



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:44 PM UTC

PDB ID : 7VY1 / pdb_00007vy1
EMDB ID : EMD-32191
Title : Membrane arm of deactive state CI from Q10 dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-13
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

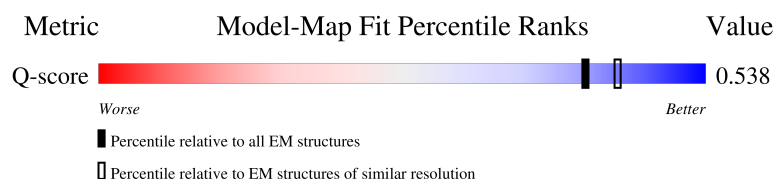
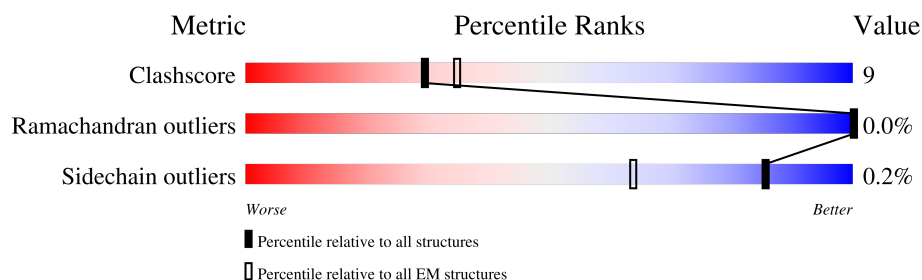
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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.



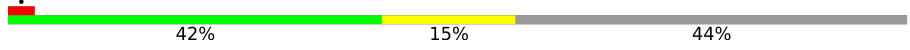
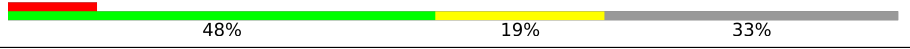
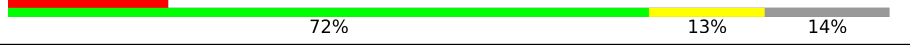
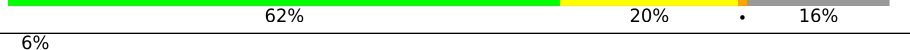
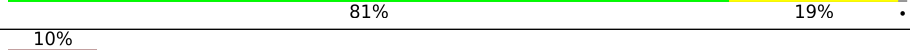
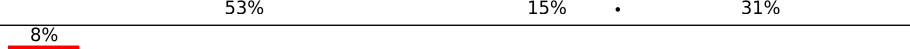
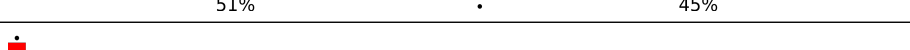
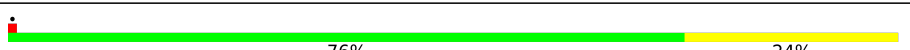
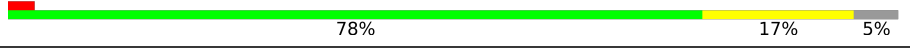
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	Q	473	 7% . 92%
2	S	70	 87% 13%
3	U	84	 5% 90% 8% .
4	V	141	 16% 85% 14% .

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Mol	Chain	Length	Quality of chain
5	W	144	
6	X	156	
7	Y	105	
8	Z	98	
9	a	189	
10	b	128	
11	c	186	
12	d	176	
13	e	154	
14	f	76	
15	g	122	
16	h	106	
17	i	347	
18	j	113	
19	k	98	
20	l	603	
21	m	175	
22	n	58	
23	o	129	
24	p	179	
25	r	459	
26	s	318	
27	u	172	
28	v	136	
29	w	357	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 38899 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] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	40	Total	C	N	O	S	0	0
			333	217	56	59	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	U	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	113	Total	C	N	O	S	0	0
			949	614	160	167	8		

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	88	Total	C	N	O	S	0	0
			699	450	103	141	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

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

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

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

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 10 is a protein called NADH dehydrogenase 1 beta subcomplex 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	103	Total	C	N	O	S	0	0
			875	571	158	145	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	156	Total	C	N	O	S	0	0
			1299	843	211	237	8		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

- Molecule 13 is a protein called Complex I-ESSS.

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

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	?	-	CYS	deletion	UNP A0A287BMW6
e	?	-	MET	deletion	UNP A0A287BMW6
e	?	-	GLY	deletion	UNP A0A287BMW6
e	?	-	CYS	deletion	UNP A0A287BMW6
e	?	-	PRO	deletion	UNP A0A287BMW6
e	?	-	ARG	deletion	UNP A0A287BMW6
e	?	-	GLU	deletion	UNP A0A287BMW6
e	?	-	TRP	deletion	UNP A0A287BMW6
e	?	-	GLY	deletion	UNP A0A287BMW6
e	?	-	GLY	deletion	UNP A0A287BMW6

- Molecule 14 is a protein called Complex I-KFYI.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	f	42	Total	C	N	O	0	0
			344	227	58	59		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

- Molecule 17 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	i	347	Total	C	N	O	S	0	0
			2710	1782	420	462	46		

- Molecule 18 is a protein called ND3.

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

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

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

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	603	Total	C	N	O	S	0	0
			4785	3173	741	820	51		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	129	Total	C	N	O	S	0	0
			951	637	138	168	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	n	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

- Molecule 23 is a protein called Complex I-B15.

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

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	p	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

- Molecule 25 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 26 is a protein called NADH-ubiquinone oxidoreductase chain 1.

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

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

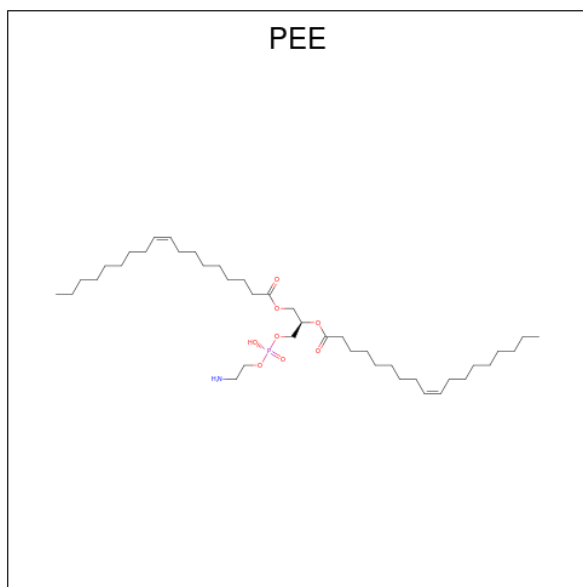
- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

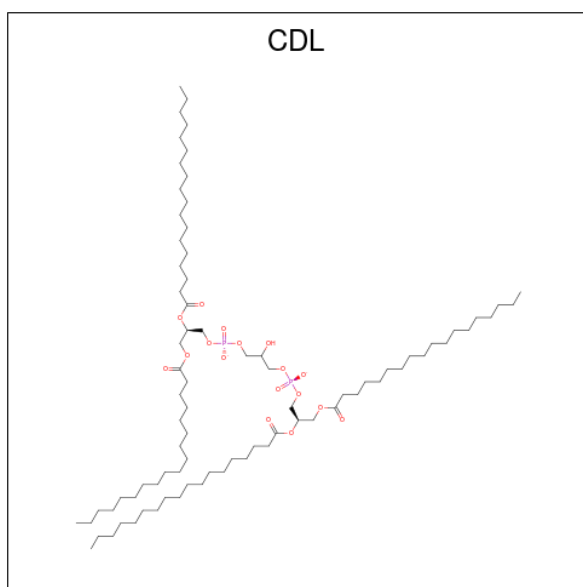
Mol	Chain	Residues	Atoms					AltConf	Trace
29	w	320	Total	C	N	O	S	0	0
			2581	1645	437	489	10		

- Molecule 30 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P) (labeled as "Ligand of Interest" by depositor).



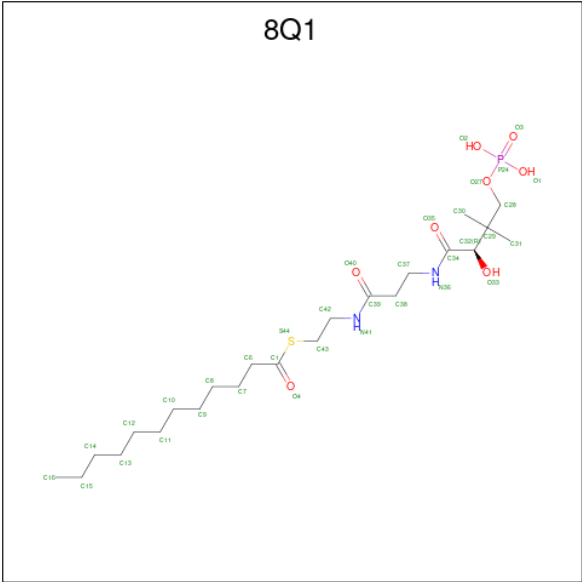
Mol	Chain	Residues	Atoms					AltConf
30	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
30	b	1	Total	C	N	O	P	0
			46	36	1	8	1	
30	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
30	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	l	1	Total	C	N	O	P	0
			40	30	1	8	1	
30	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
30	r	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 31 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



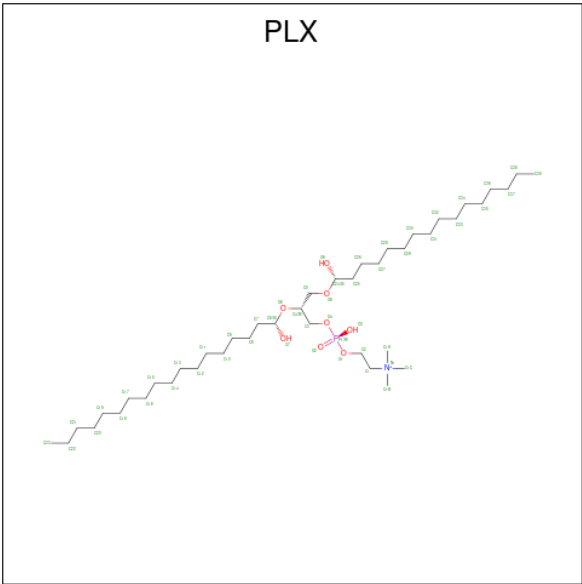
Mol	Chain	Residues	Atoms				AltConf
31	V	1	Total	C	O	P	0
			94	75	17	2	
31	a	1	Total	C	O	P	0
			91	72	17	2	
31	g	1	Total	C	O	P	0
			95	76	17	2	
31	i	1	Total	C	O	P	0
			66	47	17	2	
31	l	1	Total	C	O	P	0
			100	81	17	2	
31	o	1	Total	C	O	P	0
			68	49	17	2	
31	r	1	Total	C	O	P	0
			99	80	17	2	
31	u	1	Total	C	O	P	0
			78	59	17	2	

- Molecule 32 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 33 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-TRIOX (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



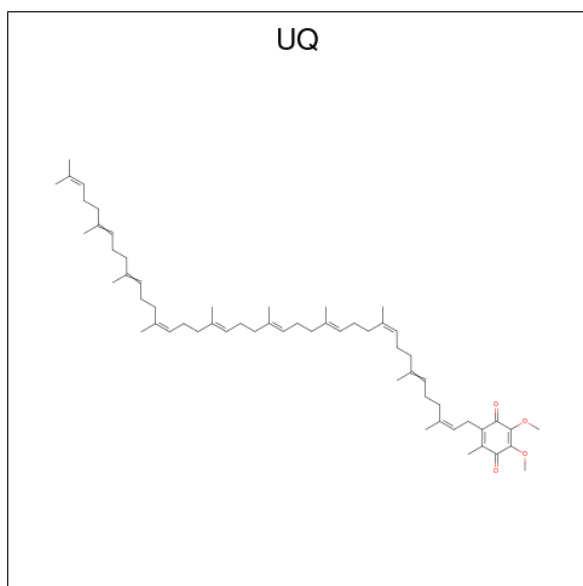
Mol	Chain	Residues	Atoms					AltConf
33	a	1	Total	C	N	O	P	0
			52	42	1	8	1	

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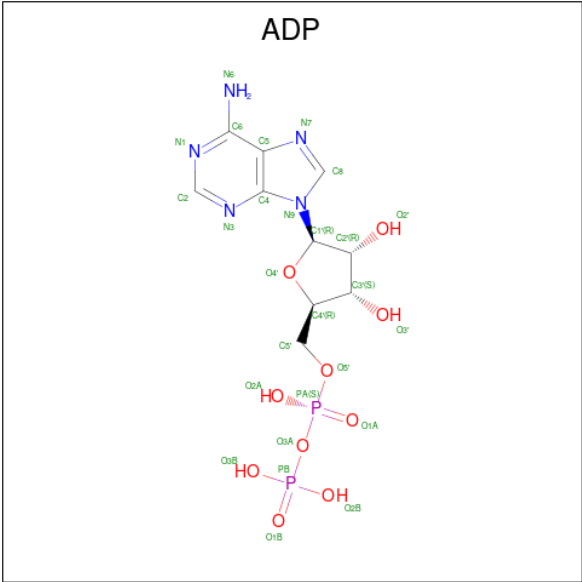
Mol	Chain	Residues	Atoms					AltConf
33	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 34 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
34	s	1	Total	C	O	0
			28	24	4	

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

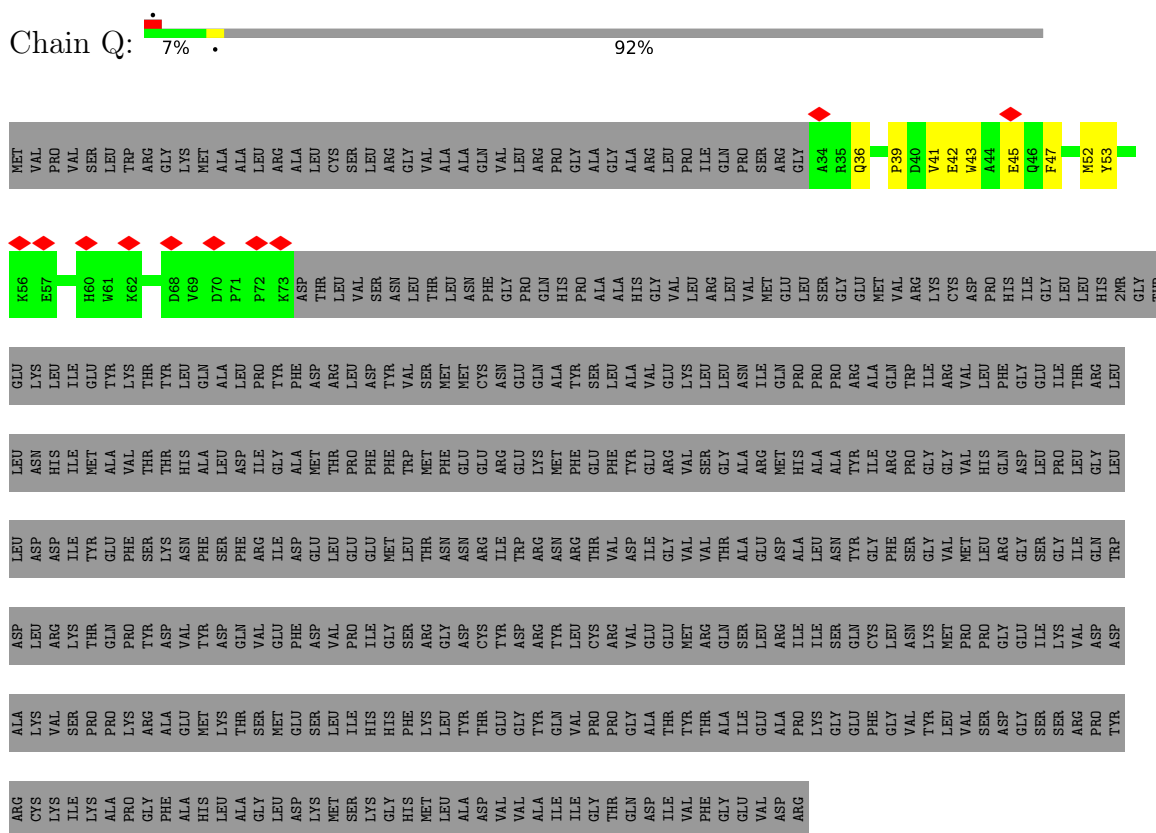


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
35	w	1	27	10	5	10	2	0

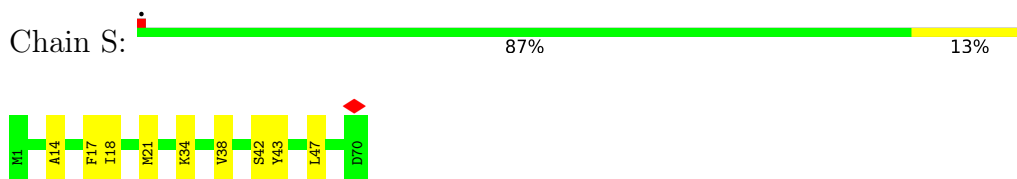
3 Residue-property plots

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

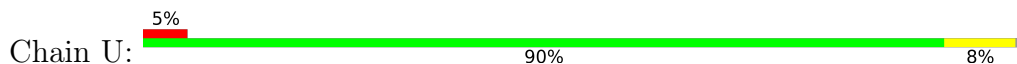
- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



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

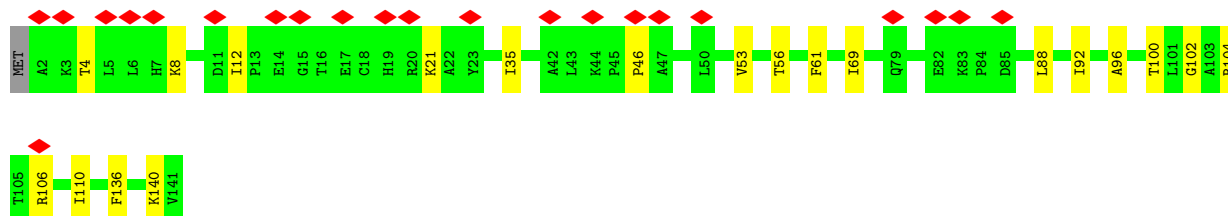
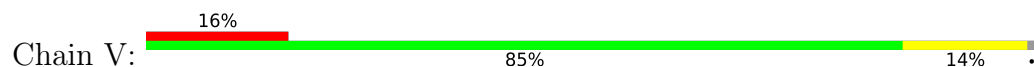


- Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

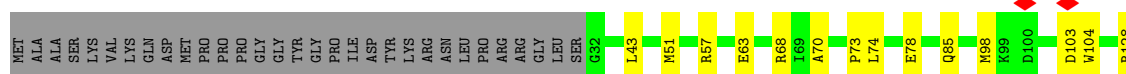




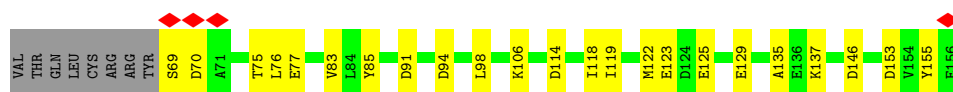
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



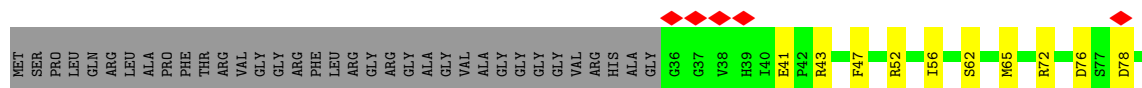
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



- Molecule 6: Acyl carrier protein



- Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

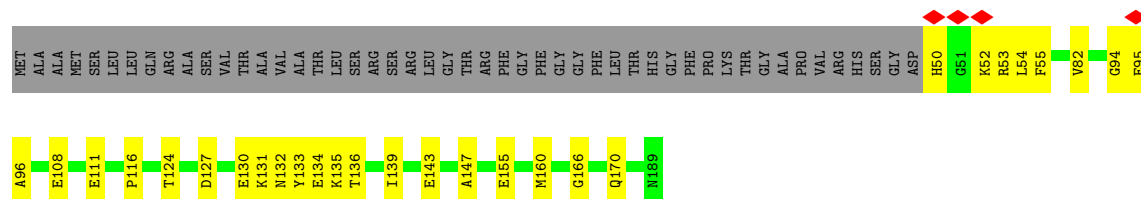


- Molecule 8: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

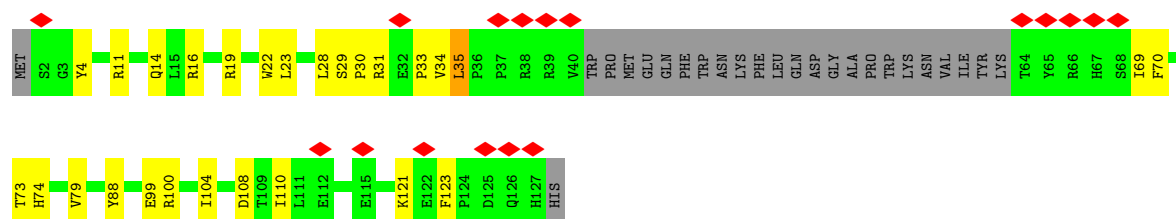




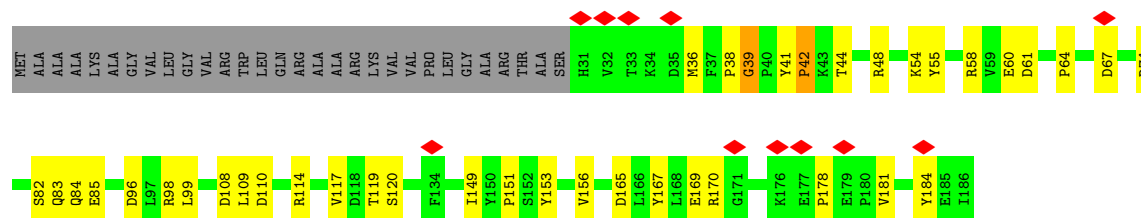
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



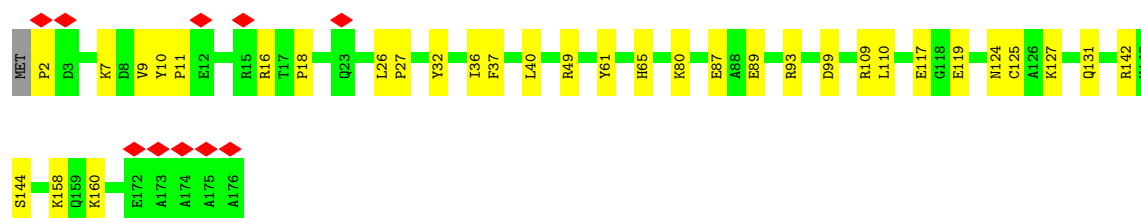
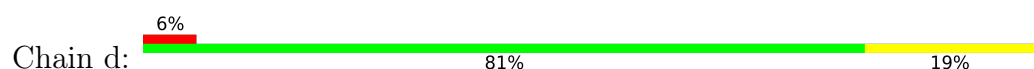
- Molecule 10: NADH dehydrogenase 1 beta subcomplex 6



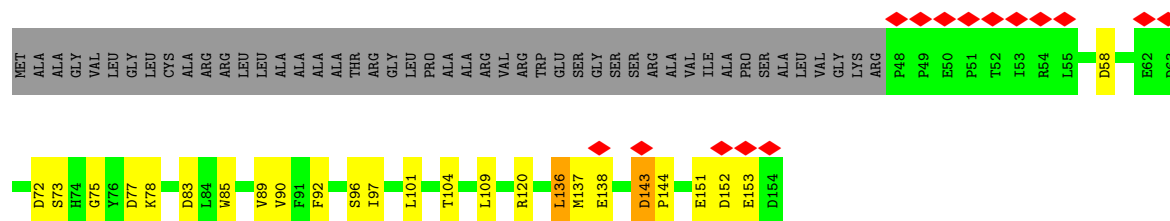
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



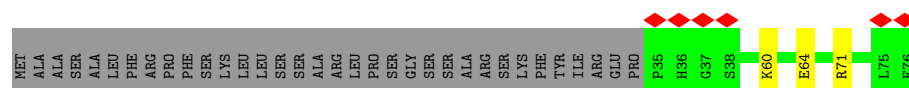
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



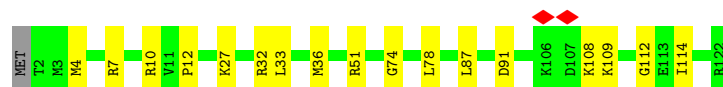
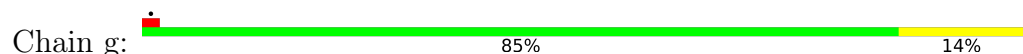
- Molecule 13: Complex I-ESSS



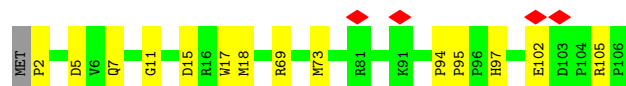
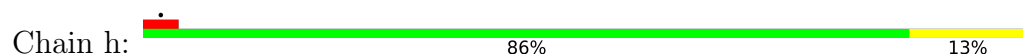
• Molecule 14: Complex I-KFYI



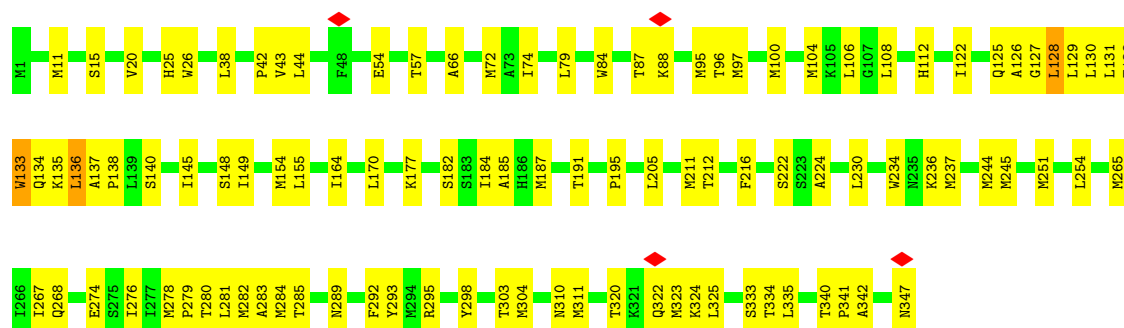
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2



• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

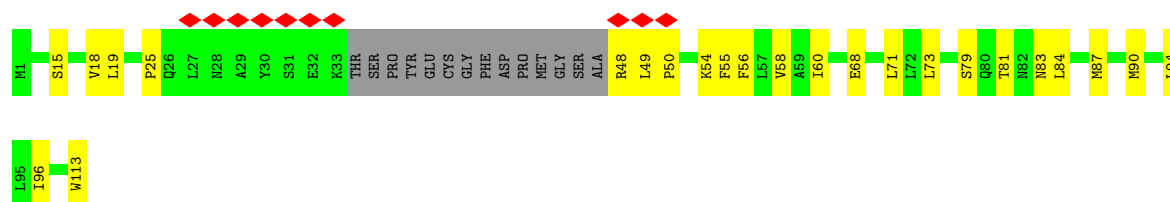


• Molecule 17: NADH-ubiquinone oxidoreductase chain 2

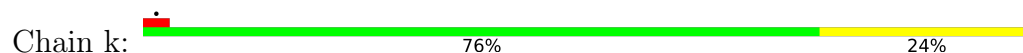


• Molecule 18: ND3

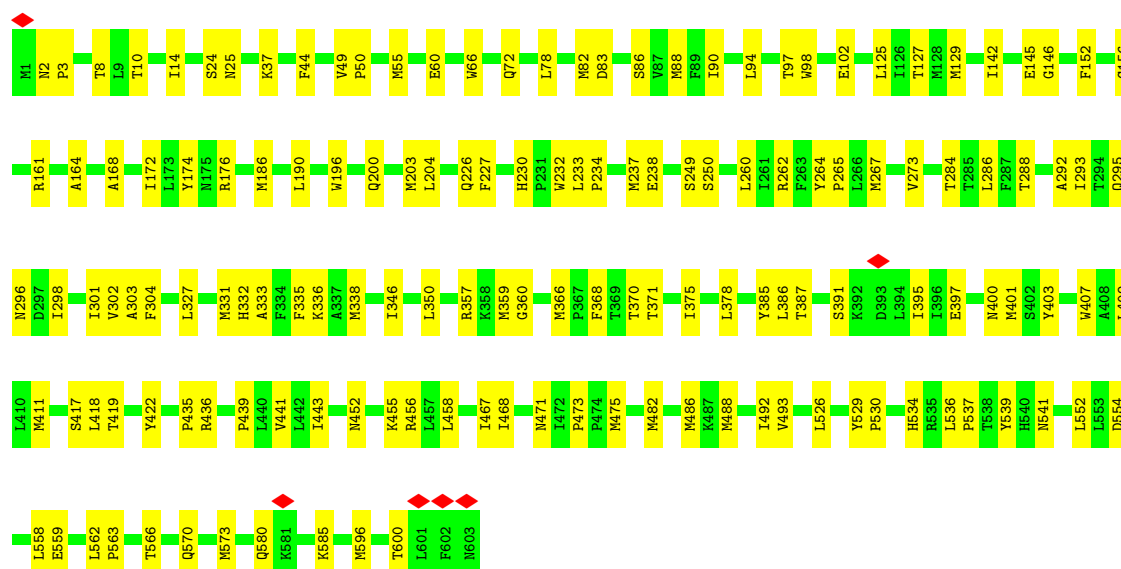
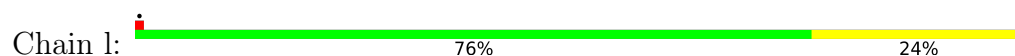




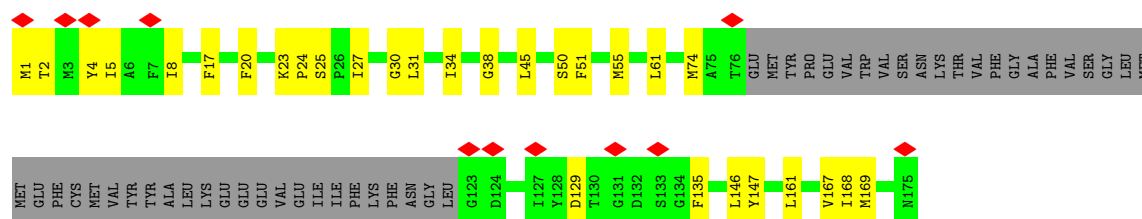
- Molecule 19: NADH-ubiquinone oxidoreductase chain 4L



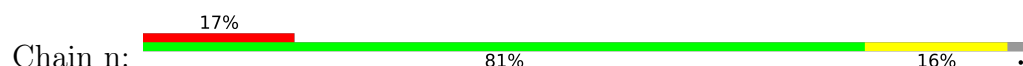
- Molecule 20: NADH-ubiquinone oxidoreductase chain 5

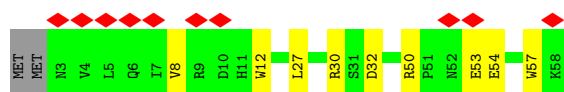


- Molecule 21: NADH-ubiquinone oxidoreductase chain 6

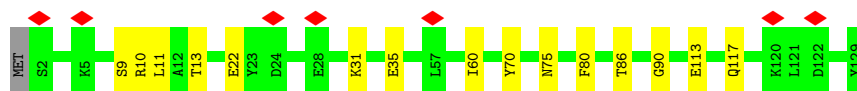
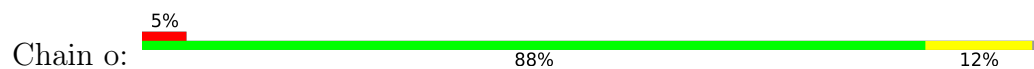


- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

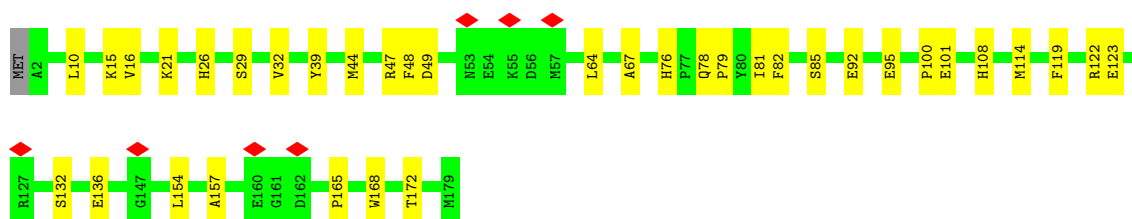
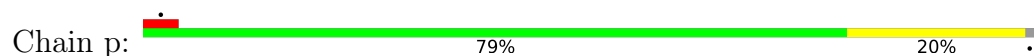




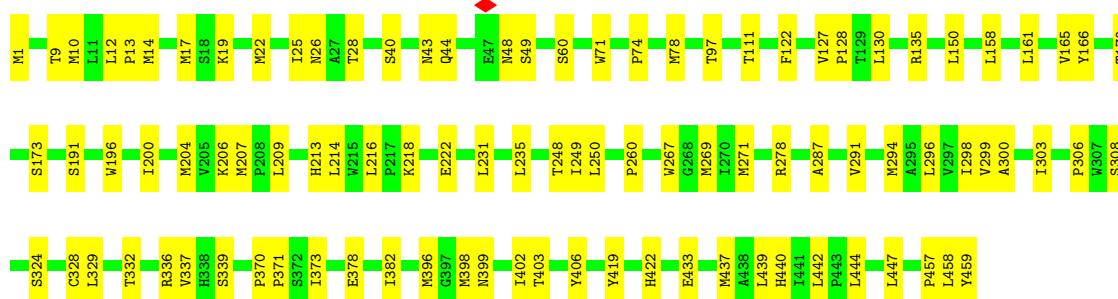
- Molecule 23: Complex I-B15



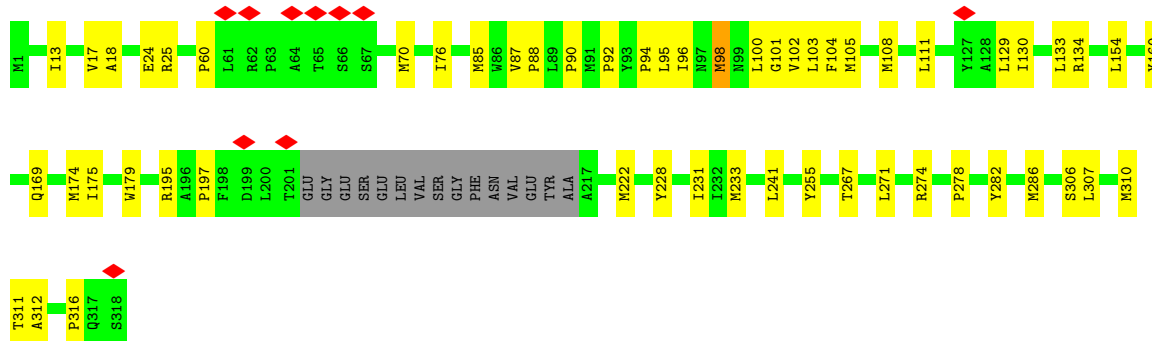
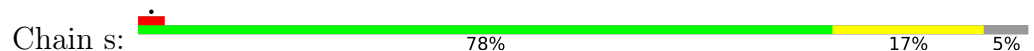
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 25: NADH-ubiquinone oxidoreductase chain 4



- Molecule 26: NADH-ubiquinone oxidoreductase chain 1



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:  83% 17%



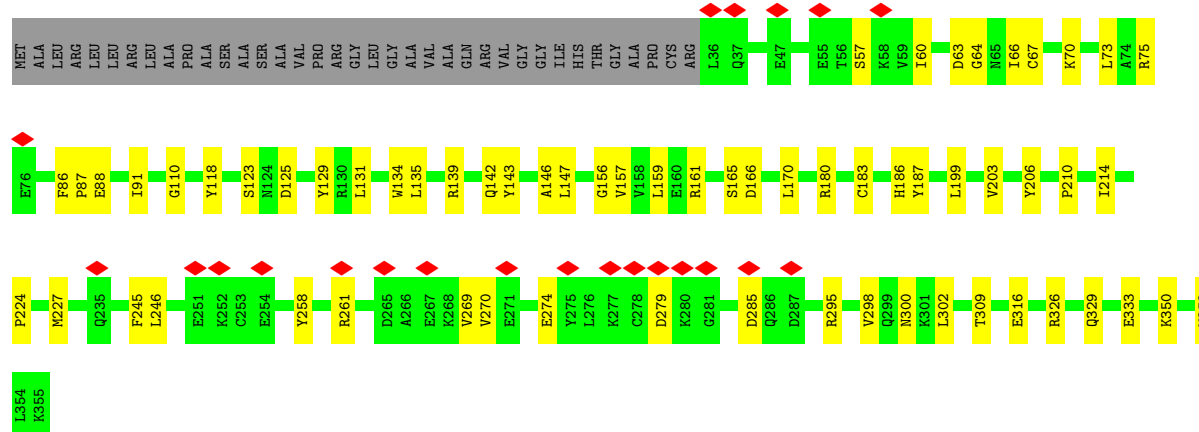
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v:  12% 71% 20% 9%



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain w:  6% 72% 18% 10%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	193234	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	0.108	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0238	Depositor
Map size ($\text{\AA}$)	354.48602, 354.48602, 354.48602	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, PEE, UQ, PLX, 8Q1, ADP

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	Q	0.15	0/350	0.33	0/483
2	S	0.17	0/582	0.32	0/783
3	U	0.13	0/664	0.24	0/912
4	V	0.14	0/1042	0.27	0/1411
5	W	0.17	0/973	0.30	0/1312
6	X	0.14	0/711	0.33	0/963
7	Y	0.15	0/623	0.30	0/853
8	Z	0.13	0/695	0.32	0/939
9	a	0.17	0/1199	0.31	0/1623
10	b	0.18	0/902	0.40	0/1227
11	c	0.20	0/1355	0.51	4/1857 (0.2%)
12	d	0.15	0/1494	0.29	0/2015
13	e	0.18	0/916	0.53	3/1246 (0.2%)
14	f	0.13	0/353	0.25	0/477
15	g	0.15	0/1031	0.26	0/1394
16	h	0.15	0/889	0.26	0/1190
17	i	0.20	0/2773	0.41	2/3768 (0.1%)
18	j	0.18	0/819	0.34	0/1117
19	k	0.19	0/759	0.32	0/1029
20	l	0.18	0/4914	0.35	0/6683
21	m	0.19	0/973	0.39	0/1320
22	n	0.13	0/491	0.29	0/663
23	o	0.15	0/1092	0.29	0/1481
24	p	0.16	0/1590	0.29	0/2155
25	r	0.20	0/3723	0.37	0/5078
26	s	0.18	0/2464	0.34	0/3369
27	u	0.15	0/1436	0.30	0/1938
28	v	0.14	0/1052	0.37	0/1411
29	w	0.16	0/2641	0.34	0/3577
All	All	0.17	0/38506	0.35	9/52274 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	e	143	ASP	CA-C-N	7.45	127.31	119.05
13	e	143	ASP	C-N-CA	7.45	127.31	119.05
17	i	136	LEU	N-CA-C	5.58	117.36	111.28
13	e	136	LEU	CB-CA-C	-5.41	110.31	116.54
11	c	44	THR	CA-C-N	5.34	124.98	119.05
11	c	44	THR	C-N-CA	5.34	124.98	119.05
17	i	133	TRP	N-CA-C	5.14	116.96	111.36
11	c	39	GLY	CA-C-N	5.01	124.94	119.78
11	c	39	GLY	C-N-CA	5.01	124.94	119.78

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	333	0	301	6	0
2	S	567	0	565	6	0
3	U	643	0	642	6	0
4	V	1021	0	1027	13	0
5	W	949	0	935	21	0
6	X	699	0	682	18	0
7	Y	597	0	537	19	0
8	Z	674	0	643	9	0
9	a	1165	0	1174	29	0
10	b	875	0	895	34	0
11	c	1299	0	1178	34	0
12	d	1461	0	1429	26	0
13	e	890	0	837	19	0
14	f	344	0	347	2	0
15	g	1000	0	994	14	0
16	h	867	0	871	13	0
17	i	2710	0	2874	97	0
18	j	800	0	855	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	k	748	0	799	21	0
20	l	4785	0	4933	114	0
21	m	951	0	962	29	0
22	n	479	0	486	9	0
23	o	1062	0	1072	12	0
24	p	1534	0	1470	30	0
25	r	3631	0	3839	82	0
26	s	2394	0	2508	41	0
27	u	1398	0	1378	20	0
28	v	1028	0	980	28	0
29	w	2581	0	2540	46	0
30	U	51	0	82	1	0
30	W	41	0	59	1	0
30	b	46	0	69	3	0
30	i	47	0	71	2	0
30	j	51	0	82	1	0
30	l	86	0	123	5	0
30	r	51	0	82	3	0
31	V	94	0	138	4	0
31	a	91	0	132	1	0
31	g	95	0	143	10	0
31	i	66	0	76	4	0
31	l	100	0	156	4	0
31	o	68	0	83	4	0
31	r	99	0	151	13	0
31	u	78	0	103	7	0
32	X	35	0	0	2	0
33	a	52	0	88	12	0
33	g	52	0	88	4	0
33	j	52	0	88	3	0
33	r	104	0	176	7	0
34	s	28	0	31	2	0
35	w	27	0	11	2	0
All	All	38899	0	39785	720	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 (720) 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)
11:c:39:GLY:O	11:c:74:ASP:HB3	1.48	1.13
33:a:202:PLX:H81	25:r:40:SER:HB3	1.30	1.11
29:w:67:CYS:HB3	29:w:214:ILE:HD11	1.37	1.07
17:i:135:LYS:HD2	17:i:187:MET:HE3	1.40	1.00
33:a:202:PLX:H81	25:r:40:SER:CB	2.01	0.91
9:a:127:ASP:OD1	33:a:202:PLX:H12	1.71	0.90
17:i:135:LYS:CD	17:i:187:MET:HE3	2.02	0.89
33:a:202:PLX:C8	25:r:40:SER:HB3	2.01	0.88
10:b:29:SER:HB2	10:b:30:PRO:HD2	1.58	0.85
17:i:122:ILE:HD12	17:i:126:ALA:CB	2.07	0.84
10:b:34:VAL:O	24:p:114:MET:HG2	1.78	0.84
6:X:123:GLU:HG2	6:X:129:GLU:HA	1.59	0.82
17:i:87:THR:HG22	17:i:88:LYS:H	1.46	0.81
11:c:39:GLY:O	11:c:74:ASP:CB	2.28	0.80
17:i:131:LEU:HD12	17:i:216:PHE:CE2	2.16	0.80
21:m:55:MET:HA	21:m:55:MET:HE2	1.65	0.78
29:w:261:ARG:O	29:w:261:ARG:NH1	2.16	0.77
26:s:195:ARG:HD3	26:s:231:ILE:HD11	1.66	0.77
13:e:109:LEU:HD13	25:r:43:ASN:HB2	1.65	0.77
29:w:67:CYS:HB3	29:w:214:ILE:CD1	2.13	0.76
12:d:26:LEU:HD12	12:d:27:PRO:HD2	1.67	0.76
17:i:122:ILE:HD12	17:i:126:ALA:HB3	1.68	0.75
31:r:504:CDL:H621	31:r:504:CDL:H432	1.68	0.75
17:i:324:LYS:O	17:i:325:LEU:HB2	1.87	0.75
10:b:35:LEU:N	10:b:35:LEU:HD12	2.01	0.74
17:i:135:LYS:HG3	17:i:187:MET:CE	2.17	0.74
20:l:360:GLY:HA3	20:l:435:PRO:HA	1.70	0.73
13:e:151:GLU:OE2	13:e:152:ASP:OD1	2.06	0.73
25:r:191:SER:HB3	30:r:501:PEE:H3	1.70	0.73
24:p:101:GLU:OE2	24:p:122:ARG:NH1	2.22	0.72
21:m:30:GLY:O	21:m:34:ILE:HD12	1.89	0.72
16:h:97:HIS:HA	16:h:102:GLU:HB3	1.71	0.72
17:i:283:ALA:HB1	25:r:158:LEU:HD13	1.70	0.72
33:a:202:PLX:H282	33:a:202:PLX:H322	1.70	0.72
20:l:237:MET:HE2	20:l:303:ALA:HB2	1.72	0.72
11:c:99:LEU:HD11	11:c:109:LEU:HD11	1.73	0.71
17:i:128:LEU:C	17:i:128:LEU:HD23	2.16	0.71
17:i:211:MET:HG3	17:i:333:SER:HB2	1.73	0.70
10:b:99:GLU:OE1	20:l:2:ASN:ND2	2.24	0.69
5:W:85:GLN:OE1	16:h:105:ARG:NH1	2.25	0.69
22:n:54:GLU:N	22:n:54:GLU:OE1	2.25	0.69
11:c:108:ASP:OD1	25:r:278:ARG:NH2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:s:169:GLN:HE21	26:s:174:MET:HE2	1.58	0.68
6:X:114:ASP:O	6:X:118:ILE:HD12	1.94	0.68
29:w:75:ARG:HB2	29:w:75:ARG:NH1	2.09	0.68
10:b:11:ARG:NH2	24:p:165:PRO:O	2.26	0.68
29:w:139:ARG:NH1	29:w:166:ASP:OD2	2.27	0.68
9:a:54:LEU:C	10:b:28:LEU:HD13	2.19	0.67
20:l:558:LEU:HB3	25:r:214:LEU:HD21	1.77	0.67
9:a:54:LEU:C	10:b:28:LEU:CD1	2.67	0.67
5:W:51:MET:HE2	26:s:311:THR:HB	1.76	0.67
13:e:77:ASP:OD1	13:e:78:LYS:N	2.27	0.67
17:i:135:LYS:CG	17:i:187:MET:CE	2.73	0.67
20:l:573:MET:HE2	30:l:701:PEE:H21	1.75	0.67
11:c:38:PRO:HB2	23:o:75:ASN:HD22	1.59	0.67
20:l:102:GLU:OE1	20:l:456:ARG:NH2	2.27	0.67
17:i:131:LEU:HD12	17:i:216:PHE:CZ	2.30	0.66
26:s:18:ALA:HB2	34:s:401:UQ:H152	1.76	0.66
18:j:18:VAL:HG22	26:s:222:MET:HG3	1.76	0.66
17:i:177:LYS:NZ	19:k:97:GLN:O	2.25	0.66
28:v:51:LEU:O	28:v:52:MET:HG2	1.96	0.66
31:o:201:CDL:H582	31:o:201:CDL:H742	1.78	0.65
33:a:202:PLX:H282	33:a:202:PLX:C32	2.26	0.65
11:c:58:ARG:NH2	11:c:60:GLU:OE2	2.30	0.65
33:a:202:PLX:C8	25:r:40:SER:CB	2.70	0.64
18:j:60:ILE:HG21	21:m:168:ILE:HG21	1.79	0.64
20:l:145:GLU:OE1	20:l:176:ARG:NH1	2.30	0.64
13:e:151:GLU:OE2	13:e:153:GLU:N	2.29	0.64
10:b:108:ASP:OD2	28:v:71:ARG:NH2	2.31	0.64
20:l:357:ARG:HG3	24:p:32:VAL:HG13	1.79	0.64
25:r:378:GLU:O	25:r:382:ILE:HG12	1.98	0.64
18:j:90:MET:HE1	33:j:202:PLX:H281	1.79	0.64
17:i:135:LYS:CD	17:i:187:MET:CE	2.76	0.63
20:l:375:ILE:HD12	20:l:458:LEU:HD11	1.79	0.63
29:w:224:PRO:HA	29:w:227:MET:HE1	1.80	0.63
9:a:131:LYS:NZ	22:n:32:ASP:OD2	2.30	0.63
30:i:402:PEE:H37	30:i:402:PEE:H60	1.80	0.63
5:W:68:ARG:HD2	21:m:135:PHE:HD2	1.63	0.63
12:d:125:CYS:HB2	20:l:203:MET:HE1	1.79	0.63
20:l:331:MET:HB3	20:l:387:THR:HG22	1.81	0.62
9:a:135:LYS:NZ	22:n:32:ASP:OD1	2.22	0.62
19:k:98:CYS:HB2	20:l:580:GLN:HB2	1.80	0.62
12:d:2:PRO:O	12:d:7:LYS:NZ	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:p:29:SER:HB3	24:p:76:HIS:HD2	1.65	0.61
17:i:135:LYS:HD2	17:i:187:MET:CE	2.25	0.61
9:a:170:GLN:OE1	27:u:151:ASN:ND2	2.33	0.61
17:i:211:MET:HE3	17:i:251:MET:HG2	1.81	0.61
27:u:49:GLU:OE1	27:u:135:ARG:NH2	2.33	0.61
11:c:184:TYR:HA	28:v:34:ARG:HH12	1.65	0.61
6:X:118:ILE:O	6:X:122:MET:HG2	2.00	0.61
10:b:104:ILE:HD13	12:d:18:PRO:HG3	1.83	0.61
17:i:135:LYS:HG3	17:i:187:MET:HE1	1.81	0.61
5:W:70:ALA:HB2	27:u:125:LEU:HD13	1.83	0.61
17:i:125:GLN:N	17:i:125:GLN:OE1	2.33	0.60
17:i:84:TRP:HH2	19:k:59:MET:HE2	1.65	0.60
21:m:5:ILE:HA	21:m:8:ILE:HD12	1.84	0.60
26:s:87:VAL:HG23	26:s:88:PRO:HD3	1.83	0.60
5:W:130:ASN:OD1	21:m:1:MET:HB2	2.01	0.60
11:c:82:SER:OG	11:c:83:GLN:N	2.33	0.60
12:d:99:ASP:OD2	12:d:142:ARG:NH1	2.34	0.60
18:j:68:GLU:HG3	21:m:161:LEU:HD13	1.84	0.60
11:c:119:THR:HG22	23:o:11:LEU:HA	1.83	0.60
19:k:23:ARG:HG2	21:m:23:LYS:HE2	1.83	0.60
11:c:110:ASP:OD1	25:r:278:ARG:NE	2.34	0.60
20:l:97:THR:HG21	20:l:125:LEU:HD22	1.84	0.60
20:l:250:SER:HB2	20:l:333:ALA:HA	1.84	0.60
9:a:53:ARG:HH12	10:b:33:PRO:HG3	1.67	0.60
11:c:153:TYR:HB3	20:l:403:TYR:HD1	1.67	0.60
17:i:135:LYS:CG	17:i:187:MET:HE1	2.33	0.59
10:b:100:ARG:HB2	20:l:60:GLU:HB2	1.84	0.59
17:i:122:ILE:HD12	17:i:126:ALA:HB1	1.82	0.59
19:k:22:TYR:HB3	20:l:585:LYS:HG2	1.83	0.59
17:i:278:MET:O	17:i:282:MET:HG3	2.02	0.59
20:l:401:MET:SD	20:l:482:MET:HG2	2.42	0.59
6:X:91:ASP:HB3	8:Z:47:ARG:HH12	1.67	0.59
25:r:269:MET:HE1	25:r:296:LEU:HD13	1.85	0.59
31:V:201:CDL:H741	31:V:201:CDL:H611	1.85	0.58
6:X:153:ASP:OD1	10:b:19:ARG:NH2	2.35	0.58
24:p:10:LEU:O	24:p:15:LYS:NZ	2.36	0.58
25:r:1:MET:SD	25:r:111:THR:HG21	2.43	0.58
12:d:144:SER:O	12:d:158:LYS:NZ	2.33	0.58
23:o:9:SER:OG	23:o:10:ARG:N	2.37	0.58
32:X:201:8Q1:N36	32:X:201:8Q1:O40	2.36	0.58
20:l:55:MET:HE2	20:l:471:ASN:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:r:503:PLX:H222	31:r:504:CDL:H521	1.86	0.58
20:l:127:THR:HG21	20:l:146:GLY:HA3	1.86	0.58
6:X:85:TYR:OH	8:Z:22:TRP:NE1	2.30	0.57
11:c:41:TYR:HE1	11:c:64:PRO:HG2	1.69	0.57
19:k:5:TYR:O	19:k:9:ILE:HG13	2.04	0.57
28:v:33:GLU:OE2	28:v:33:GLU:N	2.31	0.57
9:a:82:VAL:HG11	13:e:104:THR:HG21	1.86	0.57
11:c:38:PRO:HB2	23:o:75:ASN:ND2	2.18	0.57
24:p:119:PHE:O	24:p:123:GLU:HG2	2.05	0.57
25:r:216:LEU:HD22	25:r:291:VAL:HG23	1.85	0.57
6:X:83:VAL:HA	6:X:122:MET:HE1	1.86	0.57
31:r:504:CDL:H541	31:r:504:CDL:HA61	1.85	0.57
10:b:121:LYS:HE2	28:v:40:VAL:HG12	1.86	0.57
16:h:105:ARG:NH2	27:u:17:GLU:OE2	2.36	0.57
4:V:96:ALA:O	4:V:100:THR:HG23	2.05	0.57
7:Y:62:SER:OG	20:l:371:THR:OG1	2.22	0.57
10:b:88:TYR:CE1	12:d:49:ARG:HG2	2.38	0.57
17:i:280:THR:O	17:i:284:MET:HG2	2.04	0.57
17:i:42:PRO:HG2	21:m:167:VAL:HG22	1.87	0.57
20:l:391:SER:O	20:l:395:ILE:HG12	2.04	0.57
20:l:558:LEU:HD11	31:o:201:CDL:H852	1.86	0.57
26:s:24:GLU:OE2	26:s:274:ARG:NH1	2.36	0.57
20:l:419:THR:HA	20:l:422:TYR:CE2	2.41	0.56
20:l:552:LEU:HD21	23:o:90:GLY:HA2	1.85	0.56
4:V:88:LEU:O	4:V:92:ILE:HG13	2.05	0.56
9:a:132:ASN:ND2	25:r:49:SER:O	2.29	0.56
17:i:132:THR:HG22	17:i:212:THR:HG21	1.87	0.56
29:w:135:LEU:HD13	35:w:401:ADP:C5	2.40	0.56
25:r:328:CYS:HB3	25:r:437:MET:HE1	1.87	0.56
28:v:52:MET:HB2	28:v:55:GLN:HB2	1.87	0.56
12:d:11:PRO:HD2	12:d:109:ARG:HD2	1.87	0.56
20:l:359:MET:O	20:l:436:ARG:NH2	2.39	0.56
25:r:324:SER:OG	25:r:440:HIS:NE2	2.29	0.56
10:b:31:ARG:HG3	10:b:31:ARG:O	2.05	0.56
13:e:72:ASP:OD1	24:p:108:HIS:NE2	2.38	0.56
20:l:338:MET:HE2	20:l:458:LEU:HA	1.87	0.56
31:u:201:CDL:H161	31:u:201:CDL:HB31	1.88	0.56
29:w:91:ILE:HD11	29:w:131:LEU:HD12	1.88	0.56
10:b:104:ILE:HB	28:v:48:ASP:HB3	1.86	0.56
18:j:79:SER:HA	18:j:87:MET:HE2	1.87	0.56
9:a:55:PHE:CA	10:b:28:LEU:HD11	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:69:ILE:O	10:b:73:THR:HG22	2.06	0.56
17:i:96:THR:O	17:i:100:MET:HG2	2.06	0.55
20:l:417:SER:HB2	20:l:493:VAL:HG22	1.88	0.55
25:r:336:ARG:NH2	25:r:433:GLU:OE1	2.39	0.55
29:w:227:MET:SD	29:w:227:MET:N	2.79	0.55
25:r:207:MET:HE3	25:r:298:ILE:HG12	1.88	0.55
25:r:403:THR:HA	25:r:406:TYR:CE2	2.42	0.55
4:V:102:GLY:HA2	4:V:110:ILE:HG23	1.87	0.55
9:a:147:ALA:HB2	25:r:173:SER:HB2	1.89	0.55
29:w:129:TYR:HD1	29:w:129:TYR:O	1.88	0.55
7:Y:43:ARG:NH1	7:Y:47:PHE:O	2.40	0.55
17:i:20:VAL:HG11	17:i:137:ALA:HB1	1.88	0.55
17:i:130:LEU:HD12	17:i:134:GLN:HG3	1.88	0.55
9:a:160:MET:HE2	9:a:166:GLY:HA3	1.87	0.55
17:i:149:ILE:HD11	17:i:195:PRO:HG3	1.89	0.55
28:v:12:ASP:OD1	28:v:15:LYS:N	2.39	0.55
5:W:98:MET:HG3	5:W:104:TRP:CD1	2.42	0.55
17:i:44:LEU:HD22	17:i:122:ILE:HD13	1.89	0.55
25:r:78:MET:HE1	25:r:439:LEU:HD12	1.89	0.55
25:r:196:TRP:CD1	25:r:250:LEU:HB3	2.42	0.55
6:X:125:GLU:HG2	20:l:439:PRO:HG2	1.88	0.55
1:Q:47:PHE:HD1	1:Q:52:MET:HE1	1.71	0.55
20:l:397:GLU:HG2	20:l:482:MET:HE1	1.88	0.55
30:l:701:PEE:H58	30:l:701:PEE:H23	1.89	0.55
23:o:31:LYS:O	23:o:35:GLU:HG3	2.06	0.55
25:r:204:MET:HG3	25:r:209:LEU:HB2	1.88	0.55
27:u:83:THR:HA	27:u:86:TRP:CD1	2.42	0.55
29:w:129:TYR:HE2	29:w:183:CYS:HA	1.71	0.55
8:Z:64:VAL:O	8:Z:68:LEU:HD12	2.08	0.54
15:g:32:ARG:O	15:g:36:MET:HG2	2.07	0.54
20:l:161:ARG:NH1	20:l:238:GLU:OE2	2.40	0.54
30:r:501:PEE:H74	30:r:501:PEE:H34	1.90	0.54
18:j:56:PHE:HB2	21:m:74:MET:HE1	1.89	0.54
11:c:84:GLN:HA	11:c:114:ARG:HG2	1.90	0.54
13:e:85:TRP:O	13:e:89:VAL:HG13	2.08	0.54
17:i:230:LEU:HD11	17:i:244:MET:HE1	1.89	0.54
26:s:100:LEU:HD23	26:s:103:LEU:HD12	1.88	0.54
17:i:87:THR:HG22	17:i:88:LYS:N	2.19	0.54
21:m:45:LEU:HD23	21:m:50:SER:HA	1.88	0.54
7:Y:90:SER:OG	7:Y:91:GLN:NE2	2.40	0.54
18:j:15:SER:O	18:j:19:LEU:HG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:w:60:ILE:HG12	29:w:203:VAL:HB	1.90	0.54
12:d:109:ARG:NH2	12:d:131:GLN:OE1	2.41	0.54
20:l:418:LEU:HD23	31:l:702:CDL:H562	1.90	0.54
16:h:7:GLN:O	16:h:11:GLY:N	2.41	0.54
5:W:128:ARG:NH1	16:h:102:GLU:OE2	2.33	0.53
9:a:130:GLU:OE1	9:a:130:GLU:N	2.29	0.53
11:c:96:ASP:OD1	11:c:96:ASP:N	2.41	0.53
17:i:26:TRP:HB3	17:i:74:ILE:HD13	1.89	0.53
5:W:103:ASP:OD1	5:W:103:ASP:N	2.33	0.53
20:l:467:ILE:O	20:l:471:ASN:HB2	2.08	0.53
21:m:31:LEU:HD12	26:s:70:MET:HE2	1.90	0.53
29:w:123:SER:OG	29:w:125:ASP:OD1	2.21	0.53
9:a:108:GLU:N	9:a:111:GLU:OE1	2.38	0.53
11:c:36:MET:O	11:c:54:LYS:HD2	2.08	0.53
27:u:155:GLU:N	27:u:155:GLU:OE1	2.42	0.53
16:h:18:MET:HE3	19:k:56:ALA:HA	1.90	0.53
20:l:566:THR:O	20:l:570:GLN:HG2	2.08	0.53
30:l:701:PEE:H13	30:l:701:PEE:H49	1.91	0.53
19:k:8:ILE:HG21	19:k:43:MET:HB2	1.90	0.53
19:k:58:MET:SD	21:m:146:LEU:HA	2.49	0.53
28:v:15:LYS:NZ	28:v:110:GLN:HE22	2.06	0.53
7:Y:41:GLU:OE2	7:Y:41:GLU:N	2.42	0.53
5:W:144:THR:HB	26:s:96:ILE:HG23	1.91	0.53
12:d:119:GLU:HG2	28:v:52:MET:HA	1.91	0.53
5:W:134:LEU:HD21	21:m:2:THR:HG23	1.91	0.52
20:l:72:GLN:NE2	25:r:459:TYR:O	2.42	0.52
21:m:27:ILE:HG13	26:s:70:MET:HE1	1.91	0.52
9:a:96:ALA:HB2	12:d:61:TYR:CE1	2.45	0.52
20:l:142:ILE:HG12	25:r:370:PRO:HB2	1.91	0.52
20:l:596:MET:O	20:l:600:THR:HG23	2.09	0.52
25:r:371:PRO:HD2	31:r:504:CDL:H391	1.92	0.52
2:S:17:PHE:HB3	2:S:21:MET:HE3	1.91	0.52
17:i:11:MET:O	17:i:15:SER:OG	2.24	0.52
20:l:227:PHE:O	20:l:230:HIS:ND1	2.42	0.52
20:l:327:LEU:O	20:l:331:MET:HG2	2.09	0.52
6:X:77:GLU:OE2	6:X:77:GLU:N	2.28	0.52
26:s:24:GLU:HA	26:s:271:LEU:HD13	1.91	0.52
20:l:441:VAL:HG13	20:l:443:ILE:HG12	1.91	0.52
21:m:25:SER:O	21:m:27:ILE:N	2.42	0.52
26:s:130:ILE:O	26:s:134:ARG:HG3	2.09	0.52
3:U:42:ALA:HB2	26:s:312:ALA:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:g:202:CDL:H391	17:i:334:THR:HG21	1.91	0.52
19:k:30:LEU:O	19:k:34:GLU:HG2	2.10	0.52
20:l:400:ASN:HA	20:l:409:LEU:HD11	1.91	0.52
20:l:473:PRO:HG2	20:l:475:MET:HE3	1.92	0.52
25:r:44:GLN:HG3	25:r:60:SER:HA	1.91	0.52
8:Z:39:ARG:HG3	8:Z:41:LEU:HD12	1.92	0.52
12:d:32:TYR:O	12:d:36:ILE:HG22	2.10	0.52
12:d:110:LEU:HD11	20:l:203:MET:HG2	1.92	0.52
33:j:202:PLX:H322	33:j:202:PLX:H381	1.92	0.52
20:l:200:GLN:HG3	20:l:204:LEU:HD23	1.91	0.52
20:l:284:THR:O	20:l:288:THR:HG23	2.10	0.52
25:r:328:CYS:O	25:r:332:THR:HG23	2.09	0.52
26:s:307:LEU:HA	26:s:310:MET:HE3	1.91	0.52
28:v:15:LYS:HZ2	28:v:110:GLN:HE22	1.58	0.52
29:w:129:TYR:OH	29:w:186:HIS:ND1	2.25	0.52
5:W:57:ARG:HB3	26:s:316:PRO:HG3	1.92	0.51
9:a:134:GLU:OE1	22:n:57:TRP:NE1	2.40	0.51
11:c:55:TYR:OH	11:c:74:ASP:O	2.25	0.51
33:a:202:PLX:C32	33:a:202:PLX:C28	2.85	0.51
17:i:132:THR:HG22	17:i:212:THR:CG2	2.40	0.51
25:r:12:LEU:HB2	25:r:13:PRO:HD3	1.93	0.51
7:Y:94:ASP:OD1	28:v:107:ARG:NH1	2.43	0.51
25:r:161:LEU:O	25:r:165:VAL:HG22	2.10	0.51
9:a:96:ALA:HB2	12:d:61:TYR:HE1	1.75	0.51
15:g:109:LYS:HB3	15:g:114:ILE:HD11	1.93	0.51
17:i:79:LEU:HB2	19:k:47:ILE:HD13	1.91	0.51
29:w:75:ARG:HB2	29:w:75:ARG:CZ	2.40	0.51
32:X:201:8Q1:O27	32:X:201:8Q1:O33	2.29	0.51
31:g:202:CDL:H742	31:g:202:CDL:H271	1.93	0.51
29:w:180:ARG:NH1	29:w:316:GLU:OE2	2.43	0.51
4:V:35:ILE:HG21	31:V:201:CDL:H781	1.92	0.51
20:l:296:ASN:HD22	20:l:357:ARG:CZ	2.23	0.51
8:Z:25:GLU:HA	8:Z:30:GLU:OE1	2.10	0.51
11:c:38:PRO:HD2	23:o:70:TYR:CD1	2.46	0.51
18:j:25:PRO:HB2	26:s:60:PRO:HD3	1.92	0.51
24:p:16:VAL:HG22	24:p:64:LEU:HD13	1.92	0.51
3:U:56:PRO:HG2	27:u:45:LEU:HB2	1.93	0.51
6:X:155:TYR:CE1	10:b:23:LEU:HB3	2.46	0.51
9:a:127:ASP:OD1	33:a:202:PLX:C1	2.53	0.51
22:n:27:LEU:HD21	31:u:201:CDL:H112	1.93	0.51
26:s:87:VAL:HG12	26:s:95:LEU:HD23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:559:GLU:O	20:l:563:PRO:HD2	2.10	0.50
20:l:526:LEU:HD12	20:l:530:PRO:HG2	1.93	0.50
25:r:337:VAL:HG12	25:r:339:SER:HB3	1.92	0.50
4:V:69:ILE:HG13	4:V:100:THR:HG21	1.93	0.50
33:a:202:PLX:O1	33:a:202:PLX:H1A2	2.11	0.50
20:l:83:ASP:OD2	20:l:262:ARG:NH1	2.44	0.50
33:g:201:PLX:H352	17:i:342:ALA:HB3	1.93	0.50
19:k:37:MET:HG3	19:k:67:ALA:HB1	1.92	0.50
24:p:100:PRO:HG3	25:r:419:TYR:CE1	2.46	0.50
6:X:146:ASP:OD2	10:b:16:ARG:NH1	2.45	0.50
20:l:366:MET:O	20:l:370:THR:HG22	2.11	0.50
20:l:562:LEU:HB3	20:l:563:PRO:HD3	1.93	0.50
24:p:26:HIS:CD2	24:p:79:PRO:HB3	2.47	0.50
8:Z:24:ILE:HG23	8:Z:29:LEU:HB2	1.94	0.50
11:c:184:TYR:HA	28:v:34:ARG:NH1	2.27	0.50
13:e:97:ILE:O	13:e:101:LEU:HB2	2.12	0.50
20:l:292:ALA:HB2	20:l:304:PHE:HB3	1.94	0.50
23:o:22:GLU:OE1	23:o:22:GLU:N	2.37	0.50
24:p:81:ILE:HG22	24:p:85:SER:HB2	1.93	0.50
24:p:100:PRO:HG3	25:r:419:TYR:CZ	2.46	0.50
26:s:13:ILE:O	26:s:17:VAL:HG13	2.12	0.50
16:h:15:ASP:OD2	17:i:25:HIS:HB2	2.11	0.50
18:j:54:LYS:HD3	18:j:113:TRP:HA	1.92	0.50
31:u:201:CDL:H251	31:u:201:CDL:H792	1.94	0.50
31:r:504:CDL:H312	31:r:504:CDL:H742	1.93	0.49
28:v:42:THR:OG1	28:v:45:GLU:OE2	2.29	0.49
5:W:134:LEU:HD11	21:m:1:MET:HA	1.94	0.49
11:c:58:ARG:HB2	11:c:61:ASP:HB2	1.93	0.49
27:u:106:LYS:O	27:u:109:GLU:HG3	2.13	0.49
9:a:133:TYR:OH	12:d:87:GLU:OE1	2.22	0.49
17:i:88:LYS:HD2	17:i:148:SER:OG	2.12	0.49
25:r:248:THR:HG23	25:r:249:ILE:HG23	1.95	0.49
20:l:264:TYR:CD2	20:l:265:PRO:HD3	2.47	0.49
1:Q:39:PRO:HB3	1:Q:43:TRP:CD1	2.48	0.49
10:b:35:LEU:HD12	10:b:35:LEU:H	1.74	0.49
17:i:155:LEU:HD12	17:i:278:MET:SD	2.52	0.49
17:i:170:LEU:O	17:i:295:ARG:NH2	2.40	0.49
20:l:293:ILE:HG13	20:l:418:LEU:HD22	1.94	0.49
4:V:4:THR:O	4:V:8:LYS:HG3	2.13	0.49
17:i:95:MET:HE1	17:i:145:ILE:HD12	1.94	0.49
17:i:289:ASN:HA	17:i:292:PHE:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:s:25:ARG:HD3	34:s:401:UQ:HM21	1.94	0.49
7:Y:65:MET:HE1	20:l:378:LEU:HD12	1.94	0.49
13:e:89:VAL:HG21	25:r:25:ILE:HG23	1.94	0.49
13:e:90:VAL:HG22	25:r:28:THR:HG21	1.95	0.49
2:S:47:LEU:HD22	27:u:22:SER:HB2	1.94	0.48
7:Y:94:ASP:HB3	7:Y:99:ILE:HB	1.94	0.48
9:a:55:PHE:N	10:b:28:LEU:HD11	2.29	0.48
20:l:90:ILE:HD13	20:l:129:MET:SD	2.53	0.48
7:Y:83:HIS:O	7:Y:83:HIS:ND1	2.41	0.48
7:Y:92:TRP:O	28:v:107:ARG:NH2	2.42	0.48
13:e:58:ASP:OD2	29:w:326:ARG:NE	2.47	0.48
17:i:236:LYS:HE2	29:w:302:LEU:HD11	1.95	0.48
20:l:286:LEU:HD22	20:l:411:MET:SD	2.53	0.48
9:a:50:HIS:HB3	9:a:52:LYS:HZ2	1.78	0.48
19:k:85:TYR:CD2	19:k:92:ASN:HB3	2.49	0.48
20:l:488:MET:O	20:l:492:ILE:HG12	2.14	0.48
4:V:53:VAL:HA	4:V:56:THR:HG22	1.95	0.48
25:r:260:PRO:HG2	33:r:502:PLX:H132	1.96	0.48
9:a:136:THR:HG21	25:r:48:ASN:HD22	1.78	0.48
25:r:130:LEU:HD22	25:r:150:LEU:HD13	1.94	0.48
4:V:140:LYS:NZ	17:i:274:GLU:OE2	2.42	0.48
29:w:86:PHE:HB2	29:w:159:LEU:HD23	1.96	0.48
6:X:119:ILE:HG21	6:X:135:ALA:HB1	1.96	0.48
9:a:95:GLU:OE1	31:a:201:CDL:O1	2.31	0.48
19:k:23:ARG:HD3	21:m:23:LYS:HB2	1.95	0.48
19:k:25:HIS:O	19:k:28:SER:N	2.40	0.48
20:l:346:ILE:HA	20:l:366:MET:HE1	1.94	0.48
24:p:92:GLU:HB3	24:p:95:GLU:HG3	1.96	0.48
5:W:134:LEU:HD11	21:m:1:MET:HG2	1.96	0.47
29:w:270:VAL:O	29:w:274:GLU:HG2	2.14	0.47
17:i:268:GLN:HG3	27:u:168:PHE:HZ	1.79	0.47
25:r:382:ILE:HD12	25:r:396:MET:HB3	1.95	0.47
1:Q:41:VAL:O	1:Q:45:GLU:HG2	2.14	0.47
31:l:702:CDL:H612	31:l:702:CDL:H371	1.95	0.47
22:n:30:ARG:HG3	22:n:30:ARG:HH11	1.78	0.47
11:c:84:GLN:O	11:c:98:ARG:NH1	2.39	0.47
11:c:119:THR:HB	23:o:13:THR:HG23	1.97	0.47
17:i:211:MET:HE3	17:i:251:MET:HA	1.96	0.47
17:i:128:LEU:HD23	17:i:128:LEU:O	2.14	0.47
20:l:156:GLY:HA2	20:l:164:ALA:HB1	1.95	0.47
25:r:267:TRP:HE1	25:r:271:MET:HE2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:w:88:GLU:OE2	29:w:161:ARG:NH1	2.48	0.47
7:Y:93:THR:OG1	7:Y:96:GLU:OE1	2.23	0.47
10:b:35:LEU:N	10:b:35:LEU:CD1	2.73	0.47
10:b:110:ILE:HG12	12:d:16:ARG:HB2	1.97	0.47
17:i:254:LEU:HD23	25:r:127:VAL:HG22	1.97	0.47
21:m:23:LYS:N	21:m:24:PRO:HD3	2.30	0.47
31:o:201:CDL:H872	31:o:201:CDL:H841	1.77	0.47
25:r:166:TYR:O	25:r:170:THR:HG23	2.14	0.47
4:V:12:ILE:HB	4:V:21:LYS:HD3	1.96	0.47
4:V:61:PHE:HD2	4:V:104:ARG:HH21	1.62	0.47
17:i:128:LEU:C	17:i:128:LEU:CD2	2.85	0.47
23:o:80:PHE:HE1	23:o:86:THR:HG21	1.79	0.47
11:c:41:TYR:CD2	11:c:67:ASP:HB2	2.50	0.47
33:g:201:PLX:H301	17:i:347:ASN:HB3	1.96	0.47
20:l:298:ILE:O	20:l:302:VAL:HG23	2.15	0.47
20:l:482:MET:HE3	20:l:486:MET:HG2	1.97	0.47
25:r:44:GLN:HG3	25:r:60:SER:CA	2.45	0.47
31:r:504:CDL:H312	31:r:504:CDL:H761	1.97	0.47
8:Z:68:LEU:HB3	8:Z:71:PHE:HB2	1.96	0.46
17:i:276:ILE:HG21	30:r:501:PEE:H14	1.97	0.46
20:l:338:MET:CE	20:l:458:LEU:HA	2.45	0.46
26:s:88:PRO:HG2	26:s:105:MET:SD	2.55	0.46
13:e:143:ASP:HA	13:e:144:PRO:HD3	1.73	0.46
29:w:57:SER:O	29:w:156:GLY:HA3	2.15	0.46
26:s:102:VAL:HG21	26:s:154:LEU:HD11	1.98	0.46
29:w:258:TYR:HE2	29:w:269:VAL:HG13	1.80	0.46
11:c:85:GLU:OE2	11:c:120:SER:HA	2.16	0.46
29:w:66:ILE:O	29:w:214:ILE:CD1	2.63	0.46
17:i:267:ILE:HG12	17:i:279:PRO:HB3	1.96	0.46
33:r:503:PLX:H121	33:r:503:PLX:H152	1.51	0.46
20:l:186:MET:HG2	20:l:196:TRP:NE1	2.31	0.46
24:p:10:LEU:HB2	24:p:15:LYS:HZ2	1.81	0.46
22:n:50:ARG:HB2	22:n:53:GLU:HB2	1.98	0.46
26:s:197:PRO:HB3	26:s:278:PRO:O	2.16	0.46
17:i:133:TRP:HE3	31:i:401:CDL:H381	1.80	0.46
25:r:122:PHE:HE1	25:r:206:LYS:HD2	1.81	0.46
20:l:401:MET:HE3	20:l:401:MET:HB3	1.75	0.46
24:p:76:HIS:O	24:p:78:GLN:N	2.49	0.46
25:r:447:LEU:HD11	33:r:503:PLX:H371	1.97	0.46
25:r:457:PRO:HG2	25:r:458:LEU:HD12	1.98	0.46
5:W:73:PRO:HG2	27:u:40:ASN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:g:202:CDL:H582	25:r:13:PRO:HB3	1.97	0.45
18:j:49:LEU:N	18:j:50:PRO:HD2	2.31	0.45
25:r:74:PRO:O	25:r:78:MET:HG3	2.15	0.45
33:r:502:PLX:H301	33:r:502:PLX:H331	1.70	0.45
27:u:85:TYR:CZ	27:u:104:GLN:HB2	2.52	0.45
24:p:29:SER:HB3	24:p:76:HIS:CD2	2.47	0.45
25:r:14:MET:SD	25:r:26:ASN:HB3	2.56	0.45
25:r:22:MET:O	25:r:26:ASN:ND2	2.49	0.45
31:r:504:CDL:H611	31:r:504:CDL:H581	1.67	0.45
9:a:94:GLY:HA2	9:a:116:PRO:HG3	1.97	0.45
10:b:14:GLN:NE2	24:p:157:ALA:HB3	2.31	0.45
31:g:202:CDL:H792	31:g:202:CDL:H761	1.90	0.45
31:g:202:CDL:H171	17:i:245:MET:HE1	1.97	0.45
11:c:165:ASP:OD1	11:c:170:ARG:NH2	2.50	0.45
12:d:160:LYS:NZ	15:g:112:GLY:O	2.35	0.45
19:k:84:THR:HG22	19:k:85:TYR:CD1	2.52	0.45
20:l:78:LEU:HD11	31:r:504:CDL:H251	1.99	0.45
29:w:279:ASP:OD1	29:w:279:ASP:N	2.47	0.45
33:j:202:PLX:H372	33:j:202:PLX:H342	1.81	0.45
19:k:37:MET:HG3	19:k:67:ALA:CB	2.46	0.45
25:r:48:ASN:N	25:r:48:ASN:OD1	2.47	0.45
1:Q:36:GLN:NE2	25:r:135:ARG:O	2.48	0.45
6:X:94:ASP:OD1	6:X:94:ASP:N	2.40	0.45
30:b:201:PEE:H60	30:b:201:PEE:H55	1.75	0.45
31:g:202:CDL:H812	31:g:202:CDL:H241	1.99	0.45
26:s:306:SER:OG	26:s:310:MET:HE2	2.16	0.45
20:l:536:LEU:HB3	20:l:537:PRO:HD3	1.98	0.45
33:r:502:PLX:H51	33:r:502:PLX:H6	1.51	0.45
29:w:165:SER:HB3	29:w:245:PHE:CE1	2.51	0.45
6:X:123:GLU:OE1	24:p:21:LYS:NZ	2.36	0.45
7:Y:76:ASP:O	20:l:385:TYR:OH	2.23	0.45
28:v:33:GLU:H	28:v:33:GLU:CD	2.21	0.45
29:w:64:GLY:N	29:w:70:LYS:HD3	2.31	0.45
7:Y:87:PRO:HG2	28:v:96:VAL:HG22	1.98	0.45
13:e:137:MET:HE2	13:e:137:MET:HB2	1.91	0.45
20:l:554:ASP:OD1	25:r:213:HIS:NE2	2.50	0.45
21:m:51:PHE:HD2	26:s:100:LEU:HD21	1.82	0.45
26:s:24:GLU:OE1	26:s:228:TYR:OH	2.31	0.45
4:V:106:ARG:HA	4:V:106:ARG:NE	2.32	0.45
6:X:137:LYS:HD3	10:b:4:TYR:CE1	2.52	0.45
7:Y:72:ARG:HH21	7:Y:76:ASP:CG	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:222:SER:O	17:i:224:ALA:N	2.50	0.45
20:l:145:GLU:HA	20:l:145:GLU:OE2	2.17	0.45
25:r:267:TRP:NE1	25:r:271:MET:HE2	2.32	0.45
29:w:350:LYS:HA	29:w:350:LYS:HD3	1.77	0.45
8:Z:18:ASP:OD1	8:Z:18:ASP:N	2.41	0.44
15:g:51:ARG:CZ	17:i:322:GLN:HB3	2.47	0.44
17:i:320:THR:HG21	29:w:300:ASN:HA	2.00	0.44
20:l:350:LEU:HD23	20:l:350:LEU:HA	1.79	0.44
20:l:407:TRP:O	20:l:411:MET:HG2	2.17	0.44
25:r:269:MET:HE2	25:r:399:ASN:ND2	2.32	0.44
26:s:92:PRO:HB3	26:s:255:TYR:CD2	2.52	0.44
2:S:42:SER:O	2:S:42:SER:OG	2.33	0.44
12:d:127:LYS:HB3	12:d:127:LYS:HE3	1.83	0.44
31:g:202:CDL:H211	31:g:202:CDL:H401	1.98	0.44
17:i:38:LEU:HD12	19:k:73:LEU:HD22	1.99	0.44
17:i:298:TYR:O	17:i:303:THR:OG1	2.35	0.44
18:j:73:LEU:O	26:s:160:TYR:OH	2.36	0.44
20:l:529:TYR:HB3	20:l:530:PRO:HD3	1.99	0.44
15:g:51:ARG:NE	17:i:322:GLN:HG3	2.33	0.44
20:l:152:PHE:CD1	20:l:168:ALA:HB1	2.52	0.44
27:u:80:GLU:O	27:u:84:GLU:HG3	2.17	0.44
17:i:11:MET:HE3	31:i:401:CDL:H542	1.98	0.44
18:j:71:LEU:HD23	18:j:71:LEU:HA	1.83	0.44
31:l:702:CDL:H781	31:l:702:CDL:H751	1.53	0.44
31:o:201:CDL:H721	31:o:201:CDL:H752	1.49	0.44
27:u:38:LYS:HB3	27:u:39:PRO:HD3	1.99	0.44
9:a:155:GLU:HA	9:a:155:GLU:OE1	2.17	0.44
16:h:2:PRO:HA	17:i:140:SER:HB2	2.00	0.44
17:i:43:VAL:HG11	17:i:129:LEU:HD23	1.99	0.44
20:l:161:ARG:HA	24:p:92:GLU:HB2	1.99	0.44
20:l:172:ILE:O	20:l:176:ARG:HG2	2.16	0.44
20:l:226:GLN:OE1	20:l:284:THR:HG21	2.18	0.44
25:r:300:ALA:O	25:r:308:SER:HB3	2.18	0.44
29:w:170:LEU:HD22	29:w:187:TYR:CD1	2.53	0.44
7:Y:65:MET:HE3	20:l:386:LEU:HD11	1.98	0.44
11:c:169:GLU:HB3	28:v:53:LEU:HD11	1.98	0.44
15:g:12:PRO:HB3	16:h:5:ASP:HB3	1.99	0.44
18:j:48:ARG:HB2	18:j:49:LEU:H	1.70	0.44
20:l:249:SER:OG	20:l:336:LYS:HG3	2.17	0.44
20:l:541:ASN:OD1	30:l:703:PEE:H57	2.17	0.44
25:r:218:LYS:O	25:r:222:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:30:ILE:HD11	18:j:96:ILE:HD11	2.00	0.44
10:b:29:SER:HB2	10:b:30:PRO:CD	2.40	0.44
18:j:15:SER:HA	26:s:76:ILE:HD12	2.00	0.44
21:m:169:MET:HE3	21:m:169:MET:HB3	1.77	0.44
25:r:299:VAL:O	25:r:303:ILE:HG12	2.18	0.44
17:i:42:PRO:HG3	21:m:167:VAL:HG13	2.00	0.44
20:l:233:LEU:HB3	20:l:234:PRO:HD3	1.98	0.44
31:l:702:CDL:H591	31:l:702:CDL:H622	1.54	0.44
24:p:82:PHE:HB2	24:p:85:SER:OG	2.18	0.44
26:s:169:GLN:NE2	26:s:241:LEU:O	2.48	0.44
3:U:14:ALA:O	3:U:15:LYS:HG2	2.18	0.44
5:W:43:LEU:HG	26:s:179:TRP:HE1	1.83	0.44
7:Y:97:LEU:O	28:v:104:ARG:HG3	2.18	0.44
23:o:113:GLU:O	23:o:117:GLN:HG2	2.18	0.44
1:Q:53:TYR:HE1	30:i:402:PEE:H2	1.82	0.43
7:Y:65:MET:SD	20:l:375:ILE:HG12	2.57	0.43
33:g:201:PLX:H22	33:g:201:PLX:H1C3	1.72	0.43
20:l:234:PRO:O	20:l:237:MET:HG2	2.18	0.43
31:r:504:CDL:H311	31:r:504:CDL:H561	2.00	0.43
7:Y:92:TRP:CE2	28:v:100:LYS:HE3	2.52	0.43
11:c:117:VAL:HG21	20:l:539:TYR:HB2	2.00	0.43
14:f:60:LYS:NZ	14:f:64:GLU:OE1	2.43	0.43
17:i:149:ILE:CD1	17:i:154:MET:HG3	2.48	0.43
17:i:236:LYS:HG2	17:i:237:MET:HG3	1.99	0.43
10:b:123:PHE:HB3	28:v:40:VAL:HG11	1.99	0.43
12:d:65:HIS:ND1	13:e:120:ARG:HD2	2.34	0.43
15:g:74:GLY:O	15:g:78:LEU:HG	2.18	0.43
20:l:8:THR:HB	20:l:82:MET:SD	2.58	0.43
25:r:158:LEU:HD23	25:r:158:LEU:HA	1.77	0.43
28:v:103:GLU:HA	28:v:103:GLU:OE1	2.18	0.43
4:V:140:LYS:HB3	4:V:140:LYS:HE2	1.65	0.43
6:X:69:SER:OG	6:X:70:ASP:N	2.51	0.43
20:l:332:HIS:HA	20:l:335:PHE:CZ	2.54	0.43
21:m:1:MET:HE1	21:m:4:TYR:HA	1.99	0.43
5:W:63:GLU:OE2	27:u:119:ARG:NH2	2.51	0.43
11:c:48:ARG:NH2	11:c:64:PRO:HD2	2.33	0.43
24:p:168:TRP:O	24:p:172:THR:OG1	2.24	0.43
27:u:137:LEU:HD12	27:u:138:PRO:HD2	2.00	0.43
11:c:41:TYR:HA	11:c:42:PRO:HD3	1.87	0.43
17:i:136:LEU:HD23	17:i:205:LEU:HD21	2.00	0.43
19:k:2:PRO:HD2	19:k:5:TYR:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:m:17:PHE:HA	21:m:20:PHE:CD1	2.53	0.43
25:r:17:MET:HE3	25:r:17:MET:HB3	1.87	0.43
25:r:127:VAL:HB	25:r:128:PRO:HD3	1.99	0.43
31:V:201:CDL:H622	31:V:201:CDL:H592	1.91	0.43
5:W:98:MET:HG3	5:W:104:TRP:NE1	2.34	0.43
33:a:202:PLX:H1C3	33:a:202:PLX:H22	1.80	0.43
15:g:87:LEU:HD23	15:g:87:LEU:HA	1.86	0.43
31:g:202:CDL:H632	25:r:10:MET:HE1	1.99	0.43
13:e:83:ASP:OD1	13:e:83:ASP:C	2.62	0.43
17:i:108:LEU:HD11	17:i:191:THR:HG21	2.00	0.43
18:j:84:LEU:HD23	18:j:84:LEU:HA	1.84	0.43
18:j:94:LEU:HD12	21:m:147:TYR:HE1	1.83	0.43
20:l:127:THR:HG21	20:l:146:GLY:C	2.44	0.43
26:s:24:GLU:HG3	26:s:271:LEU:HD22	2.01	0.43
29:w:143:TYR:OH	29:w:199:LEU:O	2.30	0.43
29:w:261:ARG:HH11	29:w:261:ARG:C	2.22	0.43
10:b:88:TYR:CZ	12:d:49:ARG:HG2	2.54	0.43
20:l:452:ASN:HA	20:l:455:LYS:HG2	2.01	0.43
24:p:44:MET:HA	24:p:47:ARG:HG2	2.00	0.43
24:p:132:SER:HB3	24:p:136:GLU:OE2	2.17	0.43
10:b:11:ARG:HE	24:p:154:LEU:HB2	1.83	0.43
17:i:135:LYS:CB	17:i:187:MET:HE1	2.49	0.43
31:i:401:CDL:H142	31:i:401:CDL:H171	1.66	0.43
20:l:127:THR:HG21	20:l:146:GLY:CA	2.48	0.43
22:n:30:ARG:HG3	22:n:30:ARG:NH1	2.34	0.43
9:a:55:PHE:N	10:b:28:LEU:CD1	2.81	0.42
15:g:4:MET:O	15:g:10:ARG:NH1	2.52	0.42
17:i:265:MET:HE3	17:i:340:THR:HG21	2.00	0.42
20:l:331:MET:HG3	20:l:391:SER:HB3	2.00	0.42
22:n:8:VAL:O	22:n:12:TRP:HB3	2.19	0.42
24:p:49:ASP:OD1	24:p:49:ASP:C	2.62	0.42
27:u:121:ASP:N	27:u:124:GLU:OE1	2.46	0.42
28:v:35:LYS:HA	28:v:35:LYS:HD2	1.70	0.42
7:Y:52:ARG:O	7:Y:56:ILE:HG23	2.18	0.42
30:b:201:PEE:H38	20:l:66:TRP:HZ3	1.84	0.42
17:i:122:ILE:HD11	17:i:127:GLY:HA2	2.00	0.42
17:i:334:THR:HG22	17:i:335:LEU:HG	2.01	0.42
20:l:292:ALA:HB2	20:l:304:PHE:CB	2.49	0.42
25:r:9:THR:HG21	31:u:201:CDL:H242	2.01	0.42
5:W:128:ARG:HB3	5:W:132:GLU:OE2	2.19	0.42
8:Z:32:VAL:HG13	24:p:39:TYR:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:37:PHE:CE2	20:l:3:PRO:HB3	2.54	0.42
17:i:66:ALA:HB2	17:i:104:MET:HB3	2.01	0.42
17:i:323:MET:H	17:i:323:MET:HG2	1.59	0.42
17:i:340:THR:N	17:i:341:PRO:HD2	2.33	0.42
20:l:190:LEU:HB2	20:l:196:TRP:NE1	2.34	0.42
20:l:295:GLN:HB2	20:l:301:ILE:HG12	2.01	0.42
20:l:411:MET:HA	20:l:411:MET:HE2	2.00	0.42
29:w:73:LEU:HD12	29:w:73:LEU:O	2.19	0.42
33:g:201:PLX:H131	33:g:201:PLX:H102	1.40	0.42
31:g:202:CDL:H262	31:g:202:CDL:H231	1.83	0.42
19:k:22:TYR:O	20:l:585:LYS:NZ	2.38	0.42
25:r:398:MET:O	25:r:402:ILE:HG13	2.19	0.42
12:d:89:GLU:O	12:d:93:ARG:HG2	2.19	0.42
31:g:202:CDL:H242	25:r:97:THR:HG21	2.01	0.42
31:u:201:CDL:H762	31:u:201:CDL:H121	2.01	0.42
17:i:112:HIS:CE1	17:i:164:ILE:HG21	2.54	0.42
1:Q:42:GLU:OE1	1:Q:42:GLU:HA	2.18	0.42
17:i:182:SER:HG	17:i:293:TYR:HH	1.60	0.42
18:j:55:PHE:O	18:j:58:VAL:HG12	2.20	0.42
25:r:206:LYS:HE3	25:r:206:LYS:HB2	1.93	0.42
25:r:306:PRO:HA	25:r:458:LEU:HD22	2.00	0.42
26:s:90:PRO:HB3	26:s:94:PRO:HD3	2.02	0.42
17:i:281:LEU:O	17:i:285:THR:OG1	2.31	0.42
17:i:323:MET:HE2	17:i:323:MET:HB3	1.87	0.42
20:l:10:THR:O	20:l:14:ILE:HG22	2.20	0.42
20:l:44:PHE:HB2	20:l:94:LEU:HB3	2.02	0.42
20:l:86:SER:O	20:l:90:ILE:HG12	2.20	0.42
20:l:267:MET:HE1	20:l:273:VAL:HG12	2.02	0.42
30:W:201:PEE:H40	21:m:38:GLY:HA3	2.02	0.42
17:i:185:ALA:CB	17:i:289:ASN:HD21	2.33	0.42
21:m:129:ASP:OD1	21:m:129:ASP:N	2.50	0.42
26:s:282:TYR:O	26:s:286:MET:HG2	2.20	0.42
7:Y:78:ASP:HB2	7:Y:83:HIS:HB2	2.02	0.42
20:l:172:ILE:HD13	20:l:172:ILE:HA	1.95	0.42
20:l:260:LEU:HD23	20:l:260:LEU:HA	1.86	0.42
25:r:214:LEU:HD13	25:r:214:LEU:HA	1.94	0.42
31:u:201:CDL:H712	31:u:201:CDL:H741	1.60	0.42
12:d:142:ARG:NE	13:e:138:GLU:O	2.51	0.41
17:i:125:GLN:HG2	31:i:401:CDL:HA21	2.02	0.41
17:i:131:LEU:CD1	17:i:216:PHE:CE2	2.97	0.41
17:i:135:LYS:HB3	17:i:187:MET:HE1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:324:LYS:O	17:i:325:LEU:CB	2.60	0.41
18:j:81:THR:C	18:j:83:ASN:H	2.28	0.41
29:w:329:GLN:O	29:w:333:GLU:HG2	2.21	0.41
2:S:14:ALA:O	2:S:18:ILE:HG12	2.20	0.41
17:i:54:GLU:O	17:i:57:THR:HG22	2.20	0.41
20:l:534:HIS:CD2	30:l:703:PEE:H13	2.55	0.41
26:s:267:THR:O	26:s:271:LEU:HG	2.19	0.41
27:u:47:ARG:NH2	27:u:53:PRO:HG3	2.35	0.41
13:e:92:PHE:O	13:e:96:SER:HB2	2.19	0.41
17:i:72:MET:HG3	17:i:97:MET:SD	2.60	0.41
19:k:23:ARG:HG3	19:k:24:SER:H	1.84	0.41
29:w:118:TYR:OH	35:w:401:ADP:O2'	2.38	0.41
29:w:295:ARG:HA	29:w:298:VAL:HG22	2.02	0.41
2:S:43:TYR:CZ	5:W:68:ARG:HG3	2.55	0.41
5:W:133:ILE:O	5:W:137:THR:HG22	2.20	0.41
10:b:22:TRP:CE2	24:p:172:THR:HG22	2.55	0.41
11:c:149:ILE:HD13	11:c:149:ILE:HA	1.88	0.41
11:c:156:VAL:HG11	28:v:95:TYR:CZ	2.55	0.41
13:e:73:SER:C	13:e:75:GLY:H	2.27	0.41
15:g:108:LYS:HA	15:g:108:LYS:HD3	1.84	0.41
17:i:310:ASN:HB2	29:w:309:THR:HG22	2.00	0.41
20:l:174:TYR:CD2	20:l:232:TRP:HB3	2.54	0.41
20:l:250:SER:CB	20:l:333:ALA:HA	2.49	0.41
25:r:71:TRP:O	25:r:74:PRO:HD2	2.20	0.41
11:c:167:TYR:CD2	11:c:178:PRO:HG3	2.55	0.41
15:g:33:LEU:HD23	15:g:33:LEU:HA	1.88	0.41
20:l:88:MET:HE3	20:l:468:ILE:HG23	2.02	0.41
25:r:442:LEU:HD23	25:r:442:LEU:HA	1.88	0.41
3:U:25:ILE:HD11	30:U:401:PEE:H31	2.03	0.41
12:d:117:GLU:HG3	12:d:124:ASN:HB2	2.03	0.41
14:f:71:ARG:HD2	14:f:71:ARG:C	2.46	0.41
16:h:17:TRP:CE3	16:h:18:MET:HB2	2.55	0.41
20:l:37:LYS:HD3	20:l:98:TRP:HE1	1.86	0.41
23:o:60:ILE:HD12	25:r:422:HIS:HB2	2.02	0.41
25:r:216:LEU:HD23	25:r:287:ALA:HB1	2.03	0.41
11:c:149:ILE:O	11:c:151:PRO:HD3	2.20	0.41
15:g:7:ARG:NH1	15:g:91:ASP:OD1	2.54	0.41
20:l:24:SER:OG	20:l:25:ASN:N	2.54	0.41
25:r:373:ILE:HD11	25:r:444:LEU:HD23	2.02	0.41
27:u:152:PRO:C	27:u:153:GLU:HG3	2.46	0.41
29:w:63:ASP:O	29:w:206:TYR:HD1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:w:146:ALA:HB1	29:w:157:VAL:HG21	2.03	0.41
3:U:19:LEU:HD23	3:U:19:LEU:HA	1.90	0.41
9:a:139:ILE:O	9:a:143:GLU:HG2	2.21	0.41
13:e:136:LEU:HB3	13:e:137:MET:H	1.57	0.41
16:h:69:ARG:O	16:h:73:MET:HG3	2.20	0.41
20:l:49:VAL:HB	20:l:50:PRO:HD3	2.02	0.41
26:s:98:MET:HE2	26:s:101:GLY:HA2	2.02	0.41
2:S:34:LYS:HE3	2:S:34:LYS:HB2	1.94	0.41
6:X:106:LYS:HB3	6:X:106:LYS:HE3	1.92	0.41
12:d:9:VAL:HG13	12:d:10:TYR:CD2	2.56	0.41
12:d:80:LYS:HD3	12:d:80:LYS:HA	1.80	0.41
15:g:36:MET:HE3	15:g:36:MET:HB3	1.88	0.41
16:h:94:PRO:HA	16:h:95:PRO:HD3	1.94	0.41
17:i:106:LEU:HG	17:i:138:PRO:HB2	2.02	0.41
17:i:112:HIS:HB2	17:i:184:ILE:HD13	2.03	0.41
17:i:234:TRP:CZ2	17:i:304:MET:HB3	2.56	0.41
20:l:386:LEU:HD23	20:l:386:LEU:HA	1.93	0.41
25:r:200:ILE:HD13	25:r:200:ILE:HA	1.90	0.41
25:r:329:LEU:HD23	25:r:437:MET:HE3	2.03	0.41
33:r:503:PLX:H212	31:r:504:CDL:H801	2.02	0.41
28:v:26:PRO:HA	28:v:27:PRO:HD3	1.99	0.41
28:v:46:MET:HG2	28:v:56:ARG:HG2	2.02	0.41
29:w:75:ARG:NH1	29:w:75:ARG:CB	2.82	0.41
29:w:87:PRO:O	29:w:142:GLN:NE2	2.51	0.41
29:w:210:PRO:O	29:w:214:ILE:HG22	2.20	0.41
29:w:353:TRP:CD1	29:w:353:TRP:H	2.39	0.41
30:b:201:PEE:H33	31:r:504:CDL:H241	2.02	0.41
15:g:27:LYS:HZ2	15:g:27:LYS:HG2	1.79	0.41
17:i:132:THR:CG2	17:i:212:THR:CG2	2.99	0.41
20:l:304:PHE:CZ	20:l:526:LEU:HD22	2.56	0.41
26:s:85:MET:CE	26:s:233:MET:HE2	2.51	0.41
26:s:104:PHE:O	26:s:108:MET:HG2	2.21	0.41
26:s:175:ILE:HD12	26:s:175:ILE:HA	1.84	0.41
31:u:201:CDL:H201	31:u:201:CDL:H171	1.86	0.41
29:w:147:LEU:HD23	29:w:147:LEU:HA	1.88	0.41
31:V:201:CDL:H322	31:V:201:CDL:H352	1.48	0.40
17:i:347:ASN:OD1	17:i:347:ASN:N	2.51	0.40
20:l:368:PHE:O	20:l:371:THR:HG22	2.20	0.40
21:m:61:LEU:HB3	26:s:111:LEU:HD21	2.03	0.40
24:p:44:MET:O	24:p:48:PHE:HB2	2.21	0.40
25:r:207:MET:O	25:r:294:MET:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:u:83:THR:HA	27:u:86:TRP:NE1	2.35	0.40
4:V:136:PHE:CE1	17:i:278:MET:HE1	2.56	0.40
5:W:74:LEU:O	5:W:78:GLU:HG3	2.21	0.40
25:r:19:LYS:HB3	25:r:19:LYS:HE2	1.68	0.40
31:r:504:CDL:H572	31:r:504:CDL:H871	2.03	0.40
28:v:76:ASN:OD1	28:v:78:LEU:HD12	2.22	0.40
29:w:110:GLY:HA2	29:w:134:TRP:CD2	2.56	0.40
9:a:124:THR:O	33:a:202:PLX:H1A3	2.22	0.40
9:a:136:THR:HG21	25:r:48:ASN:ND2	2.36	0.40
10:b:70:PHE:O	10:b:74:HIS:HB2	2.21	0.40
10:b:79:VAL:HG22	20:l:10:THR:HG21	2.04	0.40
25:r:207:MET:HG2	25:r:298:ILE:HG13	2.03	0.40
11:c:184:TYR:OH	28:v:104:ARG:NH1	2.54	0.40
24:p:64:LEU:HA	24:p:67:ALA:HB3	2.04	0.40
25:r:231:LEU:HA	25:r:235:LEU:HB2	2.04	0.40
31:r:504:CDL:H762	31:r:504:CDL:H792	1.87	0.40
26:s:129:LEU:O	26:s:133:LEU:HG	2.21	0.40
6:X:75:THR:OG1	6:X:76:LEU:N	2.54	0.40
16:h:17:TRP:CZ3	16:h:18:MET:HB2	2.56	0.40
17:i:311:MET:HE2	17:i:311:MET:HB2	1.90	0.40
30:j:201:PEE:H35	30:j:201:PEE:H30	1.85	0.40
29:w:245:PHE:HD2	29:w:246:LEU:HD22	1.85	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	Q	38/473 (8%)	37 (97%)	1 (3%)	0	100	100
2	S	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
3	U	81/84 (96%)	78 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	V	138/141 (98%)	129 (94%)	8 (6%)	1 (1%)	18	49
5	W	111/144 (77%)	109 (98%)	2 (2%)	0	100	100
6	X	86/156 (55%)	83 (96%)	3 (4%)	0	100	100
7	Y	68/105 (65%)	64 (94%)	4 (6%)	0	100	100
8	Z	82/98 (84%)	79 (96%)	3 (4%)	0	100	100
9	a	138/189 (73%)	134 (97%)	4 (3%)	0	100	100
10	b	99/128 (77%)	97 (98%)	2 (2%)	0	100	100
11	c	154/186 (83%)	142 (92%)	11 (7%)	1 (1%)	21	52
12	d	173/176 (98%)	169 (98%)	4 (2%)	0	100	100
13	e	105/154 (68%)	102 (97%)	3 (3%)	0	100	100
14	f	40/76 (53%)	39 (98%)	1 (2%)	0	100	100
15	g	119/122 (98%)	114 (96%)	5 (4%)	0	100	100
16	h	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
17	i	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
18	j	95/113 (84%)	88 (93%)	7 (7%)	0	100	100
19	k	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
20	l	601/603 (100%)	568 (94%)	33 (6%)	0	100	100
21	m	125/175 (71%)	112 (90%)	13 (10%)	0	100	100
22	n	54/58 (93%)	54 (100%)	0	0	100	100
23	o	126/129 (98%)	122 (97%)	4 (3%)	0	100	100
24	p	176/179 (98%)	167 (95%)	9 (5%)	0	100	100
25	r	457/459 (100%)	443 (97%)	14 (3%)	0	100	100
26	s	299/318 (94%)	288 (96%)	11 (4%)	0	100	100
27	u	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
28	v	122/136 (90%)	118 (97%)	4 (3%)	0	100	100
29	w	318/357 (89%)	302 (95%)	16 (5%)	0	100	100
All	All	4586/5552 (83%)	4384 (96%)	200 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	c	42	PRO
4	V	46	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	34/401 (8%)	34 (100%)	0	100	100
2	S	58/58 (100%)	57 (98%)	1 (2%)	53	71
3	U	69/70 (99%)	69 (100%)	0	100	100
4	V	101/102 (99%)	101 (100%)	0	100	100
5	W	99/124 (80%)	99 (100%)	0	100	100
6	X	78/132 (59%)	77 (99%)	1 (1%)	61	74
7	Y	62/84 (74%)	62 (100%)	0	100	100
8	Z	65/76 (86%)	65 (100%)	0	100	100
9	a	122/158 (77%)	122 (100%)	0	100	100
10	b	97/121 (80%)	96 (99%)	1 (1%)	68	76
11	c	137/160 (86%)	136 (99%)	1 (1%)	76	80
12	d	155/156 (99%)	154 (99%)	1 (1%)	78	81
13	e	99/129 (77%)	99 (100%)	0	100	100
14	f	36/66 (54%)	36 (100%)	0	100	100
15	g	108/109 (99%)	108 (100%)	0	100	100
16	h	93/94 (99%)	93 (100%)	0	100	100
17	i	311/311 (100%)	310 (100%)	1 (0%)	86	86
18	j	88/99 (89%)	88 (100%)	0	100	100
19	k	85/85 (100%)	85 (100%)	0	100	100
20	l	537/537 (100%)	537 (100%)	0	100	100
21	m	99/141 (70%)	99 (100%)	0	100	100
22	n	53/55 (96%)	53 (100%)	0	100	100
23	o	113/114 (99%)	113 (100%)	0	100	100
24	p	159/160 (99%)	159 (100%)	0	100	100
25	r	410/410 (100%)	410 (100%)	0	100	100
26	s	263/275 (96%)	262 (100%)	1 (0%)	84	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	u	153/154 (99%)	153 (100%)	0	100	100
28	v	104/119 (87%)	104 (100%)	0	100	100
29	w	281/307 (92%)	280 (100%)	1 (0%)	84	84
All	All	4069/4807 (85%)	4061 (100%)	8 (0%)	85	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S	38	VAL
6	X	98	LEU
10	b	35	LEU
11	c	181	VAL
12	d	40	LEU
17	i	128	LEU
26	s	98	MET
29	w	285	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
2	S	31	ASN
3	U	71	GLN
6	X	142	GLN
7	Y	54	GLN
7	Y	57	GLN
9	a	50	HIS
10	b	14	GLN
11	c	94	HIS
11	c	100	ASN
12	d	124	ASN
12	d	161	GLN
14	f	73	ASN
15	g	14	GLN
15	g	90	HIS
16	h	7	GLN
17	i	36	ASN
17	i	91	ASN
17	i	120	GLN
17	i	134	GLN
17	i	152	ASN

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Mol	Chain	Res	Type
17	i	310	ASN
18	j	28	ASN
18	j	82	ASN
19	k	50	ASN
19	k	57	ASN
20	l	59	GLN
20	l	135	ASN
20	l	194	ASN
20	l	447	ASN
20	l	524	ASN
21	m	175	ASN
22	n	3	ASN
22	n	6	GLN
23	o	52	ASN
25	r	20	HIS
27	u	30	HIS
28	v	47	ASN
28	v	110	GLN
29	w	257	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 ligands are 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$
30	PEE	U	401	-	50,50,50	1.17	6 (12%)	53,55,55	0.99	2 (3%)
30	PEE	l	703	-	45,45,50	1.24	6 (13%)	48,50,55	0.99	2 (4%)
30	PEE	j	201	-	50,50,50	1.17	6 (12%)	53,55,55	0.97	2 (3%)
33	PLX	r	502	-	51,51,51	1.18	4 (7%)	53,59,59	0.64	1 (1%)
31	CDL	l	702	-	99,99,99	1.11	9 (9%)	105,111,111	0.86	4 (3%)
30	PEE	b	201	-	45,45,50	1.24	6 (13%)	48,50,55	1.00	2 (4%)
30	PEE	i	402	-	46,46,50	1.22	6 (13%)	49,51,55	1.01	2 (4%)
33	PLX	a	202	-	51,51,51	0.61	0	53,59,59	0.68	0
31	CDL	V	201	-	93,93,99	1.14	9 (9%)	99,105,111	0.87	4 (4%)
35	ADP	w	401	-	28,29,29	3.16	9 (32%)	43,45,45	1.90	8 (18%)
33	PLX	j	202	-	51,51,51	1.20	4 (7%)	53,59,59	0.62	1 (1%)
31	CDL	g	202	-	94,94,99	1.13	8 (8%)	100,106,111	0.89	4 (4%)
30	PEE	l	701	-	39,39,50	1.33	6 (15%)	42,44,55	1.12	3 (7%)
33	PLX	g	201	-	51,51,51	1.20	3 (5%)	53,59,59	0.64	1 (1%)
34	UQ	s	401	-	28,28,63	0.53	0	36,37,79	1.11	4 (11%)
30	PEE	W	201	-	40,40,50	1.15	5 (12%)	43,45,55	1.04	2 (4%)
32	8Q1	X	201	-	32,34,34	1.61	6 (18%)	39,43,43	1.62	7 (17%)
33	PLX	r	503	-	51,51,51	1.20	4 (7%)	53,59,59	0.61	1 (1%)
31	CDL	o	201	-	67,67,99	1.27	9 (13%)	73,79,111	1.03	4 (5%)
31	CDL	a	201	-	90,90,99	1.15	8 (8%)	96,102,111	0.95	4 (4%)
31	CDL	r	504	-	98,98,99	1.11	8 (8%)	104,110,111	0.92	4 (3%)
31	CDL	u	201	-	77,77,99	1.22	8 (10%)	83,89,111	0.98	4 (4%)
30	PEE	r	501	-	50,50,50	1.18	6 (12%)	53,55,55	0.99	2 (3%)
31	CDL	i	401	-	65,65,99	1.29	8 (12%)	71,77,111	1.04	4 (5%)

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
30	PEE	U	401	-	-	24/54/54/54	-
30	PEE	l	703	-	-	21/49/49/54	-
30	PEE	j	201	-	-	26/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PLX	r	502	-	-	23/55/55/55	-
31	CDL	l	702	-	-	51/110/110/110	-
30	PEE	b	201	-	-	26/49/49/54	-
30	PEE	i	402	-	-	19/50/50/54	-
33	PLX	a	202	-	-	10/55/55/55	-
31	CDL	V	201	-	-	50/104/104/110	-
35	ADP	w	401	-	-	4/16/32/32	0/3/3/3
33	PLX	j	202	-	-	29/55/55/55	-
31	CDL	g	202	-	-	60/105/105/110	-
30	PEE	l	701	-	-	30/43/43/54	-
33	PLX	g	201	-	-	25/55/55/55	-
34	UQ	s	401	-	-	8/21/45/87	0/1/1/1
30	PEE	W	201	-	-	20/44/44/54	-
32	8Q1	X	201	-	-	17/41/41/41	-
33	PLX	r	503	-	-	34/55/55/55	-
31	CDL	o	201	-	-	42/78/78/110	-
31	CDL	a	201	-	-	47/101/101/110	-
31	CDL	r	504	-	-	53/109/109/110	-
31	CDL	u	201	-	-	37/88/88/110	-
30	PEE	r	501	-	-	29/54/54/54	-
31	CDL	i	401	-	-	41/76/76/110	-

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	w	401	ADP	C3'-C4'	-8.96	1.30	1.53
35	w	401	ADP	O4'-C4'	7.70	1.62	1.45
35	w	401	ADP	PA-O3A	6.40	1.66	1.59
35	w	401	ADP	C6-N6	5.44	1.48	1.34
32	X	201	8Q1	C39-N41	5.08	1.45	1.33
32	X	201	8Q1	C34-N36	5.00	1.45	1.33
35	w	401	ADP	O4'-C1'	-4.57	1.31	1.42
30	l	703	PEE	C18-C19	3.83	1.53	1.31
30	l	701	PEE	C18-C19	3.81	1.53	1.31
30	W	201	PEE	C18-C19	3.80	1.53	1.31
30	b	201	PEE	C18-C19	3.79	1.53	1.31
30	U	401	PEE	C18-C19	3.79	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	r	501	PEE	C18-C19	3.79	1.53	1.31
30	j	201	PEE	C18-C19	3.78	1.53	1.31
30	i	402	PEE	C18-C19	3.76	1.53	1.31
30	r	501	PEE	C39-C38	3.75	1.53	1.31
30	i	402	PEE	C39-C38	3.73	1.52	1.31
30	l	701	PEE	C39-C38	3.73	1.52	1.31
30	b	201	PEE	C39-C38	3.72	1.52	1.31
30	j	201	PEE	C39-C38	3.72	1.52	1.31
30	l	703	PEE	C39-C38	3.70	1.52	1.31
30	U	401	PEE	C39-C38	3.70	1.52	1.31
31	u	201	CDL	OA8-CA7	3.48	1.43	1.33
31	V	201	CDL	OA8-CA7	3.45	1.43	1.33
31	i	401	CDL	OA8-CA7	3.44	1.43	1.33
31	a	201	CDL	OA8-CA7	3.42	1.43	1.33
31	o	201	CDL	OA8-CA7	3.42	1.43	1.33
31	g	202	CDL	OA8-CA7	3.39	1.43	1.33
31	l	702	CDL	OA8-CA7	3.38	1.43	1.33
31	r	504	CDL	OA8-CA7	3.36	1.43	1.33
35	w	401	ADP	C8-N9	-3.35	1.31	1.37
31	V	201	CDL	OA6-CA5	3.12	1.43	1.34
35	w	401	ADP	O2'-C2'	-3.07	1.35	1.43
31	i	401	CDL	OB6-CB5	3.05	1.42	1.34
31	g	202	CDL	OB6-CB5	3.03	1.42	1.34
31	l	702	CDL	OB6-CB5	3.02	1.42	1.34
31	r	504	CDL	OB6-CB5	3.02	1.42	1.34
35	w	401	ADP	O3'-C3'	3.01	1.50	1.43
31	g	202	CDL	OB8-CB7	3.00	1.42	1.33
31	u	201	CDL	OB8-CB7	2.99	1.42	1.33
31	l	702	CDL	OA6-CA5	2.99	1.42	1.34
33	g	201	PLX	O6-C4	-2.97	1.40	1.44
31	o	201	CDL	OB6-CB5	2.97	1.42	1.34
31	r	504	CDL	OB8-CB7	2.96	1.42	1.33
31	a	201	CDL	OB6-CB5	2.95	1.42	1.34
31	o	201	CDL	OA6-CA5	2.95	1.42	1.34
31	a	201	CDL	OA6-CA5	2.95	1.42	1.34
31	i	401	CDL	OB8-CB7	2.95	1.41	1.33
31	l	702	CDL	OB8-CB7	2.95	1.41	1.33
31	V	201	CDL	OB6-CB5	2.94	1.42	1.34
31	a	201	CDL	OB8-CB7	2.94	1.41	1.33
31	V	201	CDL	OB8-CB7	2.94	1.41	1.33
33	r	503	PLX	O6-C4	-2.93	1.40	1.44
31	o	201	CDL	OB8-CB7	2.93	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	g	202	CDL	OA6-CA5	2.91	1.42	1.34
31	i	401	CDL	OA6-CA5	2.91	1.42	1.34
31	u	201	CDL	OB6-CB5	2.90	1.42	1.34
31	r	504	CDL	OA6-CA5	2.90	1.42	1.34
31	u	201	CDL	OA6-CA5	2.89	1.42	1.34
33	j	202	PLX	O6-C4	-2.72	1.41	1.44
30	U	401	PEE	O2-C2	-2.64	1.40	1.46
31	u	201	CDL	OA6-CA4	-2.63	1.40	1.46
30	l	703	PEE	O2-C2	-2.63	1.40	1.46
30	r	501	PEE	O2-C2	-2.63	1.40	1.46
31	o	201	CDL	OA6-CA4	-2.62	1.40	1.46
31	r	504	CDL	OA6-CA4	-2.61	1.40	1.46
31	g	202	CDL	OA6-CA4	-2.61	1.40	1.46
30	j	201	PEE	O2-C2	-2.60	1.40	1.46
30	i	402	PEE	O2-C2	-2.59	1.40	1.46
30	b	201	PEE	O2-C2	-2.59	1.40	1.46
31	a	201	CDL	OA6-CA4	-2.56	1.40	1.46
31	i	401	CDL	OA6-CA4	-2.55	1.40	1.46
30	b	201	PEE	O3-C30	2.51	1.40	1.33
30	W	201	PEE	O2-C2	-2.50	1.40	1.46
31	l	702	CDL	OA6-CA4	-2.50	1.40	1.46
30	j	201	PEE	O3-C30	2.48	1.40	1.33
33	r	502	PLX	C7-C6	2.47	1.55	1.50
30	l	701	PEE	O2-C2	-2.45	1.40	1.46
30	i	402	PEE	O3-C30	2.44	1.40	1.33
30	U	401	PEE	O3-C30	2.42	1.40	1.33
33	j	202	PLX	C7-C6	2.40	1.55	1.50
30	r	501	PEE	O3-C30	2.40	1.40	1.33
30	l	701	PEE	O3-C30	2.40	1.40	1.33
31	V	201	CDL	OB6-CB4	-2.40	1.41	1.46
31	o	201	CDL	OB6-CB4	-2.39	1.41	1.46
35	w	401	ADP	C5-N7	-2.39	1.34	1.39
30	l	701	PEE	O2-C10	2.38	1.41	1.34
32	X	201	8Q1	O35-C34	-2.38	1.18	1.23
31	l	702	CDL	OB6-CB4	-2.38	1.41	1.46
33	g	201	PLX	C7-C6	2.37	1.55	1.50
31	a	201	CDL	OB6-CB4	-2.36	1.41	1.46
31	u	201	CDL	OB6-CB4	-2.36	1.41	1.46
30	l	703	PEE	O3-C30	2.36	1.40	1.33
31	r	504	CDL	OB6-CB4	-2.36	1.41	1.46
33	r	503	PLX	C7-C6	2.35	1.55	1.50
30	W	201	PEE	O3-C30	2.31	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	r	502	PLX	O6-C4	-2.30	1.41	1.44
32	X	201	8Q1	C1-S44	2.30	1.81	1.76
31	i	401	CDL	OB6-CB4	-2.29	1.41	1.46
30	l	703	PEE	O3-C3	-2.29	1.40	1.45
30	U	401	PEE	O2-C10	2.29	1.40	1.34
30	b	201	PEE	O2-C10	2.29	1.40	1.34
31	o	201	CDL	PB2-OB2	2.28	1.68	1.59
32	X	201	8Q1	O40-C39	-2.27	1.18	1.23
32	X	201	8Q1	C6-C1	2.27	1.53	1.50
31	g	202	CDL	OB6-CB4	-2.26	1.41	1.46
31	V	201	CDL	OA6-CA4	-2.26	1.41	1.46
31	g	202	CDL	PB2-OB5	2.26	1.68	1.59
30	W	201	PEE	O2-C10	2.26	1.40	1.34
30	l	703	PEE	O2-C10	2.25	1.40	1.34
30	W	201	PEE	O3-C3	-2.25	1.40	1.45
31	u	201	CDL	PB2-OB2	2.24	1.68	1.59
31	V	201	CDL	PB2-OB2	2.24	1.68	1.59
30	j	201	PEE	O2-C10	2.24	1.40	1.34
30	r	501	PEE	O2-C10	2.24	1.40	1.34
31	i	401	CDL	PB2-OB2	2.24	1.68	1.59
30	i	402	PEE	O2-C10	2.23	1.40	1.34
33	j	202	PLX	P1-O4	2.21	1.68	1.59
31	r	504	CDL	PB2-OB2	2.21	1.68	1.59
31	l	702	CDL	PB2-OB2	2.21	1.68	1.59
31	i	401	CDL	PB2-OB5	2.20	1.68	1.59
31	g	202	CDL	PB2-OB2	2.20	1.68	1.59
31	u	201	CDL	PB2-OB5	2.20	1.68	1.59
31	a	201	CDL	PB2-OB2	2.19	1.68	1.59
30	j	201	PEE	O3-C3	-2.18	1.40	1.45
31	o	201	CDL	PB2-OB5	2.18	1.67	1.59
31	r	504	CDL	PB2-OB5	2.18	1.67	1.59
31	V	201	CDL	PB2-OB5	2.17	1.67	1.59
33	r	502	PLX	P1-O4	2.15	1.67	1.59
30	l	701	PEE	O3-C3	-2.14	1.40	1.45
30	r	501	PEE	O3-C3	-2.14	1.40	1.45
31	l	702	CDL	PB2-OB5	2.14	1.67	1.59
33	r	503	PLX	P1-O4	2.12	1.67	1.59
31	a	201	CDL	PB2-OB5	2.12	1.67	1.59
30	U	401	PEE	O3-C3	-2.10	1.40	1.45
33	g	201	PLX	P1-O4	2.10	1.67	1.59
30	i	402	PEE	O3-C3	-2.09	1.40	1.45
30	b	201	PEE	O3-C3	-2.05	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	r	502	PLX	P1-O1	2.05	1.67	1.59
31	l	702	CDL	C11-CA5	2.04	1.56	1.50
33	r	503	PLX	P1-O1	2.04	1.67	1.59
33	j	202	PLX	P1-O1	2.04	1.67	1.59
31	o	201	CDL	C11-CA5	2.01	1.56	1.50
31	V	201	CDL	C11-CA5	2.01	1.56	1.50

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	201	8Q1	C6-C1-S44	6.15	120.74	113.40
35	w	401	ADP	C5-C4-N3	-5.49	119.16	126.72
35	w	401	ADP	N3-C2-N1	-4.48	121.80	128.58
31	a	201	CDL	OA6-CA5-C11	4.30	120.78	111.48
35	w	401	ADP	N3-C4-N9	4.26	134.41	127.17
31	r	504	CDL	OB6-CB5-C51	4.21	120.59	111.48
31	u	201	CDL	OB6-CB5-C51	4.14	120.43	111.48
30	W	201	PEE	O2-C10-C11	4.14	120.43	111.48
31	i	401	CDL	OA6-CA5-C11	4.11	120.38	111.48
31	a	201	CDL	OB6-CB5-C51	4.10	120.34	111.48
30	l	701	PEE	O2-C10-C11	4.08	120.30	111.48
31	g	202	CDL	OB6-CB5-C51	4.06	120.27	111.48
31	r	504	CDL	OA6-CA5-C11	4.03	120.19	111.48
30	U	401	PEE	O2-C10-C11	4.01	120.16	111.48
31	l	702	CDL	OA6-CA5-C11	3.99	120.11	111.48
30	j	201	PEE	O2-C10-C11	3.95	120.03	111.48
31	i	401	CDL	OB6-CB5-C51	3.93	119.98	111.48
30	b	201	PEE	O2-C10-C11	3.93	119.97	111.48
31	u	201	CDL	OA6-CA5-C11	3.91	119.94	111.48
31	o	201	CDL	OB6-CB5-C51	3.90	119.93	111.48
30	r	501	PEE	O2-C10-C11	3.90	119.91	111.48
30	i	402	PEE	O2-C10-C11	3.87	119.84	111.48
31	o	201	CDL	OA6-CA5-C11	3.82	119.75	111.48
31	g	202	CDL	OA6-CA5-C11	3.82	119.75	111.48
31	V	201	CDL	OB6-CB5-C51	3.79	119.67	111.48
30	l	703	PEE	O2-C10-C11	3.78	119.66	111.48
31	l	702	CDL	OB6-CB5-C51	3.78	119.65	111.48
31	V	201	CDL	OA6-CA5-C11	3.76	119.61	111.48
32	X	201	8Q1	O4-C1-C6	-3.58	119.84	123.98
35	w	401	ADP	C2-N3-C4	3.54	120.49	111.83
34	s	401	UQ	C7-C6-C5	-3.51	118.88	124.89
35	w	401	ADP	N9-C8-N7	-3.48	109.00	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	w	401	ADP	C5-N7-C8	3.19	108.46	103.45
35	w	401	ADP	C4-N9-C8	3.09	108.99	105.74
35	w	401	ADP	C4-C5-N7	-3.02	107.12	110.58
30	r	501	PEE	O3-C30-C31	2.97	120.90	111.83
31	V	201	CDL	OB8-CB7-C71	2.91	120.71	111.83
30	U	401	PEE	O3-C30-C31	2.86	120.56	111.83
31	a	201	CDL	OB8-CB7-C71	2.83	120.47	111.83
31	u	201	CDL	OB8-CB7-C71	2.83	120.46	111.83
30	i	402	PEE	O3-C30-C31	2.83	120.46	111.83
31	o	201	CDL	OB8-CB7-C71	2.80	120.36	111.83
31	i	401	CDL	OB8-CB7-C71	2.78	120.32	111.83
30	b	201	PEE	O3-C30-C31	2.75	120.22	111.83
31	r	504	CDL	OB8-CB7-C71	2.74	120.20	111.83
31	r	504	CDL	OA8-CA7-C31	2.72	120.13	111.83
31	i	401	CDL	OA8-CA7-C31	2.70	120.08	111.83
30	j	201	PEE	O3-C30-C31	2.69	120.03	111.83
30	l	703	PEE	O3-C30-C31	2.68	120.00	111.83
31	l	702	CDL	OA8-CA7-C31	2.68	119.99	111.83
31	g	202	CDL	OB8-CB7-C71	2.66	119.94	111.83
30	l	701	PEE	O3-C30-C31	2.66	119.93	111.83
31	l	702	CDL	OB8-CB7-C71	2.64	119.88	111.83
31	g	202	CDL	OA8-CA7-C31	2.64	119.87	111.83
31	u	201	CDL	OA8-CA7-C31	2.63	119.87	111.83
31	o	201	CDL	OA8-CA7-C31	2.61	119.80	111.83
32	X	201	8Q1	O4-C1-S44	-2.57	119.42	122.68
31	V	201	CDL	OA8-CA7-C31	2.56	119.64	111.83
30	W	201	PEE	O3-C30-C31	2.54	119.57	111.83
33	r	502	PLX	C1A-N1-C1	2.53	119.98	109.91
31	a	201	CDL	OA8-CA7-C31	2.53	119.54	111.83
33	r	503	PLX	C1A-N1-C1	2.52	119.93	109.91
33	j	202	PLX	C1A-N1-C1	2.49	119.80	109.91
33	g	201	PLX	C1A-N1-C1	2.48	119.77	109.91
32	X	201	8Q1	C37-C38-C39	2.34	116.29	112.39
30	l	701	PEE	C20-C19-C18	-2.33	112.41	126.42
34	s	401	UQ	C7-C6-C1	2.30	121.19	118.52
32	X	201	8Q1	C38-C39-N41	2.28	120.50	116.34
32	X	201	8Q1	C43-S44-C1	2.25	108.48	101.84
34	s	401	UQ	C6-C5-C4	2.10	120.83	119.17
32	X	201	8Q1	C32-C34-N36	2.10	120.46	116.48
34	s	401	UQ	C8-C7-C6	2.08	117.21	112.08

There are no chirality outliers.

All (726) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	W	201	PEE	C4-O4P-P-O1P
30	b	201	PEE	C1-O3P-P-O1P
30	i	402	PEE	C11-C10-O2-C2
30	j	201	PEE	C1-O3P-P-O2P
30	j	201	PEE	C1-O3P-P-O1P
30	j	201	PEE	C1-O3P-P-O4P
30	j	201	PEE	C4-O4P-P-O3P
30	j	201	PEE	C4-O4P-P-O2P
30	l	701	PEE	O3P-C1-C2-O2
30	l	701	PEE	C4-O4P-P-O3P
30	l	701	PEE	C4-O4P-P-O1P
30	r	501	PEE	C1-O3P-P-O1P
30	r	501	PEE	C4-O4P-P-O3P
30	r	501	PEE	C4-O4P-P-O2P
30	r	501	PEE	C4-O4P-P-O1P
31	V	201	CDL	CA2-C1-CB2-OB2
31	V	201	CDL	CA2-OA2-PA1-OA4
31	V	201	CDL	CA2-OA2-PA1-OA5
31	V	201	CDL	CA3-OA5-PA1-OA2
31	V	201	CDL	CA3-OA5-PA1-OA4
31	V	201	CDL	CB2-OB2-PB2-OB4
31	V	201	CDL	CB2-OB2-PB2-OB5
31	V	201	CDL	CB3-OB5-PB2-OB2
31	V	201	CDL	CB3-OB5-PB2-OB3
31	V	201	CDL	CB3-OB5-PB2-OB4
31	a	201	CDL	CA2-OA2-PA1-OA3
31	a	201	CDL	CA2-OA2-PA1-OA4
31	a	201	CDL	CA2-OA2-PA1-OA5
31	a	201	CDL	CA3-OA5-PA1-OA2
31	a	201	CDL	CB2-OB2-PB2-OB3
31	a	201	CDL	CB2-OB2-PB2-OB5
31	a	201	CDL	CB3-OB5-PB2-OB2
31	a	201	CDL	CB3-OB5-PB2-OB3
31	g	202	CDL	CA2-OA2-PA1-OA3
31	g	202	CDL	CA2-OA2-PA1-OA4
31	g	202	CDL	CA2-OA2-PA1-OA5
31	g	202	CDL	CA3-OA5-PA1-OA2
31	g	202	CDL	CA3-OA5-PA1-OA4
31	g	202	CDL	CB2-OB2-PB2-OB3
31	g	202	CDL	CB3-OB5-PB2-OB2
31	g	202	CDL	CB3-OB5-PB2-OB3
31	g	202	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
31	i	401	CDL	CA2-OA2-PA1-OA4
31	i	401	CDL	CA2-OA2-PA1-OA5
31	i	401	CDL	CA3-OA5-PA1-OA3
31	i	401	CDL	CB2-OB2-PB2-OB4
31	i	401	CDL	CB2-OB2-PB2-OB5
31	l	702	CDL	O1-C1-CA2-OA2
31	l	702	CDL	CA2-C1-CB2-OB2
31	l	702	CDL	OA6-CA4-CA6-OA8
31	l	702	CDL	CB2-OB2-PB2-OB3
31	l	702	CDL	CB2-OB2-PB2-OB4
31	l	702	CDL	CB2-OB2-PB2-OB5
31	l	702	CDL	OB6-CB4-CB6-OB8
31	o	201	CDL	O1-C1-CA2-OA2
31	o	201	CDL	CA2-OA2-PA1-OA4
31	o	201	CDL	CA2-OA2-PA1-OA5
31	o	201	CDL	CB3-OB5-PB2-OB2
31	o	201	CDL	CB3-OB5-PB2-OB3
31	o	201	CDL	CB3-OB5-PB2-OB4
31	o	201	CDL	OB6-CB4-CB6-OB8
31	r	504	CDL	O1-C1-CA2-OA2
31	r	504	CDL	CA2-C1-CB2-OB2
31	r	504	CDL	CA2-OA2-PA1-OA5
31	r	504	CDL	CB2-OB2-PB2-OB3
31	r	504	CDL	CB2-OB2-PB2-OB4
31	r	504	CDL	CB2-OB2-PB2-OB5
31	r	504	CDL	CB3-OB5-PB2-OB2
31	r	504	CDL	CB3-OB5-PB2-OB3
31	u	201	CDL	O1-C1-CA2-OA2
31	u	201	CDL	CA2-OA2-PA1-OA3
31	u	201	CDL	CA2-OA2-PA1-OA4
31	u	201	CDL	CA2-OA2-PA1-OA5
31	u	201	CDL	CB2-OB2-PB2-OB3
31	u	201	CDL	CB2-OB2-PB2-OB5
31	u	201	CDL	CB3-OB5-PB2-OB2
31	u	201	CDL	CB3-OB5-PB2-OB3
32	X	201	8Q1	C1-C6-C7-C8
32	X	201	8Q1	C28-C29-C32-C34
32	X	201	8Q1	C28-C29-C32-O33
32	X	201	8Q1	C30-C29-C32-C34
32	X	201	8Q1	C30-C29-C32-O33
32	X	201	8Q1	C31-C29-C32-C34
32	X	201	8Q1	C31-C29-C32-O33

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Mol	Chain	Res	Type	Atoms
32	X	201	8Q1	C29-C32-C34-O35
32	X	201	8Q1	N36-C37-C38-C39
32	X	201	8Q1	C42-C43-S44-C1
32	X	201	8Q1	C28-O27-P24-O3
32	X	201	8Q1	C28-O27-P24-O2
32	X	201	8Q1	C28-O27-P24-O1
33	a	202	PLX	O9-C24-O8-C5
33	g	201	PLX	C3-O4-P1-O1
33	g	201	PLX	C3-O4-P1-O3
33	g	201	PLX	C25-C24-O8-C5
33	j	202	PLX	O7-C6-C7-C8
33	j	202	PLX	C3-O4-P1-O1
33	j	202	PLX	O9-C24-C25-C26
33	r	502	PLX	O7-C6-O6-C4
33	r	502	PLX	C5-C4-O6-C6
33	r	502	PLX	O9-C24-O8-C5
33	r	502	PLX	O9-C24-C25-C26
33	r	503	PLX	O7-C6-O6-C4
33	r	503	PLX	C3-O4-P1-O1
33	r	503	PLX	C3-O4-P1-O2
33	r	503	PLX	C3-O4-P1-O3
33	r	503	PLX	C2-O1-P1-O4
33	r	503	PLX	C2-O1-P1-O2
33	r	503	PLX	C2-O1-P1-O3
33	r	503	PLX	C25-C24-O8-C5
33	r	503	PLX	O9-C24-C25-C26
34	s	401	UQ	C1-C6-C7-C8
34	s	401	UQ	C5-C6-C7-C8
34	s	401	UQ	C9-C11-C12-C13
35	w	401	ADP	C5'-O5'-PA-O1A
35	w	401	ADP	C5'-O5'-PA-O2A
35	w	401	ADP	C5'-O5'-PA-O3A
31	i	401	CDL	OA9-CA7-OA8-CA6
31	r	504	CDL	OA9-CA7-OA8-CA6
30	i	402	PEE	O4-C10-O2-C2
30	l	703	PEE	O4-C10-O2-C2
31	g	202	CDL	C71-CB7-OB8-CB6
31	i	401	CDL	C31-CA7-OA8-CA6
31	r	504	CDL	C31-CA7-OA8-CA6
30	l	703	PEE	C11-C10-O2-C2
30	U	401	PEE	C37-C38-C39-C40
30	b	201	PEE	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
30	j	201	PEE	C17-C18-C19-C20
30	l	701	PEE	C17-C18-C19-C20
30	l	703	PEE	O5-C30-O3-C3
31	V	201	CDL	O1-C1-CA2-OA2
31	a	201	CDL	O1-C1-CB2-OB2
31	l	702	CDL	O1-C1-CB2-OB2
31	r	504	CDL	O1-C1-CB2-OB2
30	b	201	PEE	C31-C30-O3-C3
31	l	702	CDL	C71-CB7-OB8-CB6
30	b	201	PEE	O5-C30-O3-C3
31	g	202	CDL	OB9-CB7-OB8-CB6
30	U	401	PEE	C11-C10-O2-C2
31	V	201	CDL	C11-CA5-OA6-CA4
30	l	703	PEE	C31-C30-O3-C3
31	l	702	CDL	OB9-CB7-OB8-CB6
30	U	401	PEE	O4-C10-O2-C2
31	l	702	CDL	C75-C76-C77-C78
30	l	701	PEE	C31-C30-O3-C3
31	u	201	CDL	C71-C72-C73-C74
31	l	702	CDL	C59-C60-C61-C62
33	r	502	PLX	C9-C10-C11-C12
31	a	201	CDL	CA2-C1-CB2-OB2
31	g	202	CDL	CB2-C1-CA2-OA2
31	i	401	CDL	CB2-C1-CA2-OA2
31	l	702	CDL	CB2-C1-CA2-OA2
31	o	201	CDL	CB2-C1-CA2-OA2
31	o	201	CDL	CA2-C1-CB2-OB2
31	u	201	CDL	CB2-C1-CA2-OA2
31	u	201	CDL	CA2-C1-CB2-OB2
30	W	201	PEE	C31-C30-O3-C3
30	j	201	PEE	C31-C30-O3-C3
31	V	201	CDL	C11-C12-C13-C14
31	u	201	CDL	C52-C53-C54-C55
31	V	201	CDL	C59-C60-C61-C62
33	g	201	PLX	C10-C11-C12-C13
33	j	202	PLX	C28-C29-C30-C31
33	r	503	PLX	C12-C13-C14-C15
31	o	201	CDL	C72-C73-C74-C75
31	u	201	CDL	C75-C76-C77-C78
31	l	702	CDL	C35-C36-C37-C38
31	l	702	CDL	C11-C12-C13-C14
31	a	201	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
31	i	401	CDL	O1-C1-CA2-OA2
31	u	201	CDL	O1-C1-CB2-OB2
33	r	502	PLX	C30-C31-C32-C33
31	V	201	CDL	OA7-CA5-OA6-CA4
30	l	703	PEE	O3P-C1-C2-O2
30	j	201	PEE	C11-C10-O2-C2
31	V	201	CDL	C32-C33-C34-C35
31	V	201	CDL	C62-C63-C64-C65
31	r	504	CDL	CB7-C71-C72-C73
30	j	201	PEE	C19-C20-C21-C22
31	r	504	CDL	C55-C56-C57-C58
30	i	402	PEE	C30-C31-C32-C33
30	l	703	PEE	C30-C31-C32-C33
31	a	201	CDL	CA5-C11-C12-C13
31	i	401	CDL	CB7-C71-C72-C73
31	o	201	CDL	CB7-C71-C72-C73
30	j	201	PEE	O5-C30-O3-C3
30	r	501	PEE	C11-C10-O2-C2
31	g	202	CDL	C76-C77-C78-C79
30	l	701	PEE	C11-C12-C13-C14
33	j	202	PLX	C15-C16-C17-C18
31	V	201	CDL	O1-C1-CB2-OB2
31	g	202	CDL	O1-C1-CA2-OA2
31	o	201	CDL	O1-C1-CB2-OB2
31	g	202	CDL	C74-C75-C76-C77
30	l	701	PEE	O5-C30-O3-C3
33	r	502	PLX	C11-C12-C13-C14
31	V	201	CDL	CB7-C71-C72-C73
31	a	201	CDL	C71-CB7-OB8-CB6
31	o	201	CDL	C31-CA7-OA8-CA6
31	r	504	CDL	C71-CB7-OB8-CB6
33	g	201	PLX	C12-C13-C14-C15
30	W	201	PEE	O5-C30-O3-C3
31	g	202	CDL	CA7-C31-C32-C33
31	i	401	CDL	C14-C15-C16-C17
31	r	504	CDL	C58-C59-C60-C61
31	g	202	CDL	CA5-C11-C12-C13
30	j	201	PEE	O4-C10-O2-C2
30	r	501	PEE	O4-C10-O2-C2
31	V	201	CDL	CB2-C1-CA2-OA2
31	a	201	CDL	CB2-C1-CA2-OA2
31	r	504	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
30	l	703	PEE	C33-C34-C35-C36
31	g	202	CDL	CB5-C51-C52-C53
30	j	201	PEE	C32-C33-C34-C35
31	i	401	CDL	CA7-C31-C32-C33
31	u	201	CDL	CB7-C71-C72-C73
34	s	401	UQ	C12-C11-C9-C10
33	g	201	PLX	O8-C24-C25-C26
30	b	201	PEE	C11-C10-O2-C2
31	g	202	CDL	C51-CB5-OB6-CB4
30	b	201	PEE	O4-C10-O2-C2
30	j	201	PEE	C34-C35-C36-C37
31	o	201	CDL	C71-CB7-OB8-CB6
31	l	702	CDL	C39-C40-C41-C42
31	u	201	CDL	C17-C18-C19-C20
31	a	201	CDL	CA7-C31-C32-C33
31	a	201	CDL	C31-C32-C33-C34
31	g	202	CDL	OB7-CB5-OB6-CB4
30	l	701	PEE	C11-C10-O2-C2
31	V	201	CDL	C51-CB5-OB6-CB4
33	g	201	PLX	C31-C32-C33-C34
31	r	504	CDL	OB9-CB7-OB8-CB6
31	l	702	CDL	C37-C38-C39-C40
33	r	502	PLX	C27-C28-C29-C30
33	r	503	PLX	C25-C26-C27-C28
30	b	201	PEE	C31-C32-C33-C34
30	l	703	PEE	C34-C35-C36-C37
31	g	202	CDL	C35-C36-C37-C38
31	g	202	CDL	C59-C60-C61-C62
31	g	202	CDL	C78-C79-C80-C81
31	r	504	CDL	C52-C53-C54-C55
31	r	504	CDL	C74-C75-C76-C77
31	a	201	CDL	OB9-CB7-OB8-CB6
33	a	202	PLX	O9-C24-C25-C26
33	g	201	PLX	O9-C24-C25-C26
30	U	401	PEE	C33-C34-C35-C36
30	r	501	PEE	C13-C14-C15-C16
31	a	201	CDL	C73-C74-C75-C76
31	a	201	CDL	C75-C76-C77-C78
31	g	202	CDL	C12-C13-C14-C15
31	g	202	CDL	C56-C57-C58-C59
33	r	502	PLX	C7-C8-C9-C10
33	r	503	PLX	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	i	401	CDL	C52-C53-C54-C55
31	l	702	CDL	CB7-C71-C72-C73
31	r	504	CDL	C59-C60-C61-C62
31	o	201	CDL	C51-CB5-OB6-CB4
31	V	201	CDL	C74-C75-C76-C77
31	a	201	CDL	C21-C22-C23-C24
30	j	201	PEE	C30-C31-C32-C33
31	l	702	CDL	CB5-C51-C52-C53
31	u	201	CDL	CB5-C51-C52-C53
30	b	201	PEE	C32-C33-C34-C35
30	i	402	PEE	C11-C12-C13-C14
31	V	201	CDL	C52-C53-C54-C55
31	g	202	CDL	C32-C33-C34-C35
31	u	201	CDL	C53-C54-C55-C56
33	r	502	PLX	C15-C16-C17-C18
33	r	503	PLX	C13-C14-C15-C16
31	o	201	CDL	OA9-CA7-OA8-CA6
31	V	201	CDL	C40-C41-C42-C43
30	W	201	PEE	C13-C14-C15-C16
31	g	202	CDL	C71-C72-C73-C74
30	l	701	PEE	O4-C10-O2-C2
31	V	201	CDL	OB7-CB5-OB6-CB4
30	j	201	PEE	C41-C42-C43-C44
31	a	201	CDL	C37-C38-C39-C40
31	i	401	CDL	C11-C12-C13-C14
31	r	504	CDL	C73-C74-C75-C76
30	r	501	PEE	C10-C11-C12-C13
30	W	201	PEE	C33-C34-C35-C36
30	l	703	PEE	C23-C24-C25-C26
31	r	504	CDL	C35-C36-C37-C38
31	r	504	CDL	C56-C57-C58-C59
31	r	504	CDL	C75-C76-C77-C78
31	u	201	CDL	C13-C14-C15-C16
31	u	201	CDL	C55-C56-C57-C58
33	g	201	PLX	C11-C10-C9-C8
33	g	201	PLX	C27-C28-C29-C30
33	r	502	PLX	C13-C14-C15-C16
30	U	401	PEE	C20-C21-C22-C23
33	g	201	PLX	C25-C26-C27-C28
31	o	201	CDL	OB9-CB7-OB8-CB6
31	u	201	CDL	C11-C12-C13-C14
31	u	201	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
30	b	201	PEE	C13-C14-C15-C16
31	g	202	CDL	C73-C74-C75-C76
31	o	201	CDL	C83-C84-C85-C86
31	o	201	CDL	OB7-CB5-OB6-CB4
31	l	702	CDL	C55-C56-C57-C58
31	l	702	CDL	C73-C74-C75-C76
34	s	401	UQ	C12-C11-C9-C8
30	b	201	PEE	C34-C35-C36-C37
31	g	202	CDL	C43-C44-C45-C46
33	j	202	PLX	C10-C11-C12-C13
33	r	502	PLX	C12-C13-C14-C15
33	r	502	PLX	C31-C32-C33-C34
31	V	201	CDL	C31-CA7-OA8-CA6
31	o	201	CDL	C75-C76-C77-C78
31	r	504	CDL	C61-C62-C63-C64
31	r	504	CDL	C82-C83-C84-C85
33	g	201	PLX	C9-C10-C11-C12
33	j	202	PLX	C12-C13-C14-C15
33	r	503	PLX	C14-C15-C16-C17
31	g	202	CDL	C17-C18-C19-C20
31	o	201	CDL	C71-C72-C73-C74
30	b	201	PEE	C22-C23-C24-C25
31	g	202	CDL	C72-C73-C74-C75
33	j	202	PLX	C7-C8-C9-C10
33	r	503	PLX	C27-C28-C29-C30
30	W	201	PEE	C23-C24-C25-C26
30	i	402	PEE	C21-C22-C23-C24
31	o	201	CDL	C73-C74-C75-C76
31	u	201	CDL	C59-C60-C61-C62
33	j	202	PLX	C25-C26-C27-C28
33	j	202	PLX	C27-C28-C29-C30
33	r	502	PLX	C14-C15-C16-C17
31	V	201	CDL	C71-CB7-OB8-CB6
31	g	202	CDL	CB7-C71-C72-C73
30	U	401	PEE	C22-C23-C24-C25
31	l	702	CDL	C58-C59-C60-C61
30	U	401	PEE	C39-C40-C41-C42
30	i	402	PEE	C19-C20-C21-C22
30	i	402	PEE	C35-C36-C37-C38
31	r	504	CDL	C20-C21-C22-C23
30	U	401	PEE	C23-C24-C25-C26
31	l	702	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
30	l	703	PEE	C37-C38-C39-C40
33	r	503	PLX	C26-C27-C28-C29
33	r	503	PLX	C2-C1-N1-C1C
33	r	503	PLX	C2-C1-N1-C1A
31	r	504	CDL	C11-C12-C13-C14
33	j	202	PLX	C14-C15-C16-C17
31	g	202	CDL	C57-C58-C59-C60
31	o	201	CDL	CA7-C31-C32-C33
31	l	702	CDL	C71-C72-C73-C74
31	g	202	CDL	C41-C42-C43-C44
30	l	703	PEE	C11-C12-C13-C14
31	i	401	CDL	C37-C38-C39-C40
31	l	702	CDL	C72-C73-C74-C75
30	U	401	PEE	C35-C36-C37-C38
31	g	202	CDL	OB6-CB4-CB6-OB8
31	i	401	CDL	OB6-CB4-CB6-OB8
31	l	702	CDL	C56-C57-C58-C59
30	b	201	PEE	C33-C34-C35-C36
31	o	201	CDL	C55-C56-C57-C58
31	r	504	CDL	C32-C33-C34-C35
31	u	201	CDL	C14-C15-C16-C17
31	l	702	CDL	C60-C61-C62-C63
33	g	201	PLX	C28-C29-C30-C31
30	j	201	PEE	C36-C37-C38-C39
30	r	501	PEE	C36-C37-C38-C39
33	a	202	PLX	C25-C26-C27-C28
31	g	202	CDL	CB4-CB3-OB5-PB2
30	b	201	PEE	C23-C24-C25-C26
31	a	201	CDL	C71-C72-C73-C74
31	i	401	CDL	C33-C34-C35-C36
30	l	701	PEE	C32-C33-C34-C35
31	g	202	CDL	C75-C76-C77-C78
30	W	201	PEE	C22-C23-C24-C25
30	l	703	PEE	C31-C32-C33-C34
31	V	201	CDL	OA9-CA7-OA8-CA6
31	V	201	CDL	C31-C32-C33-C34
30	b	201	PEE	C10-C11-C12-C13
30	r	501	PEE	C40-C41-C42-C43
31	r	504	CDL	C14-C15-C16-C17
33	r	503	PLX	C31-C32-C33-C34
30	U	401	PEE	C15-C16-C17-C18
30	l	701	PEE	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
30	l	703	PEE	O3P-C1-C2-C3
31	i	401	CDL	OB5-CB3-CB4-CB6
33	j	202	PLX	O4-C3-C4-C5
31	u	201	CDL	OA7-CA5-OA6-CA4
31	V	201	CDL	C33-C34-C35-C36
31	V	201	CDL	OB9-CB7-OB8-CB6
30	j	201	PEE	C22-C23-C24-C25
31	i	401	CDL	C32-C33-C34-C35
31	r	504	CDL	C42-C43-C44-C45
30	r	501	PEE	C12-C13-C14-C15
31	o	201	CDL	C82-C83-C84-C85
33	j	202	PLX	C26-C27-C28-C29
30	W	201	PEE	C12-C13-C14-C15
30	U	401	PEE	C31-C30-O3-C3
30	U	401	PEE	C17-C18-C19-C20
30	l	701	PEE	C30-C31-C32-C33
30	W	201	PEE	C1-C2-C3-O3
30	l	701	PEE	C1-C2-C3-O3
31	g	202	CDL	CB3-CB4-CB6-OB8
31	l	702	CDL	CA3-CA4-CA6-OA8
31	l	702	CDL	CB3-CB4-CB6-OB8
31	o	201	CDL	CB3-CB4-CB6-OB8
31	u	201	CDL	CA3-CA4-CA6-OA8
30	r	501	PEE	C21-C22-C23-C24
33	r	503	PLX	C29-C30-C31-C32
30	l	701	PEE	C35-C36-C37-C38
30	r	501	PEE	C39-C40-C41-C42
31	o	201	CDL	C54-C55-C56-C57
31	o	201	CDL	C84-C85-C86-C87
33	r	503	PLX	C28-C29-C30-C31
30	U	401	PEE	C21-C22-C23-C24
33	r	503	PLX	C2-C1-N1-C1B
31	g	202	CDL	C14-C15-C16-C17
31	r	504	CDL	C23-C24-C25-C26
31	a	201	CDL	C76-C77-C78-C79
31	g	202	CDL	C37-C38-C39-C40
33	g	201	PLX	C13-C14-C15-C16
33	r	503	PLX	C16-C17-C18-C19
30	l	703	PEE	C32-C33-C34-C35
33	r	502	PLX	C33-C34-C35-C36
31	a	201	CDL	C43-C44-C45-C46
33	r	502	PLX	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
30	j	201	PEE	C31-C32-C33-C34
31	l	702	CDL	C14-C15-C16-C17
31	V	201	CDL	C35-C36-C37-C38
31	r	504	CDL	C76-C77-C78-C79
31	o	201	CDL	C74-C75-C76-C77
33	a	202	PLX	C7-C8-C9-C10
33	g	201	PLX	C33-C34-C35-C36
30	r	501	PEE	O3P-C1-C2-O2
31	a	201	CDL	OA5-CA3-CA4-OA6
31	g	202	CDL	C60-C61-C62-C63
31	i	401	CDL	C71-CB7-OB8-CB6
30	W	201	PEE	C11-C10-O2-C2
33	r	503	PLX	C15-C16-C17-C18
31	V	201	CDL	C37-C38-C39-C40
31	l	702	CDL	C41-C42-C43-C44
31	a	201	CDL	C52-C53-C54-C55
31	r	504	CDL	C36-C37-C38-C39
30	l	701	PEE	O2-C2-C3-O3
31	o	201	CDL	OA6-CA4-CA6-OA8
31	l	702	CDL	C64-C65-C66-C67
30	r	501	PEE	C41-C42-C43-C44
33	g	201	PLX	C11-C12-C13-C14
33	j	202	PLX	C9-C10-C11-C12
30	U	401	PEE	O5-C30-O3-C3
31	V	201	CDL	C54-C55-C56-C57
31	i	401	CDL	C34-C35-C36-C37
31	l	702	CDL	C52-C53-C54-C55
31	V	201	CDL	C14-C15-C16-C17
30	r	501	PEE	C17-C18-C19-C20
33	a	202	PLX	C11-C12-C13-C14
31	l	702	CDL	C54-C55-C56-C57
31	r	504	CDL	C71-C72-C73-C74
31	V	201	CDL	C58-C59-C60-C61
31	a	201	CDL	C55-C56-C57-C58
31	i	401	CDL	C73-C74-C75-C76
30	i	402	PEE	O3P-C1-C2-C3
31	a	201	CDL	OA5-CA3-CA4-CA6
31	a	201	CDL	OB5-CB3-CB4-CB6
31	o	201	CDL	OB5-CB3-CB4-CB6
31	a	201	CDL	C14-C15-C16-C17
31	o	201	CDL	C52-C53-C54-C55
30	r	501	PEE	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	r	504	CDL	C62-C63-C64-C65
32	X	201	8Q1	C29-C32-C34-N36
30	i	402	PEE	C18-C19-C20-C21
33	r	503	PLX	C30-C31-C32-C33
33	j	202	PLX	C13-C14-C15-C16
33	r	503	PLX	C7-C8-C9-C10
30	b	201	PEE	C1-C2-C3-O3
30	i	402	PEE	C1-C2-C3-O3
31	i	401	CDL	CB3-CB4-CB6-OB8
32	X	201	8Q1	O33-C32-C34-N36
33	r	502	PLX	C3-C4-C5-O8
33	r	503	PLX	C3-C4-C5-O8
31	g	202	CDL	C20-C21-C22-C23
33	j	202	PLX	C33-C34-C35-C36
33	j	202	PLX	C34-C35-C36-C37
31	g	202	CDL	C13-C14-C15-C16
31	i	401	CDL	OB9-CB7-OB8-CB6
31	V	201	CDL	OB5-CB3-CB4-OB6
31	o	201	CDL	OB5-CB3-CB4-OB6
33	g	201	PLX	O4-C3-C4-O6
33	j	202	PLX	O4-C3-C4-O6
30	W	201	PEE	O3-C30-C31-C32
32	X	201	8Q1	O4-C1-S44-C43
31	g	202	CDL	C33-C34-C35-C36
31	u	201	CDL	C54-C55-C56-C57
33	r	503	PLX	C33-C34-C35-C36
31	g	202	CDL	OA6-CA4-CA6-OA8
33	j	202	PLX	O6-C4-C5-O8
33	r	503	PLX	O6-C4-C5-O8
31	r	504	CDL	C39-C40-C41-C42
33	r	503	PLX	O8-C24-C25-C26
30	l	701	PEE	C10-C11-C12-C13
31	a	201	CDL	CB5-C51-C52-C53
31	a	201	CDL	C60-C61-C62-C63
31	l	702	CDL	C40-C41-C42-C43
31	l	702	CDL	C43-C44-C45-C46
30	r	501	PEE	C38-C39-C40-C41
32	X	201	8Q1	C6-C1-S44-C43
33	g	201	PLX	C14-C15-C16-C17
33	r	502	PLX	C28-C29-C30-C31
31	V	201	CDL	OB5-CB3-CB4-CB6
31	i	401	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
30	l	701	PEE	C33-C34-C35-C36
31	g	202	CDL	C52-C53-C54-C55
30	W	201	PEE	O4-C10-O2-C2
31	g	202	CDL	C42-C43-C44-C45
31	o	201	CDL	C32-C31-CA7-OA8
31	V	201	CDL	CA6-CA4-OA6-CA5
30	W	201	PEE	C32-C33-C34-C35
31	r	504	CDL	C60-C61-C62-C63
30	i	402	PEE	O3P-C1-C2-O2
31	a	201	CDL	OB5-CB3-CB4-OB6
31	i	401	CDL	OA5-CA3-CA4-OA6
30	r	501	PEE	C1-C2-C3-O3
31	i	401	CDL	CA3-CA4-CA6-OA8
33	j	202	PLX	C3-C4-C5-O8
30	r	501	PEE	O2-C2-C3-O3
31	i	401	CDL	OA6-CA4-CA6-OA8
31	u	201	CDL	OA6-CA4-CA6-OA8
33	r	502	PLX	O6-C4-C5-O8
33	r	503	PLX	C9-C10-C11-C12
30	b	201	PEE	C11-C12-C13-C14
30	b	201	PEE	C14-C15-C16-C17
31	l	702	CDL	CA7-C31-C32-C33
31	l	702	CDL	C12-C13-C14-C15
31	g	202	CDL	C55-C56-C57-C58
33	j	202	PLX	C25-C24-O8-C5
30	l	701	PEE	C13-C14-C15-C16
31	a	201	CDL	C17-C18-C19-C20
30	b	201	PEE	O3P-C1-C2-C3
30	r	501	PEE	O3P-C1-C2-C3
31	l	702	CDL	OA5-CA3-CA4-CA6
33	g	201	PLX	O4-C3-C4-C5
31	i	401	CDL	C35-C36-C37-C38
31	V	201	CDL	C34-C35-C36-C37
31	a	201	CDL	C36-C37-C38-C39
31	g	202	CDL	C54-C55-C56-C57
33	j	202	PLX	C31-C32-C33-C34
33	r	503	PLX	C18-C19-C20-C21
31	a	201	CDL	C54-C55-C56-C57
33	r	503	PLX	C11-C12-C13-C14
30	b	201	PEE	C16-C17-C18-C19
30	b	201	PEE	C38-C39-C40-C41
31	i	401	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
33	j	202	PLX	O6-C6-C7-C8
30	b	201	PEE	O3P-C1-C2-O2
31	i	401	CDL	OB5-CB3-CB4-OB6
31	l	702	CDL	OA5-CA3-CA4-OA6
30	r	501	PEE	C14-C15-C16-C17
31	i	401	CDL	C74-C75-C76-C77
33	g	201	PLX	C16-C17-C18-C19
30	W	201	PEE	O2-C2-C3-O3
30	b	201	PEE	O2-C2-C3-O3
30	i	402	PEE	O2-C2-C3-O3
31	g	202	CDL	C64-C65-C66-C67
31	a	201	CDL	C19-C20-C21-C22
31	g	202	CDL	CA3-CA4-CA6-OA8
31	o	201	CDL	CA3-CA4-CA6-OA8
30	i	402	PEE	C24-C25-C26-C27
30	W	201	PEE	C18-C19-C20-C21
30	l	701	PEE	C38-C39-C40-C41
30	l	703	PEE	C14-C15-C16-C17
31	V	201	CDL	C71-C72-C73-C74
30	j	201	PEE	C4-O4P-P-O1P
30	l	701	PEE	C1-O3P-P-O2P
30	l	701	PEE	C1-O3P-P-O1P
30	l	701	PEE	C1-O3P-P-O4P
30	l	701	PEE	C4-O4P-P-O2P
30	r	501	PEE	C1-O3P-P-O2P
30	r	501	PEE	C1-O3P-P-O4P
31	a	201	CDL	CA3-OA5-PA1-OA4
31	a	201	CDL	CB2-OB2-PB2-OB4
31	g	202	CDL	CA3-OA5-PA1-OA3
31	i	401	CDL	CA3-OA5-PA1-OA2
31	i	401	CDL	CA3-OA5-PA1-OA4
31	i	401	CDL	CB2-OB2-PB2-OB3
31	i	401	CDL	CB3-OB5-PB2-OB2
31	i	401	CDL	CB3-OB5-PB2-OB4
31	l	702	CDL	CB3-OB5-PB2-OB2
31	l	702	CDL	CB3-OB5-PB2-OB3
31	l	702	CDL	CB3-OB5-PB2-OB4
31	o	201	CDL	CB2-OB2-PB2-OB4
31	r	504	CDL	CA2-OA2-PA1-OA3
31	r	504	CDL	CA3-OA5-PA1-OA3
31	r	504	CDL	CB3-OB5-PB2-OB4
31	u	201	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
31	u	201	CDL	CB3-OB5-PB2-OB4
33	j	202	PLX	C3-O4-P1-O3
31	u	201	CDL	CA5-C11-C12-C13
31	V	201	CDL	C55-C56-C57-C58
31	r	504	CDL	CA7-C31-C32-C33
31	r	504	CDL	C34-C35-C36-C37
31	l	702	CDL	C32-C33-C34-C35
30	U	401	PEE	O3P-C1-C2-O2
33	a	202	PLX	C13-C14-C15-C16
31	g	202	CDL	C62-C63-C64-C65
30	l	701	PEE	C18-C19-C20-C21
33	g	201	PLX	C29-C30-C31-C32
30	l	701	PEE	C31-C32-C33-C34
30	b	201	PEE	C15-C16-C17-C18
34	s	401	UQ	C14-C16-C17-C18
30	U	401	PEE	C11-C12-C13-C14
31	o	201	CDL	C32-C33-C34-C35
33	a	202	PLX	C34-C35-C36-C37
31	i	401	CDL	C15-C16-C17-C18
31	r	504	CDL	C40-C41-C42-C43
30	j	201	PEE	C38-C39-C40-C41
31	a	201	CDL	C31-CA7-OA8-CA6
31	a	201	CDL	OA9-CA7-OA8-CA6
30	i	402	PEE	C31-C32-C33-C34
31	g	202	CDL	C23-C24-C25-C26
31	l	702	CDL	C63-C64-C65-C66
31	V	201	CDL	C53-C54-C55-C56
31	i	401	CDL	C71-C72-C73-C74
31	g	202	CDL	C39-C40-C41-C42
30	i	402	PEE	C37-C38-C39-C40
30	i	402	PEE	C2-C1-O3P-P
30	l	701	PEE	C39-C40-C41-C42
30	U	401	PEE	C34-C35-C36-C37
30	U	401	PEE	C40-C41-C42-C43
31	V	201	CDL	C75-C76-C77-C78
31	V	201	CDL	C39-C40-C41-C42
31	u	201	CDL	C61-C62-C63-C64
33	g	201	PLX	C36-C37-C38-C39
30	b	201	PEE	C18-C19-C20-C21
31	u	201	CDL	C60-C61-C62-C63
31	g	202	CDL	C11-C12-C13-C14
33	j	202	PLX	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	i	401	CDL	CB5-C51-C52-C53
31	g	202	CDL	C31-C32-C33-C34
31	r	504	CDL	C21-C22-C23-C24
30	U	401	PEE	O3P-C1-C2-C3
33	j	202	PLX	C19-C20-C21-C22
33	a	202	PLX	C10-C11-C12-C13
30	l	703	PEE	C22-C23-C24-C25
31	g	202	CDL	C44-C45-C46-C47
31	r	504	CDL	C37-C38-C39-C40
33	r	502	PLX	O8-C24-C25-C26
31	r	504	CDL	C78-C79-C80-C81
31	u	201	CDL	C72-C73-C74-C75
30	W	201	PEE	C34-C35-C36-C37
31	V	201	CDL	CA3-CA4-CA6-OA8
30	U	401	PEE	C32-C33-C34-C35
31	l	702	CDL	C57-C58-C59-C60
30	W	201	PEE	O5-C30-C31-C32
30	W	201	PEE	C16-C17-C18-C19
31	g	202	CDL	C51-C52-C53-C54
30	r	501	PEE	C20-C21-C22-C23
31	V	201	CDL	OB6-CB4-CB6-OB8
30	l	703	PEE	C13-C14-C15-C16
33	a	202	PLX	C33-C34-C35-C36
30	r	501	PEE	C31-C32-C33-C34
30	j	201	PEE	C39-C40-C41-C42
31	i	401	CDL	C13-C14-C15-C16
30	U	401	PEE	C18-C19-C20-C21
30	i	402	PEE	C38-C39-C40-C41
31	o	201	CDL	C80-C81-C82-C83
30	j	201	PEE	C16-C17-C18-C19
30	l	703	PEE	C16-C17-C18-C19
30	l	703	PEE	C15-C16-C17-C18
30	i	402	PEE	C23-C24-C25-C26
31	a	201	CDL	C15-C16-C17-C18
31	V	201	CDL	OA5-CA3-CA4-OA6
30	l	703	PEE	C19-C20-C21-C22
31	V	201	CDL	C64-C65-C66-C67
30	U	401	PEE	C14-C15-C16-C17
30	l	701	PEE	C16-C17-C18-C19
30	l	703	PEE	C36-C37-C38-C39
31	a	201	CDL	C35-C36-C37-C38
31	r	504	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
33	r	502	PLX	C25-C26-C27-C28
30	W	201	PEE	O3P-C1-C2-C3
31	l	702	CDL	C31-C32-C33-C34
33	j	202	PLX	C7-C6-O6-C4
30	U	401	PEE	C13-C14-C15-C16
31	r	504	CDL	C17-C18-C19-C20
30	i	402	PEE	C36-C37-C38-C39
35	w	401	ADP	PB-O3A-PA-O2A
31	a	201	CDL	C12-C13-C14-C15
31	V	201	CDL	C57-C58-C59-C60
30	j	201	PEE	C15-C16-C17-C18
30	W	201	PEE	O3P-C1-C2-O2
30	U	401	PEE	C44-C45-C46-C47
31	r	504	CDL	C72-C73-C74-C75
31	g	202	CDL	C36-C37-C38-C39
31	l	702	CDL	C12-C11-CA5-OA6
33	a	202	PLX	C25-C24-O8-C5
33	j	202	PLX	C2-C1-N1-C1A
33	r	502	PLX	C25-C24-O8-C5
30	l	701	PEE	O3-C30-C31-C32
31	u	201	CDL	C72-C71-CB7-OB8
31	o	201	CDL	C32-C31-CA7-OA9
33	g	201	PLX	C6-C7-C8-C9
31	o	201	CDL	C12-C11-CA5-OA6
31	l	702	CDL	OB5-CB3-CB4-CB6
31	o	201	CDL	C78-C79-C80-C81
30	j	201	PEE	O2-C10-C11-C12
31	l	702	CDL	C52-C51-CB5-OB6
30	b	201	PEE	C12-C13-C14-C15
31	a	201	CDL	C18-C19-C20-C21
34	s	401	UQ	C6-C7-C8-C9
31	u	201	CDL	C72-C71-CB7-OB9
30	r	501	PEE	C30-C31-C32-C33
31	a	201	CDL	C74-C75-C76-C77
33	r	502	PLX	C35-C36-C37-C38
33	g	201	PLX	O6-C6-C7-C8
30	b	201	PEE	O3-C30-C31-C32
30	l	701	PEE	O5-C30-C31-C32
34	s	401	UQ	C1-C2-O2-CM2
30	j	201	PEE	C40-C41-C42-C43
31	l	702	CDL	C12-C11-CA5-OA7
33	g	201	PLX	O9-C24-O8-C5

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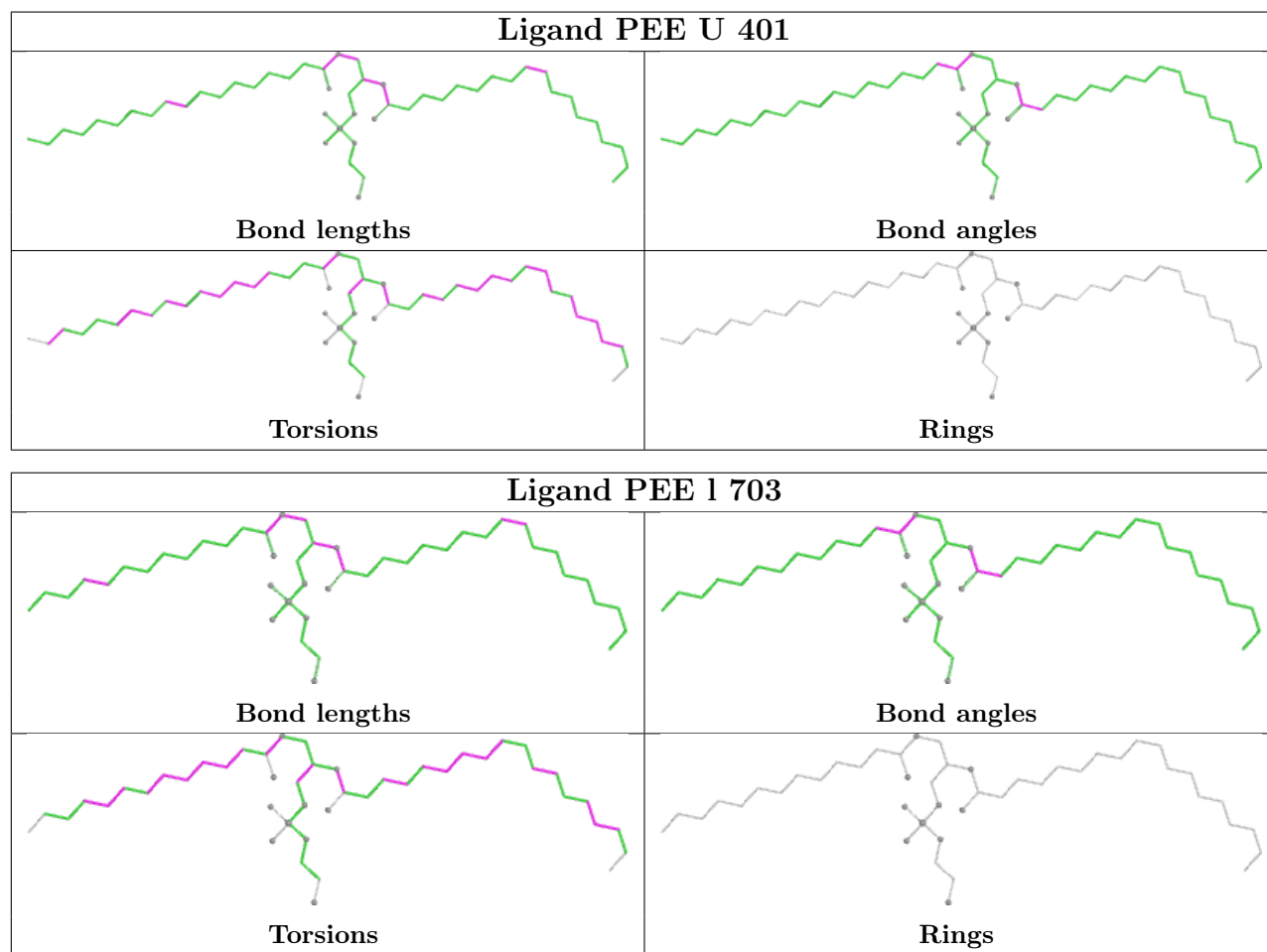
Mol	Chain	Res	Type	Atoms
33	r	503	PLX	O9-C24-O8-C5
31	o	201	CDL	C12-C11-CA5-OA7
33	j	202	PLX	C4-C5-O8-C24
31	r	504	CDL	C44-C45-C46-C47
31	r	504	CDL	C12-C11-CA5-OA6
30	l	701	PEE	C37-C38-C39-C40
30	r	501	PEE	C16-C17-C18-C19
31	a	201	CDL	C53-C54-C55-C56
31	r	504	CDL	C12-C11-CA5-OA7
30	j	201	PEE	O4-C10-C11-C12
30	r	501	PEE	C18-C19-C20-C21
31	u	201	CDL	C57-C58-C59-C60

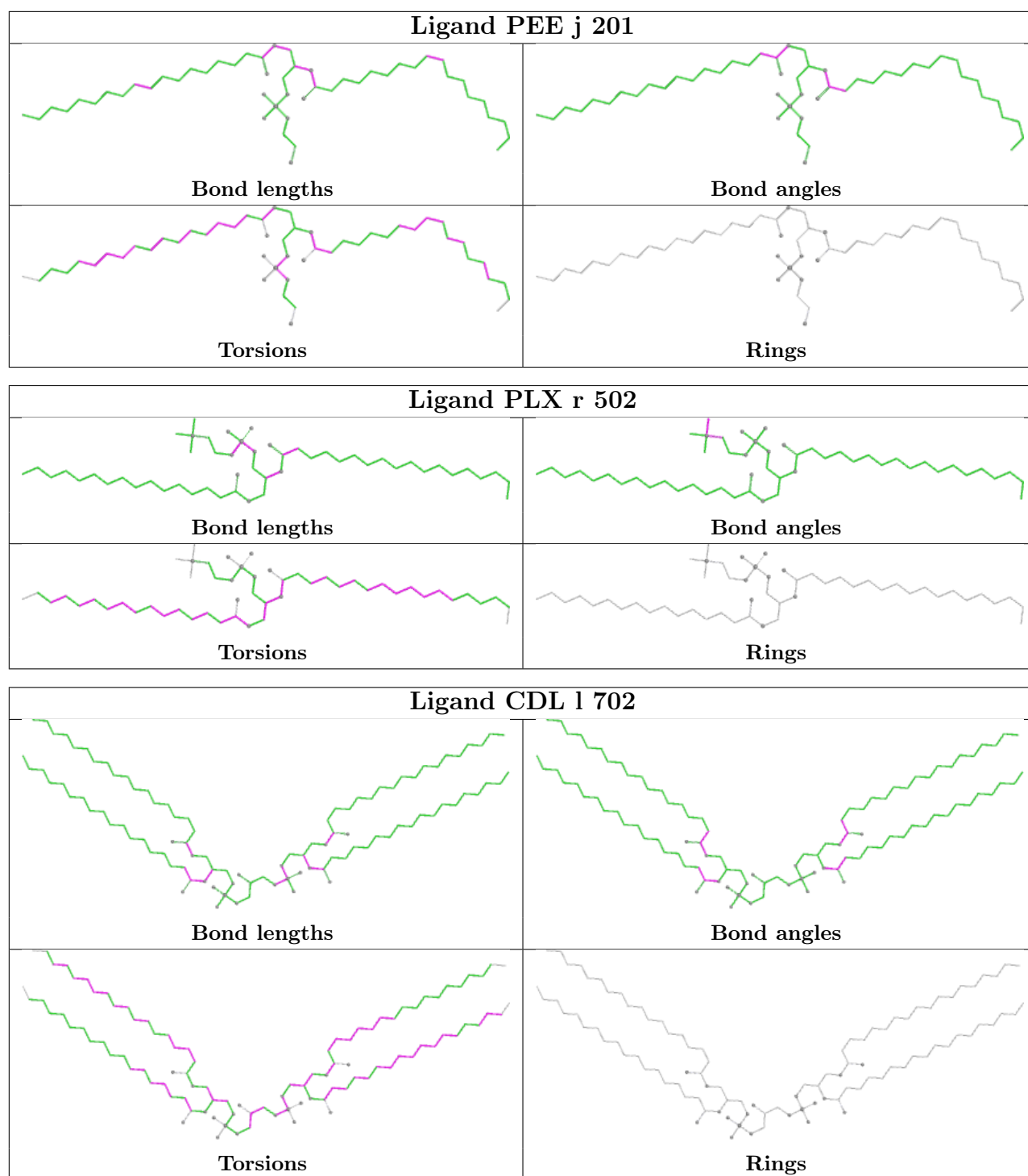
There are no ring outliers.

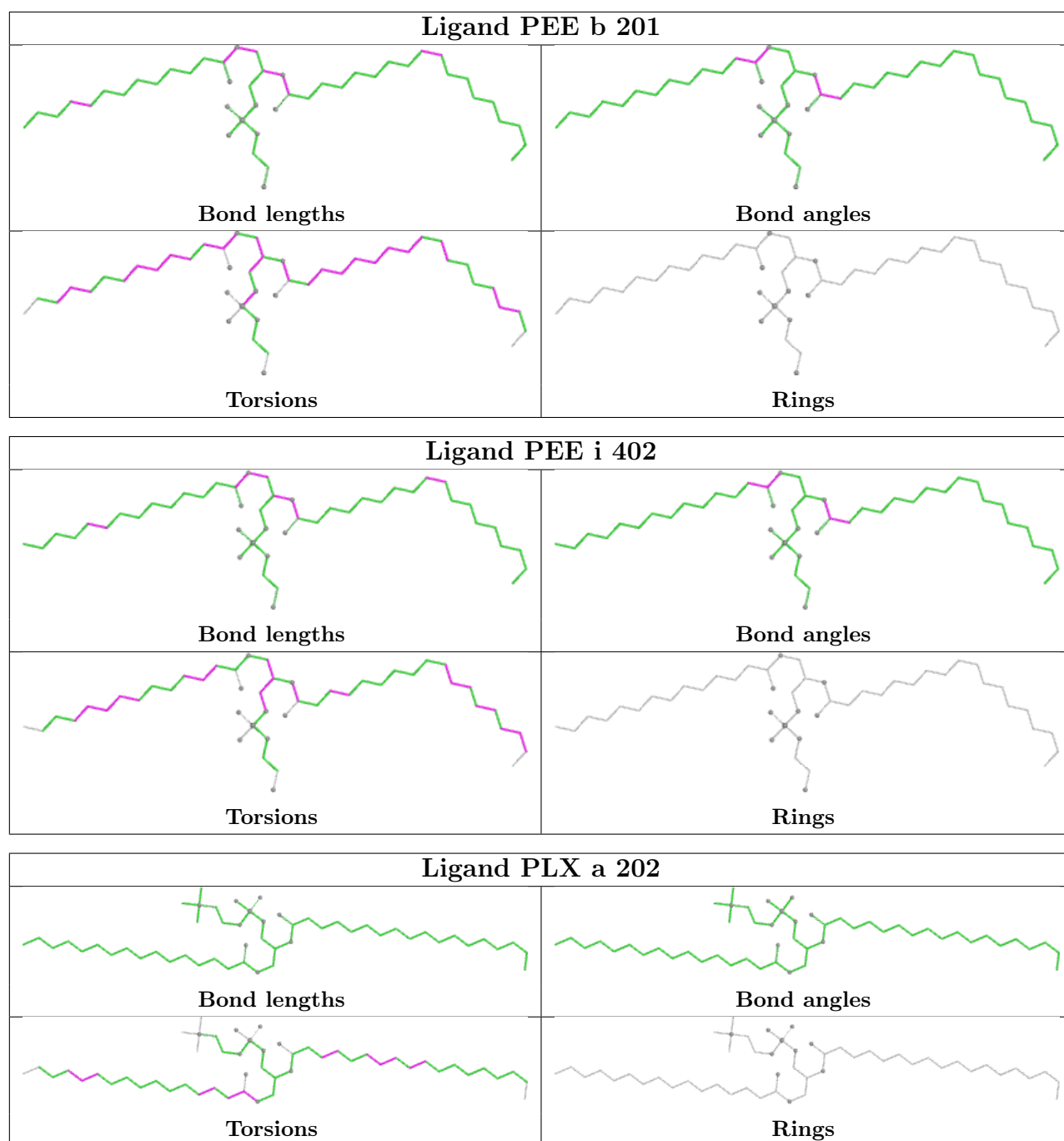
24 monomers are involved in 92 short contacts:

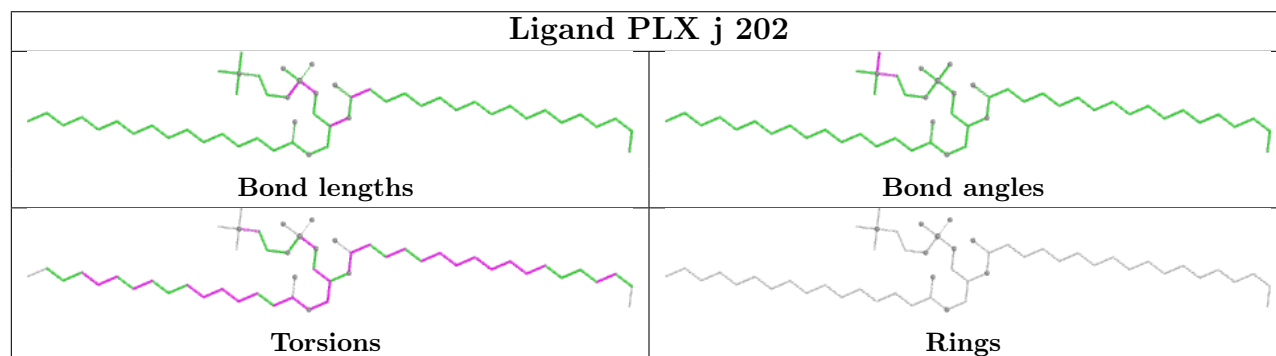
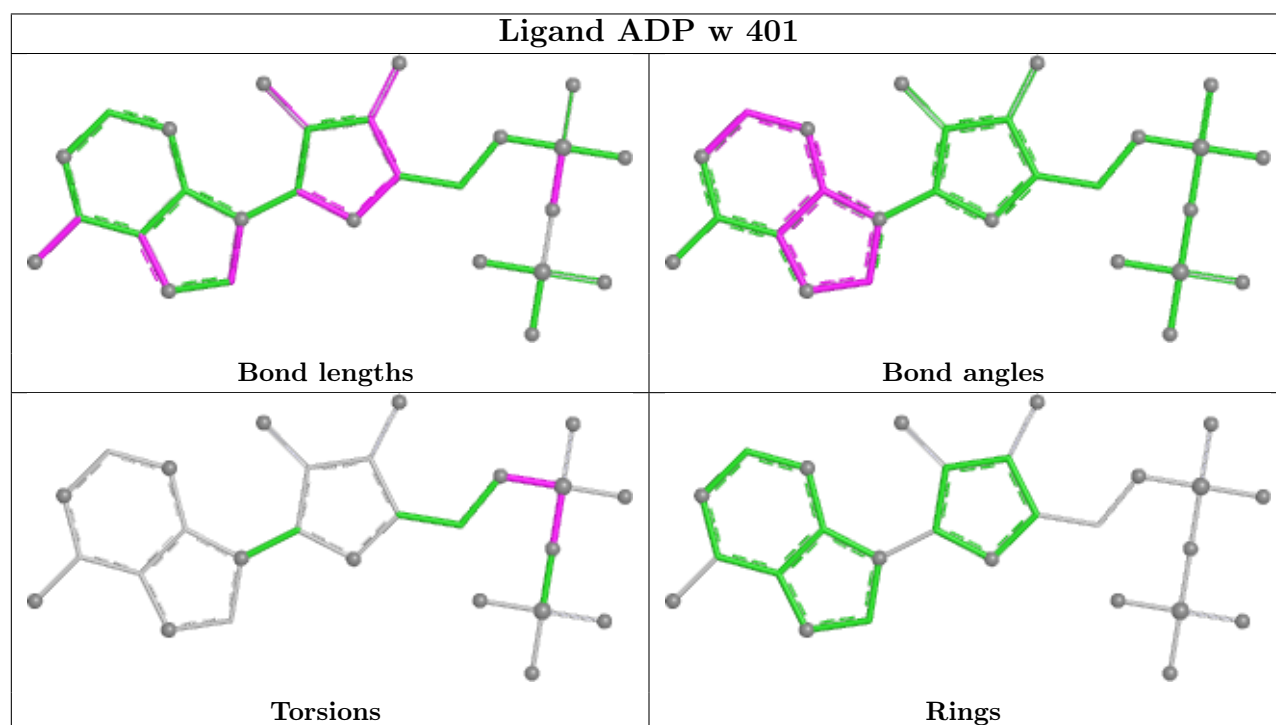
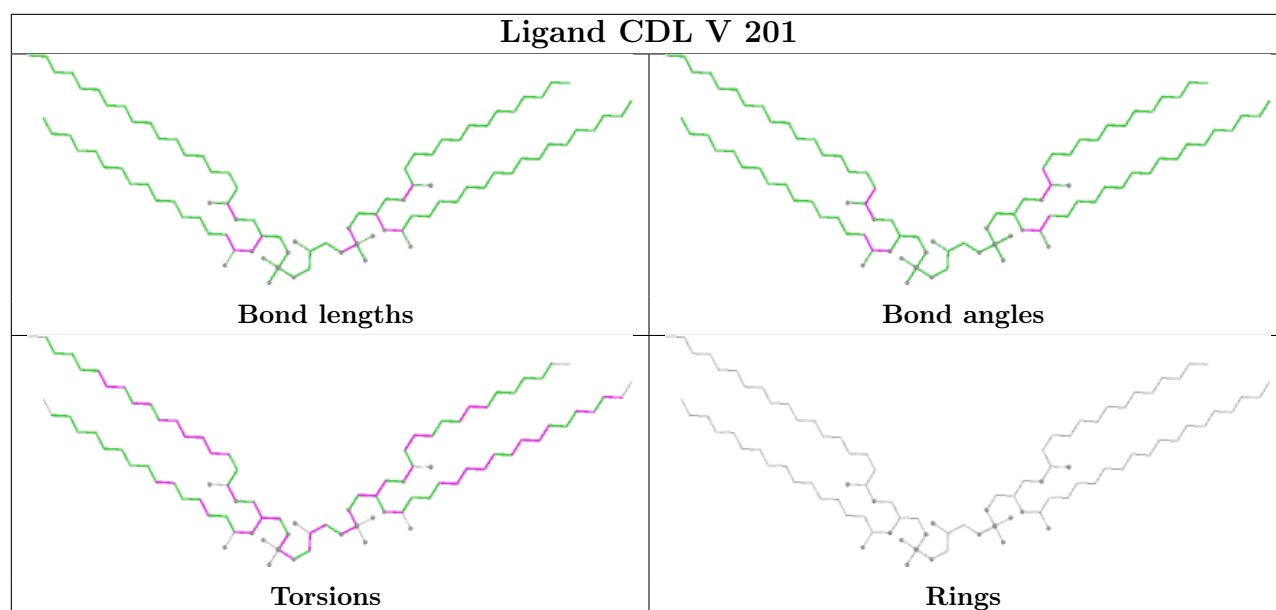
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	U	401	PEE	1	0
30	l	703	PEE	2	0
30	j	201	PEE	1	0
33	r	502	PLX	3	0
31	l	702	CDL	4	0
30	b	201	PEE	3	0
30	i	402	PEE	2	0
33	a	202	PLX	12	0
31	V	201	CDL	4	0
35	w	401	ADP	2	0
33	j	202	PLX	3	0
31	g	202	CDL	10	0
30	l	701	PEE	3	0
33	g	201	PLX	4	0
34	s	401	UQ	2	0
30	W	201	PEE	1	0
32	X	201	8Q1	2	0
33	r	503	PLX	4	0
31	o	201	CDL	4	0
31	a	201	CDL	1	0
31	r	504	CDL	13	0
31	u	201	CDL	7	0
30	r	501	PEE	3	0
31	i	401	CDL	4	0

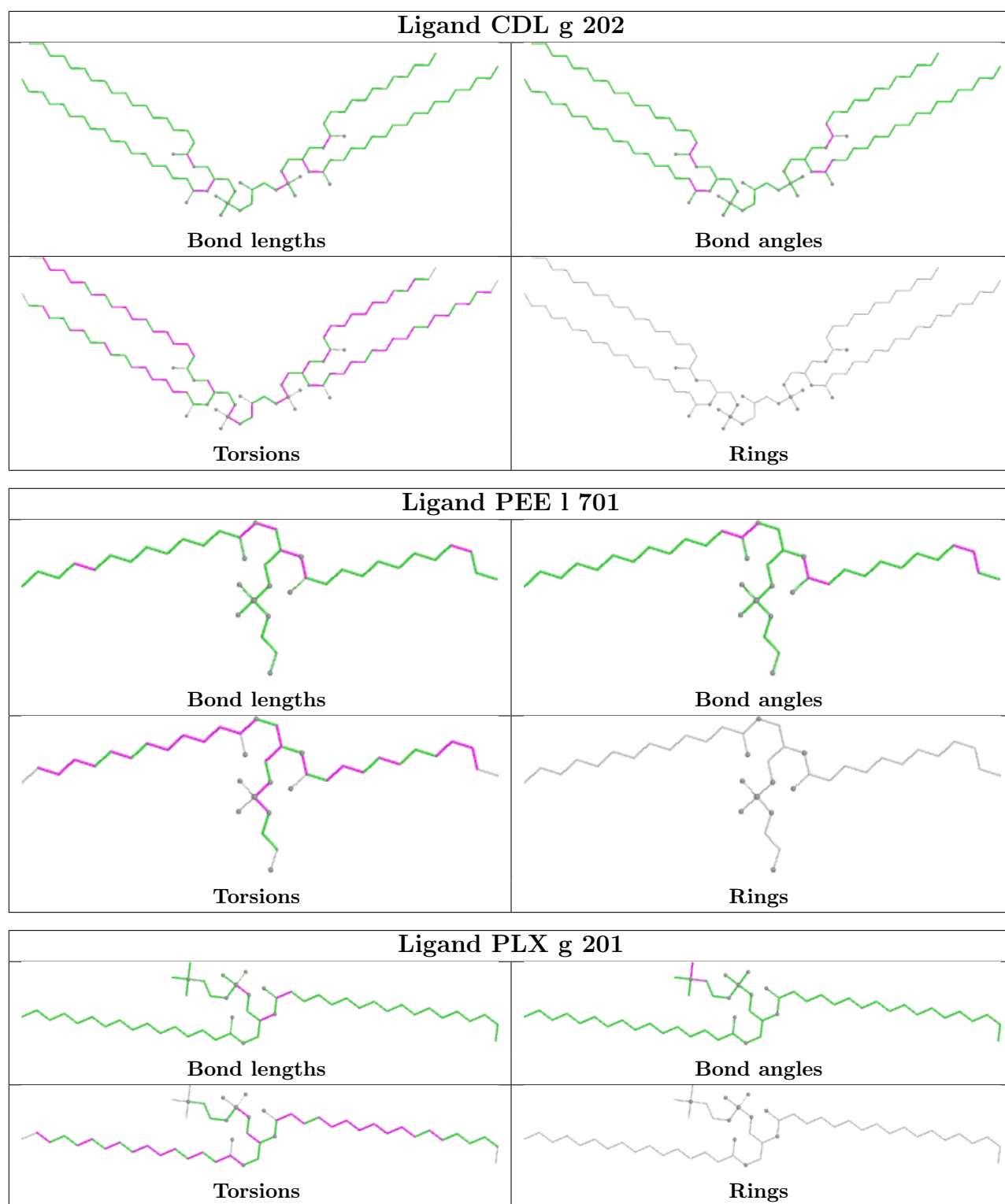
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

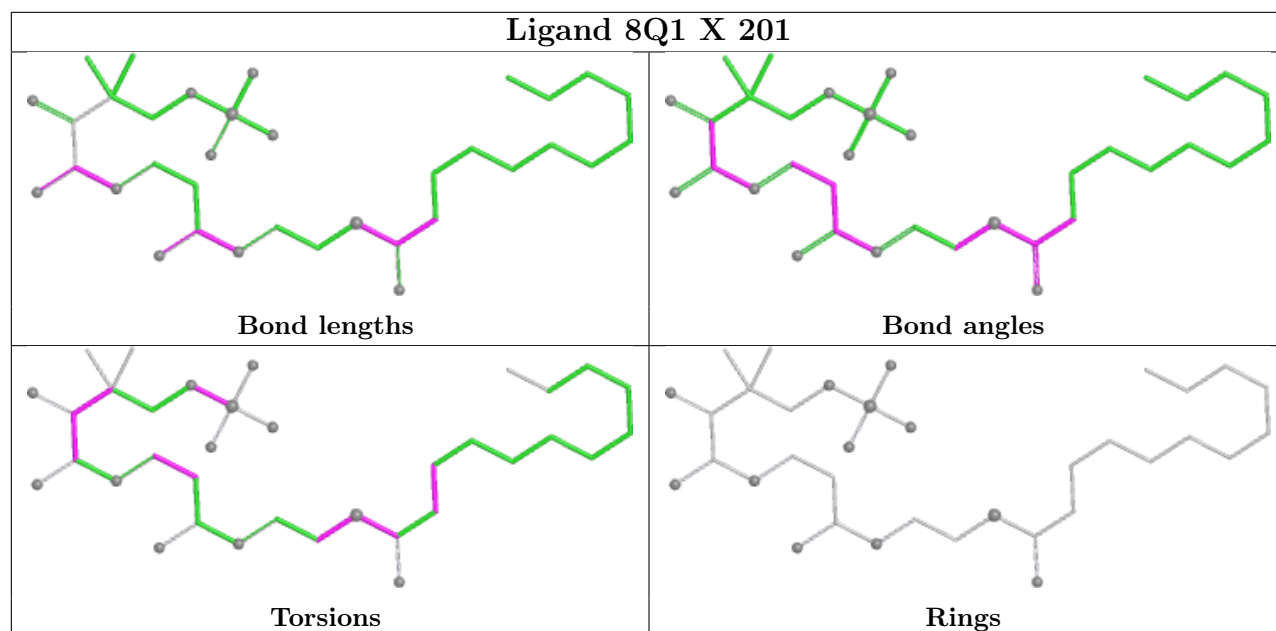
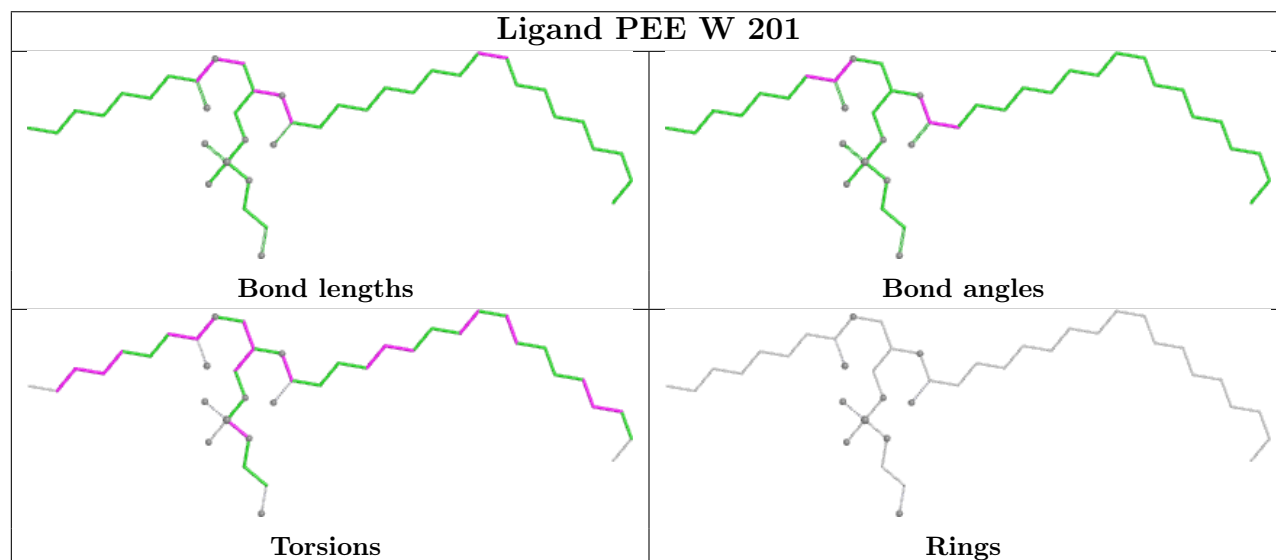
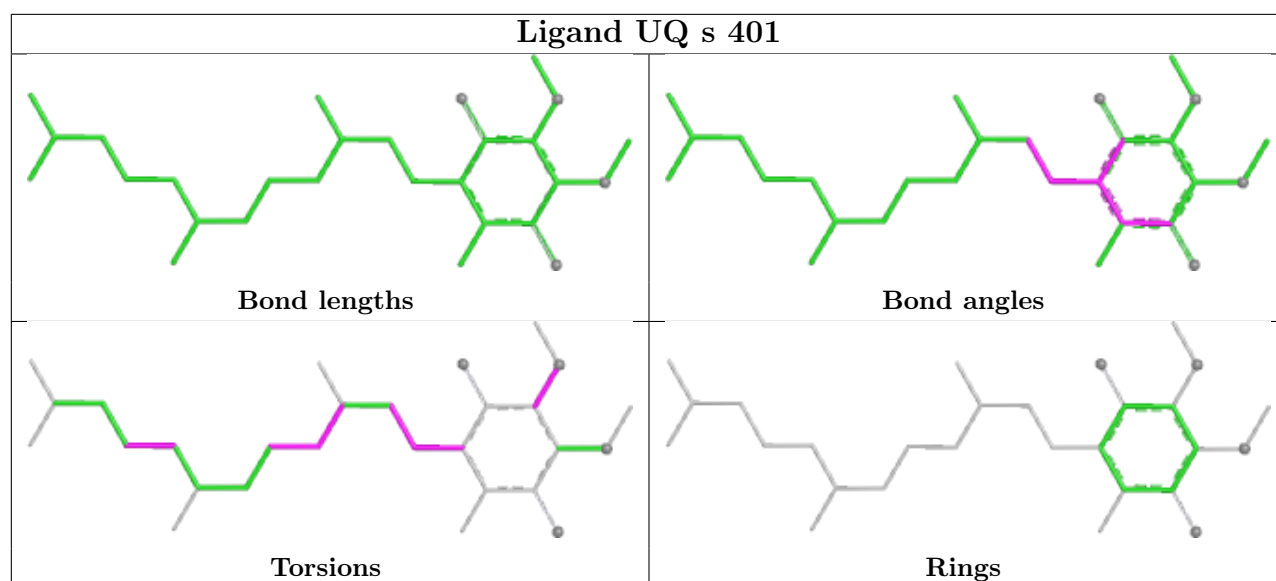


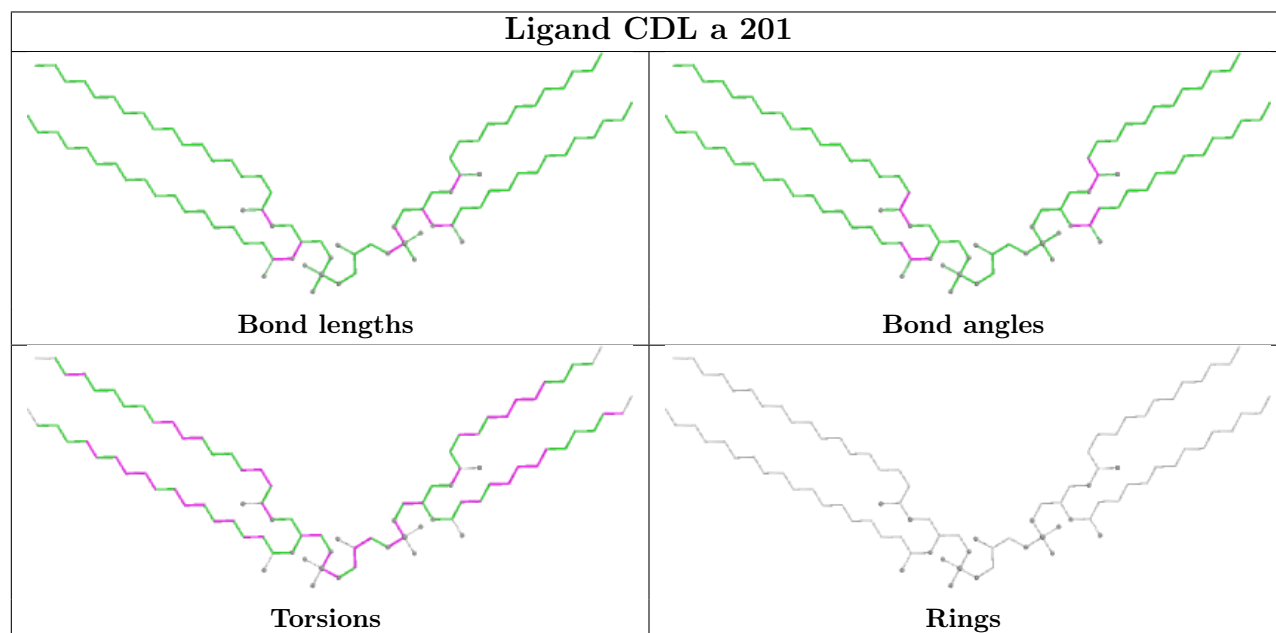
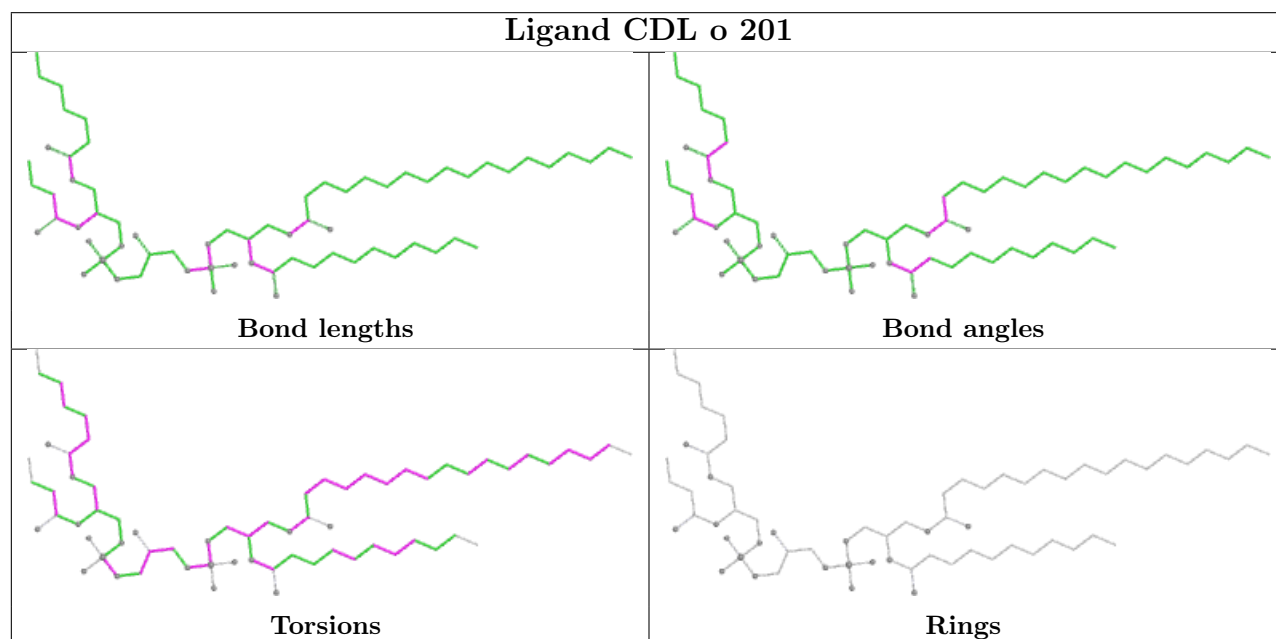
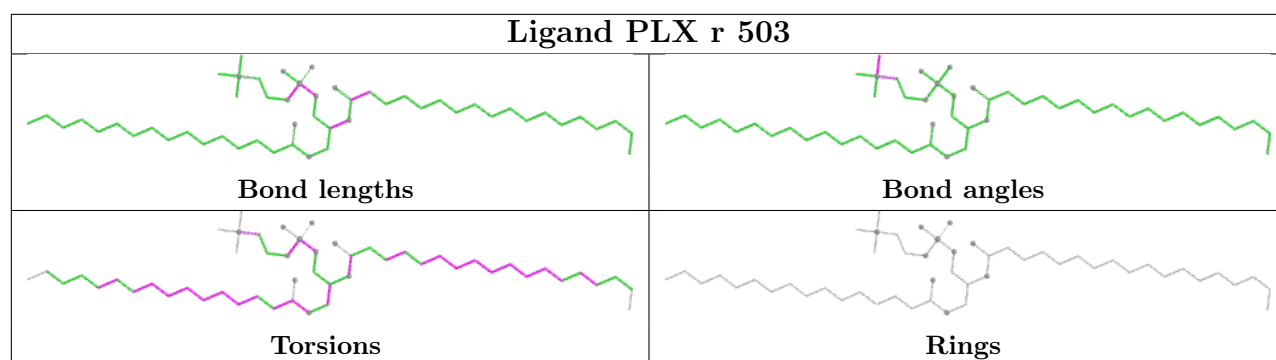


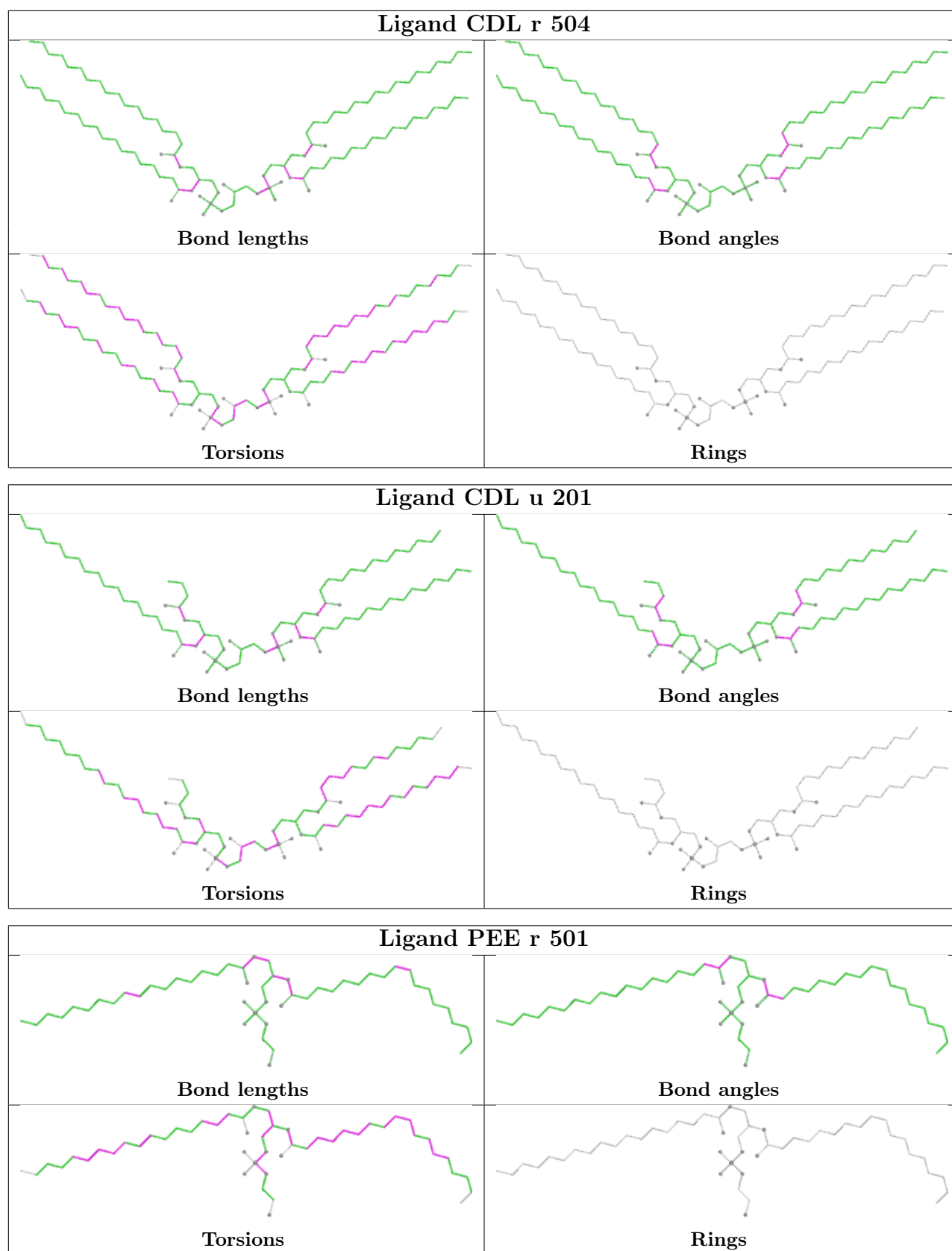


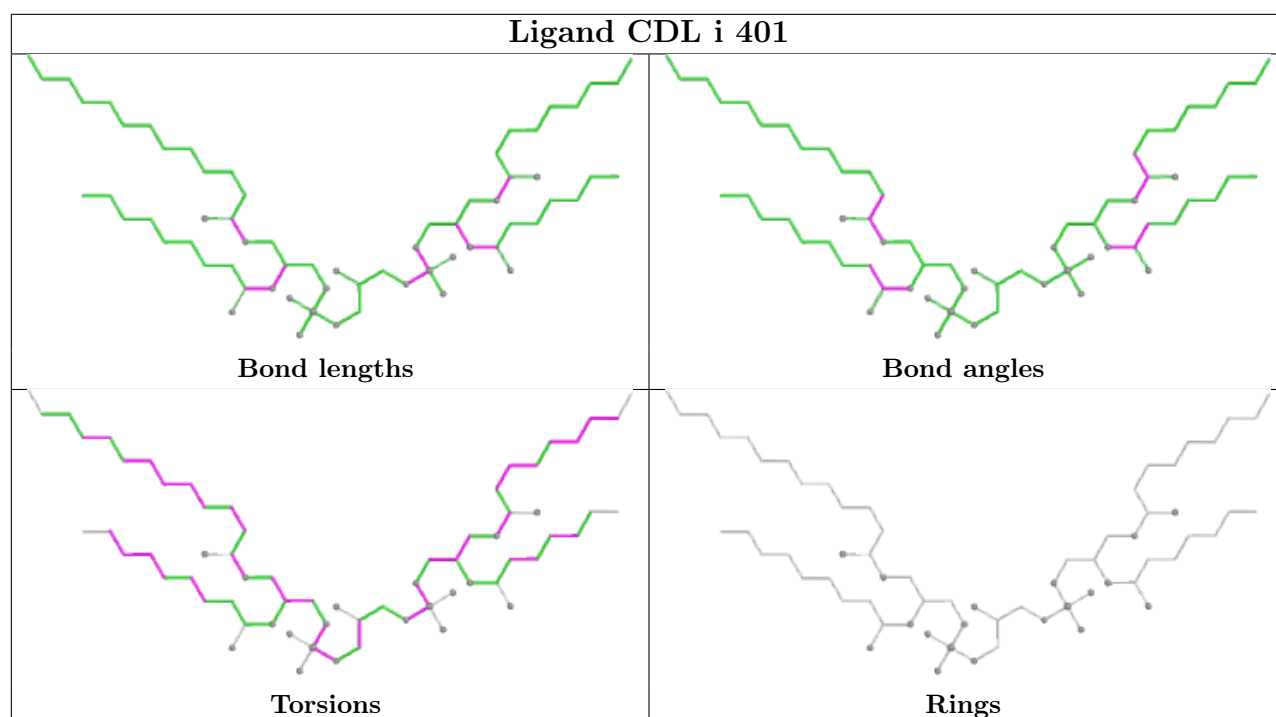












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

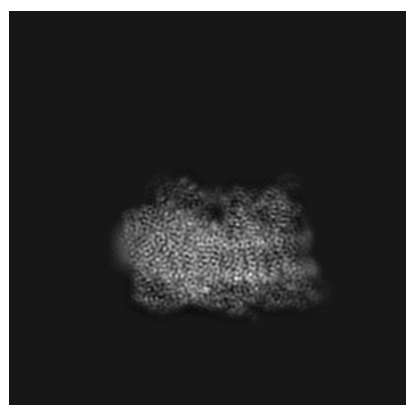
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32191. These allow visual inspection of the internal detail of the map and identification of artifacts.

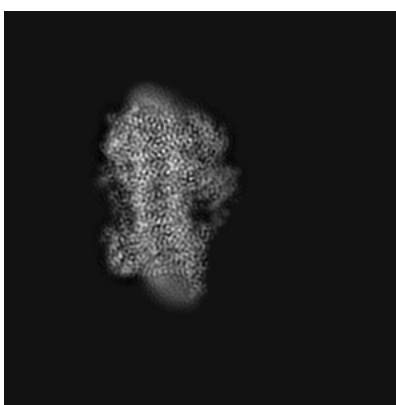
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

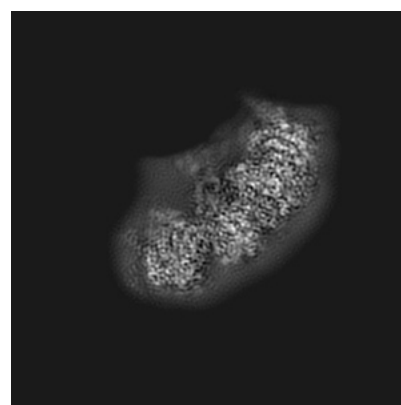
6.1.1 Primary map



X



Y

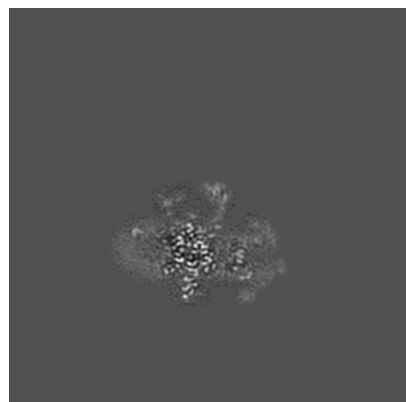


Z

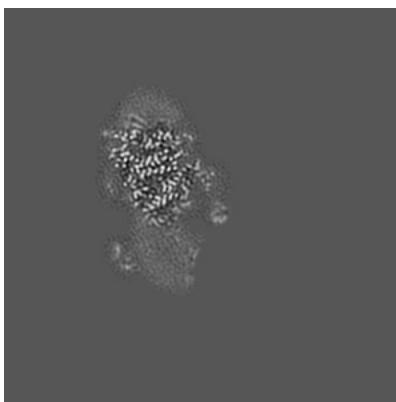
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

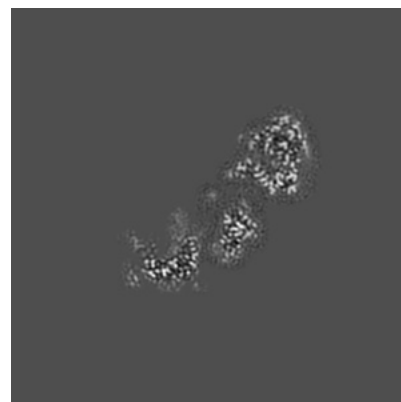
6.2.1 Primary map



X Index: 165



Y Index: 165

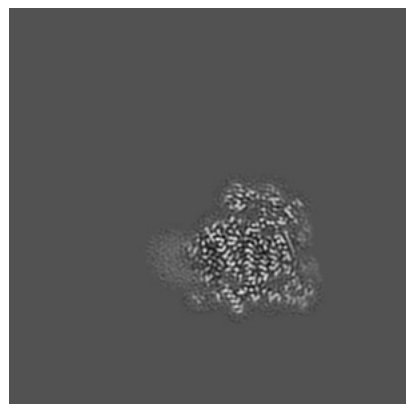


Z Index: 165

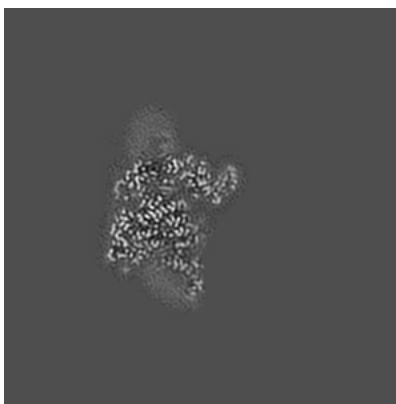
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

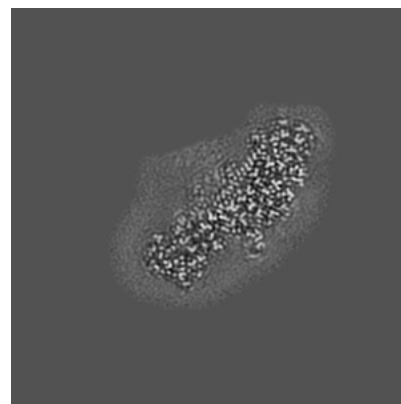
6.3.1 Primary map



X Index: 219



Y Index: 142

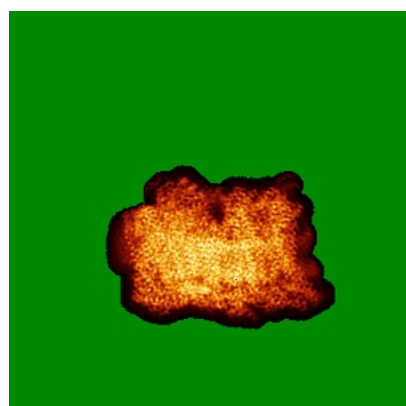


Z Index: 136

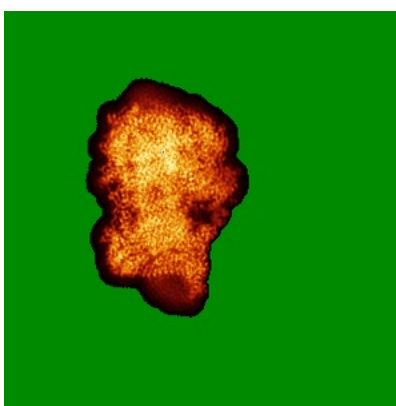
The images above show the largest variance slices of the map in three orthogonal directions.

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

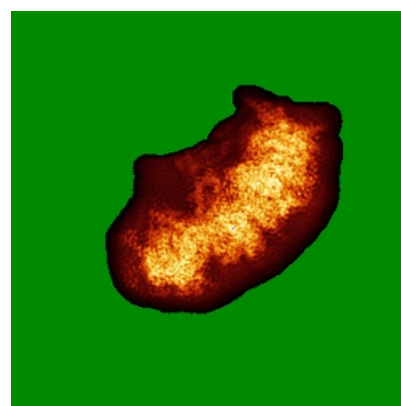
6.4.1 Primary map



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 0.0238. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

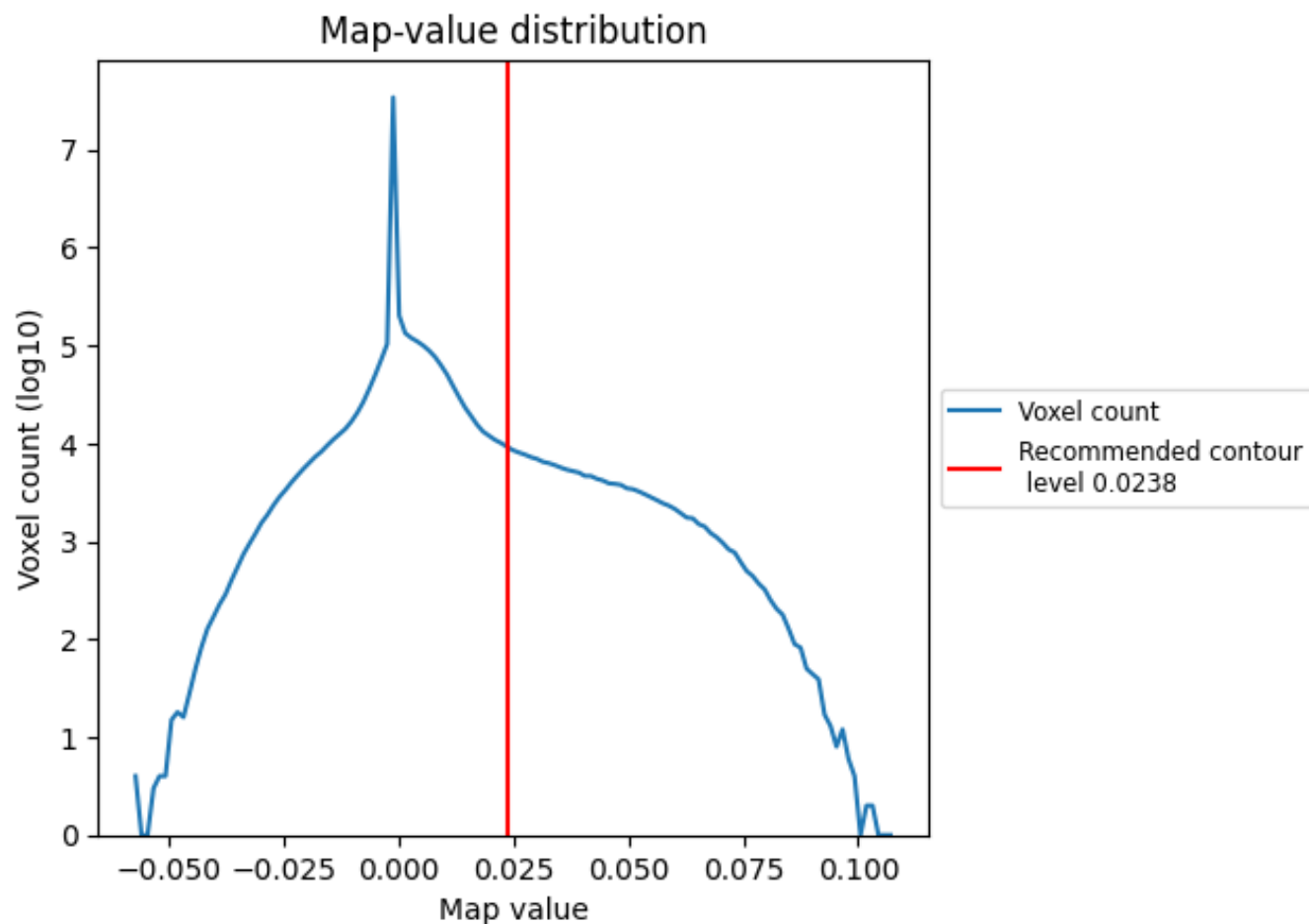
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

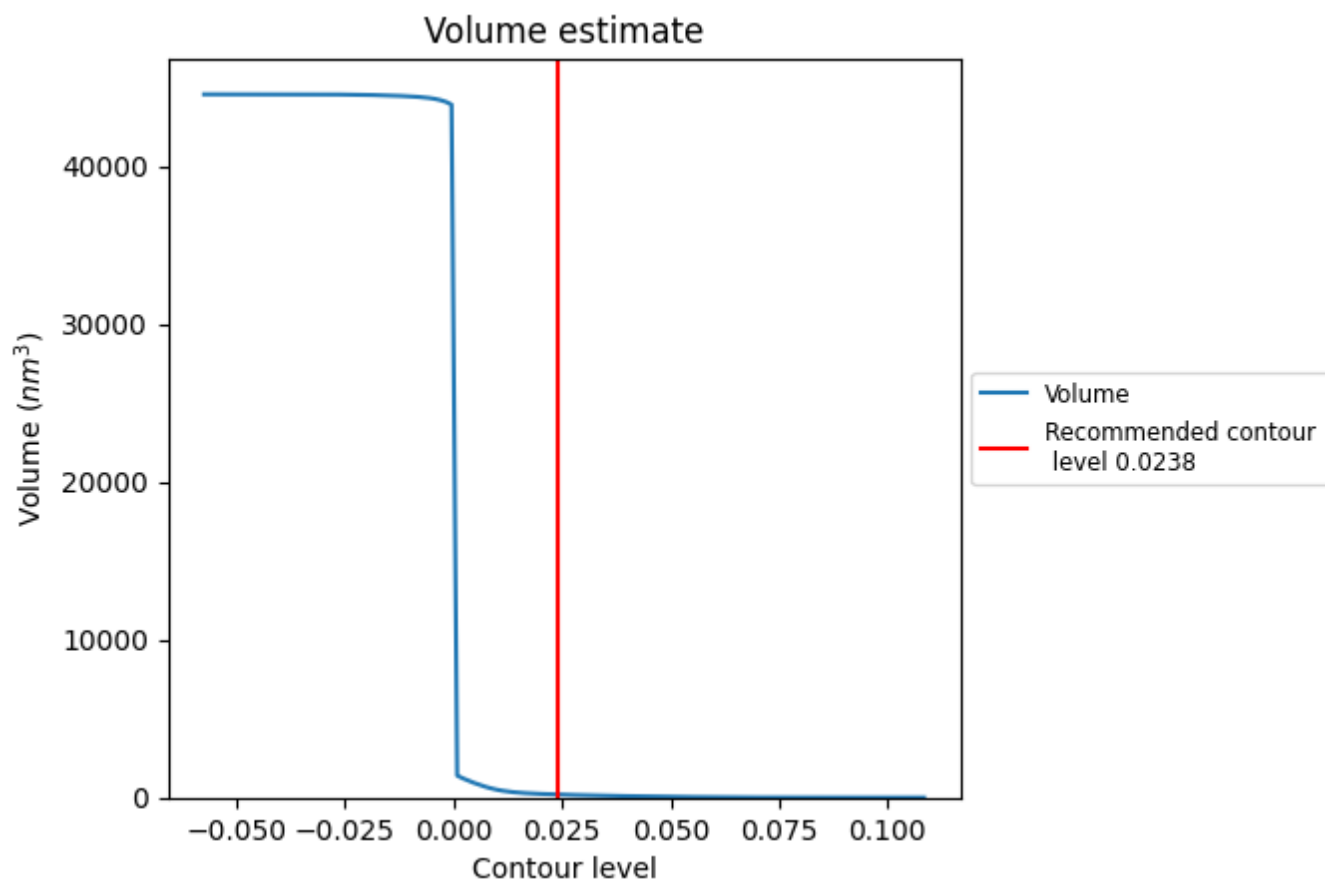
This section contains the results of statistical analysis of the map.

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.

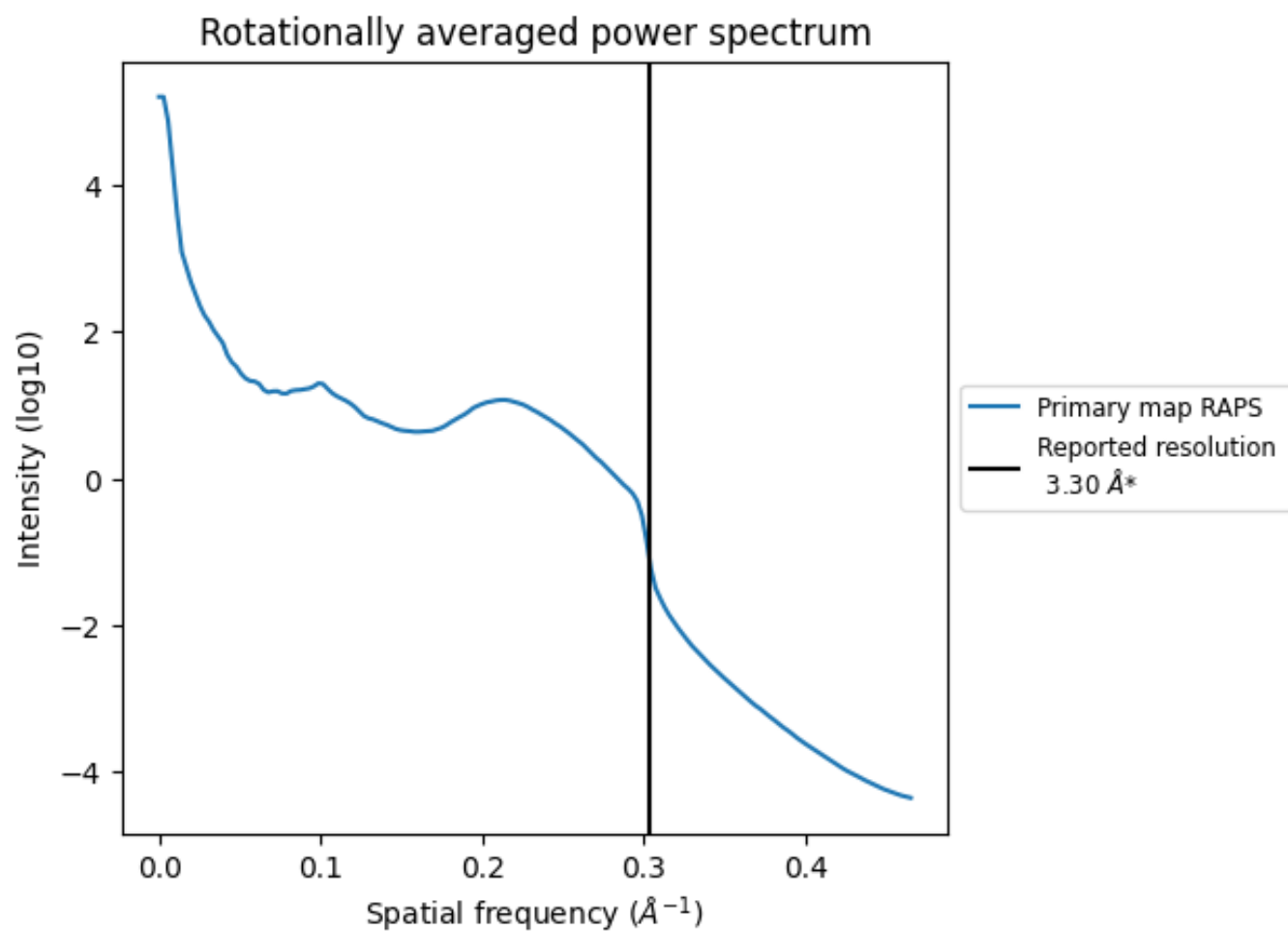
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 195 nm^3 ; this corresponds to an approximate mass of 176 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 0.303 Å⁻¹

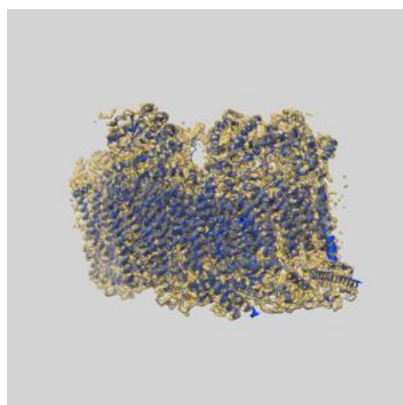
8 Fourier-Shell correlation

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

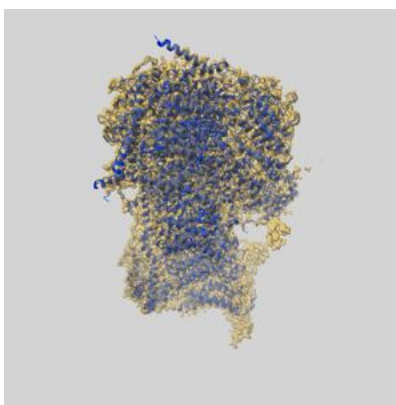
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32191 and PDB model 7VY1. Per-residue inclusion information can be found in section [3](#) on page [14](#).

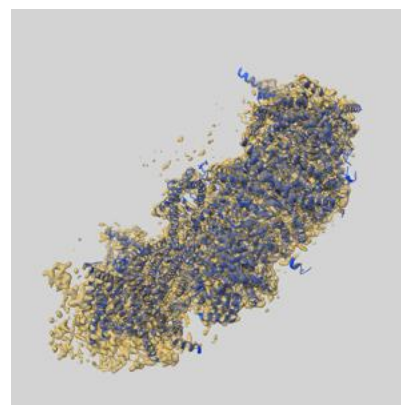
9.1 Map-model overlay [i](#)



X



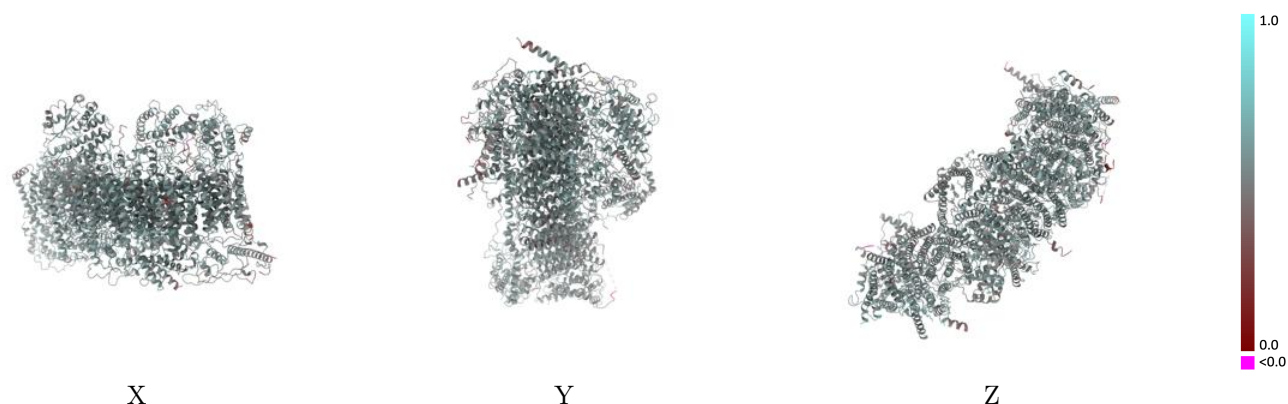
Y



Z

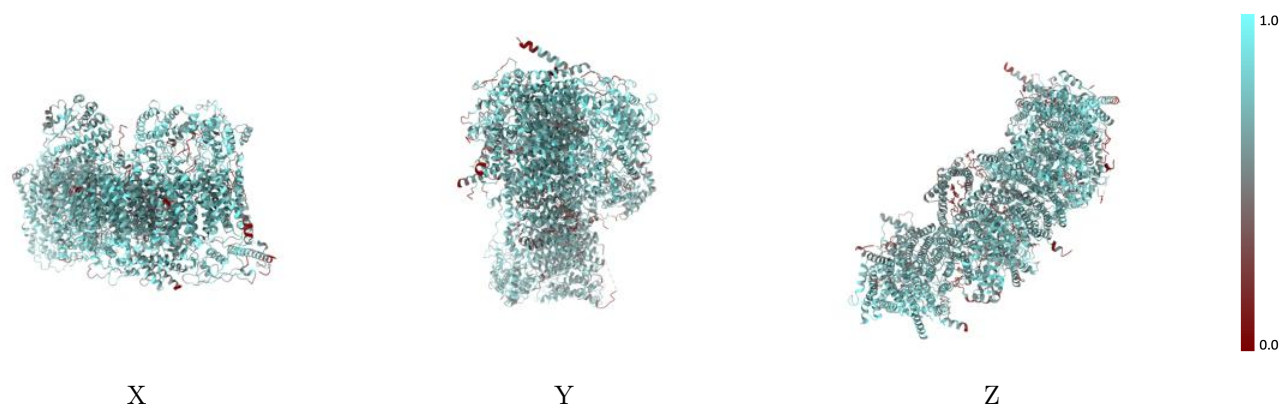
The images above show the 3D surface view of the map at the recommended contour level 0.0238 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



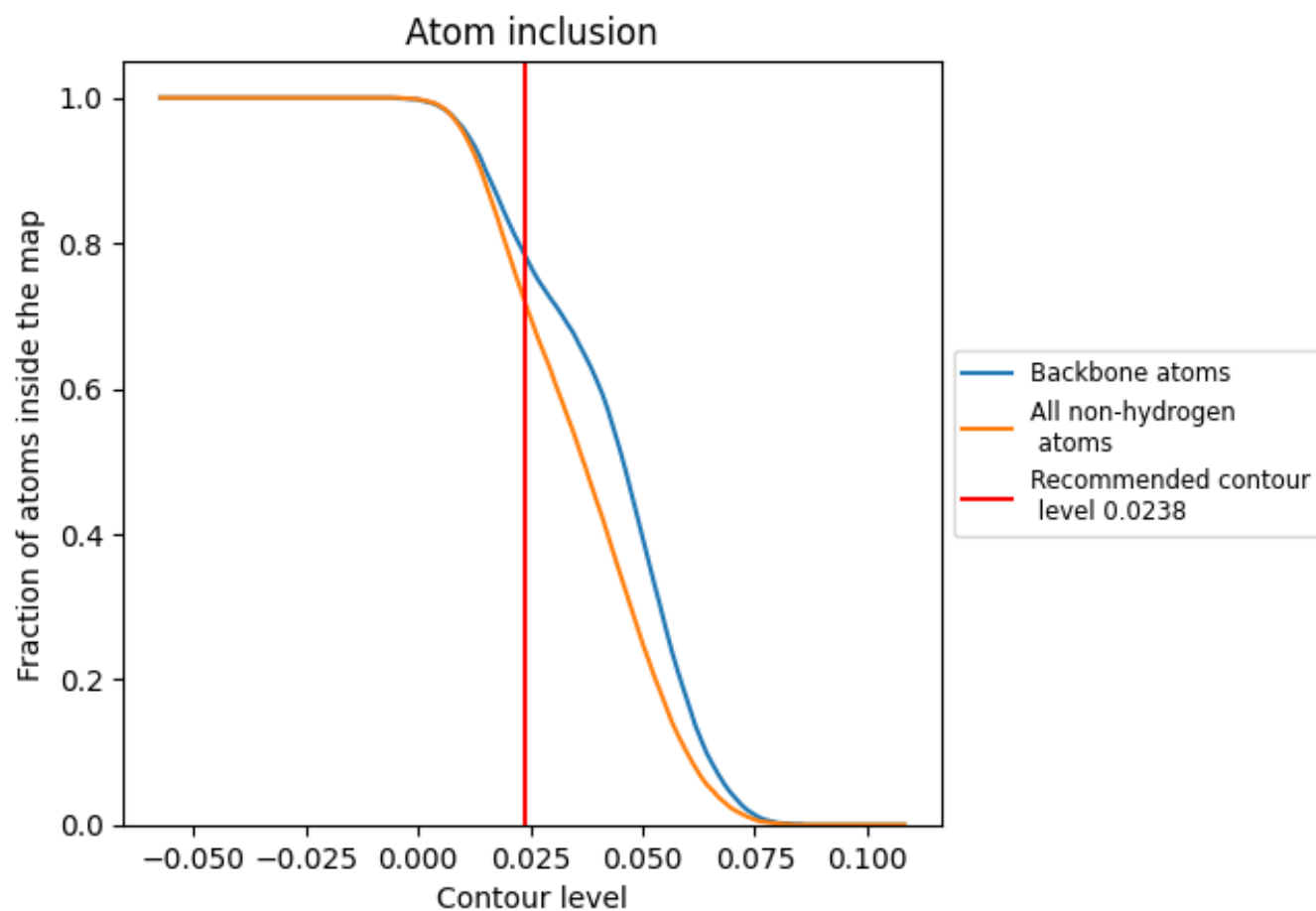
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0238).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0238) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7190	 0.5380
Q	 0.6230	 0.5400
S	 0.7880	 0.5560
U	 0.7530	 0.5410
V	 0.5390	 0.5080
W	 0.7690	 0.5520
X	 0.7090	 0.5240
Y	 0.6730	 0.5130
Z	 0.5840	 0.4800
a	 0.7480	 0.5540
b	 0.6320	 0.5140
c	 0.7430	 0.5370
d	 0.7170	 0.5290
e	 0.6670	 0.5230
f	 0.6580	 0.5210
g	 0.7410	 0.5560
h	 0.7380	 0.5480
i	 0.7670	 0.5560
j	 0.6200	 0.5130
k	 0.6930	 0.5350
l	 0.7440	 0.5470
m	 0.6870	 0.5200
n	 0.6380	 0.5180
o	 0.6760	 0.5360
p	 0.7480	 0.5400
r	 0.7680	 0.5570
s	 0.7560	 0.5450
u	 0.7510	 0.5450
v	 0.6610	 0.5010
w	 0.6980	 0.5280

