



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:29 AM UTC

PDB ID : 7VYI / pdb_00007vyi
EMDB ID : EMD-32206
Title : Membrane arm of deactive state CI from Rotenone dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-14
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

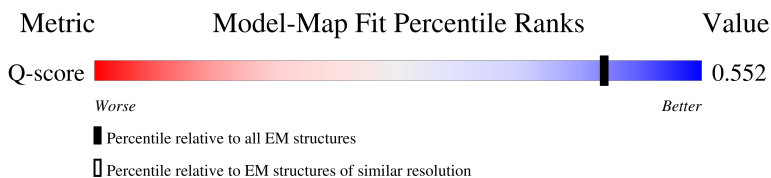
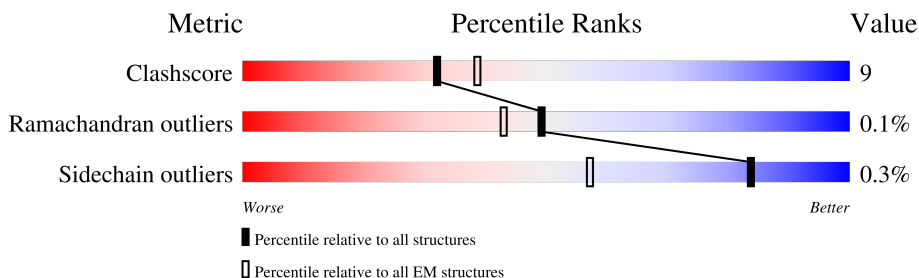
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



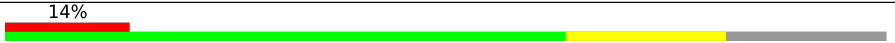
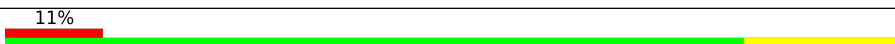
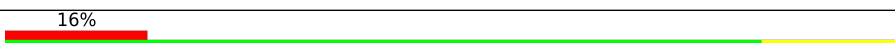
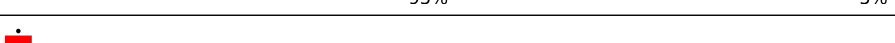
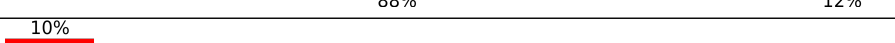
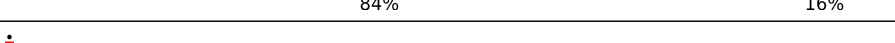
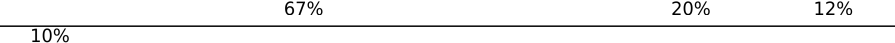
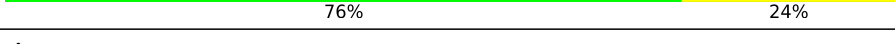
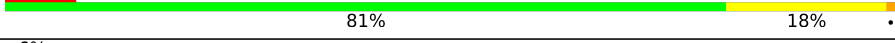
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	Q	40	40% 82% 18%
2	S	70	87% 13%
3	U	83	11% 88% 12%
4	V	140	31% 85% 15%

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Mol	Chain	Length	Quality of chain
5	W	113	
6	X	88	
7	Y	70	
8	Z	84	
9	a	140	
10	b	126	
11	c	156	
12	d	175	
13	e	107	
14	f	42	
15	g	121	
16	h	105	
17	i	347	
18	j	113	
19	k	98	
20	l	603	
21	m	175	
22	n	56	
23	o	128	
24	p	178	
25	r	459	
26	s	318	
27	u	171	
28	v	125	
29	w	320	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 38620 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	88	Total	C	N	O	S	0	0
			693	445	102	141	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	70	Total	C	N	O	S	0	0
			600	393	98	108	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	140	Total	C	N	O	S	0	0
			1161	760	199	199	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	103	Total	C	N	O	S	0	0
			879	573	158	147	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
			1303	846	212	238	7		

- 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	107	Total	C	N	O	S	0	0
			890	568	145	173	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	f	42	Total	C	N	O	0	0
			342	225	58	59		

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

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

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

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

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

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

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	n	56	Total	C	N	O	S	0	0
			456	295	83	77	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
			1530	980	279	263	8		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	v	124	Total	C	N	O	S	0	0
			992	622	180	181	9		

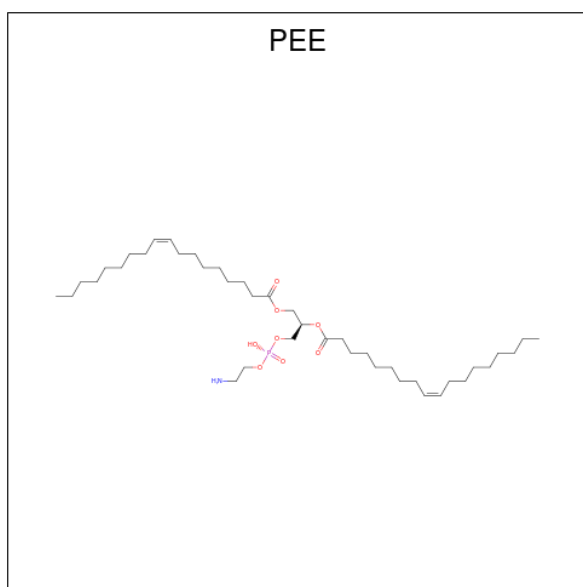
There is a discrepancy between the modelled and reference sequences:

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

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

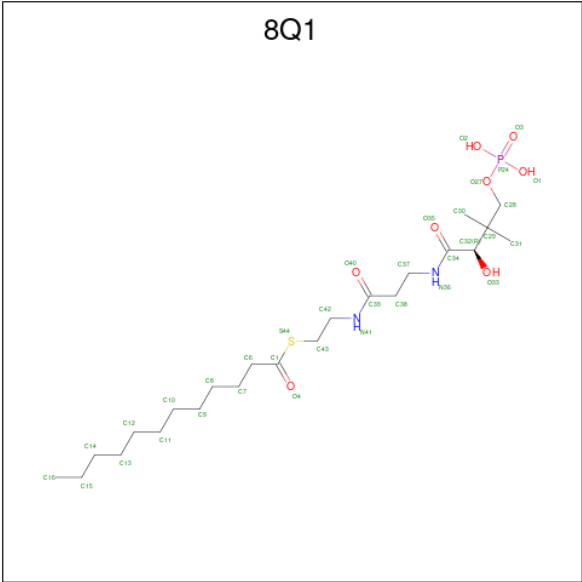
Mol	Chain	Residues	Atoms					AltConf	Trace
29	w	320	Total	C	N	O	S	0	0
			2563	1634	431	488	10		

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



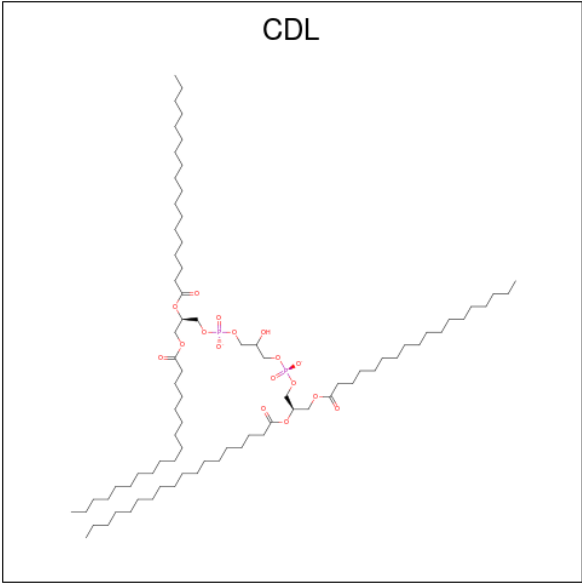
Mol	Chain	Residues	Atoms					AltConf
30	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	b	1	Total	C	N	O	P	0
			46	36	1	8	1	
30	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
30	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
30	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
30	r	1	Total	C	N	O	P	0
			51	41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

- Molecule 31 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
31	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 32 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



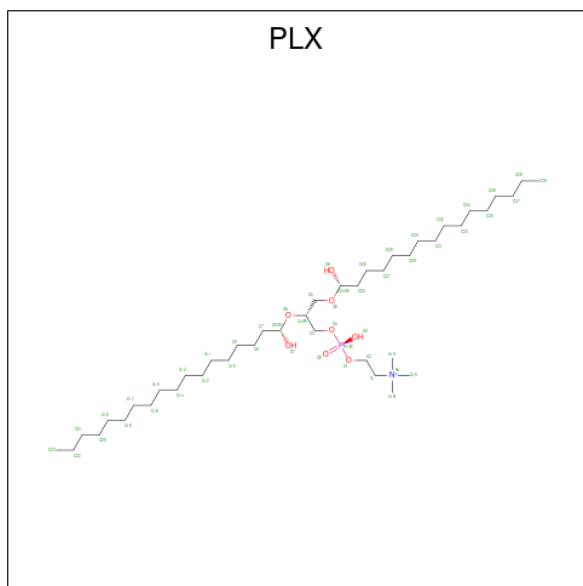
Mol	Chain	Residues	Atoms				AltConf
32	a	1	Total	C	O	P	0
			91	72	17	2	
32	g	1	Total	C	O	P	0
			78	59	17	2	

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Mol	Chain	Residues	Atoms				AltConf
32	i	1	Total	C	O	P	0
			66	47	17	2	
32	l	1	Total	C	O	P	0
			100	81	17	2	
32	r	1	Total	C	O	P	0
			99	80	17	2	
32	r	1	Total	C	O	P	0
			100	81	17	2	

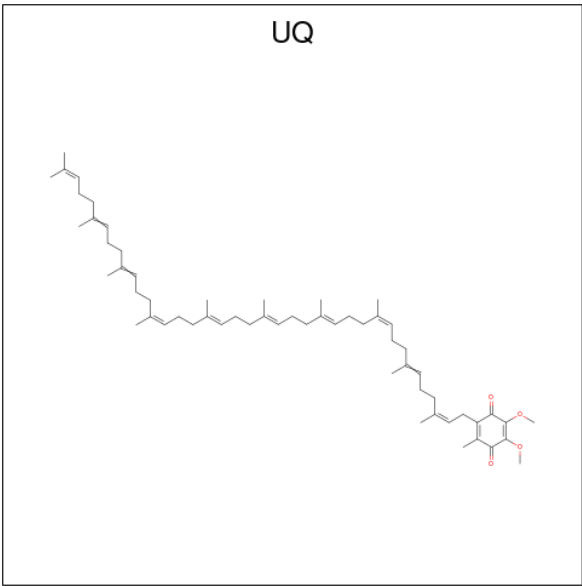
- Molecule 33 is (9R,11S)-9-([[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



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

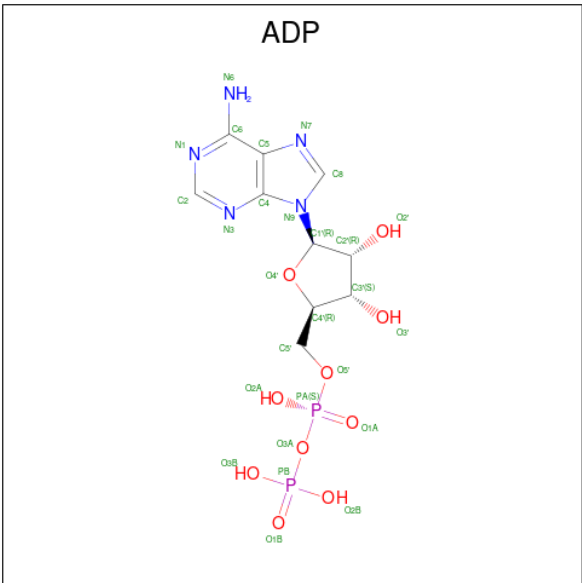
- Molecule 34 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ)

(formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
34	s	1	Total	C	O	0
			28	24	4	

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

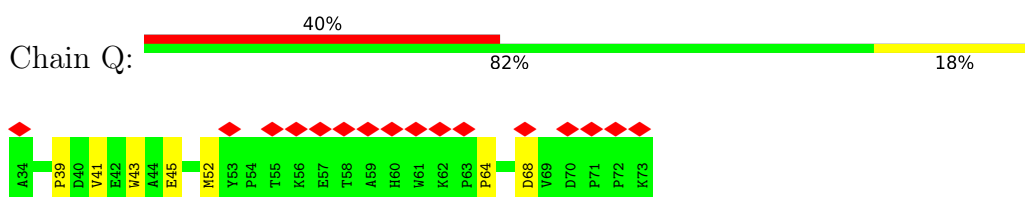


Mol	Chain	Residues	Atoms					AltConf
35	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

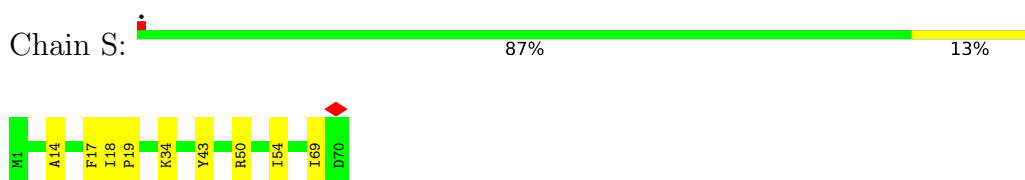
3 Residue-property plots

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

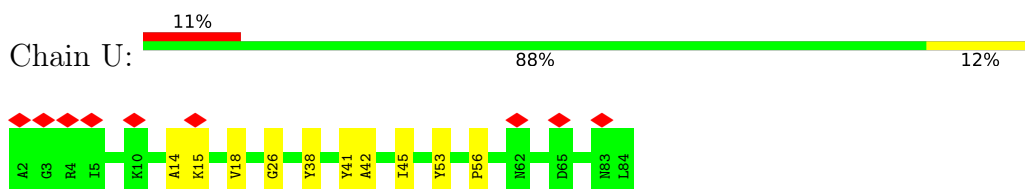
- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



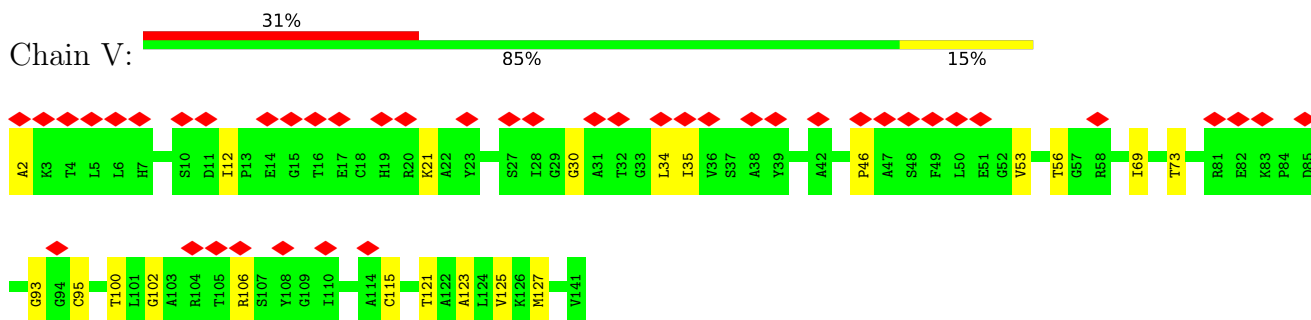
- Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



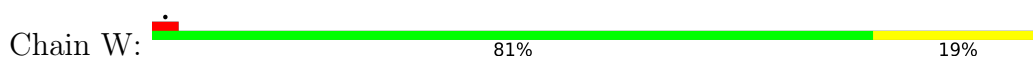
- Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



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

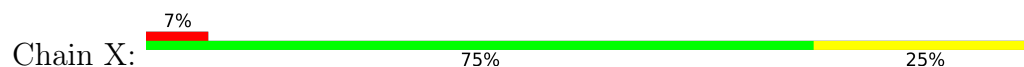


- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

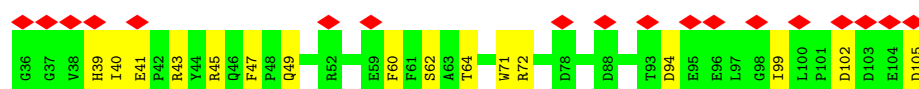
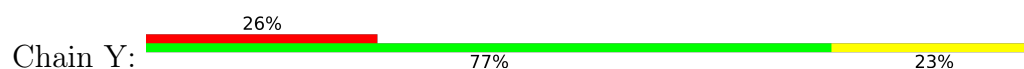




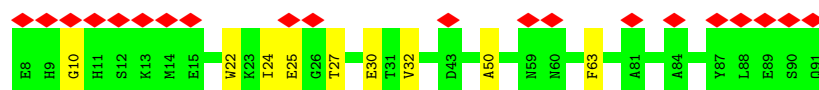
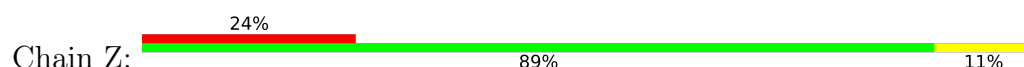
- Molecule 6: Acyl carrier protein, mitochondrial



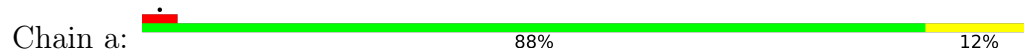
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



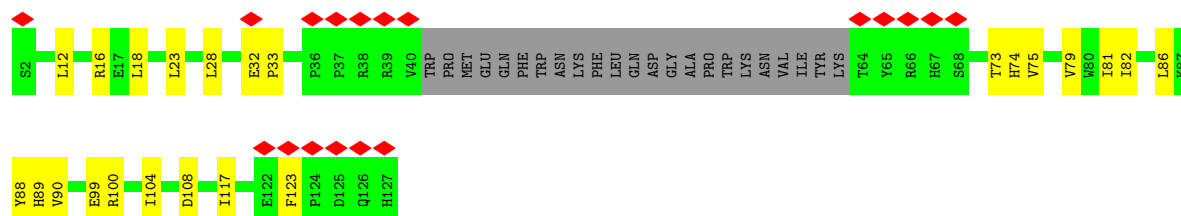
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



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

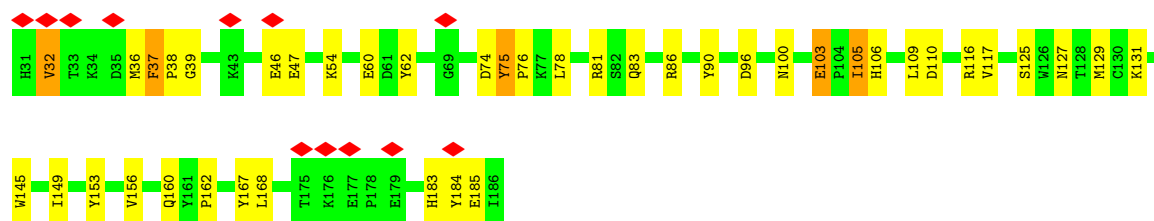


- Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

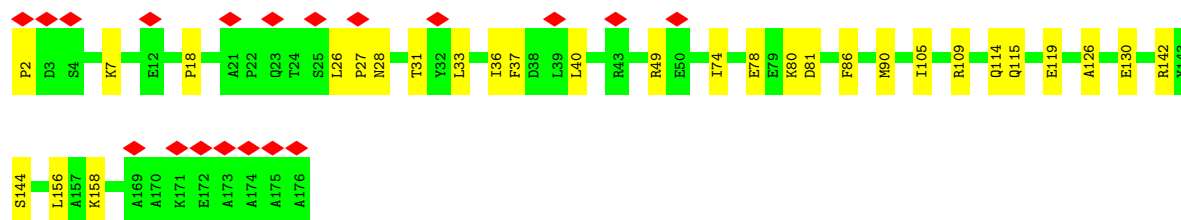
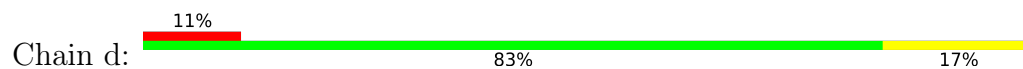


- Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

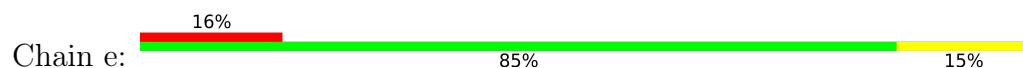




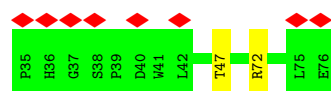
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



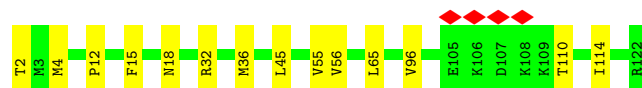
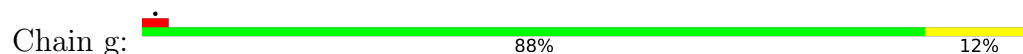
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



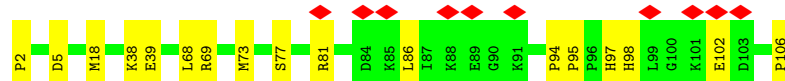
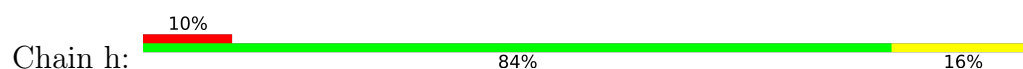
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



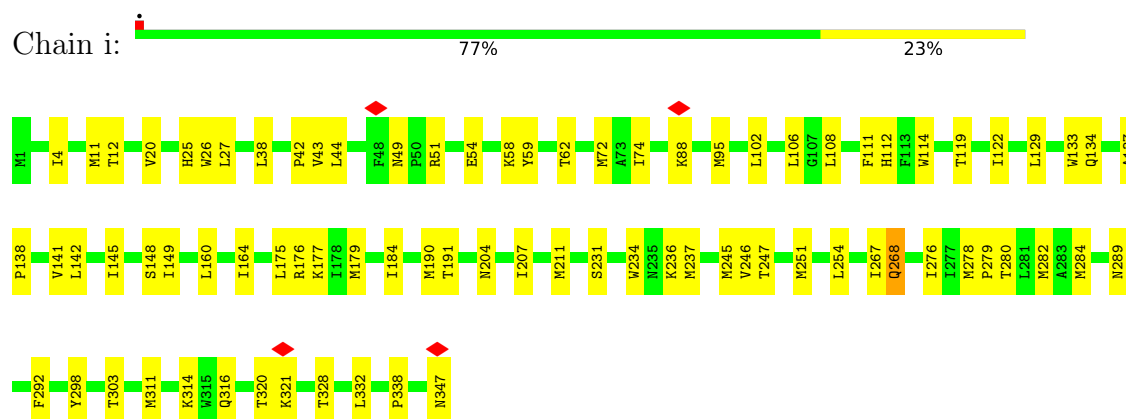
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2



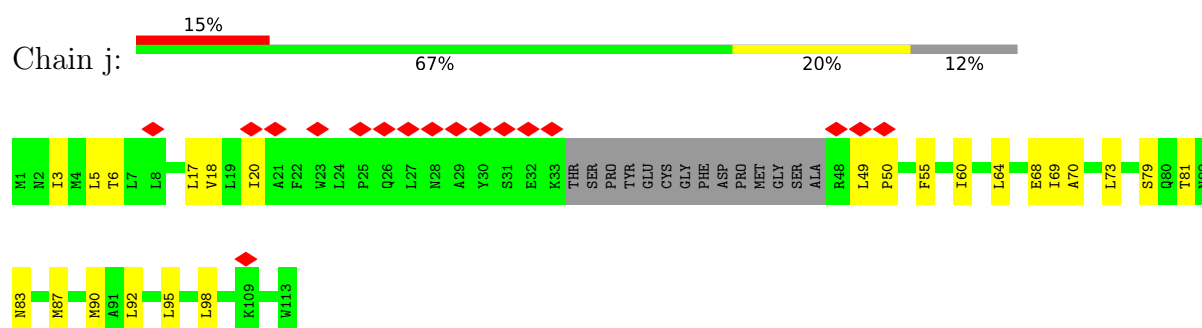
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



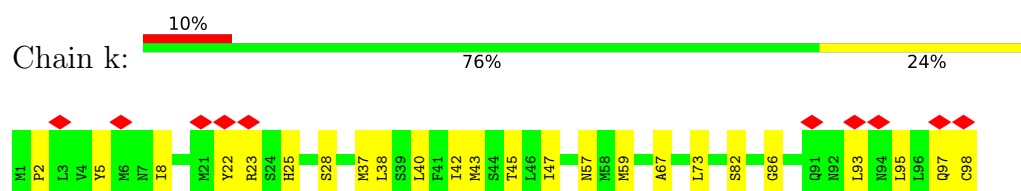
- Molecule 17: NADH-ubiquinone oxidoreductase chain 2



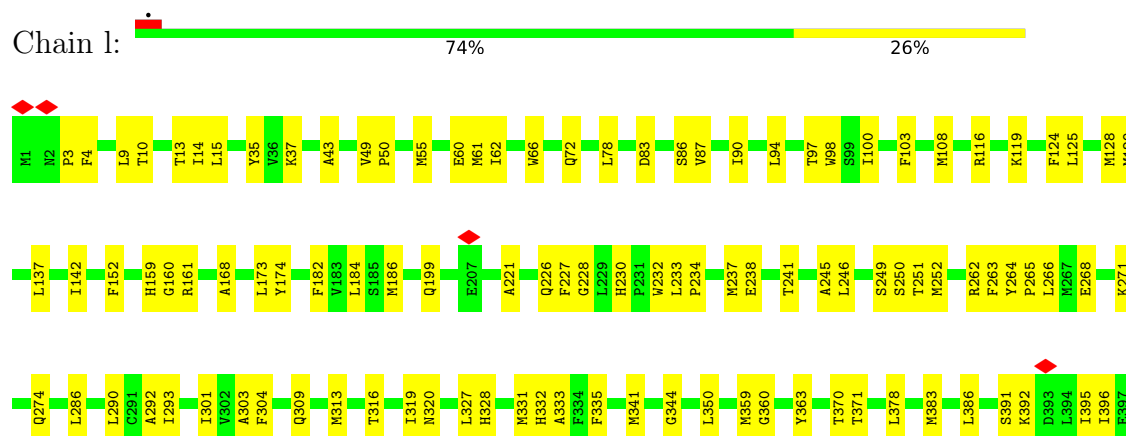
- Molecule 18: NADH-ubiquinone oxidoreductase chain 3

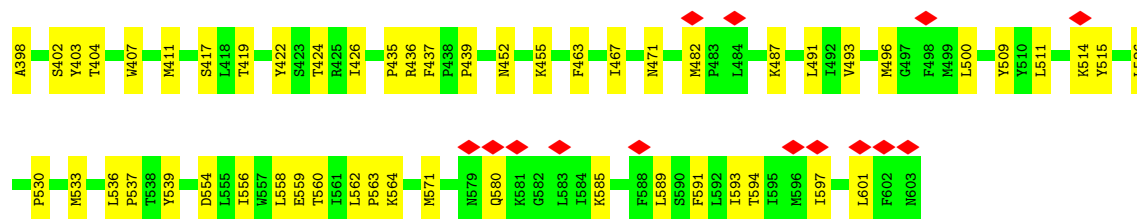


- Molecule 19: NADH-ubiquinone oxidoreductase chain 4L

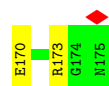
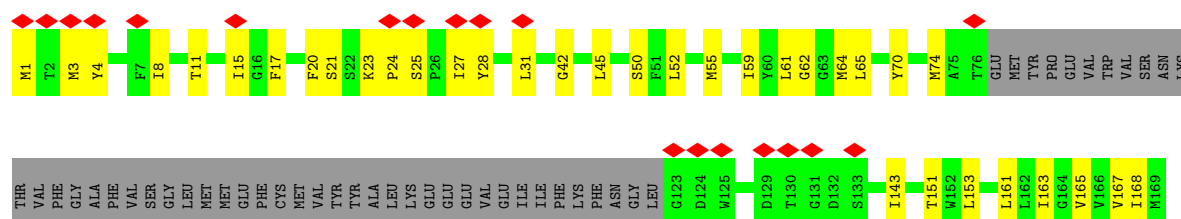


- Molecule 20: NADH-ubiquinone oxidoreductase chain 5





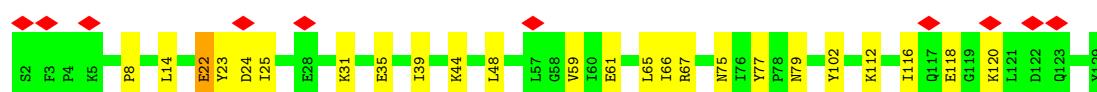
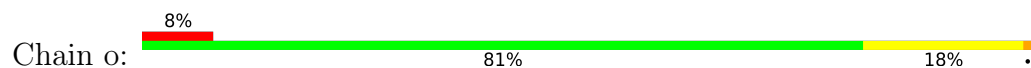
• Molecule 21: NADH-ubiquinone oxidoreductase chain 6



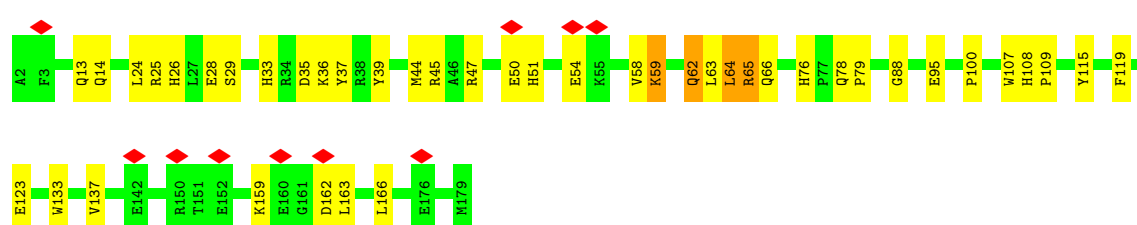
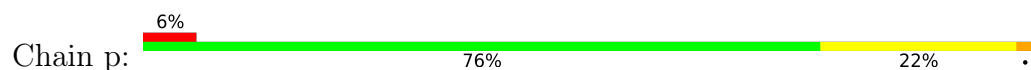
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



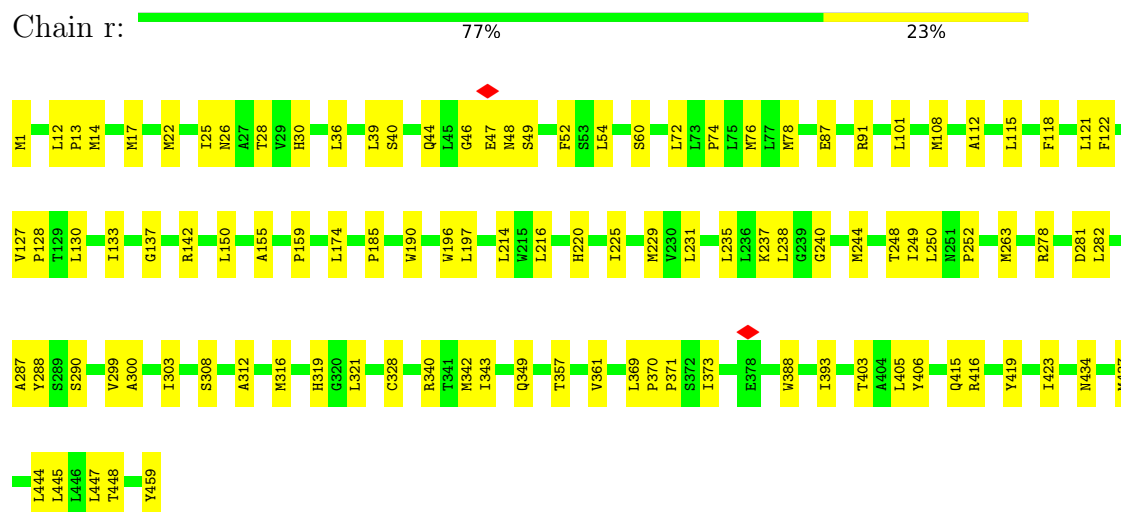
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



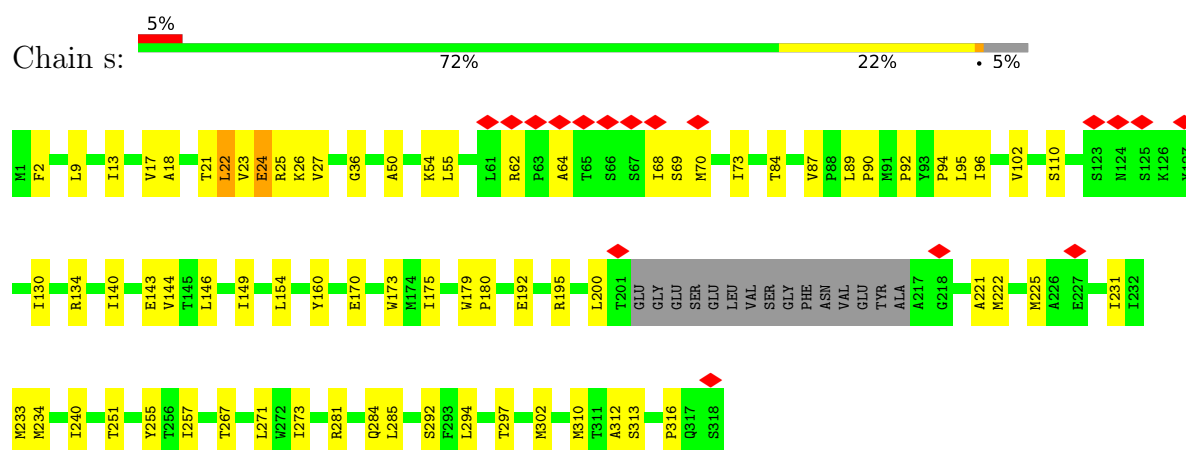
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



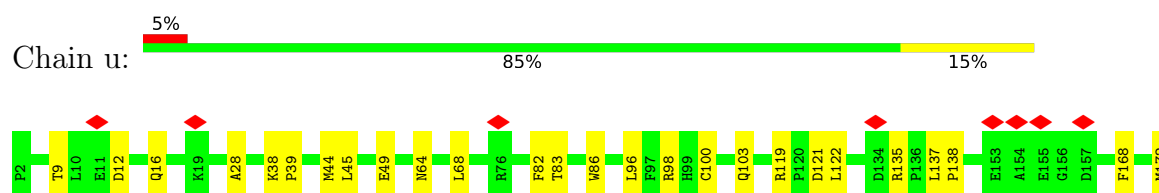
• Molecule 25: NADH-ubiquinone oxidoreductase chain 4



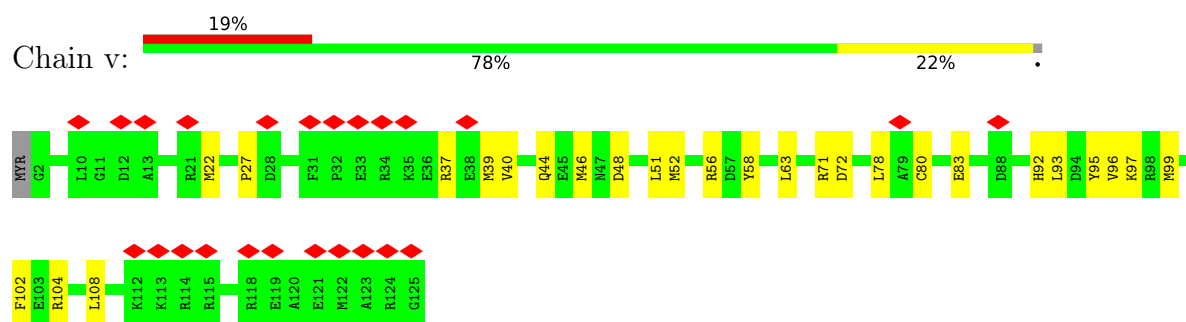
• Molecule 26: NADH-ubiquinone oxidoreductase chain 1



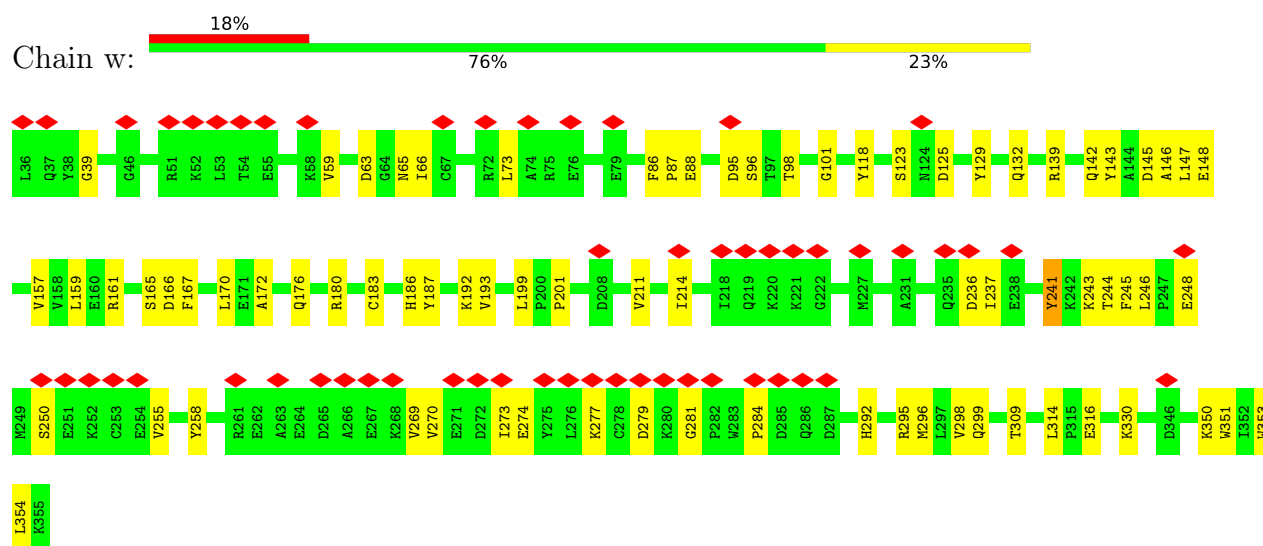
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63623	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	0.141	Depositor
Minimum map value	-0.085	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0288	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.13	0/350	0.30	0/483
2	S	0.13	0/582	0.34	0/783
3	U	0.10	0/664	0.24	0/912
4	V	0.12	0/1042	0.29	0/1411
5	W	0.11	0/973	0.27	0/1312
6	X	0.12	0/705	0.31	0/956
7	Y	0.13	0/626	0.30	0/857
8	Z	0.09	0/695	0.25	0/939
9	a	0.12	0/1195	0.31	0/1618
10	b	0.12	0/906	0.30	0/1232
11	c	0.17	0/1359	0.59	4/1861 (0.2%)
12	d	0.11	0/1494	0.28	0/2015
13	e	0.11	0/916	0.29	0/1246
14	f	0.08	0/350	0.19	0/473
15	g	0.10	0/1031	0.24	0/1394
16	h	0.10	0/889	0.32	0/1190
17	i	0.13	0/2773	0.31	0/3768
18	j	0.15	0/819	0.34	0/1117
19	k	0.14	0/759	0.32	0/1029
20	l	0.13	0/4914	0.33	0/6683
21	m	0.15	0/973	0.41	0/1320
22	n	0.18	0/468	0.45	0/633
23	o	0.12	0/1092	0.36	0/1481
24	p	0.16	0/1586	0.38	0/2150
25	r	0.13	0/3723	0.32	0/5078
26	s	0.15	0/2464	0.33	0/3369
27	u	0.10	0/1436	0.27	0/1938
28	v	0.12	0/1016	0.36	0/1370
29	w	0.13	0/2623	0.36	1/3557 (0.0%)
All	All	0.13	0/38423	0.34	5/52175 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	c	75	TYR	CA-C-N	10.20	130.15	119.85
11	c	75	TYR	C-N-CA	10.20	130.15	119.85
11	c	37	PHE	CA-C-N	7.06	127.09	119.89
11	c	37	PHE	C-N-CA	7.06	127.09	119.89
29	w	243	LYS	N-CA-C	6.28	118.20	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	333	0	301	5	0
2	S	567	0	565	8	0
3	U	643	0	642	9	0
4	V	1021	0	1027	11	0
5	W	949	0	935	17	0
6	X	693	0	664	22	0
7	Y	600	0	539	12	0
8	Z	674	0	643	7	0
9	a	1161	0	1170	14	0
10	b	879	0	899	24	0
11	c	1303	0	1183	41	0
12	d	1461	0	1429	22	0
13	e	890	0	837	13	0
14	f	342	0	341	2	0
15	g	1000	0	994	11	0
16	h	867	0	871	14	0
17	i	2710	0	2874	61	0
18	j	800	0	855	20	0
19	k	748	0	799	22	0
20	l	4785	0	4933	117	0
21	m	951	0	962	35	0
22	n	456	0	433	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	o	1062	0	1072	21	0
24	p	1530	0	1466	36	0
25	r	3631	0	3839	77	0
26	s	2394	0	2508	58	0
27	u	1398	0	1378	22	0
28	v	992	0	908	20	0
29	w	2563	0	2501	52	0
30	U	102	0	164	4	0
30	b	46	0	69	4	0
30	i	47	0	71	3	0
30	l	46	0	69	3	0
30	m	41	0	59	2	0
30	r	51	0	82	3	0
31	X	35	0	0	4	0
32	a	91	0	132	2	0
32	g	78	0	103	7	0
32	i	66	0	76	4	0
32	l	100	0	156	6	0
32	r	199	0	307	20	0
33	a	52	0	88	2	0
33	g	52	0	88	5	0
33	j	52	0	88	1	0
33	r	104	0	176	11	0
34	s	28	0	31	6	0
35	w	27	0	11	1	0
All	All	38620	0	39338	671	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 (671) 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)
6:X:112:SER:CB	31:X:201:8Q1:O1	1.65	1.40
29:w:244:THR:O	29:w:248:GLU:HG2	1.66	0.96
6:X:123:GLU:HG2	6:X:129:GLU:HA	1.47	0.95
24:p:65:ARG:HG2	24:p:65:ARG:HH11	1.37	0.85
24:p:54:GLU:OE2	24:p:59:LYS:HG2	1.76	0.85
26:s:146:LEU:HD11	26:s:192:GLU:HG3	1.60	0.81
23:o:23:TYR:CD2	24:p:65:ARG:HD2	2.16	0.81
11:c:100:ASN:HB3	11:c:103:GLU:HG2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:o:23:TYR:CE2	24:p:65:ARG:HD2	2.21	0.75
17:i:108:LEU:HD11	17:i:191:THR:HG21	1.69	0.75
12:d:78:GLU:HB2	12:d:81:ASP:HB2	1.68	0.75
29:w:63:ASP:HB2	29:w:241:TYR:OH	1.87	0.74
6:X:111:ASP:OD1	6:X:112:SER:N	2.21	0.74
26:s:23:VAL:O	26:s:27:VAL:HG23	1.88	0.74
1:Q:68:ASP:O	17:i:49:ASN:ND2	2.21	0.73
25:r:14:MET:SD	25:r:30:HIS:ND1	2.63	0.72
5:W:134:LEU:HD13	21:m:1:MET:HA	1.72	0.71
17:i:207:ILE:HG22	17:i:211:MET:HE2	1.73	0.71
10:b:82:ILE:HD11	20:l:13:THR:HG21	1.71	0.70
18:j:60:ILE:HG21	21:m:168:ILE:HG21	1.71	0.70
25:r:216:LEU:HG	25:r:220:HIS:CE1	2.27	0.69
25:r:281:ASP:OD2	25:r:340:ARG:NH1	2.26	0.69
32:r:504:CDL:H621	32:r:504:CDL:H432	1.73	0.69
9:a:152:LYS:HD3	15:g:96:VAL:HG21	1.73	0.69
20:l:496:MET:HE2	32:l:701:CDL:H401	1.74	0.68
12:d:26:LEU:HD12	12:d:27:PRO:HD2	1.73	0.68
26:s:22:LEU:HD12	26:s:22:LEU:O	1.93	0.68
10:b:104:ILE:HB	28:v:48:ASP:HB3	1.75	0.67
20:l:419:THR:HA	20:l:422:TYR:CE2	2.30	0.67
6:X:146:ASP:OD2	10:b:16:ARG:NH2	2.28	0.67
26:s:17:VAL:O	26:s:21:THR:HG23	1.95	0.67
10:b:99:GLU:HG2	20:l:61:MET:HE2	1.77	0.66
24:p:44:MET:HA	24:p:47:ARG:HG2	1.76	0.66
10:b:12:LEU:O	10:b:16:ARG:HG3	1.96	0.66
17:i:246:VAL:HG21	32:r:505:CDL:H361	1.77	0.66
11:c:39:GLY:O	11:c:74:ASP:HB2	1.95	0.65
21:m:1:MET:SD	21:m:4:TYR:N	2.67	0.65
17:i:316:GLN:NE2	29:w:95:ASP:OD1	2.30	0.65
20:l:360:GLY:HA3	20:l:435:PRO:HA	1.78	0.65
21:m:11:THR:O	21:m:15:ILE:HG12	1.97	0.64
5:W:57:ARG:HB3	26:s:316:PRO:HG3	1.80	0.64
30:i:402:PEE:H37	30:i:402:PEE:H60	1.79	0.64
20:l:514:LYS:NZ	20:l:515:TYR:O	2.30	0.64
23:o:22:GLU:HG3	23:o:22:GLU:O	1.98	0.64
11:c:105:ILE:CG2	11:c:109:LEU:HD22	2.27	0.64
11:c:116:ARG:HG2	30:l:702:PEE:H49	1.80	0.63
20:l:301:ILE:HG21	20:l:426:ILE:HD11	1.80	0.63
20:l:161:ARG:NH2	24:p:88:GLY:O	2.30	0.63
25:r:137:GLY:O	25:r:142:ARG:NH1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:w:129:TYR:CD2	29:w:183:CYS:HB3	2.34	0.63
13:e:89:VAL:HG21	25:r:25:ILE:HG23	1.80	0.62
18:j:64:LEU:HD13	21:m:165:VAL:HG22	1.79	0.62
18:j:79:SER:HA	18:j:87:MET:HE2	1.80	0.62
11:c:110:ASP:OD1	25:r:278:ARG:NH2	2.27	0.62
24:p:65:ARG:HG2	24:p:65:ARG:NH1	2.08	0.62
11:c:36:MET:O	11:c:54:LYS:HD2	1.99	0.62
11:c:117:VAL:HG21	20:l:539:TYR:HB2	1.80	0.62
24:p:62:GLN:OE1	24:p:62:GLN:HA	2.00	0.62
6:X:155:TYR:CE1	10:b:23:LEU:HB3	2.34	0.62
26:s:170:GLU:OE1	27:u:98:ARG:NH2	2.33	0.62
16:h:77:SER:OG	16:h:81:ARG:NH2	2.32	0.61
17:i:267:ILE:HG12	17:i:279:PRO:HB3	1.83	0.61
29:w:246:LEU:CD1	29:w:255:VAL:HG11	2.31	0.61
25:r:282:LEU:HG	25:r:342:MET:HG2	1.81	0.61
6:X:83:VAL:HG22	6:X:122:MET:HE1	1.82	0.61
26:s:62:ARG:HH21	26:s:68:ILE:HB	1.66	0.61
19:k:22:TYR:O	20:l:585:LYS:NZ	2.28	0.61
4:V:69:ILE:HG13	4:V:100:THR:HG21	1.83	0.60
11:c:54:LYS:NZ	11:c:74:ASP:OD2	2.26	0.60
20:l:391:SER:O	20:l:395:ILE:HG12	2.00	0.60
23:o:23:TYR:O	23:o:25:ILE:N	2.33	0.60
11:c:39:GLY:H	11:c:74:ASP:CB	2.15	0.60
11:c:162:PRO:HG3	28:v:39:MET:HE2	1.82	0.60
32:i:401:CDL:H372	32:i:401:CDL:H141	1.83	0.60
12:d:115:GLN:HG2	20:l:62:ILE:HG12	1.84	0.60
20:l:72:GLN:NE2	25:r:459:TYR:O	2.34	0.60
29:w:165:SER:HB3	29:w:245:PHE:CZ	2.37	0.60
10:b:123:PHE:HB3	28:v:40:VAL:HG11	1.82	0.60
20:l:161:ARG:NH1	20:l:238:GLU:OE1	2.34	0.60
18:j:17:LEU:HD12	18:j:20:ILE:HD11	1.82	0.60
20:l:55:MET:HE2	20:l:471:ASN:HB3	1.84	0.60
6:X:114:ASP:O	6:X:118:ILE:HG13	2.01	0.59
17:i:95:MET:HE1	17:i:145:ILE:HD12	1.84	0.59
21:m:27:ILE:O	21:m:31:LEU:HD12	2.02	0.59
29:w:139:ARG:NH1	29:w:166:ASP:OD2	2.35	0.59
20:l:264:TYR:CD1	20:l:265:PRO:HD3	2.37	0.59
27:u:121:ASP:OD1	27:u:122:LEU:N	2.34	0.59
12:d:90:MET:HE1	25:r:48:ASN:H	1.67	0.59
25:r:22:MET:O	25:r:26:ASN:ND2	2.35	0.59
25:r:447:LEU:HD11	33:r:503:PLX:H371	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:39:HIS:NE2	7:Y:41:GLU:OE2	2.35	0.59
4:V:53:VAL:HA	4:V:56:THR:HG22	1.83	0.59
26:s:200:LEU:HD11	26:s:285:LEU:HD21	1.84	0.59
26:s:233:MET:HE1	26:s:234:MET:HE2	1.85	0.59
32:r:505:CDL:H742	32:r:505:CDL:H271	1.85	0.58
2:S:19:PRO:HB3	26:s:9:LEU:HD12	1.84	0.58
9:a:131:LYS:NZ	22:n:32:ASP:OD2	2.35	0.58
2:S:54:ILE:HD11	16:h:106:PRO:HB3	1.84	0.58
21:m:3:MET:HG3	21:m:8:ILE:HD11	1.84	0.58
12:d:36:ILE:O	12:d:40:LEU:HD23	2.03	0.58
17:i:280:THR:O	17:i:284:MET:HG2	2.04	0.58
10:b:28:LEU:HG	10:b:32:GLU:HG2	1.86	0.58
11:c:105:ILE:HG21	11:c:109:LEU:HD22	1.84	0.58
10:b:18:LEU:HD11	24:p:163:LEU:HD22	1.85	0.58
10:b:104:ILE:HD13	12:d:18:PRO:HG3	1.86	0.58
25:r:371:PRO:HD2	32:r:504:CDL:H391	1.85	0.58
7:Y:40:ILE:HG23	7:Y:49:GLN:HB2	1.86	0.58
33:a:202:PLX:H102	25:r:40:SER:HB3	1.86	0.57
12:d:144:SER:O	12:d:158:LYS:NZ	2.32	0.57
19:k:23:ARG:HD3	21:m:23:LYS:HB2	1.85	0.57
29:w:87:PRO:O	29:w:142:GLN:NE2	2.37	0.57
20:l:359:MET:O	20:l:436:ARG:NH2	2.36	0.57
29:w:269:VAL:O	29:w:273:ILE:HG12	2.04	0.57
9:a:160:MET:HE2	9:a:167:PRO:HD2	1.85	0.57
29:w:176:GLN:NE2	29:w:236:ASP:OD2	2.37	0.57
9:a:139:ILE:HG23	25:r:54:LEU:HD23	1.86	0.57
32:g:202:CDL:H121	32:g:202:CDL:H762	1.87	0.57
15:g:12:PRO:HB3	16:h:5:ASP:HB3	1.87	0.57
23:o:59:VAL:HG23	25:r:423:ILE:HG12	1.86	0.57
24:p:51:HIS:CD2	24:p:63:LEU:HD11	2.39	0.57
17:i:276:ILE:HG21	30:r:501:PEE:H14	1.86	0.57
32:a:201:CDL:H772	32:a:201:CDL:H201	1.85	0.57
25:r:403:THR:HA	25:r:406:TYR:CE2	2.40	0.57
26:s:9:LEU:HD22	26:s:95:LEU:HD13	1.87	0.57
26:s:50:ALA:O	26:s:54:LYS:HG2	2.05	0.57
26:s:102:VAL:HG21	26:s:154:LEU:HD11	1.86	0.57
6:X:117:GLU:OE1	24:p:45:ARG:NH1	2.37	0.56
9:a:108:GLU:HB2	9:a:111:GLU:HG3	1.87	0.56
27:u:83:THR:HA	27:u:86:TRP:CD1	2.40	0.56
28:v:44:GLN:NE2	28:v:48:ASP:OD2	2.37	0.56
4:V:12:ILE:HB	4:V:21:LYS:HD3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:63:GLU:OE2	27:u:119:ARG:NH2	2.38	0.56
8:Z:24:ILE:O	8:Z:27:THR:OG1	2.22	0.56
9:a:82:VAL:HG11	13:e:104:THR:HG21	1.88	0.56
20:l:594:THR:HA	20:l:597:ILE:HG22	1.86	0.56
29:w:246:LEU:HD12	29:w:255:VAL:HG11	1.88	0.56
24:p:29:SER:HB3	24:p:76:HIS:HD2	1.70	0.56
12:d:28:ASN:HD21	12:d:31:THR:HG23	1.71	0.56
11:c:75:TYR:CG	11:c:76:PRO:HD2	2.39	0.56
12:d:86:PHE:O	12:d:90:MET:HG2	2.06	0.56
6:X:85:TYR:OH	8:Z:22:TRP:NE1	2.28	0.56
12:d:142:ARG:NE	13:e:138:GLU:O	2.35	0.56
20:l:173:LEU:HD12	25:r:405:LEU:HD21	1.88	0.56
2:S:50:ARG:O	2:S:54:ILE:HG12	2.06	0.56
20:l:558:LEU:HB3	25:r:214:LEU:HD21	1.88	0.56
25:r:122:PHE:HE1	25:r:238:LEU:HB3	1.71	0.56
20:l:142:ILE:HG12	25:r:370:PRO:HB2	1.88	0.55
29:w:118:TYR:OH	35:w:401:ADP:O2'	2.23	0.55
20:l:533:MET:HG3	30:l:702:PEE:H23	1.88	0.55
17:i:95:MET:HE2	17:i:149:ILE:HG22	1.87	0.55
25:r:371:PRO:O	25:r:448:THR:OG1	2.24	0.55
20:l:97:THR:HG21	20:l:125:LEU:HD22	1.88	0.55
10:b:86:LEU:HD11	20:l:9:LEU:HD12	1.88	0.55
16:h:18:MET:HE1	21:m:153:LEU:HD11	1.88	0.55
17:i:236:LYS:HG2	17:i:237:MET:HG3	1.89	0.55
17:i:314:LYS:NZ	29:w:309:THR:OG1	2.40	0.55
20:l:417:SER:HB2	20:l:493:VAL:HG22	1.88	0.55
17:i:42:PRO:HG2	21:m:167:VAL:HG22	1.88	0.55
29:w:172:ALA:HB2	29:w:237:ILE:HG12	1.88	0.55
6:X:105:MET:HE1	6:X:139:MET:SD	2.47	0.55
15:g:56:VAL:HG21	25:r:17:MET:HE1	1.89	0.54
20:l:526:LEU:HD12	20:l:530:PRO:HG2	1.89	0.54
20:l:227:PHE:O	20:l:230:HIS:ND1	2.37	0.54
23:o:112:LYS:O	23:o:116:ILE:HG12	2.06	0.54
26:s:221:ALA:O	26:s:225:MET:HG3	2.07	0.54
27:u:49:GLU:OE1	27:u:135:ARG:NH2	2.40	0.54
7:Y:94:ASP:HB3	7:Y:99:ILE:HB	1.90	0.54
26:s:195:ARG:HD3	26:s:231:ILE:HD11	1.89	0.54
8:Z:22:TRP:HB3	8:Z:50:ALA:HB3	1.89	0.54
20:l:245:ALA:O	20:l:249:SER:OG	2.24	0.54
33:r:503:PLX:H212	32:r:504:CDL:H801	1.90	0.54
4:V:2:ALA:HA	20:l:601:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:134:GLU:OE1	22:n:57:TRP:NE1	2.30	0.54
25:r:328:CYS:HB3	25:r:437:MET:HE1	1.90	0.54
12:d:2:PRO:O	12:d:7:LYS:NZ	2.41	0.54
25:r:196:TRP:CD1	25:r:250:LEU:HB3	2.43	0.54
10:b:108:ASP:HB2	10:b:117:ILE:HD12	1.89	0.54
11:c:90:TYR:OH	23:o:44:LYS:NZ	2.41	0.54
5:W:89:GLU:O	5:W:93:GLU:HG2	2.08	0.54
13:e:113:ARG:HA	25:r:46:GLY:H	1.73	0.54
20:l:15:LEU:HD11	20:l:94:LEU:HD21	1.90	0.53
19:k:45:THR:HG23	21:m:52:LEU:HD13	1.89	0.53
20:l:554:ASP:OD2	25:r:288:TYR:OH	2.24	0.53
25:r:373:ILE:HD11	25:r:444:LEU:HD23	1.89	0.53
17:i:289:ASN:HA	17:i:292:PHE:CE2	2.42	0.53
11:c:62:TYR:CE1	11:c:76:PRO:HB3	2.44	0.53
19:k:57:ASN:HB3	21:m:143:ILE:HG13	1.90	0.53
20:l:125:LEU:O	20:l:129:MET:HG2	2.07	0.53
20:l:327:LEU:O	20:l:331:MET:HG2	2.09	0.53
23:o:48:LEU:HB3	24:p:166:LEU:HD13	1.91	0.53
26:s:69:SER:O	26:s:73:ILE:HG12	2.08	0.53
11:c:184:TYR:HB2	28:v:27:PRO:HB3	1.91	0.53
12:d:119:GLU:HG2	28:v:52:MET:HA	1.90	0.53
19:k:8:ILE:HG21	19:k:43:MET:HB2	1.89	0.53
29:w:39:GLY:HA2	29:w:296:MET:HE1	1.91	0.53
7:Y:43:ARG:NH1	7:Y:47:PHE:O	2.42	0.53
20:l:78:LEU:HD11	32:r:504:CDL:H251	1.90	0.53
10:b:74:HIS:NE2	20:l:35:TYR:OH	2.32	0.53
28:v:46:MET:HE3	28:v:56:ARG:HG2	1.91	0.53
4:V:30:GLY:O	4:V:34:LEU:HG	2.09	0.52
9:a:132:ASN:ND2	25:r:49:SER:O	2.24	0.52
14:f:47:THR:HG23	15:g:65:LEU:HD22	1.91	0.52
18:j:6:THR:HG21	26:s:87:VAL:HG11	1.91	0.52
20:l:556:ILE:O	20:l:560:THR:OG1	2.20	0.52
21:m:170:GLU:OE2	21:m:173:ARG:NH2	2.42	0.52
27:u:9:THR:OG1	27:u:12:ASP:OD1	2.26	0.52
29:w:65:ASN:OD1	29:w:66:ILE:N	2.34	0.52
29:w:123:SER:OG	29:w:125:ASP:OD1	2.22	0.52
25:r:108:MET:HB3	25:r:121:LEU:HD13	1.92	0.52
5:W:97:ILE:HG23	16:h:86:LEU:HD12	1.91	0.52
28:v:22:MET:HE1	28:v:102:PHE:HA	1.90	0.52
5:W:137:THR:HG23	5:W:138:TYR:CD2	2.45	0.52
20:l:182:PHE:HD1	20:l:186:MET:HE2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:231:LEU:HA	25:r:235:LEU:HB2	1.91	0.52
10:b:86:LEU:HA	10:b:90:VAL:HB	1.90	0.52
20:l:482:MET:HG2	20:l:487:LYS:HD3	1.90	0.52
9:a:60:SER:HB3	24:p:107:TRP:HA	1.92	0.52
11:c:185:GLU:HB2	28:v:37:ARG:HG2	1.92	0.52
20:l:509:TYR:CE1	24:p:33:HIS:CE1	2.97	0.52
4:V:35:ILE:HD12	20:l:597:ILE:HD12	1.92	0.51
25:r:112:ALA:HB1	25:r:118:PHE:HB2	1.92	0.51
11:c:153:TYR:HB3	20:l:403:TYR:HD1	1.75	0.51
21:m:17:PHE:HA	21:m:20:PHE:CE1	2.44	0.51
32:r:504:CDL:H541	32:r:504:CDL:HA61	1.92	0.51
33:g:201:PLX:H301	17:i:347:ASN:HB3	1.93	0.51
19:k:37:MET:HE1	21:m:64:MET:HE1	1.91	0.51
29:w:96:SER:HA	29:w:101:GLY:HA2	1.92	0.51
9:a:141:GLN:O	9:a:145:GLU:HG3	2.10	0.51
24:p:26:HIS:CD2	24:p:79:PRO:HB3	2.46	0.51
25:r:197:LEU:HD21	33:r:502:PLX:H142	1.93	0.51
26:s:24:GLU:HA	26:s:271:LEU:HD13	1.92	0.51
4:V:123:ALA:O	4:V:127:MET:HG3	2.11	0.51
20:l:467:ILE:O	20:l:471:ASN:HB2	2.10	0.51
25:r:357:THR:O	25:r:361:VAL:HG23	2.11	0.51
19:k:43:MET:HE3	19:k:47:ILE:HD11	1.92	0.51
25:r:48:ASN:OD1	25:r:49:SER:N	2.39	0.51
29:w:88:GLU:OE2	29:w:161:ARG:NH1	2.44	0.51
3:U:26:GLY:HA3	30:U:101:PEE:H37	1.93	0.51
11:c:38:PRO:HB2	23:o:75:ASN:HD22	1.76	0.51
22:n:7:ILE:O	22:n:11:HIS:N	2.43	0.51
17:i:20:VAL:HG11	17:i:137:ALA:HB1	1.94	0.50
20:l:86:SER:OG	20:l:262:ARG:NH2	2.42	0.50
20:l:221:ALA:HA	20:l:226:GLN:HG2	1.93	0.50
18:j:68:GLU:HG2	21:m:161:LEU:HD13	1.92	0.50
32:r:504:CDL:H312	32:r:504:CDL:H761	1.93	0.50
29:w:165:SER:HB3	29:w:245:PHE:CE1	2.46	0.50
29:w:246:LEU:O	29:w:250:SER:OG	2.23	0.50
26:s:25:ARG:HD2	34:s:401:UQ:HM21	1.93	0.50
11:c:81:ARG:HG2	11:c:81:ARG:HH11	1.76	0.50
25:r:369:LEU:HD12	25:r:370:PRO:HD2	1.92	0.50
17:i:12:THR:HG21	21:m:163:ILE:HG21	1.94	0.50
17:i:328:THR:O	17:i:332:LEU:HG	2.12	0.50
20:l:100:ILE:HG21	20:l:246:LEU:HB2	1.94	0.50
26:s:21:THR:O	26:s:25:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:w:146:ALA:HB1	29:w:157:VAL:HG21	1.93	0.50
5:W:74:LEU:O	5:W:78:GLU:HG3	2.12	0.50
32:a:201:CDL:H531	30:b:201:PEE:H56	1.92	0.50
20:l:309:GLN:O	20:l:313:MET:HG3	2.12	0.50
16:h:69:ARG:O	16:h:73:MET:HG3	2.11	0.49
29:w:258:TYR:CE2	29:w:269:VAL:HG22	2.46	0.49
5:W:86:MET:SD	5:W:124:LEU:HB3	2.52	0.49
16:h:97:HIS:HA	16:h:102:GLU:HB3	1.94	0.49
17:i:54:GLU:HG3	19:k:93:LEU:HD22	1.95	0.49
11:c:39:GLY:H	11:c:74:ASP:HB2	1.77	0.49
2:S:69:ILE:HD11	27:u:68:LEU:HD23	1.94	0.49
18:j:69:ILE:HD11	26:s:144:VAL:HG13	1.94	0.49
4:V:121:THR:O	4:V:125:VAL:HG23	2.13	0.49
5:W:144:THR:HB	26:s:96:ILE:HG23	1.93	0.49
6:X:118:ILE:O	6:X:122:MET:HG2	2.12	0.49
19:k:98:CYS:HB2	20:l:580:GLN:HB2	1.94	0.49
3:U:38:TYR:HB2	26:s:310:MET:O	2.11	0.49
7:Y:62:SER:OG	20:l:371:THR:OG1	2.30	0.49
25:r:12:LEU:HB2	25:r:13:PRO:HD3	1.94	0.49
29:w:258:TYR:HE2	29:w:269:VAL:HG22	1.78	0.49
5:W:90:ASN:ND2	5:W:123:GLU:O	2.45	0.49
20:l:407:TRP:O	20:l:411:MET:HG2	2.13	0.49
25:r:237:LYS:HD2	25:r:316:MET:HB3	1.94	0.49
26:s:90:PRO:HB3	26:s:94:PRO:HD3	1.94	0.49
5:W:51:MET:HA	26:s:313:SER:HB2	1.94	0.49
9:a:67:PHE:CE2	25:r:434:ASN:HB3	2.47	0.49
4:V:102:GLY:O	4:V:106:ARG:N	2.46	0.49
19:k:22:TYR:HB3	20:l:585:LYS:HG2	1.95	0.49
24:p:133:TRP:O	24:p:137:VAL:HG23	2.13	0.49
25:r:225:ILE:O	25:r:229:MET:HG3	2.13	0.49
11:c:125:SER:O	11:c:129:MET:HG3	2.13	0.48
17:i:54:GLU:HG2	17:i:58:LYS:HE2	1.95	0.48
28:v:71:ARG:NH2	28:v:72:ASP:OD1	2.46	0.48
30:U:102:PEE:H19	26:s:180:PRO:HB3	1.94	0.48
30:U:102:PEE:H64	26:s:273:ILE:HD11	1.95	0.48
11:c:60:GLU:OE2	11:c:60:GLU:N	2.29	0.48
20:l:536:LEU:HB3	20:l:537:PRO:HD3	1.95	0.48
25:r:312:ALA:O	25:r:316:MET:HG3	2.13	0.48
20:l:496:MET:HE3	20:l:500:LEU:HD11	1.94	0.48
29:w:170:LEU:HD22	29:w:187:TYR:CD1	2.49	0.48
7:Y:45:ARG:HG2	20:l:439:PRO:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:43:VAL:HG11	17:i:129:LEU:HD23	1.96	0.48
20:l:159:HIS:HB3	25:r:416:ARG:HD2	1.96	0.48
29:w:274:GLU:O	29:w:277:LYS:NZ	2.47	0.48
11:c:78:LEU:HD12	11:c:106:HIS:HA	1.96	0.48
20:l:290:LEU:O	20:l:293:ILE:HG22	2.14	0.48
32:r:504:CDL:H311	32:r:504:CDL:H561	1.95	0.48
17:i:51:ARG:HE	19:k:95:LEU:HD23	1.79	0.48
27:u:137:LEU:HD12	27:u:138:PRO:HD2	1.96	0.48
29:w:143:TYR:OH	29:w:199:LEU:O	2.27	0.48
2:S:43:TYR:CZ	5:W:68:ARG:HG3	2.48	0.48
20:l:292:ALA:HB2	20:l:304:PHE:HB3	1.96	0.48
7:Y:71:TRP:CD1	7:Y:72:ARG:HH21	2.32	0.48
11:c:38:PRO:HD3	23:o:67:ARG:HG3	1.96	0.48
25:r:299:VAL:O	25:r:303:ILE:HG12	2.14	0.48
29:w:73:LEU:HD11	29:w:269:VAL:HG21	1.96	0.48
3:U:42:ALA:HB2	26:s:312:ALA:HA	1.96	0.48
6:X:105:MET:SD	6:X:105:MET:N	2.87	0.47
13:e:76:TYR:HB2	13:e:83:ASP:OD1	2.14	0.47
17:i:106:LEU:HG	17:i:138:PRO:HB2	1.95	0.47
25:r:229:MET:HE3	25:r:328:CYS:SG	2.54	0.47
29:w:145:ASP:O	29:w:148:GLU:HG3	2.14	0.47
5:W:93:GLU:HG3	16:h:98:HIS:NE2	2.28	0.47
6:X:120:MET:HE1	24:p:24:LEU:HB3	1.96	0.47
10:b:88:TYR:CE1	12:d:49:ARG:HG2	2.49	0.47
18:j:49:LEU:N	18:j:50:PRO:HD2	2.29	0.47
20:l:286:LEU:HD22	20:l:411:MET:SD	2.53	0.47
22:n:18:PRO:O	22:n:21:PHE:HB3	2.13	0.47
12:d:126:ALA:O	12:d:130:GLU:HG2	2.14	0.47
17:i:112:HIS:HB2	17:i:184:ILE:HD13	1.96	0.47
32:l:701:CDL:H751	32:l:701:CDL:H781	1.49	0.47
33:r:503:PLX:H122	32:r:504:CDL:H652	1.96	0.47
26:s:281:ARG:HB2	26:s:284:GLN:HG3	1.96	0.47
33:g:201:PLX:H1C2	16:h:2:PRO:HD2	1.95	0.47
17:i:278:MET:O	17:i:282:MET:HG3	2.14	0.47
25:r:101:LEU:HD13	32:r:505:CDL:H441	1.96	0.47
18:j:68:GLU:OE1	18:j:98:LEU:HD13	2.15	0.47
32:r:505:CDL:H461	32:r:505:CDL:H212	1.96	0.47
29:w:295:ARG:HA	29:w:298:VAL:HG22	1.95	0.47
7:Y:60:PHE:O	7:Y:64:THR:HG23	2.13	0.47
30:b:201:PEE:H38	20:l:66:TRP:HZ3	1.80	0.47
16:h:38:LYS:NZ	16:h:39:GLU:OE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:j:73:LEU:O	26:s:160:TYR:OH	2.32	0.47
20:l:86:SER:O	20:l:90:ILE:HG12	2.14	0.47
20:l:128:MET:HG2	20:l:251:THR:HG22	1.96	0.47
29:w:167:PHE:O	29:w:170:LEU:HB3	2.15	0.47
29:w:279:ASP:OD1	29:w:279:ASP:N	2.45	0.47
7:Y:99:ILE:HD13	28:v:108:LEU:HD23	1.97	0.47
11:c:46:GLU:HG2	11:c:47:GLU:N	2.29	0.47
32:g:202:CDL:HB62	27:u:172:MET:HE2	1.97	0.47
17:i:72:MET:HB2	19:k:40:LEU:HD21	1.97	0.47
20:l:452:ASN:HA	20:l:455:LYS:HG2	1.97	0.47
23:o:102:TYR:HB2	25:r:263:MET:HG3	1.96	0.47
25:r:74:PRO:O	25:r:78:MET:HG3	2.15	0.47
25:r:216:LEU:HD23	25:r:287:ALA:HB1	1.97	0.47
33:r:503:PLX:H222	32:r:504:CDL:H521	1.97	0.47
28:v:104:ARG:O	28:v:108:LEU:HG	2.14	0.47
20:l:237:MET:HE3	20:l:303:ALA:HB2	1.97	0.47
18:j:95:LEU:HD13	26:s:302:MET:HG3	1.97	0.47
20:l:250:SER:HB2	20:l:333:ALA:HA	1.97	0.47
22:n:35:LEU:C	22:n:37:ALA:H	2.22	0.47
25:r:130:LEU:HD22	25:r:150:LEU:HD13	1.96	0.47
25:r:248:THR:HG23	25:r:249:ILE:HG23	1.97	0.47
33:r:502:PLX:H92	33:r:502:PLX:H121	1.78	0.47
27:u:103:GLN:N	27:u:103:GLN:OE1	2.48	0.47
3:U:56:PRO:HG2	27:u:45:LEU:HB2	1.97	0.46
17:i:133:TRP:HE3	32:i:401:CDL:H392	1.80	0.46
11:c:156:VAL:HG11	28:v:95:TYR:CZ	2.50	0.46
25:r:290:SER:HA	25:r:319:HIS:HE2	1.80	0.46
6:X:79:ILE:O	6:X:83:VAL:HG23	2.15	0.46
31:X:201:8Q1:O27	31:X:201:8Q1:O33	2.31	0.46
21:m:45:LEU:HD23	21:m:50:SER:HA	1.97	0.46
4:V:73:THR:OG1	4:V:93:GLY:HA2	2.15	0.46
5:W:98:MET:HG3	5:W:104:TRP:CD1	2.50	0.46
11:c:39:GLY:C	11:c:74:ASP:HB2	2.39	0.46
21:m:25:SER:O	21:m:27:ILE:N	2.49	0.46
22:n:19:VAL:O	22:n:22:VAL:HG22	2.15	0.46
29:w:350:LYS:HB3	29:w:351:TRP:HE3	1.79	0.46
11:c:156:VAL:HG12	28:v:99:MET:HG2	1.97	0.46
20:l:363:TYR:HA	20:l:370:THR:HG21	1.96	0.46
28:v:78:LEU:HD23	28:v:78:LEU:H	1.81	0.46
29:w:132:GLN:NE2	29:w:166:ASP:OD1	2.49	0.46
29:w:292:HIS:CE1	29:w:296:MET:HE3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:w:330:LYS:HA	29:w:330:LYS:HD2	1.77	0.46
15:g:45:LEU:HD22	15:g:55:VAL:HG12	1.96	0.46
17:i:247:THR:O	17:i:251:MET:HG3	2.15	0.46
19:k:82:SER:O	19:k:86:GLY:N	2.39	0.46
24:p:65:ARG:NH1	24:p:65:ARG:CG	2.73	0.46
24:p:100:PRO:HG3	25:r:419:TYR:CE2	2.50	0.46
27:u:44:MET:HA	27:u:44:MET:HE2	1.98	0.46
20:l:383:MET:HB3	20:l:386:LEU:HD12	1.96	0.46
25:r:445:LEU:HD22	32:r:504:CDL:H401	1.98	0.46
6:X:111:ASP:HB3	6:X:114:ASP:OD1	2.16	0.46
12:d:33:LEU:HD13	20:l:49:VAL:HG13	1.98	0.46
26:s:62:ARG:HD3	26:s:64:ALA:H	1.81	0.46
31:X:201:8Q1:O40	31:X:201:8Q1:N36	2.49	0.46
9:a:179:ILE:HG21	16:h:38:LYS:HG3	1.98	0.46
10:b:81:ILE:HG23	30:b:201:PEE:H58	1.97	0.46
11:c:100:ASN:CB	11:c:103:GLU:HG2	2.41	0.46
11:c:127:ASN:O	11:c:131:LYS:HG3	2.16	0.46
13:e:90:VAL:HG22	25:r:28:THR:HG21	1.97	0.46
20:l:116:ARG:HA	20:l:119:LYS:HG2	1.98	0.46
7:Y:105:ASP:N	7:Y:105:ASP:OD1	2.47	0.46
18:j:18:VAL:HG22	26:s:222:MET:HG3	1.97	0.46
11:c:96:ASP:OD1	11:c:96:ASP:N	2.46	0.45
34:s:401:UQ:H101	34:s:401:UQ:H121	1.70	0.45
5:W:76:GLN:HG2	27:u:44:MET:HE1	1.99	0.45
24:p:58:VAL:HG12	24:p:58:VAL:O	2.16	0.45
25:r:115:LEU:HD12	25:r:174:LEU:HD22	1.99	0.45
11:c:37:PHE:HE1	23:o:66:ILE:HG22	1.81	0.45
26:s:84:THR:O	26:s:87:VAL:HG22	2.16	0.45
26:s:21:THR:HB	34:s:401:UQ:HM23	1.98	0.45
27:u:16:GLN:O	27:u:64:ASN:ND2	2.49	0.45
32:g:202:CDL:H712	32:g:202:CDL:H741	1.45	0.45
17:i:311:MET:HE2	17:i:311:MET:HB2	1.86	0.45
20:l:233:LEU:HB3	20:l:234:PRO:HD3	1.98	0.45
10:b:86:LEU:HD23	10:b:90:VAL:HG21	1.98	0.45
21:m:21:SER:O	21:m:23:LYS:NZ	2.50	0.45
29:w:281:GLY:O	29:w:284:PRO:HD2	2.17	0.45
11:c:62:TYR:CD1	11:c:76:PRO:HB3	2.51	0.45
13:e:103:SER:HA	33:r:503:PLX:H271	1.98	0.45
18:j:70:ALA:HB2	21:m:59:ILE:HG13	1.99	0.45
20:l:83:ASP:OD2	20:l:262:ARG:NH1	2.50	0.45
23:o:118:GLU:OE1	23:o:120:LYS:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:r:502:PLX:H51	33:r:502:PLX:H6	1.35	0.45
15:g:2:THR:HG22	15:g:4:MET:HG3	1.99	0.45
17:i:38:LEU:HD12	19:k:73:LEU:HD22	1.98	0.45
20:l:10:THR:HA	20:l:13:THR:HG22	1.99	0.45
11:c:38:PRO:HB2	23:o:75:ASN:ND2	2.32	0.45
20:l:562:LEU:HB3	20:l:563:PRO:HD3	1.98	0.45
7:Y:102:ASP:OD1	7:Y:102:ASP:O	2.35	0.45
17:i:102:LEU:HD13	17:i:142:LEU:HG	1.99	0.45
17:i:175:LEU:O	17:i:179:MET:HG2	2.17	0.45
18:j:73:LEU:HD12	21:m:55:MET:HE1	1.99	0.45
20:l:37:LYS:HD3	20:l:98:TRP:HE1	1.82	0.45
20:l:509:TYR:HE1	24:p:33:HIS:CE1	2.34	0.45
26:s:26:LYS:HD2	26:s:36:GLY:HA3	1.99	0.45
17:i:26:TRP:HB3	17:i:74:ILE:HD13	1.99	0.44
19:k:23:ARG:HG2	21:m:23:LYS:HE2	1.99	0.44
20:l:174:TYR:CD2	20:l:232:TRP:HB3	2.52	0.44
26:s:149:ILE:HG13	26:s:297:THR:HG23	1.99	0.44
26:s:222:MET:HE2	26:s:222:MET:HA	1.98	0.44
11:c:32:VAL:HG13	23:o:61:GLU:OE1	2.16	0.44
32:l:701:CDL:H572	32:l:701:CDL:H541	1.65	0.44
25:r:300:ALA:O	25:r:308:SER:HB3	2.17	0.44
25:r:349:GLN:HG3	25:r:415:GLN:O	2.17	0.44
28:v:51:LEU:HD13	28:v:63:LEU:HD23	1.99	0.44
17:i:62:THR:HG21	17:i:114:TRP:CD1	2.52	0.44
25:r:445:LEU:O	25:r:448:THR:HG22	2.17	0.44
2:S:14:ALA:O	2:S:18:ILE:HG12	2.17	0.44
21:m:55:MET:HA	21:m:55:MET:HE2	1.98	0.44
29:w:192:LYS:HG3	29:w:193:VAL:N	2.32	0.44
29:w:211:VAL:HA	29:w:214:ILE:HG22	1.99	0.44
30:U:102:PEE:H16	30:U:102:PEE:H21	1.74	0.44
6:X:103:HIS:HE1	6:X:105:MET:HE2	1.83	0.44
10:b:79:VAL:HG22	20:l:10:THR:HG21	1.99	0.44
33:g:201:PLX:H22	33:g:201:PLX:H1C3	1.73	0.44
17:i:111:PHE:HA	20:l:591:PHE:CE1	2.51	0.44
17:i:268:GLN:HG3	27:u:168:PHE:HZ	1.82	0.44
19:k:25:HIS:O	19:k:28:SER:N	2.49	0.44
19:k:37:MET:HG3	19:k:67:ALA:CB	2.48	0.44
10:b:100:ARG:HD3	20:l:60:GLU:HG3	1.98	0.44
17:i:119:THR:HG22	17:i:176:ARG:HB3	2.00	0.44
17:i:245:MET:HE3	17:i:245:MET:HB3	1.85	0.44
21:m:28:TYR:HA	21:m:31:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:o:35:GLU:O	23:o:39:ILE:HG22	2.18	0.44
25:r:321:LEU:HD13	25:r:444:LEU:HG	2.00	0.44
33:r:503:PLX:H121	33:r:503:PLX:H152	1.45	0.44
11:c:160:GLN:HG2	11:c:183:HIS:CD2	2.53	0.44
17:i:160:LEU:O	17:i:164:ILE:HG12	2.18	0.44
21:m:42:GLY:HA2	30:m:201:PEE:H23	2.00	0.44
21:m:62:GLY:HA3	26:s:110:SER:HB3	2.00	0.44
12:d:74:ILE:HG23	12:d:156:LEU:HD22	2.00	0.44
12:d:142:ARG:HH21	13:e:138:GLU:HB3	1.82	0.44
20:l:228:GLY:HA3	30:l:702:PEE:H39	1.99	0.44
24:p:64:LEU:C	24:p:64:LEU:HD23	2.42	0.44
26:s:140:ILE:O	26:s:143:GLU:HG2	2.18	0.44
3:U:18:VAL:HG11	26:s:292:SER:HA	2.00	0.44
32:g:202:CDL:HB21	32:g:202:CDL:H151	1.99	0.44
17:i:237:MET:HE3	17:i:237:MET:HB2	1.94	0.44
17:i:254:LEU:HD23	25:r:127:VAL:HG22	2.00	0.44
32:l:701:CDL:H622	32:l:701:CDL:H591	1.49	0.44
25:r:133:ILE:HD11	25:r:231:LEU:HD11	2.00	0.44
27:u:96:LEU:HB3	27:u:98:ARG:HG2	2.00	0.44
29:w:353:TRP:CE3	29:w:354:LEU:HG	2.53	0.44
20:l:108:MET:HE3	20:l:108:MET:HB3	1.93	0.43
6:X:83:VAL:HG22	6:X:122:MET:CE	2.47	0.43
7:Y:39:HIS:HE1	8:Z:10:GLY:HA2	1.83	0.43
22:n:13:VAL:O	22:n:16:LEU:HB2	2.17	0.43
11:c:83:GLN:HA	11:c:86:ARG:HG3	1.99	0.43
14:f:72:ARG:NH2	15:g:18:ASN:OD1	2.47	0.43
20:l:83:ASP:O	20:l:87:VAL:HG22	2.18	0.43
20:l:241:THR:HG21	20:l:344:GLY:HA3	2.01	0.43
24:p:35:ASP:OD1	24:p:36:LYS:N	2.50	0.43
25:r:87:GLU:OE2	25:r:91:ARG:HD2	2.19	0.43
30:r:501:PEE:H21	30:r:501:PEE:H28	1.91	0.43
6:X:119:ILE:HG21	6:X:135:ALA:HB1	2.01	0.43
8:Z:25:GLU:HA	8:Z:30:GLU:OE1	2.18	0.43
8:Z:63:PHE:CZ	20:l:424:THR:HG23	2.53	0.43
11:c:162:PRO:HB3	28:v:58:TYR:CE1	2.53	0.43
32:g:202:CDL:H752	32:g:202:CDL:H781	1.74	0.43
17:i:88:LYS:HD2	17:i:148:SER:OG	2.17	0.43
20:l:49:VAL:HB	20:l:50:PRO:HD3	2.01	0.43
24:p:119:PHE:O	24:p:123:GLU:OE1	2.36	0.43
26:s:9:LEU:O	26:s:13:ILE:HG12	2.19	0.43
26:s:130:ILE:O	26:s:134:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:w:86:PHE:HB2	29:w:159:LEU:HD23	2.00	0.43
5:W:130:ASN:HB3	21:m:1:MET:N	2.33	0.43
5:W:133:ILE:O	5:W:137:THR:HG22	2.19	0.43
13:e:69:LYS:HE2	13:e:69:LYS:HB2	1.91	0.43
20:l:398:ALA:O	20:l:402:SER:OG	2.31	0.43
27:u:83:THR:HA	27:u:86:TRP:NE1	2.33	0.43
20:l:559:GLU:O	20:l:563:PRO:HD2	2.18	0.43
24:p:28:GLU:HB3	24:p:37:TYR:CE1	2.54	0.43
26:s:173:TRP:HB3	26:s:175:ILE:HG22	2.01	0.43
13:e:73:SER:O	13:e:74:HIS:HB2	2.19	0.43
13:e:92:PHE:O	13:e:96:SER:HB2	2.18	0.43
16:h:18:MET:HG2	17:i:25:HIS:HE2	1.82	0.43
19:k:38:LEU:O	19:k:42:ILE:HG12	2.18	0.43
26:s:95:LEU:HD23	26:s:96:ILE:HG13	1.99	0.43
29:w:270:VAL:HG12	29:w:274:GLU:OE1	2.18	0.43
12:d:114:GLN:OE1	20:l:199:GLN:HG3	2.18	0.43
17:i:137:ALA:HB3	17:i:138:PRO:HD3	1.99	0.43
29:w:350:LYS:HA	29:w:350:LYS:HD3	1.85	0.43
17:i:4:ILE:HD13	32:i:401:CDL:H741	2.00	0.43
33:j:201:PLX:H312	33:j:201:PLX:H282	1.80	0.43
20:l:137:LEU:HD13	20:l:186:MET:HG2	2.01	0.43
21:m:23:LYS:N	21:m:24:PRO:HD3	2.33	0.43
29:w:186:HIS:HB2	29:w:314:LEU:HD11	2.00	0.43
29:w:350:LYS:HB3	29:w:351:TRP:CE3	2.54	0.43
18:j:55:PHE:HB3	21:m:70:TYR:HE2	1.83	0.43
20:l:350:LEU:HD11	20:l:437:PHE:HB3	2.01	0.43
25:r:127:VAL:HB	25:r:128:PRO:HD3	2.00	0.43
32:g:202:CDL:H611	32:r:505:CDL:H873	2.01	0.42
18:j:3:ILE:HD13	30:m:201:PEE:H50	2.00	0.42
18:j:5:LEU:HD23	26:s:2:PHE:HD2	1.84	0.42
21:m:61:LEU:HD23	21:m:65:LEU:HD12	2.01	0.42
24:p:76:HIS:O	24:p:78:GLN:N	2.52	0.42
3:U:53:TYR:CZ	27:u:44:MET:HG3	2.54	0.42
32:l:701:CDL:H872	32:l:701:CDL:H201	1.99	0.42
22:n:11:HIS:HA	22:n:14:HIS:HD2	1.84	0.42
11:c:145:TRP:CZ2	11:c:149:ILE:HD11	2.54	0.42
17:i:44:LEU:HD22	17:i:122:ILE:HG21	2.02	0.42
18:j:90:MET:SD	21:m:151:THR:HG23	2.60	0.42
20:l:271:LYS:HB2	20:l:271:LYS:HE2	1.81	0.42
20:l:313:MET:HG2	20:l:328:HIS:HD2	1.85	0.42
32:r:504:CDL:H392	32:r:504:CDL:H341	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:32:GLU:HB3	10:b:33:PRO:HD3	2.01	0.42
10:b:89:HIS:CD2	30:b:201:PEE:H49	2.54	0.42
16:h:68:LEU:HD23	16:h:68:LEU:HA	1.92	0.42
17:i:11:MET:HE2	17:i:11:MET:HA	2.01	0.42
34:s:401:UQ:H121	34:s:401:UQ:H152	1.85	0.42
27:u:28:ALA:HB2	27:u:82:PHE:CE1	2.54	0.42
27:u:38:LYS:HB3	27:u:39:PRO:HD3	2.00	0.42
29:w:246:LEU:CD1	29:w:255:VAL:CG1	2.97	0.42
33:a:202:PLX:O3	22:n:29:ARG:NH2	2.53	0.42
18:j:92:LEU:HD22	26:s:302:MET:HG2	2.02	0.42
20:l:14:ILE:HD11	20:l:43:ALA:HA	2.02	0.42
20:l:422:TYR:O	20:l:426:ILE:HG12	2.20	0.42
32:l:701:CDL:H673	32:l:701:CDL:H472	2.01	0.42
26:s:89:LEU:HD22	26:s:240:ILE:HD12	2.02	0.42
26:s:294:LEU:HD12	26:s:294:LEU:HA	1.87	0.42
3:U:14:ALA:O	3:U:15:LYS:HG2	2.20	0.42
10:b:75:VAL:O	10:b:79:VAL:HG23	2.20	0.42
20:l:319:ILE:HG22	20:l:404:THR:HG21	2.01	0.42
1:Q:39:PRO:HB3	1:Q:43:TRP:CD1	2.54	0.42
16:h:94:PRO:HA	16:h:95:PRO:HD3	1.91	0.42
20:l:263:PHE:HD2	20:l:266:LEU:HD12	1.85	0.42
31:X:201:8Q1:O3	24:p:13:GLN:NE2	2.53	0.42
20:l:571:MET:HE2	20:l:571:MET:HB3	1.89	0.42
23:o:65:LEU:HD11	25:r:343:ILE:HD11	2.02	0.42
8:Z:32:VAL:HG13	24:p:39:TYR:HB2	2.01	0.42
15:g:32:ARG:O	15:g:36:MET:HG2	2.19	0.42
20:l:332:HIS:HA	20:l:335:PHE:CZ	2.54	0.42
20:l:564:LYS:HE2	23:o:77:TYR:CE2	2.54	0.42
32:r:504:CDL:H581	32:r:504:CDL:H611	1.73	0.42
6:X:123:GLU:OE1	24:p:25:ARG:NH2	2.48	0.41
20:l:491:LEU:HD12	20:l:491:LEU:HA	1.95	0.41
9:a:168:TRP:HB3	15:g:2:THR:O	2.19	0.41
20:l:392:LYS:O	20:l:396:ILE:HG12	2.20	0.41
24:p:108:HIS:CD2	24:p:109:PRO:HD2	2.55	0.41
33:r:502:PLX:H1C3	33:r:502:PLX:H22	1.77	0.41
28:v:80:CYS:HB2	28:v:83:GLU:OE1	2.20	0.41
12:d:80:LYS:HA	12:d:80:LYS:HD3	1.69	0.41
33:g:201:PLX:H131	33:g:201:PLX:H102	1.45	0.41
17:i:27:LEU:HD22	19:k:59:MET:HG2	2.01	0.41
1:Q:41:VAL:O	1:Q:45:GLU:HG2	2.21	0.41
6:X:84:LEU:HB3	6:X:88:LYS:HE2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:136:GLU:OE1	24:p:14:GLN:NE2	2.54	0.41
13:e:98:VAL:HG22	25:r:36:LEU:HB2	2.02	0.41
17:i:42:PRO:HG3	21:m:167:VAL:HG13	2.01	0.41
17:i:231:SER:O	17:i:234:TRP:HD1	2.04	0.41
20:l:152:PHE:CD1	20:l:168:ALA:HB1	2.56	0.41
1:Q:52:MET:HE3	1:Q:52:MET:HB3	1.82	0.41
20:l:124:PHE:CE1	20:l:252:MET:HB2	2.55	0.41
20:l:304:PHE:CZ	20:l:526:LEU:HD22	2.55	0.41
20:l:316:THR:OG1	20:l:395:ILE:HD12	2.20	0.41
23:o:8:PRO:HB3	23:o:14:LEU:HB2	2.01	0.41
26:s:267:THR:O	26:s:271:LEU:HG	2.20	0.41
11:c:110:ASP:OD1	11:c:110:ASP:N	2.54	0.41
32:g:202:CDL:H552	17:i:338:PRO:HG3	2.02	0.41
20:l:184:LEU:HD13	25:r:393:ILE:HG21	2.03	0.41
20:l:463:PHE:O	20:l:467:ILE:HG12	2.20	0.41
23:o:75:ASN:OD1	23:o:79:ASN:ND2	2.53	0.41
24:p:50:GLU:HG3	24:p:51:HIS:ND1	2.36	0.41
29:w:180:ARG:NH1	29:w:316:GLU:OE2	2.50	0.41
1:Q:64:PRO:HB3	17:i:51:ARG:HH12	1.86	0.41
3:U:53:TYR:CE2	27:u:44:MET:HG3	2.56	0.41
4:V:95:CYS:HA	4:V:115:CYS:HA	2.03	0.41
20:l:103:PHE:HB2	20:l:341:MET:HE3	2.02	0.41
23:o:31:LYS:O	23:o:35:GLU:HG3	2.20	0.41
28:v:92:HIS:O	28:v:96:VAL:HG23	2.20	0.41
12:d:90:MET:HE1	25:r:47:GLU:HB3	2.02	0.41
17:i:177:LYS:NZ	19:k:97:GLN:O	2.49	0.41
25:r:1:MET:HB2	25:r:52:PHE:CD2	2.56	0.41
32:r:505:CDL:H342	32:r:505:CDL:H202	2.03	0.41
2:S:17:PHE:HE1	26:s:257:ILE:HA	1.85	0.41
2:S:34:LYS:HE3	2:S:34:LYS:HB2	1.92	0.41
6:X:83:VAL:HA	6:X:122:MET:HE1	2.02	0.41
12:d:37:PHE:CD2	20:l:3:PRO:HB3	2.56	0.41
12:d:105:ILE:O	12:d:109:ARG:HG3	2.21	0.41
13:e:97:ILE:O	13:e:101:LEU:HB2	2.20	0.41
17:i:59:TYR:OH	17:i:134:GLN:NE2	2.50	0.41
17:i:320:THR:OG1	17:i:321:LYS:N	2.53	0.41
19:k:37:MET:HG3	19:k:67:ALA:HB1	2.03	0.41
20:l:378:LEU:HD13	20:l:383:MET:SD	2.61	0.41
21:m:70:TYR:O	21:m:74:MET:HG3	2.21	0.41
25:r:185:PRO:HB3	25:r:252:PRO:HD3	2.02	0.41
25:r:303:ILE:HD12	25:r:388:TRP:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:s:18:ALA:HB2	34:s:401:UQ:H152	2.03	0.41
29:w:295:ARG:O	29:w:299:GLN:HG2	2.21	0.41
15:g:15:PHE:HD1	33:g:201:PLX:H6	1.86	0.41
15:g:110:THR:O	15:g:114:ILE:HG13	2.20	0.41
17:i:190:MET:HG2	17:i:204:ASN:HB3	2.03	0.41
25:r:190:TRP:CZ2	33:r:502:PLX:H11	2.56	0.41
26:s:92:PRO:HB3	26:s:255:TYR:CD1	2.56	0.41
29:w:59:VAL:HG23	29:w:157:VAL:HG23	2.03	0.41
29:w:59:VAL:HG13	29:w:201:PRO:HA	2.03	0.41
10:b:32:GLU:HG3	24:p:115:TYR:HD1	1.86	0.40
11:c:167:TYR:HD2	11:c:168:LEU:HD22	1.86	0.40
30:i:402:PEE:H34	25:r:155:ALA:HB2	2.03	0.40
20:l:4:PHE:HZ	20:l:87:VAL:HG11	1.85	0.40
20:l:268:GLU:HA	20:l:274:GLN:NE2	2.35	0.40
20:l:411:MET:HA	20:l:411:MET:HE2	2.02	0.40
20:l:589:LEU:O	20:l:593:ILE:HG13	2.21	0.40
26:s:55:LEU:HD11	34:s:401:UQ:HM52	2.04	0.40
3:U:41:TYR:O	3:U:45:ILE:HG13	2.22	0.40
17:i:316:GLN:HB3	29:w:98:THR:HG21	2.03	0.40
18:j:81:THR:C	18:j:83:ASN:H	2.29	0.40
19:k:2:PRO:HD2	19:k:5:TYR:CD2	2.56	0.40
20:l:511:LEU:HD23	20:l:511:LEU:HA	1.93	0.40
25:r:159:PRO:HB3	30:r:501:PEE:H25	2.02	0.40
32:r:505:CDL:H262	32:r:505:CDL:H332	2.03	0.40
30:i:402:PEE:H27	20:l:563:PRO:HA	2.03	0.40
26:s:251:THR:O	26:s:251:THR:HG23	2.20	0.40
9:a:155:GLU:HA	9:a:155:GLU:OE2	2.22	0.40
10:b:73:THR:HG23	10:b:74:HIS:ND1	2.35	0.40
17:i:11:MET:HE3	32:i:401:CDL:H542	2.03	0.40
17:i:141:VAL:O	17:i:145:ILE:HG12	2.21	0.40
17:i:246:VAL:HG11	32:r:505:CDL:H392	2.03	0.40
17:i:298:TYR:O	17:i:303:THR:OG1	2.33	0.40
20:l:232:TRP:HH2	20:l:252:MET:HE1	1.86	0.40
21:m:17:PHE:O	21:m:21:SER:OG	2.31	0.40
24:p:159:LYS:HB2	24:p:162:ASP:CG	2.46	0.40
25:r:44:GLN:HG3	25:r:60:SER:HA	2.04	0.40
25:r:122:PHE:CE1	25:r:238:LEU:HB3	2.53	0.40
20:l:160:GLY:HA3	24:p:95:GLU:HB3	2.04	0.40
20:l:274:GLN:NE2	20:l:320:ASN:HD22	2.18	0.40
25:r:39:LEU:HD23	25:r:39:LEU:HA	1.91	0.40
25:r:72:LEU:O	25:r:76:MET:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:240:GLY:O	25:r:244:MET:HG3	2.21	0.40
26:s:69:SER:OG	26:s:70:MET:N	2.54	0.40
26:s:143:GLU:HA	26:s:146:LEU:HD12	2.02	0.40
26:s:179:TRP:CG	26:s:180:PRO:HD3	2.56	0.40
27:u:100:CYS:HB2	27:u:103:GLN:OE1	2.22	0.40
28:v:93:LEU:O	28:v:97:LYS:HG3	2.22	0.40
29:w:147:LEU:HD23	29:w:147:LEU:HA	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	38/40 (95%)	36 (95%)	2 (5%)	0	100	100
2	S	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
3	U	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
4	V	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	18	49
5	W	111/113 (98%)	109 (98%)	2 (2%)	0	100	100
6	X	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
7	Y	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
8	Z	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
9	a	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
10	b	99/126 (79%)	98 (99%)	1 (1%)	0	100	100
11	c	154/156 (99%)	146 (95%)	8 (5%)	0	100	100
12	d	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
13	e	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
14	f	40/42 (95%)	39 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	g	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
16	h	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
17	i	345/347 (99%)	331 (96%)	14 (4%)	0	100	100
18	j	95/113 (84%)	89 (94%)	6 (6%)	0	100	100
19	k	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
20	l	601/603 (100%)	577 (96%)	24 (4%)	0	100	100
21	m	125/175 (71%)	114 (91%)	11 (9%)	0	100	100
22	n	54/56 (96%)	52 (96%)	1 (2%)	1 (2%)	6	27
23	o	126/128 (98%)	119 (94%)	6 (5%)	1 (1%)	16	47
24	p	176/178 (99%)	169 (96%)	7 (4%)	0	100	100
25	r	457/459 (100%)	445 (97%)	12 (3%)	0	100	100
26	s	299/318 (94%)	291 (97%)	8 (3%)	0	100	100
27	u	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
28	v	122/125 (98%)	114 (93%)	8 (7%)	0	100	100
29	w	318/320 (99%)	304 (96%)	14 (4%)	0	100	100
All	All	4586/4751 (96%)	4406 (96%)	177 (4%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	n	36	THR
23	o	24	ASP
4	V	46	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	34/34 (100%)	34 (100%)	0	100	100
2	S	58/58 (100%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	99 (100%)	0	100	100
6	X	76/81 (94%)	76 (100%)	0	100	100
7	Y	63/63 (100%)	63 (100%)	0	100	100
8	Z	65/65 (100%)	65 (100%)	0	100	100
9	a	121/122 (99%)	121 (100%)	0	100	100
10	b	98/119 (82%)	98 (100%)	0	100	100
11	c	137/141 (97%)	134 (98%)	3 (2%)	45	71
12	d	155/155 (100%)	155 (100%)	0	100	100
13	e	99/99 (100%)	99 (100%)	0	100	100
14	f	35/38 (92%)	35 (100%)	0	100	100
15	g	108/108 (100%)	108 (100%)	0	100	100
16	h	93/93 (100%)	93 (100%)	0	100	100
17	i	311/311 (100%)	310 (100%)	1 (0%)	86	87
18	j	88/99 (89%)	88 (100%)	0	100	100
19	k	85/85 (100%)	85 (100%)	0	100	100
20	l	537/537 (100%)	537 (100%)	0	100	100
21	m	99/141 (70%)	99 (100%)	0	100	100
22	n	46/53 (87%)	46 (100%)	0	100	100
23	o	113/113 (100%)	112 (99%)	1 (1%)	70	80
24	p	158/159 (99%)	153 (97%)	5 (3%)	34	64
25	r	410/410 (100%)	410 (100%)	0	100	100
26	s	263/275 (96%)	261 (99%)	2 (1%)	73	81
27	u	153/153 (100%)	153 (100%)	0	100	100
28	v	97/111 (87%)	97 (100%)	0	100	100
29	w	277/283 (98%)	276 (100%)	1 (0%)	84	86
All	All	4048/4175 (97%)	4035 (100%)	13 (0%)	84	87

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	c	32	VAL

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Mol	Chain	Res	Type
11	c	103	GLU
11	c	105	ILE
17	i	268	GLN
23	o	22	GLU
24	p	59	LYS
24	p	62	GLN
24	p	64	LEU
24	p	65	ARG
24	p	66	GLN
26	s	22	LEU
26	s	24	GLU
29	w	241	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
2	S	61	HIS
6	X	142	GLN
7	Y	49	GLN
8	Z	9	HIS
10	b	126	GLN
11	c	154	GLN
11	c	164	ASN
12	d	124	ASN
12	d	161	GLN
16	h	25	GLN
17	i	36	ASN
17	i	310	ASN
19	k	50	ASN
19	k	57	ASN
20	l	135	ASN
20	l	170	GLN
20	l	199	GLN
20	l	274	GLN
20	l	354	GLN
20	l	447	ASN
20	l	534	HIS
21	m	175	ASN
22	n	11	HIS
22	n	14	HIS
23	o	79	ASN
24	p	33	HIS

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Mol	Chain	Res	Type
26	s	247	HIS
26	s	250	HIS
27	u	30	HIS
27	u	65	GLN
29	w	107	GLN
29	w	149	HIS
29	w	239	ASN

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](#)

21 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	$\# Z > 2$
33	PLX	a	202	-	51,51,51	1.21	4 (7%)	53,59,59	0.61	1 (1%)
30	PEE	m	201	-	40,40,50	1.17	5 (12%)	43,45,55	1.00	2 (4%)
32	CDL	a	201	-	90,90,99	1.16	8 (8%)	96,102,111	0.93	4 (4%)
35	ADP	w	401	-	28,29,29	3.17	9 (32%)	43,45,45	1.90	8 (18%)
32	CDL	l	701	-	99,99,99	1.12	8 (8%)	105,111,111	0.85	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CDL	r	504	-	98,98,99	1.12	8 (8%)	104,110,111	0.89	4 (3%)
33	PLX	g	201	-	51,51,51	1.20	4 (7%)	53,59,59	0.62	1 (1%)
33	PLX	j	201	-	51,51,51	1.21	4 (7%)	53,59,59	0.60	1 (1%)
32	CDL	g	202	-	77,77,99	1.22	8 (10%)	83,89,111	0.96	4 (4%)
33	PLX	r	502	-	51,51,51	1.20	5 (9%)	53,59,59	0.61	1 (1%)
31	8Q1	X	201	-	32,34,34	1.63	6 (18%)	39,43,43	1.58	6 (15%)
34	UQ	s	401	-	28,28,63	3.34	8 (28%)	36,37,79	2.60	11 (30%)
30	PEE	U	101	-	50,50,50	1.18	6 (12%)	53,55,55	0.97	2 (3%)
30	PEE	i	402	-	46,46,50	1.23	6 (13%)	49,51,55	1.00	2 (4%)
30	PEE	U	102	-	50,50,50	1.18	6 (12%)	53,55,55	0.99	2 (3%)
30	PEE	b	201	-	45,45,50	1.24	6 (13%)	48,50,55	1.00	2 (4%)
33	PLX	r	503	-	51,51,51	1.21	5 (9%)	53,59,59	0.61	1 (1%)
32	CDL	r	505	-	99,99,99	1.12	9 (9%)	105,111,111	0.86	4 (3%)
30	PEE	r	501	-	50,50,50	1.18	6 (12%)	53,55,55	0.98	2 (3%)
30	PEE	l	702	-	45,45,50	1.24	6 (13%)	48,50,55	1.03	2 (4%)
32	CDL	i	401	-	65,65,99	1.30	8 (12%)	71,77,111	1.04	4 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PLX	a	202	-	-	29/55/55/55	-
30	PEE	m	201	-	-	18/44/44/54	-
32	CDL	a	201	-	-	50/101/101/110	-
35	ADP	w	401	-	-	3/16/32/32	0/3/3/3
32	CDL	l	701	-	-	61/110/110/110	-
32	CDL	r	504	-	-	52/109/109/110	-
33	PLX	g	201	-	-	22/55/55/55	-
33	PLX	j	201	-	-	30/55/55/55	-
32	CDL	g	202	-	-	38/88/88/110	-
33	PLX	r	502	-	-	21/55/55/55	-
31	8Q1	X	201	-	-	12/41/41/41	-
34	UQ	s	401	-	-	7/21/45/87	0/1/1/1
30	PEE	U	101	-	-	28/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PEE	i	402	-	-	21/50/50/54	-
30	PEE	U	102	-	-	24/54/54/54	-
30	PEE	b	201	-	-	31/49/49/54	-
33	PLX	r	503	-	-	31/55/55/55	-
32	CDL	r	505	-	-	65/110/110/110	-
30	PEE	r	501	-	-	24/54/54/54	-
30	PEE	l	702	-	-	24/49/49/54	-
32	CDL	i	401	-	-	37/76/76/110	-

All (135) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	s	401	UQ	C13-C14	9.69	1.55	1.33
34	s	401	UQ	C8-C9	9.34	1.54	1.33
35	w	401	ADP	C3'-C4'	-8.92	1.30	1.53
34	s	401	UQ	C18-C19	7.90	1.56	1.32
35	w	401	ADP	O4'-C4'	7.78	1.62	1.45
35	w	401	ADP	PA-O3A	6.45	1.66	1.59
35	w	401	ADP	C6-N6	5.48	1.48	1.34
31	X	201	8Q1	C39-N41	5.20	1.45	1.33
31	X	201	8Q1	C34-N36	5.06	1.45	1.33
35	w	401	ADP	O4'-C1'	-4.49	1.31	1.42
30	m	201	PEE	C18-C19	3.84	1.53	1.31
30	r	501	PEE	C18-C19	3.83	1.53	1.31
30	U	102	PEE	C18-C19	3.82	1.53	1.31
30	l	702	PEE	C18-C19	3.81	1.53	1.31
30	U	101	PEE	C18-C19	3.81	1.53	1.31
30	i	402	PEE	C18-C19	3.81	1.53	1.31
30	b	201	PEE	C18-C19	3.80	1.53	1.31
30	b	201	PEE	C39-C38	3.76	1.53	1.31
30	l	702	PEE	C39-C38	3.75	1.53	1.31
30	i	402	PEE	C39-C38	3.75	1.53	1.31
30	U	101	PEE	C39-C38	3.74	1.53	1.31
30	U	102	PEE	C39-C38	3.74	1.53	1.31
30	r	501	PEE	C39-C38	3.74	1.52	1.31
32	i	401	CDL	OA8-CA7	3.47	1.43	1.33
32	l	701	CDL	OA8-CA7	3.46	1.43	1.33
32	g	202	CDL	OA8-CA7	3.45	1.43	1.33
32	r	505	CDL	OA8-CA7	3.44	1.43	1.33
32	r	504	CDL	OA8-CA7	3.43	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	201	CDL	OA8-CA7	3.42	1.43	1.33
35	w	401	ADP	C8-N9	-3.35	1.31	1.37
35	w	401	ADP	O2'-C2'	-3.19	1.35	1.43
32	l	701	CDL	OB6-CB5	3.08	1.43	1.34
32	a	201	CDL	OB6-CB5	3.06	1.42	1.34
32	i	401	CDL	OB6-CB5	3.05	1.42	1.34
32	r	505	CDL	OB6-CB5	3.04	1.42	1.34
32	g	202	CDL	OB8-CB7	3.03	1.42	1.33
32	r	504	CDL	OB6-CB5	3.03	1.42	1.34
32	i	401	CDL	OB8-CB7	3.02	1.42	1.33
32	r	504	CDL	OB8-CB7	3.01	1.42	1.33
32	r	505	CDL	OB8-CB7	3.01	1.42	1.33
32	l	701	CDL	OA6-CA5	3.01	1.42	1.34
32	g	202	CDL	OB6-CB5	3.00	1.42	1.34
32	l	701	CDL	OB8-CB7	2.98	1.42	1.33
35	w	401	ADP	O3'-C3'	2.98	1.50	1.43
32	a	201	CDL	OA6-CA5	2.98	1.42	1.34
32	a	201	CDL	OB8-CB7	2.98	1.42	1.33
32	r	505	CDL	OA6-CA5	2.97	1.42	1.34
32	i	401	CDL	OA6-CA5	2.94	1.42	1.34
32	g	202	CDL	OA6-CA5	2.94	1.42	1.34
32	r	504	CDL	OA6-CA5	2.94	1.42	1.34
33	g	201	PLX	O6-C4	-2.84	1.41	1.44
33	a	202	PLX	O6-C4	-2.83	1.41	1.44
33	r	503	PLX	O6-C4	-2.81	1.41	1.44
34	s	401	UQ	C6-C1	2.72	1.54	1.46
33	j	201	PLX	O6-C4	-2.72	1.41	1.44
32	g	202	CDL	OA6-CA4	-2.59	1.40	1.46
30	i	402	PEE	O2-C2	-2.57	1.40	1.46
30	r	501	PEE	O2-C2	-2.56	1.40	1.46
30	U	101	PEE	O2-C2	-2.55	1.40	1.46
32	r	504	CDL	OA6-CA4	-2.54	1.40	1.46
30	l	702	PEE	O2-C2	-2.54	1.40	1.46
30	b	201	PEE	O2-C2	-2.54	1.40	1.46
32	r	505	CDL	OA6-CA4	-2.53	1.40	1.46
32	l	701	CDL	OA6-CA4	-2.51	1.40	1.46
30	U	102	PEE	O3-C30	2.50	1.40	1.33
32	i	401	CDL	OA6-CA4	-2.49	1.40	1.46
32	a	201	CDL	OA6-CA4	-2.48	1.40	1.46
30	U	102	PEE	O2-C2	-2.48	1.40	1.46
30	i	402	PEE	O3-C30	2.47	1.40	1.33
33	j	201	PLX	C7-C6	2.47	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	l	702	PEE	O3-C30	2.46	1.40	1.33
33	r	502	PLX	C7-C6	2.46	1.55	1.50
30	r	501	PEE	O3-C30	2.46	1.40	1.33
30	U	101	PEE	O3-C30	2.45	1.40	1.33
30	b	201	PEE	O3-C30	2.43	1.40	1.33
30	m	201	PEE	O3-C30	2.42	1.40	1.33
30	m	201	PEE	O2-C2	-2.40	1.41	1.46
33	r	502	PLX	O6-C4	-2.39	1.41	1.44
30	m	201	PEE	O2-C10	2.39	1.41	1.34
33	r	503	PLX	C7-C6	2.37	1.55	1.50
35	w	401	ADP	C5-N7	-2.37	1.34	1.39
33	a	202	PLX	C7-C6	2.36	1.55	1.50
30	U	102	PEE	O2-C10	2.35	1.40	1.34
31	X	201	8Q1	C1-S44	2.35	1.81	1.76
33	g	201	PLX	C7-C6	2.35	1.55	1.50
31	X	201	8Q1	C6-C1	2.33	1.53	1.50
30	U	101	PEE	O2-C10	2.30	1.40	1.34
32	a	201	CDL	OB6-CB4	-2.30	1.41	1.46
30	l	702	PEE	O2-C10	2.30	1.40	1.34
32	g	202	CDL	PB2-OB2	2.29	1.68	1.59
32	r	505	CDL	OB6-CB4	-2.29	1.41	1.46
32	i	401	CDL	PB2-OB2	2.29	1.68	1.59
32	r	504	CDL	OB6-CB4	-2.28	1.41	1.46
32	l	701	CDL	PB2-OB2	2.28	1.68	1.59
30	b	201	PEE	O2-C10	2.28	1.40	1.34
31	X	201	8Q1	O35-C34	-2.28	1.19	1.23
32	g	202	CDL	OB6-CB4	-2.28	1.41	1.46
30	i	402	PEE	O2-C10	2.28	1.40	1.34
32	r	505	CDL	PB2-OB5	2.27	1.68	1.59
32	r	504	CDL	PB2-OB2	2.26	1.68	1.59
32	i	401	CDL	PB2-OB5	2.25	1.68	1.59
32	i	401	CDL	OB6-CB4	-2.25	1.41	1.46
30	r	501	PEE	O2-C10	2.24	1.40	1.34
32	a	201	CDL	PB2-OB2	2.24	1.68	1.59
32	r	505	CDL	PB2-OB2	2.24	1.68	1.59
32	l	701	CDL	OB6-CB4	-2.23	1.41	1.46
31	X	201	8Q1	O40-C39	-2.23	1.18	1.23
32	l	701	CDL	PB2-OB5	2.22	1.68	1.59
32	g	202	CDL	PB2-OB5	2.22	1.68	1.59
32	r	504	CDL	PB2-OB5	2.22	1.68	1.59
32	a	201	CDL	PB2-OB5	2.20	1.68	1.59
34	s	401	UQ	C7-C8	2.19	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	j	201	PLX	P1-O4	2.18	1.67	1.59
33	r	502	PLX	P1-O4	2.17	1.67	1.59
33	g	201	PLX	P1-O4	2.17	1.67	1.59
33	r	503	PLX	P1-O4	2.15	1.67	1.59
30	b	201	PEE	O3-C3	-2.15	1.40	1.45
33	a	202	PLX	P1-O4	2.15	1.67	1.59
30	l	702	PEE	O3-C3	-2.14	1.40	1.45
30	U	101	PEE	O3-C3	-2.14	1.40	1.45
30	m	201	PEE	O3-C3	-2.13	1.40	1.45
34	s	401	UQ	O4-C4	-2.12	1.18	1.23
30	i	402	PEE	O3-C3	-2.12	1.40	1.45
30	r	501	PEE	O3-C3	-2.10	1.40	1.45
34	s	401	UQ	O3-CM3	-2.10	1.40	1.45
33	r	502	PLX	P1-O1	2.09	1.67	1.59
33	j	201	PLX	P1-O1	2.08	1.67	1.59
30	U	102	PEE	O3-C3	-2.08	1.40	1.45
33	r	503	PLX	P1-O1	2.08	1.67	1.59
33	a	202	PLX	P1-O1	2.06	1.67	1.59
33	r	502	PLX	C1-C2	2.02	1.57	1.51
33	r	503	PLX	C1-C2	2.02	1.57	1.51
32	r	505	CDL	C11-CA5	2.02	1.56	1.50
33	g	201	PLX	P1-O1	2.01	1.67	1.59
34	s	401	UQ	C5-C4	2.00	1.54	1.47

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	s	401	UQ	C7-C8-C9	-8.47	112.25	126.83
34	s	401	UQ	C12-C13-C14	-6.28	113.25	127.62
31	X	201	8Q1	C6-C1-S44	5.92	120.46	113.40
35	w	401	ADP	C5-C4-N3	-5.51	119.13	126.72
35	w	401	ADP	N3-C2-N1	-4.56	121.67	128.58
35	w	401	ADP	N3-C4-N9	4.32	134.51	127.17
34	s	401	UQ	C10-C9-C8	-4.29	112.61	123.63
32	a	201	CDL	OA6-CA5-C11	4.19	120.53	111.48
34	s	401	UQ	C15-C14-C13	-4.18	112.89	123.63
30	U	102	PEE	O2-C10-C11	4.14	120.45	111.48
30	m	201	PEE	O2-C10-C11	4.08	120.32	111.48
30	l	702	PEE	O2-C10-C11	4.08	120.31	111.48
32	i	401	CDL	OA6-CA5-C11	4.08	120.31	111.48
34	s	401	UQ	C17-C18-C19	-4.06	114.12	127.64
32	g	202	CDL	OB6-CB5-C51	4.03	120.19	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	r	504	CDL	OA6-CA5-C11	4.02	120.19	111.48
32	r	505	CDL	OB6-CB5-C51	3.99	120.11	111.48
30	b	201	PEE	O2-C10-C11	3.97	120.07	111.48
30	i	402	PEE	O2-C10-C11	3.97	120.06	111.48
32	i	401	CDL	OB6-CB5-C51	3.94	120.00	111.48
30	r	501	PEE	O2-C10-C11	3.94	120.00	111.48
32	r	504	CDL	OB6-CB5-C51	3.93	119.98	111.48
32	l	701	CDL	OB6-CB5-C51	3.92	119.97	111.48
32	a	201	CDL	OB6-CB5-C51	3.90	119.92	111.48
32	l	701	CDL	OA6-CA5-C11	3.90	119.92	111.48
34	s	401	UQ	C11-C9-C8	-3.87	112.48	121.17
30	U	101	PEE	O2-C10-C11	3.87	119.85	111.48
32	r	505	CDL	OA6-CA5-C11	3.86	119.84	111.48
32	g	202	CDL	OA6-CA5-C11	3.85	119.80	111.48
31	X	201	8Q1	O4-C1-C6	-3.61	119.81	123.98
35	w	401	ADP	C2-N3-C4	3.58	120.58	111.83
34	s	401	UQ	C16-C14-C13	-3.56	113.18	121.17
35	w	401	ADP	N9-C8-N7	-3.49	108.99	113.94
34	s	401	UQ	C21-C19-C18	-3.32	112.69	122.66
35	w	401	ADP	C5-N7-C8	3.18	108.45	103.45
35	w	401	ADP	C4-N9-C8	3.15	109.05	105.74
35	w	401	ADP	C4-C5-N7	-3.00	107.15	110.58
34	s	401	UQ	C20-C19-C18	-2.97	113.74	122.66
34	s	401	UQ	C7-C6-C5	-2.88	119.96	124.89
30	U	102	PEE	O3-C30-C31	2.78	120.33	111.83
30	r	501	PEE	O3-C30-C31	2.78	120.31	111.83
30	l	702	PEE	O3-C30-C31	2.78	120.30	111.83
32	g	202	CDL	OB8-CB7-C71	2.76	120.26	111.83
31	X	201	8Q1	C37-C38-C39	2.75	116.98	112.39
32	r	504	CDL	OB8-CB7-C71	2.74	120.19	111.83
32	a	201	CDL	OB8-CB7-C71	2.72	120.13	111.83
32	a	201	CDL	OA8-CA7-C31	2.71	120.11	111.83
30	U	101	PEE	O3-C30-C31	2.70	120.06	111.83
34	s	401	UQ	CM5-C5-C6	-2.69	120.02	124.45
32	i	401	CDL	OB8-CB7-C71	2.69	120.03	111.83
32	g	202	CDL	OA8-CA7-C31	2.69	120.02	111.83
32	i	401	CDL	OA8-CA7-C31	2.68	120.00	111.83
32	l	701	CDL	OA8-CA7-C31	2.67	119.98	111.83
32	r	504	CDL	OA8-CA7-C31	2.66	119.95	111.83
32	r	505	CDL	OB8-CB7-C71	2.65	119.93	111.83
30	b	201	PEE	O3-C30-C31	2.64	119.88	111.83
30	i	402	PEE	O3-C30-C31	2.63	119.86	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	l	701	CDL	OB8-CB7-C71	2.60	119.77	111.83
32	r	505	CDL	OA8-CA7-C31	2.60	119.75	111.83
33	r	503	PLX	C1A-N1-C1	2.57	120.13	109.91
30	m	201	PEE	O3-C30-C31	2.57	119.66	111.83
33	j	201	PLX	C1A-N1-C1	2.49	119.80	109.91
33	r	502	PLX	C1A-N1-C1	2.47	119.75	109.91
33	g	201	PLX	C1A-N1-C1	2.45	119.66	109.91
33	a	202	PLX	C1A-N1-C1	2.42	119.51	109.91
31	X	201	8Q1	O4-C1-S44	-2.33	119.72	122.68
31	X	201	8Q1	C43-S44-C1	2.30	108.64	101.84
31	X	201	8Q1	C38-C39-N41	2.14	120.24	116.34

There are no chirality outliers.

All (628) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	U	101	PEE	C1-O3P-P-O1P
30	U	101	PEE	C1-O3P-P-O4P
30	U	101	PEE	C4-O4P-P-O1P
30	b	201	PEE	C1-O3P-P-O2P
30	b	201	PEE	C1-O3P-P-O1P
30	b	201	PEE	C1-O3P-P-O4P
30	b	201	PEE	C4-O4P-P-O2P
30	i	402	PEE	C11-C10-O2-C2
30	l	702	PEE	C11-C10-O2-C2
30	l	702	PEE	O3P-C1-C2-O2
30	l	702	PEE	C4-O4P-P-O3P
30	m	201	PEE	C11-C10-O2-C2
30	m	201	PEE	O4-C10-O2-C2
31	X	201	8Q1	C1-C6-C7-C8
31	X	201	8Q1	C28-C29-C32-C34
31	X	201	8Q1	C28-C29-C32-O33
31	X	201	8Q1	C30-C29-C32-C34
31	X	201	8Q1	C30-C29-C32-O33
31	X	201	8Q1	C31-C29-C32-C34
31	X	201	8Q1	N36-C37-C38-C39
31	X	201	8Q1	C42-C43-S44-C1
32	a	201	CDL	O1-C1-CA2-OA2
32	a	201	CDL	CA2-C1-CB2-OB2
32	a	201	CDL	OA5-CA3-CA4-OA6
32	a	201	CDL	CB2-OB2-PB2-OB3
32	a	201	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
32	a	201	CDL	CB2-OB2-PB2-OB5
32	a	201	CDL	CB3-OB5-PB2-OB2
32	a	201	CDL	CB3-OB5-PB2-OB3
32	a	201	CDL	CB3-OB5-PB2-OB4
32	g	202	CDL	CB2-C1-CA2-OA2
32	g	202	CDL	CA2-C1-CB2-OB2
32	g	202	CDL	CA2-OA2-PA1-OA4
32	g	202	CDL	CA2-OA2-PA1-OA5
32	g	202	CDL	CA3-OA5-PA1-OA2
32	g	202	CDL	CA3-OA5-PA1-OA3
32	g	202	CDL	CA3-OA5-PA1-OA4
32	i	401	CDL	CA3-OA5-PA1-OA2
32	i	401	CDL	CA3-OA5-PA1-OA3
32	i	401	CDL	CB2-OB2-PB2-OB4
32	i	401	CDL	CB2-OB2-PB2-OB5
32	i	401	CDL	CB3-OB5-PB2-OB2
32	i	401	CDL	CB3-OB5-PB2-OB3
32	l	701	CDL	CA2-OA2-PA1-OA4
32	l	701	CDL	CA2-OA2-PA1-OA5
32	l	701	CDL	CA3-OA5-PA1-OA2
32	l	701	CDL	CA3-OA5-PA1-OA4
32	l	701	CDL	OA6-CA4-CA6-OA8
32	l	701	CDL	CB2-OB2-PB2-OB3
32	l	701	CDL	CB2-OB2-PB2-OB5
32	l	701	CDL	OB6-CB4-CB6-OB8
32	r	504	CDL	O1-C1-CA2-OA2
32	r	504	CDL	CA2-OA2-PA1-OA5
32	r	504	CDL	CB2-OB2-PB2-OB3
32	r	504	CDL	CB2-OB2-PB2-OB4
32	r	504	CDL	CB2-OB2-PB2-OB5
32	r	504	CDL	CB3-OB5-PB2-OB3
32	r	505	CDL	CA2-OA2-PA1-OA3
32	r	505	CDL	CA2-OA2-PA1-OA4
32	r	505	CDL	CA2-OA2-PA1-OA5
32	r	505	CDL	CA3-OA5-PA1-OA2
32	r	505	CDL	CA3-OA5-PA1-OA3
32	r	505	CDL	CA3-OA5-PA1-OA4
32	r	505	CDL	CB2-OB2-PB2-OB3
32	r	505	CDL	CB2-OB2-PB2-OB4
32	r	505	CDL	CB2-OB2-PB2-OB5
32	r	505	CDL	CB3-OB5-PB2-OB2
33	a	202	PLX	O7-C6-O6-C4

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Mol	Chain	Res	Type	Atoms
33	a	202	PLX	C3-O4-P1-O2
33	a	202	PLX	C2-O1-P1-O4
33	a	202	PLX	C2-O1-P1-O2
33	a	202	PLX	C25-C24-O8-C5
33	j	201	PLX	O7-C6-C7-C8
33	j	201	PLX	O9-C24-O8-C5
33	r	502	PLX	O7-C6-O6-C4
33	r	502	PLX	C5-C4-O6-C6
33	r	503	PLX	C2-O1-P1-O4
33	r	503	PLX	C2-O1-P1-O2
33	r	503	PLX	C2-O1-P1-O3
33	r	503	PLX	C25-C24-O8-C5
33	r	503	PLX	O9-C24-C25-C26
34	s	401	UQ	C7-C8-C9-C10
34	s	401	UQ	C7-C8-C9-C11
34	s	401	UQ	C12-C13-C14-C16
35	w	401	ADP	C5'-O5'-PA-O2A
35	w	401	ADP	C5'-O5'-PA-O3A
32	i	401	CDL	OA9-CA7-OA8-CA6
32	r	504	CDL	OA9-CA7-OA8-CA6
32	i	401	CDL	C31-CA7-OA8-CA6
32	r	504	CDL	C31-CA7-OA8-CA6
30	i	402	PEE	O4-C10-O2-C2
30	l	702	PEE	O4-C10-O2-C2
32	r	505	CDL	C71-CB7-OB8-CB6
34	s	401	UQ	C12-C11-C9-C10
30	l	702	PEE	C31-C30-O3-C3
30	U	101	PEE	C17-C18-C19-C20
30	U	102	PEE	C37-C38-C39-C40
32	l	701	CDL	OB9-CB7-OB8-CB6
32	l	701	CDL	C59-C60-C61-C62
34	s	401	UQ	C17-C18-C19-C21
32	l	701	CDL	O1-C1-CA2-OA2
32	r	504	CDL	O1-C1-CB2-OB2
32	r	505	CDL	OB9-CB7-OB8-CB6
30	b	201	PEE	C11-C10-O2-C2
32	r	505	CDL	C51-CB5-OB6-CB4
32	l	701	CDL	C71-CB7-OB8-CB6
30	l	702	PEE	O5-C30-O3-C3
34	s	401	UQ	C9-C11-C12-C13
32	l	701	CDL	C75-C76-C77-C78
33	a	202	PLX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	r	503	PLX	C12-C13-C14-C15
30	b	201	PEE	O4-C10-O2-C2
32	a	201	CDL	CB2-C1-CA2-OA2
32	r	505	CDL	CB2-C1-CA2-OA2
30	U	101	PEE	C31-C30-O3-C3
30	b	201	PEE	C31-C30-O3-C3
30	m	201	PEE	C31-C30-O3-C3
32	i	401	CDL	C71-CB7-OB8-CB6
32	r	504	CDL	C55-C56-C57-C58
33	j	201	PLX	C28-C29-C30-C31
32	l	701	CDL	C11-C12-C13-C14
32	l	701	CDL	C35-C36-C37-C38
33	a	202	PLX	C7-C8-C9-C10
33	r	502	PLX	C9-C10-C11-C12
33	g	201	PLX	C10-C11-C12-C13
32	a	201	CDL	O1-C1-CB2-OB2
30	b	201	PEE	O5-C30-O3-C3
30	m	201	PEE	O5-C30-O3-C3
30	U	101	PEE	O5-C30-O3-C3
33	a	202	PLX	O4-C3-C4-O6
30	U	102	PEE	C11-C10-O2-C2
32	g	202	CDL	C71-C72-C73-C74
32	g	202	CDL	CB7-C71-C72-C73
32	r	505	CDL	OB7-CB5-OB6-CB4
32	g	202	CDL	C75-C76-C77-C78
33	r	503	PLX	C2-C1-N1-C1A
30	U	102	PEE	C30-C31-C32-C33
32	i	401	CDL	CB7-C71-C72-C73
32	r	504	CDL	CB7-C71-C72-C73
32	i	401	CDL	OB9-CB7-OB8-CB6
30	U	101	PEE	C11-C10-O2-C2
30	r	501	PEE	C10-C11-C12-C13
32	a	201	CDL	CA7-C31-C32-C33
32	r	505	CDL	CB7-C71-C72-C73
33	j	201	PLX	C15-C16-C17-C18
32	g	202	CDL	O1-C1-CA2-OA2
32	i	401	CDL	O1-C1-CA2-OA2
32	r	505	CDL	O1-C1-CA2-OA2
32	r	505	CDL	CA7-C31-C32-C33
30	U	102	PEE	O4-C10-O2-C2
30	U	102	PEE	C17-C18-C19-C20
30	i	402	PEE	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
32	a	201	CDL	C71-CB7-OB8-CB6
33	g	201	PLX	C12-C13-C14-C15
33	r	502	PLX	C30-C31-C32-C33
30	U	101	PEE	O4-C10-O2-C2
32	i	401	CDL	CB2-C1-CA2-OA2
32	l	701	CDL	CB2-C1-CA2-OA2
32	r	504	CDL	CB2-C1-CA2-OA2
32	r	504	CDL	CA2-C1-CB2-OB2
30	l	702	PEE	C23-C24-C25-C26
33	j	201	PLX	C2-C1-N1-C1A
33	r	503	PLX	C2-C1-N1-C1C
30	i	402	PEE	C10-C11-C12-C13
30	r	501	PEE	C11-C10-O2-C2
32	a	201	CDL	C51-CB5-OB6-CB4
30	r	501	PEE	O4-C10-O2-C2
30	b	201	PEE	C17-C18-C19-C20
30	l	702	PEE	C37-C38-C39-C40
30	r	501	PEE	C17-C18-C19-C20
32	g	202	CDL	O1-C1-CB2-OB2
32	l	701	CDL	CB5-C51-C52-C53
32	a	201	CDL	OB9-CB7-OB8-CB6
30	m	201	PEE	C13-C14-C15-C16
32	a	201	CDL	OB7-CB5-OB6-CB4
32	r	504	CDL	C62-C63-C64-C65
30	U	101	PEE	C43-C44-C45-C46
32	a	201	CDL	C17-C18-C19-C20
32	a	201	CDL	C34-C35-C36-C37
32	i	401	CDL	C71-C72-C73-C74
32	r	505	CDL	C56-C57-C58-C59
30	r	501	PEE	C12-C13-C14-C15
32	r	504	CDL	C61-C62-C63-C64
32	r	505	CDL	C12-C13-C14-C15
33	g	201	PLX	C11-C10-C9-C8
33	j	201	PLX	C27-C28-C29-C30
33	a	202	PLX	O7-C6-C7-C8
33	a	202	PLX	O9-C24-C25-C26
30	l	702	PEE	C31-C32-C33-C34
32	a	201	CDL	C11-C12-C13-C14
32	i	401	CDL	C37-C38-C39-C40
32	r	504	CDL	C52-C53-C54-C55
33	a	202	PLX	C26-C27-C28-C29
33	g	201	PLX	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
33	r	502	PLX	C27-C28-C29-C30
33	r	503	PLX	C13-C14-C15-C16
32	a	201	CDL	C33-C34-C35-C36
33	g	201	PLX	C9-C10-C11-C12
33	g	201	PLX	C25-C26-C27-C28
32	a	201	CDL	C73-C74-C75-C76
32	r	504	CDL	C58-C59-C60-C61
32	l	701	CDL	CB7-C71-C72-C73
32	l	701	CDL	C37-C38-C39-C40
32	r	505	CDL	C43-C44-C45-C46
32	a	201	CDL	C31-C32-C33-C34
32	i	401	CDL	C52-C53-C54-C55
32	r	504	CDL	C82-C83-C84-C85
32	a	201	CDL	C75-C76-C77-C78
32	r	505	CDL	C71-C72-C73-C74
33	a	202	PLX	C11-C12-C13-C14
33	r	503	PLX	C25-C26-C27-C28
32	r	504	CDL	C74-C75-C76-C77
32	r	505	CDL	C14-C15-C16-C17
32	r	504	CDL	C71-CB7-OB8-CB6
30	b	201	PEE	C33-C34-C35-C36
30	r	501	PEE	C13-C14-C15-C16
32	l	701	CDL	C54-C55-C56-C57
32	r	504	CDL	C35-C36-C37-C38
33	j	201	PLX	C7-C8-C9-C10
32	a	201	CDL	CB5-C51-C52-C53
32	l	701	CDL	C55-C56-C57-C58
32	l	701	CDL	C60-C61-C62-C63
33	a	202	PLX	C14-C15-C16-C17
33	r	502	PLX	C10-C11-C12-C13
33	r	502	PLX	C14-C15-C16-C17
32	l	701	CDL	C39-C40-C41-C42
32	r	504	CDL	C20-C21-C22-C23
33	r	503	PLX	C2-C1-N1-C1B
32	l	701	CDL	C33-C34-C35-C36
33	a	202	PLX	C28-C29-C30-C31
33	j	201	PLX	C25-C26-C27-C28
32	r	505	CDL	C74-C75-C76-C77
30	i	402	PEE	C35-C36-C37-C38
30	b	201	PEE	C37-C38-C39-C40
32	g	202	CDL	C59-C60-C61-C62
32	r	504	CDL	C59-C60-C61-C62

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Mol	Chain	Res	Type	Atoms
33	j	201	PLX	C10-C11-C12-C13
32	g	202	CDL	C55-C56-C57-C58
32	r	504	CDL	OB9-CB7-OB8-CB6
32	r	505	CDL	C52-C53-C54-C55
30	m	201	PEE	C11-C12-C13-C14
32	l	701	CDL	C40-C41-C42-C43
32	r	505	CDL	C35-C36-C37-C38
33	r	503	PLX	C33-C34-C35-C36
32	a	201	CDL	C52-C53-C54-C55
32	r	504	CDL	C56-C57-C58-C59
32	r	505	CDL	C73-C74-C75-C76
33	a	202	PLX	C13-C14-C15-C16
33	r	503	PLX	C14-C15-C16-C17
33	r	503	PLX	C27-C28-C29-C30
33	r	503	PLX	C29-C30-C31-C32
32	a	201	CDL	C71-C72-C73-C74
32	r	504	CDL	C32-C33-C34-C35
32	r	504	CDL	C73-C74-C75-C76
32	r	504	CDL	C75-C76-C77-C78
32	r	505	CDL	C59-C60-C61-C62
32	l	701	CDL	C72-C73-C74-C75
32	r	505	CDL	C37-C38-C39-C40
32	l	701	CDL	C73-C74-C75-C76
33	a	202	PLX	C25-C26-C27-C28
32	r	505	CDL	CB5-C51-C52-C53
33	a	202	PLX	C33-C34-C35-C36
32	a	201	CDL	C35-C36-C37-C38
32	r	505	CDL	C75-C76-C77-C78
30	b	201	PEE	C22-C23-C24-C25
33	a	202	PLX	C10-C11-C12-C13
32	r	505	CDL	C79-C80-C81-C82
32	i	401	CDL	C33-C34-C35-C36
32	g	202	CDL	C73-C74-C75-C76
32	r	504	CDL	C14-C15-C16-C17
33	a	202	PLX	C31-C32-C33-C34
33	j	201	PLX	C2-C1-N1-C1C
33	j	201	PLX	C2-C1-N1-C1B
32	l	701	CDL	C56-C57-C58-C59
33	j	201	PLX	C12-C13-C14-C15
33	r	503	PLX	C10-C11-C12-C13
30	r	501	PEE	C30-C31-C32-C33
32	a	201	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
30	b	201	PEE	C32-C33-C34-C35
32	r	504	CDL	C71-C72-C73-C74
30	l	702	PEE	C19-C20-C21-C22
30	r	501	PEE	C39-C40-C41-C42
32	i	401	CDL	C11-C12-C13-C14
32	g	202	CDL	C12-C13-C14-C15
30	U	101	PEE	C21-C22-C23-C24
32	r	505	CDL	C62-C63-C64-C65
30	U	101	PEE	C36-C37-C38-C39
30	r	501	PEE	C36-C37-C38-C39
32	l	701	CDL	C62-C63-C64-C65
32	r	504	CDL	C11-C12-C13-C14
30	U	101	PEE	C22-C23-C24-C25
32	r	505	CDL	C61-C62-C63-C64
33	g	201	PLX	C31-C32-C33-C34
33	j	201	PLX	C13-C14-C15-C16
30	r	501	PEE	C31-C32-C33-C34
32	l	701	CDL	C74-C75-C76-C77
33	r	502	PLX	C28-C29-C30-C31
33	r	503	PLX	C11-C12-C13-C14
32	a	201	CDL	C22-C23-C24-C25
32	i	401	CDL	C32-C33-C34-C35
32	l	701	CDL	C71-C72-C73-C74
32	r	505	CDL	C42-C43-C44-C45
32	r	505	CDL	C32-C33-C34-C35
32	r	505	CDL	C33-C34-C35-C36
30	i	402	PEE	C18-C19-C20-C21
33	r	502	PLX	C7-C8-C9-C10
30	m	201	PEE	C19-C20-C21-C22
30	U	101	PEE	C31-C32-C33-C34
33	a	202	PLX	O4-C3-C4-C5
33	r	502	PLX	C33-C34-C35-C36
33	j	201	PLX	C26-C27-C28-C29
32	r	504	CDL	C40-C41-C42-C43
30	b	201	PEE	C12-C13-C14-C15
32	l	701	CDL	CA7-C31-C32-C33
30	b	201	PEE	C1-C2-C3-O3
30	r	501	PEE	C1-C2-C3-O3
32	g	202	CDL	CA3-CA4-CA6-OA8
32	r	505	CDL	CB3-CB4-CB6-OB8
33	r	502	PLX	C3-C4-C5-O8
30	i	402	PEE	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
32	l	701	CDL	C31-C32-C33-C34
32	l	701	CDL	C52-C53-C54-C55
32	r	505	CDL	C55-C56-C57-C58
30	U	102	PEE	C13-C14-C15-C16
32	a	201	CDL	C74-C75-C76-C77
32	i	401	CDL	C35-C36-C37-C38
30	U	102	PEE	C33-C34-C35-C36
32	a	201	CDL	C59-C60-C61-C62
32	i	401	CDL	C14-C15-C16-C17
33	r	503	PLX	C28-C29-C30-C31
30	U	102	PEE	C23-C24-C25-C26
33	g	201	PLX	C13-C14-C15-C16
30	i	402	PEE	C30-C31-C32-C33
30	U	102	PEE	C12-C13-C14-C15
32	g	202	CDL	C60-C61-C62-C63
32	r	505	CDL	C82-C83-C84-C85
32	r	505	CDL	OB6-CB4-CB6-OB8
30	r	501	PEE	C40-C41-C42-C43
33	g	201	PLX	C27-C28-C29-C30
33	j	201	PLX	C9-C10-C11-C12
32	i	401	CDL	C75-C76-C77-C78
32	r	504	CDL	C60-C61-C62-C63
30	m	201	PEE	O3-C30-C31-C32
32	g	202	CDL	C54-C55-C56-C57
30	i	402	PEE	C24-C25-C26-C27
31	X	201	8Q1	C31-C29-C32-O33
33	r	503	PLX	C9-C10-C11-C12
32	i	401	CDL	C73-C74-C75-C76
32	r	505	CDL	C17-C18-C19-C20
33	j	201	PLX	C14-C15-C16-C17
30	U	102	PEE	C34-C35-C36-C37
31	X	201	8Q1	C29-C32-C34-O35
33	g	201	PLX	C29-C30-C31-C32
30	l	702	PEE	O3P-C1-C2-C3
32	a	201	CDL	OA5-CA3-CA4-CA6
32	l	701	CDL	C64-C65-C66-C67
30	l	702	PEE	C30-C31-C32-C33
30	U	102	PEE	C14-C15-C16-C17
32	r	505	CDL	CA5-C11-C12-C13
32	l	701	CDL	C82-C83-C84-C85
30	r	501	PEE	C41-C42-C43-C44
32	a	201	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
30	i	402	PEE	C1-C2-C3-O3
30	l	702	PEE	C1-C2-C3-O3
31	X	201	8Q1	O33-C32-C34-N36
32	l	701	CDL	CA3-CA4-CA6-OA8
32	l	701	CDL	CB3-CB4-CB6-OB8
33	r	503	PLX	C3-C4-C5-O8
32	a	201	CDL	C60-C61-C62-C63
33	r	503	PLX	C26-C27-C28-C29
32	r	505	CDL	C41-C42-C43-C44
32	i	401	CDL	CA7-C31-C32-C33
30	b	201	PEE	O3P-C1-C2-O2
30	m	201	PEE	C23-C24-C25-C26
32	r	505	CDL	C76-C77-C78-C79
32	r	505	CDL	CB4-CB3-OB5-PB2
33	j	201	PLX	C33-C34-C35-C36
30	i	402	PEE	C31-C32-C33-C34
32	r	504	CDL	C36-C37-C38-C39
30	l	702	PEE	O2-C2-C3-O3
32	i	401	CDL	OB6-CB4-CB6-OB8
32	r	505	CDL	OA6-CA4-CA6-OA8
33	r	502	PLX	O6-C4-C5-O8
33	r	503	PLX	O6-C4-C5-O8
33	r	503	PLX	C16-C17-C18-C19
32	r	505	CDL	C20-C21-C22-C23
33	g	201	PLX	C14-C15-C16-C17
30	U	102	PEE	C38-C39-C40-C41
33	r	503	PLX	O8-C24-C25-C26
32	g	202	CDL	C13-C14-C15-C16
32	r	504	CDL	C37-C38-C39-C40
33	g	201	PLX	C11-C12-C13-C14
32	l	701	CDL	C17-C18-C19-C20
30	U	102	PEE	C20-C21-C22-C23
33	j	201	PLX	C34-C35-C36-C37
33	g	201	PLX	C36-C37-C38-C39
30	b	201	PEE	C23-C24-C25-C26
32	a	201	CDL	C14-C15-C16-C17
32	r	505	CDL	C54-C55-C56-C57
32	r	505	CDL	C63-C64-C65-C66
30	l	702	PEE	C21-C22-C23-C24
33	a	202	PLX	C27-C28-C29-C30
32	a	201	CDL	OB5-CB3-CB4-CB6
32	i	401	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
33	j	201	PLX	O4-C3-C4-C5
33	r	503	PLX	C31-C32-C33-C34
32	r	504	CDL	C42-C43-C44-C45
33	r	503	PLX	C15-C16-C17-C18
33	r	503	PLX	C36-C37-C38-C39
30	m	201	PEE	C3-C2-O2-C10
30	U	101	PEE	C15-C16-C17-C18
30	U	102	PEE	C15-C16-C17-C18
32	g	202	CDL	C14-C15-C16-C17
32	r	504	CDL	C72-C73-C74-C75
30	U	102	PEE	O3P-C1-C2-O2
32	a	201	CDL	OB5-CB3-CB4-OB6
32	i	401	CDL	OA5-CA3-CA4-OA6
32	l	701	CDL	OA5-CA3-CA4-OA6
33	g	201	PLX	O4-C3-C4-O6
33	j	201	PLX	O4-C3-C4-O6
33	r	502	PLX	O4-C3-C4-O6
32	r	505	CDL	CA3-CA4-CA6-OA8
33	g	201	PLX	C3-C4-C5-O8
30	b	201	PEE	C13-C14-C15-C16
30	i	402	PEE	C32-C33-C34-C35
32	l	701	CDL	C63-C64-C65-C66
30	i	402	PEE	O2-C2-C3-O3
30	r	501	PEE	O2-C2-C3-O3
32	g	202	CDL	OA6-CA4-CA6-OA8
32	i	401	CDL	OA6-CA4-CA6-OA8
33	g	201	PLX	O6-C4-C5-O8
30	i	402	PEE	C2-C1-O3P-P
32	l	701	CDL	O1-C1-CB2-OB2
30	U	102	PEE	C31-C30-O3-C3
32	l	701	CDL	C31-CA7-OA8-CA6
30	U	101	PEE	C19-C20-C21-C22
33	g	201	PLX	C28-C29-C30-C31
30	U	101	PEE	C38-C39-C40-C41
30	U	102	PEE	O3P-C1-C2-C3
30	b	201	PEE	O3P-C1-C2-C3
32	l	701	CDL	OA5-CA3-CA4-CA6
33	g	201	PLX	O4-C3-C4-C5
33	r	502	PLX	O4-C3-C4-C5
32	r	505	CDL	C83-C84-C85-C86
32	l	701	CDL	C58-C59-C60-C61
30	U	102	PEE	O5-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
32	l	701	CDL	OA9-CA7-OA8-CA6
32	g	202	CDL	C58-C59-C60-C61
33	r	502	PLX	C31-C32-C33-C34
32	i	401	CDL	CA3-CA4-CA6-OA8
30	U	101	PEE	C30-C31-C32-C33
32	r	505	CDL	C64-C65-C66-C67
30	b	201	PEE	C18-C19-C20-C21
32	r	505	CDL	C44-C45-C46-C47
30	U	101	PEE	C1-O3P-P-O2P
30	U	101	PEE	C4-O4P-P-O3P
30	U	101	PEE	C4-O4P-P-O2P
30	b	201	PEE	C4-O4P-P-O3P
30	b	201	PEE	C4-O4P-P-O1P
30	i	402	PEE	C1-O3P-P-O1P
30	l	702	PEE	C4-O4P-P-O2P
30	r	501	PEE	C1-O3P-P-O2P
30	r	501	PEE	C1-O3P-P-O1P
30	r	501	PEE	C1-O3P-P-O4P
30	r	501	PEE	C4-O4P-P-O1P
32	a	201	CDL	CA3-OA5-PA1-OA2
32	g	202	CDL	CB2-OB2-PB2-OB4
32	g	202	CDL	CB2-OB2-PB2-OB5
32	g	202	CDL	CB3-OB5-PB2-OB2
32	g	202	CDL	CB3-OB5-PB2-OB4
32	i	401	CDL	CA2-OA2-PA1-OA5
32	i	401	CDL	CA3-OA5-PA1-OA4
32	i	401	CDL	CB2-OB2-PB2-OB3
32	l	701	CDL	CB3-OB5-PB2-OB2
32	l	701	CDL	CB3-OB5-PB2-OB3
32	l	701	CDL	CB3-OB5-PB2-OB4
32	r	504	CDL	CA2-OA2-PA1-OA3
32	r	504	CDL	CA3-OA5-PA1-OA3
32	r	504	CDL	CB3-OB5-PB2-OB2
32	r	504	CDL	CB3-OB5-PB2-OB4
32	r	505	CDL	CB3-OB5-PB2-OB3
33	r	502	PLX	C3-O4-P1-O3
34	s	401	UQ	C12-C11-C9-C8
30	b	201	PEE	C34-C35-C36-C37
32	a	201	CDL	C21-C22-C23-C24
32	r	505	CDL	C13-C14-C15-C16
33	j	201	PLX	C11-C12-C13-C14
33	r	502	PLX	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
32	r	504	CDL	CA7-C31-C32-C33
33	j	201	PLX	C31-C32-C33-C34
32	l	701	CDL	C44-C45-C46-C47
30	U	102	PEE	C22-C23-C24-C25
32	a	201	CDL	C31-CA7-OA8-CA6
32	a	201	CDL	OA9-CA7-OA8-CA6
32	a	201	CDL	C13-C14-C15-C16
30	U	101	PEE	O2-C2-C3-O3
30	b	201	PEE	O2-C2-C3-O3
33	r	503	PLX	C30-C31-C32-C33
33	a	202	PLX	C6-C7-C8-C9
32	a	201	CDL	C77-C78-C79-C80
33	a	202	PLX	C24-C25-C26-C27
32	g	202	CDL	C72-C73-C74-C75
32	i	401	CDL	C38-C39-C40-C41
33	j	201	PLX	O9-C24-C25-C26
33	j	201	PLX	O6-C6-C7-C8
32	r	504	CDL	C44-C45-C46-C47
30	r	501	PEE	C38-C39-C40-C41
33	r	502	PLX	C16-C17-C18-C19
33	a	202	PLX	C29-C30-C31-C32
31	X	201	8Q1	C29-C32-C34-N36
30	m	201	PEE	O5-C30-C31-C32
30	U	102	PEE	C21-C22-C23-C24
30	U	101	PEE	C12-C13-C14-C15
32	r	504	CDL	C54-C55-C56-C57
32	r	504	CDL	C76-C77-C78-C79
32	g	202	CDL	C19-C20-C21-C22
33	r	502	PLX	C13-C14-C15-C16
30	i	402	PEE	C37-C38-C39-C40
30	i	402	PEE	C22-C23-C24-C25
33	j	201	PLX	C18-C19-C20-C21
32	r	505	CDL	C31-CA7-OA8-CA6
33	r	503	PLX	C19-C20-C21-C22
30	U	102	PEE	C16-C17-C18-C19
30	l	702	PEE	C38-C39-C40-C41
30	m	201	PEE	C22-C23-C24-C25
30	r	501	PEE	C24-C25-C26-C27
32	g	202	CDL	C11-C12-C13-C14
32	r	504	CDL	C34-C35-C36-C37
32	r	505	CDL	C72-C73-C74-C75
30	U	101	PEE	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
30	m	201	PEE	C16-C17-C18-C19
32	r	504	CDL	C53-C54-C55-C56
30	m	201	PEE	C15-C16-C17-C18
30	U	101	PEE	C34-C35-C36-C37
33	r	503	PLX	C7-C8-C9-C10
33	r	502	PLX	C18-C19-C20-C21
30	U	102	PEE	C39-C40-C41-C42
30	r	501	PEE	C31-C30-O3-C3
32	r	505	CDL	OA9-CA7-OA8-CA6
32	g	202	CDL	C17-C18-C19-C20
33	j	201	PLX	C32-C33-C34-C35
30	r	501	PEE	O5-C30-O3-C3
32	a	201	CDL	C36-C37-C38-C39
30	U	102	PEE	C44-C45-C46-C47
32	g	202	CDL	C61-C62-C63-C64
30	l	702	PEE	C16-C17-C18-C19
32	g	202	CDL	C51-C52-C53-C54
33	a	202	PLX	C16-C17-C18-C19
32	i	401	CDL	C39-C40-C41-C42
33	a	202	PLX	C30-C31-C32-C33
32	r	504	CDL	C23-C24-C25-C26
32	l	701	CDL	C80-C81-C82-C83
30	r	501	PEE	C15-C16-C17-C18
30	U	102	PEE	C18-C19-C20-C21
30	b	201	PEE	C10-C11-C12-C13
30	i	402	PEE	C36-C37-C38-C39
30	l	702	PEE	C36-C37-C38-C39
30	m	201	PEE	C18-C19-C20-C21
30	r	501	PEE	C18-C19-C20-C21
30	b	201	PEE	C15-C16-C17-C18
30	i	402	PEE	C14-C15-C16-C17
32	l	701	CDL	C61-C62-C63-C64
30	i	402	PEE	C38-C39-C40-C41
30	U	101	PEE	C1-C2-C3-O3
32	r	505	CDL	C60-C61-C62-C63
32	a	201	CDL	C76-C77-C78-C79
33	j	201	PLX	C30-C31-C32-C33
32	a	201	CDL	C43-C44-C45-C46
30	l	702	PEE	C18-C19-C20-C21
33	j	201	PLX	C7-C6-O6-C4
32	r	505	CDL	C51-C52-C53-C54
32	r	504	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
30	b	201	PEE	C38-C39-C40-C41
30	l	702	PEE	O2-C10-C11-C12
32	l	701	CDL	C14-C15-C16-C17
30	b	201	PEE	C16-C17-C18-C19
32	a	201	CDL	C37-C38-C39-C40
32	r	505	CDL	C84-C85-C86-C87
30	b	201	PEE	C24-C25-C26-C27
32	i	401	CDL	C15-C16-C17-C18
32	a	201	CDL	C32-C31-CA7-OA8
32	l	701	CDL	C32-C31-CA7-OA8
30	i	402	PEE	C20-C21-C22-C23
32	l	701	CDL	C57-C58-C59-C60
35	w	401	ADP	C4'-C5'-O5'-PA
32	g	202	CDL	C12-C11-CA5-OA6
30	m	201	PEE	C1-C2-C3-O3
32	i	401	CDL	CB3-CB4-CB6-OB8
33	j	201	PLX	C3-C4-C5-O8
32	g	202	CDL	C72-C71-CB7-OB8
32	l	701	CDL	C12-C11-CA5-OA6
33	a	202	PLX	C19-C20-C21-C22
32	r	504	CDL	C17-C18-C19-C20
32	l	701	CDL	C32-C33-C34-C35
30	b	201	PEE	O3-C30-C31-C32
32	r	504	CDL	C12-C13-C14-C15
32	r	505	CDL	C15-C16-C17-C18
33	g	201	PLX	C6-C7-C8-C9
33	g	201	PLX	C24-C25-C26-C27
32	i	401	CDL	C72-C73-C74-C75
33	a	202	PLX	O8-C24-C25-C26
33	g	201	PLX	O8-C24-C25-C26
30	U	101	PEE	C11-C12-C13-C14
30	l	702	PEE	O4-C10-C11-C12
32	l	701	CDL	C12-C11-CA5-OA7
32	r	505	CDL	C23-C24-C25-C26
32	l	701	CDL	C41-C42-C43-C44
32	r	504	CDL	C12-C11-CA5-OA7
33	a	202	PLX	O9-C24-O8-C5
33	r	502	PLX	O9-C24-O8-C5
33	r	503	PLX	O9-C24-O8-C5
32	g	202	CDL	C72-C71-CB7-OB9
33	g	201	PLX	C4-C5-O8-C24
33	j	201	PLX	C4-C5-O8-C24

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Mol	Chain	Res	Type	Atoms
30	m	201	PEE	O2-C2-C3-O3
30	U	101	PEE	C40-C41-C42-C43
32	g	202	CDL	C21-C22-C23-C24
30	b	201	PEE	O5-C30-C31-C32
30	l	702	PEE	C32-C33-C34-C35
32	l	701	CDL	C53-C54-C55-C56
32	l	701	CDL	C32-C31-CA7-OA9
32	a	201	CDL	C32-C31-CA7-OA9
32	g	202	CDL	C12-C11-CA5-OA7
30	m	201	PEE	C34-C35-C36-C37
32	a	201	CDL	C72-C71-CB7-OB8
30	l	702	PEE	C14-C15-C16-C17
30	U	101	PEE	O3-C30-C31-C32
32	r	505	CDL	C57-C58-C59-C60

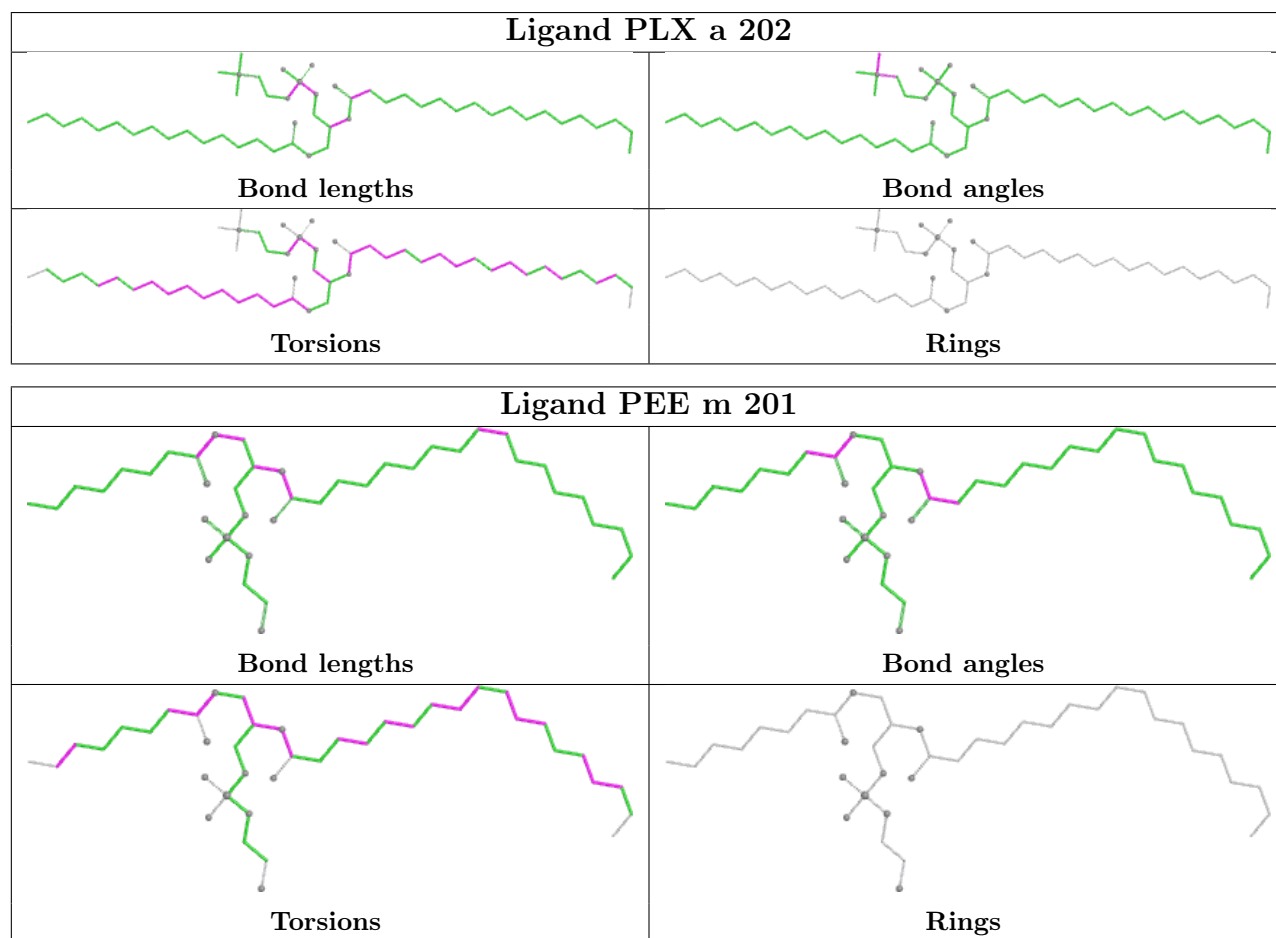
There are no ring outliers.

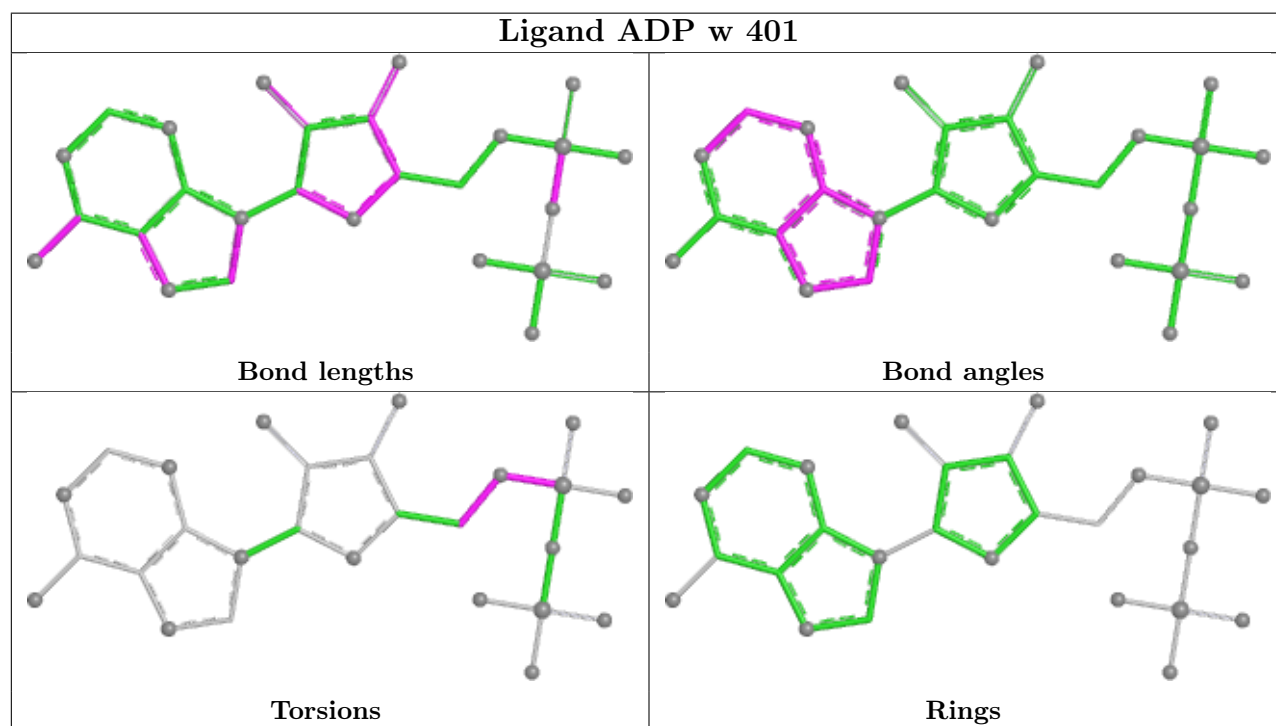
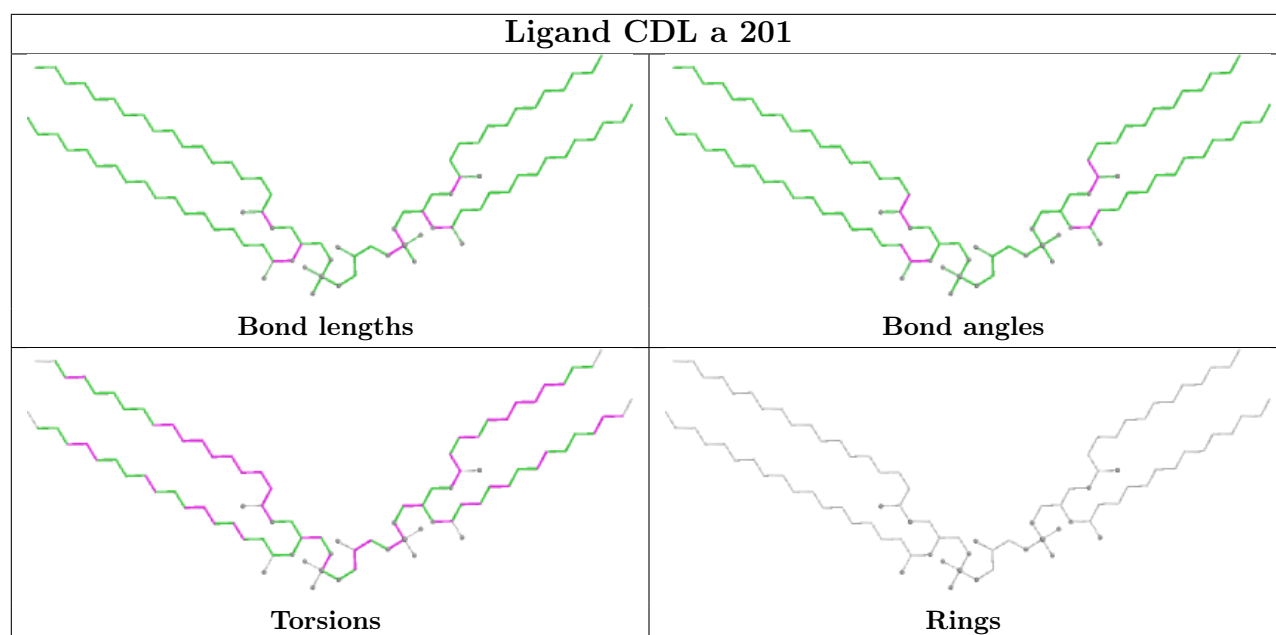
21 monomers are involved in 83 short contacts:

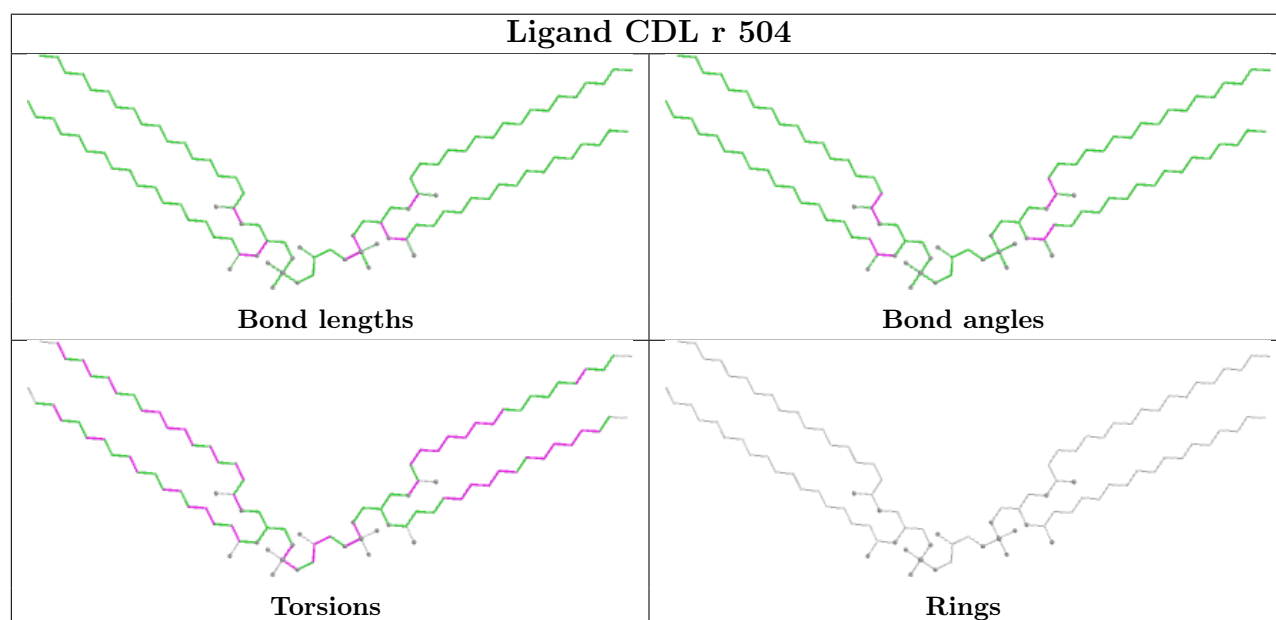
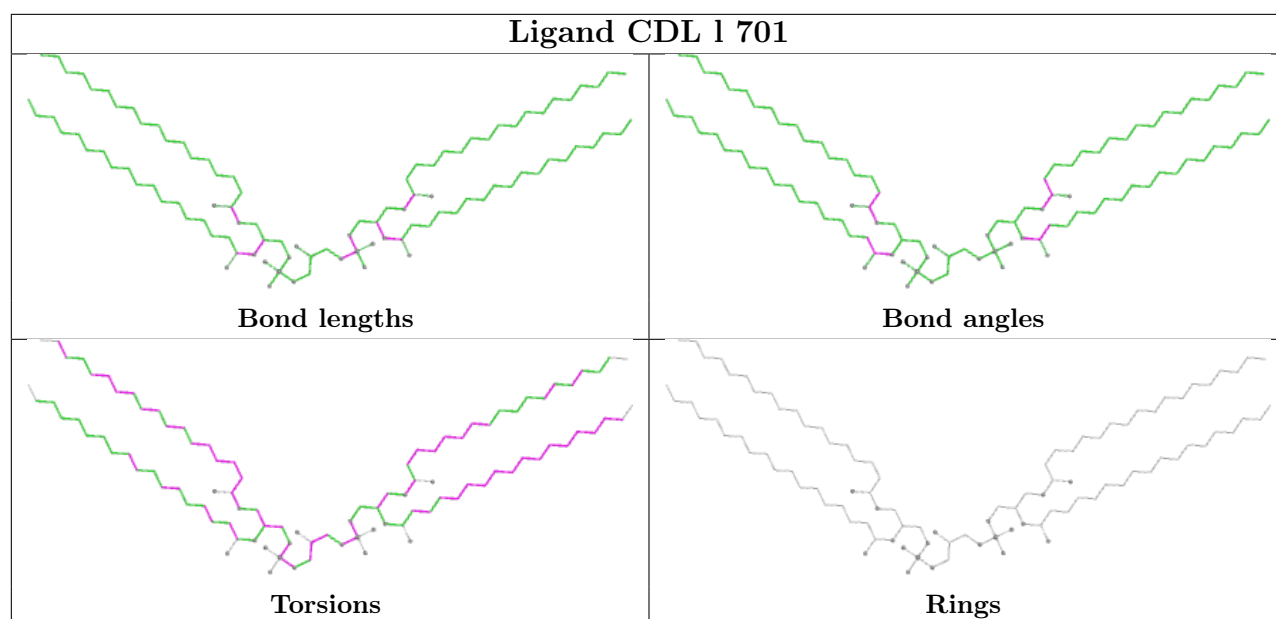
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	a	202	PLX	2	0
30	m	201	PEE	2	0
32	a	201	CDL	2	0
35	w	401	ADP	1	0
32	l	701	CDL	6	0
32	r	504	CDL	12	0
33	g	201	PLX	5	0
33	j	201	PLX	1	0
32	g	202	CDL	7	0
33	r	502	PLX	5	0
31	X	201	8Q1	4	0
34	s	401	UQ	6	0
30	U	101	PEE	1	0
30	i	402	PEE	3	0
30	U	102	PEE	3	0
30	b	201	PEE	4	0
33	r	503	PLX	6	0
32	r	505	CDL	8	0
30	r	501	PEE	3	0
30	l	702	PEE	3	0
32	i	401	CDL	4	0

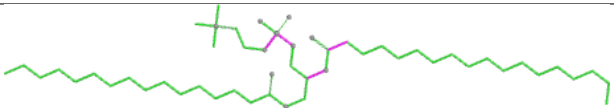
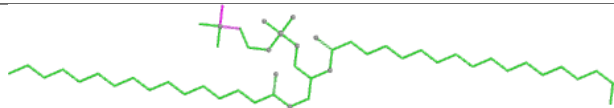
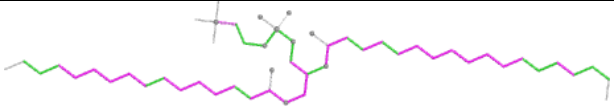
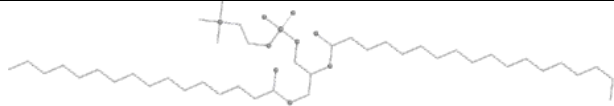
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

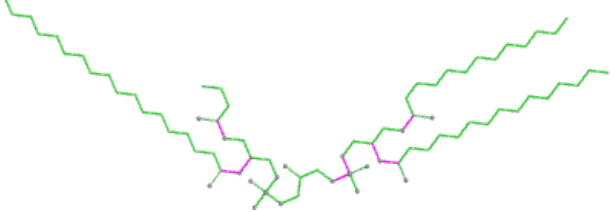
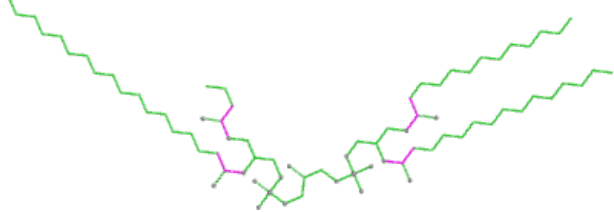
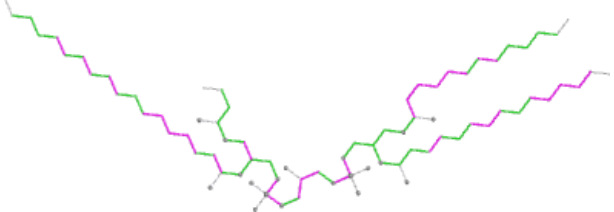
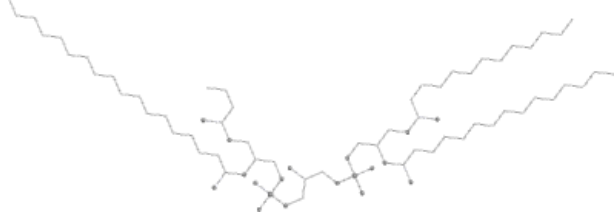
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

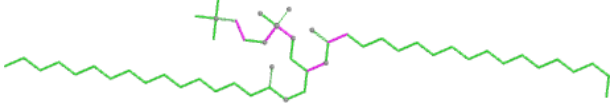
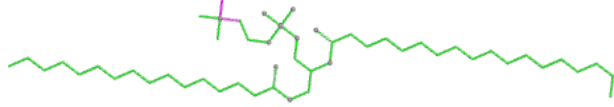
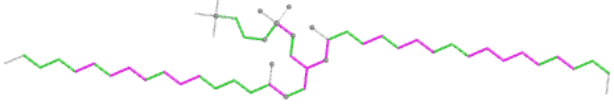
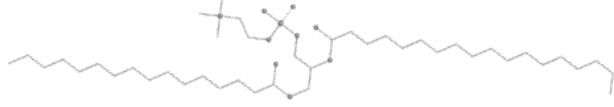


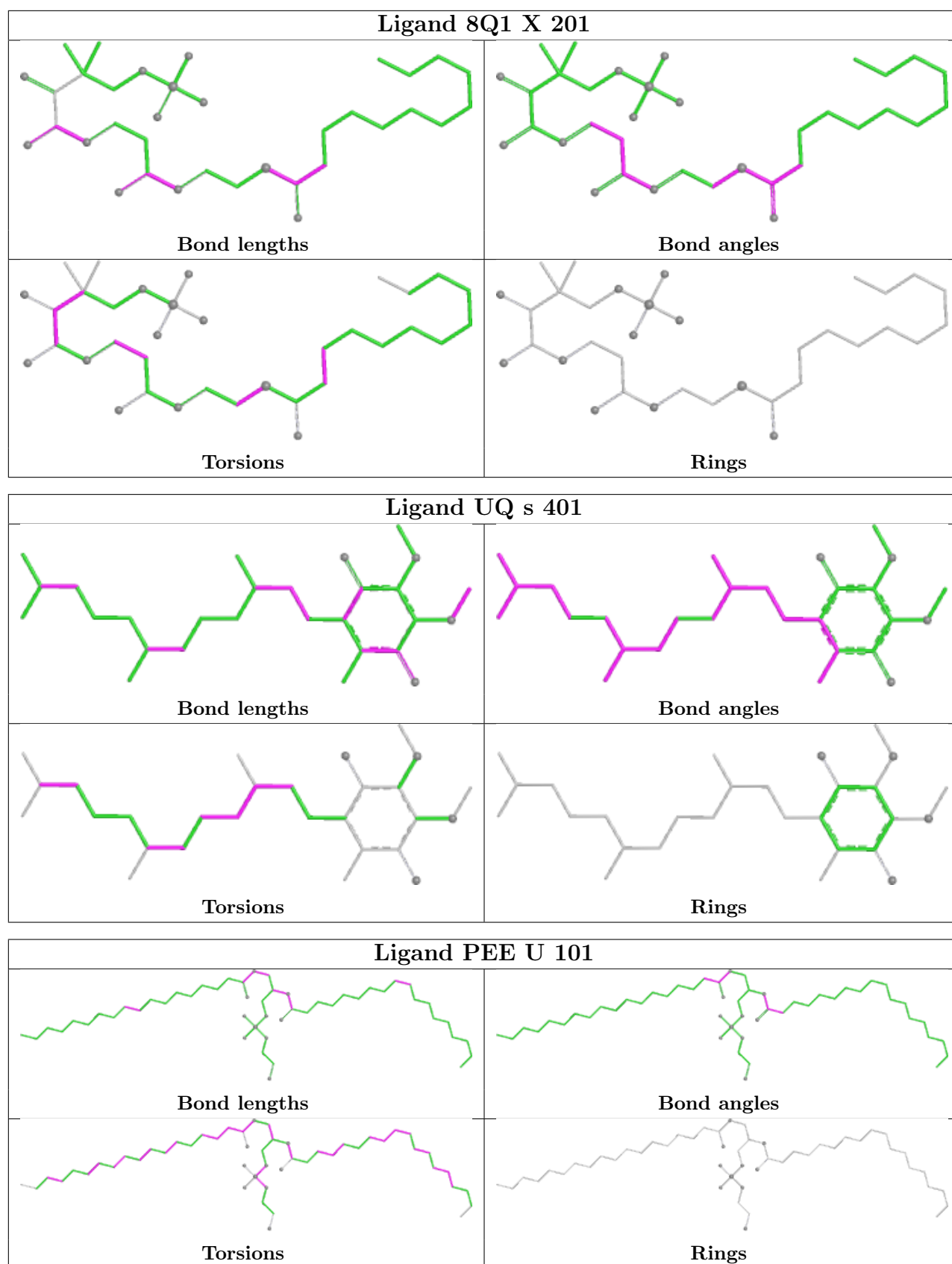


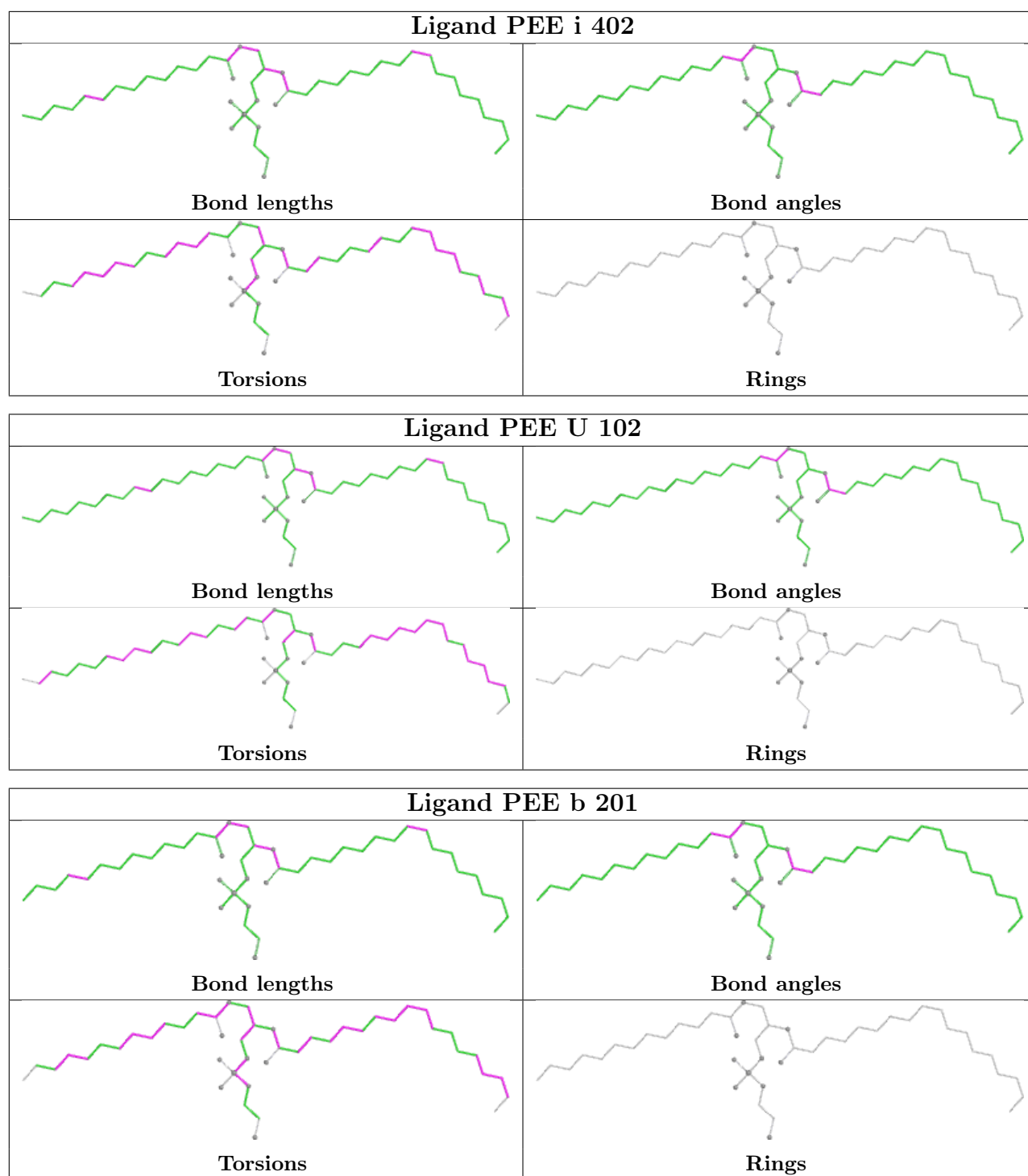


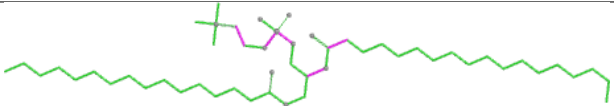
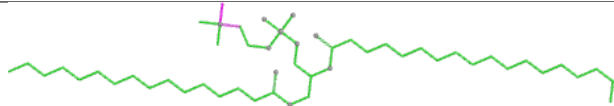
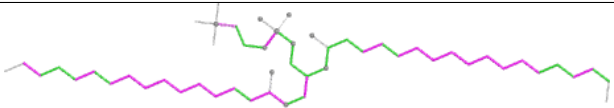
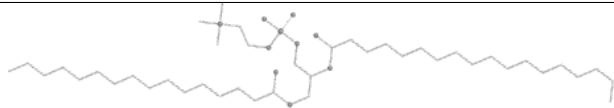
Ligand PLX j 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

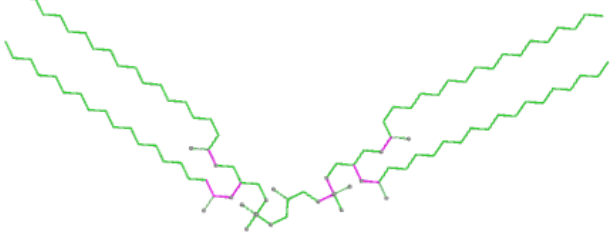
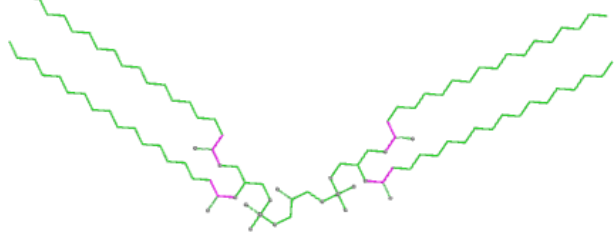
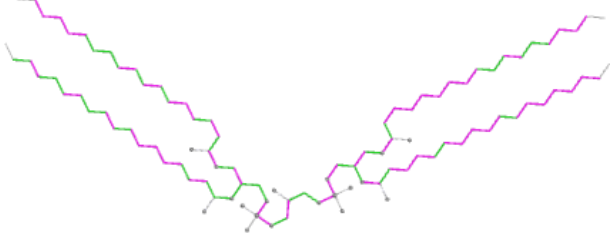
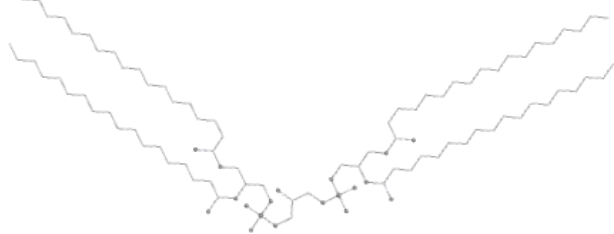
Ligand CDL g 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

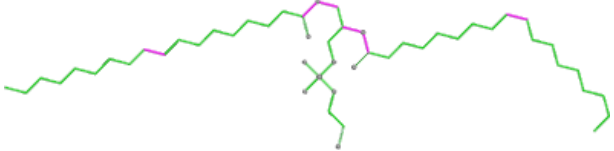
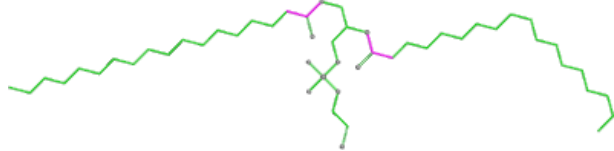
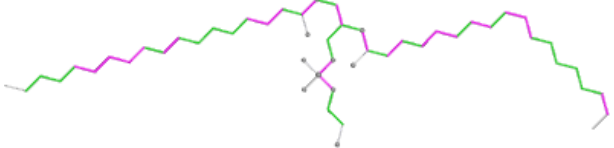
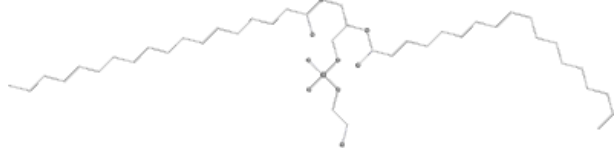
Ligand PLX r 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

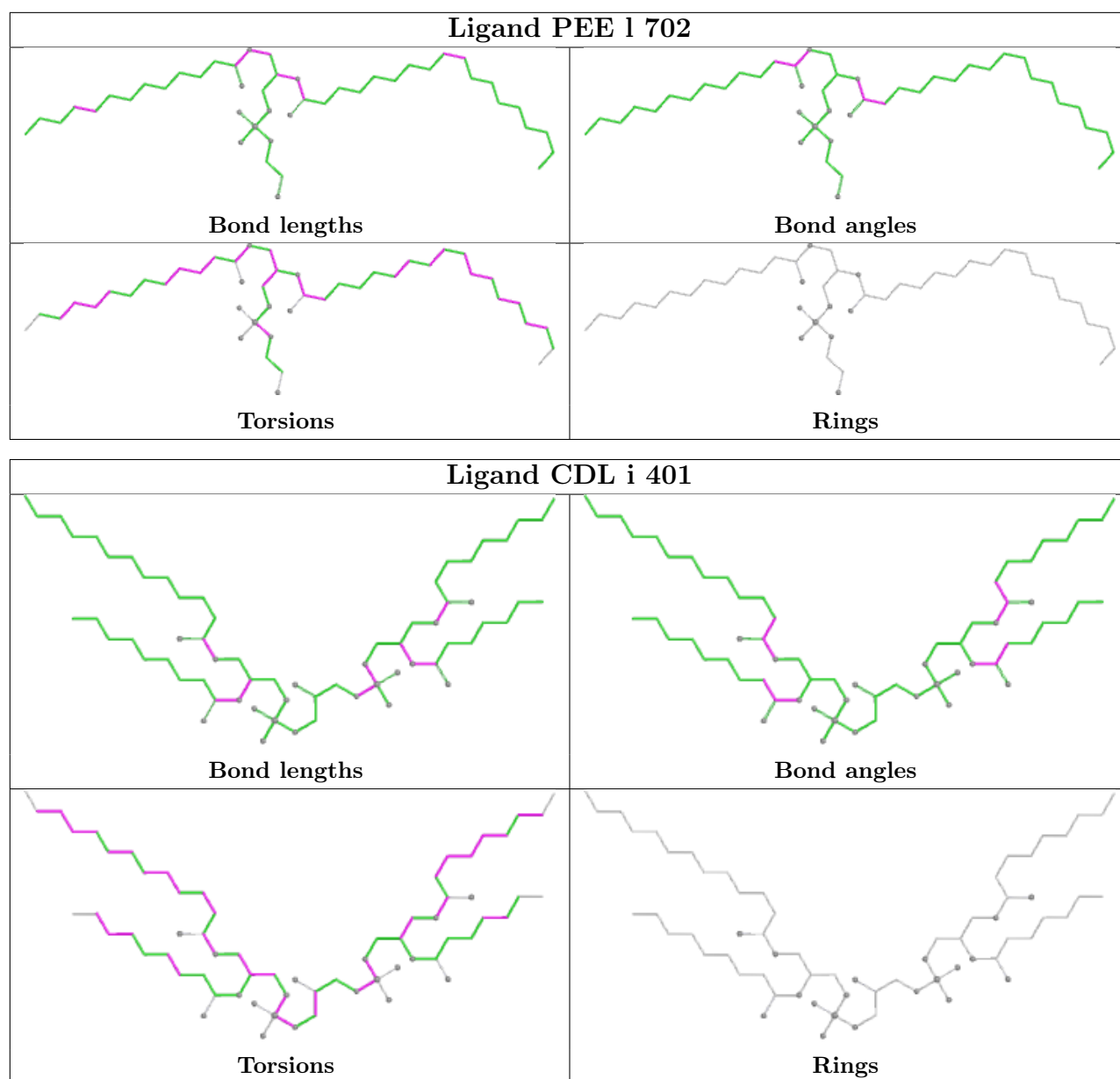




Ligand PLX r 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CDL r 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEE r 501	
	
Bond lengths	Bond angles
	
Torsions	Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

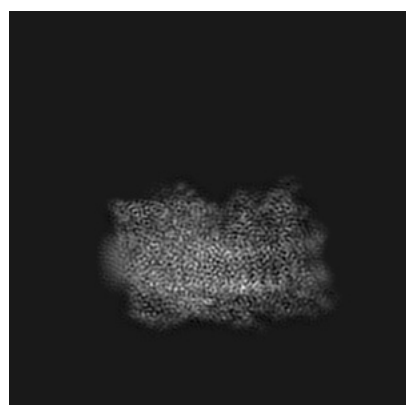
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32206. These allow visual inspection of the internal detail of the map and identification of artifacts.

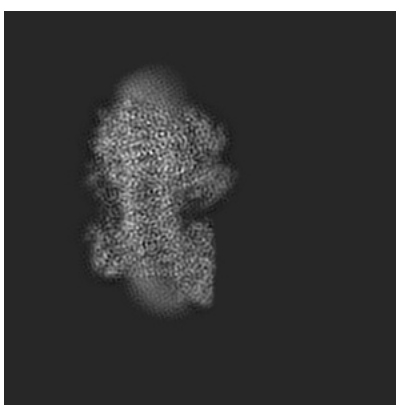
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

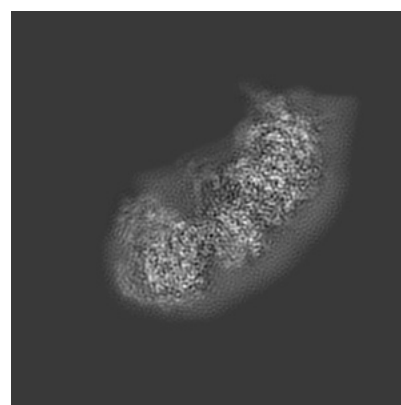
6.1.1 Primary map



X



Y

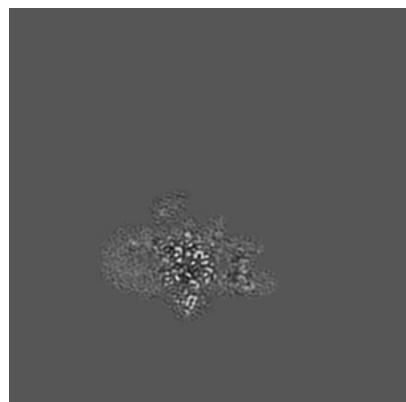


Z

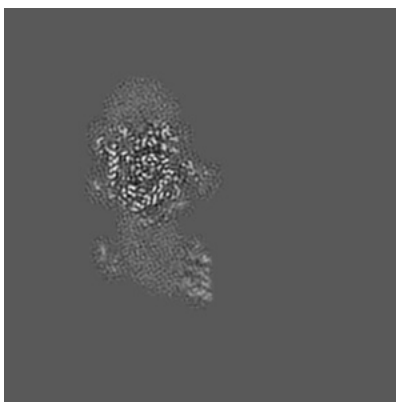
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

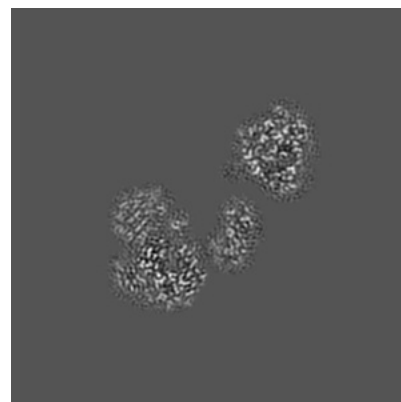
6.2.1 Primary map



X Index: 155



Y Index: 155

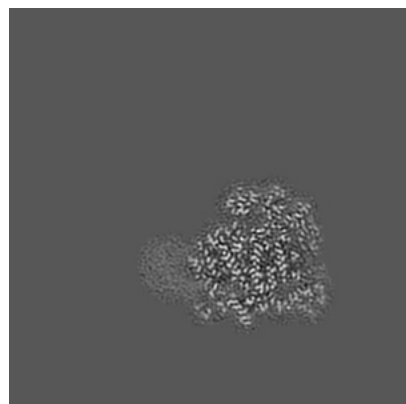


Z Index: 155

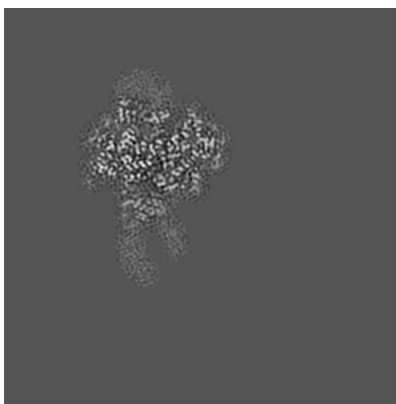
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

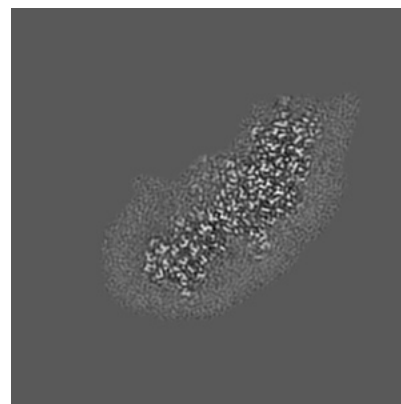
6.3.1 Primary map



X Index: 208



Y Index: 180

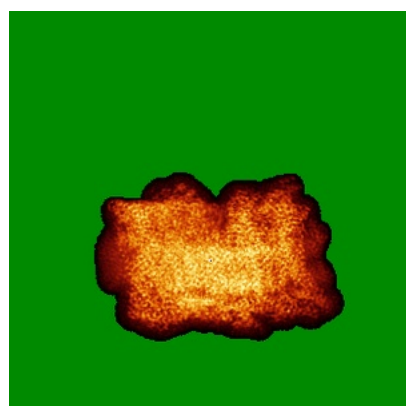


Z Index: 120

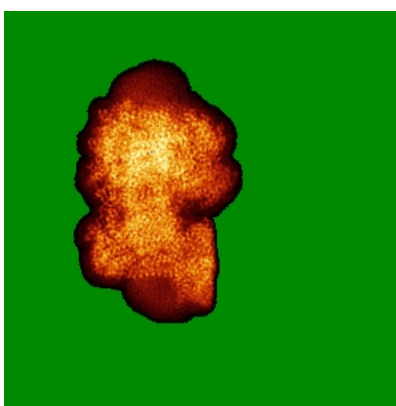
The images above show the largest variance slices of the map in three orthogonal directions.

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

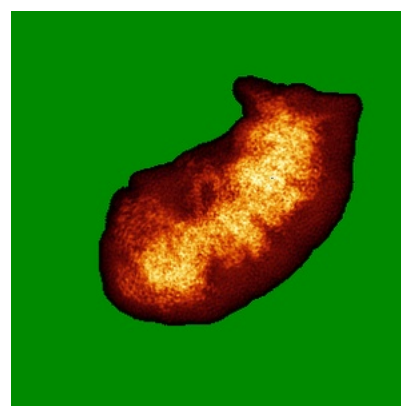
6.4.1 Primary map



X



Y

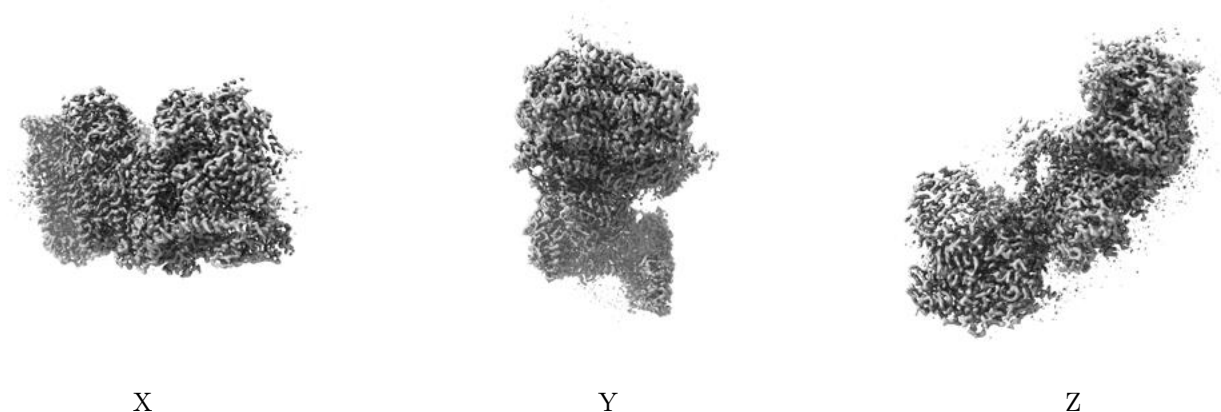


Z

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 0.0288. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

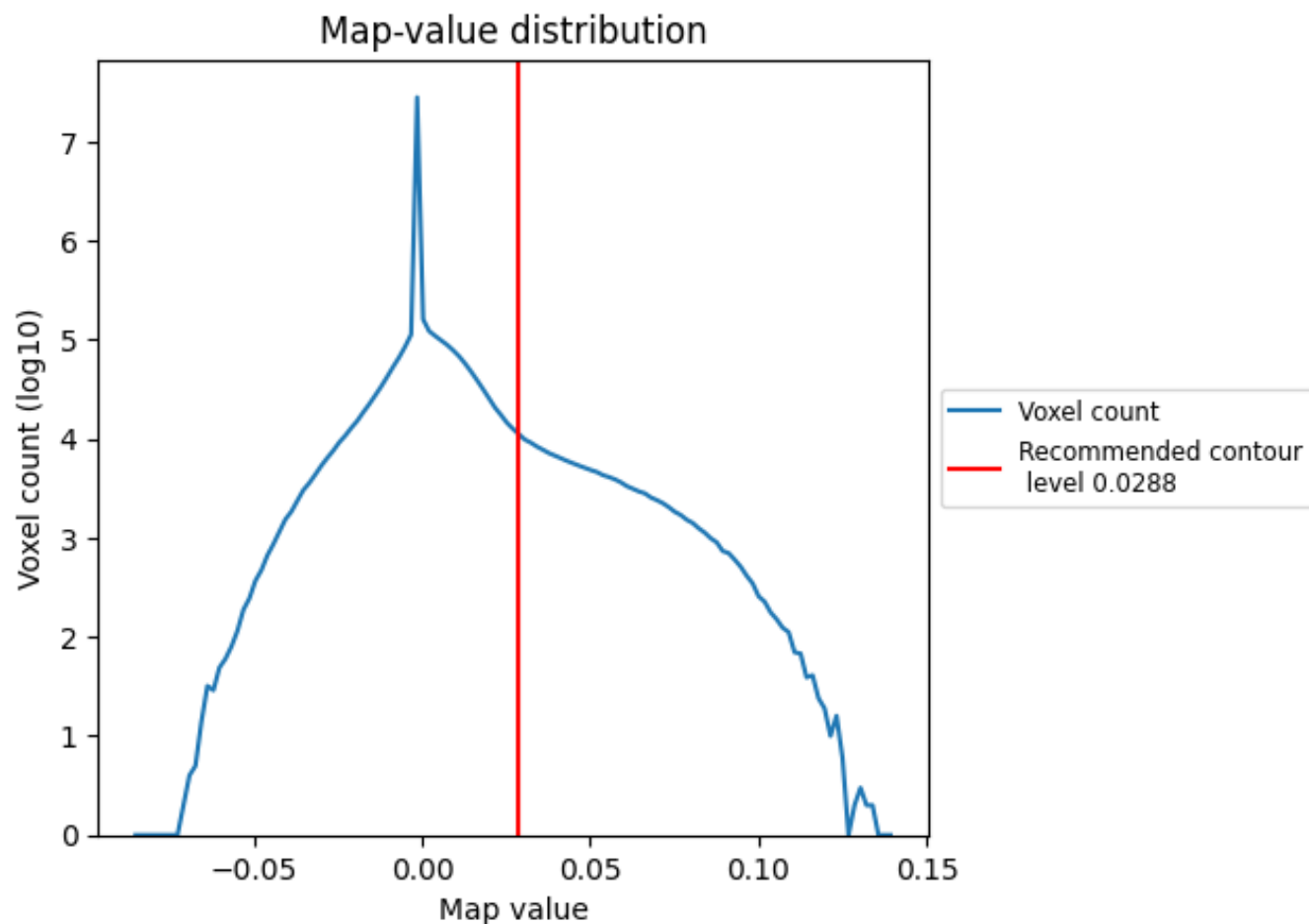
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

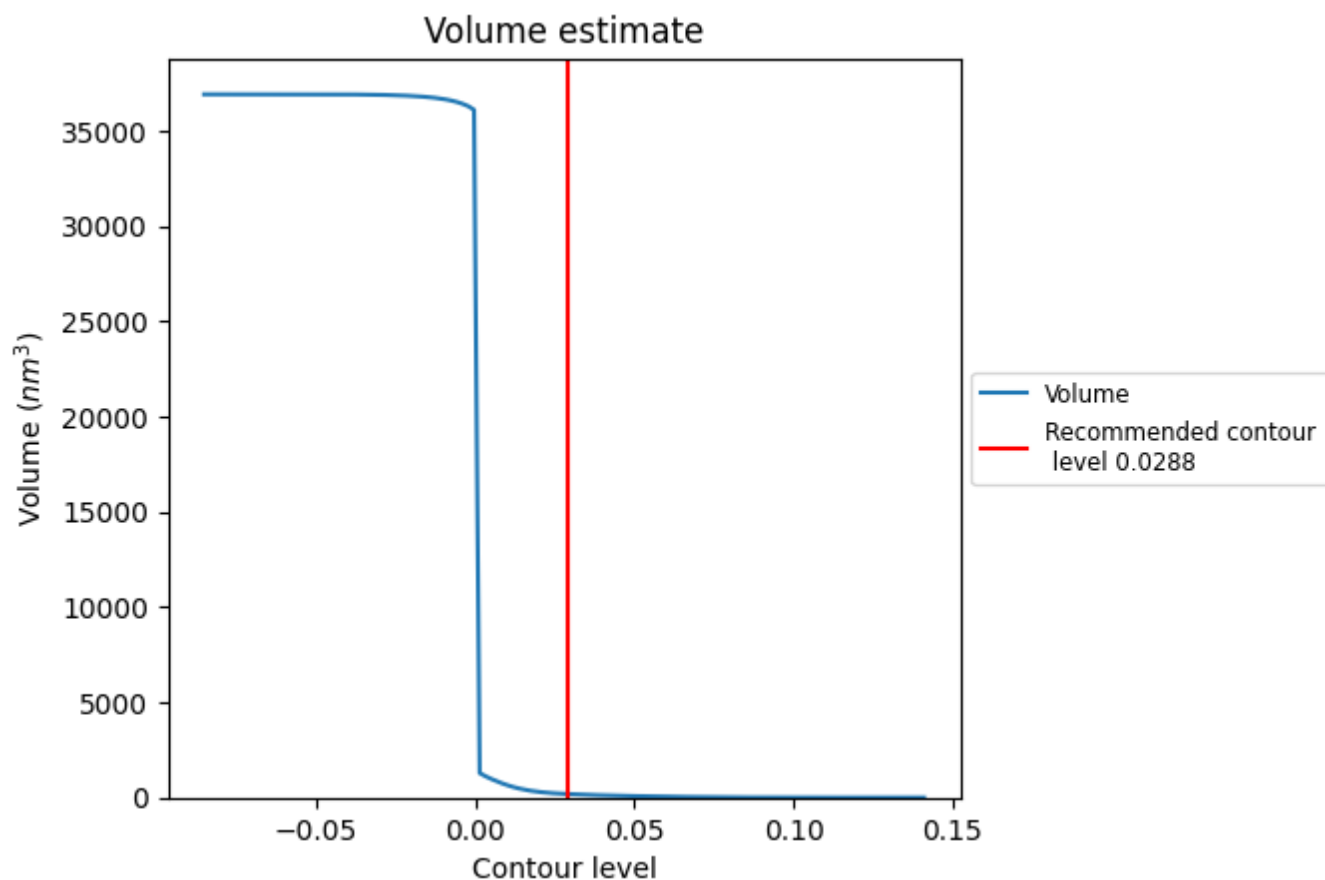
This section contains the results of statistical analysis of the map.

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.

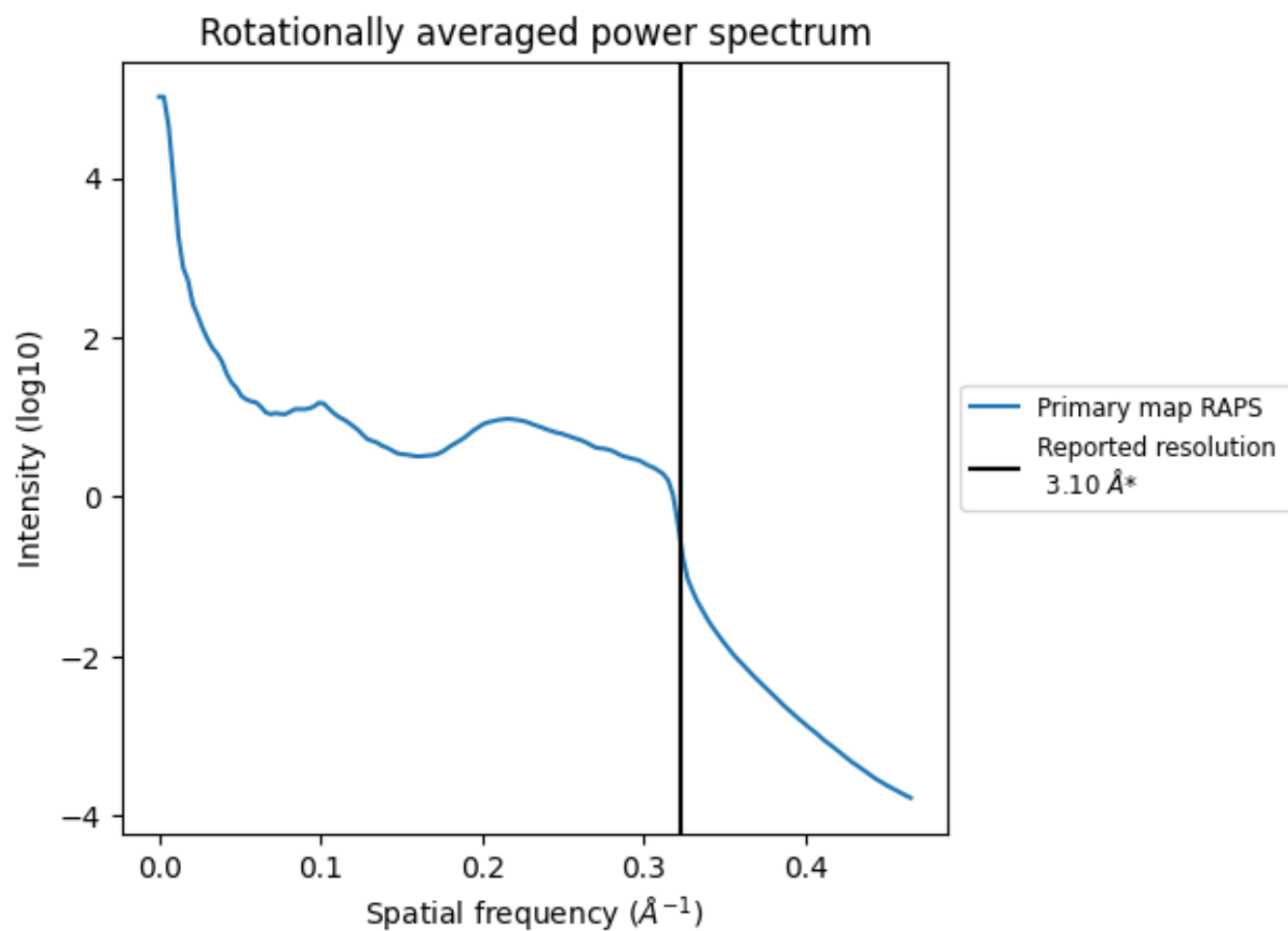
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 188 nm³; this corresponds to an approximate mass of 169 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

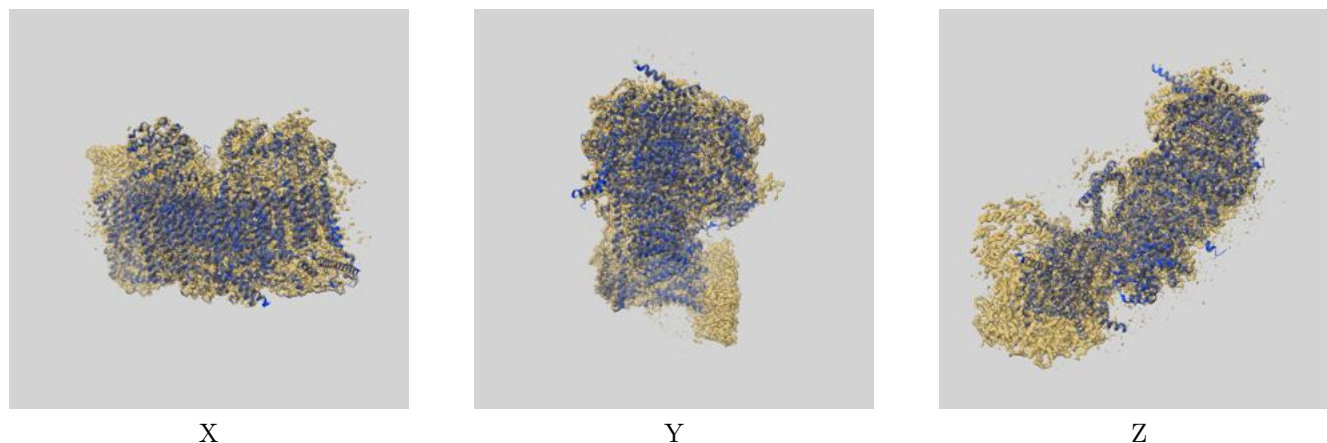
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

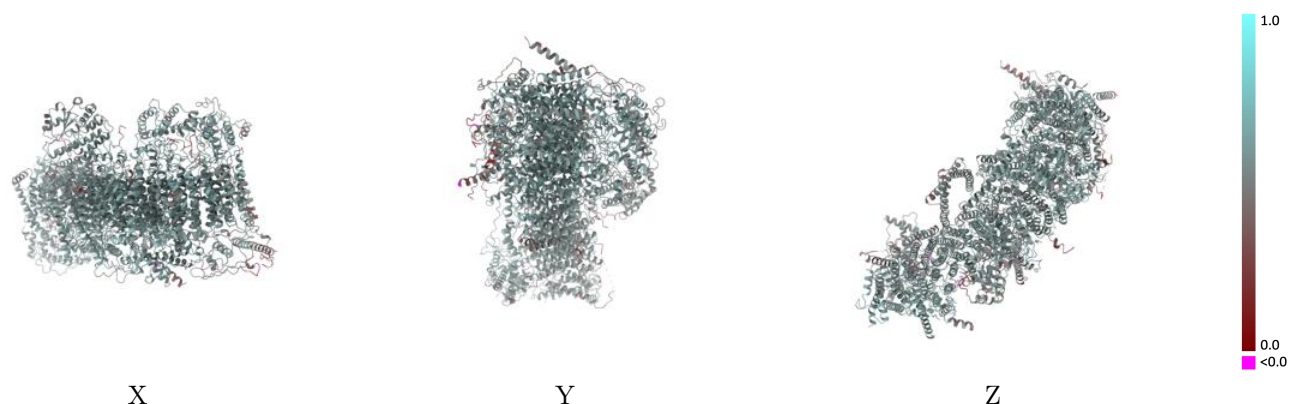
This section contains information regarding the fit between EMDB map EMD-32206 and PDB model 7VYI. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0288 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

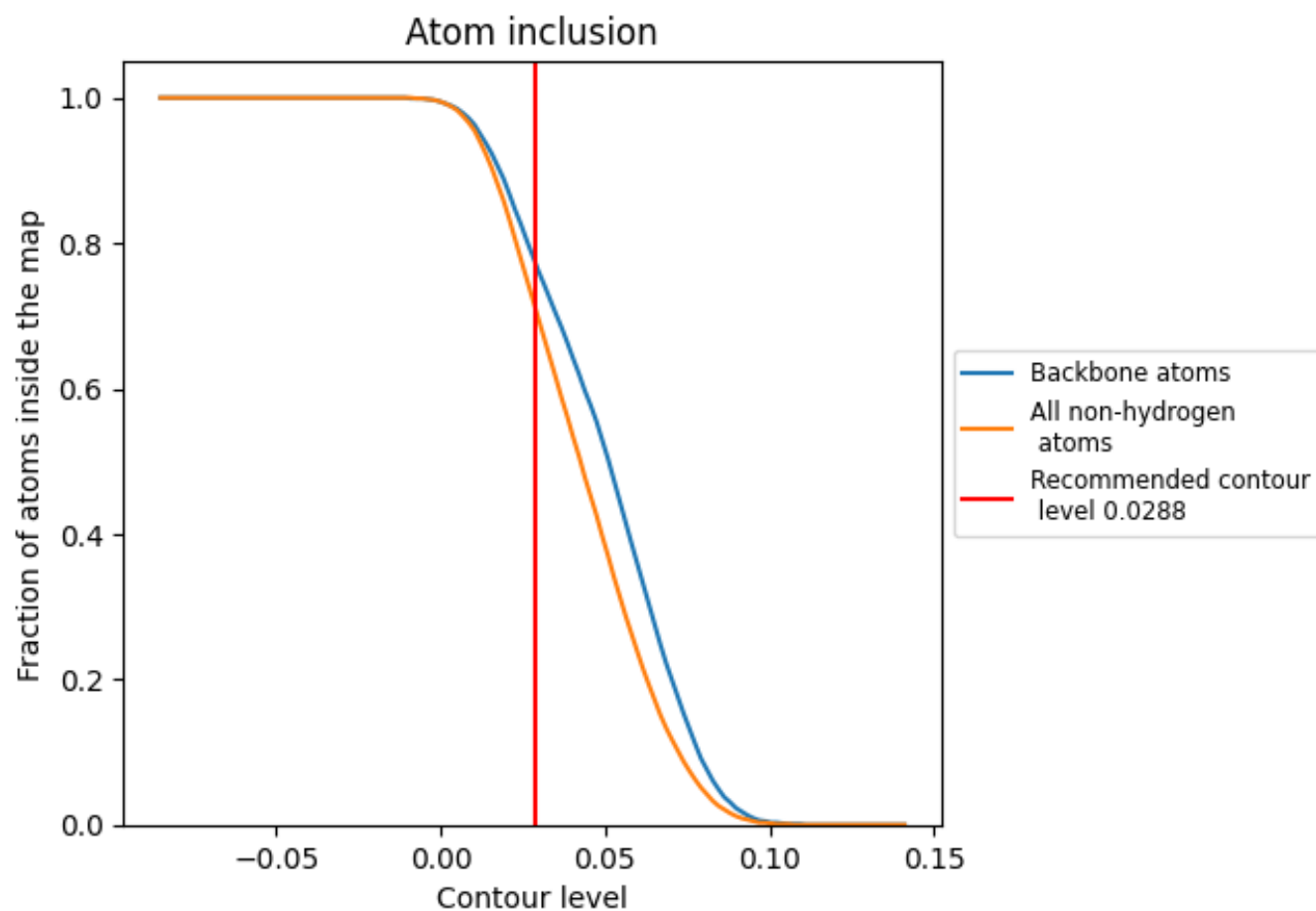


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 71% 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 (0.0288) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7100	 0.5520
Q	 0.5120	 0.5020
S	 0.7740	 0.5690
U	 0.6880	 0.5550
V	 0.5130	 0.4990
W	 0.7610	 0.5670
X	 0.6840	 0.5280
Y	 0.6050	 0.4930
Z	 0.5730	 0.5080
a	 0.7520	 0.5750
b	 0.6250	 0.5250
c	 0.7320	 0.5540
d	 0.7190	 0.5460
e	 0.6700	 0.5340
f	 0.6350	 0.5250
g	 0.7500	 0.5710
h	 0.7290	 0.5600
i	 0.7830	 0.5800
j	 0.5720	 0.5130
k	 0.6790	 0.5500
l	 0.7570	 0.5680
m	 0.6280	 0.5270
n	 0.6520	 0.5250
o	 0.7180	 0.5580
p	 0.7530	 0.5650
r	 0.7850	 0.5830
s	 0.7440	 0.5640
u	 0.7390	 0.5620
v	 0.6080	 0.4870
w	 0.6220	 0.5170

