2.32	0.53
6:G:112:SER:O	6:G:116:VAL:HG23	2.09	0.53
8:I:16:SER:O	8:I:18:ARG:NH1	2.42	0.53
26:c:81:ARG:HB3	26:c:85:GLU:OE2	2.08	0.53
27:d:50:GLU:O	27:d:54:GLN:HG3	2.09	0.53
41:s:10:ILE:HG23	41:s:83:LEU:HD22	1.91	0.53
1:A:71:LYS:HG3	1:A:75:TRP:CZ3	2.44	0.53
1:A:161:GLU:N	1:A:161:GLU:OE1	2.42	0.53
1:A:338:ASP:OD1	1:A:338:ASP:N	2.41	0.53
6:G:142:GLN:NE2	6:G:146:ASP:OD1	2.41	0.53
14:O:181:VAL:HG13	14:O:182:ASN:OD1	2.08	0.52
41:s:24:GLU:HG3	41:s:271:LEU:HD22	1.89	0.52
43:v:8:ARG:NH2	43:v:18:ASP:OD1	2.42	0.52
3:C:123:GLN:O	41:s:61:LEU:CD1	2.57	0.52
3:C:188:LYS:HE3	3:C:191:ARG:CZ	2.40	0.52
9:J:201:ILE:HG22	9:J:203:PRO:HD3	1.90	0.52
12:M:250:SER:OG	12:M:251:ILE:N	2.42	0.52
28:e:108:TYR:CE1	48:r:503:PLX:H1B2	2.43	0.52
32:i:26:TRP:HB3	32:i:74:ILE:HD13	1.91	0.52
41:s:195:ARG:HD3	41:s:231:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:TYR:OH	47:A:503:NAI:H5N	2.09	0.52
25:b:111:LEU:HD21	27:d:19:ALA:HA	1.91	0.52
27:d:24:THR:CG2	43:v:73:SER:CA	2.86	0.52
35:l:293:ILE:HD11	55:l:701:CDL:H712	1.91	0.52
9:J:369:VAL:HG12	9:J:370:LYS:HG2	1.90	0.52
11:L:99:MET:HE2	11:L:126:LEU:HD12	1.92	0.52
12:M:342:ALA:HA	12:M:548:LEU:HB3	1.90	0.52
40:r:105:PHE:O	40:r:109:THR:OG1	2.25	0.52
6:G:119:ILE:O	6:G:123:GLU:HG2	2.10	0.52
41:s:287:HIS:CD2	41:s:291:LYS:HD2	2.44	0.52
35:l:261:ILE:HG13	35:l:317:ILE:HD11	1.92	0.52
36:m:31:LEU:HD13	41:s:70:MET:HE1	1.91	0.52
40:r:87:GLU:OE1	40:r:91:ARG:HD2	2.10	0.52
11:L:77:VAL:HG23	11:L:145:PHE:HB3	1.90	0.52
16:Q:217:VAL:HG23	16:Q:236:LEU:HD23	1.91	0.52
12:M:338:VAL:HG23	12:M:363:SER:HB2	1.92	0.52
39:p:170:ILE:O	39:p:173:ARG:HD3	2.10	0.52
40:r:225:ILE:O	40:r:229:MET:HG3	2.10	0.52
1:A:159:ARG:NH2	14:O:176:CYS:O	2.38	0.52
11:L:163:ASN:O	11:L:171:ARG:HA	2.08	0.52
19:U:63:MET:O	42:u:130:LYS:NZ	2.36	0.52
28:e:120:ARG:O	28:e:124:ARG:HG3	2.10	0.52
32:i:57:THR:HA	34:k:77:LEU:HD13	1.92	0.52
35:l:400:ASN:ND2	35:l:409:LEU:HD11	2.26	0.52
26:c:127:ASN:O	26:c:131:LYS:HG3	2.10	0.51
34:k:17:ALA:O	34:k:21:MET:HG2	2.09	0.51
41:s:264:LEU:O	41:s:268:ILE:HG12	2.10	0.51
44:w:258:TYR:CE2	44:w:269:VAL:HG13	2.40	0.51
5:F:55:ILE:O	5:F:56:ARG:NH1	2.43	0.51
5:F:62:GLN:OE1	5:F:80:ASN:ND2	2.40	0.51
12:M:483:ARG:HH22	12:M:682:ASP:HB3	1.76	0.51
15:P:125:ARG:HH22	15:P:201:ASP:CG	2.18	0.51
21:W:68:ARG:HD2	36:m:135:PHE:CE2	2.45	0.51
23:Z:15:GLU:N	23:Z:15:GLU:OE1	2.43	0.51
28:e:67:TYR:HA	28:e:70:ASN:O	2.10	0.51
34:k:4:VAL:O	34:k:8:ILE:HG12	2.10	0.51
21:W:81:ARG:NH2	42:u:64:ASN:OD1	2.43	0.51
27:d:71:VAL:O	27:d:91:GLN:NE2	2.38	0.51
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.91	0.51
12:M:667:GLN:O	12:M:671:LEU:HB2	2.10	0.51
55:g:202:CDL:H391	32:i:334:THR:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:v:30:GLY:H	43:v:104:ARG:HH22	1.58	0.51
5:F:19:ILE:HG13	5:F:53:ILE:HG23	1.92	0.51
7:H:92:ARG:HH12	44:w:268:LYS:HE2	1.75	0.51
15:P:69:LEU:HD22	15:P:96:VAL:HG22	1.93	0.51
16:Q:139:LEU:HD13	16:Q:424:ILE:HG21	1.92	0.51
24:a:96:ALA:HB2	27:d:61:TYR:CE2	2.46	0.51
27:d:125:CYS:CB	35:l:203:MET:CE	2.88	0.51
28:e:144:PRO:HA	28:e:147:ILE:HD12	1.92	0.51
31:h:69:ARG:O	31:h:73:MET:HG3	2.11	0.51
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.92	0.51
42:u:153:GLU:O	42:u:154:ALA:C	2.54	0.51
15:P:179:ALA:O	15:P:180:ASN:HB2	2.11	0.51
33:j:5:LEU:HD11	41:s:3:MET:HE1	1.91	0.51
8:I:6:ARG:CZ	8:I:10:LEU:HD11	2.41	0.51
9:J:168:SER:O	9:J:202:LYS:HA	2.11	0.51
13:N:144:TYR:N	13:N:144:TYR:CD1	2.74	0.51
21:W:31:SER:O	21:W:35:MET:HG3	2.10	0.51
36:m:129:ASP:OD1	36:m:129:ASP:N	2.44	0.51
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.92	0.51
41:s:87:VAL:HG23	41:s:88:PRO:HD3	1.92	0.51
1:A:406:PRO:HA	1:A:450:MET:HE1	1.93	0.51
20:V:90:TYR:CE1	20:V:126:LYS:HE3	2.46	0.51
22:Y:43:ARG:HG3	22:Y:48:PRO:HA	1.93	0.51
12:M:483:ARG:NH2	12:M:682:ASP:HB3	2.26	0.50
14:O:152:ILE:HG12	14:O:205:ILE:HD11	1.92	0.50
24:a:141:GLN:O	24:a:145:GLU:HG3	2.11	0.50
27:d:104:ASN:HD21	35:l:73:THR:HA	1.77	0.50
32:i:84:TRP:HH2	34:k:59:MET:HE2	1.76	0.50
46:A:502:FMN:O4'	46:A:502:FMN:O2'	2.29	0.50
14:O:134:VAL:HG22	14:O:186:VAL:HG23	1.93	0.50
16:Q:262:LEU:O	16:Q:268:TRP:CD1	2.64	0.50
43:v:46:MET:HE3	43:v:56:ARG:HG2	1.93	0.50
1:A:89:GLY:O	47:A:503:NAI:H2N	2.11	0.50
14:O:218:PRO:HG3	14:O:224:SER:H	1.76	0.50
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.47	0.50
44:w:229:ILE:H	44:w:229:ILE:HD12	1.75	0.50
12:M:153:PHE:CZ	12:M:155:GLU:HB2	2.47	0.50
12:M:389:THR:HB	12:M:473:MET:HE3	1.92	0.50
24:a:189:ASN:ND2	42:u:142:TYR:OH	2.40	0.50
26:c:111:MET:HE1	35:l:543:SER:HB2	1.94	0.50
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:67:VAL:HG12	48:r:503:PLX:H382	1.93	0.50
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.94	0.50
2:B:76:TYR:CE1	41:s:33:LEU:HD13	2.42	0.50
14:O:110:MET:O	14:O:114:GLU:HG3	2.11	0.50
16:Q:198:THR:HG23	41:s:32:GLN:HG3	1.94	0.50
26:c:182:VAL:HG13	26:c:182:VAL:O	2.11	0.50
36:m:17:PHE:O	36:m:21:SER:HB2	2.12	0.50
1:A:69:LEU:HD13	1:A:147:ARG:HG2	1.94	0.50
12:M:217:GLU:OE1	12:M:217:GLU:N	2.30	0.50
12:M:304:GLN:HG2	12:M:615:LEU:HD12	1.94	0.50
12:M:476:LEU:HD22	12:M:493:VAL:HG21	1.92	0.50
6:X:90:TYR:HE1	23:Z:44:PRO:HB2	1.76	0.50
27:d:25:SER:O	27:d:26:LEU:C	2.54	0.50
35:l:589:LEU:O	35:l:593:ILE:HG13	2.11	0.50
38:o:59:VAL:HG13	40:r:422:HIS:CE1	2.46	0.50
40:r:174:LEU:HA	40:r:179:ILE:HD11	1.92	0.50
40:r:191:SER:HB3	53:r:501:PEE:H3	1.93	0.50
27:d:119:GLU:HG2	43:v:52:MET:HA	1.94	0.50
28:e:143:ASP:OD1	28:e:146:LYS:HD3	2.12	0.50
55:l:701:CDL:H673	55:l:701:CDL:H472	1.94	0.50
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.93	0.50
5:F:30:SER:OG	5:F:63:PRO:HG3	2.12	0.49
6:G:94:ASP:OD1	6:G:97:LYS:HG2	2.11	0.49
12:M:81:GLU:OE1	12:M:106:SER:OG	2.26	0.49
12:M:557:ARG:NH2	12:M:581:ASP:OD1	2.44	0.49
6:X:93:ILE:HD11	6:X:98:LEU:HD13	1.94	0.49
8:I:29:GLN:NE2	13:N:52:ASN:HB3	2.27	0.49
20:V:69:ILE:HG21	20:V:100:THR:CG2	2.42	0.49
6:X:119:ILE:HG21	6:X:135:ALA:HB1	1.95	0.49
24:a:136:THR:HG21	40:r:48:ASN:HD22	1.78	0.49
26:c:110:ASP:OD1	26:c:110:ASP:N	2.45	0.49
27:d:124:ASN:N	27:d:124:ASN:ND2	2.60	0.49
41:s:24:GLU:OE1	41:s:228:TYR:OH	2.21	0.49
12:M:460:HIS:ND1	12:M:461:PRO:HD2	2.28	0.49
31:h:47:ILE:HG22	31:h:51:ARG:HB2	1.93	0.49
39:p:29:SER:HB3	39:p:76:HIS:CD2	2.47	0.49
35:l:399:VAL:HG12	35:l:409:LEU:CD1	2.43	0.49
40:r:306:PRO:HA	40:r:458:LEU:HD13	1.94	0.49
41:s:55:LEU:HD11	56:s:401:UQ:HM52	1.93	0.49
41:s:307:LEU:HA	41:s:310:MET:HE2	1.93	0.49
3:C:44:GLU:OE1	3:C:195:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:196:ARG:O	9:J:136:THR:HG21	2.12	0.49
13:N:5:GLN:O	13:N:9:ARG:HG3	2.12	0.49
25:b:109:THR:O	27:d:19:ALA:N	2.36	0.49
36:m:57:PHE:CD1	36:m:61:LEU:HD12	2.47	0.49
44:w:143:TYR:OH	44:w:199:LEU:O	2.25	0.49
16:Q:47:PHE:CD1	16:Q:52:MET:HE1	2.48	0.49
16:Q:65:PRO:HB2	16:Q:67:ASN:O	2.13	0.49
19:U:26:GLY:HA3	53:j:202:PEE:H37	1.93	0.49
35:l:346:ILE:HD11	35:l:431:PHE:CZ	2.47	0.49
39:p:132:SER:OG	39:p:163:LEU:HB2	2.12	0.49
14:O:58:GLU:O	14:O:62:ARG:HG3	2.12	0.49
20:V:17:GLU:HB3	20:V:20:ARG:HD2	1.95	0.49
36:m:25:SER:O	36:m:27:ILE:N	2.45	0.49
41:s:9:LEU:O	41:s:13:ILE:HG12	2.12	0.49
4:E:28:ALA:HB1	4:E:79:VAL:HG11	1.95	0.49
12:M:334:GLN:HG2	12:M:361:VAL:HG22	1.95	0.49
13:N:42:ASP:HB3	13:N:46:ASN:H	1.78	0.49
28:e:99:LEU:O	28:e:103:SER:OG	2.29	0.49
40:r:12:LEU:HB2	40:r:13:PRO:HD3	1.94	0.49
43:v:25:PHE:CD2	43:v:108:LEU:HB3	2.47	0.49
9:J:87:GLU:OE1	9:J:88:PRO:HD2	2.13	0.48
12:M:367:CYS:HB2	12:M:533:GLY:O	2.12	0.48
18:T:78:GLU:OE2	18:T:119:ARG:HD2	2.12	0.48
32:i:54:GLU:OE1	34:k:95:LEU:HB2	2.13	0.48
25:b:117:ILE:HD11	27:d:16:ARG:HH22	1.78	0.48
32:i:270:MET:HE1	32:i:282:MET:SD	2.53	0.48
44:w:86:PHE:HB2	44:w:159:LEU:HD23	1.95	0.48
1:A:75:TRP:HH2	14:O:249:LEU:HD12	1.78	0.48
3:C:56:TRP:CE2	48:C:302:PLX:H92	2.49	0.48
12:M:546:PHE:CE1	12:M:567:ILE:HD13	2.48	0.48
26:c:149:ILE:O	26:c:151:PRO:HD3	2.13	0.48
27:d:24:THR:HG21	43:v:73:SER:CB	2.39	0.48
35:l:27:TYR:O	35:l:115:ASN:ND2	2.38	0.48
40:r:48:ASN:N	40:r:48:ASN:OD1	2.44	0.48
34:k:37:MET:HE1	36:m:64:MET:HE1	1.96	0.48
37:n:54:GLU:HG2	37:n:55:VAL:HG22	1.94	0.48
40:r:329:LEU:O	40:r:332:THR:OG1	2.29	0.48
44:w:123:SER:OG	44:w:125:ASP:OD1	2.21	0.48
1:A:442:PHE:HD2	1:A:445:GLU:HG3	1.79	0.48
12:M:488:ALA:HB1	12:M:679:LEU:HD22	1.96	0.48
34:k:25:HIS:O	34:k:28:SER:N	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:72:CYS:HB3	3:C:133:MET:HE2	1.96	0.48
3:C:77:MET:HE1	16:Q:185:MET:HE1	1.95	0.48
12:M:203:ASP:OD1	12:M:203:ASP:N	2.37	0.48
26:c:164:ASN:OD1	26:c:180:PRO:HA	2.14	0.48
32:i:12:THR:HA	32:i:15:SER:OG	2.14	0.48
48:j:203:PLX:H342	48:j:203:PLX:H372	1.58	0.48
1:A:290:GLU:OE2	1:A:303:HIS:NE2	2.39	0.48
4:E:25:MET:HE1	4:E:79:VAL:HG21	1.94	0.48
11:L:92:ASN:HB3	15:P:238:PRO:HA	1.96	0.48
26:c:78:LEU:HD12	26:c:106:HIS:HA	1.96	0.48
27:d:125:CYS:HB3	35:l:203:MET:HE2	1.96	0.48
28:e:53:ILE:O	44:w:315:PRO:HB3	2.13	0.48
39:p:54:GLU:HG3	39:p:55:LYS:N	2.29	0.48
40:r:403:THR:HA	40:r:406:TYR:CE2	2.48	0.48
42:u:83:THR:HA	42:u:86:TRP:CD1	2.49	0.48
42:u:88:CYS:HB3	42:u:100:CYS:SG	2.54	0.48
44:w:181:LYS:O	44:w:184:VAL:HG22	2.14	0.48
5:F:46:LYS:HE2	12:M:674:LEU:HD21	1.94	0.48
7:H:9:THR:HG23	7:H:16:VAL:HG22	1.95	0.48
7:H:15:ALA:O	7:H:78:GLU:HG2	2.14	0.48
12:M:450:LYS:HD2	12:M:453:GLN:HB2	1.96	0.48
13:N:69:ASN:OD1	13:N:112:ASN:ND2	2.46	0.48
16:Q:236:LEU:HD22	16:Q:240:LEU:CD2	2.44	0.48
19:U:11:ASN:OD1	19:U:15:LYS:NZ	2.47	0.48
33:j:28:ASN:OD1	33:j:28:ASN:N	2.44	0.48
39:p:28:GLU:OE2	39:p:34:ARG:NH1	2.43	0.48
42:u:96:LEU:HD12	42:u:99:HIS:HD2	1.77	0.48
44:w:132:GLN:HB2	44:w:173:MET:HE1	1.95	0.48
1:A:210:THR:HG23	1:A:224:ARG:H	1.78	0.48
21:W:51:MET:HA	41:s:313:SER:HB2	1.94	0.48
33:j:70:ALA:HB2	36:m:59:ILE:HG13	1.96	0.48
40:r:445:LEU:O	40:r:448:THR:HG22	2.13	0.48
44:w:330:LYS:HB2	44:w:330:LYS:HE3	1.62	0.48
6:G:93:ILE:HA	6:G:97:LYS:HZ1	1.79	0.48
11:L:90:GLY:HA3	15:P:238:PRO:HB2	1.96	0.48
14:O:222:ARG:CZ	14:O:225:CYS:HA	2.44	0.48
22:Y:51:THR:HG22	22:Y:53:SER:H	1.79	0.48
25:b:109:THR:HG23	27:d:19:ALA:CB	2.44	0.48
27:d:30:VAL:O	27:d:34:THR:HG23	2.14	0.48
33:j:103:ALA:O	33:j:107:THR:HG23	2.14	0.48
48:r:502:PLX:H51	48:r:502:PLX:H6	1.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:165:SER:HB3	44:w:245:PHE:CE1	2.48	0.48
12:M:326:VAL:HG22	12:M:582:VAL:HG11	1.96	0.47
48:g:201:PLX:H312	48:g:201:PLX:H211	1.96	0.47
39:p:63:LEU:O	39:p:64:LEU:HB3	2.13	0.47
6:G:76:LEU:HB3	6:G:80:LYS:HZ3	1.79	0.47
15:P:213:ASP:HB3	15:P:216:VAL:HG22	1.96	0.47
16:Q:217:VAL:CG2	16:Q:236:LEU:HD23	2.45	0.47
26:c:64:PRO:O	26:c:65:TYR:C	2.56	0.47
26:c:182:VAL:CG2	43:v:36:GLU:OE2	2.53	0.47
32:i:280:THR:O	32:i:284:MET:HG2	2.14	0.47
4:E:23:ARG:HH22	11:L:51:GLN:HA	1.79	0.47
16:Q:357:LYS:HD3	16:Q:364:SER:HB3	1.96	0.47
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	1.96	0.47
17:S:43:TYR:CZ	21:W:68:ARG:HG3	2.48	0.47
38:o:114:LYS:O	38:o:118:GLU:HG2	2.14	0.47
32:i:284:MET:HE1	40:r:159:PRO:HD3	1.97	0.47
35:l:526:LEU:HD12	35:l:530:PRO:HG2	1.97	0.47
38:o:35:GLU:O	38:o:39:ILE:HG22	2.14	0.47
41:s:193:THR:HG21	41:s:231:ILE:HG13	1.96	0.47
42:u:80:GLU:O	42:u:84:GLU:HG3	2.13	0.47
12:M:254:MET:HE2	12:M:289:LYS:HG2	1.96	0.47
14:O:66:ILE:HG21	14:O:81:PRO:HB2	1.96	0.47
15:P:81:PHE:HE1	15:P:83:GLU:OE2	1.96	0.47
16:Q:148:GLU:O	16:Q:152:SER:OG	2.30	0.47
21:W:5:LYS:HE2	21:W:5:LYS:HB3	1.79	0.47
33:j:68:GLU:HB2	33:j:98:LEU:HD21	1.97	0.47
35:l:233:LEU:HB3	35:l:234:PRO:HD3	1.96	0.47
35:l:277:THR:HG23	35:l:314:MET:HG3	1.97	0.47
35:l:557:TRP:O	35:l:561:ILE:HG12	2.14	0.47
46:A:502:FMN:O2'	47:A:503:NAI:O2N	2.33	0.47
24:a:168:TRP:CD2	30:g:2:THR:HG23	2.49	0.47
30:g:52:ARG:NE	32:i:318:GLU:OE1	2.39	0.47
55:g:202:CDL:H581	40:r:13:PRO:HB3	1.96	0.47
1:A:104:LYS:HG3	1:A:105:PRO:HD2	1.96	0.47
1:A:210:THR:HG22	1:A:223:PRO:HB3	1.96	0.47
1:A:366:ALA:HA	14:O:141:MET:HE1	1.97	0.47
4:E:119:LEU:HD11	12:M:628:GLU:OE1	2.15	0.47
9:J:286:ARG:HH22	9:J:358:THR:HG23	1.80	0.47
12:M:573:GLY:HA3	13:N:137:TRP:CD1	2.49	0.47
14:O:152:ILE:HG21	14:O:171:LEU:HD13	1.97	0.47
21:W:120:MET:SD	31:h:69:ARG:HD2	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:33:THR:OG1	26:c:35:ASP:OD1	2.23	0.47
26:c:113:ILE:HD11	26:c:116:ARG:HD2	1.97	0.47
35:l:338:MET:HE2	35:l:338:MET:HB3	1.84	0.47
40:r:342:MET:HE1	40:r:409:TYR:CE2	2.49	0.47
41:s:55:LEU:HD13	41:s:221:ALA:HB2	1.97	0.47
6:G:115:GLN:NE2	6:G:119:ILE:HD11	2.30	0.47
7:H:55:LYS:HA	7:H:58:MET:HG3	1.97	0.47
31:h:97:HIS:HA	31:h:102:GLU:HB3	1.96	0.47
35:l:141:PHE:HE2	40:r:375:LEU:HD11	1.79	0.47
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.50	0.47
3:C:92:VAL:HG11	56:s:401:UQ:HM32	1.96	0.47
20:V:66:ILE:HD11	20:V:101:LEU:HD13	1.97	0.47
20:V:69:ILE:HG21	20:V:100:THR:HG23	1.97	0.47
26:c:173:ASP:CG	26:c:176:LYS:HG2	2.40	0.47
34:k:37:MET:HG3	34:k:67:ALA:CB	2.45	0.47
44:w:210:PRO:O	44:w:214:ILE:HG22	2.15	0.47
2:B:150:THR:HG21	2:B:180:HIS:CD2	2.50	0.47
9:J:286:ARG:NH2	9:J:358:THR:HG23	2.30	0.47
41:s:253:GLU:O	41:s:257:ILE:HG12	2.15	0.47
44:w:171:GLU:O	44:w:175:ARG:HG2	2.15	0.47
1:A:50:ASP:OD1	10:K:74:ARG:NH1	2.48	0.46
1:A:185:ASN:C	1:A:187:CYS:H	2.23	0.46
20:V:107:SER:CB	20:V:110:ILE:HG22	2.45	0.46
27:d:43:ARG:HB3	27:d:44:PRO:HD3	1.98	0.46
32:i:72:MET:HB3	32:i:97:MET:HE1	1.96	0.46
55:i:401:CDL:H142	55:i:401:CDL:H171	1.73	0.46
16:Q:41:VAL:O	16:Q:45:GLU:HG2	2.14	0.46
16:Q:232:VAL:CG2	16:Q:356:ILE:HB	2.45	0.46
18:T:79:VAL:O	18:T:121:PRO:HD3	2.15	0.46
26:c:129:MET:HG2	35:l:528:TYR:CD1	2.50	0.46
40:r:86:LYS:HE3	40:r:86:LYS:HB2	1.55	0.46
14:O:222:ARG:NH2	14:O:226:GLU:O	2.40	0.46
53:Q:502:PEE:H16	53:Q:502:PEE:H21	1.76	0.46
6:X:141:PRO:O	6:X:145:VAL:HG23	2.16	0.46
35:l:337:ALA:O	35:l:341:MET:HG3	2.15	0.46
6:G:79:ILE:HG22	6:G:145:VAL:HG13	1.97	0.46
8:I:93:LYS:HB3	8:I:93:LYS:HE2	1.73	0.46
12:M:266:ARG:HG2	12:M:267:THR:HG23	1.96	0.46
15:P:153:ILE:O	15:P:178:PHE:HA	2.14	0.46
25:b:65:TYR:O	25:b:69:ILE:HG22	2.14	0.46
34:k:14:ILE:HD13	36:m:18:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:15:ALA:HB2	36:m:17:PHE:HE2	1.80	0.46
41:s:233:MET:HB3	41:s:233:MET:HE3	1.65	0.46
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.97	0.46
27:d:125:CYS:HB2	35:l:203:MET:HE1	1.96	0.46
32:i:41:ILE:HG13	34:k:73:LEU:HD21	1.97	0.46
32:i:213:LEU:HD11	55:i:401:CDL:H382	1.97	0.46
41:s:134:ARG:HG3	41:s:282:TYR:CZ	2.51	0.46
48:C:302:PLX:H311	48:C:302:PLX:H281	1.55	0.46
5:F:83:SER:O	5:F:87:VAL:HG22	2.16	0.46
55:a:201:CDL:HB21	53:l:703:PEE:H51	1.97	0.46
34:k:22:TYR:O	35:l:585:LYS:HG3	2.15	0.46
48:r:503:PLX:H121	48:r:503:PLX:H152	1.47	0.46
1:A:398:ARG:CG	1:A:403:ASP:HB2	2.45	0.46
9:J:192:ARG:NH1	9:J:260:GLY:O	2.49	0.46
12:M:251:ILE:HB	12:M:606:THR:HG22	1.98	0.46
55:a:201:CDL:H751	28:e:103:SER:HB2	1.98	0.46
5:F:55:ILE:HD13	12:M:381:LEU:HD23	1.97	0.46
16:Q:101:LEU:HD23	16:Q:106:VAL:HA	1.98	0.46
19:U:41:TYR:HD2	19:U:84:LEU:HD11	1.81	0.46
21:W:94:GLU:OE1	21:W:104:TRP:NE1	2.39	0.46
25:b:69:ILE:O	25:b:73:THR:HG23	2.16	0.46
26:c:126:TRP:HA	26:c:129:MET:HE2	1.98	0.46
27:d:24:THR:HG23	43:v:73:SER:HB3	1.97	0.46
35:l:127:THR:HG21	35:l:146:GLY:C	2.41	0.46
1:A:214:GLU:OE2	1:A:224:ARG:NE	2.48	0.46
13:N:85:GLU:HB2	13:N:98:PRO:HB3	1.98	0.46
14:O:208:LEU:HD23	14:O:208:LEU:HA	1.74	0.46
17:S:1:MET:O	17:S:4:GLU:HB2	2.16	0.46
25:b:81:ILE:HG23	53:l:703:PEE:H58	1.98	0.46
27:d:89:GLU:O	27:d:93:ARG:HG3	2.16	0.46
1:A:41:ILE:H	1:A:289:GLU:CD	2.24	0.46
4:E:98:LYS:HB3	4:E:102:HIS:HB2	1.98	0.46
14:O:224:SER:O	14:O:224:SER:OG	2.33	0.46
31:h:38:LYS:O	31:h:42:GLU:HG3	2.16	0.46
33:j:98:LEU:HA	33:j:98:LEU:HD23	1.66	0.46
41:s:126:LYS:O	41:s:130:ILE:HG12	2.16	0.46
44:w:180:ARG:NH1	44:w:316:GLU:OE2	2.44	0.46
4:E:80:ASP:N	4:E:80:ASP:OD1	2.42	0.45
13:N:3:LEU:O	13:N:6:VAL:HG22	2.15	0.45
15:P:103:HIS:CD2	15:P:105:ASN:HB2	2.51	0.45
17:S:68:ASN:ND2	42:u:19:LYS:HB3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:32:GLU:HG3	39:p:115:TYR:HA	1.97	0.45
34:k:80:MET:HE2	36:m:172:THR:HA	1.97	0.45
35:l:97:THR:HG22	35:l:101:MET:HE3	1.97	0.45
2:B:151:LYS:HA	3:C:141:GLY:HA2	1.97	0.45
5:F:23:LEU:O	5:F:57:GLU:HA	2.16	0.45
6:G:92:LYS:HE2	6:G:92:LYS:HB2	1.57	0.45
20:V:126:LYS:O	20:V:126:LYS:HD3	2.14	0.45
26:c:75:TYR:CG	26:c:76:PRO:HD2	2.50	0.45
42:u:82:PHE:HB2	42:u:107:PHE:CE1	2.52	0.45
1:A:117:ALA:O	1:A:118:ASP:C	2.58	0.45
2:B:135:ARG:HD3	2:B:141:ARG:HG3	1.98	0.45
8:I:66:PRO:HB3	15:P:79:SER:HA	1.97	0.45
11:L:158:LYS:NZ	12:M:67:GLU:O	2.41	0.45
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.51	0.45
17:S:54:ILE:HD11	31:h:106:PRO:HB3	1.98	0.45
20:V:41:ILE:HD13	20:V:55:ARG:HH11	1.82	0.45
34:k:23:ARG:HG2	36:m:23:LYS:HE2	1.98	0.45
34:k:57:ASN:HB3	36:m:143:ILE:HG13	1.99	0.45
36:m:57:PHE:HD1	36:m:61:LEU:HD12	1.81	0.45
40:r:126:LEU:HD21	40:r:153:THR:HG21	1.98	0.45
3:C:124:MET:HA	3:C:125:PRO:HD3	1.72	0.45
9:J:171:ASN:C	9:J:181:LEU:HD12	2.42	0.45
12:M:333:PHE:CE2	12:M:543:LYS:HD2	2.50	0.45
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.45	0.45
23:Z:31:THR:O	23:Z:35:LYS:HG2	2.15	0.45
40:r:73:LEU:HD22	40:r:103:GLN:HE21	1.82	0.45
4:E:15:THR:OG1	11:L:55:VAL:O	2.34	0.45
4:E:29:LYS:HZ1	49:G:201:8Q1:P24	2.39	0.45
10:K:87:LEU:HD12	14:O:66:ILE:HD11	1.99	0.45
53:Q:501:PEE:H37	53:Q:501:PEE:H60	1.98	0.45
20:V:26:THR:CG2	20:V:68:ALA:HB2	2.47	0.45
26:c:169:GLU:OE1	26:c:169:GLU:N	2.49	0.45
35:l:129:MET:HA	35:l:129:MET:HE2	1.97	0.45
48:r:502:PLX:H1C3	48:r:502:PLX:H22	1.62	0.45
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.98	0.45
32:i:257:LEU:HD12	32:i:334:THR:HG23	1.99	0.45
34:k:45:THR:HG23	36:m:52:LEU:HD13	1.98	0.45
35:l:511:LEU:HD23	35:l:511:LEU:HA	1.84	0.45
55:l:701:CDL:H382	55:l:701:CDL:H351	1.71	0.45
44:w:281:GLY:O	44:w:284:PRO:HD2	2.17	0.45
1:A:109:ARG:HG2	11:L:166:TRP:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ILE:HG23	1:A:235:VAL:HA	1.99	0.45
7:H:9:THR:O	7:H:76:GLN:NE2	2.50	0.45
35:l:292:ALA:HB2	35:l:304:PHE:HB3	1.97	0.45
41:s:37:PRO:O	41:s:44:GLY:HA3	2.17	0.45
43:v:39:MET:HB3	43:v:39:MET:HE2	1.54	0.45
27:d:31:THR:O	27:d:35:LYS:HG2	2.17	0.45
28:e:92:PHE:O	28:e:96:SER:HB2	2.16	0.45
7:H:77:ILE:HA	7:H:80:VAL:HG22	1.99	0.45
12:M:385:TYR:OH	12:M:527:ASP:OD1	2.27	0.45
14:O:140:CYS:HA	14:O:183:ALA:HB1	1.98	0.45
9:J:37:HIS:CE1	18:T:49:ASP:HA	2.52	0.45
14:O:132:ILE:HD11	14:O:169:PHE:HD2	1.82	0.45
14:O:197:THR:H	14:O:200:ASP:HB2	1.80	0.45
33:j:81:THR:C	33:j:83:ASN:H	2.24	0.45
35:l:452:ASN:HA	35:l:455:LYS:HG2	1.99	0.45
35:l:529:TYR:HB3	35:l:530:PRO:HD3	1.99	0.45
36:m:30:GLY:O	36:m:34:ILE:HG12	2.17	0.45
41:s:87:VAL:CG2	41:s:88:PRO:HD3	2.47	0.45
44:w:110:GLY:HA2	44:w:134:TRP:CD2	2.52	0.45
44:w:350:LYS:HA	44:w:350:LYS:HD3	1.78	0.45
3:C:71:CYS:HB3	16:Q:141:TYR:CB	2.48	0.44
26:c:38:PRO:HD2	38:o:70:TYR:CD2	2.53	0.44
27:d:117:GLU:HG3	27:d:124:ASN:HB2	1.98	0.44
38:o:61:GLU:HG2	38:o:66:ILE:HD11	1.98	0.44
41:s:141:SER:HB3	41:s:289:LEU:HD22	1.99	0.44
12:M:275:PRO:HB3	12:M:286:ILE:HG23	1.99	0.44
12:M:394:VAL:HG22	12:M:473:MET:HE1	1.98	0.44
12:M:395:GLU:OE2	12:M:417:ARG:NH1	2.33	0.44
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.49	0.44
43:v:22:MET:HE1	43:v:102:PHE:CD2	2.53	0.44
3:C:44:GLU:HB2	3:C:195:ARG:HH22	1.83	0.44
12:M:638:THR:O	12:M:642:VAL:HG23	2.18	0.44
6:X:113:LEU:O	6:X:116:VAL:HG12	2.17	0.44
24:a:70:LEU:HD22	28:e:87:MET:CE	2.43	0.44
27:d:127:LYS:HD2	27:d:127:LYS:N	2.33	0.44
32:i:117:GLU:OE1	35:l:587:TYR:HE2	2.00	0.44
32:i:326:LEU:HB3	32:i:327:PRO:HD3	2.00	0.44
33:j:104:TYR:O	33:j:108:GLN:HG2	2.17	0.44
36:m:23:LYS:N	36:m:24:PRO:HD3	2.33	0.44
8:I:70:MET:HE1	15:P:73:VAL:HG12	1.98	0.44
55:a:201:CDL:H341	55:a:201:CDL:H372	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:272:LEU:O	35:l:276:MET:HG3	2.18	0.44
1:A:134:ASP:OD1	1:A:137:LYS:HB2	2.16	0.44
1:A:267:ARG:HG3	1:A:293:SER:OG	2.18	0.44
1:A:398:ARG:HG3	1:A:403:ASP:HB2	1.99	0.44
6:G:138:LEU:HD23	6:G:143:GLU:HG3	1.98	0.44
9:J:114:ASP:O	9:J:118:LYS:HG2	2.18	0.44
14:O:158:ILE:HB	14:O:162:GLU:HG3	1.99	0.44
20:V:5:LEU:O	20:V:8:LYS:HG2	2.17	0.44
21:W:85:GLN:HG3	42:u:10:LEU:HD22	1.99	0.44
23:Z:43:ASP:OD1	39:p:38:ARG:NH2	2.43	0.44
27:d:106:ILE:HG13	27:d:135:VAL:HG21	2.00	0.44
34:k:19:LEU:HB2	34:k:32:CYS:HB3	1.99	0.44
35:l:221:ALA:HA	35:l:226:GLN:HG2	1.99	0.44
36:m:8:ILE:O	36:m:12:ILE:HG13	2.16	0.44
38:o:59:VAL:HG22	40:r:423:ILE:HG12	1.99	0.44
1:A:375:LYS:NZ	14:O:33:GLY:O	2.50	0.44
7:H:54:GLU:O	7:H:58:MET:HG3	2.18	0.44
16:Q:139:LEU:HD11	16:Q:424:ILE:HD13	1.99	0.44
55:g:202:CDL:H832	55:g:202:CDL:H862	1.70	0.44
32:i:221:HIS:HB2	32:i:323:MET:HE1	2.00	0.44
35:l:8:THR:HB	35:l:82:MET:HE2	1.99	0.44
11:L:111:LEU:O	11:L:112:MET:HB2	2.17	0.44
55:V:201:CDL:H601	55:V:201:CDL:H632	1.57	0.44
55:g:202:CDL:H362	55:g:202:CDL:H392	1.58	0.44
32:i:26:TRP:CH2	32:i:98:MET:HE3	2.53	0.44
39:p:29:SER:HB3	39:p:76:HIS:HD2	1.83	0.44
39:p:176:GLU:HG3	39:p:177:ARG:N	2.32	0.44
41:s:120:GLY:HA3	41:s:132:ALA:HB2	1.99	0.44
7:H:76:GLN:O	7:H:78:GLU:N	2.51	0.44
11:L:111:LEU:HD11	13:N:126:PRO:HG2	2.00	0.44
16:Q:184:ILE:HG21	16:Q:207:ARG:HG3	2.00	0.44
26:c:57:MET:HE2	26:c:62:TYR:HA	2.00	0.44
32:i:222:SER:O	32:i:224:ALA:N	2.51	0.44
35:l:36:VAL:HG13	35:l:122:LEU:HD22	2.00	0.44
40:r:290:SER:HA	40:r:319:HIS:HE2	1.83	0.44
9:J:166:HIS:HB3	9:J:200:ILE:HD13	1.99	0.44
15:P:75:GLN:HB3	15:P:87:PHE:CD1	2.53	0.44
35:l:108:MET:CE	35:l:240:PRO:HB3	2.48	0.44
36:m:42:GLY:HA2	53:m:201:PEE:H23	2.00	0.44
1:A:141:GLY:HA3	1:A:248:VAL:O	2.17	0.43
1:A:208:GLU:OE1	1:A:210:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:75:LYS:HE3	14:O:75:LYS:HB2	1.78	0.43
15:P:43:THR:HG23	15:P:47:ILE:HB	2.00	0.43
21:W:129:THR:HG22	21:W:132:GLU:OE2	2.18	0.43
28:e:116:GLU:O	28:e:120:ARG:HG3	2.18	0.43
30:g:15:PHE:O	30:g:80:ARG:HD2	2.18	0.43
32:i:45:MET:HE2	32:i:45:MET:HB3	1.72	0.43
33:j:69:ILE:HD11	41:s:144:VAL:HG13	1.99	0.43
1:A:75:TRP:CH2	14:O:249:LEU:HD12	2.52	0.43
1:A:338:ASP:OD1	1:A:341:ALA:HB3	2.18	0.43
12:M:185:PHE:CZ	12:M:221:ASN:HB2	2.53	0.43
26:c:94:HIS:O	26:c:98:ARG:N	2.51	0.43
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.53	0.43
55:l:701:CDL:H591	55:l:701:CDL:H622	1.67	0.43
40:r:371:PRO:O	40:r:448:THR:OG1	2.36	0.43
48:r:502:PLX:H301	48:r:502:PLX:H331	1.64	0.43
41:s:46:LEU:HD12	41:s:49:ILE:HD12	2.00	0.43
44:w:268:LYS:HZ3	44:w:272:ASP:CG	2.21	0.43
48:C:302:PLX:H1C3	48:C:302:PLX:H21	1.71	0.43
6:G:74:LEU:HD12	6:G:79:ILE:HD11	2.00	0.43
6:G:84:LEU:O	6:G:88:LYS:HG2	2.18	0.43
9:J:275:ASP:OD1	9:J:275:ASP:N	2.51	0.43
6:X:116:VAL:HG11	39:p:20:TYR:HD2	1.83	0.43
25:b:109:THR:HG23	27:d:19:ALA:HB3	2.01	0.43
27:d:140:GLN:O	27:d:144:SER:HB2	2.18	0.43
30:g:4:MET:HE2	30:g:4:MET:HB3	1.96	0.43
32:i:21:MET:HE3	32:i:136:LEU:HB3	2.00	0.43
33:j:29:ALA:HB3	53:j:201:PEE:H12	2.00	0.43
7:H:81:ILE:HG22	7:H:85:GLU:OE2	2.19	0.43
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.54	0.43
9:J:195:PHE:HB3	9:J:198:ALA:HB2	1.99	0.43
14:O:222:ARG:HH21	14:O:226:GLU:C	2.22	0.43
21:W:86:MET:HE2	21:W:124:LEU:HB3	1.99	0.43
34:k:15:ALA:HB2	36:m:17:PHE:CE2	2.53	0.43
42:u:11:GLU:HA	42:u:14:LYS:HG3	2.01	0.43
1:A:311:TRP:CD1	1:A:329:LYS:HE3	2.54	0.43
8:I:29:GLN:HE21	13:N:52:ASN:HB3	1.84	0.43
11:L:80:PHE:HE1	11:L:100:GLU:HG2	1.82	0.43
24:a:78:THR:HG21	28:e:96:SER:HA	1.99	0.43
30:g:3:MET:HE2	30:g:3:MET:HB2	1.89	0.43
32:i:95:MET:CE	32:i:149:ILE:HG22	2.48	0.43
35:l:176:ARG:HA	35:l:176:ARG:HD2	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:70:ASN:ND2	49:G:201:8Q1:O4	2.43	0.43
9:J:111:LYS:HE3	9:J:139:PHE:CE2	2.54	0.43
9:J:129:LEU:HD23	9:J:167:ILE:HG13	2.00	0.43
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	2.00	0.43
55:V:201:CDL:H312	55:V:201:CDL:HA62	1.70	0.43
43:v:70:LYS:HB3	43:v:70:LYS:HE3	1.91	0.43
3:C:44:GLU:HA	3:C:47:VAL:HG22	2.00	0.43
55:i:401:CDL:H141	55:i:401:CDL:H371	2.00	0.43
35:l:245:ALA:HB2	35:l:340:PHE:HB3	2.01	0.43
14:O:146:ASP:OD1	14:O:146:ASP:N	2.51	0.43
17:S:47:LEU:HD22	42:u:22:SER:HB2	1.99	0.43
25:b:9:LYS:HB3	25:b:9:LYS:HE3	1.79	0.43
26:c:116:ARG:HG2	53:l:702:PEE:H49	2.01	0.43
32:i:277:ILE:O	32:i:281:LEU:HG	2.19	0.43
43:v:34:ARG:O	43:v:34:ARG:HG3	2.18	0.43
43:v:46:MET:HE3	43:v:56:ARG:HB3	2.00	0.43
5:F:40:ARG:NH1	5:F:84:ALA:HB1	2.28	0.43
6:G:88:LYS:NZ	6:G:98:LEU:HD11	2.33	0.43
13:N:139:PRO:HA	13:N:140:PRO:HD3	1.84	0.43
14:O:46:GLU:N	14:O:46:GLU:OE2	2.52	0.43
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	2.00	0.43
21:W:111:PHE:CE2	31:h:65:GLU:HG3	2.53	0.43
22:Y:58:ALA:HA	35:l:371:THR:HG21	2.00	0.43
25:b:4:TYR:CB	25:b:9:LYS:HG2	2.48	0.43
27:d:80:LYS:HD3	27:d:80:LYS:HA	1.71	0.43
28:e:72:ASP:HB3	39:p:108:HIS:HE2	1.84	0.43
48:j:203:PLX:H22	48:j:203:PLX:H1C3	1.87	0.43
35:l:127:THR:HG21	35:l:147:VAL:N	2.34	0.43
38:o:59:VAL:HG22	40:r:423:ILE:HG23	2.01	0.43
39:p:44:MET:O	39:p:48:PHE:HB2	2.19	0.43
44:w:176:GLN:NE2	44:w:236:ASP:OD2	2.51	0.43
1:A:29:LYS:HE3	1:A:32:PHE:CE2	2.54	0.43
1:A:56:ALA:HB1	1:A:61:ASP:HB2	2.01	0.43
1:A:78:GLY:O	1:A:82:THR:HG23	2.19	0.43
1:A:187:CYS:HB2	1:A:189:SER:HB3	2.01	0.43
9:J:141:PHE:HE1	9:J:180:TYR:HD2	1.66	0.43
12:M:58:MET:HE2	12:M:60:ILE:HD13	2.01	0.43
21:W:88:ARG:O	21:W:92:GLU:HG2	2.18	0.43
21:W:134:LEU:HD21	36:m:1:MET:HA	2.00	0.43
23:Z:57:PHE:CG	35:l:435:PRO:HG3	2.54	0.43
26:c:62:TYR:OH	26:c:74:ASP:O	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:445:GLU:O	35:l:447:ASN:N	2.45	0.43
37:n:27:LEU:HD23	37:n:27:LEU:HA	1.84	0.43
41:s:26:LYS:HE2	41:s:37:PRO:O	2.19	0.43
41:s:51:ASP:HB3	56:s:401:UQ:H8	2.00	0.43
41:s:92:PRO:HB3	41:s:255:TYR:CD1	2.54	0.43
43:v:25:PHE:CE2	43:v:108:LEU:HB3	2.54	0.43
3:C:125:PRO:HG3	41:s:61:LEU:CD1	2.49	0.42
12:M:390:THR:HA	12:M:600:GLU:HG2	2.01	0.42
13:N:32:ASP:OD2	13:N:58:ARG:NH2	2.51	0.42
32:i:115:VAL:HB	32:i:116:PRO:HD3	2.00	0.42
32:i:128:LEU:HD12	32:i:216:PHE:HB3	2.00	0.42
35:l:7:LEU:O	35:l:11:THR:HG23	2.19	0.42
38:o:32:ALA:O	38:o:36:ARG:HG3	2.19	0.42
9:J:83:PRO:HA	9:J:106:MET:O	2.18	0.42
12:M:373:PRO:HD2	12:M:481:LEU:HD13	2.01	0.42
12:M:485:ASP:OD2	12:M:680:LEU:HB3	2.19	0.42
13:N:68:MET:SD	13:N:81:MET:HB3	2.59	0.42
27:d:100:GLN:O	27:d:104:ASN:ND2	2.48	0.42
28:e:110:PRO:HG2	28:e:112:TYR:CE1	2.53	0.42
32:i:133:TRP:HE3	55:i:401:CDL:H391	1.83	0.42
34:k:22:TYR:O	35:l:585:LYS:HE2	2.19	0.42
34:k:66:PHE:O	34:k:70:GLU:HG2	2.19	0.42
6:X:75:THR:OG1	6:X:156:GLU:O	2.28	0.42
35:l:49:VAL:HB	35:l:50:PRO:HD3	2.01	0.42
42:u:105:ALA:O	42:u:109:GLU:HG2	2.19	0.42
12:M:578:PRO:HB3	13:N:140:PRO:HG2	2.02	0.42
12:M:650:SER:OG	12:M:652:ASN:OD1	2.27	0.42
15:P:211:ARG:NH2	15:P:222:GLU:OE1	2.51	0.42
24:a:147:ALA:HB2	40:r:173:SER:HB2	2.01	0.42
27:d:24:THR:CG2	43:v:73:SER:HB3	2.47	0.42
35:l:534:HIS:CD2	53:l:702:PEE:H16	2.54	0.42
53:m:201:PEE:H53	53:m:201:PEE:H59	1.84	0.42
41:s:35:LYS:HE2	41:s:35:LYS:HB3	1.82	0.42
46:A:502:FMN:N5	47:A:503:NAI:H4N	2.35	0.42
2:B:41:VAL:HA	8:I:113:LEU:HB3	2.01	0.42
3:C:133:MET:HG3	3:C:168:PRO:HG2	2.02	0.42
5:F:64:LYS:HB2	5:F:64:LYS:HE2	1.89	0.42
6:G:94:ASP:OD2	6:G:97:LYS:HE3	2.20	0.42
7:H:94:MET:SD	7:H:99:PRO:HG3	2.60	0.42
13:N:43:LYS:HE2	13:N:111:THR:O	2.20	0.42
15:P:89:HIS:CE1	15:P:91:ASP:OD1	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:149:GLN:O	16:Q:153:LEU:HG	2.20	0.42
35:l:44:PHE:HB2	35:l:94:LEU:HB3	2.01	0.42
40:r:357:THR:O	40:r:361:VAL:HG23	2.20	0.42
1:A:388:GLY:O	1:A:392:MET:HG3	2.20	0.42
2:B:114:ILE:HD12	12:M:130:ILE:HG23	2.02	0.42
1:A:102:MET:CG	1:A:149:MET:HB3	2.49	0.42
1:A:195:VAL:O	10:K:97:ARG:NH1	2.48	0.42
12:M:178:GLN:HG2	12:M:204:MET:HE2	2.00	0.42
21:W:28:ARG:HA	21:W:28:ARG:HD2	1.91	0.42
22:Y:68:TRP:CZ2	22:Y:72:ARG:HD2	2.54	0.42
25:b:70:PHE:O	25:b:74:HIS:HB2	2.19	0.42
35:l:108:MET:HE1	35:l:240:PRO:HB3	2.02	0.42
42:u:47:ARG:NH2	42:u:53:PRO:HG3	2.35	0.42
42:u:108:ASP:O	42:u:111:VAL:HG22	2.20	0.42
44:w:223:ASN:HB3	44:w:226:GLU:HB2	2.02	0.42
1:A:391:TRP:O	1:A:395:VAL:HG23	2.20	0.42
5:F:42:VAL:O	5:F:46:LYS:HG2	2.20	0.42
9:J:73:LEU:O	9:J:78:SER:OG	2.27	0.42
10:K:73:TYR:CZ	10:K:75:ASN:HB3	2.55	0.42
6:X:82:ARG:HD2	6:X:125:GLU:OE1	2.20	0.42
40:r:197:LEU:HD21	48:r:502:PLX:H142	2.01	0.42
40:r:300:ALA:O	40:r:308:SER:HB3	2.19	0.42
3:C:76:MET:HE2	3:C:173:LEU:HD21	2.01	0.42
5:F:65:LEU:HB2	5:F:79:LEU:HD11	2.01	0.42
12:M:346:VAL:H	12:M:521:SER:HB3	1.85	0.42
13:N:53:LYS:HD3	13:N:53:LYS:HA	1.80	0.42
14:O:164:THR:CG2	14:O:169:PHE:H	2.33	0.42
19:U:78:LEU:HD23	19:U:78:LEU:HA	1.86	0.42
20:V:50:LEU:O	20:V:53:VAL:HG12	2.20	0.42
48:g:201:PLX:H22	48:g:201:PLX:H1C3	1.77	0.42
1:A:132:ARG:NH2	14:O:224:SER:HB2	2.35	0.42
1:A:185:ASN:O	1:A:187:CYS:N	2.53	0.42
4:E:40:TYR:CD1	6:G:120:MET:SD	3.13	0.42
7:H:56:LEU:HA	7:H:59:VAL:HG12	2.02	0.42
8:I:6:ARG:NH2	8:I:10:LEU:HD11	2.35	0.42
11:L:51:GLN:HB3	11:L:52:LEU:HD22	2.02	0.42
12:M:73:GLY:HA2	51:M:803:FES:S2	2.59	0.42
55:V:201:CDL:H592	55:V:201:CDL:H562	1.80	0.42
6:X:116:VAL:O	6:X:120:MET:HG3	2.20	0.42
24:a:159:LEU:HD23	24:a:159:LEU:HA	1.89	0.42
25:b:92:ALA:O	27:d:4:SER:OG	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:101:TRP:CE3	38:o:47:TYR:HB2	2.55	0.42
48:g:201:PLX:H351	32:i:339:MET:HB2	2.02	0.42
31:h:37:GLU:HB2	31:h:63:PHE:CZ	2.55	0.42
35:l:419:THR:HA	35:l:422:TYR:CE2	2.55	0.42
40:r:266:MET:O	40:r:269:MET:HG2	2.20	0.42
43:v:108:LEU:HD23	43:v:108:LEU:HA	1.93	0.42
8:I:70:MET:HE2	15:P:66:ALA:HB1	2.02	0.41
12:M:209:TYR:CZ	14:O:41:HIS:HB2	2.54	0.41
15:P:152:PRO:HB3	15:P:177:PHE:HD2	1.85	0.41
18:T:119:ARG:HG2	18:T:120:GLN:O	2.21	0.41
6:X:93:ILE:HD12	6:X:108:LEU:HD13	2.01	0.41
30:g:44:GLY:HA2	30:g:66:TYR:CD2	2.54	0.41
32:i:95:MET:HE1	32:i:145:ILE:HD12	2.02	0.41
35:l:355:ASP:CG	35:l:357:ARG:HE	2.28	0.41
55:l:701:CDL:H391	55:l:701:CDL:H421	1.71	0.41
38:o:107:THR:O	38:o:111:LYS:HG3	2.20	0.41
39:p:136:GLU:HG2	39:p:165:PRO:HA	2.02	0.41
48:r:502:PLX:H181	48:r:502:PLX:H212	1.81	0.41
48:C:302:PLX:H82	48:C:302:PLX:H252	2.02	0.41
7:H:44:TYR:HB2	15:P:68:ILE:HG23	2.00	0.41
8:I:42:PRO:HD3	21:W:6:VAL:HG13	2.03	0.41
12:M:716:GLU:O	12:M:716:GLU:HG2	2.20	0.41
33:j:25:PRO:HG3	41:s:56:PHE:O	2.20	0.41
35:l:331:MET:HE3	35:l:387:THR:O	2.19	0.41
42:u:59:GLU:O	42:u:63:VAL:HG13	2.20	0.41
1:A:201:ALA:O	14:O:119:TYR:HB3	2.20	0.41
3:C:167:PRO:HG3	16:Q:222:MET:SD	2.61	0.41
4:E:29:LYS:NZ	49:G:201:8Q1:O3	2.53	0.41
6:G:103:HIS:CD2	6:G:139:MET:HB3	2.55	0.41
6:X:87:LEU:HD23	6:X:87:LEU:HA	1.89	0.41
22:Y:98:GLY:HA3	43:v:104:ARG:NH1	2.36	0.41
26:c:109:LEU:O	26:c:113:ILE:HG23	2.20	0.41
28:e:66:LEU:HD23	28:e:66:LEU:HA	1.89	0.41
28:e:97:ILE:O	28:e:101:LEU:HB2	2.20	0.41
31:h:94:PRO:HB2	31:h:99:LEU:HD21	2.00	0.41
40:r:207:MET:HG2	40:r:298:ILE:HG12	2.00	0.41
41:s:71:PHE:CD1	41:s:71:PHE:C	2.98	0.41
41:s:137:ALA:HB3	41:s:282:TYR:OH	2.20	0.41
44:w:279:ASP:OD1	44:w:279:ASP:N	2.52	0.41
1:A:53:LEU:O	1:A:57:GLN:HG2	2.20	0.41
1:A:130:ILE:HD11	1:A:245:VAL:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:GLU:CD	1:A:210:THR:HG22	2.46	0.41
2:B:79:ARG:HA	8:I:12:ARG:NH2	2.36	0.41
27:d:43:ARG:O	27:d:47:LEU:HG	2.19	0.41
33:j:4:MET:SD	53:m:201:PEE:H21	2.61	0.41
42:u:38:LYS:HB3	42:u:39:PRO:HD3	2.01	0.41
2:B:76:TYR:CE1	41:s:33:LEU:HB2	2.55	0.41
4:E:27:GLU:H	4:E:27:GLU:HG3	1.66	0.41
4:E:29:LYS:NZ	49:G:201:8Q1:P24	2.93	0.41
5:F:89:ARG:HH11	5:F:89:ARG:HG2	1.85	0.41
12:M:354:LEU:HD12	12:M:354:LEU:HA	1.88	0.41
12:M:389:THR:O	12:M:390:THR:OG1	2.30	0.41
14:O:156:LEU:HD21	14:O:205:ILE:HD13	2.02	0.41
19:U:24:ALA:HB2	53:j:202:PEE:H72	2.02	0.41
25:b:117:ILE:HD11	27:d:16:ARG:NH2	2.35	0.41
32:i:263:LYS:HB2	32:i:263:LYS:HE3	1.84	0.41
35:l:350:LEU:HD12	35:l:359:MET:HE2	2.02	0.41
40:r:233:ALA:HA	40:r:320:GLY:HA2	2.01	0.41
40:r:455:LEU:HD23	40:r:455:LEU:HA	1.94	0.41
43:v:69:CYS:HB3	43:v:80:CYS:HB2	1.89	0.41
44:w:57:SER:O	44:w:156:GLY:HA3	2.20	0.41
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.56	0.41
4:E:87:LYS:HB2	4:E:87:LYS:HE3	1.78	0.41
5:F:88:THR:O	5:F:92:GLU:HG2	2.20	0.41
7:H:41:ASN:OD1	7:H:41:ASN:N	2.53	0.41
9:J:178:SER:HB3	9:J:181:LEU:HD23	2.02	0.41
13:N:101:LYS:HB3	13:N:101:LYS:HE2	1.77	0.41
20:V:133:TRP:CZ3	53:r:501:PEE:H51	2.55	0.41
21:W:30:LEU:HB3	21:W:35:MET:HE3	2.02	0.41
32:i:221:HIS:O	32:i:319:HIS:HE1	2.03	0.41
35:l:401:MET:HE3	35:l:401:MET:HB3	1.79	0.41
36:m:70:TYR:CE1	36:m:74:MET:HE2	2.55	0.41
44:w:314:LEU:O	44:w:318:THR:HG22	2.20	0.41
1:A:202:GLY:N	14:O:121:MET:HG3	2.36	0.41
3:C:80:ALA:HA	3:C:86:MET:HG2	2.02	0.41
3:C:192:ILE:HG21	9:J:86:CYS:HA	2.02	0.41
6:G:93:ILE:HD11	6:G:110:LEU:HD21	2.02	0.41
7:H:64:ASP:HB3	7:H:67:LYS:HG3	2.01	0.41
8:I:74:LYS:HA	8:I:74:LYS:HD2	1.79	0.41
26:c:64:PRO:O	26:c:65:TYR:O	2.38	0.41
30:g:74:GLY:O	30:g:78:LEU:HG	2.21	0.41
39:p:138:LYS:HB3	39:p:138:LYS:HE3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:172:ILE:HG13	41:s:176:PHE:HD2	1.85	0.41
41:s:221:ALA:O	41:s:225:MET:HG2	2.20	0.41
56:s:401:UQ:H111	56:s:401:UQ:H72	1.83	0.41
42:u:80:GLU:N	42:u:81:PRO:CD	2.84	0.41
47:A:503:NAI:H2D	47:A:503:NAI:H6N	1.68	0.41
5:F:41:TYR:CD1	5:F:41:TYR:C	2.98	0.41
12:M:548:LEU:HD12	12:M:548:LEU:HA	1.89	0.41
14:O:98:MET:HE2	14:O:116:ALA:CB	2.51	0.41
16:Q:393:PRO:HA	16:Q:413:SER:O	2.21	0.41
26:c:164:ASN:HA	26:c:181:VAL:CG2	2.51	0.41
32:i:284:MET:O	32:i:287:LEU:HB2	2.20	0.41
40:r:127:VAL:HB	40:r:128:PRO:HD3	2.01	0.41
1:A:73:PRO:HD3	1:A:147:ARG:NH2	2.36	0.41
2:B:210:LEU:HD23	2:B:210:LEU:HA	1.83	0.41
48:C:302:PLX:H31	13:N:75:TRP:CE3	2.55	0.41
9:J:268:PRO:HG2	9:J:344:PRO:HA	2.02	0.41
50:J:401:NDP:H2N	50:J:401:NDP:H2D	1.84	0.41
12:M:338:VAL:HG21	12:M:361:VAL:CG1	2.50	0.41
12:M:377:ALA:HB2	12:M:668:ALA:HA	2.02	0.41
12:M:405:THR:OG1	12:M:410:GLU:OE1	2.36	0.41
13:N:85:GLU:HG2	13:N:86:TRP:H	1.85	0.41
15:P:125:ARG:HD3	15:P:126:PHE:CZ	2.55	0.41
15:P:193:PHE:CE2	15:P:197:PRO:HG3	2.55	0.41
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.56	0.41
16:Q:383:LYS:HA	16:Q:383:LYS:HD2	1.93	0.41
19:U:50:PRO:HB2	21:W:69:ILE:HD11	2.03	0.41
21:W:130:ASN:HB3	36:m:1:MET:N	2.36	0.41
26:c:173:ASP:OD2	26:c:176:LYS:CG	2.69	0.41
27:d:97:LYS:HE3	27:d:97:LYS:HB3	1.88	0.41
32:i:170:LEU:HD11	32:i:288:LEU:HD22	2.03	0.41
35:l:284:THR:O	35:l:288:THR:OG1	2.32	0.41
35:l:375:ILE:HD12	35:l:458:LEU:HD11	2.03	0.41
37:n:50:ARG:HB2	37:n:53:GLU:HB2	2.02	0.41
39:p:20:TYR:HB2	39:p:48:PHE:CZ	2.56	0.41
41:s:197:PRO:HB3	41:s:278:PRO:O	2.20	0.41
42:u:60:GLY:O	42:u:63:VAL:HG22	2.20	0.41
43:v:33:GLU:OE2	43:v:35:LYS:NZ	2.38	0.41
3:C:184:ILE:O	3:C:187:GLU:HG2	2.21	0.41
7:H:90:LEU:HB2	15:P:102:ASP:HB3	2.02	0.41
9:J:270:ARG:O	9:J:374:THR:OG1	2.21	0.41
11:L:174:THR:HG21	14:O:114:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:382:ARG:HA	12:M:385:TYR:CE1	2.56	0.41
16:Q:271:ARG:NH1	41:s:279:ARG:O	2.50	0.41
20:V:51:GLU:OE2	20:V:51:GLU:N	2.54	0.41
49:X:201:8Q1:C31	39:p:52:LYS:HG3	2.51	0.41
33:j:70:ALA:HA	33:j:73:LEU:HD12	2.03	0.41
36:m:57:PHE:CZ	41:s:111:LEU:HG	2.56	0.41
40:r:6:ILE:O	40:r:10:MET:HG2	2.21	0.41
40:r:202:ALA:O	40:r:205:VAL:HG12	2.21	0.41
41:s:113:VAL:HG22	41:s:136:VAL:HG22	2.03	0.41
44:w:254:GLU:CD	44:w:276:LEU:HD13	2.46	0.41
1:A:43:THR:HB	14:O:238:PRO:HB3	2.03	0.40
1:A:326:LEU:CD1	1:A:363:ILE:HD11	2.51	0.40
14:O:69:ASN:HD22	14:O:69:ASN:HA	1.63	0.40
28:e:55:LEU:HB2	44:w:318:THR:HG23	2.03	0.40
32:i:106:LEU:HG	32:i:138:PRO:HB2	2.01	0.40
32:i:263:LYS:HG3	32:i:264:TRP:H	1.85	0.40
35:l:230:HIS:N	35:l:231:PRO:HD3	2.36	0.40
38:o:48:LEU:HB3	39:p:166:LEU:HD13	2.04	0.40
43:v:66:LEU:O	43:v:70:LYS:HG2	2.21	0.40
1:A:102:MET:O	1:A:102:MET:HG3	2.19	0.40
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.56	0.40
6:G:106:LYS:HE2	6:G:106:LYS:HB3	1.93	0.40
8:I:46:SER:O	8:I:52:ASN:ND2	2.53	0.40
14:O:187:GLN:HG3	14:O:192:TYR:CE1	2.56	0.40
16:Q:137:ASP:OD1	16:Q:144:MET:HB3	2.21	0.40
55:g:202:CDL:H121	40:r:135:ARG:HH21	1.86	0.40
35:l:407:TRP:O	35:l:411:MET:HG2	2.21	0.40
1:A:408:GLU:O	1:A:411:SER:HB3	2.21	0.40
4:E:123:TYR:CE1	12:M:320:GLU:HG3	2.56	0.40
8:I:107:SER:C	8:I:109:ASP:H	2.29	0.40
9:J:37:HIS:O	9:J:40:LEU:N	2.42	0.40
12:M:354:LEU:HD22	12:M:548:LEU:HD22	2.03	0.40
12:M:372:PHE:H	12:M:532:PRO:HB2	1.86	0.40
14:O:169:PHE:CE1	14:O:209:LYS:HG3	2.56	0.40
14:O:177:LEU:O	14:O:192:TYR:OH	2.32	0.40
53:Q:501:PEE:H67	32:i:284:MET:O	2.21	0.40
17:S:34:LYS:HB2	17:S:34:LYS:HE3	1.81	0.40
34:k:3:LEU:HD23	36:m:7:PHE:CE1	2.57	0.40
38:o:73:SER:OG	38:o:74:ALA:N	2.55	0.40
39:p:63:LEU:C	39:p:65:ARG:H	2.28	0.40
40:r:151:PHE:O	40:r:152:TYR:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:404:ALA:O	40:r:405:LEU:C	2.64	0.40
6:G:120:MET:O	6:G:123:GLU:HB2	2.22	0.40
15:P:117:VAL:HB	15:P:127:GLU:HG2	2.03	0.40
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.86	0.40
32:i:21:MET:CE	32:i:136:LEU:HB3	2.51	0.40
35:l:71:LEU:HD23	40:r:307:TRP:CH2	2.57	0.40
35:l:260:LEU:HD23	35:l:260:LEU:HA	1.89	0.40
41:s:101:GLY:O	41:s:105:MET:HG3	2.21	0.40
4:E:41:ARG:O	4:E:44:PRO:HD2	2.22	0.40
12:M:546:PHE:CD1	12:M:567:ILE:HB	2.56	0.40
13:N:42:ASP:OD2	13:N:44:TYR:HD1	2.04	0.40
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.56	0.40
18:T:84:ILE:HD12	18:T:84:ILE:HA	1.82	0.40
22:Y:62:SER:HG	35:l:371:THR:HG1	1.61	0.40
23:Z:23:LYS:HD3	23:Z:23:LYS:HA	1.90	0.40
24:a:106:VAL:HG23	37:n:50:ARG:NH2	2.32	0.40
26:c:43:LYS:HG2	26:c:47:GLU:OE1	2.21	0.40
32:i:72:MET:CE	34:k:43:MET:HE1	2.52	0.40
55:i:401:CDL:OB4	44:w:40:PRO:HG3	2.21	0.40
33:j:28:ASN:ND2	33:j:30:TYR:OH	2.55	0.40
35:l:401:MET:SD	35:l:482:MET:HG2	2.61	0.40
43:v:17:PRO:HB3	43:v:105:GLU:HG2	2.04	0.40
43:v:35:LYS:HA	43:v:35:LYS:HD3	1.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/433 (99%)	413 (96%)	16 (4%)	0	100	100
2	B	174/176 (99%)	169 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
4	E	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
5	F	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
6	G	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
8	I	93/112 (83%)	82 (88%)	11 (12%)	0	100	100
9	J	289/342 (84%)	274 (95%)	14 (5%)	1 (0%)	36	67
10	K	40/43 (93%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	661 (96%)	27 (4%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	204 (95%)	11 (5%)	0	100	100
15	P	206/208 (99%)	196 (95%)	10 (5%)	0	100	100
16	Q	412/430 (96%)	400 (97%)	12 (3%)	0	100	100
17	S	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
18	T	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
19	U	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
20	V	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	18	49
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%)	134 (97%)	4 (3%)	0	100	100
25	b	99/126 (79%)	90 (91%)	7 (7%)	2 (2%)	6	25
26	c	154/156 (99%)	142 (92%)	11 (7%)	1 (1%)	21	52
27	d	173/175 (99%)	168 (97%)	4 (2%)	1 (1%)	21	52
28	e	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
29	f	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
30	g	119/122 (98%)	114 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
32	i	345/347 (99%)	331 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	j	95/115 (83%)	89 (94%)	6 (6%)	0	100	100
34	k	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
35	l	601/603 (100%)	573 (95%)	28 (5%)	0	100	100
36	m	125/175 (71%)	111 (89%)	14 (11%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	119 (94%)	7 (6%)	0	100	100
39	p	176/178 (99%)	165 (94%)	10 (6%)	1 (1%)	21	52
40	r	457/459 (100%)	442 (97%)	15 (3%)	0	100	100
41	s	299/318 (94%)	284 (95%)	15 (5%)	0	100	100
42	u	169/171 (99%)	162 (96%)	6 (4%)	1 (1%)	21	52
43	v	122/124 (98%)	117 (96%)	5 (4%)	0	100	100
44	w	318/320 (99%)	304 (96%)	13 (4%)	1 (0%)	36	67
All	All	8029/8322 (96%)	7679 (96%)	341 (4%)	9 (0%)	49	78

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
42	u	154	ALA
9	J	38	HIS
27	d	22	PRO
44	w	123	SER
25	b	37	PRO
25	b	36	PRO
20	V	46	PRO
26	c	64	PRO
39	p	174	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	340/346 (98%)	340 (100%)	0	100	100
2	B	151/151 (100%)	149 (99%)	2 (1%)	61	77
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	75/81 (93%)	75 (100%)	0	100	100
6	X	77/81 (95%)	77 (100%)	0	100	100
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	86 (99%)	1 (1%)	65	78
9	J	253/296 (86%)	252 (100%)	1 (0%)	84	86
10	K	41/42 (98%)	41 (100%)	0	100	100
11	L	113/113 (100%)	113 (100%)	0	100	100
12	M	579/580 (100%)	578 (100%)	1 (0%)	87	89
13	N	130/130 (100%)	129 (99%)	1 (1%)	73	81
14	O	183/183 (100%)	182 (100%)	1 (0%)	81	85
15	P	190/190 (100%)	189 (100%)	1 (0%)	81	85
16	Q	361/370 (98%)	360 (100%)	1 (0%)	86	87
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	99/101 (98%)	98 (99%)	1 (1%)	68	79
21	W	123/123 (100%)	123 (100%)	0	100	100
22	Y	59/63 (94%)	58 (98%)	1 (2%)	53	74
23	Z	65/65 (100%)	65 (100%)	0	100	100
24	a	122/122 (100%)	122 (100%)	0	100	100
25	b	96/119 (81%)	95 (99%)	1 (1%)	68	79
26	c	139/141 (99%)	139 (100%)	0	100	100
27	d	154/155 (99%)	153 (99%)	1 (1%)	78	83
28	e	99/99 (100%)	99 (100%)	0	100	100
29	f	35/45 (78%)	35 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	g	107/109 (98%)	107 (100%)	0	100	100
31	h	93/93 (100%)	93 (100%)	0	100	100
32	i	310/311 (100%)	308 (99%)	2 (1%)	78	83
33	j	87/100 (87%)	87 (100%)	0	100	100
34	k	85/85 (100%)	84 (99%)	1 (1%)	63	78
35	l	535/537 (100%)	534 (100%)	1 (0%)	87	89
36	m	98/141 (70%)	96 (98%)	2 (2%)	48	72
37	n	52/53 (98%)	52 (100%)	0	100	100
38	o	112/113 (99%)	112 (100%)	0	100	100
39	p	157/159 (99%)	157 (100%)	0	100	100
40	r	410/410 (100%)	410 (100%)	0	100	100
41	s	263/275 (96%)	262 (100%)	1 (0%)	84	86
42	u	150/153 (98%)	150 (100%)	0	100	100
43	v	102/111 (92%)	102 (100%)	0	100	100
44	w	281/283 (99%)	281 (100%)	0	100	100
All	All	7033/7246 (97%)	7013 (100%)	20 (0%)	84	87

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	146	ASP
2	B	165	ASP
8	I	7	VAL
9	J	206	ILE
12	M	311	LYS
13	N	144	TYR
14	O	234	LEU
15	P	110	SER
16	Q	156	GLU
20	V	95	CYS
22	Y	90	SER
25	b	122	GLU
27	d	111	LYS
32	i	17	THR
32	i	268	GLN
34	k	91	GLN
35	l	586	LEU

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Mol	Chain	Res	Type
36	m	41	CYS
36	m	56	VAL
41	s	111	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	ASN
1	A	346	GLN
1	A	393	ASN
4	E	26	ASN
4	E	99	GLN
5	F	73	GLN
5	F	76	ASN
6	G	142	GLN
7	H	50	GLN
7	H	73	GLN
8	I	25	GLN
9	J	122	HIS
9	J	251	ASN
9	J	341	GLN
9	J	356	HIS
12	M	30	ASN
12	M	123	ASN
12	M	202	ASN
12	M	278	HIS
12	M	336	ASN
12	M	388	ASN
12	M	464	GLN
12	M	540	ASN
12	M	666	GLN
12	M	669	ASN
15	P	82	ASN
15	P	131	ASN
15	P	181	HIS
16	Q	147	ASN
16	Q	160	ASN
16	Q	233	HIS
16	Q	234	GLN
16	Q	250	ASN
18	T	63	ASN
18	T	117	GLN

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Mol	Chain	Res	Type
18	T	123	HIS
20	V	7	HIS
22	Y	46	GLN
23	Z	48	ASN
24	a	132	ASN
25	b	14	GLN
25	b	89	HIS
25	b	126	GLN
26	c	154	GLN
27	d	107	GLN
27	d	124	ASN
29	f	61	GLN
31	h	34	HIS
32	i	77	ASN
32	i	310	ASN
33	j	26	GLN
33	j	108	GLN
34	k	57	ASN
35	l	59	GLN
35	l	165	ASN
35	l	194	ASN
35	l	199	GLN
35	l	274	GLN
35	l	309	GLN
35	l	320	ASN
35	l	354	GLN
35	l	400	ASN
35	l	447	ASN
35	l	579	ASN
37	n	3	ASN
38	o	52	ASN
39	p	169	HIS
40	r	20	HIS
40	r	26	ASN
40	r	175	ASN
40	r	192	ASN
40	r	251	ASN
40	r	255	ASN
40	r	304	GLN
40	r	366	ASN
40	r	415	GLN
40	r	422	HIS

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Mol	Chain	Res	Type
41	s	47	GLN
41	s	235	ASN
41	s	317	GLN
42	u	99	HIS
42	u	151	ASN
43	v	65	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	2MR	Q	118	16	10,12,13	1.97	1 (10%)	5,13,15	5.96	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	-	2/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.67	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	12.07	130.54	119.48
16	Q	118	2MR	CD-NE-CZ	4.70	132.21	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.03	130.57	123.86

There are no chirality outliers.

All (2) 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

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 36 ligands modelled in this entry, 2 are monoatomic - leaving 34 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	$\# Z > 2$
46	FMN	A	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.21	8 (16%)
47	NAI	A	503	-	45,48,48	3.91	21 (46%)	60,73,73	1.79	12 (20%)
48	PLX	a	202	-	51,51,51	1.14	4 (7%)	55,59,59	0.63	1 (1%)
55	CDL	i	401	-	65,65,99	1.29	9 (13%)	71,77,111	0.99	4 (5%)
51	FES	O	301	14	0,4,4	-	-	-	-	-
53	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	0.95	2 (3%)
50	NDP	J	401	-	49,52,52	4.40	23 (46%)	66,80,80	2.21	15 (22%)
49	8Q1	G	201	6	31,34,34	1.73	6 (19%)	40,43,43	1.61	6 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	CDL	a	201	-	90,90,99	1.13	8 (8%)	96,102,111	0.94	5 (5%)
55	CDL	V	201	-	70,70,99	1.22	8 (11%)	76,82,111	0.97	4 (5%)
45	SF4	B	302	2	0,12,12	-	-	-	-	-
55	CDL	g	202	-	99,99,99	1.08	8 (8%)	105,111,111	0.85	4 (3%)
57	ADP	w	401	-	27,29,29	2.96	8 (29%)	42,45,45	2.01	10 (23%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
53	PEE	l	702	-	45,45,50	1.22	6 (13%)	48,50,55	1.01	2 (4%)
48	PLX	r	503	-	51,51,51	1.14	5 (9%)	55,59,59	0.59	1 (1%)
48	PLX	g	201	-	51,51,51	1.13	3 (5%)	55,59,59	0.68	1 (1%)
49	8Q1	X	201	6	31,34,34	1.67	6 (19%)	40,43,43	1.50	5 (12%)
55	CDL	l	701	-	99,99,99	1.08	9 (9%)	105,111,111	0.85	4 (3%)
45	SF4	A	501	1	0,12,12	-	-	-	-	-
53	PEE	Q	501	-	46,46,50	1.19	6 (13%)	49,51,55	1.02	2 (4%)
53	PEE	Q	502	-	50,50,50	1.17	6 (12%)	53,55,55	1.06	2 (3%)
53	PEE	j	201	-	46,46,50	1.22	6 (13%)	49,51,55	0.93	2 (4%)
48	PLX	r	502	-	51,51,51	1.14	4 (7%)	55,59,59	0.62	1 (1%)
51	FES	M	803	12	0,4,4	-	-	-	-	-
56	UQ	s	401	-	28,28,63	3.26	8 (28%)	34,37,79	2.92	10 (29%)
53	PEE	l	703	-	45,45,50	1.22	6 (13%)	48,50,55	0.96	2 (4%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-
53	PEE	m	201	-	40,40,50	1.15	5 (12%)	43,45,55	0.97	2 (4%)
48	PLX	C	302	-	51,51,51	1.15	4 (7%)	55,59,59	0.60	1 (1%)
48	PLX	j	203	-	51,51,51	1.16	4 (7%)	55,59,59	0.58	1 (1%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
45	SF4	C	301	16,3	0,12,12	-	-	-	-	-
53	PEE	j	202	-	50,50,50	1.16	6 (12%)	53,55,55	0.96	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	FMN	A	502	-	-	8/18/18/18	0/3/3/3
47	NAI	A	503	-	-	8/29/72/72	0/5/5/5
48	PLX	a	202	-	-	21/55/55/55	-
55	CDL	i	401	-	-	42/76/76/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	FES	O	301	14	-	-	0/1/1/1
53	PEE	r	501	-	-	23/54/54/54	-
50	NDP	J	401	-	-	8/34/77/77	0/4/5/5
49	8Q1	G	201	6	-	21/41/41/41	-
55	CDL	a	201	-	-	41/101/101/110	-
55	CDL	V	201	-	-	47/81/81/110	-
45	SF4	B	302	2	-	-	0/6/5/5
55	CDL	g	202	-	-	67/110/110/110	-
57	ADP	w	401	-	-	4/16/32/32	0/3/3/3
45	SF4	M	802	12	-	-	0/6/5/5
48	PLX	r	503	-	-	33/55/55/55	-
48	PLX	g	201	-	-	25/55/55/55	-
49	8Q1	X	201	6	-	20/41/41/41	-
55	CDL	l	701	-	-	63/110/110/110	-
45	SF4	A	501	1	-	-	0/6/5/5
53	PEE	Q	501	-	-	25/50/50/54	-
53	PEE	Q	502	-	-	23/54/54/54	-
53	PEE	j	202	-	-	24/54/54/54	-
53	PEE	j	201	-	-	25/50/50/54	-
48	PLX	r	502	-	-	26/55/55/55	-
51	FES	M	803	12	-	-	0/1/1/1
56	UQ	s	401	-	-	8/21/45/87	0/1/1/1
53	PEE	l	703	-	-	26/49/49/54	-
45	SF4	M	801	12	-	-	0/6/5/5
53	PEE	m	201	-	-	20/44/44/54	-
48	PLX	C	302	-	-	24/55/55/55	-
48	PLX	j	203	-	-	28/55/55/55	-
45	SF4	B	301	2	-	-	0/6/5/5
45	SF4	C	301	16,3	-	-	0/6/5/5
53	PEE	l	702	-	-	25/49/49/54	-

All (187) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	J	401	NDP	C3B-C2B	-12.84	1.24	1.52
50	J	401	NDP	C6N-C5N	12.52	1.55	1.33
50	J	401	NDP	O4D-C4D	10.68	1.68	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	C3D-C4D	-10.11	1.27	1.53
50	J	401	NDP	C3D-C4D	-9.80	1.28	1.53
47	A	503	NAI	O4B-C1B	9.25	1.63	1.42
56	s	401	UQ	C13-C14	9.20	1.55	1.33
56	s	401	UQ	C8-C9	8.88	1.54	1.33
57	w	401	ADP	C3'-C4'	-8.81	1.30	1.53
56	s	401	UQ	C18-C19	8.25	1.56	1.32
47	A	503	NAI	O4B-C4B	-8.19	1.26	1.45
50	J	401	NDP	O4B-C4B	-7.87	1.27	1.45
57	w	401	ADP	O4'-C4'	7.74	1.62	1.45
47	A	503	NAI	C2D-C1D	-7.62	1.29	1.53
50	J	401	NDP	C2N-C3N	7.50	1.55	1.34
47	A	503	NAI	C2B-C1B	-7.20	1.30	1.53
47	A	503	NAI	O4D-C4D	7.12	1.60	1.45
47	A	503	NAI	C2D-C3D	5.91	1.69	1.53
50	J	401	NDP	C6A-N6A	5.90	1.48	1.34
47	A	503	NAI	C7N-N7N	5.75	1.48	1.33
50	J	401	NDP	P2B-O2B	5.66	1.70	1.59
49	G	201	8Q1	C34-N36	5.56	1.45	1.33
50	J	401	NDP	C3B-C4B	5.47	1.67	1.53
57	w	401	ADP	C6-N6	5.46	1.47	1.34
49	G	201	8Q1	C39-N41	5.46	1.45	1.33
47	A	503	NAI	O4D-C1D	5.43	1.54	1.42
49	X	201	8Q1	C34-N36	5.42	1.45	1.33
49	X	201	8Q1	C39-N41	5.34	1.45	1.33
47	A	503	NAI	C6A-N6A	5.23	1.47	1.34
47	A	503	NAI	C4N-C3N	-5.11	1.39	1.49
50	J	401	NDP	C6N-N1N	5.04	1.49	1.37
50	J	401	NDP	O4D-C1D	-4.89	1.30	1.42
50	J	401	NDP	O4B-C1B	4.55	1.52	1.42
47	A	503	NAI	O2B-C2B	4.55	1.53	1.43
50	J	401	NDP	C1B-N9A	-4.54	1.33	1.46
57	w	401	ADP	O4'-C1'	-4.44	1.31	1.42
50	J	401	NDP	C7N-N7N	4.21	1.44	1.33
50	J	401	NDP	O2D-C2D	-4.15	1.33	1.43
46	A	502	FMN	C4A-N5	3.94	1.38	1.30
47	A	503	NAI	C6N-C5N	3.93	1.40	1.33
53	Q	502	PEE	C18-C19	3.78	1.53	1.31
53	j	201	PEE	C18-C19	3.76	1.53	1.31
53	l	702	PEE	C18-C19	3.75	1.53	1.31
53	j	202	PEE	C18-C19	3.74	1.53	1.31
53	r	501	PEE	C18-C19	3.73	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	m	201	PEE	C18-C19	3.73	1.53	1.31
53	l	703	PEE	C18-C19	3.72	1.53	1.31
53	Q	501	PEE	C18-C19	3.71	1.53	1.31
53	j	201	PEE	C39-C38	3.68	1.53	1.31
53	r	501	PEE	C39-C38	3.66	1.53	1.31
53	l	702	PEE	C39-C38	3.65	1.53	1.31
53	j	202	PEE	C39-C38	3.65	1.52	1.31
53	Q	502	PEE	C39-C38	3.65	1.52	1.31
53	l	703	PEE	C39-C38	3.64	1.52	1.31
53	Q	501	PEE	C39-C38	3.64	1.52	1.31
47	A	503	NAI	C7N-C3N	3.59	1.56	1.48
55	V	201	CDL	OA8-CA7	3.55	1.43	1.33
55	i	401	CDL	OA8-CA7	3.52	1.43	1.33
55	l	701	CDL	OA8-CA7	3.38	1.43	1.33
55	a	201	CDL	OA8-CA7	3.38	1.43	1.33
55	g	202	CDL	OA8-CA7	3.37	1.43	1.33
57	w	401	ADP	O2'-C2'	-3.37	1.35	1.43
47	A	503	NAI	C4N-C5N	-3.36	1.40	1.48
50	J	401	NDP	C7N-C3N	3.11	1.55	1.48
50	J	401	NDP	O3D-C3D	3.10	1.50	1.43
57	w	401	ADP	C8-N9	-3.10	1.32	1.37
57	w	401	ADP	O3'-C3'	3.10	1.50	1.43
55	a	201	CDL	OB6-CB5	3.10	1.43	1.34
55	l	701	CDL	OB6-CB5	3.06	1.42	1.34
55	i	401	CDL	OB6-CB5	3.06	1.42	1.34
55	g	202	CDL	OB6-CB5	3.05	1.42	1.34
55	i	401	CDL	OB8-CB7	3.04	1.42	1.33
50	J	401	NDP	C8A-N9A	-3.03	1.32	1.37
55	i	401	CDL	OA6-CA5	3.01	1.42	1.34
55	V	201	CDL	OB6-CB5	3.01	1.42	1.34
55	l	701	CDL	OB8-CB7	3.00	1.42	1.33
55	V	201	CDL	OB8-CB7	2.97	1.42	1.33
55	V	201	CDL	OA6-CA5	2.97	1.42	1.34
55	l	701	CDL	OA6-CA5	2.95	1.42	1.34
55	a	201	CDL	OA6-CA5	2.95	1.42	1.34
55	g	202	CDL	OA6-CA5	2.95	1.42	1.34
55	a	201	CDL	OB8-CB7	2.95	1.41	1.33
55	g	202	CDL	OB8-CB7	2.93	1.41	1.33
50	J	401	NDP	C5A-N7A	-2.90	1.33	1.39
48	C	302	PLX	O6-C4	-2.78	1.40	1.44
48	r	503	PLX	O6-C4	-2.73	1.41	1.44
48	g	201	PLX	O6-C4	-2.70	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	s	401	UQ	C6-C1	2.66	1.54	1.46
48	a	202	PLX	O6-C4	-2.61	1.41	1.44
47	A	503	NAI	C8A-N9A	-2.59	1.32	1.37
53	l	703	PEE	O3-C30	2.53	1.40	1.33
53	l	702	PEE	O3-C30	2.51	1.40	1.33
46	A	502	FMN	C10-N1	2.51	1.38	1.33
48	j	203	PLX	O6-C4	-2.50	1.41	1.44
53	j	201	PEE	O3-C30	2.50	1.40	1.33
53	r	501	PEE	O3-C30	2.49	1.40	1.33
53	r	501	PEE	O2-C2	-2.47	1.40	1.46
48	j	203	PLX	C7-C6	2.47	1.56	1.50
53	Q	501	PEE	O3-C30	2.47	1.40	1.33
55	g	202	CDL	OA6-CA4	-2.47	1.40	1.46
47	A	503	NAI	PN-O5D	2.46	1.69	1.59
53	l	703	PEE	O2-C2	-2.45	1.40	1.46
53	j	202	PEE	O3-C30	2.44	1.40	1.33
50	J	401	NDP	O2B-C2B	2.44	1.53	1.44
49	G	201	8Q1	C1-S44	2.43	1.82	1.76
55	a	201	CDL	OA6-CA4	-2.43	1.40	1.46
47	A	503	NAI	O3B-C3B	-2.43	1.37	1.43
53	Q	501	PEE	O2-C2	-2.42	1.40	1.46
53	m	201	PEE	O3-C30	2.42	1.40	1.33
50	J	401	NDP	C2D-C3D	2.42	1.60	1.53
53	m	201	PEE	O2-C10	2.41	1.41	1.34
53	Q	502	PEE	O3-C30	2.40	1.40	1.33
47	A	503	NAI	C5B-C4B	2.39	1.59	1.51
55	V	201	CDL	OA6-CA4	-2.38	1.40	1.46
53	l	702	PEE	O2-C10	2.37	1.41	1.34
53	j	202	PEE	O2-C2	-2.37	1.40	1.46
48	r	502	PLX	C7-C6	2.37	1.55	1.50
53	j	201	PEE	O2-C2	-2.37	1.40	1.46
55	i	401	CDL	OA6-CA4	-2.35	1.40	1.46
53	j	201	PEE	O2-C10	2.35	1.40	1.34
53	j	202	PEE	O2-C10	2.35	1.40	1.34
49	X	201	8Q1	C1-S44	2.35	1.81	1.76
55	l	701	CDL	OA6-CA4	-2.34	1.40	1.46
56	s	401	UQ	O4-C4	-2.34	1.18	1.23
48	g	201	PLX	C7-C6	2.33	1.55	1.50
49	G	201	8Q1	C6-C1	2.33	1.53	1.50
53	Q	502	PEE	O2-C10	2.32	1.40	1.34
48	r	502	PLX	O6-C4	-2.29	1.41	1.44
53	Q	502	PEE	O2-C2	-2.29	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	G	201	8Q1	O40-C39	-2.27	1.18	1.23
56	s	401	UQ	C7-C8	2.26	1.53	1.50
48	r	503	PLX	C7-C6	2.26	1.55	1.50
57	w	401	ADP	C5-N7	-2.26	1.34	1.39
48	a	202	PLX	C7-C6	2.26	1.55	1.50
53	m	201	PEE	O2-C2	-2.25	1.41	1.46
55	i	401	CDL	PB2-OB5	2.25	1.68	1.59
53	l	702	PEE	O2-C2	-2.25	1.41	1.46
48	C	302	PLX	C7-C6	2.24	1.55	1.50
48	r	502	PLX	P1-O4	2.23	1.68	1.59
55	V	201	CDL	PB2-OB2	2.22	1.68	1.59
55	g	202	CDL	PB2-OB2	2.22	1.68	1.59
53	l	703	PEE	O2-C10	2.21	1.40	1.34
53	Q	501	PEE	O2-C10	2.21	1.40	1.34
49	G	201	8Q1	O35-C34	-2.21	1.19	1.23
55	l	701	CDL	OB6-CB4	-2.21	1.41	1.46
53	r	501	PEE	O2-C10	2.21	1.40	1.34
55	g	202	CDL	PB2-OB5	2.19	1.68	1.59
55	i	401	CDL	PB2-OB2	2.19	1.68	1.59
49	X	201	8Q1	O35-C34	-2.19	1.19	1.23
48	j	203	PLX	P1-O4	2.18	1.68	1.59
53	Q	502	PEE	O3-C3	-2.17	1.40	1.45
55	V	201	CDL	OB6-CB4	-2.16	1.41	1.46
55	a	201	CDL	PB2-OB2	2.15	1.68	1.59
53	m	201	PEE	O3-C3	-2.15	1.40	1.45
53	j	202	PEE	O3-C3	-2.15	1.40	1.45
55	l	701	CDL	PB2-OB2	2.14	1.68	1.59
49	X	201	8Q1	O40-C39	-2.14	1.18	1.23
55	V	201	CDL	PB2-OB5	2.13	1.67	1.59
55	i	401	CDL	OB6-CB4	-2.13	1.41	1.46
48	C	302	PLX	P1-O4	2.12	1.67	1.59
48	a	202	PLX	P1-O4	2.12	1.67	1.59
56	s	401	UQ	O1-C1	-2.12	1.18	1.23
48	r	502	PLX	P1-O1	2.11	1.67	1.59
55	a	201	CDL	PB2-OB5	2.11	1.67	1.59
55	l	701	CDL	PB2-OB5	2.11	1.67	1.59
50	J	401	NDP	PA-O5B	2.11	1.67	1.59
55	g	202	CDL	OB6-CB4	-2.10	1.41	1.46
55	a	201	CDL	OB6-CB4	-2.09	1.41	1.46
49	X	201	8Q1	C6-C1	2.09	1.53	1.50
50	J	401	NDP	O7N-C7N	-2.08	1.19	1.24
48	r	503	PLX	P1-O4	2.07	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	j	203	PLX	P1-O1	2.07	1.67	1.59
48	g	201	PLX	P1-O4	2.06	1.67	1.59
53	r	501	PEE	O3-C3	-2.06	1.40	1.45
53	Q	501	PEE	O3-C3	-2.05	1.40	1.45
47	A	503	NAI	C2N-C3N	2.05	1.40	1.34
48	a	202	PLX	P1-O1	2.05	1.67	1.59
55	i	401	CDL	C11-CA5	2.05	1.56	1.50
48	C	302	PLX	P1-O1	2.03	1.67	1.59
53	l	702	PEE	O3-C3	-2.03	1.40	1.45
56	s	401	UQ	O3-CM3	-2.03	1.40	1.45
55	l	701	CDL	C11-CA5	2.03	1.56	1.50
48	r	503	PLX	P1-O1	2.03	1.67	1.59
53	j	201	PEE	O3-C3	-2.02	1.40	1.45
48	r	503	PLX	C1-C2	2.02	1.57	1.51
53	l	703	PEE	O3-C3	-2.01	1.40	1.45
47	A	503	NAI	C5A-N7A	-2.01	1.35	1.39

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	s	401	UQ	C7-C8-C9	-10.49	109.33	126.79
50	J	401	NDP	C3N-C2N-N1N	-7.76	112.02	123.10
50	J	401	NDP	C1D-N1N-C2N	-6.85	109.72	121.11
49	G	201	8Q1	C6-C1-S44	6.18	120.65	113.46
56	s	401	UQ	C12-C13-C14	-6.10	112.96	127.66
47	A	503	NAI	C5A-C4A-N3A	-5.92	119.03	126.75
50	J	401	NDP	C5A-C4A-N3A	-5.88	119.08	126.75
57	w	401	ADP	C5-C4-N3	-5.71	119.30	126.75
49	X	201	8Q1	C6-C1-S44	5.67	120.05	113.46
50	J	401	NDP	C1D-N1N-C6N	-5.67	108.62	120.83
56	s	401	UQ	C11-C9-C8	-5.19	110.62	121.12
56	s	401	UQ	C10-C9-C8	-5.06	110.70	123.68
53	Q	502	PEE	O2-C10-C11	4.50	121.19	111.50
55	a	201	CDL	OA6-CA5-C11	4.45	121.08	111.50
57	w	401	ADP	N3-C4-N9	4.43	134.38	127.08
57	w	401	ADP	N3-C2-N1	-4.42	121.69	128.60
47	A	503	NAI	N3A-C2A-N1A	-4.29	121.89	128.60
50	J	401	NDP	N3A-C4A-N9A	4.27	134.11	127.08
47	A	503	NAI	N3A-C4A-N9A	4.22	134.03	127.08
56	s	401	UQ	C17-C18-C19	-4.16	113.52	127.75
56	s	401	UQ	C15-C14-C13	-4.11	113.13	123.68
55	V	201	CDL	OB6-CB5-C51	4.08	120.30	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	g	202	CDL	OB6-CB5-C51	4.08	120.28	111.50
56	s	401	UQ	C16-C14-C13	-4.07	112.89	121.12
55	l	701	CDL	OA6-CA5-C11	4.05	120.22	111.50
53	l	702	PEE	O2-C10-C11	4.01	120.15	111.50
50	J	401	NDP	N3A-C2A-N1A	-4.01	122.34	128.60
53	m	201	PEE	O2-C10-C11	3.98	120.09	111.50
55	i	401	CDL	OB6-CB5-C51	3.98	120.07	111.50
53	Q	501	PEE	O2-C10-C11	3.96	120.04	111.50
53	j	202	PEE	O2-C10-C11	3.92	119.94	111.50
55	a	201	CDL	OB6-CB5-C51	3.91	119.92	111.50
47	A	503	NAI	C2A-N3A-C4A	3.86	120.87	111.75
55	i	401	CDL	OA6-CA5-C11	3.82	119.74	111.50
47	A	503	NAI	C5A-N7A-C8A	3.74	108.83	103.51
50	J	401	NDP	C2A-N3A-C4A	3.72	120.55	111.75
49	G	201	8Q1	C37-C38-C39	3.72	118.56	112.36
53	r	501	PEE	O2-C10-C11	3.70	119.47	111.50
57	w	401	ADP	C2-N3-C4	3.69	120.47	111.75
55	g	202	CDL	OA6-CA5-C11	3.69	119.45	111.50
53	j	201	PEE	O2-C10-C11	3.64	119.36	111.50
55	l	701	CDL	OB6-CB5-C51	3.63	119.33	111.50
57	w	401	ADP	N9-C8-N7	-3.63	108.95	113.91
49	G	201	8Q1	O4-C1-C6	-3.62	119.71	123.99
53	l	703	PEE	O2-C10-C11	3.62	119.30	111.50
49	X	201	8Q1	O4-C1-C6	-3.52	119.84	123.99
47	A	503	NAI	N9A-C8A-N7A	-3.42	109.23	113.91
57	w	401	ADP	C5-N7-C8	3.40	108.34	103.51
50	J	401	NDP	C5A-N7A-C8A	3.29	108.18	103.51
47	A	503	NAI	C4A-C5A-N7A	-3.25	106.66	110.62
56	s	401	UQ	C21-C19-C18	-3.24	113.29	122.65
55	V	201	CDL	OA6-CA5-C11	3.21	119.76	110.80
50	J	401	NDP	N9A-C8A-N7A	-3.21	109.52	113.91
57	w	401	ADP	C4-N9-C8	3.10	109.09	105.73
46	A	502	FMN	C4-N3-C2	-3.05	120.02	125.64
56	s	401	UQ	C20-C19-C18	-3.04	113.85	122.65
50	J	401	NDP	C2B-C1B-N9A	-3.03	108.42	113.53
53	Q	502	PEE	O3-C30-C31	2.92	121.06	111.91
47	A	503	NAI	PN-O3-PA	-2.91	122.84	132.83
50	J	401	NDP	C4A-C5A-N7A	-2.91	107.08	110.62
53	l	702	PEE	O3-C30-C31	2.88	120.94	111.91
57	w	401	ADP	PA-O3A-PB	-2.87	122.96	132.83
53	r	501	PEE	O3-C30-C31	2.81	120.72	111.91
55	V	201	CDL	OA8-CA7-C31	2.81	120.72	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	A	503	NAI	C4D-O4D-C1D	-2.75	103.40	109.47
57	w	401	ADP	C4-C5-N7	-2.72	107.30	110.62
55	i	401	CDL	OA8-CA7-C31	2.70	120.39	111.91
53	l	703	PEE	O3-C30-C31	2.65	120.21	111.91
50	J	401	NDP	C2B-C3B-C4B	2.64	107.73	101.99
46	A	502	FMN	C4A-C4-N3	2.63	119.86	113.19
48	g	201	PLX	C1A-N1-C1	2.60	120.56	109.92
55	V	201	CDL	OB8-CB7-C71	2.58	119.99	111.91
55	i	401	CDL	OB8-CB7-C71	2.56	119.95	111.91
53	Q	501	PEE	O3-C30-C31	2.56	119.94	111.91
55	a	201	CDL	OB8-CB7-C71	2.55	119.90	111.91
53	j	201	PEE	O3-C30-C31	2.54	119.89	111.91
47	A	503	NAI	C2D-C3D-C4D	2.54	107.57	102.64
48	r	503	PLX	C1A-N1-C1	2.52	120.24	109.92
55	g	202	CDL	OB8-CB7-C71	2.52	119.83	111.91
55	g	202	CDL	OA8-CA7-C31	2.51	119.78	111.91
49	X	201	8Q1	C38-C39-N41	2.50	120.63	116.42
53	j	202	PEE	O3-C30-C31	2.50	119.74	111.91
53	m	201	PEE	O3-C30-C31	2.49	119.74	111.91
55	l	701	CDL	OB8-CB7-C71	2.49	119.72	111.91
55	l	701	CDL	OA8-CA7-C31	2.49	119.72	111.91
46	A	502	FMN	O4-C4-C4A	-2.47	120.04	126.60
50	J	401	NDP	C4A-N9A-C8A	2.47	108.41	105.73
46	A	502	FMN	C4A-C10-N10	2.46	120.08	116.48
48	a	202	PLX	C1A-N1-C1	2.45	119.94	109.92
47	A	503	NAI	C4A-N9A-C8A	2.41	108.34	105.73
57	w	401	ADP	C4'-O4'-C1'	-2.39	104.19	109.47
49	G	201	8Q1	C43-S44-C1	2.39	109.32	101.87
47	A	503	NAI	C3D-C2D-C1D	2.36	105.91	101.43
49	X	201	8Q1	C38-C37-N36	-2.36	107.14	111.90
50	J	401	NDP	PN-O3-PA	-2.34	124.81	132.83
55	a	201	CDL	OA8-CA7-C31	2.32	119.19	111.91
48	C	302	PLX	C1A-N1-C1	2.32	119.39	109.92
48	j	203	PLX	C1A-N1-C1	2.31	119.37	109.92
48	r	502	PLX	C1A-N1-C1	2.30	119.32	109.92
49	G	201	8Q1	O4-C1-S44	-2.29	119.63	122.61
46	A	502	FMN	C10-C4A-N5	-2.28	120.03	124.86
49	X	201	8Q1	C43-S44-C1	2.27	108.94	101.87
46	A	502	FMN	C9A-C5A-N5	-2.26	119.98	122.43
49	G	201	8Q1	C38-C39-N41	2.20	120.12	116.42
56	s	401	UQ	CM5-C5-C6	-2.18	120.84	124.40
46	A	502	FMN	C4A-C10-N1	-2.13	119.78	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	a	201	CDL	CA4-OA6-CA5	-2.12	112.56	117.79
46	A	502	FMN	C5A-C9A-N10	2.12	120.14	117.95
50	J	401	NDP	C2D-C3D-C4D	2.04	106.61	102.64

There are no chirality outliers.

All (685) 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'
47	A	503	NAI	C5B-O5B-PA-O1A
48	C	302	PLX	O4-C3-C4-O6
48	C	302	PLX	C3-O4-P1-O1
48	C	302	PLX	C3-O4-P1-O2
48	C	302	PLX	C3-O4-P1-O3
48	a	202	PLX	O7-C6-C7-C8
48	a	202	PLX	C25-C24-O8-C5
48	g	201	PLX	O7-C6-C7-C8
48	g	201	PLX	O7-C6-O6-C4
48	g	201	PLX	C3-O4-P1-O1
48	g	201	PLX	C3-O4-P1-O2
48	j	203	PLX	O7-C6-C7-C8
48	j	203	PLX	O7-C6-O6-C4
48	j	203	PLX	C25-C24-O8-C5
48	j	203	PLX	O9-C24-C25-C26
48	r	502	PLX	O7-C6-O6-C4
48	r	502	PLX	C5-C4-O6-C6
48	r	502	PLX	O9-C24-O8-C5
48	r	502	PLX	O9-C24-C25-C26
48	r	503	PLX	C3-O4-P1-O1
48	r	503	PLX	C3-O4-P1-O2
48	r	503	PLX	C2-O1-P1-O4
48	r	503	PLX	C2-O1-P1-O2
48	r	503	PLX	C2-O1-P1-O3
48	r	503	PLX	C25-C24-O8-C5
48	r	503	PLX	O9-C24-C25-C26
49	G	201	8Q1	C1-C6-C7-C8
49	G	201	8Q1	C28-C29-C32-C34
49	G	201	8Q1	C28-C29-C32-O33
49	G	201	8Q1	C31-C29-C32-O33

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Mol	Chain	Res	Type	Atoms
49	G	201	8Q1	N41-C42-C43-S44
49	G	201	8Q1	C28-O27-P24-O2
49	G	201	8Q1	C28-O27-P24-O1
49	X	201	8Q1	C1-C6-C7-C8
49	X	201	8Q1	O27-C28-C29-C32
49	X	201	8Q1	C28-C29-C32-C34
49	X	201	8Q1	C28-C29-C32-O33
49	X	201	8Q1	C30-C29-C32-C34
49	X	201	8Q1	C30-C29-C32-O33
49	X	201	8Q1	C31-C29-C32-C34
49	X	201	8Q1	C31-C29-C32-O33
49	X	201	8Q1	N36-C37-C38-C39
49	X	201	8Q1	C42-C43-S44-C1
49	X	201	8Q1	C28-O27-P24-O3
49	X	201	8Q1	C28-O27-P24-O2
49	X	201	8Q1	C28-O27-P24-O1
50	J	401	NDP	C5B-O5B-PA-O1A
50	J	401	NDP	C5B-O5B-PA-O3
50	J	401	NDP	C2N-C3N-C7N-N7N
53	Q	501	PEE	C11-C10-O2-C2
53	Q	501	PEE	C4-O4P-P-O1P
53	Q	502	PEE	O4P-C4-C5-N
53	j	201	PEE	C1-O3P-P-O1P
53	j	201	PEE	C4-O4P-P-O1P
53	j	201	PEE	O4P-C4-C5-N
53	j	202	PEE	C17-C18-C19-C20
53	j	202	PEE	C1-O3P-P-O1P
53	l	702	PEE	C11-C10-O2-C2
53	l	702	PEE	C4-O4P-P-O2P
53	l	702	PEE	C4-O4P-P-O1P
53	l	703	PEE	C1-O3P-P-O1P
53	m	201	PEE	C11-C10-O2-C2
55	V	201	CDL	OA9-CA7-OA8-CA6
55	V	201	CDL	C31-CA7-OA8-CA6
55	a	201	CDL	CA2-OA2-PA1-OA3
55	a	201	CDL	CA2-OA2-PA1-OA4
55	a	201	CDL	CA2-OA2-PA1-OA5
55	a	201	CDL	CA3-OA5-PA1-OA2
55	a	201	CDL	CA3-OA5-PA1-OA3
55	a	201	CDL	CA3-OA5-PA1-OA4
55	a	201	CDL	OA5-CA3-CA4-OA6
55	a	201	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
55	g	202	CDL	CB2-C1-CA2-OA2
55	g	202	CDL	CA2-OA2-PA1-OA3
55	g	202	CDL	CA2-OA2-PA1-OA4
55	g	202	CDL	CA3-OA5-PA1-OA3
55	g	202	CDL	CA3-OA5-PA1-OA4
55	g	202	CDL	C51-CB5-OB6-CB4
55	i	401	CDL	CA2-OA2-PA1-OA5
55	i	401	CDL	CA3-OA5-PA1-OA3
55	i	401	CDL	CA3-OA5-PA1-OA4
55	i	401	CDL	CB2-OB2-PB2-OB3
55	i	401	CDL	CB2-OB2-PB2-OB4
55	l	701	CDL	O1-C1-CB2-OB2
55	l	701	CDL	CA2-C1-CB2-OB2
55	l	701	CDL	CA2-OA2-PA1-OA3
55	l	701	CDL	CA2-OA2-PA1-OA5
55	l	701	CDL	CA3-OA5-PA1-OA2
55	l	701	CDL	CA3-OA5-PA1-OA3
55	l	701	CDL	CA3-OA5-PA1-OA4
55	l	701	CDL	OA6-CA4-CA6-OA8
55	l	701	CDL	CB2-OB2-PB2-OB4
55	l	701	CDL	CB2-OB2-PB2-OB5
55	l	701	CDL	CB3-OB5-PB2-OB3
55	l	701	CDL	OB6-CB4-CB6-OB8
56	s	401	UQ	C7-C8-C9-C11
56	s	401	UQ	C12-C11-C9-C10
57	w	401	ADP	C5'-O5'-PA-O2A
57	w	401	ADP	C5'-O5'-PA-O3A
53	Q	501	PEE	O4-C10-O2-C2
53	l	702	PEE	O4-C10-O2-C2
53	m	201	PEE	O4-C10-O2-C2
55	g	202	CDL	OB7-CB5-OB6-CB4
55	i	401	CDL	OA9-CA7-OA8-CA6
55	l	701	CDL	C71-CB7-OB8-CB6
56	s	401	UQ	C17-C18-C19-C21
53	l	702	PEE	C31-C30-O3-C3
53	l	703	PEE	C31-C30-O3-C3
53	m	201	PEE	C31-C30-O3-C3
55	g	202	CDL	C71-CB7-OB8-CB6
55	i	401	CDL	C31-CA7-OA8-CA6
53	Q	502	PEE	C37-C38-C39-C40
53	l	703	PEE	C37-C38-C39-C40
53	r	501	PEE	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
56	s	401	UQ	C7-C8-C9-C10
53	l	703	PEE	O5-C30-O3-C3
55	g	202	CDL	OB9-CB7-OB8-CB6
55	l	701	CDL	O1-C1-CA2-OA2
53	m	201	PEE	O5-C30-O3-C3
55	l	701	CDL	OB9-CB7-OB8-CB6
48	j	203	PLX	C28-C29-C30-C31
55	l	701	CDL	C11-C12-C13-C14
50	J	401	NDP	C2D-C1D-N1N-C6N
48	C	302	PLX	C28-C29-C30-C31
53	l	702	PEE	O5-C30-O3-C3
48	j	203	PLX	C15-C16-C17-C18
48	r	502	PLX	C9-C10-C11-C12
48	r	503	PLX	C12-C13-C14-C15
50	J	401	NDP	O4B-C4B-C5B-O5B
48	r	502	PLX	C30-C31-C32-C33
55	g	202	CDL	C36-C37-C38-C39
55	l	701	CDL	C59-C60-C61-C62
55	l	701	CDL	C35-C36-C37-C38
53	m	201	PEE	C33-C34-C35-C36
55	V	201	CDL	C60-C61-C62-C63
55	V	201	CDL	CA2-C1-CB2-OB2
53	j	202	PEE	C31-C30-O3-C3
55	a	201	CDL	C71-CB7-OB8-CB6
55	i	401	CDL	C71-CB7-OB8-CB6
55	i	401	CDL	C31-C32-C33-C34
53	j	202	PEE	O5-C30-O3-C3
48	j	203	PLX	C34-C35-C36-C37
55	V	201	CDL	C74-C75-C76-C77
55	V	201	CDL	O1-C1-CB2-OB2
55	l	701	CDL	CB7-C71-C72-C73
55	g	202	CDL	C74-C75-C76-C77
53	j	202	PEE	C11-C10-O2-C2
53	m	201	PEE	C13-C14-C15-C16
55	i	401	CDL	CB7-C71-C72-C73
55	i	401	CDL	OB9-CB7-OB8-CB6
48	g	201	PLX	C7-C8-C9-C10
55	g	202	CDL	CB5-C51-C52-C53
55	g	202	CDL	CB7-C71-C72-C73
55	i	401	CDL	CA7-C31-C32-C33
55	a	201	CDL	CA7-C31-C32-C33
55	a	201	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
55	g	202	CDL	C78-C79-C80-C81
55	V	201	CDL	O1-C1-CA2-OA2
55	g	202	CDL	O1-C1-CA2-OA2
55	i	401	CDL	O1-C1-CA2-OA2
55	l	701	CDL	C39-C40-C41-C42
53	j	202	PEE	C30-C31-C32-C33
55	g	202	CDL	CA7-C31-C32-C33
53	Q	501	PEE	C17-C18-C19-C20
48	a	202	PLX	C29-C30-C31-C32
53	Q	501	PEE	C22-C23-C24-C25
48	r	502	PLX	C3-O4-P1-O1
53	j	201	PEE	C1-O3P-P-O4P
53	l	702	PEE	C4-O4P-P-O3P
53	m	201	PEE	C4-O4P-P-O3P
53	r	501	PEE	C1-O3P-P-O4P
55	V	201	CDL	CB2-OB2-PB2-OB5
55	a	201	CDL	CB3-OB5-PB2-OB2
55	g	202	CDL	CA2-OA2-PA1-OA5
55	g	202	CDL	CA3-OA5-PA1-OA2
55	g	202	CDL	CB2-OB2-PB2-OB5
55	g	202	CDL	CB3-OB5-PB2-OB2
55	i	401	CDL	CA3-OA5-PA1-OA2
55	i	401	CDL	CB2-OB2-PB2-OB5
55	l	701	CDL	CB3-OB5-PB2-OB2
56	s	401	UQ	C12-C13-C14-C15
55	g	202	CDL	C76-C77-C78-C79
55	V	201	CDL	CB2-C1-CA2-OA2
55	i	401	CDL	CB2-C1-CA2-OA2
53	j	202	PEE	O4-C10-O2-C2
53	r	501	PEE	C41-C42-C43-C44
48	a	202	PLX	O6-C6-C7-C8
53	Q	502	PEE	C12-C13-C14-C15
48	g	201	PLX	C30-C31-C32-C33
53	r	501	PEE	C12-C13-C14-C15
53	j	201	PEE	C11-C10-O2-C2
48	C	302	PLX	C17-C18-C19-C20
48	j	203	PLX	C27-C28-C29-C30
48	r	502	PLX	C16-C17-C18-C19
48	r	503	PLX	C16-C17-C18-C19
48	r	503	PLX	C25-C26-C27-C28
53	Q	502	PEE	C14-C15-C16-C17
55	i	401	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
49	X	201	8Q1	O27-C28-C29-C30
49	X	201	8Q1	O27-C28-C29-C31
48	C	302	PLX	C33-C34-C35-C36
48	a	202	PLX	C28-C29-C30-C31
48	a	202	PLX	C31-C32-C33-C34
48	g	201	PLX	C33-C34-C35-C36
48	j	203	PLX	C14-C15-C16-C17
48	r	502	PLX	C27-C28-C29-C30
49	G	201	8Q1	C7-C8-C9-C10
53	j	201	PEE	C14-C15-C16-C17
55	V	201	CDL	C55-C56-C57-C58
55	a	201	CDL	C17-C18-C19-C20
53	j	201	PEE	O4-C10-O2-C2
53	r	501	PEE	C10-C11-C12-C13
46	A	502	FMN	O2'-C2'-C3'-C4'
53	m	201	PEE	C11-C12-C13-C14
55	a	201	CDL	C37-C38-C39-C40
48	g	201	PLX	C14-C15-C16-C17
53	Q	501	PEE	C32-C33-C34-C35
53	j	202	PEE	C40-C41-C42-C43
55	V	201	CDL	C52-C53-C54-C55
48	C	302	PLX	C7-C8-C9-C10
48	g	201	PLX	C11-C10-C9-C8
55	g	202	CDL	C17-C18-C19-C20
48	j	203	PLX	C25-C26-C27-C28
55	a	201	CDL	C22-C23-C24-C25
48	a	202	PLX	C11-C10-C9-C8
48	g	201	PLX	C25-C26-C27-C28
48	j	203	PLX	C12-C13-C14-C15
48	r	502	PLX	C7-C8-C9-C10
49	X	201	8Q1	C10-C11-C12-C13
53	j	201	PEE	C32-C33-C34-C35
53	j	202	PEE	C21-C22-C23-C24
55	V	201	CDL	C59-C60-C61-C62
55	g	202	CDL	C73-C74-C75-C76
53	Q	502	PEE	C32-C33-C34-C35
53	Q	502	PEE	C33-C34-C35-C36
55	i	401	CDL	C11-C12-C13-C14
48	g	201	PLX	C32-C33-C34-C35
48	r	503	PLX	C29-C30-C31-C32
53	r	501	PEE	C13-C14-C15-C16
55	g	202	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
53	Q	501	PEE	C19-C20-C21-C22
53	j	201	PEE	C15-C16-C17-C18
53	l	702	PEE	C19-C20-C21-C22
53	j	201	PEE	C30-C31-C32-C33
48	j	203	PLX	C10-C11-C12-C13
48	j	203	PLX	C7-C8-C9-C10
48	r	503	PLX	C9-C10-C11-C12
48	r	503	PLX	C33-C34-C35-C36
53	j	201	PEE	C13-C14-C15-C16
53	j	201	PEE	C33-C34-C35-C36
53	l	703	PEE	C33-C34-C35-C36
53	r	501	PEE	C31-C32-C33-C34
55	V	201	CDL	C62-C63-C64-C65
55	g	202	CDL	C75-C76-C77-C78
55	l	701	CDL	C73-C74-C75-C76
49	G	201	8Q1	C11-C12-C13-C14
53	m	201	PEE	C31-C32-C33-C34
55	a	201	CDL	C11-C12-C13-C14
53	r	501	PEE	O4P-C4-C5-N
48	C	302	PLX	C25-C26-C27-C28
48	C	302	PLX	C27-C28-C29-C30
48	g	201	PLX	C28-C29-C30-C31
48	r	502	PLX	C28-C29-C30-C31
53	l	702	PEE	C31-C32-C33-C34
55	a	201	CDL	C71-C72-C73-C74
48	g	201	PLX	C27-C28-C29-C30
48	r	503	PLX	C27-C28-C29-C30
48	r	503	PLX	C28-C29-C30-C31
53	l	703	PEE	C39-C40-C41-C42
55	g	202	CDL	C71-C72-C73-C74
55	l	701	CDL	C40-C41-C42-C43
55	V	201	CDL	C56-C57-C58-C59
53	Q	502	PEE	C34-C35-C36-C37
55	i	401	CDL	C71-C72-C73-C74
55	a	201	CDL	C32-C33-C34-C35
55	l	701	CDL	C72-C73-C74-C75
53	l	703	PEE	C17-C18-C19-C20
48	C	302	PLX	C16-C17-C18-C19
53	Q	501	PEE	C10-C11-C12-C13
48	a	202	PLX	C26-C27-C28-C29
48	C	302	PLX	O7-C6-C7-C8
48	a	202	PLX	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
48	j	203	PLX	C26-C27-C28-C29
55	l	701	CDL	C37-C38-C39-C40
55	V	201	CDL	CA7-C31-C32-C33
55	i	401	CDL	C52-C53-C54-C55
55	g	202	CDL	CA5-C11-C12-C13
55	a	201	CDL	C31-C32-C33-C34
48	C	302	PLX	C14-C15-C16-C17
53	r	501	PEE	C11-C12-C13-C14
55	a	201	CDL	C75-C76-C77-C78
55	g	202	CDL	C33-C34-C35-C36
55	i	401	CDL	C32-C33-C34-C35
53	j	202	PEE	C41-C42-C43-C44
55	l	701	CDL	C55-C56-C57-C58
53	l	702	PEE	C30-C31-C32-C33
48	C	302	PLX	C13-C14-C15-C16
53	l	702	PEE	C14-C15-C16-C17
55	g	202	CDL	C62-C63-C64-C65
53	Q	501	PEE	C31-C30-O3-C3
55	g	202	CDL	C31-CA7-OA8-CA6
48	C	302	PLX	C26-C27-C28-C29
55	g	202	CDL	C43-C44-C45-C46
53	l	703	PEE	C12-C13-C14-C15
53	Q	502	PEE	O4-C10-O2-C2
55	a	201	CDL	C35-C36-C37-C38
48	a	202	PLX	C13-C14-C15-C16
53	j	202	PEE	C22-C23-C24-C25
55	g	202	CDL	C59-C60-C61-C62
55	l	701	CDL	C52-C53-C54-C55
55	l	701	CDL	C75-C76-C77-C78
48	C	302	PLX	C11-C12-C13-C14
48	g	201	PLX	C10-C11-C12-C13
48	r	503	PLX	C13-C14-C15-C16
48	r	502	PLX	C12-C13-C14-C15
49	G	201	8Q1	C12-C13-C14-C15
55	V	201	CDL	C54-C55-C56-C57
55	a	201	CDL	CB5-C51-C52-C53
53	Q	502	PEE	C11-C10-O2-C2
53	l	703	PEE	C11-C10-O2-C2
55	V	201	CDL	C11-CA5-OA6-CA4
55	V	201	CDL	C51-CB5-OB6-CB4
53	l	702	PEE	O3P-C1-C2-O2
48	a	202	PLX	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
55	g	202	CDL	C42-C43-C44-C45
55	g	202	CDL	C52-C53-C54-C55
55	V	201	CDL	OA7-CA5-OA6-CA4
55	i	401	CDL	CB5-C51-C52-C53
55	V	201	CDL	C84-C85-C86-C87
55	g	202	CDL	C35-C36-C37-C38
55	g	202	CDL	OB6-CB4-CB6-OB8
53	r	501	PEE	C20-C21-C22-C23
55	g	202	CDL	C41-C42-C43-C44
48	a	202	PLX	C15-C16-C17-C18
49	X	201	8Q1	C11-C10-C9-C8
46	A	502	FMN	O2'-C2'-C3'-O3'
48	r	502	PLX	C10-C11-C12-C13
55	V	201	CDL	C64-C65-C66-C67
55	l	701	CDL	C14-C15-C16-C17
48	r	503	PLX	C14-C15-C16-C17
53	Q	501	PEE	O5-C30-O3-C3
55	g	202	CDL	OA9-CA7-OA8-CA6
53	l	703	PEE	O4-C10-O2-C2
53	j	201	PEE	C42-C43-C44-C45
53	Q	501	PEE	C18-C19-C20-C21
53	j	202	PEE	C1-O3P-P-O4P
53	l	703	PEE	C31-C32-C33-C34
55	i	401	CDL	C74-C75-C76-C77
48	C	302	PLX	O4-C3-C4-C5
53	Q	502	PEE	O3P-C1-C2-C3
55	a	201	CDL	OA5-CA3-CA4-CA6
55	l	701	CDL	C77-C78-C79-C80
55	l	701	CDL	CB5-C51-C52-C53
55	a	201	CDL	C34-C35-C36-C37
53	Q	502	PEE	C20-C21-C22-C23
55	g	202	CDL	C37-C38-C39-C40
53	Q	502	PEE	C39-C40-C41-C42
55	i	401	CDL	CA5-C11-C12-C13
49	G	201	8Q1	C11-C10-C9-C8
48	g	201	PLX	C16-C17-C18-C19
55	V	201	CDL	C58-C59-C60-C61
55	g	202	CDL	C56-C57-C58-C59
48	a	202	PLX	C3-C4-C5-O8
48	g	201	PLX	C3-C4-C5-O8
48	j	203	PLX	C3-C4-C5-O8
48	r	503	PLX	C3-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
53	Q	501	PEE	C1-C2-C3-O3
53	l	703	PEE	C1-C2-C3-O3
55	g	202	CDL	CB3-CB4-CB6-OB8
55	V	201	CDL	C77-C78-C79-C80
55	g	202	CDL	C11-C12-C13-C14
48	r	502	PLX	C15-C16-C17-C18
48	r	503	PLX	C18-C19-C20-C21
53	Q	501	PEE	C35-C36-C37-C38
53	Q	502	PEE	C15-C16-C17-C18
48	C	302	PLX	C9-C10-C11-C12
48	r	502	PLX	C31-C32-C33-C34
53	Q	501	PEE	C21-C22-C23-C24
55	l	701	CDL	C64-C65-C66-C67
55	a	201	CDL	C60-C61-C62-C63
55	i	401	CDL	C33-C34-C35-C36
55	i	401	CDL	C35-C36-C37-C38
53	j	202	PEE	C36-C37-C38-C39
49	G	201	8Q1	C28-O27-P24-O3
49	X	201	8Q1	C7-C8-C9-C10
55	V	201	CDL	OB5-CB3-CB4-OB6
53	Q	502	PEE	C17-C18-C19-C20
48	g	201	PLX	C13-C14-C15-C16
53	Q	501	PEE	C31-C32-C33-C34
55	V	201	CDL	C78-C79-C80-C81
48	j	203	PLX	C33-C34-C35-C36
55	i	401	CDL	C15-C16-C17-C18
48	r	503	PLX	O6-C4-C5-O8
55	g	202	CDL	OA6-CA4-CA6-OA8
55	i	401	CDL	OB6-CB4-CB6-OB8
53	l	702	PEE	C23-C24-C25-C26
48	j	203	PLX	C13-C14-C15-C16
48	j	203	PLX	C9-C10-C11-C12
53	r	501	PEE	C22-C23-C24-C25
55	g	202	CDL	C83-C84-C85-C86
55	V	201	CDL	OB7-CB5-OB6-CB4
55	i	401	CDL	C75-C76-C77-C78
48	a	202	PLX	C7-C8-C9-C10
48	r	503	PLX	C31-C32-C33-C34
53	l	703	PEE	C13-C14-C15-C16
53	Q	502	PEE	C30-C31-C32-C33
53	l	702	PEE	O3P-C1-C2-C3
55	g	202	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
55	g	202	CDL	C64-C65-C66-C67
55	a	201	CDL	C59-C60-C61-C62
55	g	202	CDL	C20-C21-C22-C23
53	l	703	PEE	C16-C17-C18-C19
48	r	502	PLX	C33-C34-C35-C36
53	r	501	PEE	C1-C2-C3-O3
55	g	202	CDL	CA3-CA4-CA6-OA8
55	l	701	CDL	CA3-CA4-CA6-OA8
55	l	701	CDL	CB3-CB4-CB6-OB8
53	j	201	PEE	C37-C38-C39-C40
48	r	502	PLX	C18-C19-C20-C21
53	l	702	PEE	C32-C33-C34-C35
48	j	203	PLX	C3-O4-P1-O1
48	r	503	PLX	C5-C4-O6-C6
53	j	201	PEE	C4-O4P-P-O3P
53	l	703	PEE	C1-O3P-P-O4P
55	V	201	CDL	CA2-OA2-PA1-OA5
47	A	503	NAI	C2D-C1D-N1N-C2N
53	Q	502	PEE	C22-C23-C24-C25
55	g	202	CDL	C31-C32-C33-C34
48	r	503	PLX	C36-C37-C38-C39
53	Q	502	PEE	O3P-C1-C2-O2
48	r	502	PLX	C29-C30-C31-C32
48	r	503	PLX	C26-C27-C28-C29
55	i	401	CDL	C14-C15-C16-C17
48	g	201	PLX	O6-C4-C5-O8
55	V	201	CDL	OB6-CB4-CB6-OB8
53	r	501	PEE	C11-C10-O2-C2
55	l	701	CDL	CB2-C1-CA2-OA2
48	g	201	PLX	C9-C10-C11-C12
48	r	502	PLX	C13-C14-C15-C16
55	a	201	CDL	C52-C53-C54-C55
53	m	201	PEE	C20-C21-C22-C23
55	l	701	CDL	C62-C63-C64-C65
48	g	201	PLX	C11-C12-C13-C14
49	G	201	8Q1	O4-C1-S44-C43
49	X	201	8Q1	O4-C1-S44-C43
53	l	703	PEE	C30-C31-C32-C33
53	r	501	PEE	O4-C10-O2-C2
55	a	201	CDL	C11-CA5-OA6-CA4
53	j	202	PEE	C32-C33-C34-C35
48	r	503	PLX	O8-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
53	Q	501	PEE	O3P-C1-C2-C3
55	l	701	CDL	OA5-CA3-CA4-CA6
53	r	501	PEE	C36-C37-C38-C39
48	a	202	PLX	C30-C31-C32-C33
48	C	302	PLX	C11-C10-C9-C8
55	l	701	CDL	C82-C83-C84-C85
50	J	401	NDP	C3B-C4B-C5B-O5B
53	Q	502	PEE	C31-C30-O3-C3
48	g	201	PLX	C36-C37-C38-C39
55	a	201	CDL	C33-C34-C35-C36
53	j	202	PEE	C38-C39-C40-C41
53	l	703	PEE	C18-C19-C20-C21
49	G	201	8Q1	C6-C1-S44-C43
49	X	201	8Q1	C6-C1-S44-C43
53	m	201	PEE	C3-C2-O2-C10
55	l	701	CDL	C34-C35-C36-C37
49	G	201	8Q1	N36-C37-C38-C39
48	j	203	PLX	C7-C6-O6-C4
48	r	502	PLX	C3-C4-C5-O8
53	Q	501	PEE	C2-C1-O3P-P
55	l	701	CDL	C44-C45-C46-C47
55	i	401	CDL	OA5-CA3-CA4-OA6
55	l	701	CDL	C57-C58-C59-C60
49	G	201	8Q1	C31-C29-C32-C34
55	l	701	CDL	C60-C61-C62-C63
53	r	501	PEE	O2-C2-C3-O3
53	m	201	PEE	O3-C30-C31-C32
55	a	201	CDL	C73-C74-C75-C76
47	A	503	NAI	C5B-O5B-PA-O3
48	r	503	PLX	C10-C11-C12-C13
55	a	201	CDL	OA7-CA5-OA6-CA4
55	l	701	CDL	C78-C79-C80-C81
55	i	401	CDL	CB3-OB5-PB2-OB2
55	g	202	CDL	C23-C24-C25-C26
55	l	701	CDL	C51-C52-C53-C54
55	l	701	CDL	C54-C55-C56-C57
55	g	202	CDL	CB4-CB3-OB5-PB2
56	s	401	UQ	C12-C11-C9-C8
46	A	502	FMN	C3'-C4'-C5'-O5'
48	r	502	PLX	C3-O4-P1-O2
48	r	502	PLX	C3-O4-P1-O3
53	j	201	PEE	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
53	j	201	PEE	C4-O4P-P-O2P
53	j	202	PEE	C1-O3P-P-O2P
53	m	201	PEE	C4-O4P-P-O2P
53	m	201	PEE	C4-O4P-P-O1P
53	r	501	PEE	C1-O3P-P-O2P
53	r	501	PEE	C1-O3P-P-O1P
55	V	201	CDL	CB2-OB2-PB2-OB3
55	V	201	CDL	CB2-OB2-PB2-OB4
55	g	202	CDL	CB2-OB2-PB2-OB3
55	g	202	CDL	CB2-OB2-PB2-OB4
55	g	202	CDL	CB3-OB5-PB2-OB3
55	l	701	CDL	CB2-OB2-PB2-OB3
57	w	401	ADP	C5'-O5'-PA-O1A
55	g	202	CDL	OB5-CB3-CB4-CB6
55	i	401	CDL	OA5-CA3-CA4-CA6
53	j	201	PEE	C17-C18-C19-C20
53	Q	502	PEE	O5-C30-O3-C3
55	V	201	CDL	C81-C82-C83-C84
53	Q	501	PEE	C39-C40-C41-C42
53	j	201	PEE	C39-C40-C41-C42
55	g	202	CDL	C34-C35-C36-C37
55	l	701	CDL	C12-C13-C14-C15
47	A	503	NAI	C3D-C4D-C5D-O5D
48	g	201	PLX	O4-C3-C4-O6
55	g	202	CDL	OB5-CB3-CB4-OB6
55	l	701	CDL	OA5-CA3-CA4-OA6
48	r	503	PLX	C2-C1-N1-C1A
47	A	503	NAI	C2D-C1D-N1N-C6N
48	C	302	PLX	N1-C1-C2-O1
50	J	401	NDP	C2N-C3N-C7N-O7N
55	i	401	CDL	CA3-CA4-CA6-OA8
48	a	202	PLX	O6-C4-C5-O8
48	j	203	PLX	O6-C4-C5-O8
53	l	703	PEE	O2-C2-C3-O3
55	i	401	CDL	OA6-CA4-CA6-OA8
55	i	401	CDL	C73-C74-C75-C76
48	a	202	PLX	C10-C11-C12-C13
53	l	702	PEE	C21-C22-C23-C24
55	a	201	CDL	C16-C17-C18-C19
55	l	701	CDL	C32-C33-C34-C35
48	C	302	PLX	C18-C19-C20-C21
55	g	202	CDL	C61-C62-C63-C64

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	C24-C25-C26-C27
53	l	702	PEE	C20-C21-C22-C23
55	l	701	CDL	C17-C18-C19-C20
48	g	201	PLX	O4-C3-C4-C5
48	j	203	PLX	O4-C3-C4-C5
55	V	201	CDL	OB5-CB3-CB4-CB6
48	r	503	PLX	C17-C18-C19-C20
53	Q	501	PEE	C14-C15-C16-C17
46	A	502	FMN	C5'-O5'-P-O1P
48	r	502	PLX	C14-C15-C16-C17
55	i	401	CDL	C13-C14-C15-C16
55	l	701	CDL	C31-C32-C33-C34
48	j	203	PLX	O4-C3-C4-O6
48	r	503	PLX	C2-C1-N1-C1C
47	A	503	NAI	O4D-C1D-N1N-C2N
55	l	701	CDL	C58-C59-C60-C61
48	r	502	PLX	O6-C4-C5-O8
53	Q	501	PEE	O2-C2-C3-O3
49	G	201	8Q1	C6-C7-C8-C9
53	Q	501	PEE	C24-C25-C26-C27
53	r	501	PEE	C24-C25-C26-C27
48	a	202	PLX	C2-O1-P1-O4
55	V	201	CDL	CA3-OA5-PA1-OA2
55	g	202	CDL	C60-C61-C62-C63
49	G	201	8Q1	C30-C29-C32-O33
53	Q	502	PEE	C21-C22-C23-C24
55	i	401	CDL	CB3-CB4-CB6-OB8
55	l	701	CDL	C56-C57-C58-C59
53	j	201	PEE	C44-C45-C46-C47
48	r	503	PLX	C2-C1-N1-C1B
55	V	201	CDL	C75-C76-C77-C78
55	a	201	CDL	C57-C58-C59-C60
48	a	202	PLX	C11-C12-C13-C14
48	C	302	PLX	C31-C32-C33-C34
55	a	201	CDL	C54-C55-C56-C57
53	j	202	PEE	C37-C38-C39-C40
55	g	202	CDL	C82-C83-C84-C85
53	j	201	PEE	C18-C19-C20-C21
56	s	401	UQ	C14-C16-C17-C18
55	V	201	CDL	C82-C83-C84-C85
53	Q	502	PEE	C13-C14-C15-C16
55	l	701	CDL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
53	m	201	PEE	C24-C25-C26-C27
48	r	503	PLX	C24-C25-C26-C27
55	a	201	CDL	C44-C45-C46-C47
48	j	203	PLX	O6-C6-C7-C8
48	j	203	PLX	O8-C24-C25-C26
55	V	201	CDL	C12-C11-CA5-OA7
57	w	401	ADP	C4'-C5'-O5'-PA
48	j	203	PLX	C35-C36-C37-C38
55	l	701	CDL	C23-C24-C25-C26
49	G	201	8Q1	C9-C10-C11-C12
53	j	201	PEE	C1-C2-C3-O3
55	a	201	CDL	C43-C44-C45-C46
49	G	201	8Q1	O27-C28-C29-C30
48	r	503	PLX	C7-C8-C9-C10
53	l	703	PEE	C32-C33-C34-C35
53	j	202	PEE	C24-C25-C26-C27
53	Q	501	PEE	C38-C39-C40-C41
55	V	201	CDL	C12-C11-CA5-OA6
55	i	401	CDL	C37-C38-C39-C40
55	a	201	CDL	C41-C42-C43-C44
53	Q	501	PEE	O3P-C1-C2-O2
53	r	501	PEE	C18-C19-C20-C21
55	l	701	CDL	C20-C21-C22-C23
55	l	701	CDL	C71-C72-C73-C74
55	V	201	CDL	C83-C84-C85-C86
55	g	202	CDL	C44-C45-C46-C47
48	r	503	PLX	C11-C12-C13-C14
55	l	701	CDL	C79-C80-C81-C82
53	m	201	PEE	C17-C18-C19-C20
53	j	202	PEE	C31-C32-C33-C34
53	m	201	PEE	C32-C33-C34-C35
53	l	703	PEE	C22-C23-C24-C25
48	a	202	PLX	C19-C20-C21-C22
55	l	701	CDL	C63-C64-C65-C66
50	J	401	NDP	PN-O3-PA-O1A
55	V	201	CDL	OB9-CB7-OB8-CB6
55	V	201	CDL	CB3-CB4-CB6-OB8
55	V	201	CDL	CB7-C71-C72-C73
47	A	503	NAI	O4D-C1D-N1N-C6N
53	l	702	PEE	C16-C17-C18-C19
53	l	703	PEE	C10-C11-C12-C13
53	j	202	PEE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
48	C	302	PLX	O8-C24-C25-C26
48	g	201	PLX	O8-C24-C25-C26
48	a	202	PLX	C27-C28-C29-C30
56	s	401	UQ	C9-C11-C12-C13
53	l	703	PEE	O4P-C4-C5-N
48	j	203	PLX	C31-C32-C33-C34
48	r	502	PLX	C4-C3-O4-P1
55	i	401	CDL	CA4-CA3-OA5-PA1
53	j	202	PEE	C44-C45-C46-C47
55	V	201	CDL	C71-CB7-OB8-CB6
48	r	502	PLX	C11-C12-C13-C14
53	l	702	PEE	C13-C14-C15-C16
49	G	201	8Q1	O27-C28-C29-C31
48	C	302	PLX	C30-C31-C32-C33
55	l	701	CDL	C32-C31-CA7-OA8
53	j	201	PEE	C38-C39-C40-C41
53	l	702	PEE	C36-C37-C38-C39
53	l	703	PEE	C38-C39-C40-C41
53	m	201	PEE	C16-C17-C18-C19
55	l	701	CDL	C33-C34-C35-C36
55	V	201	CDL	C71-C72-C73-C74
55	V	201	CDL	C32-C31-CA7-OA8
53	Q	501	PEE	C36-C37-C38-C39
53	Q	502	PEE	C18-C19-C20-C21
53	j	201	PEE	C16-C17-C18-C19
53	Q	501	PEE	C15-C16-C17-C18
53	l	702	PEE	C1-C2-C3-O3
55	g	202	CDL	C52-C51-CB5-OB6
48	g	201	PLX	C18-C19-C20-C21
53	m	201	PEE	C18-C19-C20-C21
53	r	501	PEE	C32-C33-C34-C35
53	l	702	PEE	C22-C23-C24-C25
53	j	202	PEE	O2-C10-C11-C12
53	l	702	PEE	O2-C2-C3-O3
55	g	202	CDL	C81-C82-C83-C84
55	a	201	CDL	C15-C16-C17-C18
53	j	201	PEE	C36-C37-C38-C39
47	A	503	NAI	O4D-C4D-C5D-O5D
55	V	201	CDL	C32-C31-CA7-OA9
53	Q	502	PEE	C42-C43-C44-C45
53	r	501	PEE	C40-C41-C42-C43
55	g	202	CDL	C52-C51-CB5-OB7

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	CB3-CB4-CB6-OB8
53	j	202	PEE	O4-C10-C11-C12
53	l	702	PEE	O2-C10-C11-C12
55	l	701	CDL	C32-C31-CA7-OA9
48	j	203	PLX	C3-O4-P1-O3
53	r	501	PEE	C4-O4P-P-O1P
55	V	201	CDL	CA3-OA5-PA1-OA3
55	V	201	CDL	CB3-OB5-PB2-OB3
55	i	401	CDL	CA2-OA2-PA1-OA4
55	i	401	CDL	CB3-OB5-PB2-OB3
55	a	201	CDL	OB6-CB4-CB6-OB8
55	g	202	CDL	C80-C81-C82-C83
53	l	703	PEE	C5-C4-O4P-P
53	l	703	PEE	O3-C30-C31-C32
55	g	202	CDL	C72-C71-CB7-OB8
55	l	701	CDL	C12-C11-CA5-OA6
53	l	702	PEE	O4-C10-C11-C12
53	m	201	PEE	C12-C13-C14-C15
55	g	202	CDL	C72-C71-CB7-OB9
53	l	703	PEE	O2-C10-C11-C12
53	j	202	PEE	C16-C17-C18-C19

There are no ring outliers.

27 monomers are involved in 90 short contacts:

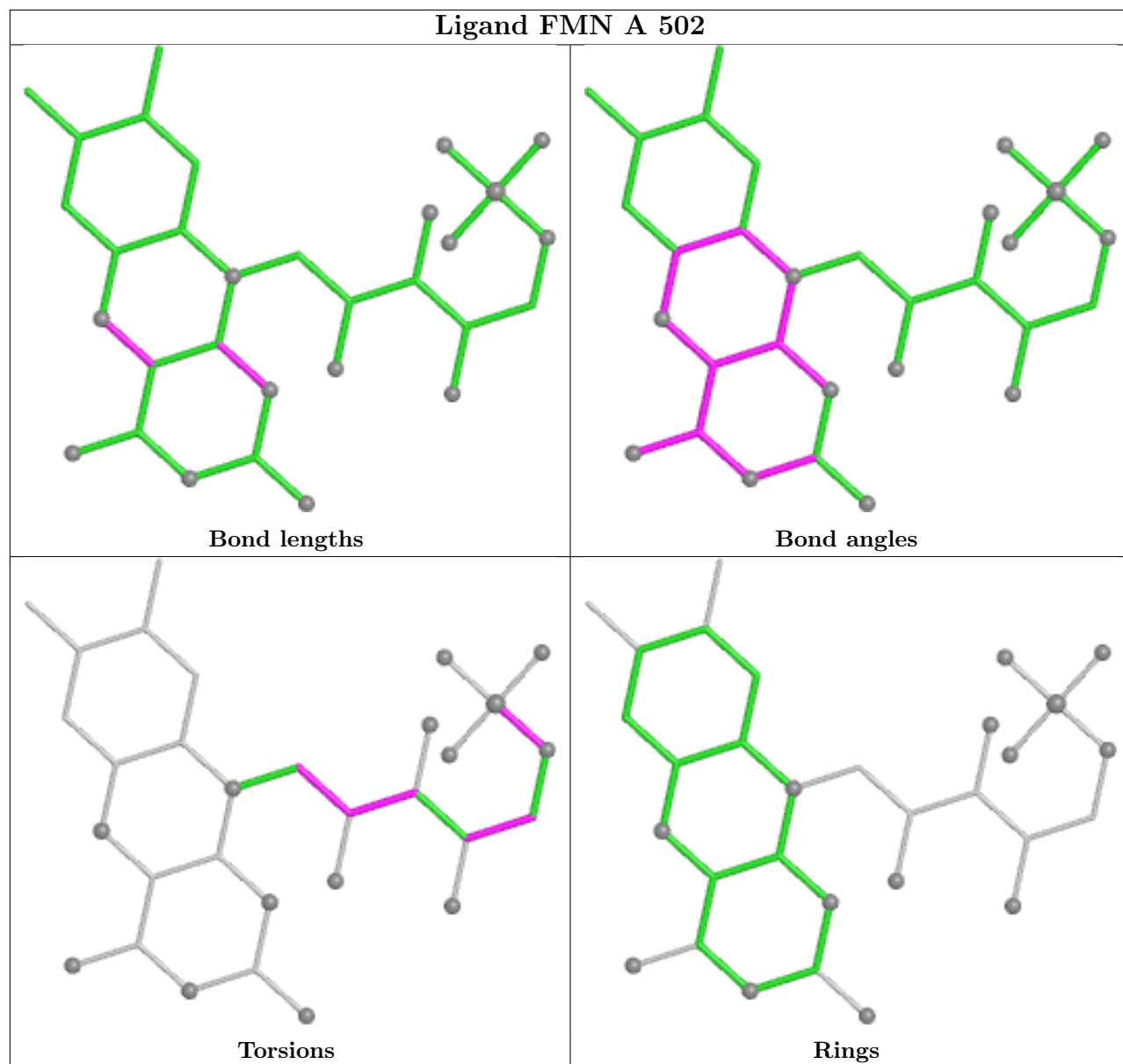
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	A	502	FMN	4	0
47	A	503	NAI	7	0
55	i	401	CDL	5	0
53	r	501	PEE	2	0
50	J	401	NDP	3	0
49	G	201	8Q1	5	0
55	a	201	CDL	4	0
55	V	201	CDL	4	0
55	g	202	CDL	10	0
53	l	702	PEE	2	0
48	r	503	PLX	3	0
48	g	201	PLX	3	0
49	X	201	8Q1	3	0
55	l	701	CDL	5	0
45	A	501	SF4	1	0
53	Q	501	PEE	2	0

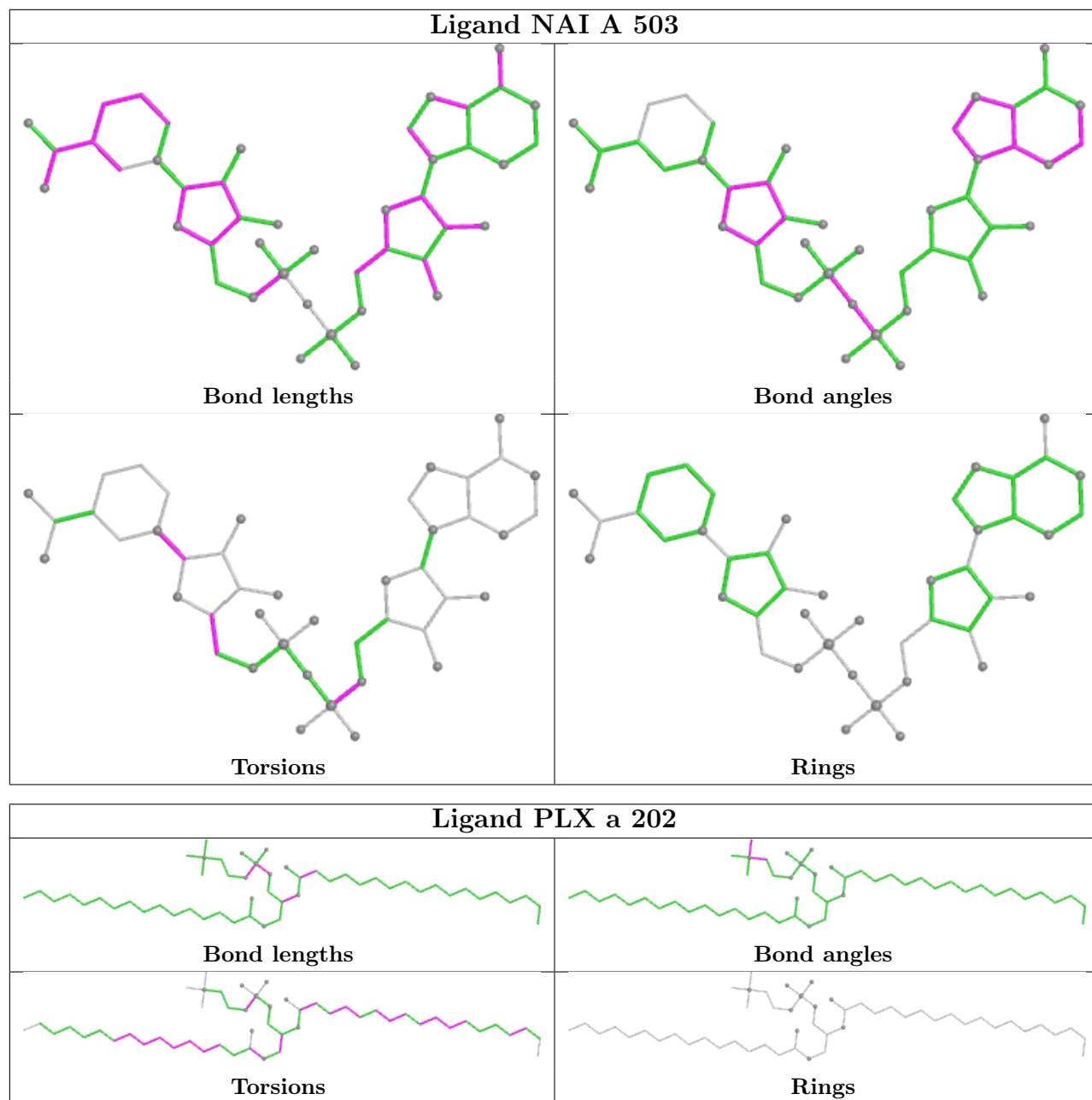
Continued on next page...

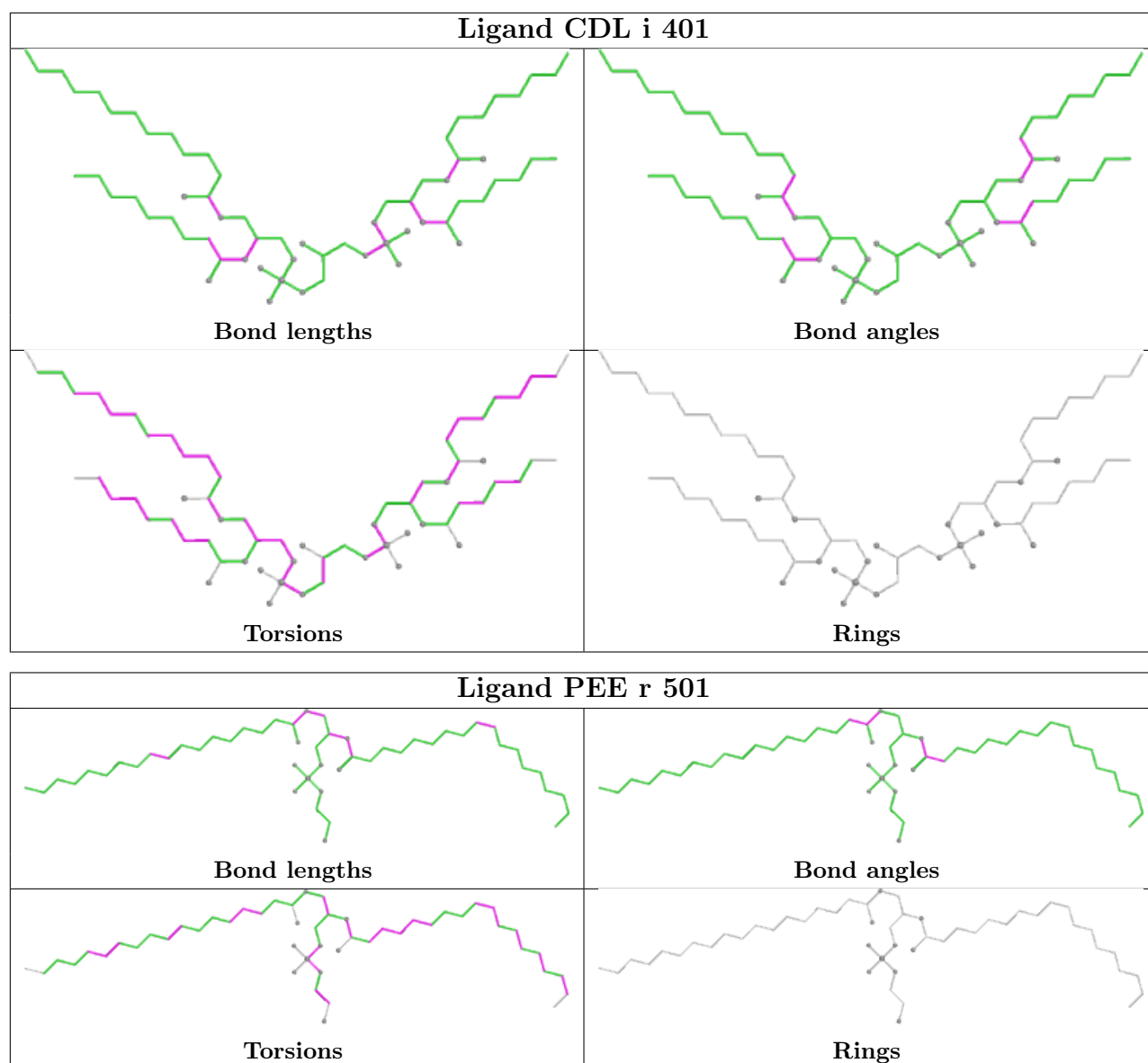
Continued from previous page...

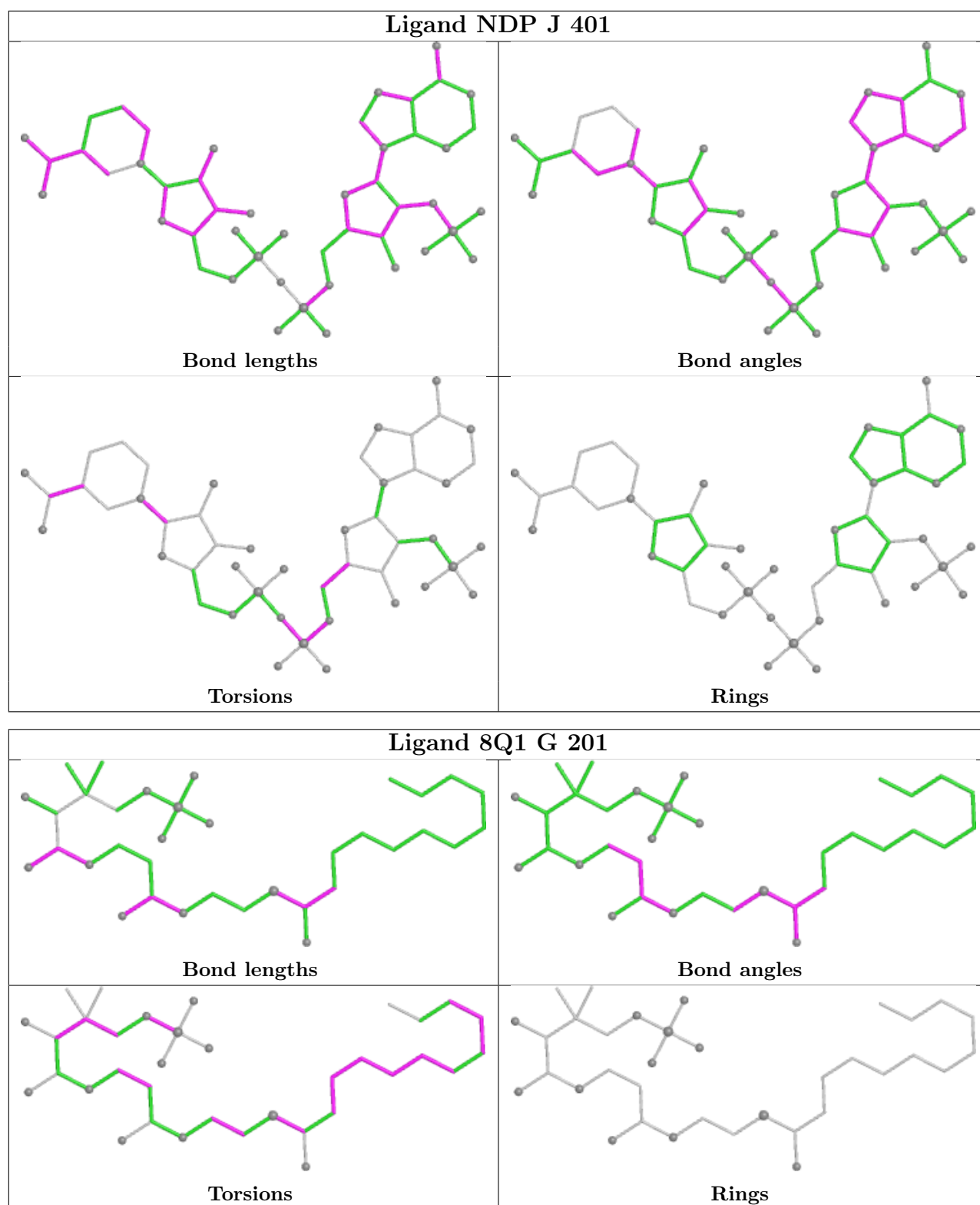
Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	Q	502	PEE	1	0
53	j	201	PEE	2	0
48	r	502	PLX	6	0
51	M	803	FES	1	0
56	s	401	UQ	4	0
53	l	703	PEE	3	0
53	m	201	PEE	3	0
48	C	302	PLX	6	0
48	j	203	PLX	2	0
45	C	301	SF4	1	0
53	j	202	PEE	2	0

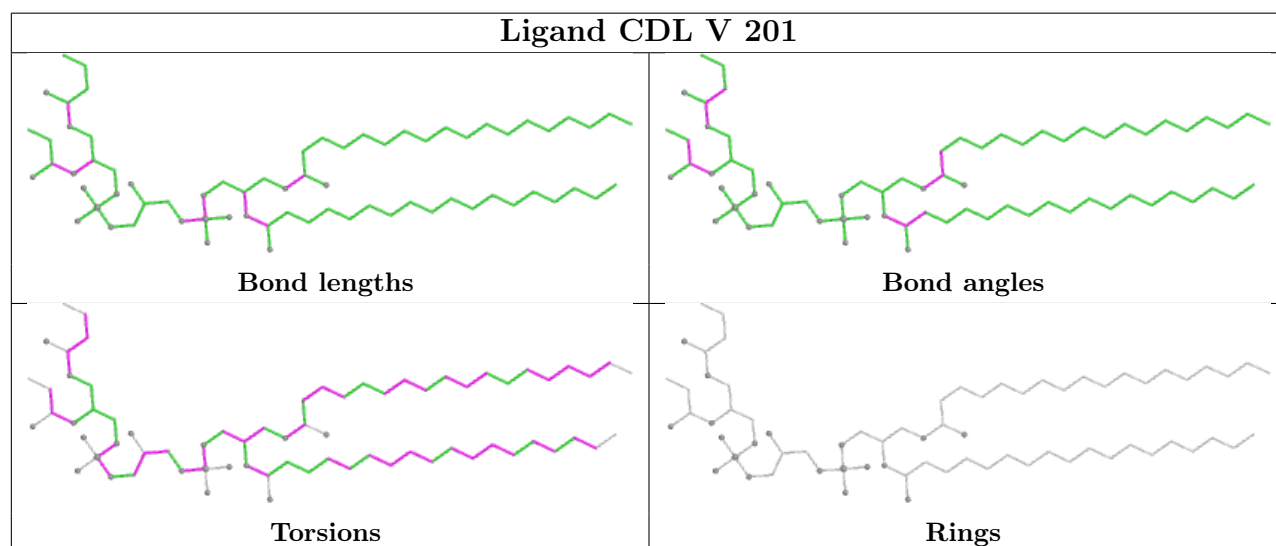
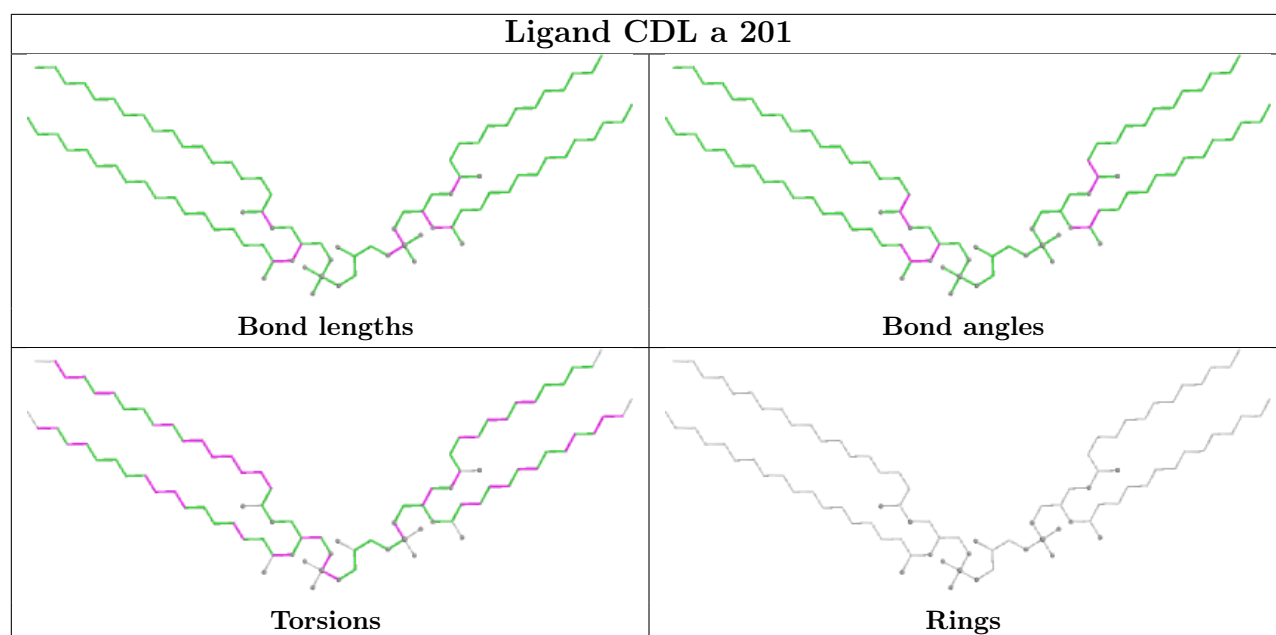
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

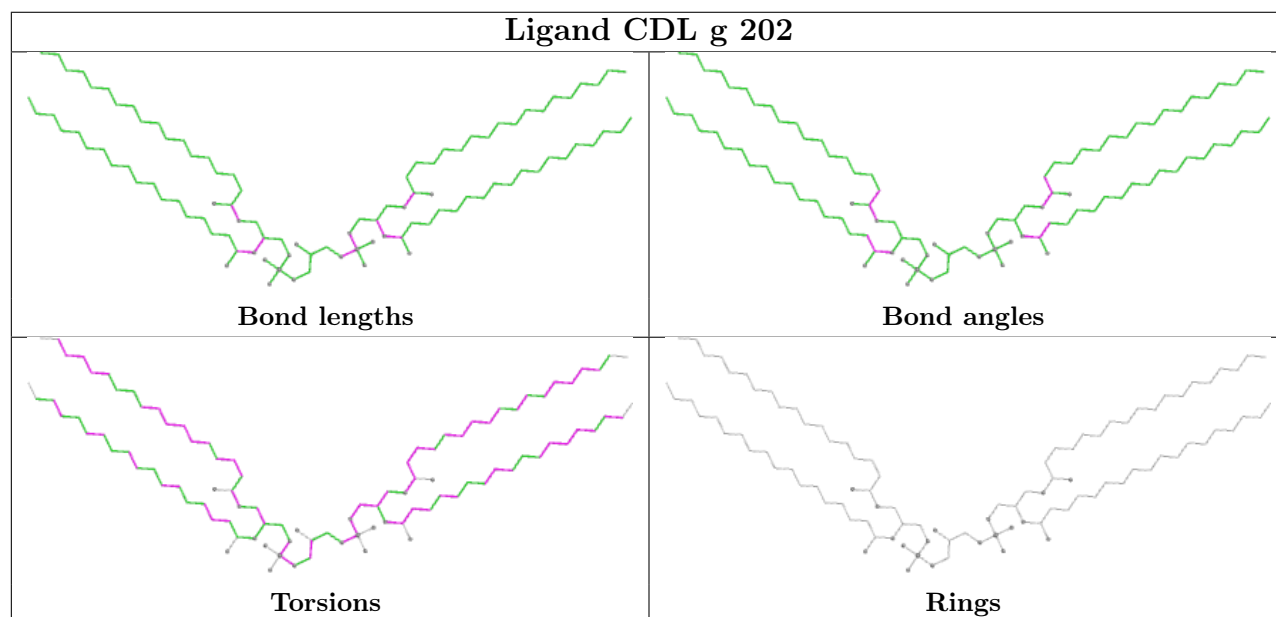
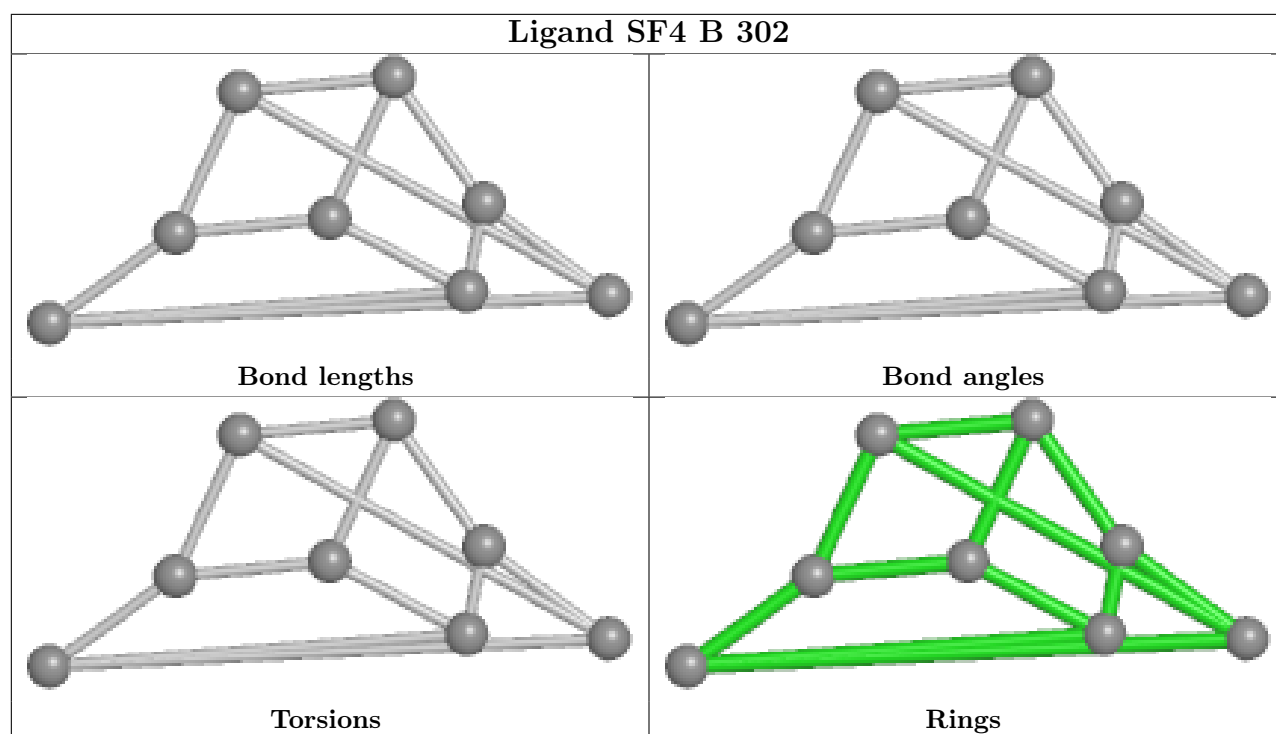


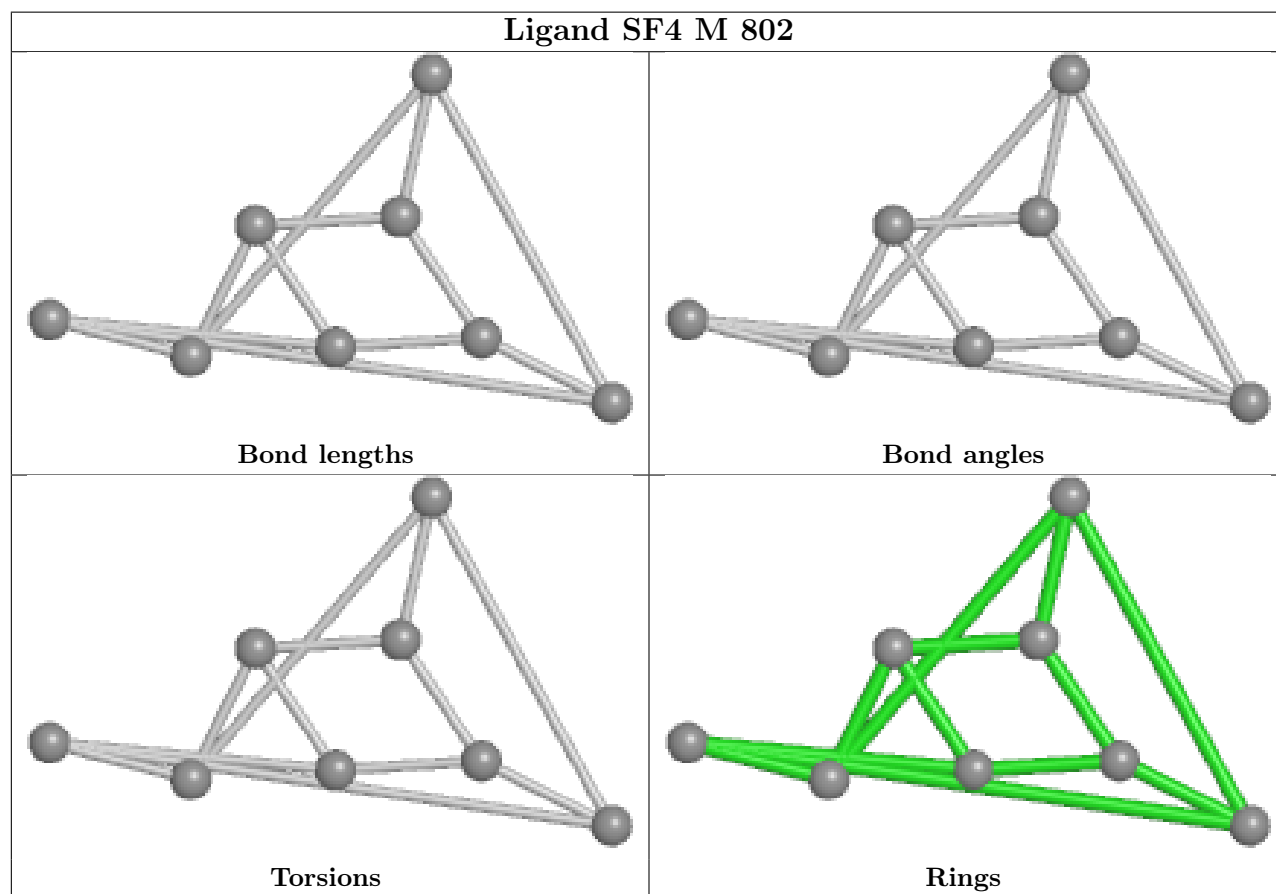
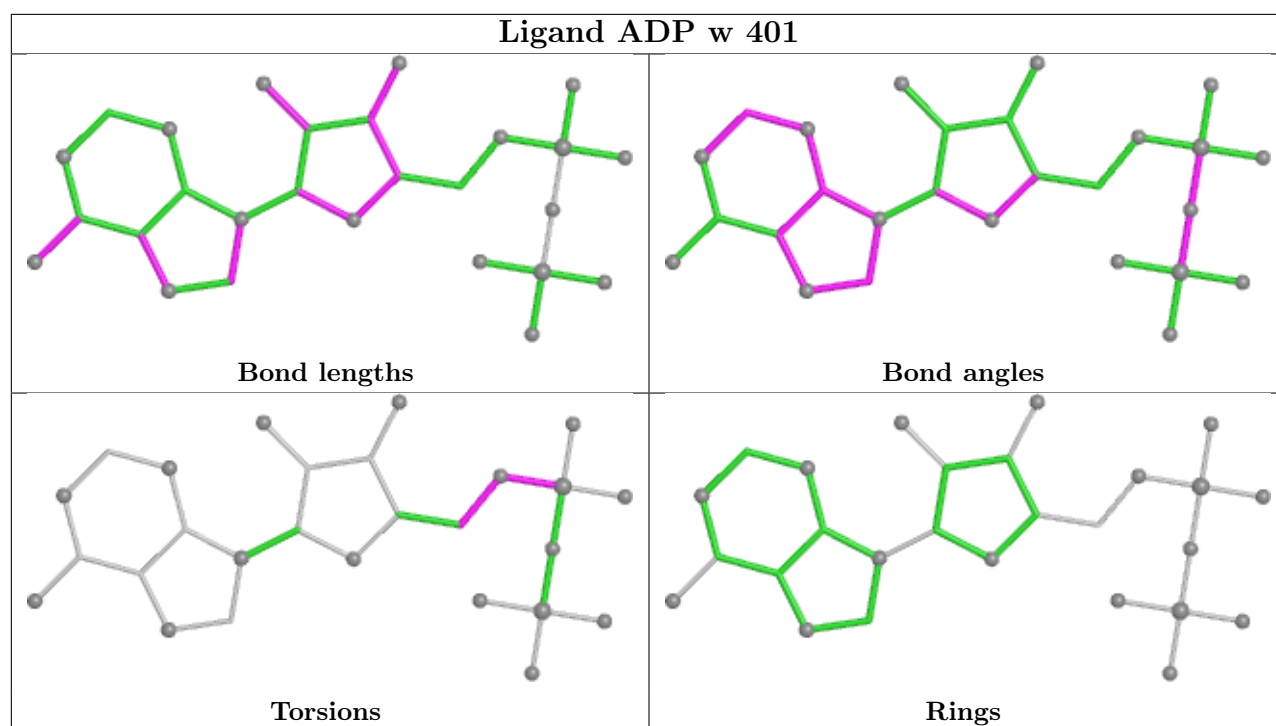


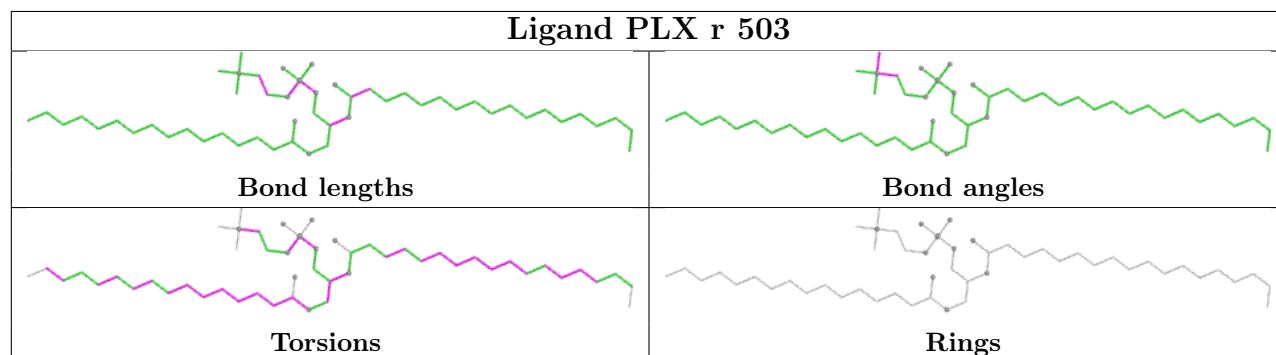
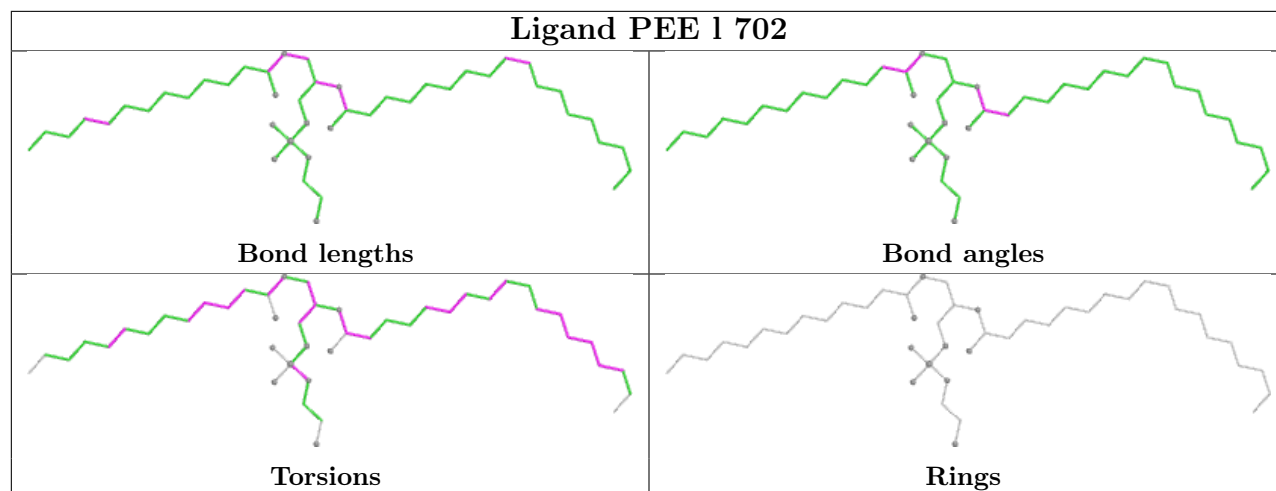


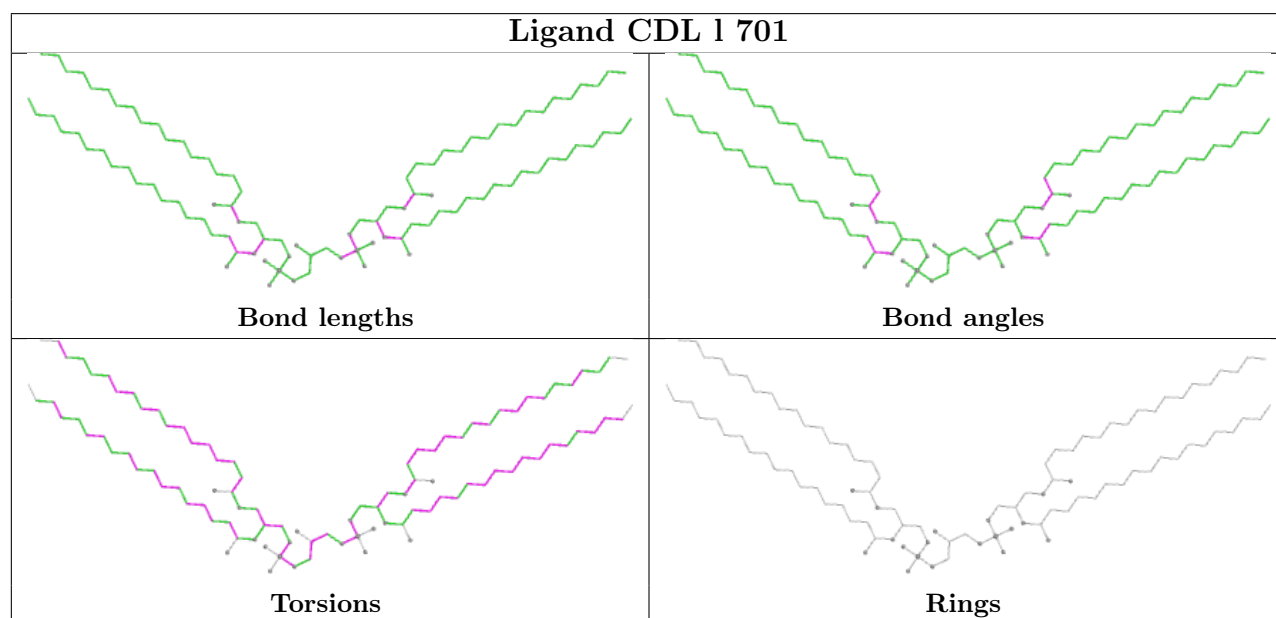
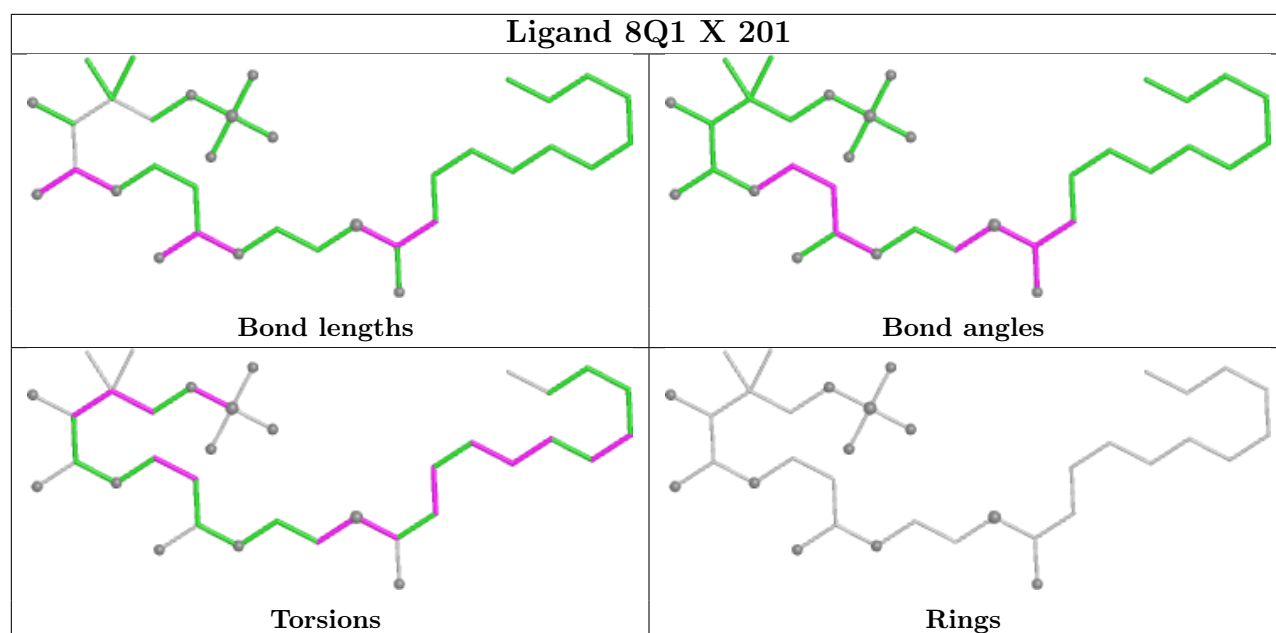


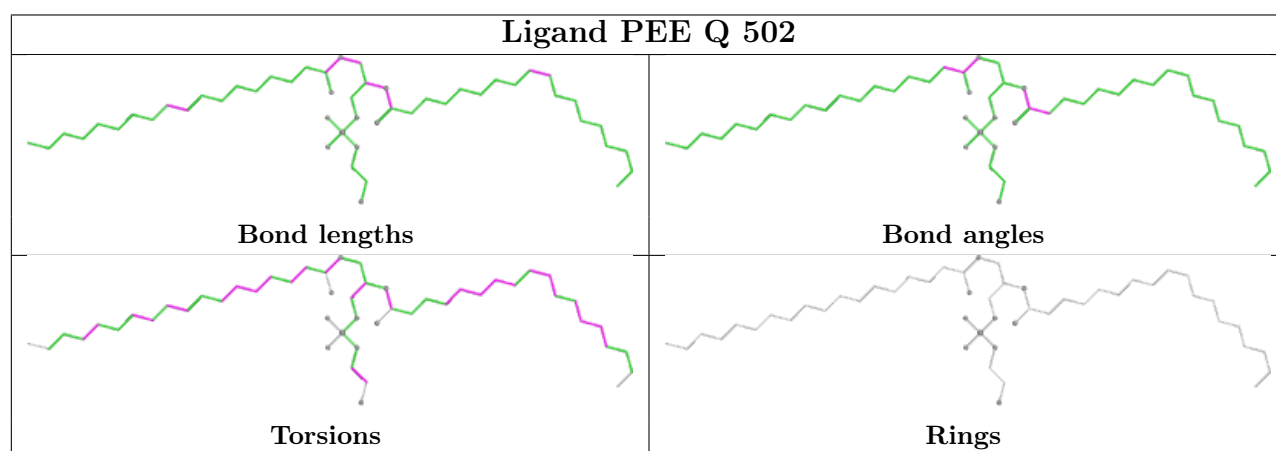
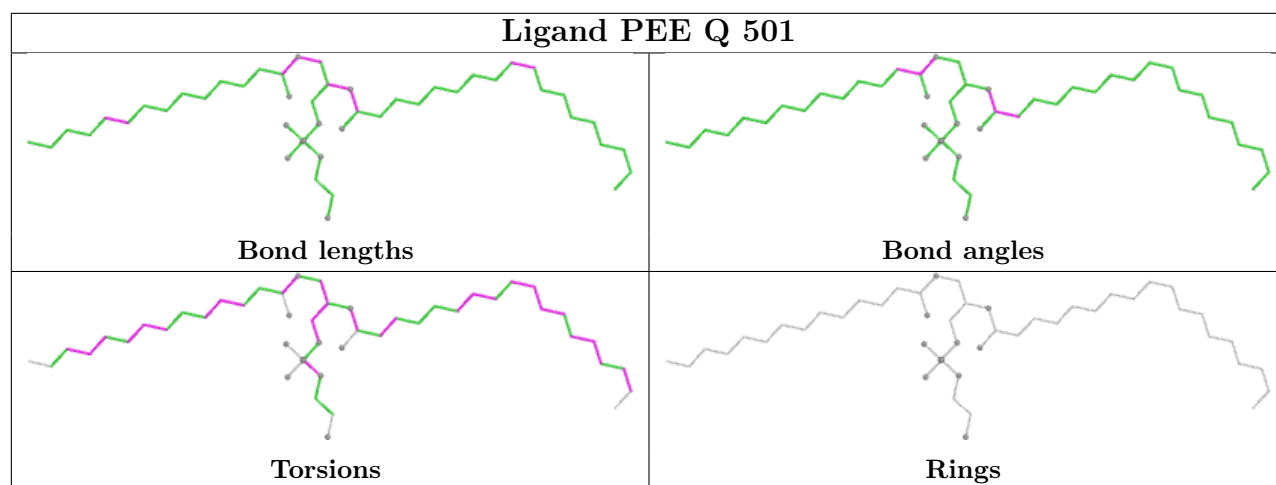
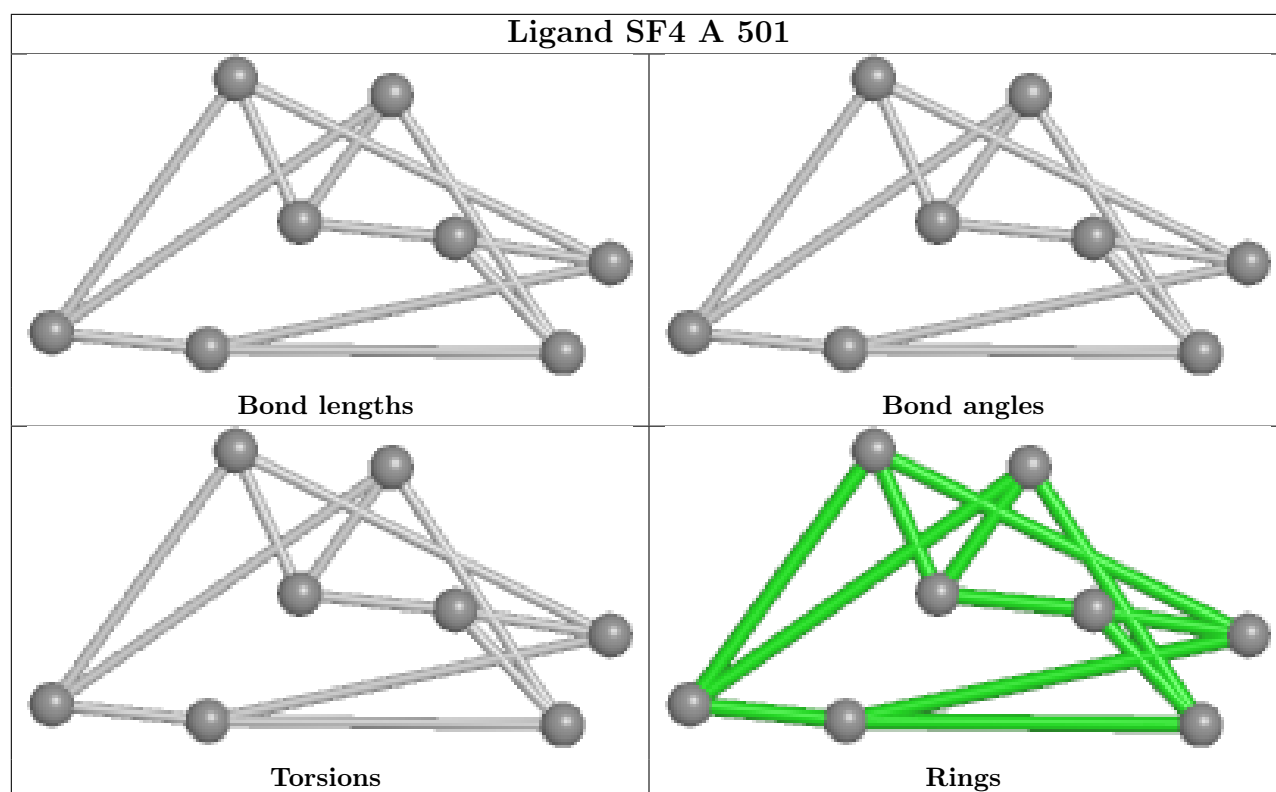


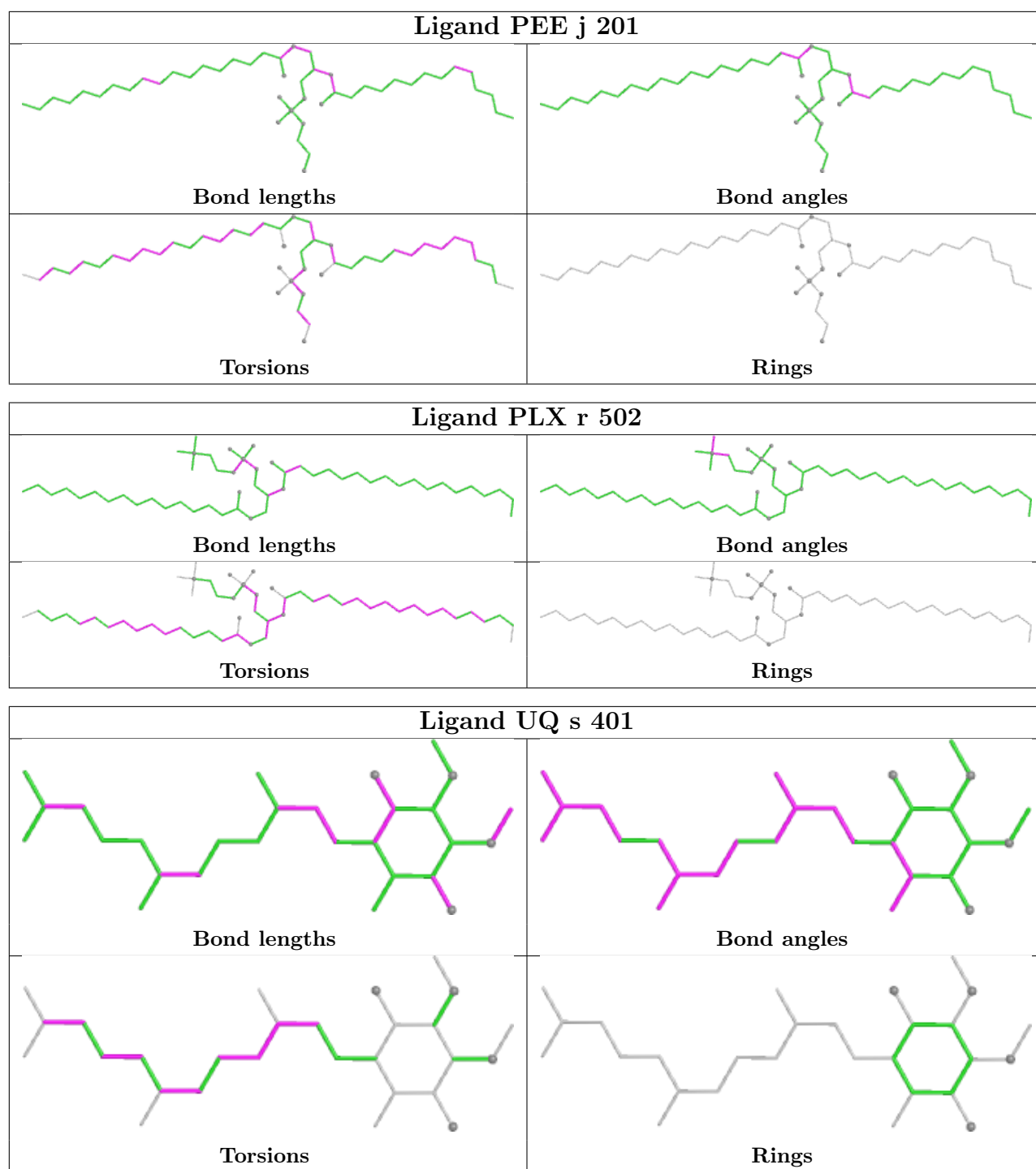


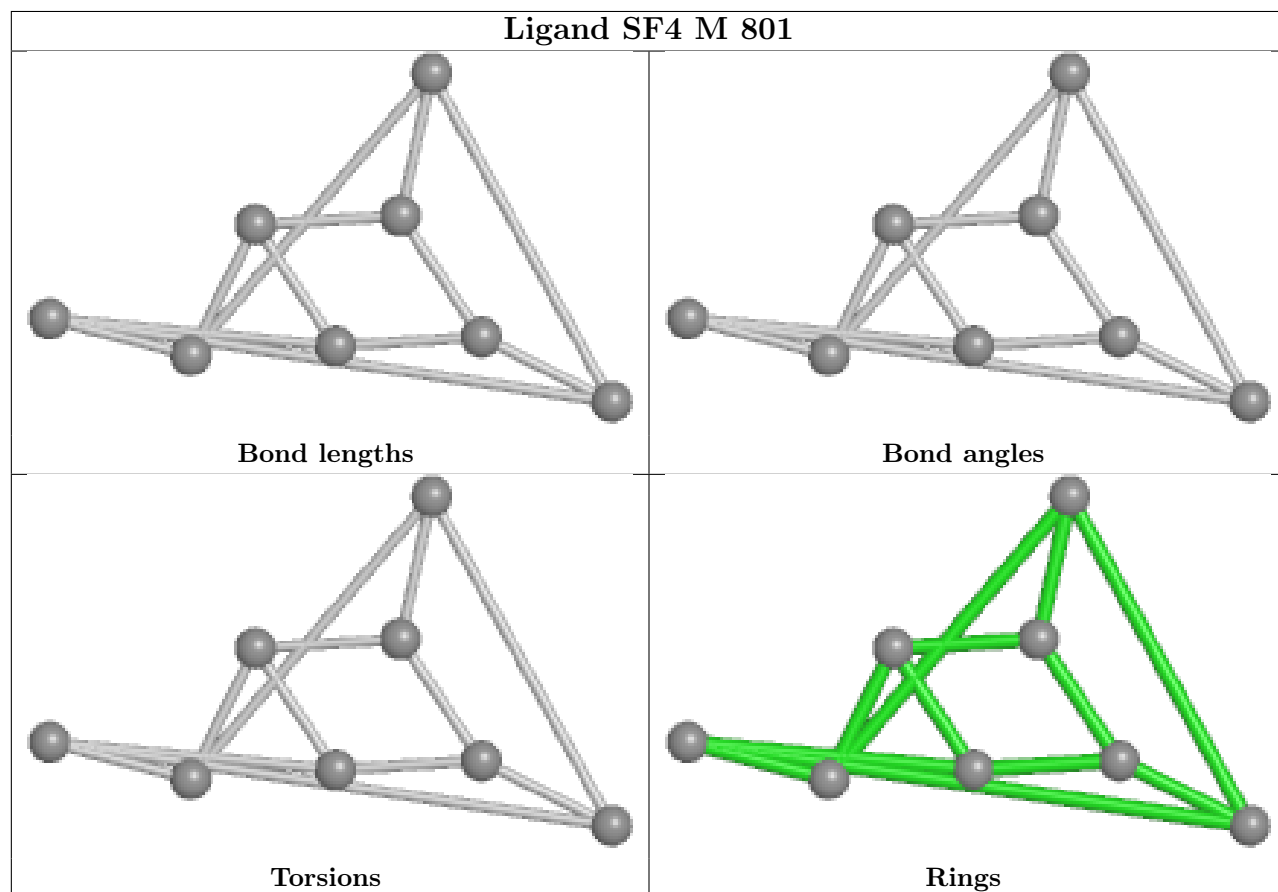
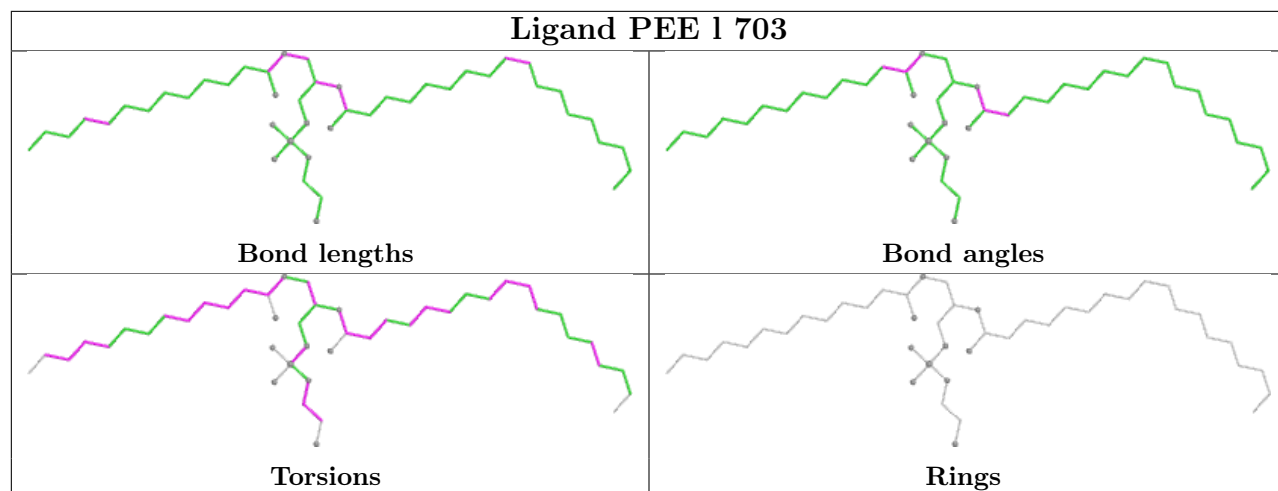


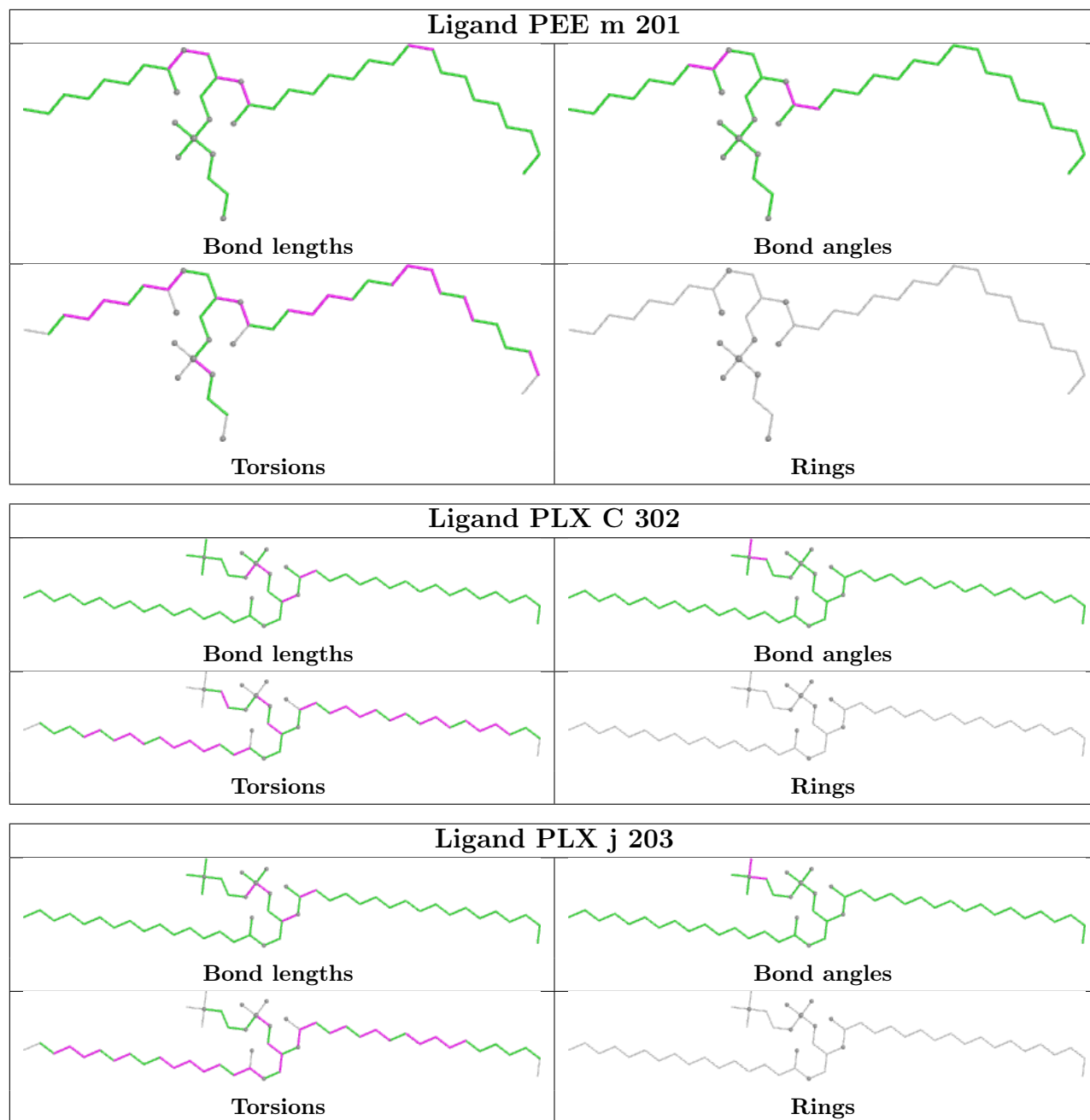


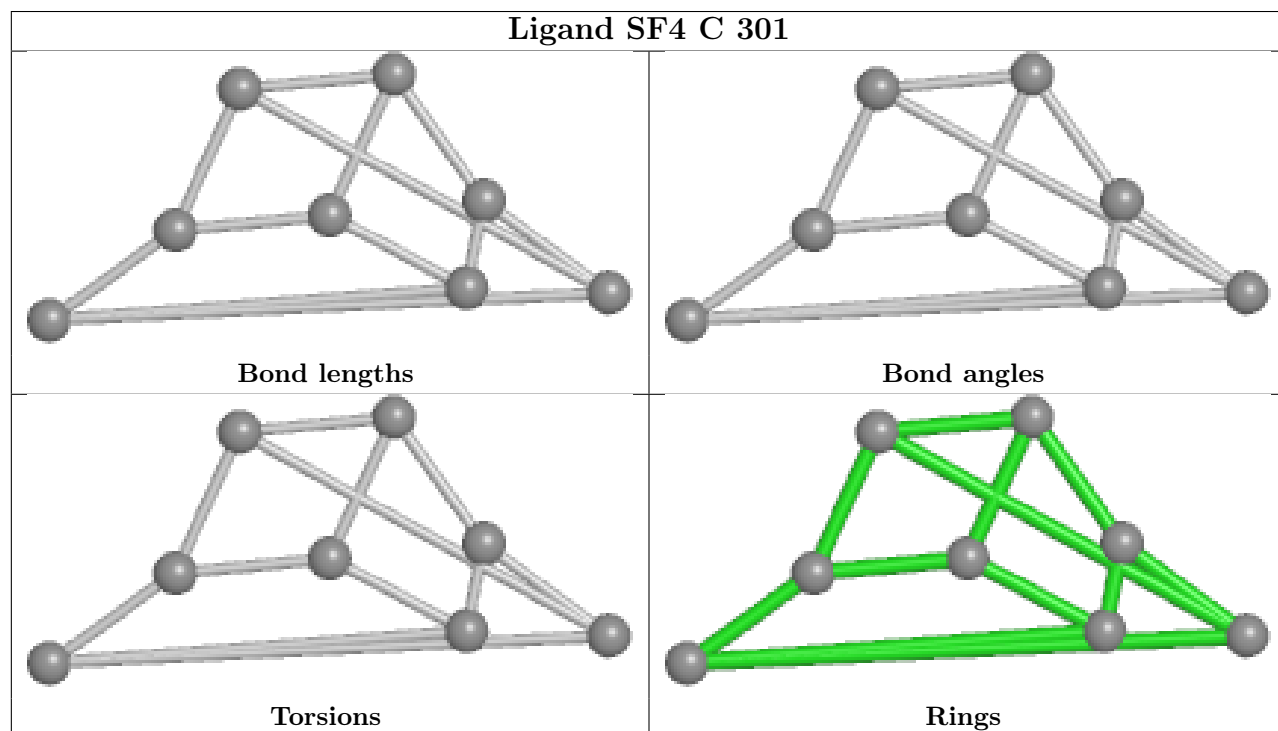
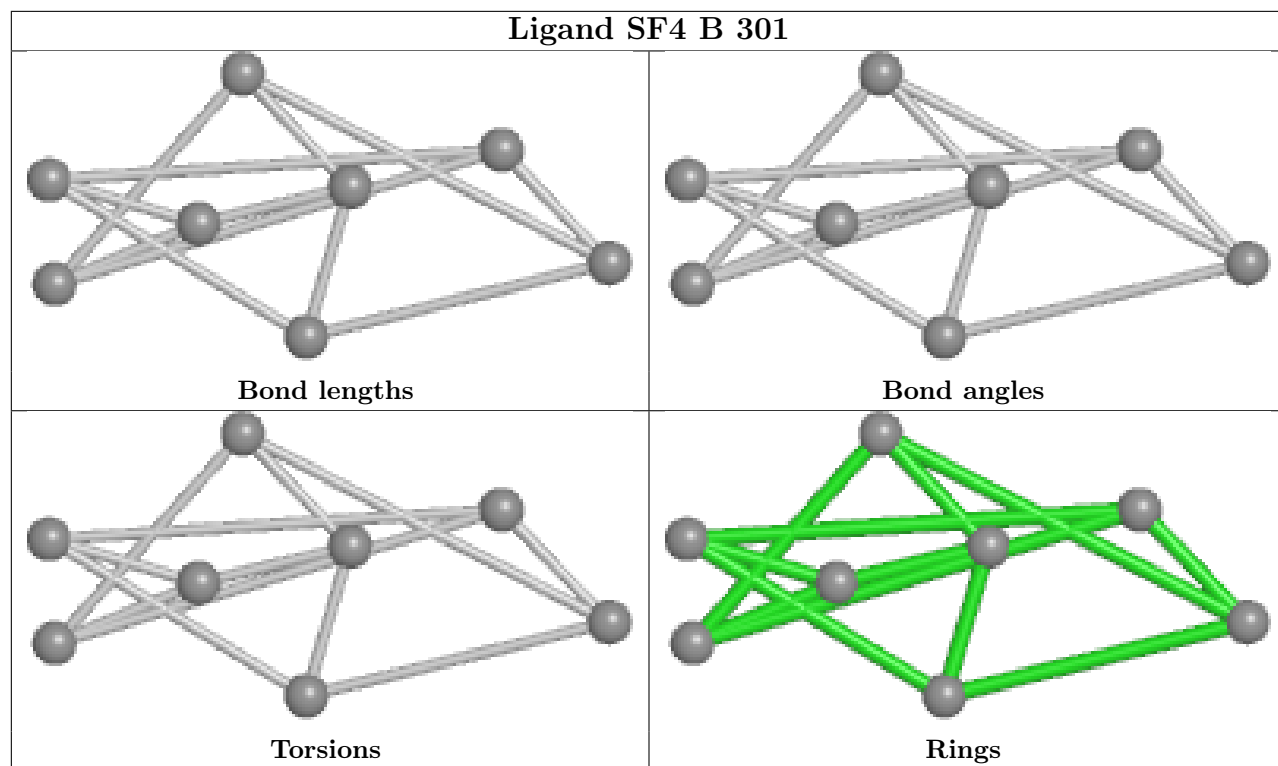


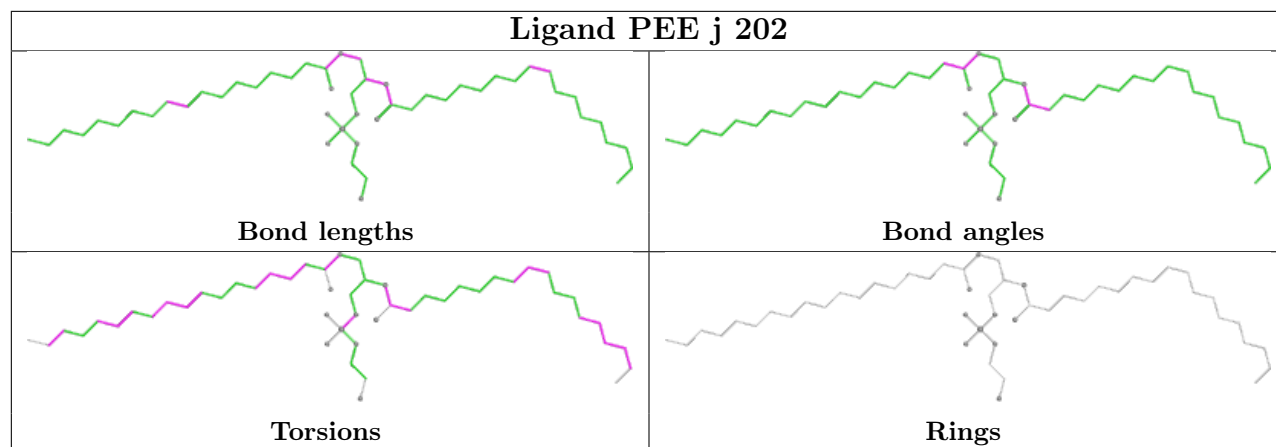












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

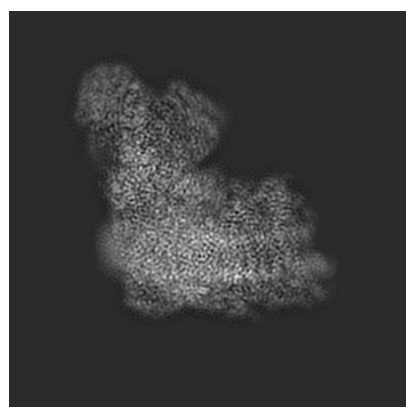
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32307. These allow visual inspection of the internal detail of the map and identification of artifacts.

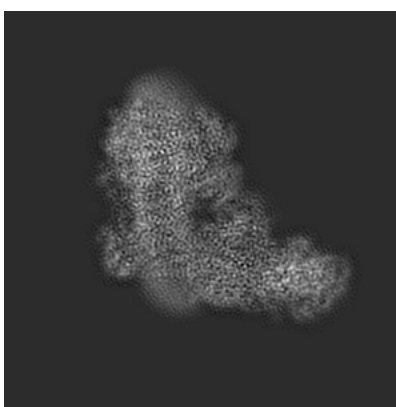
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

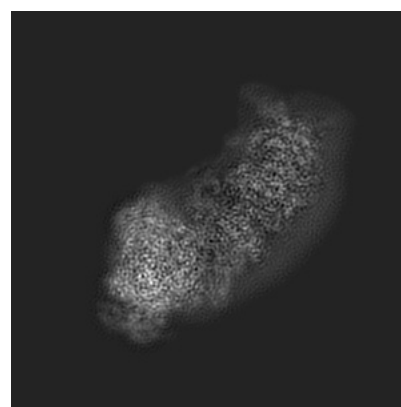
6.1.1 Primary map



X



Y

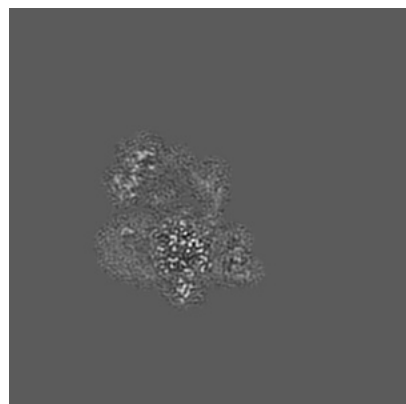


Z

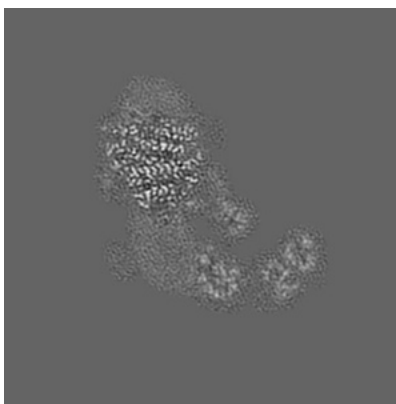
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

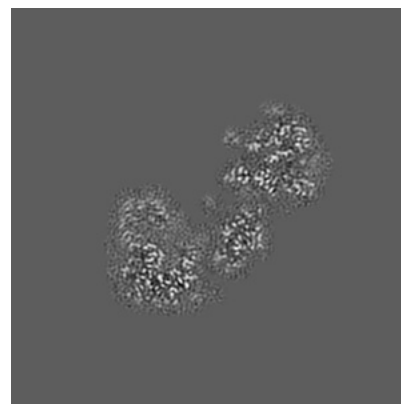
6.2.1 Primary map



X Index: 152



Y Index: 152

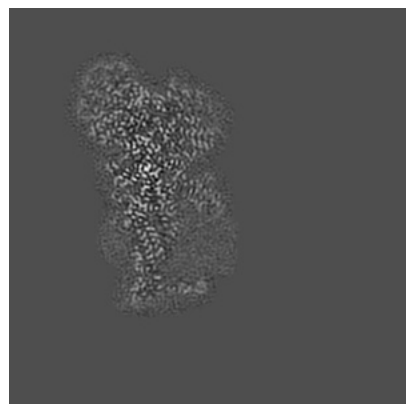


Z Index: 152

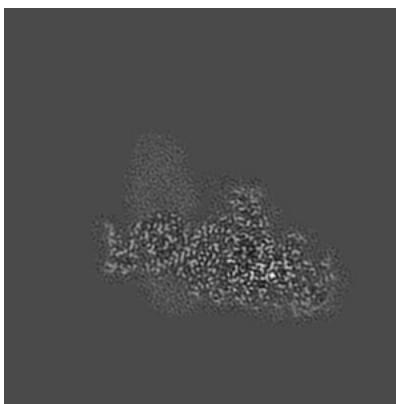
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

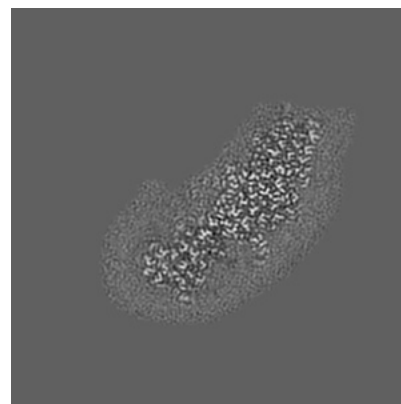
6.3.1 Primary map



X Index: 105



Y Index: 98

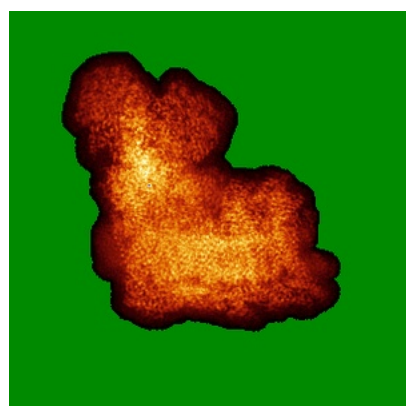


Z Index: 127

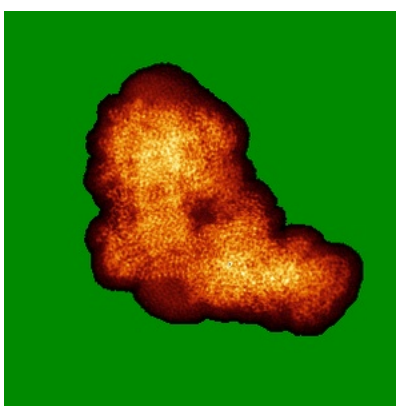
The images above show the largest variance slices of the map in three orthogonal directions.

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

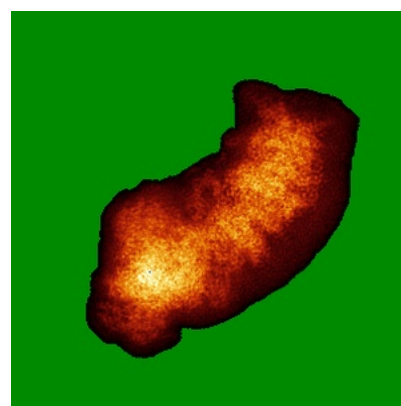
6.4.1 Primary map



X



Y

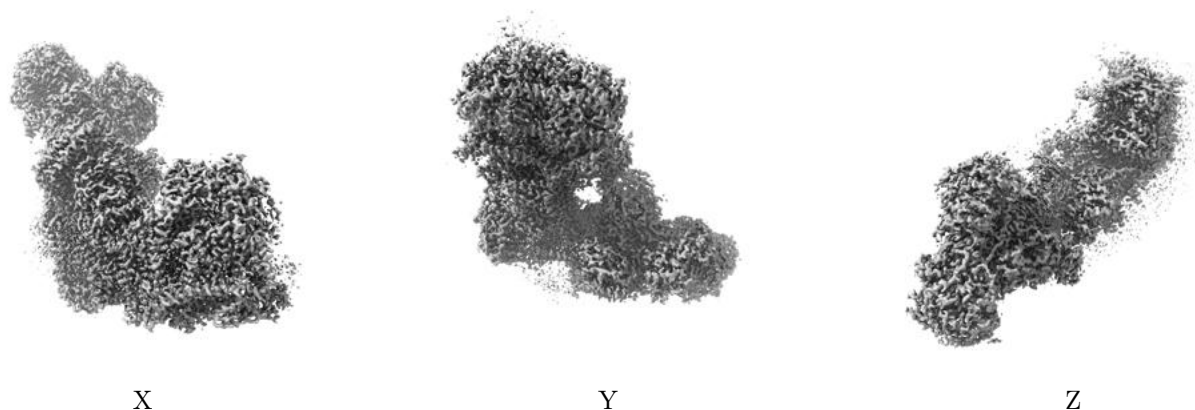


Z

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 0.0296. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

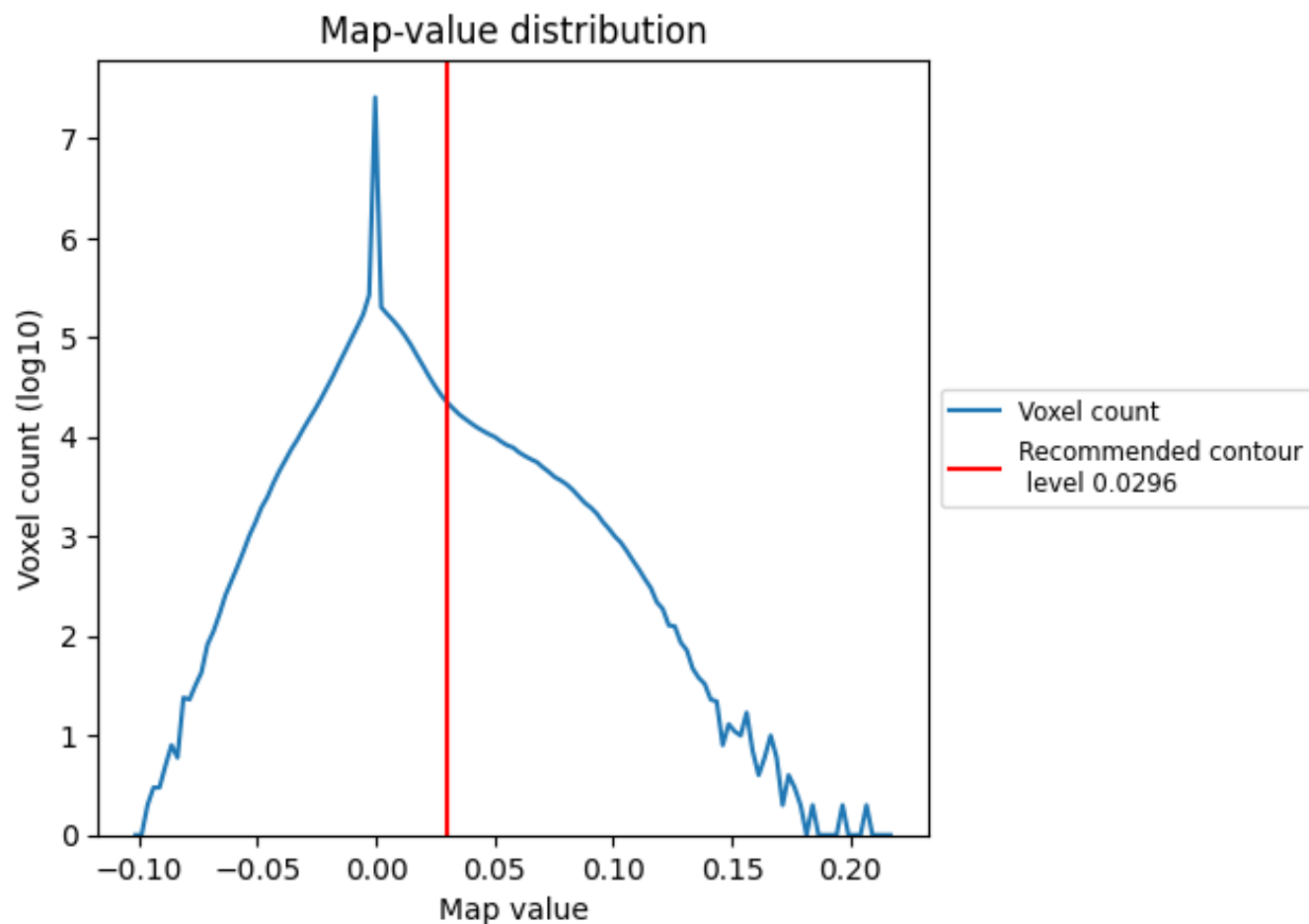
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

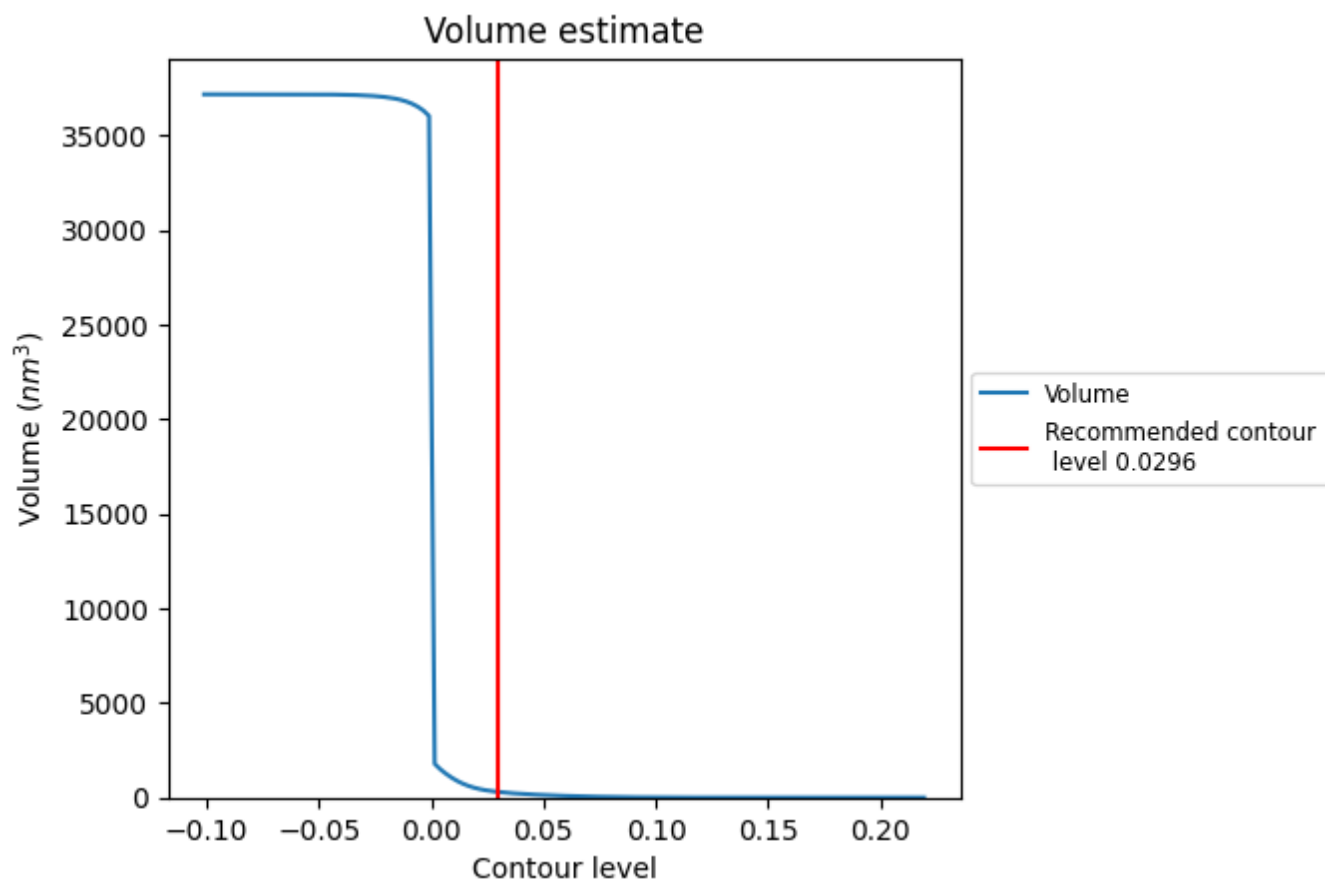
This section contains the results of statistical analysis of the map.

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.

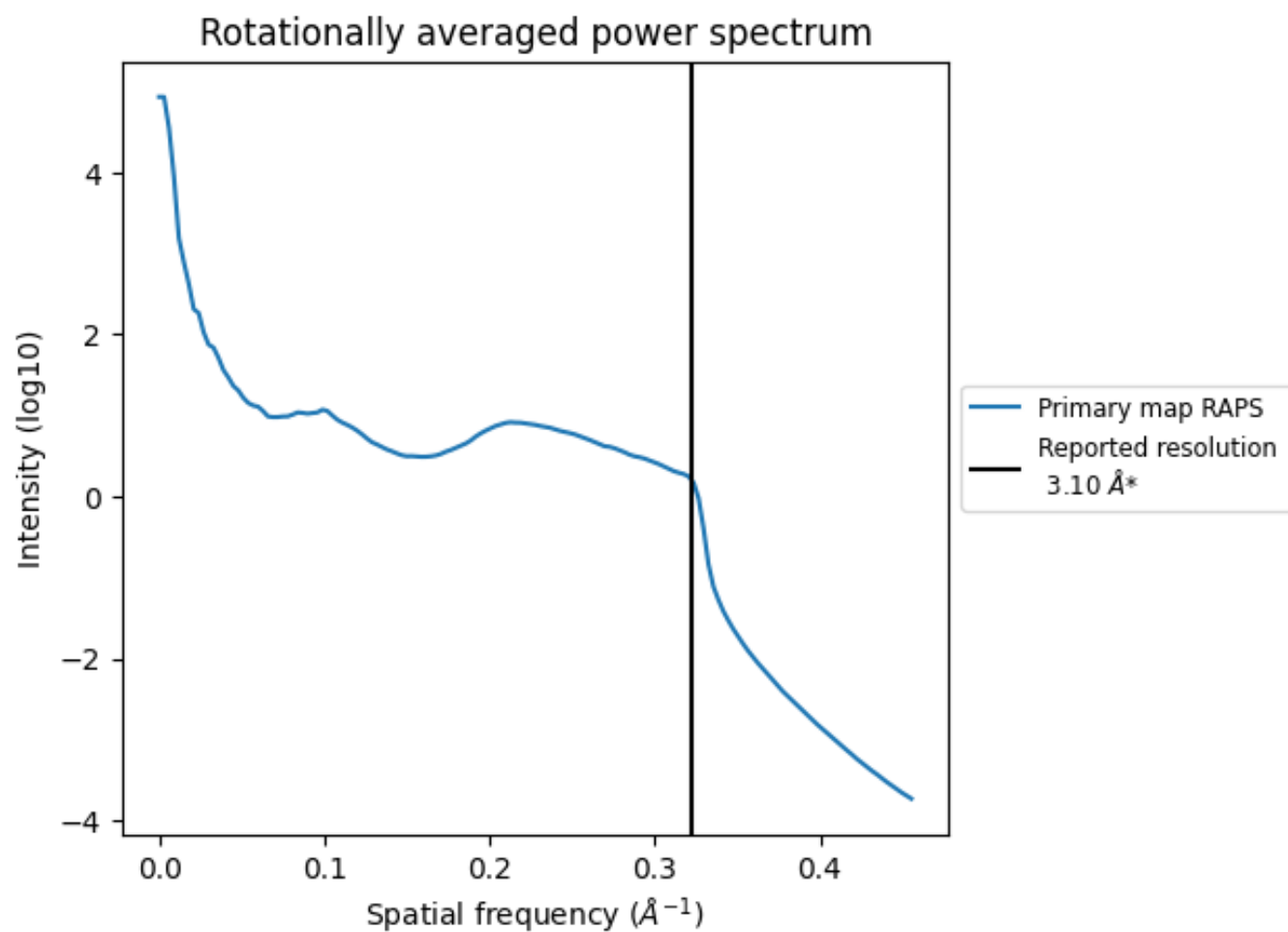
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 300 nm³; this corresponds to an approximate mass of 271 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 0.323 Å⁻¹

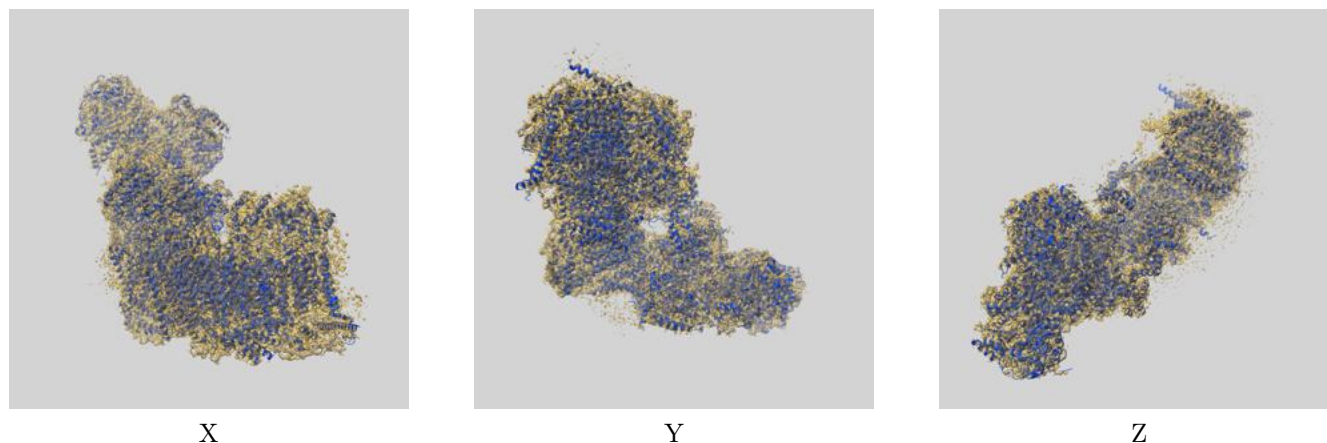
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

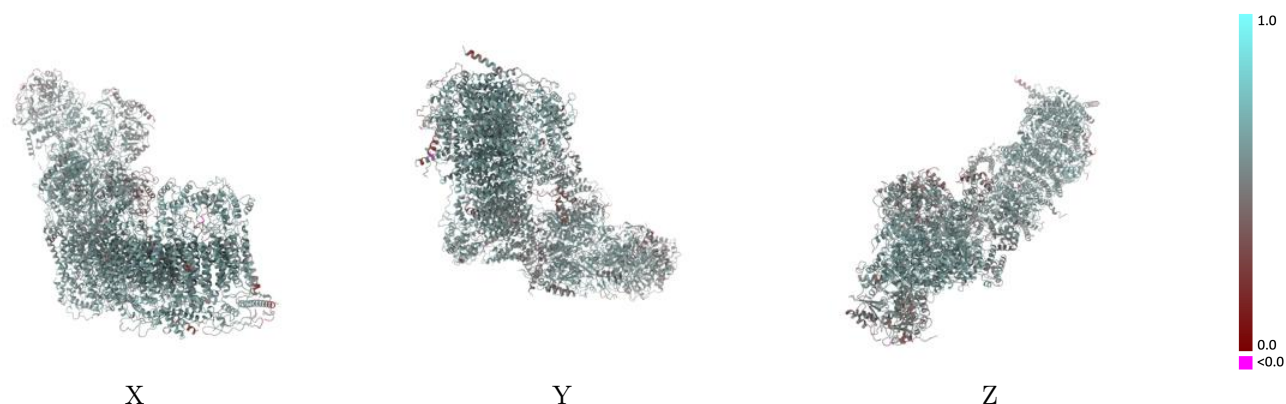
This section contains information regarding the fit between EMDB map EMD-32307 and PDB model 7W4L. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



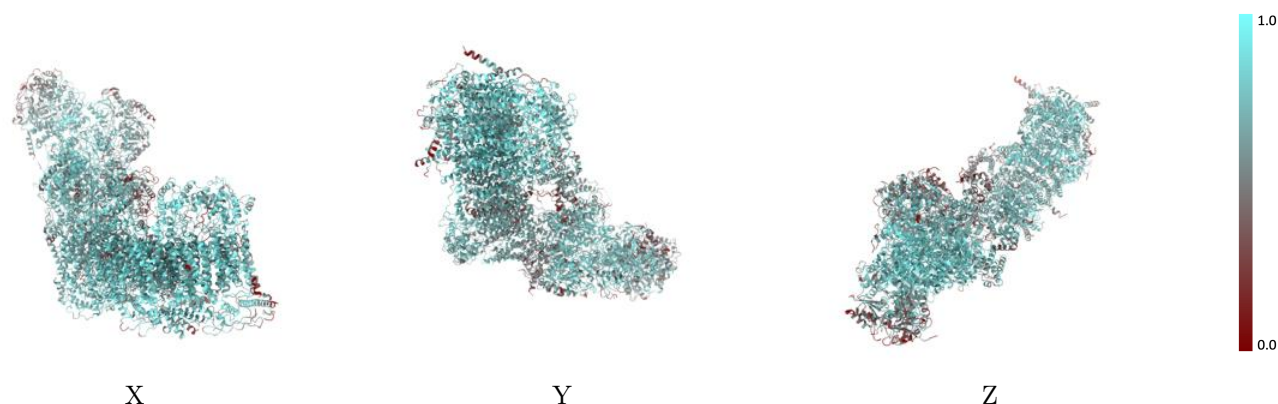
The images above show the 3D surface view of the map at the recommended contour level 0.0296 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



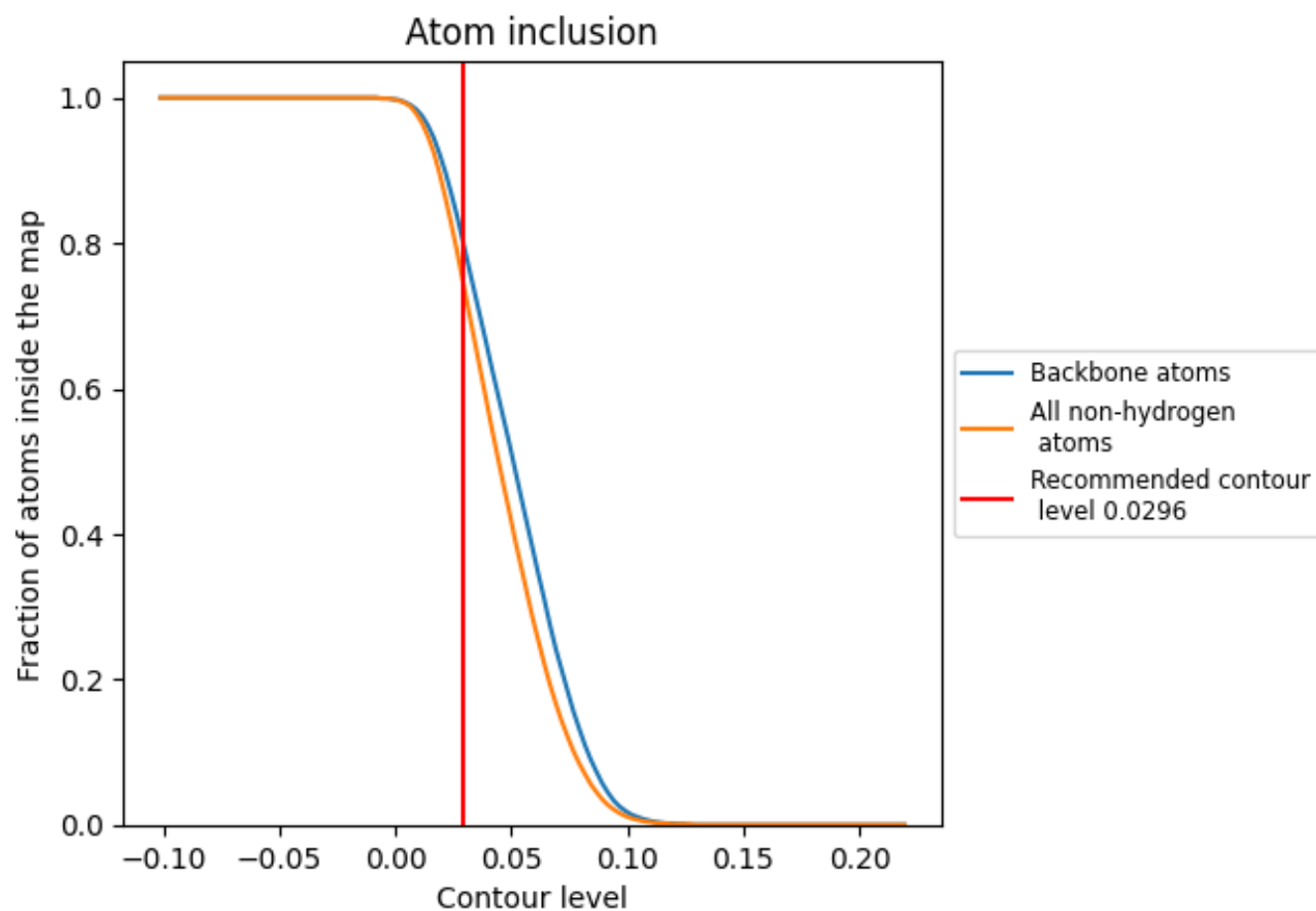
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0296).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 74% 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 (0.0296) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7390	 0.5650
A	 0.6120	 0.5170
B	 0.8870	 0.6130
C	 0.8270	 0.5960
E	 0.6920	 0.5630
F	 0.4910	 0.4760
G	 0.3620	 0.3940
H	 0.6650	 0.5350
I	 0.7350	 0.5670
J	 0.6160	 0.5250
K	 0.5410	 0.4980
L	 0.7870	 0.5800
M	 0.7370	 0.5640
N	 0.7640	 0.5830
O	 0.5720	 0.5030
P	 0.8530	 0.6030
Q	 0.8420	 0.6060
S	 0.8140	 0.5880
T	 0.7330	 0.5800
U	 0.7280	 0.5610
V	 0.5260	 0.5160
W	 0.7560	 0.5700
X	 0.7260	 0.5480
Y	 0.6450	 0.5380
Z	 0.5990	 0.5020
a	 0.7820	 0.5900
b	 0.6800	 0.5330
c	 0.7780	 0.5750
d	 0.7440	 0.5590
e	 0.7040	 0.5550
f	 0.6290	 0.5240
g	 0.7750	 0.5810
h	 0.7640	 0.5720
i	 0.8500	 0.6050
j	 0.6200	 0.5370



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Chain	Atom inclusion	Q-score
k	 0.7220	 0.5720
l	 0.8050	 0.5930
m	 0.6870	 0.5470
n	 0.6650	 0.5450
o	 0.7700	 0.5850
p	 0.7840	 0.5750
r	 0.8580	 0.6060
s	 0.7900	 0.5770
u	 0.7700	 0.5730
v	 0.6850	 0.5290
w	 0.7040	 0.5500