Full wwPDB EM Validation Report ⓘ

Sep 10, 2024 – 07:29 PM JST

PDB ID	:	8IC4
EMDB ID	:	EMD-35354
Title	:	Respiratory complex Membrane domain of CI, focus-refined of type I, PERK -/- mouse under cold temperature
Authors	:	Shin, Y.-C.; Liao, M.
Deposited on	:	2023-02-10
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

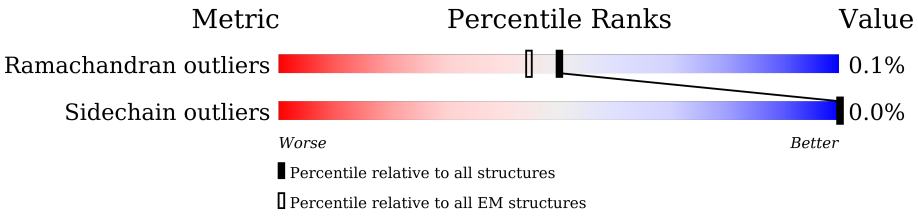
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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.



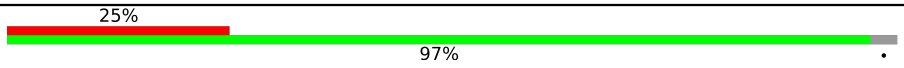
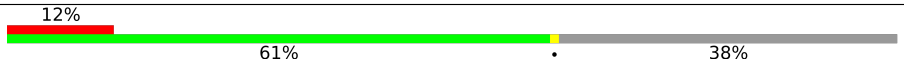
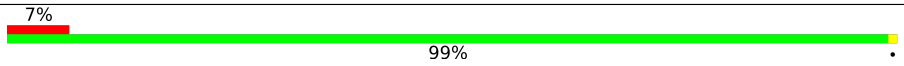
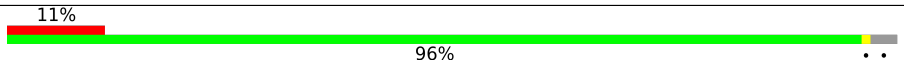
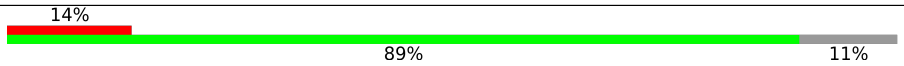
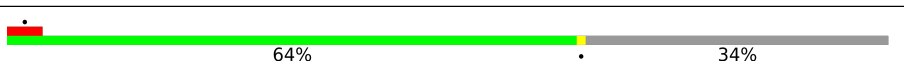
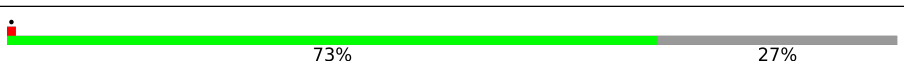
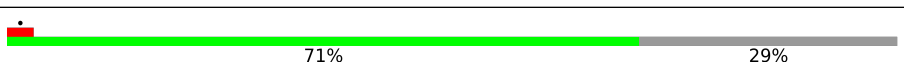
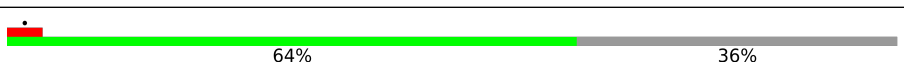
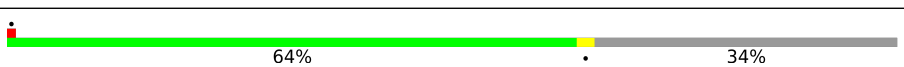
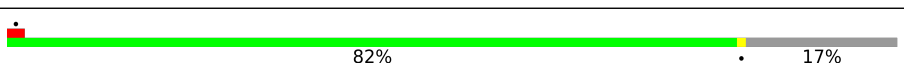
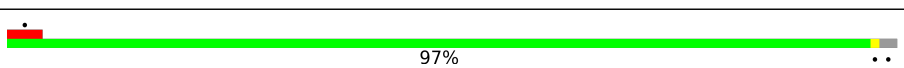
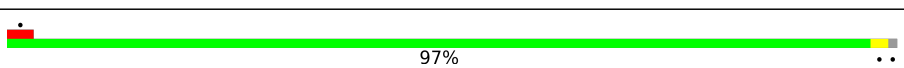
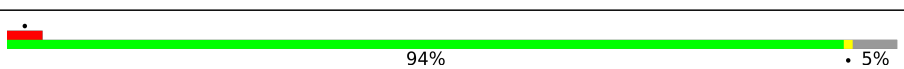
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	D	463	9% 91%
2	J	172	28% 90% 10%
3	K	98	7% 96%
4	L	607	97%
5	M	459	97%
6	N	345	98%
7	O	355	15% 88% 10%
8	U	156	54% 44%
9	X	172	16% 84%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	Y	143	
11	c	76	
12	d	120	
13	e	106	
14	f	57	
15	g	151	
16	h	189	
17	i	128	
18	j	105	
19	k	104	
20	l	186	
21	m	129	
22	n	179	
23	o	137	
24	p	176	

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 31638 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	42	Total	C	N	O	S	0	0
			355	231	59	64	1		

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	155	Total	C	N	O	S	0	0
			1178	797	167	199	15		

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	96	Total	C	N	O	S	0	0
			721	468	110	134	9		

- Molecule 4 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	606	Total	C	N	O	S	0	0
			4798	3181	746	826	45		

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	459	Total	C	N	O	S	0	0
			3630	2407	567	616	40		

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	344	Total	C	N	O	S	0	0
			2694	1790	416	451	37		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	318	Total	C	N	O	S	0	0
			2588	1662	426	490	10		

- Molecule 8 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	87	Total	C	N	O	S	0	0
			700	450	103	142	5		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	X	27	Total	C	N	O	0	0
			221	146	39	36		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Y	139	Total	C	N	O	S	0	0
			1030	657	174	191	8		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	47	Total	C	N	O	S	0	0
			389	255	67	66	1		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	103	Total	C	N	O	S	0	0
			859	544	157	150	8		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	f	51	Total	C	N	O	S	0	0
			439	284	79	74	2		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	99	Total	C	N	O	S	0	0
			835	541	134	156	4		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	138	Total	C	N	O	S	0	0
			1162	762	194	203	3		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	i	91	Total	C	N	O	S	0	0
			765	500	131	131	3		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	67	Total	C	N	O	S	0	0
			574	376	95	102	1		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	k	69	Total	C	N	O	S	0	0
			560	370	97	91	2		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	155	Total	C	N	O	S	0	0
			1304	840	218	235	11		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	m	126	Total	C	N	O	0	0
			1050	676	189	185		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	n	177	Total	C	N	O	S	0	0
			1534	981	275	267	11		

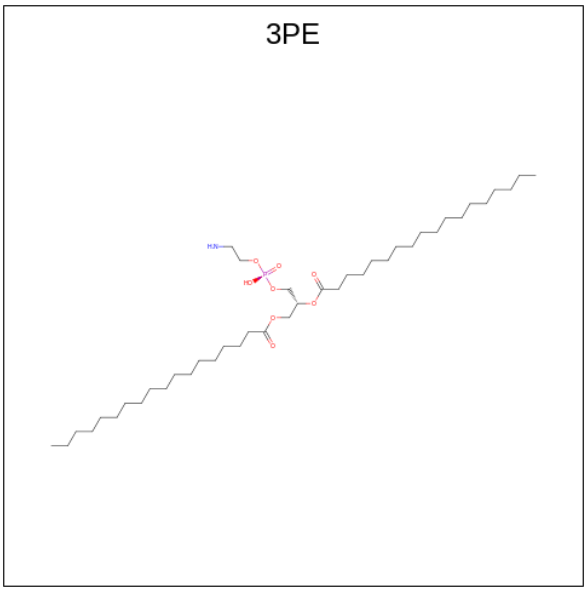
- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	o	121	Total	C	N	O	S	0	0
			1038	654	196	180	8		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

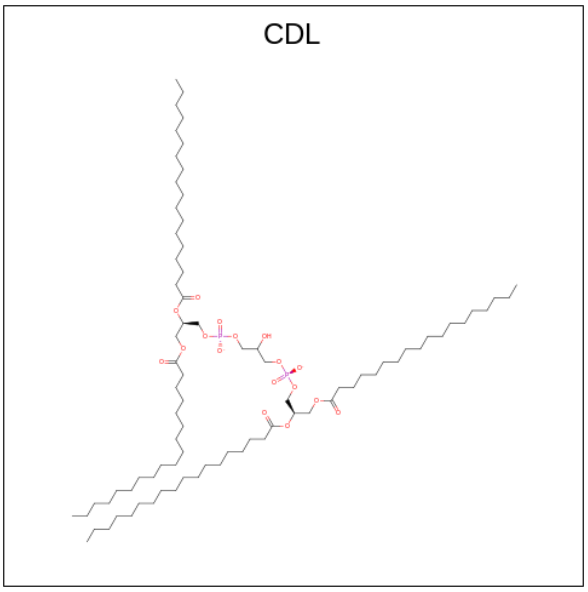
Mol	Chain	Residues	Atoms					AltConf	Trace
24	p	167	Total	C	N	O	S	0	0
			1415	891	254	262	8		

- Molecule 25 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
25	D	1	Total	C	N	O	P	0
			38	28	1	8	1	
25	J	1	Total	C	N	O	P	0
			46	36	1	8	1	
25	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
25	L	1	Total	C	N	O	P	0
			44	34	1	8	1	
25	M	1	Total	C	N	O	P	0
			37	27	1	8	1	
25	M	1	Total	C	N	O	P	0
			49	39	1	8	1	
25	i	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	m	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).

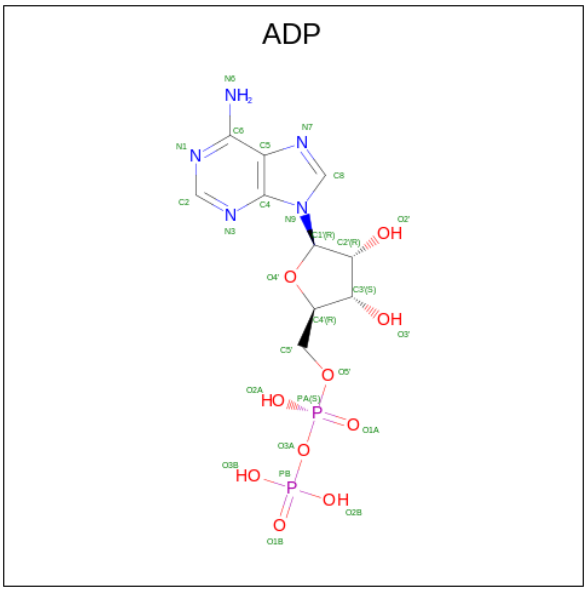


Mol	Chain	Residues	Atoms				AltConf
26	L	1	Total	C	O	P	0
			73	54	17	2	
26	M	1	Total	C	O	P	0
			82	63	17	2	
26	Y	1	Total	C	O	P	0
			71	52	17	2	
26	d	1	Total	C	O	P	0
			65	46	17	2	
26	h	1	Total	C	O	P	0
			68	49	17	2	

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

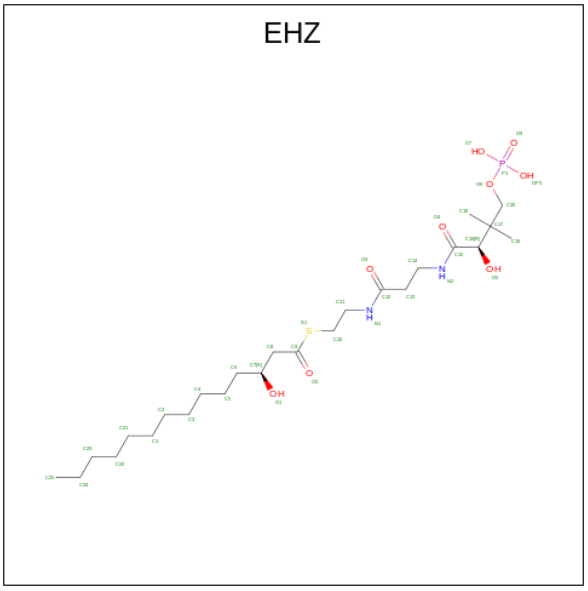
Mol	Chain	Residues	Atoms		AltConf
27	L	1	Total	Zn	0
			1	1	

- Molecule 28 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 29 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$) (labeled as "Ligand of Interest" by depositor).



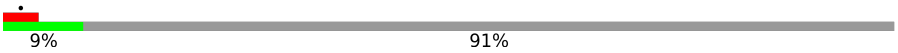
Mol	Chain	Residues	Atoms						AltConf
29	n	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	

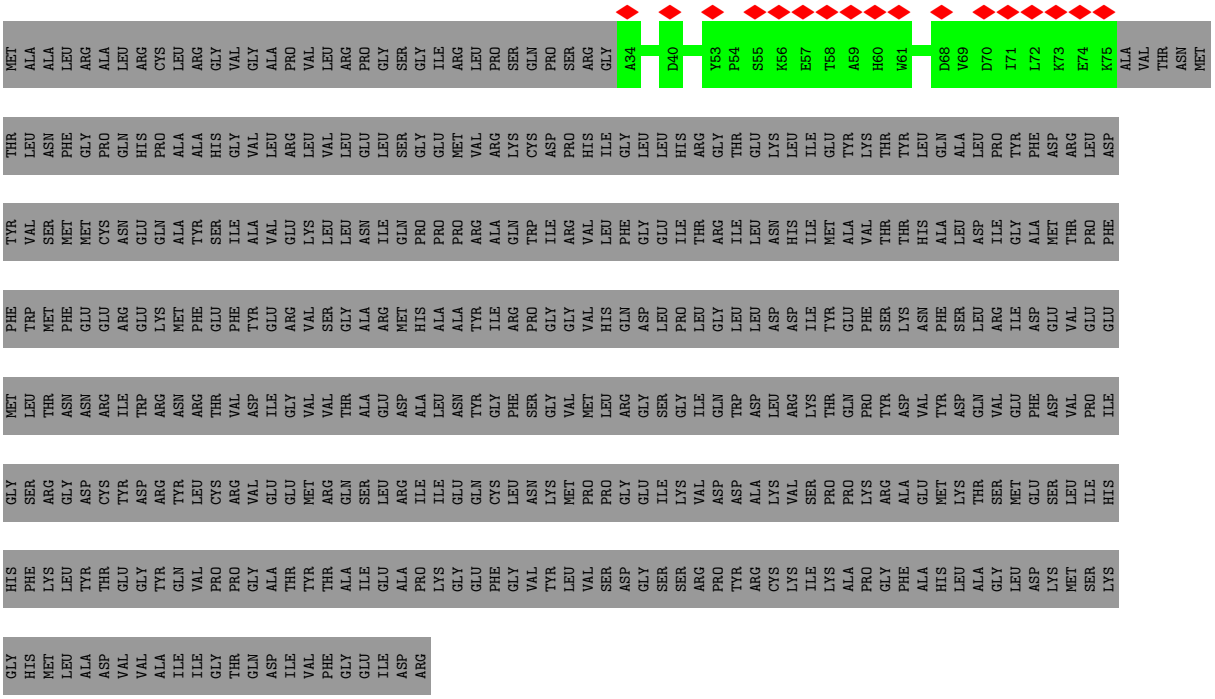
3 Residue-property plots (i)

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

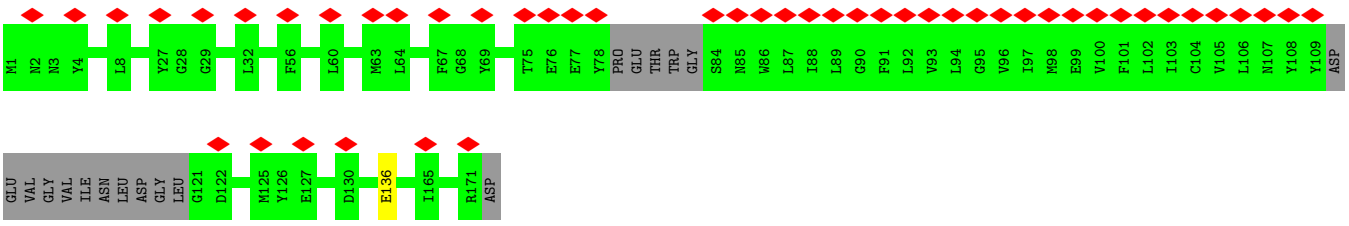
Chain D:





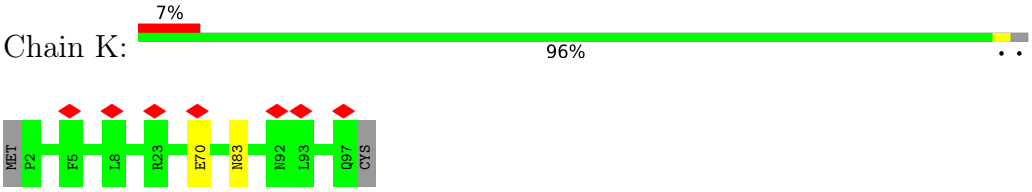
• Molecule 2: NADH-ubiquinone oxidoreductase chain 6

Chain J:



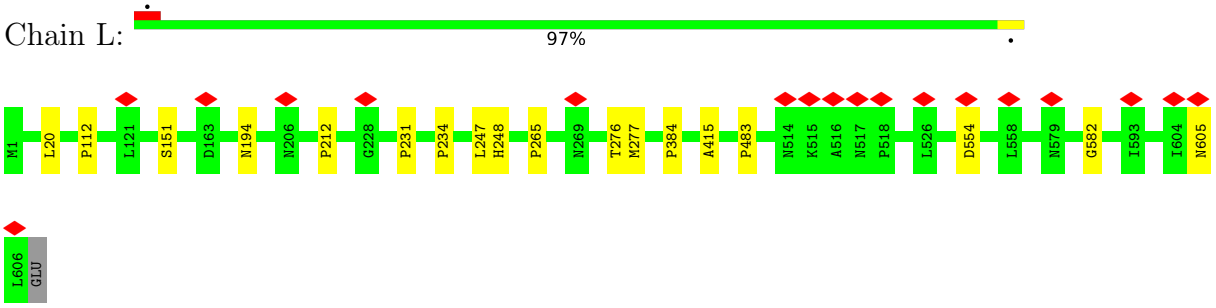
• Molecule 3: NADH-ubiquinone oxidoreductase chain 4L

Chain K:



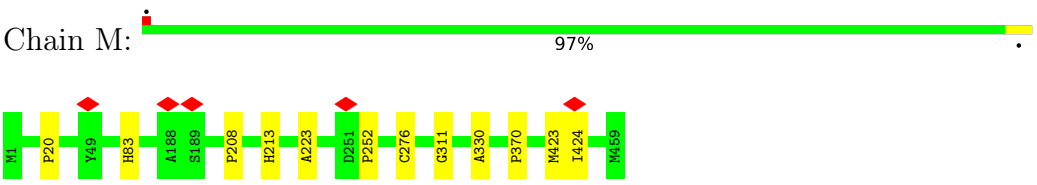
• Molecule 4: NADH-ubiquinone oxidoreductase chain 5

Chain L:



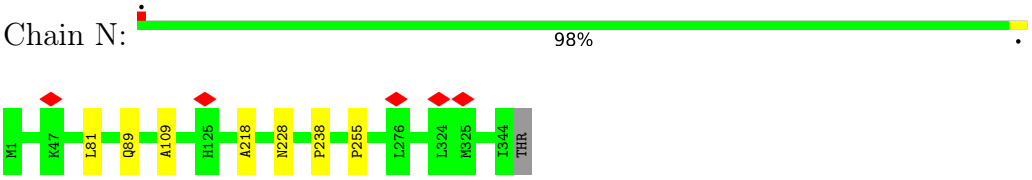
• Molecule 5: NADH-ubiquinone oxidoreductase chain 4

Chain M:



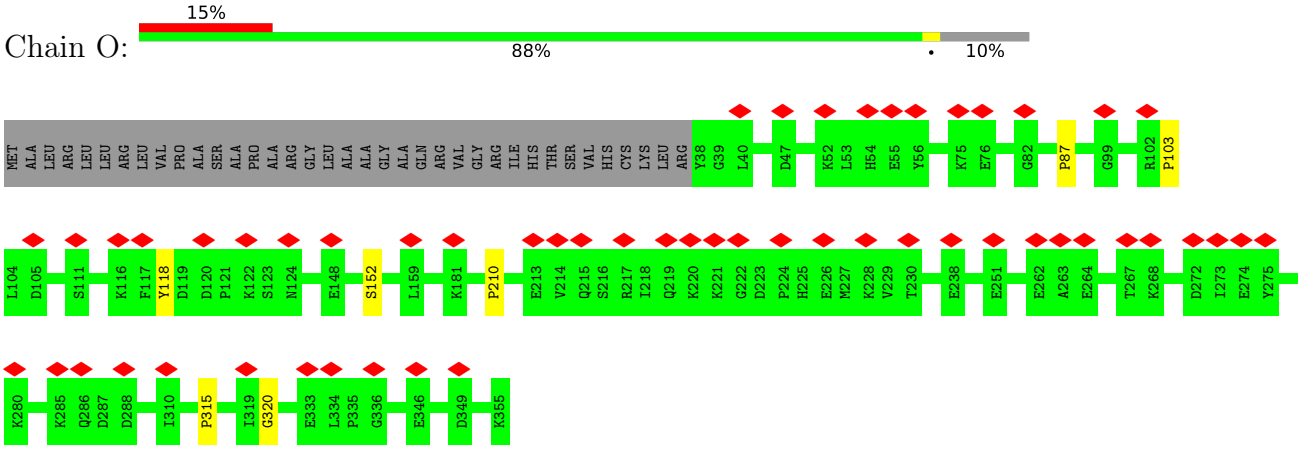
• Molecule 6: NADH-ubiquinone oxidoreductase chain 2

Chain N:



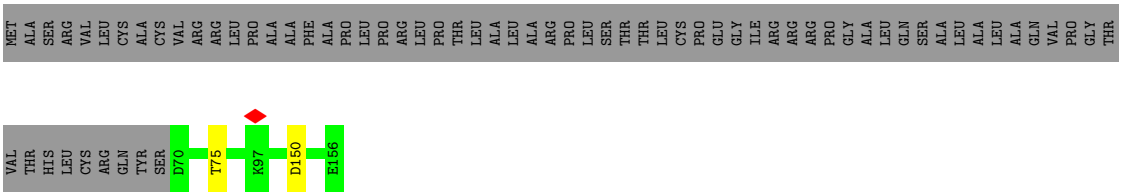
• Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:



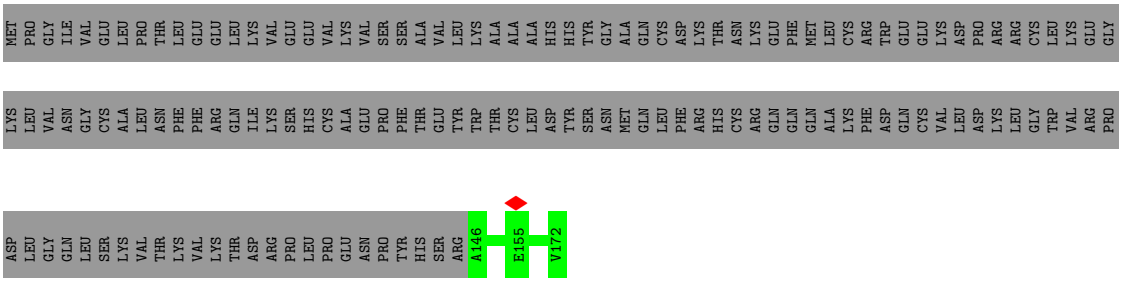
• Molecule 8: Acyl carrier protein, mitochondrial

Chain U:



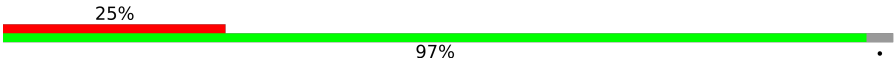
• Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

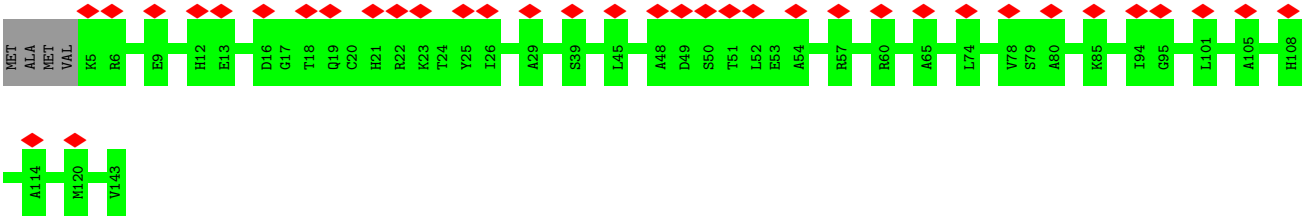
Chain X:



• Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

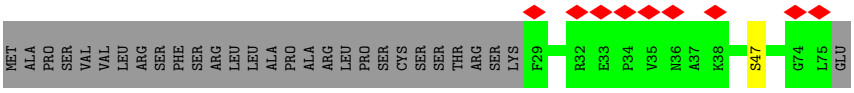
Chain Y:





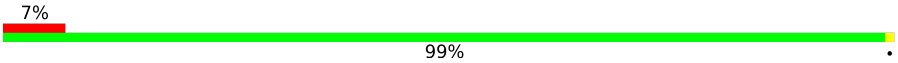
• Molecule 11: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

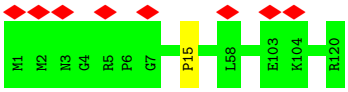
Chain c:



• Molecule 12: NADH dehydrogenase [ubiquinone] 1 subunit C2

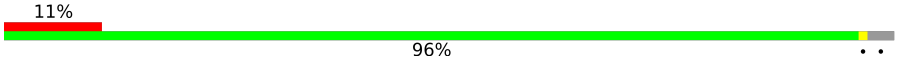
Chain d:

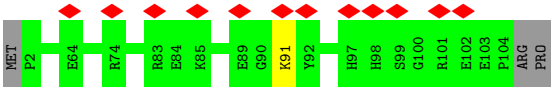




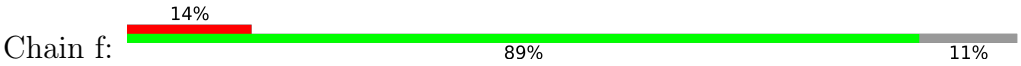
• Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

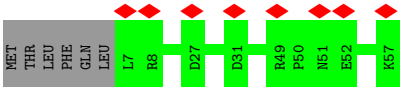
Chain e:



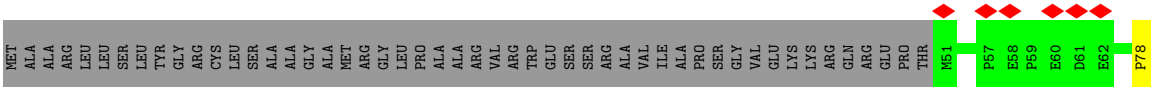


• Molecule 14: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

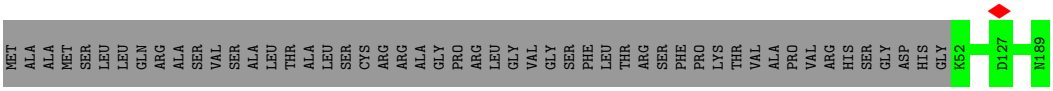




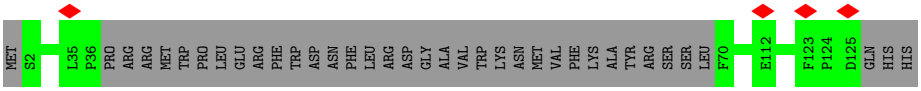
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



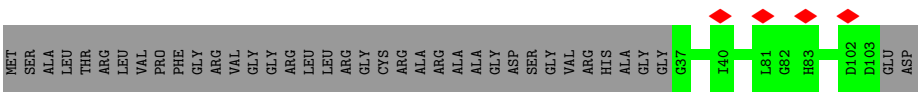
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



• Molecule 17: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

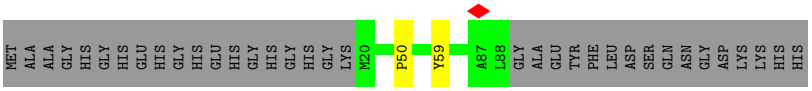


• Molecule 18: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



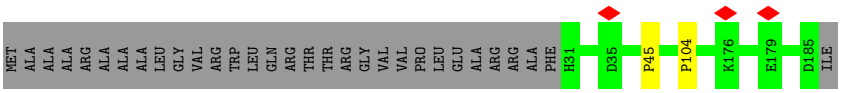
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



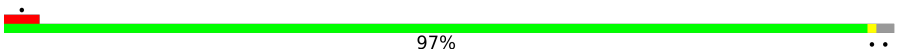
• Molecule 20: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

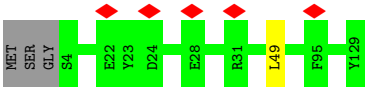
Chain l:



• Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

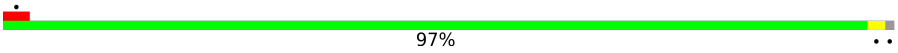
Chain m:

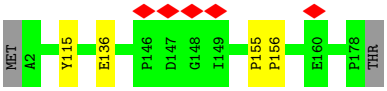




• Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

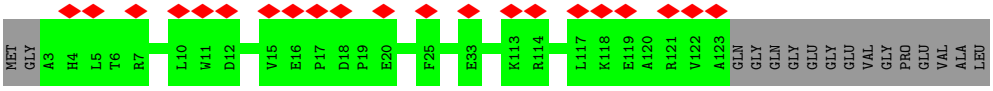
Chain n:





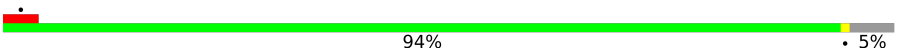
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

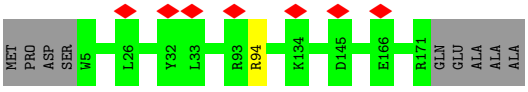
Chain o:



• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45095	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 ($e^-/Å^2$)	50.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.147	Depositor
Minimum map value	-1.164	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: EHZ, 3PE, ZN, CDL, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	D	0.39	0/370	0.59	0/506
2	J	0.39	0/1205	0.59	1/1633 (0.1%)
3	K	0.57	0/732	0.79	2/994 (0.2%)
4	L	0.67	5/4921 (0.1%)	0.90	19/6696 (0.3%)
5	M	0.69	4/3717 (0.1%)	0.90	10/5062 (0.2%)
6	N	0.67	2/2756 (0.1%)	0.85	7/3751 (0.2%)
7	O	0.63	4/2655 (0.2%)	0.74	8/3601 (0.2%)
8	U	0.61	0/712	0.79	2/962 (0.2%)
9	X	0.54	0/230	0.72	0/313
10	Y	0.52	0/1054	0.59	0/1429
11	c	0.46	0/400	0.76	1/544 (0.2%)
12	d	0.61	1/1028 (0.1%)	0.63	2/1387 (0.1%)
13	e	0.51	1/881 (0.1%)	0.64	1/1173 (0.1%)
14	f	0.40	0/451	0.44	0/607
15	g	0.63	1/863 (0.1%)	0.92	3/1175 (0.3%)
16	h	0.52	0/1197	0.74	0/1621
17	i	0.56	0/790	0.74	0/1074
18	j	0.51	0/599	0.69	0/820
19	k	0.82	1/578 (0.2%)	0.94	3/782 (0.4%)
20	l	0.69	2/1359 (0.1%)	0.76	1/1855 (0.1%)
21	m	0.55	0/1079	0.75	0/1463
22	n	0.64	1/1589 (0.1%)	0.74	2/2152 (0.1%)
23	o	0.50	0/1063	0.63	0/1427
24	p	0.53	0/1448	0.71	1/1957 (0.1%)
All	All	0.61	22/31677 (0.1%)	0.79	63/42984 (0.1%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	265	PRO	N-CD	13.75	1.67	1.47
19	k	50	PRO	N-CD	-13.70	1.28	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	255	PRO	N-CD	-13.52	1.28	1.47
7	O	315	PRO	N-CD	-12.22	1.30	1.47
7	O	210	PRO	N-CD	-11.38	1.31	1.47
4	L	234	PRO	N-CD	11.11	1.63	1.47
5	M	370	PRO	N-CD	-10.70	1.32	1.47
15	g	78	PRO	N-CD	-9.68	1.34	1.47
12	d	15	PRO	N-CD	-9.44	1.34	1.47
5	M	20	PRO	N-CD	8.44	1.59	1.47
4	L	212	PRO	N-CD	-8.33	1.36	1.47
22	n	155	PRO	N-CD	8.12	1.59	1.47
13	e	91	LYS	C-N	7.49	1.51	1.34
20	l	104	PRO	N-CD	-7.23	1.37	1.47
5	M	208	PRO	N-CD	7.16	1.57	1.47
6	N	238	PRO	N-CD	-6.99	1.38	1.47
4	L	384	PRO	N-CD	6.24	1.56	1.47
4	L	112	PRO	N-CD	5.95	1.56	1.47
20	l	45	PRO	N-CD	-5.81	1.39	1.47
7	O	87	PRO	N-CD	-5.77	1.39	1.47
5	M	252	PRO	N-CD	-5.61	1.40	1.47
7	O	103	PRO	N-CD	-5.43	1.40	1.47

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	k	50	PRO	CA-N-CD	9.93	125.61	111.70
6	N	255	PRO	CA-N-CD	9.86	125.50	111.70
7	O	315	PRO	CA-N-CD	8.77	123.98	111.70
19	k	50	PRO	N-CA-CB	-8.13	93.54	103.30
7	O	210	PRO	CA-N-CD	7.79	122.60	111.70
4	L	265	PRO	CA-N-CD	-7.43	101.09	111.50
7	O	210	PRO	N-CA-CB	-7.23	94.62	103.30
6	N	255	PRO	N-CA-CB	-7.14	94.73	103.30
15	g	78	PRO	CA-N-CD	7.01	121.52	111.70
4	L	265	PRO	N-CA-CB	7.00	111.70	103.30
11	c	47	SER	N-CA-CB	6.87	120.80	110.50
5	M	213	HIS	CB-CA-C	-6.78	96.84	110.40
7	O	320	GLY	N-CA-C	-6.61	96.57	113.10
12	d	15	PRO	CA-N-CD	6.59	120.92	111.70
19	k	59	TYR	N-CA-CB	-6.52	98.86	110.60
22	n	115	TYR	N-CA-CB	6.42	122.15	110.60
5	M	370	PRO	N-CA-C	6.29	128.46	112.10
5	M	424	ILE	N-CA-C	-6.28	94.03	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	370	PRO	CA-N-CD	6.23	120.42	111.70
6	N	255	PRO	N-CA-C	6.22	128.28	112.10
15	g	137	SER	N-CA-CB	-6.15	101.28	110.50
6	N	81	LEU	N-CA-C	-6.15	94.40	111.00
4	L	231	PRO	N-CA-C	6.05	127.82	112.10
8	U	75	THR	N-CA-CB	6.03	121.77	110.30
7	O	315	PRO	N-CA-CB	-6.01	95.99	102.60
6	N	218	ALA	N-CA-CB	5.97	118.45	110.10
4	L	276	THR	N-CA-CB	5.95	121.61	110.30
4	L	234	PRO	CA-N-CD	-5.95	103.17	111.50
4	L	554	ASP	N-CA-CB	5.92	121.25	110.60
4	L	605	ASN	N-CA-CB	5.89	121.20	110.60
4	L	483	PRO	N-CA-C	-5.88	96.81	112.10
2	J	136	GLU	C-N-CA	-5.86	110.00	122.30
3	K	83	ASN	N-CA-CB	5.74	120.93	110.60
5	M	223	ALA	N-CA-CB	5.72	118.11	110.10
8	U	150	ASP	CB-CA-C	5.72	121.83	110.40
12	d	15	PRO	N-CA-CB	-5.71	96.32	102.60
6	N	89	GLN	N-CA-CB	-5.63	100.46	110.60
7	O	118	TYR	N-CA-CB	-5.57	100.58	110.60
4	L	415	ALA	N-CA-CB	5.56	117.89	110.10
7	O	118	TYR	N-CA-C	5.53	125.94	111.00
5	M	311	GLY	N-CA-C	-5.52	99.31	113.10
22	n	136	GLU	CB-CA-C	5.45	121.30	110.40
4	L	582	GLY	N-CA-C	-5.44	99.49	113.10
7	O	152	SER	N-CA-CB	5.41	118.61	110.50
4	L	194	ASN	N-CA-C	5.35	125.45	111.00
5	M	276	CYS	N-CA-CB	5.33	120.19	110.60
4	L	151	SER	N-CA-CB	5.31	118.46	110.50
24	p	94	ARG	NE-CZ-NH1	5.24	122.92	120.30
4	L	277	MET	CB-CA-C	-5.24	99.92	110.40
5	M	330	ALA	N-CA-CB	5.24	117.44	110.10
3	K	70	GLU	N-CA-CB	5.23	120.02	110.60
4	L	212	PRO	CA-N-CD	5.21	118.99	111.70
5	M	423	MET	N-CA-C	-5.21	96.94	111.00
4	L	248	HIS	CB-CA-C	5.21	120.81	110.40
4	L	212	PRO	N-CA-C	5.19	125.59	112.10
4	L	234	PRO	N-CA-CB	5.16	109.49	103.30
20	l	104	PRO	CA-N-CD	5.16	118.92	111.70
4	L	247	LEU	N-CA-CB	5.14	120.69	110.40
5	M	83	HIS	N-CA-C	-5.10	97.24	111.00
15	g	78	PRO	N-CA-CB	-5.09	97.00	102.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	e	91	LYS	C-N-CA	-5.06	109.04	121.70
4	L	20	LEU	CB-CA-C	-5.02	100.67	110.20
6	N	228	ASN	N-CA-CB	5.01	119.61	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	D	40/463 (9%)	36 (90%)	4 (10%)	0	100	100
2	J	149/172 (87%)	136 (91%)	13 (9%)	0	100	100
3	K	94/98 (96%)	92 (98%)	2 (2%)	0	100	100
4	L	604/607 (100%)	576 (95%)	28 (5%)	0	100	100
5	M	457/459 (100%)	439 (96%)	18 (4%)	0	100	100
6	N	342/345 (99%)	331 (97%)	10 (3%)	1 (0%)	37	69
7	O	316/355 (89%)	302 (96%)	14 (4%)	0	100	100
8	U	85/156 (54%)	83 (98%)	2 (2%)	0	100	100
9	X	25/172 (14%)	23 (92%)	2 (8%)	0	100	100
10	Y	137/143 (96%)	133 (97%)	4 (3%)	0	100	100
11	c	45/76 (59%)	44 (98%)	1 (2%)	0	100	100
12	d	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
13	e	101/106 (95%)	95 (94%)	6 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	f	49/57 (86%)	49 (100%)	0	0	100	100
15	g	97/151 (64%)	91 (94%)	6 (6%)	0	100	100
16	h	136/189 (72%)	130 (96%)	6 (4%)	0	100	100
17	i	87/128 (68%)	80 (92%)	7 (8%)	0	100	100
18	j	65/105 (62%)	61 (94%)	4 (6%)	0	100	100
19	k	67/104 (64%)	64 (96%)	3 (4%)	0	100	100
20	l	153/186 (82%)	141 (92%)	12 (8%)	0	100	100
21	m	124/129 (96%)	117 (94%)	7 (6%)	0	100	100
22	n	175/179 (98%)	165 (94%)	9 (5%)	1 (1%)	22	57
23	o	119/137 (87%)	116 (98%)	3 (2%)	0	100	100
24	p	165/176 (94%)	148 (90%)	17 (10%)	0	100	100
All	All	3750/4813 (78%)	3569 (95%)	179 (5%)	2 (0%)	50	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	N	109	ALA
22	n	156	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	D	37/395 (9%)	37 (100%)	0	100	100
2	J	124/138 (90%)	124 (100%)	0	100	100
3	K	86/88 (98%)	86 (100%)	0	100	100
4	L	549/550 (100%)	549 (100%)	0	100	100
5	M	415/415 (100%)	415 (100%)	0	100	100
6	N	307/308 (100%)	307 (100%)	0	100	100
7	O	282/309 (91%)	282 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	U	80/135 (59%)	80 (100%)	0	100	100
9	X	23/154 (15%)	23 (100%)	0	100	100
10	Y	104/107 (97%)	104 (100%)	0	100	100
11	c	41/67 (61%)	41 (100%)	0	100	100
12	d	107/107 (100%)	107 (100%)	0	100	100
13	e	91/94 (97%)	91 (100%)	0	100	100
14	f	47/53 (89%)	47 (100%)	0	100	100
15	g	90/129 (70%)	90 (100%)	0	100	100
16	h	123/162 (76%)	123 (100%)	0	100	100
17	i	86/120 (72%)	86 (100%)	0	100	100
18	j	62/87 (71%)	62 (100%)	0	100	100
19	k	54/78 (69%)	54 (100%)	0	100	100
20	l	140/161 (87%)	140 (100%)	0	100	100
21	m	112/114 (98%)	111 (99%)	1 (1%)	75	89
22	n	162/164 (99%)	162 (100%)	0	100	100
23	o	111/121 (92%)	111 (100%)	0	100	100
24	p	152/158 (96%)	152 (100%)	0	100	100
All	All	3385/4214 (80%)	3384 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	m	49	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	60	HIS
3	K	7	ASN
4	L	2	ASN
4	L	25	ASN
4	L	58	ASN
4	L	135	ASN
4	L	136	ASN
4	L	139	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L	170	GLN
4	L	199	GLN
4	L	209	ASN
4	L	226	GLN
4	L	264	HIS
4	L	321	GLN
4	L	328	HIS
4	L	332	HIS
4	L	354	GLN
4	L	400	ASN
4	L	446	ASN
4	L	452	ASN
4	L	579	ASN
5	M	26	ASN
5	M	51	ASN
5	M	81	GLN
5	M	92	GLN
5	M	170	HIS
5	M	175	ASN
5	M	184	HIS
5	M	192	ASN
5	M	213	HIS
5	M	279	GLN
5	M	293	HIS
5	M	304	GLN
5	M	349	GLN
5	M	374	ASN
5	M	390	ASN
5	M	415	GLN
5	M	421	ASN
6	N	120	GLN
6	N	134	GLN
6	N	204	ASN
6	N	273	ASN
6	N	310	ASN
7	O	54	HIS
7	O	80	GLN
7	O	132	GLN
7	O	175	ASN
7	O	219	GLN
7	O	292	HIS
7	O	299	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	O	306	ASN
7	O	323	GLN
9	X	151	ASN
10	Y	21	HIS
10	Y	91	ASN
12	d	59	HIS
12	d	88	HIS
16	h	170	GLN
17	i	74	HIS
17	i	83	HIS
18	j	41	GLN
19	k	39	GLN
19	k	66	ASN
20	l	91	GLN
20	l	106	HIS
21	m	75	ASN
21	m	79	ASN
22	n	12	HIS
22	n	14	GLN
22	n	33	HIS
22	n	53	ASN
22	n	76	HIS
23	o	54	GLN
23	o	61	HIS
24	p	67	GLN
24	p	91	GLN
24	p	100	GLN
24	p	124	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 for Mogul analysis.

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	$\#\|Z\| > 2$
28	ADP	O	401	-	24,29,29	0.94	1 (4%)	29,45,45	1.37	4 (13%)
29	EHZ	n	201	-	27,31,37	1.91	7 (25%)	37,41,47	1.56	4 (10%)
25	3PE	m	201	-	40,40,50	1.01	2 (5%)	43,45,55	1.15	3 (6%)
25	3PE	D	501	-	37,37,50	1.06	2 (5%)	40,42,55	1.08	3 (7%)
25	3PE	M	501	-	36,36,50	1.08	2 (5%)	39,41,55	1.05	3 (7%)
25	3PE	L	702	-	48,48,50	0.92	2 (4%)	51,53,55	1.10	3 (5%)
25	3PE	L	705	-	43,43,50	0.99	2 (4%)	46,48,55	1.08	3 (6%)
25	3PE	i	201	-	39,39,50	1.03	2 (5%)	42,44,55	1.14	3 (7%)
26	CDL	Y	201	-	70,70,99	1.08	4 (5%)	76,82,111	1.16	7 (9%)
26	CDL	d	201	-	64,64,99	1.13	4 (6%)	70,76,111	1.20	6 (8%)
25	3PE	J	201	-	45,45,50	0.97	2 (4%)	48,50,55	1.06	3 (6%)
26	CDL	h	201	-	67,67,99	1.10	4 (5%)	73,79,111	1.15	6 (8%)
26	CDL	M	503	-	81,81,99	1.01	4 (4%)	87,93,111	1.14	6 (6%)
25	3PE	L	701	-	39,39,50	1.02	2 (5%)	42,44,55	1.06	2 (4%)
26	CDL	L	703	-	72,72,99	1.06	4 (5%)	78,84,111	1.14	6 (7%)
25	3PE	M	502	-	48,48,50	0.93	2 (4%)	51,53,55	1.14	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	ADP	O	401	-	-	2/12/32/32	0/3/3/3
29	EHZ	n	201	-	-	21/39/39/45	-
25	3PE	m	201	-	-	11/44/44/54	-
25	3PE	D	501	-	-	10/41/41/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	3PE	M	501	-	-	10/40/40/54	-
25	3PE	L	702	-	-	13/52/52/54	-
25	3PE	L	705	-	-	13/47/47/54	-
25	3PE	i	201	-	-	9/43/43/54	-
26	CDL	Y	201	-	-	16/81/81/110	-
26	CDL	d	201	-	-	27/75/75/110	-
25	3PE	J	201	-	-	13/49/49/54	-
26	CDL	h	201	-	-	19/78/78/110	-
26	CDL	M	503	-	-	24/92/92/110	-
25	3PE	L	701	-	-	9/43/43/54	-
26	CDL	L	703	-	-	20/83/83/110	-
25	3PE	M	502	-	-	14/52/52/54	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	n	201	EHZ	C12-N1	5.51	1.45	1.33
29	n	201	EHZ	C15-N2	5.29	1.45	1.33
26	Y	201	CDL	OA8-CA7	4.30	1.45	1.33
25	M	501	3PE	O31-C31	4.30	1.45	1.33
25	J	201	3PE	O31-C31	4.29	1.45	1.33
25	D	501	3PE	O31-C31	4.26	1.45	1.33
26	L	703	CDL	OB8-CB7	4.26	1.45	1.33
25	L	705	3PE	O31-C31	4.26	1.45	1.33
25	M	502	3PE	O31-C31	4.26	1.45	1.33
25	i	201	3PE	O31-C31	4.25	1.45	1.33
26	d	201	CDL	OB8-CB7	4.24	1.45	1.33
26	M	503	CDL	OA8-CA7	4.23	1.45	1.33
25	m	201	3PE	O31-C31	4.20	1.45	1.33
26	M	503	CDL	OB8-CB7	4.19	1.45	1.33
26	d	201	CDL	OA8-CA7	4.19	1.45	1.33
26	h	201	CDL	OB8-CB7	4.17	1.45	1.33
26	h	201	CDL	OA8-CA7	4.16	1.45	1.33
25	L	701	3PE	O21-C21	4.15	1.46	1.34
25	L	702	3PE	O31-C31	4.13	1.45	1.33
26	M	503	CDL	OB6-CB5	4.11	1.45	1.34
25	L	701	3PE	O31-C31	4.10	1.45	1.33
26	h	201	CDL	OB6-CB5	4.10	1.45	1.34
26	L	703	CDL	OA8-CA7	4.10	1.45	1.33
26	Y	201	CDL	OB8-CB7	4.08	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	201	CDL	OB6-CB5	4.08	1.45	1.34
26	h	201	CDL	OA6-CA5	4.08	1.45	1.34
25	M	501	3PE	O21-C21	4.07	1.45	1.34
25	i	201	3PE	O21-C21	4.06	1.45	1.34
26	M	503	CDL	OA6-CA5	4.05	1.45	1.34
26	L	703	CDL	OB6-CB5	4.05	1.45	1.34
26	Y	201	CDL	OB6-CB5	4.04	1.45	1.34
26	Y	201	CDL	OA6-CA5	4.04	1.45	1.34
25	J	201	3PE	O21-C21	4.02	1.45	1.34
25	m	201	3PE	O21-C21	4.01	1.45	1.34
25	D	501	3PE	O21-C21	4.00	1.45	1.34
25	L	705	3PE	O21-C21	4.00	1.45	1.34
25	M	502	3PE	O21-C21	3.99	1.45	1.34
25	L	702	3PE	O21-C21	3.98	1.45	1.34
26	d	201	CDL	OA6-CA5	3.94	1.45	1.34
26	L	703	CDL	OA6-CA5	3.89	1.45	1.34
29	n	201	EHZ	P1-O7	2.67	1.65	1.54
29	n	201	EHZ	C9-S1	2.57	1.82	1.76
29	n	201	EHZ	O4-C15	-2.39	1.18	1.23
28	O	401	ADP	C5-C4	2.34	1.47	1.40
29	n	201	EHZ	O3-C12	-2.27	1.18	1.23
29	n	201	EHZ	P1-OP3	-2.17	1.46	1.54

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	n	201	EHZ	C8-C9-S1	5.56	120.50	113.63
26	M	503	CDL	OA6-CA5-C11	4.63	121.47	111.50
26	L	703	CDL	OB6-CB5-C51	4.23	120.61	111.50
26	h	201	CDL	OB6-CB5-C51	4.21	120.57	111.50
25	M	502	3PE	O21-C21-C22	4.14	120.42	111.50
26	d	201	CDL	OA6-CA5-C11	4.12	120.37	111.50
26	Y	201	CDL	OA6-CA5-C11	4.07	120.28	111.50
25	L	701	3PE	O21-C21-C22	4.02	120.17	111.50
25	J	201	3PE	O21-C21-C22	3.97	120.06	111.50
26	d	201	CDL	OB6-CB5-C51	3.97	120.05	111.50
26	M	503	CDL	OB6-CB5-C51	3.96	120.05	111.50
25	L	702	3PE	O21-C21-C22	3.92	119.96	111.50
26	Y	201	CDL	OB6-CB5-C51	3.90	119.91	111.50
25	m	201	3PE	O21-C21-C22	3.90	119.91	111.50
25	L	705	3PE	O21-C21-C22	3.86	119.83	111.50
25	i	201	3PE	O21-C21-C22	3.82	119.72	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	h	201	CDL	OA6-CA5-C11	3.64	119.35	111.50
26	L	703	CDL	OA6-CA5-C11	3.63	119.32	111.50
25	D	501	3PE	O21-C21-C22	3.60	119.27	111.50
25	M	501	3PE	O21-C21-C22	3.59	119.25	111.50
28	O	401	ADP	N3-C2-N1	-3.25	123.59	128.68
28	O	401	ADP	PA-O3A-PB	-3.25	121.68	132.83
25	M	502	3PE	O31-C31-C32	2.94	121.12	111.91
25	M	502	3PE	C2-O21-C21	-2.93	110.58	117.79
28	O	401	ADP	C3'-C2'-C1'	2.91	105.36	100.98
26	d	201	CDL	CA4-OA6-CA5	-2.87	110.72	117.79
25	L	702	3PE	C2-O21-C21	-2.86	110.75	117.79
25	L	705	3PE	O31-C31-C32	2.82	120.74	111.91
25	i	201	3PE	C2-O21-C21	-2.81	110.88	117.79
26	M	503	CDL	OA8-CA7-C31	2.77	120.61	111.91
26	d	201	CDL	OA8-CA7-C31	2.77	120.60	111.91
25	m	201	3PE	O31-C31-C32	2.75	120.55	111.91
25	J	201	3PE	C2-O21-C21	-2.75	111.03	117.79
25	m	201	3PE	C2-O21-C21	-2.75	111.03	117.79
26	Y	201	CDL	OA8-CA7-C31	2.66	120.27	111.91
25	L	702	3PE	O31-C31-C32	2.65	120.24	111.91
29	n	201	EHZ	OP3-P1-O9	-2.64	100.33	110.68
26	h	201	CDL	OB8-CB7-C71	2.61	120.11	111.91
26	Y	201	CDL	CA4-OA6-CA5	-2.60	111.39	117.79
25	J	201	3PE	O31-C31-C32	2.59	120.03	111.91
26	L	703	CDL	CB4-OB6-CB5	-2.57	111.46	117.79
26	Y	201	CDL	OB8-CB7-C71	2.57	119.96	111.91
29	n	201	EHZ	C10-S1-C9	2.56	109.85	101.87
25	i	201	3PE	O31-C31-C32	2.55	119.91	111.91
26	L	703	CDL	OA8-CA7-C31	2.53	119.86	111.91
26	h	201	CDL	OA8-CA7-C31	2.51	119.79	111.91
25	L	705	3PE	C2-O21-C21	-2.49	111.66	117.79
26	L	703	CDL	OB8-CB7-C71	2.49	119.72	111.91
28	O	401	ADP	C4-C5-N7	-2.47	106.82	109.40
26	d	201	CDL	OB8-CB7-C71	2.47	119.66	111.91
25	M	501	3PE	O31-C31-C32	2.41	119.47	111.91
26	L	703	CDL	CA4-OA6-CA5	-2.41	111.86	117.79
25	D	501	3PE	O31-C31-C32	2.39	119.42	111.91
29	n	201	EHZ	C5-C6-C7	-2.32	108.17	114.85
26	M	503	CDL	OB8-CB7-C71	2.30	119.12	111.91
25	M	501	3PE	C2-O21-C21	-2.27	112.21	117.79
26	Y	201	CDL	CB4-OB6-CB5	-2.26	112.23	117.79
26	d	201	CDL	CB4-OB6-CB5	-2.21	112.34	117.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	L	701	3PE	O31-C31-C32	2.19	118.78	111.91
26	h	201	CDL	CA4-OA6-CA5	-2.18	112.41	117.79
26	M	503	CDL	CA4-OA6-CA5	-2.10	112.63	117.79
26	M	503	CDL	OA6-CA5-OA7	-2.05	118.75	123.70
26	Y	201	CDL	OB8-CB7-OB9	-2.04	118.44	123.59
25	D	501	3PE	C2-O21-C21	-2.03	112.80	117.79
26	h	201	CDL	OA8-CA7-OA9	-2.01	118.53	123.59

There are no chirality outliers.

All (231) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	D	501	3PE	C1-O11-P-O14
25	J	201	3PE	C1-O11-P-O12
25	J	201	3PE	C1-O11-P-O13
25	J	201	3PE	C1-O11-P-O14
25	L	701	3PE	C1-O11-P-O12
25	L	701	3PE	C22-C21-O21-C2
25	L	702	3PE	C1-O11-P-O12
25	L	702	3PE	C1-O11-P-O14
25	L	702	3PE	C11-O13-P-O11
25	L	702	3PE	C11-O13-P-O12
25	L	702	3PE	C11-O13-P-O14
25	L	702	3PE	O22-C21-O21-C2
25	L	702	3PE	C22-C21-O21-C2
25	L	705	3PE	C1-O11-P-O12
25	L	705	3PE	C11-O13-P-O12
25	L	705	3PE	C11-O13-P-O14
25	L	705	3PE	O22-C21-O21-C2
25	L	705	3PE	C22-C21-O21-C2
25	M	501	3PE	C11-O13-P-O12
25	M	502	3PE	C1-O11-P-O14
25	M	502	3PE	C32-C31-O31-C3
25	M	502	3PE	C22-C21-O21-C2
25	i	201	3PE	C1-O11-P-O12
25	i	201	3PE	C1-O11-P-O13
25	i	201	3PE	C1-O11-P-O14
25	i	201	3PE	C2-C1-O11-P
25	i	201	3PE	C22-C21-O21-C2
25	m	201	3PE	C1-O11-P-O14
25	m	201	3PE	C11-O13-P-O12
26	L	703	CDL	CA3-OA5-PA1-OA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	L	703	CDL	CB2-OB2-PB2-OB5
26	L	703	CDL	CB3-OB5-PB2-OB3
26	L	703	CDL	C51-CB5-OB6-CB4
26	M	503	CDL	CA2-OA2-PA1-OA3
26	M	503	CDL	CA2-OA2-PA1-OA4
26	M	503	CDL	CA2-OA2-PA1-OA5
26	M	503	CDL	C11-CA5-OA6-CA4
26	M	503	CDL	CB2-OB2-PB2-OB3
26	M	503	CDL	CB2-OB2-PB2-OB4
26	M	503	CDL	CB2-OB2-PB2-OB5
26	M	503	CDL	CB3-OB5-PB2-OB3
26	M	503	CDL	CB3-OB5-PB2-OB4
26	M	503	CDL	C51-CB5-OB6-CB4
26	Y	201	CDL	CA2-OA2-PA1-OA3
26	Y	201	CDL	CA2-OA2-PA1-OA4
26	Y	201	CDL	CA2-OA2-PA1-OA5
26	Y	201	CDL	CB3-OB5-PB2-OB2
26	d	201	CDL	CA2-OA2-PA1-OA3
26	d	201	CDL	CA2-OA2-PA1-OA4
26	d	201	CDL	CA2-OA2-PA1-OA5
26	d	201	CDL	CB2-OB2-PB2-OB4
26	h	201	CDL	CA2-OA2-PA1-OA3
26	h	201	CDL	CA2-OA2-PA1-OA4
26	h	201	CDL	CA2-OA2-PA1-OA5
26	h	201	CDL	CA3-OA5-PA1-OA4
26	h	201	CDL	CB3-OB5-PB2-OB3
26	h	201	CDL	C51-CB5-OB6-CB4
29	n	201	EHZ	O1-C7-C8-C9
29	n	201	EHZ	C7-C8-C9-S1
29	n	201	EHZ	C10-C11-N1-C12
29	n	201	EHZ	C15-C16-C17-C18
29	n	201	EHZ	C15-C16-C17-C19
29	n	201	EHZ	C15-C16-C17-C20
29	n	201	EHZ	O5-C16-C17-C18
29	n	201	EHZ	O5-C16-C17-C19
29	n	201	EHZ	O5-C16-C17-C20
29	n	201	EHZ	O2-C9-S1-C10
29	n	201	EHZ	C8-C9-S1-C10
29	n	201	EHZ	C20-O6-P1-O7
29	n	201	EHZ	C20-O6-P1-O9
29	n	201	EHZ	C20-O6-P1-OP3
25	M	502	3PE	O32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	m	201	3PE	O32-C31-O31-C3
25	m	201	3PE	C32-C31-O31-C3
25	D	501	3PE	O22-C21-O21-C2
25	L	701	3PE	O22-C21-O21-C2
25	M	502	3PE	O22-C21-O21-C2
26	L	703	CDL	OB7-CB5-OB6-CB4
26	M	503	CDL	OA7-CA5-OA6-CA4
26	h	201	CDL	OB7-CB5-OB6-CB4
25	M	501	3PE	C2-C3-O31-C31
25	D	501	3PE	C22-C21-O21-C2
25	i	201	3PE	C32-C31-O31-C3
25	i	201	3PE	O22-C21-O21-C2
26	M	503	CDL	OB7-CB5-OB6-CB4
26	L	703	CDL	C11-CA5-OA6-CA4
25	i	201	3PE	O32-C31-O31-C3
26	Y	201	CDL	C31-CA7-OA8-CA6
26	Y	201	CDL	C71-CB7-OB8-CB6
26	h	201	CDL	C71-CB7-OB8-CB6
26	h	201	CDL	OB9-CB7-OB8-CB6
25	m	201	3PE	C22-C21-O21-C2
26	Y	201	CDL	OB9-CB7-OB8-CB6
26	h	201	CDL	CA4-CA3-OA5-PA1
26	d	201	CDL	C54-C55-C56-C57
26	Y	201	CDL	OA9-CA7-OA8-CA6
26	d	201	CDL	O1-C1-CB2-OB2
26	L	703	CDL	OA7-CA5-OA6-CA4
26	d	201	CDL	C11-CA5-OA6-CA4
25	L	701	3PE	C1-O11-P-O13
25	L	702	3PE	C1-O11-P-O13
25	L	705	3PE	C1-O11-P-O13
25	L	705	3PE	C11-O13-P-O11
25	M	501	3PE	C1-O11-P-O13
25	M	501	3PE	C11-O13-P-O11
25	M	502	3PE	C1-O11-P-O13
25	M	502	3PE	C11-O13-P-O11
26	L	703	CDL	CA3-OA5-PA1-OA2
26	L	703	CDL	CB3-OB5-PB2-OB2
26	M	503	CDL	CA3-OA5-PA1-OA2
26	M	503	CDL	CB3-OB5-PB2-OB2
26	d	201	CDL	CA3-OA5-PA1-OA2
26	d	201	CDL	CB2-OB2-PB2-OB5
26	d	201	CDL	CB3-OB5-PB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	h	201	CDL	CB3-OB5-PB2-OB2
26	L	703	CDL	C71-CB7-OB8-CB6
26	d	201	CDL	CA2-C1-CB2-OB2
25	m	201	3PE	O22-C21-O21-C2
26	L	703	CDL	C11-C12-C13-C14
25	M	501	3PE	C32-C33-C34-C35
26	d	201	CDL	OA7-CA5-OA6-CA4
26	L	703	CDL	OB9-CB7-OB8-CB6
26	M	503	CDL	C62-C63-C64-C65
25	M	501	3PE	C23-C24-C25-C26
26	d	201	CDL	C71-CB7-OB8-CB6
25	J	201	3PE	C32-C31-O31-C3
25	M	501	3PE	C32-C31-O31-C3
26	h	201	CDL	C14-C15-C16-C17
26	M	503	CDL	C71-CB7-OB8-CB6
25	J	201	3PE	O32-C31-O31-C3
26	d	201	CDL	OB9-CB7-OB8-CB6
25	J	201	3PE	O22-C21-O21-C2
26	L	703	CDL	C31-CA7-OA8-CA6
26	d	201	CDL	C31-CA7-OA8-CA6
25	M	501	3PE	O32-C31-O31-C3
25	J	201	3PE	C22-C21-O21-C2
25	M	502	3PE	C2-C3-O31-C31
25	L	702	3PE	C24-C25-C26-C27
26	M	503	CDL	OB9-CB7-OB8-CB6
26	d	201	CDL	OA9-CA7-OA8-CA6
25	J	201	3PE	C2A-C2B-C2C-C2D
25	i	201	3PE	C27-C28-C29-C2A
25	L	705	3PE	C3C-C3D-C3E-C3F
26	L	703	CDL	OA9-CA7-OA8-CA6
29	n	201	EHZ	C5-C6-C7-O1
26	L	703	CDL	C74-C75-C76-C77
25	L	702	3PE	C28-C29-C2A-C2B
29	n	201	EHZ	C3-C4-C5-C6
26	h	201	CDL	C18-C19-C20-C21
25	D	501	3PE	C24-C25-C26-C27
26	Y	201	CDL	CB2-OB2-PB2-OB5
29	n	201	EHZ	C5-C6-C7-C8
25	L	701	3PE	C3-C2-O21-C21
26	h	201	CDL	CB3-CB4-OB6-CB5
26	h	201	CDL	CB4-CB3-OB5-PB2
25	L	705	3PE	C27-C28-C29-C2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	D	501	3PE	C1-O11-P-O13
25	m	201	3PE	C1-O11-P-O13
25	m	201	3PE	C11-O13-P-O11
26	h	201	CDL	CA3-OA5-PA1-OA2
26	Y	201	CDL	C1-CA2-OA2-PA1
25	L	701	3PE	C1-O11-P-O14
25	L	705	3PE	C1-O11-P-O14
25	M	501	3PE	C1-O11-P-O12
25	M	501	3PE	C1-O11-P-O14
25	M	502	3PE	C1-O11-P-O12
25	M	502	3PE	C11-O13-P-O12
25	M	502	3PE	C11-O13-P-O14
25	m	201	3PE	C11-O13-P-O14
26	L	703	CDL	CA3-OA5-PA1-OA3
26	L	703	CDL	CB2-OB2-PB2-OB4
26	L	703	CDL	CB3-OB5-PB2-OB4
26	M	503	CDL	CA3-OA5-PA1-OA3
26	Y	201	CDL	CB3-OB5-PB2-OB4
26	d	201	CDL	CA3-OA5-PA1-OA3
26	d	201	CDL	CB3-OB5-PB2-OB3
26	h	201	CDL	CB3-OB5-PB2-OB4
29	n	201	EHZ	C6-C7-C8-C9
25	L	705	3PE	C32-C31-O31-C3
26	M	503	CDL	C31-CA7-OA8-CA6
26	d	201	CDL	C51-CB5-OB6-CB4
25	L	701	3PE	C36-C37-C38-C39
25	L	705	3PE	O32-C31-O31-C3
26	M	503	CDL	OA9-CA7-OA8-CA6
25	L	701	3PE	C2-C1-O11-P
25	L	702	3PE	C33-C34-C35-C36
26	L	703	CDL	C32-C33-C34-C35
25	M	502	3PE	C2D-C2E-C2F-C2G
29	n	201	EHZ	O4-C15-C16-O5
26	d	201	CDL	OB7-CB5-OB6-CB4
25	L	705	3PE	C36-C37-C38-C39
26	M	503	CDL	CB4-CB3-OB5-PB2
26	Y	201	CDL	C55-C56-C57-C58
29	n	201	EHZ	C2-C3-C4-C5
25	J	201	3PE	C36-C37-C38-C39
25	D	501	3PE	C32-C31-O31-C3
26	M	503	CDL	C58-C59-C60-C61
25	D	501	3PE	O32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	L	702	3PE	C2-C1-O11-P
28	O	401	ADP	C4'-C5'-O5'-PA
26	Y	201	CDL	C56-C57-C58-C59
26	L	703	CDL	CA3-CA4-CA6-OA8
26	M	503	CDL	CB3-CB4-CB6-OB8
29	n	201	EHZ	C7-C8-C9-O2
25	m	201	3PE	C3-C2-O21-C21
28	O	401	ADP	O4'-C4'-C5'-O5'
26	M	503	CDL	C36-C37-C38-C39
25	M	502	3PE	C34-C35-C36-C37
25	J	201	3PE	O11-C1-C2-O21
26	d	201	CDL	CB4-CB3-OB5-PB2
25	J	201	3PE	O21-C2-C3-O31
26	Y	201	CDL	OA7-CA5-OA6-CA4
25	M	502	3PE	C32-C33-C34-C35
25	J	201	3PE	C38-C39-C3A-C3B
25	D	501	3PE	C32-C33-C34-C35
25	J	201	3PE	O11-C1-C2-C3
26	d	201	CDL	C32-C31-CA7-OA8
26	Y	201	CDL	C11-CA5-OA6-CA4
25	L	702	3PE	C26-C27-C28-C29
25	D	501	3PE	C34-C35-C36-C37
26	d	201	CDL	C57-C58-C59-C60
26	d	201	CDL	C1-CB2-OB2-PB2
25	m	201	3PE	C1-O11-P-O12
26	Y	201	CDL	CB2-OB2-PB2-OB4
26	h	201	CDL	CA3-OA5-PA1-OA3
26	d	201	CDL	C34-C35-C36-C37
25	L	701	3PE	C22-C23-C24-C25
25	D	501	3PE	C12-C11-O13-P
26	d	201	CDL	C56-C57-C58-C59
26	d	201	CDL	C32-C31-CA7-OA9
26	h	201	CDL	C11-C12-C13-C14

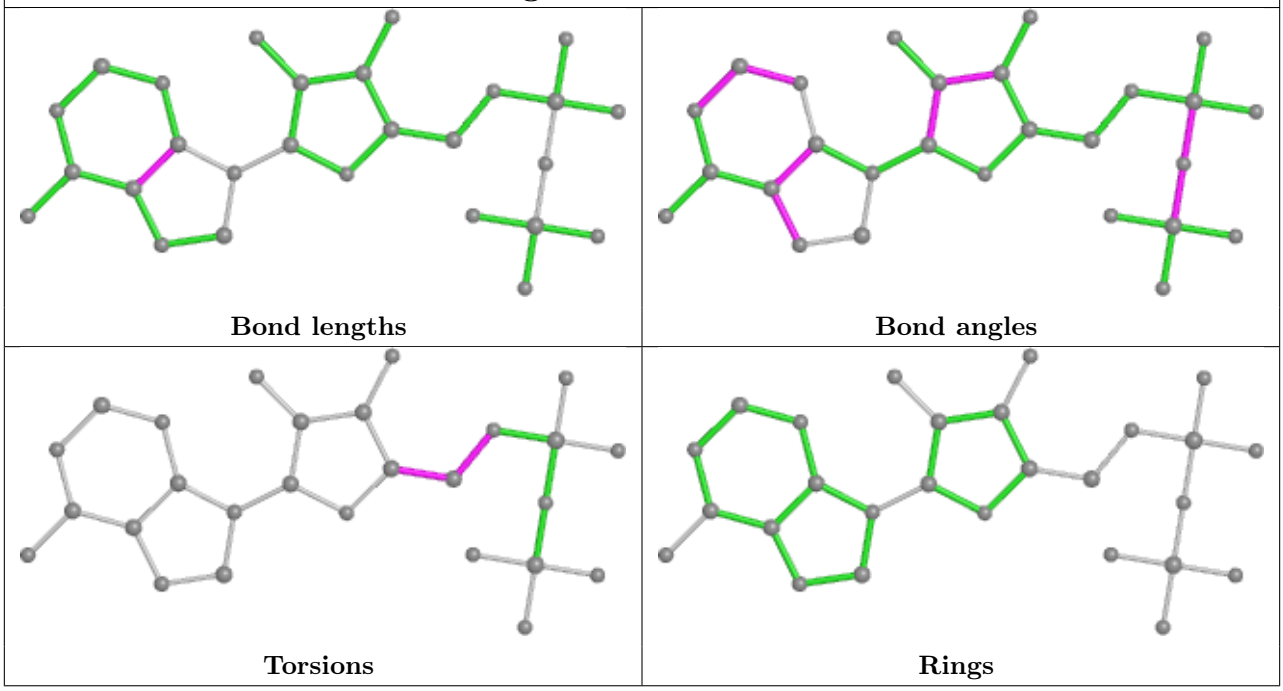
There are no ring outliers.

No monomer is involved in short contacts.

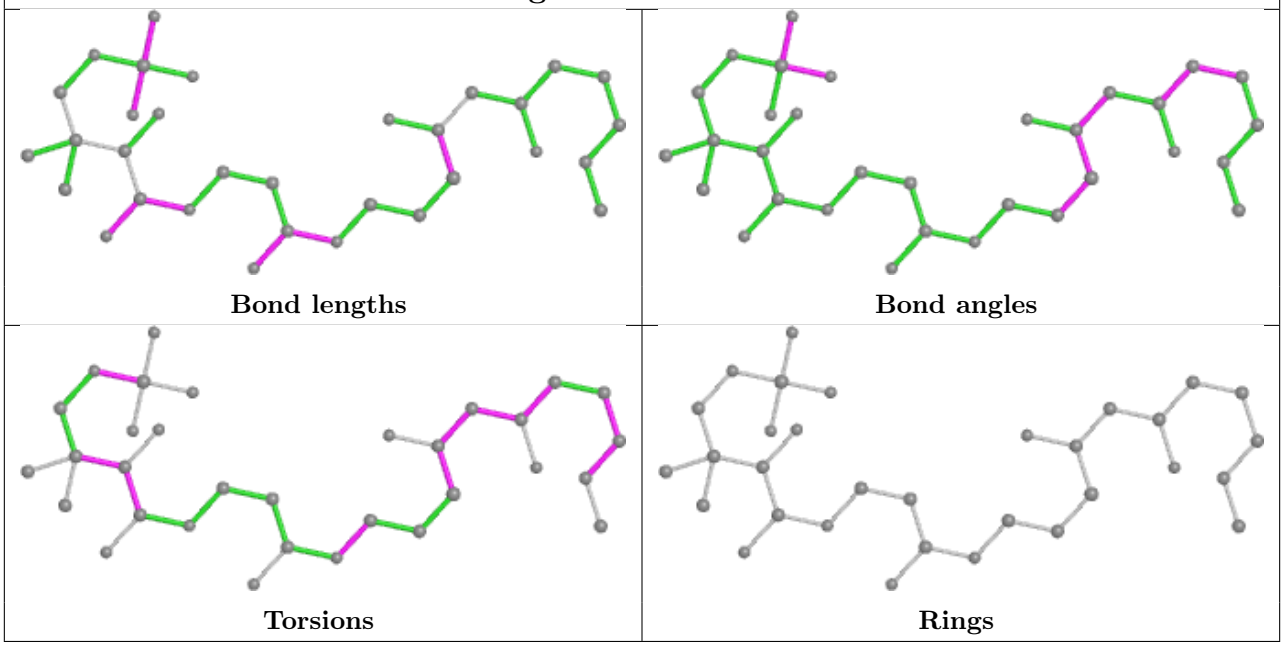
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

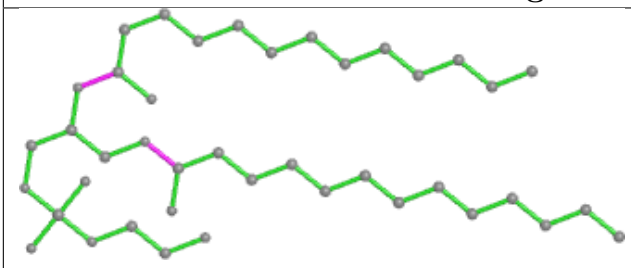
Ligand ADP O 401



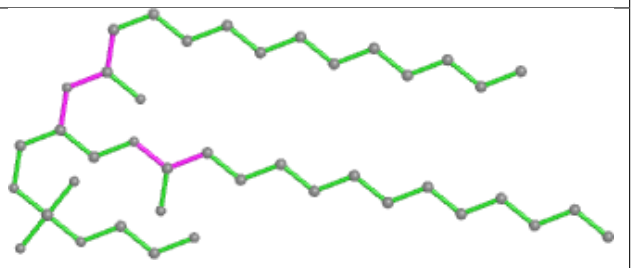
Ligand EHZ n 201



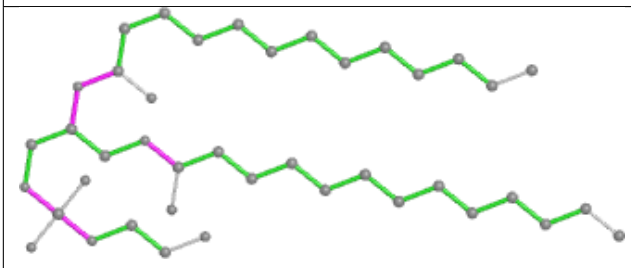
Ligand 3PE m 201



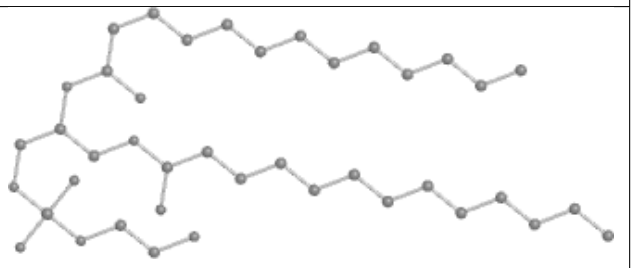
Bond lengths



Bond angles

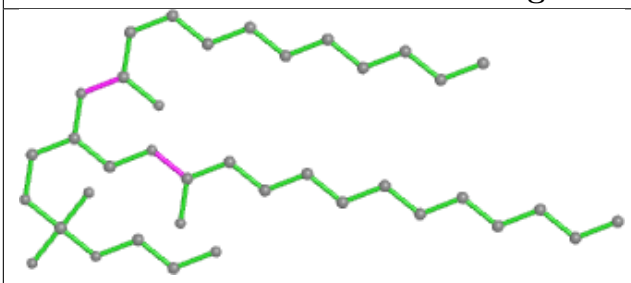


Torsions

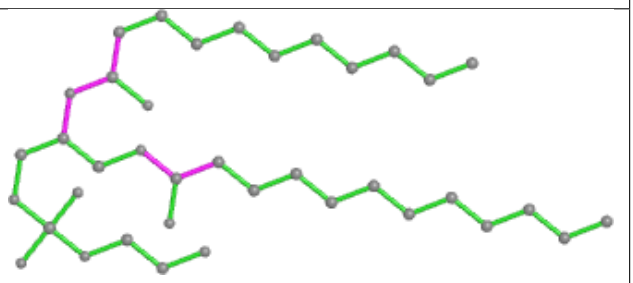


Rings

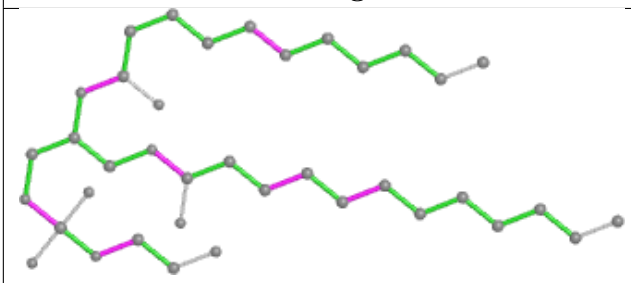
Ligand 3PE D 501



Bond lengths



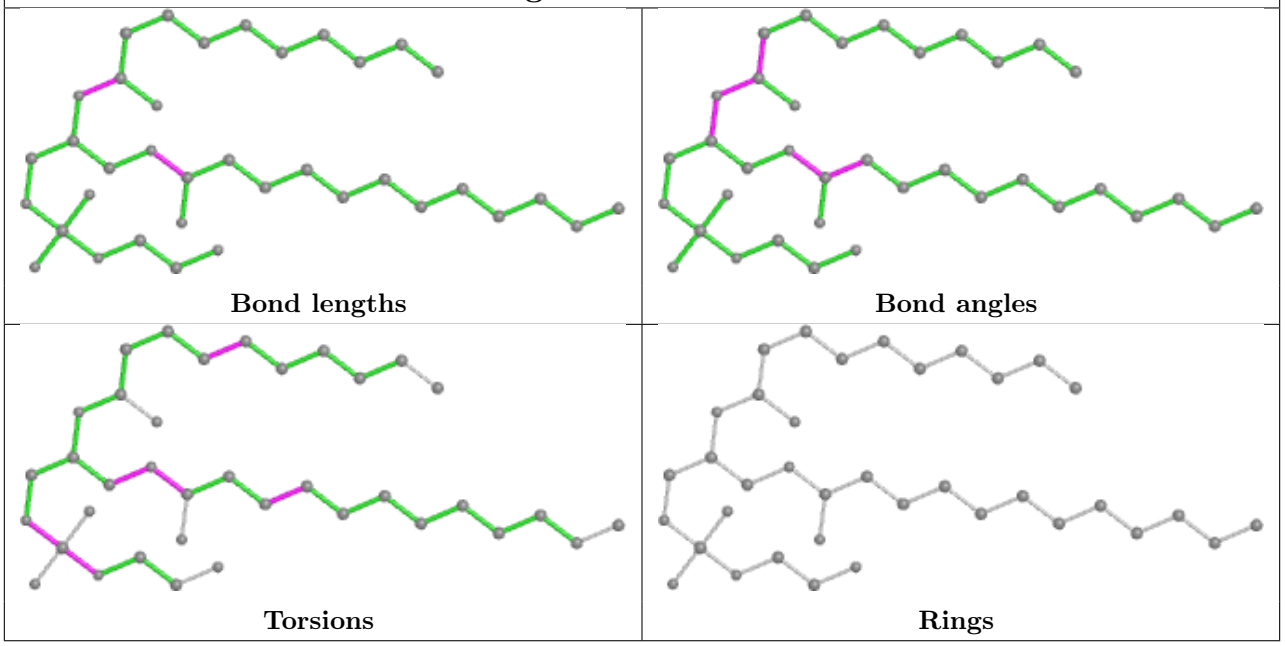
Bond angles



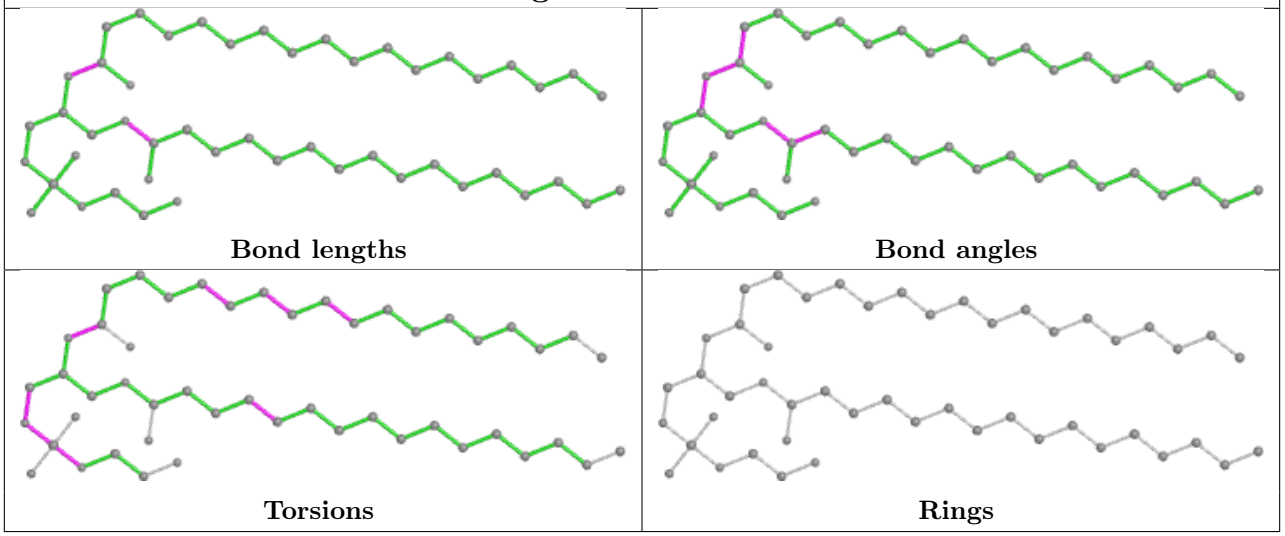
Torsions

Rings

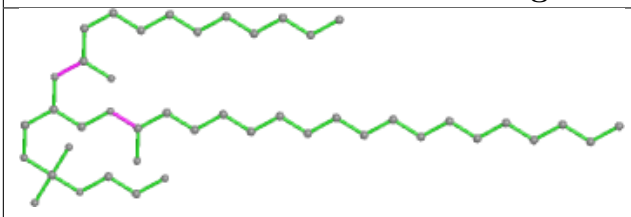
Ligand 3PE M 501



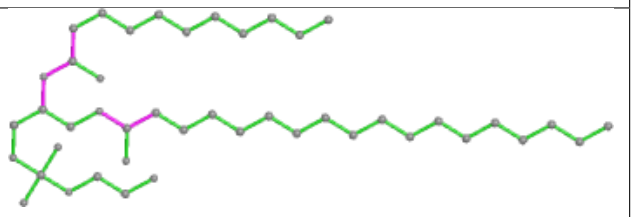
Ligand 3PE L 702



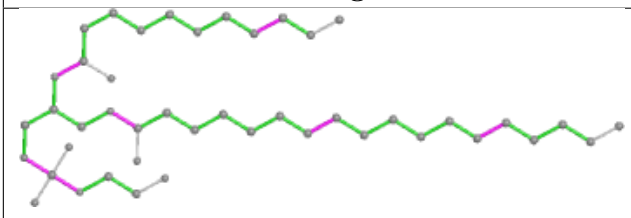
Ligand 3PE L 705



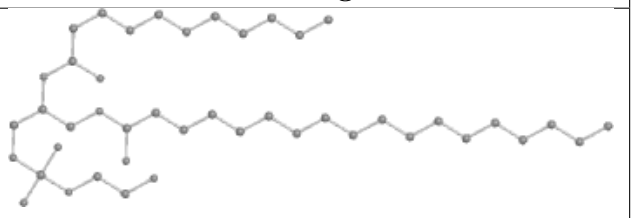
Bond lengths



Bond angles

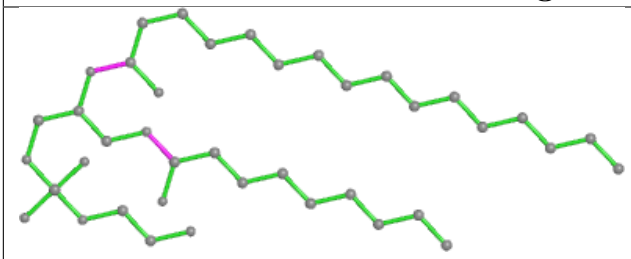


Torsions

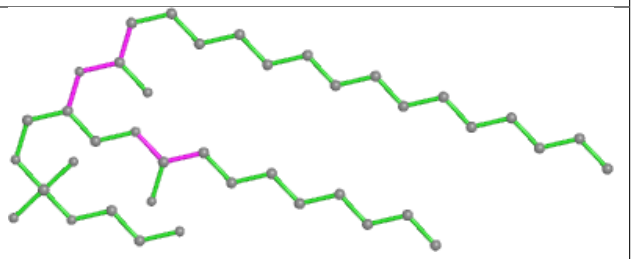


Rings

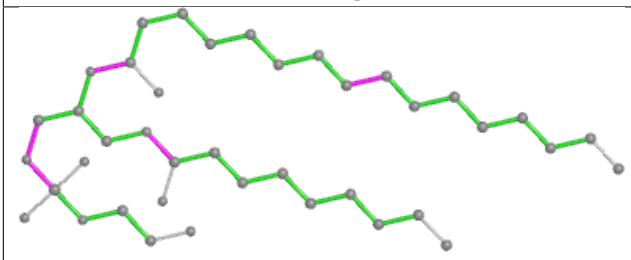
Ligand 3PE i 201



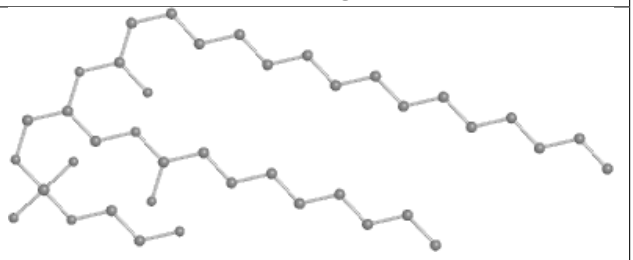
Bond lengths



Bond angles

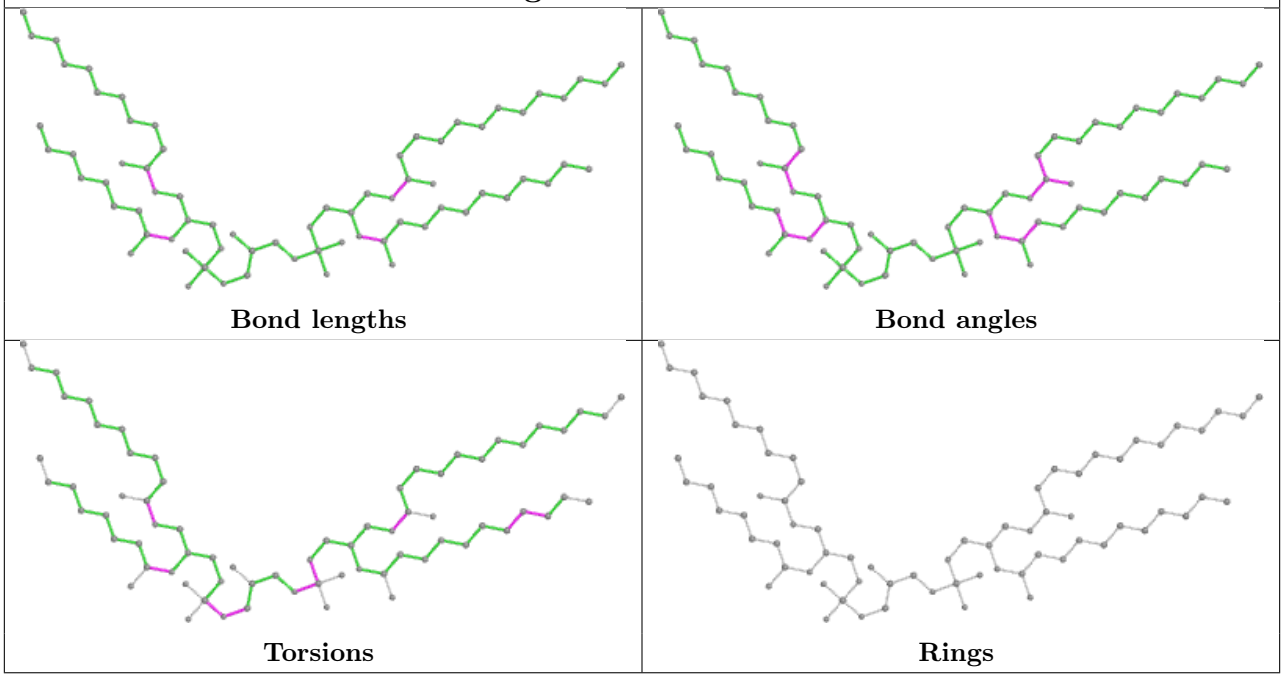


Torsions

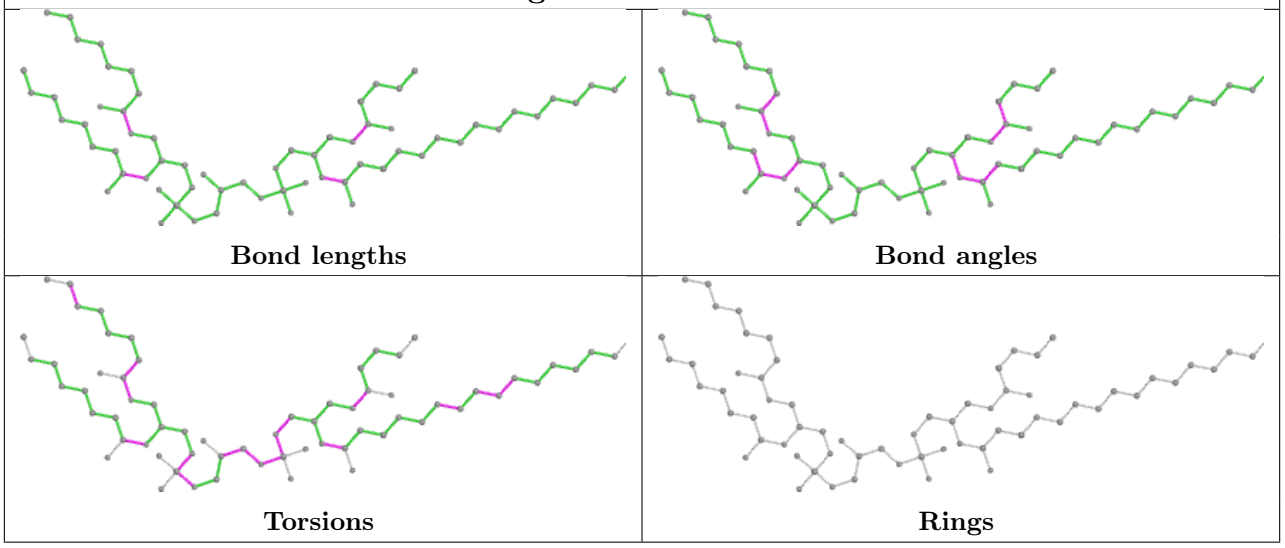


Rings

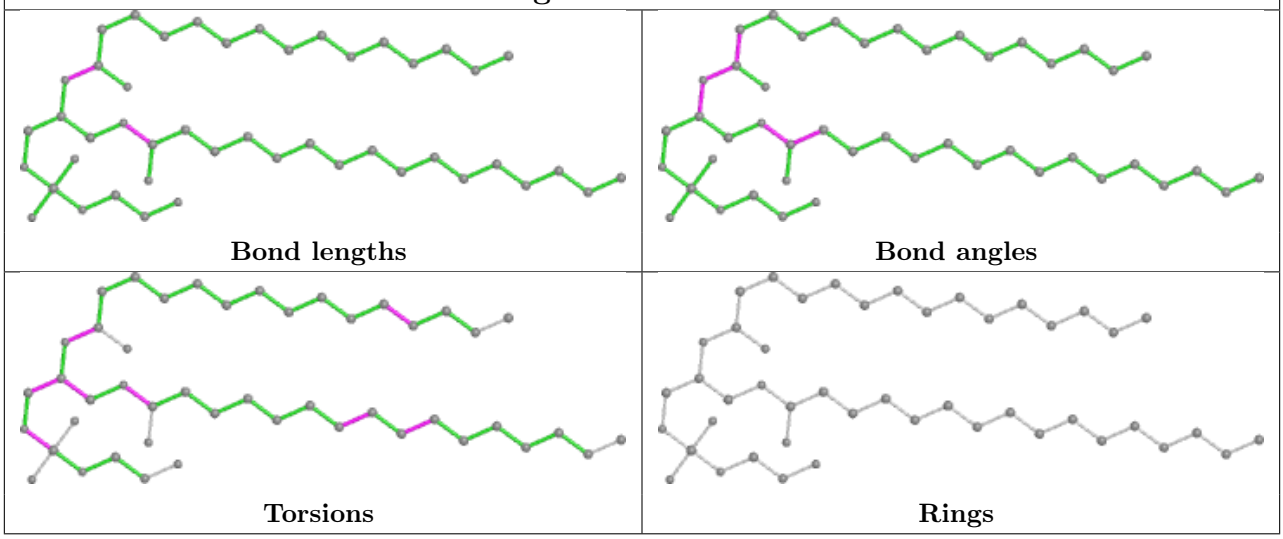
Ligand CDL Y 201



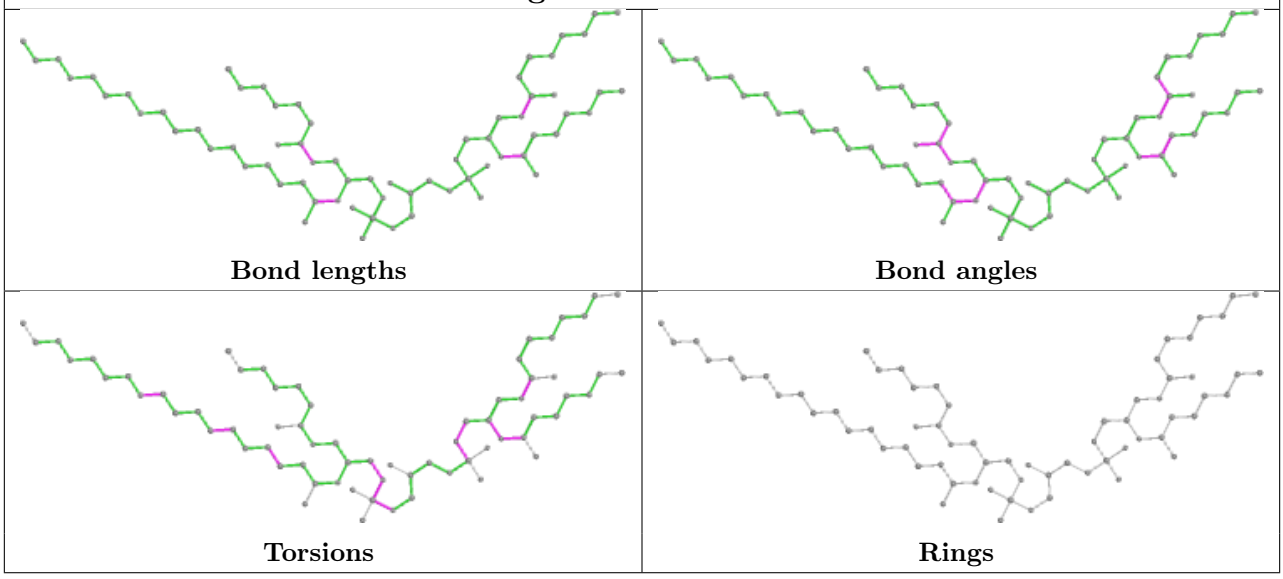
Ligand CDL d 201



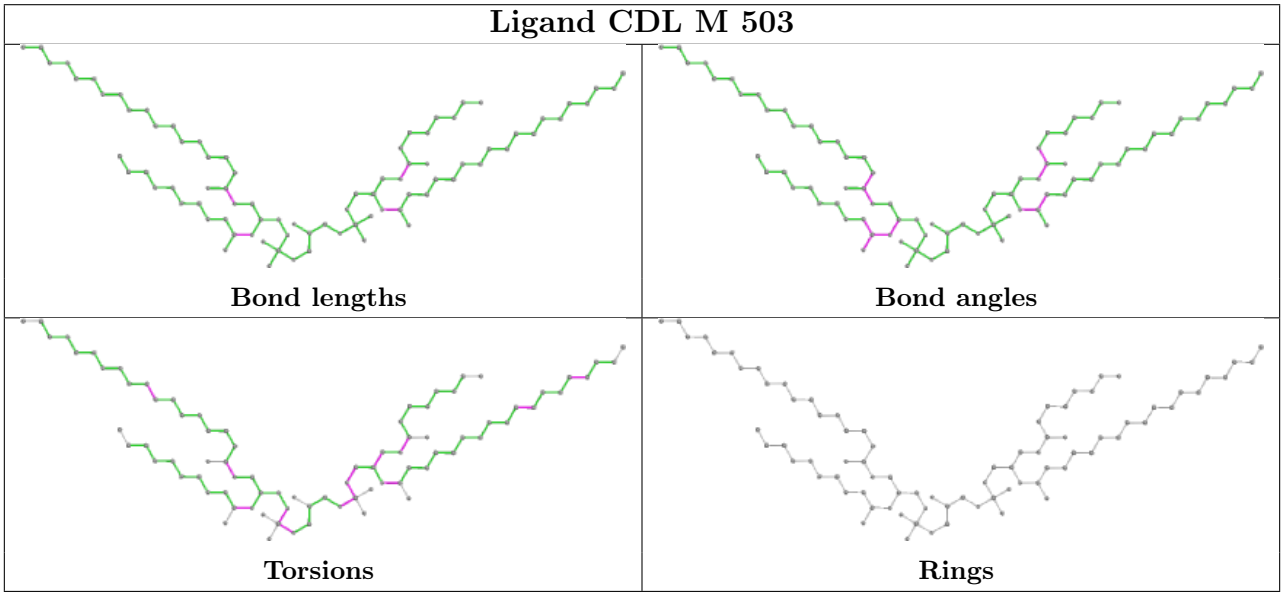
Ligand 3PE J 201



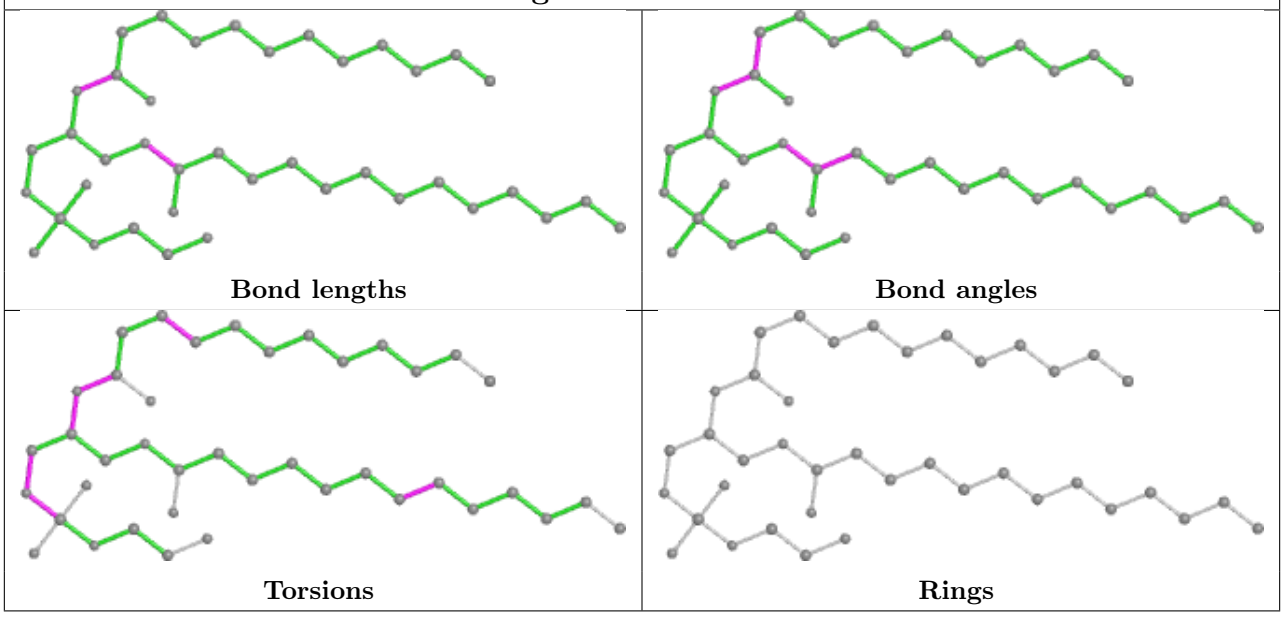
Ligand CDL h 201



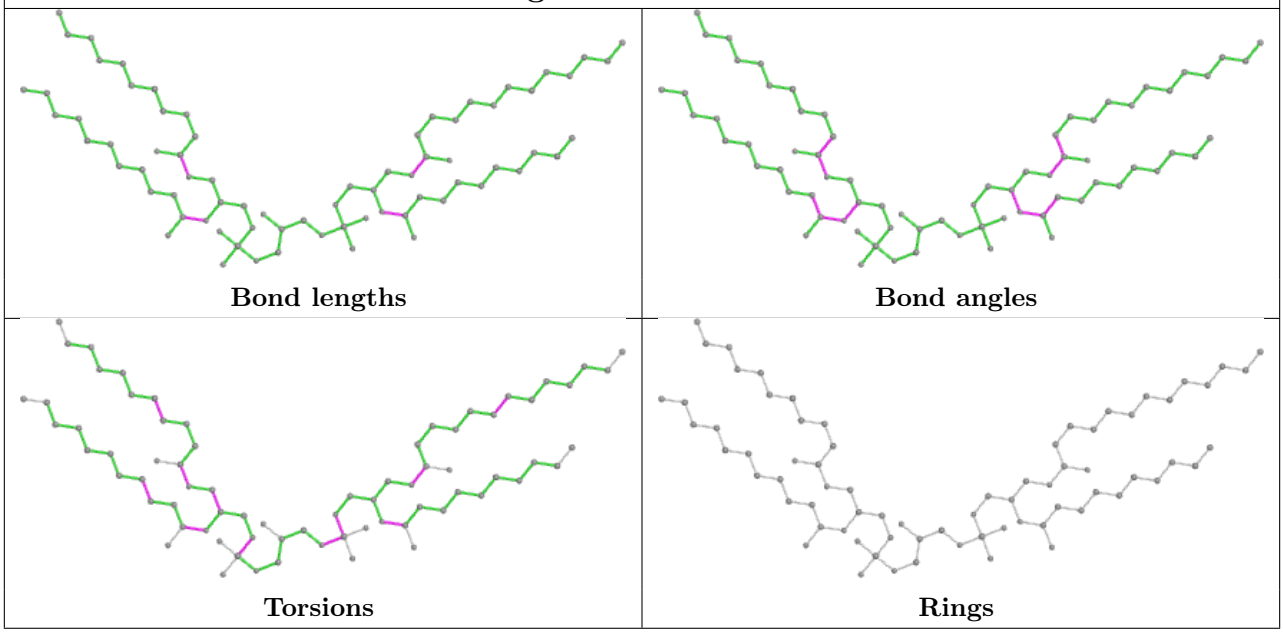
Ligand CDL M 503



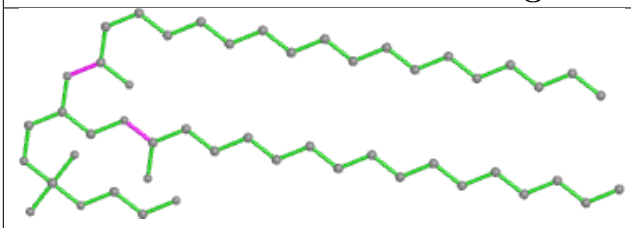
Ligand 3PE L 701



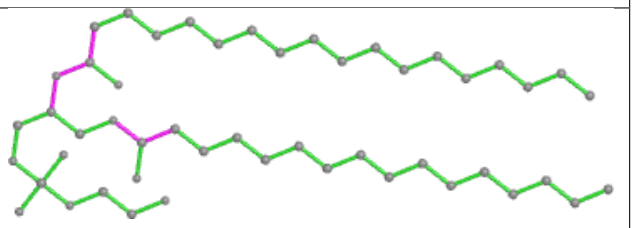
Ligand CDL L 703



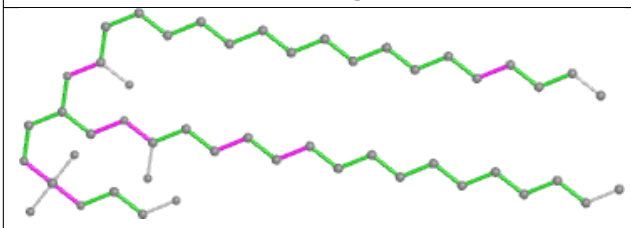
Ligand 3PE M 502



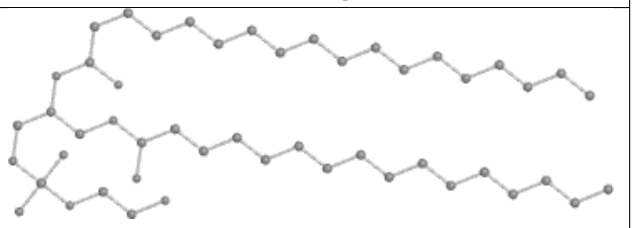
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

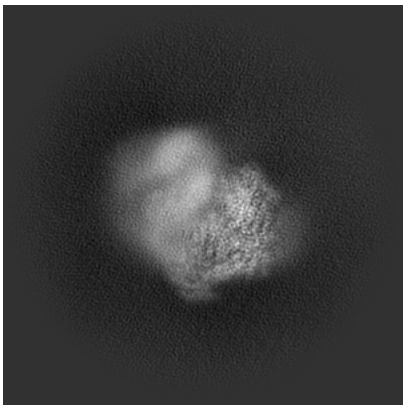
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35354. These allow visual inspection of the internal detail of the map and identification of artifacts.

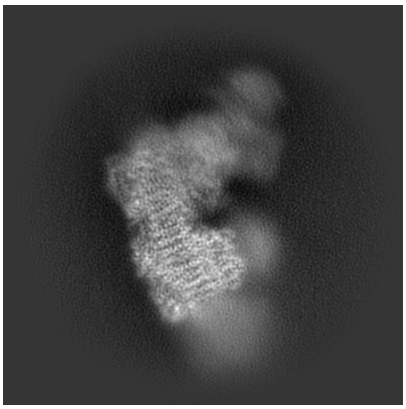
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

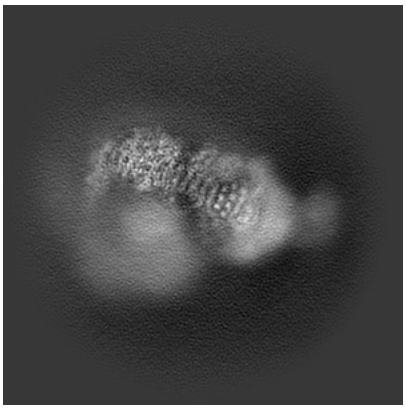
6.1.1 Primary map



X

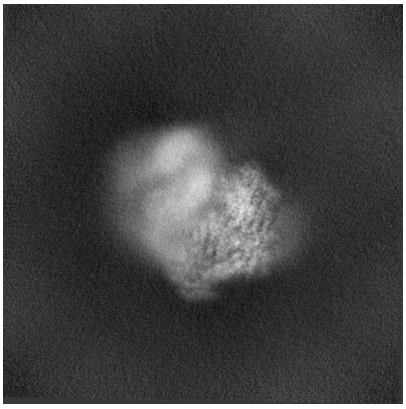


Y

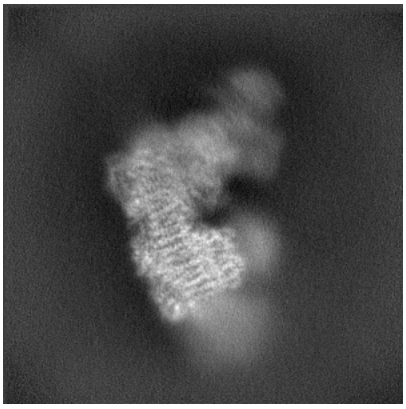


Z

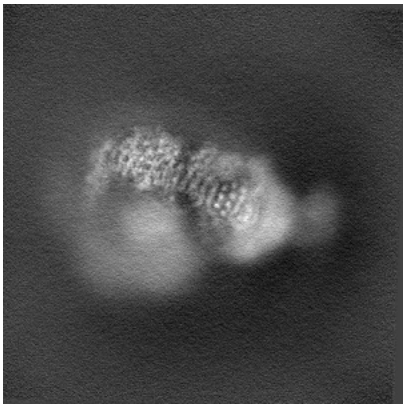
6.1.2 Raw map



X



Y

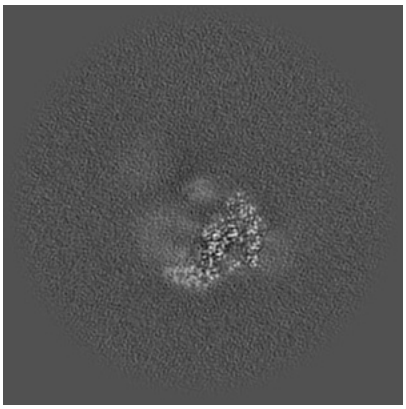


Z

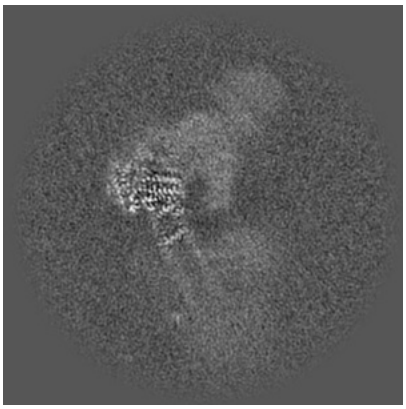
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

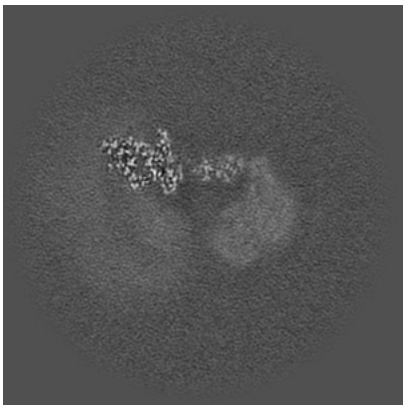
6.2.1 Primary map



X Index: 256

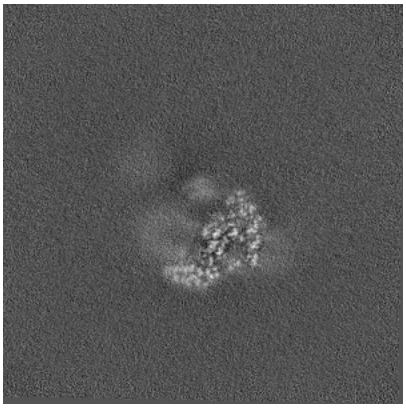


Y Index: 256

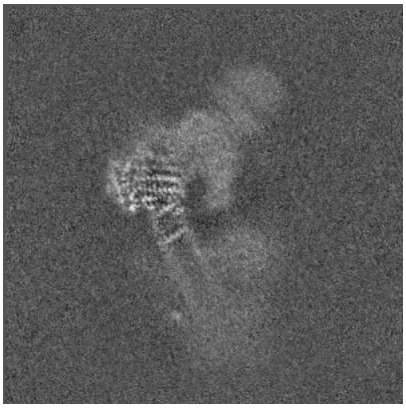


Z Index: 256

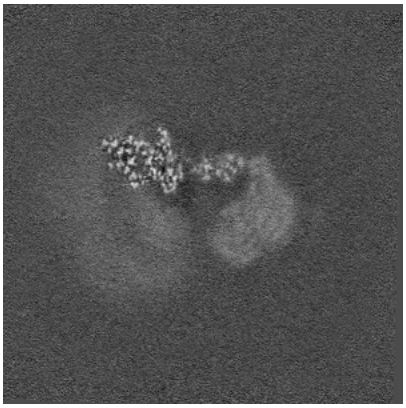
6.2.2 Raw map



X Index: 256



Y Index: 256

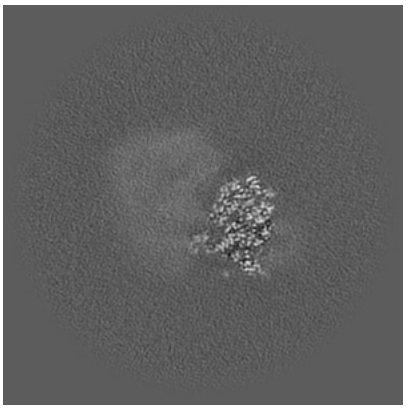


Z Index: 256

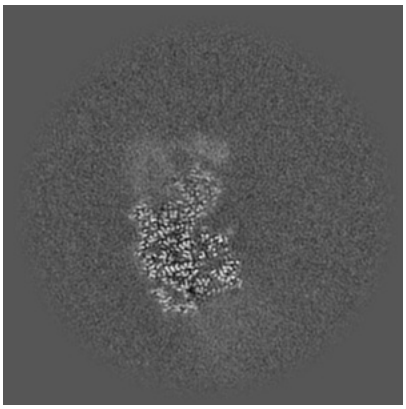
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

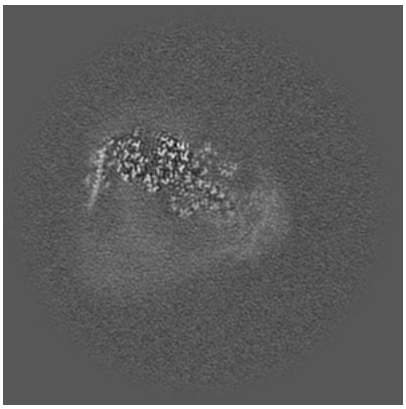
6.3.1 Primary map



X Index: 211

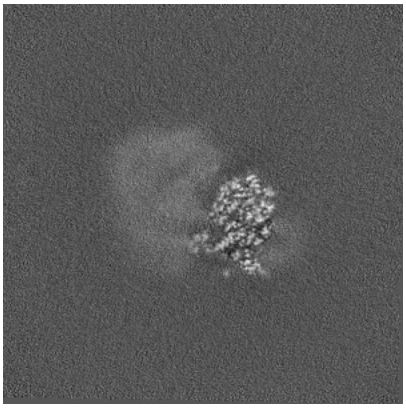


Y Index: 300

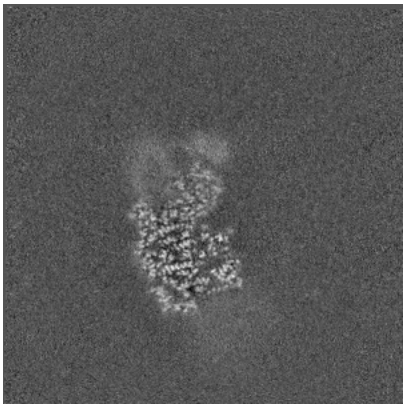


Z Index: 224

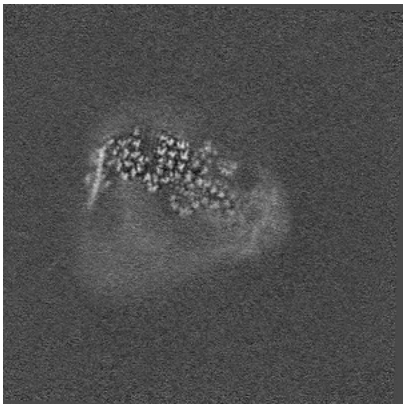
6.3.2 Raw map



X Index: 211



Y Index: 300

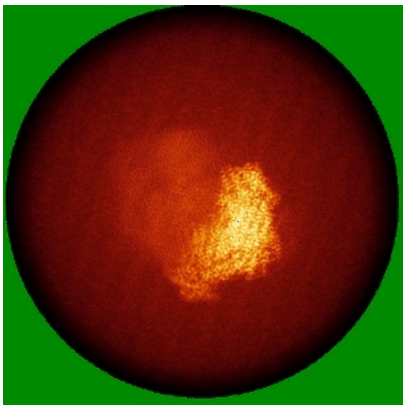


Z Index: 224

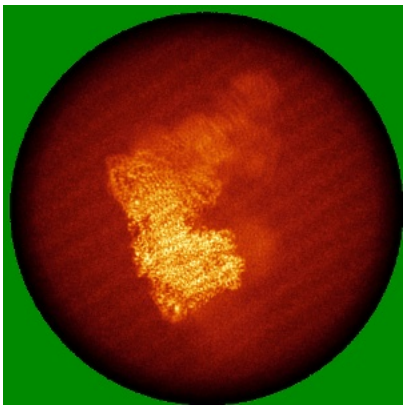
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

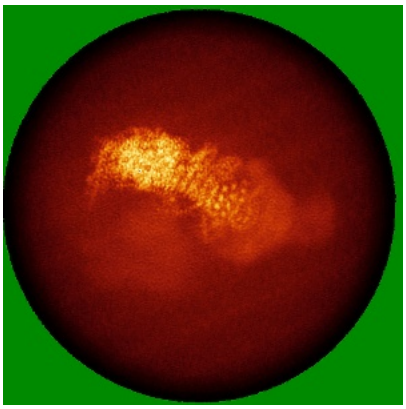
6.4.1 Primary map



X

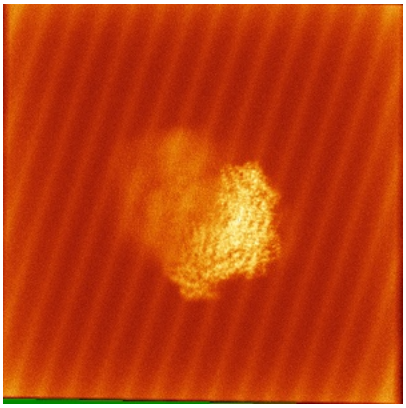


Y

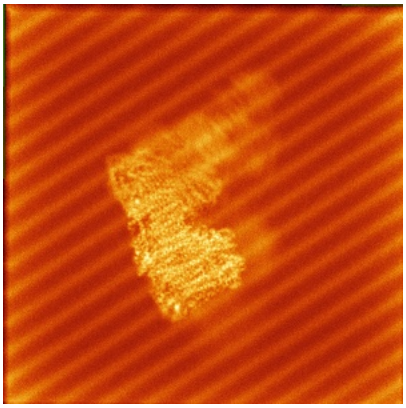


Z

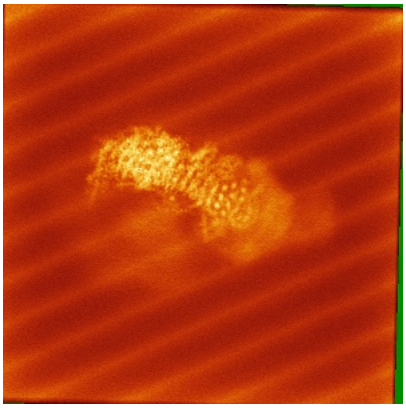
6.4.2 Raw map



X



Y



Z

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

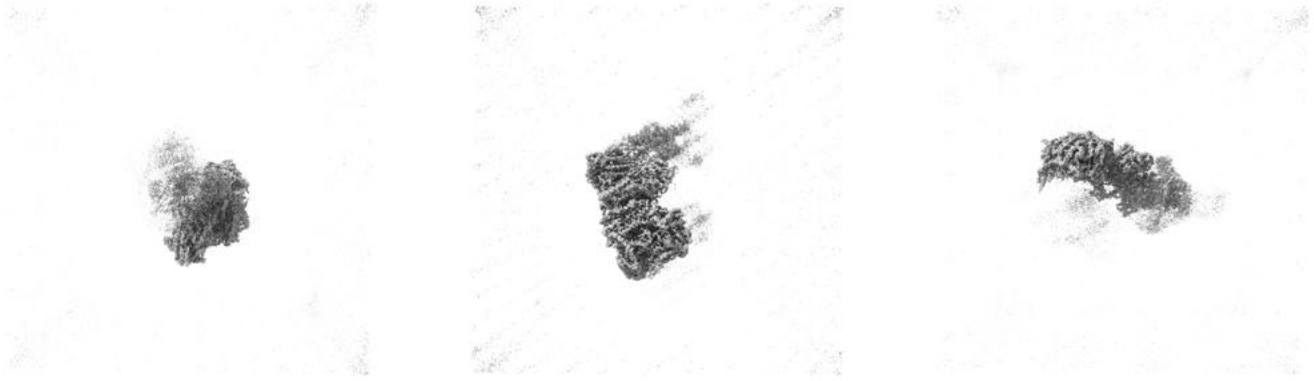
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

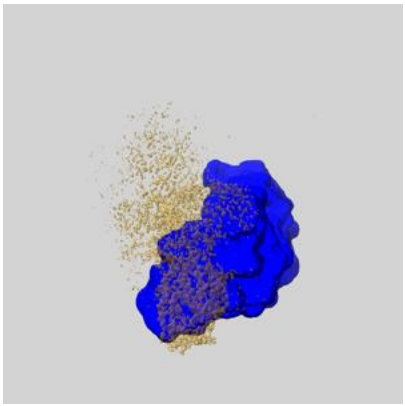
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

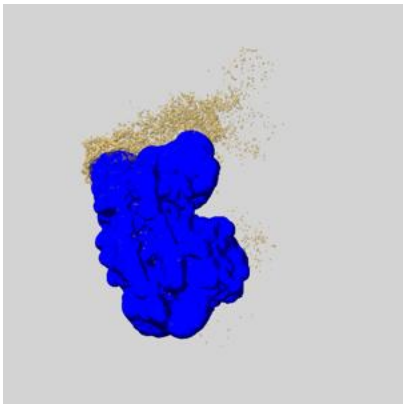
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

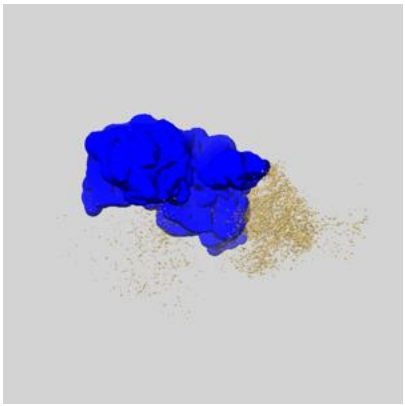
6.6.1 emd_35354_msk_1.map (i)



X



Y

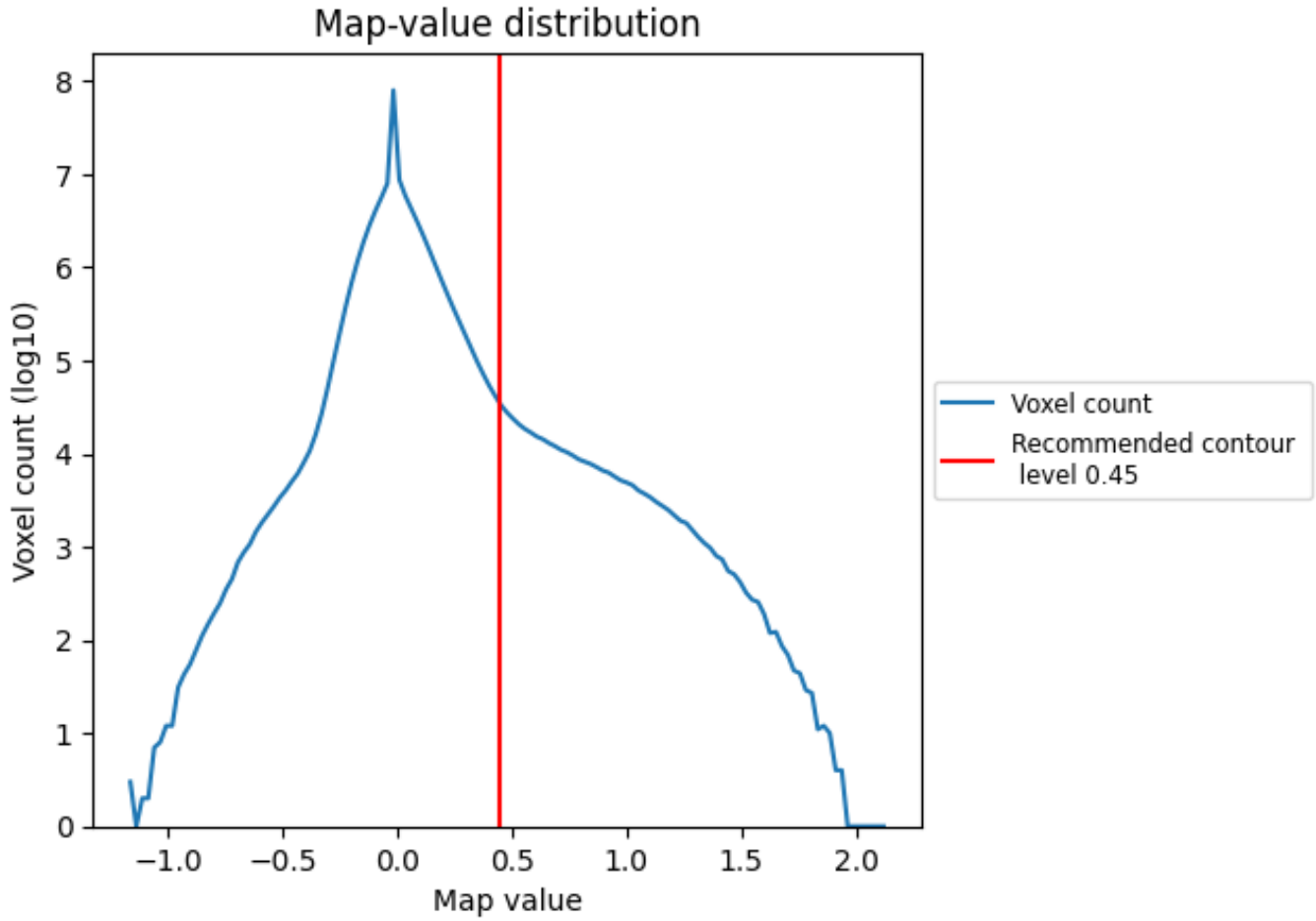


Z

7 Map analysis

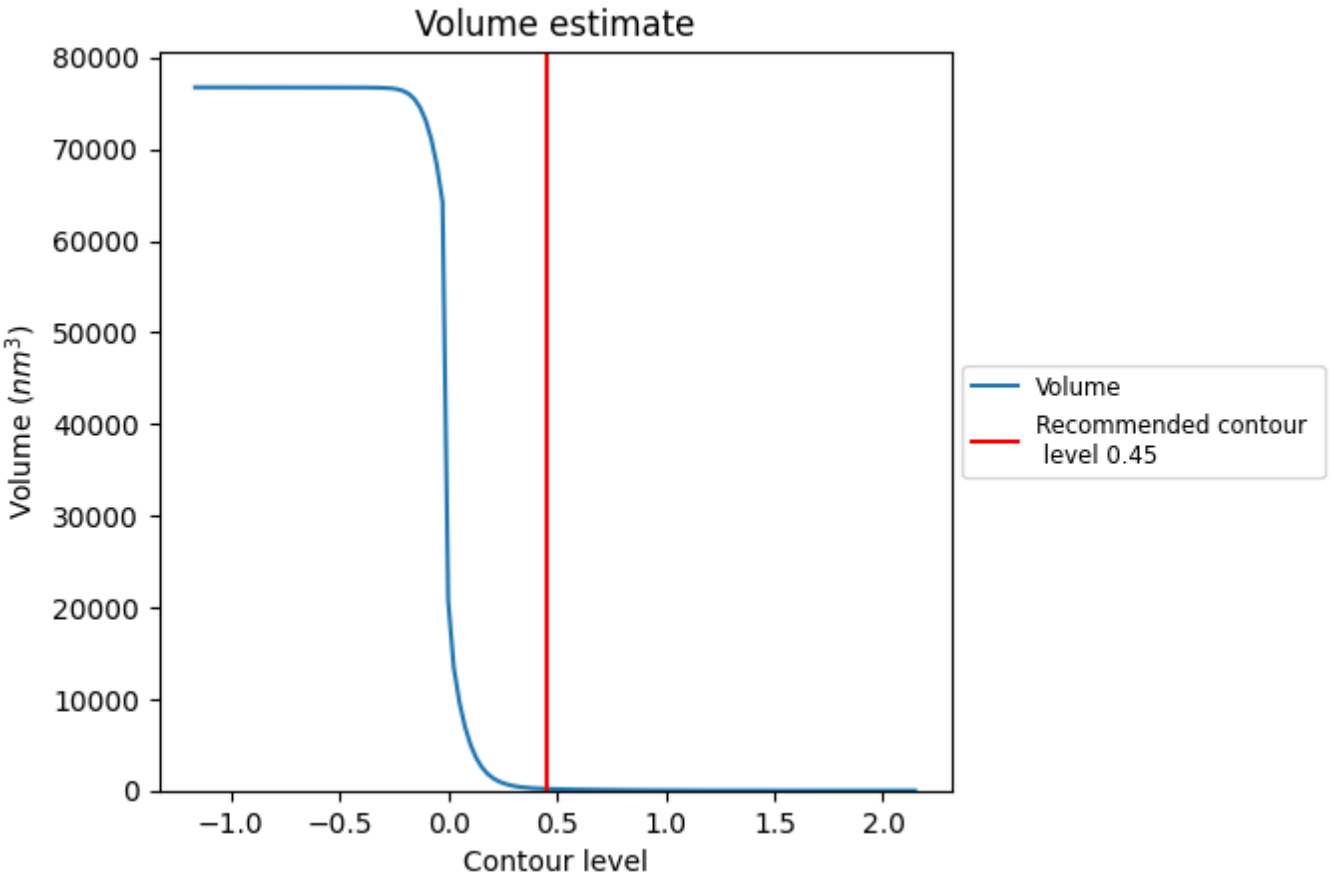
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

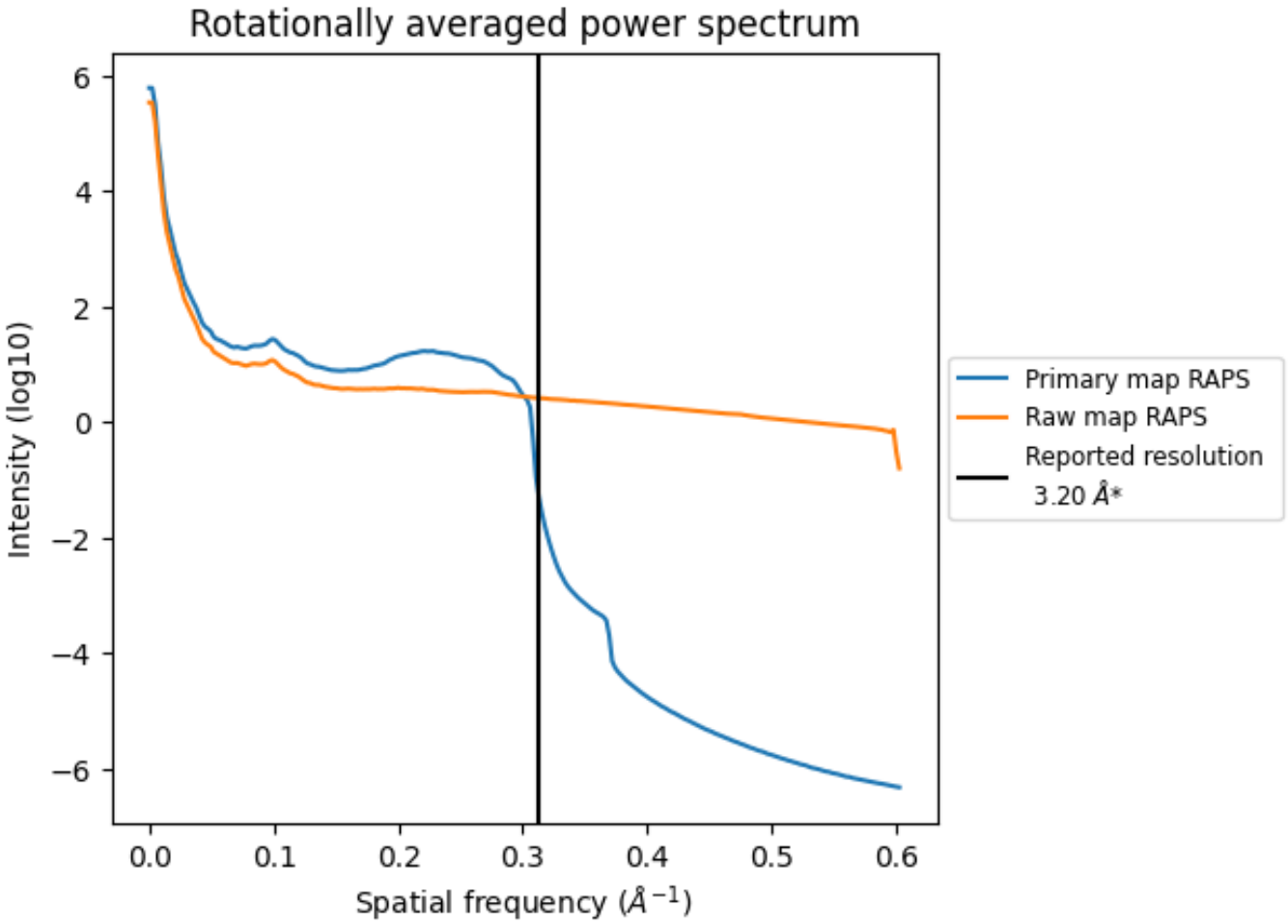
7.2 Volume estimate



The volume at the recommended contour level is 189 nm^3; this corresponds to an approximate mass of 171 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)

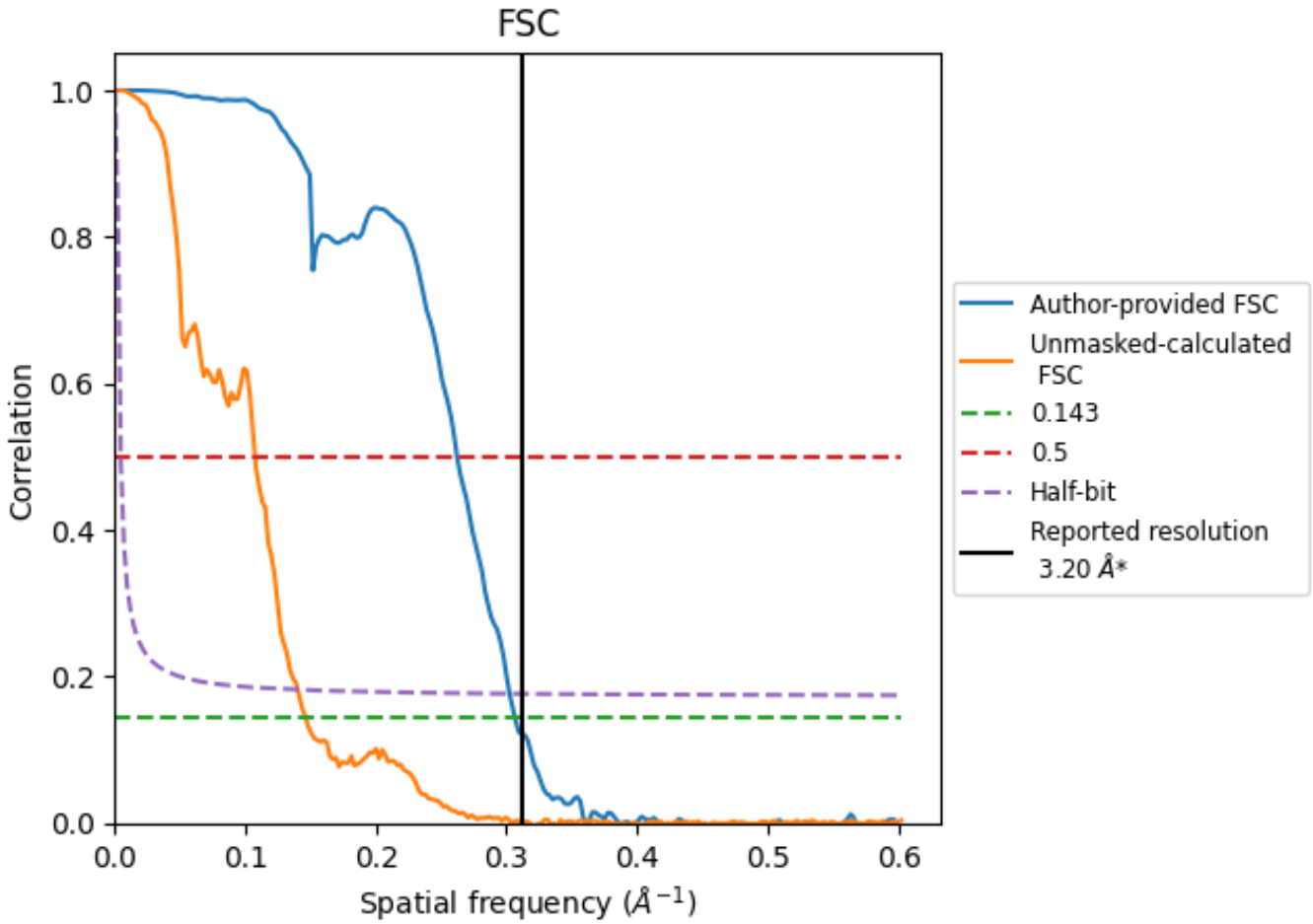


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

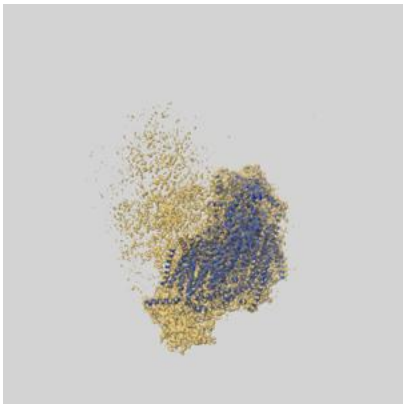
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.26	3.81	3.31
Unmasked-calculated*	6.84	9.31	7.14

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.84 differs from the reported value 3.2 by more than 10 %

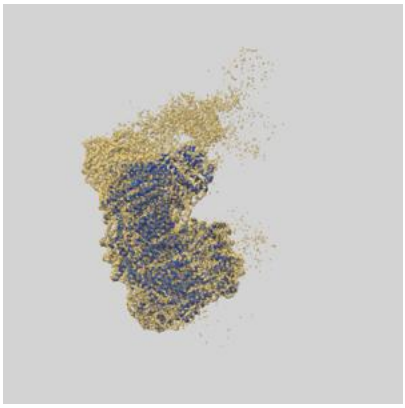
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35354 and PDB model 8IC4. Per-residue inclusion information can be found in section 3 on page 11.

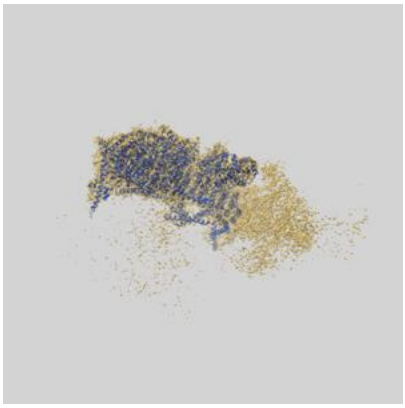
9.1 Map-model overlay



X



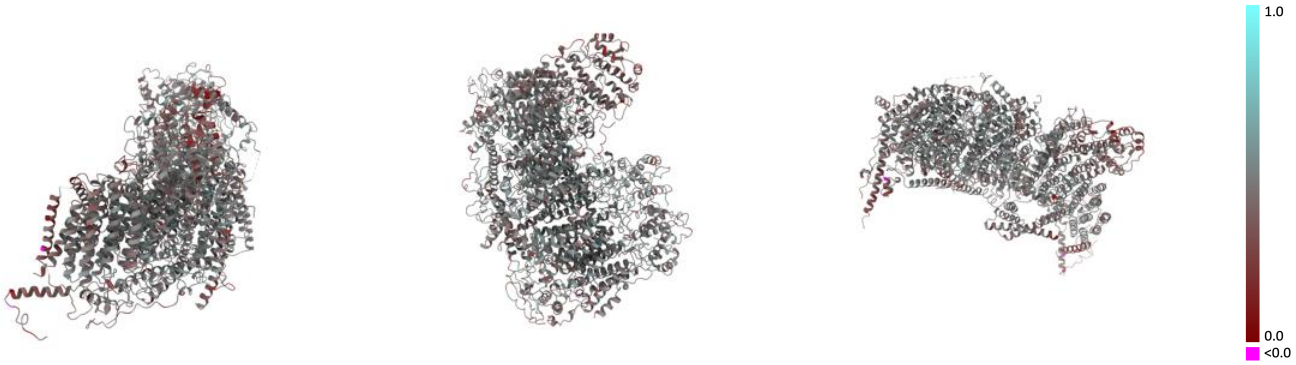
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45 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.

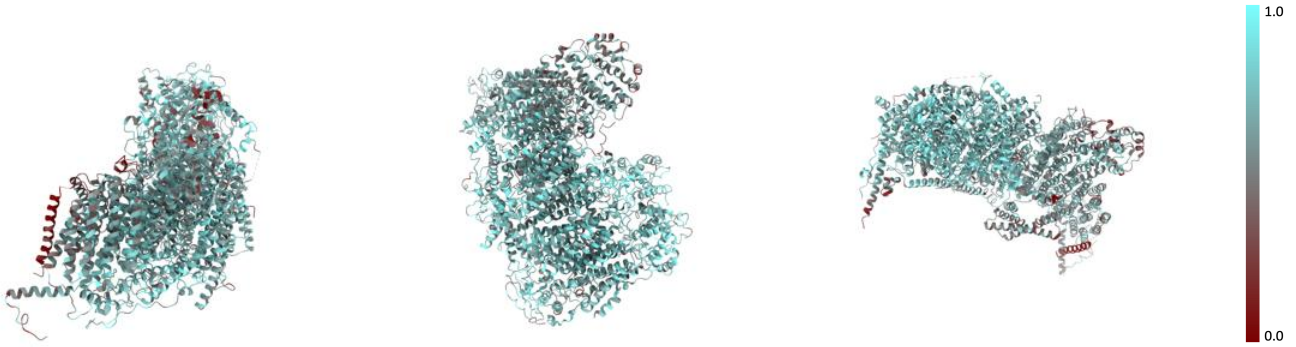
9.2 Q-score mapped to coordinate model (i)



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.

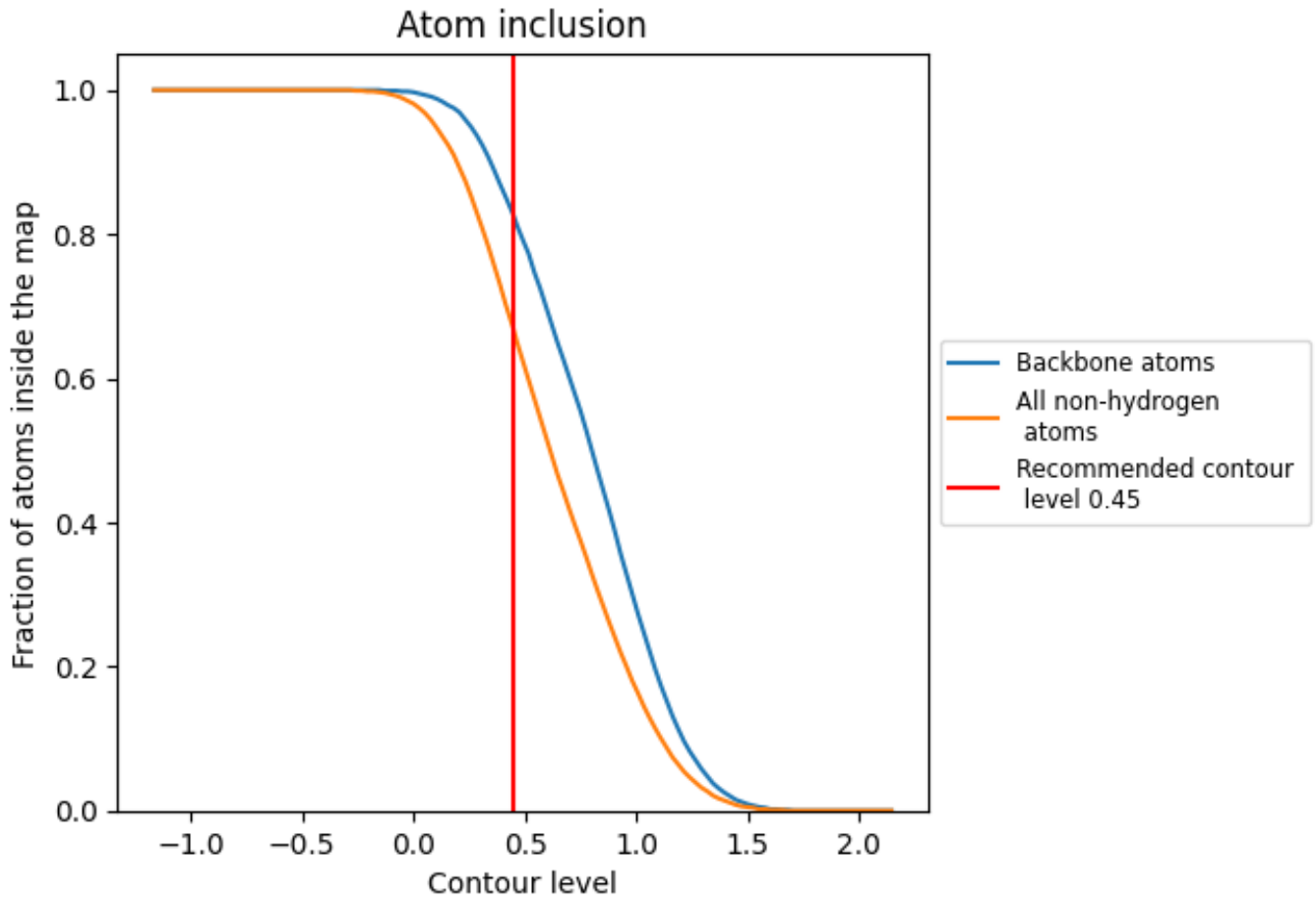
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.45).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6680	0.4500
D	0.4170	0.4180
J	0.4460	0.4010
K	0.6210	0.4630
L	0.6960	0.4680
M	0.7040	0.4860
N	0.6940	0.4770
O	0.5680	0.3830
U	0.7420	0.4720
X	0.7450	0.4480
Y	0.4880	0.4150
c	0.5820	0.4040
d	0.7030	0.4670
e	0.6030	0.3850
f	0.6640	0.4600
g	0.7100	0.4560
h	0.7180	0.4630
i	0.7060	0.4560
j	0.6920	0.4160
k	0.7520	0.4620
l	0.7480	0.4710
m	0.6850	0.4550
n	0.7610	0.4750
o	0.6540	0.4080
p	0.7070	0.4380