Full wwPDB EM Validation Report (i)

Dec 7, 2022 – 09:50 AM JST

PDB ID	:	5XTC
EMDB ID	:	EMD-6772
Title	:	Cryo-EM structure of human respiratory complex I transmembrane arm
Authors	:	Gu, J.; Wu, M.; Yang, M.
Deposited on	:	2017-06-19
Resolution	:	3.70 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 (i) 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 (1)) were used in the production of this report:

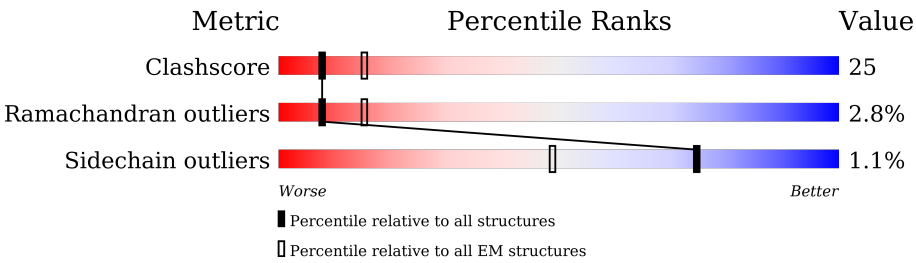
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	46	89%, 76%, 22%, •
2	S	70	13%, 74%, 24%, •
3	U	83	16%, 84%, 16%
4	V	140	31%, 66%, 33%, •
5	W	116	8%, 79%, 20%, •
6	X	85	5%, 58%, 40%, •
7	Y	59	7%, 47%, 32%, 19%, •
8	Z	80	15%, 79%, 21%

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Mol	Chain	Length	Quality of chain
9	a	138	96%
10	b	128	28%, 87%, 9%
11	c	153	7%, 95%, 5%
12	d	171	6%, 95%, 5%
13	e	97	10%, 97%
14	f	47	30%, 98%
15	g	119	95%, 5%
16	h	104	9%, 94%, 6%
17	i	347	7%, 98%
18	j	115	50%, 97%
19	k	97	18%, 93%, 6%
20	l	603	9%, 94%, 5%
21	m	174	26%, 94%, 6%
22	n	56	21%, 96%
23	o	128	5%, 97%
24	p	172	5%, 98%
25	r	459	98%
26	s	318	16%, 97%
27	u	169	97%
28	v	122	18%, 86%, 5%, 9%
29	w	320	57%, 97%

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 38835 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
			Total	C	N	O	S		
1	Q	46	381	247	65	68	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	S	70	568	367	101	96	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	U	83	647	427	105	113	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	V	140	1038	668	178	187	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	W	116	956	614	167	170	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	X	85	686	442	101	138	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	Y	59	533	354	87	91	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	Z	80	648	426	110	110	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	a	138	1174	771	199	202	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	b	124	1059	697	181	176	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	c	153	1236	795	208	222	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	d	171	1418	885	262	259	12	0	0

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	e	97	810	522	132	152	4	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	f	47	405	269	69	67	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	g	119	1004	658	173	169	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	h	104	863	546	161	150	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	i	347	2735	1819	421	470	25	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	j	115	919	626	132	152	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	k	97	740	487	113	127	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	l	603	4717	3119	742	823	33	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	m	174	1313	879	194	229	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	n	56	473	305	85	80	3	0	0

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	o	128	1066	685	192	187	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	p	172	1495	961	265	261	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	r	459	3629	2411	569	619	30	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	s	318	2509	1678	380	435	16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	u	169	1394	886	247	252	9	0	0

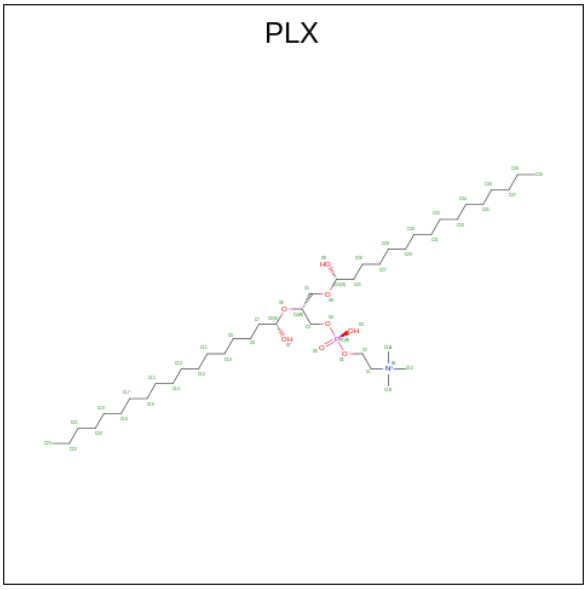
- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	v	111	921	569	187	156	9	0	0

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

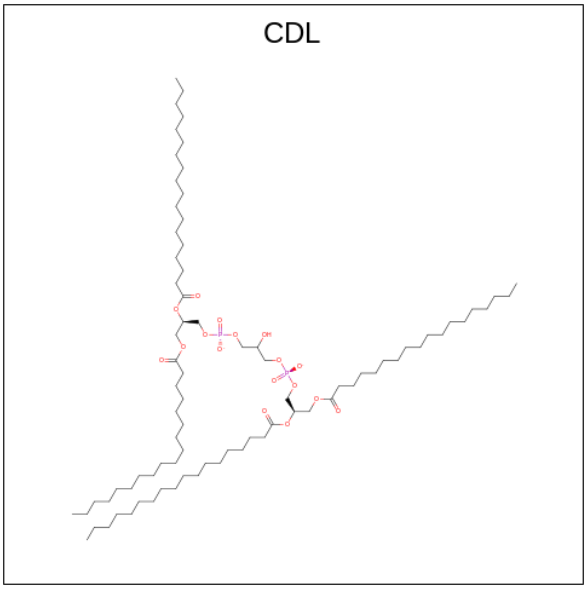
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	w	320	2474	1573	429	464	8	0	0

- Molecule 30 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 (three-letter code: PLX) (formula: $C_{42}H_{89}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
30	U	1	52	42	1	8	1	0
30	V	1	52	42	1	8	1	0
30	b	1	52	42	1	8	1	0
30	g	1	156	126	3	24	3	0
30	g	1	156	126	3	24	3	0
30	g	1	156	126	3	24	3	0
30	r	1	104	84	2	16	2	0
30	r	1	104	84	2	16	2	0
30	s	1	52	42	1	8	1	0

- Molecule 31 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
31	V	1	63	44	17	2	0
31	i	1	64	45	17	2	0
31	l	1	128	90	34	4	0

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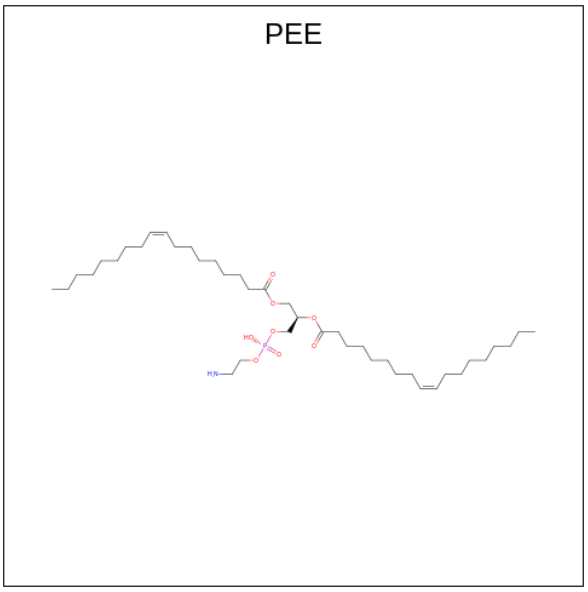
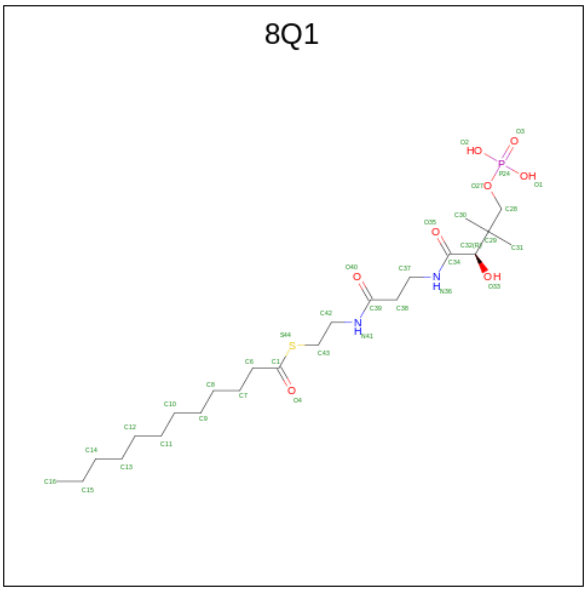
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
31	l	1	128	90	34	4	0
			Total	C	O	P	
31	n	1	64	45	17	2	0

- Molecule 32 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
32	V	1	51	41	1	8	1	0
			Total	C	N	O	P	
32	W	1	51	41	1	8	1	0
			Total	C	N	O	P	
32	l	1	100	80	2	16	2	0
			Total	C	N	O	P	
32	l	1	100	80	2	16	2	0

- Molecule 33 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).



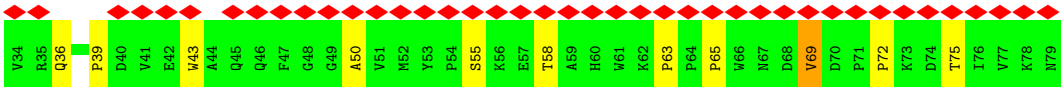
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
33	p	1	35	23	2	8	1	1	0

3 Residue-property plots (i)

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

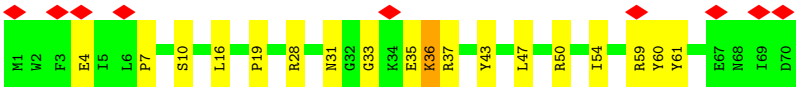
• Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain Q:



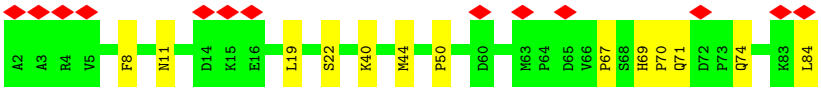
• Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S:



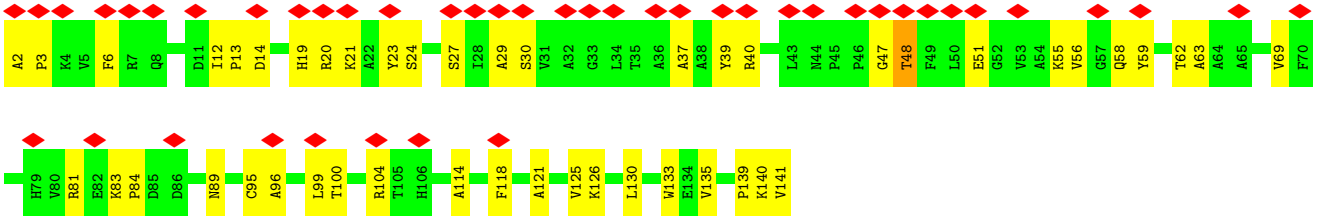
• Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:



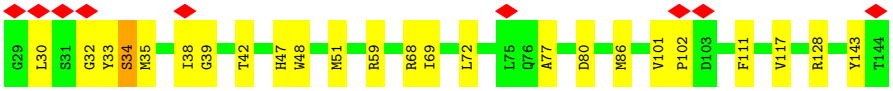
• Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:



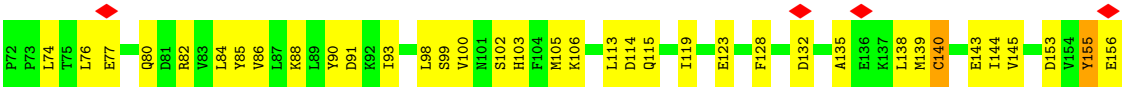
• Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:



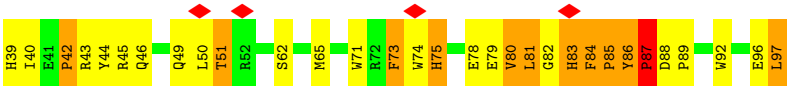
• Molecule 6: Acyl carrier protein, mitochondrial

Chain X:



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

Chain Y:

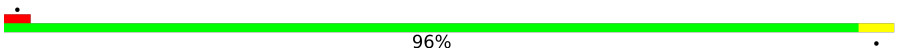


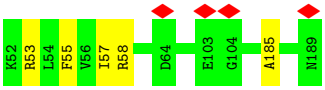
• Molecule 8: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z:

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

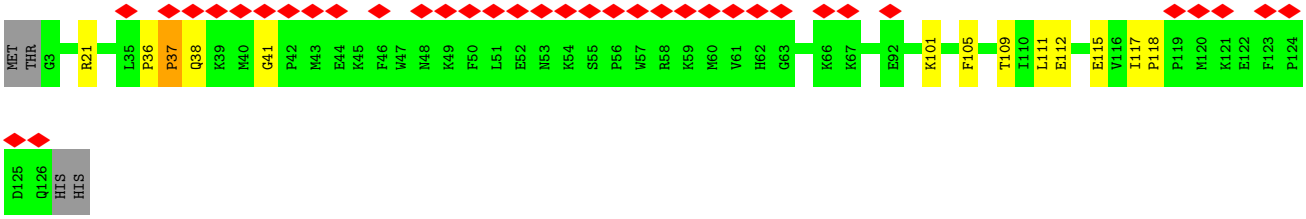
Chain a:





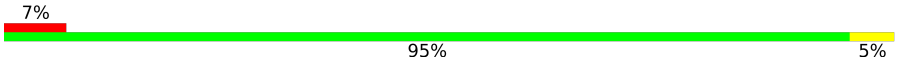
• Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

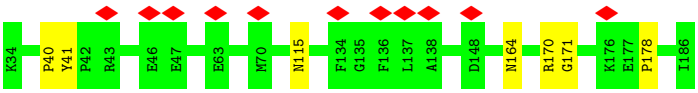
Chain b:



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

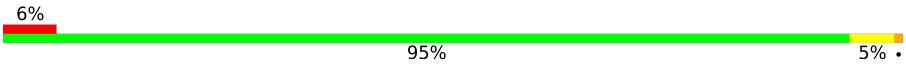
Chain c:

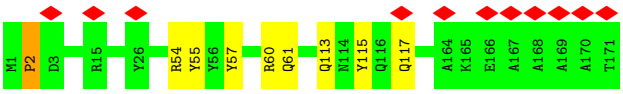




• Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

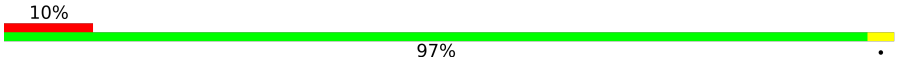
Chain d:

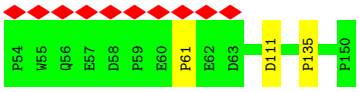




• Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

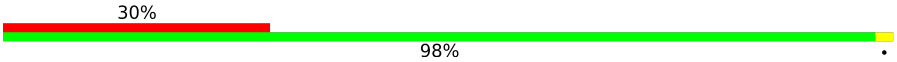
Chain e:

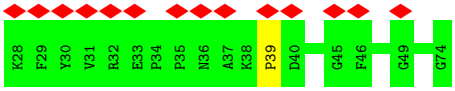




• Molecule 14: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

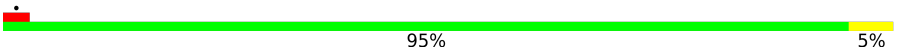
Chain f:

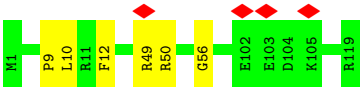




• Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2

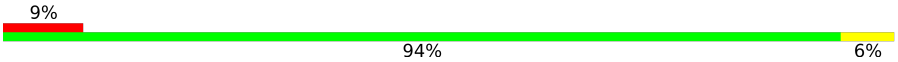
Chain g:

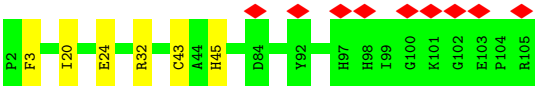




• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

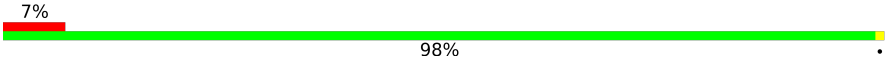
Chain h:

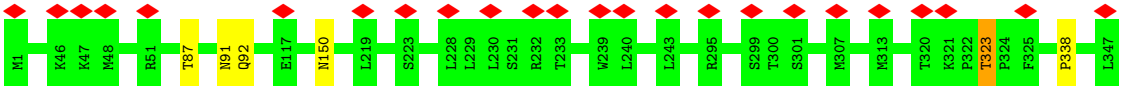




• Molecule 17: NADH-ubiquinone oxidoreductase chain 2

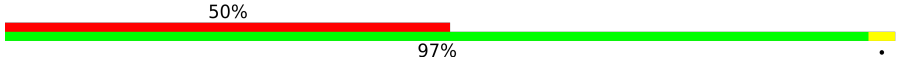
Chain i:

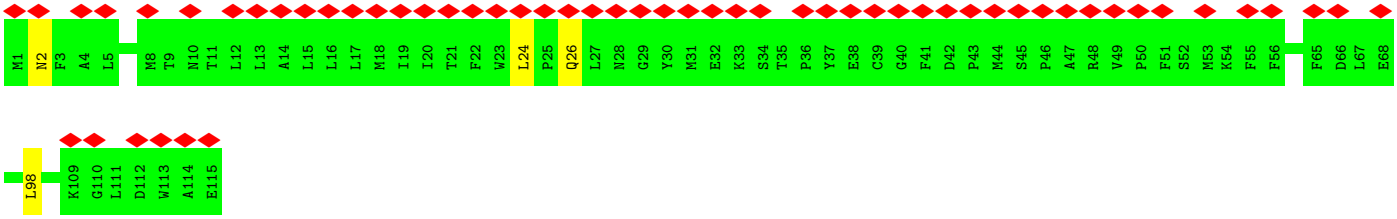




- Molecule 18: NADH-ubiquinone oxidoreductase chain 3

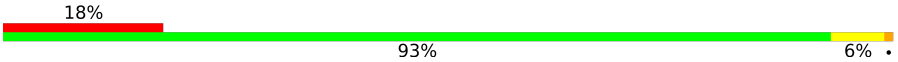
Chain j:

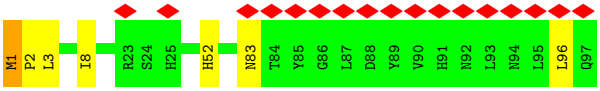




- Molecule 19: NADH-ubiquinone oxidoreductase chain 4L

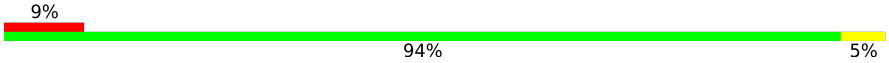
Chain k:

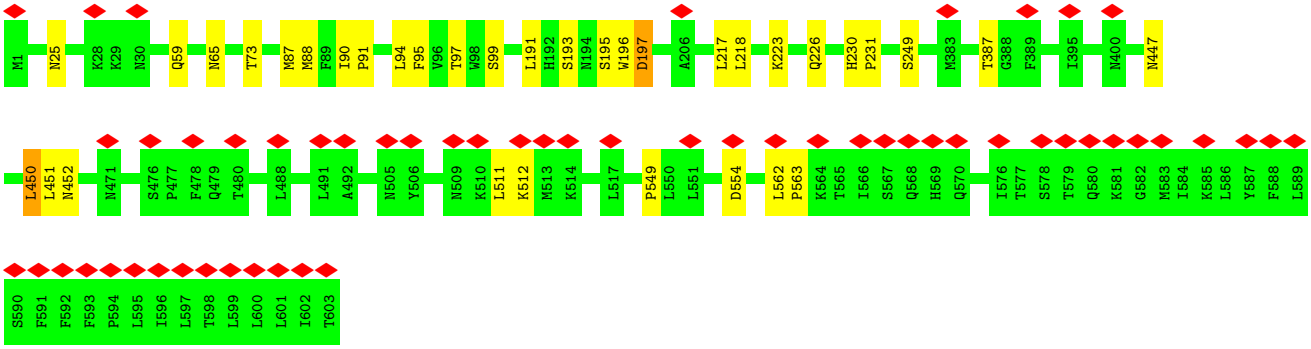




- Molecule 20: NADH-ubiquinone oxidoreductase chain 5

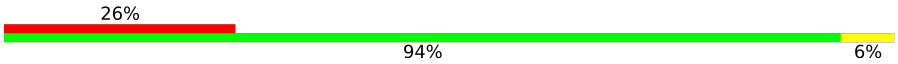
Chain l:

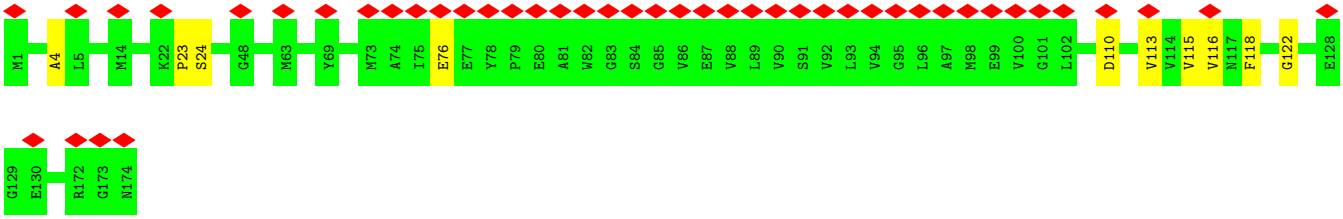




- Molecule 21: NADH-ubiquinone oxidoreductase chain 6

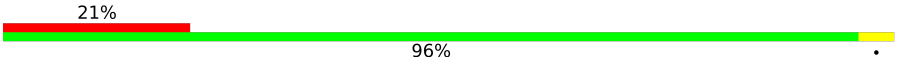
Chain m:

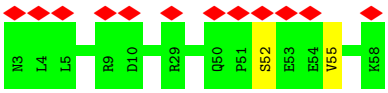




- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

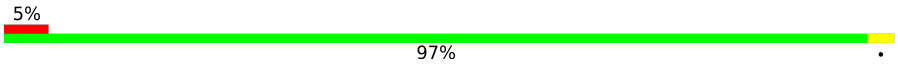
Chain n:

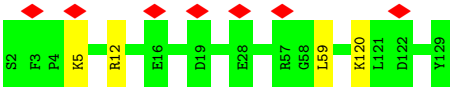




• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

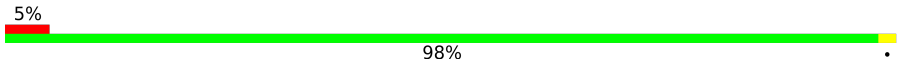
Chain o:

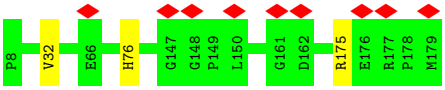




• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

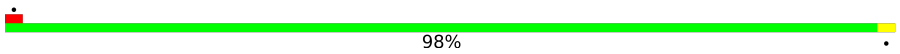
Chain p:

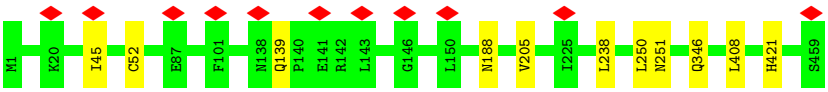




• Molecule 25: NADH-ubiquinone oxidoreductase chain 4

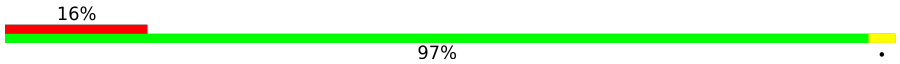
Chain r:

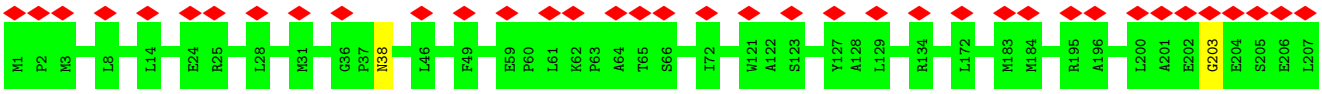


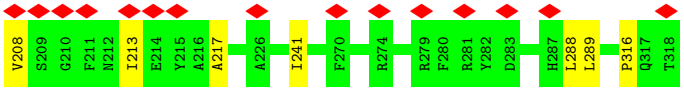


• Molecule 26: NADH-ubiquinone oxidoreductase chain 1

Chain s:

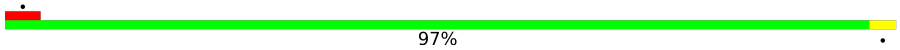


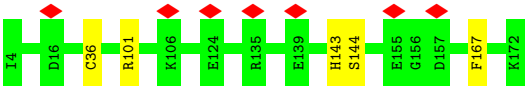




• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

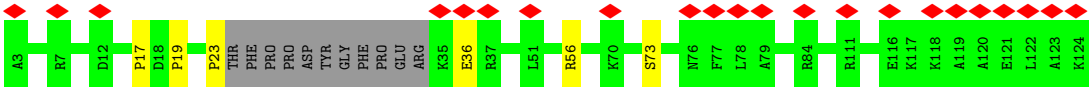
Chain u:





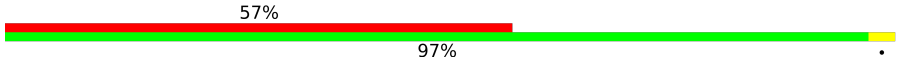
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

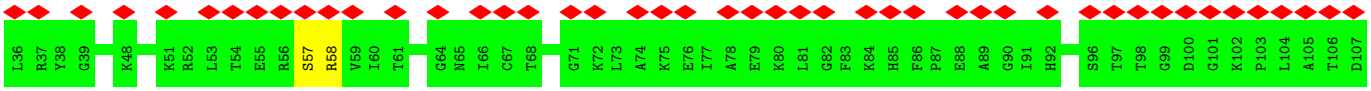
Chain v:

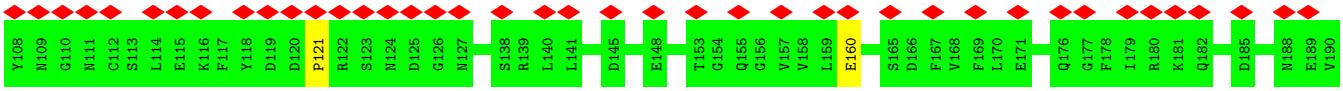


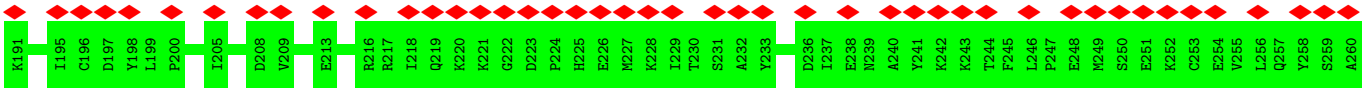
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

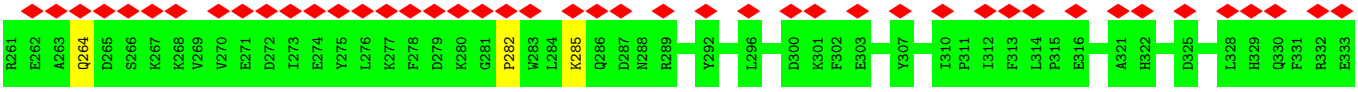
Chain w:

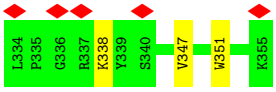












4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	167761	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.305	Depositor
Minimum map value	-0.154	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0677	Depositor
Map size (Å)	519.83997, 519.83997, 519.83997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.083, 1.083, 1.083	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.33	0/398	0.51	0/548
2	S	0.60	0/583	0.64	0/785
3	U	0.52	0/670	0.63	0/920
4	V	0.51	0/1065	0.61	0/1450
5	W	0.60	0/980	0.66	0/1327
6	X	0.57	0/698	0.61	0/942
7	Y	0.52	0/559	0.73	3/763 (0.4%)
8	Z	0.45	0/669	0.53	0/899
9	a	0.68	0/1209	0.65	0/1639
10	b	0.59	1/1095 (0.1%)	0.69	4/1480 (0.3%)
11	c	0.58	0/1287	0.58	0/1761
12	d	0.63	0/1445	0.65	1/1945 (0.1%)
13	e	0.61	0/835	0.61	0/1134
14	f	0.48	0/418	0.58	0/566
15	g	0.64	0/1035	0.63	0/1398
16	h	0.62	0/884	0.65	0/1182
17	i	0.67	0/2808	0.77	2/3843 (0.1%)
18	j	0.55	0/945	0.69	1/1292 (0.1%)
19	k	0.68	1/751 (0.1%)	0.79	1/1019 (0.1%)
20	l	0.61	2/4840 (0.0%)	0.69	3/6611 (0.0%)
21	m	0.68	0/1346	0.67	0/1832
22	n	0.49	0/484	0.62	0/652
23	o	0.54	0/1093	0.60	0/1479
24	p	0.58	0/1549	0.59	0/2098
25	r	0.70	0/3723	0.76	2/5089 (0.0%)
26	s	0.62	0/2580	0.73	0/3539
27	u	0.57	0/1433	0.60	0/1937
28	v	0.48	0/934	0.67	3/1241 (0.2%)
29	w	0.44	0/2533	0.56	0/3440
All	All	0.60	4/38849 (0.0%)	0.67	20/52811 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
29	w	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	b	118	PRO	N-CD	5.14	1.55	1.47
19	k	2	PRO	N-CD	5.14	1.55	1.47
20	l	231	PRO	N-CD	5.04	1.54	1.47
20	l	91	PRO	N-CD	5.00	1.54	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	i	323	THR	C-N-CD	-7.37	104.39	120.60
7	Y	92	TRP	N-CA-C	-6.98	92.15	111.00
12	d	2	PRO	N-CA-CB	6.75	111.41	103.30
7	Y	87	PRO	CA-N-CD	-6.58	102.30	111.50
10	b	36	PRO	C-N-CD	6.21	141.45	128.40
17	i	323	THR	C-N-CA	6.05	147.40	122.00
28	v	17	PRO	N-CA-CB	5.92	110.40	103.30
20	l	197	ASP	C-N-CD	5.90	140.78	128.40
28	v	23	PRO	N-CA-CB	5.90	110.38	103.30
10	b	105	PHE	C-N-CD	5.81	140.60	128.40
19	k	1	MET	C-N-CD	5.75	140.47	128.40
20	l	90	ILE	C-N-CD	5.71	140.39	128.40
20	l	230	HIS	C-N-CD	5.69	140.34	128.40
10	b	117	ILE	C-N-CD	5.68	140.32	128.40
28	v	19	PRO	N-CA-CB	5.65	110.08	103.30
10	b	37	PRO	CA-N-CD	-5.42	103.92	111.50
18	j	98	LEU	CB-CG-CD2	-5.39	101.84	111.00
7	Y	86	TYR	C-N-CD	5.12	139.15	128.40
25	r	238	LEU	CB-CG-CD2	-5.09	102.34	111.00
25	r	408	LEU	CA-CB-CG	-5.08	103.61	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	w	338	LYS	Peptide

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	381	0	355	9	0
2	S	568	0	567	13	0
3	U	647	0	653	9	0
4	V	1038	0	1027	34	0
5	W	956	0	949	21	0
6	X	686	0	676	24	0
7	Y	533	0	475	45	0
8	Z	648	0	627	13	0
9	a	1174	0	1177	0	0
10	b	1059	0	1079	0	0
11	c	1236	0	1092	0	0
12	d	1418	0	1375	0	0
13	e	810	0	772	0	0
14	f	405	0	407	0	0
15	g	1004	0	1008	0	0
16	h	863	0	861	0	0
17	i	2735	0	2893	0	0
18	j	919	0	968	0	0
19	k	740	0	792	0	0
20	l	4717	0	4893	0	0
21	m	1313	0	1330	0	0
22	n	473	0	480	0	0
23	o	1066	0	1086	0	0
24	p	1495	0	1440	0	0
25	r	3629	0	3825	0	0
26	s	2509	0	2617	0	0
27	u	1394	0	1367	0	0
28	v	921	0	892	0	0
29	w	2474	0	2304	0	0
30	U	52	0	88	1	0
30	V	52	0	88	2	0
30	b	52	0	88	0	0
30	g	156	0	264	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	r	104	0	176	0	0
30	s	52	0	88	0	0
31	V	63	0	68	8	0
31	i	64	0	72	0	0
31	l	128	0	144	0	0
31	n	64	0	72	0	0
32	V	51	0	82	12	0
32	W	51	0	82	5	0
32	l	100	0	157	0	0
33	p	35	0	0	0	0
All	All	38835	0	39456	181	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 25.

All (181) 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)
7:Y:84:PHE:CD1	7:Y:85:PRO:HD3	1.84	1.13
7:Y:71:TRP:CH2	7:Y:75:HIS:CD2	2.42	1.08
7:Y:71:TRP:CH2	7:Y:75:HIS:HD2	1.76	1.04
32:V:202:PEE:C25	32:V:202:PEE:H60	1.92	0.99
6:X:99:SER:HG	6:X:102:SER:HG	1.09	0.96
7:Y:83:HIS:O	7:Y:84:PHE:HB2	1.67	0.91
7:Y:84:PHE:CG	7:Y:85:PRO:CD	2.57	0.87
7:Y:84:PHE:CD1	7:Y:85:PRO:CD	2.58	0.86
32:W:201:PEE:O2P	32:W:201:PEE:N	2.08	0.85
4:V:84:PRO:O	4:V:89:ASN:ND2	2.10	0.84
7:Y:74:TRP:HZ3	7:Y:75:HIS:HD1	1.29	0.80
7:Y:74:TRP:CE3	7:Y:75:HIS:HA	2.16	0.79
7:Y:83:HIS:O	7:Y:84:PHE:CB	2.31	0.78
7:Y:84:PHE:CG	7:Y:85:PRO:HD2	2.19	0.77
7:Y:96:GLU:O	7:Y:97:LEU:HD23	1.84	0.77
4:V:40:ARG:HH22	4:V:55:LYS:HD3	1.50	0.75
7:Y:71:TRP:CZ2	7:Y:75:HIS:CD2	2.74	0.74
7:Y:84:PHE:CG	7:Y:85:PRO:HD3	2.22	0.74
32:V:202:PEE:H60	32:V:202:PEE:H41	1.67	0.74
32:V:202:PEE:H39	32:V:202:PEE:H32	1.70	0.73
7:Y:43:ARG:HG3	7:Y:46:GLN:HB2	1.72	0.72
32:V:202:PEE:H60	32:V:202:PEE:H42	1.73	0.71
7:Y:86:TYR:HB3	7:Y:87:PRO:CA	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:91:ASP:OD1	8:Z:47:ARG:NH1	2.24	0.70
7:Y:86:TYR:CB	7:Y:87:PRO:HA	2.22	0.69
6:X:84:LEU:HD22	6:X:98:LEU:HD21	1.74	0.69
32:W:201:PEE:H24	32:W:201:PEE:H53	1.74	0.69
4:V:81:ARG:HG2	4:V:83:LYS:HG3	1.75	0.68
7:Y:86:TYR:HB3	7:Y:87:PRO:HA	1.75	0.68
7:Y:84:PHE:CD2	7:Y:85:PRO:HD2	2.30	0.67
5:W:86:MET:SD	5:W:128:ARG:NH1	2.66	0.66
7:Y:81:LEU:HD23	7:Y:81:LEU:C	2.15	0.66
7:Y:79:GLU:O	7:Y:80:VAL:HG13	1.96	0.64
4:V:27:SER:O	4:V:30:SER:OG	2.14	0.63
32:V:202:PEE:H32	32:V:202:PEE:C24	2.25	0.63
7:Y:74:TRP:HE3	7:Y:75:HIS:HA	1.62	0.63
8:Z:24:ILE:HD11	8:Z:47:ARG:HG2	1.80	0.62
7:Y:96:GLU:O	7:Y:97:LEU:HB2	1.98	0.62
7:Y:81:LEU:HD23	7:Y:82:GLY:N	2.14	0.61
6:X:138:LEU:HD21	6:X:144:ILE:HG12	1.83	0.61
31:V:201:CDL:OA7	31:V:201:CDL:O1	2.15	0.61
7:Y:73:PHE:O	7:Y:73:PHE:HD1	1.84	0.61
5:W:39:GLY:O	5:W:42:THR:OG1	2.15	0.60
5:W:111:PHE:HE2	5:W:117:VAL:HG11	1.66	0.60
7:Y:45:ARG:HG3	8:Z:52:ARG:HB2	1.84	0.59
4:V:40:ARG:HA	31:V:201:CDL:OB3	2.02	0.59
8:Z:25:GLU:HA	8:Z:30:GLU:HG3	1.84	0.59
6:X:84:LEU:O	6:X:88:LYS:HG2	2.03	0.58
3:U:67:PRO:HB3	3:U:74:GLN:HB2	1.86	0.57
4:V:40:ARG:HD3	4:V:59:TYR:HE2	1.68	0.57
7:Y:39:HIS:ND1	7:Y:40:ILE:HG13	2.20	0.57
4:V:139:PRO:O	4:V:141:VAL:N	2.38	0.56
32:V:202:PEE:H57	32:V:202:PEE:H40	1.87	0.56
2:S:59:ARG:O	2:S:61:TYR:N	2.36	0.56
4:V:40:ARG:NH2	4:V:55:LYS:HD3	2.20	0.56
8:Z:51:TRP:O	8:Z:53:TYR:N	2.37	0.56
4:V:62:THR:HG22	4:V:104:ARG:HE	1.69	0.56
8:Z:22:TRP:CE3	8:Z:51:TRP:HA	2.41	0.56
4:V:3:PRO:HA	4:V:6:PHE:HB3	1.88	0.56
32:V:202:PEE:H60	32:V:202:PEE:C24	2.36	0.55
4:V:40:ARG:HD3	4:V:59:TYR:CE2	2.41	0.55
3:U:67:PRO:HA	3:U:74:GLN:OE1	2.07	0.55
7:Y:74:TRP:HE3	7:Y:75:HIS:CA	2.19	0.55
6:X:84:LEU:HD11	6:X:100:VAL:HG22	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:96:GLU:O	7:Y:97:LEU:CB	2.55	0.54
7:Y:96:GLU:O	7:Y:97:LEU:CD2	2.54	0.54
1:Q:72:PRO:O	1:Q:75:THR:OG1	2.18	0.54
1:Q:69:VAL:HG12	1:Q:72:PRO:HD2	1.90	0.53
8:Z:24:ILE:HG22	8:Z:30:GLU:HB2	1.90	0.53
32:V:202:PEE:C24	32:V:202:PEE:H57	2.39	0.53
6:X:93:ILE:HG21	6:X:98:LEU:HD12	1.91	0.53
3:U:69:HIS:ND1	3:U:70:PRO:HA	2.24	0.53
1:Q:39:PRO:HB3	1:Q:43:TRP:CE3	2.45	0.52
5:W:33:TYR:CG	5:W:34:SER:N	2.77	0.52
5:W:35:MET:HA	5:W:38:ILE:HD12	1.91	0.52
2:S:37:ARG:O	5:W:143:TYR:OH	2.27	0.52
4:V:58:GLN:O	4:V:62:THR:HG23	2.10	0.52
3:U:84:LEU:O	5:W:59:ARG:NH1	2.41	0.51
4:V:12:ILE:HG22	4:V:13:PRO:O	2.11	0.51
6:X:77:GLU:HB2	8:Z:13:LYS:HE2	1.93	0.51
7:Y:86:TYR:HB3	7:Y:87:PRO:HB3	1.93	0.51
6:X:85:TYR:HE2	7:Y:45:ARG:NH1	2.09	0.51
7:Y:86:TYR:HB3	7:Y:87:PRO:CB	2.40	0.50
7:Y:74:TRP:CE3	7:Y:74:TRP:C	2.85	0.50
1:Q:65:PRO:HG2	1:Q:69:VAL:HG22	1.94	0.50
4:V:14:ASP:O	4:V:21:LYS:NZ	2.45	0.50
6:X:103:HIS:HB2	6:X:106:LYS:HB3	1.94	0.50
32:V:202:PEE:H40	32:V:202:PEE:C35	2.42	0.49
4:V:62:THR:HG22	4:V:104:ARG:NE	2.27	0.49
6:X:90:TYR:HD2	6:X:93:ILE:HD12	1.77	0.49
4:V:39:TYR:HD2	31:V:201:CDL:H721	1.76	0.49
32:V:202:PEE:H41	32:V:202:PEE:C37	2.40	0.49
6:X:76:LEU:HD12	6:X:156:GLU:HB2	1.94	0.49
4:V:62:THR:HG22	4:V:104:ARG:HD3	1.95	0.48
8:Z:28:PRO:O	8:Z:31:THR:OG1	2.22	0.48
2:S:50:ARG:CZ	2:S:54:ILE:HD11	2.43	0.48
4:V:29:ALA:O	4:V:63:ALA:HB1	2.14	0.48
5:W:47:HIS:O	5:W:51:MET:HG3	2.13	0.48
2:S:28:ARG:O	2:S:33:GLY:N	2.47	0.48
4:V:47:GLY:O	4:V:48:THR:OG1	2.25	0.48
5:W:30:LEU:HB2	5:W:32:GLY:H	1.78	0.48
7:Y:71:TRP:CE3	7:Y:71:TRP:C	2.87	0.48
6:X:102:SER:O	6:X:140:CYS:HA	2.14	0.48
32:W:201:PEE:N	32:W:201:PEE:P	2.87	0.47
4:V:37:ALA:HB1	4:V:56:VAL:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:40:ARG:HG3	31:V:201:CDL:HB22	1.97	0.47
31:V:201:CDL:H552	31:V:201:CDL:H522	1.70	0.47
6:X:80:GLN:HG3	6:X:145:VAL:HG11	1.95	0.47
4:V:96:ALA:HA	4:V:99:LEU:HD12	1.95	0.47
7:Y:50:LEU:O	7:Y:51:THR:OG1	2.27	0.47
32:W:201:PEE:H28	32:W:201:PEE:H22	1.50	0.47
7:Y:73:PHE:CD1	7:Y:73:PHE:C	2.88	0.47
5:W:101:VAL:HG13	5:W:102:PRO:HD2	1.96	0.47
2:S:35:GLU:HG2	2:S:35:GLU:O	2.14	0.47
5:W:48:TRP:O	5:W:51:MET:HB2	2.15	0.47
7:Y:88:ASP:N	7:Y:89:PRO:CD	2.78	0.47
2:S:4:GLU:O	2:S:7:PRO:HD2	2.15	0.46
7:Y:74:TRP:CE3	7:Y:75:HIS:CA	2.91	0.46
5:W:77:ALA:O	5:W:80:ASP:HB3	2.16	0.46
6:X:82:ARG:O	6:X:86:VAL:HG23	2.15	0.46
2:S:47:LEU:HA	2:S:50:ARG:HB3	1.98	0.46
4:V:121:ALA:O	4:V:125:VAL:HG23	2.15	0.46
2:S:43:TYR:CZ	5:W:68:ARG:HD2	2.51	0.46
7:Y:42:PRO:HD2	8:Z:14:MET:HG3	1.98	0.46
8:Z:31:THR:O	8:Z:34:LYS:HB3	2.16	0.46
6:X:132:ASP:HA	6:X:135:ALA:HB3	1.98	0.45
5:W:111:PHE:CD2	5:W:117:VAL:HG21	2.51	0.45
2:S:16:LEU:O	2:S:19:PRO:HD2	2.16	0.45
4:V:2:ALA:O	4:V:6:PHE:N	2.45	0.45
31:V:201:CDL:H541	31:V:201:CDL:H572	1.46	0.45
7:Y:74:TRP:HE3	7:Y:75:HIS:N	2.15	0.45
6:X:138:LEU:CD2	6:X:144:ILE:HG12	2.47	0.45
32:V:202:PEE:H60	32:V:202:PEE:H40	1.99	0.44
2:S:31:ASN:HD21	2:S:36:LYS:HD3	1.83	0.44
4:V:69:VAL:HG21	4:V:100:THR:HG21	1.98	0.44
5:W:111:PHE:CE2	5:W:117:VAL:HG11	2.49	0.44
7:Y:85:PRO:O	7:Y:86:TYR:CD1	2.70	0.44
4:V:40:ARG:HE	31:V:201:CDL:CA2	2.30	0.44
32:W:201:PEE:H51	32:W:201:PEE:H56	1.33	0.44
1:Q:55:SER:N	1:Q:58:THR:OG1	2.51	0.44
4:V:51:GLU:HB3	4:V:55:LYS:NZ	2.34	0.43
2:S:43:TYR:CE2	5:W:68:ARG:HD2	2.53	0.43
6:X:123:GLU:HB2	6:X:128:PHE:O	2.18	0.43
8:Z:65:ASP:O	8:Z:69:LYS:HB2	2.19	0.43
30:V:203:PLX:H332	30:V:203:PLX:H141	2.01	0.43
4:V:19:HIS:CD2	4:V:20:ARG:HG3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:69:VAL:HG12	1:Q:72:PRO:CD	2.48	0.43
5:W:33:TYR:O	5:W:34:SER:OG	2.27	0.43
4:V:62:THR:HG22	4:V:104:ARG:CD	2.49	0.42
4:V:95:CYS:O	4:V:99:LEU:HG	2.19	0.42
4:V:133:TRP:CG	32:V:202:PEE:H7	2.54	0.42
8:Z:18:ASP:OD1	8:Z:19:TYR:N	2.52	0.42
2:S:7:PRO:O	2:S:10:SER:OG	2.23	0.42
5:W:72:LEU:HD23	5:W:72:LEU:HA	1.84	0.42
3:U:40:LYS:O	3:U:44:MET:HG2	2.18	0.42
3:U:69:HIS:CE1	3:U:70:PRO:HA	2.54	0.42
6:X:155:TYR:CD2	6:X:155:TYR:O	2.73	0.42
3:U:19:LEU:O	3:U:22:SER:OG	2.29	0.41
4:V:23:TYR:O	4:V:24:SER:HB2	2.20	0.41
4:V:126:LYS:HE3	4:V:130:LEU:HD11	2.02	0.41
6:X:105:MET:CE	6:X:139:MET:HG3	2.50	0.41
6:X:115:GLN:HE21	6:X:119:ILE:HD11	1.84	0.41
31:V:201:CDL:H722	31:V:201:CDL:H752	1.75	0.41
5:W:86:MET:HG2	5:W:128:ARG:HH22	1.86	0.41
4:V:114:ALA:HB1	4:V:118:PHE:CE2	2.56	0.41
6:X:140:CYS:HB2	6:X:143:GLU:CD	2.41	0.41
2:S:47:LEU:O	2:S:50:ARG:HB3	2.20	0.41
6:X:88:LYS:HZ2	6:X:98:LEU:HD13	1.85	0.41
6:X:113:LEU:HD12	6:X:114:ASP:N	2.36	0.41
7:Y:62:SER:O	7:Y:65:MET:HB3	2.21	0.41
1:Q:65:PRO:CG	1:Q:69:VAL:HG22	2.51	0.40
30:V:203:PLX:H371	30:V:203:PLX:H342	1.76	0.40
7:Y:45:ARG:O	7:Y:45:ARG:HG2	2.22	0.40
30:U:101:PLX:H22	30:U:101:PLX:H1B3	1.86	0.40
7:Y:43:ARG:HH11	7:Y:49:GLN:HG2	1.86	0.40
7:Y:74:TRP:CZ3	7:Y:75:HIS:HA	2.53	0.40
3:U:50:PRO:HB2	5:W:69:ILE:HD11	2.03	0.40
5:W:111:PHE:CE2	5:W:117:VAL:HG21	2.56	0.40
1:Q:50:ALA:HB2	1:Q:63:PRO:HB3	2.03	0.40
1:Q:69:VAL:O	1:Q:72:PRO:HD2	2.22	0.40
3:U:8:PHE:O	3:U:11:ASN:HB3	2.21	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	44/46 (96%)	40 (91%)	2 (4%)	2 (4%)	2	23
2	S	68/70 (97%)	61 (90%)	5 (7%)	2 (3%)	4	32
3	U	81/83 (98%)	76 (94%)	4 (5%)	1 (1%)	13	48
4	V	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	6	37
5	W	114/116 (98%)	109 (96%)	4 (4%)	1 (1%)	17	54
6	X	83/85 (98%)	73 (88%)	6 (7%)	4 (5%)	2	22
7	Y	57/59 (97%)	50 (88%)	1 (2%)	6 (10%)	0	6
8	Z	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
9	a	136/138 (99%)	121 (89%)	12 (9%)	3 (2%)	6	37
10	b	122/128 (95%)	107 (88%)	10 (8%)	5 (4%)	3	26
11	c	151/153 (99%)	129 (85%)	15 (10%)	7 (5%)	2	23
12	d	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	25	62
13	e	95/97 (98%)	84 (88%)	8 (8%)	3 (3%)	4	31
14	f	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	6	37
15	g	117/119 (98%)	105 (90%)	6 (5%)	6 (5%)	2	21
16	h	102/104 (98%)	87 (85%)	9 (9%)	6 (6%)	1	18
17	i	345/347 (99%)	324 (94%)	15 (4%)	6 (2%)	9	42
18	j	113/115 (98%)	103 (91%)	7 (6%)	3 (3%)	5	33
19	k	95/97 (98%)	88 (93%)	4 (4%)	3 (3%)	4	31
20	l	601/603 (100%)	551 (92%)	38 (6%)	12 (2%)	7	39
21	m	172/174 (99%)	150 (87%)	12 (7%)	10 (6%)	1	19
22	n	54/56 (96%)	50 (93%)	2 (4%)	2 (4%)	3	28
23	o	126/128 (98%)	113 (90%)	9 (7%)	4 (3%)	4	31
24	p	170/172 (99%)	157 (92%)	10 (6%)	3 (2%)	8	41
25	r	457/459 (100%)	420 (92%)	28 (6%)	9 (2%)	7	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	s	316/318 (99%)	286 (90%)	21 (7%)	9 (3%)	5	33
27	u	167/169 (99%)	152 (91%)	10 (6%)	5 (3%)	4	32
28	v	107/122 (88%)	90 (84%)	14 (13%)	3 (3%)	5	33
29	w	318/320 (99%)	281 (88%)	28 (9%)	9 (3%)	5	33
All	All	4641/4716 (98%)	4217 (91%)	295 (6%)	129 (3%)	8	33

All (129) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S	60	TYR
3	U	71	GLN
5	W	34	SER
6	X	155	TYR
7	Y	84	PHE
9	a	58	ARG
11	c	115	ASN
11	c	178	PRO
12	d	2	PRO
16	h	20	ILE
17	i	91	ASN
17	i	323	THR
18	j	24	LEU
18	j	26	GLN
19	k	52	HIS
20	l	450	LEU
21	m	115	VAL
21	m	116	VAL
21	m	118	PHE
22	n	55	VAL
25	r	52	CYS
25	r	346	GLN
29	w	57	SER
29	w	264	GLN
29	w	282	PRO
29	w	347	VAL
4	V	135	VAL
4	V	140	LYS
7	Y	44	TYR
7	Y	51	THR
9	a	57	ILE
9	a	185	ALA

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Mol	Chain	Res	Type
10	b	101	LYS
11	c	170	ARG
15	g	9	PRO
16	h	3	PHE
16	h	24	GLU
16	h	43	CYS
18	j	2	ASN
20	l	73	THR
20	l	512	LYS
21	m	122	GLY
22	n	52	SER
25	r	45	ILE
25	r	188	ASN
25	r	250	LEU
25	r	421	HIS
26	s	203	GLY
26	s	213	ILE
26	s	217	ALA
26	s	316	PRO
28	v	56	ARG
29	w	285	LYS
1	Q	36	GLN
6	X	140	CYS
7	Y	85	PRO
10	b	37	PRO
10	b	109	THR
11	c	164	ASN
13	e	61	PRO
13	e	111	ASP
15	g	10	LEU
15	g	12	PHE
15	g	50	ARG
17	i	87	THR
19	k	83	ASN
19	k	96	LEU
20	l	65	ASN
20	l	451	LEU
20	l	511	LEU
20	l	549	PRO
20	l	554	ASP
20	l	563	PRO
21	m	4	ALA

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Mol	Chain	Res	Type
21	m	76	GLU
21	m	110	ASP
23	o	5	LYS
23	o	12	ARG
25	r	139	GLN
26	s	38	ASN
27	u	36	CYS
27	u	101	ARG
27	u	143	HIS
28	v	73	SER
29	w	351	TRP
2	S	36	LYS
6	X	74	LEU
7	Y	42	PRO
7	Y	87	PRO
10	b	115	GLU
11	c	40	PRO
11	c	41	TYR
15	g	49	ARG
15	g	56	GLY
16	h	32	ARG
16	h	45	HIS
17	i	150	ASN
20	l	249	SER
20	l	387	THR
20	l	562	LEU
23	o	59	LEU
23	o	120	LYS
24	p	76	HIS
25	r	251	ASN
26	s	208	VAL
26	s	288	LEU
26	s	289	LEU
27	u	167	PHE
28	v	36	GLU
4	V	48	THR
6	X	153	ASP
11	c	171	GLY
17	i	92	GLN
21	m	113	VAL
24	p	175	ARG
27	u	144	SER

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Mol	Chain	Res	Type
29	w	58	ARG
29	w	121	PRO
29	w	160	GLU
10	b	41	GLY
14	f	39	PRO
21	m	24	SER
24	p	32	VAL
25	r	205	VAL
26	s	241	ILE
21	m	23	PRO
1	Q	69	VAL
17	i	338	PRO
13	e	135	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Q	41/41 (100%)	41 (100%)	0	100 100
2	S	59/59 (100%)	59 (100%)	0	100 100
3	U	72/72 (100%)	72 (100%)	0	100 100
4	V	102/102 (100%)	102 (100%)	0	100 100
5	W	100/100 (100%)	100 (100%)	0	100 100
6	X	78/79 (99%)	78 (100%)	0	100 100
7	Y	57/57 (100%)	49 (86%)	8 (14%)	3 20
8	Z	62/63 (98%)	62 (100%)	0	100 100
9	a	124/124 (100%)	122 (98%)	2 (2%)	62 80
10	b	118/122 (97%)	114 (97%)	4 (3%)	37 64
11	c	124/137 (90%)	124 (100%)	0	100 100
12	d	145/154 (94%)	137 (94%)	8 (6%)	21 53
13	e	90/90 (100%)	90 (100%)	0	100 100
14	f	43/43 (100%)	43 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	g	105/105 (100%)	105 (100%)	0	100	100
16	h	90/90 (100%)	90 (100%)	0	100	100
17	i	314/314 (100%)	314 (100%)	0	100	100
18	j	102/103 (99%)	102 (100%)	0	100	100
19	k	85/85 (100%)	82 (96%)	3 (4%)	36	63
20	l	531/532 (100%)	511 (96%)	20 (4%)	33	61
21	m	137/137 (100%)	137 (100%)	0	100	100
22	n	53/53 (100%)	53 (100%)	0	100	100
23	o	114/114 (100%)	114 (100%)	0	100	100
24	p	157/157 (100%)	157 (100%)	0	100	100
25	r	416/416 (100%)	416 (100%)	0	100	100
26	s	278/278 (100%)	278 (100%)	0	100	100
27	u	153/153 (100%)	153 (100%)	0	100	100
28	v	89/111 (80%)	89 (100%)	0	100	100
29	w	249/288 (86%)	249 (100%)	0	100	100
All	All	4088/4179 (98%)	4043 (99%)	45 (1%)	74	85

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	Y	73	PHE
7	Y	75	HIS
7	Y	78	GLU
7	Y	80	VAL
7	Y	81	LEU
7	Y	83	HIS
7	Y	87	PRO
7	Y	97	LEU
9	a	53	ARG
9	a	55	PHE
10	b	21	ARG
10	b	38	GLN
10	b	111	LEU
10	b	112	GLU
12	d	54	ARG
12	d	55	TYR
12	d	57	TYR

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Mol	Chain	Res	Type
12	d	60	ARG
12	d	61	GLN
12	d	113	GLN
12	d	115	TYR
12	d	117	GLN
19	k	1	MET
19	k	3	LEU
19	k	8	ILE
20	l	25	ASN
20	l	59	GLN
20	l	87	MET
20	l	88	MET
20	l	94	LEU
20	l	95	PHE
20	l	97	THR
20	l	99	SER
20	l	191	LEU
20	l	193	SER
20	l	195	SER
20	l	196	TRP
20	l	197	ASP
20	l	217	LEU
20	l	218	LEU
20	l	223	LYS
20	l	226	GLN
20	l	447	ASN
20	l	450	LEU
20	l	452	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	38	GLN
2	S	44	HIS
2	S	68	ASN
5	W	61	GLN
5	W	112	HIS
5	W	135	HIS
7	Y	75	HIS
9	a	90	ASN
9	a	189	ASN
10	b	14	GLN

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Mol	Chain	Res	Type
10	b	83	HIS
10	b	89	HIS
10	b	126	GLN
11	c	56	ASN
11	c	84	HIS
11	c	154	GLN
12	d	59	HIS
12	d	61	GLN
12	d	85	GLN
12	d	113	GLN
12	d	117	GLN
12	d	138	GLN
15	g	60	GLN
15	g	96	HIS
17	i	83	GLN
17	i	112	HIS
17	i	150	ASN
17	i	186	HIS
17	i	222	ASN
18	j	10	ASN
19	k	7	ASN
19	k	94	ASN
20	l	4	HIS
20	l	59	GLN
20	l	139	GLN
20	l	192	HIS
20	l	199	GLN
20	l	205	ASN
20	l	226	GLN
20	l	248	HIS
20	l	274	GLN
20	l	296	ASN
20	l	320	ASN
20	l	332	HIS
20	l	348	HIS
20	l	394	HIS
20	l	400	ASN
20	l	442	ASN
20	l	446	ASN
20	l	534	HIS
20	l	569	HIS
20	l	580	GLN

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Mol	Chain	Res	Type
21	m	45	ASN
21	m	117	ASN
22	n	40	ASN
23	o	62	ASN
23	o	126	HIS
24	p	75	GLN
25	r	48	ASN
25	r	168	HIS
25	r	390	ASN
25	r	415	GLN
25	r	425	ASN
26	s	93	ASN
26	s	169	GLN
26	s	235	ASN
27	u	30	HIS
27	u	31	HIS
27	u	64	ASN
27	u	77	HIS
27	u	99	HIS
27	u	104	GLN
27	u	143	HIS
28	v	43	GLN
28	v	61	HIS
28	v	85	HIS
28	v	92	HIS
29	w	85	HIS
29	w	111	ASN
29	w	132	GLN
29	w	149	HIS
29	w	257	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

19 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
31	CDL	n	101	-	63,63,99	1.24	5 (7%)	69,75,111	1.06	4 (5%)
31	CDL	i	401	-	63,63,99	1.21	5 (7%)	69,75,111	1.04	5 (7%)
30	PLX	g	203	-	51,51,51	0.78	1 (1%)	55,59,59	0.58	1 (1%)
31	CDL	l	704	-	63,63,99	1.26	5 (7%)	69,75,111	1.01	4 (5%)
30	PLX	r	502	-	51,51,51	0.64	0	55,59,59	0.67	1 (1%)
30	PLX	V	203	-	51,51,51	0.78	1 (1%)	55,59,59	0.59	1 (1%)
31	CDL	l	703	-	63,63,99	1.21	5 (7%)	69,75,111	1.07	4 (5%)
32	PEE	l	702	-	50,50,50	1.17	6 (12%)	53,55,55	0.99	2 (3%)
30	PLX	r	501	-	51,51,51	0.74	1 (1%)	55,59,59	0.65	1 (1%)
30	PLX	s	401	-	51,51,51	0.76	1 (1%)	55,59,59	0.68	1 (1%)
32	PEE	l	701	-	48,48,50	1.34	4 (8%)	51,53,55	0.96	2 (3%)
30	PLX	g	201	-	51,51,51	0.82	1 (1%)	55,59,59	0.69	1 (1%)
33	8Q1	p	201	-	31,34,34	1.67	5 (16%)	40,43,43	1.57	5 (12%)
31	CDL	V	201	-	61,61,99	1.21	5 (8%)	64,71,111	0.94	3 (4%)
30	PLX	b	201	-	51,51,51	0.57	0	55,59,59	0.64	0
30	PLX	U	101	-	51,51,51	0.74	1 (1%)	55,59,59	0.72	2 (3%)
32	PEE	W	201	-	50,50,50	1.14	6 (12%)	53,55,55	0.97	2 (3%)
32	PEE	V	202	-	50,50,50	1.16	6 (12%)	53,55,55	0.90	2 (3%)
30	PLX	g	202	-	51,51,51	0.75	1 (1%)	55,59,59	0.61	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CDL	n	101	-	-	33/74/74/110	-
31	CDL	i	401	-	-	39/74/74/110	-
30	PLX	g	203	-	-	24/55/55/55	-
31	CDL	l	704	-	-	44/74/74/110	-
30	PLX	r	502	-	-	36/55/55/55	-
30	PLX	V	203	-	-	26/55/55/55	-
31	CDL	l	703	-	-	38/74/74/110	-
32	PEE	l	702	-	-	27/54/54/54	-
30	PLX	r	501	-	-	28/55/55/55	-
30	PLX	s	401	-	-	21/55/55/55	-
32	PEE	l	701	-	-	32/52/52/54	-
30	PLX	g	201	-	-	25/55/55/55	-
33	8Q1	p	201	-	-	19/41/41/41	-
31	CDL	V	201	-	-	42/69/69/110	-
30	PLX	b	201	-	-	27/55/55/55	-
30	PLX	U	101	-	-	22/55/55/55	-
32	PEE	W	201	-	-	32/54/54/54	-
32	PEE	V	202	-	-	27/54/54/54	-
30	PLX	g	202	-	-	25/55/55/55	-

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	p	201	8Q1	C34-N36	5.30	1.45	1.33
33	p	201	8Q1	C39-N41	5.27	1.45	1.33
31	l	704	CDL	OB8-CB7	4.35	1.46	1.33
31	n	101	CDL	OA6-CA5	4.30	1.46	1.34
31	l	703	CDL	OA6-CA5	4.29	1.46	1.34
31	V	201	CDL	OA6-CA5	4.26	1.46	1.34
31	l	703	CDL	OB8-CB7	4.23	1.45	1.33
32	l	701	PEE	C39-C38	4.17	1.55	1.31
31	V	201	CDL	OB8-CB7	4.16	1.45	1.33
31	l	704	CDL	OA6-CA5	4.14	1.46	1.34
31	l	704	CDL	OA8-CA7	4.13	1.45	1.33
32	l	701	PEE	O3-C30	4.12	1.45	1.33
31	n	101	CDL	OB8-CB7	4.12	1.45	1.33
32	l	701	PEE	C19-C18	4.12	1.55	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	i	401	CDL	OB8-CB7	4.07	1.45	1.33
31	i	401	CDL	OA6-CA5	4.01	1.45	1.34
31	n	101	CDL	OA8-CA7	3.92	1.44	1.33
31	l	703	CDL	OA8-CA7	3.80	1.44	1.33
32	l	702	PEE	C19-C18	3.77	1.53	1.31
32	V	202	PEE	C19-C18	3.75	1.53	1.31
32	W	201	PEE	C19-C18	3.74	1.53	1.31
31	i	401	CDL	OA8-CA7	3.74	1.44	1.33
32	V	202	PEE	C39-C38	3.71	1.53	1.31
32	l	702	PEE	C39-C38	3.70	1.53	1.31
32	W	201	PEE	C39-C38	3.66	1.53	1.31
31	l	704	CDL	OB6-CB5	3.31	1.43	1.34
32	l	701	PEE	O2-C10	3.31	1.43	1.34
31	n	101	CDL	OB6-CB5	3.28	1.43	1.34
31	l	703	CDL	OB6-CB5	3.25	1.43	1.34
31	i	401	CDL	OB6-CB5	3.13	1.43	1.34
31	V	201	CDL	OB6-CB5	3.12	1.43	1.34
31	V	201	CDL	OA8-CA7	3.02	1.45	1.33
30	s	401	PLX	O6-C4	-2.93	1.40	1.44
30	g	203	PLX	O6-C4	-2.90	1.40	1.44
30	g	201	PLX	O6-C4	-2.79	1.40	1.44
30	V	203	PLX	O6-C4	-2.77	1.40	1.44
31	n	101	CDL	OB6-CB4	-2.74	1.39	1.46
31	V	201	CDL	OB6-CB4	-2.60	1.40	1.46
31	i	401	CDL	OB6-CB4	-2.54	1.40	1.46
30	U	101	PLX	O6-C4	-2.51	1.41	1.44
30	g	202	PLX	O6-C4	-2.46	1.41	1.44
33	p	201	8Q1	O35-C34	-2.44	1.18	1.23
32	l	702	PEE	O2-C10	2.39	1.41	1.34
32	V	202	PEE	O2-C10	2.39	1.41	1.34
30	r	501	PLX	O6-C4	-2.38	1.41	1.44
31	l	703	CDL	OB6-CB4	-2.37	1.40	1.46
32	l	702	PEE	O3-C30	2.36	1.40	1.33
31	l	704	CDL	OB6-CB4	-2.35	1.40	1.46
33	p	201	8Q1	O40-C39	-2.34	1.18	1.23
32	l	702	PEE	O2-C2	-2.28	1.40	1.46
32	V	202	PEE	O3-C3	-2.26	1.40	1.45
32	V	202	PEE	O3-C30	2.25	1.39	1.33
32	V	202	PEE	O2-C2	-2.25	1.41	1.46
32	W	201	PEE	O2-C10	2.25	1.40	1.34
33	p	201	8Q1	C1-S44	2.24	1.81	1.76
32	W	201	PEE	O3-C30	2.23	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	201	PEE	O2-C2	-2.20	1.41	1.46
32	l	702	PEE	O3-C3	-2.19	1.40	1.45
32	W	201	PEE	O3-C3	-2.14	1.40	1.45

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	p	201	8Q1	C6-C1-S44	6.02	120.47	113.46
32	l	702	PEE	O2-C10-C11	4.39	120.96	111.50
31	l	703	CDL	OA6-CA5-C11	4.18	120.51	111.50
31	i	401	CDL	OA6-CA5-C11	4.14	120.42	111.50
31	l	704	CDL	OA6-CA5-C11	4.11	120.36	111.50
31	V	201	CDL	OB6-CB5-C51	4.09	120.31	111.50
31	n	101	CDL	OB6-CB5-C51	4.08	120.29	111.50
32	l	701	PEE	O2-C10-C11	4.01	120.14	111.50
31	l	703	CDL	OB6-CB5-C51	3.94	120.00	111.50
31	l	704	CDL	OB6-CB5-C51	3.92	119.96	111.50
31	n	101	CDL	OA6-CA5-C11	3.90	119.91	111.50
32	W	201	PEE	O2-C10-C11	3.68	119.43	111.50
33	p	201	8Q1	O4-C1-C6	-3.62	119.71	123.99
32	V	202	PEE	O2-C10-C11	3.57	119.20	111.50
31	i	401	CDL	OB6-CB5-C51	3.52	119.09	111.50
31	V	201	CDL	OA6-CA5-C11	3.43	118.89	111.50
31	l	703	CDL	OA8-CA7-C31	2.99	121.28	111.91
32	V	202	PEE	O3-C30-C31	2.85	120.86	111.91
32	l	702	PEE	O3-C30-C31	2.84	120.83	111.91
31	i	401	CDL	OB8-CB7-C71	2.75	120.54	111.91
31	n	101	CDL	OA8-CA7-C31	2.74	120.50	111.91
31	l	704	CDL	OA8-CA7-C31	2.72	120.46	111.91
32	W	201	PEE	O3-C30-C31	2.71	120.41	111.91
33	p	201	8Q1	C43-S44-C1	2.71	110.30	101.87
31	n	101	CDL	OB8-CB7-C71	2.70	120.39	111.91
31	l	703	CDL	OB8-CB7-C71	2.69	120.35	111.91
31	l	704	CDL	OB8-CB7-C71	2.66	120.26	111.91
33	p	201	8Q1	C38-C39-N41	2.54	120.71	116.42
31	V	201	CDL	OB8-CB7-C71	2.53	119.83	111.91
31	i	401	CDL	OA8-CA7-C31	2.39	119.40	111.91
30	s	401	PLX	C1C-N1-C1	2.37	119.59	109.92
30	V	203	PLX	C1C-N1-C1	2.32	119.41	109.92
32	l	701	PEE	O3-C30-C31	2.30	119.14	111.91
30	U	101	PLX	C1C-N1-C1	2.30	119.31	109.92
30	g	203	PLX	C1C-N1-C1	2.26	119.15	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	g	201	PLX	C1C-N1-C1	2.20	118.92	109.92
30	g	202	PLX	C1C-N1-C1	2.20	118.91	109.92
33	p	201	8Q1	O4-C1-S44	-2.15	119.82	122.61
30	r	502	PLX	C2-C1-N1	-2.10	108.76	115.78
30	r	501	PLX	C1C-N1-C1	2.06	118.36	109.92
30	U	101	PLX	C5-C4-C3	-2.06	106.91	111.79
31	i	401	CDL	OA6-CA5-OA7	-2.01	118.84	123.70

There are no chirality outliers.

All (567) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	U	101	PLX	O7-C6-C7-C8
30	U	101	PLX	O7-C6-O6-C4
30	U	101	PLX	C3-O4-P1-O2
30	U	101	PLX	N1-C1-C2-O1
30	U	101	PLX	O9-C24-C25-C26
30	V	203	PLX	O7-C6-C7-C8
30	V	203	PLX	N1-C1-C2-O1
30	V	203	PLX	O9-C24-C25-C26
30	b	201	PLX	O7-C6-O6-C4
30	b	201	PLX	N1-C1-C2-O1
30	b	201	PLX	O9-C24-O8-C5
30	g	201	PLX	O7-C6-C7-C8
30	g	201	PLX	O7-C6-O6-C4
30	g	201	PLX	C3-C4-O6-C6
30	g	202	PLX	C2-O1-P1-O4
30	g	202	PLX	C2-O1-P1-O2
30	g	202	PLX	C2-O1-P1-O3
30	g	202	PLX	O9-C24-O8-C5
30	g	203	PLX	O7-C6-O6-C4
30	g	203	PLX	C2-O1-P1-O2
30	g	203	PLX	C25-C24-O8-C5
30	r	501	PLX	C3-O4-P1-O1
30	r	501	PLX	C3-O4-P1-O2
30	r	501	PLX	C3-O4-P1-O3
30	r	501	PLX	O8-C24-C25-C26
30	r	502	PLX	C7-C6-O6-C4
30	r	502	PLX	C3-O4-P1-O1
30	r	502	PLX	C3-O4-P1-O2
30	r	502	PLX	C3-O4-P1-O3
30	r	502	PLX	C2-O1-P1-O2

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Mol	Chain	Res	Type	Atoms
30	r	502	PLX	N1-C1-C2-O1
30	r	502	PLX	O9-C24-C25-C26
30	s	401	PLX	C2-O1-P1-O2
30	s	401	PLX	N1-C1-C2-O1
31	V	201	CDL	CB2-C1-CA2-OA2
31	V	201	CDL	CA2-OA2-PA1-OA3
31	V	201	CDL	CA2-OA2-PA1-OA4
31	V	201	CDL	CA2-OA2-PA1-OA5
31	V	201	CDL	CA3-OA5-PA1-OA3
31	V	201	CDL	CA3-OA5-PA1-OA4
31	V	201	CDL	OA9-CA7-OA8-CA6
31	V	201	CDL	C51-CB5-OB6-CB4
31	i	401	CDL	O1-C1-CA2-OA2
31	i	401	CDL	CB2-C1-CA2-OA2
31	i	401	CDL	CA2-OA2-PA1-OA3
31	i	401	CDL	CA2-OA2-PA1-OA4
31	i	401	CDL	CA2-OA2-PA1-OA5
31	i	401	CDL	CA3-OA5-PA1-OA3
31	i	401	CDL	CA3-OA5-PA1-OA4
31	i	401	CDL	OA6-CA4-CA6-OA8
31	i	401	CDL	CB2-OB2-PB2-OB4
31	i	401	CDL	CB3-OB5-PB2-OB3
31	i	401	CDL	CB3-OB5-PB2-OB4
31	l	703	CDL	CA2-OA2-PA1-OA3
31	l	704	CDL	CA2-OA2-PA1-OA3
31	l	704	CDL	CA2-OA2-PA1-OA4
31	l	704	CDL	CA3-OA5-PA1-OA2
31	l	704	CDL	CA3-OA5-PA1-OA4
31	l	704	CDL	C11-CA5-OA6-CA4
31	l	704	CDL	CB2-OB2-PB2-OB3
31	n	101	CDL	CA2-OA2-PA1-OA3
31	n	101	CDL	CA2-OA2-PA1-OA4
31	n	101	CDL	CA2-OA2-PA1-OA5
31	n	101	CDL	OA7-CA5-OA6-CA4
31	n	101	CDL	C11-CA5-OA6-CA4
31	n	101	CDL	CB2-OB2-PB2-OB3
31	n	101	CDL	CB2-OB2-PB2-OB4
31	n	101	CDL	C51-CB5-OB6-CB4
32	V	202	PEE	C2-C1-O3P-P
32	V	202	PEE	O4P-C4-C5-N
32	W	201	PEE	C4-O4P-P-O1P
32	W	201	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
32	l	701	PEE	C11-C10-O2-C2
32	l	701	PEE	C4-O4P-P-O1P
32	l	701	PEE	C4-O4P-P-O2P
33	p	201	8Q1	C1-C6-C7-C8
33	p	201	8Q1	O4-C1-S44-C43
33	p	201	8Q1	C6-C1-S44-C43
33	p	201	8Q1	C28-C29-C32-C34
33	p	201	8Q1	C28-C29-C32-O33
33	p	201	8Q1	C30-C29-C32-C34
33	p	201	8Q1	C31-C29-C32-C34
33	p	201	8Q1	C31-C29-C32-O33
33	p	201	8Q1	C28-O27-P24-O2
33	p	201	8Q1	C28-O27-P24-O1
31	l	704	CDL	OA9-CA7-OA8-CA6
31	l	704	CDL	OB9-CB7-OB8-CB6
31	n	101	CDL	OA9-CA7-OA8-CA6
31	V	201	CDL	OB7-CB5-OB6-CB4
31	l	703	CDL	OB7-CB5-OB6-CB4
31	l	704	CDL	OA7-CA5-OA6-CA4
31	n	101	CDL	OB7-CB5-OB6-CB4
32	l	701	PEE	O4-C10-O2-C2
31	l	704	CDL	C31-CA7-OA8-CA6
31	l	704	CDL	C71-CB7-OB8-CB6
31	n	101	CDL	C31-CA7-OA8-CA6
31	n	101	CDL	C71-CB7-OB8-CB6
31	l	703	CDL	C51-CB5-OB6-CB4
32	W	201	PEE	C17-C18-C19-C20
32	l	701	PEE	C37-C38-C39-C40
32	l	702	PEE	C37-C38-C39-C40
31	n	101	CDL	OB9-CB7-OB8-CB6
32	l	702	PEE	O5-C30-O3-C3
31	l	703	CDL	O1-C1-CA2-OA2
31	l	704	CDL	O1-C1-CA2-OA2
31	i	401	CDL	C11-CA5-OA6-CA4
32	W	201	PEE	C21-C22-C23-C24
32	V	202	PEE	C20-C21-C22-C23
30	r	502	PLX	C16-C17-C18-C19
32	l	701	PEE	C32-C33-C34-C35
32	l	702	PEE	C31-C30-O3-C3
30	g	203	PLX	C26-C27-C28-C29
30	b	201	PLX	C4-C3-O4-P1
30	r	501	PLX	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
30	b	201	PLX	C14-C15-C16-C17
30	g	203	PLX	C30-C31-C32-C33
30	r	502	PLX	C30-C31-C32-C33
32	W	201	PEE	C32-C33-C34-C35
30	g	202	PLX	C10-C11-C12-C13
31	l	703	CDL	CB2-C1-CA2-OA2
30	r	502	PLX	C12-C13-C14-C15
31	i	401	CDL	C31-C32-C33-C34
32	W	201	PEE	C31-C30-O3-C3
31	l	703	CDL	C73-C74-C75-C76
31	l	703	CDL	OB5-CB3-CB4-OB6
32	W	201	PEE	C12-C13-C14-C15
32	l	701	PEE	C34-C35-C36-C37
31	V	201	CDL	O1-C1-CA2-OA2
31	l	703	CDL	O1-C1-CB2-OB2
30	r	501	PLX	C12-C13-C14-C15
32	W	201	PEE	O5-C30-O3-C3
31	V	201	CDL	C54-C55-C56-C57
31	i	401	CDL	OA7-CA5-OA6-CA4
30	V	203	PLX	C13-C14-C15-C16
31	l	704	CDL	CB5-C51-C52-C53
31	n	101	CDL	CA7-C31-C32-C33
32	l	702	PEE	C10-C11-C12-C13
32	l	702	PEE	C17-C18-C19-C20
32	W	201	PEE	C15-C16-C17-C18
31	i	401	CDL	CA5-C11-C12-C13
32	V	202	PEE	C10-C11-C12-C13
32	l	701	PEE	C30-C31-C32-C33
30	r	501	PLX	C27-C28-C29-C30
31	n	101	CDL	C31-C32-C33-C34
31	i	401	CDL	C31-CA7-OA8-CA6
32	l	701	PEE	C39-C40-C41-C42
32	V	202	PEE	C17-C18-C19-C20
32	l	701	PEE	C17-C18-C19-C20
30	U	101	PLX	C3-O4-P1-O1
30	b	201	PLX	C3-O4-P1-O1
30	g	201	PLX	C3-O4-P1-O1
30	g	202	PLX	C3-O4-P1-O1
30	g	203	PLX	C2-O1-P1-O4
30	r	502	PLX	C2-O1-P1-O4
30	s	401	PLX	C2-O1-P1-O4
31	V	201	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
31	V	201	CDL	CB3-OB5-PB2-OB2
31	i	401	CDL	CA3-OA5-PA1-OA2
31	i	401	CDL	CB2-OB2-PB2-OB5
31	i	401	CDL	CB3-OB5-PB2-OB2
31	l	703	CDL	CB3-OB5-PB2-OB2
31	l	704	CDL	CA2-OA2-PA1-OA5
31	n	101	CDL	CB2-OB2-PB2-OB5
32	V	202	PEE	C1-O3P-P-O4P
32	W	201	PEE	C1-O3P-P-O4P
32	l	701	PEE	C4-O4P-P-O3P
32	V	202	PEE	C31-C30-O3-C3
31	l	703	CDL	CA2-C1-CB2-OB2
31	l	703	CDL	C71-CB7-OB8-CB6
30	U	101	PLX	O6-C6-C7-C8
30	g	203	PLX	O8-C24-C25-C26
30	s	401	PLX	O6-C6-C7-C8
31	l	704	CDL	C51-CB5-OB6-CB4
30	g	201	PLX	C13-C14-C15-C16
30	g	201	PLX	C7-C8-C9-C10
30	g	202	PLX	C7-C8-C9-C10
30	g	203	PLX	C29-C30-C31-C32
30	g	203	PLX	C34-C35-C36-C37
30	s	401	PLX	C27-C28-C29-C30
31	n	101	CDL	C12-C13-C14-C15
31	n	101	CDL	C13-C14-C15-C16
32	W	201	PEE	C14-C15-C16-C17
32	l	701	PEE	C22-C23-C24-C25
31	l	704	CDL	C31-C32-C33-C34
32	l	702	PEE	C20-C21-C22-C23
33	p	201	8Q1	C11-C12-C13-C14
31	l	704	CDL	OB7-CB5-OB6-CB4
31	n	101	CDL	CB5-C51-C52-C53
31	V	201	CDL	C71-C72-C73-C74
32	l	701	PEE	C21-C22-C23-C24
30	r	501	PLX	C13-C14-C15-C16
30	r	502	PLX	C14-C15-C16-C17
32	V	202	PEE	C12-C13-C14-C15
32	V	202	PEE	C40-C41-C42-C43
32	l	702	PEE	C33-C34-C35-C36
31	l	703	CDL	CB7-C71-C72-C73
31	l	704	CDL	CB7-C71-C72-C73
30	U	101	PLX	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
31	l	704	CDL	C51-C52-C53-C54
30	U	101	PLX	C12-C13-C14-C15
30	U	101	PLX	C10-C11-C12-C13
30	U	101	PLX	C35-C36-C37-C38
30	b	201	PLX	C16-C17-C18-C19
30	b	201	PLX	C29-C30-C31-C32
30	g	203	PLX	C15-C16-C17-C18
30	r	502	PLX	C11-C12-C13-C14
30	r	502	PLX	C10-C11-C12-C13
33	p	201	8Q1	C6-C7-C8-C9
30	U	101	PLX	C19-C20-C21-C22
30	U	101	PLX	C9-C10-C11-C12
30	V	203	PLX	C10-C11-C12-C13
30	b	201	PLX	C27-C28-C29-C30
30	g	202	PLX	C14-C15-C16-C17
30	s	401	PLX	C28-C29-C30-C31
31	i	401	CDL	C13-C14-C15-C16
32	l	702	PEE	C40-C41-C42-C43
30	r	502	PLX	C9-C10-C11-C12
30	s	401	PLX	C9-C10-C11-C12
31	l	704	CDL	C32-C33-C34-C35
30	V	203	PLX	C25-C26-C27-C28
30	g	201	PLX	C16-C17-C18-C19
32	V	202	PEE	C14-C15-C16-C17
32	l	702	PEE	C34-C35-C36-C37
31	l	704	CDL	CA7-C31-C32-C33
30	U	101	PLX	C7-C8-C9-C10
30	b	201	PLX	C18-C19-C20-C21
30	g	201	PLX	C10-C11-C12-C13
31	l	703	CDL	C51-C52-C53-C54
32	l	702	PEE	C21-C22-C23-C24
30	b	201	PLX	C25-C26-C27-C28
31	l	703	CDL	C11-C12-C13-C14
30	V	203	PLX	C32-C33-C34-C35
30	g	202	PLX	C9-C10-C11-C12
31	n	101	CDL	C51-C52-C53-C54
31	n	101	CDL	CB7-C71-C72-C73
32	l	701	PEE	C20-C21-C22-C23
30	r	502	PLX	C32-C33-C34-C35
30	g	203	PLX	C10-C11-C12-C13
30	s	401	PLX	C12-C13-C14-C15
32	V	202	PEE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
32	V	202	PEE	O5-C30-O3-C3
30	g	203	PLX	C17-C18-C19-C20
30	r	502	PLX	C26-C27-C28-C29
32	W	201	PEE	C37-C38-C39-C40
30	g	203	PLX	C7-C8-C9-C10
30	r	502	PLX	C25-C26-C27-C28
31	i	401	CDL	C34-C35-C36-C37
31	i	401	CDL	OA9-CA7-OA8-CA6
30	g	202	PLX	C11-C12-C13-C14
30	g	203	PLX	C14-C15-C16-C17
33	p	201	8Q1	C7-C8-C9-C10
30	g	203	PLX	O9-C24-C25-C26
30	r	501	PLX	O9-C24-C25-C26
30	r	502	PLX	O7-C6-C7-C8
30	s	401	PLX	O7-C6-C7-C8
30	r	501	PLX	C7-C8-C9-C10
31	i	401	CDL	C11-C12-C13-C14
31	l	703	CDL	C33-C34-C35-C36
31	i	401	CDL	C32-C33-C34-C35
30	r	501	PLX	C35-C36-C37-C38
31	l	703	CDL	OB9-CB7-OB8-CB6
32	V	202	PEE	C43-C44-C45-C46
32	l	701	PEE	C13-C14-C15-C16
32	l	701	PEE	C41-C42-C43-C44
31	V	201	CDL	OA7-CA5-OA6-CA4
30	V	203	PLX	C11-C12-C13-C14
33	p	201	8Q1	C12-C13-C14-C15
32	W	201	PEE	C23-C24-C25-C26
31	l	703	CDL	C31-CA7-OA8-CA6
31	V	201	CDL	C11-CA5-OA6-CA4
30	g	201	PLX	C32-C33-C34-C35
30	r	501	PLX	C26-C27-C28-C29
31	V	201	CDL	CB5-C51-C52-C53
31	i	401	CDL	CB5-C51-C52-C53
31	n	101	CDL	C55-C56-C57-C58
30	r	502	PLX	C36-C37-C38-C39
31	i	401	CDL	C73-C74-C75-C76
32	W	201	PEE	C41-C42-C43-C44
32	l	701	PEE	C15-C16-C17-C18
32	l	702	PEE	C19-C20-C21-C22
30	r	502	PLX	C20-C21-C22-C23
30	r	502	PLX	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
32	V	202	PEE	C31-C32-C33-C34
31	n	101	CDL	C71-C72-C73-C74
32	l	702	PEE	C31-C32-C33-C34
31	i	401	CDL	C71-CB7-OB8-CB6
30	b	201	PLX	C30-C31-C32-C33
30	g	202	PLX	C26-C27-C28-C29
32	W	201	PEE	C43-C44-C45-C46
31	i	401	CDL	C51-CB5-OB6-CB4
30	r	502	PLX	C35-C36-C37-C38
31	V	201	CDL	C14-C15-C16-C17
30	b	201	PLX	C32-C33-C34-C35
30	s	401	PLX	C29-C30-C31-C32
32	V	202	PEE	C19-C20-C21-C22
32	W	201	PEE	C19-C20-C21-C22
30	g	203	PLX	C35-C36-C37-C38
30	r	501	PLX	C9-C10-C11-C12
30	b	201	PLX	C11-C12-C13-C14
32	l	701	PEE	C23-C24-C25-C26
31	l	703	CDL	OA9-CA7-OA8-CA6
30	g	202	PLX	C11-C10-C9-C8
30	r	502	PLX	C17-C18-C19-C20
31	l	704	CDL	C13-C14-C15-C16
32	l	701	PEE	C40-C41-C42-C43
32	l	701	PEE	C16-C17-C18-C19
30	g	201	PLX	C2-O1-P1-O4
31	l	703	CDL	CA2-OA2-PA1-OA5
30	s	401	PLX	C15-C16-C17-C18
31	n	101	CDL	C34-C35-C36-C37
31	l	704	CDL	OB5-CB3-CB4-CB6
32	l	701	PEE	O3P-C1-C2-C3
30	r	502	PLX	C15-C16-C17-C18
32	l	702	PEE	C42-C43-C44-C45
30	s	401	PLX	C11-C10-C9-C8
31	l	704	CDL	CB2-C1-CA2-OA2
31	i	401	CDL	OB7-CB5-OB6-CB4
31	V	201	CDL	C12-C13-C14-C15
31	n	101	CDL	C33-C34-C35-C36
32	W	201	PEE	C33-C34-C35-C36
30	r	501	PLX	C3-C4-C5-O8
31	l	703	CDL	CA3-CA4-CA6-OA8
32	V	202	PEE	C41-C42-C43-C44
30	g	201	PLX	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
30	r	501	PLX	C18-C19-C20-C21
32	W	201	PEE	C44-C45-C46-C47
30	U	101	PLX	O8-C24-C25-C26
32	l	702	PEE	C12-C13-C14-C15
33	p	201	8Q1	C13-C14-C15-C16
31	i	401	CDL	OB9-CB7-OB8-CB6
30	b	201	PLX	C20-C21-C22-C23
30	V	203	PLX	C7-C8-C9-C10
32	l	701	PEE	C42-C43-C44-C45
32	l	702	PEE	C44-C45-C46-C47
32	l	701	PEE	C2-C1-O3P-P
31	V	201	CDL	OA5-CA3-CA4-OA6
30	U	101	PLX	C26-C27-C28-C29
32	W	201	PEE	O2-C2-C3-O3
31	l	703	CDL	C75-C76-C77-C78
33	p	201	8Q1	C30-C29-C32-O33
31	i	401	CDL	C52-C51-CB5-OB6
30	V	203	PLX	C16-C17-C18-C19
31	i	401	CDL	C35-C36-C37-C38
30	U	101	PLX	C11-C10-C9-C8
31	V	201	CDL	C72-C73-C74-C75
32	W	201	PEE	C34-C35-C36-C37
30	V	203	PLX	C12-C13-C14-C15
30	g	201	PLX	C17-C18-C19-C20
30	g	201	PLX	C27-C28-C29-C30
31	l	703	CDL	OB5-CB3-CB4-CB6
32	W	201	PEE	O3P-C1-C2-C3
30	V	203	PLX	C31-C32-C33-C34
30	r	501	PLX	C25-C26-C27-C28
31	V	201	CDL	C52-C53-C54-C55
30	U	101	PLX	C28-C29-C30-C31
30	b	201	PLX	C13-C14-C15-C16
30	s	401	PLX	C30-C31-C32-C33
32	l	702	PEE	C11-C10-O2-C2
30	b	201	PLX	C11-C10-C9-C8
30	b	201	PLX	C36-C37-C38-C39
30	U	101	PLX	C27-C28-C29-C30
30	g	201	PLX	C3-C4-C5-O8
31	V	201	CDL	CB3-CB4-CB6-OB8
31	i	401	CDL	CA3-CA4-CA6-OA8
32	W	201	PEE	C1-C2-C3-O3
30	r	502	PLX	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
33	p	201	8Q1	C10-C11-C12-C13
30	r	501	PLX	C28-C29-C30-C31
32	W	201	PEE	C13-C14-C15-C16
30	b	201	PLX	C5-C4-O6-C6
30	g	202	PLX	C5-C4-O6-C6
31	V	201	CDL	C53-C54-C55-C56
30	r	501	PLX	O7-C6-C7-C8
30	b	201	PLX	C35-C36-C37-C38
31	l	704	CDL	OA5-CA3-CA4-OA6
30	V	203	PLX	C26-C27-C28-C29
31	l	703	CDL	OA6-CA4-CA6-OA8
31	V	201	CDL	C12-C11-CA5-OA6
30	g	201	PLX	C20-C21-C22-C23
30	g	203	PLX	C4-C3-O4-P1
30	r	501	PLX	C4-C3-O4-P1
31	l	704	CDL	C73-C74-C75-C76
30	r	501	PLX	C19-C20-C21-C22
31	l	703	CDL	C15-C16-C17-C18
31	n	101	CDL	CA5-C11-C12-C13
32	W	201	PEE	O4-C10-O2-C2
32	l	702	PEE	O4-C10-O2-C2
32	W	201	PEE	C11-C10-O2-C2
30	s	401	PLX	C11-C12-C13-C14
30	s	401	PLX	C32-C33-C34-C35
32	l	701	PEE	C31-C32-C33-C34
31	V	201	CDL	C75-C76-C77-C78
30	r	501	PLX	C30-C31-C32-C33
30	g	202	PLX	C30-C31-C32-C33
30	g	202	PLX	O4-C3-C4-O6
31	V	201	CDL	OB5-CB3-CB4-OB6
31	l	703	CDL	OA5-CA3-CA4-OA6
32	V	202	PEE	C33-C34-C35-C36
32	V	202	PEE	C32-C33-C34-C35
30	b	201	PLX	O6-C4-C5-O8
30	r	501	PLX	O6-C4-C5-O8
31	V	201	CDL	OA6-CA4-CA6-OA8
31	V	201	CDL	OB6-CB4-CB6-OB8
31	l	704	CDL	C12-C13-C14-C15
30	r	502	PLX	C24-C25-C26-C27
30	r	502	PLX	C34-C35-C36-C37
30	g	201	PLX	C35-C36-C37-C38
32	l	701	PEE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
32	l	702	PEE	C11-C12-C13-C14
30	r	501	PLX	C31-C32-C33-C34
31	n	101	CDL	C35-C36-C37-C38
31	n	101	CDL	C11-C12-C13-C14
32	W	201	PEE	C31-C32-C33-C34
31	l	704	CDL	CB2-OB2-PB2-OB5
30	r	502	PLX	C4-C3-O4-P1
31	l	704	CDL	CA4-CA3-OA5-PA1
30	b	201	PLX	C3-O4-P1-O2
30	g	201	PLX	C3-O4-P1-O3
30	g	202	PLX	C3-O4-P1-O2
30	g	202	PLX	C3-O4-P1-O3
30	r	502	PLX	C2-O1-P1-O3
31	V	201	CDL	CB3-OB5-PB2-OB4
31	i	401	CDL	CB2-OB2-PB2-OB3
31	l	703	CDL	CA2-OA2-PA1-OA4
31	l	703	CDL	CB3-OB5-PB2-OB4
31	l	704	CDL	CA3-OA5-PA1-OA3
31	n	101	CDL	CA3-OA5-PA1-OA3
32	V	202	PEE	C1-O3P-P-O1P
30	r	501	PLX	C15-C16-C17-C18
30	g	202	PLX	O4-C3-C4-C5
31	V	201	CDL	OA5-CA3-CA4-CA6
31	V	201	CDL	OB5-CB3-CB4-CB6
31	l	703	CDL	OA5-CA3-CA4-CA6
31	l	704	CDL	OA5-CA3-CA4-CA6
30	V	203	PLX	C19-C20-C21-C22
30	g	203	PLX	C19-C20-C21-C22
30	U	101	PLX	C25-C24-O8-C5
30	b	201	PLX	C1-C2-O1-P1
30	g	203	PLX	C1-C2-O1-P1
30	r	501	PLX	C25-C24-O8-C5
32	W	201	PEE	C10-C11-C12-C13
31	V	201	CDL	C74-C75-C76-C77
31	l	704	CDL	OB5-CB3-CB4-OB6
32	l	701	PEE	O3P-C1-C2-O2
30	V	203	PLX	C14-C15-C16-C17
30	g	203	PLX	C3-C4-C5-O8
30	r	502	PLX	C3-C4-C5-O8
30	g	203	PLX	O6-C4-C5-O8
30	r	502	PLX	O6-C4-C5-O8
31	l	704	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
30	g	201	PLX	C24-C25-C26-C27
30	r	502	PLX	O8-C24-C25-C26
30	U	101	PLX	C36-C37-C38-C39
30	g	202	PLX	O7-C6-C7-C8
31	l	704	CDL	C15-C16-C17-C18
30	s	401	PLX	C20-C21-C22-C23
30	r	502	PLX	C11-C10-C9-C8
31	i	401	CDL	C32-C31-CA7-OA8
30	g	201	PLX	C14-C15-C16-C17
31	n	101	CDL	C73-C74-C75-C76
31	V	201	CDL	CA3-CA4-OA6-CA5
31	l	703	CDL	CB6-CB4-OB6-CB5
31	l	704	CDL	CA6-CA4-OA6-CA5
32	l	701	PEE	C3-C2-O2-C10
32	l	702	PEE	C3-C2-O2-C10
31	V	201	CDL	CB7-C71-C72-C73
31	V	201	CDL	C55-C56-C57-C58
31	n	101	CDL	C53-C54-C55-C56
31	l	703	CDL	CA7-C31-C32-C33
32	V	202	PEE	C11-C10-O2-C2
31	n	101	CDL	C15-C16-C17-C18
30	U	101	PLX	C2-O1-P1-O4
30	V	203	PLX	C3-O4-P1-O1
30	g	203	PLX	C3-O4-P1-O1
31	V	201	CDL	CB2-OB2-PB2-OB5
31	l	703	CDL	CB2-OB2-PB2-OB5
32	V	202	PEE	C4-O4P-P-O3P
32	l	701	PEE	C1-O3P-P-O4P
32	l	702	PEE	C4-O4P-P-O3P
30	b	201	PLX	C28-C29-C30-C31
30	V	203	PLX	C3-C4-C5-O8
30	V	203	PLX	C29-C30-C31-C32
30	r	501	PLX	C11-C10-C9-C8
31	l	703	CDL	C34-C35-C36-C37
31	l	704	CDL	C1-CB2-OB2-PB2
32	V	202	PEE	C23-C24-C25-C26
32	V	202	PEE	O4-C10-O2-C2
32	V	202	PEE	C35-C36-C37-C38
32	l	702	PEE	C23-C24-C25-C26
32	l	701	PEE	O4P-C4-C5-N
30	g	202	PLX	C15-C16-C17-C18
30	g	201	PLX	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
30	V	203	PLX	O6-C6-C7-C8
30	g	201	PLX	O6-C6-C7-C8
31	i	401	CDL	C1-CB2-OB2-PB2
31	i	401	CDL	CB4-CB3-OB5-PB2
31	l	703	CDL	CA4-CA3-OA5-PA1
32	W	201	PEE	C11-C12-C13-C14
30	V	203	PLX	C6-C7-C8-C9
30	s	401	PLX	C6-C7-C8-C9
31	l	703	CDL	CB5-C51-C52-C53
30	g	201	PLX	C25-C26-C27-C28
33	p	201	8Q1	O27-C28-C29-C31
31	V	201	CDL	C11-C12-C13-C14
30	g	203	PLX	C3-C4-O6-C6
30	r	501	PLX	C5-C4-O6-C6
32	V	202	PEE	C21-C22-C23-C24
30	V	203	PLX	C33-C34-C35-C36
33	p	201	8Q1	C42-C43-S44-C1
30	g	201	PLX	O6-C4-C5-O8
31	i	401	CDL	C72-C71-CB7-OB8
30	s	401	PLX	C7-C8-C9-C10
31	i	401	CDL	C52-C51-CB5-OB7
30	b	201	PLX	C3-C4-C5-O8
31	l	704	CDL	CA3-CA4-CA6-OA8
31	V	201	CDL	C73-C74-C75-C76
30	r	502	PLX	C28-C29-C30-C31
30	g	202	PLX	C16-C17-C18-C19
30	g	201	PLX	O4-C3-C4-O6
30	V	203	PLX	C24-C25-C26-C27
31	l	704	CDL	C32-C31-CA7-OA8
32	W	201	PEE	C35-C36-C37-C38
31	l	703	CDL	C32-C31-CA7-OA8
30	g	202	PLX	C27-C28-C29-C30
32	W	201	PEE	C1-C2-O2-C10
30	V	203	PLX	C35-C36-C37-C38
32	V	202	PEE	C30-C31-C32-C33
30	s	401	PLX	C14-C15-C16-C17
31	V	201	CDL	CA3-CA4-CA6-OA8
30	r	502	PLX	C33-C34-C35-C36
31	l	704	CDL	C35-C36-C37-C38
30	s	401	PLX	O9-C24-C25-C26
32	l	701	PEE	C38-C39-C40-C41
31	l	703	CDL	C32-C31-CA7-OA9

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Mol	Chain	Res	Type	Atoms
32	l	702	PEE	C18-C19-C20-C21
31	l	703	CDL	C32-C33-C34-C35
32	l	702	PEE	C1-C2-C3-O3
30	b	201	PLX	C24-C25-C26-C27
32	l	702	PEE	C22-C23-C24-C25
30	s	401	PLX	C4-C3-O4-P1
30	V	203	PLX	C17-C18-C19-C20
30	V	203	PLX	C3-O4-P1-O2
30	g	201	PLX	C3-O4-P1-O2
31	l	703	CDL	CA3-OA5-PA1-OA3
31	l	704	CDL	CB3-OB5-PB2-OB3
31	n	101	CDL	CB3-OB5-PB2-OB3
32	l	702	PEE	C4-O4P-P-O1P
32	l	701	PEE	C33-C34-C35-C36
31	V	201	CDL	C12-C11-CA5-OA7
31	l	704	CDL	C32-C31-CA7-OA9
30	r	501	PLX	C14-C15-C16-C17
30	b	201	PLX	C25-C24-O8-C5
30	g	202	PLX	C25-C24-O8-C5
32	W	201	PEE	C5-C4-O4P-P
32	V	202	PEE	C39-C40-C41-C42
32	l	702	PEE	C41-C42-C43-C44
31	l	704	CDL	C52-C51-CB5-OB6
32	l	702	PEE	C32-C33-C34-C35
30	g	202	PLX	C6-C7-C8-C9
30	g	202	PLX	C24-C25-C26-C27
31	l	704	CDL	C74-C75-C76-C77
32	l	701	PEE	C11-C12-C13-C14
30	V	203	PLX	C15-C16-C17-C18
30	g	203	PLX	C36-C37-C38-C39
32	W	201	PEE	C42-C43-C44-C45
31	l	704	CDL	C52-C51-CB5-OB7
31	V	201	CDL	C52-C51-CB5-OB6

There are no ring outliers.

5 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	V	203	PLX	2	0
31	V	201	CDL	8	0
30	U	101	PLX	1	0
32	W	201	PEE	5	0

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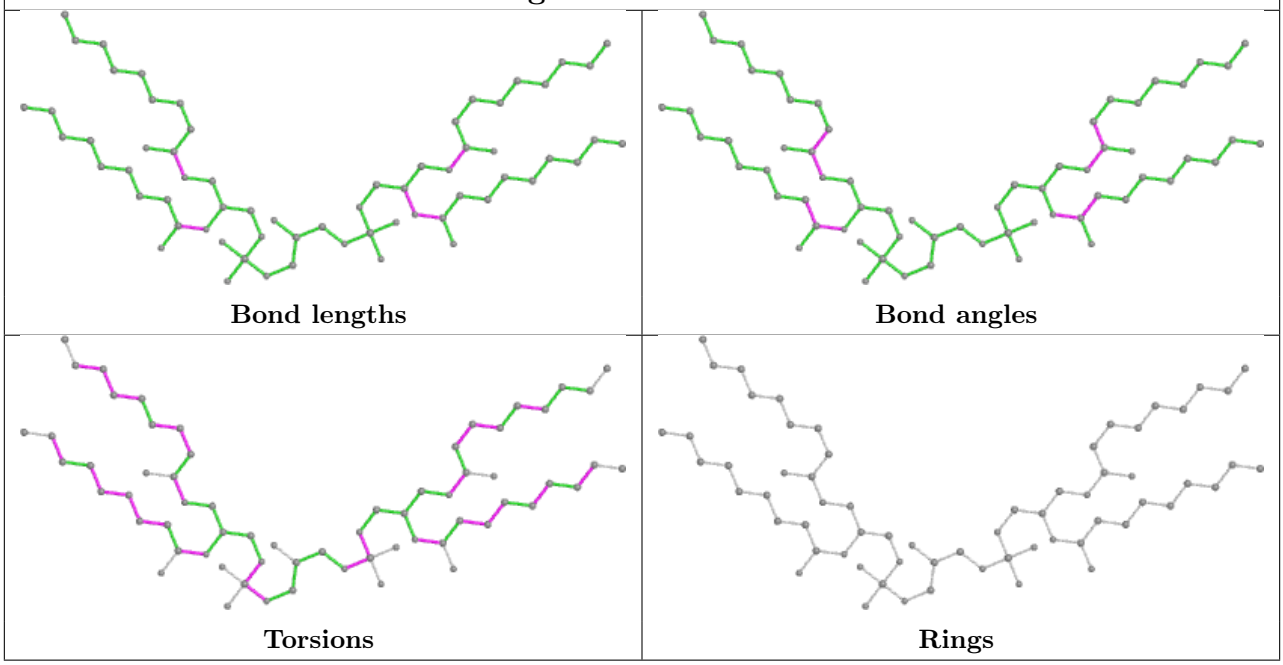
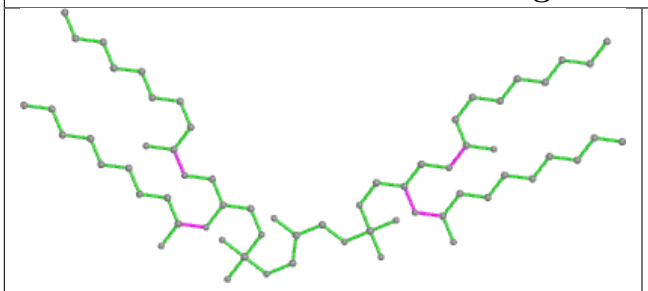
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	V	202	PEE	12	0

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 then 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.

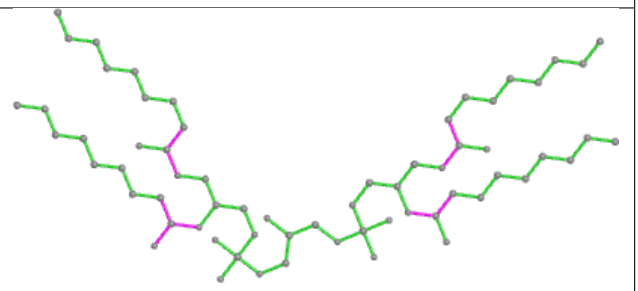
Ligand CDL n 101



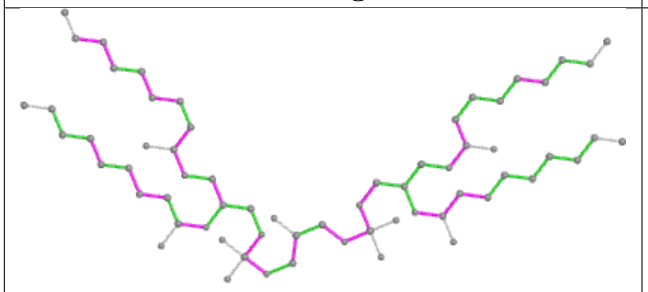
Ligand CDL i 401



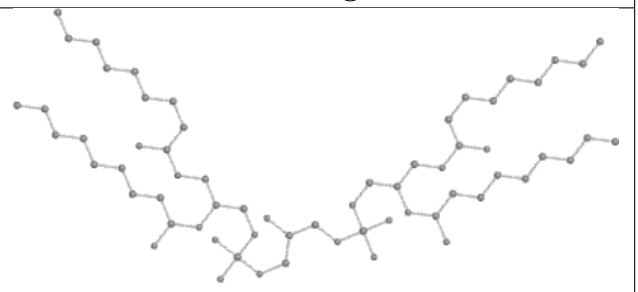
Bond lengths



Bond angles

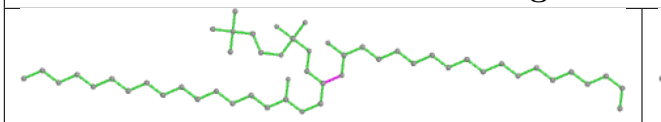


Torsions

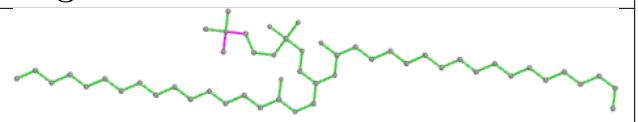


Rings

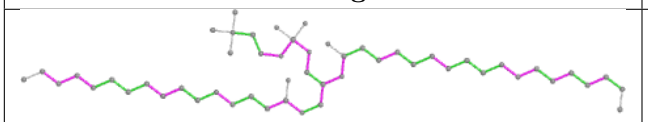
Ligand PLX g 203



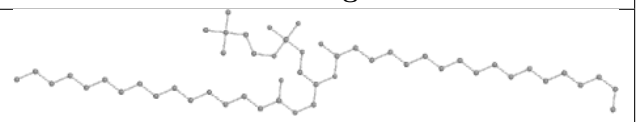
Bond lengths



Bond angles

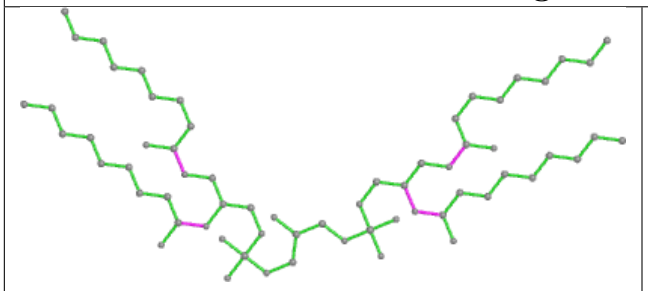


Torsions

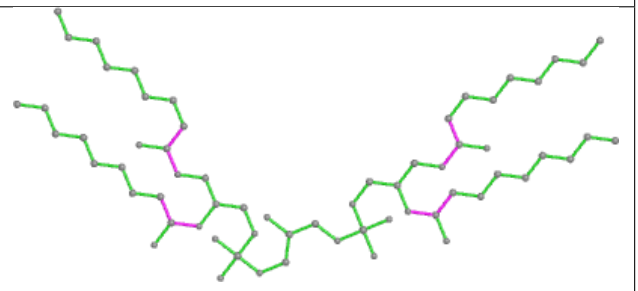


Rings

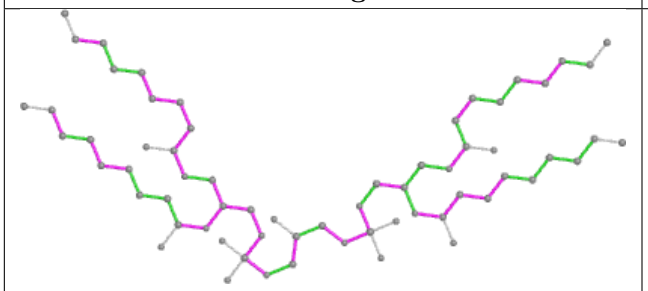
Ligand CDL l 704



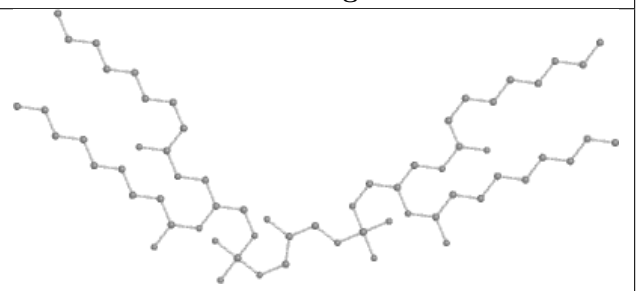
Bond lengths



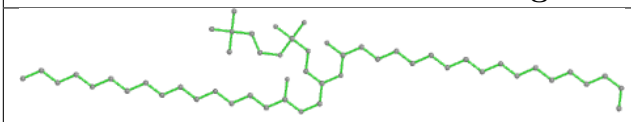
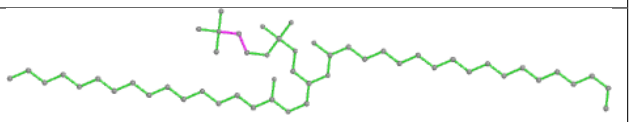
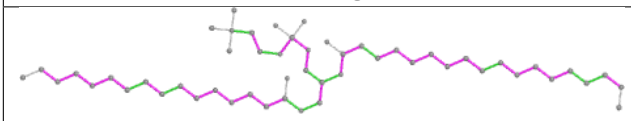
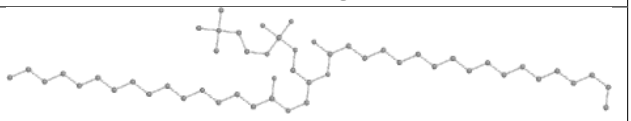
Bond angles

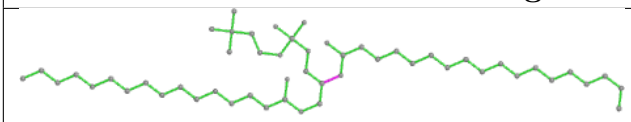
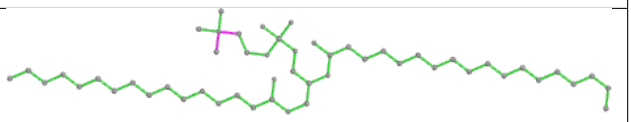
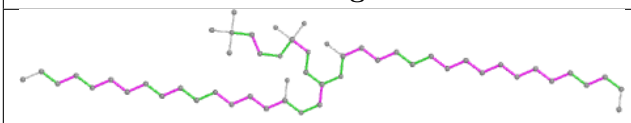
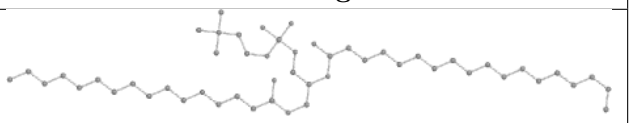


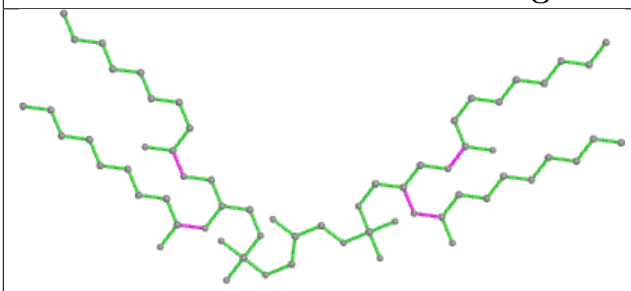
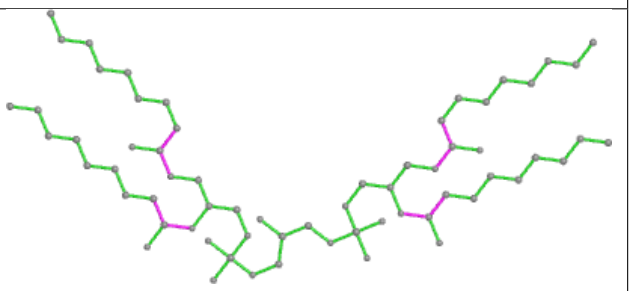
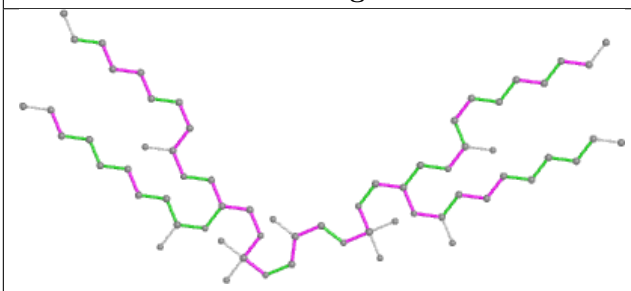
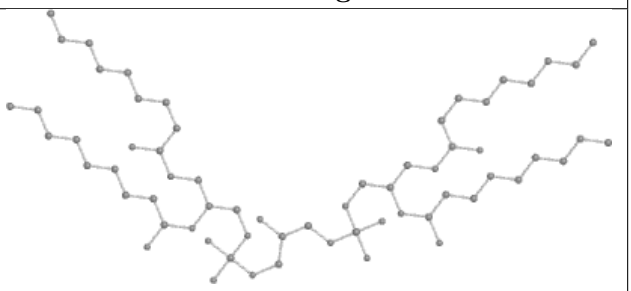
Torsions



Rings

Ligand PLX r 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLX V 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL l 703	
 Bond lengths	 Bond angles
 Torsions	 Rings

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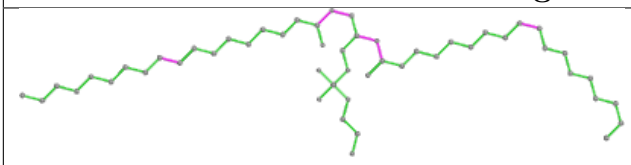
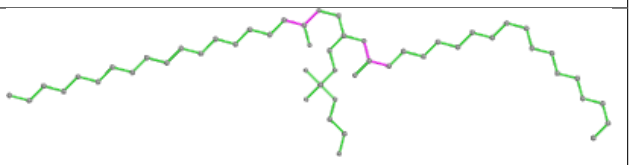
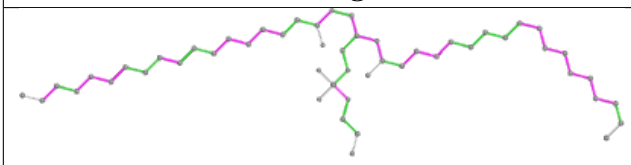
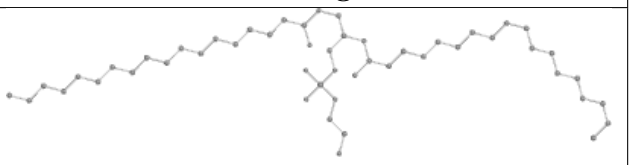
 Bond lengths	 Bond angles
 Torsions	 Rings

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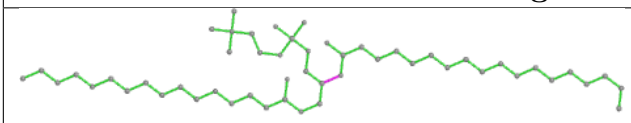
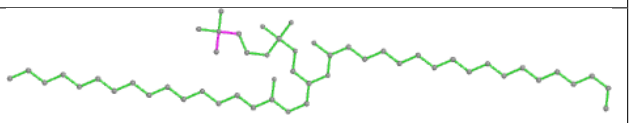
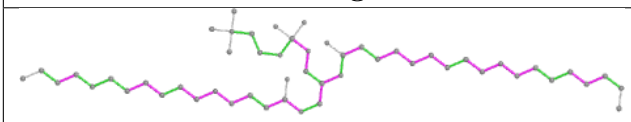
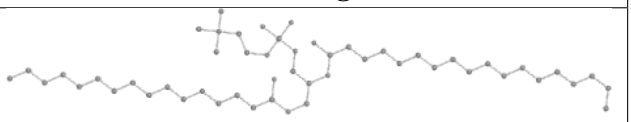
 Bond lengths	 Bond angles
 Torsions	 Rings

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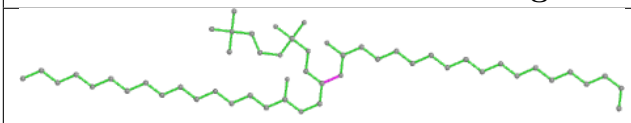
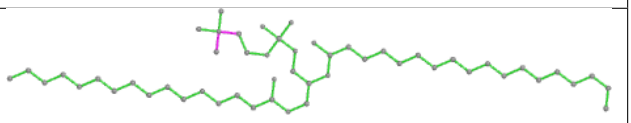
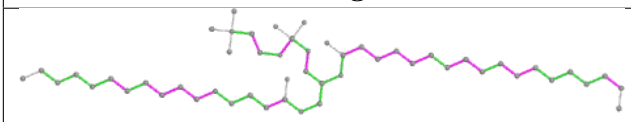
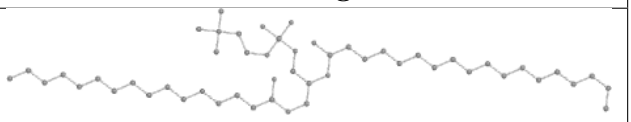
 Bond lengths	 Bond angles
 Torsions	 Rings

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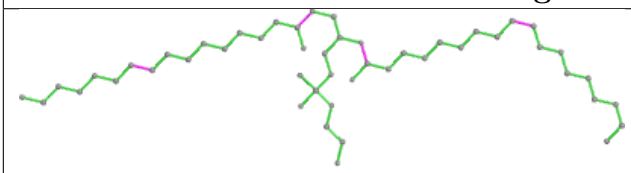
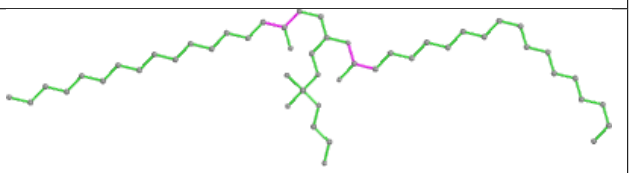
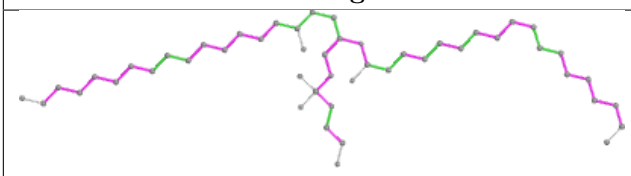
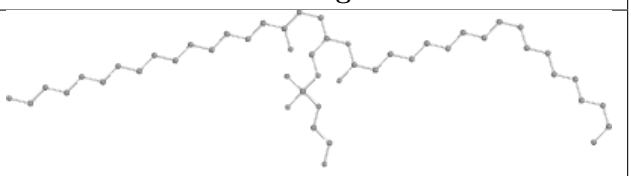
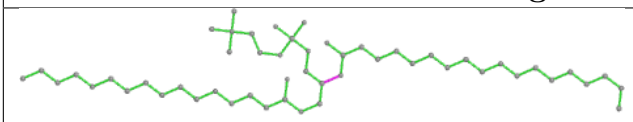
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLX g 201



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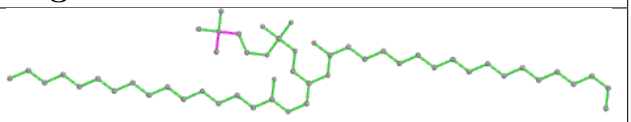

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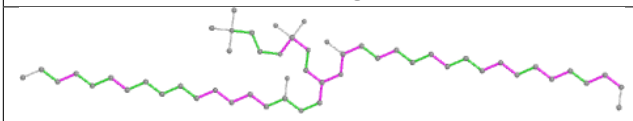

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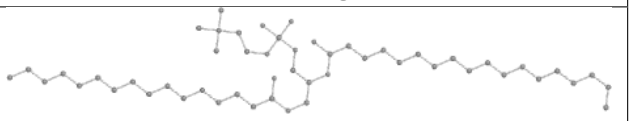
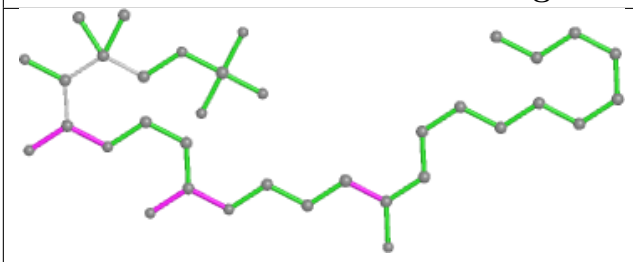


Rings

Ligand 8Q1 p 201



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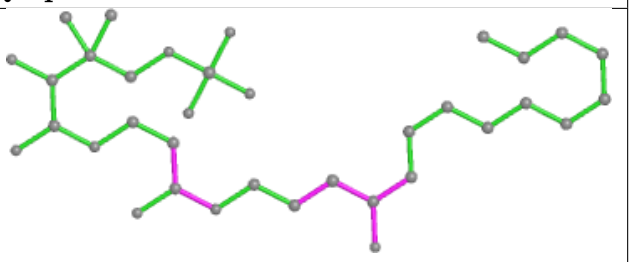

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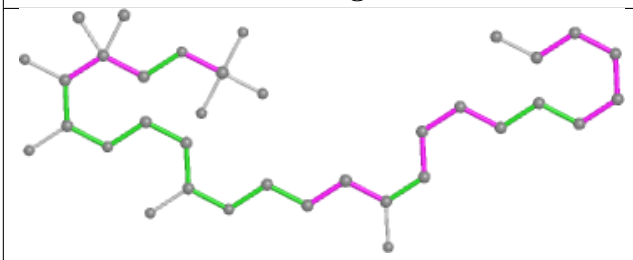

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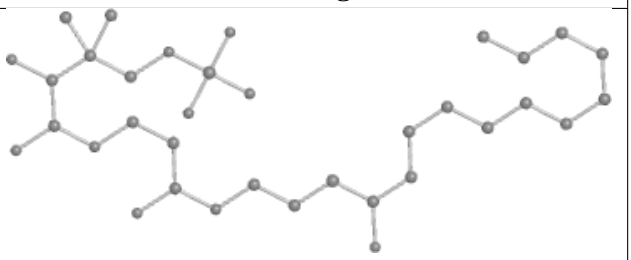
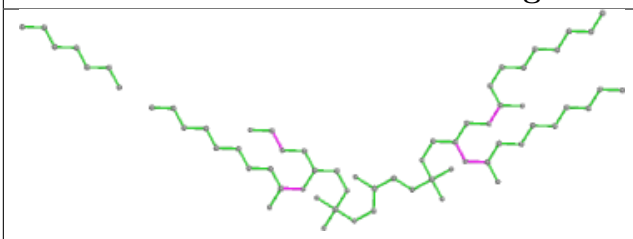


Rings

Ligand CDL V 201



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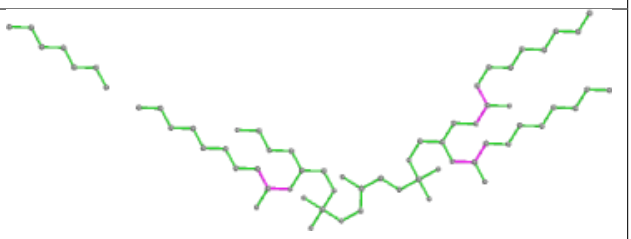

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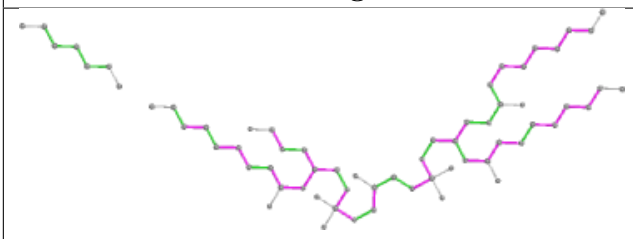

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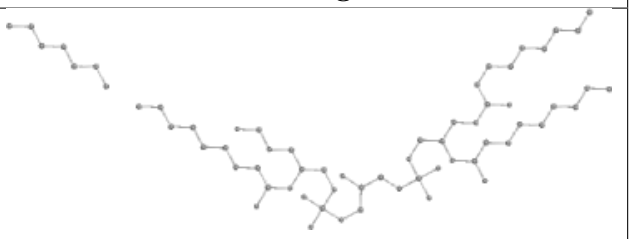
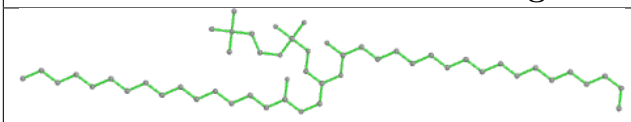


Rings

Ligand PLX b 201



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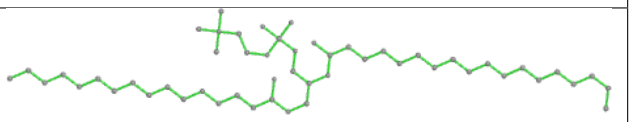

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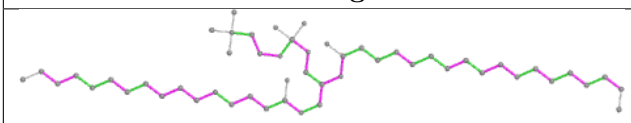

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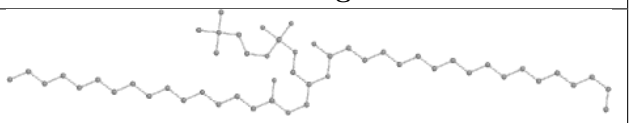
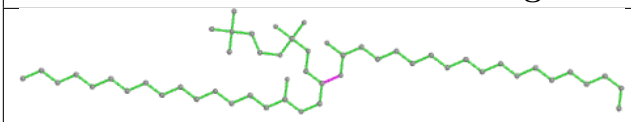


Rings

Ligand PLX U 101



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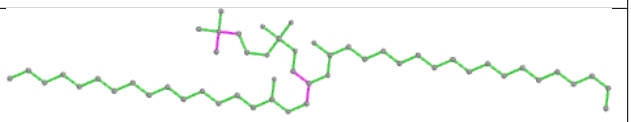

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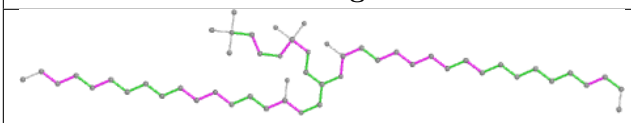

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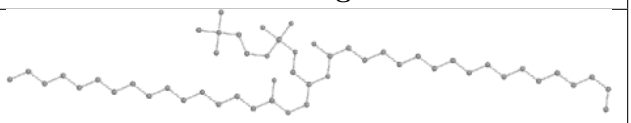
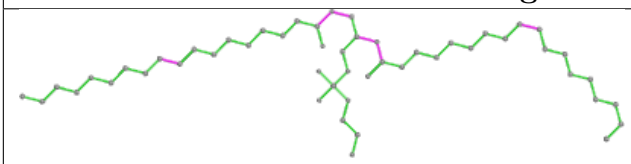


Rings

Ligand PEE W 201



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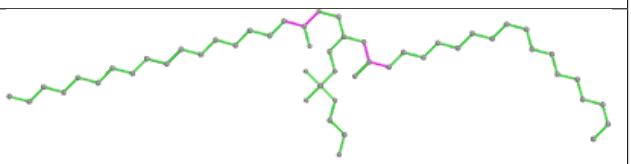
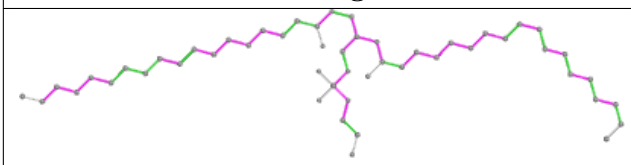


Bond angles



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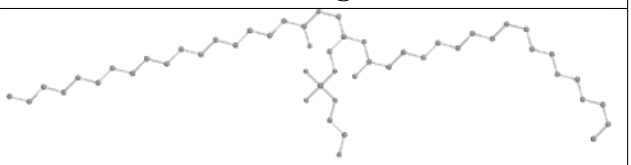
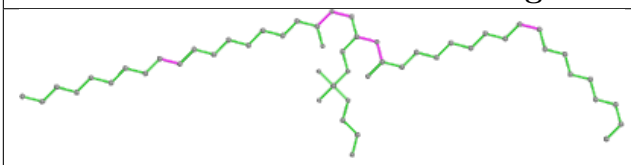


Rings

Ligand PEE V 202



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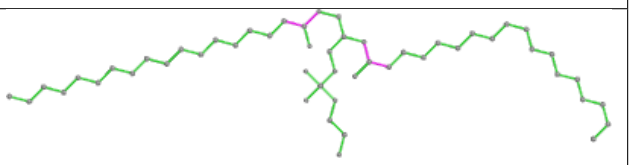

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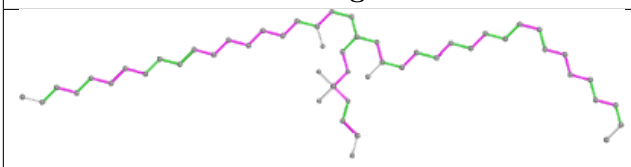

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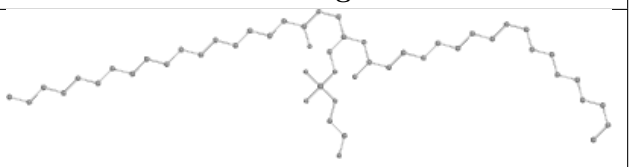
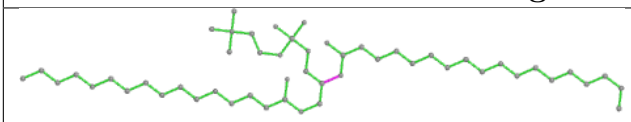
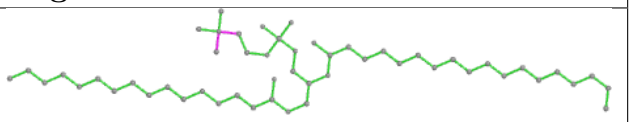
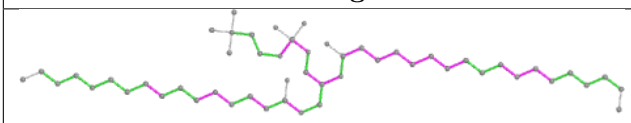
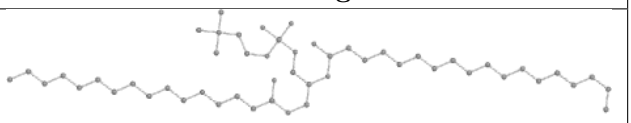


Rings

Ligand PLX g 202	
 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.

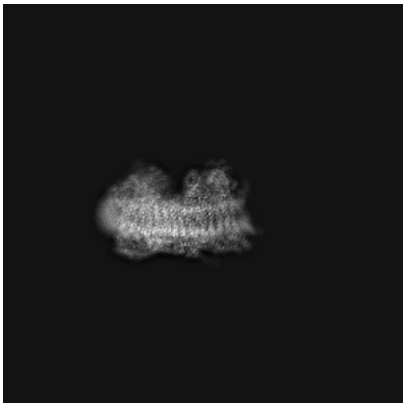
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-6772. These allow visual inspection of the internal detail of the map and identification of artifacts.

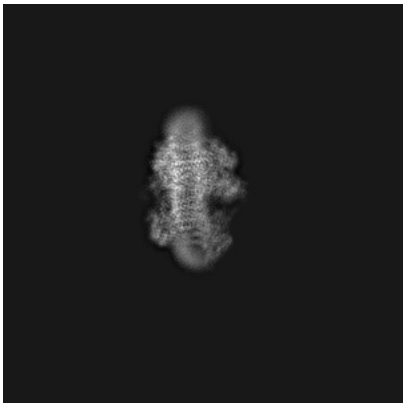
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

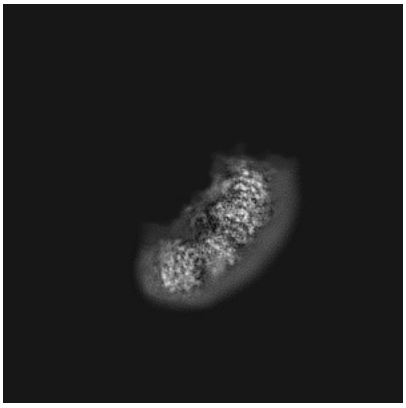
6.1.1 Primary map



X



Y

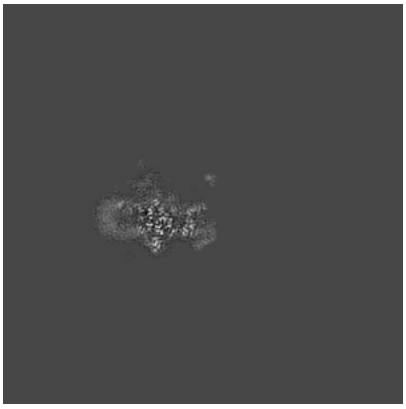


Z

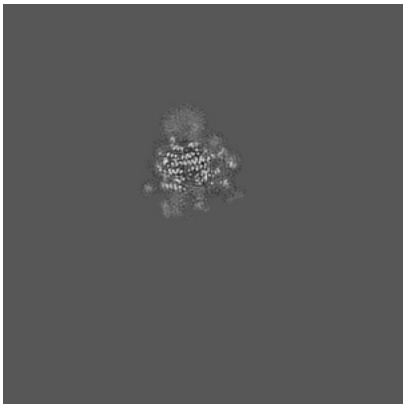
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

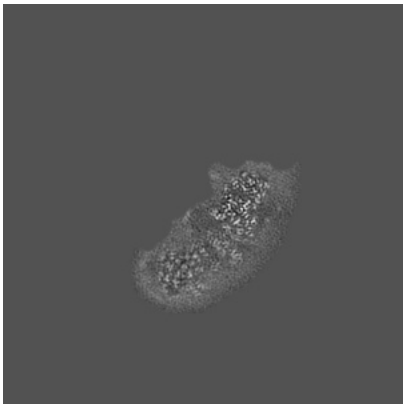
6.2.1 Primary map



X Index: 240



Y Index: 240

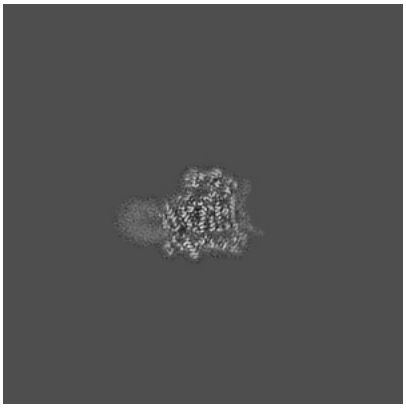


Z Index: 240

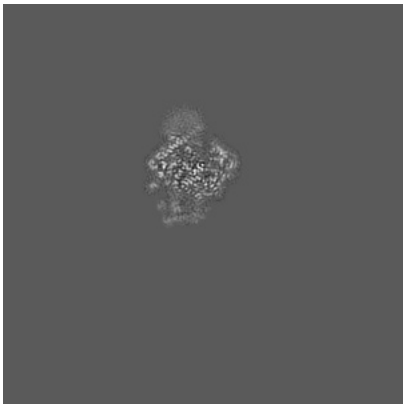
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

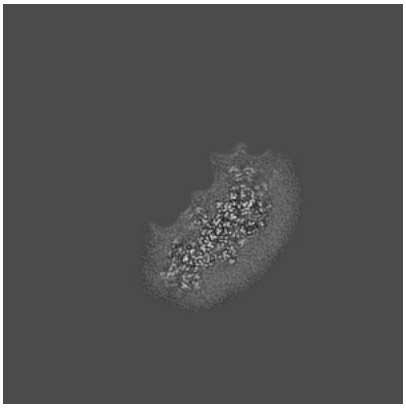
6.3.1 Primary map



X Index: 290



Y Index: 232

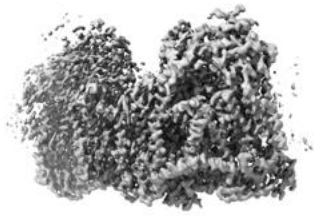


Z Index: 207

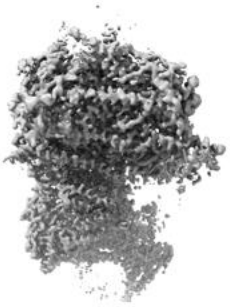
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0677. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

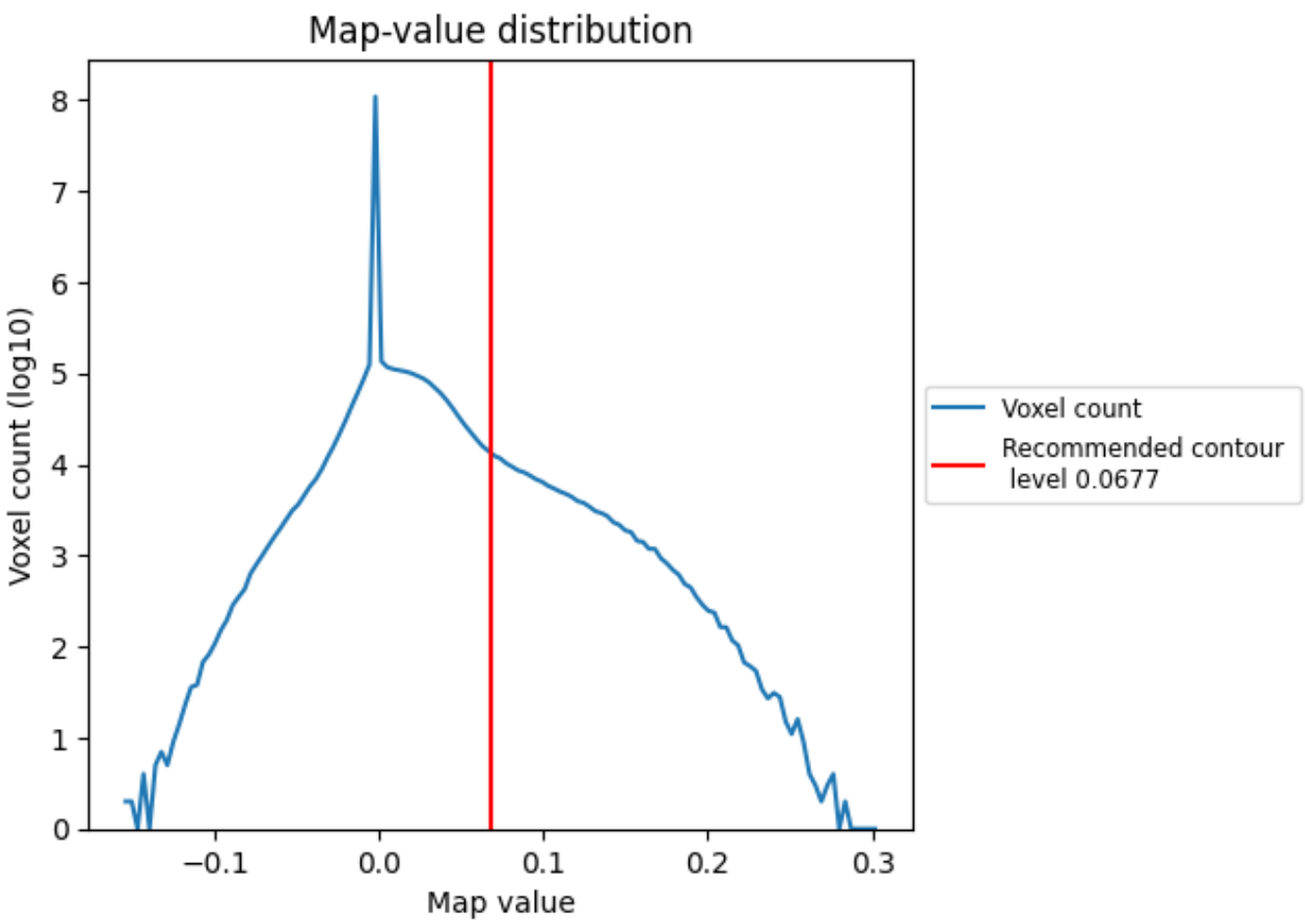
6.5 Mask visualisation (i)

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

7 Map analysis (i)

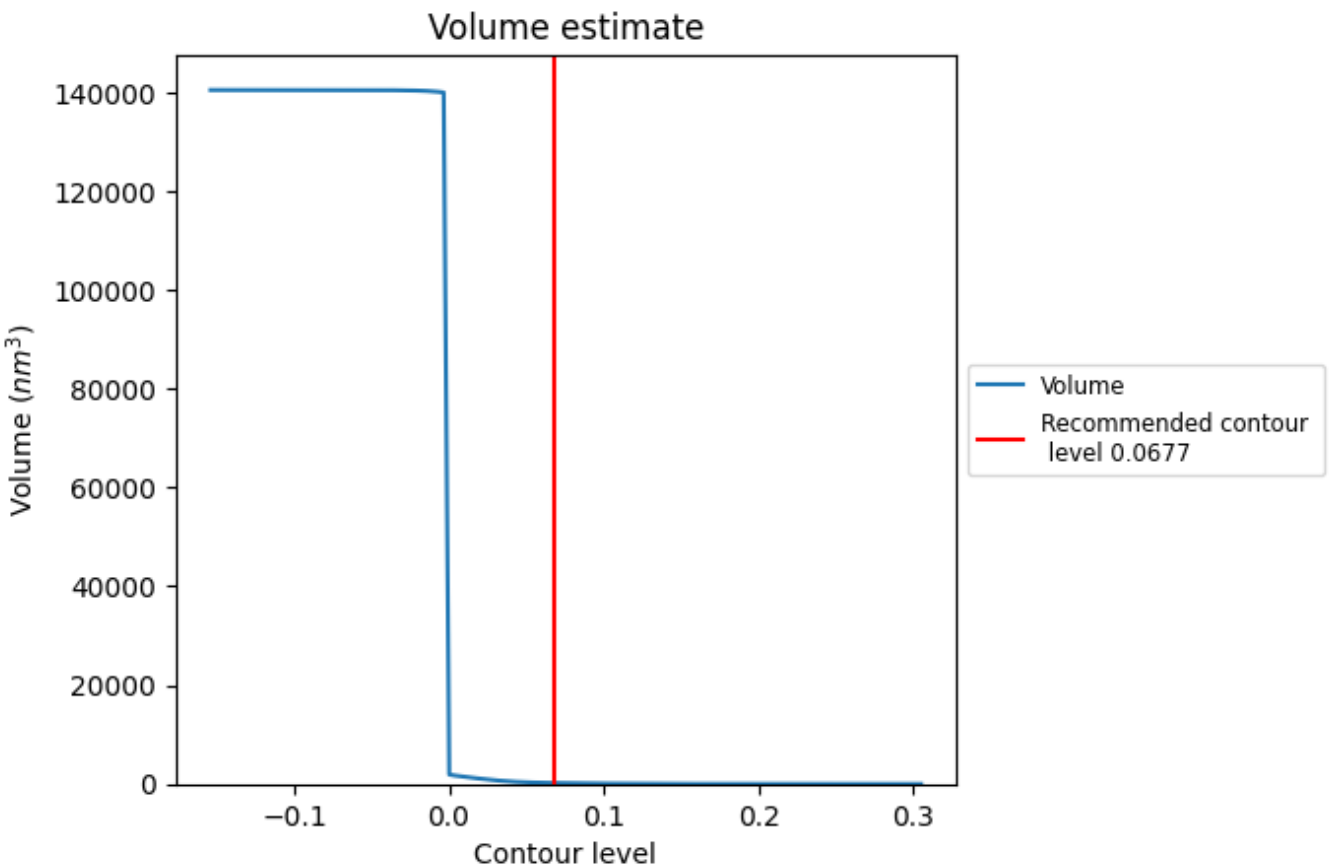
This section contains the results of statistical analysis of the map.

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.

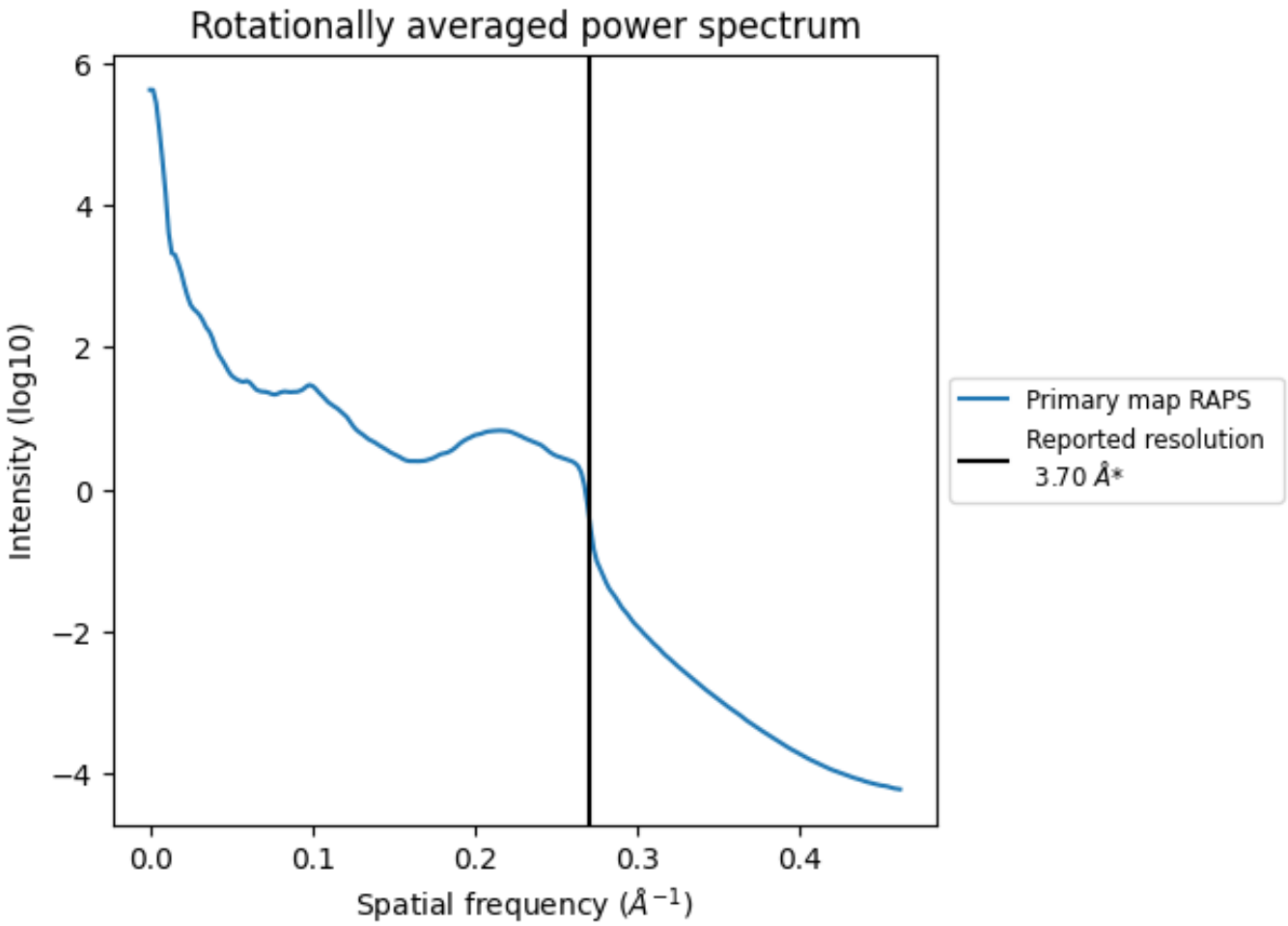
7.2 Volume estimate (i)



The volume at the recommended contour level is 198 nm^3; this corresponds to an approximate mass of 179 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 (i)



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

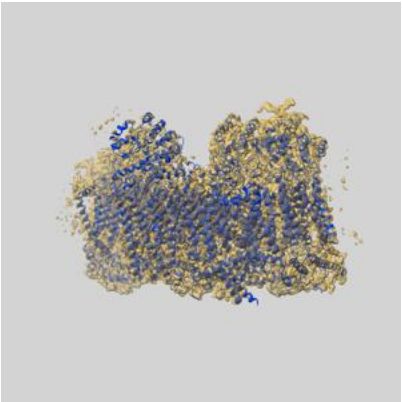
8 Fourier-Shell correlation (i)

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

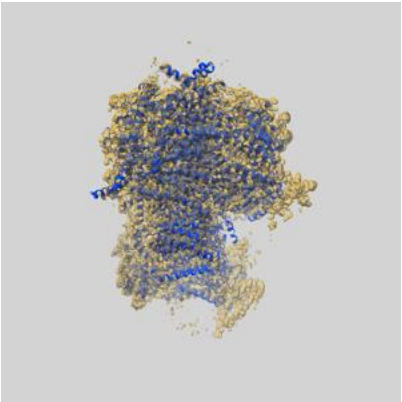
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6772 and PDB model 5XTC. Per-residue inclusion information can be found in section 3 on page 12.

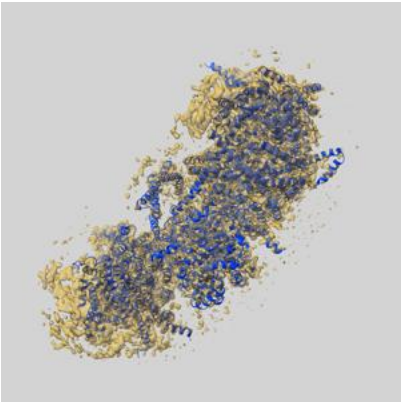
9.1 Map-model overlay (i)



X



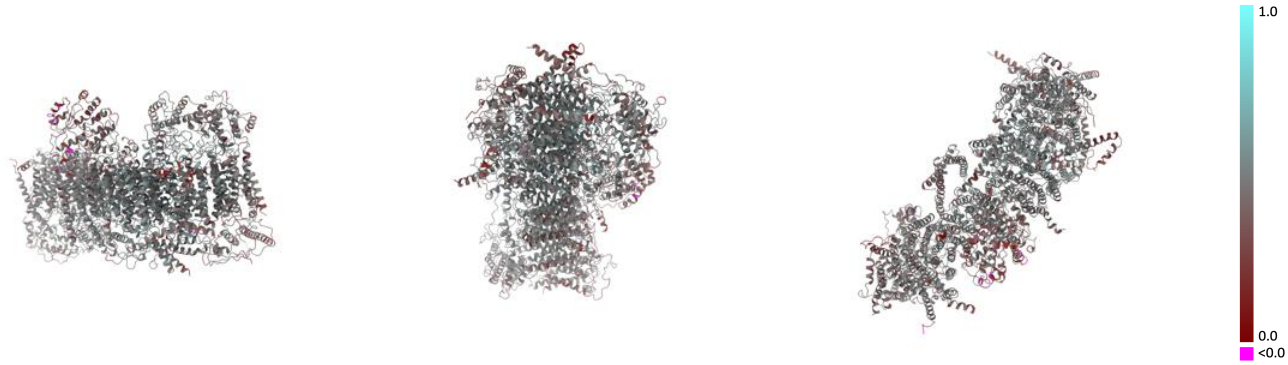
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0677 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.

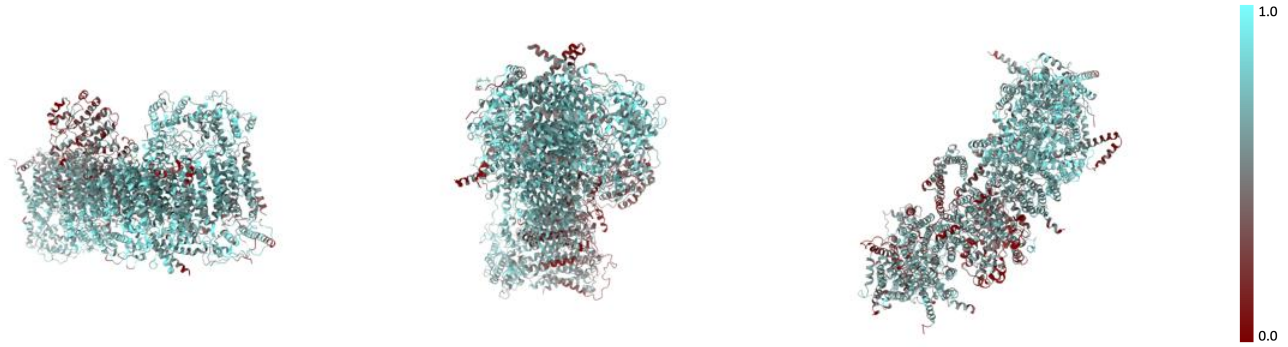
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

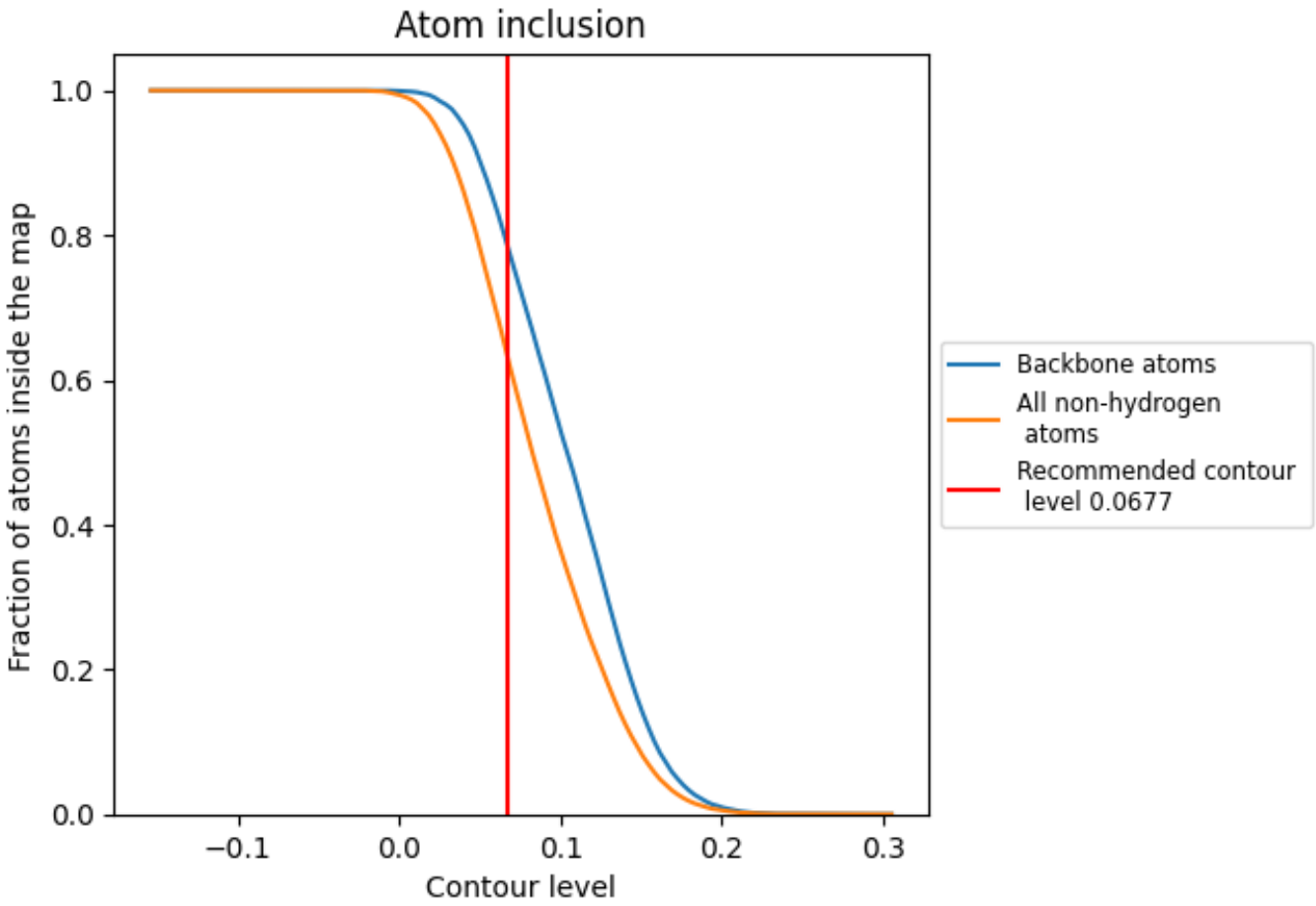
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0677).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0677) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6257	0.4550
Q	0.1604	0.3760
S	0.6491	0.4460
U	0.5820	0.4320
V	0.4691	0.4430
W	0.6984	0.4530
X	0.6868	0.4460
Y	0.7124	0.4390
Z	0.6145	0.4280
a	0.7784	0.4990
b	0.5622	0.4050
c	0.7206	0.4830
d	0.7255	0.4660
e	0.6582	0.4670
f	0.5355	0.3810
g	0.6658	0.4870
h	0.7157	0.4550
i	0.6628	0.4960
j	0.4022	0.3850
k	0.5777	0.4600
l	0.6486	0.4770
m	0.5345	0.4350
n	0.6050	0.4470
o	0.6722	0.4730
p	0.7263	0.4700
r	0.7262	0.5070
s	0.5711	0.4410
u	0.6958	0.4390
v	0.6052	0.3870
w	0.3809	0.3740