



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:21 PM UTC

PDB ID : 7P61 / pdb_00007p61
EMDB ID : EMD-13214
Title : Complex I from E. coli, DDM-purified, with NADH, Resting state
Authors : Kravchuk, V.; Kampjut, D.; Sazanov, L.
Deposited on : 2021-07-15
Resolution : 3.20 Å (reported)
Based on initial models : 3RKO, 4HEA

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

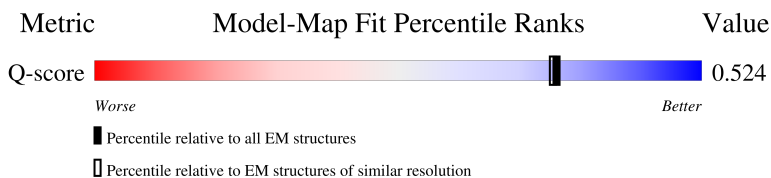
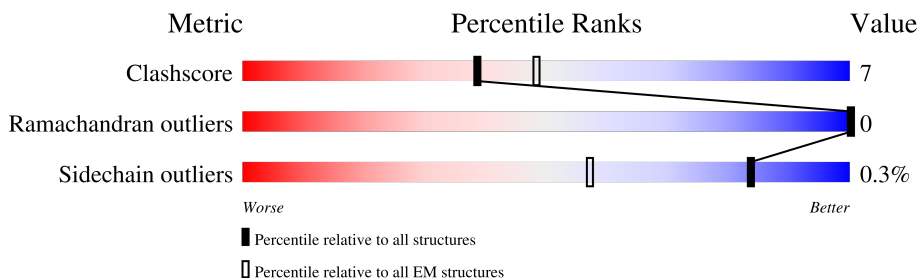
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



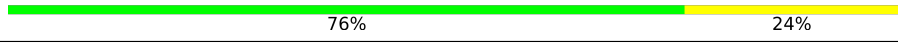
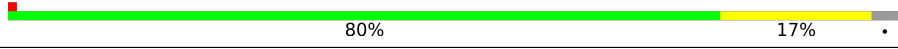
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	F	442	
2	E	156	
3	G	905	
4	C	600	

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Mol	Chain	Length	Quality of chain
5	B	220	
6	I	147	
7	L	613	
8	M	504	
9	N	485	
10	H	325	
11	A	147	
12	K	100	
13	J	175	

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
14	SF4	G	1001	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 36690 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-quinone oxidoreductase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	442	Total	C	N	O	S	0	0
			3432	2177	601	633	21		

- Molecule 2 is a protein called NADH dehydrogenase I subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	156	Total	C	N	O	S	0	0
			1220	768	215	229	8		

- Molecule 3 is a protein called NADH-quinone oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	905	Total	C	N	O	S	0	0
			7022	4388	1269	1328	37		

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit C/D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	571	Total	C	N	O	S	0	0
			4606	2953	801	829	23		

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	191	Total	C	N	O	S	0	0
			1518	961	261	279	17		

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	147	Total	C	N	O	S	0	0
			1157	734	194	217	12		

- Molecule 7 is a protein called Proton-translocating NADH-quinone oxidoreductase, chain L.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	593	Total	C	N	O	S	0	0
			4525	3015	717	762	31		

- Molecule 8 is a protein called NADH dehydrogenase I subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	504	Total	C	N	O	S	0	0
			3953	2661	617	646	29		

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	479	Total	C	N	O	S	0	0
			3630	2424	573	613	20		

- Molecule 10 is a protein called NADH-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	312	Total	C	N	O	S	0	0
			2449	1648	379	404	18		

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	106	Total	C	N	O	S	0	0
			840	573	131	131	5		

- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	100	Total	C	N	O	S	0	0
			760	494	132	129	5		

- Molecule 13 is a protein called NADH-quinone oxidoreductase subunit J.

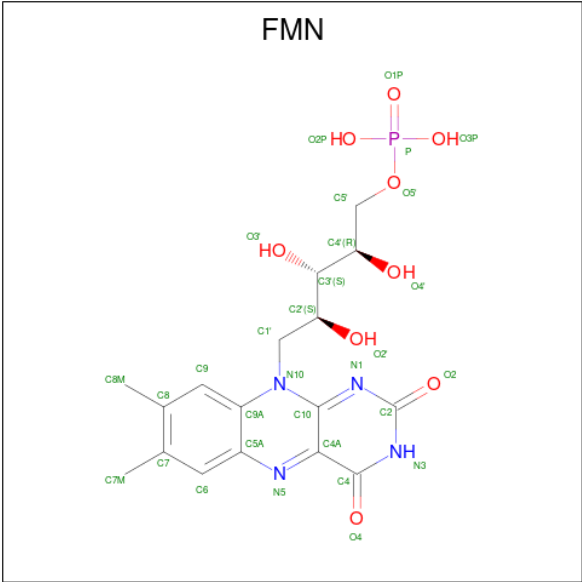
Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	175	Total	C	N	O	S	0	0
			1326	881	209	229	7		

- Molecule 14 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



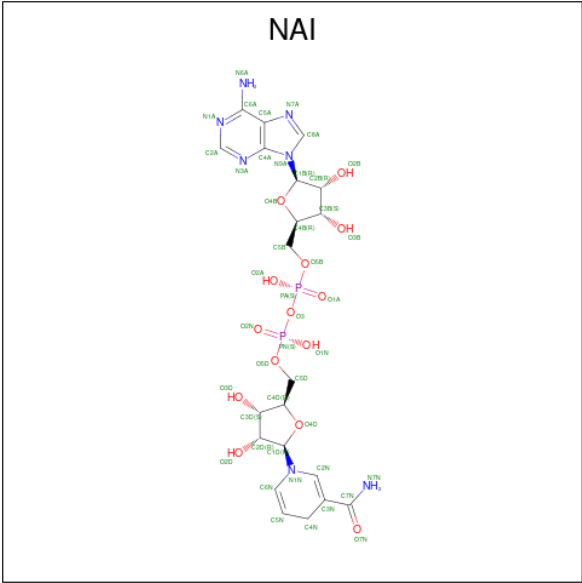
Mol	Chain	Residues	Atoms			AltConf
14	F	1	Total	Fe	S	0
			8	4	4	
14	G	1	Total	Fe	S	0
			8	4	4	
14	G	1	Total	Fe	S	0
			8	4	4	
14	G	1	Total	Fe	S	0
			8	4	4	
14	B	1	Total	Fe	S	0
			8	4	4	
14	I	1	Total	Fe	S	0
			8	4	4	
14	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 15 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



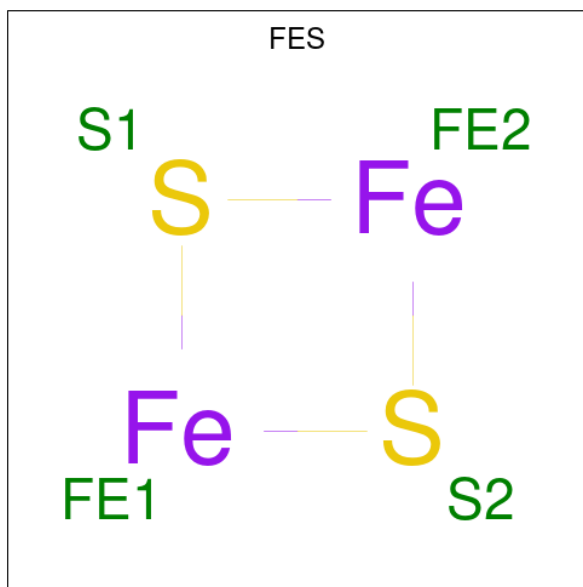
Mol	Chain	Residues	Atoms					AltConf
15	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 16 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



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

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

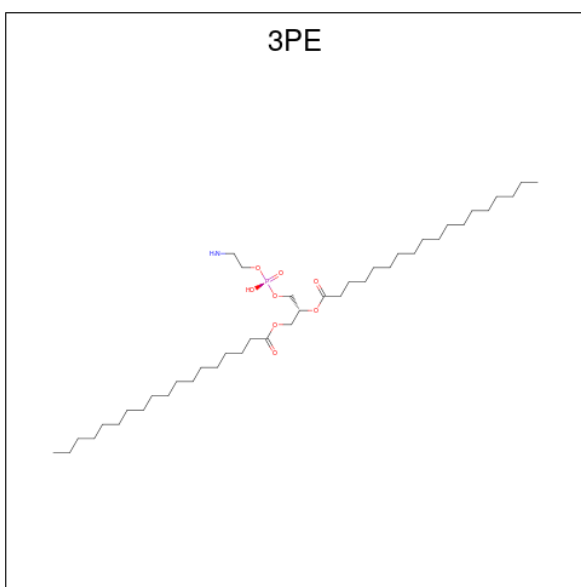


Mol	Chain	Residues	Atoms			AltConf
17	E	1	Total	Fe	S	0
			4	2	2	
17	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 18 is CALCIUM ION (CCD ID: CA) (formula: Ca).

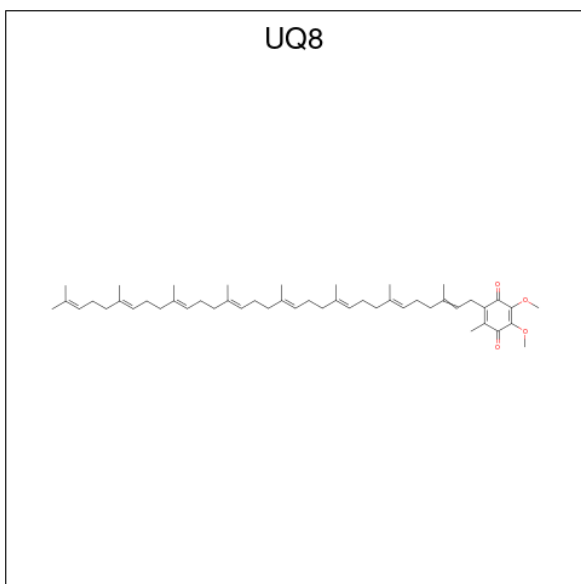
Mol	Chain	Residues	Atoms		AltConf
18	G	1	Total	Ca	0
			1	1	

- Molecule 19 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



Mol	Chain	Residues	Atoms					AltConf
19	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
19	L	1	Total	C	N	O	P	0
			37	27	1	8	1	

- Molecule 20 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$) (labeled as "Ligand of Interest" by depositor).

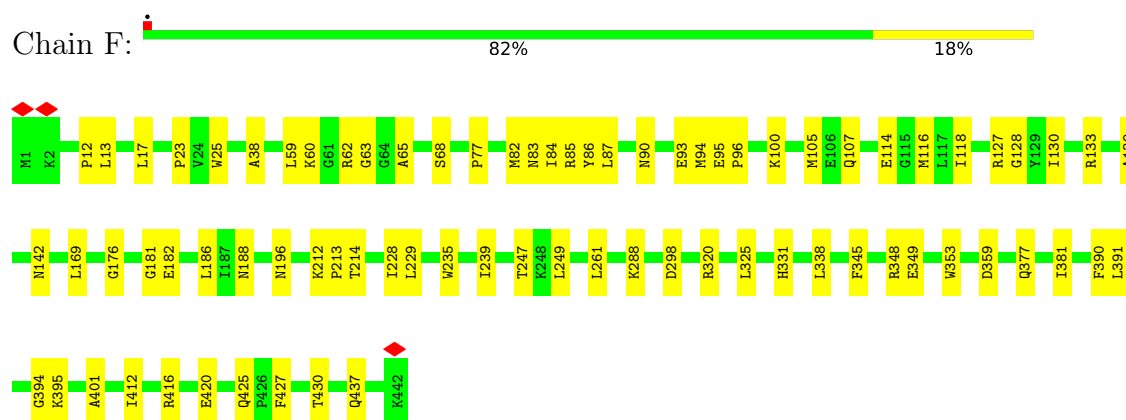


Mol	Chain	Residues	Atoms			AltConf
20	H	1	Total	C	O	0
			24	20	4	

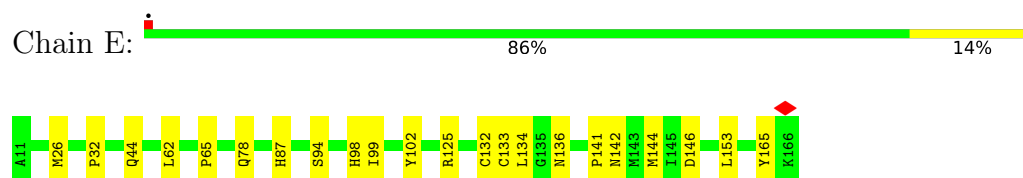
3 Residue-property plots

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.

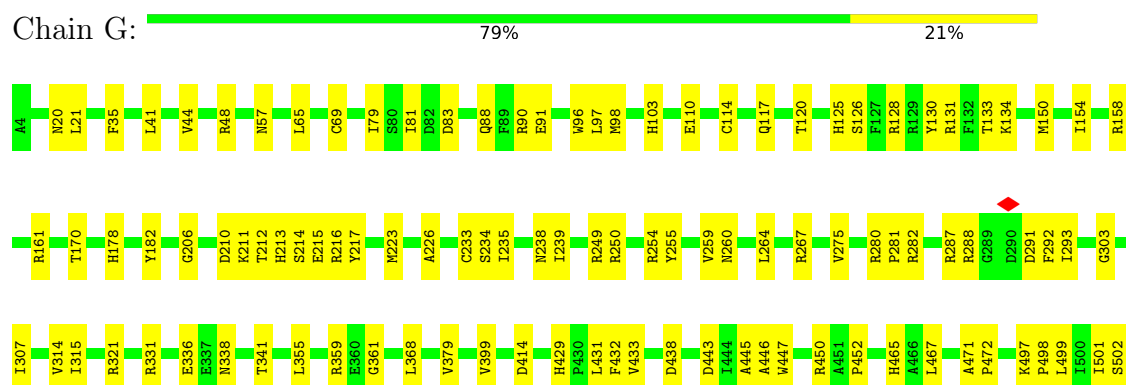
• Molecule 1: NADH-quinone oxidoreductase subunit F

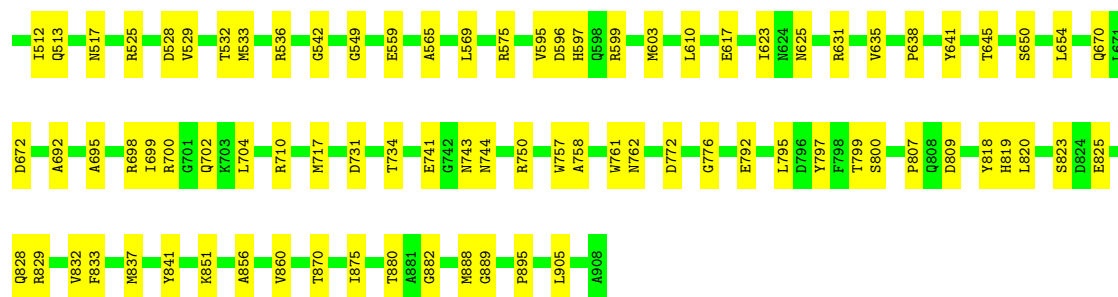


• Molecule 2: NADH dehydrogenase I subunit E

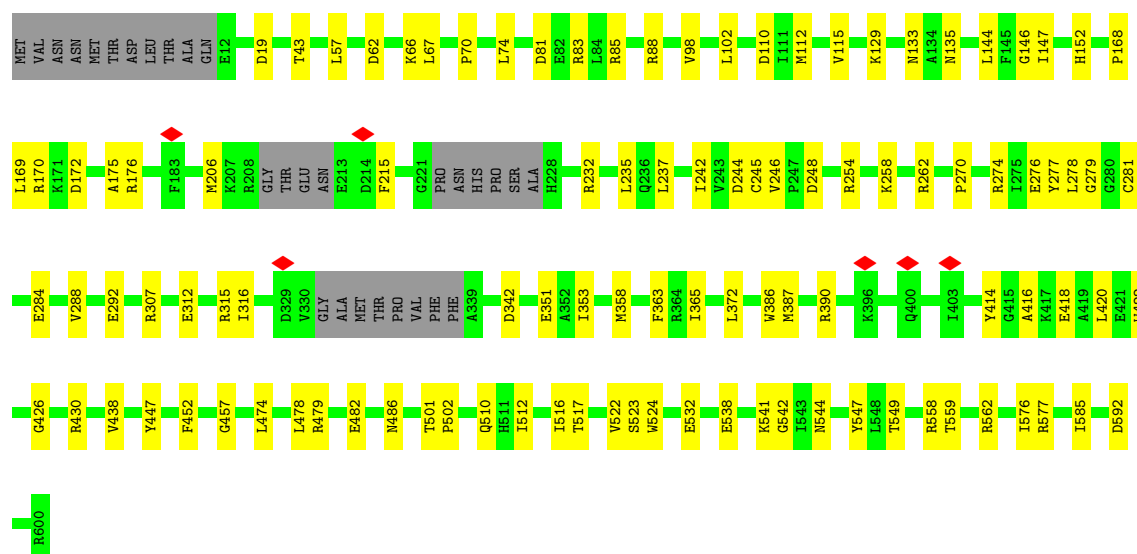
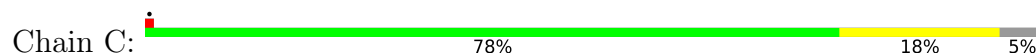


• Molecule 3: NADH-quinone oxidoreductase

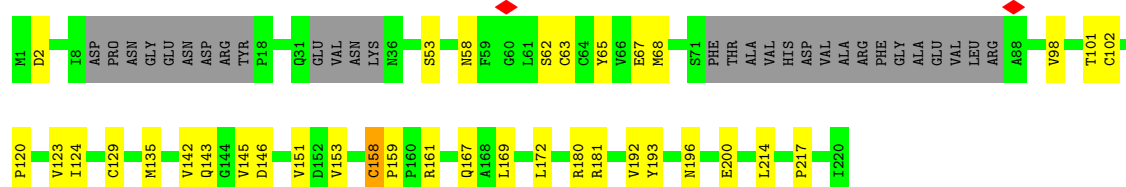




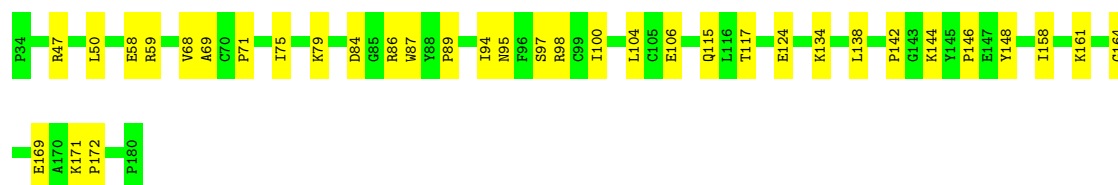
• Molecule 4: NADH-quinone oxidoreductase subunit C/D



• Molecule 5: NADH-quinone oxidoreductase subunit B



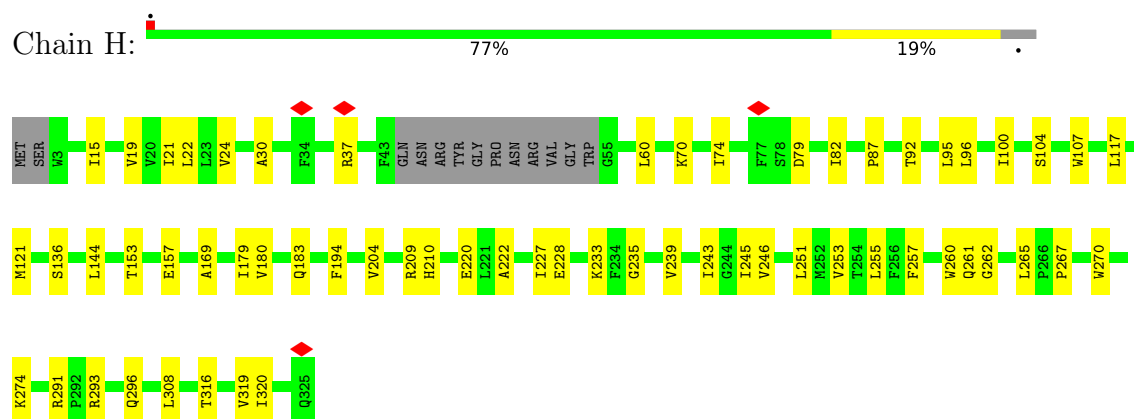
• Molecule 6: NADH-quinone oxidoreductase subunit I



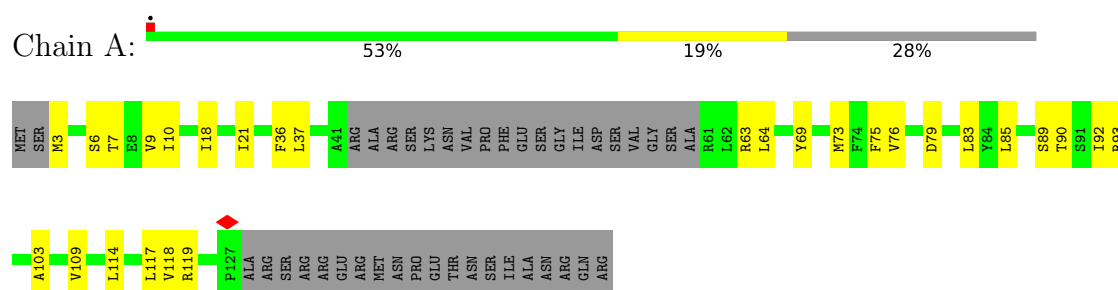
Chain L: 80% 17%



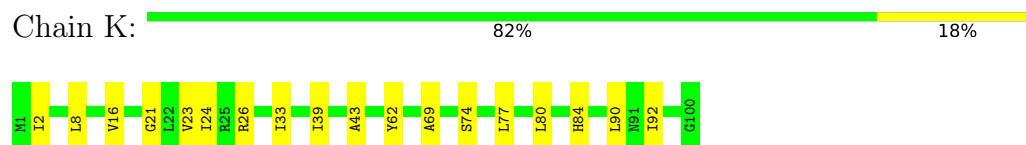
- Molecule 10: NADH-quinone oxidoreductase subunit H



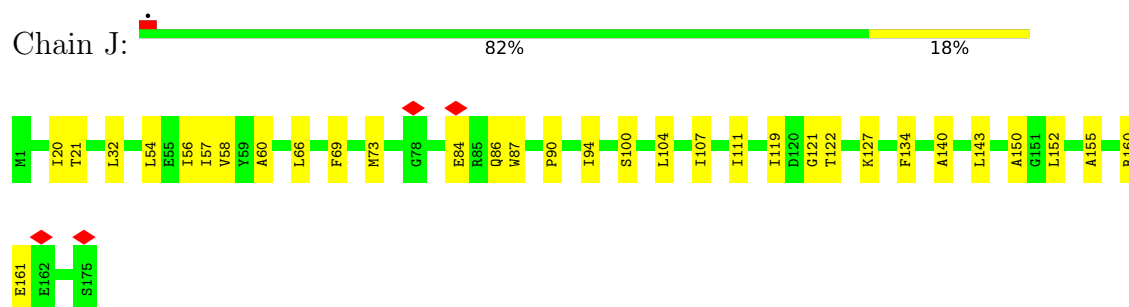
- Molecule 11: NADH-quinone oxidoreductase subunit A



- Molecule 12: NADH-quinone oxidoreductase subunit K



- Molecule 13: NADH-quinone oxidoreductase subunit J



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	145253	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 ($e^-/\text{\AA}^2$)	89	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.929	Depositor
Minimum map value	-0.129	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.075	Depositor
Map size (Å)	149.601, 220.688, 237.664	wwPDB
Map dimensions	224, 208, 141	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SF4, NAI, FMN, 3PE, FES, UQ8

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	F	0.17	0/3511	0.44	0/4745
2	E	0.15	0/1248	0.37	0/1691
3	G	0.15	0/7173	0.39	0/9726
4	C	0.17	0/4728	0.44	0/6413
5	B	0.19	0/1548	0.48	0/2092
6	I	0.16	0/1185	0.41	0/1603
7	L	0.19	0/4639	0.46	0/6322
8	M	0.20	0/4074	0.45	1/5546 (0.0%)
9	N	0.19	0/3718	0.44	3/5071 (0.1%)
10	H	0.23	0/2520	0.53	0/3427
11	A	0.20	0/865	0.50	0/1176
12	K	0.18	0/769	0.42	0/1040
13	J	0.19	0/1352	0.50	0/1841
All	All	0.18	0/37330	0.44	4/50693 (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
5	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	N	5	PRO	CA-N-CD	-5.56	104.22	112.00
8	M	136	MET	CB-CG-SD	5.33	128.68	112.70
9	N	387	PRO	CA-C-N	5.21	131.49	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	N	387	PRO	C-N-CA	5.21	131.49	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	B	158	CYS	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	F	3432	0	3405	57	0
2	E	1220	0	1188	16	0
3	G	7022	0	6825	116	0
4	C	4606	0	4516	72	0
5	B	1518	0	1513	23	0
6	I	1157	0	1121	24	0
7	L	4525	0	4668	68	0
8	M	3953	0	4053	50	0
9	N	3630	0	3799	69	0
10	H	2449	0	2503	40	0
11	A	840	0	855	26	0
12	K	760	0	817	17	0
13	J	1326	0	1394	32	0
14	B	8	0	0	0	0
14	F	8	0	0	0	0
14	G	24	0	0	2	0
14	I	16	0	0	0	0
15	F	31	0	19	2	0
16	F	44	0	27	4	0
17	E	4	0	0	0	0
17	G	4	0	0	0	0
18	G	1	0	0	0	0
19	L	88	0	130	6	0
20	H	24	0	25	0	0
All	All	36690	0	36858	535	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 7.

All (535) 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)
13:J:69:PHE:O	13:J:73:MET:HB2	1.78	0.82
4:C:215:PHE:HA	4:C:237:LEU:O	1.88	0.74
4:C:416:ALA:O	4:C:420:LEU:HB2	1.89	0.72
10:H:104:SER:HB3	10:H:107:TRP:HB2	1.70	0.72
10:H:227:ILE:HG13	10:H:228:GLU:HG2	1.74	0.69
1:F:85:ARG:HG2	1:F:213:PRO:HG2	1.75	0.68
1:F:94:MET:HE1	1:F:176:GLY:HA2	1.74	0.68
8:M:181:SER:HB2	8:M:230:ALA:HA	1.76	0.66
3:G:103:HIS:HA	4:C:512:ILE:HD13	1.75	0.66
8:M:338:TYR:HB3	8:M:493:ILE:HD12	1.79	0.65
1:F:430:THR:OG1	4:C:510:GLN:NE2	2.31	0.64
2:E:94:SER:OG	2:E:132:CYS:O	2.16	0.64
9:N:311:VAL:HA	9:N:314:ILE:HD12	1.80	0.64
12:K:77:LEU:HD12	13:J:66:LEU:HG	1.81	0.63
12:K:21:GLY:HA3	13:J:20:ILE:HD12	1.79	0.63
7:L:319:MET:SD	7:L:334:HIS:ND1	2.71	0.62
13:J:57:ILE:HG22	13:J:58:VAL:HG23	1.82	0.62
10:H:30:ALA:HB1	10:H:60:LEU:HD21	1.81	0.62
3:G:280:ARG:HH21	3:G:597:HIS:HB2	1.65	0.61
5:B:65:TYR:HA	5:B:68:MET:HE2	1.82	0.61
6:I:142:PRO:HB2	6:I:146:PRO:HA	1.83	0.61
1:F:90:ASN:HD22	15:F:502:FMN:HO4'	1.49	0.61
4:C:365:ILE:HD12	4:C:501:THR:HB	1.82	0.60
13:J:56:ILE:HA	13:J:60:ALA:HB3	1.83	0.60
9:N:82:LEU:HD11	9:N:334:LEU:HD21	1.84	0.60
2:E:26:MET:HE3	2:E:32:PRO:HB3	1.84	0.60
3:G:150:MET:HE2	3:G:182:TYR:HA	1.83	0.60
4:C:144:LEU:HA	4:C:168:PRO:HD2	1.83	0.60
7:L:392:VAL:HG13	7:L:393:THR:HG23	1.84	0.60
8:M:340:GLY:O	8:M:344:GLN:HB2	2.00	0.60
7:L:144:GLU:OE2	7:L:175:ARG:NH1	2.35	0.59
1:F:12:PRO:HB3	1:F:235:TRP:HH2	1.66	0.59
3:G:275:VAL:O	3:G:280:ARG:NH1	2.35	0.59
7:L:35:VAL:HG12	7:L:100:HIS:HB3	1.84	0.59
4:C:146:GLY:HA3	4:C:170:ARG:HH21	1.67	0.59
7:L:136:LEU:HB3	7:L:195:LEU:HG	1.84	0.59
11:A:69:TYR:OH	12:K:74:SER:O	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:744:ASN:OD1	3:G:750:ARG:NH2	2.37	0.58
9:N:248:ILE:HG12	9:N:330:LEU:HD22	1.85	0.58
11:A:3:MET:SD	11:A:3:MET:N	2.76	0.58
3:G:599:ARG:O	3:G:829:ARG:NH2	2.37	0.58
8:M:258:ASP:HA	8:M:262:ILE:HB	1.85	0.58
10:H:210:HIS:O	10:H:291:ARG:NH1	2.35	0.58
3:G:21:LEU:HD21	3:G:79:ILE:HG21	1.86	0.58
6:I:106:GLU:HG3	6:I:115:GLN:HA	1.85	0.58
2:E:87:HIS:ND1	2:E:146:ASP:OD2	2.35	0.58
3:G:497:LYS:HG2	3:G:528:ASP:HB3	1.86	0.57
9:N:312:ALA:HB2	9:N:398:VAL:HG23	1.86	0.57
8:M:362:LEU:HD21	8:M:374:MET:HE1	1.84	0.57
3:G:81:ILE:O	3:G:90:ARG:NH2	2.37	0.57
8:M:59:GLY:O	8:M:495:ASN:ND2	2.37	0.57
3:G:758:ALA:HB3	3:G:761:TRP:HB2	1.87	0.57
1:F:249:LEU:HB3	1:F:261:LEU:HD11	1.85	0.57
7:L:169:LYS:HG3	19:L:802:3PE:H341	1.87	0.57
3:G:670:GLN:NE2	3:G:672:ASP:OD2	2.38	0.57
1:F:84:ILE:HB	1:F:212:LYS:HG2	1.87	0.56
10:H:117:LEU:O	10:H:121:MET:HG3	2.05	0.56
3:G:856:ALA:HB2	3:G:875:ILE:HG12	1.87	0.56
3:G:569:LEU:HD11	3:G:650:SER:HB3	1.88	0.56
7:L:80:VAL:HB	7:L:134:ASP:HB2	1.88	0.56
12:K:16:VAL:HG13	13:J:100:SER:HB3	1.86	0.56
3:G:315:ILE:HG22	3:G:338:ASN:HB2	1.88	0.56
4:C:62:ASP:OD1	4:C:66:LYS:NZ	2.37	0.56
6:I:58:GLU:O	6:I:86:ARG:NH2	2.39	0.56
4:C:438:VAL:HB	4:C:538:GLU:HB2	1.88	0.56
1:F:288:LYS:HD3	1:F:331:HIS:HA	1.86	0.56
3:G:700:ARG:O	4:C:83:ARG:NH1	2.39	0.56
1:F:77:PRO:O	1:F:85:ARG:NH2	2.39	0.56
9:N:33:ASN:O	9:N:37:ASN:ND2	2.39	0.56
10:H:179:ILE:HG21	10:H:255:LEU:HD23	1.86	0.55
1:F:130:ILE:HG13	1:F:169:LEU:HD11	1.87	0.55
1:F:133:ARG:NH2	2:E:133:CYS:O	2.30	0.55
4:C:110:ASP:OD1	4:C:110:ASP:N	2.38	0.55
4:C:315:ARG:NH2	4:C:538:GLU:O	2.39	0.55
3:G:828:GLN:NE2	3:G:889:GLY:O	2.39	0.55
8:M:79:ILE:HA	8:M:138:LEU:HD22	1.89	0.55
1:F:345:PHE:O	1:F:349:GLU:HB2	2.07	0.55
3:G:641:TYR:OH	3:G:717:MET:SD	2.62	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:482:GLU:OE2	4:C:486:ASN:ND2	2.40	0.55
5:B:101:THR:HA	5:B:129:CYS:HB3	1.88	0.55
1:F:17:LEU:HD11	1:F:107:GLN:HG3	1.89	0.54
4:C:19:ASP:OD1	4:C:19:ASP:N	2.38	0.54
4:C:206:MET:HE2	4:C:246:VAL:HG23	1.90	0.54
6:I:164:GLY:HA2	6:I:169:GLU:HG2	1.88	0.54
7:L:45:THR:HA	7:L:48:ILE:HG12	1.89	0.54
9:N:217:LYS:HB3	9:N:250:ILE:HD13	1.88	0.54
3:G:41:LEU:O	3:G:161:ARG:NH1	2.39	0.54
3:G:704:LEU:HA	3:G:743:ASN:H	1.72	0.54
3:G:223:MET:HE1	3:G:250:ARG:HB3	1.89	0.54
10:H:79:ASP:OD1	10:H:79:ASP:N	2.37	0.54
12:K:39:ILE:HG21	12:K:69:ALA:HB2	1.89	0.54
3:G:212:THR:HG22	3:G:832:VAL:HG21	1.90	0.54
4:C:558:ARG:NH1	4:C:559:THR:O	2.41	0.54
8:M:71:TRP:HB2	8:M:79:ILE:HG13	1.88	0.54
9:N:219:SER:HB3	9:N:303:ILE:HG12	1.90	0.54
11:A:75:PHE:O	11:A:79:ASP:HB2	2.08	0.54
5:B:143:GLN:OE1	6:I:98:ARG:NH2	2.38	0.54
8:M:72:ILE:HB	8:M:77:ILE:HB	1.89	0.54
10:H:183:GLN:NE2	10:H:257:PHE:O	2.41	0.54
2:E:125:ARG:NH2	2:E:165:TYR:O	2.39	0.54
2:E:136:ASN:O	2:E:142:ASN:ND2	2.41	0.54
7:L:200:MET:HE3	7:L:272:LEU:HD11	1.88	0.53
8:M:45:GLN:NE2	8:M:49:GLN:OE1	2.41	0.53
9:N:67:MET:HG2	9:N:121:ASN:HB3	1.90	0.53
3:G:860:VAL:O	3:G:870:THR:HA	2.07	0.53
9:N:139:LEU:HD11	9:N:242:LEU:HB3	1.91	0.53
1:F:95:GLU:HB2	16:F:503:NAI:H42N	1.89	0.53
9:N:70:ASP:OD1	9:N:256:ARG:NH2	2.41	0.53
1:F:320:ARG:NH1	16:F:503:NAI:O2D	2.40	0.53
3:G:126:SER:HB3	4:C:517:THR:HG21	1.89	0.53
3:G:499:LEU:HD11	3:G:532:THR:HG23	1.89	0.53
9:N:119:LEU:HD22	9:N:253:VAL:HG11	1.90	0.53
1:F:377:GLN:HG2	1:F:427:PHE:HA	1.91	0.53
7:L:240:ALA:O	7:L:306:ARG:NH1	2.41	0.53
10:H:180:VAL:O	10:H:261:GLN:NE2	2.42	0.53
3:G:321:ARG:NH2	3:G:596:ASP:OD1	2.42	0.53
1:F:437:GLN:NE2	4:C:372:LEU:O	2.42	0.52
3:G:215:GLU:HG3	3:G:216:ARG:HG2	1.91	0.52
4:C:281:CYS:HA	4:C:284:GLU:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:309:LEU:HD11	9:N:330:LEU:HD21	1.90	0.52
3:G:226:ALA:HB3	3:G:635:VAL:HG22	1.92	0.52
8:M:137:PHE:HB2	8:M:205:PHE:HD2	1.74	0.52
9:N:125:LEU:HD13	9:N:174:MET:HB3	1.92	0.52
10:H:144:LEU:HD22	10:H:222:ALA:HB2	1.91	0.52
1:F:59:LEU:HD12	1:F:228:ILE:HD12	1.91	0.52
3:G:97:LEU:HD22	3:G:154:ILE:HB	1.90	0.52
3:G:206:GLY:N	14:G:1001:SF4:S2	2.83	0.52
4:C:81:ASP:OD2	4:C:83:ARG:NH2	2.43	0.52
1:F:96:PRO:HB3	2:E:94:SER:HB3	1.92	0.52
7:L:222:LEU:HD22	7:L:265:LEU:HD11	1.91	0.52
10:H:320:ILE:HD11	11:A:92:ILE:HG12	1.91	0.52
8:M:134:ILE:HD12	8:M:207:TYR:HB3	1.92	0.52
9:N:174:MET:HA	9:N:177:VAL:HG22	1.92	0.52
3:G:438:ASP:OD1	3:G:450:ARG:NH1	2.42	0.52
11:A:117:LEU:HD11	13:J:152:LEU:HD11	1.92	0.52
8:M:392:ALA:O	8:M:396:LEU:HB2	2.10	0.52
12:K:26:ARG:HH22	13:J:86:GLN:HG3	1.75	0.52
1:F:93:GLU:O	1:F:133:ARG:NH1	2.43	0.51
6:I:158:ILE:HB	6:I:161:LYS:HB3	1.91	0.51
9:N:369:ARG:NH1	9:N:450:TYR:OH	2.43	0.51
9:N:77:THR:HG23	9:N:117:ILE:HG12	1.90	0.51
4:C:133:ASN:HB3	4:C:422:TRP:HA	1.92	0.51
8:M:184:VAL:HG11	8:M:229:ILE:HD11	1.92	0.51
1:F:82:MET:O	1:F:85:ARG:NH1	2.44	0.51
4:C:277:TYR:CD2	5:B:63:CYS:HB3	2.46	0.51
8:M:175:PHE:HD2	9:N:422:LEU:HD13	1.75	0.51
3:G:757:TRP:NE1	3:G:762:ASN:OD1	2.43	0.51
7:L:92:VAL:HG22	7:L:257:THR:HG22	1.93	0.51
8:M:432:ALA:HA	8:M:435:TYR:CE2	2.46	0.51
3:G:234:SER:HB2	3:G:625:ASN:HB3	1.91	0.51
1:F:377:GLN:OE1	3:G:131:ARG:NE	2.44	0.51
3:G:452:PRO:HD3	3:G:880:THR:HG21	1.92	0.51
4:C:244:ASP:OD1	4:C:577:ARG:NH1	2.43	0.51
9:N:270:ARG:NH1	9:N:314:ILE:O	2.44	0.51
9:N:376:MET:HE3	9:N:380:MET:HE3	1.92	0.51
7:L:89:LEU:HD22	7:L:132:LEU:HD11	1.93	0.51
3:G:35:PHE:O	3:G:158:ARG:NH2	2.44	0.50
9:N:159:TYR:O	9:N:163:SER:OG	2.20	0.50
1:F:416:ARG:NH1	1:F:420:GLU:OE1	2.44	0.50
3:G:888:MET:HB3	3:G:895:PRO:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:118:LEU:HD22	13:J:143:LEU:HD13	1.92	0.50
9:N:244:THR:HB	9:N:334:LEU:HD12	1.93	0.50
10:H:100:ILE:HD11	10:H:251:LEU:HD21	1.93	0.50
4:C:544:ASN:ND2	4:C:562:ARG:O	2.43	0.50
5:B:217:PRO:HG3	6:I:144:LYS:HD2	1.93	0.50
7:L:609:LEU:HD22	9:N:204:LEU:HD12	1.92	0.50
8:M:6:LEU:HD21	8:M:91:VAL:HG11	1.92	0.50
4:C:98:VAL:HG22	4:C:147:ILE:HD13	1.93	0.50
7:L:315:GLN:O	7:L:319:MET:HG2	2.12	0.50
3:G:282:ARG:HE	3:G:645:THR:HG21	1.76	0.50
19:L:802:3PE:H242	8:M:434:VAL:HG21	1.93	0.50
9:N:79:LEU:HD22	9:N:334:LEU:HD22	1.94	0.50
1:F:118:ILE:HG21	1:F:229:LEU:HD13	1.93	0.50
3:G:617:GLU:HG2	3:G:638:PRO:HG3	1.94	0.50
4:C:274:ARG:NH2	5:B:158:CYS:SG	2.85	0.50
5:B:153:VAL:HG21	5:B:172:LEU:HB2	1.93	0.50
1:F:348:ARG:HH22	2:E:132:CYS:HA	1.77	0.50
3:G:287:ARG:HA	3:G:291:ASP:O	2.12	0.50
4:C:452:PHE:HA	4:C:479:ARG:HH21	1.76	0.50
10:H:169:ALA:HB1	11:A:92:ILE:HD13	1.93	0.50
1:F:188:ASN:ND2	1:F:196:ASN:O	2.40	0.49
3:G:260:ASN:H	3:G:368:LEU:HD23	1.77	0.49
4:C:426:GLY:HA2	4:C:542:GLY:HA2	1.92	0.49
8:M:153:LEU:HD23	8:M:257:VAL:HG22	1.94	0.49
7:L:550:VAL:HG13	19:L:802:3PE:H232	1.93	0.49
3:G:120:THR:HB	4:C:516:ILE:HG21	1.94	0.49
6:I:75:ILE:HG12	6:I:94:ILE:HG12	1.95	0.49
3:G:399:VAL:HA	3:G:429:HIS:HB2	1.93	0.49
8:M:84:ASP:N	8:M:84:ASP:OD1	2.42	0.49
9:N:423:TYR:O	9:N:427:ARG:HB2	2.12	0.49
4:C:522:VAL:HG13	6:I:69:ALA:HB2	1.94	0.49
6:I:71:PRO:HD3	6:I:104:LEU:HD12	1.95	0.49
7:L:4:LEU:HD21	7:L:81:LEU:HD22	1.95	0.49
7:L:174:THR:HB	7:L:229:LYS:HE2	1.95	0.49
3:G:98:MET:HE1	4:C:512:ILE:HG13	1.95	0.49
4:C:85:ARG:HB3	4:C:88:ARG:HD2	1.95	0.49
3:G:809:ASP:N	3:G:809:ASP:OD1	2.43	0.49
9:N:259:LEU:HB2	9:N:316:LEU:HD21	1.94	0.49
9:N:387:PRO:O	9:N:388:MET:HG2	2.12	0.49
11:A:3:MET:HE1	13:J:121:GLY:HA3	1.93	0.49
11:A:90:THR:O	13:J:127:LYS:NZ	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:239:ILE:HD12	1:F:247:THR:HG23	1.94	0.49
4:C:276:GLU:HG2	4:C:279:GLY:H	1.77	0.49
7:L:584:LEU:HD22	9:N:287:MET:HG2	1.95	0.49
6:I:171:LYS:HG2	6:I:172:PRO:HD2	1.95	0.49
4:C:288:VAL:HG21	4:C:363:PHE:HB3	1.93	0.48
4:C:532:GLU:OE1	4:C:547:TYR:OH	2.28	0.48
5:B:124:ILE:HD11	5:B:172:LEU:HD22	1.94	0.48
7:L:22:ARG:HH22	7:L:24:ARG:HH21	1.61	0.48
9:N:112:ALA:HB2	9:N:138:PRO:HB2	1.95	0.48
9:N:421:GLY:HA2	9:N:424:TYR:CE2	2.47	0.48
12:K:16:VAL:HG21	13:J:104:LEU:HB2	1.94	0.48
12:K:43:ALA:HB1	12:K:62:TYR:HD1	1.78	0.48
8:M:144:GLU:HB2	9:N:387:PRO:HG2	1.94	0.48
1:F:62:ARG:NH1	1:F:247:THR:O	2.44	0.48
3:G:467:LEU:O	3:G:525:ARG:NH2	2.44	0.48
3:G:807:PRO:HB3	3:G:882:GLY:HA3	1.94	0.48
7:L:192:LEU:HD22	7:L:200:MET:HG3	1.94	0.48
7:L:329:ASP:OD1	7:L:329:ASP:N	2.45	0.48
8:M:123:ILE:HG13	8:M:149:PRO:HB2	1.95	0.48
7:L:3:MET:HG2	7:L:6:LEU:HD13	1.94	0.48
3:G:128:ARG:HH22	3:G:134:LYS:HE2	1.78	0.48
3:G:255:TYR:OH	3:G:776:GLY:O	2.27	0.48
4:C:312:GLU:OE2	4:C:315:ARG:NH1	2.46	0.48
9:N:288:ALA:HB2	9:N:300:TYR:HB2	1.96	0.48
11:A:85:LEU:O	11:A:89:SER:OG	2.29	0.48
1:F:298:ASP:OD1	1:F:298:ASP:N	2.42	0.48
3:G:361:GLY:HA2	3:G:795:LEU:HG	1.94	0.48
4:C:135:ASN:HA	4:C:152:HIS:HE1	1.78	0.48
8:M:315:ILE:HD13	8:M:355:LEU:HB3	1.96	0.48
3:G:431:LEU:HB3	3:G:445:ALA:HA	1.96	0.48
3:G:443:ASP:OD1	3:G:443:ASP:N	2.47	0.48
7:L:243:MET:SD	7:L:243:MET:N	2.87	0.48
12:K:24:ILE:HD12	13:J:87:TRP:HB2	1.96	0.48
3:G:414:ASP:OD1	3:G:414:ASP:N	2.46	0.47
8:M:234:LYS:HB3	8:M:267:ALA:HB2	1.96	0.47
10:H:265:LEU:HB2	10:H:270:TRP:CD1	2.49	0.47
2:E:132:CYS:SG	2:E:133:CYS:N	2.87	0.47
10:H:253:VAL:HG23	10:H:257:PHE:HB2	1.96	0.47
3:G:91:GLU:HG3	3:G:125:HIS:HB2	1.96	0.47
5:B:180:ARG:HB2	5:B:193:TYR:HB2	1.96	0.47
6:I:84:ASP:OD1	6:I:84:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:209:ARG:HG3	10:H:245:ILE:HD13	1.97	0.47
4:C:67:LEU:HB2	4:C:70:PRO:HA	1.97	0.47
9:N:334:LEU:O	9:N:338:LEU:HB2	2.13	0.47
10:H:239:VAL:O	10:H:243:ILE:HG12	2.14	0.47
12:K:26:ARG:HH12	13:J:86:GLN:HG3	1.79	0.47
4:C:549:THR:HB	4:C:558:ARG:HB3	1.97	0.47
7:L:227:VAL:HB	7:L:232:GLN:HB2	1.97	0.47
7:L:273:PHE:HB3	7:L:280:LEU:HD13	1.97	0.47
19:L:802:3PE:H292	19:L:802:3PE:H391	1.97	0.47
1:F:381:ILE:HG23	1:F:412:ILE:HD12	1.96	0.47
3:G:110:GLU:HB3	3:G:114:CYS:HB2	1.97	0.47
11:A:103:ALA:HB2	13:J:134:PHE:HE2	1.80	0.47
2:E:134:LEU:HD11	2:E:144:MET:HB2	1.96	0.47
3:G:117:GLN:NE2	14:G:1001:SF4:S3	2.88	0.47
9:N:22:VAL:HG11	11:A:109:VAL:HG12	1.97	0.47
3:G:233:CYS:SG	3:G:234:SER:N	2.88	0.47
5:B:200:GLU:HB2	6:I:124:GLU:HG2	1.97	0.47
7:L:85:SER:OG	7:L:268:ARG:NH2	2.48	0.47
7:L:238:TRP:HZ3	7:L:253:ILE:HD11	1.80	0.47
2:E:141:PRO:HB2	2:E:153:LEU:HB2	1.95	0.47
10:H:293:ARG:HE	10:H:296:GLN:HE22	1.61	0.47
3:G:211:LYS:HA	3:G:214:SER:HB2	1.97	0.46
8:M:7:ILE:HG13	8:M:132:LEU:HD22	1.96	0.46
9:N:214:LEU:HD13	9:N:254:VAL:HG22	1.96	0.46
4:C:292:GLU:OE2	4:C:307:ARG:NH2	2.48	0.46
7:L:103:ALA:HA	7:L:106:TYR:HB3	1.96	0.46
7:L:141:LEU:HA	8:M:399:PRO:HG2	1.97	0.46
10:H:316:THR:HA	10:H:319:VAL:HG22	1.96	0.46
3:G:288:ARG:HH22	3:G:293:ILE:HD13	1.80	0.46
7:L:550:VAL:HG22	19:L:802:3PE:H252	1.97	0.46
9:N:283:PHE:O	9:N:287:MET:HB2	2.15	0.46
3:G:303:GLY:O	3:G:307:ILE:HG12	2.16	0.46
7:L:82:ASP:N	7:L:82:ASP:OD1	2.48	0.46
8:M:374:MET:H	8:M:374:MET:HG2	1.59	0.46
9:N:71:GLY:HA2	9:N:74:MET:HE3	1.97	0.46
3:G:575:ARG:HD2	3:G:825:GLU:HB3	1.98	0.46
5:B:135:MET:HB3	6:I:100:ILE:HG21	1.96	0.46
10:H:235:GLY:O	10:H:239:VAL:HG22	2.15	0.46
1:F:90:ASN:ND2	1:F:181:GLY:O	2.32	0.46
4:C:342:ASP:HA	4:C:386:TRP:HH2	1.81	0.46
7:L:291:LEU:HD22	7:L:318:TYR:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:168:ILE:HG12	9:N:430:VAL:HG11	1.97	0.46
11:A:83:LEU:HD23	13:J:58:VAL:HG21	1.96	0.46
1:F:359:ASP:HB2	3:G:96:TRP:HB3	1.98	0.46
3:G:741:GLU:OE1	4:C:262:ARG:NE	2.46	0.46
9:N:70:ASP:OD1	9:N:70:ASP:N	2.47	0.46
9:N:134:LEU:HD11	13:J:143:LEU:HB3	1.98	0.46
11:A:18:ILE:HA	11:A:21:ILE:HG22	1.97	0.46
3:G:83:ASP:OD1	3:G:83:ASP:N	2.48	0.46
3:G:472:PRO:HG3	3:G:799:THR:HA	1.98	0.46
6:I:47:ARG:O	6:I:117:THR:OG1	2.32	0.46
5:B:181:ARG:HG2	5:B:192:VAL:HG13	1.98	0.45
9:N:248:ILE:HD11	9:N:334:LEU:HB2	1.98	0.45
10:H:243:ILE:HA	10:H:246:VAL:HG12	1.98	0.45
1:F:86:TYR:HB2	1:F:214:THR:HG22	1.98	0.45
4:C:387:MET:HE3	4:C:478:LEU:HD11	1.98	0.45
7:L:98:LEU:HD23	7:L:460:LEU:HG	1.98	0.45
7:L:592:ARG:NE	12:K:23:VAL:O	2.42	0.45
9:N:305:HIS:ND1	9:N:329:TYR:OH	2.35	0.45
9:N:363:ARG:NH1	9:N:435:HIS:O	2.50	0.45
3:G:695:ALA:O	3:G:698:ARG:NH1	2.49	0.45
4:C:235:LEU:HD23	4:C:245:CYS:HB3	1.98	0.45
6:I:50:LEU:HB2	6:I:138:LEU:HA	1.99	0.45
2:E:32:PRO:HB2	2:E:62:LEU:HG	1.99	0.45
3:G:699:ILE:HD11	3:G:750:ARG:HB3	1.98	0.45
1:F:377:GLN:NE2	1:F:425:GLN:HE21	2.15	0.45
3:G:431:LEU:O	3:G:446:ALA:N	2.49	0.45
4:C:254:ARG:NH2	5:B:62:SER:OG	2.50	0.45
5:B:67:GLU:HG2	5:B:159:PRO:HB2	1.98	0.45
7:L:143:TRP:O	7:L:229:LYS:NZ	2.50	0.45
8:M:137:PHE:HB2	8:M:205:PHE:CD2	2.52	0.45
8:M:237:VAL:HG11	8:M:327:LEU:HD22	1.98	0.45
9:N:386:ILE:HD11	9:N:426:LEU:HD11	1.99	0.45
13:J:90:PRO:O	13:J:94:ILE:HB	2.16	0.45
1:F:65:ALA:HB2	16:F:503:NAI:H4D	1.99	0.45
4:C:144:LEU:HB3	4:C:169:LEU:HB2	1.98	0.45
6:I:95:ASN:OD1	6:I:97:SER:OG	2.35	0.45
9:N:32:ARG:NH2	9:N:101:ASN:OD1	2.50	0.45
9:N:72:PHE:HB3	9:N:256:ARG:HH21	1.82	0.45
1:F:86:TYR:HE1	1:F:127:ARG:HD2	1.82	0.45
4:C:242:ILE:HD11	4:C:576:ILE:HG22	1.99	0.45
4:C:316:ILE:HG12	4:C:474:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:120:PRO:HD2	10:H:70:LYS:HD2	1.99	0.45
10:H:15:ILE:HG23	11:A:18:ILE:HG21	1.99	0.45
1:F:62:ARG:O	1:F:100:LYS:NZ	2.41	0.45
7:L:227:VAL:HG23	7:L:235:LEU:HD12	1.99	0.45
9:N:100:ASP:OD1	13:J:160:ARG:NH2	2.46	0.45
9:N:426:LEU:HA	9:N:429:ALA:HB3	1.99	0.45
11:A:69:TYR:HB2	13:J:73:MET:HE1	1.99	0.45
5:B:98:VAL:HG11	5:B:145:VAL:HG11	1.98	0.45
8:M:396:LEU:HG	8:M:433:SER:HA	1.98	0.45
10:H:21:ILE:HA	10:H:24:VAL:HG12	1.99	0.45
4:C:541:LYS:HG2	4:C:592:ASP:HB3	1.99	0.44
3:G:819:HIS:NE2	3:G:841:TYR:OH	2.30	0.44
4:C:351:GLU:OE2	5:B:161:ARG:NH1	2.49	0.44
4:C:353:ILE:HD12	4:C:372:LEU:HD22	1.97	0.44
6:I:79:LYS:HE3	6:I:87:TRP:CE2	2.52	0.44
1:F:395:LYS:HD2	3:G:65:LEU:HD12	2.00	0.44
3:G:281:PRO:HG2	3:G:603:MET:HE1	1.99	0.44
4:C:43:THR:HB	4:C:532:GLU:HB2	1.99	0.44
5:B:123:VAL:HB	5:B:151:VAL:HA	2.00	0.44
8:M:130:VAL:HG11	8:M:266:THR:HB	1.99	0.44
3:G:536:ARG:NH1	3:G:818:TYR:OH	2.38	0.44
4:C:585:ILE:HD12	10:H:220:GLU:HG3	2.00	0.44
13:J:84:GLU:HB3	13:J:86:GLN:HG2	2.00	0.44
3:G:498:PRO:O	3:G:529:VAL:HA	2.18	0.44
8:M:236:PRO:HB2	8:M:320:VAL:HG22	1.99	0.44
9:N:361:SER:O	9:N:361:SER:OG	2.30	0.44
11:A:93:ARG:HE	11:A:93:ARG:HB3	1.65	0.44
3:G:512:ILE:HG23	3:G:533:MET:HE1	1.99	0.44
5:B:58:ASN:HB3	5:B:68:MET:HE3	2.00	0.44
9:N:455:ILE:O	9:N:459:ILE:HG12	2.17	0.44
10:H:262:GLY:HA3	10:H:270:TRP:CD1	2.52	0.44
13:J:122:THR:O	13:J:122:THR:OG1	2.27	0.44
1:F:60:LYS:HA	1:F:68:SER:HA	2.00	0.44
3:G:217:TYR:HB3	6:I:79:LYS:HD2	1.98	0.44
3:G:239:ILE:HG22	3:G:264:LEU:HD21	2.00	0.44
3:G:259:VAL:HA	3:G:368:LEU:HB3	1.99	0.44
3:G:379:VAL:HG22	3:G:501:ILE:HB	1.99	0.44
4:C:57:LEU:HD22	4:C:115:VAL:HG21	1.99	0.44
8:M:192:LEU:HB2	8:M:223:LEU:HD13	2.00	0.44
4:C:430:ARG:O	4:C:457:GLY:N	2.44	0.44
7:L:318:TYR:OH	7:L:418:GLY:O	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:6:SER:HB3	11:A:9:VAL:HG22	1.99	0.44
8:M:341:ALA:HA	8:M:410:ILE:HD11	2.00	0.44
9:N:216:PHE:HE2	9:N:217:LYS:HE3	1.82	0.44
12:K:84:HIS:HB2	12:K:90:LEU:HD21	2.00	0.44
5:B:2:ASP:OD1	5:B:196:ASN:ND2	2.49	0.43
7:L:59:THR:HG23	7:L:82:ASP:HB3	1.99	0.43
7:L:263:VAL:HG13	7:L:323:LEU:HD11	1.99	0.43
8:M:365:ARG:NH2	8:M:459:GLY:O	2.42	0.43
1:F:325:LEU:HD23	1:F:325:LEU:HA	1.81	0.43
3:G:851:LYS:HB3	3:G:851:LYS:HE3	1.81	0.43
7:L:31:ALA:O	7:L:35:VAL:HG22	2.18	0.43
3:G:210:ASP:HB3	3:G:213:HIS:HB3	2.00	0.43
1:F:348:ARG:HA	3:G:178:HIS:CD2	2.54	0.43
3:G:513:GLN:OE1	3:G:800:SER:OG	2.37	0.43
3:G:595:VAL:HG22	3:G:610:LEU:HD12	1.99	0.43
4:C:277:TYR:HB2	4:C:358:MET:HE2	2.00	0.43
7:L:143:TRP:CE2	7:L:229:LYS:HG3	2.53	0.43
10:H:22:LEU:HD11	10:H:95:LEU:HD21	2.00	0.43
1:F:63:GLY:O	16:F:503:NAI:H2N	2.19	0.43
7:L:5:ALA:O	7:L:9:ILE:HG12	2.19	0.43
7:L:291:LEU:HD13	7:L:318:TYR:HE1	1.83	0.43
9:N:73:ALA:O	9:N:77:THR:OG1	2.33	0.43
9:N:264:GLY:O	9:N:270:ARG:NH2	2.52	0.43
3:G:130:TYR:OH	3:G:133:THR:O	2.32	0.43
3:G:341:THR:N	3:G:549:GLY:O	2.51	0.43
3:G:631:ARG:HD2	3:G:692:ALA:HB3	2.01	0.43
3:G:772:ASP:OD1	3:G:772:ASP:N	2.51	0.43
4:C:414:TYR:HB2	4:C:418:GLU:HB2	2.00	0.43
10:H:92:THR:O	10:H:96:LEU:HG	2.18	0.43
10:H:144:LEU:HG	11:A:64:LEU:HD11	2.01	0.43
3:G:216:ARG:HH21	3:G:249:ARG:HH22	1.65	0.43
7:L:524:ASN:O	7:L:529:ARG:NH2	2.51	0.43
10:H:260:TRP:HB2	10:H:267:PRO:HB3	2.00	0.43
3:G:287:ARG:HB3	3:G:292:PHE:CD1	2.54	0.43
7:L:260:THR:HB	7:L:335:LEU:HD11	2.01	0.43
9:N:135:ILE:HD13	9:N:246:SER:HA	2.01	0.43
1:F:87:LEU:O	1:F:128:GLY:HA2	2.19	0.43
4:C:74:LEU:HA	4:C:102:LEU:HD23	2.01	0.43
7:L:28:ASN:O	7:L:32:ILE:HG23	2.18	0.43
7:L:91:VAL:HG21	7:L:336:MET:HG2	2.00	0.43
7:L:413:ASN:HA	7:L:416:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:ASN:OD1	1:F:83:ASN:N	2.51	0.43
3:G:355:LEU:O	3:G:359:ARG:HG2	2.19	0.43
4:C:175:ALA:HB2	4:C:258:LYS:HE3	2.00	0.43
3:G:710:ARG:HG3	4:C:524:TRP:HA	2.00	0.42
5:B:53:SER:O	5:B:53:SER:OG	2.37	0.42
8:M:124:LEU:HA	8:M:127:VAL:HG22	2.01	0.42
9:N:66:LEU:HD11	13:J:140:ALA:HB2	2.01	0.42
11:A:63:ARG:NH2	13:J:161:GLU:OE1	2.52	0.42
12:K:33:ILE:HG23	13:J:32:LEU:HD22	2.01	0.42
1:F:105:MET:HB3	1:F:139:ALA:HB1	2.01	0.42
7:L:425:THR:HA	7:L:428:TYR:CE2	2.55	0.42
11:A:83:LEU:HD22	13:J:54:LEU:HD22	2.01	0.42
1:F:90:ASN:ND2	15:F:502:FMN:O4'	2.37	0.42
3:G:233:CYS:SG	3:G:235:ILE:HG12	2.59	0.42
3:G:517:ASN:HD22	3:G:797:TYR:HD1	1.66	0.42
7:L:179:VAL:HG21	8:M:430:VAL:HG23	2.01	0.42
10:H:74:ILE:HD13	10:H:74:ILE:HA	1.94	0.42
12:K:8:LEU:HD23	13:J:111:ILE:HD12	2.01	0.42
7:L:183:PHE:HB3	7:L:221:MET:HG3	2.02	0.42
8:M:295:VAL:HG23	8:M:328:ILE:HD11	2.02	0.42
1:F:390:PHE:HZ	3:G:88:GLN:HG3	1.84	0.42
8:M:136:MET:HA	8:M:136:MET:HE3	2.00	0.42
4:C:175:ALA:O	4:C:176:ARG:HD3	2.19	0.42
7:L:196:ASN:O	7:L:200:MET:N	2.46	0.42
9:N:339:GLY:HA3	9:N:379:MET:HE3	2.02	0.42
1:F:116:MET:HE3	1:F:116:MET:HB3	1.83	0.42
2:E:44:GLN:NE2	2:E:78:GLN:O	2.49	0.42
8:M:235:MET:HA	8:M:236:PRO:HD3	1.92	0.42
10:H:204:VAL:HG13	10:H:209:ARG:HB2	2.01	0.42
1:F:394:GLY:O	3:G:48:ARG:NH2	2.50	0.42
3:G:833:PHE:O	3:G:837:MET:HG3	2.20	0.42
4:C:576:ILE:HD12	4:C:576:ILE:HG23	1.80	0.42
5:B:214:LEU:HD11	6:I:117:THR:HG22	2.02	0.42
7:L:12:LEU:HD11	19:L:801:3PE:H3H1	2.01	0.42
8:M:335:GLN:HG3	8:M:493:ILE:HG22	2.01	0.42
8:M:464:GLU:H	8:M:464:GLU:HG2	1.69	0.42
9:N:170:LEU:O	9:N:174:MET:HG3	2.20	0.42
11:A:114:LEU:O	11:A:118:VAL:HG23	2.19	0.42
5:B:102:CYS:O	5:B:142:VAL:N	2.46	0.42
9:N:12:LEU:HD12	9:N:12:LEU:HA	1.87	0.42
9:N:143:VAL:O	9:N:152:SER:OG	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:194:PHE:HB3	10:H:308:LEU:HD21	2.01	0.42
3:G:792:GLU:OE1	3:G:792:GLU:N	2.52	0.42
7:L:458:ILE:O	7:L:462:ILE:HG12	2.20	0.42
3:G:502:SER:O	3:G:533:MET:HA	2.19	0.41
7:L:467:VAL:HA	7:L:470:LEU:HD12	2.02	0.41
10:H:82:ILE:HG13	10:H:136:SER:HB3	2.02	0.41
12:K:2:ILE:HB	13:J:119:ILE:HB	2.02	0.41
13:J:107:ILE:O	13:J:111:ILE:HG12	2.20	0.41
7:L:88:MET:HE2	7:L:264:TYR:HB2	2.02	0.41
8:M:91:VAL:HA	8:M:94:THR:HG22	2.02	0.41
9:N:111:ILE:HG21	13:J:150:ALA:HB2	2.02	0.41
10:H:15:ILE:O	10:H:19:VAL:HG23	2.20	0.41
3:G:238:ASN:OD1	3:G:254:ARG:NH2	2.53	0.41
11:A:119:ARG:HE	11:A:119:ARG:HB3	1.68	0.41
1:F:38:ALA:HB2	1:F:114:GLU:HG3	2.03	0.41
3:G:569:LEU:HD13	3:G:654:LEU:HD11	2.03	0.41
3:G:837:MET:HG3	3:G:837:MET:H	1.68	0.41
4:C:342:ASP:OD1	4:C:390:ARG:NH1	2.53	0.41
4:C:523:SER:HA	6:I:68:VAL:HG11	2.03	0.41
10:H:153:THR:O	10:H:157:GLU:HB3	2.20	0.41
12:K:80:LEU:HD11	12:K:90:LEU:HD13	2.03	0.41
3:G:731:ASP:OD2	3:G:734:THR:OG1	2.30	0.41
7:L:82:ASP:H	7:L:85:SER:HB2	1.84	0.41
7:L:232:GLN:HA	7:L:290:THR:HG21	2.01	0.41
8:M:22:ARG:H	8:M:22:ARG:HG2	1.71	0.41
3:G:20:ASN:ND2	3:G:69:CYS:O	2.41	0.41
3:G:238:ASN:O	3:G:260:ASN:ND2	2.54	0.41
3:G:331:ARG:NE	3:G:336:GLU:OE1	2.54	0.41
6:I:158:ILE:HD13	6:I:158:ILE:HA	1.87	0.41
9:N:162:LEU:HD13	9:N:226:TRP:HB3	2.03	0.41
1:F:13:LEU:HD23	1:F:13:LEU:HA	1.94	0.41
3:G:267:ARG:HB2	3:G:820:LEU:HG	2.03	0.41
3:G:314:VAL:HG12	3:G:565:ALA:HB3	2.02	0.41
4:C:278:LEU:HB2	4:C:541:LYS:HZ2	1.85	0.41
7:L:560:LEU:HD12	8:M:303:TRP:HB3	2.03	0.41
8:M:357:ILE:O	8:M:361:GLN:HG3	2.20	0.41
13:J:21:THR:O	13:J:21:THR:OG1	2.39	0.41
1:F:338:LEU:HD11	2:E:99:ILE:HD11	2.01	0.41
4:C:232:ARG:NH2	4:C:248:ASP:OD2	2.54	0.41
4:C:312:GLU:OE2	4:C:447:TYR:OH	2.30	0.41
7:L:42:ALA:HA	7:L:45:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:345:MET:HE2	8:M:345:MET:HB3	1.83	0.41
9:N:422:LEU:HA	9:N:425:TYR:HB2	2.02	0.41
3:G:542:GLY:HA2	3:G:623:ILE:HD12	2.01	0.41
3:G:905:LEU:HD23	3:G:905:LEU:HA	1.94	0.41
4:C:501:THR:HA	4:C:502:PRO:HA	1.92	0.41
7:L:68:MET:HE2	7:L:68:MET:HB3	1.93	0.41
7:L:501:ALA:O	7:L:505:ILE:HG12	2.21	0.41
8:M:423:VAL:O	8:M:426:THR:OG1	2.36	0.41
9:N:386:ILE:O	9:N:389:THR:OG1	2.35	0.41
9:N:485:MET:HE3	9:N:485:MET:HB2	1.91	0.41
10:H:253:VAL:HG21	10:H:274:LYS:HB3	2.03	0.41
10:H:293:ARG:HE	10:H:296:GLN:NE2	2.18	0.41
11:A:73:MET:SD	13:J:155:ALA:HB3	2.60	0.41
3:G:702:GLN:HB3	4:C:172:ASP:HA	2.04	0.41
4:C:129:LYS:HA	4:C:129:LYS:HD3	1.91	0.41
7:L:380:LEU:HD13	7:L:380:LEU:HA	1.89	0.41
8:M:46:LEU:HA	8:M:49:GLN:HG2	2.03	0.41
9:N:108:LEU:HD13	9:N:141:GLY:HA3	2.03	0.41
9:N:300:TYR:HA	9:N:303:ILE:HD12	2.03	0.41
11:A:73:MET:HA	11:A:76:VAL:HG12	2.02	0.41
1:F:25:TRP:HH2	1:F:142:ASN:HD22	1.68	0.40
3:G:432:PHE:HD1	3:G:447:TRP:HB3	1.85	0.40
10:H:87:PRO:HG2	10:H:233:LYS:HG2	2.03	0.40
1:F:353:TRP:HZ2	3:G:44:VAL:HB	1.86	0.40
2:E:65:PRO:HB3	3:G:170:THR:HB	2.03	0.40
3:G:465:HIS:HA	3:G:471:ALA:HB3	2.03	0.40
6:I:59:ARG:NH1	6:I:148:TYR:O	2.54	0.40
6:I:89:PRO:O	6:I:134:LYS:NZ	2.52	0.40
7:L:372:ILE:HD12	7:L:375:VAL:HB	2.03	0.40
9:N:197:MET:HE2	9:N:197:MET:HB3	1.98	0.40
11:A:36:PHE:HB3	11:A:37:LEU:HD12	2.03	0.40
1:F:23:PRO:HA	1:F:107:GLN:HA	2.04	0.40
7:L:131:VAL:HG23	7:L:132:LEU:HG	2.03	0.40
7:L:232:GLN:O	7:L:236:GLN:HB3	2.21	0.40
10:H:37:ARG:HA	10:H:37:ARG:HD3	1.92	0.40
12:K:92:ILE:HD12	12:K:92:ILE:HA	1.92	0.40
1:F:391:LEU:HD22	1:F:401:ALA:HB1	2.04	0.40
4:C:270:PRO:O	4:C:274:ARG:HD3	2.21	0.40
7:L:327:ALA:HB1	7:L:330:ALA:HB3	2.04	0.40
9:N:171:LEU:HD12	9:N:171:LEU:HA	1.90	0.40
1:F:182:GLU:O	1:F:186:LEU:N	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:98:HIS:HA	2:E:102:TYR:HD1	1.86	0.40
3:G:117:GLN:HG2	4:C:516:ILE:HD12	2.04	0.40
3:G:379:VAL:HB	3:G:433:VAL:HG12	2.03	0.40
3:G:823:SER:OG	3:G:888:MET:O	2.23	0.40
9:N:221:VAL:HG12	9:N:224:HIS:CG	2.56	0.40
11:A:7:THR:HA	11:A:10:ILE:HG12	2.04	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	F	440/442 (100%)	427 (97%)	13 (3%)	0	100	100
2	E	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
3	G	903/905 (100%)	866 (96%)	37 (4%)	0	100	100
4	C	563/600 (94%)	543 (96%)	20 (4%)	0	100	100
5	B	183/220 (83%)	172 (94%)	11 (6%)	0	100	100
6	I	145/147 (99%)	137 (94%)	8 (6%)	0	100	100
7	L	585/613 (95%)	563 (96%)	22 (4%)	0	100	100
8	M	502/504 (100%)	484 (96%)	18 (4%)	0	100	100
9	N	473/485 (98%)	460 (97%)	13 (3%)	0	100	100
10	H	308/325 (95%)	292 (95%)	16 (5%)	0	100	100
11	A	102/147 (69%)	95 (93%)	7 (7%)	0	100	100
12	K	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
13	J	173/175 (99%)	163 (94%)	10 (6%)	0	100	100
All	All	4629/4819 (96%)	4447 (96%)	182 (4%)	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	F	356/356 (100%)	356 (100%)	0	100	100
2	E	129/129 (100%)	129 (100%)	0	100	100
3	G	732/732 (100%)	730 (100%)	2 (0%)	86	88
4	C	489/519 (94%)	488 (100%)	1 (0%)	87	89
5	B	168/192 (88%)	165 (98%)	3 (2%)	51	74
6	I	124/126 (98%)	124 (100%)	0	100	100
7	L	470/486 (97%)	468 (100%)	2 (0%)	84	86
8	M	413/413 (100%)	413 (100%)	0	100	100
9	N	381/385 (99%)	378 (99%)	3 (1%)	73	82
10	H	258/269 (96%)	258 (100%)	0	100	100
11	A	84/119 (71%)	84 (100%)	0	100	100
12	K	79/79 (100%)	79 (100%)	0	100	100
13	J	139/139 (100%)	139 (100%)	0	100	100
All	All	3822/3944 (97%)	3811 (100%)	11 (0%)	84	88

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	57	ASN
3	G	559	GLU
4	C	112	MET
5	B	146	ASP
5	B	167	GLN
5	B	169	LEU
7	L	372	ILE
7	L	400	ASP
9	N	67	MET
9	N	82	LEU

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Mol	Chain	Res	Type
9	N	287	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	52	ASN
1	F	107	GLN
1	F	142	ASN
1	F	331	HIS
1	F	425	GLN
2	E	100	ASN
3	G	7	HIS
3	G	57	ASN
3	G	117	GLN
3	G	253	ASN
3	G	260	ASN
3	G	276	ASN
3	G	352	GLN
3	G	429	HIS
3	G	673	HIS
3	G	702	GLN
3	G	730	GLN
3	G	834	GLN
3	G	901	HIS
4	C	16	GLN
4	C	20	HIS
4	C	31	ASN
4	C	120	ASN
4	C	252	HIS
4	C	370	HIS
4	C	476	GLN
4	C	510	GLN
5	B	58	ASN
5	B	131	ASN
7	L	78	ASN
7	L	135	ASN
7	L	409	ASN
8	M	19	GLN
8	M	62	GLN
8	M	80	HIS
8	M	117	HIS
8	M	212	ASN

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Mol	Chain	Res	Type
8	M	250	GLN
8	M	361	GLN
8	M	497	GLN
9	N	6	GLN
10	H	170	GLN
10	H	183	GLN
10	H	188	ASN
13	J	24	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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	$\# Z > 2$
14	SF4	F	501	1	0,12,12	-	-	-		
15	FMN	F	502	-	33,33,33	1.04	2 (6%)	48,50,50	1.24	9 (18%)
14	SF4	B	301	5	0,12,12	-	-	-		
14	SF4	G	1001	3	0,12,12	-	-	-		
14	SF4	I	201	6	0,12,12	-	-	-		
14	SF4	I	202	6	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	NAI	F	503	-	47,48,48	0.26	0	64,73,73	0.34	0
20	UQ8	H	401	-	24,24,53	0.31	0	30,32,67	0.97	2 (6%)
14	SF4	G	1002	3	0,12,12	-	-	-		
14	SF4	G	1003	3	0,12,12	-	-	-		
17	FES	E	201	2	0,4,4	-	-	-		
19	3PE	L	802	-	36,36,50	0.36	0	39,41,55	0.33	0
19	3PE	L	801	-	50,50,50	0.30	0	53,55,55	0.28	0
17	FES	G	1004	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
14	SF4	F	501	1	-	-	0/6/5/5
15	FMN	F	502	-	-	5/18/18/18	0/3/3/3
14	SF4	B	301	5	-	-	0/6/5/5
16	NAI	F	503	-	-	5/29/72/72	0/5/5/5
14	SF4	G	1001	3	-	-	0/6/5/5
14	SF4	I	201	6	-	-	0/6/5/5
14	SF4	I	202	6	-	-	0/6/5/5
20	UQ8	H	401	-	-	5/17/41/75	0/1/1/1
14	SF4	G	1002	3	-	-	0/6/5/5
14	SF4	G	1003	3	-	-	0/6/5/5
17	FES	E	201	2	-	-	0/1/1/1
19	3PE	L	802	-	-	6/40/40/54	-
19	3PE	L	801	-	-	5/54/54/54	-
17	FES	G	1004	3	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	502	FMN	C4A-N5	3.28	1.37	1.30
15	F	502	FMN	C10-N1	2.48	1.38	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	401	UQ8	C8-C7-C6	4.12	122.23	112.08
15	F	502	FMN	C4-N3-C2	-3.34	119.71	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	F	502	FMN	O4-C4-C4A	-2.68	119.46	126.53
15	F	502	FMN	C4A-C4-N3	2.64	119.97	113.25
15	F	502	FMN	C4A-C10-N10	2.59	120.19	116.48
20	H	401	UQ8	C7-C6-C5	-2.34	115.79	118.52
15	F	502	FMN	C10-C4A-N5	-2.18	120.35	124.81
15	F	502	FMN	C4A-C10-N1	-2.18	119.25	124.59
15	F	502	FMN	C5A-C9A-N10	2.09	119.86	117.97
15	F	502	FMN	C9A-C5A-N5	-2.01	120.32	122.45
15	F	502	FMN	C4-C4A-C10	2.00	120.37	116.93

There are no chirality outliers.

All (26) torsion outliers are listed below:

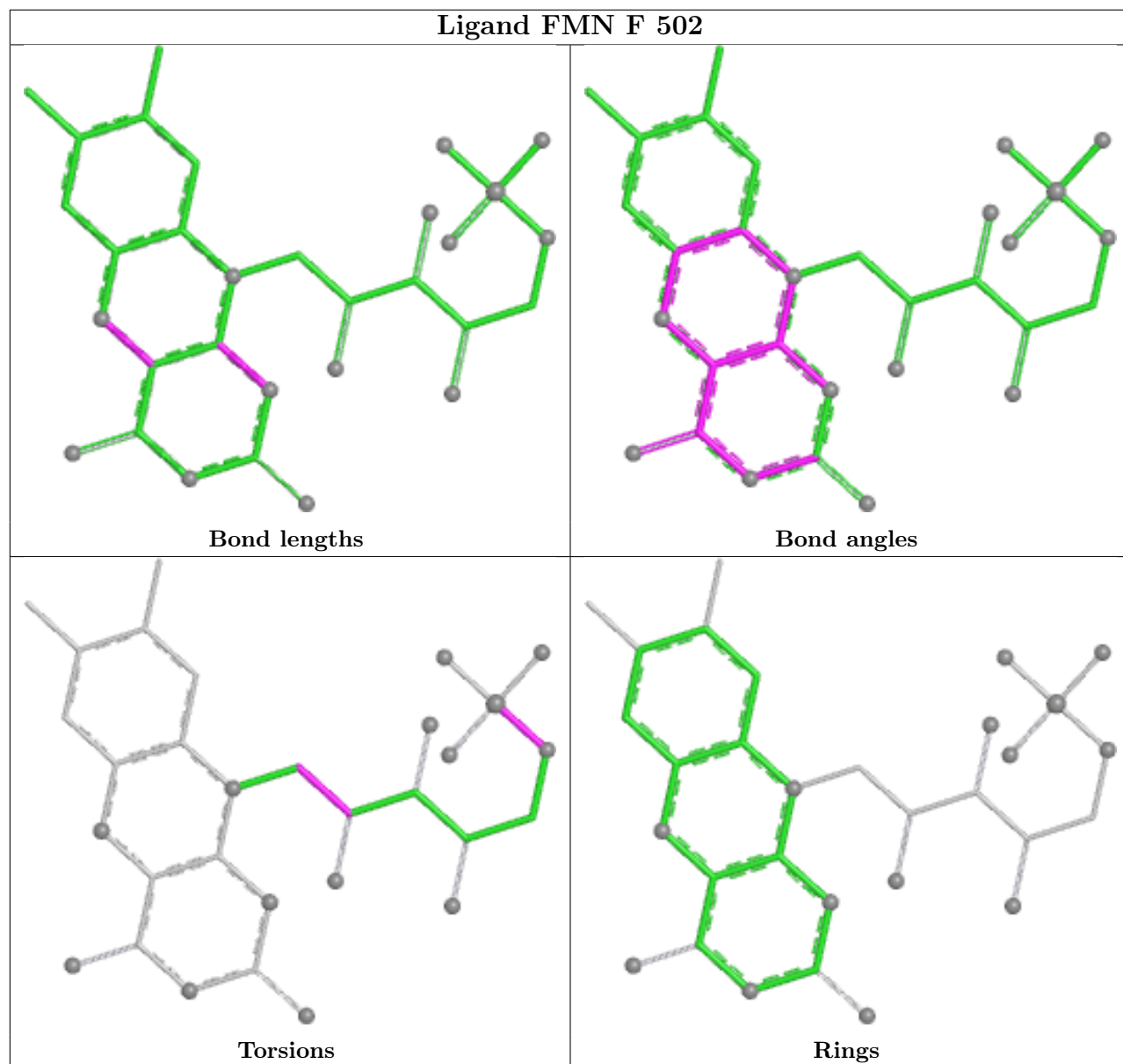
Mol	Chain	Res	Type	Atoms
15	F	502	FMN	N10-C1'-C2'-O2'
15	F	502	FMN	N10-C1'-C2'-C3'
15	F	502	FMN	C5'-O5'-P-O2P
15	F	502	FMN	C5'-O5'-P-O3P
19	L	802	3PE	C1-O11-P-O12
19	L	802	3PE	C11-O13-P-O11
19	L	802	3PE	C11-O13-P-O14
20	H	401	UQ8	C9-C11-C12-C13
19	L	802	3PE	C31-C32-C33-C34
19	L	801	3PE	C37-C38-C39-C3A
19	L	801	3PE	C2C-C2D-C2E-C2F
15	F	502	FMN	C5'-O5'-P-O1P
16	F	503	NAI	PN-O3-PA-O1A
16	F	503	NAI	PN-O3-PA-O5B
19	L	801	3PE	C23-C24-C25-C26
19	L	801	3PE	C25-C26-C27-C28
19	L	801	3PE	C1-O11-P-O14
19	L	802	3PE	C1-O11-P-O13
19	L	802	3PE	C1-O11-P-O14
20	H	401	UQ8	C2-C3-O3-C3M
20	H	401	UQ8	C12-C11-C9-C10
20	H	401	UQ8	C12-C11-C9-C8
16	F	503	NAI	O4D-C1D-N1N-C2N
16	F	503	NAI	C2D-C1D-N1N-C2N
20	H	401	UQ8	C4-C3-O3-C3M
16	F	503	NAI	PA-O3-PN-O1N

There are no ring outliers.

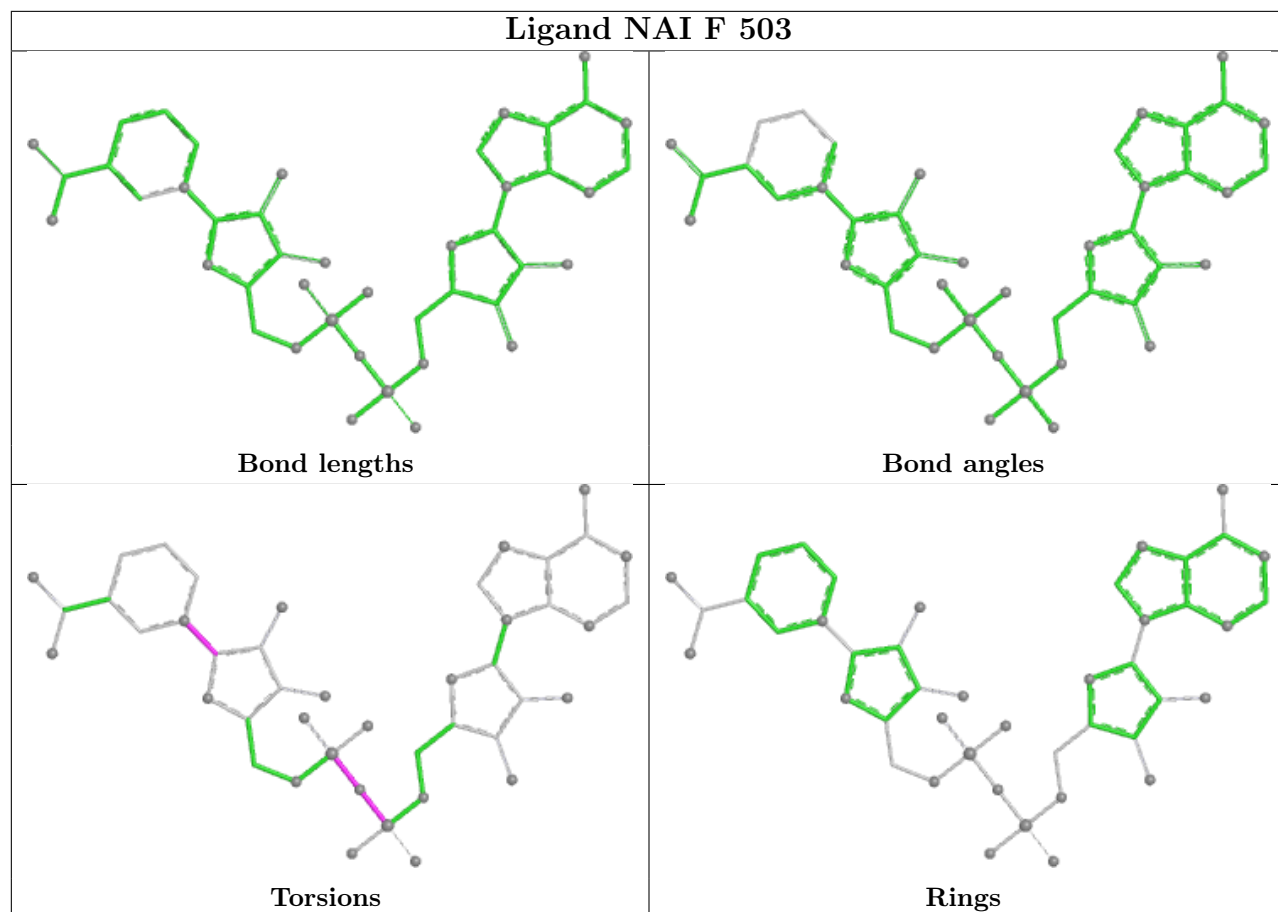
5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	F	502	FMN	2	0
14	G	1001	SF4	2	0
16	F	503	NAI	4	0
19	L	802	3PE	5	0
19	L	801	3PE	1	0

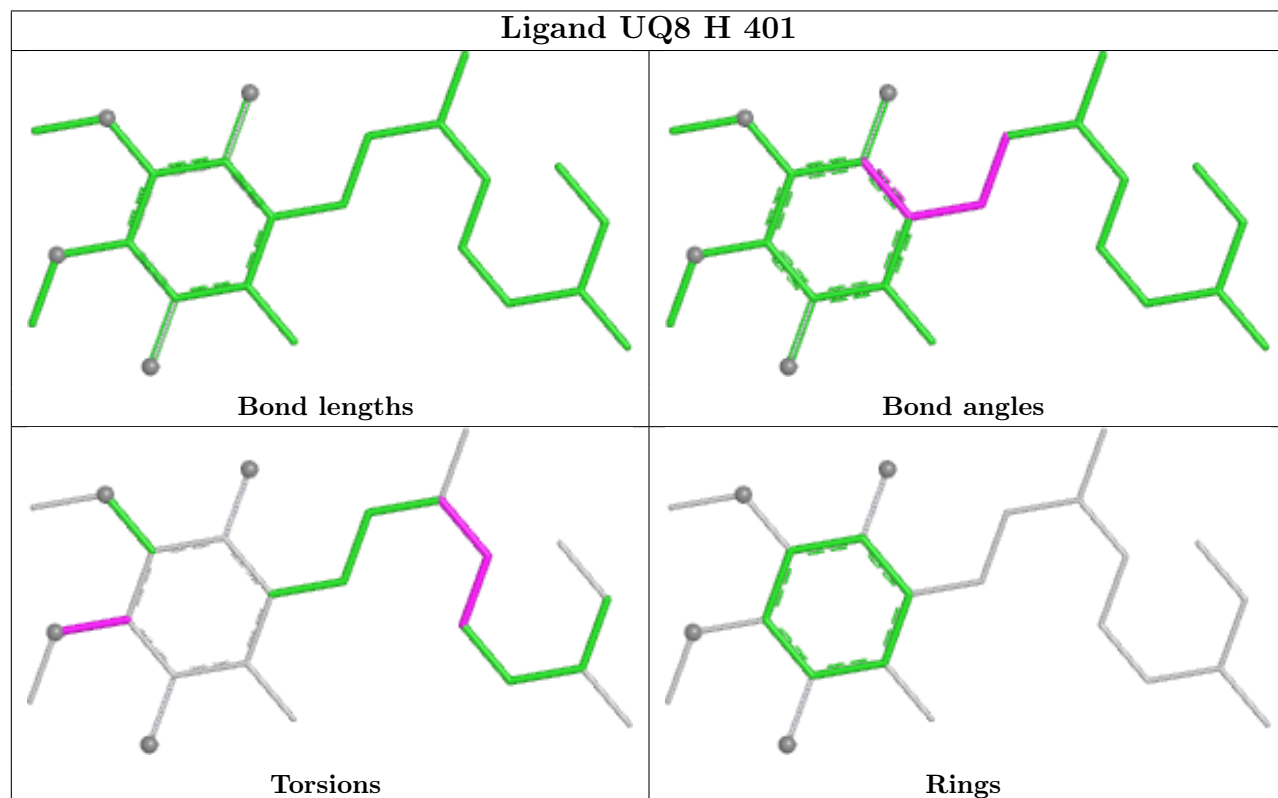
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

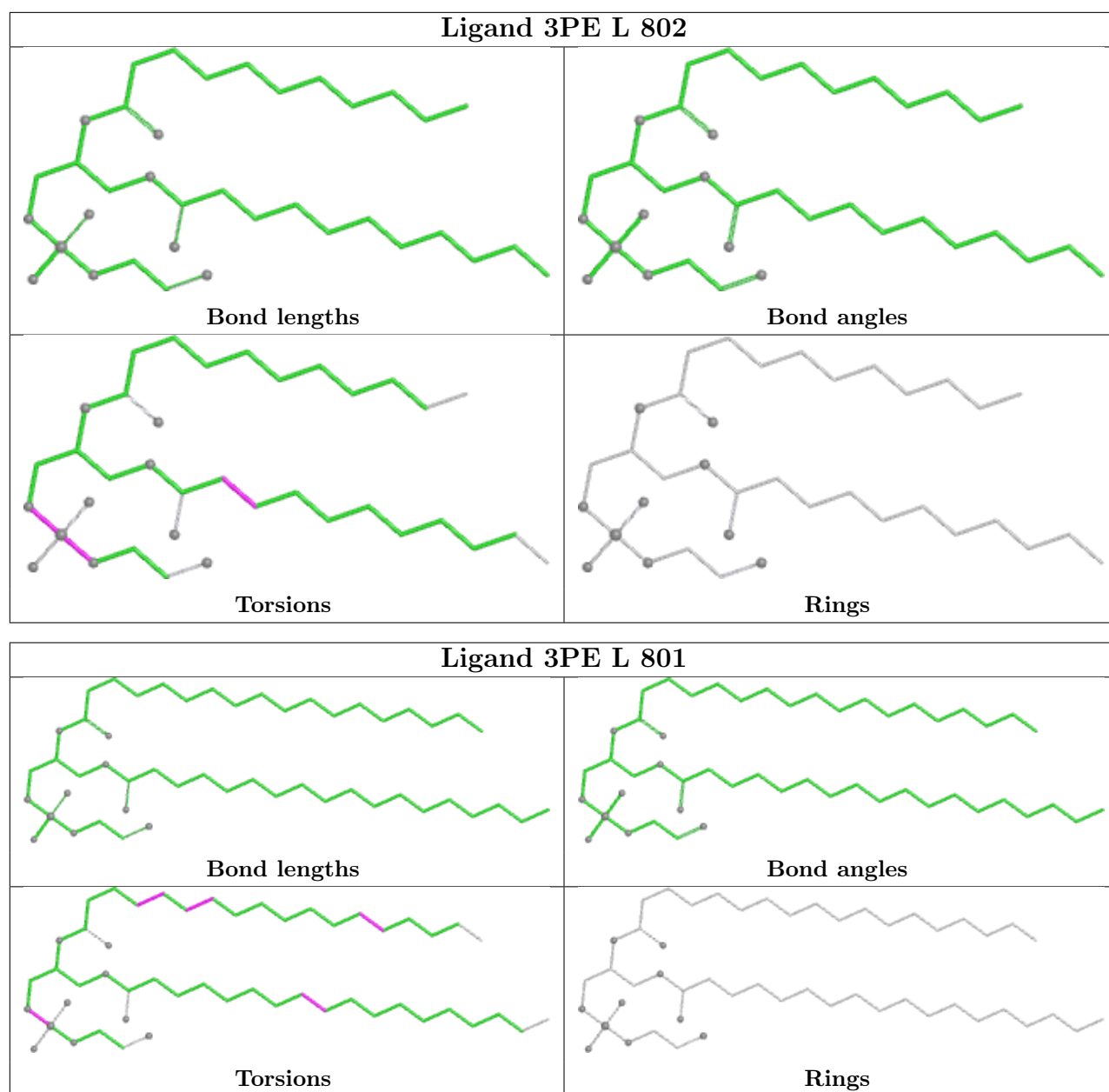


Ligand NAI F 503



Ligand UQ8 H 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.

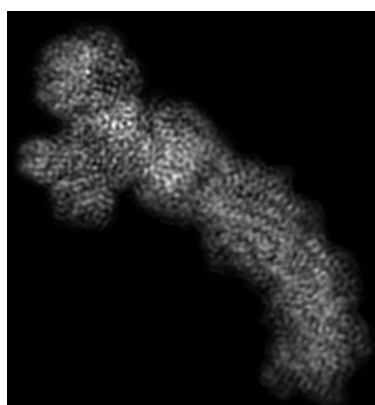
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13214. These allow visual inspection of the internal detail of the map and identification of artifacts.

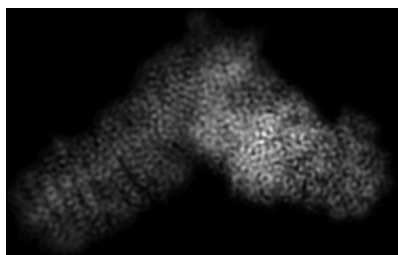
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

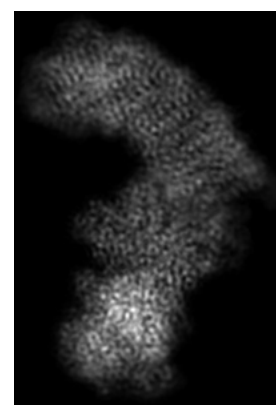
6.1.1 Primary map



X



Y

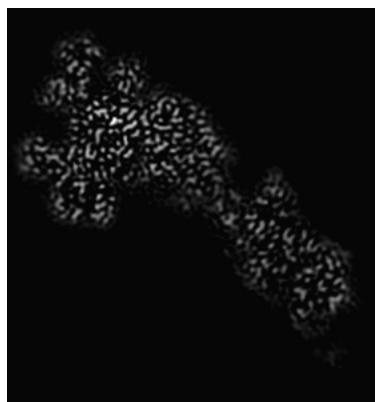


Z

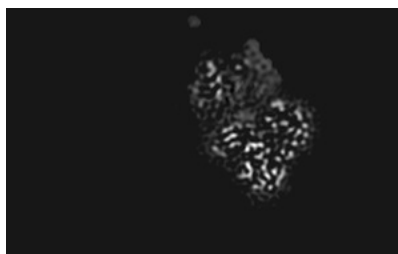
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

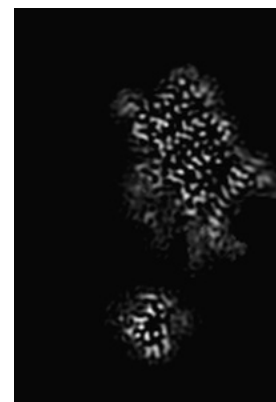
6.2.1 Primary map



X Index: 70



Y Index: 104

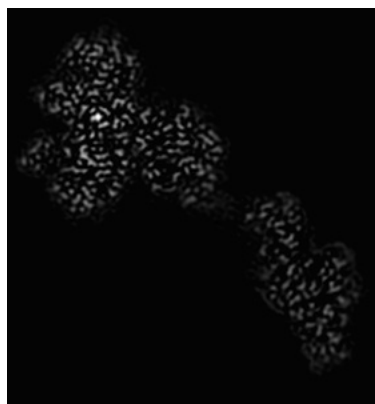


Z Index: 112

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: 62



Y Index: 59

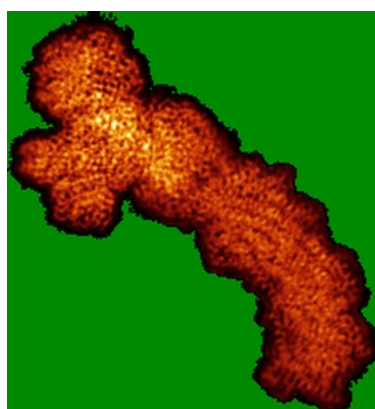


Z Index: 143

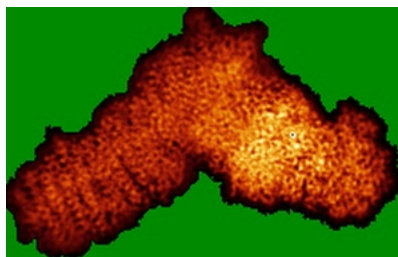
The images above show the largest variance slices of the map in three orthogonal directions.

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

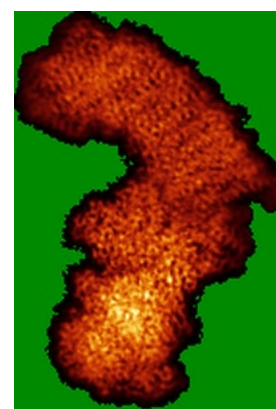
6.4.1 Primary map



X



Y

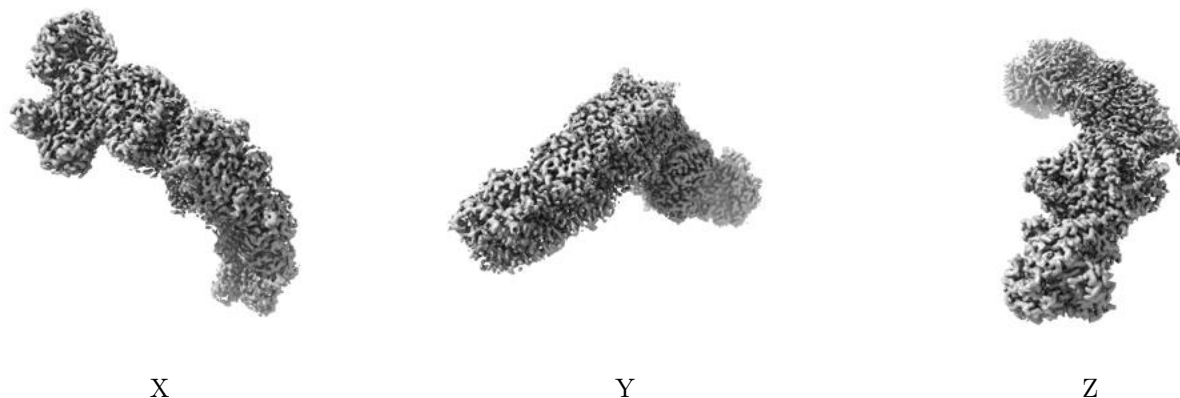


Z

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

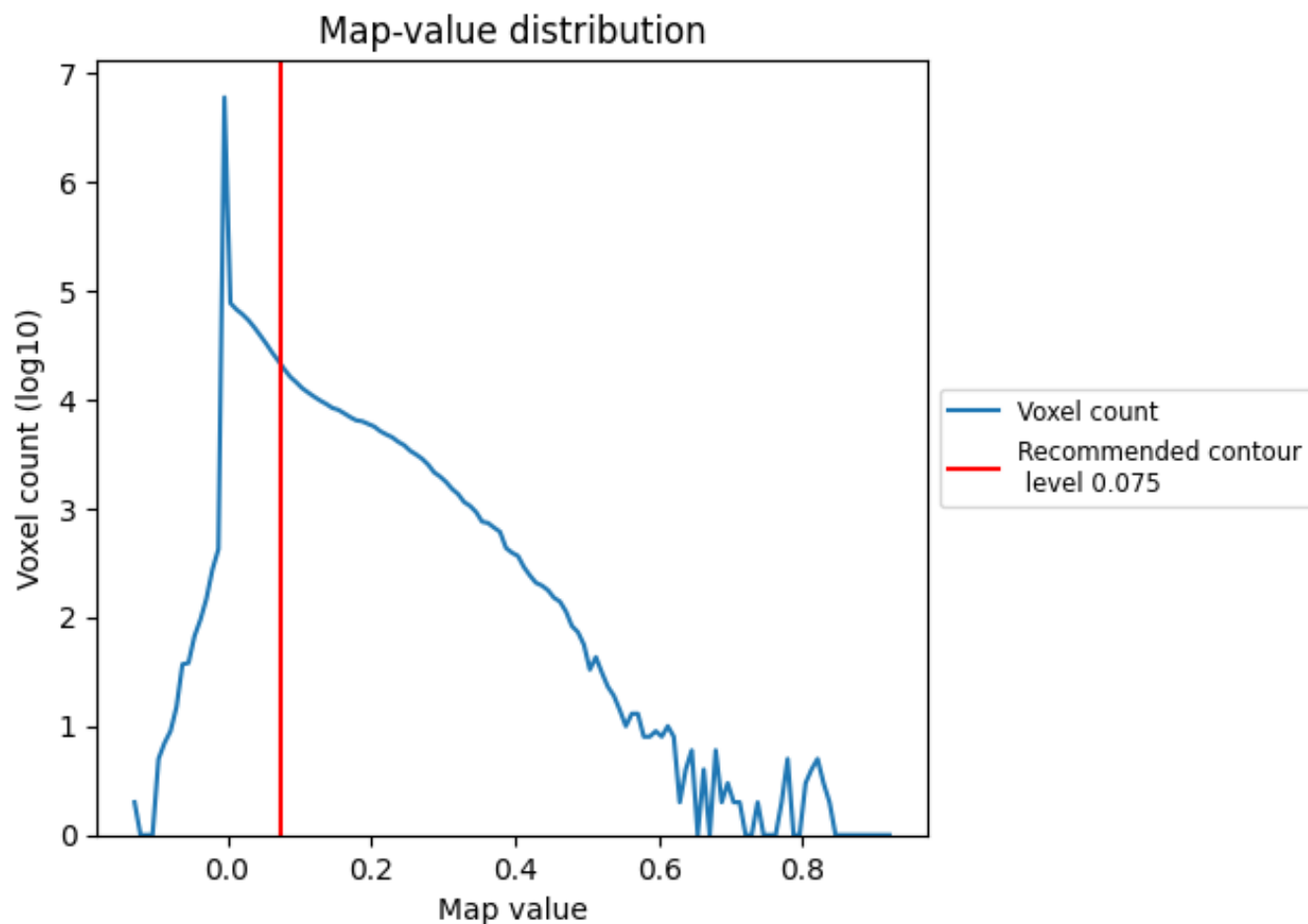
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

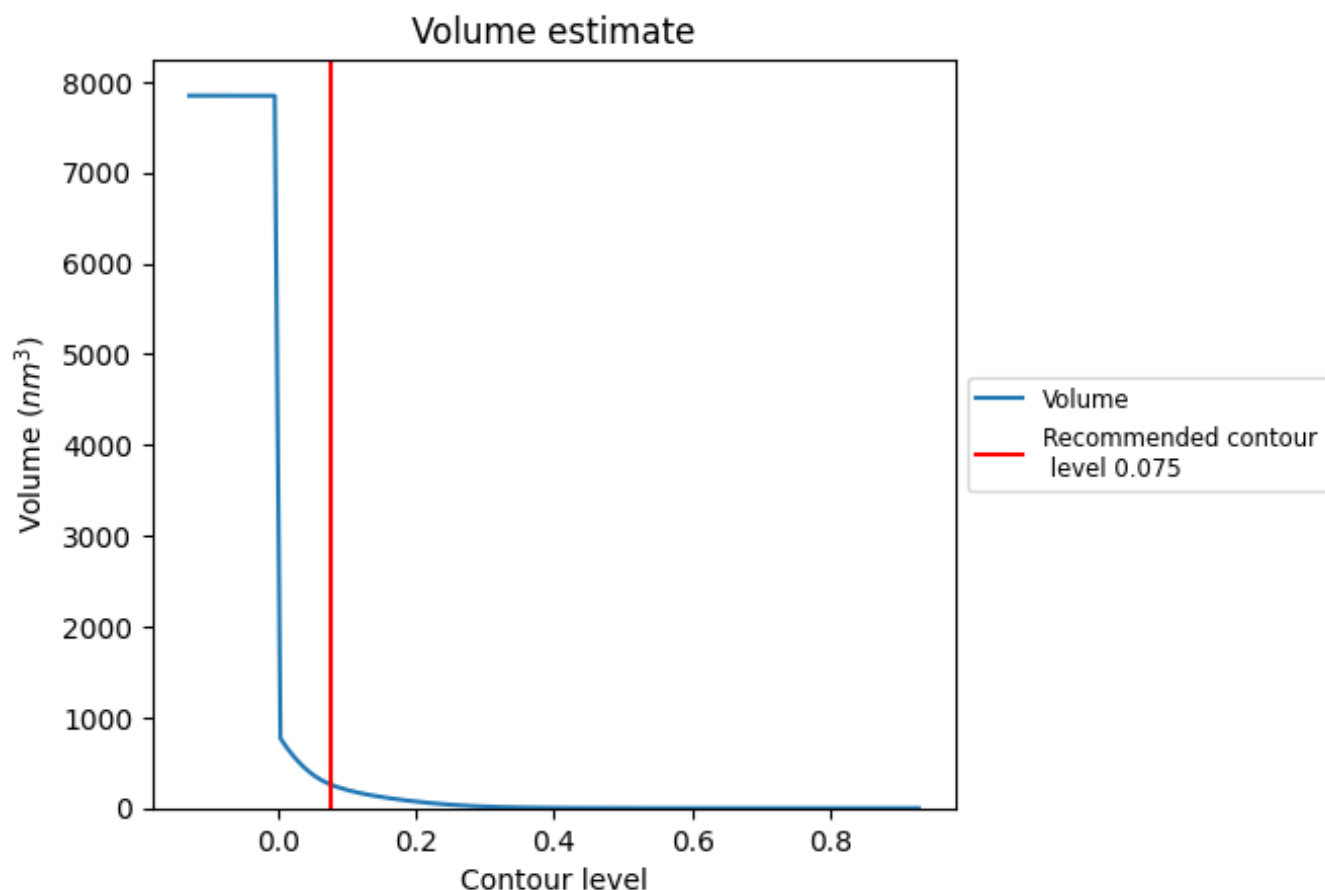
This section contains the results of statistical analysis of the map.

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 264 nm³; this corresponds to an approximate mass of 239 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.

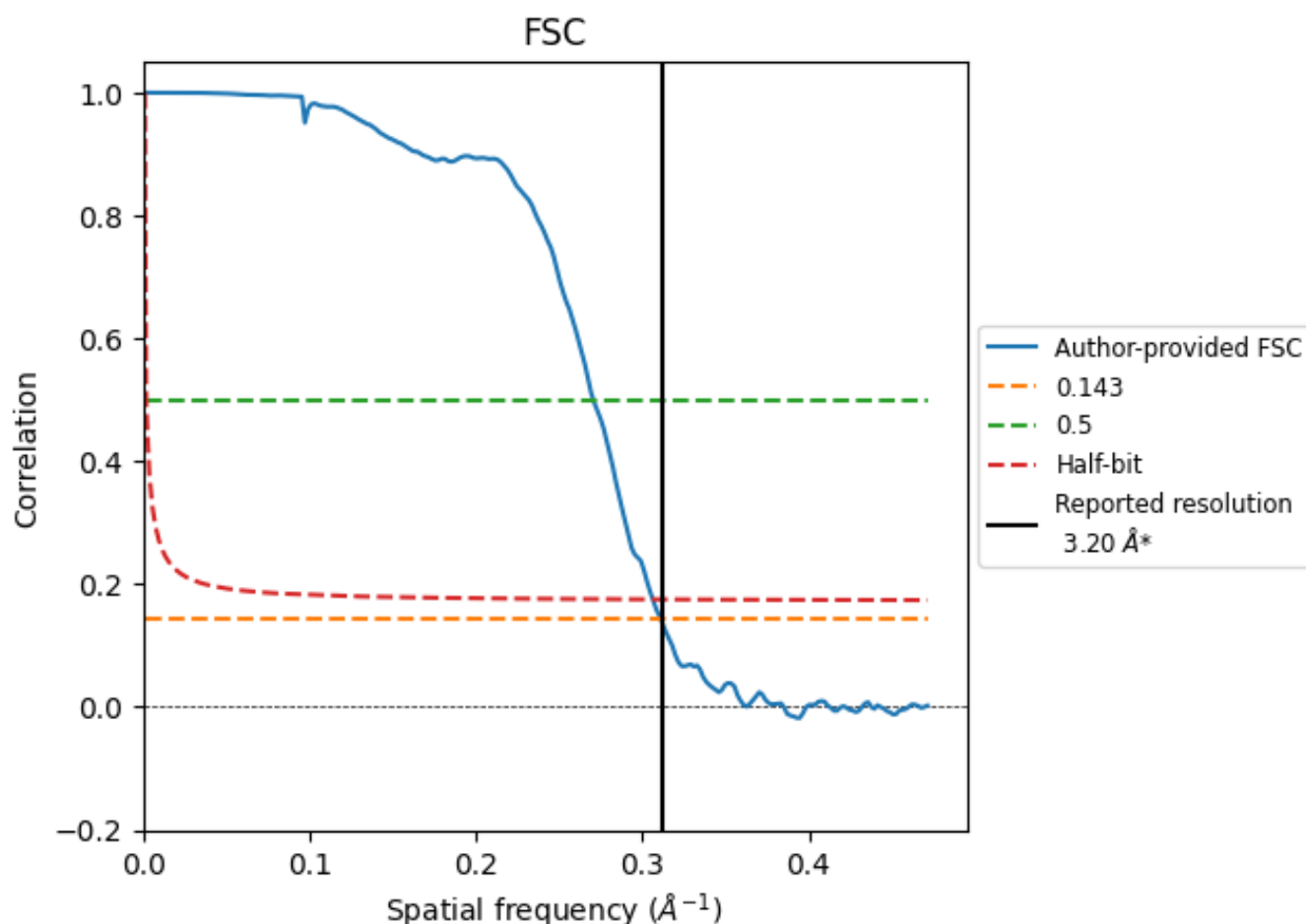
7.3 Rotationally averaged power spectrum [i](#)

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

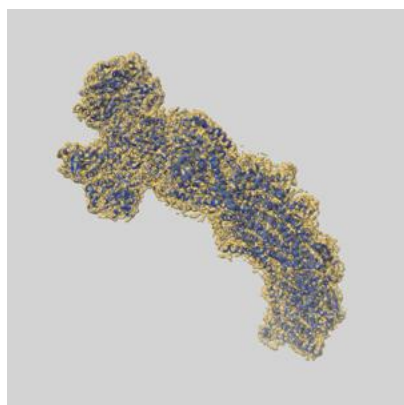
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.21	3.70	3.26
Unmasked-calculated*	-	-	-

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

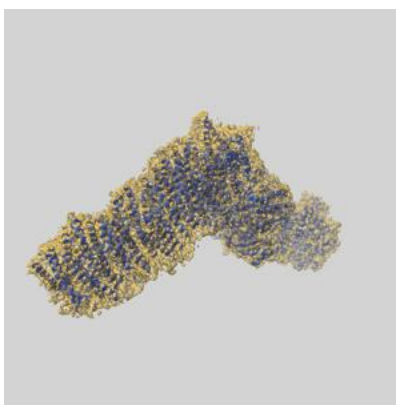
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13214 and PDB model 7P61. Per-residue inclusion information can be found in section 3 on page 10.

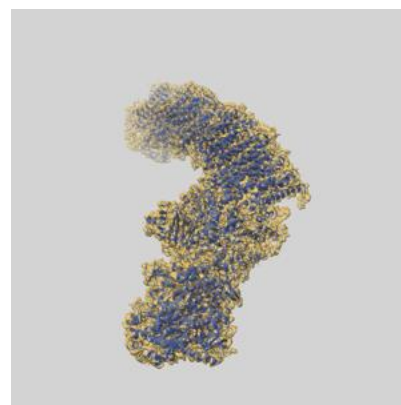
9.1 Map-model overlay [i](#)



X



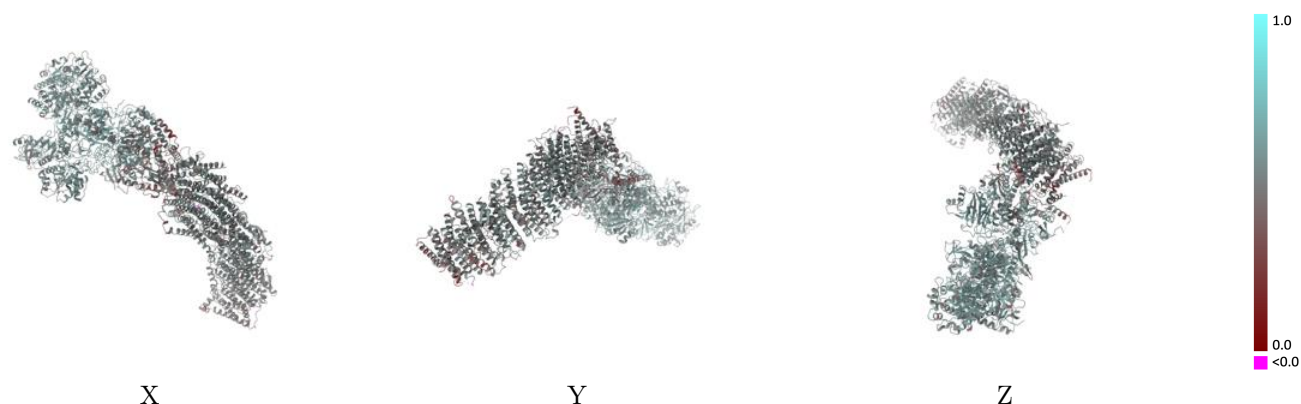
Y



Z

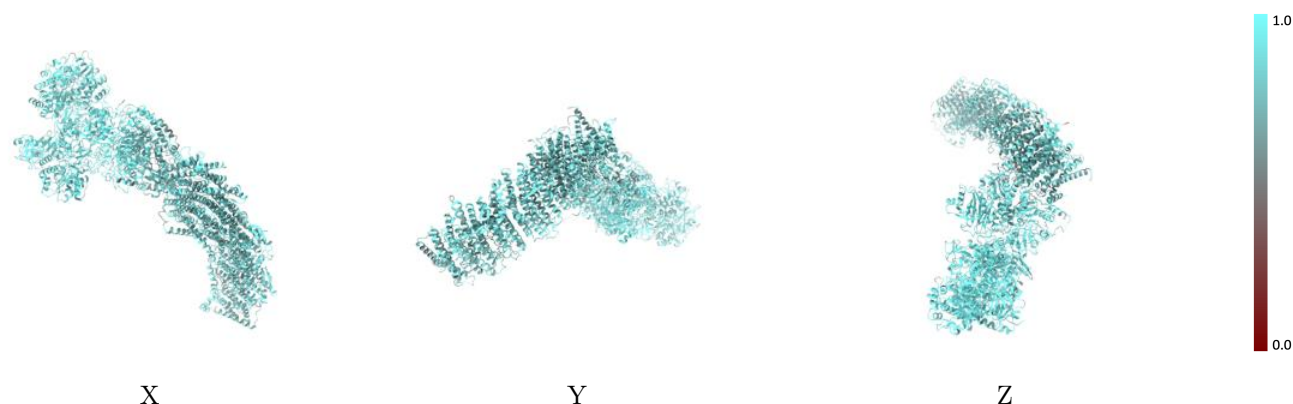
The images above show the 3D surface view of the map at the recommended contour level 0.075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



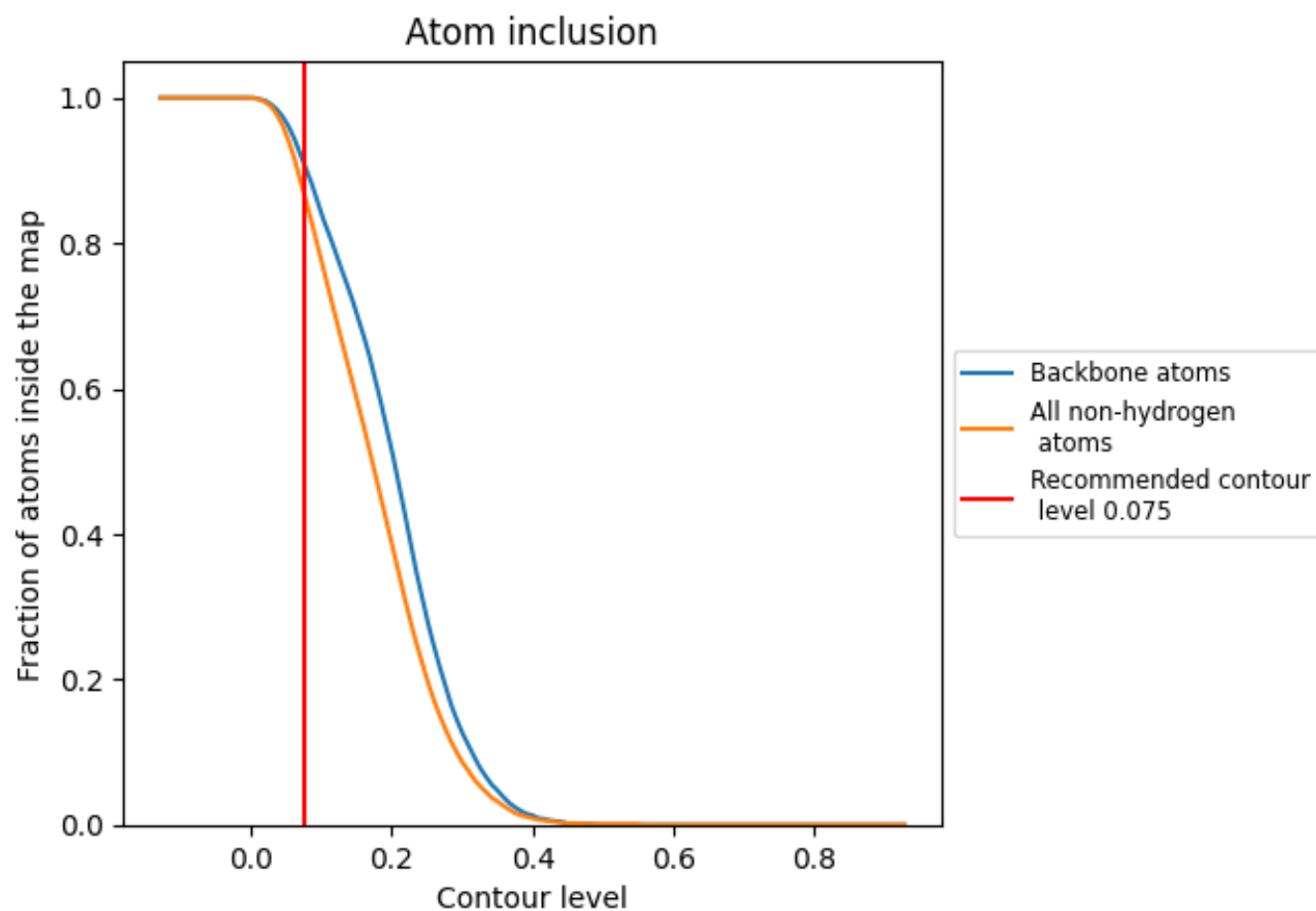
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.075).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 87% 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 (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8680	 0.5240
A	 0.8190	 0.4820
B	 0.8800	 0.5230
C	 0.8850	 0.5410
E	 0.9110	 0.5520
F	 0.9130	 0.5530
G	 0.9280	 0.5690
H	 0.8150	 0.4680
I	 0.9300	 0.5770
J	 0.8080	 0.4810
K	 0.8560	 0.5230
L	 0.8070	 0.4680
M	 0.8460	 0.5090
N	 0.8260	 0.5100

