



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 02:03 AM UTC

PDB ID : 7VXS / pdb_00007vxs
EMDB ID : EMD-32187
Title : Membrane arm of active state CI from Q10 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:

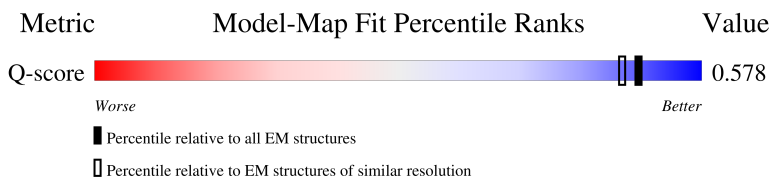
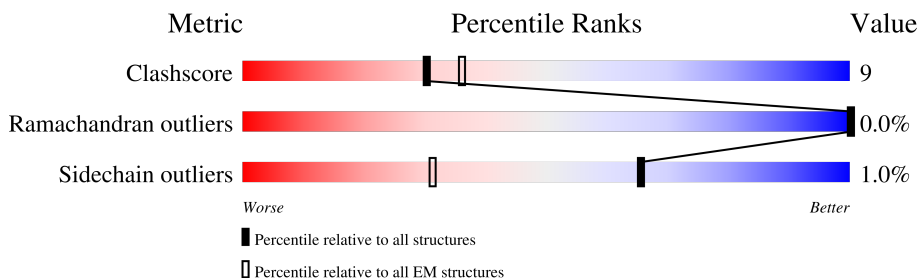
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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



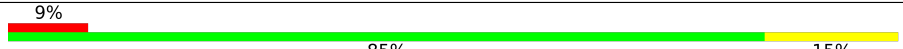
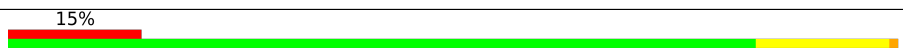
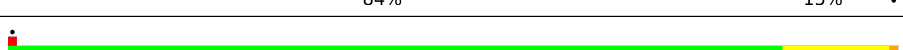
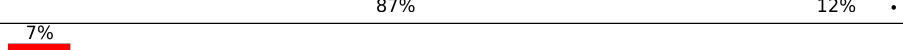
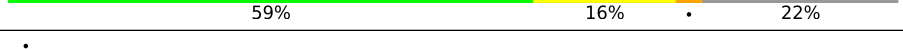
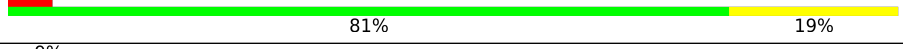
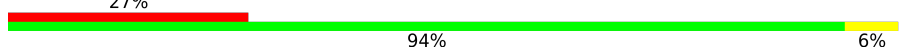
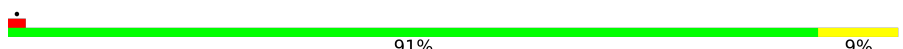
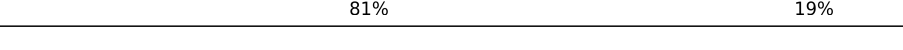
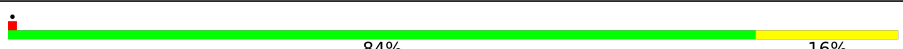
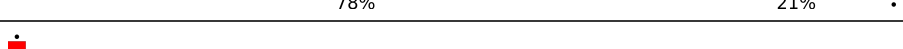
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	9% 82% 18%
2	S	70	86% 14%
3	U	83	6% 81% 19%
4	V	140	85% 15%

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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	124	
29	w	320	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CDL	i	401	-	-	X	-
30	CDL	l	702	-	-	X	-

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 39674 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
			694	447	103	139	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 Complex I-B17.

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
			4816	3193	746	826	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
			1291	861	188	229	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		

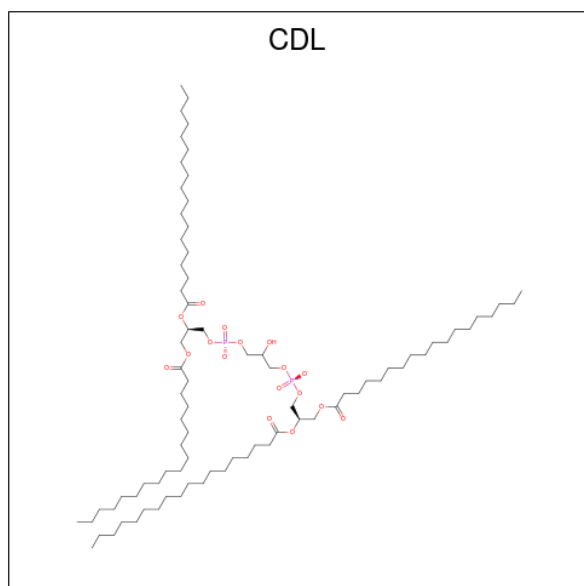
- Molecule 28 is a protein called Complex I-B18.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	w	320	Total	C	N	O	S	0	0
			2590	1649	440	491	10		

- Molecule 30 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



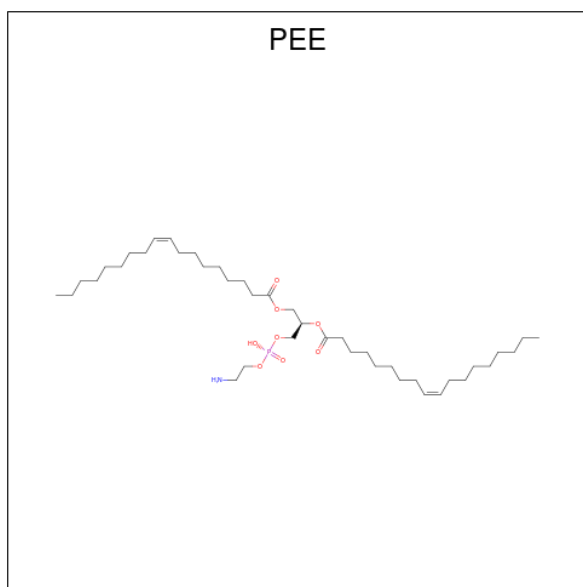
Mol	Chain	Residues	Atoms				AltConf
30	V	1	Total	C	O	P	0
			94	75	17	2	
30	V	1	Total	C	O	P	0
			100	81	17	2	

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Mol	Chain	Residues	Atoms				AltConf
30	a	1	Total	C	O	P	0
			100	81	17	2	
30	i	1	Total	C	O	P	0
			68	49	17	2	
30	l	1	Total	C	O	P	0
			99	80	17	2	
30	l	1	Total	C	O	P	0
			100	81	17	2	
30	m	1	Total	C	O	P	0
			100	81	17	2	
30	n	1	Total	C	O	P	0
			55	36	17	2	
30	r	1	Total	C	O	P	0
			100	81	17	2	
30	s	1	Total	C	O	P	0
			89	70	17	2	

- Molecule 31 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



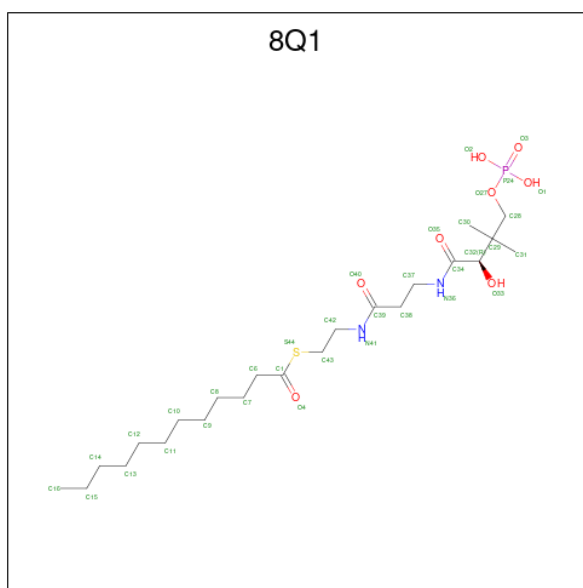
Mol	Chain	Residues	Atoms					AltConf
31	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
31	b	1	Total	C	N	O	P	0
			46	36	1	8	1	
31	i	1	Total	C	N	O	P	0
			47	37	1	8	1	

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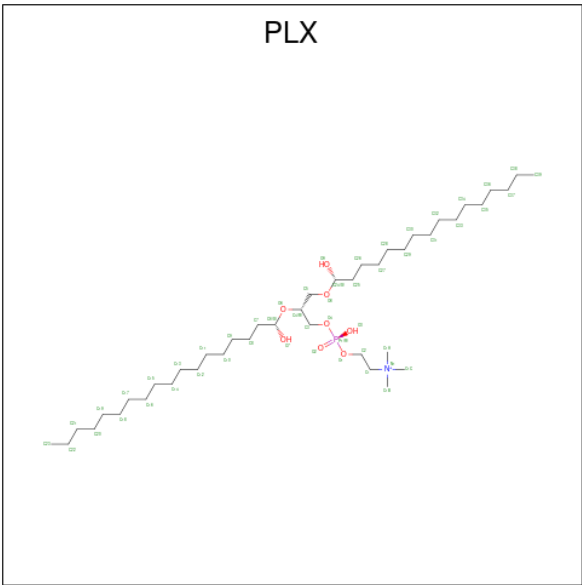
Mol	Chain	Residues	Atoms					AltConf
31	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
31	l	1	Total	C	N	O	P	0
			40	30	1	8	1	
31	l	1	Total	C	N	O	P	0
			51	41	1	8	1	
31	r	1	Total	C	N	O	P	0
			51	41	1	8	1	
31	s	1	Total	C	N	O	P	0
			41	31	1	8	1	
31	s	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 32 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
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-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



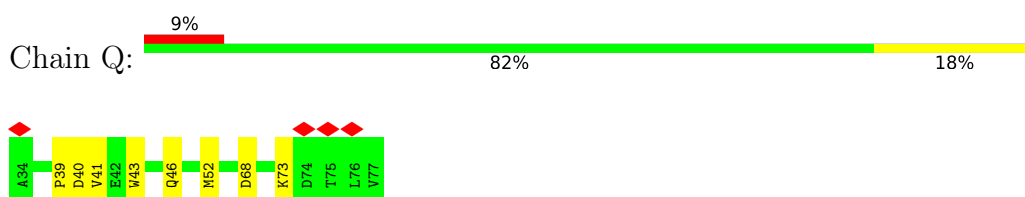
Mol	Chain	Residues	Atoms					AltConf
33	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	n	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 34 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

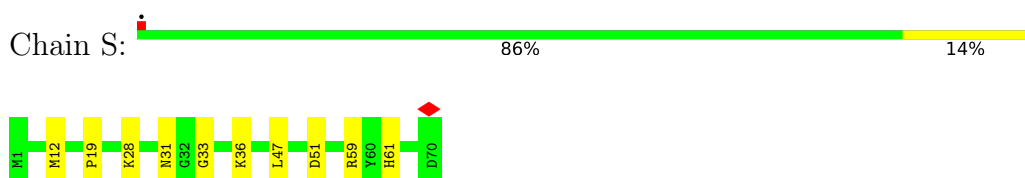
3 Residue-property plots [i](#)

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.

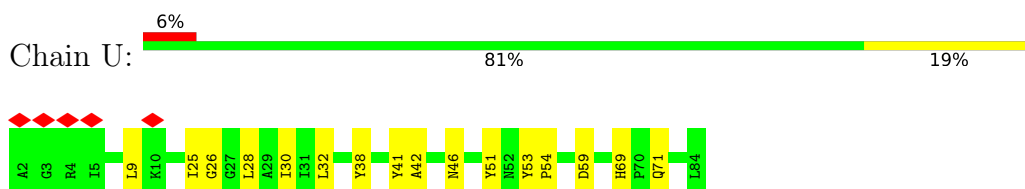
- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



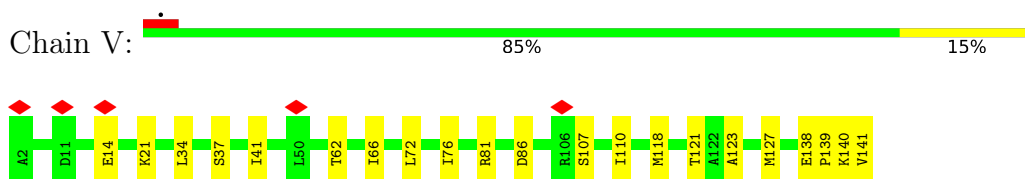
- Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



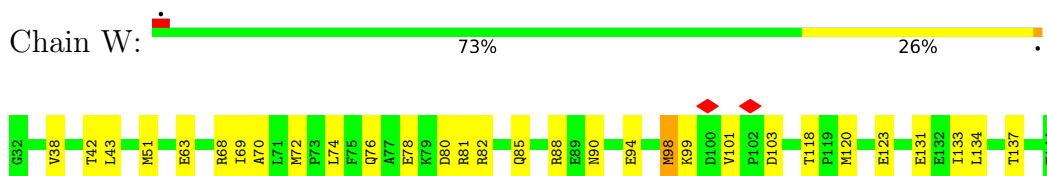
- Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



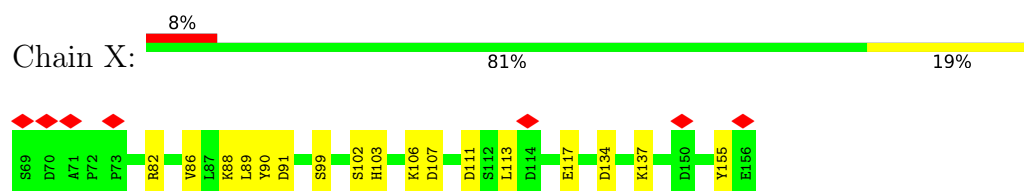
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



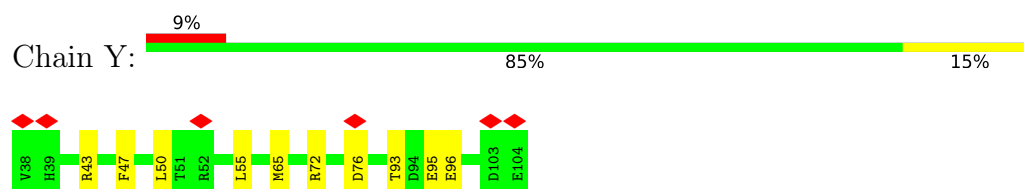
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



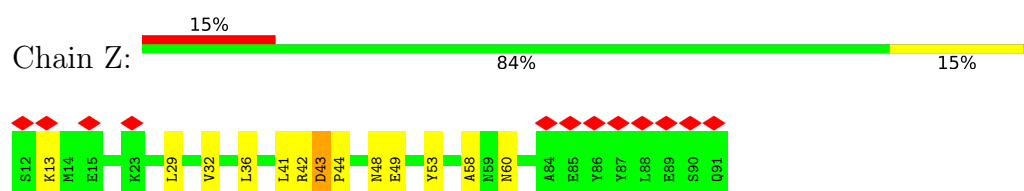
- Molecule 6: Acyl carrier protein



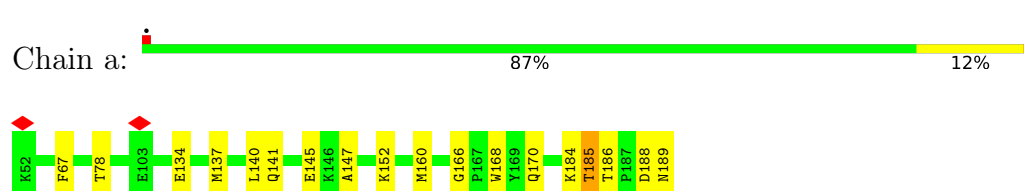
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



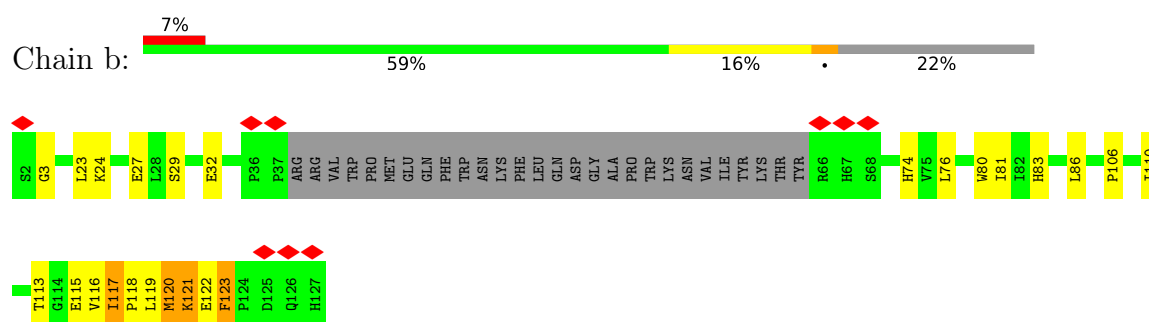
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



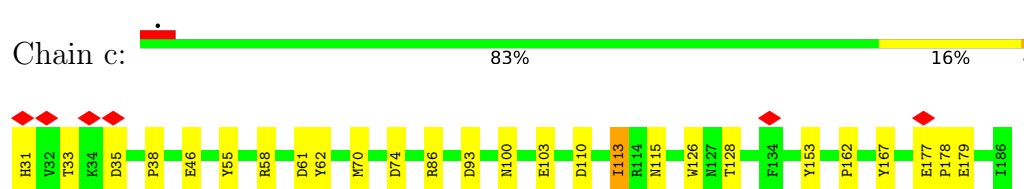
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



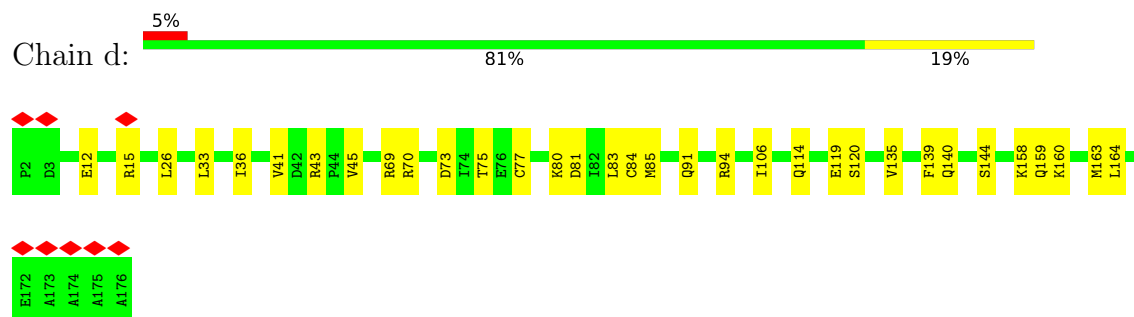
- Molecule 10: Complex I-B17



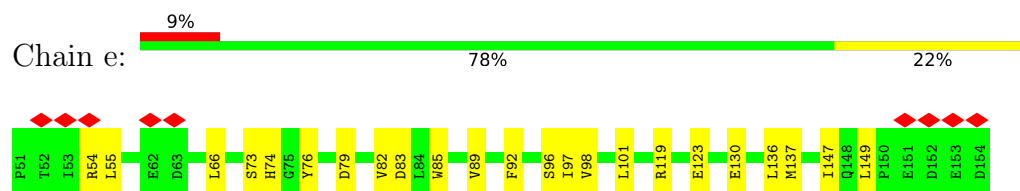
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



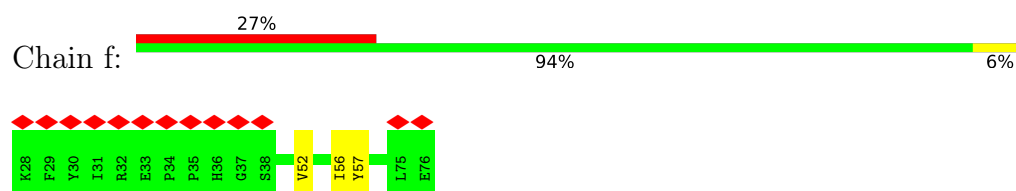
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



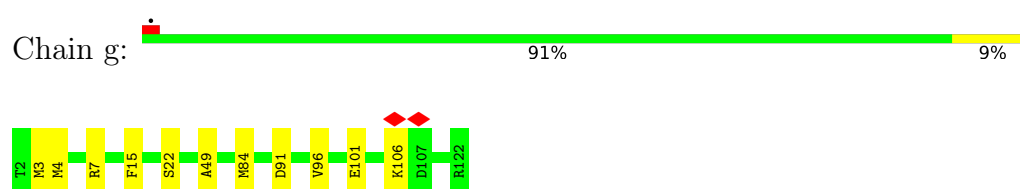
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



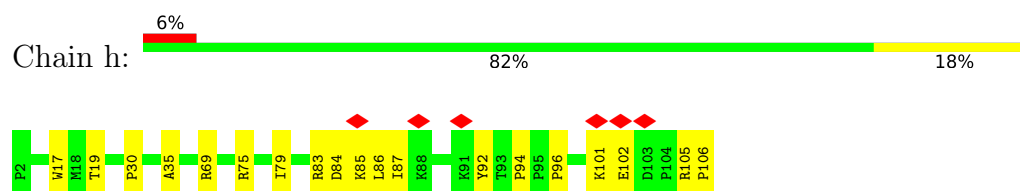
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



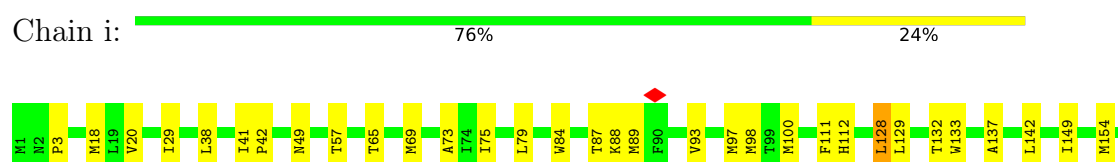
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2

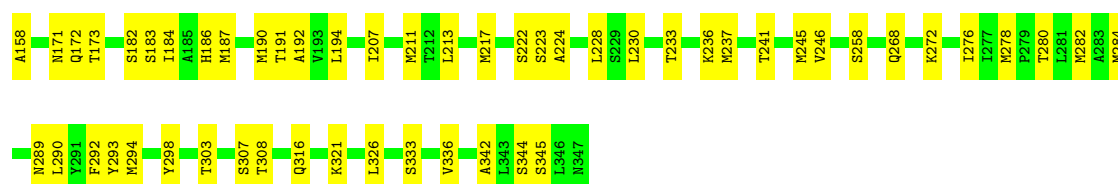


- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

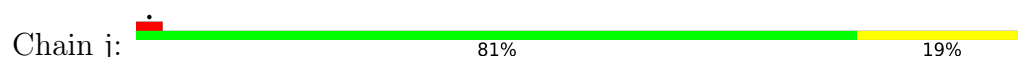


- Molecule 17: NADH-ubiquinone oxidoreductase chain 2





- Molecule 18: NADH-ubiquinone oxidoreductase chain 3



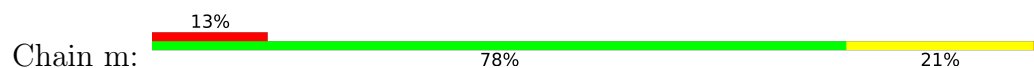
- Molecule 19: NADH-ubiquinone oxidoreductase chain 4L

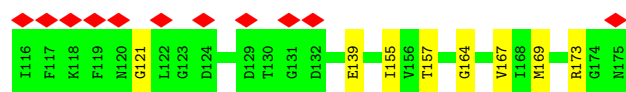


- Molecule 20: NADH-ubiquinone oxidoreductase chain 5

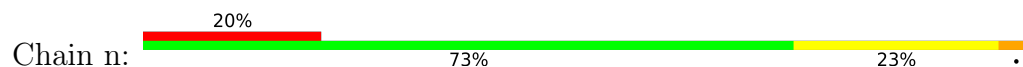


- Molecule 21: NADH-ubiquinone oxidoreductase chain 6

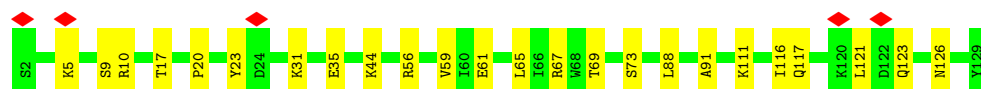
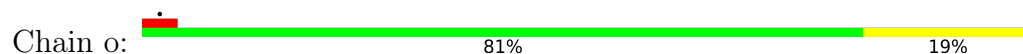




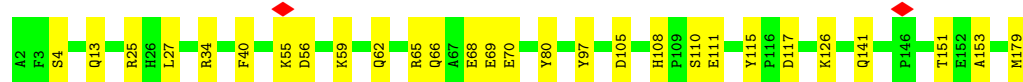
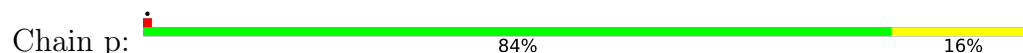
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



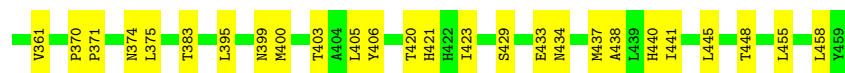
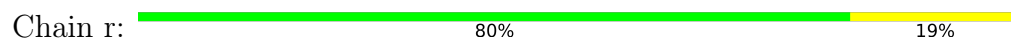
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



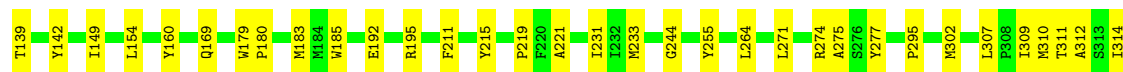
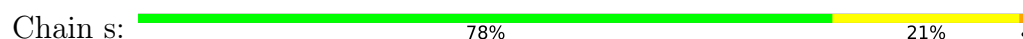
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 25: NADH-ubiquinone oxidoreductase chain 4



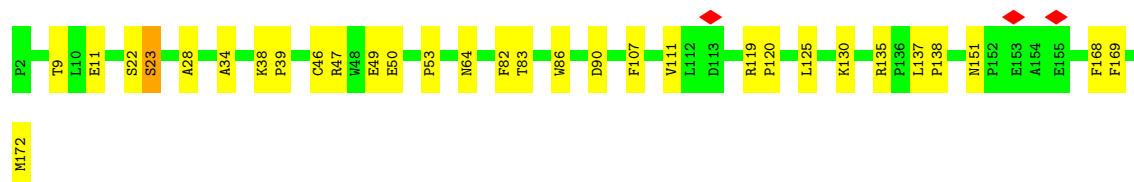
- Molecule 26: NADH-ubiquinone oxidoreductase chain 1





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

Chain u: 82% 18%



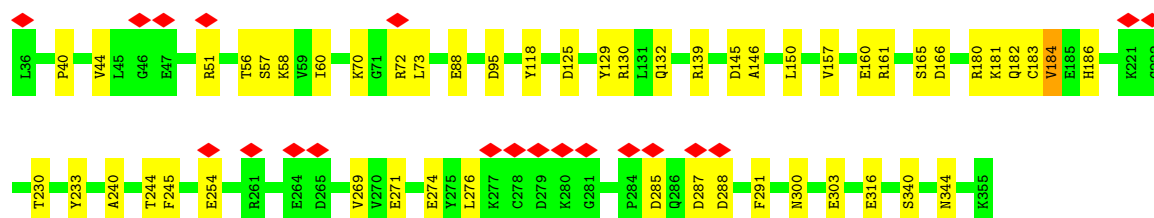
- Molecule 28: Complex I-B18

Chain v: 10% 80% 19%



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

Chain w: 6% 84% 16%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	252573	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	0.129	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.027	Depositor
Map size ($\text{\AA}$)	354.48602, 354.48602, 354.48602	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLX, 8Q1, PEE, CDL, 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	0.09	0/380	0.25	0/525
2	S	0.12	0/581	0.35	0/781
3	U	0.11	0/664	0.26	0/912
4	V	0.11	0/1042	0.23	0/1411
5	W	0.12	0/973	0.26	0/1312
6	X	0.11	0/705	0.31	0/954
7	Y	0.13	0/610	0.34	0/836
8	Z	0.18	0/660	0.70	2/892 (0.2%)
9	a	0.15	0/1184	0.34	0/1603
10	b	0.17	0/844	0.60	6/1149 (0.5%)
11	c	0.11	0/1371	0.32	0/1875
12	d	0.12	0/1494	0.29	0/2015
13	e	0.12	0/891	0.30	0/1210
14	f	0.10	0/386	0.24	0/523
15	g	0.11	0/1031	0.28	0/1394
16	h	0.12	0/889	0.31	0/1190
17	i	0.16	0/2773	0.37	0/3768
18	j	0.14	0/938	0.32	0/1281
19	k	0.15	0/759	0.32	0/1029
20	l	0.14	0/4947	0.33	1/6728 (0.0%)
21	m	0.14	0/1323	0.34	0/1797
22	n	0.18	0/491	0.40	0/663
23	o	0.12	0/1092	0.29	0/1481
24	p	0.10	0/1590	0.25	0/2155
25	r	0.14	0/3723	0.31	0/5078
26	s	0.16	0/2581	0.48	4/3529 (0.1%)
27	u	0.13	0/1436	0.32	0/1938
28	v	0.12	0/1052	0.34	0/1411
29	w	0.11	0/2650	0.29	0/3588
All	All	0.13	0/39060	0.35	13/53028 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Z	43	ASP	CA-C-N	11.79	131.71	118.85
8	Z	43	ASP	C-N-CA	11.79	131.71	118.85
26	s	68	ILE	N-CA-C	7.80	118.58	110.62
26	s	62	ARG	CA-C-N	7.70	127.72	119.78
26	s	62	ARG	C-N-CA	7.70	127.72	119.78
10	b	120	MET	N-CA-C	7.42	121.19	109.39
10	b	121	LYS	N-CA-C	7.06	121.47	112.86
20	l	26	ILE	N-CA-C	-7.00	107.06	113.71
26	s	73	ILE	N-CA-C	6.67	117.42	110.62
10	b	117	ILE	CA-C-N	5.99	125.90	119.85
10	b	117	ILE	C-N-CA	5.99	125.90	119.85
10	b	123	PHE	CA-C-N	5.49	125.42	119.76
10	b	123	PHE	C-N-CA	5.49	125.42	119.76

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	10	0
3	U	643	0	642	14	0
4	V	1021	0	1025	12	0
5	W	949	0	935	26	0
6	X	694	0	674	13	0
7	Y	584	0	529	9	0
8	Z	641	0	620	16	0
9	a	1151	0	1164	22	0
10	b	819	0	835	27	0
11	c	1315	0	1208	21	0
12	d	1461	0	1429	28	0
13	e	867	0	817	19	0
14	f	378	0	356	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	g	1000	0	994	9	0
16	h	867	0	871	20	0
17	i	2710	0	2874	76	0
18	j	914	0	951	22	0
19	k	748	0	799	21	0
20	l	4816	0	4955	101	0
21	m	1291	0	1265	35	0
22	n	479	0	486	13	0
23	o	1062	0	1072	18	0
24	p	1534	0	1470	19	0
25	r	3631	0	3839	70	0
26	s	2508	0	2607	76	0
27	u	1398	0	1374	32	0
28	v	1028	0	982	23	0
29	w	2590	0	2553	38	0
30	V	194	0	294	10	0
30	a	100	0	156	1	0
30	i	68	0	80	23	0
30	l	199	0	307	38	0
30	m	100	0	156	11	0
30	n	55	0	54	6	0
30	r	100	0	156	7	0
30	s	89	0	125	15	0
31	W	41	0	59	2	0
31	b	46	0	69	1	0
31	i	47	0	71	2	0
31	j	51	0	82	5	0
31	l	91	0	136	3	0
31	r	51	0	82	2	0
31	s	92	0	141	19	0
32	X	35	0	0	1	0
33	g	52	0	88	4	0
33	j	104	0	176	2	0
33	n	52	0	88	0	0
33	r	52	0	88	3	0
34	w	27	0	11	1	0
All	All	39674	0	40638	725	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (725) 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)
9:a:189:ASN:ND2	16:h:35:ALA:HB2	1.41	1.33
18:j:34:THR:HG22	26:s:61:LEU:HD11	1.16	1.16
17:i:129:LEU:HD13	30:i:401:CDL:H331	1.29	1.11
26:s:70:MET:HE1	26:s:121:TRP:CE3	1.88	1.08
9:a:189:ASN:HD21	16:h:35:ALA:CB	1.67	1.08
26:s:72:ILE:HD13	31:s:401:PEE:H13	1.28	1.06
30:l:702:CDL:H312	30:l:702:CDL:H742	1.37	1.04
30:l:702:CDL:HA62	30:l:702:CDL:H541	1.40	1.03
30:i:401:CDL:HB31	29:w:40:PRO:CB	1.89	1.03
26:s:70:MET:CE	26:s:121:TRP:CE3	2.44	1.00
30:l:702:CDL:C66	30:l:702:CDL:H852	1.93	0.98
30:l:702:CDL:H742	30:l:702:CDL:C31	1.95	0.97
20:l:383:MET:HE3	20:l:384:PRO:HD2	1.47	0.96
30:i:401:CDL:HB31	29:w:40:PRO:HB3	1.45	0.95
18:j:34:THR:HG22	26:s:61:LEU:CD1	1.99	0.92
26:s:77:LEU:CD1	31:s:401:PEE:H40	2.01	0.91
17:i:129:LEU:CD1	30:i:401:CDL:H331	2.02	0.89
9:a:189:ASN:ND2	16:h:35:ALA:CB	2.32	0.89
8:Z:49:GLU:OE2	24:p:34:ARG:NE	2.07	0.86
26:s:62:ARG:HH11	26:s:68:ILE:HD11	1.42	0.85
26:s:70:MET:CE	26:s:121:TRP:CZ3	2.60	0.84
26:s:77:LEU:HD13	31:s:401:PEE:H40	1.61	0.83
9:a:188:ASP:OD1	27:u:47:ARG:NH2	2.12	0.83
9:a:137:MET:HE1	22:n:42:SER:HB3	1.60	0.82
8:Z:49:GLU:OE2	24:p:34:ARG:NH2	2.12	0.82
22:n:3:ASN:N	22:n:3:ASN:HD22	1.79	0.81
30:n:102:CDL:H551	27:u:169:PHE:HE1	1.47	0.80
26:s:70:MET:HE2	26:s:121:TRP:CZ3	2.17	0.79
20:l:5:ALA:HB2	20:l:61:MET:HE1	1.63	0.79
9:a:184:LYS:O	16:h:30:PRO:HD3	1.84	0.78
26:s:70:MET:CE	26:s:121:TRP:HE3	1.94	0.77
23:o:59:VAL:HG22	25:r:423:ILE:HG12	1.64	0.77
5:W:81:ARG:NH2	27:u:64:ASN:OD1	2.19	0.76
17:i:213:LEU:O	17:i:217:MET:HG3	1.86	0.75
26:s:68:ILE:HG21	30:s:402:CDL:H111	1.68	0.75
18:j:34:THR:CG2	26:s:61:LEU:HD11	2.09	0.75
19:k:21:MET:HB3	30:m:201:CDL:HB61	1.67	0.75
30:l:702:CDL:H452	25:r:445:LEU:HB3	1.69	0.74
26:s:62:ARG:HD2	26:s:68:ILE:HD12	1.70	0.73
17:i:321:LYS:NZ	30:i:401:CDL:OA3	2.20	0.73
25:r:191:SER:HB3	31:r:501:PEE:H3	1.70	0.73
11:c:46:GLU:OE1	11:c:46:GLU:N	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:s:62:ARG:HH11	26:s:68:ILE:CD1	2.02	0.72
30:l:702:CDL:H312	30:l:702:CDL:C74	2.17	0.72
30:l:702:CDL:H541	30:l:702:CDL:CA6	2.17	0.72
10:b:119:LEU:HD22	10:b:119:LEU:N	2.05	0.71
30:i:401:CDL:OB9	29:w:44:VAL:HG21	1.89	0.71
31:s:401:PEE:H38	30:s:402:CDL:H592	1.70	0.71
26:s:77:LEU:HD12	31:s:401:PEE:H40	1.70	0.71
9:a:168:TRP:HB3	15:g:3:MET:HB2	1.73	0.70
17:i:132:THR:HG21	30:i:401:CDL:H371	1.73	0.69
30:n:102:CDL:HB31	27:u:172:MET:HE2	1.73	0.69
23:o:23:TYR:OH	24:p:68:GLU:OE2	2.10	0.69
17:i:128:LEU:C	17:i:128:LEU:HD23	2.17	0.69
26:s:72:ILE:HD13	31:s:401:PEE:C11	2.16	0.69
18:j:90:MET:HE3	18:j:90:MET:HA	1.73	0.69
30:l:702:CDL:H391	25:r:371:PRO:HD2	1.75	0.69
26:s:70:MET:HE2	26:s:121:TRP:HZ3	1.56	0.68
13:e:98:VAL:HG22	25:r:36:LEU:HB2	1.76	0.68
20:l:119:LYS:NZ	30:l:702:CDL:OA3	2.27	0.68
19:k:27:MET:HG2	21:m:71:THR:HG22	1.75	0.68
21:m:55:MET:HA	21:m:55:MET:HE2	1.75	0.68
21:m:67:VAL:O	21:m:71:THR:HG23	1.93	0.68
27:u:47:ARG:HH11	27:u:53:PRO:HA	1.59	0.67
8:Z:49:GLU:OE2	24:p:34:ARG:CZ	2.42	0.67
22:n:54:GLU:OE2	22:n:54:GLU:N	2.27	0.67
10:b:120:MET:HE1	28:v:61:HIS:HA	1.76	0.67
17:i:93:VAL:HG13	20:l:599:MET:HE1	1.77	0.67
10:b:119:LEU:HD22	10:b:119:LEU:H	1.61	0.66
12:d:15:ARG:HG3	12:d:15:ARG:O	1.95	0.66
12:d:139:PHE:HB2	13:e:137:MET:HE3	1.78	0.66
21:m:72:THR:HG21	26:s:133:LEU:HD21	1.77	0.65
24:p:151:THR:HG23	24:p:153:ALA:H	1.62	0.65
25:r:269:MET:HE1	25:r:296:LEU:HD13	1.78	0.65
25:r:210:TYR:O	25:r:213:HIS:ND1	2.26	0.65
12:d:69:ARG:NH2	22:n:46:LYS:O	2.29	0.65
7:Y:72:ARG:NH1	7:Y:76:ASP:OD2	2.30	0.65
17:i:132:THR:CG2	30:i:401:CDL:H371	2.25	0.65
3:U:9:LEU:HD11	31:j:201:PEE:H68	1.79	0.65
18:j:18:VAL:HG12	31:s:401:PEE:H16	1.79	0.64
2:S:12:MET:HE3	26:s:264:LEU:HD22	1.78	0.64
7:Y:76:ASP:O	20:l:385:TYR:OH	2.15	0.64
20:l:102:GLU:OE1	20:l:456:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:134:GLU:OE1	22:n:57:TRP:NE1	2.29	0.64
15:g:3:MET:HG3	15:g:4:MET:HG2	1.80	0.64
28:v:83:GLU:OE2	28:v:83:GLU:N	2.23	0.64
27:u:11:GLU:OE1	27:u:11:GLU:N	2.30	0.64
30:l:702:CDL:H742	30:l:702:CDL:H311	1.80	0.63
22:n:27:LEU:HD12	25:r:6:ILE:HD11	1.81	0.63
17:i:142:LEU:HB3	17:i:194:LEU:HD21	1.79	0.62
30:l:702:CDL:H422	25:r:448:THR:CG2	2.29	0.62
25:r:255:ASN:OD1	25:r:256:TYR:N	2.31	0.62
20:l:150:MET:HE3	20:l:150:MET:HA	1.81	0.62
10:b:121:LYS:O	10:b:121:LYS:HG2	1.98	0.62
30:i:401:CDL:HB62	29:w:40:PRO:HB2	1.80	0.62
8:Z:60:ASN:ND2	20:l:433:GLY:O	2.33	0.62
21:m:25:SER:O	21:m:27:ILE:N	2.32	0.62
6:X:91:ASP:HB2	8:Z:44:PRO:HA	1.81	0.62
29:w:125:ASP:O	29:w:130:ARG:NH2	2.33	0.62
5:W:63:GLU:OE2	27:u:119:ARG:NH2	2.33	0.62
26:s:72:ILE:HG21	31:s:401:PEE:H18	1.82	0.62
30:s:402:CDL:H221	30:s:402:CDL:H552	1.82	0.62
30:r:503:CDL:H401	30:r:503:CDL:H221	1.82	0.62
17:i:42:PRO:HG2	21:m:167:VAL:HG22	1.82	0.62
30:l:703:CDL:H712	30:l:703:CDL:H312	1.81	0.62
27:u:83:THR:HA	27:u:86:TRP:CD1	2.35	0.61
17:i:278:MET:O	17:i:282:MET:HG3	1.99	0.61
19:k:31:LEU:HD21	21:m:67:VAL:HG11	1.82	0.61
30:l:702:CDL:H611	30:l:702:CDL:C79	2.30	0.61
27:u:47:ARG:NH1	27:u:53:PRO:HA	2.15	0.61
24:p:97:TYR:HB3	24:p:179:MET:HG3	1.83	0.61
29:w:139:ARG:NH1	29:w:166:ASP:OD2	2.33	0.61
6:X:90:TYR:HE1	8:Z:44:PRO:HB2	1.66	0.61
25:r:207:MET:HE3	25:r:240:GLY:N	2.16	0.61
5:W:76:GLN:NE2	5:W:80:ASP:OD1	2.33	0.60
12:d:135:VAL:HG13	13:e:137:MET:HE2	1.83	0.60
26:s:215:TYR:HD2	26:s:219:PRO:HB2	1.65	0.60
27:u:47:ARG:NH1	27:u:53:PRO:CA	2.65	0.60
5:W:85:GLN:OE1	16:h:105:ARG:NH1	2.33	0.60
30:l:702:CDL:C66	30:l:702:CDL:H872	2.31	0.60
20:l:360:GLY:HA3	20:l:435:PRO:HA	1.84	0.60
30:n:102:CDL:CB3	27:u:172:MET:HE2	2.31	0.60
26:s:195:ARG:HD3	26:s:231:ILE:HD11	1.84	0.60
18:j:18:VAL:CG1	31:s:401:PEE:H16	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:419:THR:HA	20:l:422:TYR:CE2	2.37	0.60
10:b:29:SER:H	10:b:32:GLU:HG3	1.67	0.59
18:j:6:THR:HG21	26:s:87:VAL:HG11	1.84	0.59
30:l:702:CDL:H471	30:l:702:CDL:H772	1.84	0.59
12:d:159:GLN:O	12:d:163:MET:HG3	2.01	0.59
25:r:72:LEU:HD21	25:r:233:ALA:HB3	1.84	0.59
9:a:184:LYS:HB3	16:h:30:PRO:HB3	1.84	0.59
20:l:517:SER:HB3	30:l:703:CDL:HA32	1.84	0.59
21:m:61:LEU:O	26:s:114:TYR:OH	2.17	0.59
28:v:33:GLU:OE2	28:v:33:GLU:N	2.35	0.59
20:l:483:PRO:HD2	20:l:486:MET:HE2	1.84	0.59
22:n:3:ASN:N	22:n:3:ASN:ND2	2.51	0.59
4:V:123:ALA:O	4:V:127:MET:HG3	2.02	0.59
30:l:702:CDL:H631	30:l:702:CDL:H811	1.84	0.59
28:v:103:GLU:O	28:v:107:ARG:HG2	2.03	0.59
5:W:94:GLU:HG3	16:h:79:ILE:HD13	1.84	0.59
9:a:152:LYS:HD3	15:g:96:VAL:HG21	1.85	0.59
4:V:81:ARG:NH2	4:V:86:ASP:OD2	2.35	0.59
17:i:186:HIS:O	17:i:190:MET:HG3	2.02	0.59
8:Z:36:LEU:HB3	8:Z:41:LEU:O	2.03	0.59
17:i:87:THR:HG23	17:i:88:LYS:HD3	1.85	0.58
29:w:73:LEU:HD11	29:w:269:VAL:HG21	1.85	0.58
24:p:105:ASP:OD1	24:p:126:LYS:NZ	2.36	0.58
1:Q:52:MET:O	17:i:171:ASN:ND2	2.30	0.58
25:r:336:ARG:NH1	25:r:433:GLU:OE2	2.32	0.58
20:l:257:VAL:HG13	20:l:317:ILE:HD11	1.85	0.58
17:i:89:MET:HE1	17:i:98:MET:HE3	1.85	0.58
5:W:120:MET:O	5:W:120:MET:HG2	2.03	0.58
10:b:86:LEU:HD11	20:l:9:LEU:HD12	1.86	0.58
12:d:120:SER:HB3	28:v:56:ARG:HH22	1.68	0.58
27:u:137:LEU:HD12	27:u:138:PRO:HD2	1.86	0.58
27:u:49:GLU:OE1	27:u:135:ARG:NH2	2.37	0.57
30:l:702:CDL:C61	30:l:702:CDL:H791	2.35	0.57
25:r:371:PRO:O	25:r:448:THR:OG1	2.20	0.57
9:a:189:ASN:HD21	16:h:35:ALA:HB2	0.71	0.57
11:c:38:PRO:HD3	23:o:67:ARG:HG3	1.86	0.57
2:S:51:ASP:OD2	27:u:22:SER:OG	2.22	0.57
28:v:17:PRO:HB2	28:v:22:MET:HE2	1.87	0.57
21:m:82:VAL:HG13	21:m:84:VAL:H	1.70	0.57
26:s:66:SER:HB2	26:s:122:ALA:O	2.05	0.57
30:s:402:CDL:H321	30:s:402:CDL:HB61	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:70:ALA:HB2	27:u:125:LEU:HD13	1.87	0.57
19:k:23:ARG:HG3	21:m:23:LYS:HE2	1.86	0.57
17:i:20:VAL:HG11	17:i:137:ALA:HB1	1.86	0.57
30:i:401:CDL:CB3	29:w:40:PRO:HB3	2.30	0.57
26:s:62:ARG:HD2	26:s:68:ILE:CD1	2.33	0.57
10:b:113:THR:OG1	10:b:115:GLU:HG2	2.03	0.57
13:e:85:TRP:O	13:e:89:VAL:HG13	2.05	0.57
20:l:585:LYS:NZ	30:m:201:CDL:OB3	2.37	0.57
10:b:83:HIS:HD2	12:d:45:VAL:HG21	1.69	0.56
10:b:123:PHE:HB3	28:v:40:VAL:HG11	1.87	0.56
33:g:201:PLX:H361	33:g:201:PLX:H311	1.87	0.56
20:l:173:LEU:HD12	25:r:405:LEU:HD21	1.86	0.56
20:l:76:LEU:HD21	20:l:196:TRP:HE3	1.69	0.56
3:U:53:TYR:HB2	5:W:72:MET:HE1	1.88	0.56
3:U:26:GLY:HA3	31:j:201:PEE:H37	1.87	0.56
19:k:65:VAL:HG11	21:m:157:THR:HG23	1.87	0.56
27:u:46:CYS:O	27:u:50:GLU:HG2	2.06	0.56
5:W:80:ASP:OD2	27:u:47:ARG:NH1	2.39	0.56
6:X:155:TYR:CE1	10:b:23:LEU:HB3	2.40	0.56
26:s:70:MET:HE1	26:s:121:TRP:CZ3	2.33	0.56
11:c:110:ASP:OD2	25:r:278:ARG:NE	2.32	0.56
12:d:160:LYS:HE2	13:e:147:ILE:HG23	1.87	0.56
17:i:112:HIS:HB2	17:i:184:ILE:HD13	1.88	0.55
17:i:217:MET:HB2	17:i:326:LEU:HD13	1.87	0.55
20:l:7:LEU:HD22	20:l:46:LEU:HD11	1.87	0.55
25:r:133:ILE:HD11	25:r:231:LEU:HD11	1.89	0.55
26:s:77:LEU:CD1	31:s:401:PEE:H43	2.36	0.55
29:w:88:GLU:OE2	29:w:161:ARG:NH1	2.40	0.55
19:k:17:ALA:O	19:k:21:MET:HG2	2.07	0.55
25:r:31:SER:HB3	25:r:73:LEU:HD23	1.89	0.55
30:V:202:CDL:H591	30:V:202:CDL:H192	1.89	0.55
10:b:24:LYS:NZ	10:b:27:GLU:OE1	2.37	0.55
32:X:201:8Q1:O2	24:p:13:GLN:NE2	2.39	0.55
20:l:561:ILE:HG13	20:l:562:LEU:H	1.71	0.55
3:U:51:TYR:O	5:W:68:ARG:NH1	2.40	0.55
20:l:228:GLY:HA3	31:l:704:PEE:H38	1.89	0.55
2:S:51:ASP:CG	27:u:22:SER:HG	2.15	0.55
10:b:122:GLU:HA	10:b:122:GLU:OE2	2.07	0.55
17:i:289:ASN:HA	17:i:292:PHE:CE2	2.41	0.55
23:o:5:LYS:NZ	24:p:69:GLU:OE1	2.39	0.55
4:V:62:THR:O	4:V:66:ILE:HG12	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:74:LEU:O	5:W:78:GLU:HG3	2.07	0.54
11:c:93:ASP:OD1	23:o:44:LYS:NZ	2.39	0.54
30:i:401:CDL:HB31	29:w:40:PRO:HB2	1.85	0.54
31:s:401:PEE:H44	30:s:402:CDL:H622	1.88	0.54
14:f:52:VAL:O	14:f:56:ILE:HG23	2.08	0.54
17:i:42:PRO:HG3	21:m:167:VAL:HG13	1.88	0.54
10:b:119:LEU:H	10:b:119:LEU:CD2	2.20	0.54
20:l:227:PHE:O	20:l:230:HIS:ND1	2.41	0.54
22:n:16:LEU:HD12	25:r:14:MET:HB3	1.88	0.54
25:r:403:THR:HA	25:r:406:TYR:CE2	2.42	0.54
13:e:119:ARG:O	13:e:123:GLU:HG3	2.07	0.54
5:W:133:ILE:O	5:W:137:THR:HG22	2.08	0.54
27:u:107:PHE:O	27:u:111:VAL:HG22	2.08	0.54
2:S:19:PRO:HB3	26:s:9:LEU:HD12	1.90	0.53
30:a:201:CDL:H712	30:a:201:CDL:H172	1.89	0.53
25:r:67:VAL:HG12	33:r:502:PLX:H362	1.89	0.53
26:s:68:ILE:CG2	30:s:402:CDL:H111	2.38	0.53
4:V:140:LYS:HG3	4:V:141:VAL:HG23	1.90	0.53
18:j:39:CYS:SG	26:s:127:TYR:OH	2.63	0.53
22:n:47:ARG:NH2	22:n:53:GLU:OE2	2.42	0.53
17:i:258:SER:HB2	17:i:336:VAL:HG12	1.90	0.53
9:a:137:MET:HG2	12:d:83:LEU:HD22	1.89	0.53
25:r:218:LYS:O	25:r:222:GLU:HG2	2.09	0.53
28:v:12:ASP:OD1	28:v:14:SER:OG	2.24	0.53
17:i:18:MET:HA	17:i:18:MET:HE3	1.90	0.52
31:i:402:PEE:H37	31:i:402:PEE:H61	1.91	0.52
31:W:201:PEE:H59	26:s:108:MET:HE1	1.91	0.52
19:k:18:GLY:O	21:m:23:LYS:NZ	2.37	0.52
20:l:190:LEU:HD12	25:r:383:THR:HG21	1.91	0.52
30:l:702:CDL:OA9	30:l:702:CDL:H121	2.09	0.52
23:o:20:PRO:HB3	24:p:65:ARG:HH22	1.73	0.52
31:s:401:PEE:H26	30:s:402:CDL:C16	2.38	0.52
28:v:22:MET:HG2	28:v:23:PRO:HA	1.92	0.52
10:b:80:TRP:HD1	12:d:41:VAL:HG13	1.75	0.52
26:s:307:LEU:HA	26:s:310:MET:HE3	1.90	0.52
5:W:90:ASN:ND2	5:W:123:GLU:O	2.41	0.52
19:k:55:LEU:O	19:k:58:MET:HE3	2.10	0.52
5:W:51:MET:HE2	26:s:311:THR:HB	1.92	0.52
7:Y:95:GLU:N	7:Y:95:GLU:OE1	2.42	0.52
10:b:74:HIS:NE2	20:l:35:TYR:OH	2.30	0.52
20:l:171:ALA:O	20:l:175:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:93:THR:HG23	7:Y:96:GLU:HG2	1.92	0.52
11:c:153:TYR:OH	28:v:8:ARG:NH1	2.39	0.52
12:d:12:GLU:N	12:d:12:GLU:OE1	2.43	0.52
20:l:526:LEU:HD12	20:l:530:PRO:HG2	1.91	0.52
26:s:28:LEU:HD22	26:s:275:ALA:HB2	1.92	0.52
26:s:87:VAL:HG12	26:s:95:LEU:HD23	1.91	0.52
17:i:65:THR:O	17:i:69:MET:HG3	2.10	0.52
20:l:504:LEU:O	20:l:507:THR:OG1	2.28	0.52
4:V:107:SER:HB3	4:V:110:ILE:HB	1.92	0.52
29:w:132:GLN:NE2	29:w:166:ASP:OD1	2.43	0.52
2:S:59:ARG:HG3	2:S:59:ARG:HH11	1.75	0.51
7:Y:50:LEU:HD13	7:Y:55:LEU:HD21	1.91	0.51
28:v:115:ARG:HG3	28:v:115:ARG:HH11	1.75	0.51
13:e:89:VAL:HG21	25:r:25:ILE:HG23	1.92	0.51
17:i:158:ALA:HB2	17:i:191:THR:HG22	1.92	0.51
5:W:103:ASP:OD1	5:W:103:ASP:N	2.43	0.51
17:i:233:THR:HG23	17:i:241:THR:HG22	1.92	0.51
18:j:73:LEU:O	26:s:160:TYR:OH	2.26	0.51
18:j:95:LEU:HD13	26:s:302:MET:HG3	1.91	0.51
15:g:15:PHE:HB2	33:g:201:PLX:H6	1.91	0.51
29:w:72:ARG:HB3	29:w:72:ARG:NH1	2.26	0.51
1:Q:39:PRO:HB3	1:Q:43:TRP:CD1	2.45	0.51
6:X:90:TYR:CE1	8:Z:44:PRO:HB2	2.46	0.51
25:r:324:SER:OG	25:r:440:HIS:NE2	2.37	0.51
29:w:118:TYR:OH	34:w:401:ADP:O2'	2.28	0.51
30:l:702:CDL:H791	30:l:702:CDL:H612	1.92	0.51
26:s:128:ALA:HA	26:s:211:PHE:HA	1.91	0.51
28:v:42:THR:OG1	28:v:45:GLU:OE1	2.28	0.51
5:W:82:ARG:NH2	16:h:106:PRO:O	2.42	0.51
17:i:133:TRP:CZ3	30:i:401:CDL:H392	2.46	0.51
20:l:562:LEU:HB3	20:l:563:PRO:HD3	1.92	0.51
17:i:268:GLN:NE2	17:i:272:LYS:HE3	2.26	0.51
25:r:189:SER:OG	25:r:192:ASN:OD1	2.29	0.51
7:Y:43:ARG:NH1	7:Y:47:PHE:O	2.44	0.50
15:g:101:GLU:OE2	15:g:101:GLU:N	2.25	0.50
26:s:75:PRO:HG3	26:s:219:PRO:HB3	1.93	0.50
2:S:28:LYS:O	2:S:33:GLY:N	2.42	0.50
3:U:54:PRO:HD3	5:W:69:ILE:HD13	1.93	0.50
1:Q:41:VAL:HG23	13:e:55:LEU:HD21	1.93	0.50
4:V:37:SER:O	4:V:41:ILE:HG13	2.11	0.50
20:l:51:LEU:O	20:l:55:MET:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:445:LEU:O	25:r:448:THR:HG22	2.11	0.50
10:b:29:SER:HB2	10:b:32:GLU:HG2	1.94	0.50
13:e:97:ILE:O	13:e:101:LEU:HB2	2.12	0.50
17:i:246:VAL:HG11	30:r:503:CDL:H392	1.94	0.50
17:i:57:THR:HA	19:k:77:LEU:HD13	1.94	0.50
21:m:17:PHE:HA	21:m:20:PHE:CE2	2.45	0.50
28:v:46:MET:HE3	28:v:56:ARG:HD3	1.93	0.50
28:v:51:LEU:HD13	28:v:63:LEU:HD23	1.93	0.50
16:h:84:ASP:HA	16:h:87:ILE:HG12	1.93	0.50
17:i:268:GLN:HE22	17:i:272:LYS:HE3	1.77	0.50
9:a:78:THR:HG21	13:e:96:SER:HA	1.94	0.50
25:r:282:LEU:HD13	25:r:342:MET:HG3	1.94	0.50
28:v:51:LEU:O	28:v:52:MET:HG2	2.12	0.50
20:l:536:LEU:HB3	20:l:537:PRO:HD3	1.93	0.50
5:W:134:LEU:HD21	21:m:2:THR:HB	1.94	0.50
11:c:86:ARG:NH2	11:c:103:GLU:OE1	2.45	0.50
30:m:201:CDL:H222	30:m:201:CDL:H331	1.94	0.50
26:s:317:GLN:OE1	26:s:317:GLN:HA	2.12	0.50
29:w:254:GLU:OE2	29:w:254:GLU:N	2.45	0.50
26:s:24:GLU:HA	26:s:271:LEU:HD13	1.93	0.49
8:Z:29:LEU:HA	8:Z:32:VAL:HG12	1.94	0.49
10:b:119:LEU:N	10:b:119:LEU:CD2	2.73	0.49
11:c:55:TYR:OH	11:c:74:ASP:O	2.22	0.49
3:U:38:TYR:HD1	3:U:41:TYR:HD2	1.60	0.49
22:n:29:ARG:O	22:n:33:GLU:HG3	2.12	0.49
20:l:65:ASN:OD1	20:l:66:TRP:N	2.46	0.49
26:s:179:TRP:O	26:s:183:MET:HG3	2.11	0.49
30:V:201:CDL:H751	30:V:201:CDL:H381	1.94	0.49
18:j:63:LEU:HD21	21:m:63:GLY:HA2	1.93	0.49
12:d:140:GLN:O	12:d:144:SER:HB3	2.13	0.49
17:i:129:LEU:HD13	30:i:401:CDL:C33	2.21	0.49
20:l:293:ILE:HD13	20:l:418:LEU:HD22	1.95	0.49
25:r:306:PRO:HB3	25:r:458:LEU:HD12	1.95	0.49
5:W:131:GLU:CD	5:W:131:GLU:H	2.21	0.49
20:l:97:THR:HG21	20:l:125:LEU:HD22	1.94	0.49
21:m:16:GLY:HA2	30:s:402:CDL:H791	1.95	0.49
30:r:503:CDL:H232	30:r:503:CDL:H782	1.95	0.49
5:W:38:VAL:O	5:W:42:THR:HG23	2.12	0.48
16:h:75:ARG:O	16:h:79:ILE:HG13	2.13	0.48
4:V:110:ILE:HD11	31:l:701:PEE:H1	1.94	0.48
8:Z:58:ALA:O	20:l:434:LYS:NZ	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:i:401:CDL:OA7	30:i:401:CDL:HA62	2.11	0.48
22:n:34:LYS:HE2	30:n:102:CDL:H1	1.95	0.48
26:s:277:TYR:HE2	31:s:403:PEE:H59	1.77	0.48
27:u:50:GLU:OE2	27:u:135:ARG:NE	2.44	0.48
29:w:240:ALA:O	29:w:244:THR:OG1	2.29	0.48
6:X:82:ARG:O	6:X:86:VAL:HG12	2.13	0.48
17:i:192:ALA:HB1	17:i:282:MET:HE1	1.94	0.48
20:l:401:MET:HE3	20:l:401:MET:HB3	1.71	0.48
30:l:702:CDL:H432	30:l:702:CDL:H602	1.94	0.48
30:l:702:CDL:H472	25:r:445:LEU:HB2	1.95	0.48
9:a:186:THR:HG22	16:h:30:PRO:HG3	1.95	0.48
17:i:20:VAL:HG13	17:i:29:ILE:HG23	1.96	0.48
17:i:38:LEU:HD11	21:m:164:GLY:HA2	1.95	0.48
17:i:342:ALA:O	17:i:345:SER:OG	2.29	0.48
20:l:264:TYR:CD2	20:l:265:PRO:HD3	2.48	0.48
23:o:117:GLN:OE1	23:o:117:GLN:HA	2.14	0.48
31:s:401:PEE:H26	30:s:402:CDL:H161	1.96	0.48
29:w:230:THR:HG23	29:w:233:TYR:H	1.77	0.48
10:b:122:GLU:O	10:b:122:GLU:HG3	2.13	0.48
30:n:102:CDL:H551	27:u:169:PHE:CE1	2.37	0.48
30:V:202:CDL:H852	20:l:558:LEU:HD21	1.95	0.48
13:e:79:ASP:HB3	13:e:82:VAL:HG12	1.94	0.48
5:W:98:MET:HG3	5:W:101:VAL:HG21	1.96	0.48
20:l:41:SER:O	20:l:45:THR:HG22	2.13	0.48
31:j:201:PEE:H26	26:s:295:PRO:HB3	1.96	0.47
20:l:384:PRO:HG3	20:l:491:LEU:HD21	1.94	0.47
17:i:182:SER:HB2	17:i:293:TYR:OH	2.14	0.47
20:l:136:ASN:HA	20:l:197:ASP:HA	1.95	0.47
20:l:221:ALA:HA	20:l:226:GLN:HG2	1.97	0.47
25:r:225:ILE:O	25:r:229:MET:HG3	2.14	0.47
2:S:47:LEU:HD22	27:u:22:SER:HB3	1.95	0.47
6:X:111:ASP:OD1	6:X:111:ASP:N	2.45	0.47
17:i:128:LEU:C	17:i:128:LEU:CD2	2.87	0.47
19:k:23:ARG:HG2	30:m:201:CDL:HB62	1.96	0.47
20:l:121:LEU:HD22	20:l:246:LEU:HD23	1.96	0.47
26:s:46:LEU:HD23	26:s:49:ILE:HD12	1.95	0.47
26:s:68:ILE:HG22	30:s:402:CDL:H132	1.95	0.47
11:c:33:THR:HG23	11:c:35:ASP:H	1.80	0.47
11:c:179:GLU:OE2	11:c:179:GLU:N	2.31	0.47
18:j:10:ASN:ND2	26:s:84:THR:OG1	2.44	0.47
30:l:702:CDL:H611	30:l:702:CDL:H791	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:p:62:GLN:O	24:p:66:GLN:HG3	2.15	0.47
26:s:135:ALA:O	26:s:139:THR:HG22	2.14	0.47
5:W:98:MET:HE1	16:h:79:ILE:HA	1.96	0.47
18:j:19:LEU:HD11	31:s:401:PEE:H56	1.97	0.47
5:W:120:MET:HE2	16:h:69:ARG:HD2	1.96	0.47
2:S:31:ASN:CG	2:S:36:LYS:HB2	2.40	0.47
12:d:70:ARG:NH1	12:d:91:GLN:OE1	2.48	0.47
20:l:8:THR:HB	20:l:82:MET:HE3	1.97	0.47
29:w:180:ARG:NH2	29:w:182:GLN:OE1	2.48	0.47
33:j:203:PLX:H352	21:m:155:ILE:HG23	1.96	0.47
30:r:503:CDL:H741	30:r:503:CDL:H772	1.47	0.47
29:w:146:ALA:HB1	29:w:157:VAL:HG21	1.97	0.47
12:d:43:ARG:HG3	12:d:43:ARG:HH11	1.80	0.47
17:i:133:TRP:HE3	30:i:401:CDL:H362	1.78	0.47
17:i:237:MET:HE3	17:i:237:MET:HB2	1.78	0.47
17:i:268:GLN:HG3	27:u:168:PHE:HZ	1.78	0.47
23:o:9:SER:OG	23:o:10:ARG:N	2.48	0.47
25:r:229:MET:HE3	25:r:324:SER:OG	2.14	0.47
7:Y:65:MET:HE3	20:l:386:LEU:HD11	1.96	0.46
16:h:84:ASP:OD1	16:h:85:LYS:N	2.47	0.46
30:i:401:CDL:H141	30:i:401:CDL:H112	1.73	0.46
17:i:133:TRP:CE3	30:i:401:CDL:H362	2.50	0.46
17:i:245:MET:HB3	17:i:245:MET:HE3	1.84	0.46
30:l:702:CDL:H611	30:l:702:CDL:C81	2.45	0.46
23:o:111:LYS:NZ	23:o:111:LYS:HB3	2.31	0.46
3:U:46:ASN:HD21	26:s:314:ILE:HD12	1.81	0.46
8:Z:42:ARG:NH1	8:Z:42:ARG:HB2	2.30	0.46
17:i:307:SER:OG	17:i:308:THR:N	2.48	0.46
19:k:3:LEU:HD23	21:m:121:GLY:HA2	1.97	0.46
20:l:123:LEU:CD1	30:l:702:CDL:OA7	2.64	0.46
28:v:107:ARG:HA	28:v:110:GLN:HG2	1.96	0.46
20:l:290:LEU:HD11	30:l:703:CDL:H731	1.98	0.46
21:m:88:THR:HG23	30:m:201:CDL:H521	1.98	0.46
21:m:173:ARG:HG3	21:m:173:ARG:HH11	1.80	0.46
3:U:32:LEU:HB3	26:s:310:MET:SD	2.55	0.46
3:U:42:ALA:HB2	26:s:312:ALA:HA	1.97	0.46
6:X:103:HIS:HB3	6:X:106:LYS:HB2	1.98	0.46
20:l:298:ILE:O	20:l:302:VAL:HG22	2.16	0.46
25:r:231:LEU:HA	25:r:235:LEU:HB2	1.97	0.46
29:w:129:TYR:OH	29:w:186:HIS:ND1	2.34	0.46
9:a:185:THR:O	9:a:185:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:j:38:GLU:HB2	18:j:41:PHE:O	2.16	0.46
24:p:55:LYS:HE2	24:p:55:LYS:HB2	1.70	0.46
20:l:327:LEU:O	20:l:331:MET:HG2	2.16	0.46
24:p:27:LEU:HD21	24:p:40:PHE:HB3	1.97	0.46
8:Z:42:ARG:HB2	8:Z:42:ARG:CZ	2.46	0.46
11:c:62:TYR:OH	11:c:74:ASP:OD1	2.26	0.46
20:l:378:LEU:HD23	20:l:378:LEU:HA	1.84	0.46
20:l:529:TYR:HB3	20:l:530:PRO:HD3	1.98	0.46
28:v:17:PRO:HB3	28:v:105:GLU:HG2	1.98	0.46
6:X:113:LEU:O	6:X:117:GLU:HG3	2.16	0.46
7:Y:65:MET:HE1	20:l:378:LEU:HD12	1.97	0.46
9:a:141:GLN:O	9:a:145:GLU:HG3	2.15	0.46
11:c:58:ARG:NH1	11:c:61:ASP:OD2	2.48	0.46
17:i:41:ILE:HG13	19:k:73:LEU:HD21	1.97	0.46
17:i:278:MET:HE3	17:i:282:MET:HE3	1.98	0.46
26:s:139:THR:HA	26:s:142:TYR:CE2	2.50	0.46
26:s:142:TYR:CE1	26:s:192:GLU:HG2	2.51	0.46
26:s:179:TRP:CG	26:s:180:PRO:HD3	2.51	0.46
5:W:43:LEU:HG	26:s:179:TRP:HE1	1.80	0.45
31:j:201:PEE:H39	26:s:302:MET:HE1	1.97	0.45
33:j:203:PLX:H132	33:j:203:PLX:H161	1.62	0.45
17:i:183:SER:O	17:i:187:MET:HG2	2.16	0.45
18:j:53:MET:HE3	18:j:55:PHE:CE2	2.51	0.45
25:r:196:TRP:CD1	25:r:250:LEU:HG	2.51	0.45
28:v:19:PRO:HA	28:v:22:MET:HE3	1.99	0.45
11:c:167:TYR:CG	11:c:178:PRO:HG3	2.52	0.45
20:l:313:MET:HG3	20:l:328:HIS:HD2	1.82	0.45
30:l:703:CDL:H351	30:l:703:CDL:H382	1.68	0.45
25:r:370:PRO:HG3	25:r:375:LEU:HD22	1.97	0.45
29:w:58:LYS:O	29:w:60:ILE:HG13	2.16	0.45
29:w:285:ASP:OD1	29:w:285:ASP:N	2.49	0.45
9:a:147:ALA:HB2	25:r:173:SER:HB2	1.97	0.45
10:b:81:ILE:HG23	31:b:201:PEE:H58	1.99	0.45
18:j:88:LEU:HD13	26:s:309:ILE:HD12	1.99	0.45
19:k:44:SER:OG	19:k:59:MET:SD	2.71	0.45
10:b:110:ILE:HD11	10:b:117:ILE:HD11	1.97	0.45
13:e:76:TYR:HB2	13:e:83:ASP:OD1	2.17	0.45
20:l:392:LYS:HE2	20:l:416:THR:HG23	1.98	0.45
25:r:266:MET:HB3	25:r:395:LEU:HD13	1.98	0.45
6:X:99:SER:H	6:X:102:SER:HB2	1.82	0.45
30:i:401:CDL:CB3	29:w:40:PRO:CB	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:197:ASP:OD1	20:l:197:ASP:N	2.45	0.45
20:l:593:ILE:HD11	30:m:201:CDL:H192	1.98	0.45
30:l:702:CDL:H231	30:l:702:CDL:H202	1.70	0.45
21:m:49:GLY:HA2	21:m:139:GLU:OE1	2.16	0.45
11:c:177:GLU:OE1	11:c:177:GLU:HA	2.16	0.45
12:d:73:ASP:OD1	12:d:75:THR:OG1	2.31	0.45
20:l:97:THR:HG22	20:l:101:MET:HE3	1.98	0.45
20:l:332:HIS:HA	20:l:335:PHE:CZ	2.51	0.45
5:W:88:ARG:HH21	27:u:9:THR:HG22	1.82	0.45
12:d:33:LEU:HD13	20:l:49:VAL:HG13	1.98	0.45
17:i:294:MET:SD	25:r:130:LEU:HD21	2.57	0.45
23:o:17:THR:O	23:o:23:TYR:OH	2.35	0.45
23:o:65:LEU:O	23:o:69:THR:HG23	2.16	0.45
10:b:120:MET:HE2	28:v:61:HIS:CB	2.47	0.45
30:m:201:CDL:H652	30:m:201:CDL:H622	1.73	0.45
30:n:102:CDL:HB62	27:u:172:MET:HE2	1.99	0.45
10:b:116:VAL:HG23	10:b:116:VAL:O	2.15	0.45
26:s:102:VAL:HG21	26:s:154:LEU:HD11	1.99	0.45
30:s:402:CDL:H312	30:s:402:CDL:H341	1.74	0.45
11:c:100:ASN:HB2	11:c:103:GLU:OE2	2.17	0.44
18:j:67:LEU:HD22	21:m:59:ILE:HD12	1.99	0.44
20:l:253:VAL:HB	20:l:310:LEU:HD11	1.99	0.44
23:o:116:ILE:HG12	23:o:121:LEU:HD22	1.99	0.44
25:r:139:GLN:OE1	25:r:340:ARG:NH1	2.49	0.44
30:s:402:CDL:H141	30:s:402:CDL:H171	1.71	0.44
30:V:202:CDL:H752	30:V:202:CDL:H721	1.62	0.44
10:b:106:PRO:HB3	10:b:118:PRO:O	2.16	0.44
12:d:94:ARG:NE	25:r:47:GLU:OE2	2.37	0.44
20:l:515:TYR:OH	24:p:70:GLU:OE2	2.17	0.44
24:p:56:ASP:HB3	24:p:59:LYS:HB2	1.98	0.44
19:k:41:PHE:O	19:k:45:THR:HG22	2.18	0.44
20:l:484:LEU:HD23	20:l:484:LEU:HA	1.83	0.44
30:l:702:CDL:H422	25:r:448:THR:HG21	1.99	0.44
30:l:702:CDL:H521	33:r:502:PLX:H211	1.99	0.44
29:w:181:LYS:O	29:w:184:VAL:HG22	2.17	0.44
12:d:119:GLU:HG2	28:v:52:MET:HA	2.00	0.44
21:m:24:PRO:HG3	21:m:83:TRP:NE1	2.33	0.44
30:m:201:CDL:H432	30:m:201:CDL:H462	1.83	0.44
23:o:123:GLN:OE1	23:o:126:ASN:ND2	2.50	0.44
4:V:118:MET:HA	4:V:121:THR:HG22	1.99	0.44
30:V:202:CDL:H441	30:V:202:CDL:H242	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:32:GLU:HB3	24:p:115:TYR:HD1	1.82	0.44
20:l:49:VAL:HB	20:l:50:PRO:HD3	1.99	0.44
20:l:557:TRP:O	20:l:561:ILE:HG12	2.17	0.44
30:l:702:CDL:H812	30:l:702:CDL:H841	1.81	0.44
13:e:54:ARG:O	13:e:55:LEU:HD23	2.18	0.44
22:n:15:ILE:C	22:n:18:PRO:HD2	2.42	0.44
26:s:149:ILE:HG21	26:s:185:TRP:HB2	1.99	0.44
29:w:271:GLU:HA	29:w:274:GLU:HG2	1.99	0.44
17:i:222:SER:O	17:i:224:ALA:N	2.51	0.44
20:l:16:THR:HG22	20:l:126:ILE:HD13	2.00	0.44
20:l:78:LEU:HD11	30:l:702:CDL:H273	2.00	0.44
30:l:702:CDL:C66	30:l:702:CDL:H622	2.48	0.44
30:s:402:CDL:H331	30:s:402:CDL:H362	1.83	0.44
4:V:72:LEU:O	4:V:76:ILE:HD13	2.18	0.44
13:e:73:SER:O	13:e:74:HIS:HB2	2.17	0.44
17:i:172:GLN:OE1	20:l:578:SER:OG	2.25	0.44
17:i:230:LEU:O	17:i:233:THR:HG22	2.18	0.44
20:l:356:ILE:HA	20:l:359:MET:HE2	2.00	0.44
17:i:111:PHE:HA	20:l:591:PHE:CE1	2.53	0.44
23:o:31:LYS:O	23:o:35:GLU:HG3	2.18	0.44
25:r:27:ALA:O	25:r:31:SER:OG	2.22	0.44
20:l:435:PRO:HB3	20:l:437:PHE:CZ	2.53	0.43
27:u:28:ALA:HB2	27:u:82:PHE:CE1	2.53	0.43
16:h:96:PRO:HB2	16:h:101:LYS:HB2	1.99	0.43
20:l:230:HIS:N	20:l:231:PRO:HD3	2.33	0.43
21:m:26:PRO:HB2	21:m:71:THR:HG21	2.01	0.43
25:r:31:SER:HB2	25:r:74:PRO:HG3	2.00	0.43
26:s:84:THR:O	26:s:87:VAL:HG22	2.18	0.43
26:s:169:GLN:HG3	26:s:244:GLY:HA3	2.00	0.43
29:w:165:SER:HB3	29:w:245:PHE:CE1	2.53	0.43
29:w:287:ASP:OD1	29:w:288:ASP:N	2.48	0.43
20:l:33:PRO:HB3	20:l:118:PHE:CZ	2.53	0.43
20:l:358:LYS:HG3	24:p:80:TYR:CE1	2.52	0.43
26:s:70:MET:HE3	26:s:121:TRP:HE3	1.78	0.43
3:U:28:LEU:HD22	3:U:32:LEU:HD13	1.98	0.43
9:a:170:GLN:NE2	27:u:151:ASN:OD1	2.50	0.43
17:i:280:THR:O	17:i:284:MET:HG2	2.18	0.43
20:l:129:MET:HA	20:l:129:MET:HE2	1.99	0.43
20:l:132:VAL:O	20:l:262:ARG:NH2	2.51	0.43
20:l:249:SER:OG	20:l:336:LYS:HG3	2.19	0.43
25:r:336:ARG:NH2	25:r:429:SER:HA	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:107:ASP:OD1	6:X:107:ASP:N	2.50	0.43
19:k:55:LEU:HD23	19:k:55:LEU:HA	1.91	0.43
20:l:213:LEU:HB3	20:l:273:VAL:HG11	2.00	0.43
25:r:269:MET:HE2	25:r:399:ASN:ND2	2.33	0.43
30:V:201:CDL:H322	30:V:201:CDL:H352	1.54	0.43
11:c:113:ILE:HD12	11:c:115:ASN:HB2	2.00	0.43
30:i:401:CDL:OB4	29:w:40:PRO:HG3	2.19	0.43
26:s:86:TRP:NE1	26:s:233:MET:HB2	2.34	0.43
8:Z:13:LYS:HD2	8:Z:13:LYS:HA	1.85	0.43
11:c:153:TYR:HB3	20:l:403:TYR:HD1	1.84	0.43
12:d:26:LEU:HD23	12:d:26:LEU:HA	1.89	0.43
20:l:12:LEU:HD22	20:l:129:MET:HB3	2.00	0.43
20:l:297:ASP:O	20:l:301:ILE:HG13	2.19	0.43
25:r:281:ASP:OD1	25:r:282:LEU:N	2.50	0.43
3:U:59:ASP:CG	27:u:130:LYS:HD3	2.44	0.43
5:W:99:LYS:HE3	5:W:99:LYS:HB3	1.81	0.43
17:i:3:PRO:HB3	30:i:401:CDL:HB32	2.01	0.43
21:m:82:VAL:HG22	21:m:83:TRP:H	1.84	0.43
23:o:116:ILE:HD11	23:o:123:GLN:HE21	1.83	0.43
26:s:85:MET:SD	26:s:108:MET:HB2	2.58	0.43
27:u:34:ALA:HB2	27:u:120:PRO:HG3	2.01	0.43
29:w:51:ARG:HE	29:w:51:ARG:HB3	1.57	0.43
17:i:149:ILE:HD13	17:i:154:MET:SD	2.59	0.43
31:i:402:PEE:H36	20:l:566:THR:HG21	2.01	0.43
30:l:703:CDL:H641	30:l:703:CDL:H612	1.72	0.43
31:l:704:PEE:H58	31:l:704:PEE:H53	1.84	0.43
21:m:33:LEU:HD23	21:m:64:MET:HE3	2.01	0.43
25:r:207:MET:HE3	25:r:240:GLY:H	1.80	0.43
25:r:307:TRP:HA	25:r:310:MET:HE2	1.99	0.43
15:g:106:LYS:H	15:g:106:LYS:HG2	1.66	0.42
17:i:207:ILE:HG22	17:i:211:MET:HE2	2.01	0.42
17:i:268:GLN:HG3	27:u:168:PHE:CZ	2.54	0.42
17:i:298:TYR:O	17:i:303:THR:OG1	2.34	0.42
3:U:69:HIS:CE1	3:U:71:GLN:HG3	2.54	0.42
11:c:70:MET:HE3	11:c:70:MET:HA	2.00	0.42
12:d:81:ASP:O	12:d:85:MET:HG3	2.19	0.42
17:i:73:ALA:HB2	17:i:97:MET:HB2	2.01	0.42
17:i:79:LEU:HB2	19:k:47:ILE:HD13	2.01	0.42
17:i:128:LEU:HD23	17:i:128:LEU:O	2.19	0.42
30:V:202:CDL:H772	23:o:91:ALA:HB2	2.01	0.42
8:Z:43:ASP:HA	8:Z:44:PRO:HD3	1.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:77:CYS:SG	12:d:84:CYS:HB3	2.59	0.42
17:i:316:GLN:NE2	29:w:95:ASP:OD1	2.48	0.42
20:l:420:ALA:O	20:l:424:THR:HG22	2.19	0.42
29:w:300:ASN:OD1	29:w:303:GLU:HB2	2.19	0.42
1:Q:40:ASP:OD1	1:Q:40:ASP:N	2.53	0.42
4:V:14:GLU:HA	4:V:21:LYS:HE3	2.00	0.42
12:d:36:ILE:HD13	12:d:36:ILE:HA	1.94	0.42
33:g:201:PLX:H102	33:g:201:PLX:H71	1.61	0.42
20:l:517:SER:OG	20:l:518:GLN:N	2.52	0.42
30:l:702:CDL:H611	30:l:702:CDL:H792	2.00	0.42
30:l:702:CDL:C79	30:l:702:CDL:C61	2.95	0.42
24:p:25:ARG:HD3	24:p:25:ARG:HA	1.87	0.42
25:r:328:CYS:HB3	25:r:437:MET:HE1	2.01	0.42
26:s:92:PRO:HB3	26:s:255:TYR:CD2	2.55	0.42
21:m:65:LEU:HD11	26:s:139:THR:HG21	2.01	0.42
31:s:401:PEE:H26	30:s:402:CDL:H162	2.00	0.42
29:w:70:LYS:NZ	29:w:160:GLU:OE1	2.53	0.42
1:Q:68:ASP:O	17:i:49:ASN:ND2	2.53	0.42
16:h:92:TYR:CE2	16:h:94:PRO:HB3	2.54	0.42
18:j:73:LEU:HD23	18:j:73:LEU:HA	1.86	0.42
20:l:241:THR:HG21	20:l:344:GLY:HA3	2.01	0.42
30:m:201:CDL:H161	30:m:201:CDL:H191	1.66	0.42
30:r:503:CDL:H271	30:r:503:CDL:H721	2.01	0.42
2:S:31:ASN:ND2	2:S:36:LYS:HB2	2.35	0.42
4:V:34:LEU:HD22	30:m:201:CDL:H261	2.01	0.42
13:e:130:GLU:HG3	13:e:136:LEU:HD21	2.02	0.42
20:l:7:LEU:O	20:l:11:THR:HG23	2.20	0.42
25:r:249:ILE:HG13	25:r:250:LEU:HD13	2.01	0.42
26:s:1:MET:HE2	26:s:1:MET:HB2	1.85	0.42
29:w:276:LEU:HD23	29:w:276:LEU:HA	1.92	0.42
8:Z:53:TYR:CE2	20:l:434:LYS:HG3	2.54	0.42
20:l:295:GLN:O	20:l:425:ARG:NH1	2.53	0.42
25:r:357:THR:O	25:r:361:VAL:HG23	2.19	0.42
26:s:77:LEU:HD12	31:s:401:PEE:H43	2.01	0.42
26:s:142:TYR:CZ	26:s:192:GLU:HG2	2.55	0.42
11:c:31:HIS:N	23:o:61:GLU:OE2	2.52	0.42
30:i:401:CDL:HB31	29:w:40:PRO:CG	2.46	0.42
20:l:314:MET:HE3	20:l:314:MET:HB3	1.94	0.42
15:g:84:MET:HG2	17:i:344:SER:O	2.19	0.42
16:h:83:ARG:O	16:h:87:ILE:HG23	2.19	0.42
19:k:19:LEU:HD13	19:k:33:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:144:TRP:HH2	20:l:256:GLY:HA2	1.83	0.42
20:l:233:LEU:HB3	20:l:234:PRO:HD3	2.02	0.42
30:l:702:CDL:C39	25:r:371:PRO:HD2	2.48	0.42
25:r:420:THR:HB	25:r:423:ILE:HD12	2.01	0.42
29:w:129:TYR:CG	29:w:183:CYS:HB3	2.55	0.42
7:Y:43:ARG:HA	7:Y:43:ARG:HD3	1.86	0.41
9:a:160:MET:SD	9:a:166:GLY:HA3	2.60	0.41
17:i:75:ILE:HD12	19:k:40:LEU:HD22	2.02	0.41
20:l:292:ALA:HB2	20:l:304:PHE:HB3	2.02	0.41
30:l:702:CDL:OB7	33:r:502:PLX:H233	2.20	0.41
26:s:215:TYR:CD2	26:s:219:PRO:HB2	2.52	0.41
30:s:402:CDL:H401	30:s:402:CDL:H372	1.75	0.41
29:w:340:SER:O	29:w:344:ASN:ND2	2.53	0.41
12:d:164:LEU:HD23	13:e:149:LEU:HD13	2.00	0.41
16:h:19:THR:HA	17:i:84:TRP:HB2	2.02	0.41
17:i:154:MET:HE2	17:i:191:THR:HG23	2.02	0.41
17:i:236:LYS:HG3	17:i:237:MET:HG3	2.01	0.41
17:i:290:LEU:HD21	25:r:150:LEU:HD21	2.02	0.41
20:l:377:SER:HB2	20:l:423:SER:OG	2.20	0.41
27:u:38:LYS:HB3	27:u:39:PRO:HD3	2.02	0.41
10:b:120:MET:HB3	28:v:45:GLU:OE2	2.20	0.41
13:e:66:LEU:HD23	13:e:66:LEU:HA	1.91	0.41
17:i:132:THR:HG22	30:i:401:CDL:H371	2.01	0.41
17:i:211:MET:HG2	17:i:333:SER:OG	2.20	0.41
25:r:1:MET:SD	25:r:111:THR:HG21	2.61	0.41
29:w:180:ARG:NH1	29:w:316:GLU:OE2	2.39	0.41
1:Q:73:LYS:HE3	1:Q:73:LYS:HB3	1.77	0.41
15:g:7:ARG:HH21	15:g:91:ASP:CG	2.28	0.41
20:l:79:SER:HB2	20:l:135:ASN:HD22	1.84	0.41
24:p:108:HIS:HB3	24:p:111:GLU:HG3	2.02	0.41
27:u:23:SER:OG	27:u:90:ASP:OD1	2.36	0.41
1:Q:43:TRP:O	1:Q:46:GLN:HG3	2.19	0.41
12:d:80:LYS:HD2	12:d:80:LYS:HA	1.76	0.41
17:i:190:MET:HG3	17:i:190:MET:H	1.73	0.41
31:j:201:PEE:H35	31:j:201:PEE:H30	1.73	0.41
19:k:4:VAL:O	19:k:8:ILE:HG12	2.19	0.41
21:m:23:LYS:N	21:m:24:PRO:HD3	2.35	0.41
21:m:35:VAL:O	21:m:39:VAL:HG23	2.20	0.41
26:s:59:GLU:HA	26:s:60:PRO:HD3	1.92	0.41
26:s:62:ARG:HA	26:s:63:PRO:HD3	1.75	0.41
13:e:76:TYR:HB2	13:e:83:ASP:CG	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:h:17:TRP:CD1	16:h:17:TRP:H	2.37	0.41
17:i:276:ILE:HG21	31:r:501:PEE:H7	2.03	0.41
25:r:420:THR:O	25:r:421:HIS:HB2	2.21	0.41
2:S:59:ARG:HB3	2:S:61:HIS:CE1	2.56	0.41
6:X:89:LEU:CD2	8:Z:48:ASN:HA	2.51	0.41
12:d:106:ILE:HG13	12:d:135:VAL:HG21	2.02	0.41
17:i:258:SER:HB3	17:i:333:SER:O	2.21	0.41
20:l:33:PRO:HB3	20:l:118:PHE:CE1	2.56	0.41
20:l:176:ARG:HD3	20:l:179:ASP:HB2	2.03	0.41
25:r:87:GLU:OE2	25:r:91:ARG:HD2	2.21	0.41
20:l:398:ALA:O	20:l:402:SER:OG	2.31	0.41
26:s:55:LEU:HD13	26:s:221:ALA:HB2	2.01	0.41
30:V:201:CDL:H402	30:V:201:CDL:H762	2.03	0.41
9:a:140:LEU:HD21	25:r:177:LEU:HB3	2.03	0.41
11:c:58:ARG:HB2	11:c:61:ASP:HB2	2.02	0.41
11:c:126:TRP:C	11:c:128:THR:H	2.29	0.41
17:i:228:LEU:HD23	17:i:228:LEU:HA	1.94	0.41
18:j:69:ILE:O	18:j:73:LEU:HG	2.21	0.41
19:k:64:LEU:O	19:k:67:ALA:HB3	2.21	0.41
20:l:51:LEU:HD22	20:l:91:PRO:HG3	2.03	0.41
20:l:53:MET:HE2	20:l:53:MET:HB3	1.79	0.41
20:l:332:HIS:HA	20:l:335:PHE:CE2	2.56	0.41
20:l:399:VAL:HG12	20:l:409:LEU:HD13	2.03	0.41
25:r:216:LEU:HD23	25:r:287:ALA:HB1	2.03	0.41
25:r:455:LEU:HD23	25:r:455:LEU:HA	1.89	0.41
28:v:115:ARG:HG3	28:v:115:ARG:NH1	2.36	0.41
29:w:57:SER:HB3	29:w:150:LEU:HD11	2.01	0.41
31:W:201:PEE:H32	31:W:201:PEE:H38	1.97	0.41
18:j:63:LEU:HA	18:j:63:LEU:HD23	1.85	0.41
25:r:154:LEU:HD23	25:r:154:LEU:HA	1.84	0.41
25:r:400:MET:HE3	25:r:400:MET:HB3	1.88	0.41
25:r:438:ALA:HA	25:r:441:ILE:HG22	2.03	0.41
10:b:76:LEU:HD12	10:b:76:LEU:HA	1.89	0.40
13:e:92:PHE:O	13:e:96:SER:HB2	2.21	0.40
15:g:49:ALA:HB2	30:r:503:CDL:H711	2.03	0.40
26:s:62:ARG:NH1	26:s:68:ILE:HG13	2.36	0.40
3:U:30:ILE:HD11	18:j:96:ILE:HD11	2.02	0.40
6:X:88:LYS:HB3	6:X:88:LYS:HE3	1.81	0.40
33:g:201:PLX:H181	33:g:201:PLX:H151	1.91	0.40
19:k:38:LEU:HB2	21:m:60:TYR:CZ	2.56	0.40
30:m:201:CDL:H161	30:m:201:CDL:H131	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:97:THR:HG21	30:r:503:CDL:H242	2.03	0.40
30:V:201:CDL:H371	30:V:201:CDL:H341	1.85	0.40
30:V:202:CDL:H561	23:o:88:LEU:HD12	2.02	0.40
11:c:162:PRO:HA	28:v:58:TYR:CZ	2.57	0.40
12:d:73:ASP:OD1	12:d:75:THR:N	2.47	0.40
14:f:56:ILE:HG13	14:f:57:TYR:N	2.36	0.40
20:l:336:LYS:HD3	20:l:336:LYS:HA	1.88	0.40
21:m:24:PRO:HB3	21:m:89:VAL:HG11	2.04	0.40
22:n:24:GLY:HA2	25:r:6:ILE:HD12	2.03	0.40
25:r:346:ARG:NH2	25:r:420:THR:HG23	2.36	0.40
31:s:403:PEE:H61	31:s:403:PEE:H55	1.68	0.40
29:w:291:PHE:HD1	29:w:291:PHE:HA	1.80	0.40
3:U:25:ILE:HG12	31:s:403:PEE:H38	2.04	0.40
4:V:138:GLU:HG2	4:V:139:PRO:HD2	2.02	0.40
9:a:67:PHE:CE2	25:r:434:ASN:HB3	2.57	0.40
9:a:134:GLU:HA	9:a:137:MET:HE3	2.02	0.40
12:d:114:GLN:CG	20:l:203:MET:HG2	2.50	0.40
12:d:144:SER:OG	12:d:158:LYS:NZ	2.35	0.40
18:j:57:LEU:HD21	21:m:169:MET:SD	2.62	0.40
25:r:318:ALA:HB1	25:r:374:ASN:CG	2.46	0.40
1:Q:52:MET:HG2	17:i:173:THR:HG22	2.02	0.40
6:X:137:LYS:HA	10:b:3:GLY:HA2	2.04	0.40
17:i:133:TRP:HZ3	30:i:401:CDL:H392	1.84	0.40
20:l:504:LEU:HA	20:l:504:LEU:HD12	1.89	0.40
21:m:82:VAL:HG12	21:m:85:SER:HB3	2.02	0.40
25:r:178:ILE:HD13	25:r:178:ILE:HA	1.91	0.40
25:r:216:LEU:HD22	25:r:291:VAL:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
2	S	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
3	U	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
4	V	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
5	W	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
6	X	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
7	Y	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
8	Z	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
9	a	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
10	b	94/126 (75%)	92 (98%)	2 (2%)	0	100	100
11	c	154/156 (99%)	142 (92%)	12 (8%)	0	100	100
12	d	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
13	e	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
14	f	47/49 (96%)	42 (89%)	5 (11%)	0	100	100
15	g	119/121 (98%)	112 (94%)	7 (6%)	0	100	100
16	h	103/105 (98%)	97 (94%)	6 (6%)	0	100	100
17	i	345/347 (99%)	328 (95%)	17 (5%)	0	100	100
18	j	113/115 (98%)	110 (97%)	3 (3%)	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%)	164 (95%)	8 (5%)	1 (1%)	21	51
22	n	54/56 (96%)	54 (100%)	0	0	100	100
23	o	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
24	p	176/178 (99%)	171 (97%)	5 (3%)	0	100	100
25	r	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
26	s	316/318 (99%)	305 (96%)	11 (4%)	0	100	100
27	u	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
28	v	122/124 (98%)	116 (95%)	6 (5%)	0	100	100
29	w	318/320 (99%)	304 (96%)	14 (4%)	0	100	100
All	All	4666/4754 (98%)	4489 (96%)	176 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	m	26	PRO

5.3.2 Protein sidechains [i](#)

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%)	57 (100%)	0	100	100
3	U	69/69 (100%)	69 (100%)	0	100	100
4	V	101/101 (100%)	101 (100%)	0	100	100
5	W	99/99 (100%)	97 (98%)	2 (2%)	48	78
6	X	76/81 (94%)	75 (99%)	1 (1%)	61	86
7	Y	62/62 (100%)	62 (100%)	0	100	100
8	Z	62/62 (100%)	62 (100%)	0	100	100
9	a	121/121 (100%)	120 (99%)	1 (1%)	73	90
10	b	90/119 (76%)	90 (100%)	0	100	100
11	c	141/141 (100%)	140 (99%)	1 (1%)	76	92
12	d	155/155 (100%)	155 (100%)	0	100	100
13	e	96/96 (100%)	96 (100%)	0	100	100
14	f	36/45 (80%)	36 (100%)	0	100	100
15	g	108/108 (100%)	107 (99%)	1 (1%)	70	90
16	h	93/93 (100%)	91 (98%)	2 (2%)	45	77
17	i	311/311 (100%)	308 (99%)	3 (1%)	68	89
18	j	100/100 (100%)	97 (97%)	3 (3%)	36	70
19	k	85/85 (100%)	85 (100%)	0	100	100
20	l	540/540 (100%)	532 (98%)	8 (2%)	57	84
21	m	130/141 (92%)	129 (99%)	1 (1%)	73	90
22	n	53/53 (100%)	51 (96%)	2 (4%)	29	64
23	o	113/113 (100%)	111 (98%)	2 (2%)	51	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	p	159/159 (100%)	155 (98%)	4 (2%)	42	74
25	r	410/410 (100%)	406 (99%)	4 (1%)	68	89
26	s	275/275 (100%)	273 (99%)	2 (1%)	76	92
27	u	153/153 (100%)	152 (99%)	1 (1%)	76	92
28	v	104/111 (94%)	102 (98%)	2 (2%)	50	79
29	w	283/283 (100%)	280 (99%)	3 (1%)	65	88
All	All	4120/4182 (98%)	4077 (99%)	43 (1%)	65	89

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	W	98	MET
5	W	118	THR
6	X	134	ASP
9	a	185	THR
11	c	113	ILE
15	g	22	SER
16	h	86	LEU
16	h	102	GLU
17	i	100	MET
17	i	128	LEU
17	i	223	SER
18	j	16	LEU
18	j	79	SER
18	j	87	MET
20	l	70	THR
20	l	71	LEU
20	l	108	MET
20	l	109	HIS
20	l	140	LEU
20	l	343	SER
20	l	426	ILE
20	l	544	MET
21	m	108	LEU
22	n	3	ASN
22	n	42	SER
23	o	56	ARG
23	o	73	SER
24	p	4	SER
24	p	110	SER

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Mol	Chain	Res	Type
24	p	117	ASP
24	p	141	GLN
25	r	31	SER
25	r	179	ILE
25	r	246	ILE
25	r	250	LEU
26	s	81	LEU
26	s	274	ARG
27	u	23	SER
28	v	14	SER
28	v	69	CYS
29	w	56	THR
29	w	145	ASP
29	w	184	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	60	HIS
2	S	61	HIS
3	U	46	ASN
6	X	142	GLN
7	Y	49	GLN
8	Z	21	GLN
8	Z	91	GLN
9	a	181	HIS
9	a	189	ASN
11	c	127	ASN
12	d	149	HIS
13	e	140	ASN
16	h	97	HIS
17	i	174	GLN
20	l	23	ASN
20	l	59	GLN
20	l	135	ASN
20	l	175	ASN
20	l	199	GLN
20	l	309	GLN
20	l	470	ASN
23	o	50	GLN
23	o	52	ASN
23	o	75	ASN

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Mol	Chain	Res	Type
24	p	33	HIS
24	p	62	GLN
24	p	75	GLN
25	r	251	ASN
25	r	279	GLN
25	r	304	GLN
26	s	171	HIS
27	u	65	GLN
27	u	163	HIS
28	v	55	GLN
28	v	65	GLN
29	w	176	GLN
29	w	286	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](#)

26 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	PEE	s	401	-	40,40,50	1.17	5 (12%)	43,45,55	0.99	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEE	i	402	-	46,46,50	1.22	6 (13%)	49,51,55	1.01	2 (4%)
34	ADP	w	401	-	28,29,29	3.17	9 (32%)	43,45,45	1.91	9 (20%)
31	PEE	l	704	-	50,50,50	1.19	6 (12%)	53,55,55	0.94	2 (3%)
30	CDL	a	201	-	99,99,99	1.11	8 (8%)	105,111,111	0.88	4 (3%)
30	CDL	s	402	-	88,88,99	1.17	8 (9%)	94,100,111	0.92	4 (4%)
31	PEE	W	201	-	40,40,50	1.16	5 (12%)	43,45,55	1.04	2 (4%)
31	PEE	j	201	-	50,50,50	1.18	6 (12%)	53,55,55	0.97	2 (3%)
31	PEE	r	501	-	50,50,50	1.19	6 (12%)	53,55,55	0.98	2 (3%)
31	PEE	b	201	-	45,45,50	1.25	6 (13%)	48,50,55	1.01	2 (4%)
30	CDL	i	401	-	67,67,99	1.12	4 (5%)	73,79,111	1.17	5 (6%)
30	CDL	l	703	-	99,99,99	1.11	8 (8%)	105,111,111	0.87	4 (3%)
30	CDL	l	702	-	98,98,99	0.93	4 (4%)	104,110,111	1.10	7 (6%)
33	PLX	n	101	-	51,51,51	1.21	4 (7%)	53,59,59	0.60	1 (1%)
33	PLX	j	203	-	51,51,51	1.22	5 (9%)	53,59,59	0.60	1 (1%)
33	PLX	r	502	-	51,51,51	1.21	5 (9%)	53,59,59	0.59	1 (1%)
31	PEE	s	403	-	50,50,50	1.18	6 (12%)	53,55,55	0.99	2 (3%)
32	8Q1	X	201	-	32,34,34	1.61	6 (18%)	39,43,43	1.56	7 (17%)
30	CDL	m	201	-	99,99,99	1.12	8 (8%)	105,111,111	0.86	4 (3%)
30	CDL	r	503	-	99,99,99	1.11	8 (8%)	105,111,111	0.87	4 (3%)
30	CDL	n	102	-	54,54,99	1.24	4 (7%)	60,66,111	1.25	4 (6%)
30	CDL	V	201	-	93,93,99	1.14	9 (9%)	99,105,111	0.87	4 (4%)
31	PEE	l	701	-	39,39,50	1.33	6 (15%)	42,44,55	1.09	3 (7%)
33	PLX	g	201	-	51,51,51	1.20	4 (7%)	53,59,59	0.65	1 (1%)
33	PLX	j	202	-	51,51,51	1.21	4 (7%)	53,59,59	0.59	1 (1%)
30	CDL	V	202	-	99,99,99	1.11	9 (9%)	105,111,111	0.87	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	PEE	s	401	-	-	16/44/44/54	-
31	PEE	i	402	-	-	26/50/50/54	-
34	ADP	w	401	-	-	4/16/32/32	0/3/3/3
31	PEE	l	704	-	-	27/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CDL	a	201	-	-	61/110/110/110	-
30	CDL	s	402	-	-	50/99/99/110	-
31	PEE	W	201	-	-	24/44/44/54	-
31	PEE	j	201	-	-	26/54/54/54	-
31	PEE	r	501	-	-	26/54/54/54	-
31	PEE	b	201	-	-	27/49/49/54	-
30	CDL	i	401	-	-	30/78/78/110	-
30	CDL	l	703	-	-	54/110/110/110	-
30	CDL	l	702	-	-	37/109/109/110	-
33	PLX	n	101	-	-	26/55/55/55	-
33	PLX	j	203	-	-	25/55/55/55	-
33	PLX	r	502	-	-	28/55/55/55	-
31	PEE	s	403	-	-	25/54/54/54	-
32	8Q1	X	201	-	-	17/41/41/41	-
30	CDL	m	201	-	-	60/110/110/110	-
30	CDL	r	503	-	-	56/110/110/110	-
30	CDL	n	102	-	-	23/65/65/110	-
30	CDL	V	201	-	-	49/104/104/110	-
31	PEE	l	701	-	-	23/43/43/54	-
33	PLX	g	201	-	-	28/55/55/55	-
33	PLX	j	202	-	-	37/55/55/55	-
30	CDL	V	202	-	-	59/110/110/110	-

All (159) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	w	401	ADP	C3'-C4'	-8.95	1.30	1.53
34	w	401	ADP	O4'-C4'	7.71	1.62	1.45
34	w	401	ADP	PA-O3A	6.54	1.66	1.59
34	w	401	ADP	C6-N6	5.42	1.48	1.34
32	X	201	8Q1	C39-N41	5.09	1.45	1.33
32	X	201	8Q1	C34-N36	5.07	1.45	1.33
34	w	401	ADP	O4'-C1'	-4.60	1.31	1.42
30	i	401	CDL	OB8-CB7	4.28	1.45	1.33
30	i	401	CDL	OA8-CA7	4.28	1.45	1.33
30	n	102	CDL	OA8-CA7	4.24	1.45	1.33
30	l	702	CDL	OA8-CA7	4.23	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	l	702	CDL	OB8-CB7	4.21	1.45	1.33
30	n	102	CDL	OB8-CB7	4.21	1.45	1.33
30	l	702	CDL	OA6-CA5	4.20	1.46	1.34
30	n	102	CDL	OB6-CB5	4.18	1.46	1.34
30	i	401	CDL	OA6-CA5	4.18	1.46	1.34
30	i	401	CDL	OB6-CB5	4.16	1.46	1.34
30	n	102	CDL	OA6-CA5	4.12	1.45	1.34
30	l	702	CDL	OB6-CB5	4.05	1.45	1.34
31	r	501	PEE	C18-C19	3.84	1.53	1.31
31	l	701	PEE	C18-C19	3.84	1.53	1.31
31	j	201	PEE	C18-C19	3.83	1.53	1.31
31	s	401	PEE	C18-C19	3.82	1.53	1.31
31	b	201	PEE	C18-C19	3.82	1.53	1.31
31	l	704	PEE	C18-C19	3.82	1.53	1.31
31	s	403	PEE	C18-C19	3.82	1.53	1.31
31	W	201	PEE	C18-C19	3.81	1.53	1.31
31	i	402	PEE	C18-C19	3.80	1.53	1.31
31	l	701	PEE	C39-C38	3.75	1.53	1.31
31	r	501	PEE	C39-C38	3.75	1.53	1.31
31	j	201	PEE	C39-C38	3.75	1.53	1.31
31	i	402	PEE	C39-C38	3.74	1.52	1.31
31	l	704	PEE	C39-C38	3.73	1.52	1.31
31	b	201	PEE	C39-C38	3.73	1.52	1.31
31	s	403	PEE	C39-C38	3.73	1.52	1.31
30	s	402	CDL	OA8-CA7	3.48	1.43	1.33
30	m	201	CDL	OA8-CA7	3.47	1.43	1.33
30	V	201	CDL	OA8-CA7	3.46	1.43	1.33
30	V	202	CDL	OA8-CA7	3.45	1.43	1.33
30	a	201	CDL	OA8-CA7	3.43	1.43	1.33
30	r	503	CDL	OA8-CA7	3.40	1.43	1.33
30	l	703	CDL	OA8-CA7	3.37	1.43	1.33
34	w	401	ADP	C8-N9	-3.34	1.31	1.37
30	V	201	CDL	OA6-CA5	3.15	1.43	1.34
34	w	401	ADP	O2'-C2'	-3.13	1.35	1.43
30	m	201	CDL	OA6-CA5	3.13	1.43	1.34
30	r	503	CDL	OB6-CB5	3.07	1.42	1.34
30	a	201	CDL	OB6-CB5	3.06	1.42	1.34
30	m	201	CDL	OB8-CB7	3.05	1.42	1.33
30	s	402	CDL	OB6-CB5	3.03	1.42	1.34
30	V	202	CDL	OB6-CB5	3.02	1.42	1.34
30	m	201	CDL	OB6-CB5	3.02	1.42	1.34
30	s	402	CDL	OA6-CA5	3.00	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	V	201	CDL	OB8-CB7	3.00	1.42	1.33
30	r	503	CDL	OB8-CB7	3.00	1.42	1.33
30	a	201	CDL	OB8-CB7	2.99	1.42	1.33
30	l	703	CDL	OB8-CB7	2.99	1.42	1.33
30	l	703	CDL	OB6-CB5	2.99	1.42	1.34
30	V	201	CDL	OB6-CB5	2.97	1.42	1.34
30	a	201	CDL	OA6-CA5	2.96	1.42	1.34
34	w	401	ADP	O3'-C3'	2.96	1.50	1.43
30	V	202	CDL	OB8-CB7	2.96	1.42	1.33
30	s	402	CDL	OB8-CB7	2.94	1.41	1.33
30	r	503	CDL	OA6-CA5	2.94	1.42	1.34
30	V	202	CDL	OA6-CA5	2.94	1.42	1.34
30	l	703	CDL	OA6-CA5	2.94	1.42	1.34
33	n	101	PLX	O6-C4	-2.88	1.40	1.44
33	r	502	PLX	O6-C4	-2.81	1.41	1.44
33	g	201	PLX	O6-C4	-2.79	1.41	1.44
33	j	203	PLX	O6-C4	-2.74	1.41	1.44
31	s	401	PEE	O3-C30	2.65	1.41	1.33
30	a	201	CDL	OA6-CA4	-2.60	1.40	1.46
31	s	403	PEE	O2-C2	-2.58	1.40	1.46
30	l	703	CDL	OA6-CA4	-2.56	1.40	1.46
31	i	402	PEE	O2-C2	-2.56	1.40	1.46
31	l	704	PEE	O2-C2	-2.56	1.40	1.46
31	j	201	PEE	O2-C2	-2.56	1.40	1.46
31	r	501	PEE	O2-C2	-2.56	1.40	1.46
31	s	401	PEE	O2-C2	-2.55	1.40	1.46
30	r	503	CDL	OA6-CA4	-2.55	1.40	1.46
30	s	402	CDL	OA6-CA4	-2.54	1.40	1.46
30	V	202	CDL	OA6-CA4	-2.54	1.40	1.46
31	l	701	PEE	O2-C2	-2.54	1.40	1.46
31	b	201	PEE	O3-C30	2.50	1.40	1.33
31	b	201	PEE	O2-C2	-2.50	1.40	1.46
33	j	202	PLX	O6-C4	-2.50	1.41	1.44
31	r	501	PEE	O3-C30	2.50	1.40	1.33
31	l	701	PEE	O3-C30	2.49	1.40	1.33
31	W	201	PEE	O2-C2	-2.49	1.40	1.46
33	j	202	PLX	C7-C6	2.45	1.55	1.50
33	j	203	PLX	C7-C6	2.45	1.55	1.50
31	s	403	PEE	O3-C30	2.44	1.40	1.33
33	r	502	PLX	C7-C6	2.44	1.55	1.50
31	j	201	PEE	O3-C30	2.43	1.40	1.33
31	l	704	PEE	O3-C30	2.43	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	i	402	PEE	O3-C30	2.42	1.40	1.33
32	X	201	8Q1	C1-S44	2.42	1.81	1.76
34	w	401	ADP	C5-N7	-2.41	1.34	1.39
31	W	201	PEE	O3-C30	2.39	1.40	1.33
33	n	101	PLX	C7-C6	2.38	1.55	1.50
33	g	201	PLX	C7-C6	2.36	1.55	1.50
30	V	201	CDL	OB6-CB4	-2.35	1.41	1.46
30	m	201	CDL	OB6-CB4	-2.35	1.41	1.46
31	l	704	PEE	O2-C10	2.34	1.40	1.34
30	l	703	CDL	OB6-CB4	-2.34	1.41	1.46
31	b	201	PEE	O2-C10	2.32	1.40	1.34
31	s	401	PEE	O2-C10	2.30	1.40	1.34
30	a	201	CDL	OB6-CB4	-2.29	1.41	1.46
30	s	402	CDL	OB6-CB4	-2.29	1.41	1.46
31	W	201	PEE	O2-C10	2.28	1.40	1.34
31	s	403	PEE	O2-C10	2.28	1.40	1.34
30	s	402	CDL	PB2-OB2	2.28	1.68	1.59
30	V	201	CDL	PB2-OB2	2.27	1.68	1.59
32	X	201	8Q1	O35-C34	-2.27	1.19	1.23
31	l	701	PEE	O2-C10	2.27	1.40	1.34
32	X	201	8Q1	O40-C39	-2.27	1.18	1.23
30	a	201	CDL	PB2-OB2	2.27	1.68	1.59
31	j	201	PEE	O2-C10	2.26	1.40	1.34
30	m	201	CDL	OA6-CA4	-2.26	1.41	1.46
30	V	202	CDL	PB2-OB2	2.26	1.68	1.59
30	l	703	CDL	PB2-OB2	2.26	1.68	1.59
30	V	202	CDL	OB6-CB4	-2.26	1.41	1.46
30	m	201	CDL	PB2-OB2	2.26	1.68	1.59
30	r	503	CDL	PB2-OB2	2.26	1.68	1.59
30	V	202	CDL	PB2-OB5	2.25	1.68	1.59
31	r	501	PEE	O2-C10	2.24	1.40	1.34
30	m	201	CDL	PB2-OB5	2.23	1.68	1.59
31	i	402	PEE	O2-C10	2.23	1.40	1.34
30	r	503	CDL	OB6-CB4	-2.23	1.41	1.46
30	V	201	CDL	PB2-OB5	2.22	1.68	1.59
31	l	704	PEE	O3-C3	-2.22	1.40	1.45
33	j	202	PLX	P1-O4	2.22	1.68	1.59
30	V	201	CDL	OA6-CA4	-2.22	1.41	1.46
30	l	703	CDL	PB2-OB5	2.21	1.68	1.59
30	a	201	CDL	PB2-OB5	2.21	1.68	1.59
32	X	201	8Q1	C6-C1	2.20	1.53	1.50
33	g	201	PLX	P1-O4	2.20	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	r	503	CDL	PB2-OB5	2.20	1.68	1.59
30	s	402	CDL	PB2-OB5	2.20	1.68	1.59
33	j	203	PLX	P1-O4	2.19	1.68	1.59
31	W	201	PEE	O3-C3	-2.18	1.40	1.45
33	n	101	PLX	P1-O4	2.16	1.67	1.59
31	i	402	PEE	O3-C3	-2.15	1.40	1.45
33	r	502	PLX	P1-O4	2.14	1.67	1.59
31	j	201	PEE	O3-C3	-2.13	1.40	1.45
31	r	501	PEE	O3-C3	-2.12	1.40	1.45
31	l	701	PEE	O3-C3	-2.11	1.40	1.45
31	s	403	PEE	O3-C3	-2.10	1.40	1.45
33	j	203	PLX	P1-O1	2.10	1.67	1.59
31	b	201	PEE	O3-C3	-2.10	1.40	1.45
33	j	202	PLX	P1-O1	2.08	1.67	1.59
33	n	101	PLX	P1-O1	2.07	1.67	1.59
30	V	201	CDL	C11-CA5	2.07	1.56	1.50
33	r	502	PLX	P1-O1	2.07	1.67	1.59
33	g	201	PLX	P1-O1	2.04	1.67	1.59
33	r	502	PLX	C1-C2	2.02	1.57	1.51
30	V	202	CDL	C11-CA5	2.02	1.56	1.50
31	s	401	PEE	O3-C3	-2.02	1.40	1.45
33	j	203	PLX	C1-C2	2.01	1.57	1.51

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	201	8Q1	C6-C1-S44	5.43	119.88	113.40
34	w	401	ADP	C5-C4-N3	-5.33	119.38	126.72
34	w	401	ADP	N3-C2-N1	-4.60	121.62	128.58
30	l	702	CDL	OA6-CA5-C11	4.52	121.25	111.48
30	i	401	CDL	OA6-CA5-C11	4.25	120.68	111.48
34	w	401	ADP	N3-C4-N9	4.13	134.19	127.17
30	a	201	CDL	OB6-CB5-C51	4.08	120.31	111.48
31	b	201	PEE	O2-C10-C11	4.06	120.27	111.48
30	s	402	CDL	OB6-CB5-C51	4.03	120.21	111.48
31	W	201	PEE	O2-C10-C11	4.03	120.21	111.48
30	V	201	CDL	OA6-CA5-C11	4.01	120.15	111.48
30	l	702	CDL	OB6-CB5-C51	4.01	120.15	111.48
31	s	403	PEE	O2-C10-C11	3.99	120.11	111.48
31	j	201	PEE	O2-C10-C11	3.98	120.10	111.48
30	s	402	CDL	OA6-CA5-C11	3.98	120.09	111.48
30	m	201	CDL	OB6-CB5-C51	3.97	120.08	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	n	102	CDL	OB6-CB5-C51	3.96	120.06	111.48
31	r	501	PEE	O2-C10-C11	3.96	120.06	111.48
31	s	401	PEE	O2-C10-C11	3.96	120.06	111.48
30	V	202	CDL	OB6-CB5-C51	3.95	120.03	111.48
30	r	503	CDL	OA6-CA5-C11	3.94	120.01	111.48
30	l	703	CDL	OA6-CA5-C11	3.94	120.00	111.48
31	i	402	PEE	O2-C10-C11	3.92	119.95	111.48
30	n	102	CDL	OA6-CA5-C11	3.89	119.90	111.48
30	r	503	CDL	OB6-CB5-C51	3.87	119.84	111.48
31	l	701	PEE	O2-C10-C11	3.86	119.83	111.48
30	i	401	CDL	OB6-CB5-C51	3.86	119.83	111.48
30	l	703	CDL	OB6-CB5-C51	3.85	119.81	111.48
30	V	202	CDL	OA6-CA5-C11	3.84	119.79	111.48
30	a	201	CDL	OA6-CA5-C11	3.83	119.77	111.48
30	V	201	CDL	OB6-CB5-C51	3.81	119.71	111.48
31	l	704	PEE	O2-C10-C11	3.76	119.61	111.48
30	m	201	CDL	OA6-CA5-C11	3.58	119.23	111.48
34	w	401	ADP	C2-N3-C4	3.54	120.47	111.83
34	w	401	ADP	N9-C8-N7	-3.54	108.92	113.94
32	X	201	8Q1	O4-C1-C6	-3.49	119.95	123.98
34	w	401	ADP	C5-N7-C8	3.18	108.45	103.45
34	w	401	ADP	C4-N9-C8	3.14	109.04	105.74
30	l	702	CDL	OB8-CB7-C71	3.02	121.05	111.83
34	w	401	ADP	C4-C5-N7	-2.99	107.16	110.58
30	l	702	CDL	OA8-CA7-C31	2.99	120.95	111.83
30	n	102	CDL	OA8-CA7-C31	2.95	120.11	111.15
30	n	102	CDL	OB8-CB7-C71	2.91	120.71	111.83
30	m	201	CDL	OB8-CB7-C71	2.84	120.51	111.83
31	s	403	PEE	O3-C30-C31	2.83	120.47	111.83
30	a	201	CDL	OB8-CB7-C71	2.83	120.46	111.83
31	r	501	PEE	O3-C30-C31	2.83	120.46	111.83
30	r	503	CDL	OB8-CB7-C71	2.80	120.38	111.83
30	m	201	CDL	OA8-CA7-C31	2.79	120.33	111.83
30	i	401	CDL	OA8-CA7-C31	2.76	120.25	111.83
30	s	402	CDL	OA8-CA7-C31	2.75	120.23	111.83
30	V	202	CDL	OA8-CA7-C31	2.74	120.20	111.83
30	V	202	CDL	OB8-CB7-C71	2.74	120.19	111.83
31	j	201	PEE	O3-C30-C31	2.73	120.15	111.83
31	l	704	PEE	O3-C30-C31	2.72	120.13	111.83
31	l	701	PEE	O3-C30-C31	2.72	120.13	111.83
30	V	201	CDL	OB8-CB7-C71	2.70	120.08	111.83
31	b	201	PEE	O3-C30-C31	2.70	120.05	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	201	CDL	OA8-CA7-C31	2.69	120.04	111.83
30	l	703	CDL	OB8-CB7-C71	2.68	120.00	111.83
31	i	402	PEE	O3-C30-C31	2.68	119.99	111.83
32	X	201	8Q1	C37-C38-C39	2.67	116.85	112.39
31	s	401	PEE	O3-C30-C31	2.66	119.96	111.83
31	W	201	PEE	O3-C30-C31	2.66	119.94	111.83
33	g	201	PLX	C1A-N1-C1	2.65	120.44	109.91
30	i	401	CDL	OB8-CB7-C71	2.64	119.90	111.83
30	r	503	CDL	OA8-CA7-C31	2.64	119.89	111.83
30	s	402	CDL	OB8-CB7-C71	2.59	119.74	111.83
30	l	702	CDL	CA4-OA6-CA5	-2.58	111.62	117.80
30	V	201	CDL	OA8-CA7-C31	2.58	119.69	111.83
34	w	401	ADP	C4'-O4'-C1'	-2.52	103.90	109.47
30	l	702	CDL	CB4-OB6-CB5	-2.52	111.77	117.80
33	j	203	PLX	C1A-N1-C1	2.48	119.76	109.91
30	l	703	CDL	OA8-CA7-C31	2.45	119.31	111.83
32	X	201	8Q1	C43-S44-C1	2.45	109.07	101.84
33	r	502	PLX	C1A-N1-C1	2.41	119.51	109.91
33	n	101	PLX	C1A-N1-C1	2.41	119.48	109.91
33	j	202	PLX	C1A-N1-C1	2.35	119.24	109.91
31	l	701	PEE	C20-C19-C18	-2.31	112.51	126.42
32	X	201	8Q1	C38-C39-N41	2.28	120.50	116.34
30	i	401	CDL	CA4-OA6-CA5	-2.28	112.34	117.80
32	X	201	8Q1	C42-N41-C39	-2.07	118.98	122.82
30	l	702	CDL	OB8-CB7-OB9	-2.03	118.54	123.63
32	X	201	8Q1	O27-C28-C29	-2.00	107.33	110.55

There are no chirality outliers.

All (864) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	V	201	CDL	CA2-OA2-PA1-OA5
30	V	201	CDL	OA7-CA5-OA6-CA4
30	V	201	CDL	C11-CA5-OA6-CA4
30	V	201	CDL	CB2-OB2-PB2-OB3
30	V	201	CDL	CB2-OB2-PB2-OB5
30	V	201	CDL	CB3-OB5-PB2-OB2
30	V	201	CDL	CB3-OB5-PB2-OB3
30	V	201	CDL	CB3-OB5-PB2-OB4
30	V	202	CDL	CA3-OA5-PA1-OA2
30	V	202	CDL	CA3-OA5-PA1-OA3
30	V	202	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
30	V	202	CDL	C51-CB5-OB6-CB4
30	a	201	CDL	CB2-C1-CA2-OA2
30	a	201	CDL	CA2-OA2-PA1-OA3
30	a	201	CDL	CB2-OB2-PB2-OB3
30	a	201	CDL	CB2-OB2-PB2-OB5
30	a	201	CDL	CB3-OB5-PB2-OB2
30	a	201	CDL	CB3-OB5-PB2-OB3
30	a	201	CDL	CB3-OB5-PB2-OB4
30	a	201	CDL	OB7-CB5-OB6-CB4
30	a	201	CDL	C51-CB5-OB6-CB4
30	i	401	CDL	CA2-OA2-PA1-OA3
30	i	401	CDL	CA3-OA5-PA1-OA2
30	i	401	CDL	CA3-OA5-PA1-OA4
30	i	401	CDL	CB2-OB2-PB2-OB3
30	i	401	CDL	CB2-OB2-PB2-OB4
30	i	401	CDL	CB2-OB2-PB2-OB5
30	i	401	CDL	CB3-OB5-PB2-OB2
30	l	702	CDL	CA2-OA2-PA1-OA3
30	l	702	CDL	CA2-OA2-PA1-OA4
30	l	702	CDL	CA2-OA2-PA1-OA5
30	l	702	CDL	CA3-OA5-PA1-OA3
30	l	702	CDL	CB3-OB5-PB2-OB2
30	l	702	CDL	CB3-OB5-PB2-OB4
30	l	703	CDL	O1-C1-CA2-OA2
30	l	703	CDL	CB2-C1-CA2-OA2
30	l	703	CDL	CA2-OA2-PA1-OA4
30	l	703	CDL	CA2-OA2-PA1-OA5
30	l	703	CDL	CA3-OA5-PA1-OA2
30	l	703	CDL	CA3-OA5-PA1-OA4
30	l	703	CDL	CB2-OB2-PB2-OB4
30	l	703	CDL	CB2-OB2-PB2-OB5
30	m	201	CDL	CB2-C1-CA2-OA2
30	m	201	CDL	CA2-OA2-PA1-OA3
30	m	201	CDL	CA2-OA2-PA1-OA4
30	m	201	CDL	CA2-OA2-PA1-OA5
30	m	201	CDL	CA3-OA5-PA1-OA2
30	m	201	CDL	CA3-OA5-PA1-OA3
30	m	201	CDL	CB3-OB5-PB2-OB2
30	m	201	CDL	CB3-OB5-PB2-OB3
30	m	201	CDL	CB3-OB5-PB2-OB4
30	n	102	CDL	O1-C1-CB2-OB2
30	n	102	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
30	n	102	CDL	CA2-OA2-PA1-OA5
30	n	102	CDL	CA3-OA5-PA1-OA2
30	n	102	CDL	CA3-OA5-PA1-OA4
30	n	102	CDL	CB3-OB5-PB2-OB2
30	n	102	CDL	CB3-OB5-PB2-OB4
30	r	503	CDL	CA2-OA2-PA1-OA3
30	r	503	CDL	CA2-OA2-PA1-OA5
30	r	503	CDL	CA3-OA5-PA1-OA3
30	r	503	CDL	CB2-OB2-PB2-OB3
30	r	503	CDL	CB2-OB2-PB2-OB4
30	r	503	CDL	CB2-OB2-PB2-OB5
30	r	503	CDL	CB3-OB5-PB2-OB2
30	r	503	CDL	CB3-OB5-PB2-OB3
30	r	503	CDL	C51-CB5-OB6-CB4
30	s	402	CDL	CB2-C1-CA2-OA2
30	s	402	CDL	CA2-OA2-PA1-OA3
30	s	402	CDL	CA2-OA2-PA1-OA4
30	s	402	CDL	CA2-OA2-PA1-OA5
30	s	402	CDL	CB3-OB5-PB2-OB2
30	s	402	CDL	CB3-OB5-PB2-OB4
30	s	402	CDL	OB6-CB4-CB6-OB8
31	W	201	PEE	C4-O4P-P-O3P
31	W	201	PEE	C4-O4P-P-O1P
31	W	201	PEE	O4P-C4-C5-N
31	b	201	PEE	O4P-C4-C5-N
31	i	402	PEE	C11-C10-O2-C2
31	i	402	PEE	C4-O4P-P-O3P
31	i	402	PEE	C4-O4P-P-O1P
31	j	201	PEE	C1-O3P-P-O1P
31	j	201	PEE	C1-O3P-P-O4P
31	l	701	PEE	C11-C10-O2-C2
31	l	701	PEE	C1-O3P-P-O2P
31	l	701	PEE	C1-O3P-P-O1P
31	l	701	PEE	C1-O3P-P-O4P
31	l	701	PEE	C4-O4P-P-O3P
31	l	701	PEE	C4-O4P-P-O2P
31	l	704	PEE	O3P-C1-C2-O2
31	l	704	PEE	C4-O4P-P-O3P
31	l	704	PEE	C4-O4P-P-O2P
31	r	501	PEE	C1-O3P-P-O1P
31	r	501	PEE	C1-O3P-P-O4P
31	s	403	PEE	C11-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
32	X	201	8Q1	C1-C6-C7-C8
32	X	201	8Q1	O4-C1-S44-C43
32	X	201	8Q1	C6-C1-S44-C43
32	X	201	8Q1	N41-C42-C43-S44
32	X	201	8Q1	C42-C43-S44-C1
32	X	201	8Q1	C28-O27-P24-O3
32	X	201	8Q1	C28-O27-P24-O2
33	g	201	PLX	C2-O1-P1-O4
33	j	202	PLX	O7-C6-O6-C4
33	j	202	PLX	C2-O1-P1-O4
33	j	202	PLX	C2-O1-P1-O2
33	j	203	PLX	O7-C6-C7-C8
33	n	101	PLX	O7-C6-C7-C8
33	n	101	PLX	O7-C6-O6-C4
33	n	101	PLX	C3-O4-P1-O3
33	r	502	PLX	C3-O4-P1-O1
33	r	502	PLX	C3-O4-P1-O2
33	r	502	PLX	C3-O4-P1-O3
34	w	401	ADP	C5'-O5'-PA-O2A
30	i	401	CDL	OA9-CA7-OA8-CA6
30	s	402	CDL	OA9-CA7-OA8-CA6
30	V	202	CDL	OB7-CB5-OB6-CB4
30	r	503	CDL	OB7-CB5-OB6-CB4
30	s	402	CDL	OB7-CB5-OB6-CB4
31	l	701	PEE	O4-C10-O2-C2
31	l	704	PEE	O4-C10-O2-C2
31	s	403	PEE	O4-C10-O2-C2
30	s	402	CDL	C51-CB5-OB6-CB4
31	l	704	PEE	C11-C10-O2-C2
30	i	401	CDL	C31-CA7-OA8-CA6
30	s	402	CDL	C31-CA7-OA8-CA6
31	i	402	PEE	C31-C30-O3-C3
31	l	704	PEE	C31-C30-O3-C3
31	W	201	PEE	C17-C18-C19-C20
31	i	402	PEE	O5-C30-O3-C3
31	i	402	PEE	O4-C10-O2-C2
33	g	201	PLX	C2-C1-N1-C1A
30	a	201	CDL	O1-C1-CA2-OA2
30	a	201	CDL	O1-C1-CB2-OB2
30	l	702	CDL	O1-C1-CA2-OA2
30	r	503	CDL	O1-C1-CA2-OA2
30	s	402	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
30	s	402	CDL	O1-C1-CB2-OB2
30	V	201	CDL	C71-CB7-OB8-CB6
31	l	704	PEE	O5-C30-O3-C3
31	b	201	PEE	C11-C10-O2-C2
30	V	201	CDL	OB9-CB7-OB8-CB6
30	l	703	CDL	C71-CB7-OB8-CB6
31	b	201	PEE	C37-C38-C39-C40
31	j	201	PEE	C17-C18-C19-C20
30	m	201	CDL	C11-CA5-OA6-CA4
31	b	201	PEE	O4-C10-O2-C2
30	a	201	CDL	CA2-C1-CB2-OB2
30	n	102	CDL	CA2-C1-CB2-OB2
30	s	402	CDL	CA2-C1-CB2-OB2
30	l	702	CDL	C31-CA7-OA8-CA6
31	W	201	PEE	C31-C30-O3-C3
31	j	201	PEE	C31-C30-O3-C3
31	l	701	PEE	C31-C30-O3-C3
30	V	201	CDL	C62-C63-C64-C65
30	r	503	CDL	C74-C75-C76-C77
33	j	203	PLX	C13-C14-C15-C16
30	V	202	CDL	C32-C33-C34-C35
30	s	402	CDL	C37-C38-C39-C40
30	V	202	CDL	C11-C12-C13-C14
30	m	201	CDL	C73-C74-C75-C76
33	g	201	PLX	C9-C10-C11-C12
33	g	201	PLX	C7-C8-C9-C10
30	V	201	CDL	C32-C33-C34-C35
30	l	702	CDL	OA9-CA7-OA8-CA6
31	j	201	PEE	O5-C30-O3-C3
31	l	701	PEE	O5-C30-O3-C3
31	j	201	PEE	C11-C10-O2-C2
30	V	202	CDL	CB7-C71-C72-C73
30	l	703	CDL	C35-C36-C37-C38
30	V	201	CDL	C59-C60-C61-C62
30	m	201	CDL	C62-C63-C64-C65
30	s	402	CDL	CA7-C31-C32-C33
31	r	501	PEE	C10-C11-C12-C13
30	i	401	CDL	CA7-C31-C32-C33
30	a	201	CDL	CA5-C11-C12-C13
30	a	201	CDL	CA7-C31-C32-C33
30	s	402	CDL	CB7-C71-C72-C73
31	W	201	PEE	O5-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
31	s	403	PEE	C42-C43-C44-C45
30	s	402	CDL	C31-C32-C33-C34
30	l	703	CDL	OB9-CB7-OB8-CB6
30	m	201	CDL	OA7-CA5-OA6-CA4
30	m	201	CDL	C36-C37-C38-C39
31	i	402	PEE	C37-C38-C39-C40
31	l	701	PEE	C17-C18-C19-C20
31	l	704	PEE	C37-C38-C39-C40
31	s	403	PEE	C17-C18-C19-C20
30	r	503	CDL	C60-C61-C62-C63
30	n	102	CDL	C54-C55-C56-C57
31	b	201	PEE	C31-C30-O3-C3
30	s	402	CDL	C14-C15-C16-C17
31	j	201	PEE	O4-C10-O2-C2
30	r	503	CDL	CB2-C1-CA2-OA2
30	l	703	CDL	C17-C18-C19-C20
33	g	201	PLX	C2-C1-N1-C1C
30	a	201	CDL	C71-CB7-OB8-CB6
30	V	201	CDL	C51-CB5-OB6-CB4
31	r	501	PEE	C11-C10-O2-C2
31	r	501	PEE	O4-C10-O2-C2
31	i	402	PEE	C30-C31-C32-C33
30	l	703	CDL	O1-C1-CB2-OB2
30	m	201	CDL	O1-C1-CA2-OA2
30	V	202	CDL	C71-CB7-OB8-CB6
30	V	202	CDL	C72-C73-C74-C75
30	r	503	CDL	CA5-C11-C12-C13
31	b	201	PEE	O5-C30-O3-C3
30	m	201	CDL	C13-C14-C15-C16
33	g	201	PLX	C2-C1-N1-C1B
30	V	201	CDL	C74-C75-C76-C77
30	V	202	CDL	C33-C34-C35-C36
30	s	402	CDL	C71-C72-C73-C74
33	j	202	PLX	C31-C32-C33-C34
30	V	201	CDL	C58-C59-C60-C61
30	a	201	CDL	C75-C76-C77-C78
30	l	702	CDL	C71-C72-C73-C74
30	m	201	CDL	C32-C33-C34-C35
30	m	201	CDL	C55-C56-C57-C58
30	m	201	CDL	C60-C61-C62-C63
31	W	201	PEE	C21-C22-C23-C24
33	j	202	PLX	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
33	j	203	PLX	C31-C32-C33-C34
31	i	402	PEE	C17-C18-C19-C20
31	r	501	PEE	C37-C38-C39-C40
30	V	201	CDL	C52-C53-C54-C55
33	n	101	PLX	C31-C32-C33-C34
30	V	201	CDL	C31-CA7-OA8-CA6
33	j	202	PLX	O9-C24-C25-C26
30	V	202	CDL	C37-C38-C39-C40
30	a	201	CDL	C17-C18-C19-C20
30	a	201	CDL	C62-C63-C64-C65
30	l	703	CDL	C11-C12-C13-C14
33	g	201	PLX	C11-C12-C13-C14
33	g	201	PLX	C32-C33-C34-C35
33	j	202	PLX	C28-C29-C30-C31
33	j	202	PLX	C30-C31-C32-C33
33	j	203	PLX	C16-C17-C18-C19
33	r	502	PLX	C25-C26-C27-C28
30	V	201	CDL	OB7-CB5-OB6-CB4
30	a	201	CDL	C60-C61-C62-C63
30	s	402	CDL	C75-C76-C77-C78
31	l	704	PEE	C21-C22-C23-C24
30	V	201	CDL	C37-C38-C39-C40
33	r	502	PLX	C13-C14-C15-C16
30	V	202	CDL	C59-C60-C61-C62
31	W	201	PEE	C11-C10-O2-C2
31	b	201	PEE	C31-C32-C33-C34
31	b	201	PEE	C33-C34-C35-C36
33	g	201	PLX	C27-C28-C29-C30
30	m	201	CDL	C11-C12-C13-C14
30	l	702	CDL	CA5-C11-C12-C13
30	l	702	CDL	CB5-C51-C52-C53
30	i	401	CDL	C37-C38-C39-C40
30	m	201	CDL	C61-C62-C63-C64
30	r	503	CDL	C32-C33-C34-C35
30	r	503	CDL	C35-C36-C37-C38
33	j	203	PLX	C7-C8-C9-C10
33	n	101	PLX	C10-C11-C12-C13
30	V	201	CDL	C33-C34-C35-C36
30	m	201	CDL	C79-C80-C81-C82
30	s	402	CDL	C73-C74-C75-C76
33	n	101	PLX	C13-C14-C15-C16
30	V	201	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
30	r	503	CDL	CB7-C71-C72-C73
30	V	202	CDL	C17-C18-C19-C20
30	m	201	CDL	C59-C60-C61-C62
30	a	201	CDL	C33-C34-C35-C36
30	m	201	CDL	C34-C35-C36-C37
30	r	503	CDL	C57-C58-C59-C60
33	g	201	PLX	C14-C15-C16-C17
30	s	402	CDL	C71-CB7-OB8-CB6
30	r	503	CDL	C62-C63-C64-C65
31	i	402	PEE	C21-C22-C23-C24
31	l	701	PEE	C11-C12-C13-C14
33	j	203	PLX	C14-C15-C16-C17
30	a	201	CDL	C73-C74-C75-C76
30	r	503	CDL	C14-C15-C16-C17
31	b	201	PEE	C22-C23-C24-C25
32	X	201	8Q1	C11-C12-C13-C14
30	V	202	CDL	OB9-CB7-OB8-CB6
30	a	201	CDL	OB9-CB7-OB8-CB6
30	l	703	CDL	C55-C56-C57-C58
30	s	402	CDL	C17-C18-C19-C20
30	l	703	CDL	C14-C15-C16-C17
33	n	101	PLX	C25-C26-C27-C28
30	V	202	CDL	C14-C15-C16-C17
30	V	202	CDL	C42-C43-C44-C45
30	l	703	CDL	C74-C75-C76-C77
31	s	401	PEE	C13-C14-C15-C16
33	g	201	PLX	C30-C31-C32-C33
33	j	202	PLX	C32-C33-C34-C35
30	V	202	CDL	C82-C83-C84-C85
30	m	201	CDL	C75-C76-C77-C78
33	r	502	PLX	C10-C11-C12-C13
31	W	201	PEE	C15-C16-C17-C18
31	l	701	PEE	C35-C36-C37-C38
30	r	503	CDL	C71-CB7-OB8-CB6
31	r	501	PEE	C13-C14-C15-C16
33	g	201	PLX	C25-C26-C27-C28
33	n	101	PLX	C27-C28-C29-C30
33	j	203	PLX	C28-C29-C30-C31
30	V	202	CDL	CA7-C31-C32-C33
33	n	101	PLX	C14-C15-C16-C17
30	V	201	CDL	OA9-CA7-OA8-CA6
30	s	402	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
30	V	201	CDL	C11-C12-C13-C14
31	W	201	PEE	O4-C10-O2-C2
31	r	501	PEE	C40-C41-C42-C43
33	j	203	PLX	C9-C10-C11-C12
30	V	202	CDL	C52-C53-C54-C55
30	l	702	CDL	C32-C33-C34-C35
30	r	503	CDL	C43-C44-C45-C46
31	W	201	PEE	C12-C13-C14-C15
31	s	401	PEE	C23-C24-C25-C26
30	V	202	CDL	CB5-C51-C52-C53
30	a	201	CDL	C37-C38-C39-C40
30	m	201	CDL	C71-C72-C73-C74
33	j	202	PLX	C14-C15-C16-C17
33	j	202	PLX	C9-C10-C11-C12
30	r	503	CDL	C73-C74-C75-C76
30	s	402	CDL	C82-C83-C84-C85
33	j	203	PLX	C33-C34-C35-C36
30	r	503	CDL	C11-C12-C13-C14
33	j	202	PLX	C33-C34-C35-C36
33	j	203	PLX	C25-C26-C27-C28
30	r	503	CDL	C37-C38-C39-C40
33	g	201	PLX	C13-C14-C15-C16
30	l	703	CDL	C11-CA5-OA6-CA4
32	X	201	8Q1	N36-C37-C38-C39
31	W	201	PEE	C10-C11-C12-C13
30	l	702	CDL	C52-C53-C54-C55
33	j	202	PLX	C34-C35-C36-C37
30	r	503	CDL	C75-C76-C77-C78
31	r	501	PEE	C12-C13-C14-C15
33	j	202	PLX	C13-C14-C15-C16
33	j	203	PLX	C29-C30-C31-C32
30	s	402	CDL	C33-C34-C35-C36
33	r	502	PLX	C11-C10-C9-C8
30	V	202	CDL	C35-C36-C37-C38
30	r	503	CDL	C41-C42-C43-C44
30	s	402	CDL	CB5-C51-C52-C53
30	V	201	CDL	C72-C73-C74-C75
30	l	703	CDL	C51-C52-C53-C54
30	l	703	CDL	C59-C60-C61-C62
30	s	402	CDL	C52-C53-C54-C55
33	j	203	PLX	C12-C13-C14-C15
33	r	502	PLX	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
30	V	202	CDL	C74-C75-C76-C77
31	l	701	PEE	C10-C11-C12-C13
31	W	201	PEE	C24-C25-C26-C27
30	V	201	CDL	OB5-CB3-CB4-OB6
30	m	201	CDL	OA5-CA3-CA4-OA6
31	l	704	PEE	C43-C44-C45-C46
30	r	503	CDL	C31-C32-C33-C34
30	r	503	CDL	C71-C72-C73-C74
31	l	704	PEE	C31-C32-C33-C34
31	s	401	PEE	C19-C20-C21-C22
31	s	403	PEE	C39-C40-C41-C42
33	g	201	PLX	O6-C4-C5-O8
30	r	503	CDL	OB9-CB7-OB8-CB6
30	s	402	CDL	C59-C60-C61-C62
30	s	402	CDL	C55-C56-C57-C58
33	r	502	PLX	C11-C12-C13-C14
31	s	403	PEE	C36-C37-C38-C39
31	s	403	PEE	C12-C13-C14-C15
30	V	201	CDL	C14-C15-C16-C17
30	V	201	CDL	C71-C72-C73-C74
30	V	202	CDL	C13-C14-C15-C16
30	V	202	CDL	C73-C74-C75-C76
30	m	201	CDL	C14-C15-C16-C17
31	W	201	PEE	C13-C14-C15-C16
33	r	502	PLX	C14-C15-C16-C17
33	r	502	PLX	C27-C28-C29-C30
31	r	501	PEE	C20-C21-C22-C23
33	g	201	PLX	C28-C29-C30-C31
30	l	702	CDL	CB2-C1-CA2-OA2
30	a	201	CDL	C21-C22-C23-C24
33	j	202	PLX	C11-C12-C13-C14
30	V	201	CDL	C55-C56-C57-C58
30	r	503	CDL	C77-C78-C79-C80
30	a	201	CDL	C71-C72-C73-C74
30	n	102	CDL	C11-CA5-OA6-CA4
30	V	202	CDL	C75-C76-C77-C78
30	l	703	CDL	C31-C32-C33-C34
30	m	201	CDL	C18-C19-C20-C21
31	s	403	PEE	C31-C32-C33-C34
31	l	704	PEE	C34-C35-C36-C37
30	V	202	CDL	C34-C35-C36-C37
30	s	402	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
31	l	701	PEE	C32-C33-C34-C35
31	r	501	PEE	C36-C37-C38-C39
31	r	501	PEE	C39-C40-C41-C42
30	a	201	CDL	OB5-CB3-CB4-CB6
31	i	402	PEE	O3P-C1-C2-C3
31	l	704	PEE	O3P-C1-C2-C3
33	j	202	PLX	C11-C10-C9-C8
30	m	201	CDL	C41-C42-C43-C44
30	n	102	CDL	CB5-C51-C52-C53
30	a	201	CDL	C15-C16-C17-C18
30	l	703	CDL	C32-C33-C34-C35
33	g	201	PLX	C12-C13-C14-C15
30	a	201	CDL	C31-C32-C33-C34
30	l	703	CDL	C37-C38-C39-C40
30	l	703	CDL	C73-C74-C75-C76
30	l	703	CDL	C79-C80-C81-C82
31	j	201	PEE	C23-C24-C25-C26
31	s	401	PEE	C11-C12-C13-C14
30	V	202	CDL	C84-C85-C86-C87
31	j	201	PEE	C38-C39-C40-C41
31	s	403	PEE	C22-C23-C24-C25
30	l	703	CDL	OA7-CA5-OA6-CA4
30	a	201	CDL	C52-C53-C54-C55
31	r	501	PEE	C41-C42-C43-C44
33	r	502	PLX	C29-C30-C31-C32
30	m	201	CDL	CA3-CA4-CA6-OA8
30	n	102	CDL	CA3-CA4-CA6-OA8
31	W	201	PEE	C1-C2-C3-O3
33	j	202	PLX	C3-C4-C5-O8
33	j	203	PLX	C3-C4-C5-O8
33	n	101	PLX	C3-C4-C5-O8
33	r	502	PLX	C3-C4-C5-O8
31	j	201	PEE	C34-C35-C36-C37
31	i	402	PEE	C19-C20-C21-C22
31	l	704	PEE	C15-C16-C17-C18
31	s	403	PEE	C35-C36-C37-C38
30	s	402	CDL	C35-C36-C37-C38
31	b	201	PEE	C13-C14-C15-C16
32	X	201	8Q1	C6-C7-C8-C9
30	V	202	CDL	C60-C61-C62-C63
30	V	202	CDL	C62-C63-C64-C65
30	r	503	CDL	C83-C84-C85-C86

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Mol	Chain	Res	Type	Atoms
33	j	202	PLX	C27-C28-C29-C30
33	n	101	PLX	C9-C10-C11-C12
30	m	201	CDL	C16-C17-C18-C19
30	m	201	CDL	C71-CB7-OB8-CB6
30	m	201	CDL	CA6-CA4-OA6-CA5
31	i	402	PEE	C20-C21-C22-C23
33	j	203	PLX	C27-C28-C29-C30
30	s	402	CDL	C51-C52-C53-C54
30	V	201	CDL	C54-C55-C56-C57
31	W	201	PEE	O3P-C1-C2-O2
30	n	102	CDL	C52-C53-C54-C55
30	V	202	CDL	C40-C41-C42-C43
30	m	201	CDL	C19-C20-C21-C22
30	m	201	CDL	C20-C21-C22-C23
30	r	503	CDL	C59-C60-C61-C62
31	s	401	PEE	C12-C13-C14-C15
33	n	101	PLX	C28-C29-C30-C31
30	V	202	CDL	OA6-CA4-CA6-OA8
30	i	401	CDL	OB6-CB4-CB6-OB8
30	m	201	CDL	OB6-CB4-CB6-OB8
33	n	101	PLX	O6-C4-C5-O8
33	j	203	PLX	C11-C12-C13-C14
30	m	201	CDL	C33-C34-C35-C36
33	j	202	PLX	C25-C26-C27-C28
30	l	703	CDL	C75-C76-C77-C78
33	g	201	PLX	C10-C11-C12-C13
33	g	201	PLX	C11-C10-C9-C8
33	r	502	PLX	C31-C32-C33-C34
30	a	201	CDL	C11-C12-C13-C14
30	l	703	CDL	CB7-C71-C72-C73
31	r	501	PEE	C21-C22-C23-C24
30	a	201	CDL	C32-C33-C34-C35
33	r	502	PLX	C28-C29-C30-C31
33	j	202	PLX	C12-C13-C14-C15
30	s	402	CDL	C40-C41-C42-C43
31	l	704	PEE	C24-C25-C26-C27
30	V	202	CDL	C64-C65-C66-C67
31	r	501	PEE	C17-C18-C19-C20
30	r	503	CDL	C64-C65-C66-C67
30	r	503	CDL	C56-C57-C58-C59
33	g	201	PLX	O9-C24-C25-C26
30	l	703	CDL	C82-C83-C84-C85

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Mol	Chain	Res	Type	Atoms
33	r	502	PLX	C18-C19-C20-C21
30	r	503	CDL	C33-C34-C35-C36
33	n	101	PLX	C26-C27-C28-C29
30	V	201	CDL	C1-CB2-OB2-PB2
30	m	201	CDL	CA4-CA3-OA5-PA1
30	r	503	CDL	C1-CB2-OB2-PB2
30	V	202	CDL	C41-C42-C43-C44
33	g	201	PLX	C33-C34-C35-C36
33	n	101	PLX	C16-C17-C18-C19
31	s	403	PEE	C23-C24-C25-C26
30	V	201	CDL	OB5-CB3-CB4-CB6
30	l	703	CDL	OB5-CB3-CB4-CB6
30	m	201	CDL	OA5-CA3-CA4-CA6
31	r	501	PEE	C31-C32-C33-C34
31	j	201	PEE	C32-C33-C34-C35
31	i	402	PEE	C18-C19-C20-C21
31	s	403	PEE	C34-C35-C36-C37
31	j	201	PEE	C30-C31-C32-C33
30	r	503	CDL	C54-C55-C56-C57
30	a	201	CDL	C38-C39-C40-C41
30	m	201	CDL	OB9-CB7-OB8-CB6
31	l	704	PEE	C11-C12-C13-C14
30	r	503	CDL	C84-C85-C86-C87
30	r	503	CDL	C42-C43-C44-C45
30	s	402	CDL	C34-C35-C36-C37
30	s	402	CDL	C54-C55-C56-C57
31	l	704	PEE	C30-C31-C32-C33
31	s	403	PEE	C44-C45-C46-C47
30	m	201	CDL	CB3-CB4-CB6-OB8
31	b	201	PEE	C1-C2-C3-O3
31	i	402	PEE	C1-C2-C3-O3
31	l	704	PEE	C1-C2-C3-O3
31	r	501	PEE	C1-C2-C3-O3
33	g	201	PLX	C3-C4-C5-O8
32	X	201	8Q1	C10-C11-C12-C13
30	m	201	CDL	C64-C65-C66-C67
30	a	201	CDL	C35-C36-C37-C38
30	m	201	CDL	C17-C18-C19-C20
33	n	101	PLX	C29-C30-C31-C32
33	n	101	PLX	C30-C31-C32-C33
30	V	201	CDL	OA5-CA3-CA4-OA6
30	a	201	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
30	n	102	CDL	OB5-CB3-CB4-OB6
31	b	201	PEE	O3P-C1-C2-O2
30	m	201	CDL	C52-C53-C54-C55
31	l	704	PEE	C32-C33-C34-C35
31	r	501	PEE	C14-C15-C16-C17
30	V	201	CDL	C75-C76-C77-C78
30	i	401	CDL	C71-C72-C73-C74
30	m	201	CDL	C82-C83-C84-C85
30	s	402	CDL	C12-C13-C14-C15
31	s	401	PEE	C22-C23-C24-C25
30	r	503	CDL	CA7-C31-C32-C33
31	b	201	PEE	O2-C2-C3-O3
31	i	402	PEE	O2-C2-C3-O3
31	r	501	PEE	O2-C2-C3-O3
33	r	502	PLX	O6-C4-C5-O8
30	a	201	CDL	C36-C37-C38-C39
31	s	403	PEE	C38-C39-C40-C41
33	j	203	PLX	O6-C6-C7-C8
30	l	703	CDL	C12-C13-C14-C15
30	i	401	CDL	C71-CB7-OB8-CB6
30	l	703	CDL	C51-CB5-OB6-CB4
30	l	703	CDL	C61-C62-C63-C64
31	s	403	PEE	C13-C14-C15-C16
31	s	403	PEE	C21-C22-C23-C24
33	j	202	PLX	C26-C27-C28-C29
30	l	703	CDL	C64-C65-C66-C67
33	r	502	PLX	C36-C37-C38-C39
31	j	201	PEE	C36-C37-C38-C39
31	r	501	PEE	C38-C39-C40-C41
30	V	202	CDL	C31-C32-C33-C34
31	l	701	PEE	C18-C19-C20-C21
31	i	402	PEE	C24-C25-C26-C27
30	s	402	CDL	C84-C85-C86-C87
31	l	704	PEE	C42-C43-C44-C45
32	X	201	8Q1	C12-C13-C14-C15
33	n	101	PLX	C15-C16-C17-C18
30	V	202	CDL	CB2-C1-CA2-OA2
30	V	202	CDL	CA2-C1-CB2-OB2
30	l	702	CDL	C51-C52-C53-C54
30	l	703	CDL	C62-C63-C64-C65
30	V	202	CDL	C15-C16-C17-C18
33	j	202	PLX	O4-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
33	n	101	PLX	C12-C13-C14-C15
30	m	201	CDL	C84-C85-C86-C87
30	V	202	CDL	C55-C56-C57-C58
31	s	401	PEE	C24-C25-C26-C27
30	m	201	CDL	C31-C32-C33-C34
32	X	201	8Q1	C28-O27-P24-O1
30	n	102	CDL	OA7-CA5-OA6-CA4
30	r	503	CDL	C51-C52-C53-C54
30	n	102	CDL	CA6-CA4-OA6-CA5
31	s	403	PEE	C20-C21-C22-C23
31	W	201	PEE	C11-C12-C13-C14
30	i	401	CDL	OB9-CB7-OB8-CB6
30	V	202	CDL	O1-C1-CB2-OB2
30	V	202	CDL	OB5-CB3-CB4-OB6
30	l	703	CDL	OB5-CB3-CB4-OB6
30	m	201	CDL	OB5-CB3-CB4-OB6
31	i	402	PEE	O3P-C1-C2-O2
31	j	201	PEE	O3P-C1-C2-O2
31	l	701	PEE	O3P-C1-C2-O2
31	r	501	PEE	O3P-C1-C2-O2
33	j	202	PLX	O4-C3-C4-O6
33	j	202	PLX	C10-C11-C12-C13
31	b	201	PEE	C10-C11-C12-C13
30	a	201	CDL	C54-C55-C56-C57
31	i	402	PEE	C31-C32-C33-C34
31	W	201	PEE	C5-C4-O4P-P
30	V	201	CDL	CA7-C31-C32-C33
31	s	403	PEE	C37-C38-C39-C40
30	r	503	CDL	C39-C40-C41-C42
30	m	201	CDL	OA6-CA4-CA6-OA8
30	n	102	CDL	OA6-CA4-CA6-OA8
31	l	704	PEE	O2-C2-C3-O3
30	V	202	CDL	C12-C13-C14-C15
33	g	201	PLX	C31-C32-C33-C34
30	r	503	CDL	C82-C83-C84-C85
33	r	502	PLX	C26-C27-C28-C29
30	m	201	CDL	C15-C16-C17-C18
33	n	101	PLX	C11-C12-C13-C14
30	l	703	CDL	C21-C22-C23-C24
30	l	703	CDL	C15-C16-C17-C18
31	W	201	PEE	C20-C21-C22-C23
33	j	202	PLX	N1-C1-C2-O1

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Mol	Chain	Res	Type	Atoms
30	a	201	CDL	C84-C85-C86-C87
30	V	202	CDL	O1-C1-CA2-OA2
30	a	201	CDL	C22-C23-C24-C25
33	j	202	PLX	C35-C36-C37-C38
33	g	201	PLX	O7-C6-C7-C8
30	i	401	CDL	C15-C16-C17-C18
33	g	201	PLX	C25-C24-O8-C5
33	j	203	PLX	C25-C24-O8-C5
33	r	502	PLX	C7-C8-C9-C10
31	b	201	PEE	C15-C16-C17-C18
30	n	102	CDL	OB5-CB3-CB4-CB6
31	b	201	PEE	O3P-C1-C2-C3
31	j	201	PEE	O3P-C1-C2-C3
31	l	701	PEE	O3P-C1-C2-C3
30	l	703	CDL	OB7-CB5-OB6-CB4
30	i	401	CDL	O1-C1-CB2-OB2
30	l	702	CDL	CA4-CA3-OA5-PA1
30	n	102	CDL	C1-CB2-OB2-PB2
33	g	201	PLX	O6-C6-C7-C8
30	a	201	CDL	OA5-CA3-CA4-OA6
33	n	101	PLX	O4-C3-C4-O6
31	j	201	PEE	C19-C20-C21-C22
30	r	503	CDL	C52-C53-C54-C55
30	l	702	CDL	C75-C76-C77-C78
31	W	201	PEE	O2-C2-C3-O3
33	j	202	PLX	O6-C4-C5-O8
33	j	203	PLX	O6-C4-C5-O8
30	V	202	CDL	CA3-CA4-CA6-OA8
30	i	401	CDL	CB3-CB4-CB6-OB8
30	s	402	CDL	CB3-CB4-CB6-OB8
31	s	401	PEE	C31-C32-C33-C34
30	i	401	CDL	C35-C36-C37-C38
30	l	702	CDL	C55-C56-C57-C58
31	i	402	PEE	C11-C12-C13-C14
30	V	202	CDL	C58-C59-C60-C61
30	l	702	CDL	C82-C83-C84-C85
30	V	201	CDL	CA3-OA5-PA1-OA3
30	V	201	CDL	CB2-OB2-PB2-OB4
30	V	202	CDL	CB2-OB2-PB2-OB4
30	V	202	CDL	CB2-OB2-PB2-OB5
30	V	202	CDL	CB3-OB5-PB2-OB2
30	V	202	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
30	V	202	CDL	CB3-OB5-PB2-OB4
30	a	201	CDL	CA2-OA2-PA1-OA5
30	a	201	CDL	CB2-OB2-PB2-OB4
30	i	401	CDL	CA2-OA2-PA1-OA5
30	i	401	CDL	CB3-OB5-PB2-OB3
30	l	702	CDL	CA3-OA5-PA1-OA2
30	l	702	CDL	CA3-OA5-PA1-OA4
30	l	702	CDL	CB2-OB2-PB2-OB3
30	l	703	CDL	CB2-OB2-PB2-OB3
30	m	201	CDL	CA3-OA5-PA1-OA4
30	n	102	CDL	CB3-OB5-PB2-OB3
30	r	503	CDL	CA2-OA2-PA1-OA4
30	r	503	CDL	CA3-OA5-PA1-OA2
30	r	503	CDL	CB3-OB5-PB2-OB4
30	s	402	CDL	CA3-OA5-PA1-OA2
30	s	402	CDL	CA3-OA5-PA1-OA3
30	s	402	CDL	CA3-OA5-PA1-OA4
31	W	201	PEE	C4-O4P-P-O2P
31	b	201	PEE	C1-O3P-P-O2P
31	b	201	PEE	C1-O3P-P-O1P
31	b	201	PEE	C1-O3P-P-O4P
31	i	402	PEE	C4-O4P-P-O2P
31	j	201	PEE	C1-O3P-P-O2P
31	r	501	PEE	C1-O3P-P-O2P
31	s	401	PEE	C1-O3P-P-O2P
33	j	202	PLX	C3-C4-O6-C6
33	j	202	PLX	C5-C4-O6-C6
33	j	202	PLX	C3-O4-P1-O1
33	j	202	PLX	C3-O4-P1-O2
33	j	202	PLX	C3-O4-P1-O3
33	j	202	PLX	C2-O1-P1-O3
33	j	203	PLX	C2-O1-P1-O4
33	j	203	PLX	C2-O1-P1-O3
33	n	101	PLX	C3-O4-P1-O1
33	n	101	PLX	C3-O4-P1-O2
33	n	101	PLX	C2-O1-P1-O3
34	w	401	ADP	C5'-O5'-PA-O1A
34	w	401	ADP	C5'-O5'-PA-O3A
30	V	201	CDL	C34-C35-C36-C37
30	a	201	CDL	C74-C75-C76-C77
33	r	502	PLX	C16-C17-C18-C19
30	l	703	CDL	C81-C82-C83-C84

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Mol	Chain	Res	Type	Atoms
30	V	202	CDL	C32-C31-CA7-OA8
30	l	703	CDL	C44-C45-C46-C47
30	l	702	CDL	C76-C77-C78-C79
30	l	703	CDL	C71-C72-C73-C74
30	l	703	CDL	C12-C11-CA5-OA6
30	V	202	CDL	C71-C72-C73-C74
32	X	201	8Q1	C9-C10-C11-C12
30	r	503	CDL	C13-C14-C15-C16
30	V	201	CDL	CA6-CA4-OA6-CA5
30	i	401	CDL	CA6-CA4-OA6-CA5
30	l	702	CDL	CA6-CA4-OA6-CA5
31	l	704	PEE	C1-C2-O2-C10
30	V	201	CDL	OA5-CA3-CA4-CA6
30	V	202	CDL	OB5-CB3-CB4-CB6
31	W	201	PEE	O3P-C1-C2-C3
31	r	501	PEE	O3P-C1-C2-C3
33	n	101	PLX	O4-C3-C4-C5
33	r	502	PLX	O4-C3-C4-C5
30	l	702	CDL	C20-C21-C22-C23
31	j	201	PEE	C16-C17-C18-C19
33	r	502	PLX	O4-C3-C4-O6
30	i	401	CDL	CA5-C11-C12-C13
30	i	401	CDL	C38-C39-C40-C41
30	V	201	CDL	OB6-CB4-CB6-OB8
30	l	702	CDL	C36-C37-C38-C39
31	j	201	PEE	C41-C42-C43-C44
33	j	203	PLX	C32-C33-C34-C35
31	i	402	PEE	C39-C40-C41-C42
31	s	401	PEE	C15-C16-C17-C18
31	r	501	PEE	C11-C12-C13-C14
33	g	201	PLX	C15-C16-C17-C18
32	X	201	8Q1	C11-C10-C9-C8
30	s	402	CDL	C72-C71-CB7-OB8
30	V	201	CDL	C40-C41-C42-C43
33	r	502	PLX	C33-C34-C35-C36
33	r	502	PLX	O9-C24-C25-C26
32	X	201	8Q1	C13-C14-C15-C16
31	i	402	PEE	C15-C16-C17-C18
30	V	202	CDL	C57-C58-C59-C60
30	a	201	CDL	OA5-CA3-CA4-CA6
30	l	702	CDL	C11-C12-C13-C14
30	a	201	CDL	C64-C65-C66-C67

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Mol	Chain	Res	Type	Atoms
30	i	401	CDL	O1-C1-CA2-OA2
30	a	201	CDL	C12-C13-C14-C15
31	b	201	PEE	C18-C19-C20-C21
31	b	201	PEE	C16-C17-C18-C19
30	m	201	CDL	C42-C43-C44-C45
33	j	203	PLX	C18-C19-C20-C21
31	W	201	PEE	C34-C35-C36-C37
30	V	201	CDL	C64-C65-C66-C67
30	V	201	CDL	C21-C22-C23-C24
30	V	202	CDL	C54-C55-C56-C57
31	l	704	PEE	C13-C14-C15-C16
30	V	201	CDL	CB2-C1-CA2-OA2
32	X	201	8Q1	C7-C8-C9-C10
30	m	201	CDL	CA5-C11-C12-C13
30	a	201	CDL	C14-C15-C16-C17
30	l	702	CDL	C13-C14-C15-C16
31	s	401	PEE	C14-C15-C16-C17
30	a	201	CDL	C55-C56-C57-C58
33	r	502	PLX	C34-C35-C36-C37
31	s	403	PEE	C24-C25-C26-C27
33	j	203	PLX	C30-C31-C32-C33
30	a	201	CDL	C43-C44-C45-C46
31	s	401	PEE	C18-C19-C20-C21
30	V	201	CDL	CA4-CA3-OA5-PA1
30	a	201	CDL	C13-C14-C15-C16
30	n	102	CDL	C57-C58-C59-C60
30	m	201	CDL	C77-C78-C79-C80
31	b	201	PEE	C23-C24-C25-C26
31	b	201	PEE	C38-C39-C40-C41
31	s	401	PEE	O2-C2-C3-O3
31	i	402	PEE	C33-C34-C35-C36
30	r	503	CDL	C15-C16-C17-C18
31	j	201	PEE	C12-C13-C14-C15
30	a	201	CDL	C16-C17-C18-C19
30	l	702	CDL	C62-C63-C64-C65
30	l	702	CDL	OB7-CB5-OB6-CB4
33	j	202	PLX	O8-C24-C25-C26
30	l	702	CDL	C51-CB5-OB6-CB4
31	b	201	PEE	C11-C12-C13-C14
30	V	202	CDL	C44-C45-C46-C47
31	l	701	PEE	C14-C15-C16-C17
31	l	701	PEE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
31	s	403	PEE	C31-C30-O3-C3
31	s	403	PEE	O5-C30-O3-C3
30	m	201	CDL	C74-C75-C76-C77
30	r	503	CDL	C20-C21-C22-C23
30	a	201	CDL	C44-C45-C46-C47
33	r	502	PLX	O7-C6-C7-C8
30	V	201	CDL	C60-C61-C62-C63
31	W	201	PEE	C16-C17-C18-C19
30	n	102	CDL	C71-C72-C73-C74
30	l	703	CDL	CA2-C1-CB2-OB2
31	l	704	PEE	C19-C20-C21-C22
30	m	201	CDL	OB5-CB3-CB4-CB6
30	l	703	CDL	CB5-C51-C52-C53
30	l	703	CDL	C41-C42-C43-C44
31	i	402	PEE	C34-C35-C36-C37
30	a	201	CDL	C53-C54-C55-C56
30	s	402	CDL	C74-C75-C76-C77
30	n	102	CDL	C74-C75-C76-C77
31	r	501	PEE	C16-C17-C18-C19
31	s	401	PEE	C16-C17-C18-C19
30	l	702	CDL	CA3-CA4-OA6-CA5
31	l	704	PEE	C3-C2-O2-C10
31	s	403	PEE	C16-C17-C18-C19
31	l	701	PEE	C2-C1-O3P-P
30	r	503	CDL	C72-C71-CB7-OB8
30	l	703	CDL	C39-C40-C41-C42
31	s	403	PEE	C10-C11-C12-C13
31	i	402	PEE	C36-C37-C38-C39
31	l	701	PEE	O3-C30-C31-C32
30	a	201	CDL	C51-C52-C53-C54
33	j	203	PLX	C24-C25-C26-C27
30	i	401	CDL	C12-C11-CA5-OA6
31	j	201	PEE	O2-C10-C11-C12
30	i	401	CDL	OA6-CA4-CA6-OA8
31	s	403	PEE	C18-C19-C20-C21
30	s	402	CDL	C19-C20-C21-C22
30	l	703	CDL	C72-C71-CB7-OB8
30	s	402	CDL	C12-C11-CA5-OA6
33	j	203	PLX	C7-C6-O6-C4
30	s	402	CDL	C15-C16-C17-C18
33	j	202	PLX	C29-C30-C31-C32
30	l	702	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
30	s	402	CDL	C16-C17-C18-C19
31	l	701	PEE	C38-C39-C40-C41
31	l	704	PEE	C18-C19-C20-C21
34	w	401	ADP	PB-O3A-PA-O2A
30	V	202	CDL	C63-C64-C65-C66
31	j	201	PEE	C24-C25-C26-C27
30	l	703	CDL	C56-C57-C58-C59
30	l	702	CDL	C38-C39-C40-C41
30	a	201	CDL	C32-C31-CA7-OA8
30	i	401	CDL	C32-C33-C34-C35
30	a	201	CDL	C39-C40-C41-C42
31	s	401	PEE	O3-C30-C31-C32
30	r	503	CDL	C21-C22-C23-C24
33	r	502	PLX	C9-C10-C11-C12
30	V	201	CDL	O1-C1-CA2-OA2
30	i	401	CDL	CA3-CA4-CA6-OA8
30	a	201	CDL	C76-C77-C78-C79
30	a	201	CDL	C12-C11-CA5-OA6
30	l	702	CDL	C72-C71-CB7-OB8
30	m	201	CDL	C12-C11-CA5-OA6
31	b	201	PEE	O3-C30-C31-C32
30	a	201	CDL	C82-C83-C84-C85
30	r	503	CDL	OA6-CA4-CA6-OA8
31	j	201	PEE	C44-C45-C46-C47
30	l	703	CDL	C43-C44-C45-C46
30	V	202	CDL	C22-C23-C24-C25
31	s	403	PEE	C41-C42-C43-C44
30	s	402	CDL	C12-C11-CA5-OA7
30	l	703	CDL	OA5-CA3-CA4-OA6
30	r	503	CDL	C12-C13-C14-C15
30	a	201	CDL	C12-C11-CA5-OA7
30	a	201	CDL	C32-C31-CA7-OA9
31	s	401	PEE	O5-C30-C31-C32
30	i	401	CDL	C12-C11-CA5-OA7
33	j	202	PLX	C36-C37-C38-C39
30	l	702	CDL	C72-C71-CB7-OB9
30	a	201	CDL	C18-C19-C20-C21
31	j	201	PEE	O4-C10-C11-C12
31	l	701	PEE	O5-C30-C31-C32
33	n	101	PLX	C4-C5-O8-C24
33	g	201	PLX	C18-C19-C20-C21
30	l	703	CDL	C72-C71-CB7-OB9

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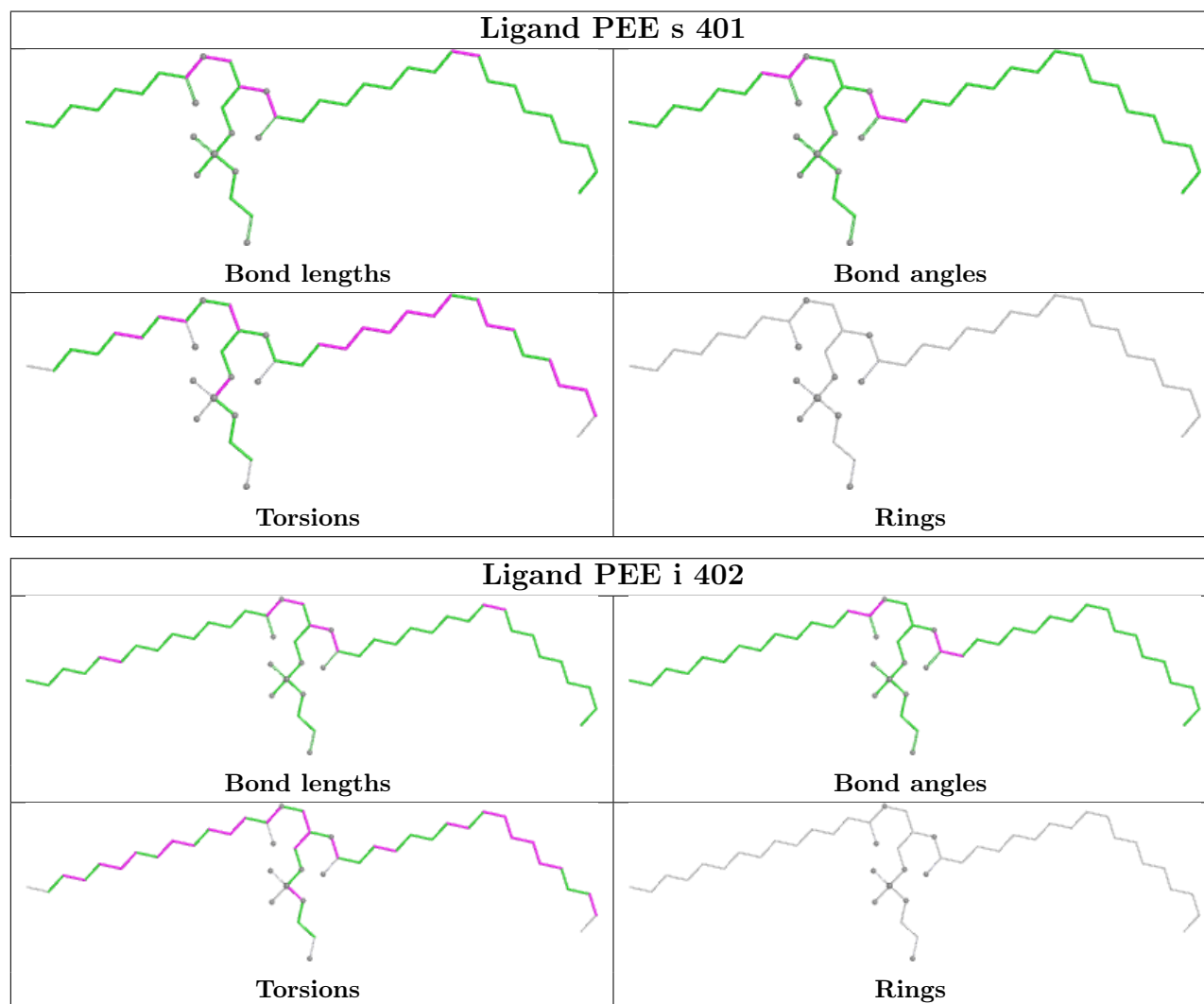
Mol	Chain	Res	Type	Atoms
30	m	201	CDL	C12-C11-CA5-OA7
31	b	201	PEE	C34-C35-C36-C37
30	m	201	CDL	C35-C36-C37-C38
30	V	202	CDL	C24-C25-C26-C27
30	V	201	CDL	CB3-CB4-CB6-OB8
31	l	704	PEE	C22-C23-C24-C25
31	b	201	PEE	O5-C30-C31-C32
31	j	201	PEE	O3-C30-C31-C32
33	g	201	PLX	C6-C7-C8-C9
33	j	202	PLX	C6-C7-C8-C9
30	l	703	CDL	C36-C37-C38-C39
31	r	501	PEE	C44-C45-C46-C47
31	j	201	PEE	C40-C41-C42-C43

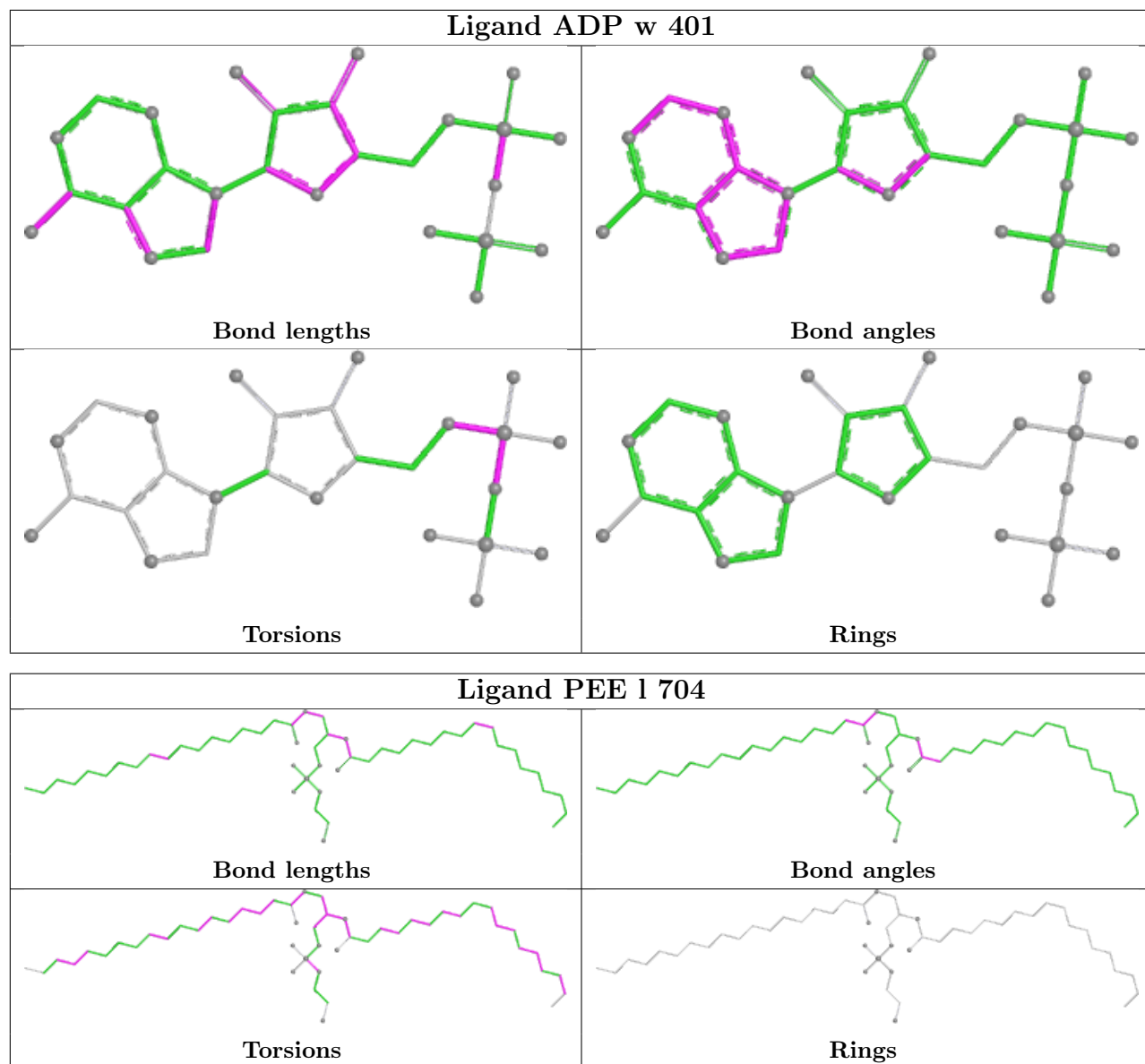
There are no ring outliers.

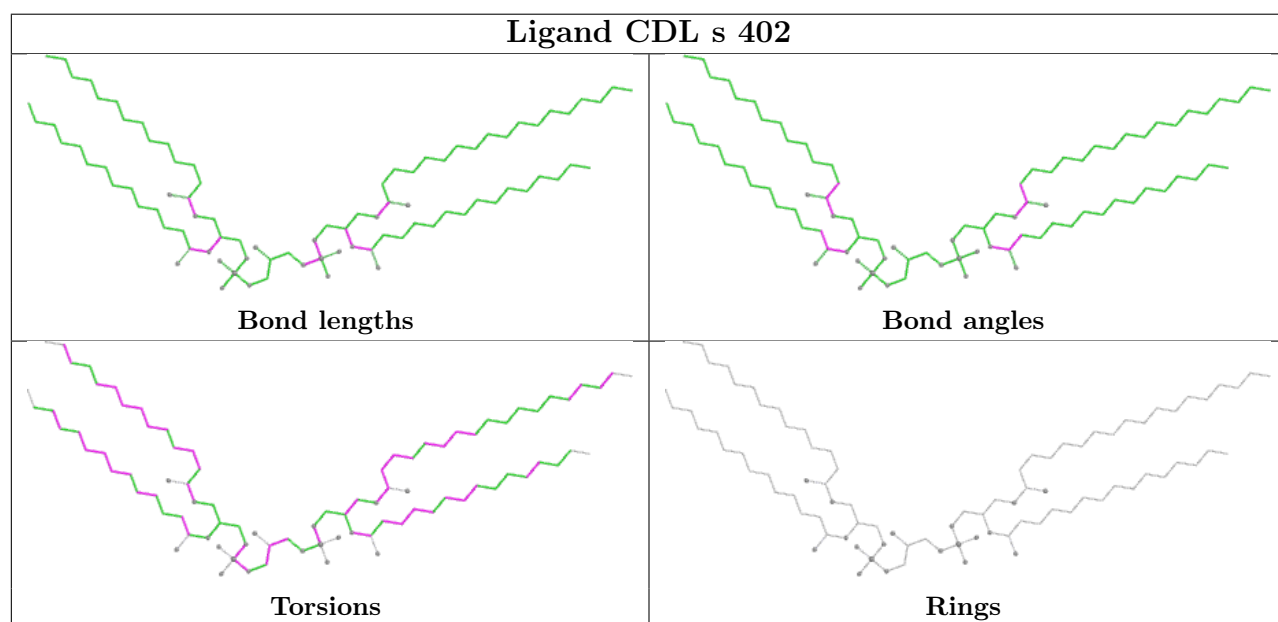
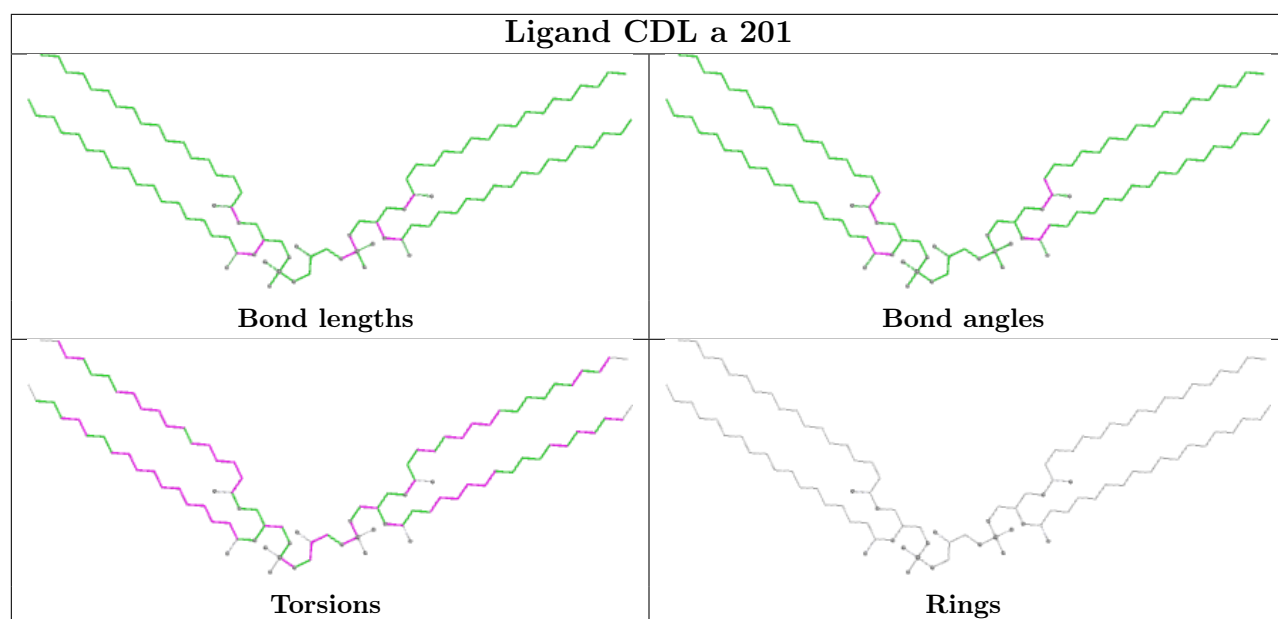
24 monomers are involved in 149 short contacts:

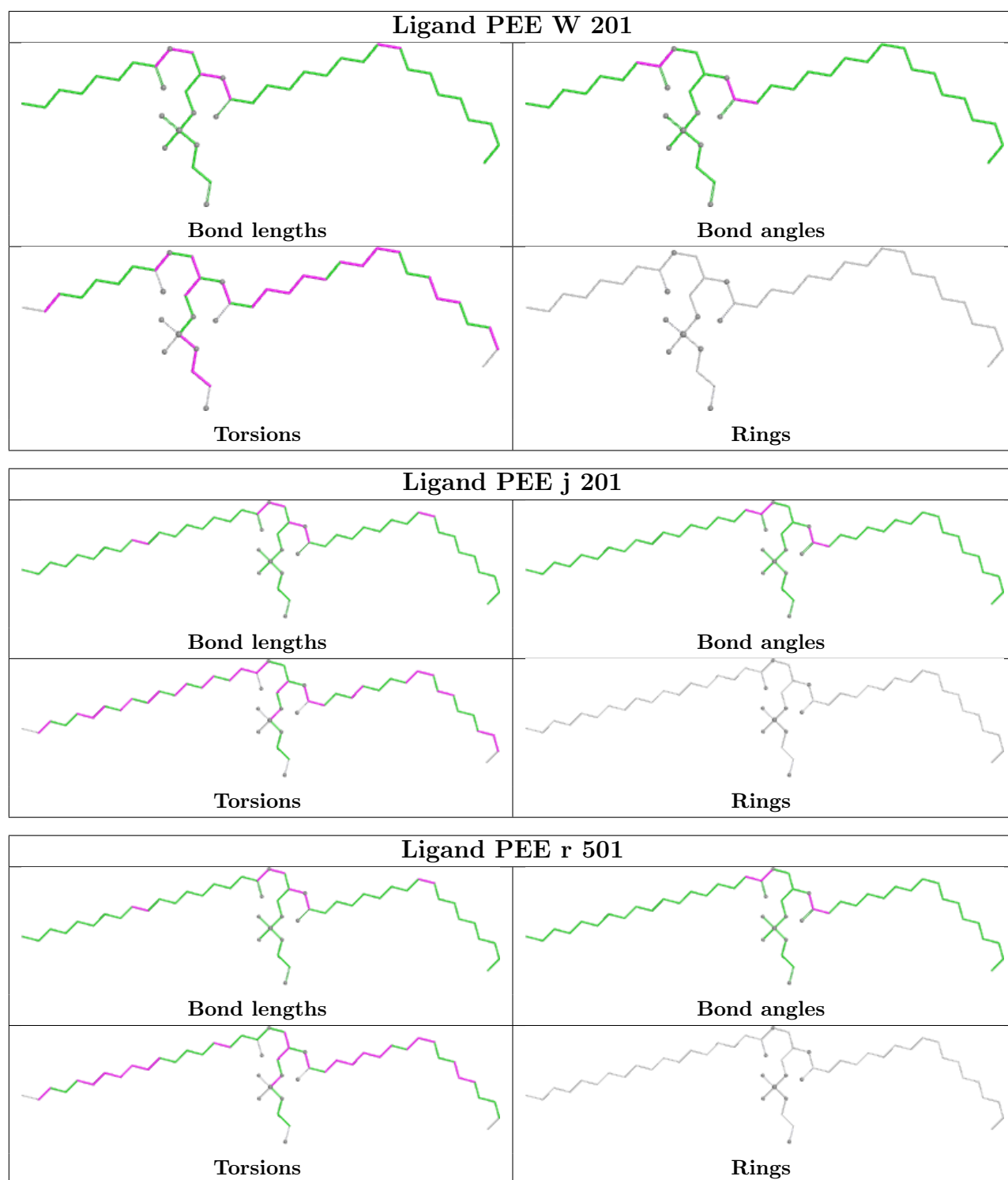
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	s	401	PEE	16	0
31	i	402	PEE	2	0
34	w	401	ADP	1	0
31	l	704	PEE	2	0
30	a	201	CDL	1	0
30	s	402	CDL	15	0
31	W	201	PEE	2	0
31	j	201	PEE	5	0
31	r	501	PEE	2	0
31	b	201	PEE	1	0
30	i	401	CDL	23	0
30	l	703	CDL	5	0
30	l	702	CDL	33	0
33	j	203	PLX	2	0
33	r	502	PLX	3	0
31	s	403	PEE	3	0
32	X	201	8Q1	1	0
30	m	201	CDL	11	0
30	r	503	CDL	7	0
30	n	102	CDL	6	0
30	V	201	CDL	4	0
31	l	701	PEE	1	0
33	g	201	PLX	4	0
30	V	202	CDL	6	0

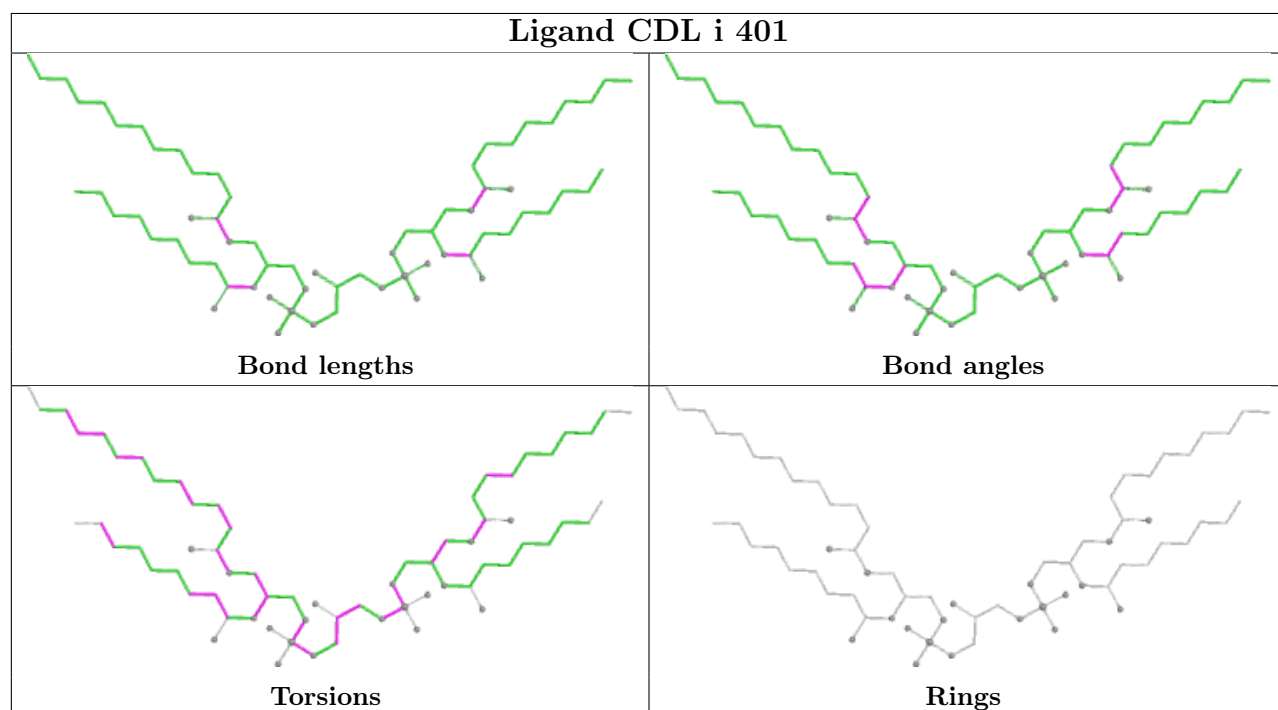
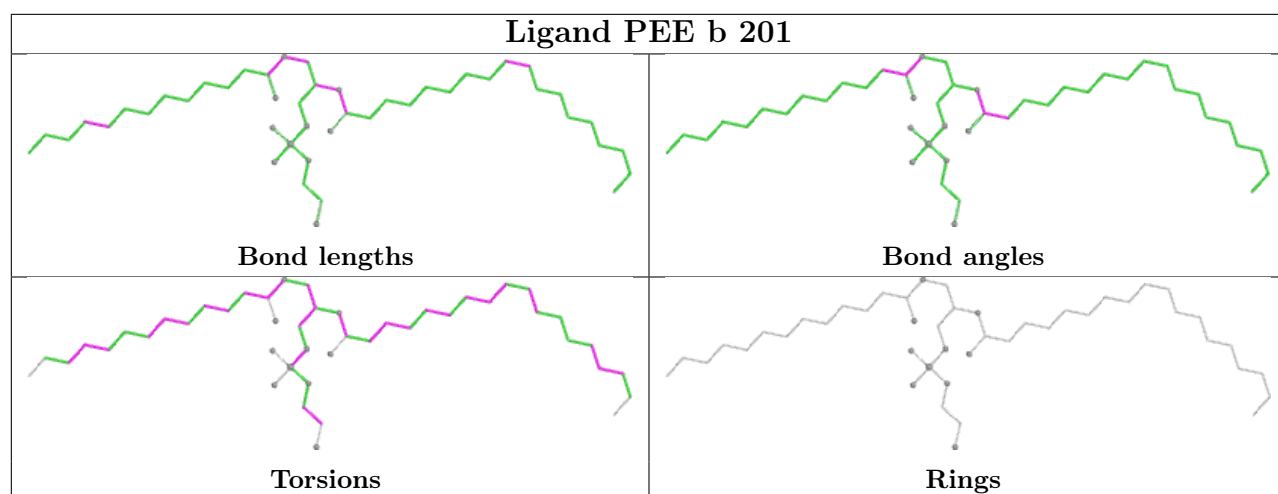
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

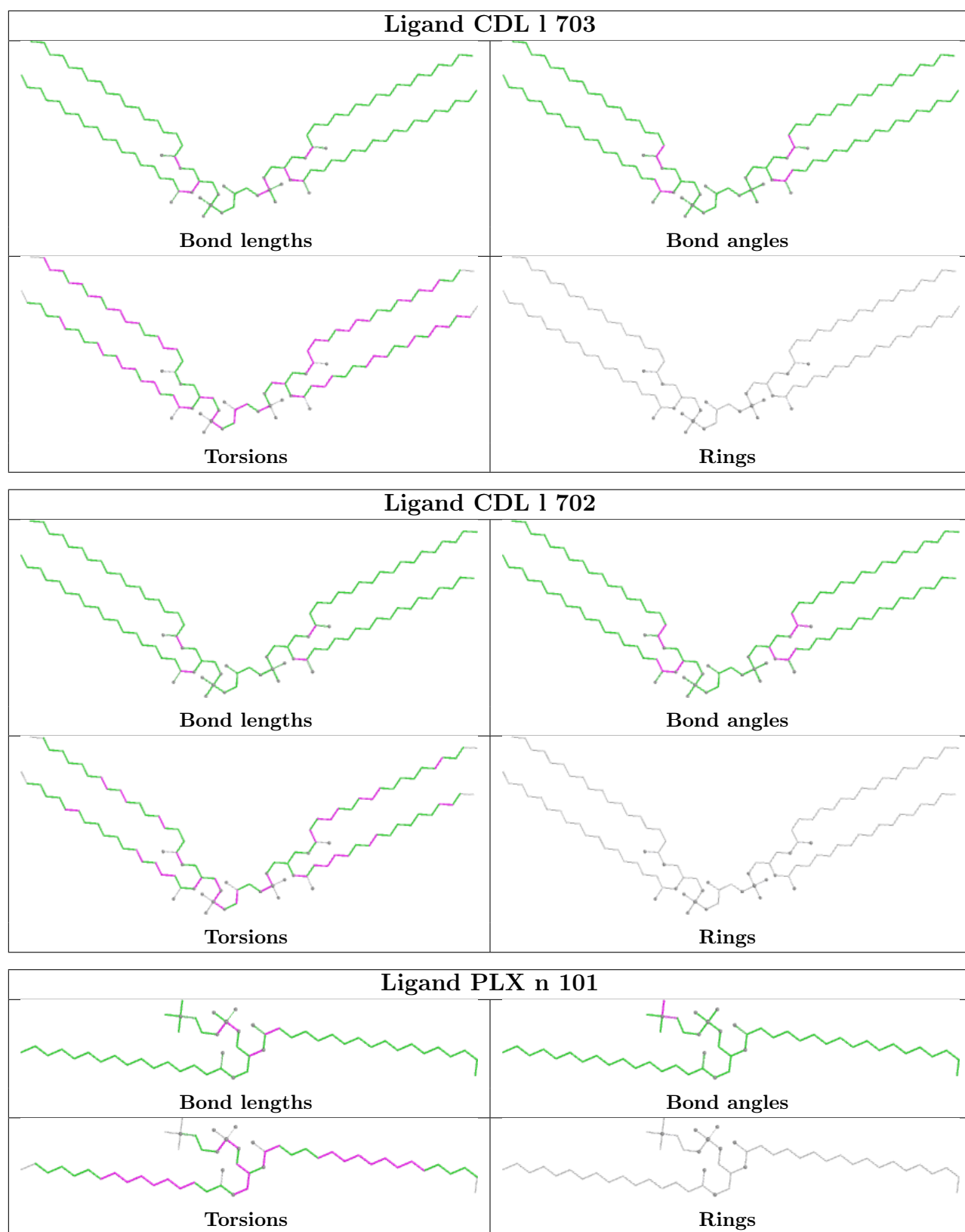


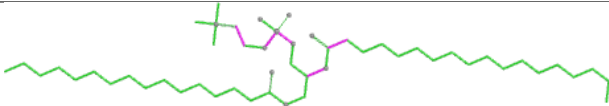
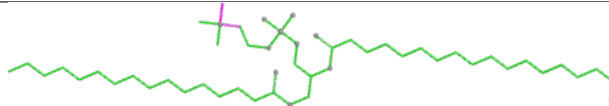
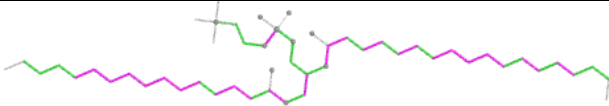
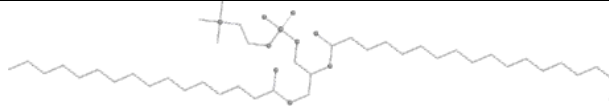


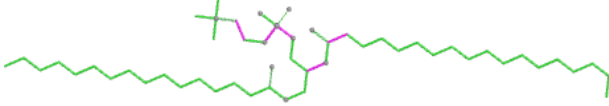
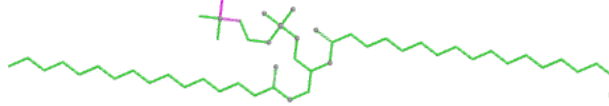
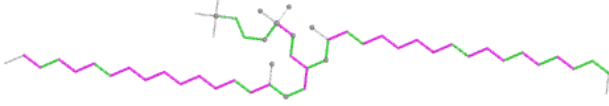
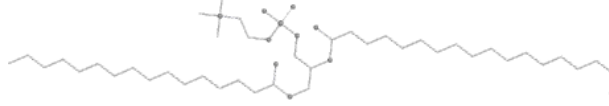


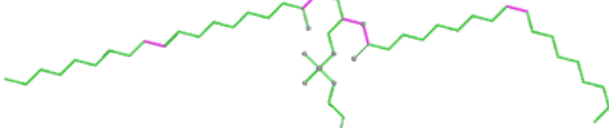
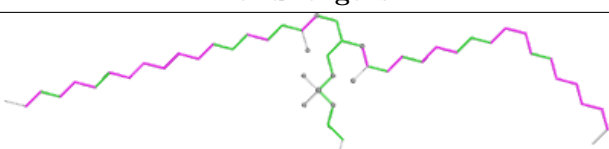
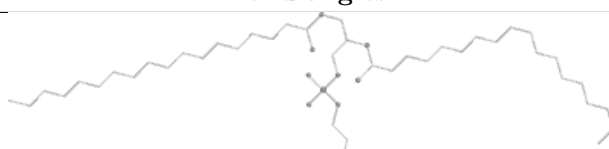


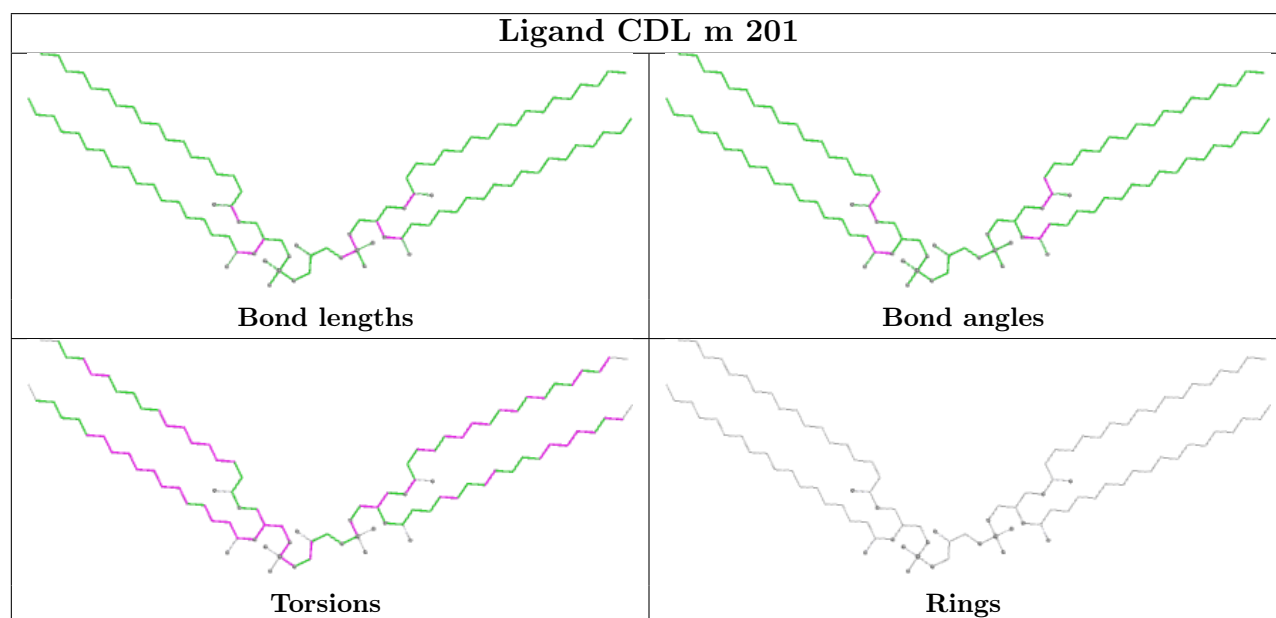
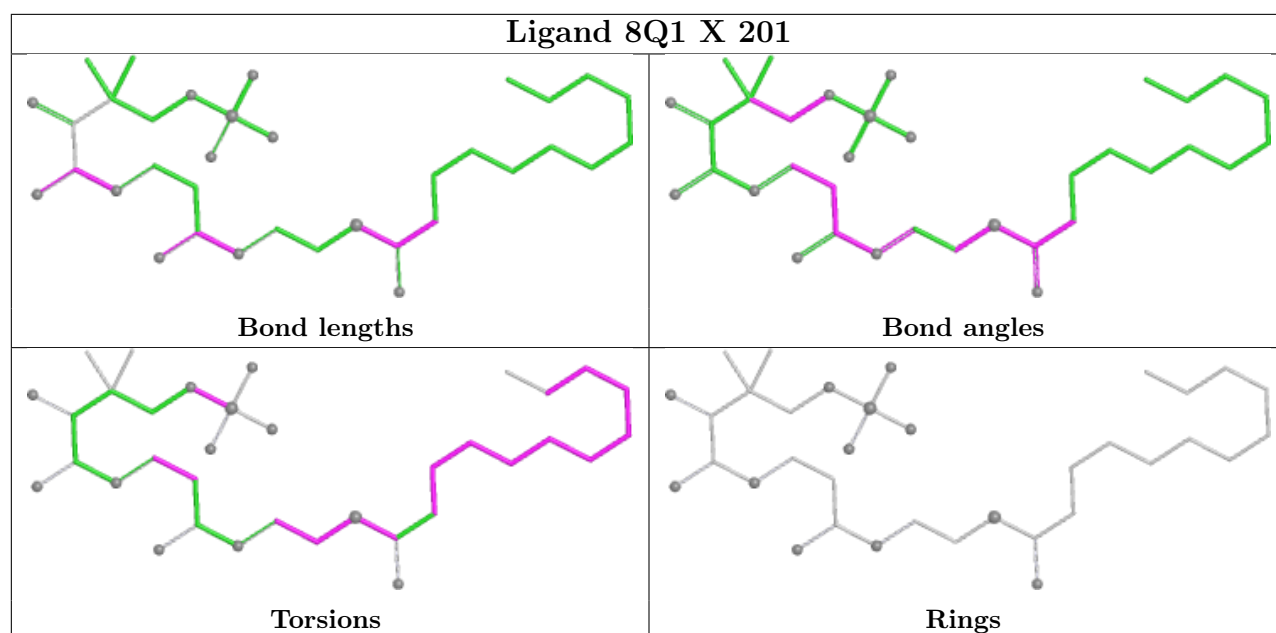


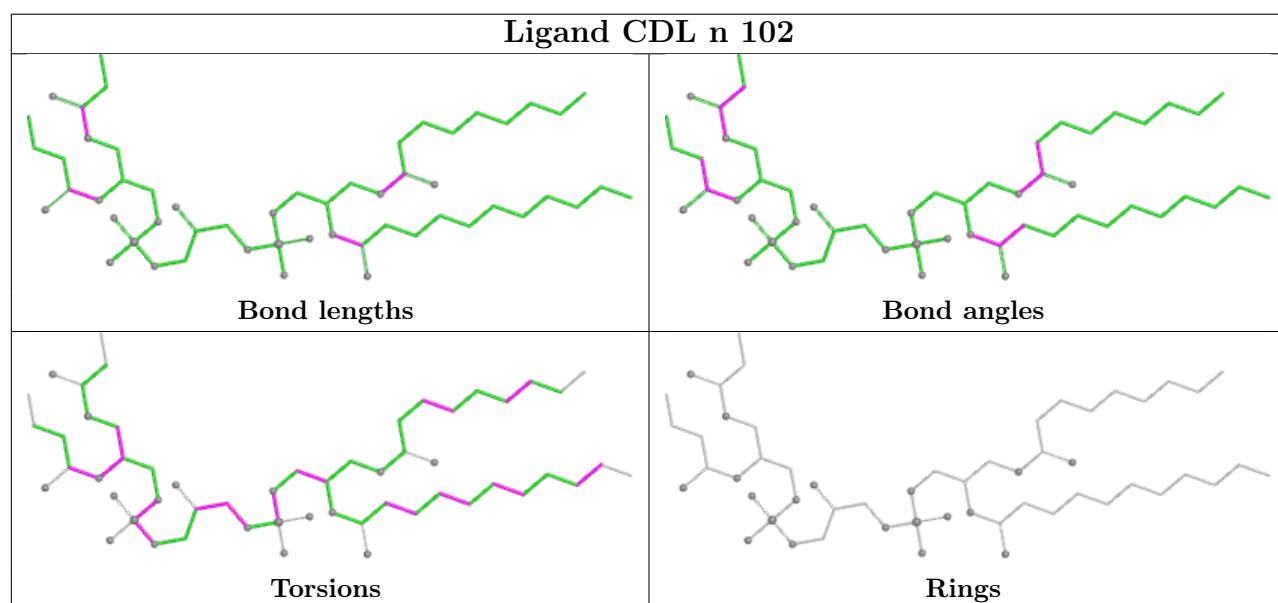
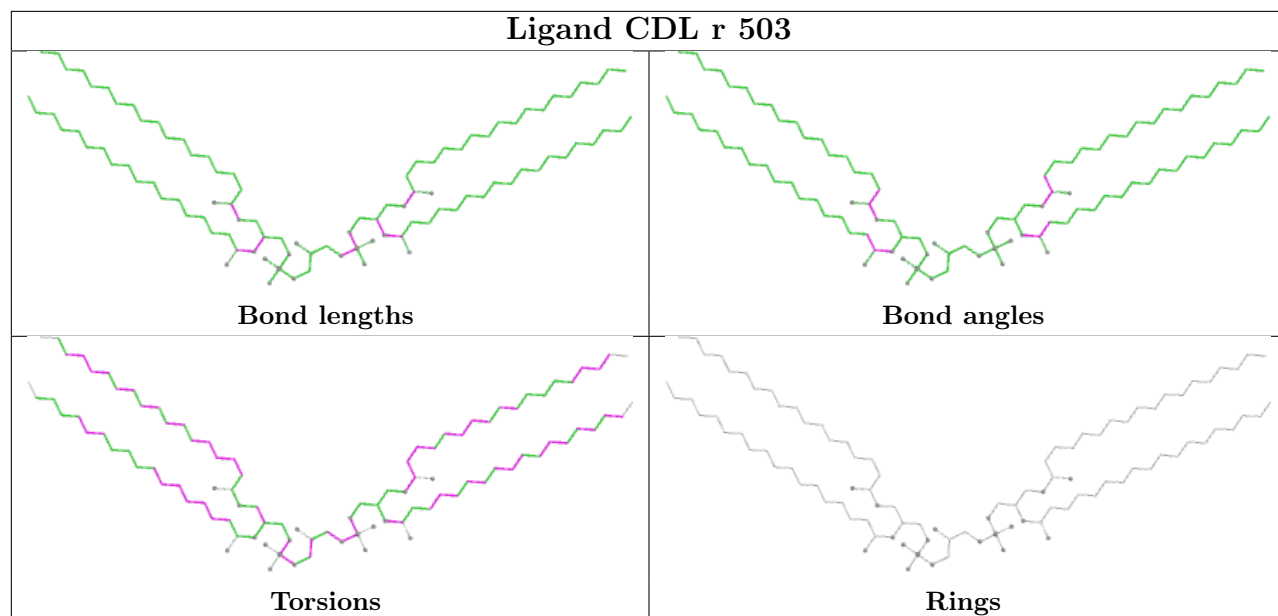


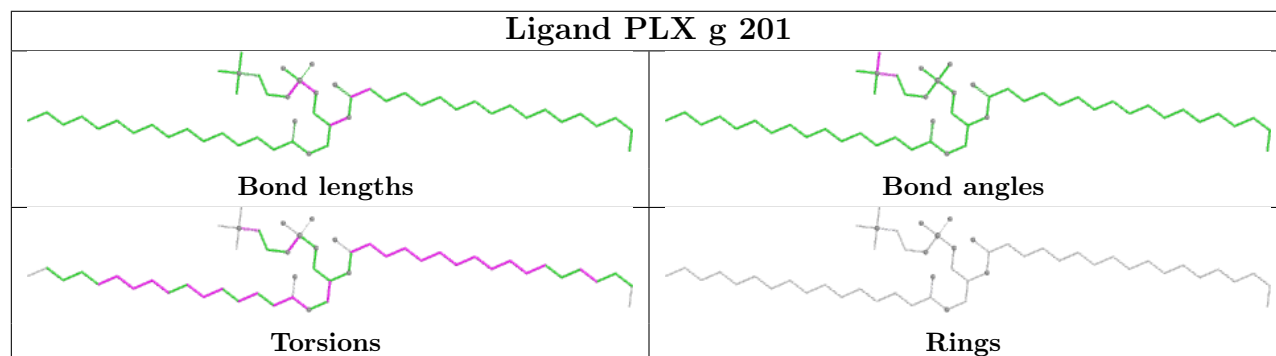
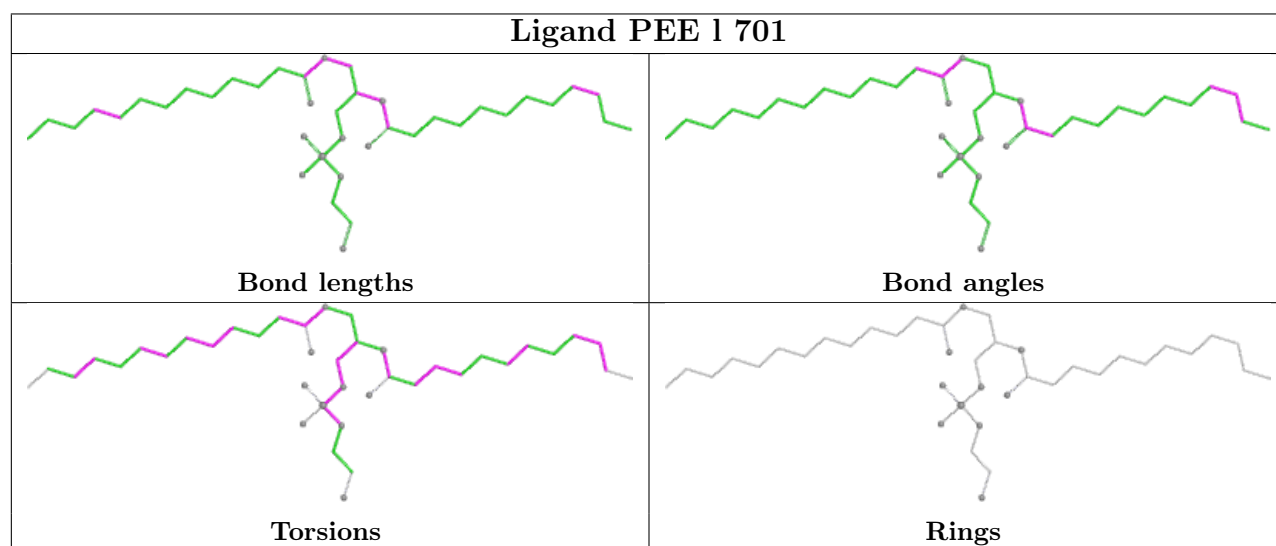
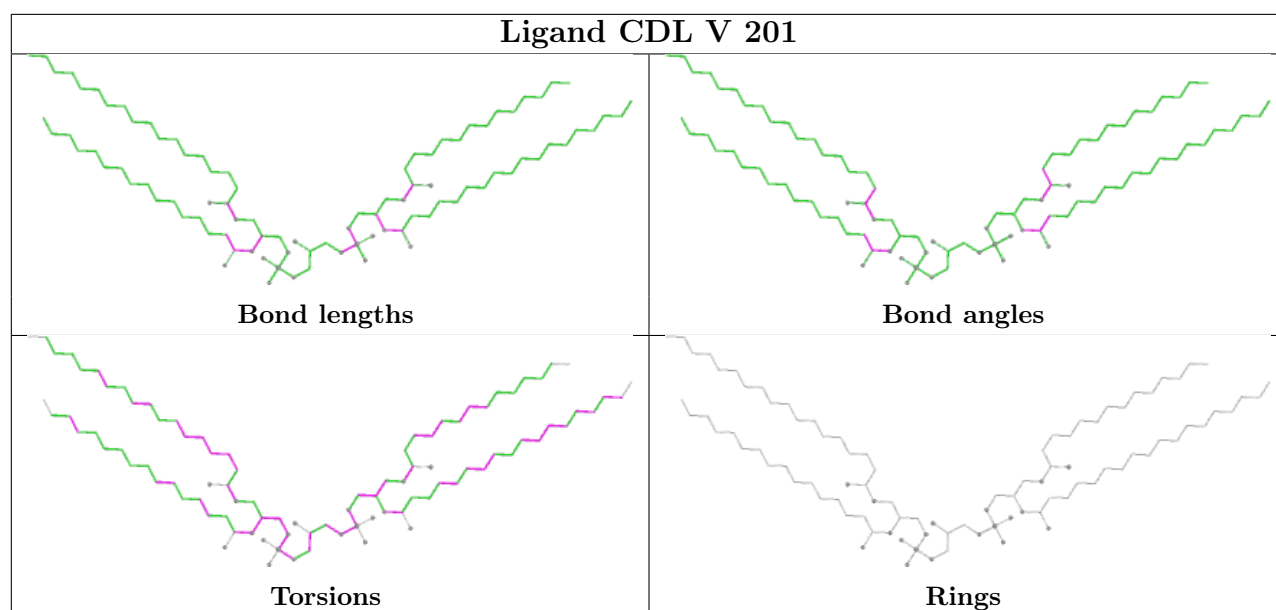
Ligand PLX j 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

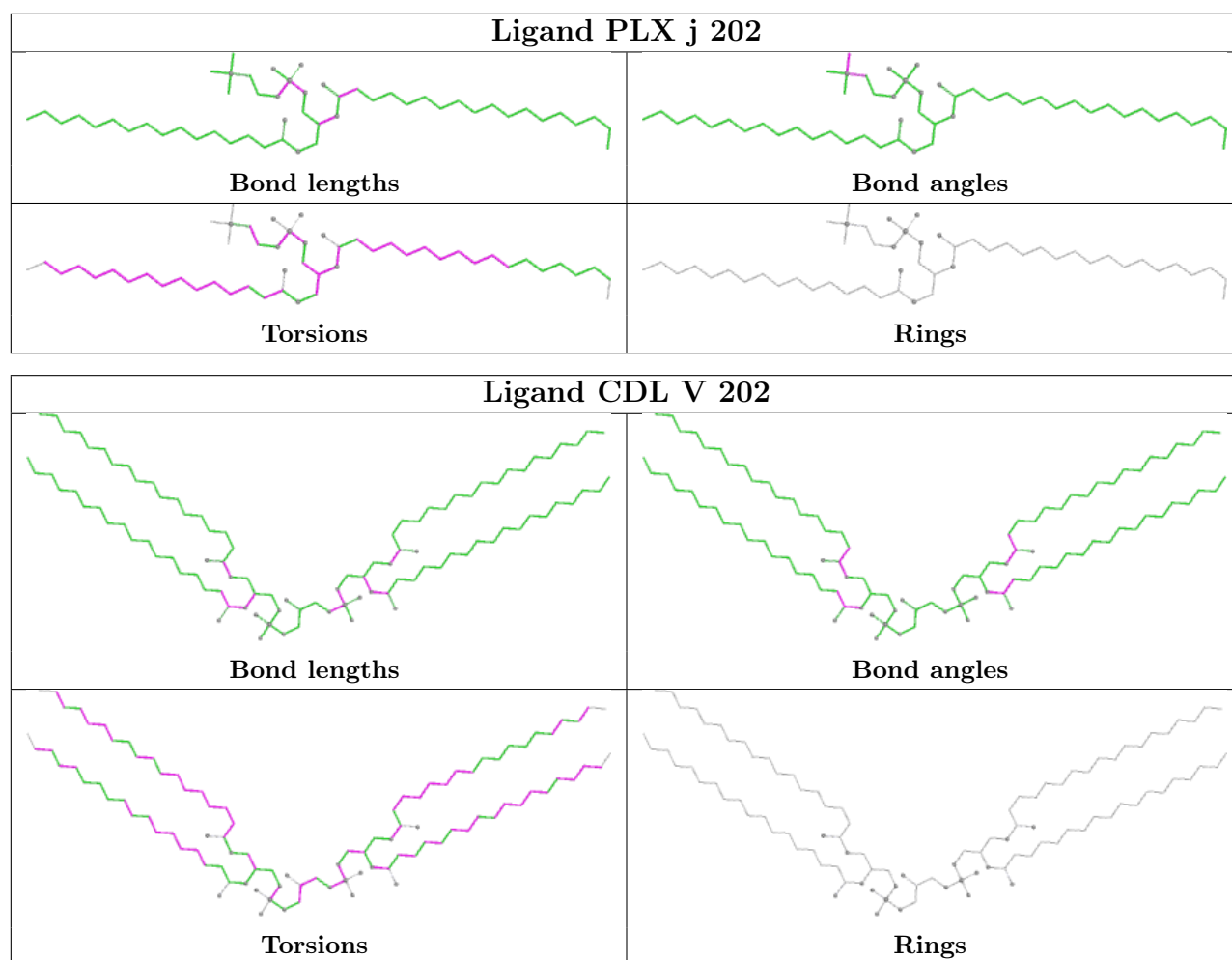
Ligand PLX r 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEE s 403	
	
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.

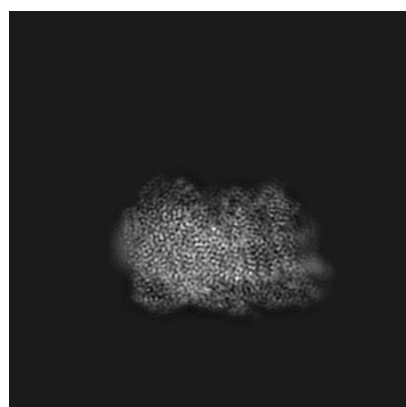
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32187. These allow visual inspection of the internal detail of the map and identification of artifacts.

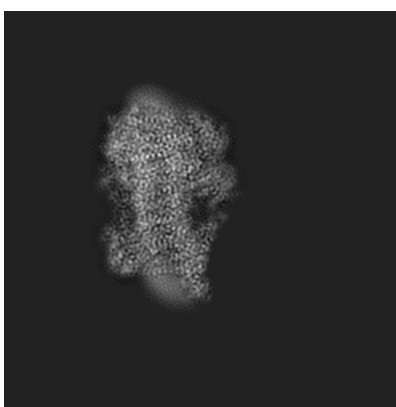
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

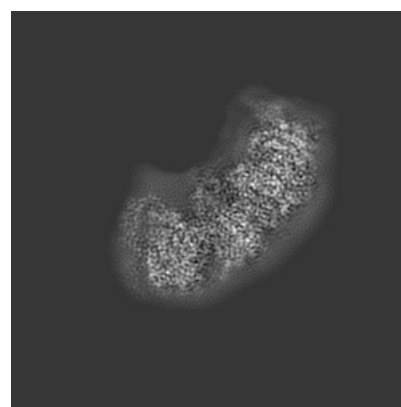
6.1.1 Primary map



X



Y

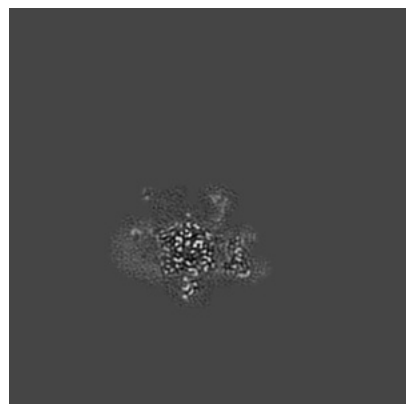


Z

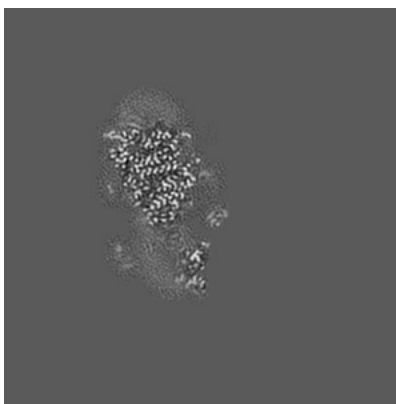
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

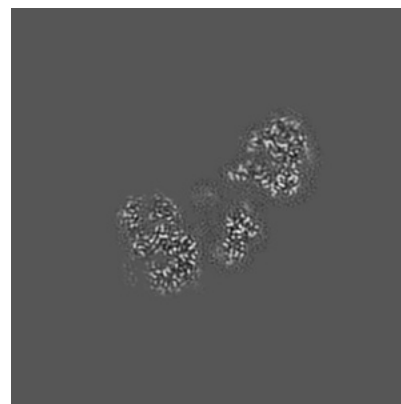
6.2.1 Primary map



X Index: 165



Y Index: 165

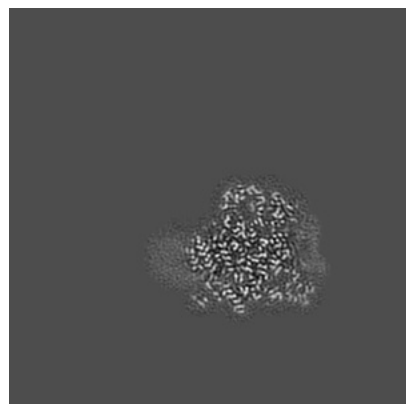


Z Index: 165

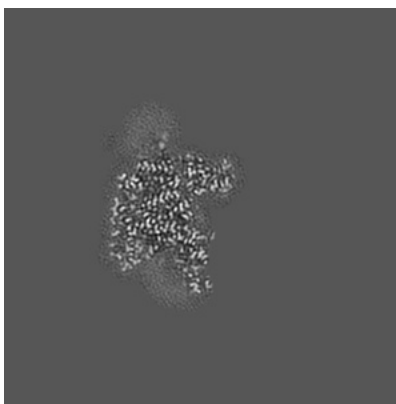
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

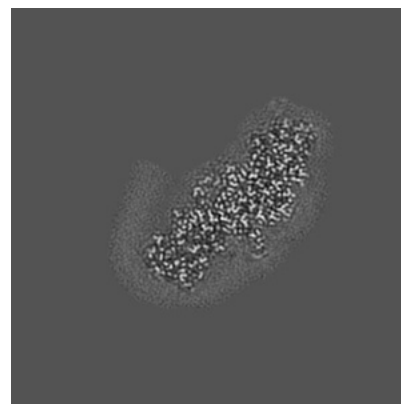
6.3.1 Primary map



X Index: 217



Y Index: 146

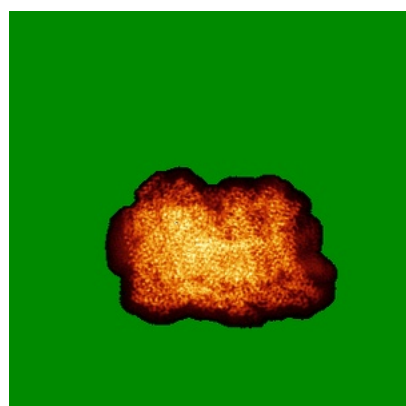


Z Index: 136

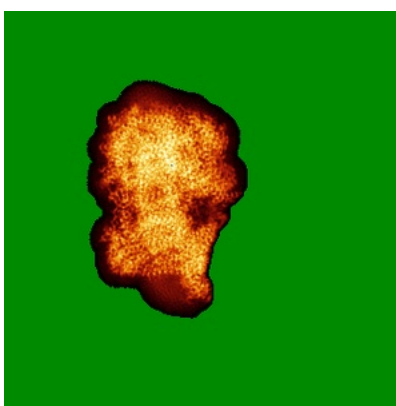
The images above show the largest variance slices of the map in three orthogonal directions.

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

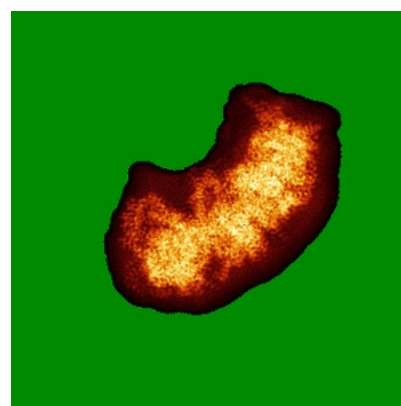
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

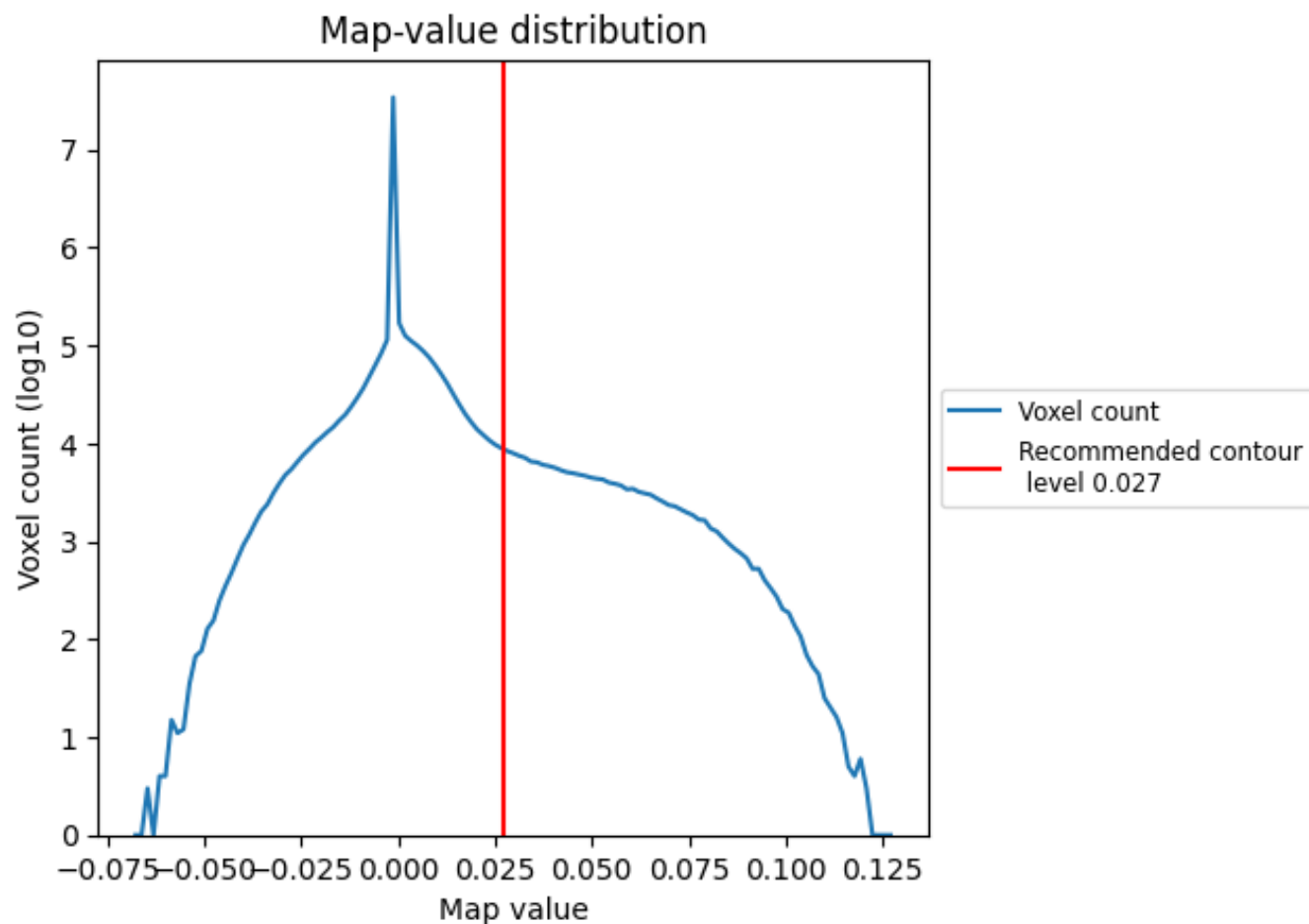
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

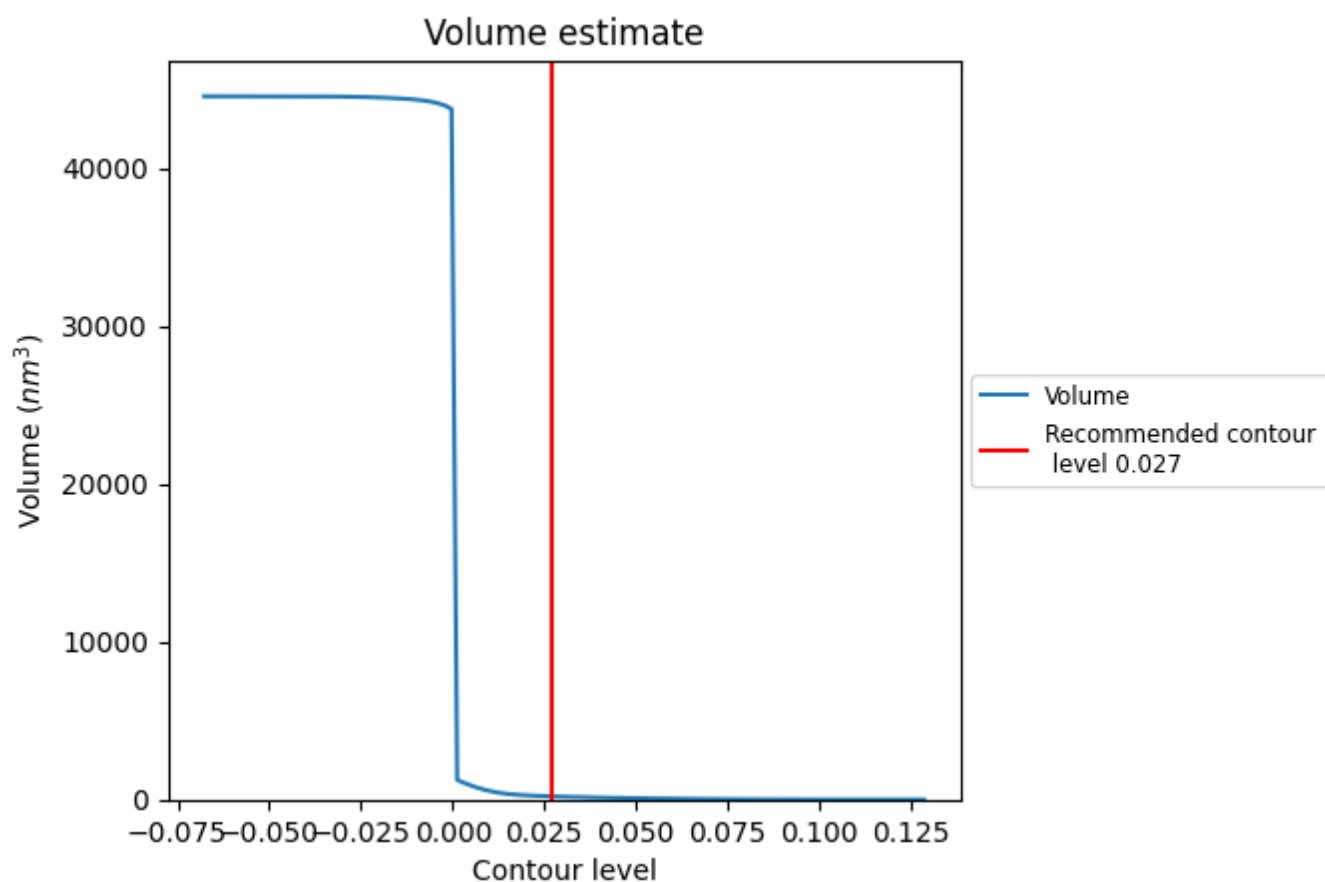
This section contains the results of statistical analysis of the map.

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.

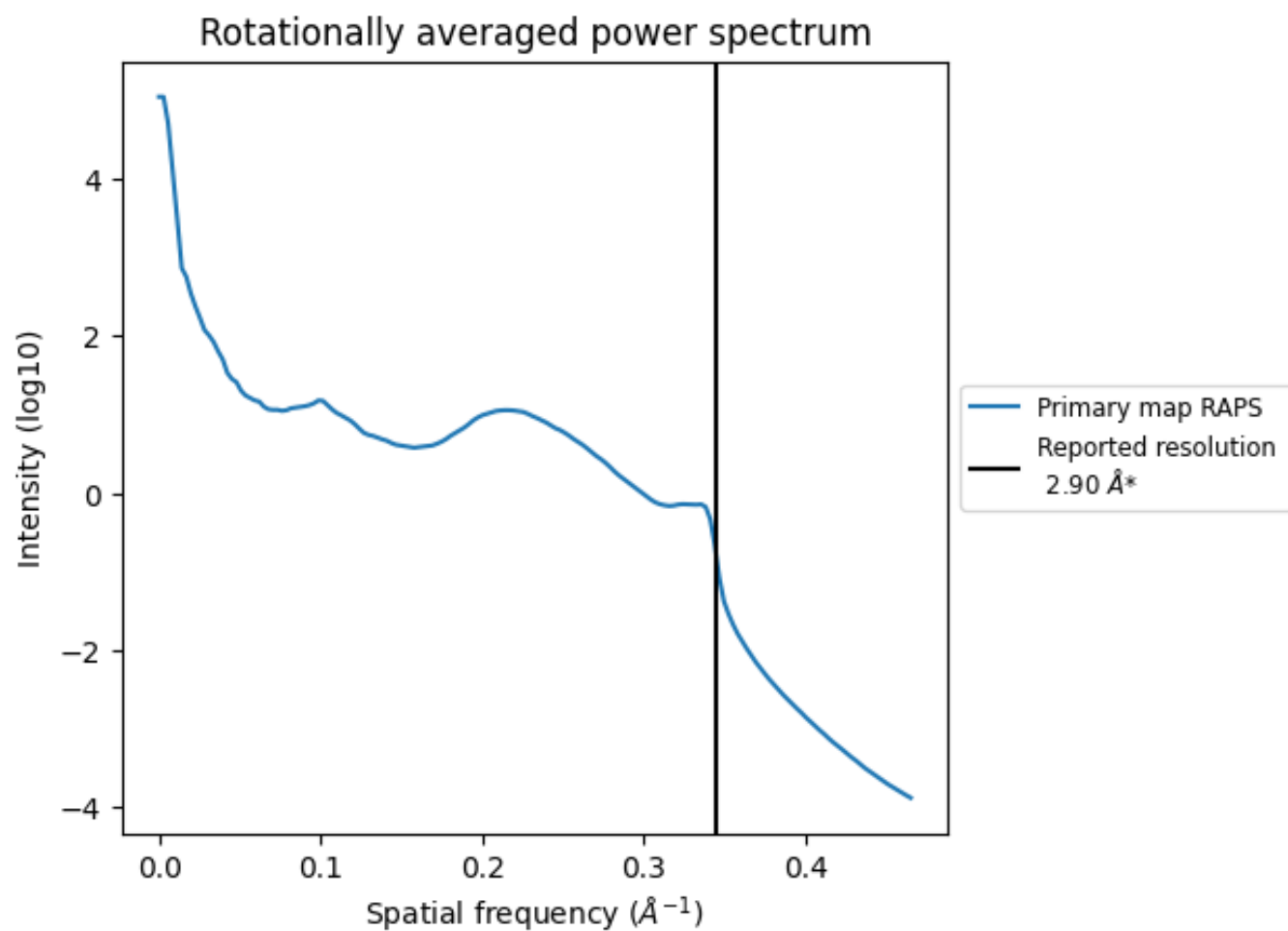
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 201 nm^3 ; this corresponds to an approximate mass of 182 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.

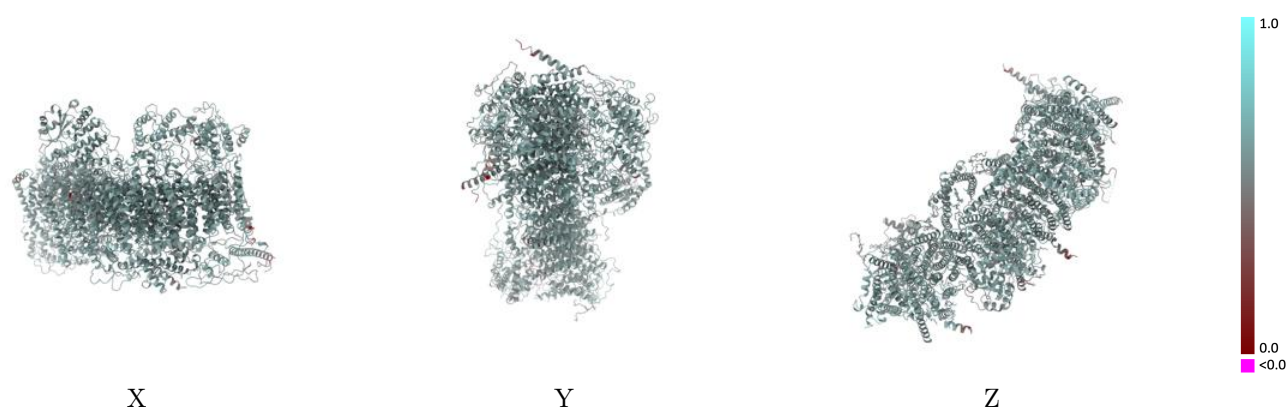
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-32187 and PDB model 7VXS. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)

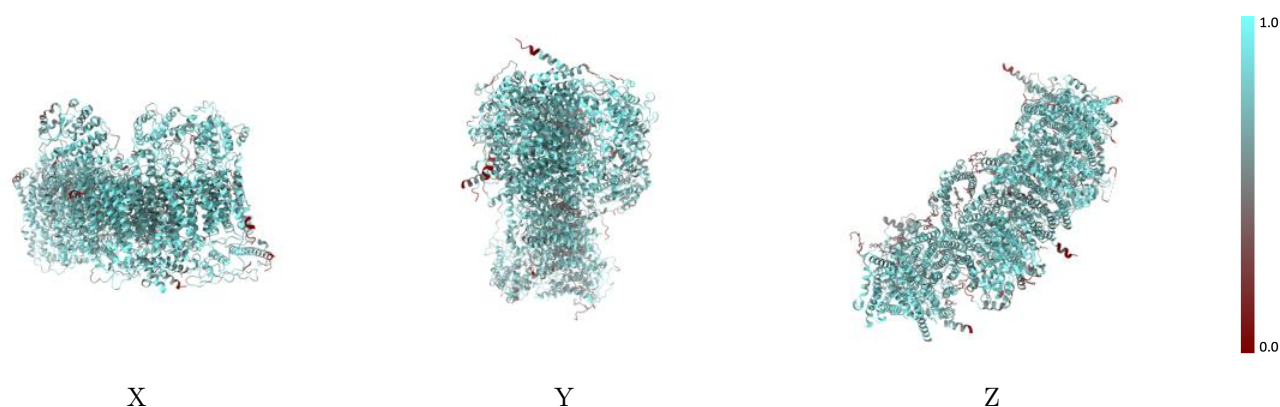
This section was not generated.

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



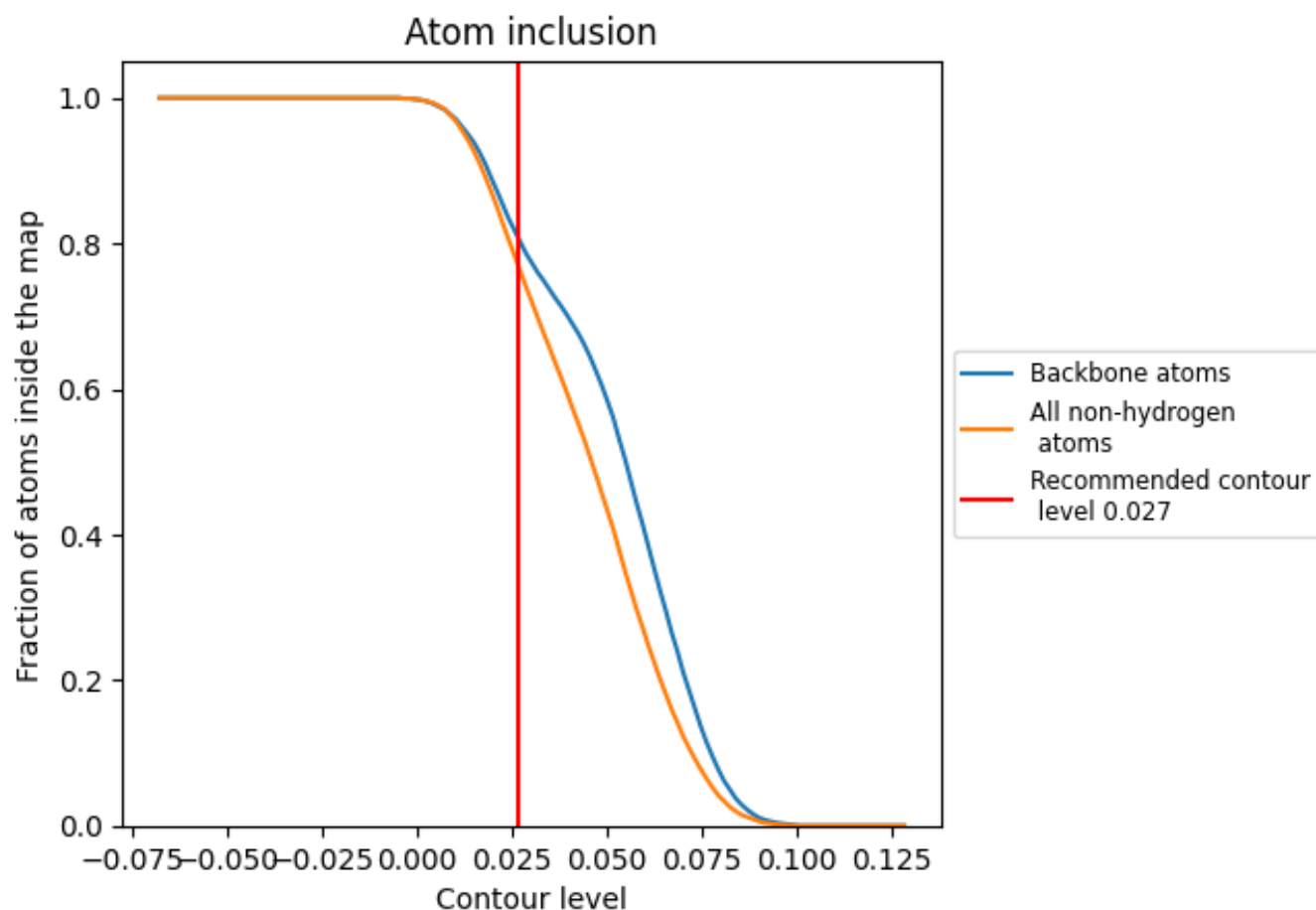
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.027).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 77% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7670	 0.5780
Q	 0.7360	 0.5790
S	 0.7990	 0.5860
U	 0.7420	 0.5710
V	 0.6630	 0.5620
W	 0.7810	 0.5830
X	 0.7460	 0.5560
Y	 0.7140	 0.5520
Z	 0.6530	 0.5370
a	 0.8020	 0.5890
b	 0.6990	 0.5620
c	 0.7790	 0.5800
d	 0.7420	 0.5580
e	 0.7290	 0.5670
f	 0.6110	 0.5350
g	 0.8090	 0.5890
h	 0.7440	 0.5640
i	 0.8210	 0.5950
j	 0.7060	 0.5760
k	 0.8300	 0.5930
l	 0.7870	 0.5860
m	 0.6960	 0.5580
n	 0.6300	 0.5550
o	 0.7580	 0.5780
p	 0.7890	 0.5860
r	 0.8220	 0.5950
s	 0.8100	 0.5920
u	 0.7720	 0.5790
v	 0.7090	 0.5520
w	 0.7570	 0.5720

