



Full wwPDB EM Validation Report ⓘ

Oct 1, 2022 – 09:22 am BST

PDB ID : 7P62
EMDB ID : EMD-13215
Title : Complex I from E. coli, DDM-purified, Apo, Resting state
Authors : Kravchuk, V.; Kampjut, D.; Sazanov, L.
Deposited on : 2021-07-15
Resolution : 3.60 Å(reported)
Based on initial models : 4HEA, 3RKO

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

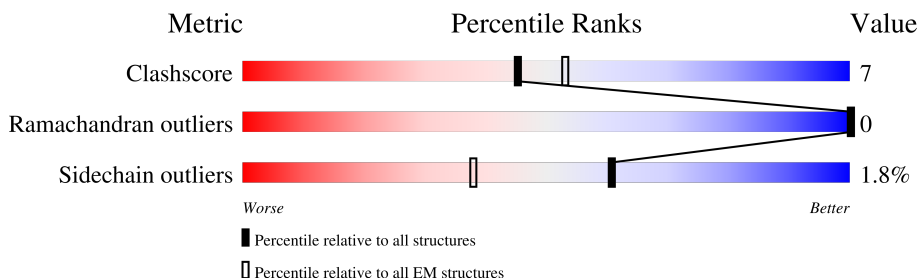
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
5	B	220	
6	I	144	
7	L	613	
8	M	504	

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Mol	Chain	Length	Quality of chain
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 [i](#)

There are 18 unique types of molecules in this entry. The entry contains 36597 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
			Total	C	N	O	S		
1	F	442	3432	2177	601	633	21	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	574	4644	2982	803	835	24	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	192	1529	970	262	280	17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	I	144	1140	723	191	214	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	L	595	4530	3018	717	763	32	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	N	480	3638	2428	574	616	20	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	H	308	2422	1629	375	400	18	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	A	100	797	549	122	122	4	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	J	175	1312	874	206	225	7	0	0

- Molecule 14 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



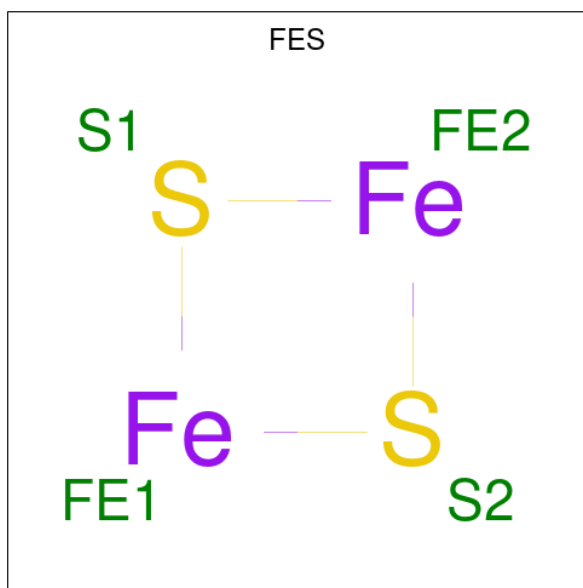
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
14	F	1	8	4	4	0
14	G	1	24	12	12	0
14	G	1	24	12	12	0
14	G	1	24	12	12	0
14	B	1	8	4	4	0
14	I	1	16	8	8	0
14	I	1	16	8	8	0

- Molecule 15 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



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

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).

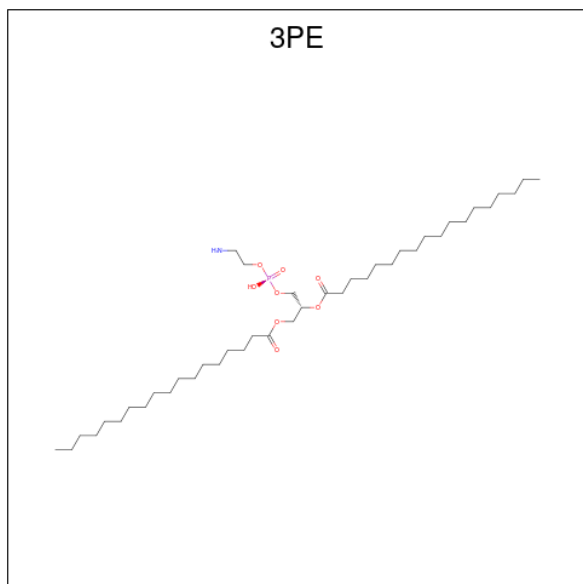


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
16	E	1	4	2	2	0
16	G	1	4	2	2	0

- Molecule 17 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 18 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).

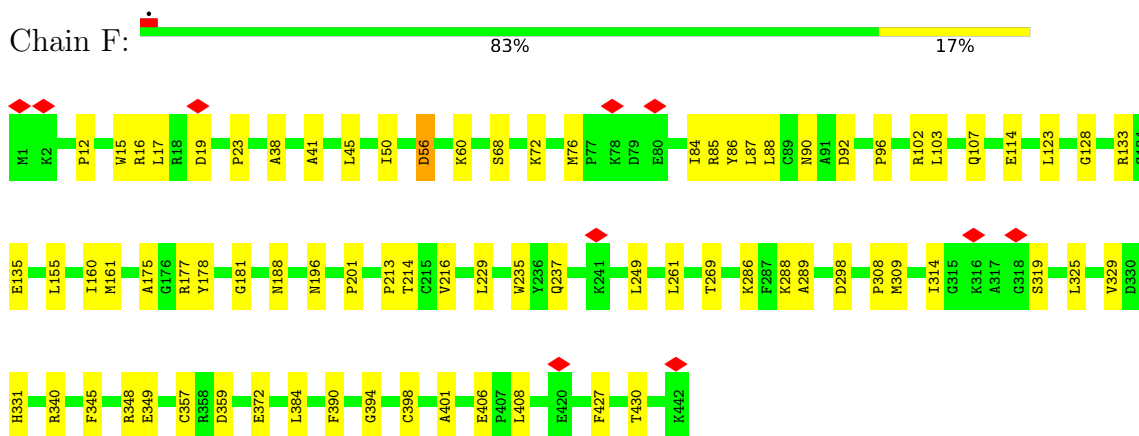


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
18	L	1	102	82	2	16	2	0
18	L	1	Total	C	N	O	P	0
			102	82	2	16	2	

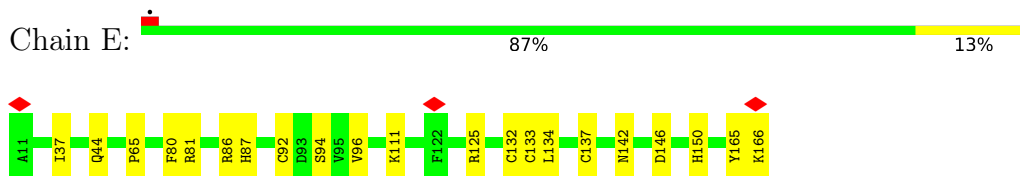
3 Residue-property plots

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.

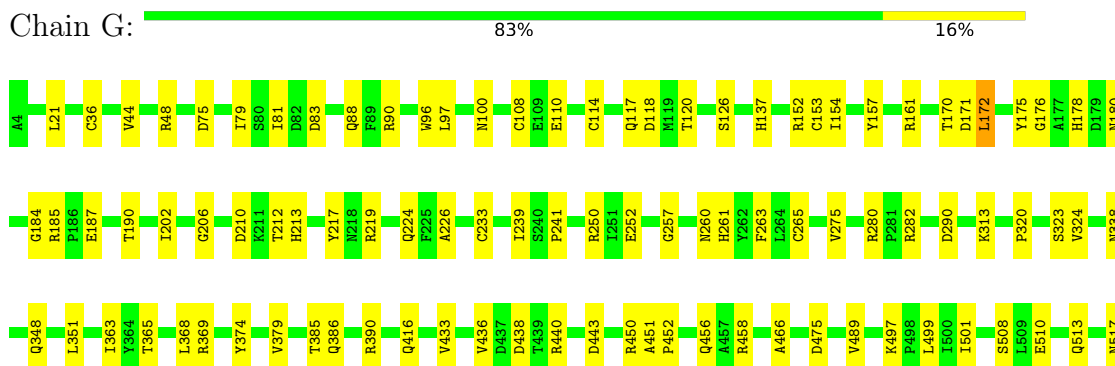
- Molecule 1: NADH-quinone oxidoreductase subunit F



- Molecule 2: NADH dehydrogenase I subunit E

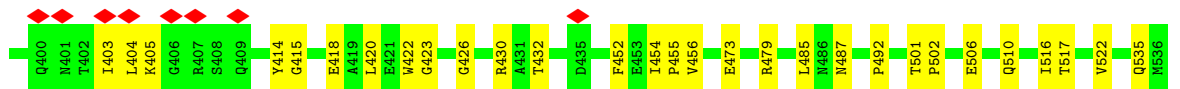
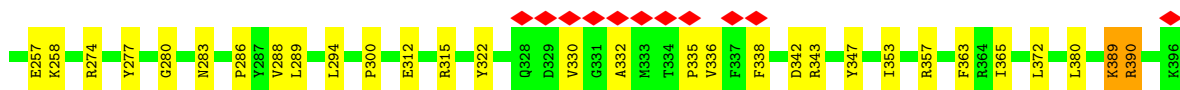
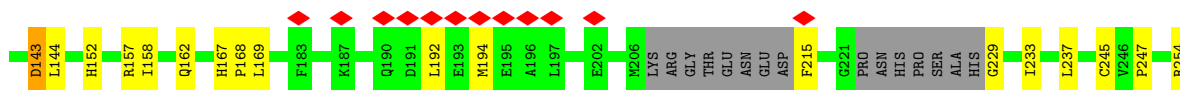
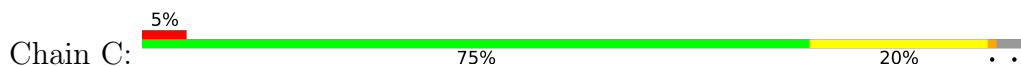


- Molecule 3: NADH-quinone oxidoreductase

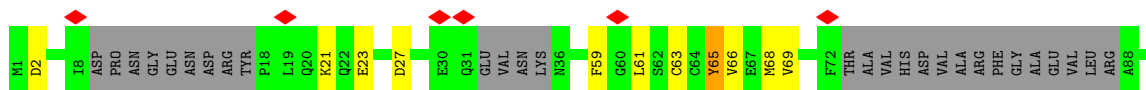




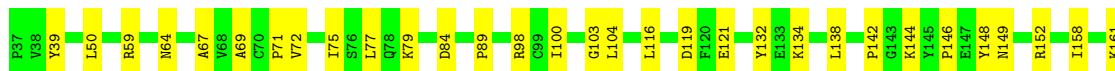
- Molecule 4: NADH-quinone oxidoreductase subunit C/D




- Molecule 5: NADH-quinone oxidoreductase subunit B

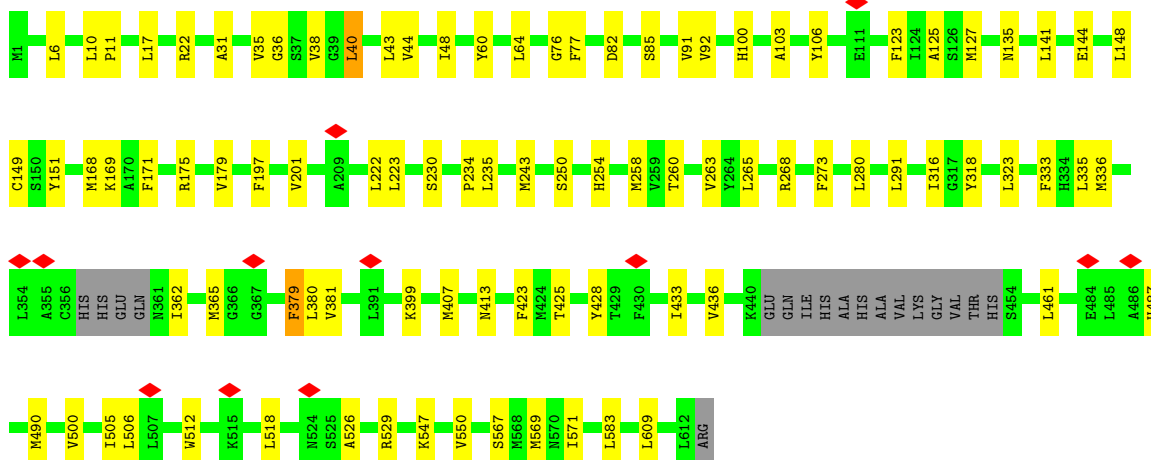


- Molecule 6: NADH-quinone oxidoreductase subunit I




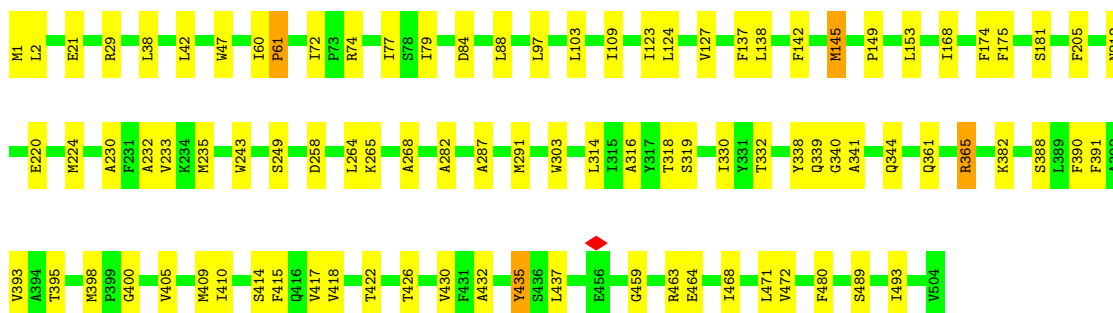
- Molecule 7: Proton-translocating NADH-quinone oxidoreductase, chain L

Chain L:  82% 15%



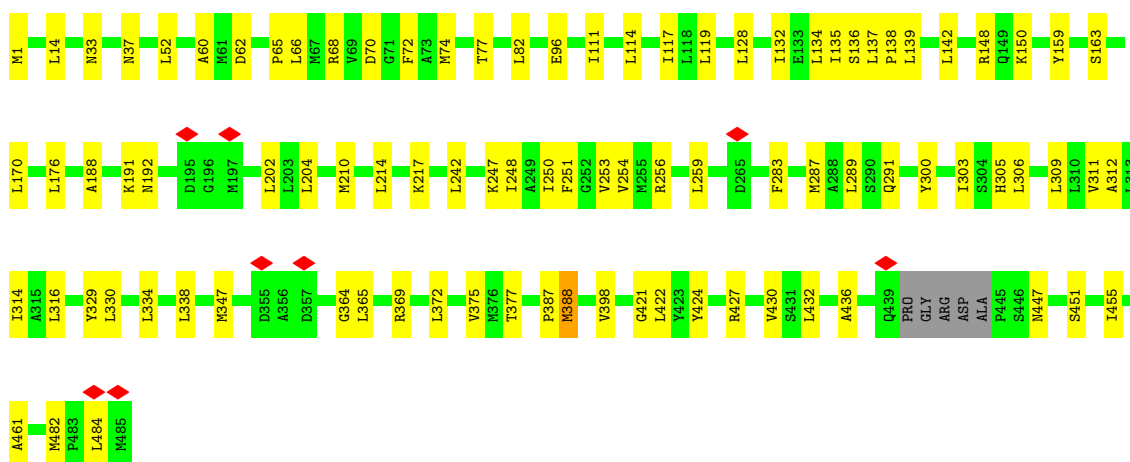
• Molecule 8: NADH dehydrogenase I subunit M

Chain M:  82% 17%




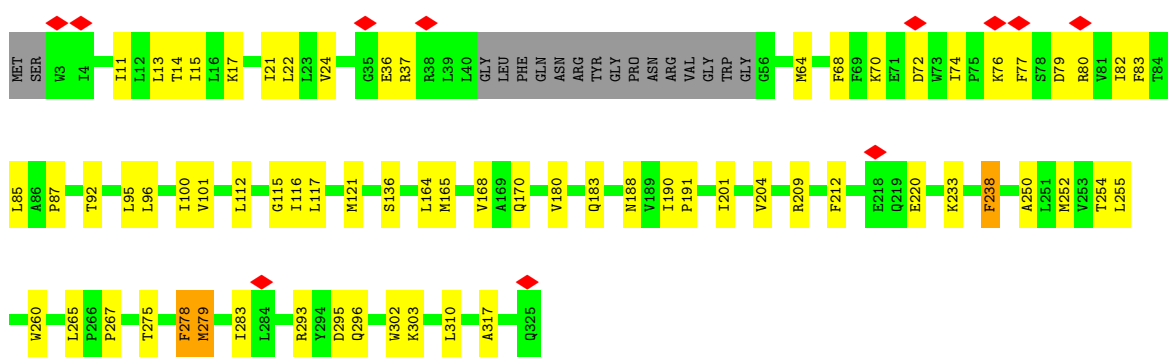
• Molecule 9: NADH-quinone oxidoreductase subunit N

Chain N:  80% 19%



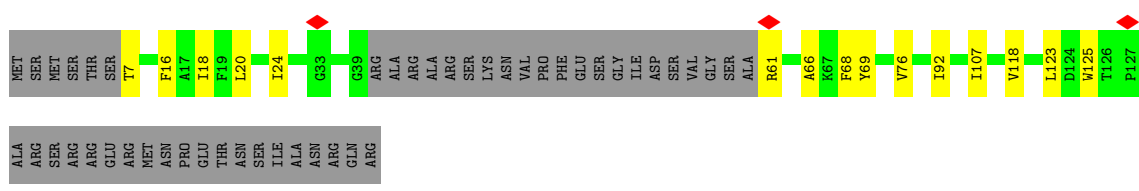
• Molecule 10: NADH-quinone oxidoreductase subunit H

Chain H:  74% 20% 5%




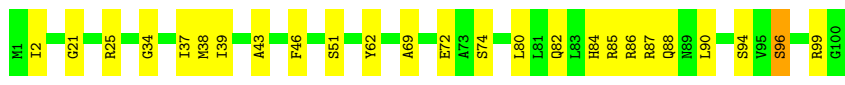
• Molecule 11: NADH-quinone oxidoreductase subunit A

Chain A:  58% 10% 32%




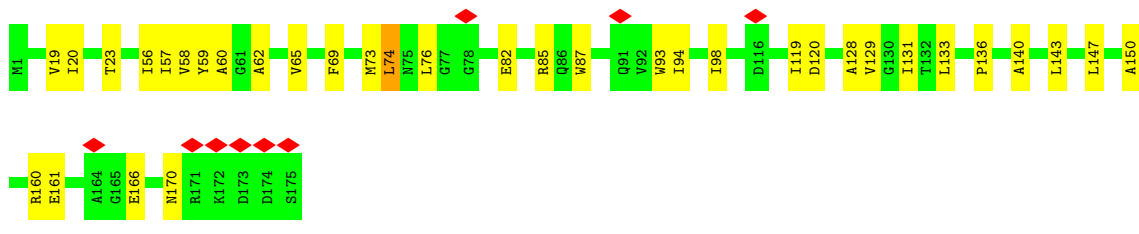
• Molecule 12: NADH-quinone oxidoreductase subunit K

Chain K:  75% 24%



• Molecule 13: NADH-quinone oxidoreductase subunit J

Chain J:  5% 80% 19%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	120909	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	0.971	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.085	Depositor
Map size (Å)	155.967, 211.13899, 245.091	wwPDB
Map dimensions	231, 199, 147	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.27	0/3511	0.57	2/4745 (0.0%)
2	E	0.25	0/1248	0.53	0/1691
3	G	0.26	0/7173	0.53	1/9726 (0.0%)
4	C	0.26	0/4769	0.56	1/6468 (0.0%)
5	B	0.28	0/1560	0.56	0/2108
6	I	0.27	0/1167	0.56	1/1577 (0.1%)
7	L	0.28	0/4644	0.60	4/6330 (0.1%)
8	M	0.28	0/4074	0.53	1/5546 (0.0%)
9	N	0.27	0/3727	0.51	1/5085 (0.0%)
10	H	0.30	0/2492	0.59	0/3390
11	A	0.30	0/822	0.60	0/1119
12	K	0.28	0/769	0.55	0/1040
13	J	0.29	0/1338	0.61	0/1824
All	All	0.27	0/37294	0.56	11/50649 (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
1	F	0	1
5	B	0	1
All	All	0	2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	597	ASP	CB-CG-OD1	6.99	124.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	56	ASP	CB-CG-OD1	6.66	124.30	118.30
7	L	40	LEU	CA-CB-CG	6.19	129.54	115.30
7	L	17	LEU	CA-CB-CG	5.77	128.57	115.30
7	L	223	LEU	CA-CB-CG	5.70	128.40	115.30
1	F	84	ILE	CG1-CB-CG2	-5.63	99.02	111.40
6	I	119	ASP	CB-CG-OD1	5.34	123.11	118.30
3	G	840	PRO	CA-N-CD	-5.24	104.17	111.50
8	M	61	PRO	CA-N-CD	-5.15	104.29	111.50
7	L	243	MET	CG-SD-CE	5.13	108.41	100.20
9	N	242	LEU	CA-CB-CG	5.13	127.09	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	B	158	CYS	Peptide
1	F	201	PRO	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	46	0
2	E	1220	0	1187	16	0
3	G	7022	0	6824	95	0
4	C	4644	0	4575	77	0
5	B	1529	0	1522	31	0
6	I	1140	0	1109	23	0
7	L	4530	0	4671	55	0
8	M	3953	0	4053	56	0
9	N	3638	0	3804	62	0
10	H	2422	0	2477	42	0
11	A	797	0	811	16	0
12	K	760	0	817	18	0
13	J	1312	0	1375	31	0
14	B	8	0	0	0	0
14	F	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	G	24	0	0	3	0
14	I	16	0	0	0	0
15	F	31	0	19	0	0
16	E	4	0	0	1	0
16	G	4	0	0	0	0
17	G	1	0	0	0	0
18	L	102	0	164	7	0
All	All	36597	0	36813	494	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 (494) 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:129:VAL:O	13:J:133:LEU:HB2	1.83	0.78
3:G:172:LEU:HA	3:G:184:GLY:O	1.89	0.73
7:L:92:VAL:HG21	7:L:127:MET:HG2	1.72	0.71
1:F:86:TYR:HB2	1:F:214:THR:HG22	1.75	0.68
4:C:389:LYS:HE3	4:C:390:ARG:HH21	1.59	0.68
7:L:487:HIS:HA	7:L:490:MET:HG2	1.76	0.67
12:K:21:GLY:HA3	13:J:20:ILE:HD12	1.78	0.66
9:N:14:LEU:HD21	13:J:143:LEU:HD11	1.79	0.65
7:L:230:SER:HB3	7:L:316:ILE:HG21	1.77	0.65
10:H:116:ILE:HG23	10:H:164:LEU:HD23	1.79	0.65
3:G:517:ASN:HD21	3:G:798:PHE:HB2	1.62	0.64
8:M:338:TYR:HB3	8:M:493:ILE:HD12	1.79	0.64
4:C:454:ILE:HD12	4:C:455:PRO:HD2	1.79	0.64
2:E:44:GLN:HE22	2:E:80:PHE:H	1.44	0.63
10:H:204:VAL:HG13	10:H:209:ARG:HB3	1.79	0.63
4:C:585:ILE:HG13	10:H:220:GLU:HG3	1.81	0.63
1:F:85:ARG:HG2	1:F:213:PRO:HG2	1.81	0.62
2:E:142:ASN:ND2	16:E:201:FES:S1	2.72	0.62
4:C:140:GLU:OE1	4:C:600:ARG:NH2	2.31	0.62
1:F:430:THR:OG1	4:C:510:GLN:NE2	2.33	0.61
8:M:142:PHE:HA	8:M:145:MET:HB2	1.83	0.61
4:C:257:GLU:OE2	4:C:600:ARG:NH1	2.33	0.61
1:F:60:LYS:HA	1:F:68:SER:HA	1.82	0.61
11:A:76:VAL:HG22	13:J:62:ALA:HB1	1.83	0.61
9:N:77:THR:HG23	9:N:117:ILE:HG12	1.81	0.61
1:F:249:LEU:HB3	1:F:261:LEU:HD11	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:33:ASN:O	9:N:37:ASN:ND2	2.34	0.60
3:G:108:CYS:SG	3:G:152:ARG:NH1	2.74	0.60
8:M:414:SER:O	8:M:418:VAL:N	2.33	0.60
9:N:217:LYS:HB3	9:N:250:ILE:HD13	1.82	0.60
8:M:60:ILE:HG23	8:M:61:PRO:HD2	1.82	0.60
4:C:288:VAL:HG21	4:C:363:PHE:HB3	1.83	0.60
2:E:87:HIS:ND1	2:E:146:ASP:OD2	2.34	0.60
9:N:72:PHE:HB3	9:N:256:ARG:HH21	1.66	0.60
3:G:758:ALA:HB3	3:G:761:TRP:HB2	1.84	0.59
3:G:695:ALA:O	3:G:698:ARG:NH1	2.35	0.59
9:N:114:LEU:HD21	13:J:143:LEU:HD22	1.85	0.59
3:G:736:PHE:HE2	3:G:754:PRO:HG3	1.67	0.59
8:M:97:LEU:HD12	8:M:265:LYS:HE3	1.85	0.59
6:I:158:ILE:HB	6:I:161:LYS:HB3	1.84	0.59
8:M:340:GLY:O	8:M:344:GLN:HB2	2.03	0.58
9:N:375:VAL:HG23	9:N:461:ALA:HB2	1.85	0.58
9:N:305:HIS:ND1	9:N:329:TYR:OH	2.32	0.58
3:G:324:VAL:HG23	3:G:539:ASN:HD21	1.67	0.58
10:H:14:THR:HA	10:H:17:LYS:HD3	1.85	0.58
3:G:260:ASN:ND2	3:G:263:PHE:O	2.36	0.58
3:G:365:THR:OG1	3:G:786:ARG:NH2	2.36	0.58
7:L:85:SER:OG	7:L:268:ARG:NH2	2.37	0.58
1:F:309:MET:HA	1:F:314:ILE:HD11	1.86	0.57
7:L:179:VAL:HG21	8:M:430:VAL:HG23	1.87	0.57
3:G:369:ARG:NH2	3:G:775:GLY:O	2.37	0.57
1:F:177:ARG:HH22	3:G:178:HIS:HD2	1.52	0.57
4:C:353:ILE:HD12	4:C:372:LEU:HD22	1.85	0.57
4:C:103:ILE:HG12	4:C:110:ASP:HB3	1.85	0.57
4:C:37:ALA:O	4:C:56:GLN:NE2	2.38	0.57
3:G:365:THR:O	3:G:786:ARG:NH2	2.38	0.56
3:G:451:ALA:O	3:G:456:GLN:NE2	2.38	0.56
3:G:458:ARG:NH2	3:G:475:ASP:O	2.38	0.56
7:L:22:ARG:HH21	8:M:382:LYS:HD2	1.68	0.56
9:N:364:GLY:HA3	9:N:436:ALA:HB2	1.86	0.56
3:G:117:GLN:NE2	14:G:1001:SF4:S3	2.77	0.56
3:G:807:PRO:HB3	3:G:882:GLY:HA3	1.87	0.56
13:J:56:ILE:HA	13:J:60:ALA:HB3	1.88	0.56
3:G:569:LEU:HD11	3:G:650:SER:HB3	1.88	0.56
5:B:126:MET:HG2	5:B:155:ILE:HD12	1.87	0.56
10:H:117:LEU:O	10:H:121:MET:HG3	2.05	0.56
4:C:229:GLY:HA3	4:C:595:MET:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:550:VAL:HG21	18:L:802:3PE:H332	1.88	0.56
7:L:144:GLU:OE1	7:L:175:ARG:NH1	2.39	0.56
7:L:609:LEU:HD22	9:N:204:LEU:HD12	1.88	0.56
7:L:263:VAL:HG13	7:L:323:LEU:HD11	1.87	0.56
8:M:365:ARG:NH2	8:M:459:GLY:O	2.39	0.56
9:N:111:ILE:HG21	13:J:150:ALA:HB2	1.87	0.56
10:H:260:TRP:HB2	10:H:267:PRO:HB3	1.88	0.56
6:I:149:ASN:HB3	6:I:152:ARG:HG3	1.88	0.56
9:N:65:PRO:HG2	13:J:136:PRO:HB3	1.88	0.56
10:H:15:ILE:HG23	11:A:18:ILE:HG21	1.88	0.56
1:F:41:ALA:HA	1:F:45:LEU:HB2	1.88	0.55
9:N:148:ARG:HD2	12:K:86:ARG:HH22	1.71	0.55
9:N:347:MET:HG3	9:N:365:LEU:HD11	1.87	0.55
7:L:168:MET:HG2	8:M:437:LEU:HB3	1.89	0.55
4:C:332:ALA:HA	4:C:335:PRO:HG3	1.89	0.55
10:H:317:ALA:HA	11:A:92:ILE:HD11	1.89	0.55
4:C:403:ILE:HD11	10:H:293:ARG:HE	1.72	0.54
3:G:217:TYR:HB3	6:I:79:LYS:HE3	1.88	0.54
9:N:259:LEU:HB2	9:N:316:LEU:HD21	1.89	0.54
8:M:417:VAL:HG12	8:M:418:VAL:HG13	1.89	0.54
9:N:248:ILE:HD11	9:N:334:LEU:HB2	1.89	0.54
10:H:82:ILE:HA	10:H:85:LEU:HB3	1.89	0.54
4:C:558:ARG:NH1	4:C:559:THR:O	2.41	0.54
7:L:151:TYR:HB2	7:L:171:PHE:HB2	1.89	0.54
1:F:175:ALA:H	2:E:37:ILE:HD11	1.73	0.53
4:C:48:PRO:HG2	4:C:111:ILE:HG22	1.91	0.53
10:H:180:VAL:HG21	10:H:260:TRP:HE1	1.73	0.53
3:G:641:TYR:OH	3:G:717:MET:SD	2.59	0.53
4:C:135:ASN:OD1	4:C:152:HIS:NE2	2.42	0.53
10:H:116:ILE:HD11	10:H:255:LEU:HD21	1.91	0.53
1:F:288:LYS:HD3	1:F:331:HIS:HA	1.90	0.53
9:N:369:ARG:HD2	9:N:372:LEU:HD12	1.90	0.53
13:J:23:THR:HG22	13:J:82:GLU:HG2	1.91	0.53
4:C:233:ILE:HD11	4:C:245:CYS:HB2	1.90	0.53
3:G:206:GLY:N	14:G:1001:SF4:S2	2.80	0.53
3:G:466:ALA:HB3	3:G:489:VAL:HG11	1.91	0.53
5:B:148:PHE:HD1	5:B:149:ILE:HG23	1.73	0.53
6:I:84:ASP:OD1	6:I:84:ASP:N	2.41	0.53
9:N:70:ASP:OD1	9:N:256:ARG:NH2	2.41	0.53
9:N:312:ALA:HB2	9:N:398:VAL:HG22	1.90	0.53
12:K:96:SER:O	12:K:99:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:137:HIS:NE2	3:G:180:ASN:OD1	2.39	0.53
4:C:37:ALA:HB1	4:C:56:GLN:HE22	1.73	0.53
8:M:393:VAL:HG13	8:M:398:MET:HE3	1.91	0.52
9:N:247:LYS:HD3	9:N:306:LEU:HD21	1.91	0.52
7:L:35:VAL:HG12	7:L:100:HIS:HB3	1.90	0.52
3:G:890:MET:HB2	3:G:893:ILE:HB	1.91	0.52
8:M:181:SER:HB2	8:M:230:ALA:HA	1.90	0.52
8:M:415:PHE:HB2	8:M:422:THR:HG21	1.91	0.52
3:G:275:VAL:O	3:G:280:ARG:NH1	2.40	0.52
3:G:513:GLN:O	3:G:517:ASN:ND2	2.43	0.52
3:G:185:ARG:NH1	3:G:190:THR:O	2.42	0.52
8:M:332:THR:HB	8:M:417:VAL:HG21	1.92	0.52
13:J:65:VAL:O	13:J:69:PHE:HB2	2.09	0.52
4:C:594:VAL:HG12	4:C:597:ASP:H	1.75	0.52
1:F:298:ASP:HB3	1:F:406:GLU:HB3	1.92	0.52
3:G:210:ASP:HB3	3:G:213:HIS:HB3	1.92	0.52
3:G:617:GLU:HG2	3:G:638:PRO:HG3	1.92	0.52
5:B:125:SER:OG	5:B:131:ASN:OD1	2.28	0.52
5:B:217:PRO:HG3	6:I:144:LYS:HD2	1.92	0.52
9:N:188:ALA:HA	9:N:191:LYS:HG3	1.92	0.52
9:N:309:LEU:HD11	9:N:330:LEU:HD21	1.91	0.52
8:M:29:ARG:HD3	8:M:109:ILE:HD11	1.92	0.52
10:H:165:MET:HA	10:H:168:VAL:HB	1.91	0.52
4:C:67:LEU:HB2	4:C:70:PRO:HA	1.91	0.52
4:C:274:ARG:NH2	5:B:158:CYS:SG	2.81	0.52
10:H:83:PHE:HD1	10:H:136:SER:HB3	1.74	0.51
7:L:505:ILE:HG23	7:L:506:LEU:HD23	1.92	0.51
1:F:394:GLY:O	3:G:48:ARG:NH2	2.44	0.51
4:C:144:LEU:HA	4:C:168:PRO:HD2	1.91	0.51
4:C:312:GLU:OE2	4:C:315:ARG:NH1	2.43	0.51
5:B:208:ARG:NH1	6:I:132:TYR:OH	2.42	0.51
2:E:125:ARG:NH1	2:E:165:TYR:O	2.43	0.51
3:G:21:LEU:HD21	3:G:79:ILE:HG21	1.92	0.51
9:N:137:LEU:HD22	13:J:147:LEU:HD11	1.92	0.51
3:G:320:PRO:HB2	3:G:537:SER:HB3	1.91	0.51
11:A:7:THR:O	11:A:7:THR:OG1	2.29	0.51
4:C:426:GLY:HA2	4:C:542:GLY:HA2	1.93	0.51
6:I:59:ARG:NH1	6:I:148:TYR:O	2.44	0.51
18:L:801:3PE:H362	8:M:390:PHE:HD1	1.74	0.51
10:H:13:LEU:HD23	10:H:17:LYS:HD2	1.92	0.51
3:G:536:ARG:NH1	3:G:818:TYR:OH	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:LEU:HD11	1:F:107:GLN:HG3	1.93	0.51
6:I:89:PRO:HG2	6:I:134:LYS:HE3	1.91	0.51
9:N:176:LEU:HD22	9:N:202:LEU:HD11	1.93	0.51
4:C:157:ARG:O	4:C:162:GLN:NE2	2.44	0.50
9:N:134:LEU:HD11	13:J:143:LEU:HB3	1.93	0.50
9:N:283:PHE:O	9:N:287:MET:HG2	2.11	0.50
1:F:103:LEU:HD13	1:F:261:LEU:HD23	1.93	0.50
3:G:108:CYS:O	3:G:219:ARG:NH1	2.42	0.50
3:G:212:THR:HG22	3:G:832:VAL:HG21	1.92	0.50
5:B:135:MET:HA	6:I:72:VAL:HG22	1.93	0.50
7:L:148:LEU:HD22	8:M:398:MET:HG2	1.93	0.50
7:L:291:LEU:HD13	7:L:318:TYR:HE1	1.76	0.50
1:F:178:TYR:HB3	1:F:349:GLU:HB3	1.94	0.50
4:C:380:LEU:HD23	4:C:485:LEU:HD13	1.92	0.50
8:M:361:GLN:OE1	8:M:365:ARG:NH1	2.41	0.50
9:N:334:LEU:O	9:N:338:LEU:HB2	2.10	0.50
12:K:39:ILE:HG21	12:K:69:ALA:HB2	1.93	0.50
3:G:250:ARG:HE	3:G:252:GLU:HG2	1.75	0.50
6:I:142:PRO:HB2	6:I:146:PRO:HA	1.93	0.50
13:J:94:ILE:HG22	13:J:98:ILE:HD13	1.93	0.50
3:G:81:ILE:O	3:G:90:ARG:NH2	2.45	0.50
9:N:82:LEU:HD11	9:N:334:LEU:HD21	1.94	0.50
10:H:170:GLN:OE1	10:H:188:ASN:ND2	2.45	0.50
1:F:88:LEU:HD12	1:F:216:VAL:HG22	1.92	0.50
2:E:65:PRO:HB3	3:G:170:THR:HB	1.94	0.50
3:G:282:ARG:HE	3:G:645:THR:HG21	1.76	0.50
11:A:68:PHE:HB3	13:J:69:PHE:HE2	1.76	0.50
7:L:11:PRO:HB2	7:L:125:ALA:HB2	1.93	0.50
7:L:413:ASN:OD1	7:L:413:ASN:N	2.45	0.50
8:M:405:VAL:O	8:M:409:MET:HG3	2.11	0.50
9:N:387:PRO:O	9:N:388:MET:HG2	2.12	0.49
10:H:96:LEU:HD13	11:A:20:LEU:HD22	1.94	0.49
11:A:61:ARG:HG3	13:J:170:ASN:HD22	1.76	0.49
1:F:340:ARG:NE	1:F:372:GLU:OE1	2.43	0.49
3:G:497:LYS:HG2	3:G:528:ASP:HB3	1.94	0.49
8:M:168:ILE:HG12	9:N:430:VAL:HG11	1.93	0.49
12:K:80:LEU:HD11	12:K:90:LEU:HD13	1.95	0.49
2:E:92:CYS:SG	2:E:94:SER:OG	2.70	0.49
5:B:66:VAL:HA	5:B:69:VAL:HB	1.94	0.49
8:M:123:ILE:HG13	8:M:149:PRO:HB2	1.94	0.49
1:F:38:ALA:HB2	1:F:114:GLU:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:343:ARG:NH2	4:C:347:TYR:OH	2.45	0.49
7:L:179:VAL:HG22	8:M:426:THR:HG22	1.94	0.49
10:H:101:VAL:HG11	10:H:250:ALA:HB1	1.94	0.49
3:G:694:ASP:OD1	3:G:695:ALA:N	2.45	0.49
5:B:107:ALA:HA	5:B:110:ILE:HD12	1.94	0.49
3:G:452:PRO:HD3	3:G:880:THR:HG21	1.93	0.49
4:C:286:PRO:HG3	4:C:537:ILE:HG12	1.94	0.49
18:L:801:3PE:H3B1	8:M:400:GLY:HA3	1.94	0.49
3:G:443:ASP:OD1	3:G:443:ASP:N	2.46	0.49
5:B:65:TYR:O	5:B:69:VAL:N	2.43	0.49
9:N:119:LEU:HD11	9:N:132:ILE:HG22	1.95	0.49
7:L:82:ASP:N	7:L:82:ASP:OD1	2.45	0.49
9:N:421:GLY:HA2	9:N:424:TYR:CE2	2.48	0.49
3:G:436:VAL:HG11	3:G:815:ALA:HB1	1.94	0.49
8:M:2:LEU:HB3	8:M:42:LEU:HD21	1.94	0.49
8:M:432:ALA:HA	8:M:435:TYR:CE2	2.48	0.49
4:C:289:LEU:HB2	4:C:535:GLN:HG2	1.95	0.48
11:A:125:TRP:NE1	13:J:166:GLU:OE2	2.43	0.48
5:B:27:ASP:OD1	5:B:27:ASP:N	2.44	0.48
7:L:169:LYS:HG3	18:L:802:3PE:H342	1.95	0.48
10:H:100:ILE:HD12	10:H:115:GLY:HA2	1.94	0.48
12:K:34:GLY:O	12:K:38:MET:HG3	2.13	0.48
3:G:260:ASN:H	3:G:368:LEU:HD23	1.78	0.48
4:C:365:ILE:HD12	4:C:501:THR:HB	1.94	0.48
3:G:239:ILE:HG13	3:G:241:PRO:HD3	1.95	0.48
4:C:144:LEU:HB3	4:C:169:LEU:HB2	1.94	0.48
7:L:362:ILE:HA	7:L:365:MET:HG2	1.95	0.48
2:E:125:ARG:NH1	2:E:166:LYS:O	2.41	0.48
18:L:801:3PE:H281	8:M:472:VAL:HG11	1.95	0.48
10:H:72:ASP:OD1	10:H:72:ASP:N	2.45	0.48
7:L:103:ALA:HA	7:L:106:TYR:HB3	1.96	0.48
1:F:12:PRO:HB3	1:F:235:TRP:HH2	1.79	0.48
3:G:323:SER:OG	3:G:621:THR:N	2.44	0.48
6:I:71:PRO:HD3	6:I:104:LEU:HD12	1.94	0.48
1:F:359:ASP:HB2	3:G:96:TRP:HB3	1.96	0.48
3:G:595:VAL:HG22	3:G:610:LEU:HD12	1.95	0.48
3:G:772:ASP:OD1	3:G:772:ASP:N	2.46	0.48
5:B:204:LYS:NZ	6:I:121:GLU:O	2.46	0.48
9:N:96:GLU:OE2	9:N:447:ASN:ND2	2.47	0.48
13:J:128:ALA:HA	13:J:131:ILE:HG12	1.95	0.48
1:F:188:ASN:ND2	1:F:196:ASN:O	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:430:ARG:HG2	4:C:456:VAL:HG12	1.96	0.47
10:H:37:ARG:HH22	10:H:238:PHE:HZ	1.62	0.47
10:H:302:TRP:HB3	11:A:123:LEU:HD21	1.96	0.47
3:G:348:GLN:NE2	3:G:548:GLY:O	2.40	0.47
4:C:330:VAL:HG21	4:C:404:LEU:HB2	1.97	0.47
10:H:79:ASP:OD1	10:H:79:ASP:N	2.43	0.47
8:M:84:ASP:N	8:M:84:ASP:OD1	2.47	0.47
12:K:43:ALA:HB1	12:K:62:TYR:HD1	1.78	0.47
1:F:286:LYS:HE2	1:F:331:HIS:HB3	1.96	0.47
12:K:2:ILE:O	13:J:119:ILE:N	2.41	0.47
4:C:522:VAL:HG13	6:I:69:ALA:HB2	1.96	0.47
5:B:2:ASP:OD1	5:B:2:ASP:N	2.36	0.47
8:M:316:ALA:O	8:M:319:SER:OG	2.25	0.47
13:J:93:TRP:HE3	13:J:94:ILE:HD13	1.79	0.47
1:F:384:LEU:HD22	1:F:408:LEU:HD21	1.97	0.47
3:G:363:ILE:HA	3:G:523:LYS:HE3	1.96	0.47
4:C:133:ASN:HB3	4:C:422:TRP:HA	1.95	0.47
4:C:548:LEU:HD22	4:C:559:THR:HG22	1.96	0.47
7:L:6:LEU:HD22	7:L:44:VAL:HG21	1.97	0.47
9:N:66:LEU:HD11	13:J:140:ALA:HB2	1.97	0.47
10:H:92:THR:O	10:H:96:LEU:HG	2.15	0.47
7:L:273:PHE:HB3	7:L:280:LEU:HD13	1.97	0.47
4:C:105:ILE:HD13	4:C:420:LEU:HD11	1.97	0.47
4:C:107:ARG:HB3	4:C:109:ARG:HG3	1.97	0.47
4:C:280:GLY:N	4:C:283:ASN:OD1	2.46	0.46
8:M:175:PHE:HD2	9:N:422:LEU:HD13	1.79	0.46
4:C:322:TYR:OH	4:C:590:SER:O	2.32	0.46
5:B:101:THR:HA	5:B:129:CYS:HB3	1.97	0.46
1:F:87:LEU:O	1:F:128:GLY:HA2	2.14	0.46
2:E:96:VAL:HG11	2:E:137:CYS:HB3	1.97	0.46
4:C:143:ASP:OD2	4:C:158:ILE:N	2.42	0.46
10:H:310:LEU:HD23	11:A:107:ILE:HG23	1.97	0.46
12:K:82:GLN:OE1	12:K:85:ARG:NH2	2.48	0.46
4:C:215:PHE:HA	4:C:237:LEU:O	2.16	0.46
10:H:15:ILE:HD12	11:A:18:ILE:HG21	1.97	0.46
3:G:508:SER:OG	3:G:510:GLU:OE1	2.34	0.46
4:C:19:ASP:OD1	4:C:19:ASP:N	2.46	0.46
9:N:248:ILE:HG12	9:N:330:LEU:HD22	1.97	0.46
3:G:638:PRO:HG2	3:G:647:MET:HB3	1.96	0.46
7:L:44:VAL:O	7:L:48:ILE:HG13	2.16	0.46
3:G:257:GLY:HA3	3:G:777:LYS:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:379:VAL:HG22	3:G:501:ILE:HB	1.97	0.46
4:C:192:LEU:HD12	5:B:108:PRO:HB2	1.97	0.46
4:C:487:ASN:OD1	4:C:487:ASN:N	2.48	0.46
7:L:222:LEU:HD22	7:L:265:LEU:HD11	1.97	0.46
3:G:219:ARG:HG3	6:I:64:ASN:HB2	1.98	0.46
3:G:619:ASP:OD1	3:G:634:GLN:N	2.49	0.46
4:C:415:GLY:HA2	4:C:432:THR:HG22	1.97	0.46
7:L:567:SER:O	7:L:571:ILE:HG23	2.16	0.46
9:N:300:TYR:HA	9:N:303:ILE:HD12	1.98	0.46
12:K:84:HIS:HB2	12:K:90:LEU:HD21	1.97	0.46
4:C:300:PRO:HG3	4:C:492:PRO:HG2	1.97	0.46
7:L:64:LEU:HB2	7:L:77:PHE:HB3	1.97	0.46
9:N:70:ASP:OD1	9:N:70:ASP:N	2.49	0.45
1:F:269:THR:HA	1:F:308:PRO:HA	1.98	0.45
8:M:232:ALA:HA	8:M:235:MET:HB3	1.98	0.45
9:N:330:LEU:HD23	9:N:330:LEU:HA	1.73	0.45
10:H:275:THR:O	10:H:279:MET:HG3	2.15	0.45
5:B:125:SER:HB3	5:B:151:VAL:HG11	1.99	0.45
3:G:97:LEU:HD22	3:G:154:ILE:HB	1.98	0.45
5:B:143:GLN:OE1	6:I:98:ARG:NH2	2.42	0.45
2:E:81:ARG:HB2	6:I:176:LYS:HB3	1.98	0.45
8:M:47:TRP:HA	8:M:88:LEU:HD21	1.98	0.45
10:H:74:ILE:HG21	10:H:80:ARG:HG2	1.99	0.45
3:G:157:TYR:N	14:G:1002:SF4:S4	2.85	0.45
7:L:91:VAL:HG21	7:L:336:MET:HA	1.99	0.45
1:F:72:LYS:NZ	1:F:216:VAL:O	2.49	0.45
7:L:291:LEU:HD22	7:L:318:TYR:CD1	2.52	0.45
10:H:201:ILE:HG23	10:H:212:PHE:HE2	1.82	0.45
4:C:551:ASP:HB2	4:C:557:TYR:HB2	1.97	0.45
5:B:61:LEU:HB3	5:B:100:GLY:HA3	1.98	0.45
7:L:175:ARG:HD2	7:L:175:ARG:HA	1.73	0.44
8:M:287:ALA:O	8:M:291:MET:HG3	2.17	0.44
8:M:314:LEU:O	8:M:318:THR:HG23	2.17	0.44
9:N:60:ALA:HB1	9:N:70:ASP:HA	1.99	0.44
9:N:139:LEU:HA	9:N:142:LEU:HB2	1.99	0.44
9:N:170:LEU:HD12	9:N:210:MET:HA	1.99	0.44
1:F:390:PHE:HZ	3:G:88:GLN:HG3	1.81	0.44
4:C:430:ARG:NH1	4:C:473:GLU:OE2	2.50	0.44
9:N:138:PRO:HG3	13:J:150:ALA:HB1	1.99	0.44
3:G:36:CYS:O	3:G:161:ARG:NH2	2.51	0.44
5:B:59:PHE:HE2	5:B:110:ILE:HG12	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:303:LYS:HG2	11:A:118:VAL:HG22	1.98	0.44
1:F:23:PRO:HA	1:F:107:GLN:HA	2.00	0.44
3:G:374:TYR:HD2	3:G:499:LEU:HB2	1.82	0.44
4:C:53:LYS:HG3	4:C:56:GLN:HG2	1.99	0.44
5:B:217:PRO:HD3	6:I:144:LYS:HB3	2.00	0.44
7:L:423:PHE:HB2	7:L:500:VAL:HG13	1.99	0.44
18:L:801:3PE:H121	8:M:382:LYS:HA	1.99	0.44
13:J:23:THR:HG23	13:J:87:TRP:HZ2	1.82	0.44
3:G:379:VAL:HB	3:G:433:VAL:HG12	2.00	0.44
5:B:169:LEU:HD23	5:B:169:LEU:HA	1.86	0.44
7:L:171:PHE:HB3	8:M:437:LEU:HD11	1.99	0.44
7:L:379:PHE:HB3	7:L:433:ILE:HD11	2.00	0.44
8:M:72:ILE:HB	8:M:77:ILE:HB	1.98	0.44
8:M:493:ILE:HD13	8:M:493:ILE:HA	1.89	0.44
3:G:120:THR:HB	4:C:516:ILE:HG21	1.99	0.44
4:C:76:ASP:OD1	4:C:560:ARG:NH2	2.43	0.44
9:N:132:ILE:O	9:N:136:SER:OG	2.30	0.44
3:G:812:TRP:O	3:G:902:LEU:N	2.51	0.44
8:M:220:GLU:HG2	8:M:282:ALA:HB2	2.00	0.44
10:H:21:ILE:HA	10:H:24:VAL:HG12	1.99	0.44
2:E:142:ASN:HA	2:E:150:HIS:O	2.18	0.44
3:G:100:ASN:OD1	3:G:100:ASN:N	2.50	0.44
3:G:338:ASN:OD1	3:G:338:ASN:N	2.51	0.44
3:G:730:GLN:H	3:G:730:GLN:HG3	1.64	0.44
5:B:135:MET:HB3	6:I:100:ILE:HG21	2.00	0.44
3:G:83:ASP:N	3:G:83:ASP:OD1	2.50	0.43
3:G:569:LEU:HD13	3:G:654:LEU:HD11	1.99	0.43
5:B:127:GLY:O	5:B:131:ASN:ND2	2.51	0.43
7:L:36:GLY:O	7:L:40:LEU:HD12	2.18	0.43
12:K:88:GLN:HE22	13:J:170:ASN:HB3	1.83	0.43
1:F:155:LEU:HA	1:F:160:ILE:HG23	1.99	0.43
9:N:451:SER:O	9:N:455:ILE:HG12	2.18	0.43
1:F:133:ARG:HE	1:F:135:GLU:HB2	1.83	0.43
1:F:357:CYS:HB2	1:F:401:ALA:HB2	2.00	0.43
5:B:158:CYS:HB2	6:I:100:ILE:HB	2.00	0.43
7:L:234:PRO:HB2	7:L:235:LEU:HD12	2.00	0.43
9:N:214:LEU:HD13	9:N:254:VAL:HG22	2.00	0.43
9:N:291:GLN:O	9:N:427:ARG:NH2	2.51	0.43
13:J:57:ILE:HG22	13:J:58:VAL:HG23	2.00	0.43
1:F:56:ASP:O	1:F:237:GLN:NE2	2.51	0.43
5:B:23:GLU:OE1	5:B:23:GLU:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:251:PHE:CZ	9:N:309:LEU:HB3	2.53	0.43
3:G:809:ASP:N	3:G:809:ASP:OD1	2.44	0.43
4:C:74:LEU:HA	4:C:102:LEU:HD23	1.99	0.43
4:C:405:LYS:HD3	4:C:405:LYS:HA	1.76	0.43
7:L:260:THR:HB	7:L:335:LEU:HD11	1.99	0.43
9:N:68:ARG:HH12	9:N:484:LEU:HD22	1.84	0.43
9:N:311:VAL:HA	9:N:314:ILE:HD12	2.00	0.43
11:A:66:ALA:HB3	13:J:161:GLU:HB2	1.99	0.43
7:L:31:ALA:O	7:L:35:VAL:HG22	2.18	0.43
8:M:149:PRO:O	8:M:153:LEU:HB2	2.17	0.43
9:N:119:LEU:HD12	9:N:135:ILE:HD12	2.01	0.43
3:G:595:VAL:HG12	3:G:612:ALA:HB2	2.01	0.43
7:L:365:MET:HG3	7:L:436:VAL:HG13	2.01	0.43
3:G:368:LEU:HD21	3:G:390:ARG:HB3	2.01	0.43
10:H:183:GLN:NE2	10:H:255:LEU:O	2.51	0.43
3:G:118:ASP:OD1	3:G:762:ASN:ND2	2.51	0.43
7:L:38:VAL:HG21	7:L:100:HIS:CD2	2.53	0.43
8:M:233:VAL:O	8:M:243:TRP:NE1	2.47	0.43
1:F:15:TRP:HE1	1:F:16:ARG:HH21	1.67	0.42
8:M:79:ILE:HA	8:M:138:LEU:HD22	2.00	0.42
8:M:361:GLN:NE2	8:M:464:GLU:OE1	2.52	0.42
9:N:150:LYS:HA	12:K:87:ARG:HH12	1.84	0.42
9:N:159:TYR:O	9:N:163:SER:OG	2.23	0.42
8:M:124:LEU:HA	8:M:127:VAL:HG22	2.00	0.42
8:M:268:ALA:HB1	8:M:330:ILE:HD11	2.01	0.42
11:A:20:LEU:O	11:A:24:ILE:HG12	2.19	0.42
13:J:74:LEU:HD21	13:J:76:LEU:HD23	2.00	0.42
3:G:171:ASP:OD2	3:G:185:ARG:NH1	2.53	0.42
3:G:385:THR:HG23	3:G:386:GLN:HG2	2.02	0.42
4:C:85:ARG:HB3	4:C:88:ARG:HD2	2.01	0.42
5:B:123:VAL:HB	5:B:151:VAL:HA	2.00	0.42
6:I:67:ALA:HA	6:I:75:ILE:HB	2.01	0.42
7:L:250:SER:O	7:L:254:HIS:ND1	2.47	0.42
3:G:176:GLY:HA2	6:I:175:VAL:HG13	2.01	0.42
4:C:44:ARG:NH1	4:C:294:LEU:O	2.52	0.42
7:L:526:ALA:HA	7:L:529:ARG:HG2	2.01	0.42
7:L:547:LYS:HE3	7:L:547:LYS:HB3	1.68	0.42
8:M:341:ALA:HA	8:M:410:ILE:HD11	2.01	0.42
11:A:69:TYR:OH	12:K:74:SER:O	2.38	0.42
4:C:258:LYS:HB3	5:B:138:ILE:HD11	2.01	0.42
10:H:36:GLU:HB2	10:H:283:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:185:ARG:HG2	3:G:187:GLU:H	1.85	0.42
3:G:888:MET:N	3:G:888:MET:SD	2.93	0.42
4:C:506:GLU:O	4:C:510:GLN:HG2	2.20	0.42
8:M:391:PHE:O	8:M:395:THR:HG23	2.19	0.42
13:J:160:ARG:HG2	13:J:160:ARG:HH11	1.85	0.42
1:F:133:ARG:NH2	2:E:133:CYS:O	2.53	0.42
1:F:348:ARG:HH22	2:E:132:CYS:HA	1.84	0.42
5:B:124:ILE:HG12	5:B:153:VAL:HB	2.01	0.42
8:M:471:LEU:HD23	8:M:471:LEU:HA	1.91	0.42
6:I:103:GLY:HA2	6:I:116:LEU:HD11	2.02	0.42
4:C:168:PRO:HB3	5:B:139:TYR:CZ	2.54	0.42
6:I:50:LEU:HB2	6:I:138:LEU:HA	2.01	0.42
8:M:103:LEU:O	8:M:463:ARG:NH1	2.53	0.42
8:M:318:THR:HG22	8:M:435:TYR:CE1	2.55	0.42
11:A:68:PHE:HB2	13:J:73:MET:HE1	2.01	0.42
1:F:102:ARG:NH2	2:E:134:LEU:O	2.53	0.42
3:G:313:LYS:HE3	3:G:338:ASN:HD22	1.85	0.42
8:M:38:LEU:HD23	8:M:38:LEU:HA	1.89	0.42
9:N:217:LYS:HD3	9:N:217:LYS:HA	1.87	0.42
10:H:250:ALA:O	10:H:254:THR:OG1	2.31	0.42
2:E:86:ARG:NH1	2:E:166:LYS:OXT	2.52	0.41
4:C:12:GLU:HA	4:C:13:PRO:HD3	1.91	0.41
1:F:314:ILE:HG22	1:F:319:SER:HB3	2.01	0.41
10:H:76:LYS:HG3	10:H:77:PHE:HD1	1.85	0.41
13:J:82:GLU:O	13:J:85:ARG:NH2	2.52	0.41
1:F:76:MET:HE2	1:F:123:LEU:HD22	2.02	0.41
1:F:289:ALA:HB3	1:F:329:VAL:HB	2.02	0.41
1:F:345:PHE:O	1:F:349:GLU:HB2	2.19	0.41
4:C:423:GLY:HA3	4:C:567:ALA:HB1	2.01	0.41
7:L:381:VAL:HG11	7:L:461:LEU:HD13	2.02	0.41
9:N:52:LEU:HD11	9:N:74:MET:HA	2.02	0.41
9:N:377:THR:HB	9:N:432:LEU:HD11	2.02	0.41
3:G:390:ARG:HA	3:G:390:ARG:HD2	1.85	0.41
3:G:438:ASP:OD1	3:G:450:ARG:NE	2.52	0.41
4:C:167:HIS:HA	4:C:168:PRO:HD3	1.93	0.41
7:L:425:THR:HA	7:L:428:TYR:CE2	2.54	0.41
9:N:1:MET:HG3	9:N:65:PRO:HD3	2.03	0.41
1:F:92:ASP:OD1	1:F:133:ARG:HB3	2.21	0.41
4:C:549:THR:HB	4:C:558:ARG:HB3	2.01	0.41
3:G:224:GLN:NE2	3:G:635:VAL:O	2.53	0.41
4:C:233:ILE:HA	4:C:247:PRO:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:539:ALA:HB2	4:C:544:ASN:HB2	2.02	0.41
7:L:280:LEU:HD12	7:L:280:LEU:HA	1.94	0.41
8:M:468:ILE:HD13	8:M:468:ILE:HA	1.95	0.41
9:N:128:LEU:HD12	9:N:253:VAL:HG22	2.02	0.41
1:F:50:ILE:HG23	1:F:229:LEU:HD11	2.03	0.41
1:F:96:PRO:HB3	2:E:94:SER:HB2	2.02	0.41
3:G:44:VAL:HG13	3:G:161:ARG:HH11	1.84	0.41
3:G:385:THR:HG21	3:G:440:ARG:HB2	2.02	0.41
4:C:57:LEU:HD22	4:C:115:VAL:HG21	2.01	0.41
12:K:37:ILE:HD11	13:J:19:VAL:HG11	2.03	0.41
3:G:759:PRO:HB3	4:C:553:SER:HA	2.03	0.41
5:B:65:TYR:HA	5:B:68:MET:HE2	2.02	0.41
7:L:76:GLY:O	7:L:135:ASN:ND2	2.35	0.41
8:M:137:PHE:HB2	8:M:205:PHE:CD2	2.56	0.41
3:G:202:ILE:HD11	3:G:263:PHE:HE1	1.86	0.41
4:C:77:LEU:HB3	4:C:137:TYR:HB3	2.03	0.41
4:C:335:PRO:HG2	4:C:336:VAL:HG23	2.02	0.41
4:C:539:ALA:N	4:C:542:GLY:O	2.53	0.41
7:L:380:LEU:HD13	7:L:380:LEU:HA	1.91	0.41
7:L:550:VAL:HG22	18:L:802:3PE:H252	2.02	0.41
7:L:583:LEU:HB3	9:N:287:MET:HE3	2.02	0.41
8:M:339:GLN:NE2	8:M:489:SER:OG	2.53	0.41
10:H:22:LEU:HD11	10:H:95:LEU:HD21	2.03	0.41
12:K:96:SER:O	12:K:96:SER:OG	2.33	0.41
3:G:261:HIS:CE1	3:G:390:ARG:HH22	2.38	0.41
4:C:452:PHE:HA	4:C:479:ARG:HH21	1.86	0.41
7:L:141:LEU:HD11	8:M:480:PHE:HE1	1.86	0.41
12:K:2:ILE:HB	13:J:119:ILE:HB	2.02	0.41
3:G:290:ASP:OD1	3:G:290:ASP:N	2.53	0.40
8:M:264:LEU:O	8:M:265:LYS:HG2	2.20	0.40
9:N:289:LEU:HD23	9:N:289:LEU:HA	1.94	0.40
10:H:87:PRO:HG2	10:H:233:LYS:HG2	2.02	0.40
1:F:19:ASP:OD1	1:F:19:ASP:N	2.50	0.40
1:F:325:LEU:HD23	1:F:325:LEU:HA	1.95	0.40
3:G:153:CYS:SG	3:G:154:ILE:N	2.95	0.40
3:G:351:LEU:HD11	3:G:541:MET:HA	2.03	0.40
3:G:739:SER:OG	3:G:741:GLU:OE1	2.22	0.40
10:H:190:ILE:HG13	10:H:191:PRO:HD3	2.04	0.40
12:K:25:ARG:HD3	12:K:25:ARG:HA	1.92	0.40
4:C:254:ARG:NH2	5:B:63:CYS:SG	2.72	0.40
4:C:342:ASP:OD1	4:C:390:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:197:PHE:O	7:L:201:VAL:HG23	2.22	0.40
10:H:170:GLN:HE22	10:H:191:PRO:HB2	1.86	0.40
10:H:295:ASP:OD1	10:H:296:GLN:N	2.53	0.40
1:F:90:ASN:ND2	1:F:181:GLY:O	2.37	0.40
3:G:110:GLU:HB3	3:G:114:CYS:HB2	2.04	0.40
3:G:226:ALA:HB3	3:G:635:VAL:HG22	2.03	0.40
4:C:414:TYR:HB2	4:C:418:GLU:HB2	2.03	0.40
7:L:10:LEU:HD23	7:L:10:LEU:HA	1.90	0.40
7:L:399:LYS:HE2	7:L:399:LYS:HB2	1.86	0.40
9:N:192:ASN:OD1	9:N:192:ASN:N	2.54	0.40
10:H:11:ILE:O	10:H:15:ILE:HG12	2.20	0.40
10:H:252:MET:HG2	10:H:278:PHE:CE2	2.57	0.40
3:G:126:SER:HB2	4:C:517:THR:HG21	2.03	0.40
4:C:110:ASP:OD1	4:C:110:ASP:N	2.55	0.40
4:C:501:THR:HA	4:C:502:PRO:HA	1.90	0.40
9:N:62:ASP:HA	9:N:68:ARG:HA	2.04	0.40
12:K:43:ALA:HB1	12:K:62:TYR:CD1	2.55	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%)	421 (96%)	19 (4%)	0	100	100
2	E	154/156 (99%)	151 (98%)	3 (2%)	0	100	100
3	G	903/905 (100%)	861 (95%)	42 (5%)	0	100	100
4	C	568/600 (95%)	537 (94%)	31 (6%)	0	100	100
5	B	184/220 (84%)	175 (95%)	9 (5%)	0	100	100
6	I	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
7	L	589/613 (96%)	565 (96%)	24 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	M	502/504 (100%)	486 (97%)	16 (3%)	0	100	100
9	N	476/485 (98%)	466 (98%)	10 (2%)	0	100	100
10	H	304/325 (94%)	291 (96%)	13 (4%)	0	100	100
11	A	96/147 (65%)	90 (94%)	6 (6%)	0	100	100
12	K	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
13	J	173/175 (99%)	167 (96%)	6 (4%)	0	100	100
All	All	4629/4816 (96%)	4441 (96%)	188 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	356/356 (100%)	353 (99%)	3 (1%)	81	91
2	E	129/129 (100%)	128 (99%)	1 (1%)	81	91
3	G	732/732 (100%)	726 (99%)	6 (1%)	81	91
4	C	496/519 (96%)	488 (98%)	8 (2%)	62	83
5	B	169/192 (88%)	164 (97%)	5 (3%)	41	71
6	I	123/123 (100%)	120 (98%)	3 (2%)	49	75
7	L	469/486 (96%)	458 (98%)	11 (2%)	50	76
8	M	413/413 (100%)	400 (97%)	13 (3%)	40	71
9	N	382/385 (99%)	380 (100%)	2 (0%)	88	95
10	H	256/269 (95%)	248 (97%)	8 (3%)	40	71
11	A	79/119 (66%)	78 (99%)	1 (1%)	69	86
12	K	79/79 (100%)	74 (94%)	5 (6%)	18	53
13	J	136/139 (98%)	133 (98%)	3 (2%)	52	77
All	All	3819/3941 (97%)	3750 (98%)	69 (2%)	61	81

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	161	MET
1	F	398	CYS
1	F	427	PHE
2	E	111	LYS
3	G	75	ASP
3	G	172	LEU
3	G	175	TYR
3	G	233	CYS
3	G	265	CYS
3	G	416	GLN
4	C	143	ASP
4	C	194	MET
4	C	277	TYR
4	C	338	PHE
4	C	357	ARG
4	C	389	LYS
4	C	390	ARG
4	C	600	ARG
5	B	21	LYS
5	B	65	TYR
5	B	94	ASP
5	B	146	ASP
5	B	180	ARG
6	I	39	TYR
6	I	77	LEU
6	I	162	ASP
7	L	43	LEU
7	L	60	TYR
7	L	123	PHE
7	L	149	CYS
7	L	258	MET
7	L	333	PHE
7	L	379	PHE
7	L	407	MET
7	L	512	TRP
7	L	518	LEU
7	L	569	MET
8	M	1	MET
8	M	21	GLU
8	M	74	ARG
8	M	145	MET
8	M	174	PHE

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Mol	Chain	Res	Type
8	M	212	ASN
8	M	224	MET
8	M	249	SER
8	M	258	ASP
8	M	303	TRP
8	M	365	ARG
8	M	388	SER
8	M	435	TYR
9	N	388	MET
9	N	482	MET
10	H	64	MET
10	H	68	PHE
10	H	70	LYS
10	H	112	LEU
10	H	238	PHE
10	H	265	LEU
10	H	278	PHE
10	H	279	MET
11	A	16	PHE
12	K	46	PHE
12	K	51	SER
12	K	72	GLU
12	K	94	SER
12	K	96	SER
13	J	59	TYR
13	J	74	LEU
13	J	120	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	44	GLN
3	G	178	HIS
3	G	539	ASN
4	C	56	GLN
4	C	359	HIS
8	M	339	GLN
10	H	170	GLN
10	H	188	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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
15	FMN	F	502	-	33,33,33	1.06	2 (6%)	48,50,50	1.21	7 (14%)
18	3PE	L	801	-	50,50,50	0.31	0	53,55,55	0.29	0
14	SF4	G	1003	3	0,12,12	-	-	-		
14	SF4	G	1001	3	0,12,12	-	-	-		
14	SF4	F	501	1	0,12,12	-	-	-		
16	FES	E	201	2	0,4,4	-	-	-		
16	FES	G	1004	3	0,4,4	-	-	-		
14	SF4	G	1002	3	0,12,12	-	-	-		
14	SF4	B	301	5	0,12,12	-	-	-		
18	3PE	L	802	-	50,50,50	0.31	0	53,55,55	0.28	0
14	SF4	I	201	6	0,12,12	-	-	-		
14	SF4	I	202	6	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	3PE	L	801	-	-	9/54/54/54	-
14	SF4	G	1003	3	-	-	0/6/5/5
14	SF4	G	1001	3	-	-	0/6/5/5
14	SF4	F	501	1	-	-	0/6/5/5
16	FES	E	201	2	-	-	0/1/1/1
16	FES	G	1004	3	-	-	0/1/1/1
14	SF4	G	1002	3	-	-	0/6/5/5
14	SF4	B	301	5	-	-	0/6/5/5
18	3PE	L	802	-	-	11/54/54/54	-
15	FMN	F	502	-	-	9/18/18/18	0/3/3/3
14	SF4	I	201	6	-	-	0/6/5/5
14	SF4	I	202	6	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	502	FMN	C4A-N5	3.57	1.37	1.30
15	F	502	FMN	C10-N1	2.43	1.38	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	F	502	FMN	C4-N3-C2	-3.29	119.57	125.64
15	F	502	FMN	O4-C4-C4A	-2.87	119.00	126.60
15	F	502	FMN	C4A-C4-N3	2.73	120.11	113.19
15	F	502	FMN	C4A-C10-N10	2.59	120.27	116.48
15	F	502	FMN	C4A-C10-N1	-2.36	119.26	124.73
15	F	502	FMN	C10-C4A-N5	-2.08	120.44	124.86
15	F	502	FMN	C4-C4A-C10	2.08	120.28	116.79

There are no chirality outliers.

All (29) 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	C1'-C2'-C3'-C4'
15	F	502	FMN	C5'-O5'-P-O2P
15	F	502	FMN	C5'-O5'-P-O3P
18	L	801	3PE	C11-O13-P-O11
18	L	801	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
18	L	801	3PE	C11-O13-P-O14
18	L	801	3PE	O13-C11-C12-N
18	L	802	3PE	C11-O13-P-O11
18	L	802	3PE	C1-O11-P-O13
15	F	502	FMN	O2'-C2'-C3'-O3'
18	L	802	3PE	C3C-C3D-C3E-C3F
15	F	502	FMN	O2'-C2'-C3'-C4'
18	L	801	3PE	C38-C39-C3A-C3B
18	L	802	3PE	C2-C1-O11-P
15	F	502	FMN	C5'-O5'-P-O1P
18	L	801	3PE	C36-C37-C38-C39
18	L	802	3PE	C1-O11-P-O12
18	L	802	3PE	C1-O11-P-O14
18	L	802	3PE	C11-O13-P-O12
15	F	502	FMN	C1'-C2'-C3'-O3'
18	L	801	3PE	C2B-C2C-C2D-C2E
18	L	802	3PE	O21-C2-C3-O31
18	L	802	3PE	O21-C21-C22-C23
18	L	801	3PE	C1-O11-P-O14
18	L	801	3PE	C3A-C3B-C3C-C3D
18	L	802	3PE	C12-C11-O13-P
18	L	802	3PE	O31-C31-C32-C33

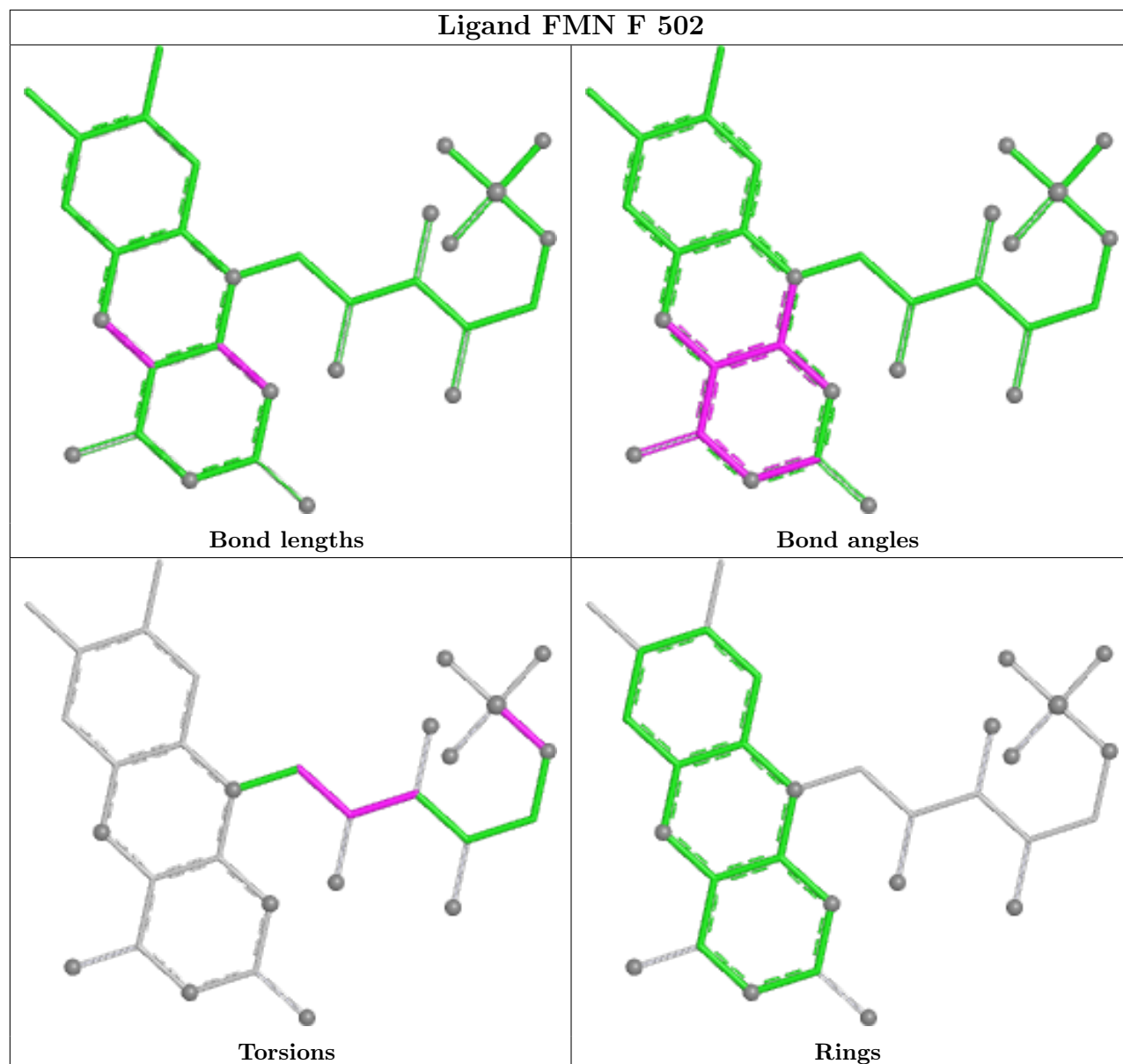
There are no ring outliers.

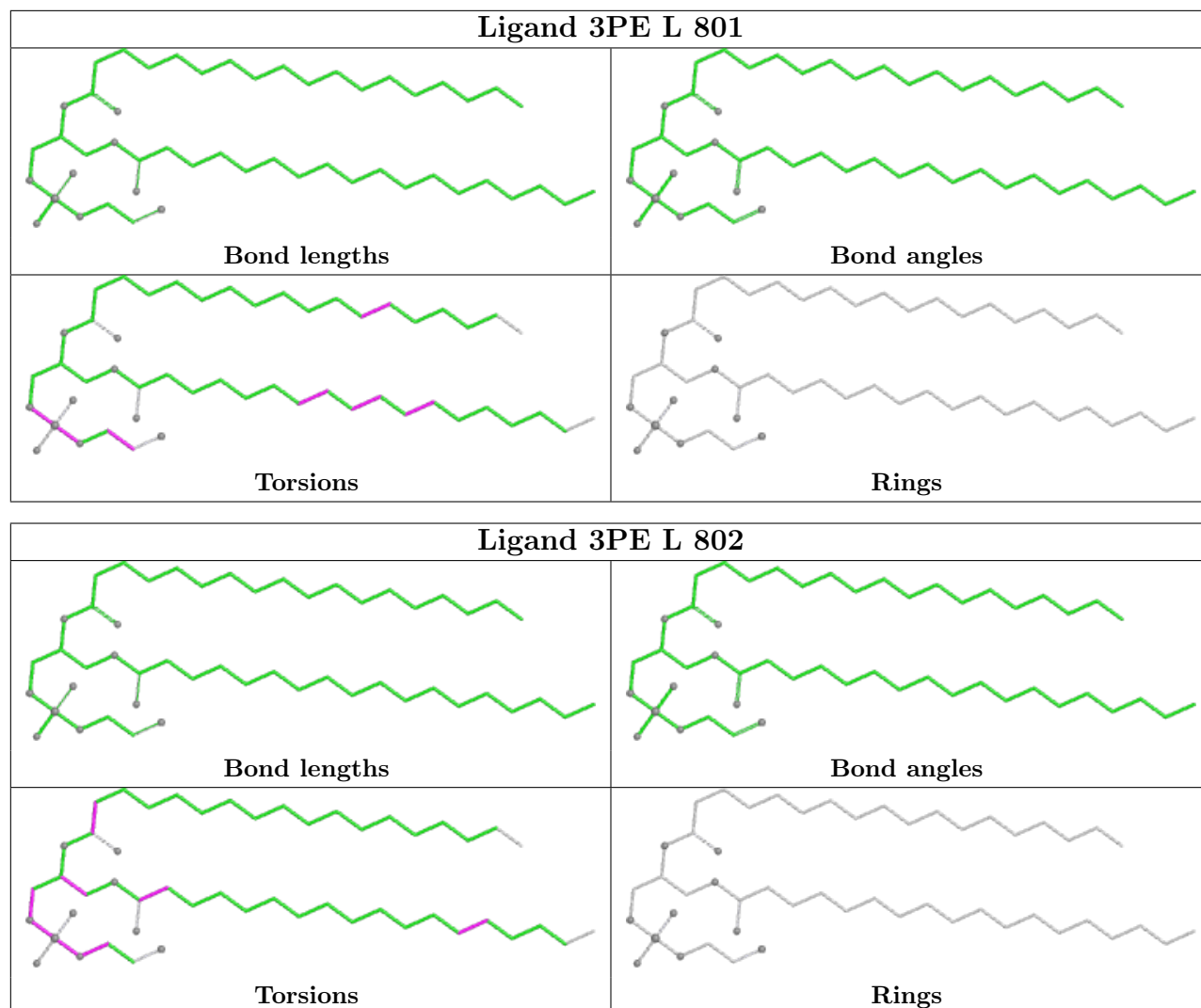
5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	L	801	3PE	4	0
14	G	1001	SF4	2	0
16	E	201	FES	1	0
14	G	1002	SF4	1	0
18	L	802	3PE	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.

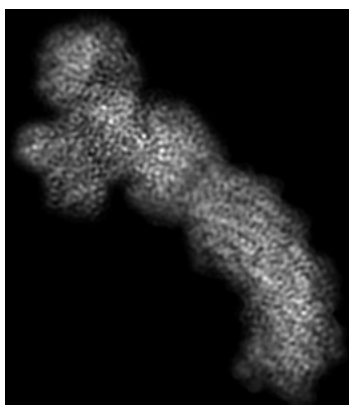
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13215. These allow visual inspection of the internal detail of the map and identification of artifacts.

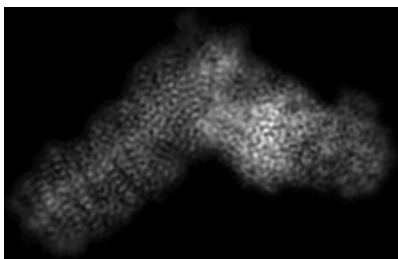
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

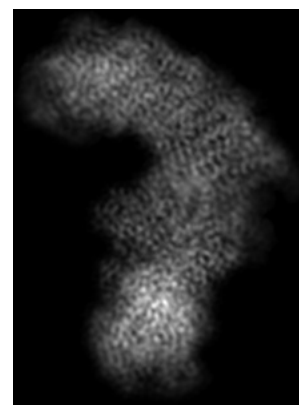
6.1.1 Primary map



X



Y

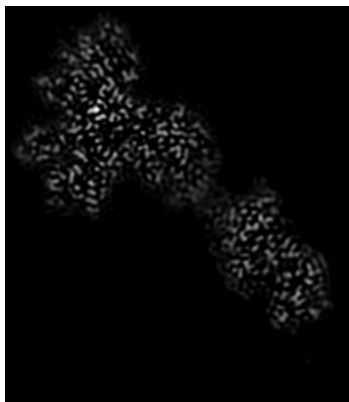


Z

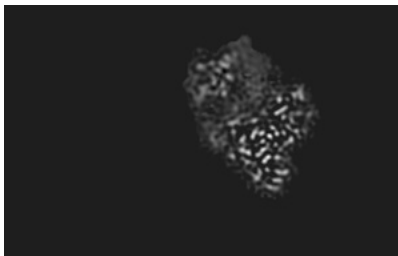
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

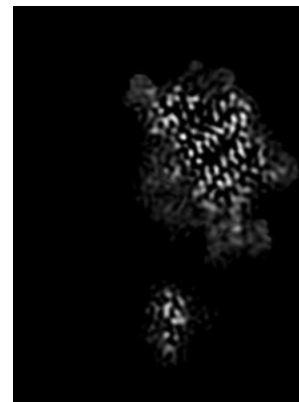
6.2.1 Primary map



X Index: 73



Y Index: 99



Z Index: 115

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: 75



Y Index: 53

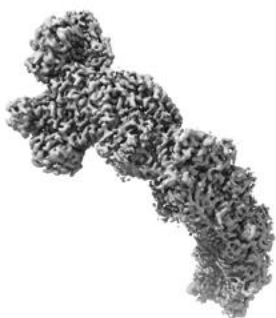


Z Index: 154

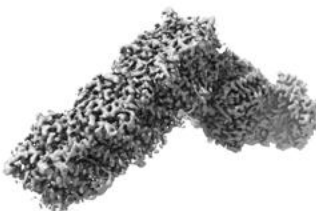
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.085. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

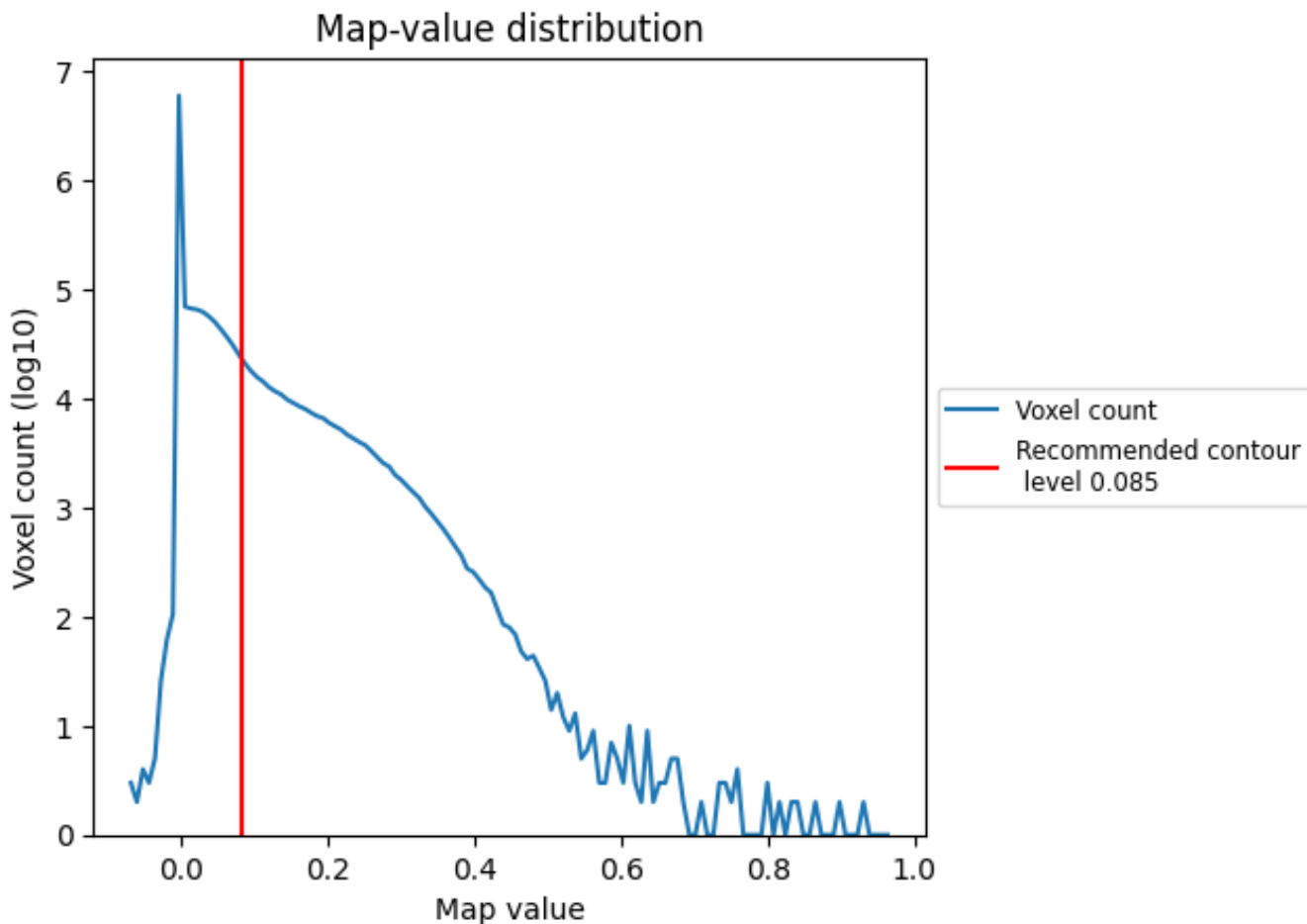
6.5 Mask visualisation

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

7 Map analysis [i](#)

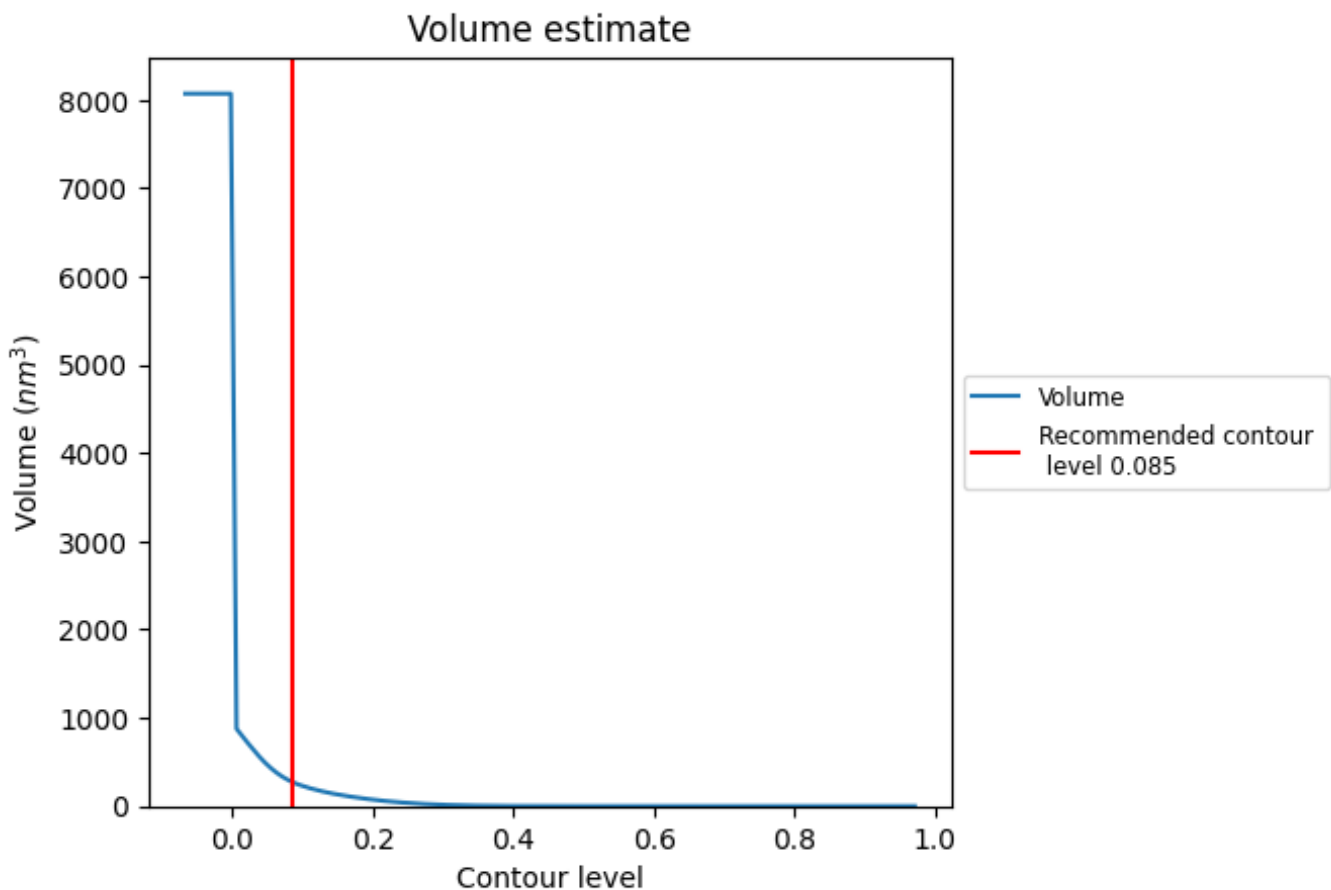
This section contains the results of statistical analysis of the map.

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 276 nm^3 ; this corresponds to an approximate mass of 249 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.

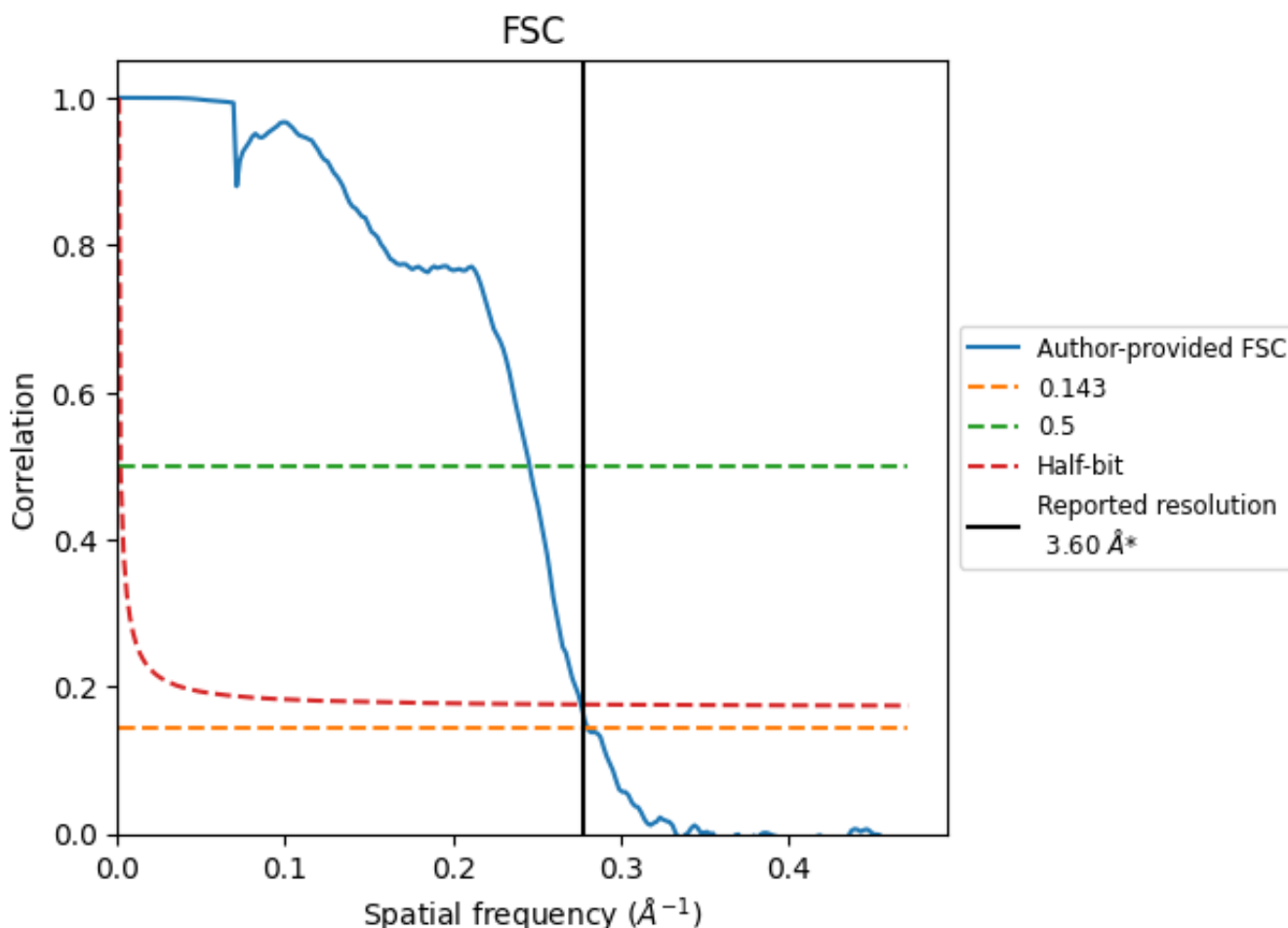
7.3 Rotationally averaged power spectrum [i](#)

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

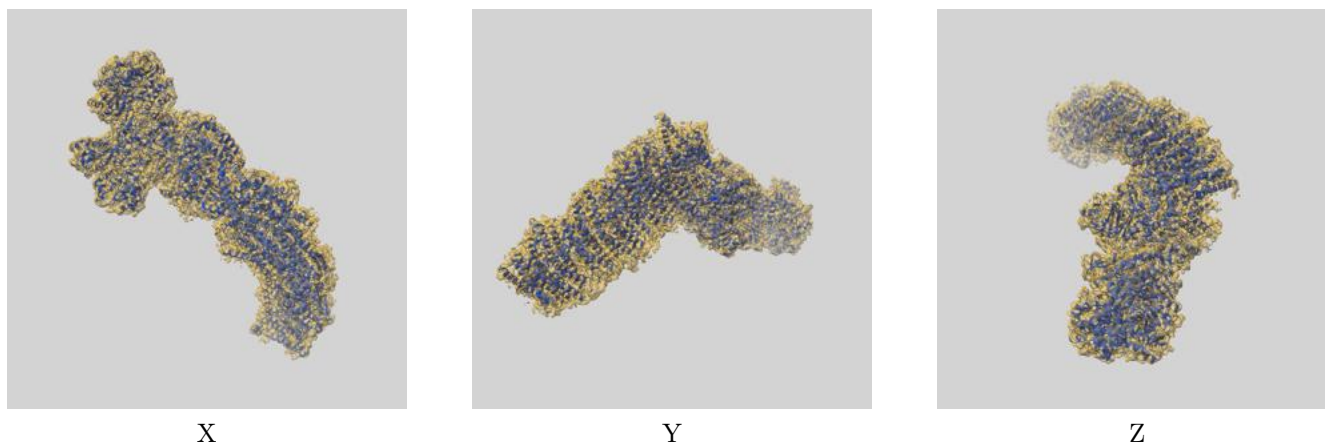
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.57	4.07	3.62
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

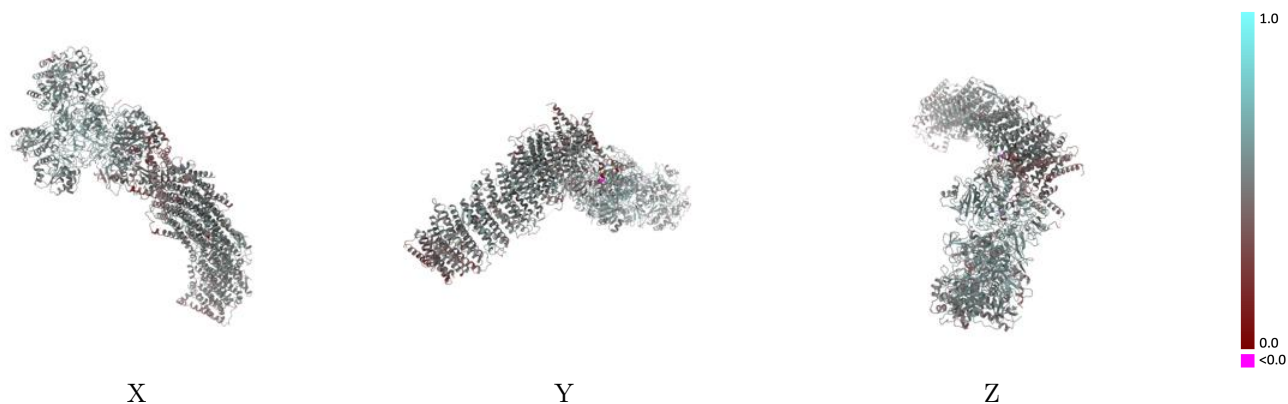
This section contains information regarding the fit between EMDB map EMD-13215 and PDB model 7P62. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



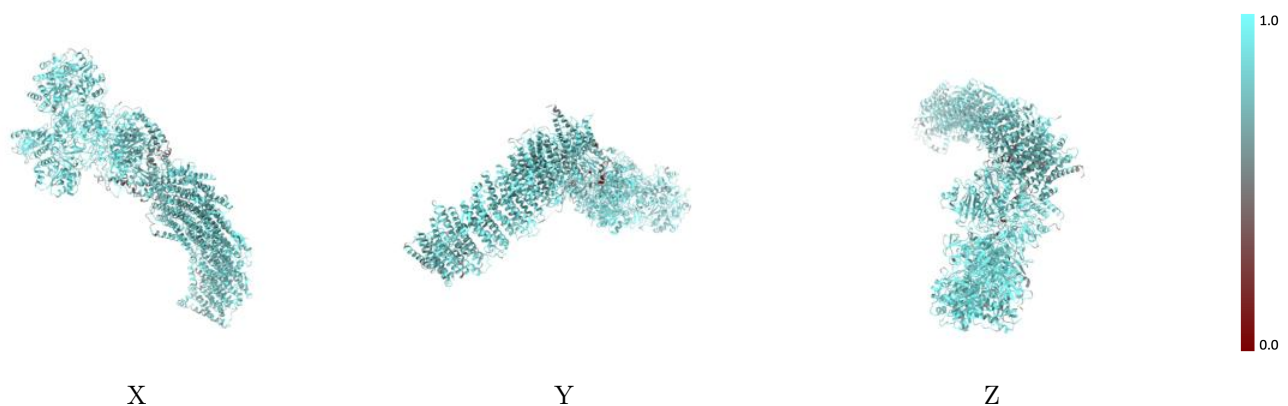
The images above show the 3D surface view of the map at the recommended contour level 0.085 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



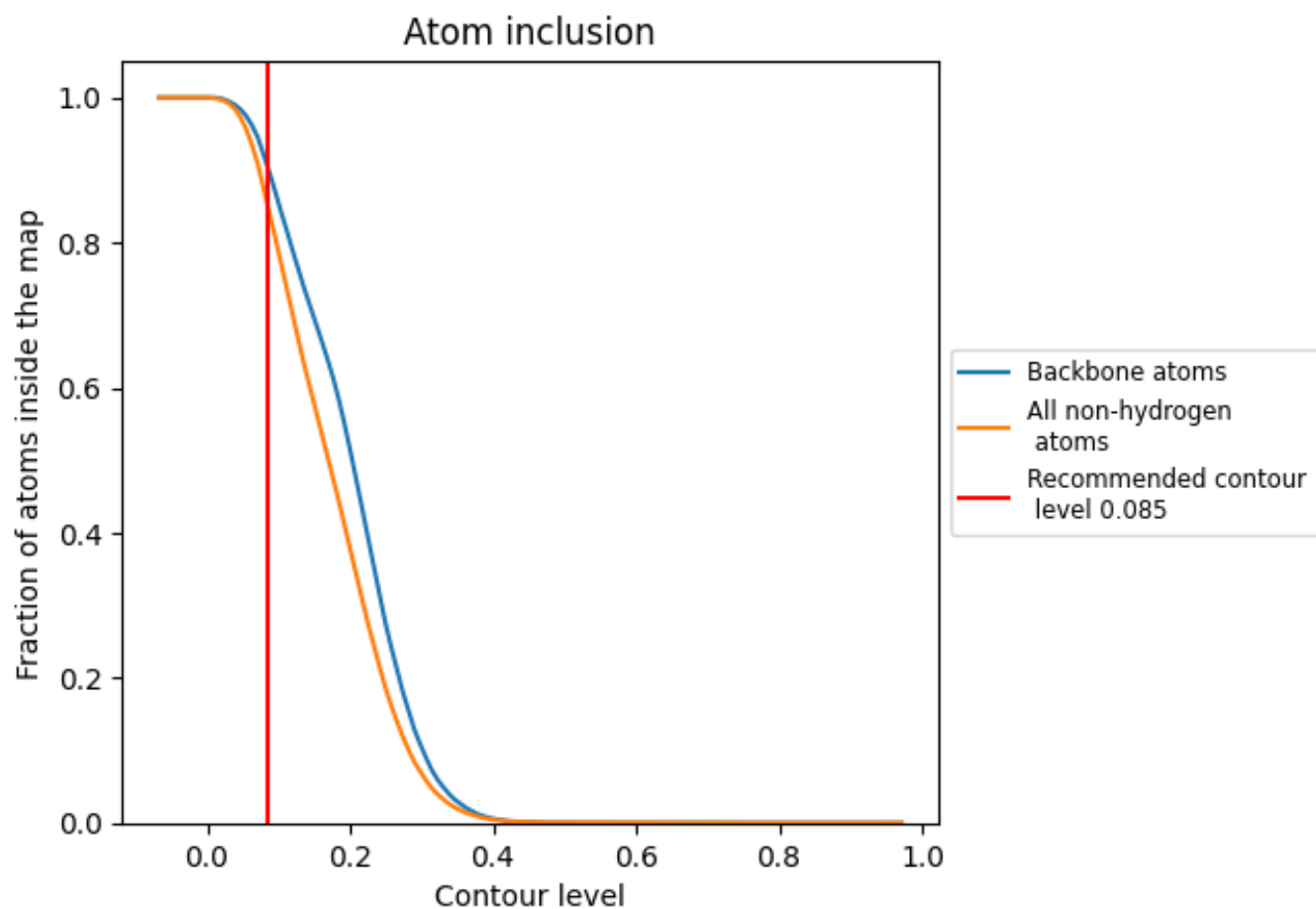
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.085).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 85% 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 (0.085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8500	 0.4960
A	 0.8079	 0.4590
B	 0.8224	 0.4790
C	 0.8328	 0.5040
E	 0.8710	 0.5120
F	 0.8646	 0.5020
G	 0.8961	 0.5350
H	 0.7858	 0.4390
I	 0.9157	 0.5560
J	 0.7863	 0.4480
K	 0.8456	 0.5110
L	 0.8109	 0.4510
M	 0.8738	 0.5000
N	 0.8532	 0.5000

