



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:42 PM UTC

PDB ID : 6ZK9 / pdb_00006zk9
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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

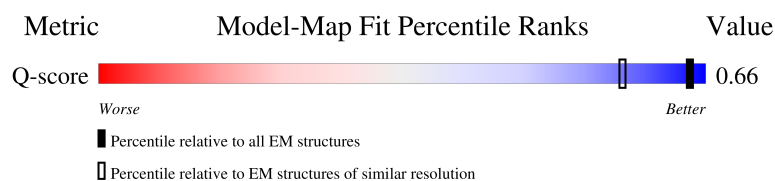
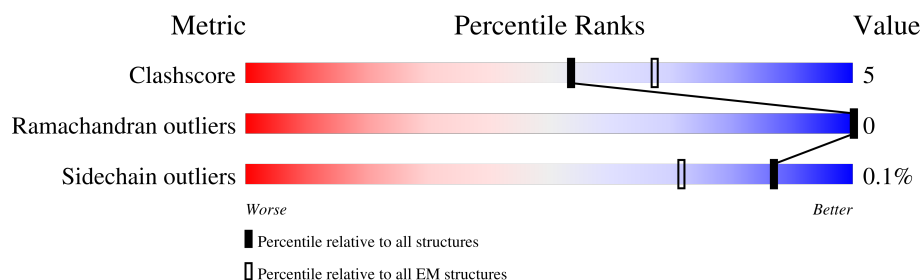
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4254 (1.80 - 2.80)

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

Mol	Chain	Length	Quality of chain
1	1	464	
2	2	246	
3	3	727	
4	4	463	

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Mol	Chain	Length	Quality of chain
5	5	266	
6	6	223	
7	9	217	
8	a	109	
9	b	124	
10	c	170	
11	d	380	
12	e	99	
13	f	116	
14	g	140	
15	h	114	
16	i	145	
17	j	157	
18	q	144	

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

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
1	1	430	Total	C	N	O	S	0	0
			3312	2086	593	613	20		

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

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

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

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

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

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

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

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

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

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

- 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		

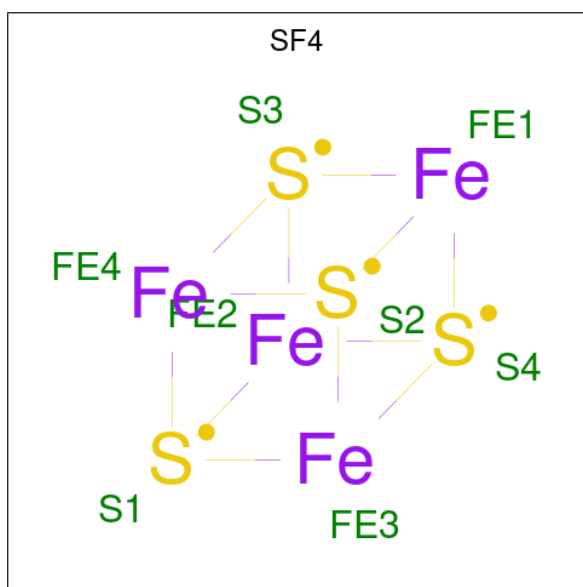
- Molecule 17 is a protein called Acyl carrier protein.

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.

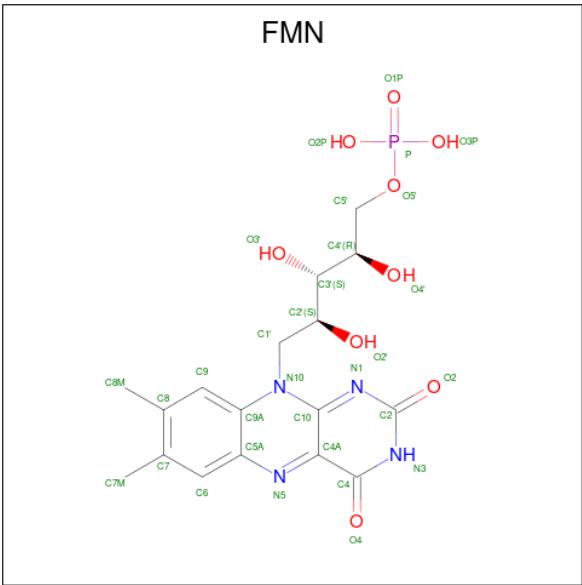
Mol	Chain	Residues	Atoms					AltConf	Trace
18	q	31	Total	C	N	O	S	0	0
			245	157	44	42	2		

- Molecule 19 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



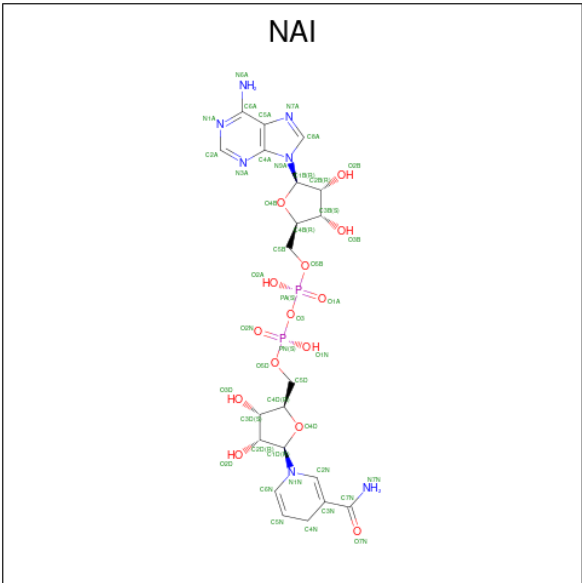
Mol	Chain	Residues	Atoms			AltConf
19	1	1	Total	Fe	S	0
			8	4	4	
19	3	1	Total	Fe	S	0
			8	4	4	
19	3	1	Total	Fe	S	0
			8	4	4	
19	6	1	Total	Fe	S	0
			8	4	4	
19	9	1	Total	Fe	S	0
			8	4	4	
19	9	1	Total	Fe	S	0
			8	4	4	

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



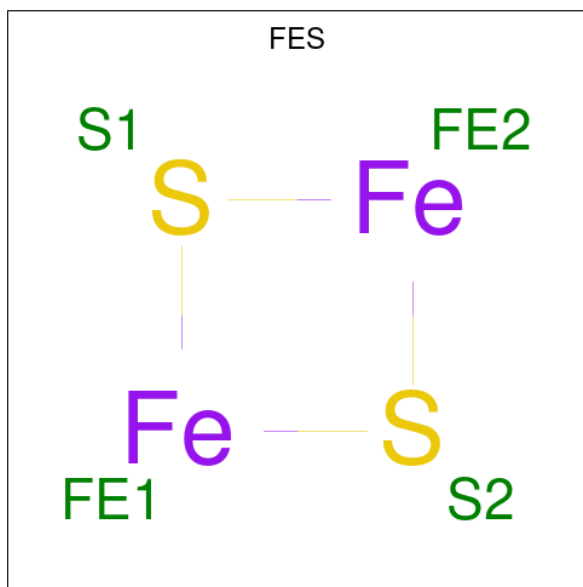
Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 21 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: 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 (CCD ID: FES) (formula: Fe_2S_2).

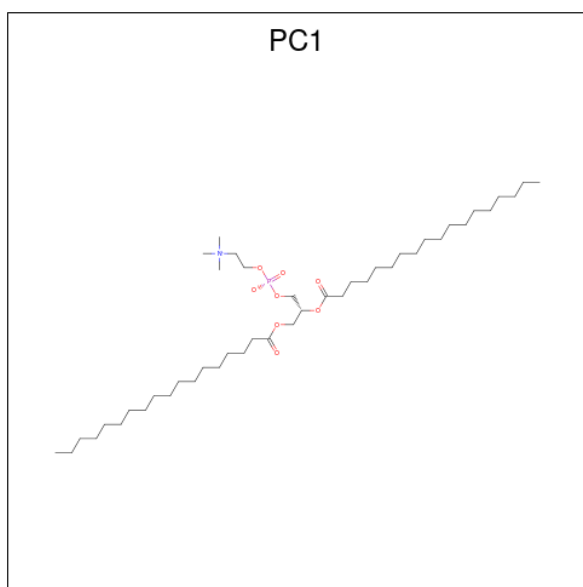


Mol	Chain	Residues	Atoms			AltConf
22	2	1	Total	Fe	S	0
			4	2	2	
22	3	1	Total	Fe	S	0
			4	2	2	

- Molecule 23 is POTASSIUM ION (CCD ID: K) (formula: K).

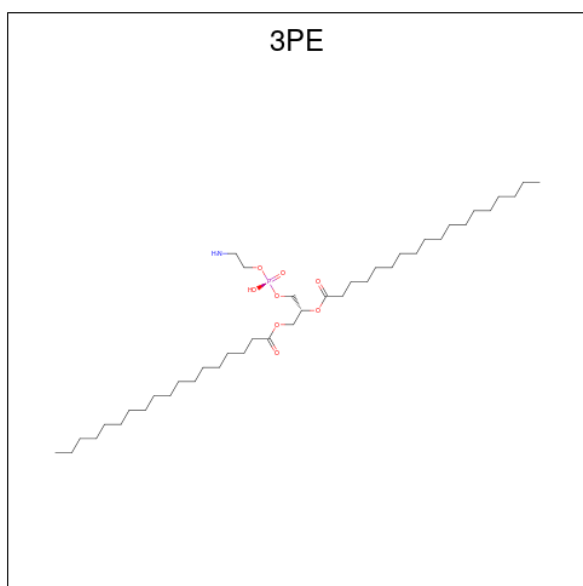
Mol	Chain	Residues	Atoms		AltConf
23	3	1	Total	K	0
			1	1	

- Molecule 24 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



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-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 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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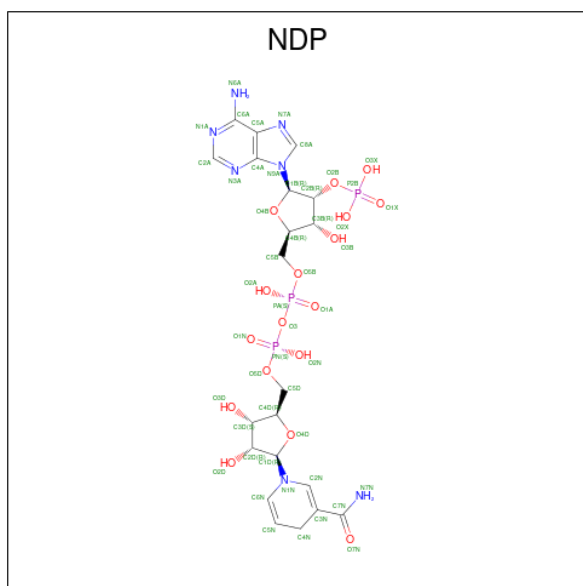
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Mol	Chain	Residues	Atoms					AltConf
25	i	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

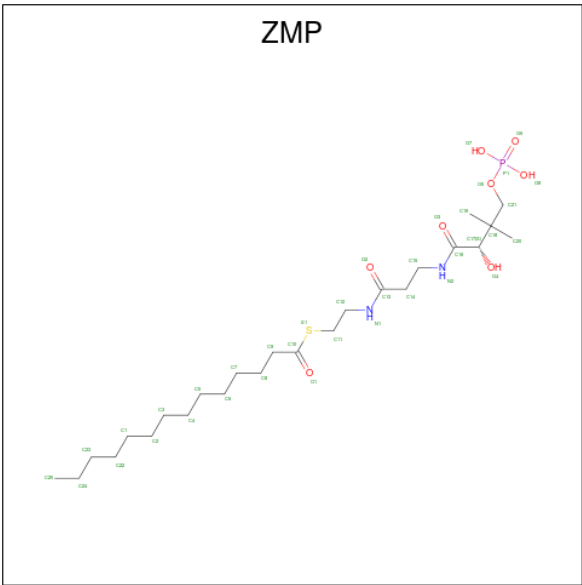
Mol	Chain	Residues	Atoms		AltConf
26	b	1	Total	Zn	0
			1	1	

- Molecule 27 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



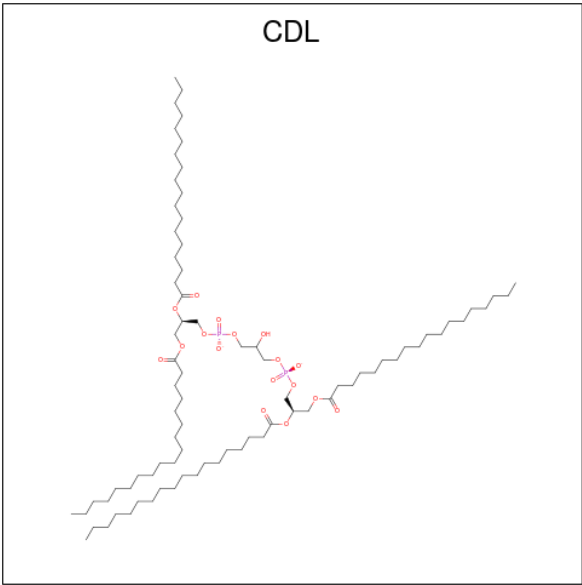
Mol	Chain	Residues	Atoms					AltConf
27	d	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 28 is S-[2-(N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



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 (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

- Molecule 30 is water.

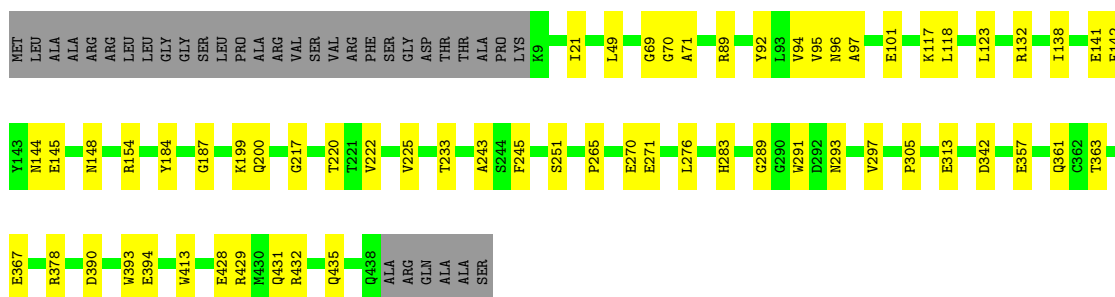
Mol	Chain	Residues	Atoms		AltConf
30	1	123	Total 123	O 123	0
30	2	44	Total 44	O 44	0
30	3	285	Total 285	O 285	0
30	4	200	Total 200	O 200	0
30	5	129	Total 129	O 129	0
30	6	81	Total 81	O 81	0
30	9	110	Total 110	O 110	0
30	a	6	Total 6	O 6	0
30	b	67	Total 67	O 67	0
30	c	109	Total 109	O 109	0
30	d	79	Total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

3 Residue-property plots

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

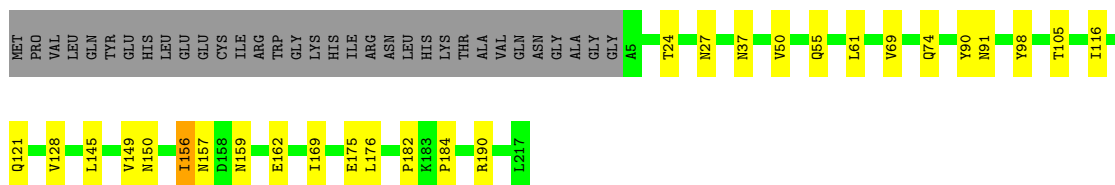
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1: 



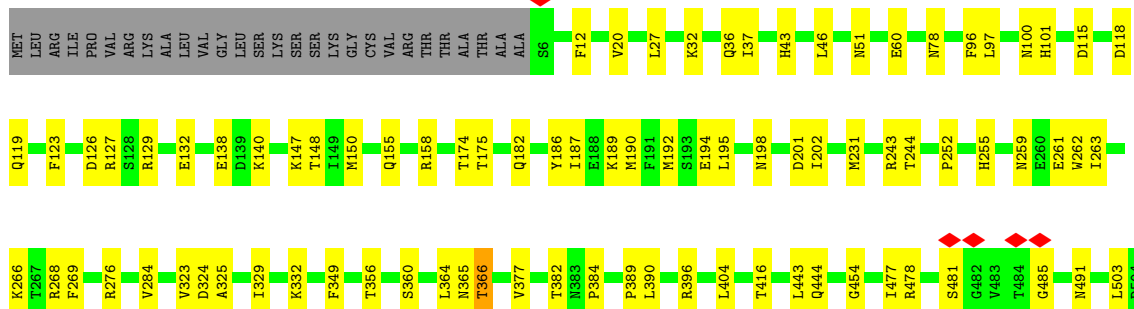
- Molecule 2: Mitochondrial complex I, 24 kDa subunit

Chain 2: 



- Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

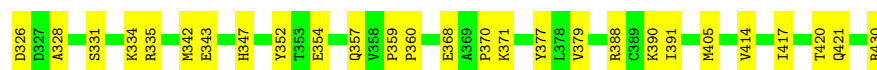
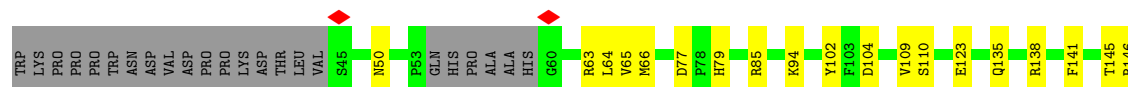
Chain 3: 





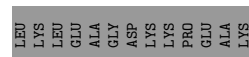
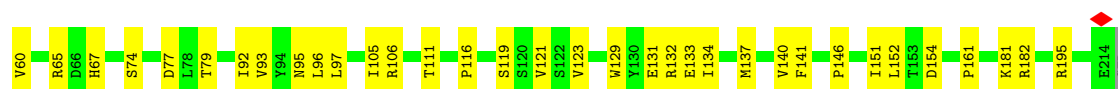
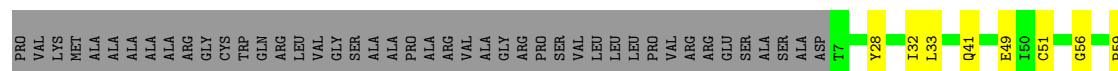
- Molecule 4: Mitochondrial complex I, 49 kDa subunit

Chain 4: 65% 17% 18%



- Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3

Chain 5: 62% 16% 22%



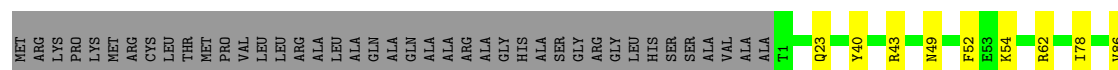
- Molecule 6: Mitochondrial complex I, PSST subunit

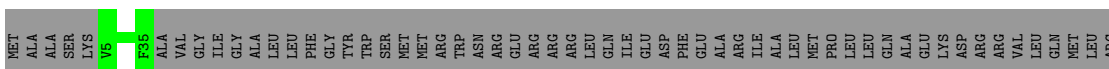
Chain 6: 62% 8% 30%



- Molecule 7: Mitochondrial complex I, TYKY subunit

Chain 9: 69% 12% 19%





GLU	ASN	LEU	GLU	GLU	GLU	ALA	THR	ILE	MET	LYS	ASP	VAL	PRO	GLY	TRP	LYS	VAL	GLY	GLU	SER	PHE	HIS	THR	THR	ARG	TRP	VAL	THR	PRO	MET	MET	GLY	GLU	LEU	TYR	GLY	LEU	ARG	THR	GLY	GLU	GLU	ILE	LEU	SER	SER	THR	TYR	GLY	PHE	ILE	TRP	TYR	THR
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4 Experimental information

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 ($e^-/\text{\AA}^2$)	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, FES, AYA, FMN, ZN, NAI, 2MR, K, NDP, PC1, CDL, 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	0.31	0/3386	0.56	0/4575
2	2	0.30	0/1695	0.58	2/2306 (0.1%)
3	3	0.32	0/5362	0.55	2/7266 (0.0%)
4	4	0.35	0/3103	0.57	0/4190
5	5	0.32	0/1776	0.56	0/2417
6	6	0.35	0/1278	0.57	0/1728
7	9	0.35	0/1445	0.57	0/1956
8	a	0.22	0/383	0.40	0/518
9	b	0.26	0/749	0.46	0/1009
10	c	0.29	0/1047	0.46	0/1415
11	d	0.27	0/2424	0.50	2/3276 (0.1%)
12	e	0.24	0/702	0.46	0/945
13	f	0.25	0/937	0.50	0/1271
14	g	0.27	0/993	0.51	0/1336
15	h	0.29	0/779	0.53	0/1053
16	i	0.28	0/1250	0.45	0/1698
17	j	0.20	0/670	0.45	0/902
18	q	0.27	0/252	0.44	0/338
All	All	0.30	0/28231	0.54	6/38199 (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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	366	THR	CA-C-N	6.17	133.33	121.54
3	3	366	THR	C-N-CA	6.17	133.33	121.54
11	d	112	LYS	CA-C-N	5.12	123.47	120.24
11	d	112	LYS	C-N-CA	5.12	123.47	120.24
2	2	156	ILE	CA-C-N	5.08	131.25	121.54
2	2	156	ILE	C-N-CA	5.08	131.25	121.54

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

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	44	0
2	2	1655	0	1668	17	0
3	3	5275	0	5300	74	0
4	4	3047	0	3021	53	0
5	5	1726	0	1676	27	0
6	6	1247	0	1259	17	0
7	9	1414	0	1371	22	0
8	a	371	0	344	4	0
9	b	737	0	710	4	0
10	c	1024	0	1023	12	0
11	d	2372	0	2407	18	0
12	e	691	0	706	6	0
13	f	917	0	958	6	0
14	g	969	0	980	8	0
15	h	769	0	780	8	0
16	i	1209	0	1182	13	0
17	j	660	0	663	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	q	245	0	244	0	0
19	1	8	0	0	1	0
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	5	0
30	4	200	0	0	6	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	1	0
30	d	79	0	0	3	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	1	0
30	i	83	0	0	1	0
30	q	1	0	0	0	0
All	All	29587	0	28054	289	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 (289) 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
3:3:632:ARG:HH12	12:e:59:ASP:H	1.38	0.70
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
1:1:132:ARG:NH2	8:a:64:PRO:O	2.29	0.65
3:3:118:ASP:OD2	10:c:46:GLN:NE2	2.30	0.65
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
12:e:19:ARG:HB2	12:e:65:TRP:HB2	1.82	0.60
16:i:34:ARG:NH2	16:i:58:ARG:O	2.33	0.60
7:9:43:ARG:HG2	15:h:11:ARG:HD2	1.83	0.60
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
16:i:60:ARG:HH22	16:i:95:ASP:HA	1.67	0.59
7:9:164:GLU:HG3	16:i:88:ARG:HG3	1.83	0.59
7:9:155:LEU:HB3	9:b:36:ASN:HD22	1.68	0.58
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
11:d:167:LYS:HB2	11:d:229:ALA:HA	1.87	0.56
17:j:48:VAL:HG12	17:j:52:MET:HE2	1.87	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
1:1:21:ILE:O	1:1:117:LYS:NZ	2.36	0.55
3:3:396:ARG:NH1	3:3:416:THR:O	2.39	0.55
3:3:332:LYS:NZ	3:3:505:LEU:O	2.37	0.55
17:j:37:MET:HE1	17:j:44:SER:HA	1.88	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
13:f:34:LEU:HD12	13:f:37:ILE:HD12	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:b:32:GLN:HE22	9:b:34:GLU:HB2	1.71	0.54
3:3:148:THR:HG23	3:3:150:MET:HE3	1.91	0.53
4:4:391:ILE:O	4:4:430:ARG:NH1	2.41	0.53
16:i:26:VAL:O	16:i:30:ALA:HB3	2.08	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
12:e:13:LEU:HD22	12:e:16:ARG:HH22	1.74	0.53
7:9:92:ILE:HG12	7:9:111:ILE:HG12	1.89	0.52
11:d:44:GLN:NE2	30:d:507:HOH:O	2.42	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
1:1:142:PHE:HB3	1:1:145:GLU:HB2	1.91	0.52
4:4:176:LYS:NZ	30:4:536:HOH:O	2.42	0.52
3:3:261:GLU:OE1	10:c:42:ARG:NH2	2.43	0.52
4:4:233:ARG:NH2	7:9:23:GLN:O	2.42	0.52
2:2:74:GLN:O	8:a:74:ARG:NH2	2.43	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
7:9:52:PHE:HE1	16:i:77:VAL:HG21	1.74	0.51
3:3:46:LEU:O	10:c:116:LYS:NZ	2.35	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
15:h:11:ARG:NH2	15:h:20:GLN:OE1	2.43	0.51
1:1:154:ARG:HA	8:a:58:LEU:HD21	1.92	0.51
8:a:57:ASP:OD1	8:a:60:LYS:NZ	2.44	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
11:d:72:ASP:O	11:d:83:ARG:NH2	2.44	0.51
10:c:8:THR:OG1	14:g:22:ARG:NH1	2.43	0.50
16:i:78:ASP:HB3	16:i:81:MET:HG3	1.93	0.50
11:d:48:PRO:HA	11:d:71:MET:O	2.11	0.50
4:4:226:GLU:OE1	4:4:305:ARG:NH2	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:65:ARG:NH1	5:5:123:VAL:O	2.44	0.50
11:d:60:ARG:NH1	30:d:518:HOH: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
11:d:100:GLU:HB2	11:d:105:ASP:HA	1.93	0.49
11:d:10:LYS:NZ	14:g:126:ASP:OD2	2.44	0.49
16:i:44:TYR:OH	16:i:113:HIS:N	2.41	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
7:9:108:ARG:NH2	16:i:128:SER:OG	2.45	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
5:5:119:SER:OG	5:5:131:GLU:OE2	2.28	0.49
13:f:71:LEU:HD13	13:f:79:VAL:HG11	1.95	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
13:f:37:ILE:O	13:f:44:ARG:NH1	2.44	0.49
3:3:582:GLN:NE2	30:c:201:HOH:O	2.46	0.48
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
11:d:135:LEU:HA	11:d:167:LYS:HB3	1.96	0.48
3:3:119:GLN:HB2	3:3:123:PHE:HD2	1.79	0.48
10:c:33:ARG:NH1	10:c:77:ASP:OD1	2.40	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
5:5:154:ASP:OD1	14:g:101:HIS:NE2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:140:LYS:HB2	3:3:148:THR:HG21	1.95	0.48
11:d:26:ALA:HA	11:d:31:GLY:HA3	1.96	0.47
4:4:65:VAL:HB	4:4:77:ASP:HB3	1.96	0.47
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
9:b:49:VAL:HG22	9:b:90:GLN:HG3	1.96	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
4:4:66:MET:HE1	4:4:414:VAL:HG11	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
16:i:50:GLU:HG3	16:i:89:TRP:HZ2	1.80	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
3:3:101:HIS:HD2	4:4:342:MET:HE2	1.80	0.46
3:3:182:GLN:NE2	30:3:936:HOH:O	2.41	0.46
14:g:42:VAL:HG11	14:g:59:ARG:HG3	1.96	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
15:h:45:SER:O	15:h:51:ASN:ND2	2.37	0.46
3:3:582:GLN:OE1	3:3:620:ARG:NH1	2.48	0.46
11:d:26:ALA:HB3	11:d:47:VAL:HG13	1.97	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
16:i:58:ARG:NH1	30:i:315:HOH:O	2.49	0.45
11:d:155:GLU:HA	11:d:158:GLU:HG2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:e:23:CYS:SG	12:e:24:GLN:N	2.90	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
5:5:181:LYS:NZ	30:d:501:HOH:O	2.49	0.45
14:g:21:SER:OG	14:g:30:ARG:NH1	2.50	0.45
17:j:11:ILE:HG22	17:j:77:VAL:HG23	1.98	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
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
3:3:147:LYS:NZ	30:3:960:HOH:O	2.50	0.44
11:d:94:LEU:HD23	11:d:132:ILE:HG13	2.00	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
1:1:199:LYS:NZ	30:1:633:HOH:O	2.49	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
11:d:280:THR:HG23	11:d:283:LYS:H	1.83	0.43
14:g:34:LEU:HD21	14:g:85:GLY:HA3	2.01	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
3:3:201:ASP:HA	10:c:45:MET:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:e:17:GLU:HG2	12:e:67:ARG:HB3	2.00	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
15:h:8:GLN:NE2	15:h:20:GLN:HG3	2.34	0.43
5:5:28:TYR:OH	5:5:67:HIS:NE2	2.42	0.42
5:5:51:CYS:HB3	13:f:111:TRP:CE2	2.54	0.42
1:1:96:ASN:ND2	20:1:502:FMN:O4'	2.52	0.42
3:3:138:GLU:N	9:b:74:ASN:HD22	2.18	0.42
3:3:382:THR:HB	3:3:454:GLY:HA3	2.00	0.42
4:4:64:LEU:HB3	4:4:66:MET:HE2	2.01	0.42
5:5:92:ILE:HD11	5:5:111:THR:HG22	2.02	0.42
10:c:59:PHE:HE2	10:c:82:LEU:HD23	1.84	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
15:h:11:ARG:HG2	15:h:19:LEU:HD12	2.02	0.42
15:h:95:SER:OG	15:h:97:ALA:O	2.34	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
3:3:36:GLN:NE2	10:c:47:SER:O	2.47	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
3:3:276:ARG:HA	16:i:135:GLN:HB2	2.02	0.41
5:5:182:ARG:HD2	14:g:100:THR:HA	2.02	0.41
6:6:127:HIS:CD2	7:9:115:LYS:HE2	2.55	0.41
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
5:5:32:ILE:HG23	13:f:43:TYR:HB2	2.00	0.41
6:6:63:ALA:HB2	6:6:69:MET:HE3	2.02	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
16:i:9:ARG:HA	16:i:12:GLN:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:j:17:TYR:HA	17:j:20:LYS:HG2	2.02	0.41
1:1:95:VAL:HG11	1:1:118:LEU:HD11	2.02	0.41
3:3:244:THR:HB	10:c:73:ALA:HB2	2.01	0.41
4:4:291:GLY:O	4:4:296:ARG:NH1	2.52	0.41
10:c:42:ARG:NH1	10:c:46:GLN:O	2.51	0.41
6:6:29:VAL:HG22	25:6:203:3PE:H3I3	2.03	0.41
10:c:77:ASP:HB3	10:c:80:SER:HB3	2.03	0.41
2:2:24:THR:OG1	2:2:27:ASN:OD1	2.34	0.41
3:3:444:GLN:O	3:3:481:SER:OG	2.32	0.41
4:4:270:ARG:HG3	4:4:368:GLU:HB3	2.03	0.41
14:g:114:PRO:HG2	14:g:123:VAL:HG21	2.03	0.41
16:i:114:LYS:HD2	16:i:117:LEU:HD11	2.02	0.41
3:3:325:ALA:HB1	3:3:623:LEU:HD11	2.03	0.41
3:3:622:ARG:NH2	12:e:73:GLU:OE2	2.53	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
11:d:98:GLU:HG3	11:d:177:ARG:HE	1.85	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
5:5:137:MET:HE3	5:5:152:LEU:HB2	2.03	0.41
11:d:91:VAL:HG23	11:d:126:VAL:HG11	2.02	0.41
11:d:133:SER:HB3	11:d:167:LYS:HD3	2.03	0.41
13:f:49:GLN:HE22	15:h:92:LYS:HA	1.85	0.41
1:1:342:ASP:OD1	1:1:429:ARG:NH2	2.49	0.40
11:d:157:ARG:NH2	11:d:163:ALA:O	2.54	0.40
11:d:311:GLU:HG2	11:d:336:PRO:HB3	2.02	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
10:c:28:GLU:O	10:c:32:THR:OG1	2.28	0.40
15:h:59:ARG:NH2	30:h:317:HOH:O	2.54	0.40
3:3:20:VAL:HG12	3:3:32:LYS:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:116:PRO:HB3	5:5:141:PHE:HD2	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	662/727 (91%)	642 (97%)	20 (3%)	0	100	100
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	3409/4304 (79%)	3301 (97%)	108 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	344/368 (94%)	344 (100%)	0	100	100
2	2	183/210 (87%)	183 (100%)	0	100	100
3	3	560/608 (92%)	560 (100%)	0	100	100
4	4	328/391 (84%)	328 (100%)	0	100	100
5	5	189/230 (82%)	189 (100%)	0	100	100
6	6	132/181 (73%)	131 (99%)	1 (1%)	73	86
7	9	151/179 (84%)	150 (99%)	1 (1%)	76	87
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%)	255 (100%)	0	100	100
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	2978/3631 (82%)	2976 (100%)	2 (0%)	87	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	6	54	CYS
7	9	78	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	148	ASN
1	1	150	GLN
1	1	293	ASN
2	2	101	GLN
2	2	121	GLN
2	2	155	GLN
3	3	237	ASN
3	3	535	GLN
3	3	581	GLN
3	3	643	GLN
4	4	149	ASN
4	4	252	ASN
5	5	19	HIS
5	5	160	HIS
8	a	40	ASN
9	b	16	GLN
9	b	36	ASN
11	d	103	ASN
11	d	148	ASN
11	d	296	HIS
12	e	47	ASN
13	f	49	GLN
14	g	125	HIS
15	h	24	GLN
16	i	69	ASN
16	i	72	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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%)	6,8,10	0.91	0
4	2MR	4	85	4	10,12,13	2.38	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	-	0/5/6/8	-
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	4.97	1.43	1.33
4	4	85	2MR	CZ-NE	4.45	1.43	1.34
15	h	1	AYA	CA-N	-2.46	1.43	1.46
4	4	85	2MR	CQ1-NH1	-2.19	1.42	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	85	2MR	NE-CZ-NH2	-3.91	115.90	119.48
4	4	85	2MR	CD-NE-CZ	-2.40	118.86	123.36

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 oligosaccharides 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
19	SF4	3	801	3	0,12,12	-	-	-		
19	SF4	3	802	3	0,12,12	-	-	-		
19	SF4	9	403	7	0,12,12	-	-	-		
22	FES	2	300	2	0,4,4	-	-	-		
25	3PE	i	201	-	50,50,50	0.30	0	53,55,55	0.30	0
27	NDP	d	401	-	51,52,52	0.42	0	71,80,80	0.37	0
21	NAI	1	503	-	47,48,48	0.38	0	64,73,73	1.82	4 (6%)
24	PC1	6	202	-	45,45,53	0.31	0	51,53,61	0.34	0
25	3PE	6	203	-	50,50,50	0.30	0	53,55,55	0.30	0
20	FMN	1	502	-	33,33,33	1.12	3 (9%)	48,50,50	1.37	7 (14%)
19	SF4	1	501	1	0,12,12	-	-	-		
19	SF4	9	402	7	0,12,12	-	-	-		
24	PC1	9	401	-	53,53,53	0.31	0	59,61,61	0.55	1 (1%)
29	CDL	h	201	-	57,57,99	0.35	0	63,69,111	0.30	0
19	SF4	6	201	6	0,12,12	-	-	-		
28	ZMP	g	201	-	28,33,36	0.66	0	32,40,45	1.28	3 (9%)
22	FES	3	803	3	0,4,4	-	-	-		

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
19	SF4	3	801	3	-	-	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
19	SF4	9	403	7	-	-	0/6/5/5
22	FES	2	300	2	-	-	0/1/1/1
25	3PE	i	201	-	-	6/54/54/54	-
27	NDP	d	401	-	-	3/34/77/77	0/5/5/5
21	NAI	1	503	-	-	6/29/72/72	0/5/5/5
24	PC1	6	202	-	-	10/49/49/57	-
25	3PE	6	203	-	-	11/54/54/54	-
20	FMN	1	502	-	-	10/18/18/18	0/3/3/3
24	PC1	9	401	-	-	9/57/57/57	-
29	CDL	h	201	-	-	17/68/68/110	-
19	SF4	1	501	1	-	-	0/6/5/5
19	SF4	9	402	7	-	-	0/6/5/5
19	SF4	6	201	6	-	-	0/6/5/5
28	ZMP	g	201	-	-	5/38/40/43	-
22	FES	3	803	3	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	502	FMN	C4A-N5	2.89	1.37	1.30
20	1	502	FMN	C10-N1	2.14	1.37	1.33
20	1	502	FMN	C4A-C10	-2.05	1.38	1.44

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	503	NAI	O5B-PA-O1A	-9.76	70.25	108.94
21	1	503	NAI	O2A-PA-O1A	-8.29	73.86	112.44
21	1	503	NAI	O3-PA-O1A	-5.69	93.58	110.70
20	1	502	FMN	C4-N3-C2	-3.80	118.89	125.64
28	g	201	ZMP	C15-C14-C13	-3.04	107.33	112.39
28	g	201	ZMP	C14-C15-N2	-3.03	105.55	112.00
20	1	502	FMN	O4-C4-C4A	-2.84	119.04	126.53
20	1	502	FMN	C4A-C10-N10	2.81	120.50	116.48
20	1	502	FMN	C4A-C4-N3	2.77	120.30	113.25
28	g	201	ZMP	O1-C10-C9	-2.76	120.80	123.98
20	1	502	FMN	C4A-C10-N1	-2.49	118.48	124.59
21	1	503	NAI	O2A-PA-O5B	2.48	118.80	107.57
20	1	502	FMN	C10-C4A-N5	-2.25	120.22	124.81
20	1	502	FMN	C4-C4A-C10	2.18	120.67	116.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	9	401	PC1	C2-O21-C21	2.04	122.67	117.80

There are no chirality outliers.

All (77) 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	C11-O13-P-O11
24	6	202	PC1	C1-O11-P-O14
24	6	202	PC1	C1-O11-P-O13
24	9	401	PC1	C11-O13-P-O12
24	9	401	PC1	C11-O13-P-O14
24	9	401	PC1	C11-O13-P-O11
25	6	203	3PE	C1-O11-P-O12
25	6	203	3PE	C1-O11-P-O13
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	CB2-OB2-PB2-OB5
29	h	201	CDL	CB3-OB5-PB2-OB2
29	h	201	CDL	CB3-OB5-PB2-OB3
29	h	201	CDL	CB3-OB5-PB2-OB4
29	h	201	CDL	O1-C1-CB2-OB2
25	i	201	3PE	C29-C2A-C2B-C2C
29	h	201	CDL	C56-C57-C58-C59
24	9	401	PC1	C2E-C2F-C2G-C2H
24	6	202	PC1	C3B-C3C-C3D-C3E
25	6	203	3PE	C3C-C3D-C3E-C3F
20	1	502	FMN	C2'-C3'-C4'-O4'
25	6	203	3PE	C36-C37-C38-C39
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
28	g	201	ZMP	O1-C10-S1-C11

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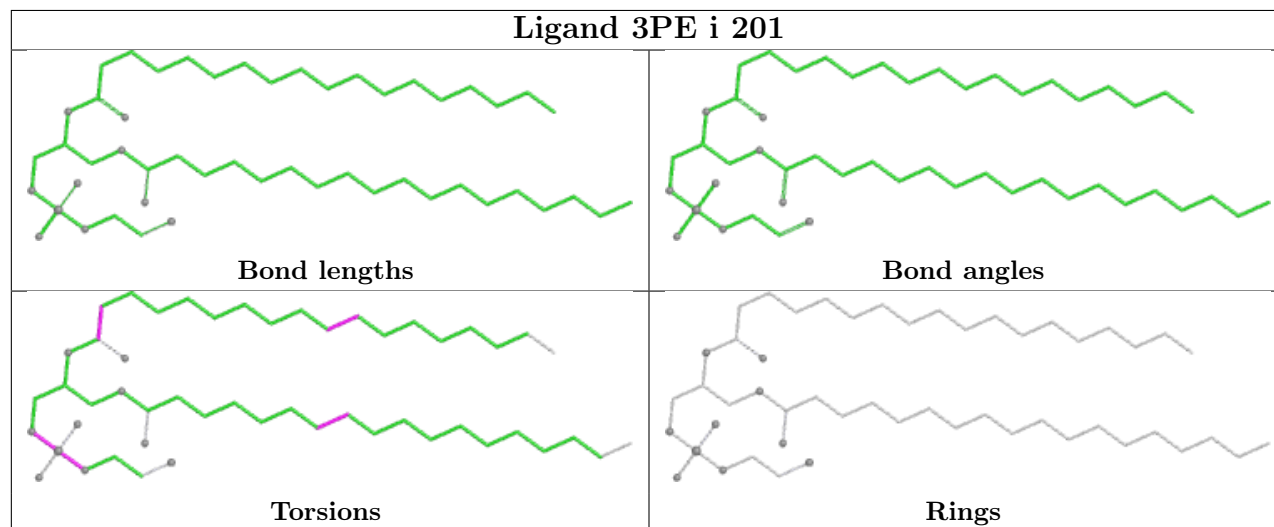
Mol	Chain	Res	Type	Atoms
25	6	203	3PE	C2D-C2E-C2F-C2G
21	1	503	NAI	PN-O3-PA-O5B
20	1	502	FMN	O3'-C3'-C4'-C5'
28	g	201	ZMP	C9-C10-S1-C11
24	9	401	PC1	O22-C21-O21-C2
29	h	201	CDL	CB3-CB4-CB6-OB8
24	9	401	PC1	C34-C35-C36-C37
24	9	401	PC1	O13-C11-C12-N
20	1	502	FMN	N10-C1'-C2'-C3'
20	1	502	FMN	C4'-C5'-O5'-P
29	h	201	CDL	C1-CB2-OB2-PB2
20	1	502	FMN	O3'-C3'-C4'-O4'
20	1	502	FMN	C2'-C3'-C4'-C5'
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	6	203	3PE	C11-O13-P-O14
25	i	201	3PE	C1-O11-P-O12
25	i	201	3PE	C11-O13-P-O14
29	h	201	CDL	CB4-CB3-OB5-PB2
25	6	203	3PE	C33-C34-C35-C36
27	d	401	NDP	O4D-C1D-N1N-C6N
21	1	503	NAI	O4D-C1D-N1N-C2N
27	d	401	NDP	O4B-C4B-C5B-O5B
24	9	401	PC1	C3-C2-O21-C21
29	h	201	CDL	OB6-CB4-CB6-OB8
21	1	503	NAI	C2N-C3N-C7N-N7N
21	1	503	NAI	C2D-C1D-N1N-C2N
25	6	203	3PE	O11-C1-C2-O21
25	i	201	3PE	C36-C37-C38-C39
25	6	203	3PE	C3D-C3E-C3F-C3G
25	i	201	3PE	O21-C21-C22-C23
29	h	201	CDL	C52-C51-CB5-OB6
20	1	502	FMN	N10-C1'-C2'-O2'
29	h	201	CDL	CB7-C71-C72-C73
25	i	201	3PE	O22-C21-C22-C23
27	d	401	NDP	C2D-C1D-N1N-C6N
29	h	201	CDL	C52-C51-CB5-OB7
28	g	201	ZMP	N2-C16-C17-O4
24	6	202	PC1	C3A-C3B-C3C-C3D
24	6	202	PC1	C38-C39-C3A-C3B

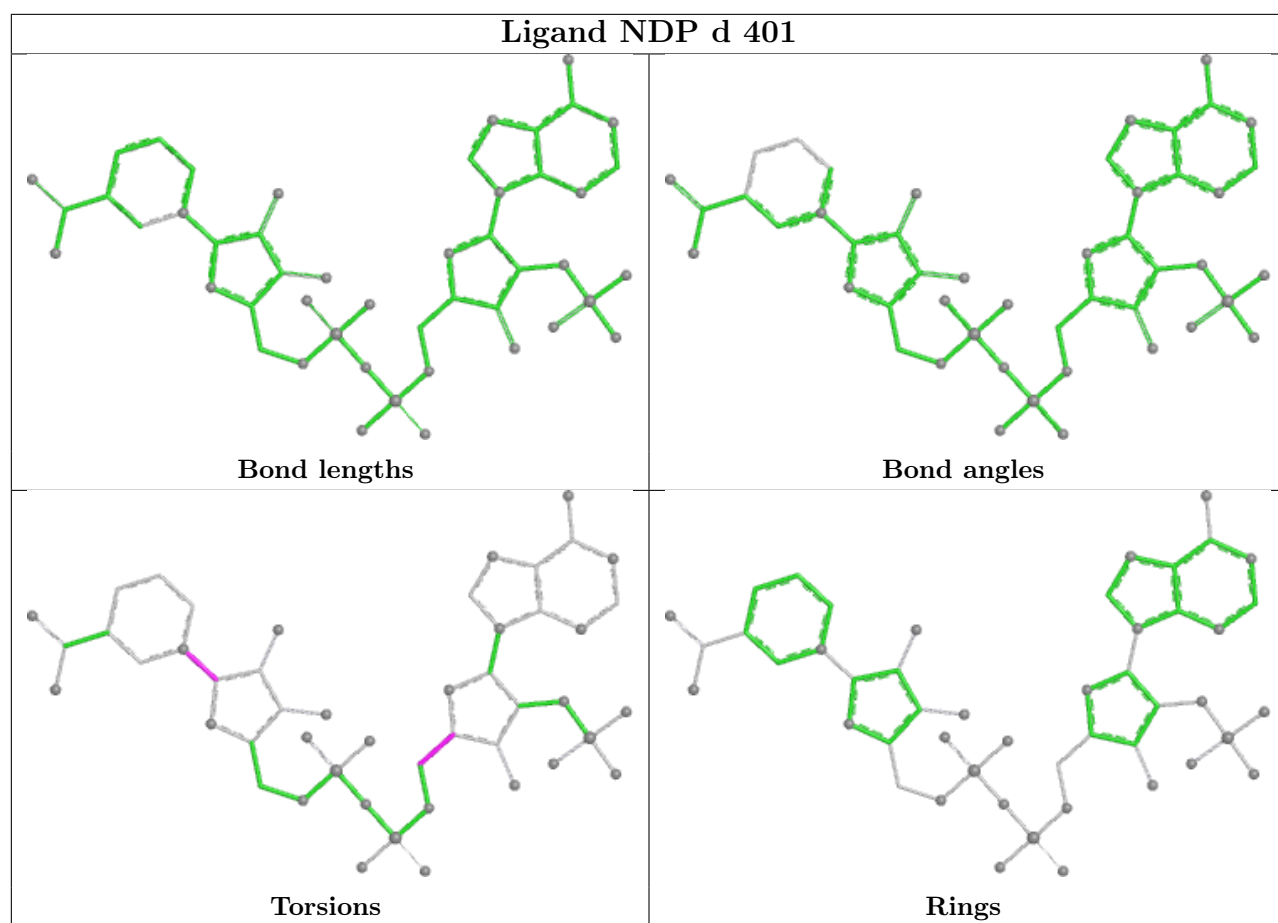
There are no ring outliers.

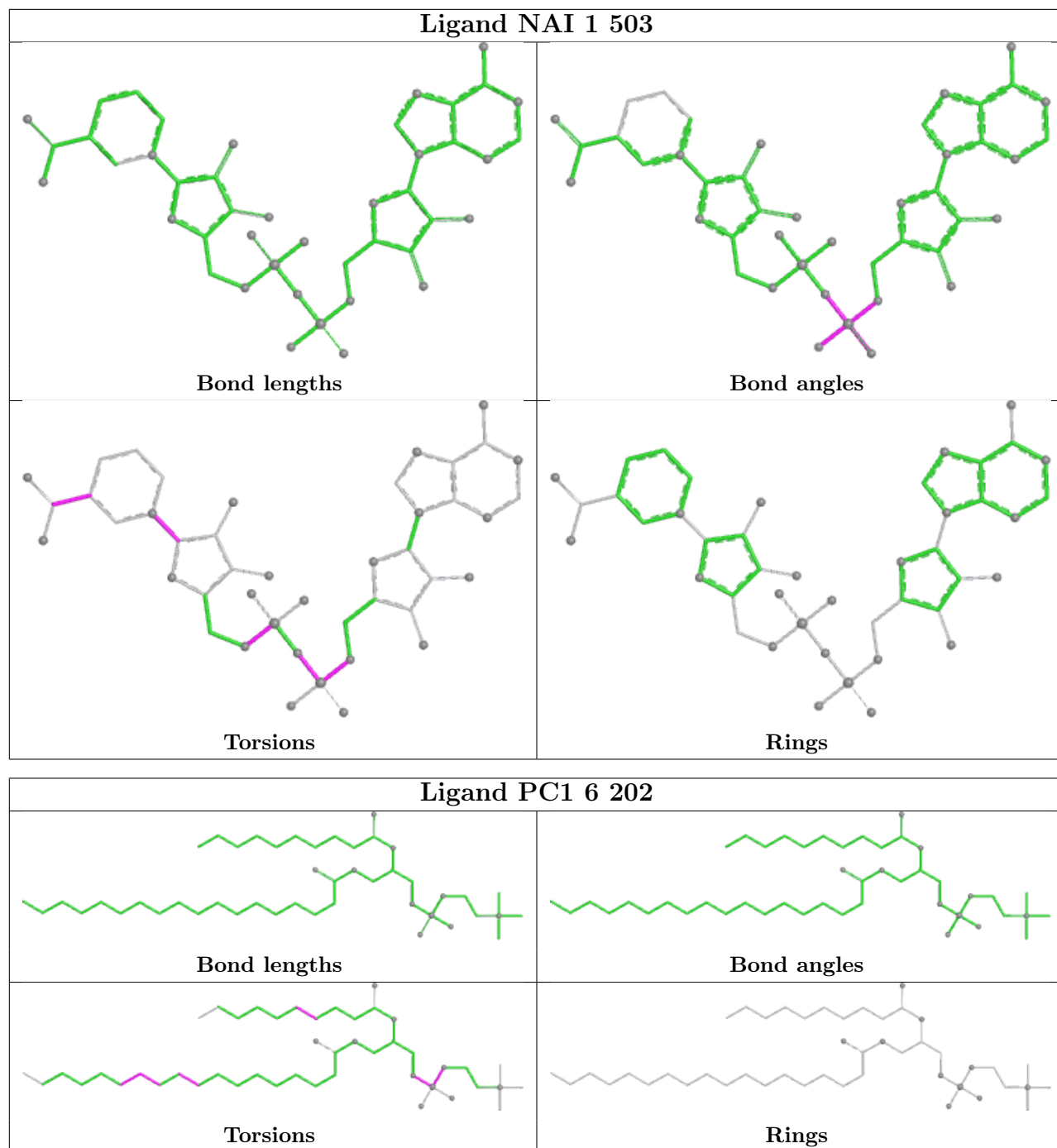
7 monomers are involved in 14 short contacts:

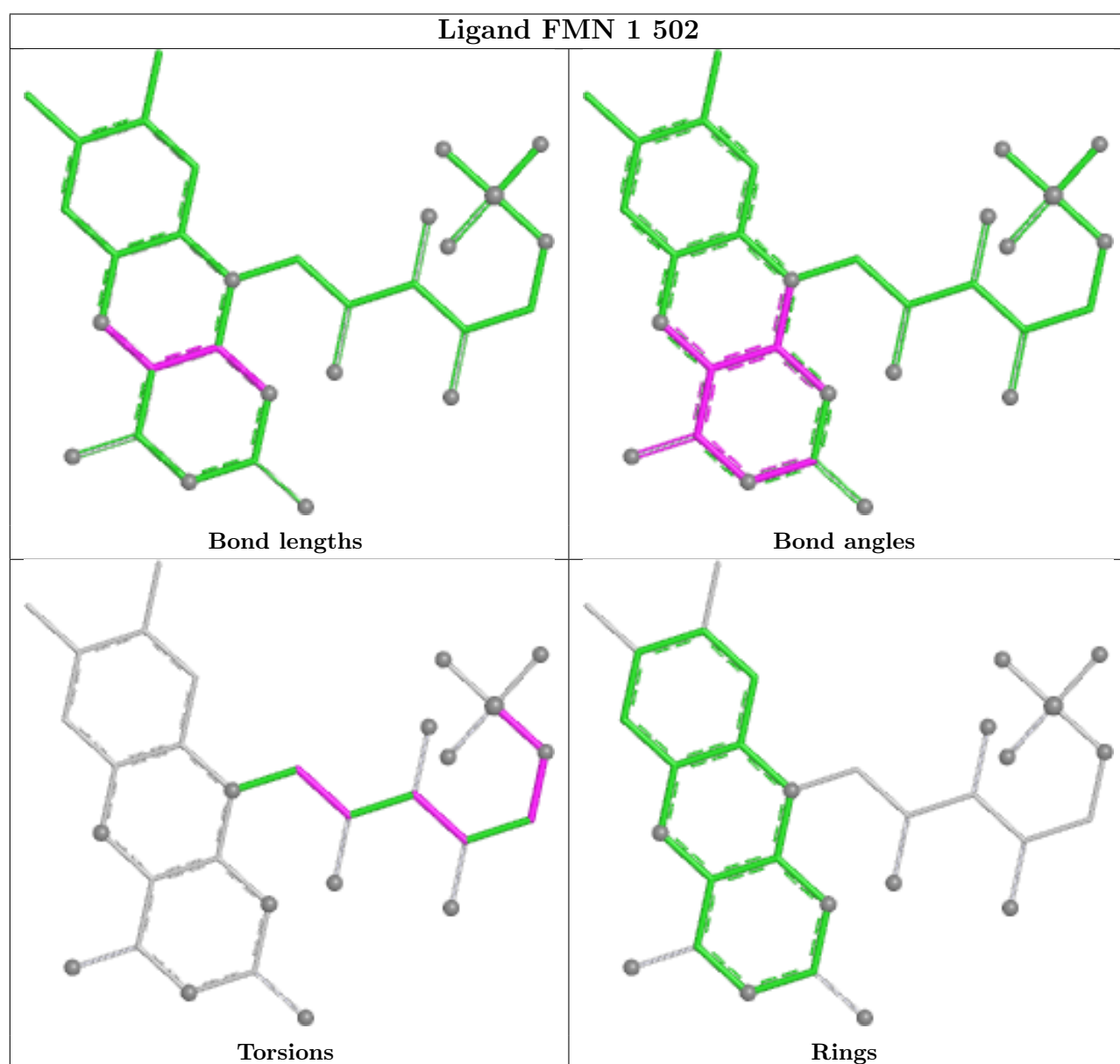
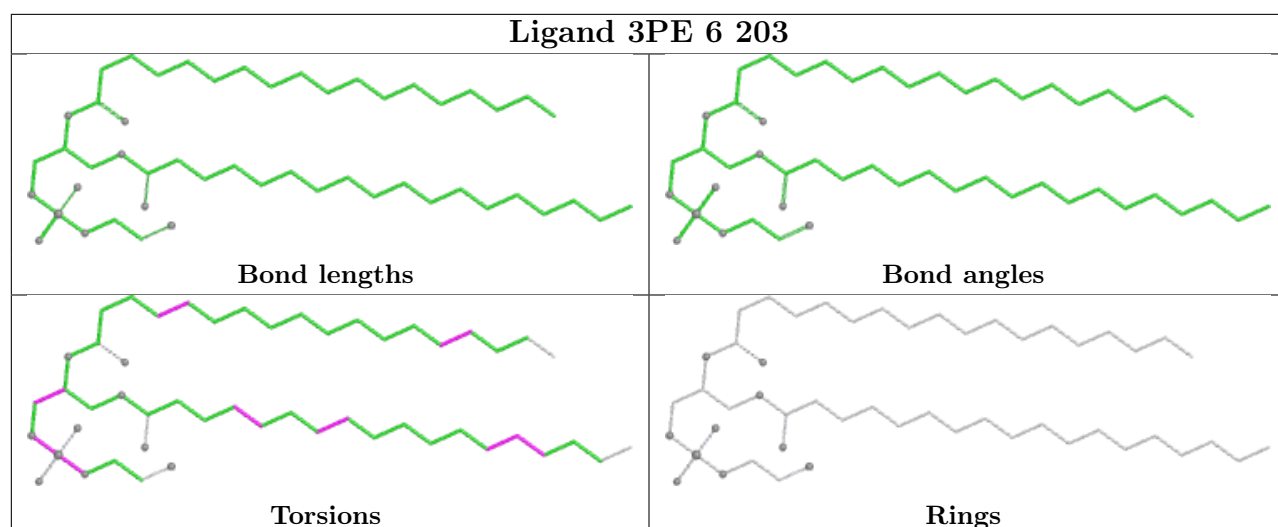
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	2	300	FES	1	0
21	1	503	NAI	4	0
25	6	203	3PE	3	0
20	1	502	FMN	1	0
19	1	501	SF4	1	0
24	9	401	PC1	1	0
19	6	201	SF4	3	0

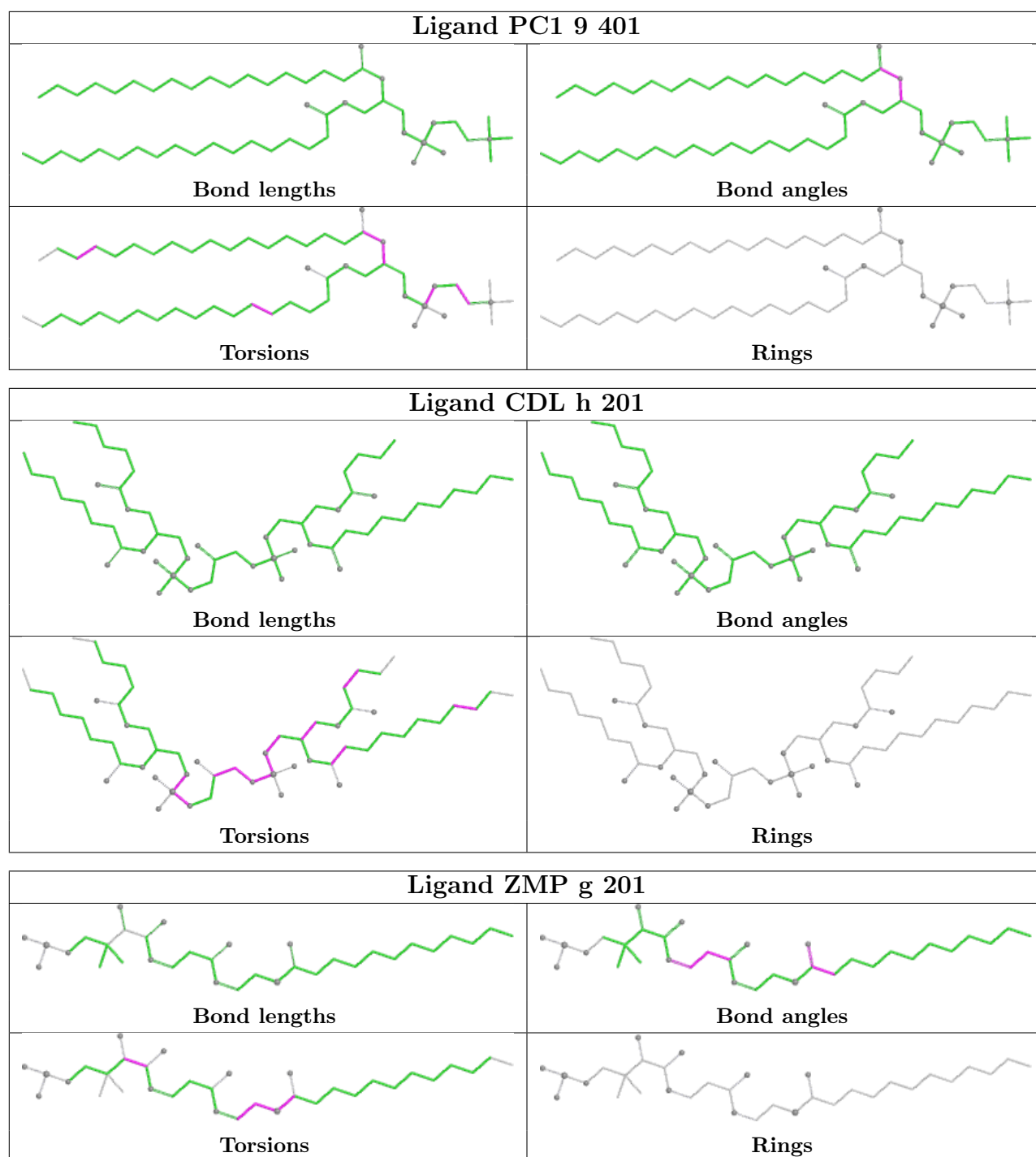
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

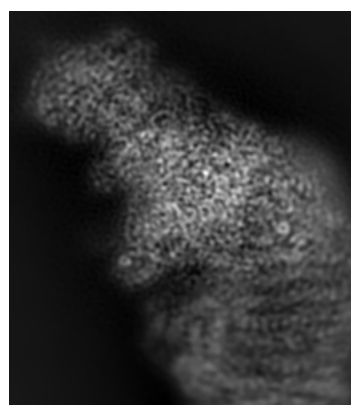
6 Map visualisation [i](#)

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

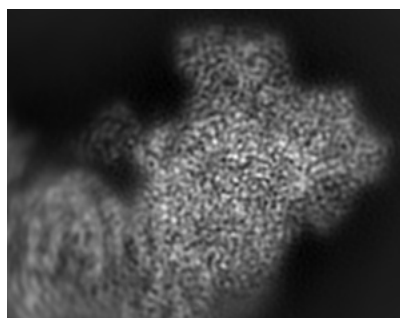
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

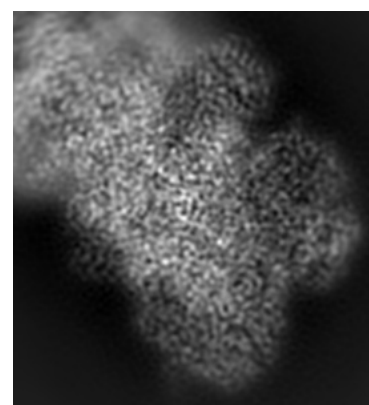
6.1.1 Primary map



X



Y

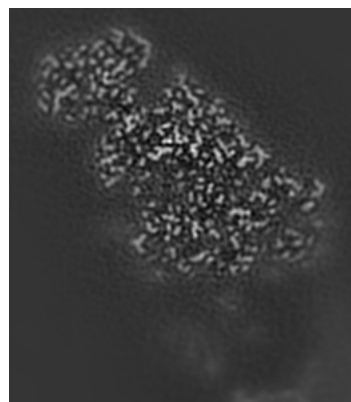


Z

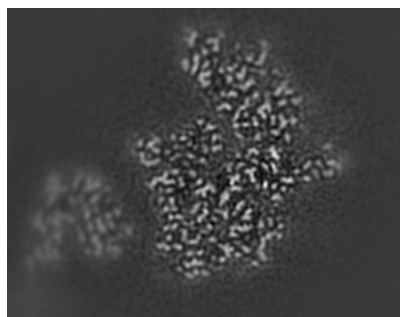
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

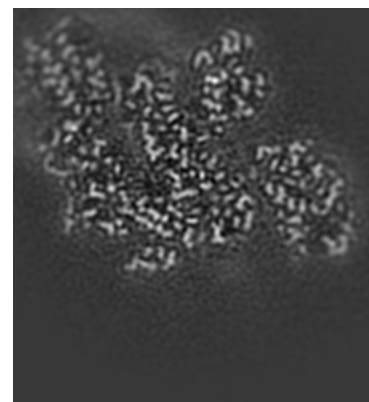
6.2.1 Primary map



X Index: 147



Y Index: 160

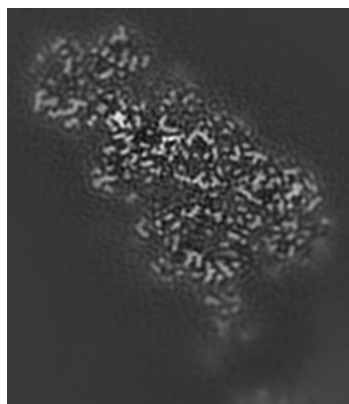


Z Index: 187

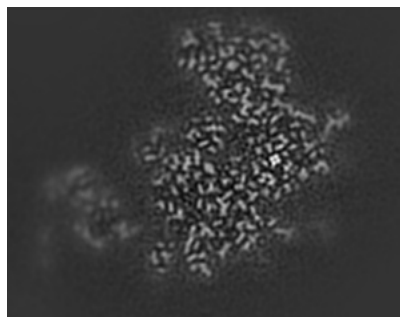
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

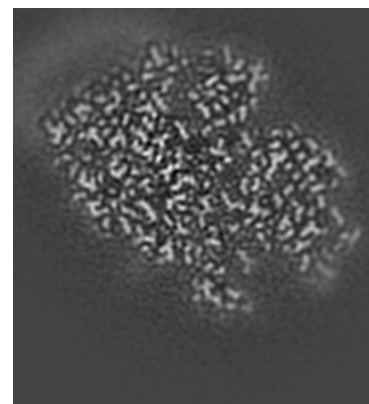
6.3.1 Primary map



X Index: 155



Y Index: 149

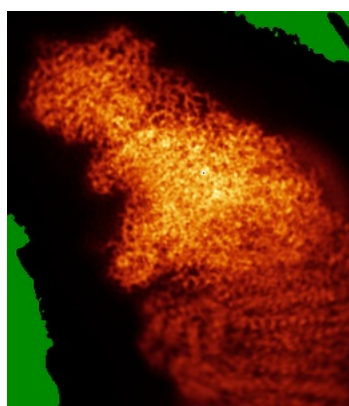


Z Index: 215

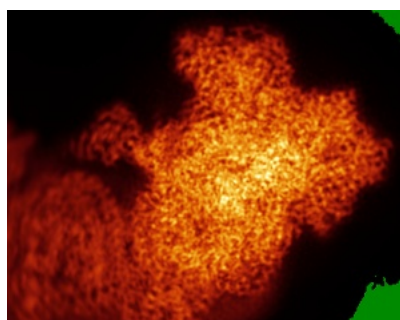
The images above show the largest variance slices of the map in three orthogonal directions.

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

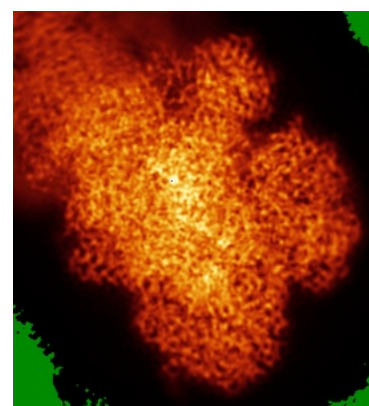
6.4.1 Primary map



X



Y

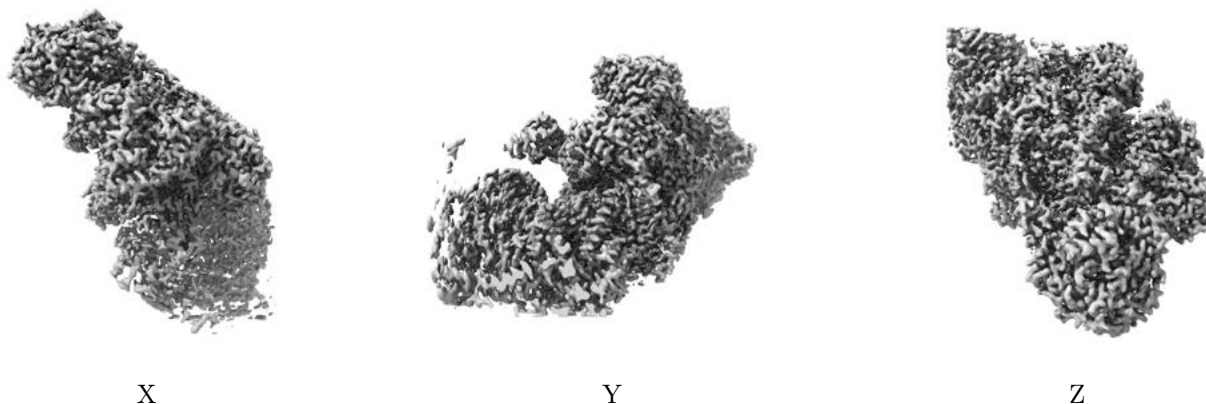


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

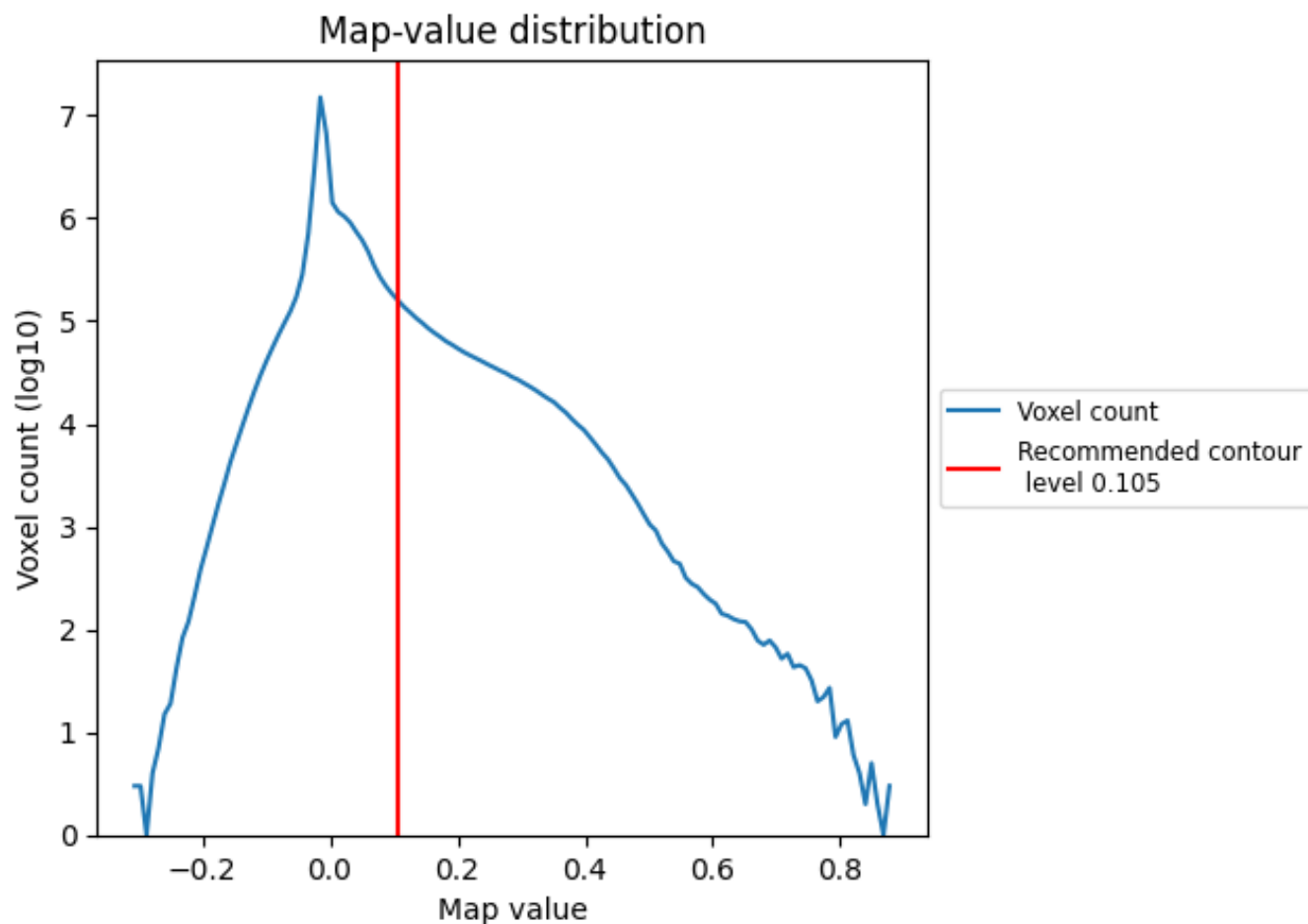
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

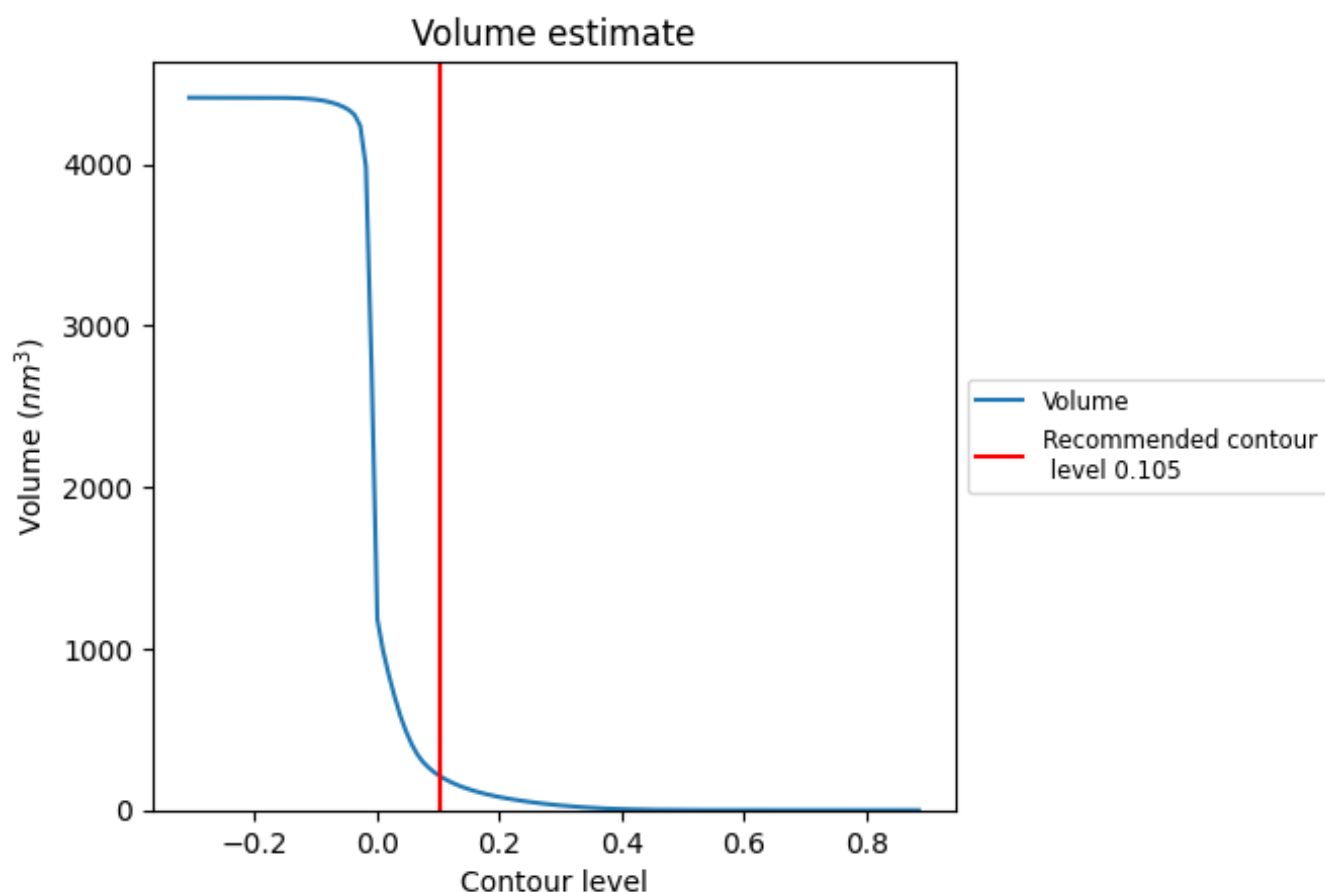
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 208 nm³; 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.

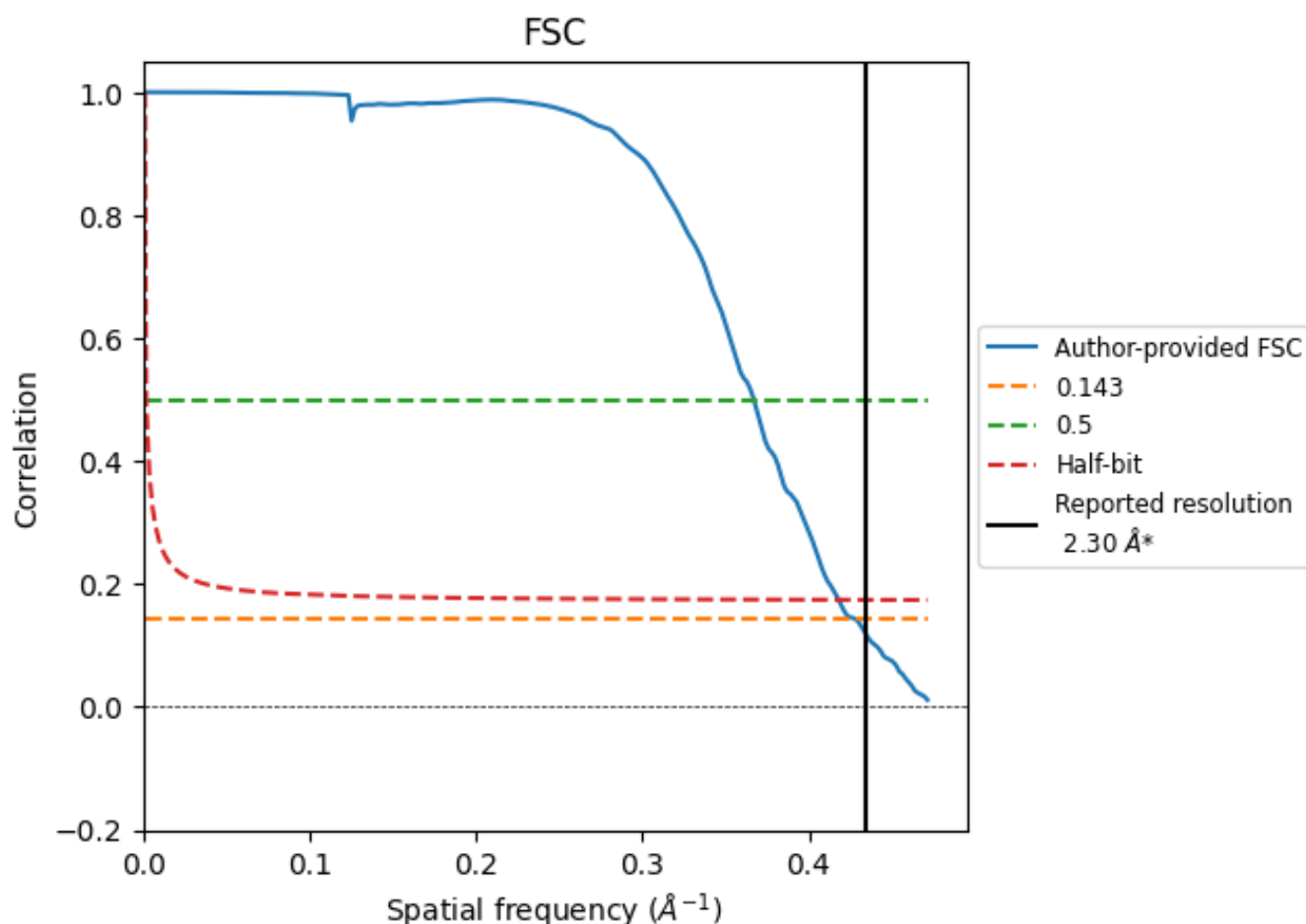
7.3 Rotationally averaged power spectrum [i](#)

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

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

8.2 Resolution estimates [i](#)

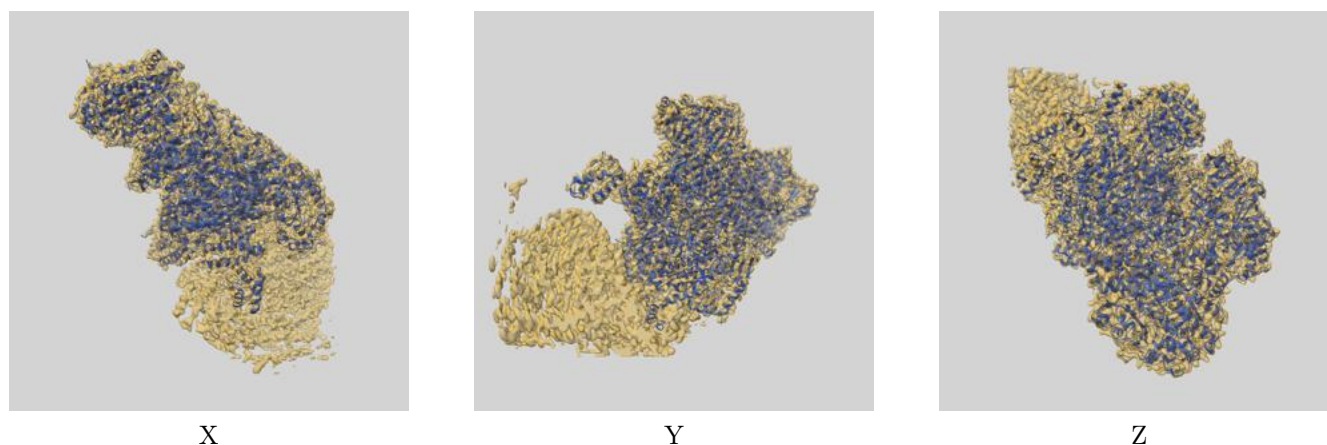
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.34	2.72	2.39
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

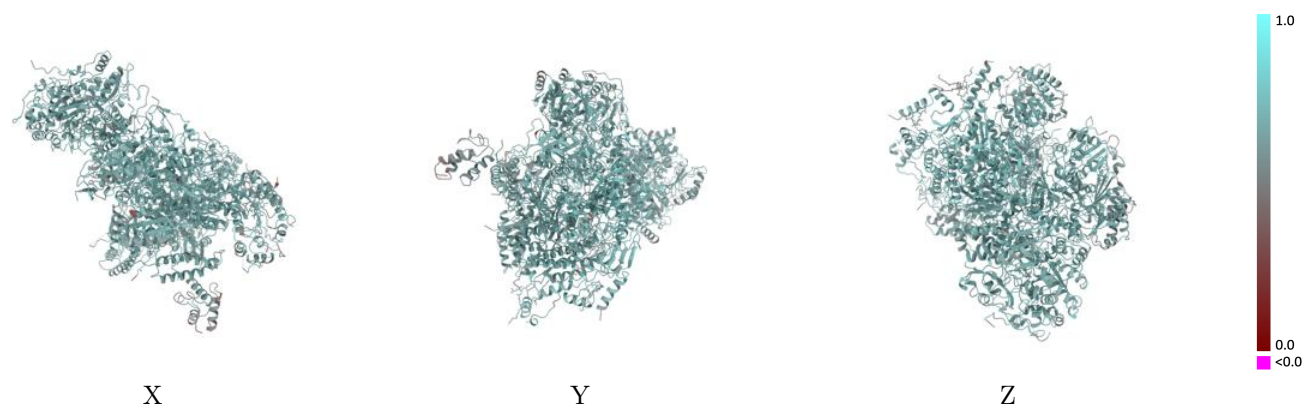
This section contains information regarding the fit between EMDB map EMD-11241 and PDB model 6ZK9. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



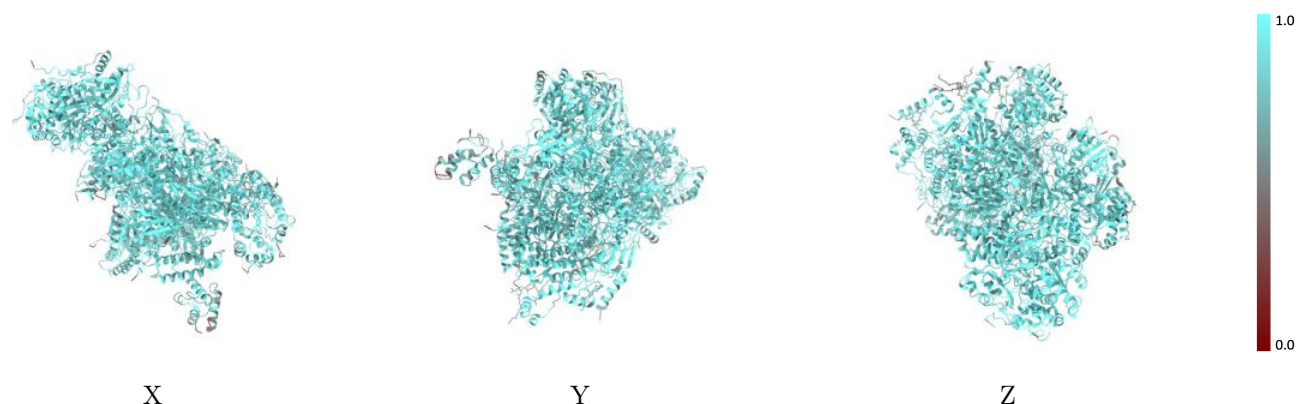
The images above show the 3D surface view of the map at the recommended contour level 0.105 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



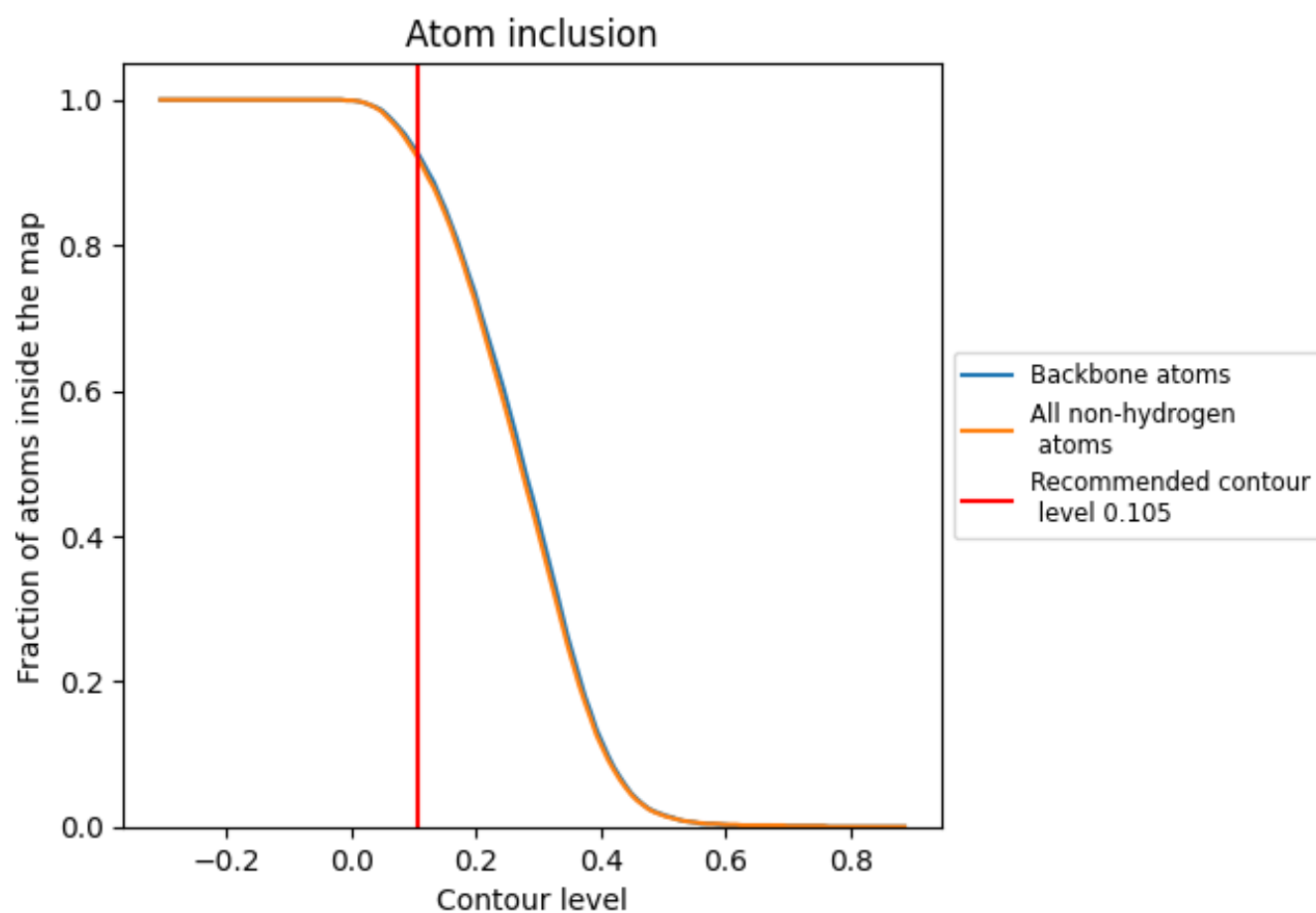
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.105).

9.4 Atom inclusion ⓘ



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	0.9220	0.6600
1	0.9510	0.6560
2	0.9220	0.6370
3	0.9320	0.6660
4	0.9600	0.6980
5	0.9590	0.6970
6	0.9320	0.6780
9	0.9520	0.6940
a	0.9230	0.6330
b	0.9280	0.6730
c	0.9320	0.6830
d	0.8930	0.6300
e	0.8820	0.6050
f	0.8970	0.6370
g	0.9010	0.6460
h	0.9040	0.6530
i	0.9150	0.6620
j	0.6900	0.5180
q	0.9190	0.6300

1.0
0.0
<0.0