



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 06:24 PM UTC

PDB ID : 7VY9 / pdb_00007vy9
EMDB ID : EMD-32197
Title : Membrane arm of active state CI from Q10-NADH dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-13
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

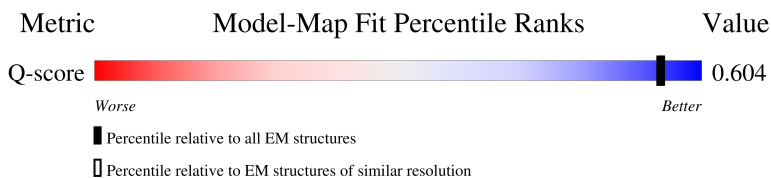
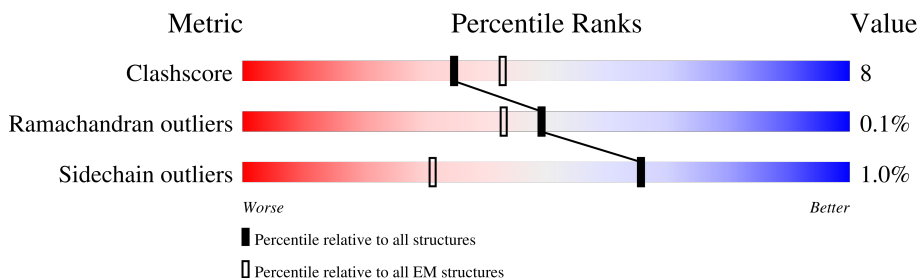
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 Å.

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



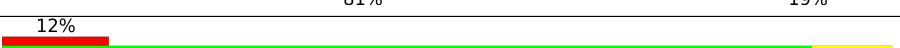
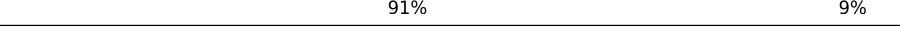
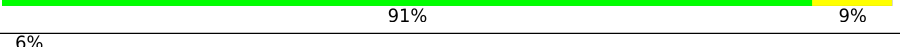
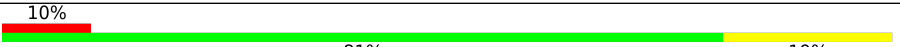
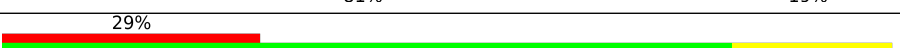
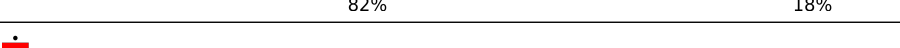
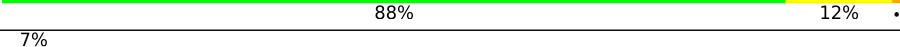
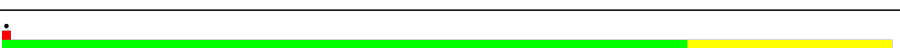
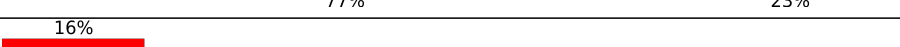
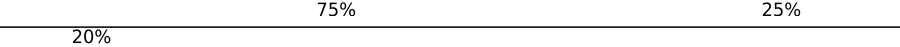
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	44	11% 73% 27%
2	S	70	81% 17% .
3	U	83	5% 83% 17%
4	V	140	6% 85% 14% .

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Mol	Chain	Length	Quality of chain
5	W	113	
6	X	88	
7	Y	67	
8	Z	80	
9	a	138	
10	b	126	
11	c	156	
12	d	175	
13	e	104	
14	f	49	
15	g	121	
16	h	105	
17	i	347	
18	j	115	
19	k	98	
20	l	606	
21	m	175	
22	n	56	
23	o	128	
24	p	178	
25	r	459	
26	s	318	
27	u	171	
28	v	125	
29	w	320	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 39717 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	44	Total	C	N	O	S	0	0
			363	236	60	66	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
			566	364	103	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
			704	454	104	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	67	Total	C	N	O	S	0	0
			584	385	95	103	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	80	Total	C	N	O	S	0	0
			641	418	108	114	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	98	Total	C	N	O	S	0	0
			819	537	144	137	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
			1315	853	213	241	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 NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	104	Total	C	N	O	S	0	0
			867	553	142	168	4		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	f	49	Total	C	N	O	0	0
			378	246	65	67		

- 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 NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	115	Total	C	N	O	S	0	0
			914	615	134	158	7		

- 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	606	Total	C	N	O	S	0	0
			4800	3182	744	823	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	175	Total	C	N	O	S	0	0
			1295	864	188	230	13		

- 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 NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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	318	Total	C	N	O	S	0	0
			2508	1678	385	424	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
			1059	658	202	189	10		

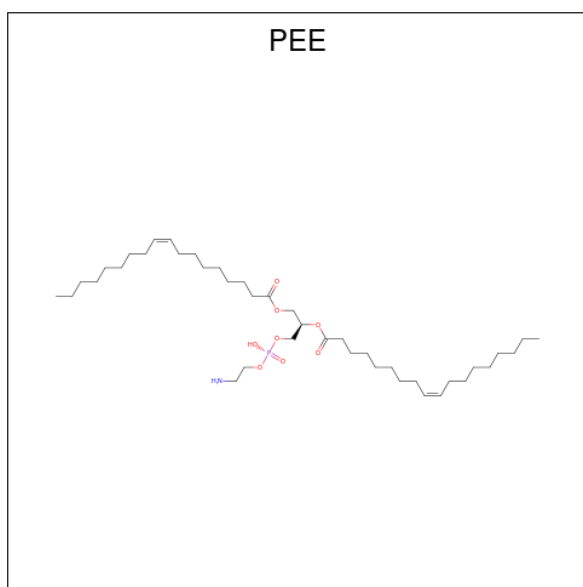
There is a discrepancy between the modelled and reference sequences:

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

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

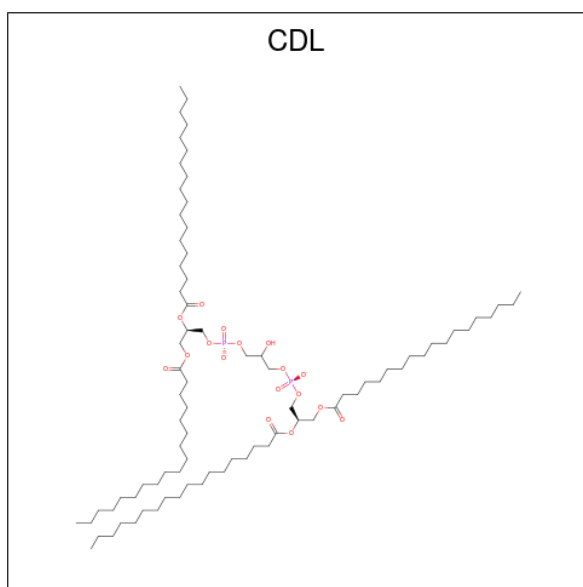
Mol	Chain	Residues	Atoms					AltConf	Trace
29	w	320	Total	C	N	O	S	0	0
			2582	1643	438	491	10		

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



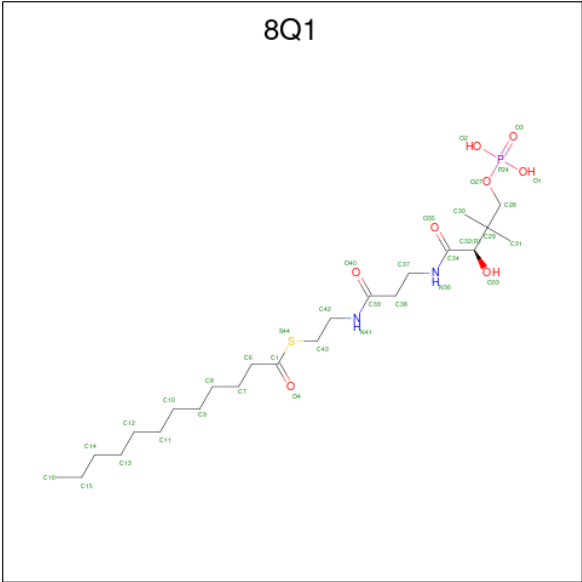
Mol	Chain	Residues	Atoms					AltConf
30	Q	1	Total	C	N	O	P	0
			47	37	1	8	1	
30	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
30	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	l	1	Total	C	N	O	P	0
			40	30	1	8	1	
30	l	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
30	r	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	s	1	Total	C	N	O	P	0
			41	31	1	8	1	
30	s	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).



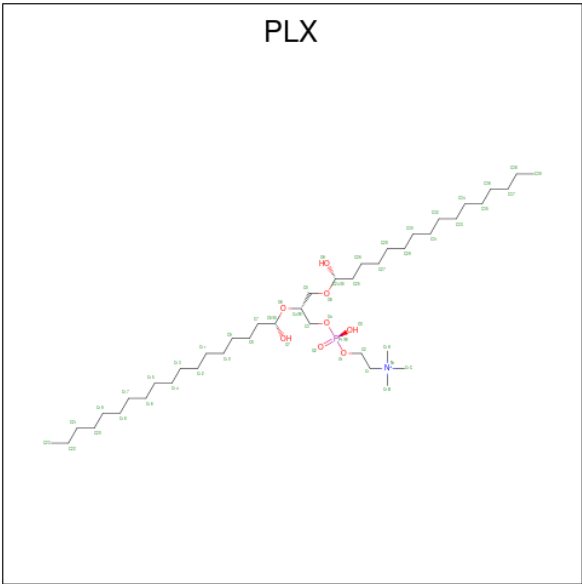
Mol	Chain	Residues	Atoms				AltConf
31	V	1	Total	C	O	P	0
			94	75	17	2	
31	V	1	Total	C	O	P	0
			100	81	17	2	
31	a	1	Total	C	O	P	0
			100	81	17	2	
31	g	1	Total	C	O	P	0
			100	81	17	2	
31	k	1	Total	C	O	P	0
			100	81	17	2	
31	l	1	Total	C	O	P	0
			99	80	17	2	
31	l	1	Total	C	O	P	0
			100	81	17	2	
31	n	1	Total	C	O	P	0
			55	36	17	2	
31	s	1	Total	C	O	P	0
			89	70	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	

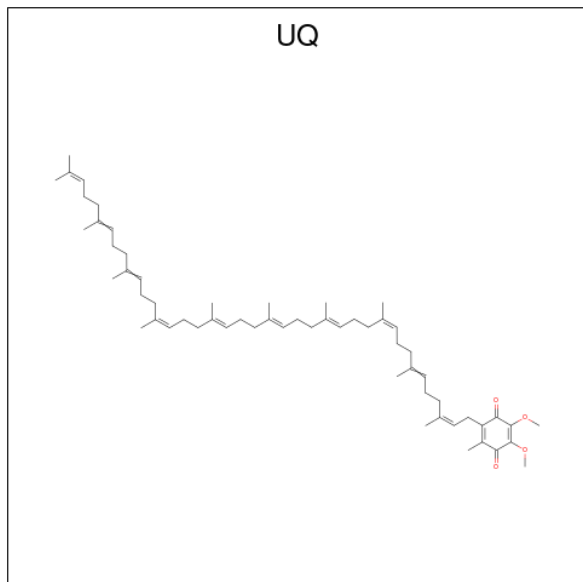
- Molecule 33 is (9R,11S)-9-([[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOX (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



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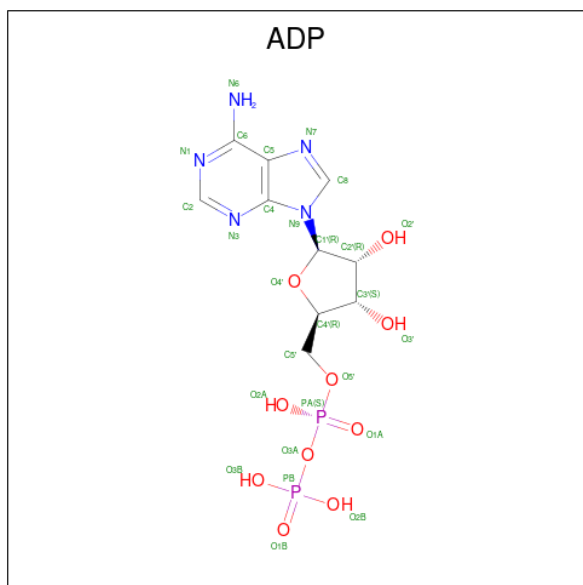
Mol	Chain	Residues	Atoms					AltConf
33	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- 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
			38	34	4	

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

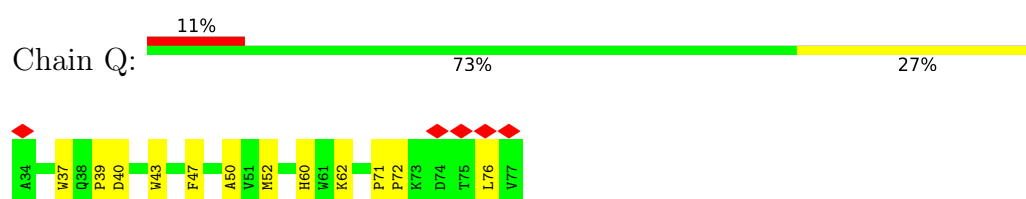


Mol	Chain	Residues	Atoms					AltConf
35	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

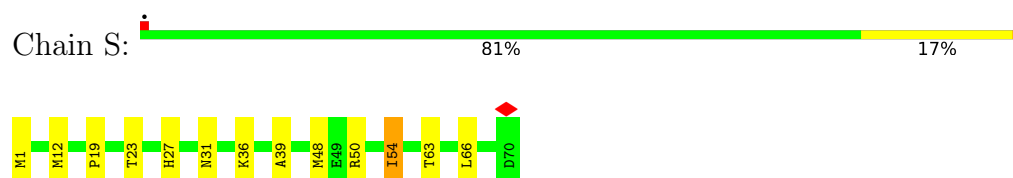
3 Residue-property plots [i](#)

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

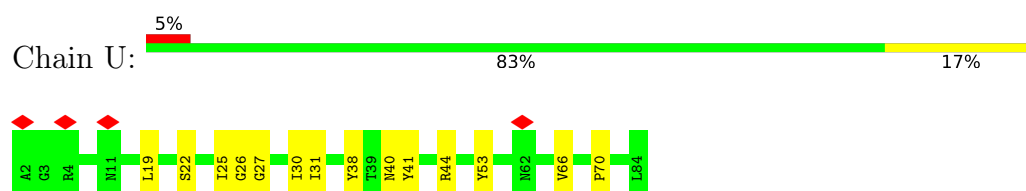
- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



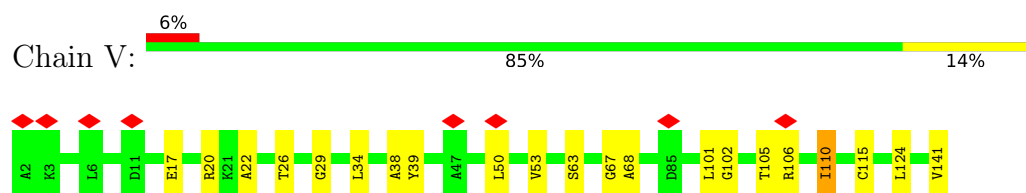
- Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



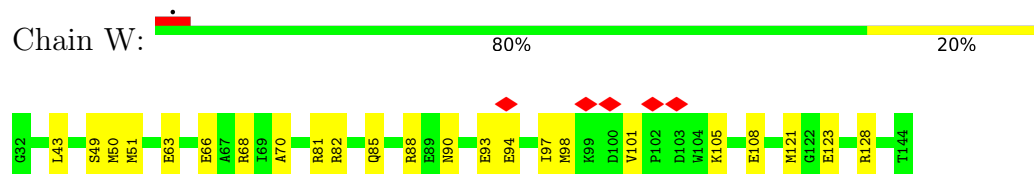
- Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



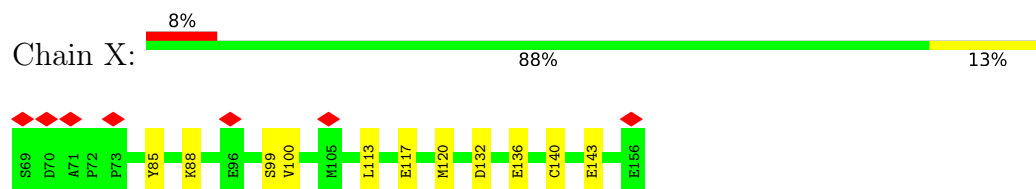
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



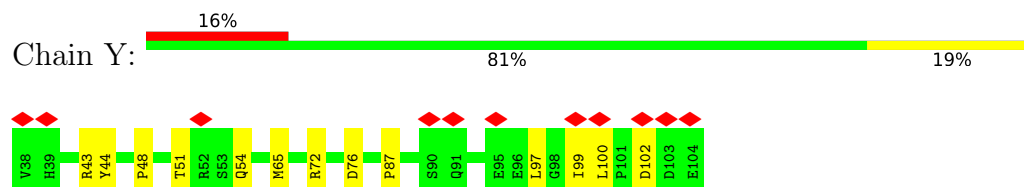
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



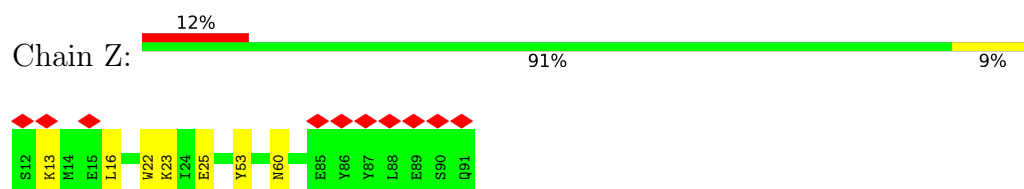
- Molecule 6: Acyl carrier protein



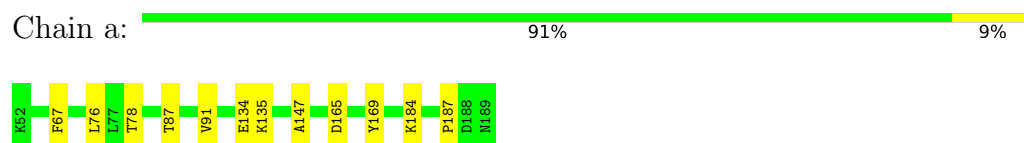
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



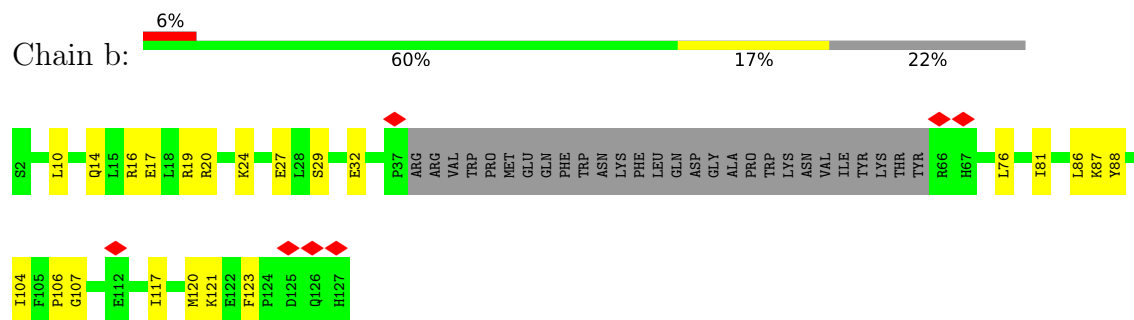
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



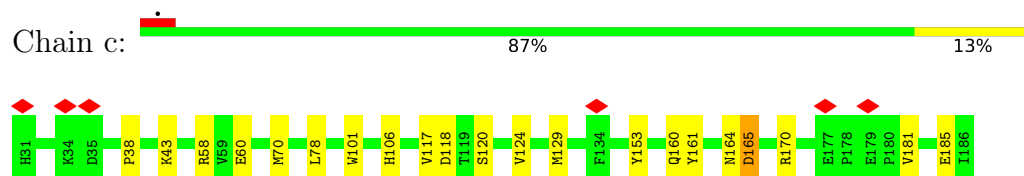
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



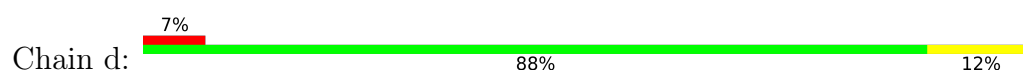
- Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



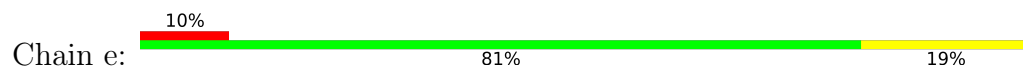
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



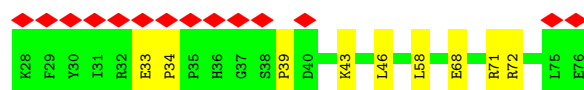
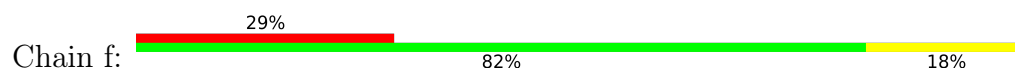
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



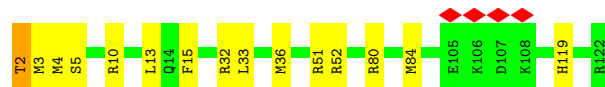
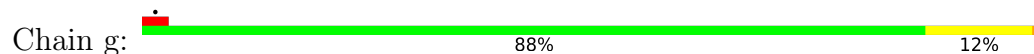
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



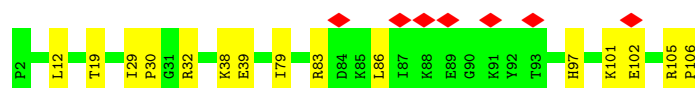
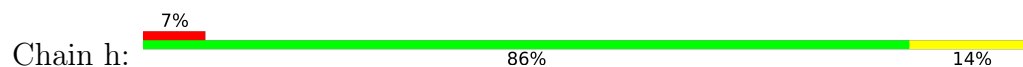
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



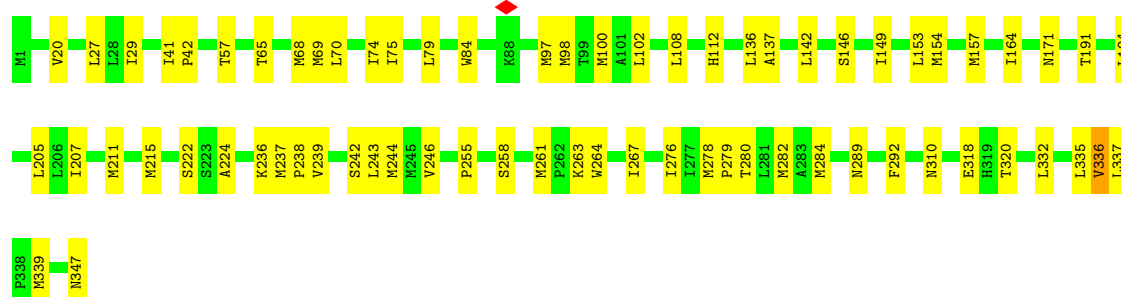
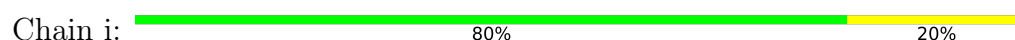
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2



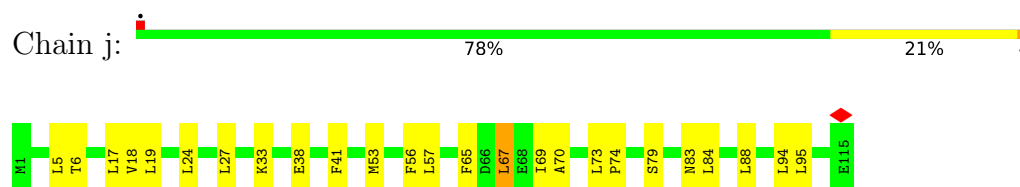
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



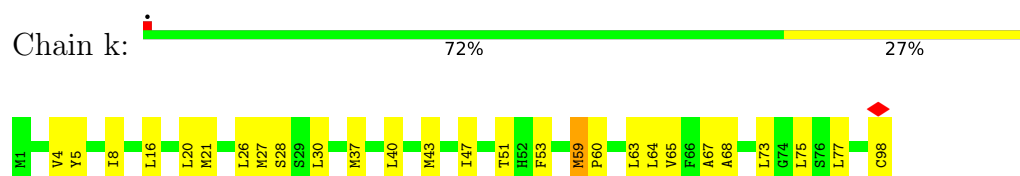
- Molecule 17: NADH-ubiquinone oxidoreductase chain 2



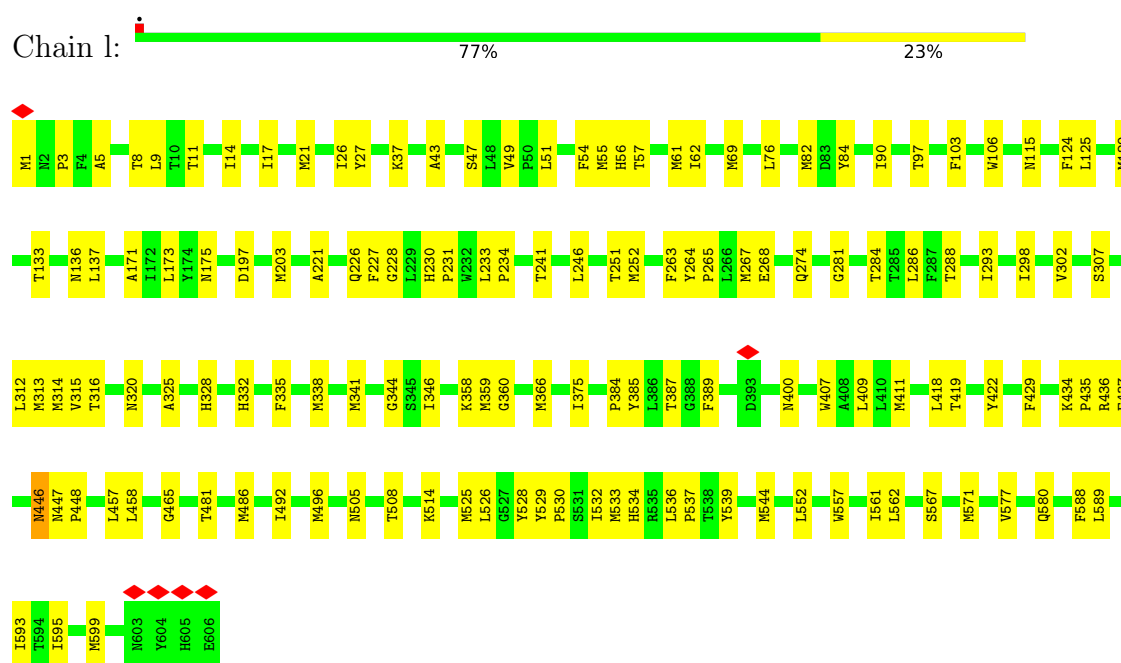
- Molecule 18: NADH-ubiquinone oxidoreductase chain 3



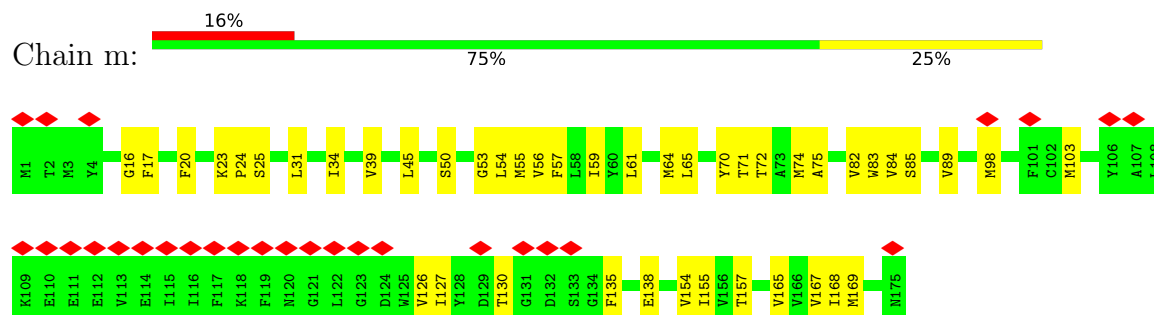
- Molecule 19: NADH-ubiquinone oxidoreductase chain 4L



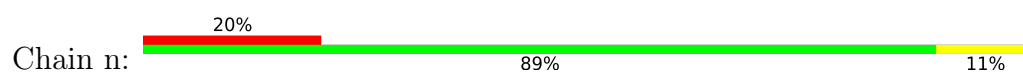
- Molecule 20: NADH-ubiquinone oxidoreductase chain 5



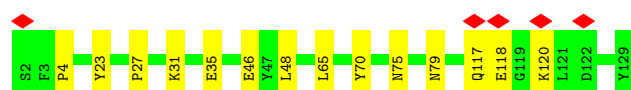
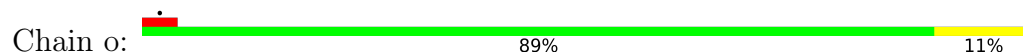
- Molecule 21: NADH-ubiquinone oxidoreductase chain 6



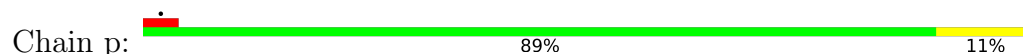
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



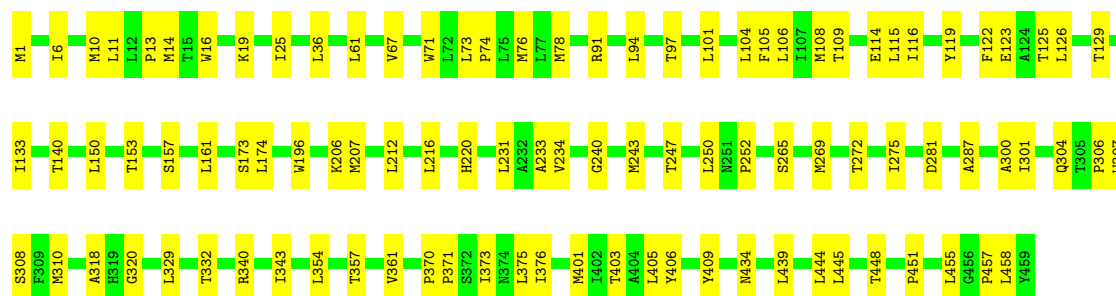
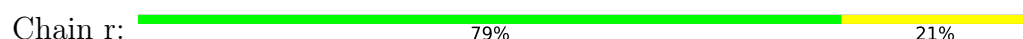
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



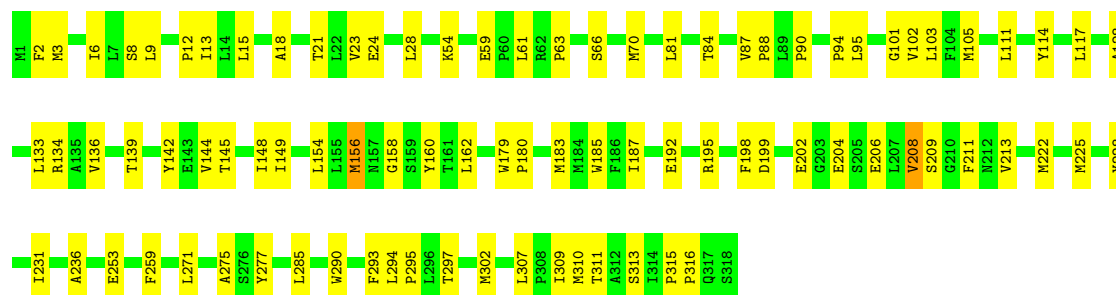
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 25: NADH-ubiquinone oxidoreductase chain 4

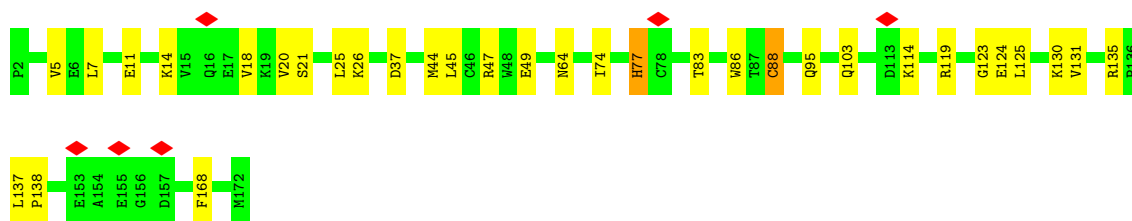


- Molecule 26: NADH-ubiquinone oxidoreductase chain 1



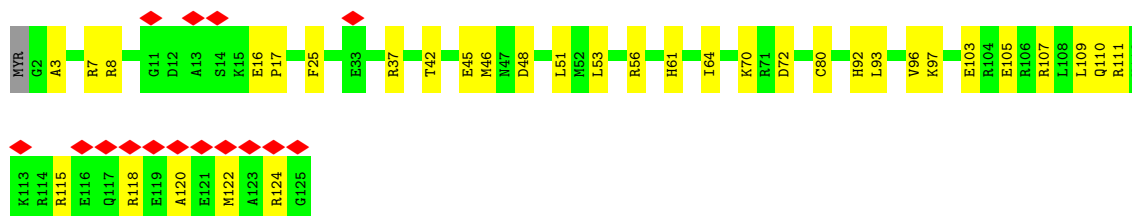
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:  81% 18%



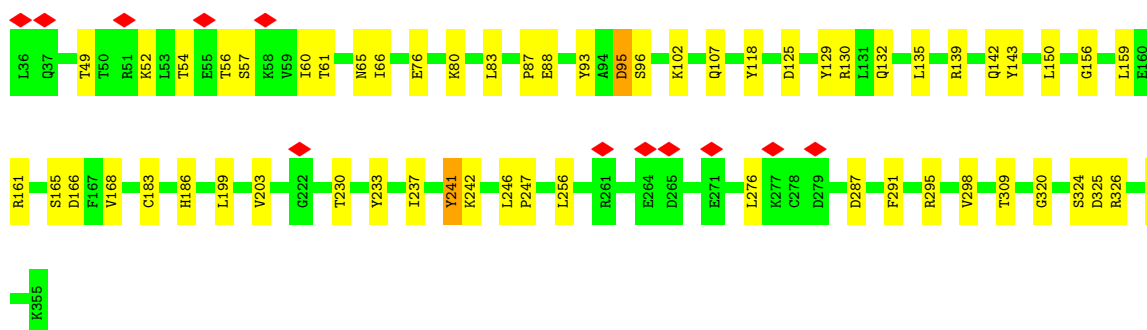
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v:  12% 72% 27%



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

Chain w:  82% 18%



R355

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	152604	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	0.155	Depositor
Minimum map value	-0.081	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0301	Depositor
Map size ($\text{\AA}$)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	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, PLX, 8Q1, PEE, UQ, 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	0.11	0/380	0.27	0/525
2	S	0.12	0/581	0.38	0/781
3	U	0.11	0/664	0.28	0/912
4	V	0.11	0/1042	0.25	0/1411
5	W	0.14	0/973	0.30	0/1312
6	X	0.11	0/716	0.27	0/968
7	Y	0.14	0/610	0.35	0/836
8	Z	0.11	0/660	0.26	0/892
9	a	0.11	0/1184	0.25	0/1603
10	b	0.14	0/844	0.35	0/1149
11	c	0.12	0/1371	0.33	0/1875
12	d	0.12	0/1494	0.31	0/2015
13	e	0.11	0/891	0.31	0/1210
14	f	0.17	0/386	0.42	0/523
15	g	0.10	0/1031	0.26	0/1394
16	h	0.13	0/889	0.33	0/1190
17	i	0.14	0/2773	0.32	0/3768
18	j	0.22	0/938	0.48	0/1281
19	k	0.16	0/759	0.36	0/1029
20	l	0.12	0/4929	0.32	1/6704 (0.0%)
21	m	0.18	0/1328	0.39	0/1804
22	n	0.09	0/491	0.25	0/663
23	o	0.12	0/1092	0.29	0/1481
24	p	0.18	0/1590	0.37	0/2155
25	r	0.14	0/3723	0.34	0/5078
26	s	0.20	0/2581	0.44	1/3529 (0.0%)
27	u	0.11	0/1436	0.32	0/1938
28	v	0.12	0/1083	0.36	0/1448
29	w	0.11	0/2642	0.28	0/3580
All	All	0.14	0/39081	0.33	2/53054 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	l	26	ILE	N-CA-C	-7.19	106.88	113.71
26	s	290	TRP	N-CA-C	5.09	116.91	111.36

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	363	0	332	8	0
2	S	566	0	561	12	0
3	U	643	0	642	11	0
4	V	1021	0	1025	14	0
5	W	949	0	935	20	0
6	X	704	0	695	7	0
7	Y	584	0	529	14	0
8	Z	641	0	620	5	0
9	a	1151	0	1164	11	0
10	b	819	0	835	17	0
11	c	1315	0	1208	18	0
12	d	1461	0	1429	18	0
13	e	867	0	817	17	0
14	f	378	0	356	8	0
15	g	1000	0	994	14	0
16	h	867	0	873	14	0
17	i	2710	0	2874	51	0
18	j	914	0	951	34	0
19	k	748	0	799	27	0
20	l	4800	0	4939	105	0
21	m	1295	0	1263	40	0
22	n	479	0	486	5	0
23	o	1062	0	1072	11	0
24	p	1534	0	1470	21	0
25	r	3631	0	3839	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	s	2508	0	2607	72	0
27	u	1398	0	1374	26	0
28	v	1059	0	1029	30	0
29	w	2582	0	2531	37	0
30	Q	47	0	71	2	0
30	W	41	0	59	1	0
30	j	51	0	82	6	0
30	l	137	0	205	6	0
30	r	51	0	82	3	0
30	s	92	0	141	8	0
31	V	194	0	294	9	0
31	a	100	0	156	5	0
31	g	100	0	156	10	0
31	k	100	0	156	13	0
31	l	199	0	307	11	0
31	n	55	0	54	2	0
31	s	89	0	125	5	0
32	X	35	0	0	5	0
33	a	52	0	88	0	0
33	g	52	0	88	5	0
33	j	104	0	176	3	0
33	r	104	0	176	7	0
34	s	38	0	47	3	0
35	w	27	0	11	1	0
All	All	39717	0	40723	640	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 8.

All (640) 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)
26:s:156:MET:HE3	26:s:156:MET:HA	1.37	1.04
18:j:73:LEU:HD12	21:m:55:MET:SD	2.03	0.99
18:j:79:SER:O	18:j:84:LEU:HD21	1.73	0.88
26:s:156:MET:HA	26:s:156:MET:CE	2.11	0.80
26:s:81:LEU:HD11	26:s:111:LEU:HG	1.64	0.79
17:i:68:MET:HE1	19:k:37:MET:HE2	1.65	0.77
28:v:16:GLU:HG3	28:v:17:PRO:HD2	1.66	0.76
31:V:202:CDL:H712	31:V:202:CDL:H512	1.68	0.76
21:m:72:THR:HG21	26:s:133:LEU:HD21	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:360:GLY:HA3	20:l:435:PRO:HA	1.67	0.75
10:b:106:PRO:HG2	10:b:120:MET:HE2	1.69	0.75
32:X:201:8Q1:C11	24:p:70:GLU:HG2	2.16	0.75
5:W:81:ARG:NH2	27:u:64:ASN:OD1	2.20	0.74
17:i:146:SER:HA	17:i:149:ILE:HG12	1.69	0.74
18:j:67:LEU:CD2	19:k:68:ALA:HB2	2.18	0.74
24:p:54:GLU:OE2	24:p:59:LYS:HG2	1.88	0.73
15:g:2:THR:N	15:g:5:SER:HG	1.87	0.72
12:d:38:ASP:OD1	12:d:39:LEU:N	2.23	0.72
18:j:69:ILE:HD11	26:s:144:VAL:HG13	1.70	0.72
23:o:75:ASN:O	23:o:79:ASN:ND2	2.23	0.71
18:j:73:LEU:CD1	21:m:55:MET:SD	2.78	0.71
29:w:57:SER:HB3	29:w:150:LEU:HD11	1.70	0.71
11:c:185:GLU:OE2	28:v:97:LYS:NZ	2.22	0.70
30:Q:101:PEE:H37	30:Q:101:PEE:H60	1.75	0.69
15:g:3:MET:HG2	15:g:4:MET:HG2	1.73	0.69
25:r:307:TRP:HA	25:r:310:MET:HE2	1.74	0.69
21:m:64:MET:HE2	21:m:64:MET:HA	1.76	0.68
20:l:173:LEU:HD12	25:r:405:LEU:HD21	1.76	0.68
20:l:525:MET:HE2	24:p:77:PRO:HB3	1.76	0.68
25:r:11:LEU:HD23	25:r:14:MET:HE1	1.76	0.68
15:g:15:PHE:HB2	33:g:201:PLX:H6	1.75	0.68
18:j:73:LEU:N	18:j:74:PRO:HD2	2.09	0.67
31:s:402:CDL:H332	31:s:402:CDL:H182	1.77	0.67
17:i:215:MET:HE1	17:i:244:MET:HG3	1.74	0.67
20:l:228:GLY:HA3	30:l:704:PEE:H38	1.77	0.66
20:l:387:THR:HG22	20:l:465:GLY:H	1.60	0.66
3:U:26:GLY:O	3:U:30:ILE:HD12	1.96	0.65
6:X:140:CYS:HB2	6:X:143:GLU:HG3	1.76	0.65
19:k:59:MET:HG3	19:k:60:PRO:HD3	1.78	0.65
20:l:5:ALA:HB2	20:l:61:MET:HE1	1.79	0.65
2:S:19:PRO:HB3	26:s:9:LEU:HD12	1.78	0.64
11:c:165:ASP:OD1	11:c:170:ARG:NH1	2.30	0.64
26:s:81:LEU:HD11	26:s:111:LEU:CG	2.28	0.64
23:o:23:TYR:OH	24:p:68:GLU:HG3	1.97	0.64
29:w:132:GLN:NE2	29:w:166:ASP:OD1	2.30	0.64
18:j:67:LEU:HD21	19:k:68:ALA:HB2	1.79	0.64
10:b:86:LEU:HD11	20:l:9:LEU:HD12	1.78	0.64
13:e:89:VAL:HG21	25:r:25:ILE:HG23	1.79	0.64
31:l:703:CDL:H592	31:l:703:CDL:H762	1.79	0.64
5:W:121:MET:HB2	21:m:130:THR:HG22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:s:253:GLU:N	26:s:253:GLU:OE1	2.29	0.63
7:Y:100:LEU:HB2	28:v:111:ARG:HH12	1.64	0.63
28:v:92:HIS:O	28:v:96:VAL:HG23	1.98	0.63
31:g:202:CDL:H241	31:g:202:CDL:H782	1.79	0.63
17:i:280:THR:O	17:i:284:MET:HG2	1.99	0.62
29:w:60:ILE:HG12	29:w:203:VAL:HB	1.81	0.62
20:l:103:PHE:HB2	20:l:341:MET:HE3	1.81	0.62
21:m:34:ILE:HG13	21:m:64:MET:HG3	1.81	0.62
25:r:67:VAL:HG12	33:r:503:PLX:H362	1.80	0.62
10:b:87:LYS:HG3	20:l:1:MET:HG2	1.82	0.61
18:j:19:LEU:HD11	30:s:401:PEE:H56	1.82	0.61
21:m:82:VAL:HG21	31:s:402:CDL:HB31	1.82	0.61
4:V:26:THR:HB	4:V:68:ALA:HB2	1.82	0.61
17:i:142:LEU:HB3	17:i:194:LEU:HD21	1.82	0.61
4:V:124:LEU:HD11	30:r:501:PEE:H64	1.82	0.61
18:j:56:PHE:HB2	21:m:70:TYR:OH	2.00	0.61
5:W:90:ASN:ND2	5:W:123:GLU:O	2.34	0.61
26:s:87:VAL:HG12	26:s:95:LEU:HD23	1.83	0.61
26:s:28:LEU:HD22	26:s:275:ALA:HB2	1.82	0.60
2:S:66:LEU:HD11	27:u:74:ILE:HG22	1.83	0.60
31:l:702:CDL:H621	31:l:702:CDL:H432	1.83	0.60
18:j:6:THR:HG21	26:s:87:VAL:HG11	1.82	0.60
23:o:65:LEU:HD11	25:r:343:ILE:HD11	1.84	0.60
25:r:272:THR:HA	25:r:275:ILE:HD12	1.82	0.60
29:w:139:ARG:NH1	29:w:166:ASP:OD2	2.35	0.60
11:c:70:MET:HE3	11:c:70:MET:HA	1.82	0.60
20:l:106:TRP:CD1	20:l:447:ASN:HD22	2.20	0.60
31:l:702:CDL:H452	25:r:445:LEU:HB3	1.84	0.59
3:U:25:ILE:HG12	30:s:403:PEE:H38	1.84	0.59
17:i:108:LEU:HD11	17:i:191:THR:HG21	1.83	0.59
21:m:71:THR:HA	21:m:75:ALA:HB3	1.83	0.59
10:b:10:LEU:HG	10:b:14:GLN:HE21	1.68	0.59
25:r:73:LEU:HA	25:r:76:MET:HE2	1.85	0.59
5:W:128:ARG:NH1	16:h:102:GLU:OE2	2.35	0.59
31:l:702:CDL:H391	25:r:371:PRO:HD2	1.85	0.59
18:j:65:PHE:O	18:j:69:ILE:HD13	2.02	0.59
23:o:31:LYS:O	23:o:35:GLU:HG2	2.03	0.58
20:l:227:PHE:O	20:l:230:HIS:ND1	2.36	0.58
17:i:276:ILE:HG21	30:r:501:PEE:H7	1.85	0.58
29:w:125:ASP:O	29:w:130:ARG:NH2	2.36	0.58
21:m:61:LEU:O	26:s:114:TYR:OH	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:23:LYS:HB3	8:Z:25:GLU:HG2	1.84	0.58
17:i:42:PRO:HG3	21:m:167:VAL:HG13	1.84	0.58
25:r:212:LEU:HD21	33:r:502:PLX:H212	1.86	0.58
27:u:49:GLU:OE1	27:u:135:ARG:NH2	2.36	0.58
9:a:134:GLU:OE1	22:n:57:TRP:NE1	2.26	0.58
26:s:63:PRO:HB2	26:s:66:SER:HB3	1.85	0.58
31:g:202:CDL:H361	17:i:243:LEU:HD23	1.85	0.58
28:v:103:GLU:O	28:v:107:ARG:HG2	2.04	0.58
26:s:117:LEU:HD21	26:s:136:VAL:HG23	1.87	0.57
17:i:154:MET:HE3	17:i:154:MET:HA	1.86	0.57
17:i:236:LYS:HG3	17:i:237:MET:HG3	1.86	0.57
31:a:201:CDL:H401	12:d:44:PRO:HB3	1.87	0.57
25:r:78:MET:HE1	25:r:439:LEU:HD12	1.87	0.57
12:d:60:ARG:HH11	12:d:60:ARG:HG3	1.68	0.57
31:g:202:CDL:HA31	17:i:238:PRO:HB2	1.87	0.57
19:k:65:VAL:HG11	21:m:157:THR:HG23	1.85	0.57
26:s:307:LEU:HA	26:s:310:MET:HE2	1.87	0.57
25:r:122:PHE:HZ	25:r:206:LYS:HG3	1.70	0.56
18:j:70:ALA:CB	21:m:55:MET:HE2	2.35	0.56
17:i:207:ILE:HG22	17:i:211:MET:HE2	1.88	0.56
5:W:85:GLN:OE1	16:h:105:ARG:NH1	2.33	0.56
18:j:33:LYS:HG2	26:s:61:LEU:HD11	1.88	0.56
31:k:101:CDL:H462	31:k:101:CDL:H402	1.88	0.56
20:l:274:GLN:NE2	20:l:320:ASN:OD1	2.39	0.56
14:f:68:GLU:OE1	14:f:72:ARG:HG3	2.05	0.55
11:c:129:MET:HB3	20:l:528:TYR:CG	2.42	0.55
9:a:78:THR:HG21	13:e:96:SER:HA	1.88	0.55
20:l:359:MET:O	20:l:436:ARG:NH2	2.40	0.55
7:Y:87:PRO:HG3	28:v:96:VAL:HG13	1.88	0.55
17:i:289:ASN:HA	17:i:292:PHE:CE2	2.41	0.55
5:W:93:GLU:O	5:W:97:ILE:HG13	2.06	0.55
10:b:81:ILE:HG23	30:l:705:PEE:H58	1.88	0.55
20:l:481:THR:OG1	28:v:92:HIS:ND1	2.27	0.54
17:i:57:THR:HA	19:k:77:LEU:HD13	1.90	0.54
20:l:69:MET:HG3	20:l:76:LEU:HB2	1.89	0.54
20:l:492:ILE:O	20:l:496:MET:HG2	2.08	0.54
29:w:54:THR:HG23	29:w:56:THR:HG22	1.90	0.54
4:V:22:ALA:O	4:V:26:THR:HG22	2.07	0.54
4:V:38:ALA:HB2	31:k:101:CDL:H251	1.89	0.54
28:v:17:PRO:HB3	28:v:105:GLU:HG2	1.88	0.54
26:s:198:PHE:CD1	26:s:285:LEU:HD13	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:c:58:ARG:NH2	11:c:60:GLU:OE2	2.41	0.53
4:V:17:GLU:OE1	4:V:20:ARG:NH1	2.36	0.53
6:X:85:TYR:OH	8:Z:22:TRP:NE1	2.26	0.53
10:b:121:LYS:O	10:b:121:LYS:HG3	2.08	0.53
3:U:27:GLY:O	3:U:31:ILE:HG23	2.09	0.53
17:i:42:PRO:HG2	21:m:167:VAL:HG22	1.89	0.53
29:w:256:LEU:HD11	29:w:276:LEU:HD11	1.90	0.53
19:k:28:SER:HB3	21:m:23:LYS:HG2	1.90	0.53
21:m:17:PHE:HA	21:m:20:PHE:CE2	2.43	0.53
7:Y:97:LEU:HD12	28:v:107:ARG:HD2	1.91	0.53
20:l:69:MET:HE3	25:r:451:PRO:HG2	1.91	0.53
12:d:127:LYS:NZ	12:d:127:LYS:HB3	2.24	0.53
13:e:98:VAL:HG22	25:r:36:LEU:HB2	1.90	0.53
15:g:10:ARG:NH2	17:i:347:ASN:O	2.42	0.52
5:W:82:ARG:NH1	16:h:106:PRO:O	2.43	0.52
13:e:55:LEU:HD23	29:w:320:GLY:HA2	1.90	0.52
18:j:67:LEU:HD23	19:k:68:ALA:CB	2.39	0.52
19:k:51:THR:O	19:k:53:PHE:N	2.42	0.52
25:r:91:ARG:NH2	29:w:325:ASP:OD2	2.42	0.52
2:S:54:ILE:HD11	16:h:106:PRO:HB3	1.90	0.52
31:k:101:CDL:H632	31:k:101:CDL:H802	1.90	0.52
26:s:18:ALA:O	26:s:21:THR:OG1	2.27	0.52
25:r:196:TRP:CD1	25:r:250:LEU:HB3	2.44	0.52
25:r:310:MET:HB3	25:r:455:LEU:HD22	1.90	0.52
20:l:536:LEU:HB3	20:l:537:PRO:HD3	1.91	0.52
20:l:544:MET:HE2	20:l:544:MET:HA	1.92	0.52
29:w:65:ASN:OD1	29:w:66:ILE:N	2.39	0.52
20:l:264:TYR:O	20:l:268:GLU:HG2	2.09	0.52
25:r:403:THR:HA	25:r:406:TYR:CE2	2.45	0.52
26:s:24:GLU:HA	26:s:271:LEU:HD13	1.91	0.52
6:X:99:SER:OG	6:X:100:VAL:N	2.42	0.52
21:m:82:VAL:HG13	21:m:84:VAL:H	1.74	0.52
26:s:149:ILE:HG21	26:s:185:TRP:HB2	1.92	0.52
32:X:201:8Q1:C10	24:p:70:GLU:HG2	2.39	0.52
31:l:702:CDL:H242	30:l:705:PEE:H34	1.92	0.52
23:o:118:GLU:OE2	23:o:120:LYS:HG2	2.10	0.52
27:u:83:THR:HA	27:u:86:TRP:CD1	2.44	0.52
20:l:56:HIS:CD2	20:l:57:THR:HG23	2.44	0.51
17:i:278:MET:O	17:i:282:MET:HG3	2.11	0.51
5:W:63:GLU:OE2	27:u:119:ARG:NH2	2.44	0.51
5:W:97:ILE:HD13	16:h:83:ARG:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:j:88:LEU:HD13	26:s:309:ILE:HD12	1.92	0.51
19:k:21:MET:HB3	31:k:101:CDL:HB61	1.92	0.51
18:j:83:ASN:OD1	18:j:83:ASN:N	2.43	0.51
26:s:12:PRO:HA	26:s:15:LEU:HD12	1.93	0.51
5:W:88:ARG:NH2	27:u:7:LEU:O	2.44	0.51
12:d:69:ARG:NH2	22:n:46:LYS:O	2.43	0.51
20:l:298:ILE:O	20:l:302:VAL:HG23	2.10	0.51
26:s:102:VAL:HG23	26:s:160:TYR:O	2.09	0.51
31:a:201:CDL:H772	31:a:201:CDL:H212	1.93	0.51
18:j:24:LEU:HD13	33:j:202:PLX:H101	1.92	0.51
20:l:346:ILE:HA	20:l:366:MET:HE1	1.92	0.51
29:w:49:THR:HG21	29:w:291:PHE:HB3	1.93	0.51
6:X:120:MET:HE1	24:p:24:LEU:HB3	1.93	0.51
11:c:160:GLN:OE1	28:v:37:ARG:NH1	2.43	0.51
7:Y:72:ARG:NE	7:Y:76:ASP:OD2	2.39	0.50
33:j:203:PLX:H352	21:m:155:ILE:HG23	1.93	0.50
20:l:532:ILE:HG22	20:l:533:MET:HE2	1.93	0.50
33:g:201:PLX:H232	17:i:332:LEU:HB3	1.93	0.50
1:Q:39:PRO:HB3	1:Q:43:TRP:CD1	2.47	0.50
5:W:98:MET:HE3	5:W:101:VAL:HG21	1.94	0.50
20:l:407:TRP:O	20:l:411:MET:HG2	2.11	0.50
2:S:50:ARG:NH2	27:u:18:VAL:O	2.44	0.50
17:i:112:HIS:CE1	17:i:164:ILE:HD13	2.47	0.50
18:j:73:LEU:N	18:j:74:PRO:CD	2.75	0.50
21:m:55:MET:O	21:m:59:ILE:HG12	2.12	0.50
11:c:117:VAL:HG11	20:l:539:TYR:HB2	1.93	0.50
13:e:97:ILE:O	13:e:101:LEU:HB2	2.12	0.50
15:g:80:ARG:O	15:g:84:MET:HG2	2.11	0.50
20:l:246:LEU:O	20:l:251:THR:OG1	2.30	0.50
27:u:26:LYS:NZ	27:u:95:GLN:O	2.36	0.50
27:u:11:GLU:HA	27:u:14:LYS:HG3	1.94	0.50
18:j:67:LEU:HD23	19:k:68:ALA:HB2	1.93	0.50
26:s:102:VAL:HG21	26:s:154:LEU:HD11	1.93	0.50
10:b:123:PHE:CZ	28:v:61:HIS:HB2	2.47	0.50
21:m:24:PRO:HG3	21:m:83:TRP:NE1	2.27	0.50
27:u:77:HIS:ND1	27:u:114:LYS:HB3	2.27	0.50
28:v:46:MET:HE3	28:v:56:ARG:HD3	1.94	0.50
11:c:124:VAL:HG23	20:l:525:MET:HE1	1.94	0.50
17:i:27:LEU:HD22	19:k:59:MET:HB2	1.94	0.50
1:Q:47:PHE:HD1	1:Q:52:MET:HE1	1.77	0.49
25:r:119:TYR:CZ	25:r:161:LEU:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:s:187:ILE:HD12	30:s:403:PEE:H52	1.94	0.49
12:d:115:GLN:HG2	20:l:62:ILE:HG12	1.94	0.49
18:j:57:LEU:HD21	21:m:169:MET:SD	2.52	0.49
13:e:78:LYS:HB2	13:e:78:LYS:NZ	2.27	0.49
26:s:294:LEU:HB3	26:s:295:PRO:HD3	1.94	0.49
32:X:201:8Q1:C13	24:p:71:PHE:HA	2.43	0.49
15:g:10:ARG:NH1	33:g:201:PLX:O3	2.45	0.49
17:i:136:LEU:HD23	17:i:205:LEU:HD21	1.95	0.49
19:k:5:TYR:HB3	19:k:43:MET:HE1	1.94	0.49
29:w:118:TYR:OH	35:w:401:ADP:O2'	2.30	0.49
4:V:53:VAL:HG12	31:k:101:CDL:H341	1.94	0.49
31:V:201:CDL:H532	20:l:577:VAL:HG22	1.93	0.49
11:c:38:PRO:HG2	23:o:70:TYR:HD2	1.78	0.49
11:c:161:TYR:HB2	11:c:165:ASP:HA	1.95	0.49
17:i:75:ILE:HD12	19:k:40:LEU:HD22	1.94	0.49
20:l:129:MET:O	20:l:133:THR:OG1	2.26	0.49
20:l:97:THR:HG21	20:l:125:LEU:HD22	1.95	0.49
20:l:375:ILE:HD12	20:l:458:LEU:HD11	1.94	0.49
25:r:216:LEU:HD23	25:r:287:ALA:HB1	1.95	0.49
25:r:243:MET:HB3	25:r:301:ILE:HG21	1.95	0.49
26:s:134:ARG:NH1	26:s:206:GLU:OE1	2.44	0.49
31:V:201:CDL:H512	20:l:580:GLN:HE22	1.78	0.48
20:l:526:LEU:HD12	20:l:530:PRO:HG2	1.95	0.48
26:s:209:SER:HB3	26:s:213:VAL:HA	1.94	0.48
5:W:43:LEU:HG	26:s:179:TRP:HE1	1.78	0.48
34:s:404:UQ:H221	34:s:404:UQ:H262	1.68	0.48
17:i:261:MET:HB2	17:i:337:LEU:HD12	1.94	0.48
20:l:400:ASN:HB3	20:l:486:MET:HE3	1.94	0.48
20:l:136:ASN:HA	20:l:197:ASP:HA	1.94	0.48
20:l:530:PRO:O	20:l:534:HIS:HB2	2.13	0.48
25:r:445:LEU:HA	25:r:448:THR:HG22	1.95	0.48
31:a:201:CDL:H782	13:e:100:VAL:HG22	1.95	0.48
31:s:402:CDL:H171	31:s:402:CDL:H141	1.67	0.48
26:s:179:TRP:O	26:s:183:MET:HG3	2.13	0.48
5:W:66:GLU:OE2	27:u:123:GLY:N	2.37	0.48
9:a:184:LYS:HB3	16:h:30:PRO:HB3	1.96	0.48
18:j:94:LEU:HD13	21:m:154:VAL:HG13	1.94	0.48
20:l:171:ALA:O	20:l:175:ASN:ND2	2.47	0.48
31:g:202:CDL:H392	17:i:246:VAL:HG11	1.95	0.47
20:l:561:ILE:HG13	20:l:562:LEU:H	1.79	0.47
27:u:137:LEU:HD12	27:u:138:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:101:GLU:OE1	12:d:101:GLU:HA	2.14	0.47
13:e:58:ASP:OD2	29:w:326:ARG:NE	2.38	0.47
31:V:202:CDL:H792	31:V:202:CDL:H761	1.68	0.47
11:c:78:LEU:HB2	11:c:106:HIS:HD2	1.78	0.47
15:g:32:ARG:HB3	17:i:339:MET:HE1	1.96	0.47
13:e:125:LEU:HD23	13:e:129:ARG:HH21	1.79	0.47
5:W:105:LYS:HB3	5:W:108:GLU:HB2	1.96	0.47
10:b:104:ILE:HB	28:v:48:ASP:HB3	1.96	0.47
17:i:97:MET:HG2	20:l:599:MET:HE1	1.95	0.47
25:r:281:ASP:OD1	25:r:340:ARG:HB3	2.14	0.47
25:r:354:LEU:O	25:r:357:THR:HG22	2.14	0.47
26:s:148:ILE:CG2	26:s:297:THR:HG22	2.44	0.47
26:s:198:PHE:CE1	26:s:285:LEU:HD13	2.49	0.47
5:W:50:MET:HE2	26:s:156:MET:HG3	1.97	0.47
17:i:20:VAL:HG13	17:i:29:ILE:HG23	1.96	0.47
26:s:236:ALA:HB1	26:s:259:PHE:HZ	1.79	0.47
28:v:93:LEU:O	28:v:97:LYS:HG3	2.14	0.47
4:V:34:LEU:HG	31:k:101:CDL:H261	1.97	0.47
12:d:114:GLN:HG3	20:l:203:MET:HG2	1.96	0.47
18:j:67:LEU:CD2	19:k:68:ALA:CB	2.89	0.47
20:l:387:THR:HG22	20:l:465:GLY:N	2.27	0.47
24:p:132:SER:OG	24:p:136:GLU:OE2	2.23	0.47
25:r:104:LEU:HG	25:r:108:MET:HE2	1.96	0.47
18:j:79:SER:O	18:j:84:LEU:CD2	2.55	0.47
20:l:429:PHE:HE1	24:p:32:VAL:HG21	1.79	0.47
20:l:338:MET:HB2	20:l:457:LEU:HB3	1.96	0.47
33:j:202:PLX:H12	33:j:202:PLX:H31	1.95	0.47
7:Y:100:LEU:O	28:v:111:ARG:NH1	2.48	0.46
18:j:18:VAL:HG12	30:s:401:PEE:H16	1.97	0.46
19:k:27:MET:HE1	19:k:75:LEU:HD21	1.97	0.46
20:l:313:MET:HG3	20:l:328:HIS:HD2	1.80	0.46
33:r:502:PLX:H101	33:r:502:PLX:H72	1.65	0.46
31:s:402:CDL:H362	31:s:402:CDL:H331	1.55	0.46
20:l:221:ALA:HA	20:l:226:GLN:HG2	1.97	0.46
30:l:701:PEE:H58	30:l:701:PEE:H19	1.97	0.46
26:s:128:ALA:HA	26:s:211:PHE:HA	1.98	0.46
28:v:120:ALA:O	28:v:124:ARG:HG2	2.14	0.46
29:w:61:THR:HG22	29:w:159:LEU:HD12	1.96	0.46
29:w:88:GLU:OE2	29:w:161:ARG:NH1	2.43	0.46
11:c:164:ASN:HA	11:c:181:VAL:HB	1.95	0.46
14:f:71:ARG:HG2	14:f:71:ARG:HH11	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:41:ILE:HG13	19:k:73:LEU:HD21	1.97	0.46
28:v:122:MET:HE3	28:v:122:MET:O	2.15	0.46
24:p:68:GLU:OE1	24:p:68:GLU:HA	2.15	0.46
25:r:122:PHE:CZ	25:r:206:LYS:HG3	2.49	0.46
27:u:88:CYS:SG	27:u:103:GLN:NE2	2.89	0.46
29:w:93:TYR:O	29:w:96:SER:OG	2.34	0.46
29:w:242:LYS:HA	29:w:246:LEU:HD12	1.97	0.46
28:v:3:ALA:O	28:v:7:ARG:HG3	2.16	0.46
5:W:51:MET:HA	26:s:313:SER:HB2	1.98	0.46
7:Y:65:MET:HE3	20:l:375:ILE:HG12	1.98	0.46
17:i:244:MET:HE2	17:i:244:MET:HB2	1.77	0.46
31:k:101:CDL:H161	31:k:101:CDL:H191	1.73	0.46
20:l:446:ASN:OD1	20:l:446:ASN:N	2.48	0.46
26:s:101:GLY:O	26:s:105:MET:HG2	2.15	0.46
28:v:115:ARG:HG3	28:v:118:ARG:HH21	1.81	0.46
11:c:43:LYS:HB2	11:c:43:LYS:HE3	1.60	0.46
12:d:23:GLN:HG2	28:v:72:ASP:HB3	1.97	0.46
33:r:502:PLX:H251	33:r:502:PLX:H51	1.41	0.46
21:m:74:MET:HE2	21:m:74:MET:HB3	1.76	0.46
1:Q:76:LEU:H	1:Q:76:LEU:HD23	1.80	0.46
4:V:29:GLY:O	4:V:63:SER:HB3	2.16	0.46
4:V:101:LEU:O	4:V:105:THR:HG23	2.15	0.46
16:h:32:ARG:HH21	19:k:51:THR:HG22	1.81	0.46
26:s:236:ALA:HB1	26:s:259:PHE:CZ	2.51	0.46
27:u:45:LEU:HD22	27:u:131:VAL:HG13	1.98	0.46
9:a:147:ALA:HB2	25:r:173:SER:HB2	1.98	0.46
20:l:384:PRO:HA	20:l:389:PHE:CD1	2.51	0.46
1:Q:60:HIS:O	1:Q:62:LYS:NZ	2.49	0.45
20:l:529:TYR:HB3	20:l:530:PRO:HD3	1.98	0.45
31:l:702:CDL:H812	33:r:503:PLX:H202	1.96	0.45
31:l:702:CDL:HA61	31:l:702:CDL:H312	1.59	0.45
24:p:71:PHE:CD1	24:p:71:PHE:C	2.94	0.45
29:w:230:THR:HG23	29:w:233:TYR:H	1.81	0.45
3:U:38:TYR:HD1	3:U:41:TYR:HD2	1.64	0.45
20:l:264:TYR:CD2	20:l:265:PRO:HD3	2.51	0.45
20:l:514:LYS:HB2	20:l:514:LYS:HE2	1.68	0.45
23:o:4:PRO:HD2	24:p:73:TYR:CE1	2.51	0.45
25:r:114:GLU:OE1	25:r:116:ILE:HB	2.16	0.45
21:m:82:VAL:HG12	21:m:85:SER:HB3	1.99	0.45
31:n:101:CDL:H742	31:n:101:CDL:H772	1.66	0.45
29:w:83:LEU:HD22	29:w:156:GLY:HA3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:W:201:PEE:H28	30:W:201:PEE:H57	1.99	0.45
32:X:201:8Q1:C11	24:p:44:MET:HE1	2.46	0.45
15:g:52:ARG:NH2	17:i:318:GLU:OE1	2.43	0.45
17:i:267:ILE:HG12	17:i:279:PRO:HB3	1.98	0.45
20:l:529:TYR:CZ	20:l:533:MET:HG3	2.51	0.45
27:u:103:GLN:OE1	27:u:103:GLN:N	2.47	0.45
15:g:51:ARG:HG3	15:g:51:ARG:HH11	1.81	0.45
17:i:70:LEU:HG	17:i:98:MET:SD	2.57	0.45
31:k:101:CDL:H611	31:k:101:CDL:H581	1.63	0.45
25:r:306:PRO:HA	25:r:458:LEU:HG	1.97	0.45
12:d:60:ARG:HG3	12:d:60:ARG:NH1	2.29	0.45
25:r:126:LEU:HD23	25:r:150:LEU:HD12	1.97	0.45
25:r:373:ILE:HA	25:r:376:ILE:HD12	1.98	0.45
10:b:88:TYR:CE1	12:d:49:ARG:HG2	2.52	0.45
19:k:4:VAL:O	19:k:8:ILE:HG12	2.16	0.45
19:k:16:LEU:HD23	31:k:101:CDL:H841	1.99	0.45
20:l:338:MET:HE2	20:l:338:MET:HB3	1.84	0.45
21:m:53:GLY:HA2	21:m:56:VAL:HG12	1.97	0.45
31:n:101:CDL:H581	31:n:101:CDL:H552	1.63	0.45
24:p:54:GLU:OE2	24:p:59:LYS:CG	2.62	0.45
27:u:47:ARG:HD2	27:u:47:ARG:HA	1.79	0.45
9:a:169:TYR:CZ	15:g:3:MET:HB2	2.52	0.45
15:g:36:MET:HE3	15:g:36:MET:HB3	1.84	0.45
20:l:233:LEU:HB3	20:l:234:PRO:HD3	1.98	0.45
31:l:703:CDL:H712	31:l:703:CDL:H312	1.97	0.45
23:o:48:LEU:HB3	24:p:166:LEU:HD13	1.99	0.45
28:v:110:GLN:HA	28:v:110:GLN:OE1	2.17	0.45
3:U:66:VAL:O	27:u:130:LYS:HE3	2.17	0.45
6:X:88:LYS:HE2	6:X:88:LYS:HB2	1.73	0.45
31:a:201:CDL:H361	31:a:201:CDL:H392	1.46	0.45
17:i:255:PRO:HG2	25:r:123:GLU:HB2	1.99	0.45
20:l:293:ILE:HD13	20:l:418:LEU:HD22	1.98	0.45
20:l:411:MET:HA	20:l:411:MET:HE2	1.99	0.45
21:m:57:PHE:O	21:m:61:LEU:HG	2.17	0.45
29:w:87:PRO:O	29:w:142:GLN:NE2	2.49	0.45
6:X:113:LEU:O	6:X:117:GLU:HG3	2.17	0.44
14:f:43:LYS:HA	14:f:46:LEU:HD23	1.99	0.44
20:l:281:GLY:HA3	20:l:314:MET:HB3	1.97	0.44
20:l:419:THR:HA	20:l:422:TYR:CE2	2.52	0.44
26:s:228:TYR:HA	26:s:231:ILE:HD12	2.00	0.44
16:h:19:THR:HA	17:i:84:TRP:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:153:LEU:HG	17:i:157:MET:HE2	1.98	0.44
31:k:101:CDL:H192	20:l:593:ILE:HD11	1.99	0.44
20:l:61:MET:HE3	20:l:61:MET:HB3	1.78	0.44
20:l:230:HIS:N	20:l:231:PRO:HD3	2.32	0.44
29:w:129:TYR:OH	29:w:186:HIS:ND1	2.36	0.44
4:V:67:GLY:HA2	31:V:201:CDL:H221	1.99	0.44
12:d:106:ILE:HG13	12:d:135:VAL:HG21	1.99	0.44
18:j:5:LEU:HD21	26:s:3:MET:HG2	1.99	0.44
20:l:332:HIS:HA	20:l:335:PHE:CZ	2.52	0.44
21:m:64:MET:HA	21:m:64:MET:CE	2.43	0.44
22:n:24:GLY:HA2	25:r:6:ILE:HD12	2.00	0.44
27:u:83:THR:HA	27:u:86:TRP:NE1	2.32	0.44
28:v:70:LYS:HE3	28:v:80:CYS:SG	2.58	0.44
11:c:118:ASP:OD1	11:c:120:SER:OG	2.35	0.44
33:g:201:PLX:H102	33:g:201:PLX:H71	1.64	0.44
17:i:69:MET:HE1	17:i:100:MET:HE3	1.99	0.44
25:r:19:LYS:HZ3	25:r:19:LYS:HB2	1.82	0.44
34:s:404:UQ:H202	34:s:404:UQ:H172	1.81	0.44
31:k:101:CDL:H632	31:k:101:CDL:H602	1.70	0.44
20:l:557:TRP:O	20:l:561:ILE:HG12	2.18	0.44
21:m:31:LEU:HD13	26:s:70:MET:HE2	1.99	0.44
21:m:103:MET:HE2	21:m:103:MET:HB3	1.87	0.44
25:r:105:PHE:O	25:r:109:THR:OG1	2.28	0.44
29:w:237:ILE:O	29:w:241:TYR:HB2	2.17	0.44
2:S:12:MET:HE2	26:s:23:VAL:HG21	1.98	0.44
32:X:201:8Q1:C11	24:p:70:GLU:CG	2.90	0.44
18:j:18:VAL:HG23	26:s:222:MET:HE1	2.00	0.44
19:k:20:LEU:HD23	20:l:588:PHE:HD2	1.83	0.44
20:l:54:PHE:CZ	20:l:84:TYR:HB2	2.53	0.44
23:o:27:PRO:O	23:o:31:LYS:HG2	2.18	0.44
26:s:87:VAL:HG23	26:s:88:PRO:HD3	2.00	0.44
26:s:199:ASP:OD1	26:s:199:ASP:N	2.44	0.44
16:h:38:LYS:NZ	16:h:39:GLU:OE2	2.51	0.44
17:i:20:VAL:HG11	17:i:137:ALA:HB1	1.99	0.44
22:n:39:ARG:HG3	22:n:57:TRP:CE2	2.53	0.44
26:s:313:SER:O	26:s:313:SER:OG	2.30	0.44
18:j:38:GLU:HB2	18:j:41:PHE:O	2.17	0.44
25:r:126:LEU:HD11	25:r:153:THR:HG21	2.00	0.44
4:V:39:TYR:HB3	31:V:201:CDL:H712	2.00	0.44
13:e:73:SER:O	13:e:75:GLY:N	2.51	0.44
18:j:73:LEU:O	26:s:160:TYR:OH	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:k:101:CDL:H162	20:l:589:LEU:HD11	2.00	0.44
30:s:403:PEE:H37	30:s:403:PEE:H43	1.60	0.44
9:a:165:ASP:OD1	9:a:165:ASP:N	2.51	0.43
14:f:39:PRO:HD3	29:w:351:TRP:HB3	2.00	0.43
16:h:29:ILE:HG21	21:m:138:GLU:HG2	1.99	0.43
25:r:300:ALA:O	25:r:308:SER:HB3	2.18	0.43
1:Q:40:ASP:OD1	1:Q:40:ASP:N	2.47	0.43
5:W:68:ARG:HD2	21:m:135:PHE:HD2	1.82	0.43
17:i:222:SER:O	17:i:224:ALA:N	2.51	0.43
30:j:201:PEE:H21	30:j:201:PEE:H27	1.61	0.43
25:r:406:TYR:O	25:r:409:TYR:HB3	2.17	0.43
26:s:179:TRP:CG	26:s:180:PRO:HD3	2.54	0.43
2:S:1:MET:HB3	2:S:1:MET:HE3	1.79	0.43
7:Y:72:ARG:HB3	20:l:385:TYR:CD1	2.53	0.43
9:a:87:THR:O	9:a:91:VAL:HG13	2.18	0.43
10:b:107:GLY:H	10:b:117:ILE:HB	1.83	0.43
15:g:119:HIS:CD2	25:r:252:PRO:HG3	2.53	0.43
30:j:201:PEE:H51	30:j:201:PEE:H56	1.86	0.43
25:r:61:LEU:HB2	25:r:457:PRO:HD3	1.99	0.43
30:s:403:PEE:H64	30:s:403:PEE:H58	1.89	0.43
2:S:31:ASN:ND2	2:S:36:LYS:HB2	2.32	0.43
3:U:41:TYR:HE1	3:U:44:ARG:HH21	1.66	0.43
18:j:67:LEU:HD13	18:j:67:LEU:HA	1.69	0.43
26:s:195:ARG:HD3	26:s:231:ILE:HD11	2.00	0.43
29:w:246:LEU:HB2	29:w:247:PRO:HD3	2.00	0.43
29:w:295:ARG:HA	29:w:298:VAL:HG22	2.01	0.43
2:S:27:HIS:ND1	2:S:36:LYS:HD3	2.33	0.43
20:l:227:PHE:N	20:l:284:THR:OG1	2.51	0.43
20:l:571:MET:HE2	20:l:571:MET:HB3	1.77	0.43
30:r:501:PEE:H20	30:r:501:PEE:H49	2.01	0.43
28:v:42:THR:OG1	28:v:45:GLU:HG3	2.18	0.43
31:V:202:CDL:H872	31:V:202:CDL:H841	1.82	0.43
12:d:127:LYS:O	12:d:130:GLU:HG3	2.18	0.43
17:i:65:THR:O	17:i:69:MET:HG3	2.19	0.43
17:i:100:MET:HE1	20:l:595:ILE:HG23	1.99	0.43
25:r:306:PRO:HB3	25:r:458:LEU:HD12	2.01	0.43
26:s:158:GLY:HA3	26:s:315:PRO:HB2	2.01	0.43
3:U:19:LEU:HB3	30:j:201:PEE:H57	2.00	0.43
3:U:26:GLY:HA3	30:j:201:PEE:H37	1.99	0.43
7:Y:65:MET:CE	20:l:375:ILE:HG12	2.49	0.43
9:a:187:PRO:HG3	27:u:47:ARG:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:s:9:LEU:O	26:s:13:ILE:HG12	2.19	0.43
29:w:143:TYR:OH	29:w:199:LEU:O	2.28	0.43
5:W:70:ALA:HB2	27:u:125:LEU:HD13	2.01	0.43
31:g:202:CDL:H391	17:i:335:LEU:HD21	2.01	0.43
17:i:258:SER:OG	17:i:336:VAL:HB	2.19	0.43
30:j:201:PEE:H60	30:j:201:PEE:H55	1.74	0.43
29:w:49:THR:O	29:w:52:LYS:HG2	2.18	0.43
2:S:63:THR:HG23	27:u:21:SER:HB2	2.01	0.43
5:W:128:ARG:NH1	16:h:97:HIS:O	2.52	0.43
8:Z:53:TYR:CE2	20:l:434:LYS:HG3	2.53	0.43
20:l:137:LEU:HD21	20:l:263:PHE:HZ	1.84	0.43
25:r:133:ILE:HD11	25:r:231:LEU:HD11	2.01	0.43
26:s:204:GLU:HA	26:s:208:VAL:O	2.17	0.43
28:v:51:LEU:HD21	28:v:64:ILE:HG12	2.00	0.43
4:V:141:VAL:O	9:a:169:TYR:OH	2.23	0.43
7:Y:43:ARG:HD3	7:Y:48:PRO:HA	2.01	0.43
11:c:118:ASP:CG	11:c:120:SER:HG	2.27	0.43
13:e:129:ARG:HB2	13:e:136:LEU:HD12	2.00	0.43
30:j:201:PEE:H59	30:j:201:PEE:H64	1.73	0.43
4:V:102:GLY:HA2	4:V:110:ILE:HG22	2.00	0.42
10:b:87:LYS:HD3	10:b:88:TYR:CZ	2.53	0.42
12:d:37:PHE:CD2	20:l:3:PRO:HB3	2.54	0.42
21:m:16:GLY:HA2	31:s:402:CDL:H791	2.01	0.42
25:r:373:ILE:HD11	25:r:444:LEU:HD23	2.00	0.42
29:w:52:LYS:HE2	29:w:52:LYS:HB3	1.82	0.42
20:l:8:THR:HB	20:l:82:MET:HE3	2.01	0.42
20:l:457:LEU:HD23	20:l:457:LEU:HA	1.89	0.42
25:r:106:LEU:HD13	25:r:234:VAL:HG11	2.01	0.42
26:s:156:MET:O	26:s:315:PRO:HG3	2.19	0.42
17:i:102:LEU:HD13	17:i:142:LEU:HG	2.01	0.42
18:j:73:LEU:HD23	18:j:73:LEU:HA	1.87	0.42
20:l:505:ASN:O	20:l:508:THR:OG1	2.31	0.42
21:m:24:PRO:HB3	21:m:89:VAL:HG11	2.02	0.42
24:p:138:LYS:HD2	24:p:138:LYS:O	2.20	0.42
25:r:370:PRO:HG3	25:r:375:LEU:HD22	2.01	0.42
26:s:277:TYR:CE2	30:s:403:PEE:H59	2.53	0.42
1:Q:50:ALA:HB1	19:k:98:CYS:SG	2.60	0.42
31:V:201:CDL:H371	31:V:201:CDL:H342	1.71	0.42
20:l:27:TYR:O	20:l:115:ASN:ND2	2.49	0.42
26:s:2:PHE:O	26:s:6:ILE:HG13	2.19	0.42
30:s:403:PEE:H55	30:s:403:PEE:H61	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:v:25:PHE:HE1	28:v:109:LEU:HG	1.84	0.42
7:Y:102:ASP:HA	28:v:115:ARG:HH22	1.85	0.42
10:b:19:ARG:HA	24:p:171:VAL:HG13	2.02	0.42
10:b:24:LYS:O	10:b:27:GLU:HG3	2.20	0.42
20:l:14:ILE:HD11	20:l:43:ALA:HA	2.01	0.42
9:a:67:PHE:CE2	25:r:434:ASN:HB3	2.55	0.42
13:e:73:SER:C	13:e:75:GLY:H	2.27	0.42
20:l:17:ILE:O	20:l:21:MET:HG3	2.20	0.42
29:w:165:SER:O	29:w:168:VAL:HG22	2.19	0.42
8:Z:13:LYS:HA	8:Z:13:LYS:HD2	1.75	0.42
12:d:48:ALA:O	12:d:52:ILE:HD12	2.20	0.42
12:d:164:LEU:HD23	13:e:149:LEU:HD13	2.01	0.42
20:l:264:TYR:HA	20:l:267:MET:HB2	2.02	0.42
20:l:447:ASN:OD1	20:l:448:PRO:HD2	2.20	0.42
24:p:140:LEU:O	24:p:144:THR:HG23	2.20	0.42
7:Y:51:THR:OG1	20:l:446:ASN:ND2	2.52	0.42
20:l:241:THR:HG21	20:l:344:GLY:HA3	2.01	0.42
20:l:288:THR:HG21	20:l:307:SER:HB3	2.01	0.42
4:V:106:ARG:HG3	4:V:106:ARG:HH11	1.82	0.42
25:r:329:LEU:O	25:r:332:THR:OG1	2.33	0.42
30:Q:101:PEE:H7	20:l:567:SER:HB3	2.01	0.42
31:g:202:CDL:H362	17:i:246:VAL:HG21	2.01	0.42
17:i:263:LYS:HG3	17:i:264:TRP:N	2.34	0.42
33:r:503:PLX:H1C3	33:r:503:PLX:H22	1.74	0.42
26:s:54:LYS:HE3	26:s:54:LYS:HB3	1.76	0.42
7:Y:44:TYR:CD2	8:Z:16:LEU:HD22	2.54	0.41
10:b:10:LEU:O	10:b:14:GLN:HG3	2.19	0.41
26:s:307:LEU:O	26:s:311:THR:OG1	2.29	0.41
28:v:48:ASP:OD1	28:v:48:ASP:N	2.52	0.41
3:U:40:ASN:O	3:U:44:ARG:HG3	2.19	0.41
12:d:127:LYS:HB3	12:d:127:LYS:HZ2	1.83	0.41
20:l:286:LEU:HD13	20:l:411:MET:SD	2.60	0.41
25:r:115:LEU:HD12	25:r:174:LEU:HD22	2.02	0.41
25:r:122:PHE:O	25:r:125:THR:OG1	2.37	0.41
26:s:90:PRO:HB3	26:s:94:PRO:HD3	2.02	0.41
29:w:95:ASP:OD1	29:w:95:ASP:N	2.51	0.41
13:e:119:ARG:O	13:e:123:GLU:HG3	2.21	0.41
13:e:129:ARG:HD2	13:e:136:LEU:HA	2.01	0.41
19:k:26:LEU:O	19:k:30:LEU:HG	2.20	0.41
20:l:37:LYS:HB3	20:l:37:LYS:HE3	1.88	0.41
20:l:312:LEU:O	20:l:315:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:l:702:CDL:H592	31:l:702:CDL:H202	2.02	0.41
25:r:10:MET:C	25:r:13:PRO:HD2	2.45	0.41
25:r:16:TRP:NE1	25:r:97:THR:OG1	2.53	0.41
25:r:220:HIS:NE2	25:r:231:LEU:HB3	2.35	0.41
7:Y:54:GLN:OE1	20:l:446:ASN:ND2	2.52	0.41
11:c:153:TYR:OH	28:v:8:ARG:NH1	2.53	0.41
18:j:53:MET:HE1	21:m:70:TYR:CD1	2.56	0.41
25:r:233:ALA:HA	25:r:320:GLY:HA2	2.03	0.41
2:S:39:ALA:HB2	2:S:48:MET:HE2	2.02	0.41
7:Y:99:ILE:CD1	28:v:107:ARG:HG3	2.50	0.41
10:b:29:SER:OG	10:b:32:GLU:HG2	2.20	0.41
19:k:37:MET:HE3	19:k:67:ALA:HA	2.02	0.41
19:k:64:LEU:O	19:k:67:ALA:HB3	2.20	0.41
20:l:11:THR:HG21	20:l:47:SER:HB3	2.01	0.41
20:l:435:PRO:HB3	20:l:437:PHE:CZ	2.54	0.41
25:r:1:MET:O	25:r:1:MET:HG3	2.20	0.41
25:r:207:MET:HE3	25:r:240:GLY:N	2.36	0.41
26:s:142:TYR:CZ	26:s:192:GLU:HG2	2.55	0.41
26:s:222:MET:HA	26:s:225:MET:HE3	2.03	0.41
5:W:94:GLU:HG3	16:h:79:ILE:HD13	2.02	0.41
11:c:70:MET:HE1	20:l:552:LEU:HD13	2.02	0.41
14:f:43:LYS:HA	14:f:46:LEU:CD2	2.51	0.41
15:g:13:LEU:HD23	33:g:201:PLX:H32	2.03	0.41
31:k:101:CDL:H402	31:k:101:CDL:H432	1.80	0.41
20:l:358:LYS:HG3	24:p:80:TYR:CE1	2.54	0.41
30:l:705:PEE:H3	33:r:503:PLX:H1C3	2.02	0.41
25:r:265:SER:O	25:r:269:MET:HB2	2.21	0.41
26:s:81:LEU:HD21	26:s:111:LEU:HD23	2.01	0.41
28:v:53:LEU:HA	28:v:53:LEU:HD12	1.88	0.41
2:S:23:THR:HG22	2:S:27:HIS:CD2	2.56	0.41
18:j:17:LEU:HD23	18:j:17:LEU:HA	1.89	0.41
19:k:60:PRO:O	19:k:63:LEU:HB3	2.20	0.41
20:l:51:LEU:O	20:l:55:MET:HG3	2.21	0.41
26:s:84:THR:O	26:s:87:VAL:HG22	2.21	0.41
26:s:156:MET:O	26:s:315:PRO:CG	2.69	0.41
29:w:129:TYR:CD1	29:w:183:CYS:HB3	2.55	0.41
1:Q:71:PRO:HA	1:Q:72:PRO:HD3	1.92	0.41
2:S:27:HIS:CE1	2:S:36:LYS:HD3	2.55	0.41
3:U:53:TYR:CE1	27:u:44:MET:HG3	2.56	0.41
11:c:101:TRP:CZ3	23:o:46:GLU:HG2	2.55	0.41
14:f:39:PRO:HD3	29:w:351:TRP:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:s:102:VAL:HG22	26:s:162:LEU:HD21	2.03	0.41
31:V:201:CDL:H622	31:V:201:CDL:H592	1.89	0.41
14:f:33:GLU:O	14:f:34:PRO:C	2.64	0.41
14:f:71:ARG:HG2	14:f:71:ARG:NH1	2.35	0.41
15:g:33:LEU:HD23	15:g:33:LEU:HA	1.96	0.41
17:i:74:ILE:HG13	17:i:98:MET:HE1	2.03	0.41
17:i:310:ASN:HB2	29:w:309:THR:HG22	2.02	0.41
18:j:27:LEU:HD22	26:s:59:GLU:HG3	2.02	0.41
20:l:124:PHE:CE1	20:l:252:MET:HB2	2.55	0.41
20:l:400:ASN:OD1	20:l:409:LEU:HD11	2.21	0.41
23:o:117:GLN:OE1	23:o:117:GLN:HA	2.21	0.41
9:a:135:LYS:HD2	22:n:32:ASP:HB2	2.02	0.41
10:b:16:ARG:O	10:b:20:ARG:HG3	2.21	0.41
12:d:33:LEU:HD13	20:l:49:VAL:HG13	2.02	0.41
16:h:12:LEU:HD23	16:h:12:LEU:HA	1.89	0.41
20:l:264:TYR:CG	20:l:265:PRO:HD3	2.56	0.41
20:l:534:HIS:CD2	30:l:704:PEE:H13	2.56	0.41
31:l:702:CDL:H231	31:l:702:CDL:H201	1.89	0.41
26:s:315:PRO:HA	26:s:316:PRO:HD3	1.94	0.41
29:w:102:LYS:HB2	29:w:102:LYS:HE3	1.95	0.41
29:w:135:LEU:HD23	29:w:135:LEU:HA	1.96	0.41
6:X:132:ASP:O	6:X:136:GLU:HG2	2.20	0.40
31:g:202:CDL:H381	31:g:202:CDL:H351	1.80	0.40
17:i:242:SER:O	17:i:246:VAL:HG23	2.21	0.40
21:m:34:ILE:HD11	26:s:114:TYR:CE1	2.56	0.40
21:m:45:LEU:HD12	21:m:50:SER:HA	2.02	0.40
21:m:65:LEU:HD13	26:s:139:THR:HG21	2.03	0.40
26:s:145:THR:HG21	26:s:293:PHE:HB3	2.02	0.40
13:e:87:MET:HE3	13:e:87:MET:HB3	1.92	0.40
31:g:202:CDL:H142	25:r:94:LEU:HD13	2.03	0.40
25:r:123:GLU:OE2	25:r:157:SER:OG	2.36	0.40
26:s:139:THR:HA	26:s:142:TYR:CE2	2.56	0.40
27:u:20:VAL:HG23	27:u:25:LEU:HG	2.02	0.40
29:w:76:GLU:HB3	29:w:80:LYS:HE3	2.01	0.40
31:a:201:CDL:H171	31:a:201:CDL:H712	2.04	0.40
13:e:92:PHE:O	13:e:96:SER:HB2	2.21	0.40
31:g:202:CDL:HA62	17:i:239:VAL:HG22	2.03	0.40
31:g:202:CDL:H441	25:r:101:LEU:HD13	2.03	0.40
16:h:101:LYS:HE3	16:h:101:LYS:HB2	1.79	0.40
18:j:95:LEU:HD13	26:s:302:MET:HG2	2.02	0.40
31:l:702:CDL:H352	25:r:361:VAL:HG23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:m:54:LEU:HD13	26:s:103:LEU:HB3	2.03	0.40
21:m:126:VAL:HG23	21:m:127:ILE:HG23	2.03	0.40
24:p:64:LEU:O	24:p:68:GLU:HG2	2.22	0.40
25:r:71:TRP:O	25:r:74:PRO:HD2	2.21	0.40
34:s:404:UQ:H152	34:s:404:UQ:H121	1.82	0.40
27:u:11:GLU:H	27:u:11:GLU:CD	2.29	0.40
10:b:76:LEU:HD12	10:b:76:LEU:HA	1.92	0.40
17:i:79:LEU:HB2	19:k:47:ILE:HD13	2.04	0.40
20:l:90:ILE:HG12	20:l:129:MET:SD	2.61	0.40
25:r:318:ALA:HB2	25:r:373:ILE:HG13	2.04	0.40
1:Q:37:TRP:CD2	25:r:140:THR:HB	2.56	0.40
3:U:70:PRO:HB3	27:u:124:GLU:O	2.22	0.40
20:l:316:THR:HG23	20:l:325:ALA:HB2	2.03	0.40
21:m:165:VAL:O	21:m:168:ILE:HG12	2.22	0.40
27:u:37:ASP:C	27:u:37:ASP:OD1	2.64	0.40
29:w:320:GLY:O	29:w:324:SER:OG	2.27	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
2	S	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
3	U	81/83 (98%)	81 (100%)	0	0	100	100
4	V	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
5	W	111/113 (98%)	110 (99%)	1 (1%)	0	100	100
6	X	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
7	Y	65/67 (97%)	63 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	Z	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
9	a	136/138 (99%)	131 (96%)	5 (4%)	0	100	100
10	b	94/126 (75%)	89 (95%)	5 (5%)	0	100	100
11	c	154/156 (99%)	144 (94%)	10 (6%)	0	100	100
12	d	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
13	e	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
14	f	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
15	g	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
16	h	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
17	i	345/347 (99%)	331 (96%)	14 (4%)	0	100	100
18	j	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
19	k	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
20	l	604/606 (100%)	580 (96%)	24 (4%)	0	100	100
21	m	173/175 (99%)	165 (95%)	7 (4%)	1 (1%)	21	51
22	n	54/56 (96%)	54 (100%)	0	0	100	100
23	o	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
24	p	176/178 (99%)	168 (96%)	8 (4%)	0	100	100
25	r	457/459 (100%)	449 (98%)	8 (2%)	0	100	100
26	s	316/318 (99%)	305 (96%)	10 (3%)	1 (0%)	36	65
27	u	169/171 (99%)	164 (97%)	4 (2%)	1 (1%)	21	51
28	v	122/125 (98%)	118 (97%)	4 (3%)	0	100	100
29	w	318/320 (99%)	308 (97%)	10 (3%)	0	100	100
All	All	4666/4755 (98%)	4505 (96%)	158 (3%)	3 (0%)	49	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	u	168	PHE
26	s	208	VAL
21	m	25	SER

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	38/38 (100%)	38 (100%)	0	100	100
2	S	57/58 (98%)	56 (98%)	1 (2%)	51	80
3	U	69/69 (100%)	68 (99%)	1 (1%)	59	85
4	V	101/101 (100%)	98 (97%)	3 (3%)	36	70
5	W	99/99 (100%)	98 (99%)	1 (1%)	68	89
6	X	79/81 (98%)	79 (100%)	0	100	100
7	Y	62/62 (100%)	62 (100%)	0	100	100
8	Z	62/62 (100%)	61 (98%)	1 (2%)	55	83
9	a	121/121 (100%)	120 (99%)	1 (1%)	73	90
10	b	90/119 (76%)	89 (99%)	1 (1%)	65	88
11	c	141/141 (100%)	140 (99%)	1 (1%)	76	92
12	d	155/155 (100%)	153 (99%)	2 (1%)	61	86
13	e	96/96 (100%)	95 (99%)	1 (1%)	68	89
14	f	36/45 (80%)	35 (97%)	1 (3%)	38	72
15	g	108/108 (100%)	107 (99%)	1 (1%)	70	90
16	h	93/93 (100%)	92 (99%)	1 (1%)	65	88
17	i	311/311 (100%)	308 (99%)	3 (1%)	68	89
18	j	100/100 (100%)	99 (99%)	1 (1%)	68	89
19	k	85/85 (100%)	84 (99%)	1 (1%)	63	86
20	l	537/540 (99%)	536 (100%)	1 (0%)	87	96
21	m	130/141 (92%)	128 (98%)	2 (2%)	57	84
22	n	53/53 (100%)	52 (98%)	1 (2%)	50	79
23	o	113/113 (100%)	113 (100%)	0	100	100
24	p	159/159 (100%)	157 (99%)	2 (1%)	61	86
25	r	410/410 (100%)	406 (99%)	4 (1%)	68	89
26	s	275/275 (100%)	272 (99%)	3 (1%)	65	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	u	153/153 (100%)	150 (98%)	3 (2%)	48	78
28	v	111/111 (100%)	111 (100%)	0	100	100
29	w	281/283 (99%)	277 (99%)	4 (1%)	59	85
All	All	4125/4182 (99%)	4084 (99%)	41 (1%)	65	89

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S	54	ILE
3	U	22	SER
4	V	50	LEU
4	V	110	ILE
4	V	115	CYS
5	W	49	SER
8	Z	60	ASN
9	a	76	LEU
10	b	17	GLU
11	c	165	ASP
12	d	36	ILE
12	d	144	SER
13	e	72	ASP
14	f	58	LEU
15	g	2	THR
16	h	86	LEU
17	i	171	ASN
17	i	320	THR
17	i	336	VAL
18	j	67	LEU
19	k	59	MET
20	l	446	ASN
21	m	39	VAL
21	m	98	MET
22	n	42	SER
24	p	66	GLN
24	p	70	GLU
25	r	129	THR
25	r	247	THR
25	r	304	GLN
25	r	401	MET
26	s	8	SER
26	s	156	MET

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Mol	Chain	Res	Type
26	s	202	GLU
27	u	5	VAL
27	u	77	HIS
27	u	88	CYS
29	w	95	ASP
29	w	107	GLN
29	w	241	TYR
29	w	287	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
2	S	27	HIS
5	W	54	ASN
5	W	61	GLN
5	W	76	GLN
6	X	142	GLN
7	Y	46	GLN
8	Z	60	ASN
10	b	89	HIS
11	c	84	GLN
12	d	124	ASN
12	d	140	GLN
14	f	62	HIS
14	f	73	ASN
15	g	99	HIS
16	h	34	HIS
16	h	45	HIS
16	h	98	HIS
17	i	77	ASN
17	i	112	HIS
17	i	221	HIS
17	i	232	HIS
20	l	135	ASN
20	l	175	ASN
20	l	199	GLN
20	l	226	GLN
20	l	296	ASN
20	l	348	HIS
20	l	446	ASN
20	l	471	ASN
20	l	580	GLN

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Mol	Chain	Res	Type
23	o	79	ASN
24	p	14	GLN
24	p	33	HIS
24	p	53	ASN
25	r	43	ASN
25	r	144	ASN
25	r	175	ASN
25	r	366	ASN
25	r	415	GLN
26	s	47	GLN
26	s	230	ASN
26	s	235	ASN
28	v	47	ASN
28	v	84	GLN
29	w	149	HIS
29	w	235	GLN
29	w	239	ASN
29	w	323	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](#)

27 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	$\# Z > 2$
31	CDL	s	402	-	88,88,99	1.16	9 (10%)	94,100,111	0.93	4 (4%)
30	PEE	j	201	-	50,50,50	1.18	6 (12%)	53,55,55	0.96	2 (3%)
33	PLX	j	202	-	51,51,51	1.20	4 (7%)	53,59,59	0.60	1 (1%)
30	PEE	l	701	-	39,39,50	1.33	6 (15%)	42,44,55	1.10	3 (7%)
30	PEE	l	704	-	50,50,50	1.18	6 (12%)	53,55,55	0.95	2 (3%)
30	PEE	l	705	-	45,45,50	1.24	6 (13%)	48,50,55	1.01	2 (4%)
30	PEE	Q	101	-	46,46,50	1.22	6 (13%)	49,51,55	1.01	2 (4%)
31	CDL	a	201	-	99,99,99	1.12	9 (9%)	105,111,111	0.86	4 (3%)
31	CDL	l	702	-	98,98,99	1.12	8 (8%)	104,110,111	0.89	4 (3%)
32	8Q1	X	201	-	32,34,34	1.62	6 (18%)	39,43,43	1.69	7 (17%)
34	UQ	s	404	-	38,38,63	3.63	12 (31%)	48,49,79	2.81	17 (35%)
33	PLX	a	202	-	51,51,51	1.22	5 (9%)	53,59,59	0.59	1 (1%)
31	CDL	l	703	-	99,99,99	1.12	9 (9%)	105,111,111	0.88	4 (3%)
35	ADP	w	401	-	28,29,29	3.17	9 (32%)	43,45,45	1.90	9 (20%)
31	CDL	k	101	-	99,99,99	1.11	9 (9%)	105,111,111	0.86	4 (3%)
33	PLX	j	203	-	51,51,51	1.21	4 (7%)	53,59,59	0.62	1 (1%)
31	CDL	V	202	-	99,99,99	1.12	8 (8%)	105,111,111	0.87	4 (3%)
30	PEE	W	201	-	40,40,50	1.17	5 (12%)	43,45,55	0.97	2 (4%)
33	PLX	g	201	-	51,51,51	1.20	4 (7%)	53,59,59	0.64	1 (1%)
30	PEE	s	401	-	40,40,50	1.17	5 (12%)	43,45,55	1.06	3 (6%)
33	PLX	r	502	-	51,51,51	1.22	5 (9%)	53,59,59	0.61	1 (1%)
33	PLX	r	503	-	51,51,51	1.21	4 (7%)	53,59,59	0.61	1 (1%)
30	PEE	r	501	-	50,50,50	1.18	6 (12%)	53,55,55	0.99	2 (3%)
31	CDL	V	201	-	93,93,99	1.14	9 (9%)	99,105,111	0.87	4 (4%)
31	CDL	n	101	-	54,54,99	1.38	9 (16%)	60,66,111	1.10	4 (6%)
30	PEE	s	403	-	50,50,50	1.18	6 (12%)	53,55,55	1.01	2 (3%)
31	CDL	g	202	-	99,99,99	1.11	9 (9%)	105,111,111	0.89	4 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CDL	s	402	-	-	49/99/99/110	-
30	PEE	j	201	-	-	29/54/54/54	-
33	PLX	j	202	-	-	31/55/55/55	-
30	PEE	l	701	-	-	26/43/43/54	-
30	PEE	l	704	-	-	31/54/54/54	-
30	PEE	l	705	-	-	27/49/49/54	-
30	PEE	Q	101	-	-	21/50/50/54	-
31	CDL	a	201	-	-	56/110/110/110	-
31	CDL	l	702	-	-	57/109/109/110	-
32	8Q1	X	201	-	-	13/41/41/41	-
34	UQ	s	404	-	-	9/33/57/87	0/1/1/1
33	PLX	a	202	-	-	31/55/55/55	-
31	CDL	l	703	-	-	55/110/110/110	-
35	ADP	w	401	-	-	5/16/32/32	0/3/3/3
31	CDL	k	101	-	-	61/110/110/110	-
33	PLX	j	203	-	-	24/55/55/55	-
31	CDL	V	202	-	-	61/110/110/110	-
30	PEE	W	201	-	-	21/44/44/54	-
33	PLX	g	201	-	-	29/55/55/55	-
30	PEE	s	401	-	-	21/44/44/54	-
33	PLX	r	502	-	-	31/55/55/55	-
33	PLX	r	503	-	-	29/55/55/55	-
30	PEE	r	501	-	-	27/54/54/54	-
31	CDL	V	201	-	-	52/104/104/110	-
31	CDL	n	101	-	-	35/65/65/110	-
30	PEE	s	403	-	-	24/54/54/54	-
31	CDL	g	202	-	-	64/110/110/110	-

All (184) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	s	404	UQ	C18-C19	10.01	1.56	1.33
34	s	404	UQ	C13-C14	9.60	1.55	1.33
34	s	404	UQ	C23-C24	9.45	1.54	1.33
34	s	404	UQ	C8-C9	9.31	1.54	1.33
35	w	401	ADP	C3'-C4'	-8.97	1.30	1.53
35	w	401	ADP	O4'-C4'	7.71	1.62	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	s	404	UQ	C28-C29	7.33	1.54	1.32
35	w	401	ADP	PA-O3A	6.47	1.66	1.59
35	w	401	ADP	C6-N6	5.42	1.48	1.34
32	X	201	8Q1	C39-N41	5.06	1.45	1.33
32	X	201	8Q1	C34-N36	4.97	1.45	1.33
35	w	401	ADP	O4'-C1'	-4.57	1.31	1.42
30	r	501	PEE	C18-C19	3.83	1.53	1.31
30	l	701	PEE	C18-C19	3.82	1.53	1.31
30	l	705	PEE	C18-C19	3.81	1.53	1.31
30	j	201	PEE	C18-C19	3.81	1.53	1.31
30	l	704	PEE	C18-C19	3.80	1.53	1.31
30	s	403	PEE	C18-C19	3.80	1.53	1.31
30	W	201	PEE	C18-C19	3.80	1.53	1.31
30	s	401	PEE	C18-C19	3.80	1.53	1.31
30	Q	101	PEE	C18-C19	3.79	1.53	1.31
30	r	501	PEE	C39-C38	3.75	1.53	1.31
30	s	403	PEE	C39-C38	3.74	1.52	1.31
30	l	701	PEE	C39-C38	3.74	1.52	1.31
30	l	704	PEE	C39-C38	3.73	1.52	1.31
30	j	201	PEE	C39-C38	3.73	1.52	1.31
30	l	705	PEE	C39-C38	3.73	1.52	1.31
30	Q	101	PEE	C39-C38	3.72	1.52	1.31
31	l	702	CDL	OA8-CA7	3.54	1.43	1.33
31	l	703	CDL	OA8-CA7	3.49	1.43	1.33
31	s	402	CDL	OA8-CA7	3.49	1.43	1.33
31	V	202	CDL	OA8-CA7	3.47	1.43	1.33
31	a	201	CDL	OA8-CA7	3.45	1.43	1.33
31	n	101	CDL	OA8-CA7	3.43	1.43	1.33
31	g	202	CDL	OA8-CA7	3.43	1.43	1.33
31	k	101	CDL	OA8-CA7	3.42	1.43	1.33
31	V	201	CDL	OA8-CA7	3.42	1.43	1.33
35	w	401	ADP	C8-N9	-3.28	1.32	1.37
35	w	401	ADP	O2'-C2'	-3.16	1.35	1.43
31	k	101	CDL	OA6-CA5	3.14	1.43	1.34
31	V	201	CDL	OA6-CA5	3.13	1.43	1.34
31	V	202	CDL	OB6-CB5	3.08	1.43	1.34
31	a	201	CDL	OB6-CB5	3.08	1.43	1.34
31	g	202	CDL	OB6-CB5	3.04	1.42	1.34
31	k	101	CDL	OB6-CB5	3.04	1.42	1.34
31	l	702	CDL	OB6-CB5	3.03	1.42	1.34
31	l	703	CDL	OB6-CB5	3.03	1.42	1.34
31	s	402	CDL	OB6-CB5	3.01	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	V	202	CDL	OB8-CB7	3.00	1.42	1.33
31	l	703	CDL	OB8-CB7	3.00	1.42	1.33
31	n	101	CDL	OB8-CB7	3.00	1.42	1.33
31	k	101	CDL	OB8-CB7	3.00	1.42	1.33
31	l	702	CDL	OB8-CB7	3.00	1.42	1.33
31	V	201	CDL	OB6-CB5	2.99	1.42	1.34
31	a	201	CDL	OB8-CB7	2.99	1.42	1.33
35	w	401	ADP	O3'-C3'	2.99	1.50	1.43
31	n	101	CDL	OA6-CA5	2.99	1.42	1.34
31	n	101	CDL	OB6-CB5	2.98	1.42	1.34
31	s	402	CDL	OA6-CA5	2.98	1.42	1.34
31	g	202	CDL	OB8-CB7	2.97	1.42	1.33
31	V	202	CDL	OA6-CA5	2.96	1.42	1.34
31	l	703	CDL	OA6-CA5	2.94	1.42	1.34
31	g	202	CDL	OA6-CA5	2.94	1.42	1.34
31	a	201	CDL	OA6-CA5	2.93	1.42	1.34
31	V	201	CDL	OB8-CB7	2.93	1.41	1.33
31	s	402	CDL	OB8-CB7	2.91	1.41	1.33
31	l	702	CDL	OA6-CA5	2.90	1.42	1.34
33	a	202	PLX	O6-C4	-2.89	1.40	1.44
33	g	201	PLX	O6-C4	-2.85	1.41	1.44
33	r	503	PLX	O6-C4	-2.78	1.41	1.44
33	r	502	PLX	O6-C4	-2.76	1.41	1.44
34	s	404	UQ	C6-C1	2.73	1.54	1.46
33	j	203	PLX	O6-C4	-2.72	1.41	1.44
31	l	702	CDL	OA6-CA4	-2.61	1.40	1.46
31	g	202	CDL	OA6-CA4	-2.59	1.40	1.46
30	Q	101	PEE	O2-C2	-2.59	1.40	1.46
30	j	201	PEE	O2-C2	-2.58	1.40	1.46
30	s	401	PEE	O2-C2	-2.58	1.40	1.46
31	a	201	CDL	OA6-CA4	-2.57	1.40	1.46
30	W	201	PEE	O2-C2	-2.57	1.40	1.46
31	V	202	CDL	OA6-CA4	-2.55	1.40	1.46
30	s	403	PEE	O2-C2	-2.54	1.40	1.46
31	n	101	CDL	OA6-CA4	-2.54	1.40	1.46
30	l	704	PEE	O2-C2	-2.53	1.40	1.46
30	l	705	PEE	O3-C30	2.52	1.40	1.33
31	s	402	CDL	OA6-CA4	-2.51	1.40	1.46
30	r	501	PEE	O2-C2	-2.51	1.40	1.46
33	j	203	PLX	C7-C6	2.51	1.56	1.50
30	s	401	PEE	O3-C30	2.50	1.40	1.33
30	l	701	PEE	O2-C2	-2.50	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	s	403	PEE	O3-C30	2.50	1.40	1.33
30	l	705	PEE	O2-C2	-2.50	1.40	1.46
30	l	701	PEE	O3-C30	2.49	1.40	1.33
31	l	703	CDL	OA6-CA4	-2.47	1.40	1.46
30	l	704	PEE	O3-C30	2.47	1.40	1.33
30	r	501	PEE	O3-C30	2.46	1.40	1.33
30	W	201	PEE	O3-C30	2.44	1.40	1.33
30	j	201	PEE	O3-C30	2.44	1.40	1.33
33	r	502	PLX	C7-C6	2.43	1.55	1.50
32	X	201	8Q1	O35-C34	-2.43	1.18	1.23
33	j	202	PLX	C7-C6	2.42	1.55	1.50
30	Q	101	PEE	O3-C30	2.41	1.40	1.33
32	X	201	8Q1	C1-S44	2.40	1.81	1.76
33	a	202	PLX	C7-C6	2.40	1.55	1.50
33	j	202	PLX	O6-C4	-2.39	1.41	1.44
31	l	703	CDL	OB6-CB4	-2.37	1.41	1.46
32	X	201	8Q1	O40-C39	-2.37	1.18	1.23
35	w	401	ADP	C5-N7	-2.36	1.34	1.39
31	V	201	CDL	OB6-CB4	-2.35	1.41	1.46
33	r	503	PLX	C7-C6	2.35	1.55	1.50
33	g	201	PLX	C7-C6	2.35	1.55	1.50
30	l	701	PEE	O2-C10	2.35	1.40	1.34
31	k	101	CDL	OB6-CB4	-2.34	1.41	1.46
30	l	704	PEE	O2-C10	2.34	1.40	1.34
31	l	702	CDL	OB6-CB4	-2.32	1.41	1.46
31	n	101	CDL	OB6-CB4	-2.31	1.41	1.46
30	s	403	PEE	O2-C10	2.30	1.40	1.34
31	s	402	CDL	OB6-CB4	-2.29	1.41	1.46
30	l	705	PEE	O2-C10	2.29	1.40	1.34
31	V	202	CDL	PB2-OB2	2.28	1.68	1.59
30	W	201	PEE	O2-C10	2.28	1.40	1.34
31	V	201	CDL	PB2-OB2	2.27	1.68	1.59
31	l	703	CDL	PB2-OB2	2.27	1.68	1.59
31	k	101	CDL	OA6-CA4	-2.27	1.41	1.46
34	s	404	UQ	C7-C8	2.26	1.54	1.50
31	s	402	CDL	PB2-OB2	2.26	1.68	1.59
31	g	202	CDL	PB2-OB2	2.26	1.68	1.59
31	a	201	CDL	OB6-CB4	-2.25	1.41	1.46
31	n	101	CDL	PB2-OB2	2.25	1.68	1.59
31	a	201	CDL	PB2-OB2	2.25	1.68	1.59
31	l	702	CDL	PB2-OB5	2.24	1.68	1.59
30	r	501	PEE	O2-C10	2.24	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	j	201	PEE	O2-C10	2.24	1.40	1.34
31	l	702	CDL	PB2-OB2	2.23	1.68	1.59
30	Q	101	PEE	O2-C10	2.22	1.40	1.34
31	n	101	CDL	PB2-OB5	2.22	1.68	1.59
31	a	201	CDL	PB2-OB5	2.22	1.68	1.59
31	V	202	CDL	OB6-CB4	-2.22	1.41	1.46
31	V	202	CDL	PB2-OB5	2.21	1.68	1.59
31	l	703	CDL	PB2-OB5	2.21	1.68	1.59
31	g	202	CDL	OB6-CB4	-2.21	1.41	1.46
31	k	101	CDL	PB2-OB2	2.21	1.68	1.59
31	g	202	CDL	PB2-OB5	2.21	1.68	1.59
31	V	201	CDL	PB2-OB5	2.20	1.68	1.59
31	k	101	CDL	PB2-OB5	2.20	1.68	1.59
30	s	401	PEE	O2-C10	2.19	1.40	1.34
33	j	202	PLX	P1-O4	2.19	1.68	1.59
33	j	203	PLX	P1-O4	2.18	1.67	1.59
31	V	201	CDL	OA6-CA4	-2.18	1.41	1.46
33	r	502	PLX	P1-O4	2.18	1.67	1.59
33	a	202	PLX	P1-O4	2.18	1.67	1.59
33	g	201	PLX	P1-O4	2.17	1.67	1.59
33	r	503	PLX	P1-O4	2.17	1.67	1.59
31	s	402	CDL	PB2-OB5	2.16	1.67	1.59
32	X	201	8Q1	C6-C1	2.15	1.53	1.50
30	l	704	PEE	O3-C3	-2.15	1.40	1.45
30	r	501	PEE	O3-C3	-2.15	1.40	1.45
30	W	201	PEE	O3-C3	-2.13	1.40	1.45
34	s	404	UQ	O4-C4	-2.13	1.18	1.23
30	j	201	PEE	O3-C3	-2.12	1.40	1.45
30	Q	101	PEE	O3-C3	-2.12	1.40	1.45
30	s	401	PEE	O3-C3	-2.11	1.40	1.45
34	s	404	UQ	O3-CM3	-2.10	1.40	1.45
33	a	202	PLX	P1-O1	2.10	1.67	1.59
33	r	502	PLX	C25-C24	2.10	1.55	1.50
31	V	201	CDL	C11-CA5	2.09	1.56	1.50
33	r	502	PLX	P1-O1	2.09	1.67	1.59
33	j	202	PLX	P1-O1	2.09	1.67	1.59
30	l	701	PEE	O3-C3	-2.08	1.40	1.45
30	s	403	PEE	O3-C3	-2.08	1.40	1.45
33	r	503	PLX	P1-O1	2.07	1.67	1.59
33	j	203	PLX	P1-O1	2.07	1.67	1.59
30	l	705	PEE	O3-C3	-2.04	1.40	1.45
33	g	201	PLX	P1-O1	2.04	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	a	202	PLX	C1-C2	2.03	1.57	1.51
34	s	404	UQ	C21-C19	2.01	1.55	1.51
31	k	101	CDL	C11-CA5	2.01	1.56	1.50
31	s	402	CDL	C11-CA5	2.01	1.56	1.50
31	a	201	CDL	C11-CA5	2.01	1.56	1.50
34	s	404	UQ	C5-C4	2.01	1.54	1.47
31	n	101	CDL	C11-CA5	2.00	1.56	1.50
31	g	202	CDL	C11-CA5	2.00	1.56	1.50
31	l	703	CDL	C11-CA5	2.00	1.56	1.50
34	s	404	UQ	O1-C1	-2.00	1.18	1.23

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	s	404	UQ	C7-C8-C9	-8.02	113.02	126.83
34	s	404	UQ	C17-C18-C19	-6.24	113.35	127.62
34	s	404	UQ	C22-C23-C24	-6.23	113.35	127.62
34	s	404	UQ	C12-C13-C14	-6.09	113.69	127.62
32	X	201	8Q1	C6-C1-S44	5.86	120.38	113.40
35	w	401	ADP	C5-C4-N3	-5.37	119.33	126.72
35	w	401	ADP	N3-C2-N1	-4.53	121.72	128.58
34	s	404	UQ	C27-C28-C29	-4.44	112.83	127.64
34	s	404	UQ	C10-C9-C8	-4.40	112.34	123.63
30	s	401	PEE	O2-C10-C11	4.23	120.64	111.48
35	w	401	ADP	N3-C4-N9	4.21	134.32	127.17
34	s	404	UQ	C25-C24-C23	-4.20	112.83	123.63
31	V	201	CDL	OA6-CA5-C11	4.12	120.39	111.48
30	r	501	PEE	O2-C10-C11	4.11	120.36	111.48
31	V	202	CDL	OB6-CB5-C51	4.08	120.30	111.48
31	s	402	CDL	OA6-CA5-C11	4.06	120.27	111.48
31	s	402	CDL	OB6-CB5-C51	4.06	120.26	111.48
31	l	703	CDL	OB6-CB5-C51	4.04	120.22	111.48
30	s	403	PEE	O2-C10-C11	4.04	120.22	111.48
31	k	101	CDL	OB6-CB5-C51	4.03	120.20	111.48
34	s	404	UQ	C20-C19-C18	-4.02	113.29	123.63
31	l	702	CDL	OA6-CA5-C11	4.02	120.17	111.48
30	l	705	PEE	O2-C10-C11	4.02	120.17	111.48
32	X	201	8Q1	O4-C1-C6	-4.00	119.36	123.98
30	l	701	PEE	O2-C10-C11	4.00	120.13	111.48
31	n	101	CDL	OA6-CA5-C11	3.98	120.09	111.48
31	g	202	CDL	OB6-CB5-C51	3.97	120.06	111.48
31	a	201	CDL	OB6-CB5-C51	3.95	120.03	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	l	702	CDL	OB6-CB5-C51	3.93	119.98	111.48
31	l	703	CDL	OA6-CA5-C11	3.93	119.98	111.48
31	n	101	CDL	OB6-CB5-C51	3.90	119.92	111.48
31	a	201	CDL	OA6-CA5-C11	3.89	119.90	111.48
31	g	202	CDL	OA6-CA5-C11	3.89	119.89	111.48
30	W	201	PEE	O2-C10-C11	3.84	119.79	111.48
30	j	201	PEE	O2-C10-C11	3.83	119.77	111.48
31	V	201	CDL	OB6-CB5-C51	3.81	119.73	111.48
30	l	704	PEE	O2-C10-C11	3.81	119.72	111.48
34	s	404	UQ	C15-C14-C13	-3.79	113.91	123.63
31	V	202	CDL	OA6-CA5-C11	3.78	119.66	111.48
30	Q	101	PEE	O2-C10-C11	3.74	119.58	111.48
34	s	404	UQ	C11-C9-C8	-3.74	112.77	121.17
34	s	404	UQ	C21-C19-C18	-3.73	112.80	121.17
34	s	404	UQ	C26-C24-C23	-3.59	113.11	121.17
34	s	404	UQ	C16-C14-C13	-3.59	113.12	121.17
31	k	101	CDL	OA6-CA5-C11	3.57	119.21	111.48
35	w	401	ADP	N9-C8-N7	-3.54	108.92	113.94
35	w	401	ADP	C2-N3-C4	3.52	120.42	111.83
32	X	201	8Q1	C43-S44-C1	3.33	111.69	101.84
34	s	404	UQ	C30-C29-C28	-3.22	112.98	122.66
35	w	401	ADP	C4-N9-C8	3.21	109.11	105.74
35	w	401	ADP	C5-N7-C8	3.20	108.47	103.45
34	s	404	UQ	C31-C29-C28	-3.19	113.09	122.66
32	X	201	8Q1	C37-C38-C39	3.03	117.44	112.39
35	w	401	ADP	C4-C5-N7	-3.00	107.15	110.58
31	l	702	CDL	OA8-CA7-C31	2.95	120.83	111.83
31	k	101	CDL	OB8-CB7-C71	2.94	120.81	111.83
30	s	403	PEE	O3-C30-C31	2.94	120.81	111.83
30	Q	101	PEE	O3-C30-C31	2.85	120.52	111.83
31	n	101	CDL	OA8-CA7-C31	2.82	119.71	111.15
30	l	704	PEE	O3-C30-C31	2.80	120.37	111.83
31	a	201	CDL	OB8-CB7-C71	2.79	120.34	111.83
31	g	202	CDL	OB8-CB7-C71	2.78	120.30	111.83
31	k	101	CDL	OA8-CA7-C31	2.76	120.25	111.83
31	V	201	CDL	OB8-CB7-C71	2.75	120.22	111.83
30	r	501	PEE	O3-C30-C31	2.74	120.19	111.83
31	s	402	CDL	OA8-CA7-C31	2.74	120.18	111.83
31	l	703	CDL	OB8-CB7-C71	2.72	120.13	111.83
30	l	705	PEE	O3-C30-C31	2.71	120.08	111.83
31	l	703	CDL	OA8-CA7-C31	2.70	120.08	111.83
31	l	702	CDL	OB8-CB7-C71	2.70	120.07	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	V	202	CDL	OA8-CA7-C31	2.70	120.06	111.83
30	s	401	PEE	O3-C30-C31	2.69	120.04	111.83
31	a	201	CDL	OA8-CA7-C31	2.66	119.94	111.83
31	g	202	CDL	OA8-CA7-C31	2.66	119.94	111.83
31	n	101	CDL	OB8-CB7-C71	2.65	119.93	111.83
30	j	201	PEE	O3-C30-C31	2.65	119.92	111.83
31	V	202	CDL	OB8-CB7-C71	2.65	119.91	111.83
30	l	701	PEE	O3-C30-C31	2.64	119.88	111.83
31	s	402	CDL	OB8-CB7-C71	2.64	119.88	111.83
33	g	201	PLX	C1A-N1-C1	2.63	120.37	109.91
30	W	201	PEE	O3-C30-C31	2.61	119.80	111.83
33	r	503	PLX	C1A-N1-C1	2.51	119.91	109.91
33	j	203	PLX	C1A-N1-C1	2.50	119.85	109.91
34	s	404	UQ	C7-C6-C5	-2.48	120.64	124.89
31	V	201	CDL	OA8-CA7-C31	2.47	119.36	111.83
33	r	502	PLX	C1A-N1-C1	2.46	119.70	109.91
34	s	404	UQ	CM5-C5-C6	-2.42	120.47	124.45
33	a	202	PLX	C1A-N1-C1	2.39	119.42	109.91
30	l	701	PEE	C20-C19-C18	-2.34	112.37	126.42
33	j	202	PLX	C1A-N1-C1	2.32	119.14	109.91
32	X	201	8Q1	C38-C39-N41	2.22	120.40	116.34
32	X	201	8Q1	C31-C29-C28	2.22	111.89	108.22
30	s	401	PEE	C2-O2-C10	-2.20	112.54	117.80
32	X	201	8Q1	C32-C34-N36	2.12	120.50	116.48
35	w	401	ADP	C2'-C3'-C4'	2.07	106.61	102.61

There are no chirality outliers.

All (919) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	Q	101	PEE	C11-C10-O2-C2
30	Q	101	PEE	C1-O3P-P-O2P
30	W	201	PEE	C1-O3P-P-O2P
30	W	201	PEE	C1-O3P-P-O1P
30	W	201	PEE	C1-O3P-P-O4P
30	W	201	PEE	O4P-C4-C5-N
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	C11-C10-O2-C2
30	l	701	PEE	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
30	l	701	PEE	C1-O3P-P-O1P
30	l	701	PEE	C1-O3P-P-O4P
30	l	701	PEE	C4-O4P-P-O3P
30	l	704	PEE	C4-O4P-P-O3P
30	l	704	PEE	C4-O4P-P-O2P
30	l	704	PEE	C4-O4P-P-O1P
30	l	705	PEE	O4P-C4-C5-N
30	r	501	PEE	C4-O4P-P-O3P
30	r	501	PEE	C4-O4P-P-O1P
30	s	401	PEE	C4-O4P-P-O3P
30	s	401	PEE	C4-O4P-P-O2P
31	V	201	CDL	CB2-C1-CA2-OA2
31	V	201	CDL	CA2-C1-CB2-OB2
31	V	201	CDL	CA2-OA2-PA1-OA3
31	V	201	CDL	CA2-OA2-PA1-OA4
31	V	201	CDL	CA2-OA2-PA1-OA5
31	V	201	CDL	C11-CA5-OA6-CA4
31	V	201	CDL	CB2-OB2-PB2-OB3
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	V	202	CDL	CB2-C1-CA2-OA2
31	V	202	CDL	CA2-C1-CB2-OB2
31	V	202	CDL	CA2-OA2-PA1-OA4
31	V	202	CDL	CA2-OA2-PA1-OA5
31	V	202	CDL	CB2-OB2-PB2-OB3
31	V	202	CDL	CB2-OB2-PB2-OB5
31	a	201	CDL	CA2-C1-CB2-OB2
31	a	201	CDL	CB2-OB2-PB2-OB3
31	a	201	CDL	CB3-OB5-PB2-OB2
31	a	201	CDL	CB3-OB5-PB2-OB3
31	a	201	CDL	CB3-OB5-PB2-OB4
31	g	202	CDL	O1-C1-CA2-OA2
31	g	202	CDL	CA2-OA2-PA1-OA3
31	g	202	CDL	CA2-OA2-PA1-OA5
31	g	202	CDL	CB2-OB2-PB2-OB3
31	g	202	CDL	CB2-OB2-PB2-OB4
31	g	202	CDL	CB2-OB2-PB2-OB5
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	k	101	CDL	CA2-OA2-PA1-OA3
31	k	101	CDL	CA2-OA2-PA1-OA5
31	k	101	CDL	CA3-OA5-PA1-OA2
31	k	101	CDL	CA3-OA5-PA1-OA4
31	k	101	CDL	OA5-CA3-CA4-OA6
31	k	101	CDL	CB2-OB2-PB2-OB3
31	k	101	CDL	CB2-OB2-PB2-OB5
31	k	101	CDL	CB3-OB5-PB2-OB2
31	k	101	CDL	CB3-OB5-PB2-OB3
31	k	101	CDL	CB3-OB5-PB2-OB4
31	l	702	CDL	O1-C1-CA2-OA2
31	l	702	CDL	CA2-C1-CB2-OB2
31	l	702	CDL	OA9-CA7-OA8-CA6
31	l	702	CDL	C31-CA7-OA8-CA6
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	703	CDL	O1-C1-CA2-OA2
31	l	703	CDL	CB2-C1-CA2-OA2
31	l	703	CDL	CA2-OA2-PA1-OA5
31	l	703	CDL	CA3-OA5-PA1-OA2
31	l	703	CDL	CA3-OA5-PA1-OA3
31	l	703	CDL	CA3-OA5-PA1-OA4
31	n	101	CDL	CB2-C1-CA2-OA2
31	n	101	CDL	CA2-OA2-PA1-OA4
31	n	101	CDL	CA2-OA2-PA1-OA5
31	n	101	CDL	OA5-CA3-CA4-OA6
31	n	101	CDL	CB2-OB2-PB2-OB3
31	n	101	CDL	CB2-OB2-PB2-OB5
31	n	101	CDL	CB3-OB5-PB2-OB2
31	n	101	CDL	CB3-OB5-PB2-OB3
31	n	101	CDL	CB3-OB5-PB2-OB4
31	s	402	CDL	O1-C1-CB2-OB2
31	s	402	CDL	CA2-OA2-PA1-OA3
31	s	402	CDL	CA2-OA2-PA1-OA4
31	s	402	CDL	CA2-OA2-PA1-OA5
31	s	402	CDL	OA5-CA3-CA4-OA6
32	X	201	8Q1	O4-C1-S44-C43
32	X	201	8Q1	C6-C1-S44-C43
32	X	201	8Q1	O27-C28-C29-C30
32	X	201	8Q1	O27-C28-C29-C31
32	X	201	8Q1	O27-C28-C29-C32

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Mol	Chain	Res	Type	Atoms
32	X	201	8Q1	O33-C32-C34-N36
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	O7-C6-O6-C4
33	a	202	PLX	C3-O4-P1-O1
33	a	202	PLX	C3-O4-P1-O2
33	a	202	PLX	C2-O1-P1-O4
33	a	202	PLX	C2-O1-P1-O2
33	a	202	PLX	C25-C24-O8-C5
33	a	202	PLX	O9-C24-C25-C26
33	g	201	PLX	O7-C6-C7-C8
33	g	201	PLX	C2-O1-P1-O4
33	g	201	PLX	C2-O1-P1-O3
33	j	202	PLX	O7-C6-O6-C4
33	j	202	PLX	C25-C24-O8-C5
33	j	203	PLX	O7-C6-C7-C8
33	j	203	PLX	O9-C24-O8-C5
33	j	203	PLX	O9-C24-C25-C26
33	r	502	PLX	O7-C6-C7-C8
33	r	502	PLX	O7-C6-O6-C4
33	r	502	PLX	C3-O4-P1-O2
33	r	502	PLX	C2-O1-P1-O2
33	r	502	PLX	C25-C24-O8-C5
33	r	502	PLX	O9-C24-C25-C26
33	r	503	PLX	O7-C6-O6-C4
33	r	503	PLX	C2-O1-P1-O2
34	s	404	UQ	C7-C8-C9-C10
34	s	404	UQ	C7-C8-C9-C11
34	s	404	UQ	C22-C23-C24-C26
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	s	402	CDL	OA9-CA7-OA8-CA6
31	s	402	CDL	C31-CA7-OA8-CA6
30	Q	101	PEE	O5-C30-O3-C3
30	Q	101	PEE	O4-C10-O2-C2
30	l	701	PEE	O4-C10-O2-C2
30	l	704	PEE	O4-C10-O2-C2
31	V	201	CDL	OA7-CA5-OA6-CA4
31	a	201	CDL	OB7-CB5-OB6-CB4
30	Q	101	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
30	l	704	PEE	C11-C10-O2-C2
31	a	201	CDL	C51-CB5-OB6-CB4
34	s	404	UQ	C23-C24-C26-C27
30	l	704	PEE	C31-C30-O3-C3
31	l	703	CDL	C71-CB7-OB8-CB6
30	W	201	PEE	C17-C18-C19-C20
34	s	404	UQ	C17-C18-C19-C21
31	n	101	CDL	C55-C56-C57-C58
31	V	201	CDL	O1-C1-CA2-OA2
31	V	202	CDL	O1-C1-CA2-OA2
31	a	201	CDL	O1-C1-CA2-OA2
31	n	101	CDL	O1-C1-CA2-OA2
31	s	402	CDL	O1-C1-CA2-OA2
30	l	704	PEE	O5-C30-O3-C3
30	s	401	PEE	C11-C10-O2-C2
30	s	403	PEE	C11-C10-O2-C2
31	V	202	CDL	C51-CB5-OB6-CB4
31	g	202	CDL	C51-CB5-OB6-CB4
31	l	703	CDL	OB9-CB7-OB8-CB6
34	s	404	UQ	C27-C28-C29-C31
30	j	201	PEE	C31-C30-O3-C3
33	g	201	PLX	C9-C10-C11-C12
30	j	201	PEE	C17-C18-C19-C20
30	l	705	PEE	C37-C38-C39-C40
30	j	201	PEE	C11-C10-O2-C2
30	l	705	PEE	C11-C10-O2-C2
30	j	201	PEE	C30-C31-C32-C33
31	V	201	CDL	C59-C60-C61-C62
30	s	401	PEE	O4-C10-O2-C2
31	V	202	CDL	OB7-CB5-OB6-CB4
31	g	202	CDL	OB7-CB5-OB6-CB4
31	a	201	CDL	CB2-C1-CA2-OA2
31	g	202	CDL	CB2-C1-CA2-OA2
31	n	101	CDL	CA2-C1-CB2-OB2
31	s	402	CDL	CA2-C1-CB2-OB2
30	l	701	PEE	C31-C30-O3-C3
30	s	401	PEE	C31-C30-O3-C3
31	V	201	CDL	C71-CB7-OB8-CB6
31	l	702	CDL	C71-CB7-OB8-CB6
31	s	402	CDL	C71-CB7-OB8-CB6
31	g	202	CDL	C74-C75-C76-C77
31	V	202	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
31	k	101	CDL	C73-C74-C75-C76
31	s	402	CDL	C37-C38-C39-C40
33	g	201	PLX	C7-C8-C9-C10
33	g	201	PLX	C2-C1-N1-C1A
31	l	702	CDL	C55-C56-C57-C58
31	V	202	CDL	O1-C1-CB2-OB2
31	n	101	CDL	O1-C1-CB2-OB2
31	V	201	CDL	C62-C63-C64-C65
31	k	101	CDL	CB5-C51-C52-C53
31	g	202	CDL	C60-C61-C62-C63
33	r	502	PLX	C9-C10-C11-C12
30	s	401	PEE	O5-C30-O3-C3
31	V	201	CDL	OB9-CB7-OB8-CB6
31	l	702	CDL	OA5-CA3-CA4-OA6
31	k	101	CDL	C11-CA5-OA6-CA4
31	V	202	CDL	OA6-CA4-CA6-OA8
31	l	703	CDL	OA6-CA4-CA6-OA8
33	g	201	PLX	O6-C4-C5-O8
31	k	101	CDL	CA7-C31-C32-C33
31	l	703	CDL	C35-C36-C37-C38
31	l	702	CDL	OB9-CB7-OB8-CB6
30	l	705	PEE	C31-C30-O3-C3
31	a	201	CDL	C36-C37-C38-C39
33	r	502	PLX	C7-C8-C9-C10
30	W	201	PEE	C10-C11-C12-C13
31	a	201	CDL	CB5-C51-C52-C53
31	l	703	CDL	CA7-C31-C32-C33
33	g	201	PLX	C17-C18-C19-C20
33	j	203	PLX	C13-C14-C15-C16
30	s	403	PEE	O4-C10-O2-C2
33	g	201	PLX	C2-C1-N1-C1B
31	n	101	CDL	C74-C75-C76-C77
30	l	701	PEE	C10-C11-C12-C13
31	l	702	CDL	CB5-C51-C52-C53
30	l	701	PEE	O5-C30-O3-C3
31	s	402	CDL	OB9-CB7-OB8-CB6
30	r	501	PEE	C10-C11-C12-C13
31	l	702	CDL	CA7-C31-C32-C33
31	l	702	CDL	CB7-C71-C72-C73
31	n	101	CDL	CB5-C51-C52-C53
30	j	201	PEE	O5-C30-O3-C3
31	k	101	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
31	l	702	CDL	C58-C59-C60-C61
31	V	201	CDL	O1-C1-CB2-OB2
31	a	201	CDL	O1-C1-CB2-OB2
31	l	702	CDL	O1-C1-CB2-OB2
31	V	202	CDL	C71-CB7-OB8-CB6
31	a	201	CDL	C71-CB7-OB8-CB6
30	j	201	PEE	O4-C10-O2-C2
30	l	705	PEE	O4-C10-O2-C2
31	s	402	CDL	C33-C34-C35-C36
33	j	202	PLX	C11-C10-C9-C8
30	l	705	PEE	O5-C30-O3-C3
31	s	402	CDL	C14-C15-C16-C17
31	k	101	CDL	OA7-CA5-OA6-CA4
31	l	702	CDL	CB2-C1-CA2-OA2
31	s	402	CDL	CB2-C1-CA2-OA2
31	k	101	CDL	C40-C41-C42-C43
31	l	703	CDL	C11-C12-C13-C14
31	n	101	CDL	CB7-C71-C72-C73
34	s	404	UQ	C18-C19-C21-C22
33	r	502	PLX	O6-C6-C7-C8
31	V	201	CDL	C32-C33-C34-C35
30	r	501	PEE	C17-C18-C19-C20
31	k	101	CDL	O1-C1-CB2-OB2
30	l	701	PEE	C11-C12-C13-C14
31	k	101	CDL	C58-C59-C60-C61
30	l	701	PEE	C39-C40-C41-C42
31	k	101	CDL	C36-C37-C38-C39
31	a	201	CDL	OB9-CB7-OB8-CB6
30	Q	101	PEE	C11-C12-C13-C14
33	g	201	PLX	C2-C1-N1-C1C
30	l	701	PEE	C32-C33-C34-C35
31	V	202	CDL	C59-C60-C61-C62
31	l	702	CDL	C71-C72-C73-C74
33	j	203	PLX	C31-C32-C33-C34
30	l	704	PEE	C34-C35-C36-C37
31	l	702	CDL	C52-C53-C54-C55
31	l	702	CDL	C56-C57-C58-C59
31	n	101	CDL	C71-C72-C73-C74
33	j	203	PLX	C14-C15-C16-C17
31	l	703	CDL	CB7-C71-C72-C73
30	l	701	PEE	C17-C18-C19-C20
30	l	704	PEE	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
30	j	201	PEE	C21-C22-C23-C24
31	V	202	CDL	C37-C38-C39-C40
31	g	202	CDL	C75-C76-C77-C78
31	s	402	CDL	C52-C53-C54-C55
31	V	202	CDL	OB9-CB7-OB8-CB6
33	g	201	PLX	O9-C24-C25-C26
30	W	201	PEE	C21-C22-C23-C24
31	V	201	CDL	C34-C35-C36-C37
31	V	201	CDL	C52-C53-C54-C55
31	l	702	CDL	C62-C63-C64-C65
33	j	202	PLX	C25-C26-C27-C28
33	r	502	PLX	C34-C35-C36-C37
30	l	705	PEE	C33-C34-C35-C36
31	n	101	CDL	C52-C53-C54-C55
31	s	402	CDL	C75-C76-C77-C78
33	a	202	PLX	C13-C14-C15-C16
30	l	705	PEE	C22-C23-C24-C25
31	l	703	CDL	C34-C35-C36-C37
33	j	202	PLX	C13-C14-C15-C16
30	r	501	PEE	C11-C10-O2-C2
31	l	702	CDL	C36-C37-C38-C39
33	r	503	PLX	C12-C13-C14-C15
31	V	202	CDL	CB7-C71-C72-C73
30	s	403	PEE	C23-C24-C25-C26
31	V	202	CDL	C60-C61-C62-C63
31	l	702	CDL	C59-C60-C61-C62
31	l	703	CDL	C59-C60-C61-C62
33	j	202	PLX	C14-C15-C16-C17
33	j	202	PLX	C7-C8-C9-C10
33	j	203	PLX	C34-C35-C36-C37
30	j	201	PEE	C14-C15-C16-C17
30	r	501	PEE	C13-C14-C15-C16
31	a	201	CDL	C35-C36-C37-C38
33	r	503	PLX	C25-C26-C27-C28
31	n	101	CDL	C73-C74-C75-C76
31	s	402	CDL	C11-C12-C13-C14
31	g	202	CDL	C62-C63-C64-C65
31	k	101	CDL	C55-C56-C57-C58
33	g	201	PLX	C30-C31-C32-C33
31	l	702	CDL	C75-C76-C77-C78
31	k	101	CDL	C71-CB7-OB8-CB6
30	j	201	PEE	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
31	s	402	CDL	C73-C74-C75-C76
33	a	202	PLX	C14-C15-C16-C17
33	a	202	PLX	C25-C26-C27-C28
30	l	704	PEE	C30-C31-C32-C33
31	s	402	CDL	CB7-C71-C72-C73
30	s	401	PEE	C14-C15-C16-C17
31	V	201	CDL	C12-C13-C14-C15
31	V	201	CDL	C55-C56-C57-C58
31	V	202	CDL	C13-C14-C15-C16
31	V	202	CDL	C33-C34-C35-C36
31	a	201	CDL	C60-C61-C62-C63
31	k	101	CDL	C21-C22-C23-C24
31	l	702	CDL	C74-C75-C76-C77
31	l	703	CDL	C71-C72-C73-C74
31	s	402	CDL	C51-C52-C53-C54
33	g	201	PLX	C18-C19-C20-C21
33	g	201	PLX	C28-C29-C30-C31
33	j	203	PLX	C16-C17-C18-C19
33	r	503	PLX	C10-C11-C12-C13
33	r	503	PLX	C35-C36-C37-C38
33	r	502	PLX	C33-C34-C35-C36
33	r	503	PLX	C13-C14-C15-C16
31	V	202	CDL	C56-C57-C58-C59
30	l	704	PEE	C31-C32-C33-C34
31	V	201	CDL	C35-C36-C37-C38
31	V	201	CDL	C37-C38-C39-C40
31	l	703	CDL	C74-C75-C76-C77
31	s	402	CDL	C71-C72-C73-C74
33	j	203	PLX	C7-C8-C9-C10
33	r	502	PLX	C27-C28-C29-C30
33	r	503	PLX	C28-C29-C30-C31
31	l	703	CDL	CB5-C51-C52-C53
30	l	704	PEE	C32-C33-C34-C35
31	n	101	CDL	C54-C55-C56-C57
31	s	402	CDL	C17-C18-C19-C20
33	g	201	PLX	C13-C14-C15-C16
31	g	202	CDL	C43-C44-C45-C46
31	V	202	CDL	C55-C56-C57-C58
31	l	702	CDL	C19-C20-C21-C22
30	l	705	PEE	C31-C32-C33-C34
31	s	402	CDL	C36-C37-C38-C39
31	l	703	CDL	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
31	l	703	CDL	C55-C56-C57-C58
33	j	203	PLX	C29-C30-C31-C32
31	a	201	CDL	C37-C38-C39-C40
31	l	702	CDL	C51-C52-C53-C54
33	j	202	PLX	C27-C28-C29-C30
33	j	202	PLX	C29-C30-C31-C32
33	r	503	PLX	C30-C31-C32-C33
31	V	202	CDL	CA7-C31-C32-C33
30	W	201	PEE	C31-C30-O3-C3
31	g	202	CDL	C71-CB7-OB8-CB6
30	r	501	PEE	C21-C22-C23-C24
30	r	501	PEE	C11-C12-C13-C14
31	g	202	CDL	C71-C72-C73-C74
31	k	101	CDL	C59-C60-C61-C62
31	k	101	CDL	C71-C72-C73-C74
33	j	202	PLX	C31-C32-C33-C34
30	l	704	PEE	C21-C22-C23-C24
31	V	202	CDL	C52-C53-C54-C55
30	W	201	PEE	C12-C13-C14-C15
31	V	201	CDL	C58-C59-C60-C61
31	a	201	CDL	C73-C74-C75-C76
31	l	703	CDL	C15-C16-C17-C18
33	g	201	PLX	C32-C33-C34-C35
33	j	203	PLX	C33-C34-C35-C36
33	r	502	PLX	C30-C31-C32-C33
31	g	202	CDL	C31-C32-C33-C34
31	g	202	CDL	C32-C33-C34-C35
31	g	202	CDL	C83-C84-C85-C86
31	l	702	CDL	C73-C74-C75-C76
33	g	201	PLX	C10-C11-C12-C13
31	V	201	CDL	C51-CB5-OB6-CB4
31	l	702	CDL	C11-CA5-OA6-CA4
31	l	703	CDL	C51-CB5-OB6-CB4
30	r	501	PEE	O4-C10-O2-C2
31	l	703	CDL	OB7-CB5-OB6-CB4
31	l	703	CDL	C57-C58-C59-C60
33	g	201	PLX	C27-C28-C29-C30
30	Q	101	PEE	C19-C20-C21-C22
30	Q	101	PEE	C35-C36-C37-C38
30	W	201	PEE	C13-C14-C15-C16
31	a	201	CDL	C32-C33-C34-C35
33	a	202	PLX	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
30	W	201	PEE	C24-C25-C26-C27
31	k	101	CDL	C52-C53-C54-C55
31	l	703	CDL	C75-C76-C77-C78
30	s	403	PEE	C42-C43-C44-C45
31	k	101	CDL	C56-C57-C58-C59
31	l	702	CDL	C13-C14-C15-C16
31	k	101	CDL	OB9-CB7-OB8-CB6
30	j	201	PEE	C22-C23-C24-C25
30	r	501	PEE	C41-C42-C43-C44
31	a	201	CDL	C76-C77-C78-C79
31	a	201	CDL	C62-C63-C64-C65
31	V	202	CDL	C11-C12-C13-C14
31	g	202	CDL	C41-C42-C43-C44
33	g	201	PLX	C33-C34-C35-C36
33	j	202	PLX	C33-C34-C35-C36
31	g	202	CDL	CA7-C31-C32-C33
31	V	202	CDL	C34-C35-C36-C37
31	V	202	CDL	C75-C76-C77-C78
30	l	704	PEE	O3P-C1-C2-O2
31	k	101	CDL	OB5-CB3-CB4-OB6
33	r	502	PLX	C14-C15-C16-C17
33	r	502	PLX	C31-C32-C33-C34
34	s	404	UQ	C14-C16-C17-C18
30	s	401	PEE	C11-C12-C13-C14
33	j	202	PLX	C28-C29-C30-C31
30	s	403	PEE	C10-C11-C12-C13
30	s	403	PEE	C39-C40-C41-C42
31	l	702	CDL	OA6-CA4-CA6-OA8
31	s	402	CDL	OB6-CB4-CB6-OB8
31	k	101	CDL	C32-C33-C34-C35
33	j	203	PLX	C27-C28-C29-C30
30	l	701	PEE	C33-C34-C35-C36
31	k	101	CDL	C14-C15-C16-C17
31	l	702	CDL	C32-C33-C34-C35
31	l	703	CDL	C43-C44-C45-C46
33	j	202	PLX	C9-C10-C11-C12
30	j	201	PEE	C36-C37-C38-C39
30	s	403	PEE	C36-C37-C38-C39
30	s	403	PEE	C38-C39-C40-C41
31	V	201	CDL	C71-C72-C73-C74
31	V	202	CDL	C54-C55-C56-C57
31	g	202	CDL	C59-C60-C61-C62

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Mol	Chain	Res	Type	Atoms
31	k	101	CDL	C62-C63-C64-C65
31	a	201	CDL	C75-C76-C77-C78
31	l	702	CDL	C37-C38-C39-C40
31	l	703	CDL	C51-C52-C53-C54
31	s	402	CDL	C55-C56-C57-C58
33	g	201	PLX	C25-C26-C27-C28
31	s	402	CDL	C59-C60-C61-C62
31	V	201	CDL	C75-C76-C77-C78
31	g	202	CDL	C54-C55-C56-C57
31	l	702	CDL	C12-C13-C14-C15
33	a	202	PLX	C9-C10-C11-C12
33	r	502	PLX	C28-C29-C30-C31
31	a	201	CDL	C22-C23-C24-C25
33	r	502	PLX	C11-C10-C9-C8
31	a	201	CDL	C52-C53-C54-C55
31	a	201	CDL	C54-C55-C56-C57
31	n	101	CDL	C72-C73-C74-C75
33	j	203	PLX	C9-C10-C11-C12
30	r	501	PEE	C31-C32-C33-C34
30	r	501	PEE	C15-C16-C17-C18
30	s	401	PEE	C19-C20-C21-C22
30	W	201	PEE	O5-C30-O3-C3
30	l	701	PEE	C31-C32-C33-C34
31	s	402	CDL	C16-C17-C18-C19
31	s	402	CDL	C54-C55-C56-C57
31	a	201	CDL	OA5-CA3-CA4-CA6
31	l	702	CDL	OA5-CA3-CA4-CA6
31	n	101	CDL	OA5-CA3-CA4-CA6
31	l	702	CDL	OA7-CA5-OA6-CA4
33	a	202	PLX	C30-C31-C32-C33
31	s	402	CDL	CB5-C51-C52-C53
30	W	201	PEE	C11-C12-C13-C14
31	g	202	CDL	C57-C58-C59-C60
31	g	202	CDL	C63-C64-C65-C66
33	r	503	PLX	C31-C32-C33-C34
31	g	202	CDL	OB9-CB7-OB8-CB6
31	s	402	CDL	C31-C32-C33-C34
33	r	503	PLX	C14-C15-C16-C17
33	a	202	PLX	C35-C36-C37-C38
30	s	403	PEE	C17-C18-C19-C20
30	j	201	PEE	C13-C14-C15-C16
31	a	201	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
30	s	401	PEE	C1-C2-C3-O3
31	V	202	CDL	CA3-CA4-CA6-OA8
31	l	703	CDL	CA3-CA4-CA6-OA8
33	g	201	PLX	C3-C4-C5-O8
31	l	703	CDL	C32-C33-C34-C35
31	l	703	CDL	C52-C53-C54-C55
31	g	202	CDL	C11-C12-C13-C14
30	s	403	PEE	C20-C21-C22-C23
31	V	201	CDL	CA5-C11-C12-C13
31	V	201	CDL	CB7-C71-C72-C73
31	k	101	CDL	C39-C40-C41-C42
31	k	101	CDL	C74-C75-C76-C77
31	l	703	CDL	C62-C63-C64-C65
30	r	501	PEE	C36-C37-C38-C39
33	r	503	PLX	C27-C28-C29-C30
31	V	201	CDL	OB7-CB5-OB6-CB4
31	l	702	CDL	C17-C18-C19-C20
31	V	201	CDL	C72-C73-C74-C75
31	k	101	CDL	CA6-CA4-OA6-CA5
31	g	202	CDL	C23-C24-C25-C26
30	s	401	PEE	C15-C16-C17-C18
30	s	403	PEE	C35-C36-C37-C38
31	V	202	CDL	C35-C36-C37-C38
31	V	202	CDL	C62-C63-C64-C65
33	r	503	PLX	C7-C8-C9-C10
33	a	202	PLX	C16-C17-C18-C19
30	l	704	PEE	C10-C11-C12-C13
30	s	401	PEE	C12-C13-C14-C15
31	s	402	CDL	C35-C36-C37-C38
33	a	202	PLX	C28-C29-C30-C31
31	a	201	CDL	OB5-CB3-CB4-OB6
30	s	403	PEE	C34-C35-C36-C37
31	V	202	CDL	C12-C13-C14-C15
31	V	202	CDL	C73-C74-C75-C76
31	k	101	CDL	C16-C17-C18-C19
31	V	202	CDL	C17-C18-C19-C20
31	g	202	CDL	C84-C85-C86-C87
31	k	101	CDL	C37-C38-C39-C40
30	Q	101	PEE	C14-C15-C16-C17
31	V	202	CDL	C82-C83-C84-C85
31	a	201	CDL	C71-C72-C73-C74
30	j	201	PEE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
30	l	704	PEE	C11-C12-C13-C14
31	g	202	CDL	C52-C53-C54-C55
33	r	503	PLX	C16-C17-C18-C19
30	l	705	PEE	O2-C2-C3-O3
31	k	101	CDL	OB6-CB4-CB6-OB8
30	s	403	PEE	C22-C23-C24-C25
31	g	202	CDL	C55-C56-C57-C58
31	g	202	CDL	C17-C18-C19-C20
33	j	203	PLX	C11-C12-C13-C14
33	r	502	PLX	C12-C13-C14-C15
30	l	705	PEE	C13-C14-C15-C16
31	a	201	CDL	C84-C85-C86-C87
30	j	201	PEE	C38-C39-C40-C41
31	k	101	CDL	C20-C21-C22-C23
33	r	503	PLX	C15-C16-C17-C18
33	j	202	PLX	C36-C37-C38-C39
30	l	704	PEE	C42-C43-C44-C45
30	s	401	PEE	C23-C24-C25-C26
31	k	101	CDL	C11-C12-C13-C14
31	n	101	CDL	C75-C76-C77-C78
30	Q	101	PEE	C23-C24-C25-C26
30	r	501	PEE	C31-C30-O3-C3
33	r	502	PLX	C10-C11-C12-C13
31	k	101	CDL	C15-C16-C17-C18
31	l	703	CDL	C64-C65-C66-C67
31	g	202	CDL	CB5-C51-C52-C53
31	V	202	CDL	C42-C43-C44-C45
32	X	201	8Q1	N41-C42-C43-S44
31	V	201	CDL	C73-C74-C75-C76
31	l	703	CDL	C14-C15-C16-C17
31	l	703	CDL	C33-C34-C35-C36
31	s	402	CDL	C40-C41-C42-C43
33	g	201	PLX	C16-C17-C18-C19
30	l	704	PEE	O3P-C1-C2-C3
31	k	101	CDL	OA5-CA3-CA4-CA6
30	Q	101	PEE	C21-C22-C23-C24
30	l	705	PEE	C10-C11-C12-C13
31	a	201	CDL	CA5-C11-C12-C13
33	a	202	PLX	C33-C34-C35-C36
31	a	201	CDL	C11-C12-C13-C14
31	s	402	CDL	C12-C13-C14-C15
31	V	201	CDL	C64-C65-C66-C67

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Mol	Chain	Res	Type	Atoms
30	j	201	PEE	C19-C20-C21-C22
33	a	202	PLX	C7-C8-C9-C10
31	a	201	CDL	C11-CA5-OA6-CA4
30	s	403	PEE	C31-C30-O3-C3
30	l	701	PEE	C1-C2-C3-O3
30	l	705	PEE	C1-C2-C3-O3
30	r	501	PEE	C1-C2-C3-O3
31	k	101	CDL	CB3-CB4-CB6-OB8
31	l	702	CDL	CA3-CA4-CA6-OA8
31	s	402	CDL	CB3-CB4-CB6-OB8
33	a	202	PLX	C3-C4-C5-O8
33	r	502	PLX	C3-C4-C5-O8
33	r	503	PLX	C3-C4-C5-O8
31	V	201	CDL	C74-C75-C76-C77
31	V	201	CDL	C43-C44-C45-C46
31	V	202	CDL	C76-C77-C78-C79
30	j	201	PEE	C32-C33-C34-C35
31	k	101	CDL	C41-C42-C43-C44
31	g	202	CDL	C14-C15-C16-C17
30	l	704	PEE	C24-C25-C26-C27
31	l	702	CDL	C15-C16-C17-C18
30	W	201	PEE	O3P-C1-C2-O2
31	V	201	CDL	OB5-CB3-CB4-OB6
31	l	702	CDL	OB5-CB3-CB4-OB6
33	j	202	PLX	O4-C3-C4-O6
33	r	503	PLX	O4-C3-C4-O6
31	V	202	CDL	C84-C85-C86-C87
30	Q	101	PEE	C18-C19-C20-C21
30	Q	101	PEE	C24-C25-C26-C27
31	V	202	CDL	C74-C75-C76-C77
31	l	703	CDL	C54-C55-C56-C57
30	s	403	PEE	C13-C14-C15-C16
31	n	101	CDL	C51-C52-C53-C54
30	l	701	PEE	O2-C2-C3-O3
30	r	501	PEE	O2-C2-C3-O3
31	V	202	CDL	OB6-CB4-CB6-OB8
31	g	202	CDL	OA6-CA4-CA6-OA8
31	n	101	CDL	OA6-CA4-CA6-OA8
31	a	201	CDL	C18-C19-C20-C21
31	g	202	CDL	C19-C20-C21-C22
33	r	502	PLX	C16-C17-C18-C19
33	j	203	PLX	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
33	j	203	PLX	O6-C6-C7-C8
31	l	703	CDL	C38-C39-C40-C41
32	X	201	8Q1	C11-C12-C13-C14
31	l	703	CDL	C31-C32-C33-C34
31	l	703	CDL	C84-C85-C86-C87
31	l	703	CDL	C58-C59-C60-C61
31	a	201	CDL	C38-C39-C40-C41
30	s	403	PEE	C12-C13-C14-C15
31	a	201	CDL	C31-C32-C33-C34
31	g	202	CDL	C64-C65-C66-C67
31	g	202	CDL	C15-C16-C17-C18
31	V	201	CDL	C54-C55-C56-C57
30	l	701	PEE	C35-C36-C37-C38
30	l	701	PEE	O3P-C1-C2-C3
30	s	403	PEE	O3P-C1-C2-C3
31	V	201	CDL	OA5-CA3-CA4-CA6
31	k	101	CDL	OB5-CB3-CB4-CB6
31	s	402	CDL	OA5-CA3-CA4-CA6
33	j	202	PLX	O4-C3-C4-C5
31	l	703	CDL	C82-C83-C84-C85
30	r	501	PEE	C38-C39-C40-C41
33	r	502	PLX	C6-C7-C8-C9
31	l	702	CDL	C80-C81-C82-C83
31	l	703	CDL	C78-C79-C80-C81
30	s	403	PEE	O5-C30-O3-C3
30	j	201	PEE	C44-C45-C46-C47
33	a	202	PLX	C11-C12-C13-C14
33	j	202	PLX	C10-C11-C12-C13
30	r	501	PEE	O5-C30-O3-C3
31	g	202	CDL	C36-C37-C38-C39
30	l	705	PEE	C15-C16-C17-C18
33	j	203	PLX	C25-C26-C27-C28
30	l	704	PEE	C13-C14-C15-C16
30	s	403	PEE	O3P-C1-C2-O2
31	V	202	CDL	OA5-CA3-CA4-OA6
31	l	703	CDL	OA5-CA3-CA4-OA6
33	r	502	PLX	O4-C3-C4-O6
33	g	201	PLX	C12-C13-C14-C15
33	j	202	PLX	C3-C4-C5-O8
33	j	203	PLX	C12-C13-C14-C15
30	W	201	PEE	C15-C16-C17-C18
31	l	703	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
30	s	403	PEE	C21-C22-C23-C24
31	V	202	CDL	C71-C72-C73-C74
31	a	201	CDL	C12-C13-C14-C15
31	k	101	CDL	C79-C80-C81-C82
31	k	101	CDL	C33-C34-C35-C36
30	s	403	PEE	C14-C15-C16-C17
31	a	201	CDL	C20-C21-C22-C23
31	a	201	CDL	C55-C56-C57-C58
31	k	101	CDL	CA4-CA3-OA5-PA1
31	k	101	CDL	C84-C85-C86-C87
33	j	202	PLX	N1-C1-C2-O1
35	w	401	ADP	PB-O3A-PA-O1A
30	r	501	PEE	C14-C15-C16-C17
31	g	202	CDL	CA5-C11-C12-C13
31	l	703	CDL	C77-C78-C79-C80
31	a	201	CDL	OA7-CA5-OA6-CA4
33	j	203	PLX	C10-C11-C12-C13
32	X	201	8Q1	O33-C32-C34-O35
33	g	201	PLX	C25-C24-O8-C5
33	j	202	PLX	C30-C31-C32-C33
31	l	703	CDL	C12-C11-CA5-OA6
31	V	201	CDL	C44-C45-C46-C47
30	l	705	PEE	O3P-C1-C2-C3
31	V	201	CDL	OB5-CB3-CB4-CB6
31	V	202	CDL	OA5-CA3-CA4-CA6
31	a	201	CDL	OB5-CB3-CB4-CB6
31	l	703	CDL	OA5-CA3-CA4-CA6
33	r	502	PLX	O4-C3-C4-C5
33	r	503	PLX	O4-C3-C4-C5
33	r	503	PLX	C32-C33-C34-C35
31	l	703	CDL	C60-C61-C62-C63
31	V	202	CDL	C64-C65-C66-C67
31	a	201	CDL	C21-C22-C23-C24
31	V	201	CDL	CB4-CB3-OB5-PB2
31	g	202	CDL	C37-C38-C39-C40
33	g	201	PLX	O6-C6-C7-C8
33	j	203	PLX	O8-C24-C25-C26
30	l	701	PEE	O3P-C1-C2-O2
30	l	705	PEE	O3P-C1-C2-O2
31	V	201	CDL	OA5-CA3-CA4-OA6
33	g	201	PLX	C11-C10-C9-C8
31	g	202	CDL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
31	l	702	CDL	C54-C55-C56-C57
33	a	202	PLX	O6-C4-C5-O8
33	j	202	PLX	O6-C4-C5-O8
33	r	502	PLX	O6-C4-C5-O8
33	r	503	PLX	O6-C4-C5-O8
31	V	202	CDL	CB3-CB4-CB6-OB8
31	l	703	CDL	CB3-CB4-CB6-OB8
31	n	101	CDL	CA3-CA4-CA6-OA8
30	r	501	PEE	C44-C45-C46-C47
30	s	401	PEE	C24-C25-C26-C27
30	Q	101	PEE	C10-C11-C12-C13
31	k	101	CDL	C64-C65-C66-C67
31	s	402	CDL	C32-C33-C34-C35
30	Q	101	PEE	C1-O3P-P-O1P
30	Q	101	PEE	C1-O3P-P-O4P
30	Q	101	PEE	C4-O4P-P-O2P
30	j	201	PEE	C1-O3P-P-O2P
30	j	201	PEE	C4-O4P-P-O1P
30	l	701	PEE	C4-O4P-P-O1P
30	l	705	PEE	C1-O3P-P-O2P
30	l	705	PEE	C1-O3P-P-O1P
30	l	705	PEE	C1-O3P-P-O4P
30	r	501	PEE	C1-O3P-P-O2P
30	r	501	PEE	C1-O3P-P-O1P
30	r	501	PEE	C1-O3P-P-O4P
30	r	501	PEE	C4-O4P-P-O2P
30	s	401	PEE	C1-O3P-P-O4P
30	s	401	PEE	C4-O4P-P-O1P
31	V	201	CDL	CB2-OB2-PB2-OB4
31	V	202	CDL	CA3-OA5-PA1-OA2
31	V	202	CDL	CA3-OA5-PA1-OA3
31	V	202	CDL	CA3-OA5-PA1-OA4
31	V	202	CDL	CB2-OB2-PB2-OB4
31	V	202	CDL	CB3-OB5-PB2-OB2
31	V	202	CDL	CB3-OB5-PB2-OB3
31	V	202	CDL	CB3-OB5-PB2-OB4
31	a	201	CDL	CB2-OB2-PB2-OB4
31	a	201	CDL	CB2-OB2-PB2-OB5
31	g	202	CDL	CA2-OA2-PA1-OA4
31	g	202	CDL	CA3-OA5-PA1-OA3
31	k	101	CDL	CB2-OB2-PB2-OB4
31	l	702	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
31	l	702	CDL	CB3-OB5-PB2-OB4
31	n	101	CDL	CB2-OB2-PB2-OB4
33	a	202	PLX	C2-O1-P1-O3
33	g	201	PLX	C3-O4-P1-O2
33	j	202	PLX	C3-C4-O6-C6
33	j	202	PLX	C5-C4-O6-C6
33	j	202	PLX	C2-O1-P1-O3
33	r	502	PLX	C2-O1-P1-O4
33	r	502	PLX	C2-O1-P1-O3
33	r	503	PLX	C3-C4-O6-C6
33	r	503	PLX	C5-C4-O6-C6
33	r	503	PLX	C2-O1-P1-O4
33	r	503	PLX	C2-O1-P1-O3
30	l	701	PEE	C2-C1-O3P-P
31	g	202	CDL	C1-CB2-OB2-PB2
31	V	201	CDL	C14-C15-C16-C17
31	V	202	CDL	C36-C37-C38-C39
31	l	702	CDL	C35-C36-C37-C38
33	a	202	PLX	C18-C19-C20-C21
33	j	202	PLX	C24-C25-C26-C27
31	a	201	CDL	C14-C15-C16-C17
30	l	704	PEE	C3-C2-O2-C10
31	V	201	CDL	CA6-CA4-OA6-CA5
31	a	201	CDL	C82-C83-C84-C85
33	r	503	PLX	C11-C12-C13-C14
33	a	202	PLX	C27-C28-C29-C30
31	g	202	CDL	C77-C78-C79-C80
30	W	201	PEE	O3P-C1-C2-C3
30	W	201	PEE	C16-C17-C18-C19
30	W	201	PEE	O4-C10-O2-C2
31	a	201	CDL	OA5-CA3-CA4-OA6
31	V	202	CDL	C83-C84-C85-C86
31	V	202	CDL	C32-C31-CA7-OA8
31	l	703	CDL	C39-C40-C41-C42
31	g	202	CDL	C44-C45-C46-C47
34	s	404	UQ	C12-C13-C14-C16
30	s	401	PEE	O2-C2-C3-O3
30	l	701	PEE	C18-C19-C20-C21
31	g	202	CDL	C73-C74-C75-C76
33	j	202	PLX	C16-C17-C18-C19
33	j	202	PLX	C11-C12-C13-C14
30	W	201	PEE	C11-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
31	s	402	CDL	C11-CA5-OA6-CA4
31	g	202	CDL	C72-C71-CB7-OB8
31	l	703	CDL	C21-C22-C23-C24
30	r	501	PEE	C16-C17-C18-C19
31	l	702	CDL	C82-C83-C84-C85
30	l	704	PEE	C39-C40-C41-C42
31	s	402	CDL	C34-C35-C36-C37
31	s	402	CDL	OA7-CA5-OA6-CA4
31	k	101	CDL	C34-C35-C36-C37
31	V	201	CDL	C38-C39-C40-C41
31	n	101	CDL	C71-CB7-OB8-CB6
33	j	202	PLX	C12-C13-C14-C15
31	n	101	CDL	OB9-CB7-OB8-CB6
31	k	101	CDL	C78-C79-C80-C81
31	n	101	CDL	C57-C58-C59-C60
31	l	702	CDL	C12-C11-CA5-OA6
30	l	705	PEE	C16-C17-C18-C19
30	r	501	PEE	C18-C19-C20-C21
31	g	202	CDL	OB6-CB4-CB6-OB8
31	a	201	CDL	C64-C65-C66-C67
31	V	202	CDL	C57-C58-C59-C60
30	r	501	PEE	C40-C41-C42-C43
33	a	202	PLX	C34-C35-C36-C37
30	l	704	PEE	C44-C45-C46-C47
31	s	402	CDL	C74-C75-C76-C77
31	g	202	CDL	CA3-CA4-CA6-OA8
30	j	201	PEE	C40-C41-C42-C43
31	g	202	CDL	C56-C57-C58-C59
33	r	503	PLX	C18-C19-C20-C21
33	r	502	PLX	C13-C14-C15-C16
32	X	201	8Q1	C11-C10-C9-C8
30	l	705	PEE	C18-C19-C20-C21
31	s	402	CDL	C18-C19-C20-C21
31	l	703	CDL	C32-C31-CA7-OA8
31	k	101	CDL	C82-C83-C84-C85
31	V	202	CDL	C19-C20-C21-C22
31	a	201	CDL	C39-C40-C41-C42
31	l	702	CDL	C24-C25-C26-C27
30	Q	101	PEE	C16-C17-C18-C19
31	V	201	CDL	CA4-CA3-OA5-PA1
31	l	702	CDL	C20-C21-C22-C23
30	l	705	PEE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
33	g	201	PLX	C11-C12-C13-C14
30	l	701	PEE	C13-C14-C15-C16
31	g	202	CDL	C42-C43-C44-C45
31	s	402	CDL	C15-C16-C17-C18
30	l	704	PEE	C15-C16-C17-C18
31	s	402	CDL	C72-C71-CB7-OB8
30	s	401	PEE	C13-C14-C15-C16
33	a	202	PLX	O8-C24-C25-C26
33	r	502	PLX	O8-C24-C25-C26
30	j	201	PEE	C2-C3-O3-C30
33	a	202	PLX	C19-C20-C21-C22
31	l	702	CDL	CB4-CB3-OB5-PB2
31	g	202	CDL	C12-C13-C14-C15
33	j	202	PLX	O9-C24-C25-C26
31	s	402	CDL	C38-C39-C40-C41
31	g	202	CDL	OA7-CA5-OA6-CA4
31	k	101	CDL	C75-C76-C77-C78
30	j	201	PEE	O3P-C1-C2-O2
30	Q	101	PEE	C20-C21-C22-C23
31	V	202	CDL	C39-C40-C41-C42
31	g	202	CDL	C11-CA5-OA6-CA4
31	a	201	CDL	C61-C62-C63-C64
31	l	702	CDL	OB5-CB3-CB4-CB6
30	Q	101	PEE	C36-C37-C38-C39
30	s	401	PEE	C16-C17-C18-C19
30	s	403	PEE	C16-C17-C18-C19
30	l	704	PEE	C33-C34-C35-C36
31	l	703	CDL	C12-C13-C14-C15
30	j	201	PEE	C15-C16-C17-C18
33	j	202	PLX	C4-C5-O8-C24
33	j	203	PLX	C36-C37-C38-C39
31	V	202	CDL	C63-C64-C65-C66
31	a	201	CDL	C44-C45-C46-C47
31	g	202	CDL	C35-C36-C37-C38
31	l	702	CDL	C76-C77-C78-C79
30	l	701	PEE	C16-C17-C18-C19
30	l	701	PEE	C38-C39-C40-C41
30	l	705	PEE	C38-C39-C40-C41
33	a	202	PLX	C12-C13-C14-C15
30	l	704	PEE	C16-C17-C18-C19
31	k	101	CDL	C1-CB2-OB2-PB2
30	l	704	PEE	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
33	r	502	PLX	C18-C19-C20-C21
30	l	705	PEE	C20-C21-C22-C23
33	j	203	PLX	C18-C19-C20-C21
33	g	201	PLX	C14-C15-C16-C17
30	W	201	PEE	C18-C19-C20-C21
31	l	703	CDL	C72-C71-CB7-OB8
30	Q	101	PEE	C38-C39-C40-C41
30	j	201	PEE	C16-C17-C18-C19
30	s	401	PEE	C18-C19-C20-C21
31	g	202	CDL	C52-C51-CB5-OB6
31	s	402	CDL	C12-C11-CA5-OA6
30	j	201	PEE	O3P-C1-C2-C3
30	W	201	PEE	C22-C23-C24-C25
31	s	402	CDL	C77-C78-C79-C80
33	j	203	PLX	C7-C6-O6-C4
31	l	702	CDL	OB7-CB5-OB6-CB4
33	r	502	PLX	C19-C20-C21-C22
33	a	202	PLX	C15-C16-C17-C18
31	n	101	CDL	C72-C71-CB7-OB8
31	l	702	CDL	C51-CB5-OB6-CB4
33	j	203	PLX	C28-C29-C30-C31
31	k	101	CDL	C52-C51-CB5-OB6
30	l	704	PEE	C36-C37-C38-C39
31	n	101	CDL	C52-C51-CB5-OB6
31	a	201	CDL	C34-C35-C36-C37
30	l	704	PEE	C1-C2-C3-O3
31	s	402	CDL	C57-C58-C59-C60
31	a	201	CDL	C32-C31-CA7-OA8
31	V	202	CDL	C44-C45-C46-C47
31	l	703	CDL	C17-C18-C19-C20
31	a	201	CDL	C12-C11-CA5-OA6
31	k	101	CDL	CA2-C1-CB2-OB2
31	l	702	CDL	C72-C71-CB7-OB8
30	l	704	PEE	C43-C44-C45-C46
31	V	202	CDL	C52-C51-CB5-OB6
31	V	201	CDL	C31-C32-C33-C34
31	n	101	CDL	C72-C71-CB7-OB9
30	l	705	PEE	C21-C22-C23-C24
33	r	503	PLX	C9-C10-C11-C12
31	n	101	CDL	CA5-C11-C12-C13
31	l	702	CDL	C44-C45-C46-C47
31	a	201	CDL	C32-C31-CA7-OA9

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Mol	Chain	Res	Type	Atoms
31	g	202	CDL	C52-C51-CB5-OB7
30	l	705	PEE	C11-C12-C13-C14
31	a	201	CDL	C12-C11-CA5-OA7
31	s	402	CDL	C12-C11-CA5-OA7
33	a	202	PLX	O9-C24-O8-C5
33	j	202	PLX	O9-C24-O8-C5
33	r	503	PLX	O9-C24-O8-C5
31	g	202	CDL	C51-C52-C53-C54
31	k	101	CDL	C51-C52-C53-C54
33	r	503	PLX	C19-C20-C21-C22
31	V	201	CDL	C12-C11-CA5-OA6
31	k	101	CDL	C52-C51-CB5-OB7
31	l	703	CDL	C72-C71-CB7-OB9
30	l	704	PEE	O2-C2-C3-O3
31	k	101	CDL	C44-C45-C46-C47
31	n	101	CDL	C52-C51-CB5-OB7
31	g	202	CDL	CB4-CB3-OB5-PB2
30	s	401	PEE	C34-C35-C36-C37
31	V	201	CDL	C12-C11-CA5-OA7
30	l	705	PEE	O3-C30-C31-C32
35	w	401	ADP	PB-O3A-PA-O2A
33	a	202	PLX	C24-C25-C26-C27
30	s	403	PEE	C18-C19-C20-C21
30	s	403	PEE	O2-C10-C11-C12
31	l	702	CDL	C72-C71-CB7-OB9

There are no ring outliers.

26 monomers are involved in 102 short contacts:

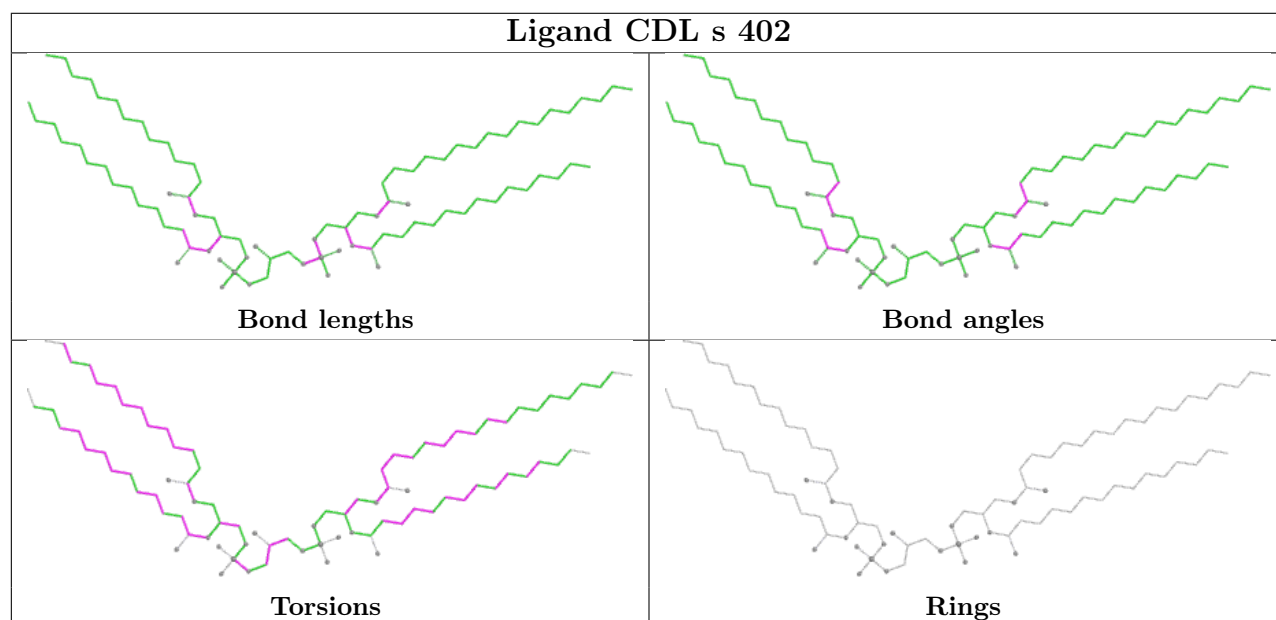
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	s	402	CDL	5	0
30	j	201	PEE	6	0
33	j	202	PLX	2	0
30	l	701	PEE	1	0
30	l	704	PEE	2	0
30	l	705	PEE	3	0
30	Q	101	PEE	2	0
31	a	201	CDL	5	0
31	l	702	CDL	9	0
32	X	201	8Q1	5	0
34	s	404	UQ	3	0
31	l	703	CDL	2	0

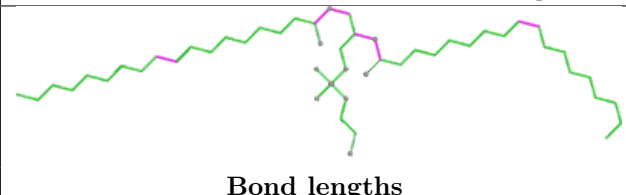
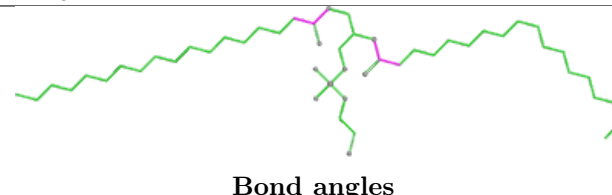
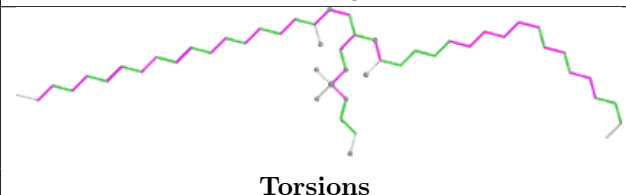
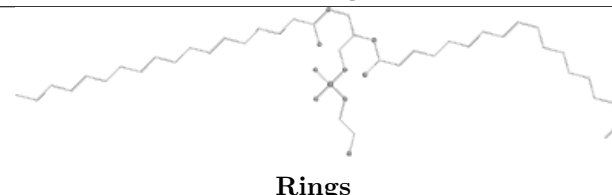
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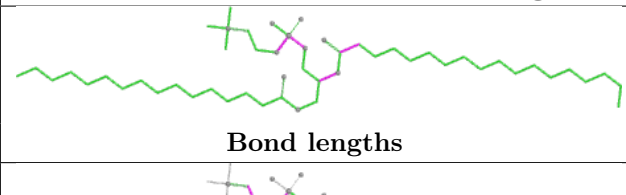
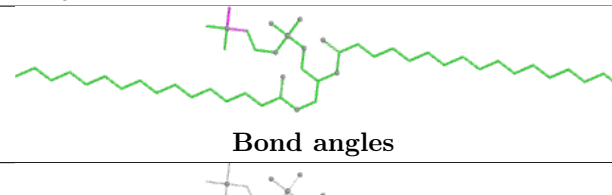
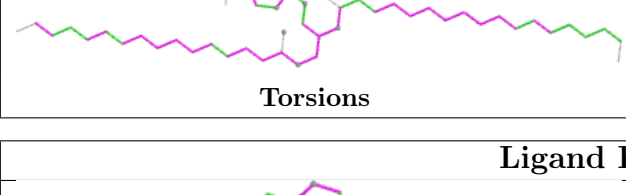
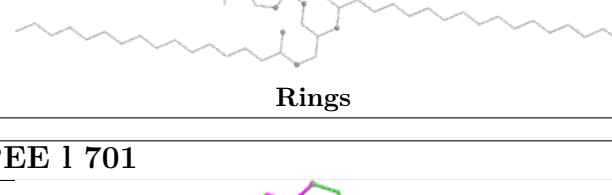
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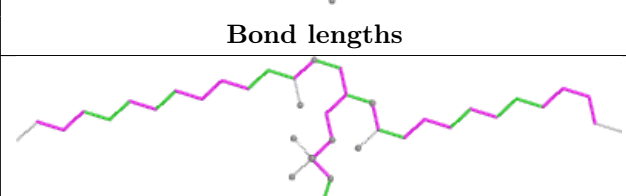
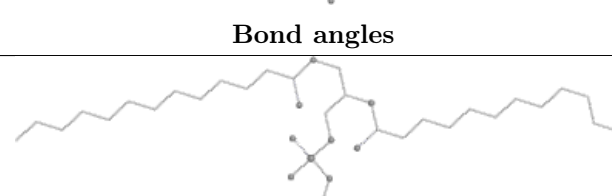
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	w	401	ADP	1	0
31	k	101	CDL	13	0
33	j	203	PLX	1	0
31	V	202	CDL	3	0
30	W	201	PEE	1	0
33	g	201	PLX	5	0
30	s	401	PEE	2	0
33	r	502	PLX	3	0
33	r	503	PLX	4	0
30	r	501	PEE	3	0
31	V	201	CDL	6	0
31	n	101	CDL	2	0
30	s	403	PEE	6	0
31	g	202	CDL	10	0

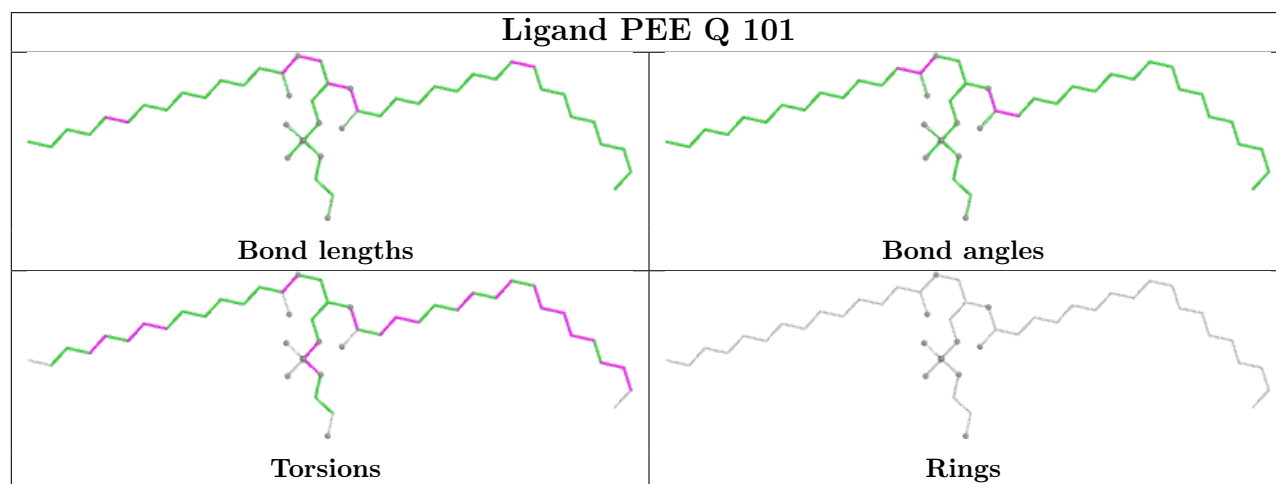
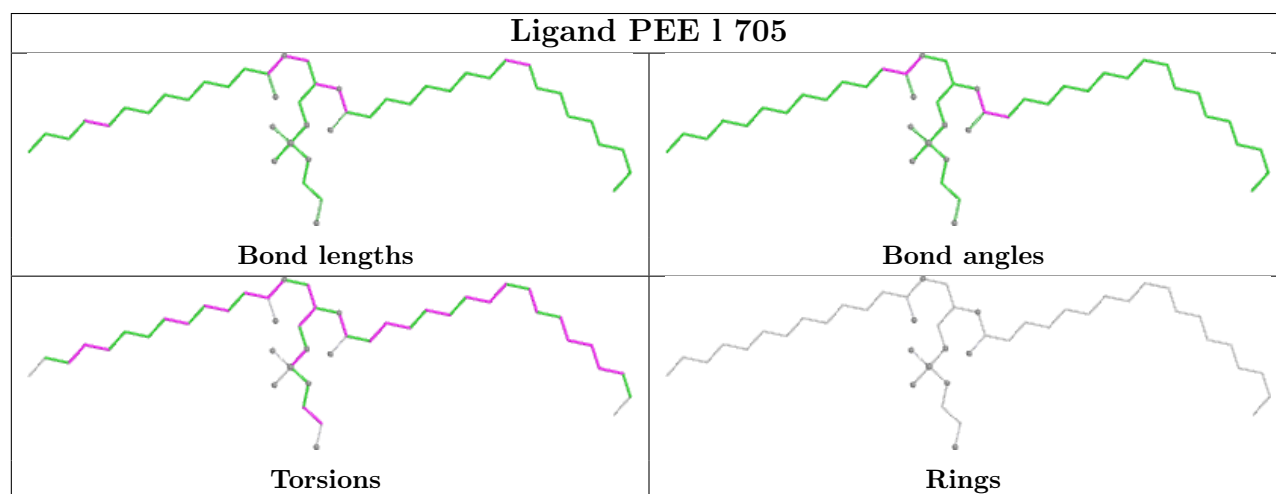
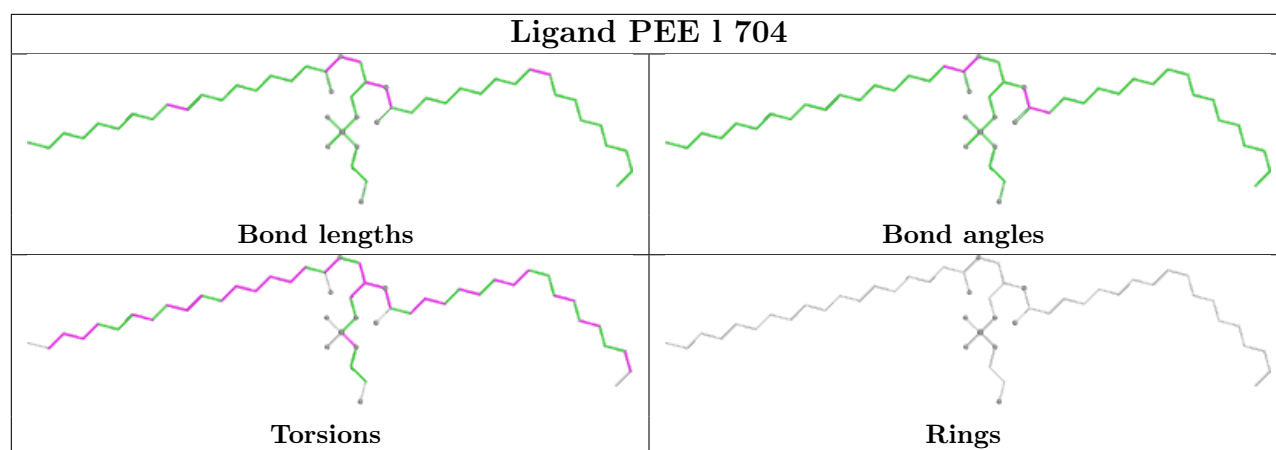
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

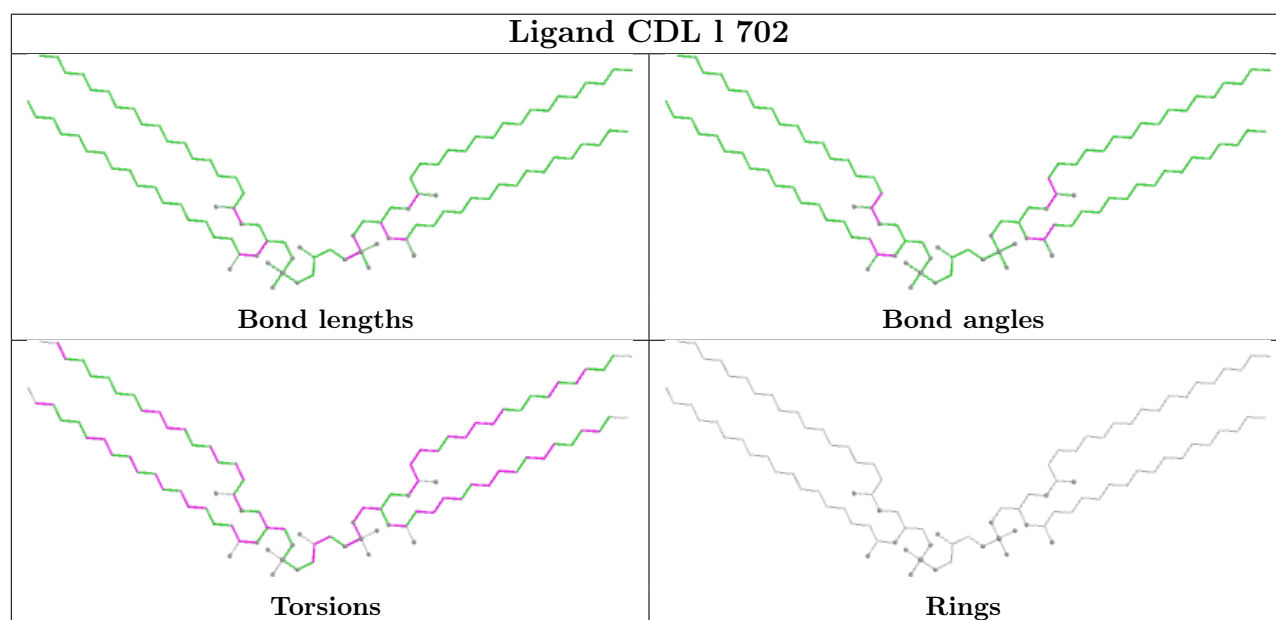
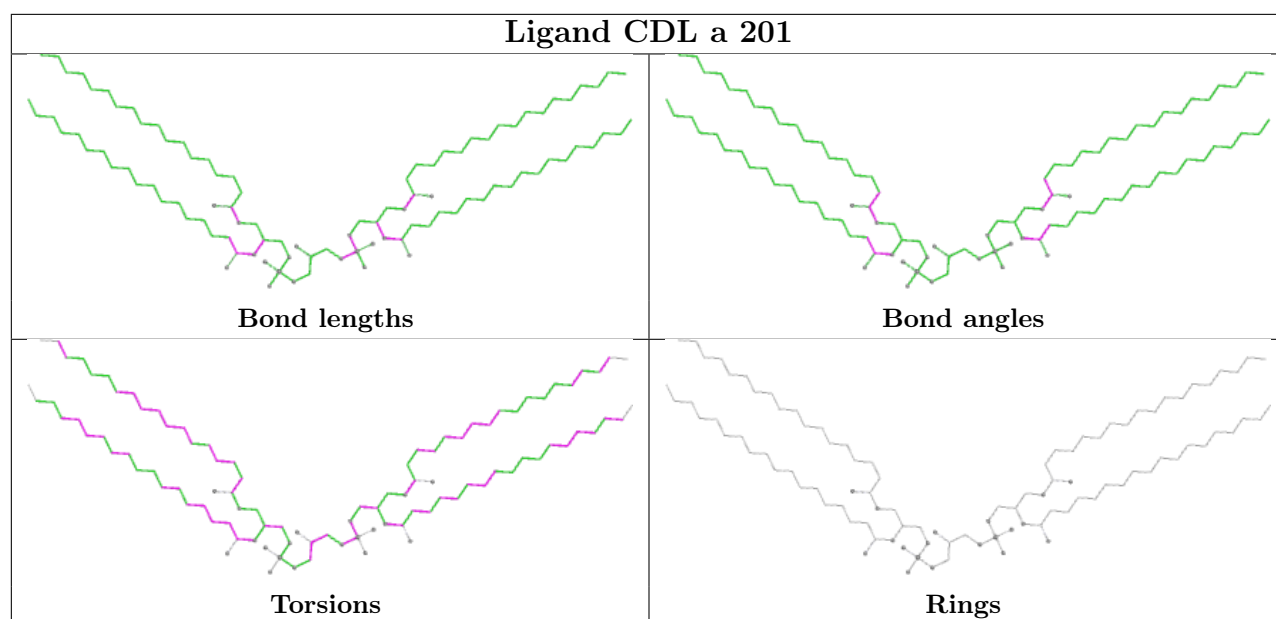


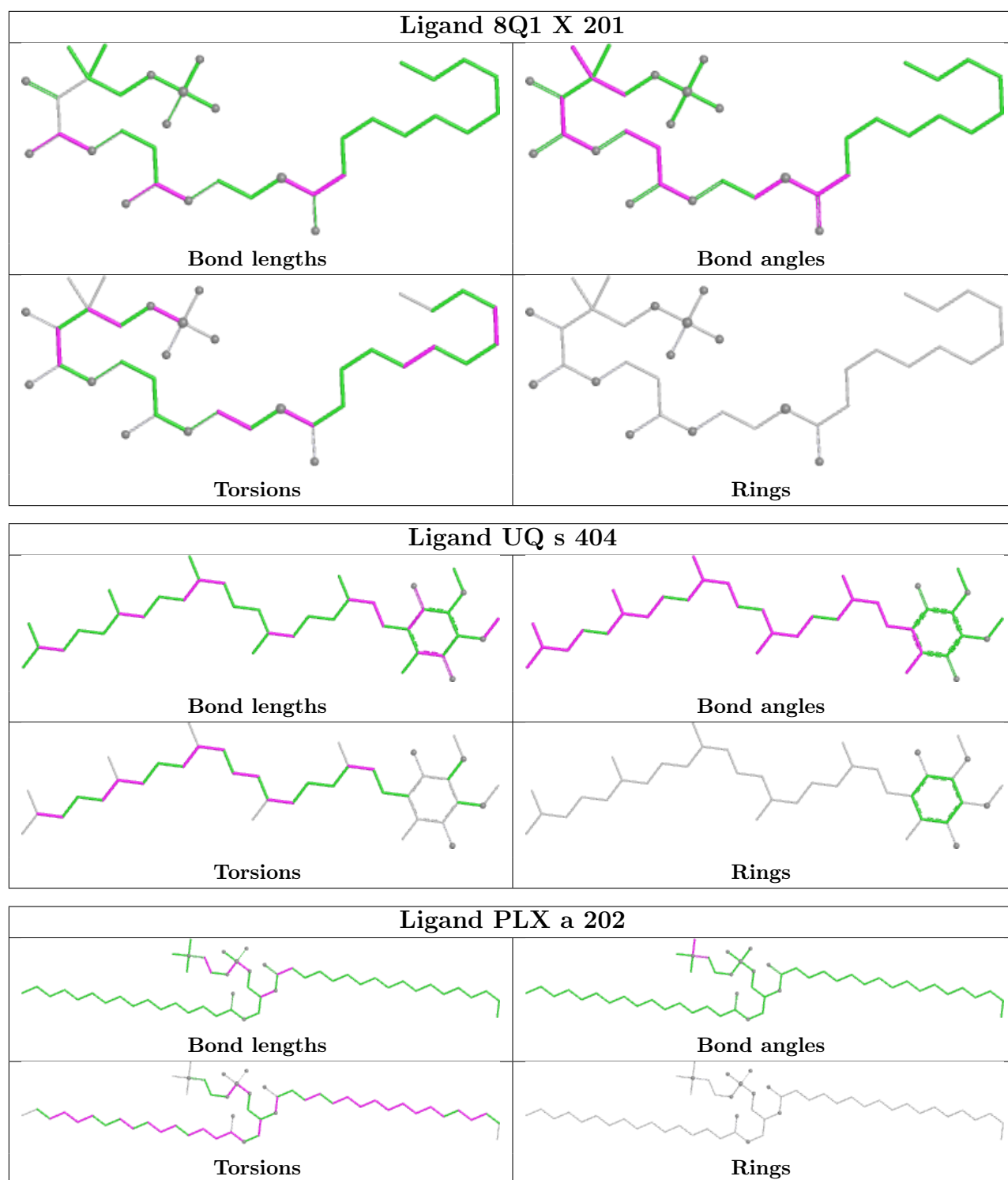
Ligand PEE j 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

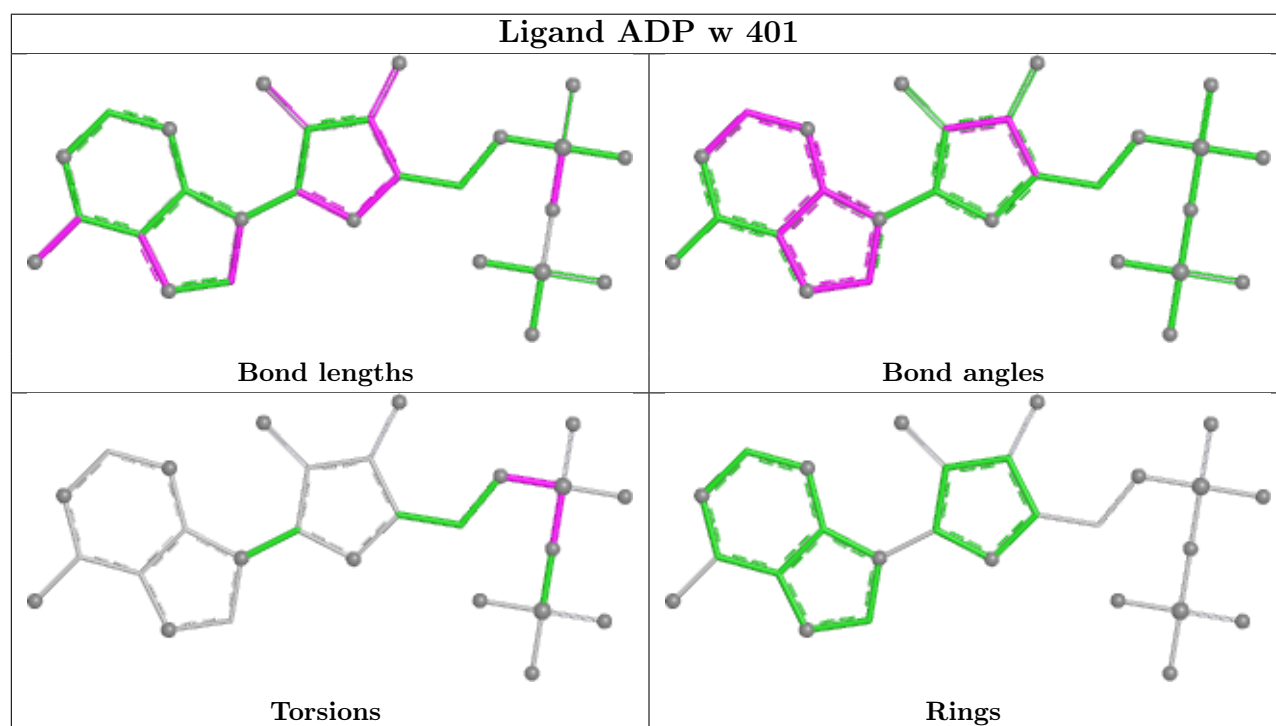
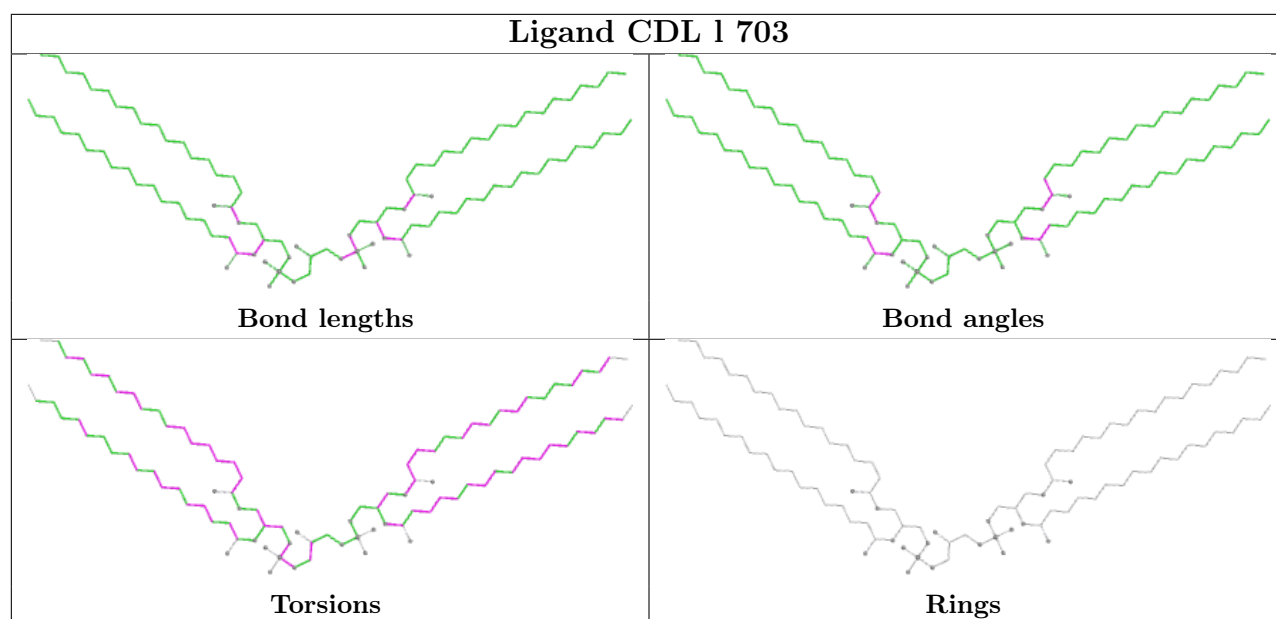
Ligand PLX j 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

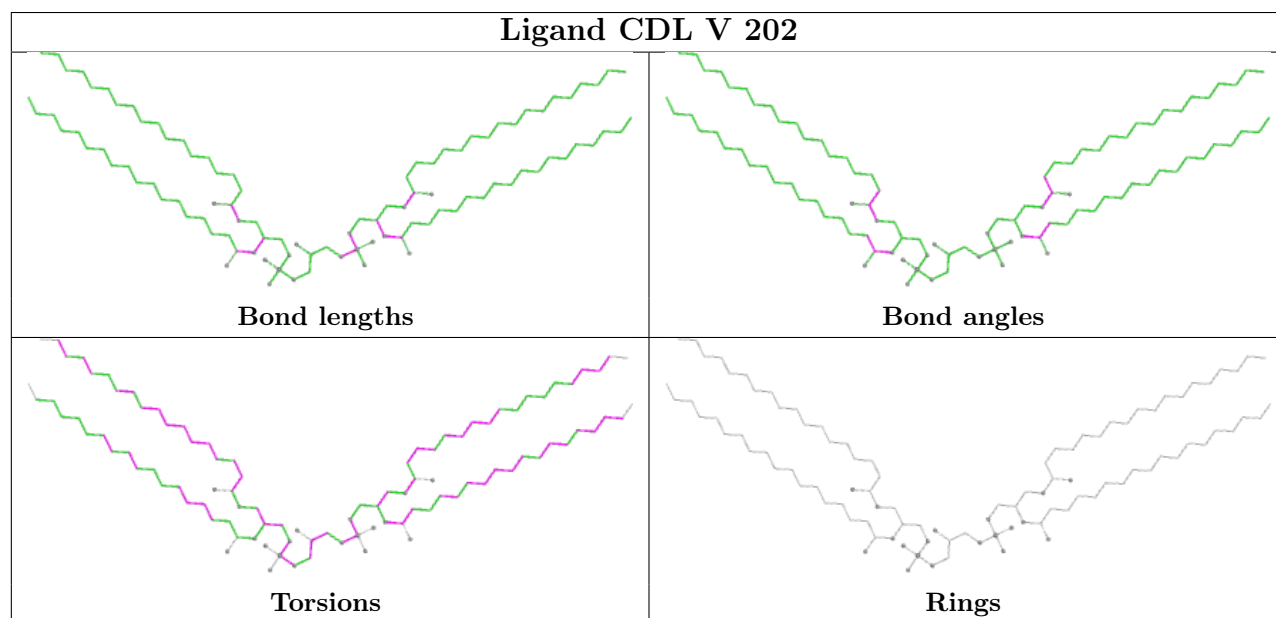
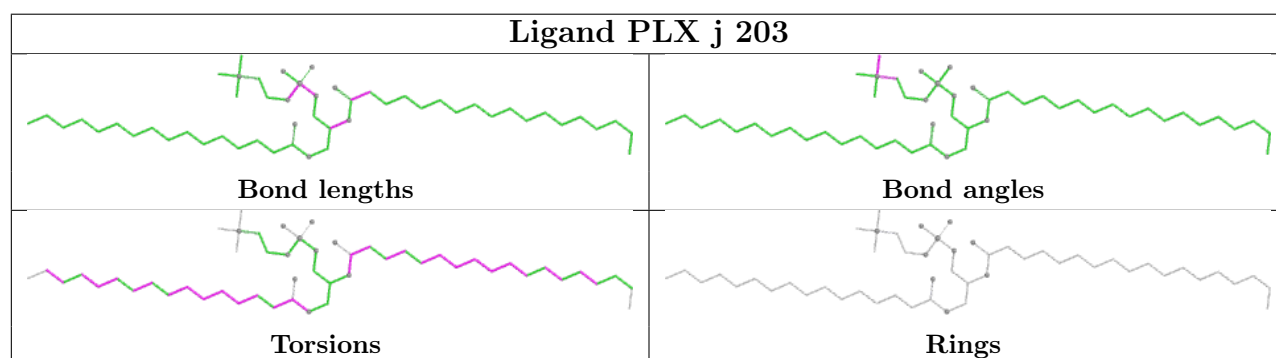
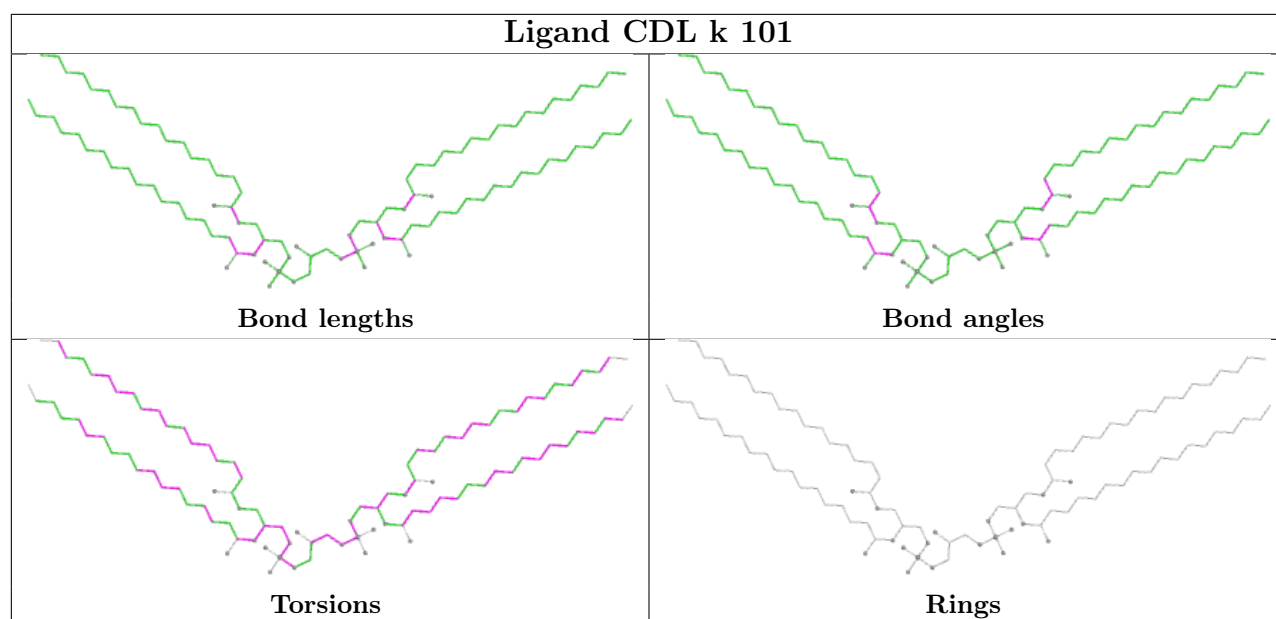
Ligand PEE l 701	
	
Bond lengths	Bond angles
	
Torsions	Rings

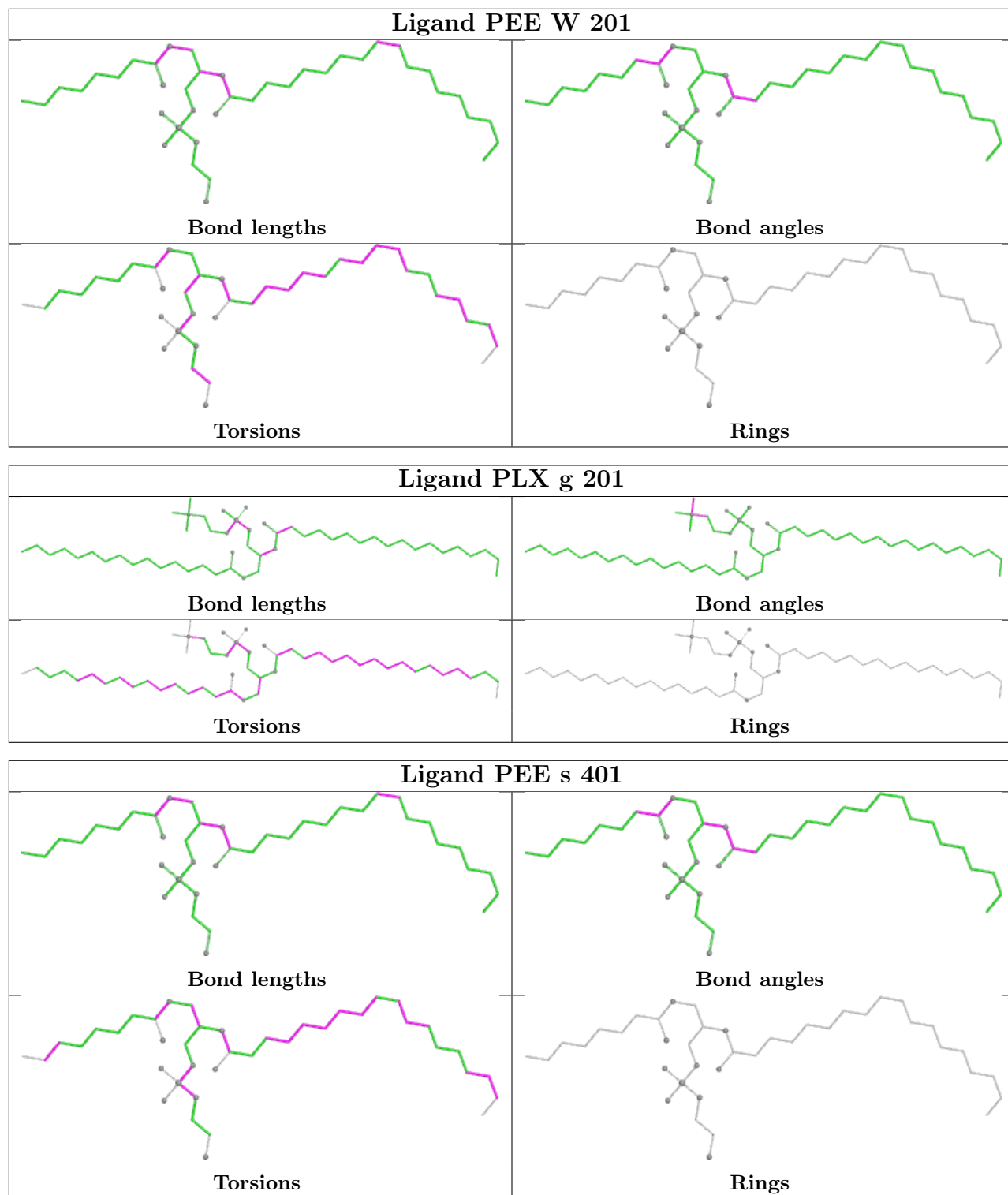


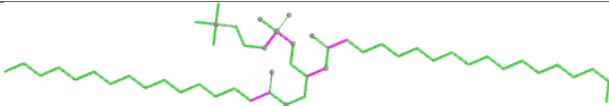
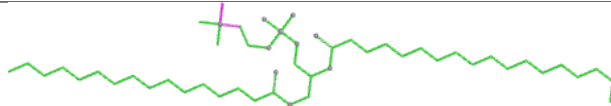
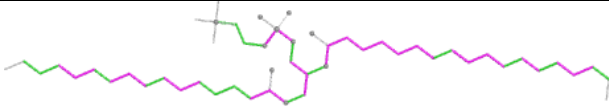
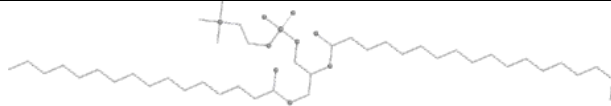


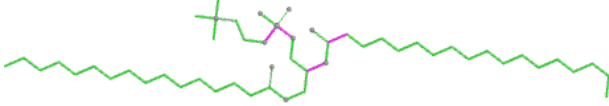
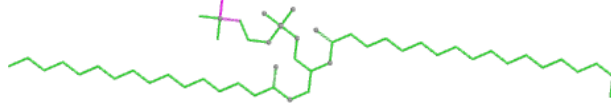
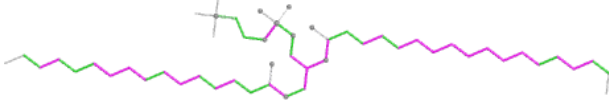
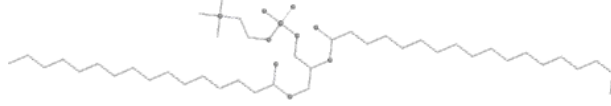


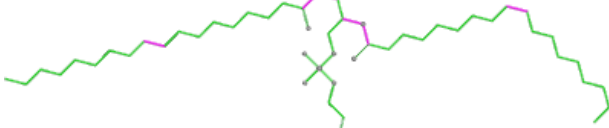
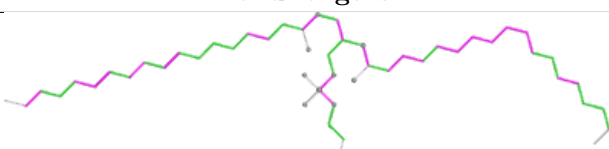
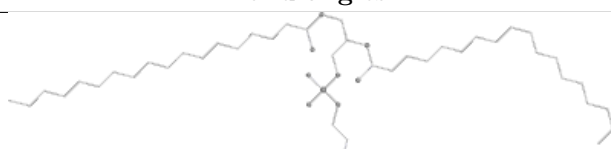


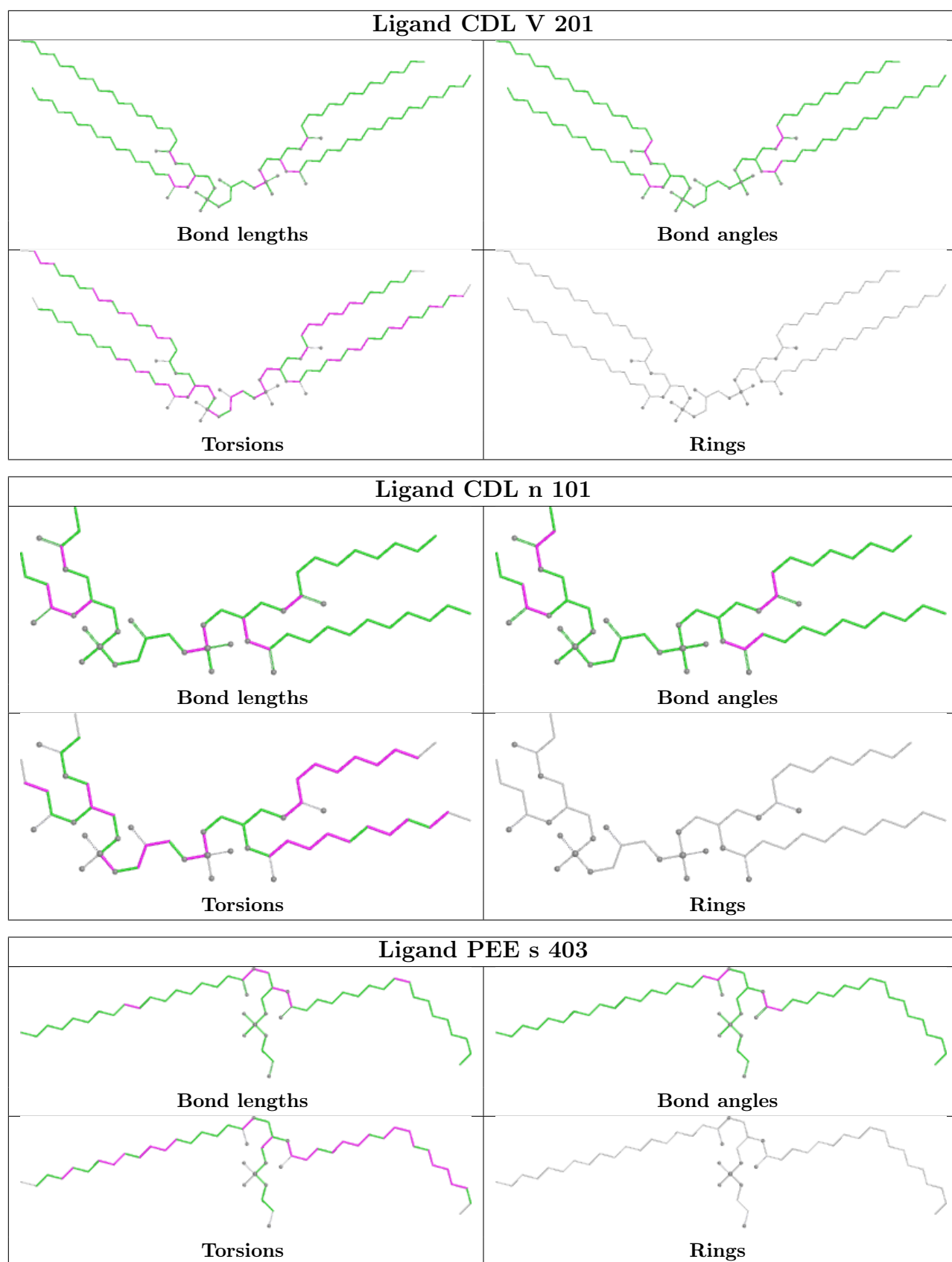


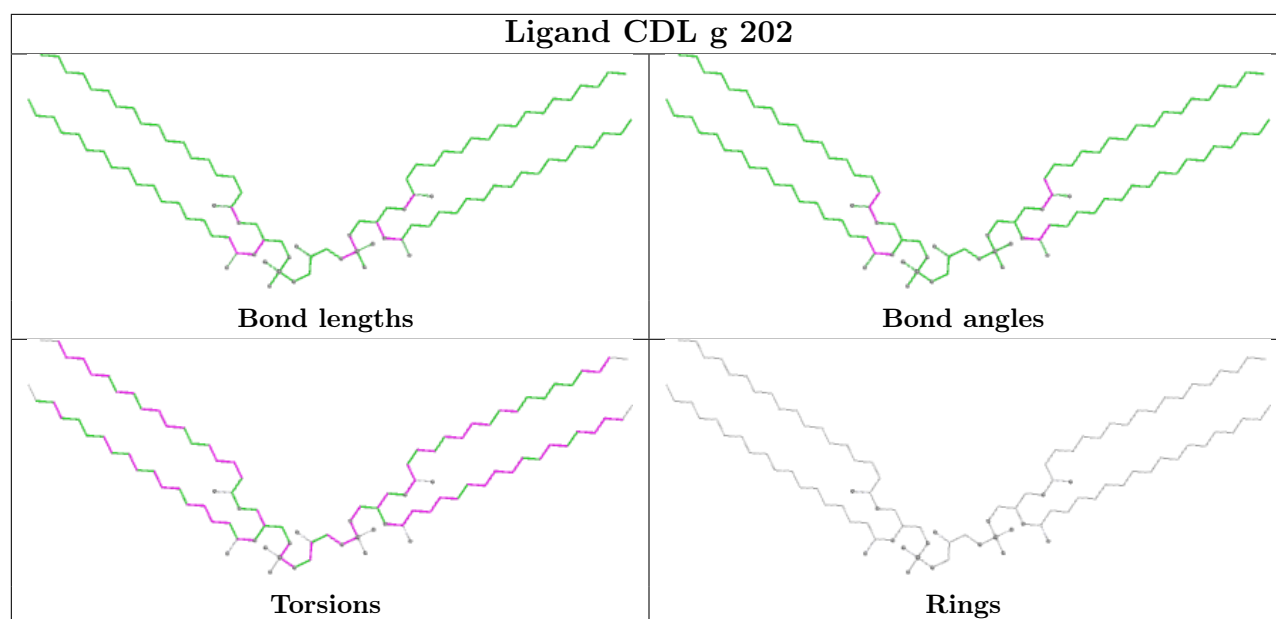


Ligand PLX r 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLX r 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEE r 501	
 Bond lengths	 Bond angles
 Torsions	 Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

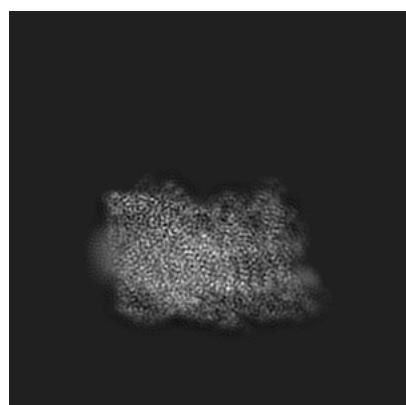
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32197. These allow visual inspection of the internal detail of the map and identification of artifacts.

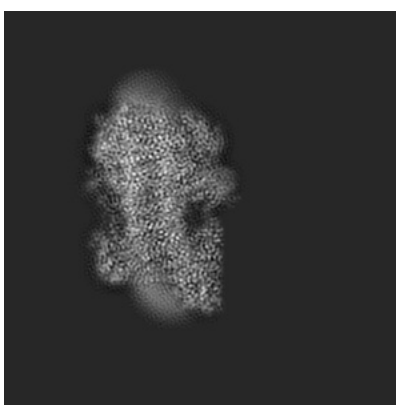
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

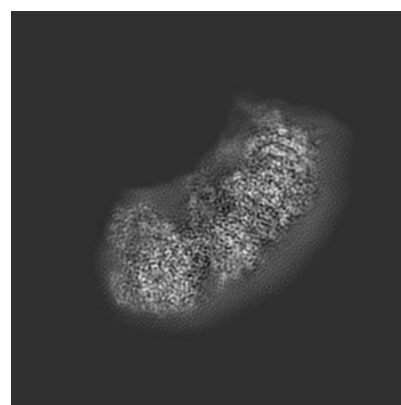
6.1.1 Primary map



X



Y

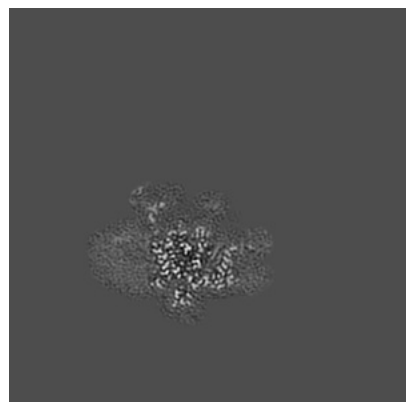


Z

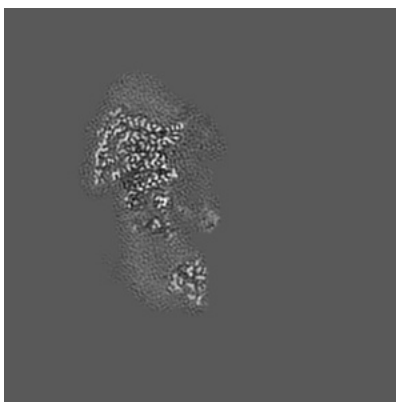
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

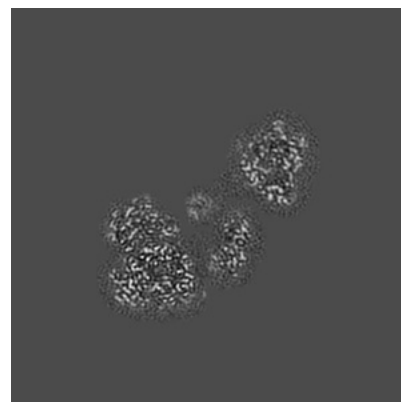
6.2.1 Primary map



X Index: 155



Y Index: 155

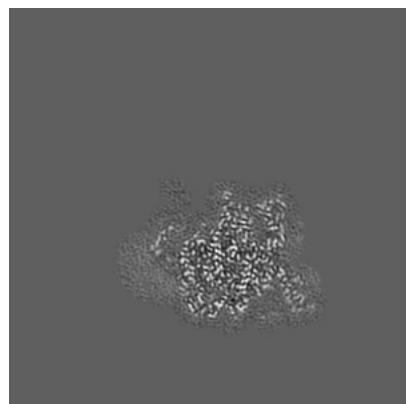


Z Index: 155

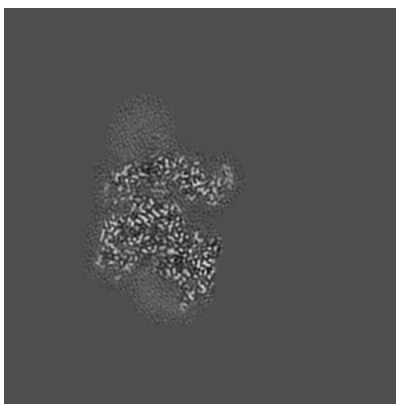
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

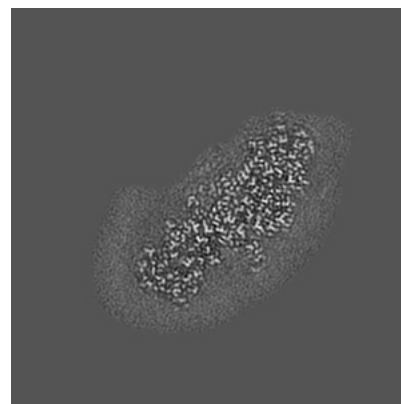
6.3.1 Primary map



X Index: 195



Y Index: 123

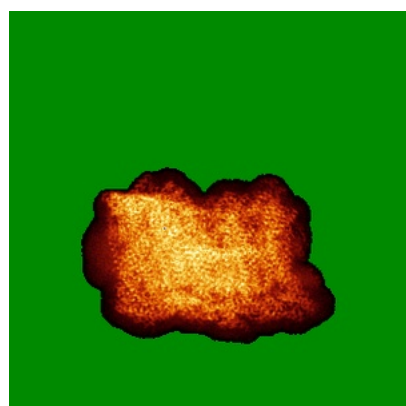


Z Index: 122

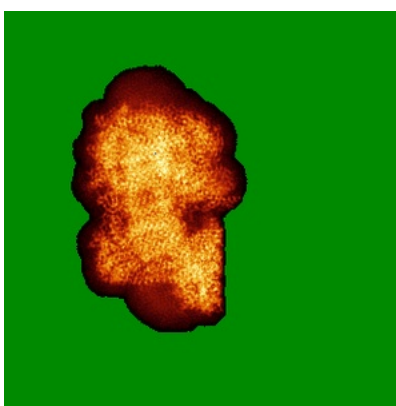
The images above show the largest variance slices of the map in three orthogonal directions.

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

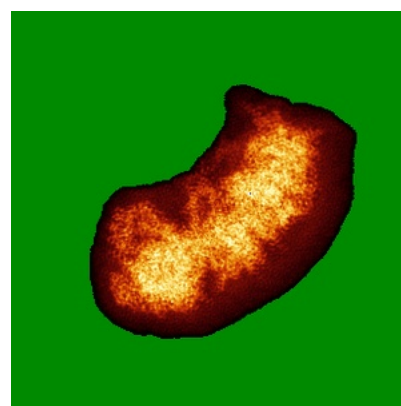
6.4.1 Primary map



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 0.0301. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

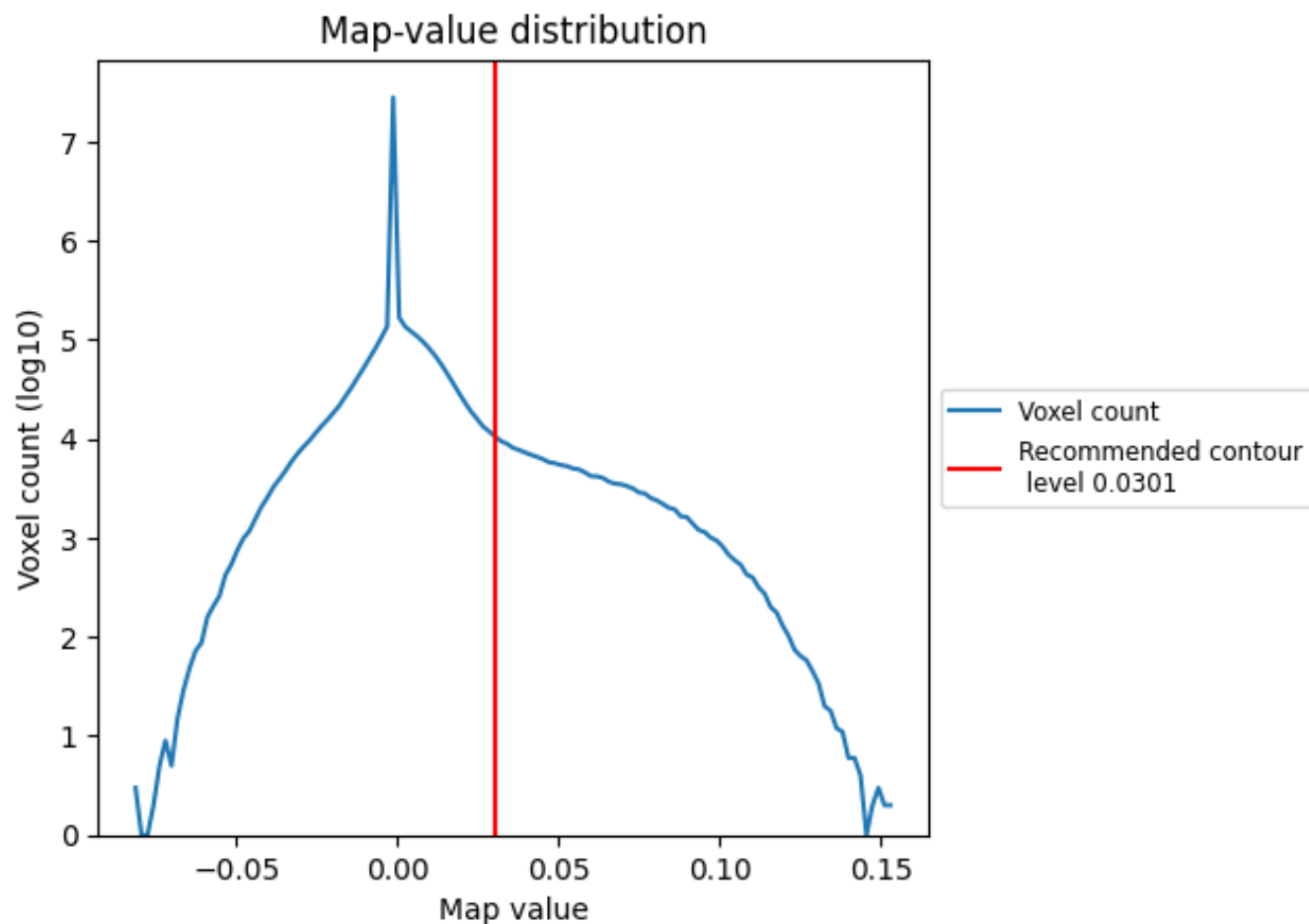
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

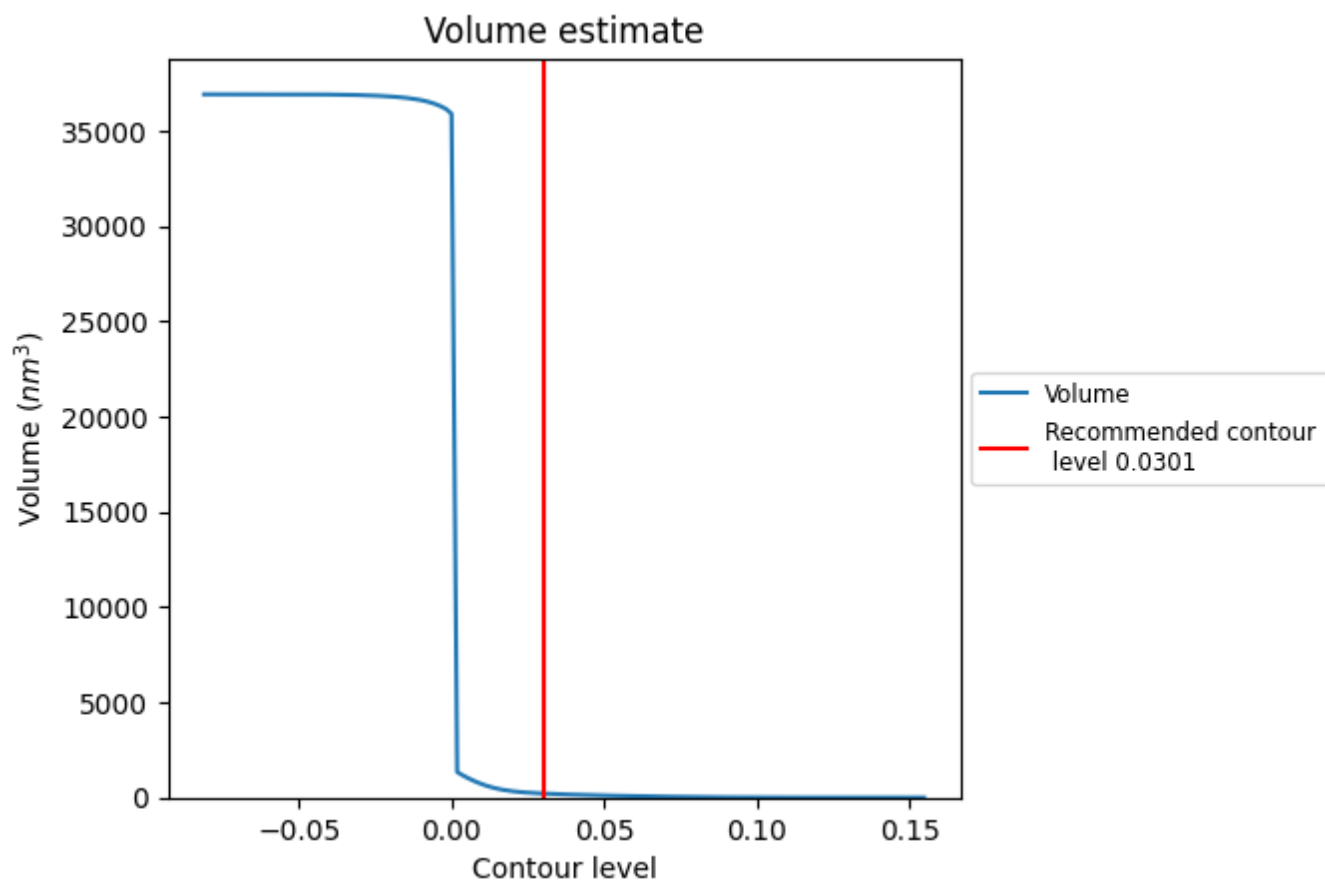
This section contains the results of statistical analysis of the map.

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.

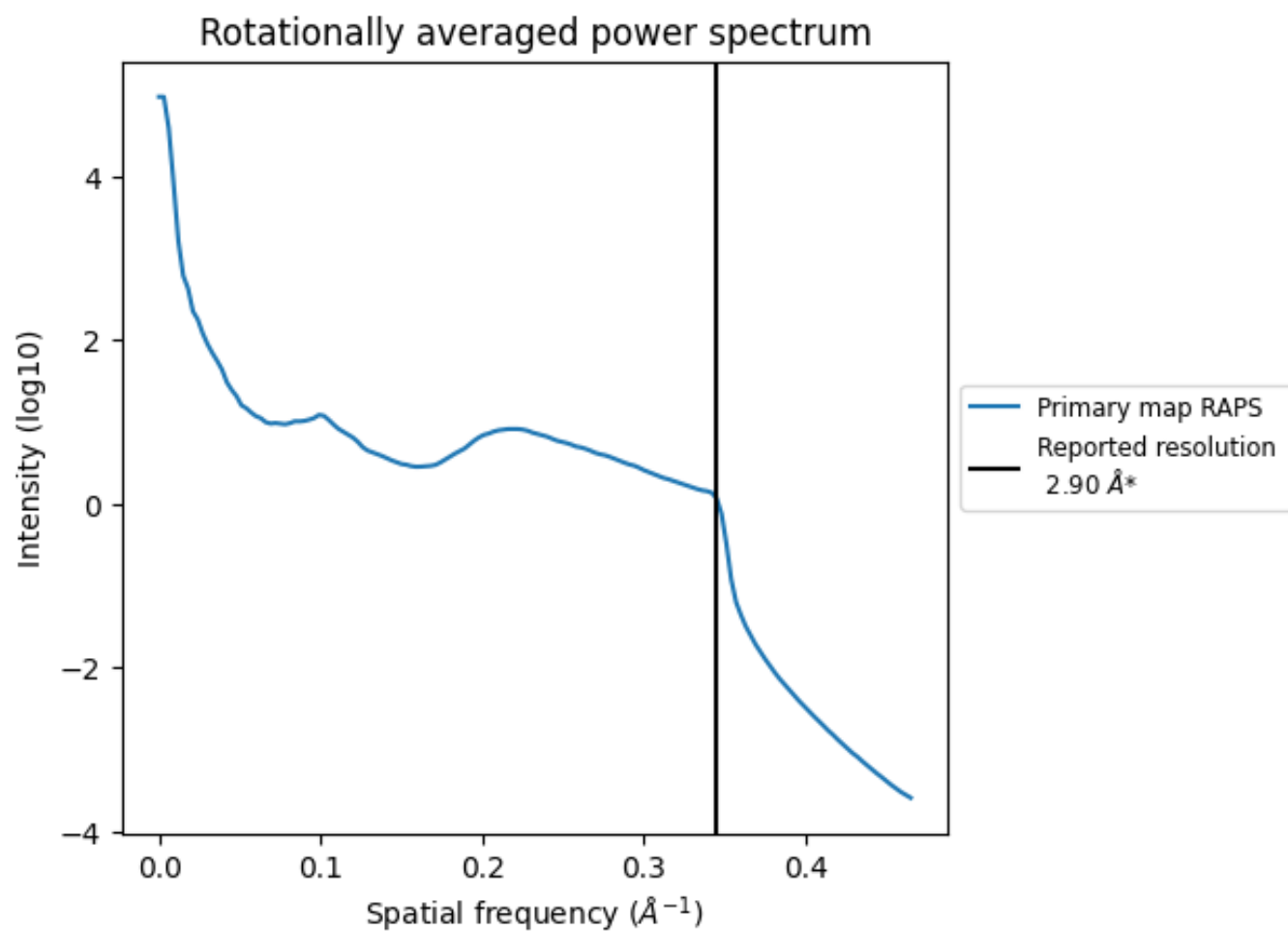
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 211 nm³; this corresponds to an approximate mass of 190 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

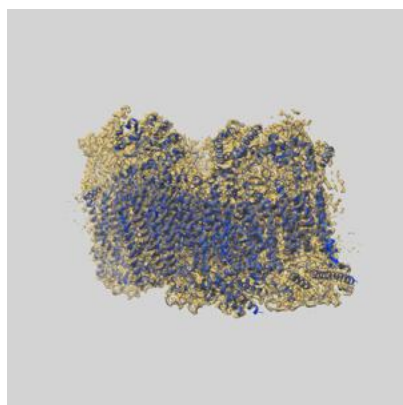
8 Fourier-Shell correlation ⓘ

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

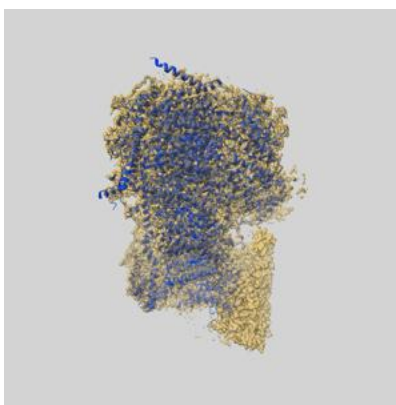
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32197 and PDB model 7VY9. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

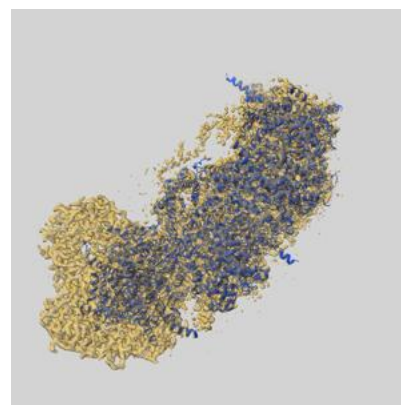
9.1 Map-model overlay [i](#)



X



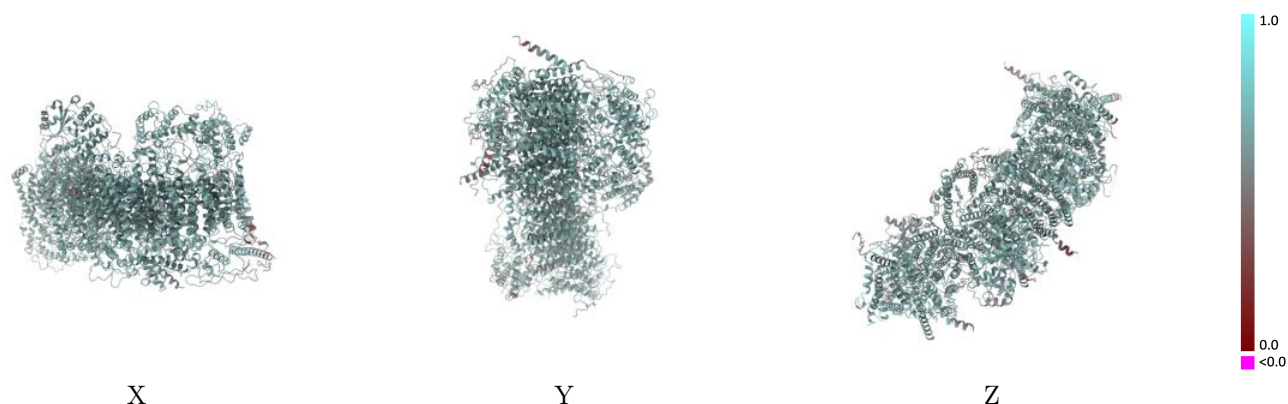
Y



Z

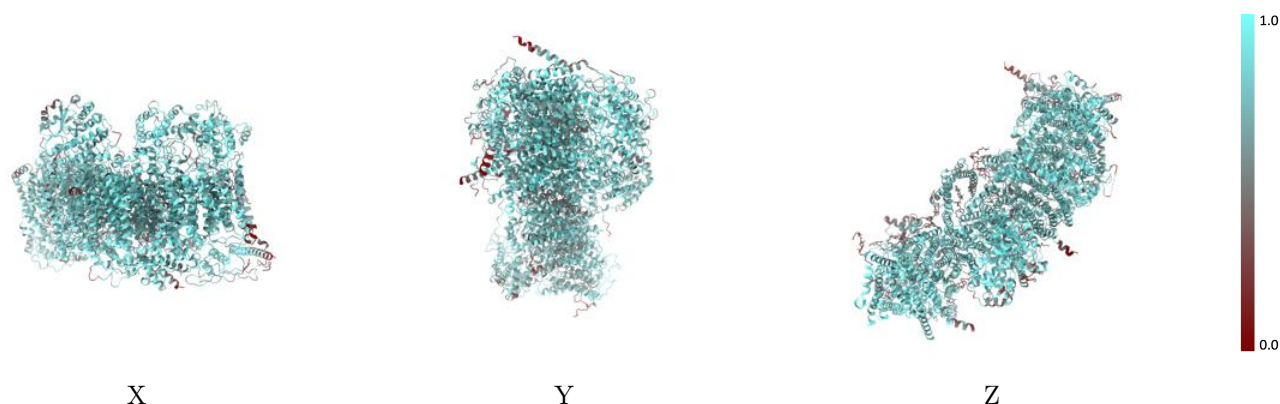
The images above show the 3D surface view of the map at the recommended contour level 0.0301 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



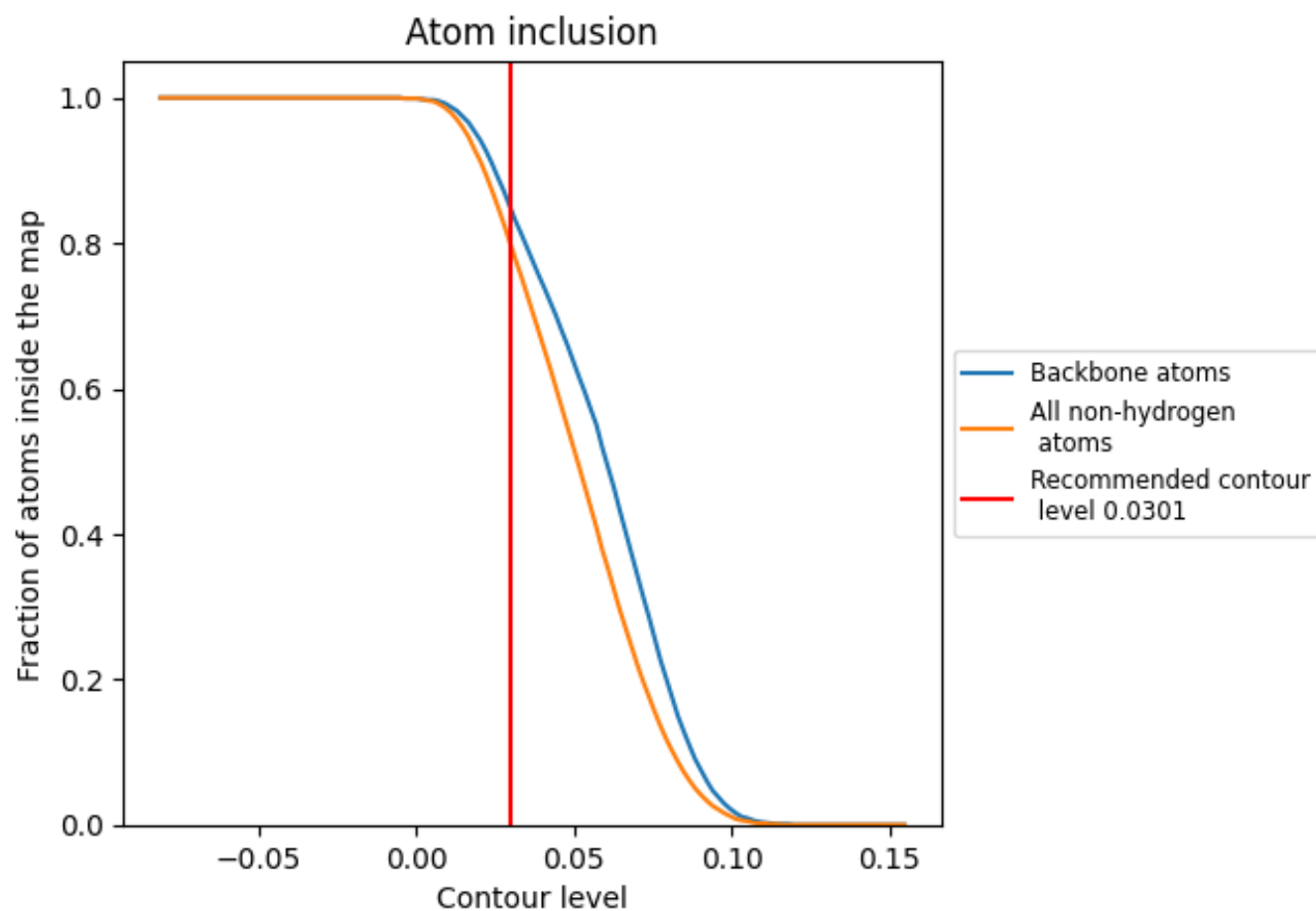
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0301).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 80% 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 (0.0301) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7950	 0.6040
Q	 0.7100	 0.5880
S	 0.8530	 0.6190
U	 0.7600	 0.5900
V	 0.6690	 0.5860
W	 0.8070	 0.6040
X	 0.7490	 0.5950
Y	 0.6780	 0.5600
Z	 0.6580	 0.5530
a	 0.8110	 0.6180
b	 0.7470	 0.5860
c	 0.8110	 0.6080
d	 0.7610	 0.5960
e	 0.7600	 0.5930
f	 0.6110	 0.5450
g	 0.7900	 0.6090
h	 0.7920	 0.5900
i	 0.8910	 0.6290
j	 0.7640	 0.6030
k	 0.7920	 0.6110
l	 0.8160	 0.6150
m	 0.7380	 0.5790
n	 0.6470	 0.5640
o	 0.8020	 0.6080
p	 0.8100	 0.6090
r	 0.8660	 0.6220
s	 0.8490	 0.6220
u	 0.7800	 0.5930
v	 0.6890	 0.5600
w	 0.8010	 0.6000

