Full wwPDB EM Validation Report ⓘ

Dec 19, 2022 – 12:38 pm GMT

PDB ID	:	6ZK9
EMDB ID	:	EMD-11241
Title	:	Peripheral domain of open complex I during turnover
Authors	:	Kampjut, D.; Sazanov, L.A.
Deposited on	:	2020-06-30
Resolution	:	2.30 Å(reported)
Based on initial model	:	5LNK

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:

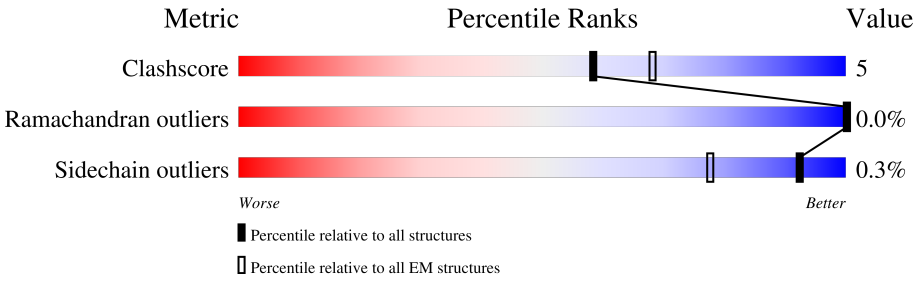
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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	1	464	80% 13% 7%
2	2	246	75% 11% 13%
3	3	727	81% 13% 5%
4	4	463	66% 16% 18%
5	5	266	65% 13% 22%
6	6	223	62% 7% 30%
7	9	217	71% 11% 19%
8	a	109	40% 60%

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Mol	Chain	Length	Quality of chain
9	b	124	77% 23%
10	c	170	74% 26%
11	d	380	78% 22%
12	e	99	87% 13%
13	f	116	97%
14	g	140	81% 19%
15	h	114	83% 16%
16	i	145	100%
17	j	157	6% 52% 48%
18	q	144	22% 78%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	SF4	6	201	-	-	X	-

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 29587 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] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	430	3312	2086	593	613	20	0	0

- Molecule 2 is a protein called Mitochondrial complex I, 24 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	213	1655	1058	278	309	10	0	0

- Molecule 3 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	688	5275	3301	922	1011	41	0	0

- Molecule 4 is a protein called Mitochondrial complex I, 49 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	380	3047	1943	523	557	24	0	0

- Molecule 5 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	208	1726	1112	296	315	3	0	0

- Molecule 6 is a protein called Mitochondrial complex I, PSST subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	156	1247	795	225	213	14	0	0

- Molecule 7 is a protein called Mitochondrial complex I, TYKY subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 8 is a protein called Mitochondrial complex I, 10 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

- Molecule 9 is a protein called Mitochondrial complex I, 13 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	b	95	Total	C	N	O	S	0	0
			737	451	139	144	3		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	c	126	Total	C	N	O	S	0	0
			1024	646	182	193	3		

- Molecule 11 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	d	297	Total	C	N	O	S	0	0
			2372	1516	432	419	5		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	e	86	Total	C	N	O	S	0	0
			691	434	129	126	2		

- Molecule 13 is a protein called Mitochondrial complex I, B13 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	f	113	Total	C	N	O	S	0	0
			917	595	153	167	2		

- Molecule 14 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	g	114	Total	C	N	O	S	0	0
			969	619	180	166	4		

- Molecule 15 is a protein called Mitochondrial complex I, B14.5a subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	h	96	Total	C	N	O	S	0	0
			769	480	146	140	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	i	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

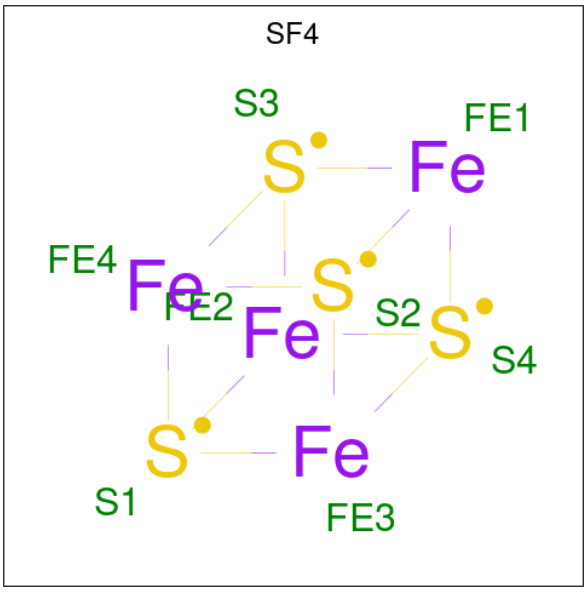
- Molecule 17 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	j	82	Total	C	N	O	S	0	0
			660	425	98	132	5		

- Molecule 18 is a protein called Mitochondrial complex I, B16.6 subunit.

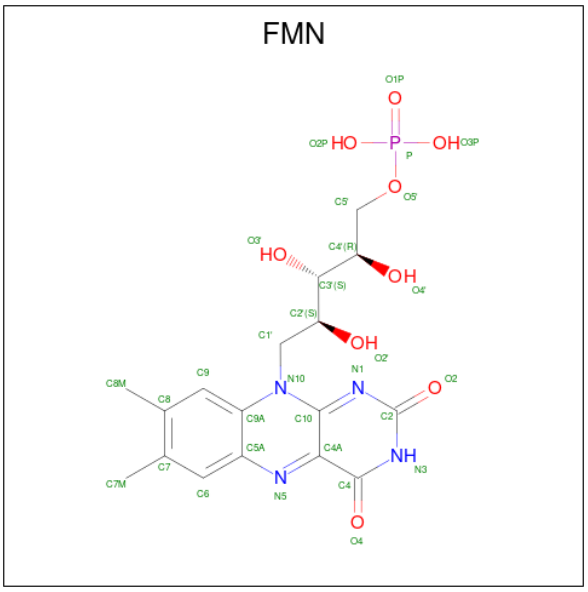
Mol	Chain	Residues	Atoms					AltConf	Trace
18	q	31	Total	C	N	O	S	0	0
			245	157	44	42	2		

- Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



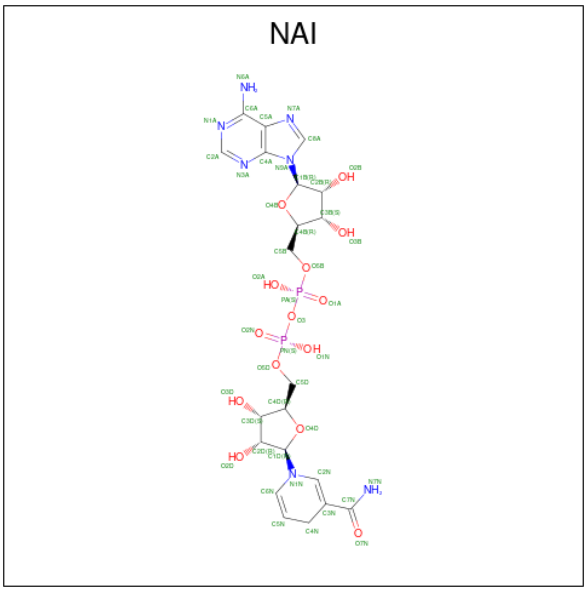
Mol	Chain	Residues	Atoms	AltConf
19	1	1	Total Fe S 8 4 4	0
19	3	1	Total Fe S 16 8 8	0
19	3	1	Total Fe S 16 8 8	0
19	6	1	Total Fe S 8 4 4	0
19	9	1	Total Fe S 16 8 8	0
19	9	1	Total Fe S 16 8 8	0

- Molecule 20 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



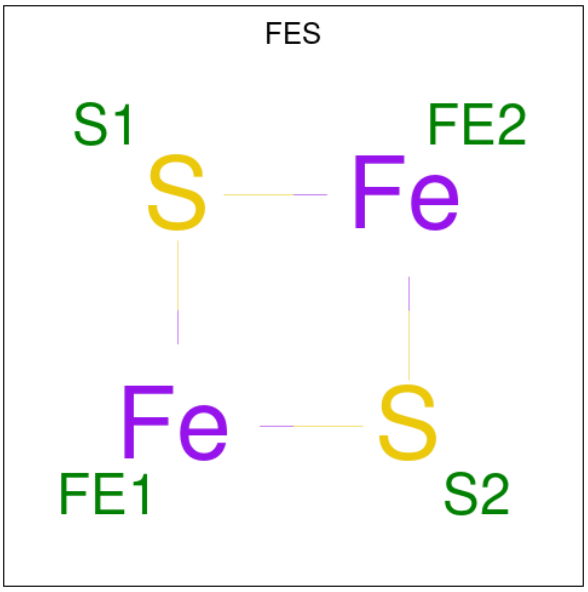
Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 21 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 22 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

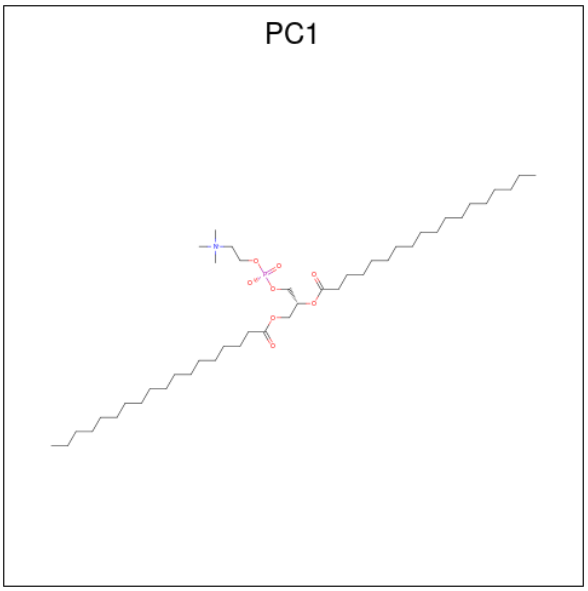


Mol	Chain	Residues	Atoms	AltConf
22	2	1	Total Fe S 4 2 2	0
22	3	1	Total Fe S 4 2 2	0

- Molecule 23 is POTASSIUM ION (three-letter code: K) (formula: K).

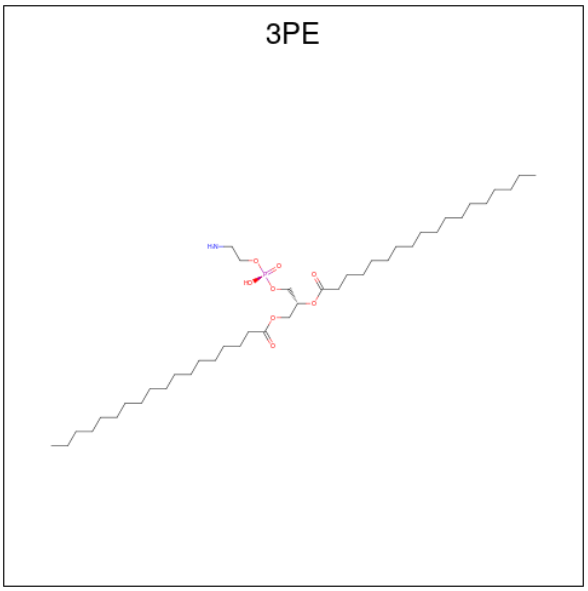
Mol	Chain	Residues	Atoms	AltConf
23	3	1	Total K 1 1	0

- Molecule 24 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
24	6	1	Total	C	N	O	P	0
			46	36	1	8	1	
24	9	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 25 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
25	6	1	Total	C	N	O	P	0
			51	41	1	8	1	

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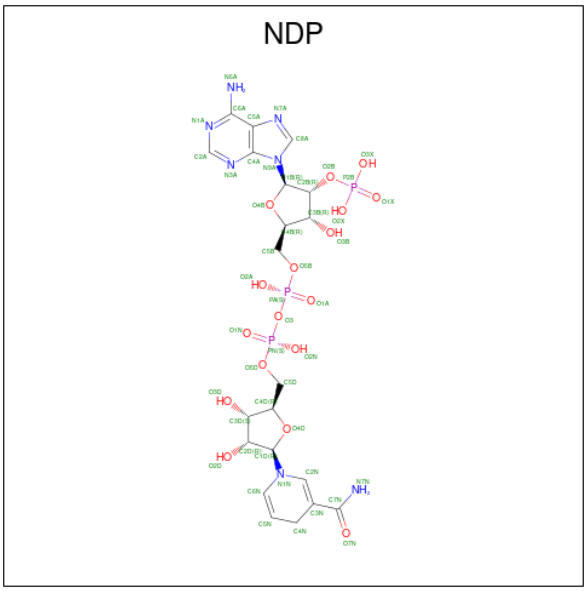
Mol	Chain	Residues	Atoms					AltConf
25	i	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
26	b	1	Total	Zn	0
			1	1	

- Molecule 27 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

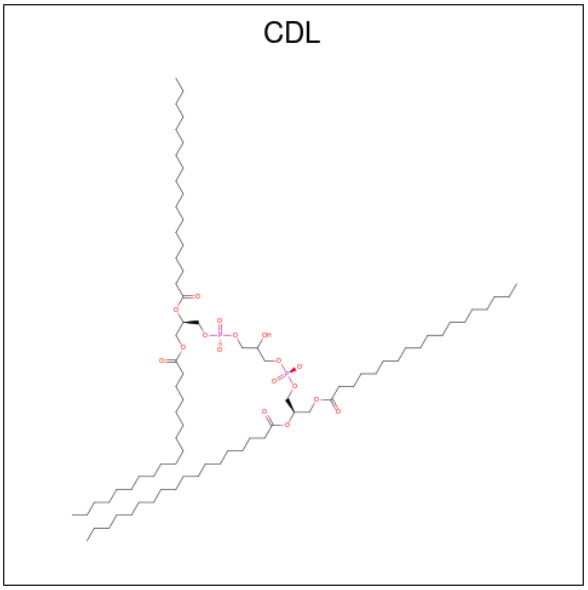


Mol	Chain	Residues	Atoms					AltConf
27	d	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 28 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).

Mol	Chain	Residues	Atoms						AltConf
28	g	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	

- Molecule 29 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
29	h	1	Total	C	O	P	0
			58	39	17	2	

- Molecule 30 is water.

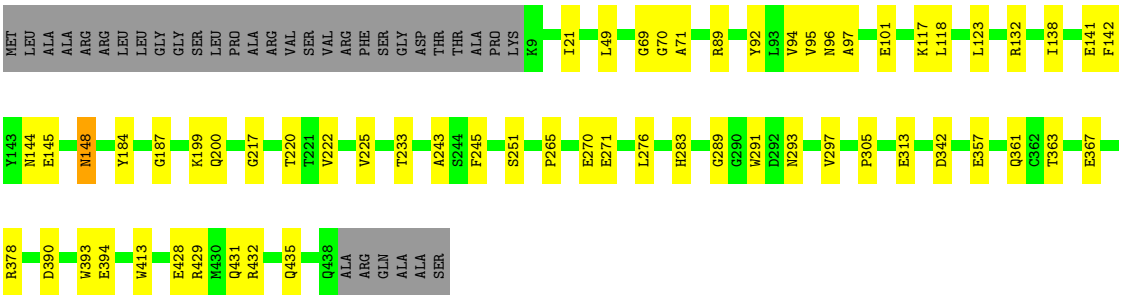
Mol	Chain	Residues	Atoms	AltConf
30	1	123	Total O 123 123	0
30	2	44	Total O 44 44	0
30	3	285	Total O 285 285	0
30	4	200	Total O 200 200	0
30	5	129	Total O 129 129	0
30	6	81	Total O 81 81	0
30	9	110	Total O 110 110	0
30	a	6	Total O 6 6	0
30	b	67	Total O 67 67	0
30	c	109	Total O 109 109	0
30	d	79	Total O 79 79	0
30	e	7	Total O 7 7	0
30	f	39	Total O 39 39	0
30	g	38	Total O 38 38	0
30	h	71	Total O 71 71	0
30	i	83	Total O 83 83	0
30	q	1	Total O 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.

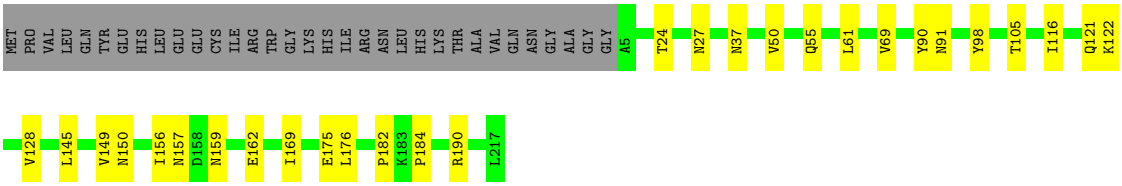
• Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1:



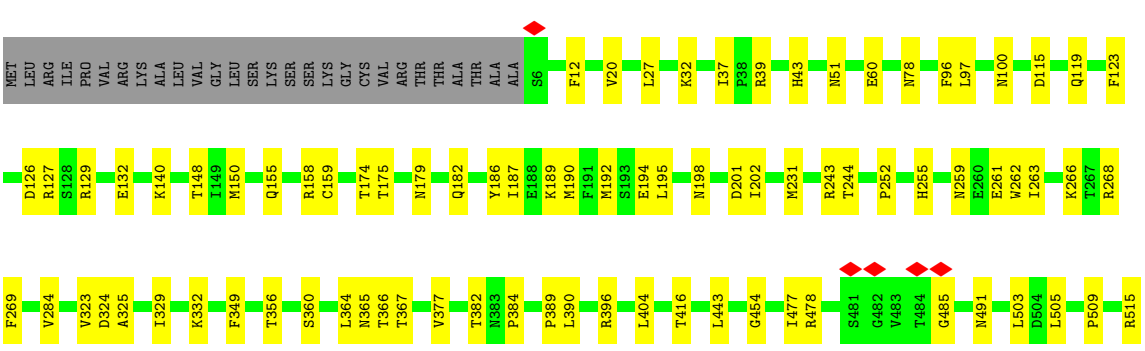
• Molecule 2: Mitochondrial complex I, 24 kDa subunit

Chain 2:



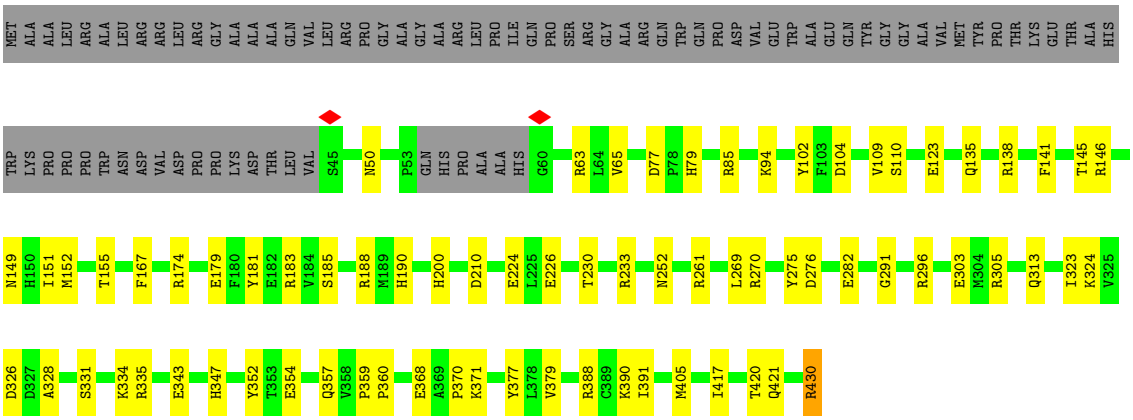
• Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

Chain 3:



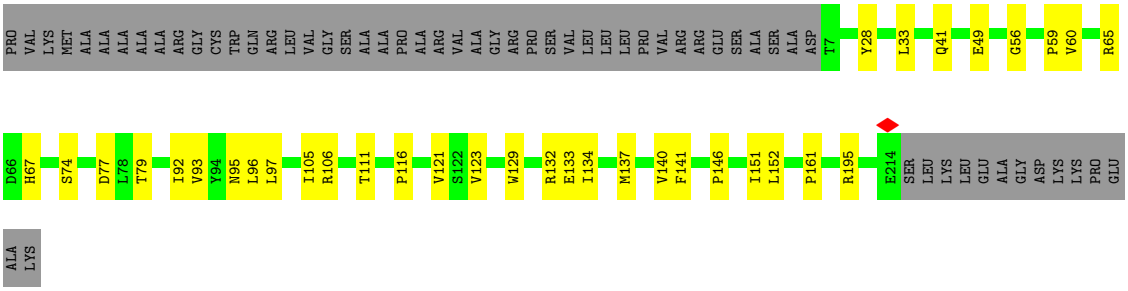
• Molecule 4: Mitochondrial complex I, 49 kDa subunit

Chain 4:



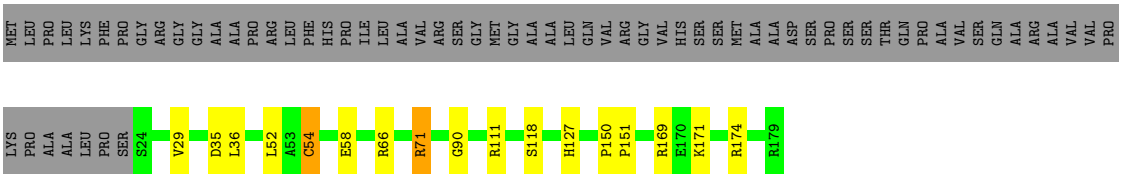
• Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3

Chain 5:



• Molecule 6: Mitochondrial complex I, PSST subunit

Chain 6:

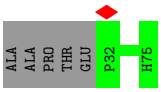


• Molecule 7: Mitochondrial complex I, TYKY subunit

Chain 9:

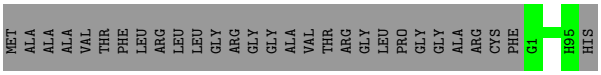
• Molecule 8: Mitochondrial complex I, 10 kDa subunit

Chain a:



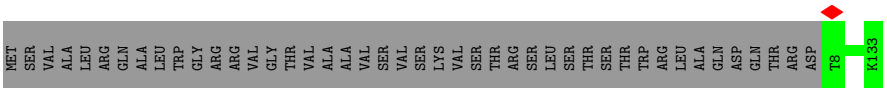
• Molecule 9: Mitochondrial complex I, 13 kDa subunit

Chain b:



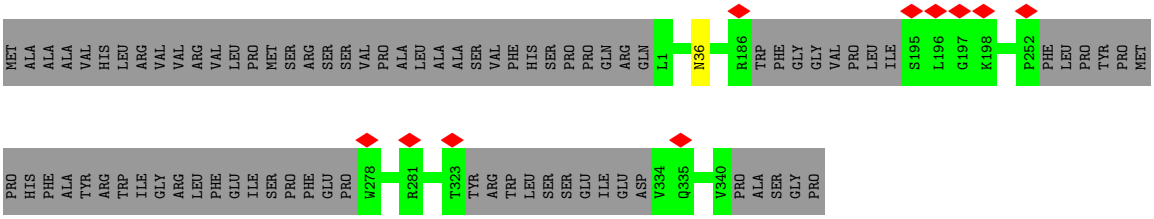
• Molecule 10: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain c:



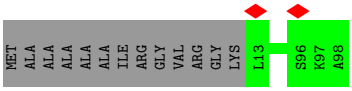
• Molecule 11: NADH:ubiquinone oxidoreductase subunit A9

Chain d:



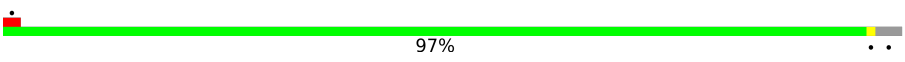
• Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

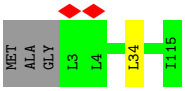
Chain e:



• Molecule 13: Mitochondrial complex I, B13 subunit

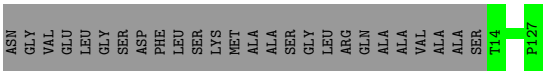
Chain f:





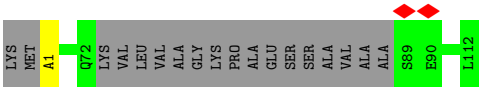
• Molecule 14: NADH:ubiquinone oxidoreductase subunit A6

Chain g:



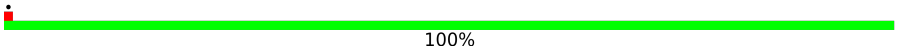
• Molecule 15: Mitochondrial complex I, B14.5a subunit

Chain h:



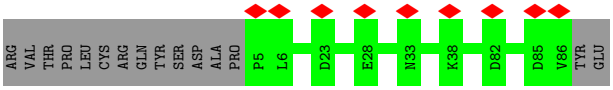
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain i:



• Molecule 17: Acyl carrier protein

Chain j:



• Molecule 18: Mitochondrial complex I, B16.6 subunit

Chain q:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	315484	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.886	Depositor
Minimum map value	-0.306	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.105	Depositor
Map size (Å)	147.0, 160.5, 187.0	wwPDB
Map dimensions	294, 321, 374	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5, 0.5, 0.5	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: K, NAI, FES, ZN, AYA, 3PE, 2MR, PC1, CDL, FMN, NDP, SF4, ZMP

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	1	0.39	0/3386	0.57	0/4575
2	2	0.36	0/1695	0.56	0/2306
3	3	0.40	1/5362 (0.0%)	0.57	0/7266
4	4	0.42	0/3103	0.58	0/4190
5	5	0.39	0/1776	0.55	0/2417
6	6	0.45	0/1278	0.55	0/1728
7	9	0.44	0/1445	0.59	0/1956
8	a	0.31	0/383	0.47	0/518
9	b	0.36	0/749	0.51	0/1009
10	c	0.34	0/1047	0.52	0/1415
11	d	0.34	0/2424	0.53	0/3276
12	e	0.31	0/702	0.51	0/945
13	f	0.32	0/937	0.52	1/1271 (0.1%)
14	g	0.35	0/993	0.53	0/1336
15	h	0.37	0/779	0.54	0/1053
16	i	0.38	0/1250	0.50	0/1698
17	j	0.30	0/670	0.50	0/902
18	q	0.36	0/252	0.52	0/338
All	All	0.38	1/28231 (0.0%)	0.55	1/38199 (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
3	3	0	2
4	4	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	159	CYS	CB-SG	-7.68	1.69	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	f	34	LEU	CA-CB-CG	5.21	127.29	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	259	ASN	Peptide
3	3	366	THR	Peptide
4	4	275	TYR	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	1	3312	0	3269	42	0
2	2	1655	0	1668	16	0
3	3	5275	0	5300	59	0
4	4	3047	0	3021	50	0
5	5	1726	0	1676	20	0
6	6	1247	0	1259	16	0
7	9	1414	0	1371	17	0
8	a	371	0	344	0	0
9	b	737	0	710	0	0
10	c	1024	0	1023	0	0
11	d	2372	0	2407	0	0
12	e	691	0	706	0	0
13	f	917	0	958	0	0
14	g	969	0	980	0	0
15	h	769	0	780	0	0
16	i	1209	0	1182	0	0
17	j	660	0	663	0	0
18	q	245	0	244	0	0
19	1	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	3	16	0	0	0	0
19	6	8	0	0	3	0
19	9	16	0	0	0	0
20	1	31	0	19	1	0
21	1	44	0	27	4	0
22	2	4	0	0	1	0
22	3	4	0	0	0	0
23	3	1	0	0	0	0
24	6	46	0	69	0	0
24	9	54	0	88	1	0
25	6	51	0	82	3	0
25	i	51	0	82	0	0
26	b	1	0	0	0	0
27	d	48	0	26	0	0
28	g	34	0	40	0	0
29	h	58	0	60	0	0
30	1	123	0	0	3	0
30	2	44	0	0	1	0
30	3	285	0	0	4	0
30	4	200	0	0	5	0
30	5	129	0	0	1	0
30	6	81	0	0	2	0
30	9	110	0	0	1	0
30	a	6	0	0	0	0
30	b	67	0	0	0	0
30	c	109	0	0	0	0
30	d	79	0	0	0	0
30	e	7	0	0	0	0
30	f	39	0	0	0	0
30	g	38	0	0	0	0
30	h	71	0	0	0	0
30	i	83	0	0	0	0
30	q	1	0	0	0	0
All	All	29587	0	28054	198	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 5.

All (198) 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)
4:4:50:ASN:HD21	4:4:63:ARG:HH21	1.33	0.76
1:1:101:GLU:HB2	21:1:503:NAI:H42N	1.76	0.68
6:6:171:LYS:HG2	6:6:174:ARG:HH11	1.61	0.66
2:2:150:ASN:HB3	2:2:162:GLU:HB3	1.80	0.62
3:3:126:ASP:HB2	4:4:328:ALA:HB3	1.81	0.62
4:4:405:MET:SD	4:4:421:GLN:NE2	2.71	0.61
4:4:174:ARG:NH2	30:4:510:HOH:O	2.34	0.61
4:4:269:LEU:HB2	4:4:368:GLU:HB2	1.84	0.60
3:3:27:LEU:HA	3:3:37:ILE:HD12	1.83	0.59
6:6:169:ARG:NH2	7:9:142:GLU:OE2	2.36	0.59
2:2:98:TYR:HA	2:2:157:ASN:HD21	1.67	0.58
3:3:262:TRP:HB2	3:3:390:LEU:HD21	1.84	0.58
2:2:175:GLU:HG3	2:2:182:PRO:HG3	1.85	0.57
3:3:127:ARG:NH2	4:4:326:ASP:O	2.37	0.57
7:9:54:LYS:NZ	30:9:509:HOH:O	2.37	0.57
3:3:201:ASP:OD2	3:3:268:ARG:NH2	2.35	0.56
4:4:110:SER:OG	4:4:149:ASN:ND2	2.37	0.56
2:2:149:VAL:O	2:2:190:ARG:NH2	2.36	0.56
3:3:194:GLU:HG3	3:3:389:PRO:HB3	1.86	0.56
3:3:515:ARG:NH2	3:3:531:CYS:O	2.38	0.55
3:3:396:ARG:NH1	3:3:416:THR:O	2.39	0.55
3:3:329:ILE:HD13	3:3:505:LEU:HD22	1.88	0.55
5:5:74:SER:HB3	5:5:97:LEU:HB3	1.88	0.55
1:1:428:GLU:HA	1:1:431:GLN:HG2	1.90	0.54
4:4:282:GLU:HB3	4:4:313:GLN:HE22	1.72	0.54
3:3:190:MET:HG2	3:3:192:MET:HG2	1.90	0.54
4:4:335:ARG:NH2	7:9:129:ASP:OD1	2.41	0.54
6:6:52:LEU:HB2	6:6:90:GLY:HA3	1.90	0.54
2:2:105:THR:OG1	22:2:300:FES:S2	2.64	0.54
3:3:158:ARG:HB3	3:3:202:ILE:HD12	1.88	0.54
3:3:364:LEU:HD12	3:3:491:ASN:HB3	1.90	0.54
3:3:601:ARG:NH2	3:3:614:ASP:OD1	2.41	0.54
5:5:77:ASP:OD2	5:5:79:THR:OG1	2.26	0.54
4:4:109:VAL:HG11	4:4:152:MET:HG2	1.89	0.54
4:4:391:ILE:O	4:4:430:ARG:NH1	2.41	0.53
4:4:352:TYR:HD1	7:9:86:VAL:HG21	1.74	0.53
5:5:151:ILE:HG23	5:5:152:LEU:HG	1.90	0.53
3:3:356:THR:HG21	3:3:503:LEU:HD22	1.91	0.53
3:3:252:PRO:HG3	3:3:263:ILE:HG12	1.90	0.53
7:9:92:ILE:HG12	7:9:111:ILE:HG12	1.89	0.52
1:1:132:ARG:NH1	30:1:618:HOH:O	2.41	0.52
3:3:198:ASN:OD1	3:3:268:ARG:NH2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:142:PHE:HB3	1:1:145:GLU:HB2	1.91	0.52
4:4:233:ARG:NH2	7:9:23:GLN:O	2.42	0.52
3:3:377:VAL:HG23	3:3:404:LEU:HD11	1.91	0.51
6:6:174:ARG:NH1	30:6:311:HOH:O	2.41	0.51
4:4:188:ARG:NH2	30:4:535:HOH:O	2.41	0.51
4:4:324:LYS:NZ	30:4:538:HOH:O	2.43	0.51
3:3:155:GLN:NE2	30:3:943:HOH:O	2.43	0.51
5:5:33:LEU:HD13	5:5:60:VAL:HG22	1.93	0.51
4:4:226:GLU:OE1	4:4:305:ARG:NH2	2.36	0.50
5:5:65:ARG:NH1	5:5:123:VAL:O	2.44	0.50
1:1:289:GLY:HA3	1:1:293:ASN:HD22	1.76	0.50
2:2:156:ILE:HD13	2:2:176:LEU:HD11	1.94	0.50
5:5:121:VAL:HG21	5:5:146:PRO:HD3	1.94	0.50
3:3:231:MET:HB3	3:3:266:LYS:HD2	1.94	0.50
3:3:349:PHE:H	3:3:509:PRO:HB2	1.77	0.50
4:4:135:GLN:HB3	4:4:276:ASP:HB3	1.94	0.49
3:3:443:LEU:HD13	3:3:477:ILE:HD11	1.92	0.49
5:5:129:TRP:O	5:5:132:ARG:HB3	2.12	0.49
3:3:12:PHE:HB2	3:3:78:ASN:HA	1.94	0.49
4:4:354:GLU:OE2	4:4:357:GLN:NE2	2.46	0.49
6:6:54:CYS:HB2	19:6:201:SF4:S2	2.52	0.49
1:1:270:GLU:OE1	1:1:283:HIS:NE2	2.45	0.49
6:6:35:ASP:HB3	25:6:203:3PE:H331	1.94	0.49
2:2:116:ILE:HG23	2:2:169:ILE:HG21	1.95	0.49
3:3:51:ASN:ND2	30:3:945:HOH:O	2.45	0.49
6:6:118:SER:N	19:6:201:SF4:S4	2.85	0.49
3:3:255:HIS:NE2	3:3:634:ASP:OD1	2.45	0.49
5:5:79:THR:HB	5:5:93:VAL:HB	1.95	0.48
6:6:36:LEU:HD13	25:6:203:3PE:H392	1.95	0.48
4:4:179:GLU:OE2	6:6:66:ARG:NH1	2.40	0.48
4:4:146:ARG:NH1	30:4:543:HOH:O	2.45	0.48
4:4:334:LYS:NZ	30:4:544:HOH:O	2.45	0.48
5:5:95:ASN:ND2	30:5:321:HOH:O	2.46	0.48
3:3:119:GLN:HB2	3:3:123:PHE:HD2	1.79	0.48
1:1:96:ASN:ND2	1:1:187:GLY:O	2.37	0.48
3:3:194:GLU:HG2	3:3:195:LEU:HG	1.95	0.48
1:1:69:GLY:O	21:1:503:NAI:H2N	2.13	0.48
4:4:123:GLU:OE2	4:4:138:ARG:NH2	2.35	0.48
3:3:140:LYS:HB2	3:3:148:THR:HG21	1.95	0.48
1:1:21:ILE:O	1:1:117:LYS:NZ	2.36	0.47
4:4:65:VAL:HB	4:4:77:ASP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:21:ILE:HG12	1:1:233:THR:HG21	1.96	0.47
1:1:71:ALA:HB2	21:1:503:NAI:H4D	1.96	0.47
3:3:60:GLU:HG2	3:3:78:ASN:HB3	1.95	0.47
5:5:56:GLY:HA2	5:5:59:PRO:HD2	1.95	0.47
3:3:382:THR:HG23	3:3:384:PRO:HD3	1.95	0.47
3:3:478:ARG:NH2	3:3:485:GLY:O	2.48	0.47
4:4:155:THR:HB	4:4:167:PHE:HA	1.96	0.47
4:4:296:ARG:HH21	4:4:420:THR:HG21	1.78	0.47
5:5:137:MET:HA	5:5:161:PRO:HD2	1.97	0.47
2:2:159:ASN:HB3	2:2:184:PRO:HB3	1.96	0.47
6:6:58:GLU:HG2	6:6:151:PRO:O	2.14	0.47
6:6:71:ARG:HH22	7:9:49:ASN:HA	1.80	0.47
3:3:182:GLN:NE2	30:3:936:HOH:O	2.41	0.46
4:4:145:THR:OG1	4:4:181:TYR:OH	2.30	0.46
2:2:37:ASN:ND2	30:2:405:HOH:O	2.48	0.46
3:3:582:GLN:OE1	3:3:620:ARG:NH1	2.48	0.46
1:1:144:ASN:O	1:1:148:ASN:HB2	2.15	0.46
2:2:121:GLN:HE21	2:2:128:VAL:HG23	1.81	0.46
24:9:401:PC1:H331	24:9:401:PC1:H362	1.78	0.46
4:4:63:ARG:HB3	4:4:79:HIS:HB2	1.98	0.46
1:1:70:GLY:HA3	21:1:503:NAI:H1D	1.98	0.46
1:1:367:GLU:OE1	3:3:100:ASN:ND2	2.42	0.46
4:4:200:HIS:NE2	7:9:124:GLU:OE1	2.48	0.46
4:4:224:GLU:OE2	7:9:40:TYR:OH	2.32	0.46
3:3:115:ASP:O	3:3:119:GLN:HG2	2.17	0.45
1:1:94:VAL:O	1:1:222:VAL:HA	2.17	0.45
3:3:175:THR:HG21	3:3:186:TYR:HB2	1.98	0.45
1:1:199:LYS:NZ	30:1:633:HOH:O	2.49	0.45
1:1:200:GLN:NE2	3:3:174:THR:O	2.47	0.45
5:5:96:LEU:HB2	5:5:105:ILE:HG22	1.99	0.45
1:1:363:THR:HG21	3:3:97:LEU:HG	1.99	0.45
2:2:50:VAL:HG12	2:2:69:VAL:HG22	1.98	0.45
2:2:55:GLN:NE2	2:2:91:ASN:OD1	2.49	0.45
3:3:569:LYS:HG3	3:3:571:ALA:HB2	1.99	0.45
3:3:243:ARG:HD2	3:3:244:THR:HG23	2.00	0.44
4:4:94:LYS:HD2	4:4:102:TYR:HE2	1.82	0.44
1:1:378:ARG:NE	3:3:132:GLU:OE2	2.43	0.44
1:1:49:LEU:HD11	1:1:123:LEU:HD21	2.00	0.44
1:1:243:ALA:HA	1:1:251:SER:HB3	2.00	0.44
4:4:190:HIS:CD2	6:6:150:PRO:HD3	2.52	0.44
5:5:195:ARG:HH12	7:9:93:THR:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:9:114:THR:HG21	7:9:144:HIS:CD2	2.52	0.44
3:3:518:PRO:HB2	3:3:538:PRO:HD3	2.00	0.44
1:1:92:TYR:O	1:1:220:THR:HA	2.17	0.44
1:1:118:LEU:HD13	1:1:225:VAL:HG13	2.00	0.44
1:1:184:TYR:HB3	1:1:357:GLU:HB3	1.98	0.44
3:3:187:ILE:HG13	3:3:189:LYS:HB2	1.98	0.44
1:1:432:ARG:HA	1:1:435:GLN:HG3	2.00	0.44
1:1:361:GLN:NE2	30:1:639:HOH:O	2.50	0.44
3:3:332:LYS:NZ	3:3:505:LEU:O	2.37	0.44
4:4:151:ILE:O	4:4:155:THR:OG1	2.31	0.44
3:3:284:VAL:HG12	3:3:559:VAL:HG22	2.00	0.43
1:1:276:LEU:HD21	1:1:297:VAL:HG11	1.99	0.43
4:4:141:PHE:O	4:4:145:THR:OG1	2.27	0.43
4:4:185:SER:O	7:9:62:ARG:NH1	2.51	0.43
4:4:324:LYS:HD3	4:4:331:SER:HB3	2.00	0.43
4:4:417:ILE:HA	4:4:420:THR:HG22	1.99	0.43
1:1:89:ARG:NH1	1:1:217:GLY:O	2.44	0.43
1:1:245:PHE:HB3	1:1:271:GLU:HG3	2.00	0.43
4:4:149:ASN:HD21	4:4:371:LYS:HG3	1.84	0.43
7:9:151:LYS:HE2	7:9:155:LEU:HD11	2.00	0.43
3:3:43:HIS:NE2	3:3:261:GLU:OE2	2.51	0.43
4:4:323:ILE:HD12	4:4:324:LYS:HG3	2.01	0.43
3:3:323:VAL:HG11	3:3:525:LEU:HD13	2.01	0.43
3:3:324:ASP:HB3	3:3:571:ALA:HB1	2.01	0.43
4:4:183:ARG:NH1	4:4:210:ASP:OD2	2.38	0.43
6:6:90:GLY:HA2	19:6:201:SF4:S3	2.59	0.43
7:9:132:VAL:HG21	7:9:165:ILE:HG21	2.00	0.43
5:5:28:TYR:OH	5:5:67:HIS:NE2	2.42	0.42
1:1:96:ASN:ND2	20:1:502:FMN:O4'	2.52	0.42
3:3:382:THR:HB	3:3:454:GLY:HA3	2.00	0.42
5:5:92:ILE:HD11	5:5:111:THR:HG22	2.02	0.42
1:1:265:PRO:O	2:2:190:ARG:NH1	2.39	0.42
4:4:104:ASP:HB3	4:4:190:HIS:ND1	2.34	0.42
4:4:359:PRO:HA	4:4:360:PRO:HD3	1.96	0.42
4:4:377:TYR:HB3	4:4:390:LYS:HB3	2.01	0.42
1:1:200:GLN:NE2	30:3:942:HOH:O	2.52	0.42
3:3:324:ASP:OD1	3:3:324:ASP:N	2.53	0.42
7:9:94:ILE:HA	7:9:108:ARG:O	2.19	0.42
4:4:226:GLU:HG3	4:4:230:THR:OG1	2.19	0.42
4:4:261:ARG:NH2	4:4:303:GLU:OE2	2.53	0.42
6:6:127:HIS:CD2	7:9:115:LYS:HE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:269:PHE:HB3	3:3:683:THR:HG21	2.01	0.41
3:3:365:ASN:N	3:3:491:ASN:OD1	2.53	0.41
1:1:97:ALA:HB3	1:1:138:ILE:HA	2.02	0.41
1:1:141:GLU:HG2	2:2:145:LEU:HD22	2.02	0.41
1:1:291:TRP:NE1	1:1:313:GLU:OE1	2.53	0.41
2:2:61:LEU:HD12	2:2:90:TYR:HB3	2.02	0.41
3:3:360:SER:O	3:3:365:ASN:ND2	2.33	0.41
4:4:379:VAL:HB	4:4:388:ARG:HB3	2.02	0.41
1:1:95:VAL:HG11	1:1:118:LEU:HD11	2.02	0.41
4:4:291:GLY:O	4:4:296:ARG:NH1	2.52	0.41
6:6:29:VAL:HG22	25:6:203:3PE:H3I3	2.03	0.41
2:2:24:THR:OG1	2:2:27:ASN:OD1	2.34	0.41
4:4:270:ARG:HG3	4:4:368:GLU:HB3	2.03	0.41
3:3:325:ALA:HB1	3:3:623:LEU:HD11	2.03	0.41
4:4:343:GLU:O	4:4:347:HIS:ND1	2.40	0.41
1:1:390:ASP:O	1:1:393:TRP:HB3	2.21	0.41
3:3:329:ILE:HD12	3:3:329:ILE:HA	1.87	0.41
3:3:503:LEU:HD21	3:3:509:PRO:HB3	2.02	0.41
4:4:149:ASN:ND2	4:4:370:PRO:HB2	2.36	0.41
4:4:430:ARG:NH2	5:5:133:GLU:OE2	2.54	0.41
5:5:134:ILE:HG22	5:5:140:VAL:HB	2.03	0.41
7:9:158:GLY:O	7:9:162:GLU:HB2	2.21	0.41
1:1:367:GLU:HB2	3:3:96:PHE:HB3	2.01	0.41
5:5:41:GLN:NE2	5:5:49:GLU:OE1	2.48	0.41
1:1:342:ASP:OD1	1:1:429:ARG:NH2	2.49	0.40
1:1:305:PRO:HG3	1:1:413:TRP:HB3	2.03	0.40
1:1:361:GLN:N	19:1:501:SF4:S4	2.94	0.40
3:3:140:LYS:HD3	3:3:150:MET:HG3	2.02	0.40
6:6:71:ARG:NH1	30:6:322:HOH:O	2.54	0.40
1:1:394:GLU:OE1	3:3:129:ARG:NH1	2.54	0.40
5:5:49:GLU:HG2	5:5:106:ARG:HB3	2.03	0.40
3:3:20:VAL:HG12	3:3:32:LYS:HD3	2.03	0.40
5:5:116:PRO:HB3	5:5:141:PHE:HD2	1.85	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	1	428/464 (92%)	412 (96%)	16 (4%)	0	100	100
2	2	211/246 (86%)	196 (93%)	15 (7%)	0	100	100
3	3	686/727 (94%)	664 (97%)	21 (3%)	1 (0%)	51	64
4	4	375/463 (81%)	365 (97%)	10 (3%)	0	100	100
5	5	206/266 (77%)	198 (96%)	8 (4%)	0	100	100
6	6	154/223 (69%)	149 (97%)	5 (3%)	0	100	100
7	9	174/217 (80%)	168 (97%)	6 (3%)	0	100	100
8	a	42/109 (38%)	41 (98%)	1 (2%)	0	100	100
9	b	93/124 (75%)	92 (99%)	1 (1%)	0	100	100
10	c	124/170 (73%)	122 (98%)	2 (2%)	0	100	100
11	d	289/380 (76%)	285 (99%)	4 (1%)	0	100	100
12	e	84/99 (85%)	81 (96%)	3 (4%)	0	100	100
13	f	111/116 (96%)	110 (99%)	1 (1%)	0	100	100
14	g	112/140 (80%)	107 (96%)	5 (4%)	0	100	100
15	h	92/114 (81%)	88 (96%)	4 (4%)	0	100	100
16	i	143/145 (99%)	142 (99%)	1 (1%)	0	100	100
17	j	80/157 (51%)	76 (95%)	4 (5%)	0	100	100
18	q	29/144 (20%)	27 (93%)	2 (7%)	0	100	100
All	All	3433/4304 (80%)	3323 (97%)	109 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	3	367	THR

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	1	344/368 (94%)	343 (100%)	1 (0%)	92 97
2	2	183/210 (87%)	182 (100%)	1 (0%)	88 95
3	3	578/608 (95%)	576 (100%)	2 (0%)	92 97
4	4	328/391 (84%)	326 (99%)	2 (1%)	86 94
5	5	189/230 (82%)	189 (100%)	0	100 100
6	6	132/181 (73%)	129 (98%)	3 (2%)	50 67
7	9	151/179 (84%)	151 (100%)	0	100 100
8	a	43/93 (46%)	43 (100%)	0	100 100
9	b	79/97 (81%)	79 (100%)	0	100 100
10	c	113/150 (75%)	113 (100%)	0	100 100
11	d	255/326 (78%)	254 (100%)	1 (0%)	91 96
12	e	76/82 (93%)	76 (100%)	0	100 100
13	f	101/102 (99%)	101 (100%)	0	100 100
14	g	107/124 (86%)	107 (100%)	0	100 100
15	h	84/96 (88%)	84 (100%)	0	100 100
16	i	131/131 (100%)	131 (100%)	0	100 100
17	j	76/141 (54%)	76 (100%)	0	100 100
18	q	26/122 (21%)	26 (100%)	0	100 100
All	All	2996/3631 (82%)	2986 (100%)	10 (0%)	92 97

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	148	ASN
2	2	122	LYS
3	3	39	ARG
3	3	179	ASN
4	4	252	ASN
4	4	430	ARG

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Mol	Chain	Res	Type
6	6	54	CYS
6	6	71	ARG
6	6	111	ARG
11	d	36	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	373	ASN
4	4	50	ASN
4	4	149	ASN
4	4	252	ASN
13	f	49	GLN
14	g	125	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
15	AYA	h	1	15	6,7,8	1.25	1 (16%)	5,8,10	1.01	0
4	2MR	4	85	4	10,12,13	2.31	3 (30%)	5,13,15	2.19	2 (40%)

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
15	AYA	h	1	15	-	0/4/6/8	-
4	2MR	4	85	4	-	1/10/13/15	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	85	2MR	CZ-NH2	4.70	1.43	1.33
4	4	85	2MR	CZ-NE	4.43	1.43	1.34
15	h	1	AYA	CA-N	-2.52	1.43	1.46
4	4	85	2MR	CQ1-NH1	-2.20	1.42	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	4	85	2MR	NE-CZ-NH2	-3.91	115.90	119.48
4	4	85	2MR	CD-NE-CZ	-2.43	118.86	123.41

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	4	85	2MR	NE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	$\#\|Z\|>2$
24	PC1	6	202	-	45,45,53	0.31	0	51,53,61	0.32	0
21	NAI	1	503	-	42,48,48	0.58	0	47,73,73	1.96	4 (8%)
19	SF4	3	801	3	0,12,12	-	-	-		
22	FES	2	300	2	0,4,4	-	-	-		
25	3PE	i	201	-	50,50,50	0.30	0	53,55,55	0.29	0
19	SF4	9	402	7	0,12,12	-	-	-		
19	SF4	6	201	6	0,12,12	-	-	-		
29	CDL	h	201	-	57,57,99	0.36	0	63,69,111	0.30	0
28	ZMP	g	201	-	27,33,36	0.66	0	32,40,45	1.28	3 (9%)
22	FES	3	803	3	0,4,4	-	-	-		
24	PC1	9	401	-	53,53,53	0.31	0	59,61,61	0.53	0
25	3PE	6	203	-	50,50,50	0.30	0	53,55,55	0.30	0
19	SF4	1	501	1	0,12,12	-	-	-		
20	FMN	1	502	-	33,33,33	1.12	3 (9%)	48,50,50	1.35	7 (14%)
27	NDP	d	401	-	45,52,52	0.58	0	53,80,80	0.54	1 (1%)
19	SF4	3	802	3	0,12,12	-	-	-		
19	SF4	9	403	7	0,12,12	-	-	-		

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
24	PC1	6	202	-	-	8/49/49/57	-
21	NAI	1	503	-	-	7/25/72/72	0/5/5/5
19	SF4	3	801	3	-	-	0/6/5/5
22	FES	2	300	2	-	-	0/1/1/1
25	3PE	i	201	-	-	7/54/54/54	-
29	CDL	h	201	-	-	19/68/68/110	-
19	SF4	6	201	6	-	-	0/6/5/5
19	SF4	9	402	7	-	-	0/6/5/5
28	ZMP	g	201	-	-	4/38/40/43	-
22	FES	3	803	3	-	-	0/1/1/1
24	PC1	9	401	-	-	10/57/57/57	-
19	SF4	1	501	1	-	-	0/6/5/5
20	FMN	1	502	-	-	10/18/18/18	0/3/3/3
27	NDP	d	401	-	-	4/30/77/77	0/5/5/5
19	SF4	9	403	7	-	-	0/6/5/5
19	SF4	3	802	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	3PE	6	203	-	-	12/54/54/54	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	502	FMN	C4A-N5	3.22	1.37	1.30
20	1	502	FMN	C10-N1	2.12	1.37	1.33
20	1	502	FMN	C4A-C10	-2.03	1.38	1.44

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	503	NAI	O5B-PA-O1A	-9.94	70.25	109.07
21	1	503	NAI	O2A-PA-O1A	-7.76	73.86	112.24
20	1	502	FMN	C4-N3-C2	-3.65	118.89	125.64
28	g	201	ZMP	C14-C15-N2	-3.14	105.55	111.90
28	g	201	ZMP	C15-C14-C13	-3.02	107.33	112.36
20	1	502	FMN	O4-C4-C4A	-2.85	119.04	126.60
20	1	502	FMN	C4A-C4-N3	2.80	120.30	113.19
20	1	502	FMN	C4A-C10-N10	2.75	120.50	116.48
28	g	201	ZMP	O1-C10-C9	-2.70	120.80	123.99
20	1	502	FMN	C4A-C10-N1	-2.69	118.48	124.73
21	1	503	NAI	O2A-PA-O5B	2.38	118.80	107.75
20	1	502	FMN	C4-C4A-C10	2.31	120.67	116.79
21	1	503	NAI	C5A-C6A-N6A	2.29	123.83	120.35
20	1	502	FMN	C10-C4A-N5	-2.19	120.22	124.86
27	d	401	NDP	C5A-C6A-N6A	2.13	123.60	120.35

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	1	502	FMN	C5'-O5'-P-O2P
20	1	502	FMN	C5'-O5'-P-O3P
21	1	503	NAI	C5D-O5D-PN-O3
24	6	202	PC1	C11-O13-P-O12
24	6	202	PC1	C11-O13-P-O14
24	6	202	PC1	C1-O11-P-O14
24	9	401	PC1	C11-O13-P-O12
24	9	401	PC1	C11-O13-P-O14
25	6	203	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
28	g	201	ZMP	S1-C11-C12-N1
28	g	201	ZMP	C12-C11-S1-C10
29	h	201	CDL	CA2-C1-CB2-OB2
29	h	201	CDL	CA2-OA2-PA1-OA3
29	h	201	CDL	CA3-OA5-PA1-OA3
29	h	201	CDL	CB2-OB2-PB2-OB3
29	h	201	CDL	CB3-OB5-PB2-OB3
29	h	201	CDL	CB3-OB5-PB2-OB4
29	h	201	CDL	O1-C1-CB2-OB2
24	6	202	PC1	C11-O13-P-O11
24	9	401	PC1	C11-O13-P-O11
29	h	201	CDL	CB2-OB2-PB2-OB5
29	h	201	CDL	CB3-OB5-PB2-OB2
25	i	201	3PE	C29-C2A-C2B-C2C
29	h	201	CDL	C56-C57-C58-C59
24	6	202	PC1	C3B-C3C-C3D-C3E
25	6	203	3PE	C3C-C3D-C3E-C3F
24	9	401	PC1	C2E-C2F-C2G-C2H
25	6	203	3PE	C36-C37-C38-C39
20	1	502	FMN	C2'-C3'-C4'-O4'
24	6	202	PC1	C1-O11-P-O13
24	9	401	PC1	C22-C21-O21-C2
20	1	502	FMN	C5'-O5'-P-O1P
25	6	203	3PE	C23-C24-C25-C26
24	6	202	PC1	C23-C24-C25-C26
25	6	203	3PE	C2D-C2E-C2F-C2G
29	h	201	CDL	CB3-CB4-CB6-OB8
25	6	203	3PE	C1-O11-P-O13
29	h	201	CDL	CA3-OA5-PA1-OA2
28	g	201	ZMP	O1-C10-S1-C11
24	9	401	PC1	O22-C21-O21-C2
21	1	503	NAI	PN-O3-PA-O5B
24	9	401	PC1	C34-C35-C36-C37
28	g	201	ZMP	C9-C10-S1-C11
20	1	502	FMN	C4'-C5'-O5'-P
29	h	201	CDL	C1-CB2-OB2-PB2
27	d	401	NDP	O4B-C4B-C5B-O5B
29	h	201	CDL	CA2-OA2-PA1-OA5
21	1	503	NAI	C5B-O5B-PA-O2A
24	6	202	PC1	C1-O11-P-O12
25	6	203	3PE	C1-O11-P-O14
25	i	201	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
20	1	502	FMN	N10-C1'-C2'-C3'
20	1	502	FMN	O3'-C3'-C4'-C5'
24	9	401	PC1	O13-C11-C12-N
29	h	201	CDL	CB4-CB3-OB5-PB2
21	1	503	NAI	O4D-C1D-N1N-C2N
25	6	203	3PE	C33-C34-C35-C36
20	1	502	FMN	C2'-C3'-C4'-C5'
24	9	401	PC1	C1-O11-P-O13
25	6	203	3PE	C11-O13-P-O11
25	i	201	3PE	C11-O13-P-O11
21	1	503	NAI	C2D-C1D-N1N-C2N
27	d	401	NDP	O4D-C1D-N1N-C6N
20	1	502	FMN	O3'-C3'-C4'-O4'
24	9	401	PC1	C3-C2-O21-C21
29	h	201	CDL	OB6-CB4-CB6-OB8
25	i	201	3PE	O21-C21-C22-C23
25	i	201	3PE	C36-C37-C38-C39
25	6	203	3PE	O11-C1-C2-O21
27	d	401	NDP	C2D-C1D-N1N-C6N
25	6	203	3PE	C3D-C3E-C3F-C3G
29	h	201	CDL	C52-C51-CB5-OB6
29	h	201	CDL	CB7-C71-C72-C73
27	d	401	NDP	C2B-O2B-P2B-O2X
25	i	201	3PE	O22-C21-C22-C23
21	1	503	NAI	C2N-C3N-C7N-N7N
25	6	203	3PE	C11-O13-P-O14
25	i	201	3PE	C1-O11-P-O14
29	h	201	CDL	C52-C51-CB5-OB7
21	1	503	NAI	C2D-C1D-N1N-C6N
20	1	502	FMN	N10-C1'-C2'-O2'

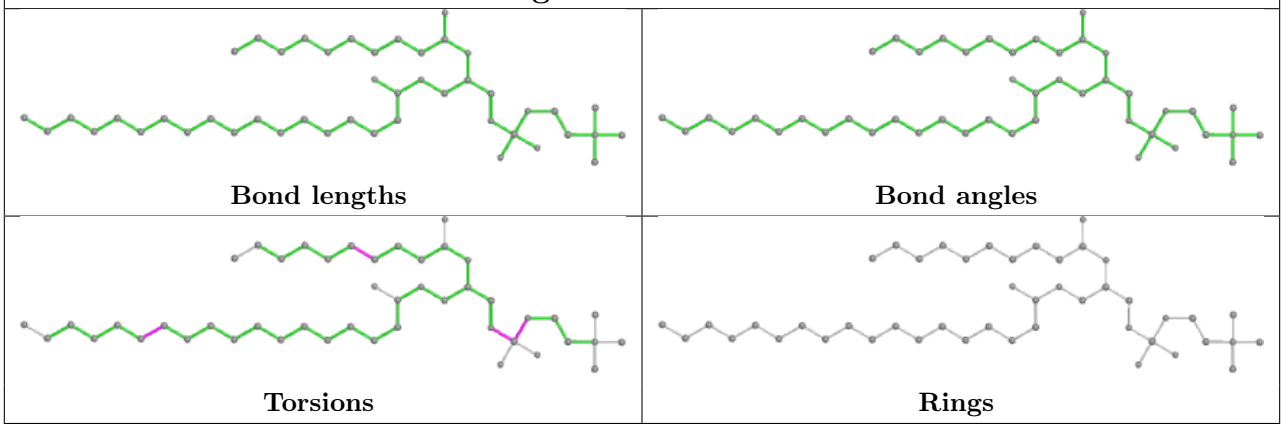
There are no ring outliers.

7 monomers are involved in 14 short contacts:

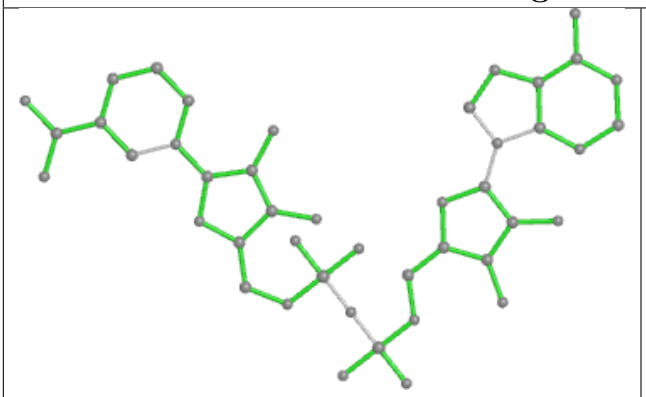
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	1	503	NAI	4	0
22	2	300	FES	1	0
19	6	201	SF4	3	0
24	9	401	PC1	1	0
25	6	203	3PE	3	0
19	1	501	SF4	1	0
20	1	502	FMN	1	0

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.

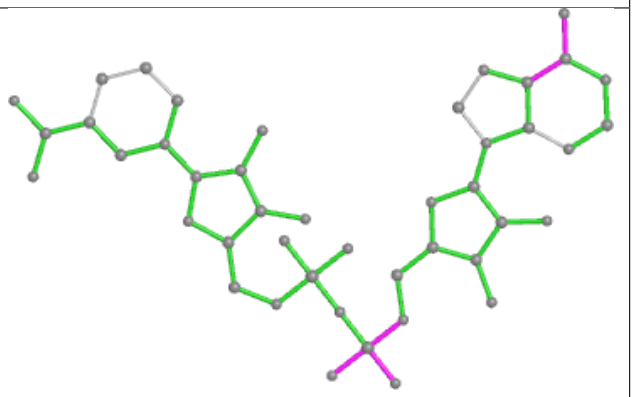
Ligand PC1 6 202



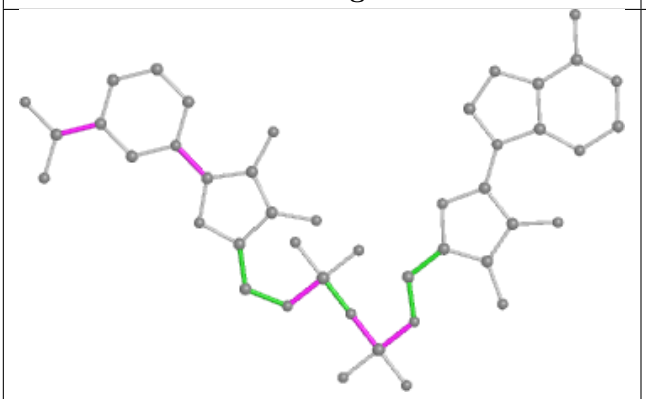
Ligand NAI 1 503



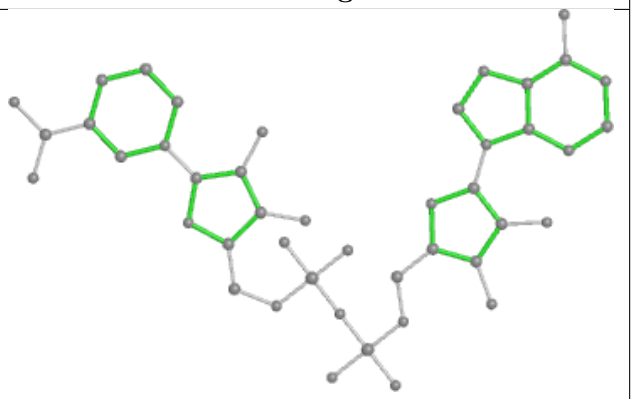
Bond lengths



Bond angles

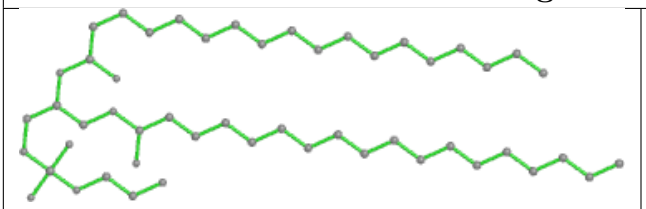


Torsions

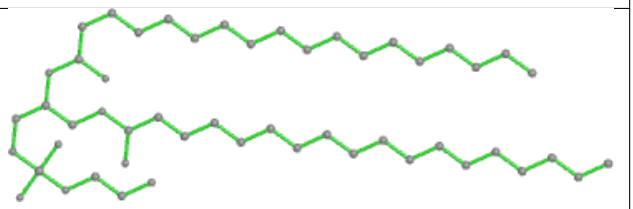


Rings

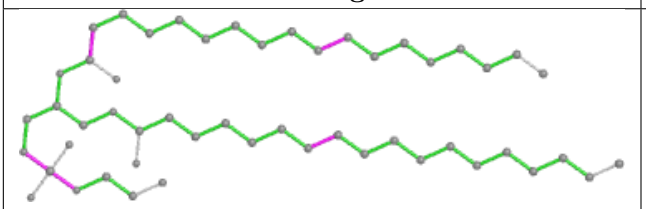
Ligand 3PE i 201



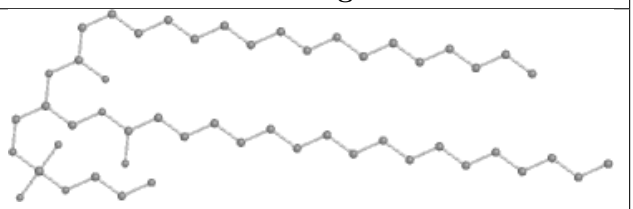
Bond lengths



Bond angles

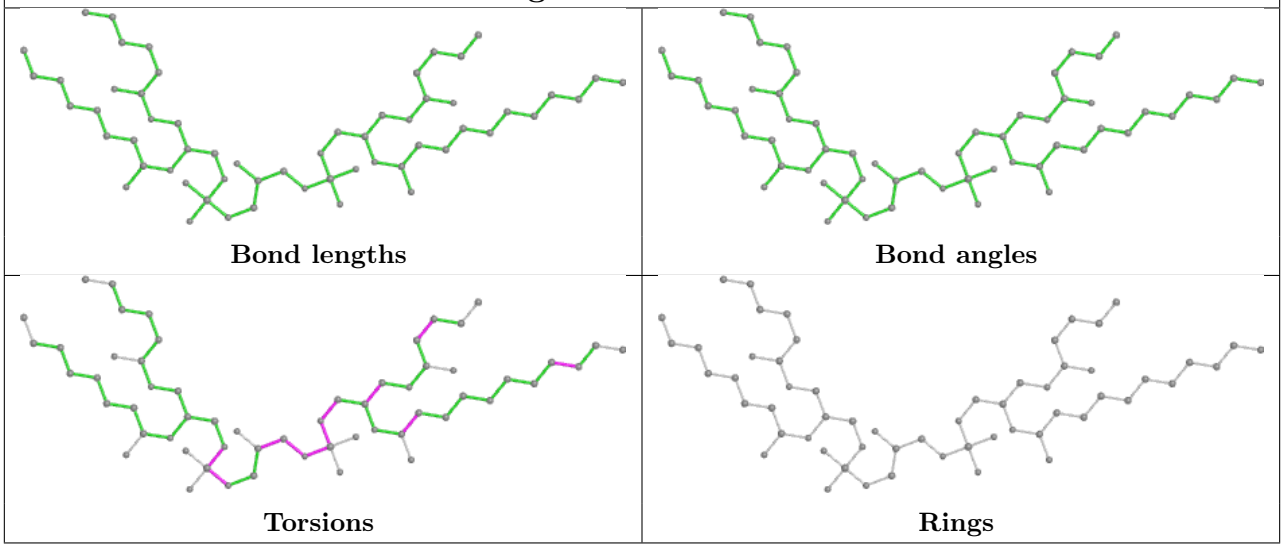


Torsions

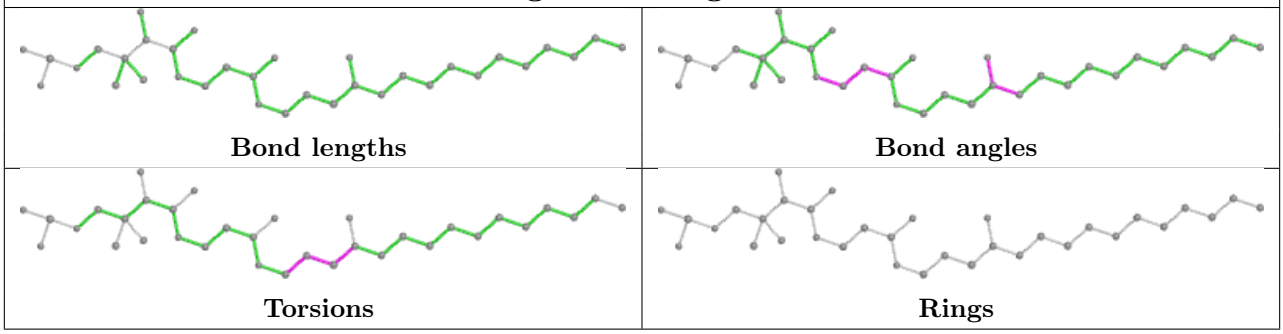


Rings

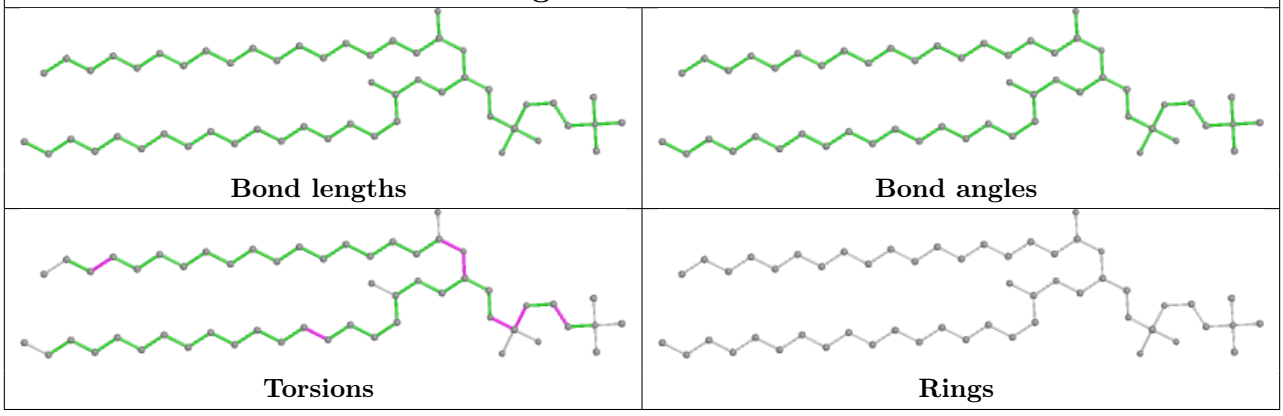
Ligand CDL h 201



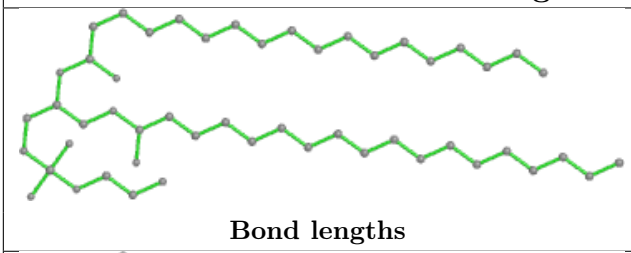
Ligand ZMP g 201



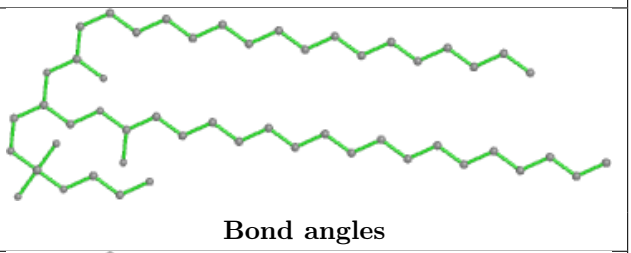
Ligand PC1 9 401



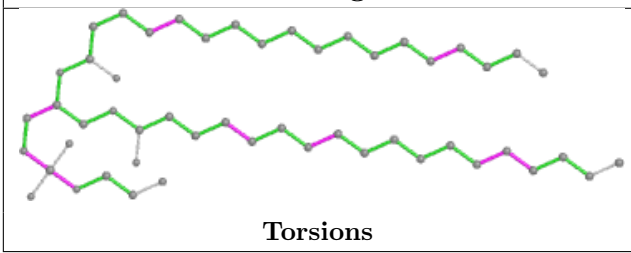
Ligand 3PE 6 203



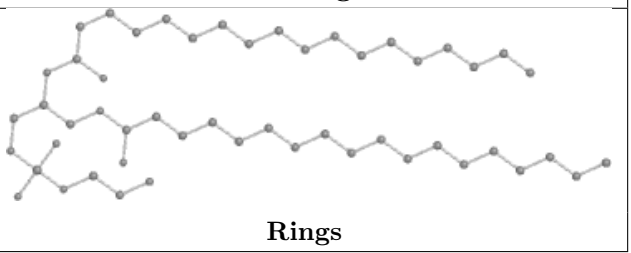
Bond lengths



Bond angles

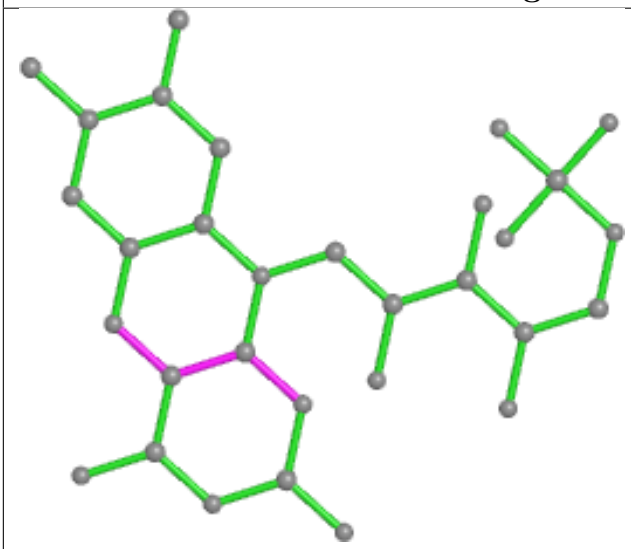


Torsions

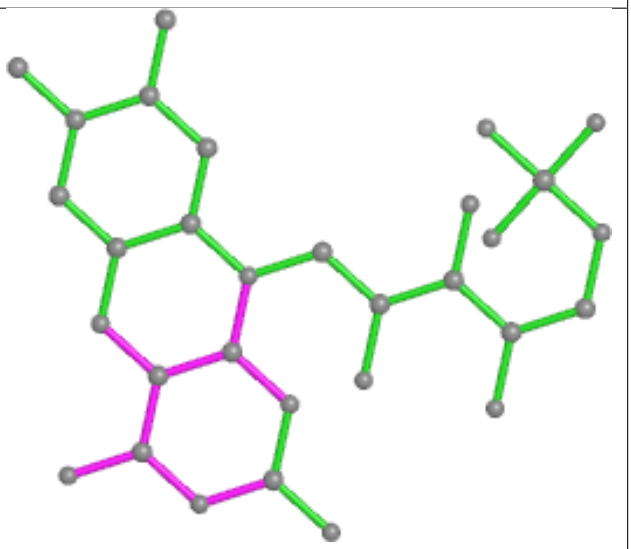


Rings

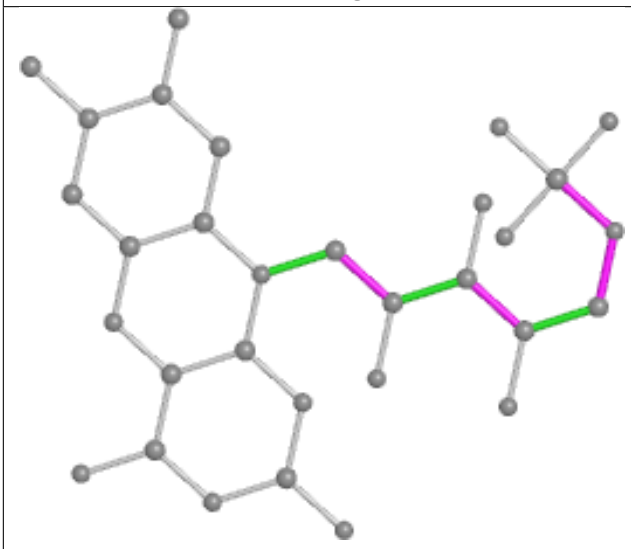
Ligand FMN 1 502



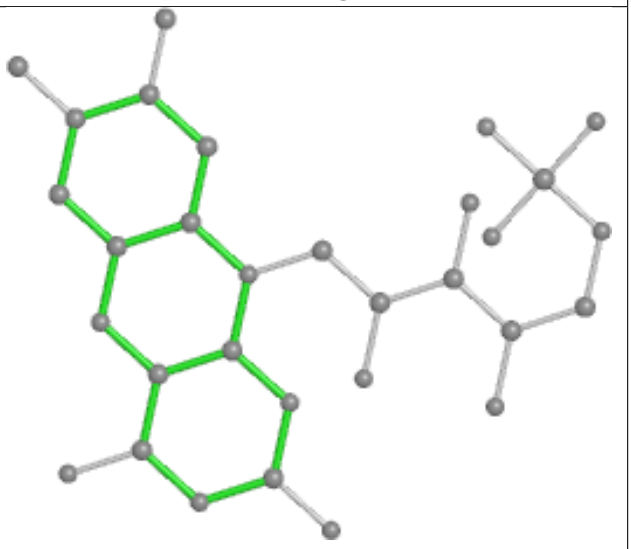
Bond lengths



Bond angles

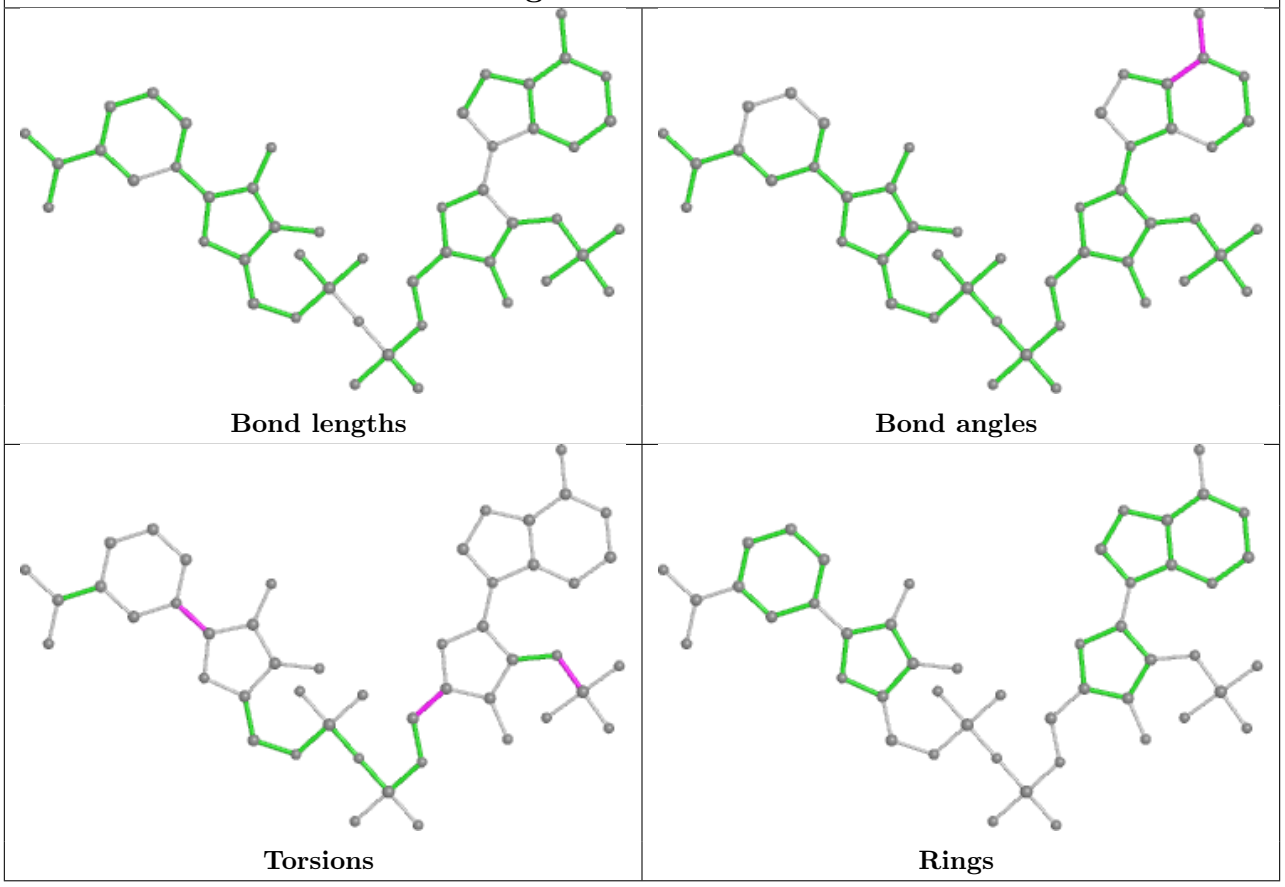


Torsions



Rings

Ligand NDP d 401



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.

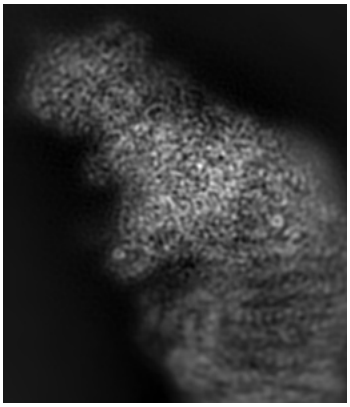
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11241. These allow visual inspection of the internal detail of the map and identification of artifacts.

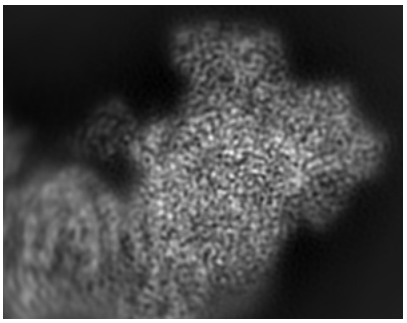
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

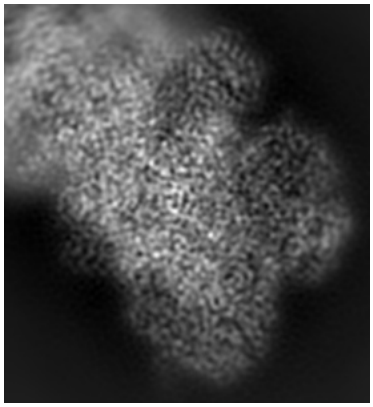
6.1.1 Primary map



X



Y

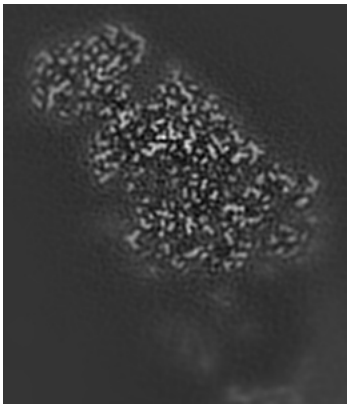


Z

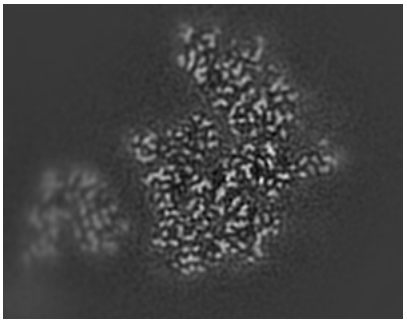
The images above show the map projected in three orthogonal directions.

6.2 Central slices

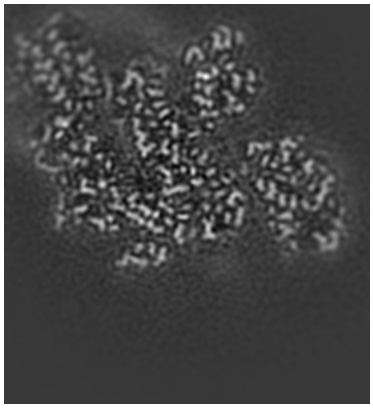
6.2.1 Primary map



X Index: 147



Y Index: 160

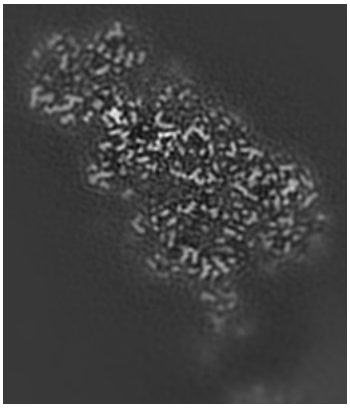


Z Index: 187

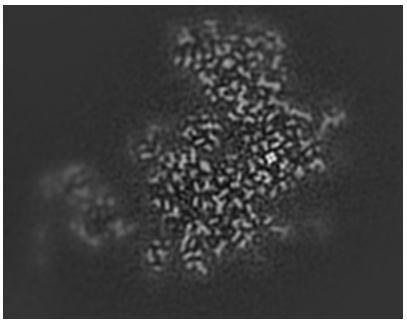
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

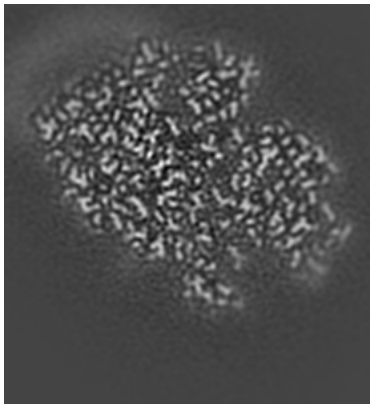
6.3.1 Primary map



X Index: 155



Y Index: 149

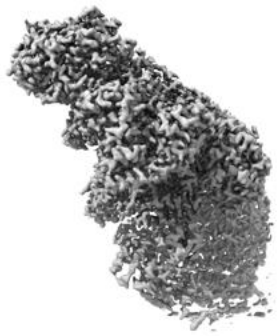


Z Index: 215

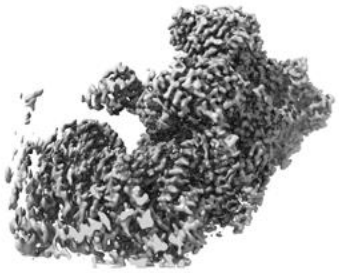
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

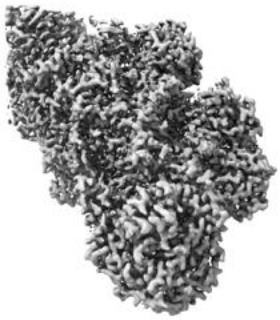
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.105. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

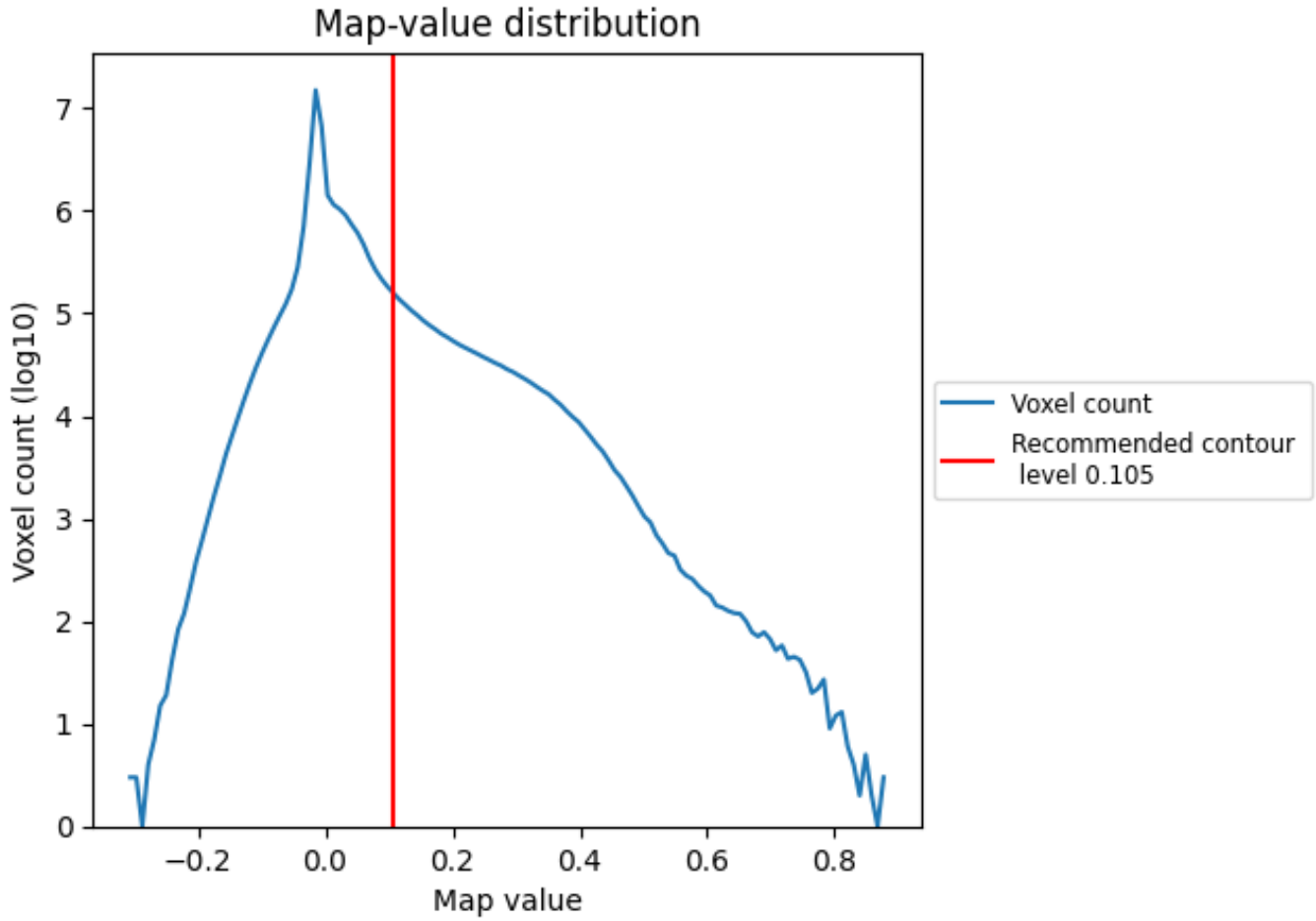
6.5 Mask visualisation (i)

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

7 Map analysis

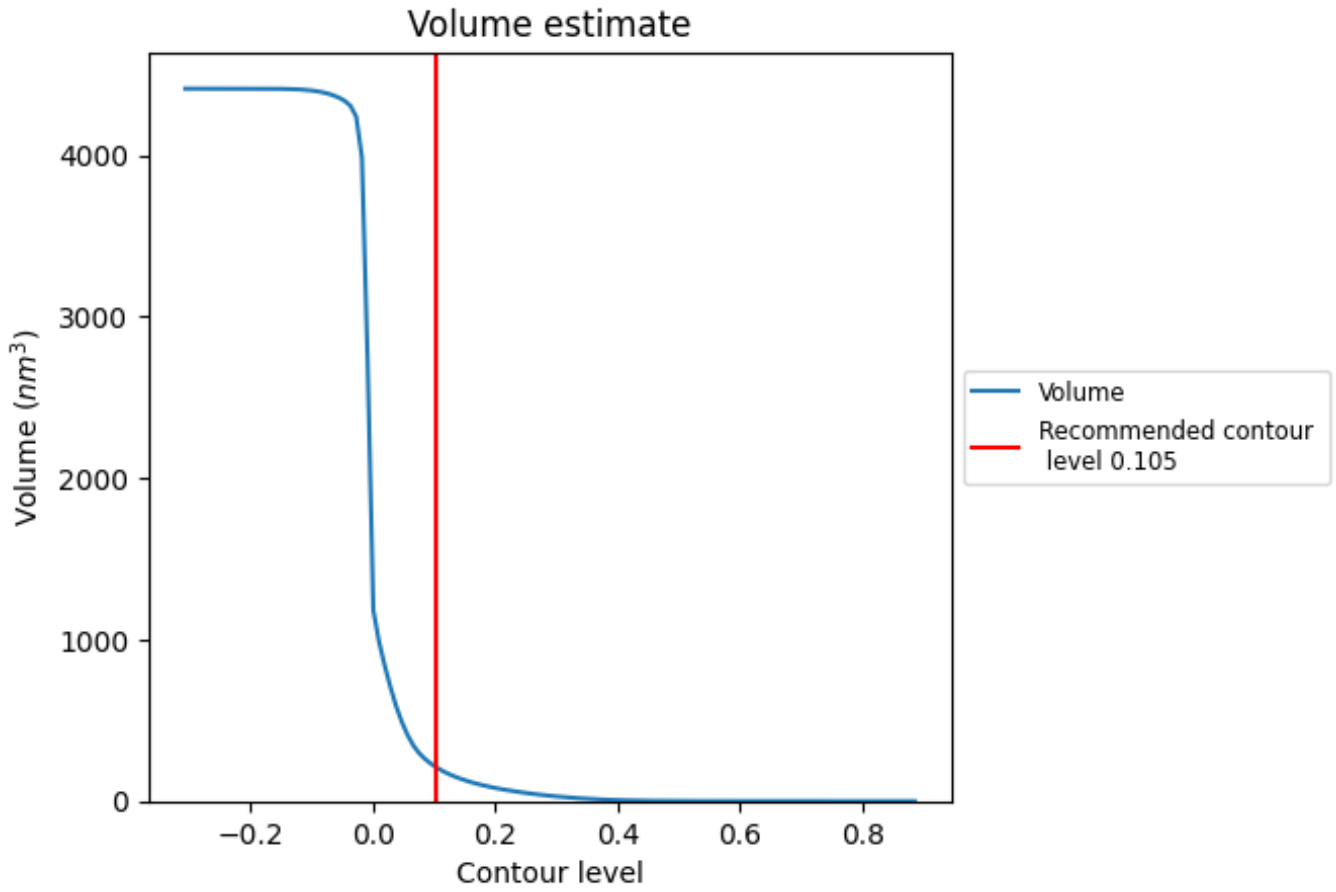
This section contains the results of statistical analysis of the map.

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 (i)



The volume at the recommended contour level is 208 nm^3; this corresponds to an approximate mass of 188 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.

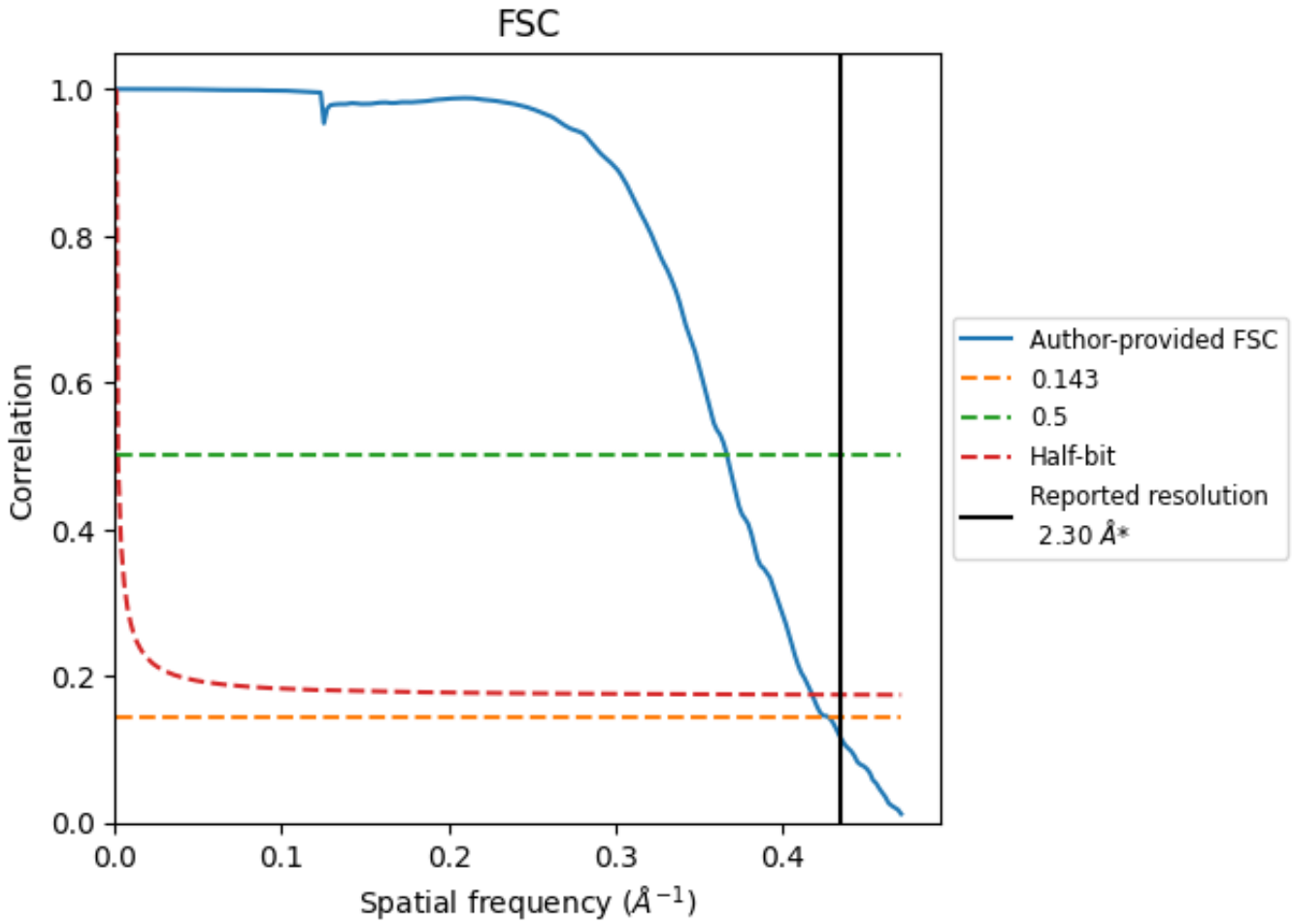
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.435 Å^{-1}

8.2 Resolution estimates (i)

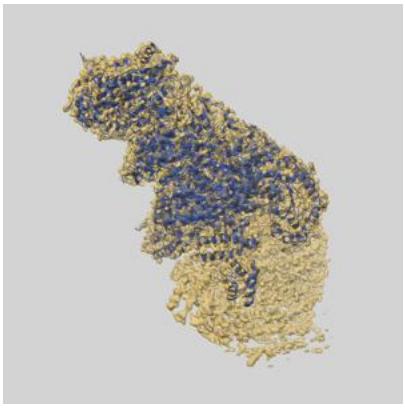
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.34	2.72	2.39
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

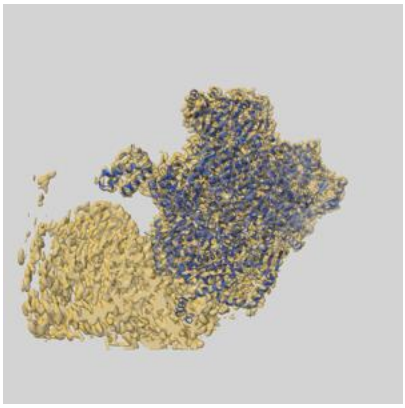
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11241 and PDB model 6ZK9. Per-residue inclusion information can be found in section 3 on page 14.

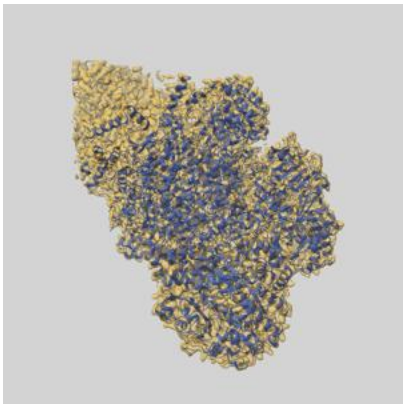
9.1 Map-model overlay



X



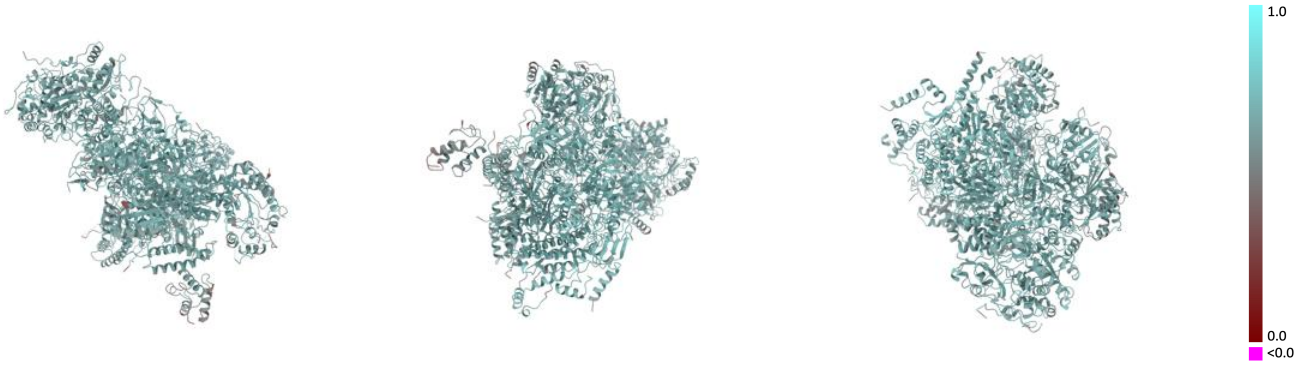
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.105 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.

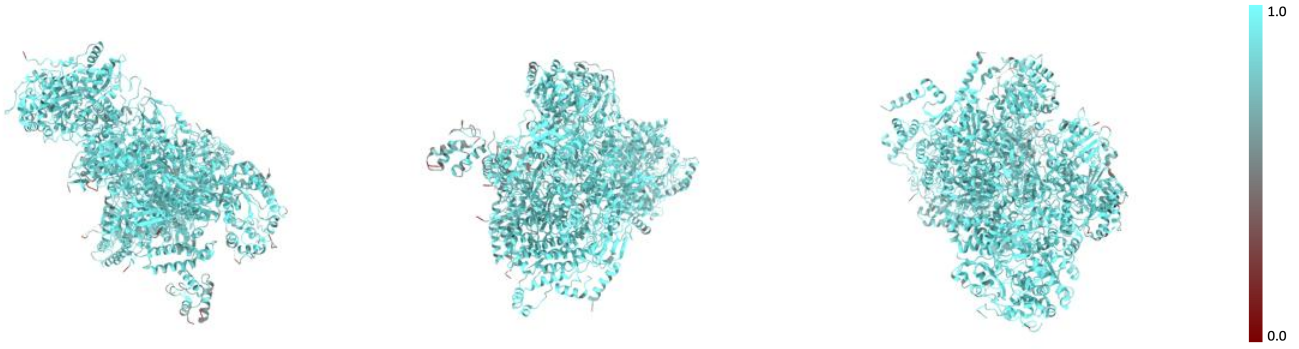
9.2 Q-score mapped to coordinate model (i)



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.

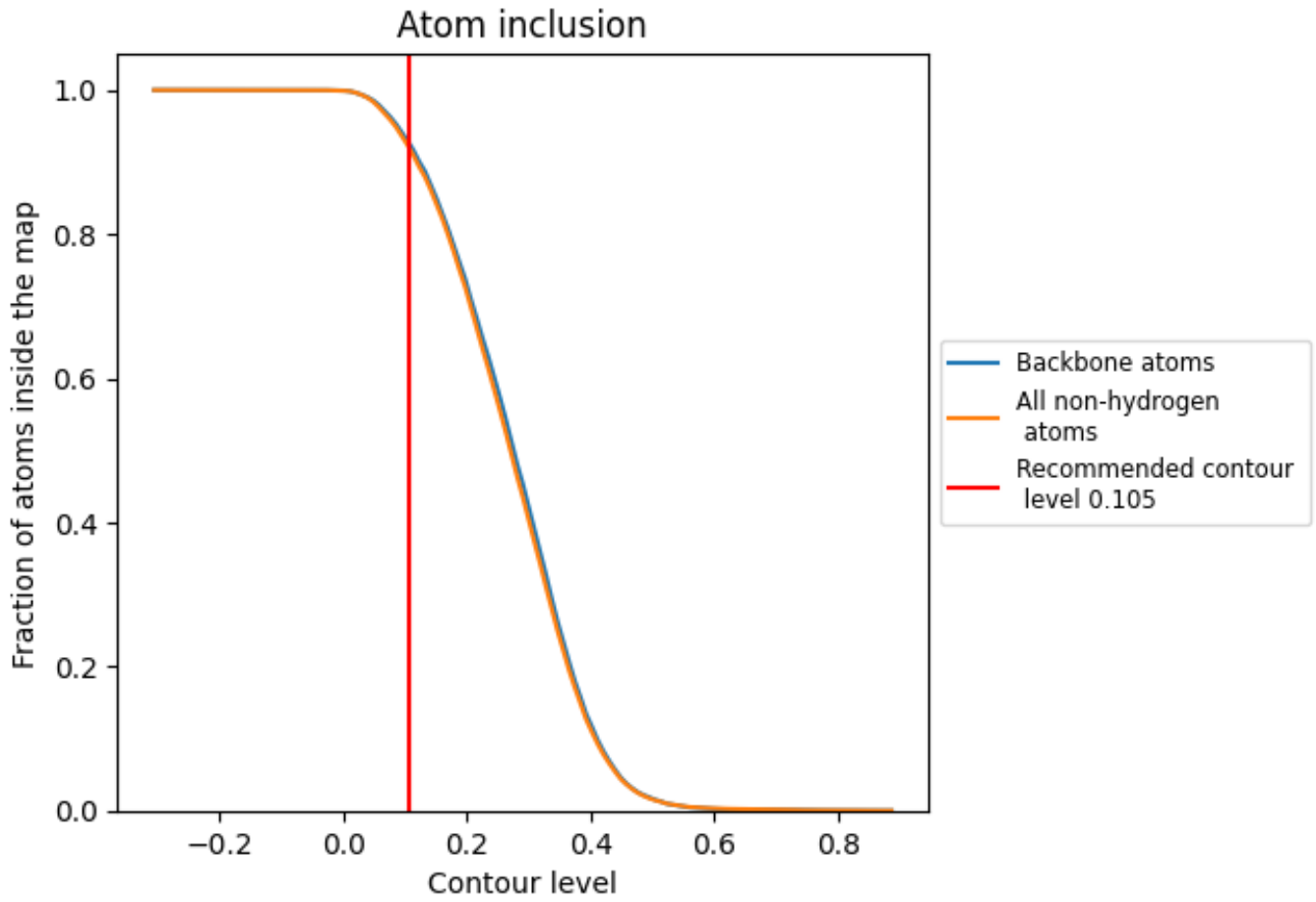
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.105).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 92% 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 (0.105) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9216	0.6600
1	0.9506	0.6560
2	0.9223	0.6370
3	0.9319	0.6660
4	0.9603	0.6980
5	0.9589	0.6970
6	0.9317	0.6780
9	0.9521	0.6940
a	0.9227	0.6330
b	0.9276	0.6730
c	0.9321	0.6830
d	0.8934	0.6300
e	0.8824	0.6050
f	0.8971	0.6370
g	0.9014	0.6460
h	0.9039	0.6530
i	0.9150	0.6620
j	0.6901	0.5180
q	0.9195	0.6300