Full wwPDB EM Validation Report ⓘ

Sep 26, 2022 – 10:57 pm BST

PDB ID	:	7Z83
EMDB ID	:	EMD-14541
Title	:	Complex I from E. coli, DDM/LMNG-purified, under Turnover at pH 8, Open state
Authors	:	Kravchuk, V.; Kampjut, D.; Sazanov, L.
Deposited on	:	2022-03-16
Resolution	:	2.88 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:

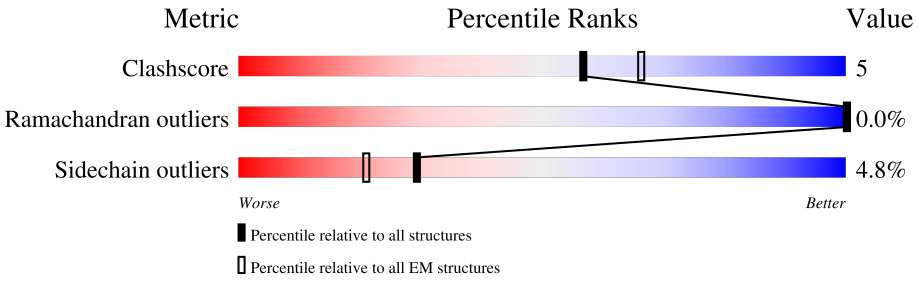
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.88 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	F	445	86% 13%
2	E	166	82% 11% 6%
3	G	908	86% 13%
4	C	600	84% 12%
5	B	220	69% 19% 10%
6	I	180	87% 13%
7	H	325	77% 18%
8	A	147	55% 14% 31%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	L	613	
10	M	509	
11	N	485	
12	K	100	
13	J	184	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 37546 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	439	3407	2162	596	629	20	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 CD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	588	4741	3039	824	854	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	198	1568	994	272	286	16	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	180	1436	915	242	264	15	0	0

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	314	Total	C	N	O	S	0	0
			2475	1666	390	401	18		

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	102	Total	C	N	O	S	0	0
			808	555	124	125	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	606	Total	C	N	O	S	0	0
			4637	3083	741	781	32		

- Molecule 10 is a protein called NADH dehydrogenase I subunit M.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	478	Total	C	N	O	S	0	0
			3620	2418	571	611	20		

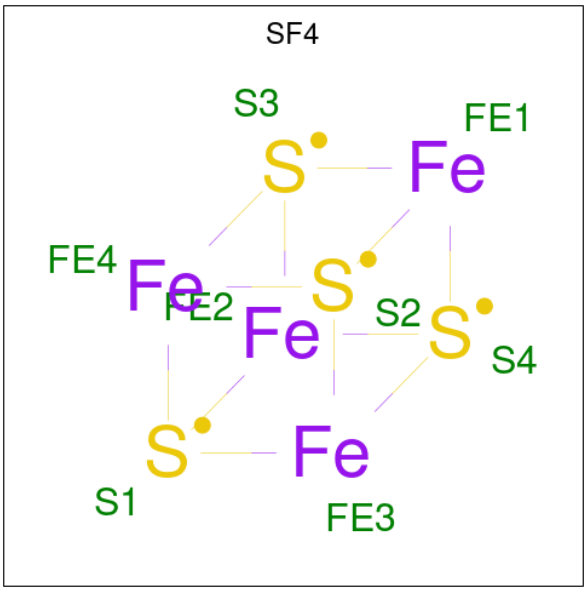
- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit K.

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.

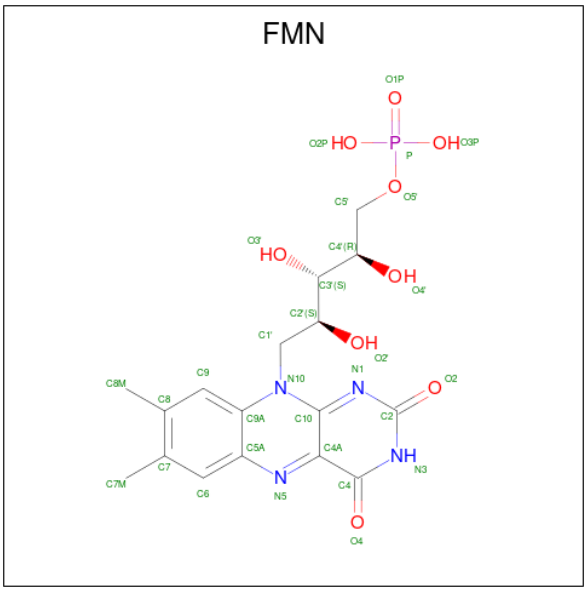
Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	162	Total	C	N	O	S	0	0
			1226	824	188	207	7		

- Molecule 14 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



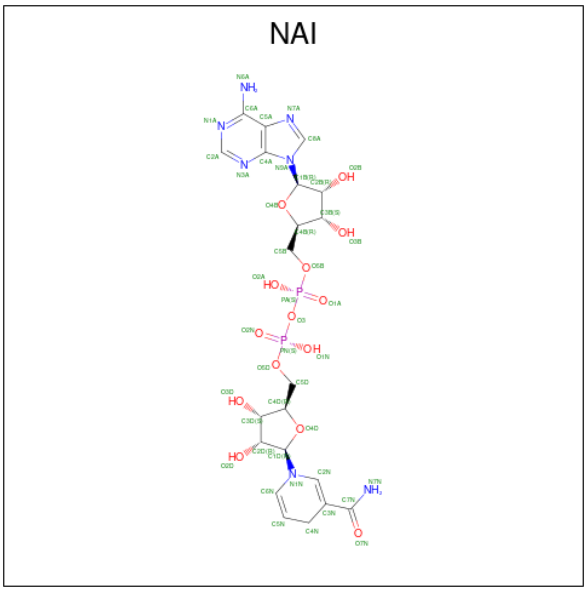
Mol	Chain	Residues	Atoms	AltConf
14	F	1	Total Fe S 8 4 4	0
14	G	1	Total Fe S 24 12 12	0
14	G	1	Total Fe S 24 12 12	0
14	G	1	Total Fe S 24 12 12	0
14	B	1	Total Fe S 8 4 4	0
14	I	1	Total Fe S 16 8 8	0
14	I	1	Total Fe S 16 8 8	0

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



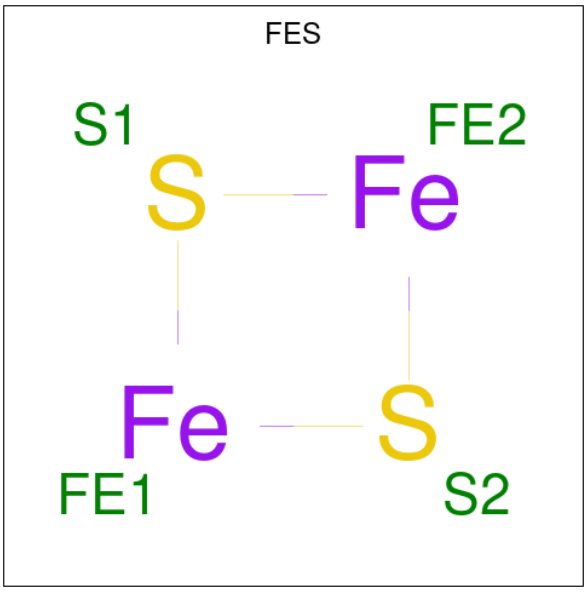
Mol	Chain	Residues	Atoms					AltConf
15	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 16 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: 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 (three-letter code: FES) (formula: Fe_2S_2).

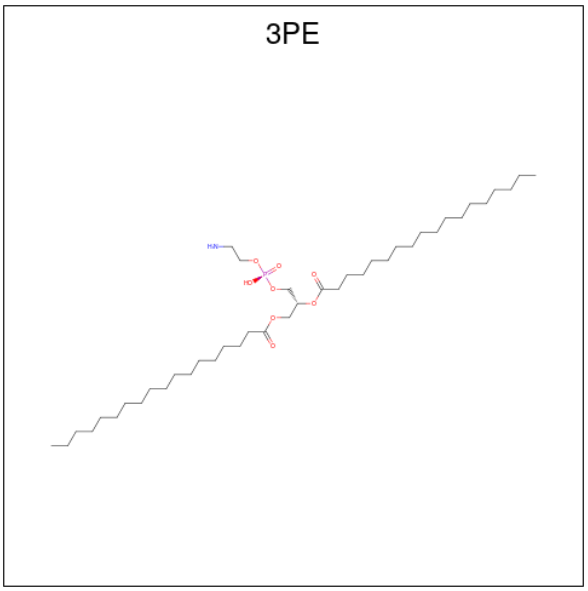


Mol	Chain	Residues	Atoms	AltConf
17	E	1	Total Fe S 4 2 2	0
17	G	1	Total Fe S 4 2 2	0

- Molecule 18 is CALCIUM ION (three-letter code: CA) (formula: Ca).

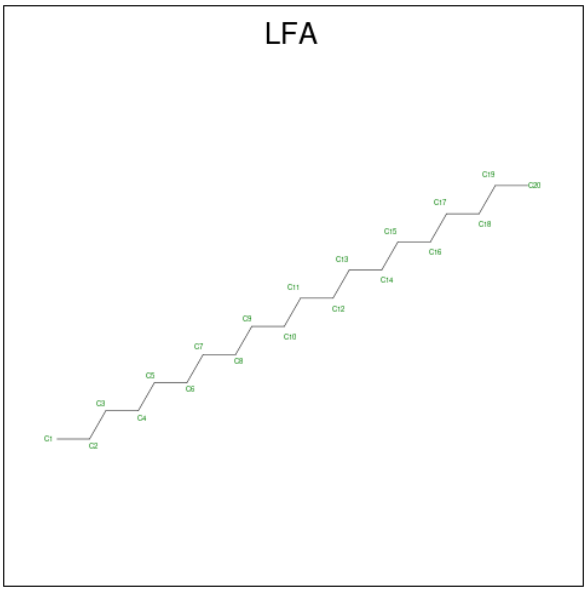
Mol	Chain	Residues	Atoms	AltConf
18	G	1	Total Ca 1 1	0

- Molecule 19 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
19	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
19	L	1	Total	C	N	O	P	0
			204	164	4	32	4	
19	L	1	Total	C	N	O	P	0
			204	164	4	32	4	
19	L	1	Total	C	N	O	P	0
			204	164	4	32	4	
19	L	1	Total	C	N	O	P	0
			204	164	4	32	4	
19	M	1	Total	C	N	O	P	0
			102	82	2	16	2	
19	M	1	Total	C	N	O	P	0
			102	82	2	16	2	
19	J	1	Total	C	N	O	P	0
			102	82	2	16	2	
19	J	1	Total	C	N	O	P	0
			102	82	2	16	2	

- Molecule 20 is EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$).

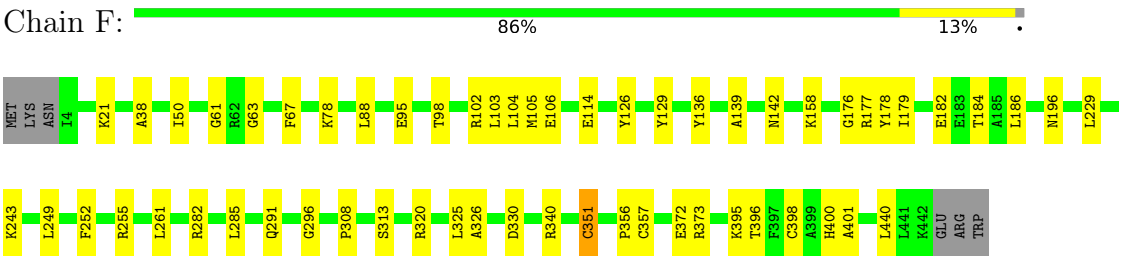


Mol	Chain	Residues	Atoms	AltConf
20	H	1	Total C 20 20	0
20	M	1	Total C 20 20	0
20	N	1	Total C 34 34	0
20	N	1	Total C 34 34	0

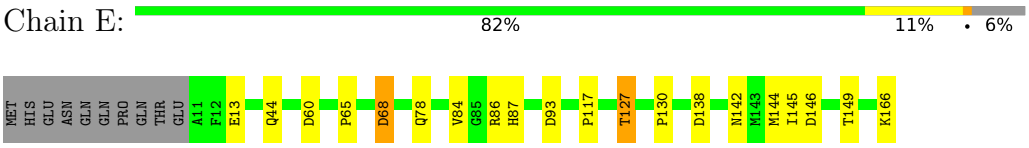
3 Residue-property plots (i)

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

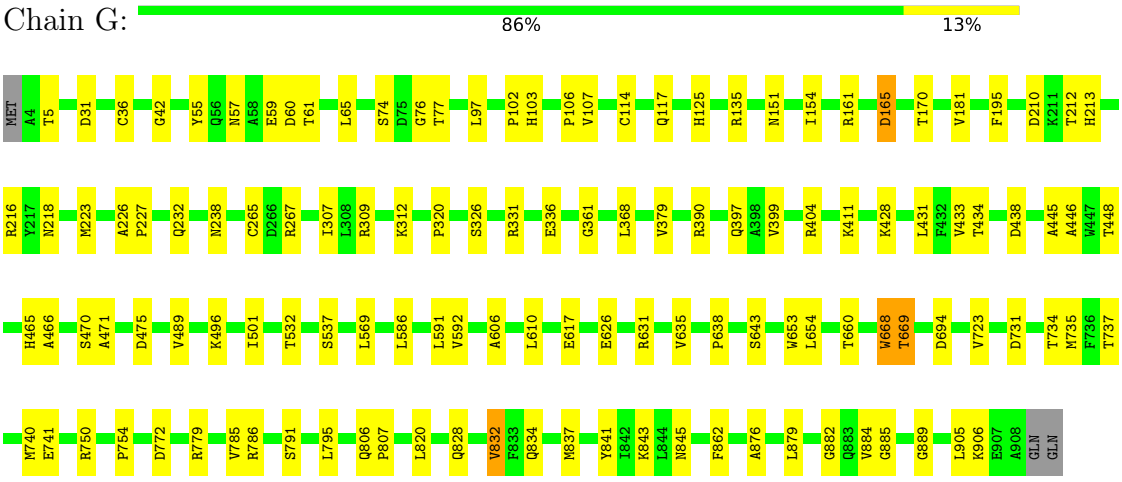
• Molecule 1: NADH-quinone oxidoreductase subunit F



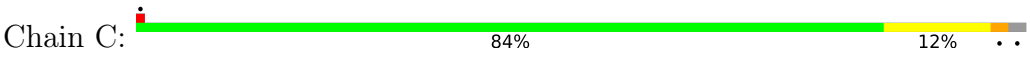
• Molecule 2: NADH dehydrogenase I subunit E

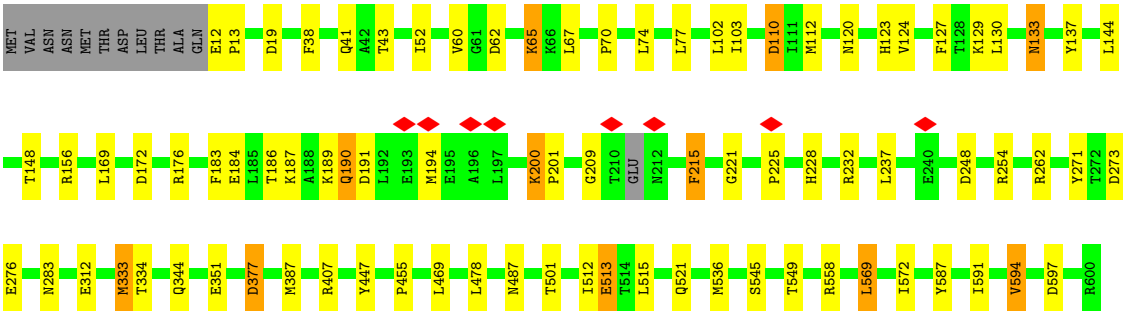


• Molecule 3: NADH-quinone oxidoreductase



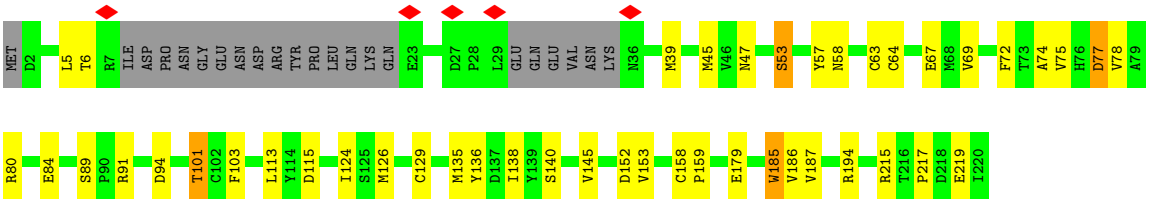
• Molecule 4: NADH-quinone oxidoreductase subunit CD





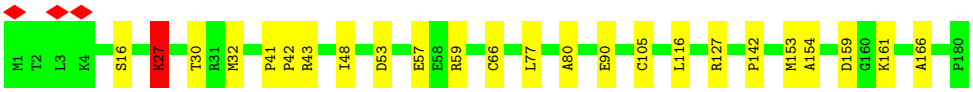
• Molecule 5: NADH-quinone oxidoreductase subunit B

Chain B:



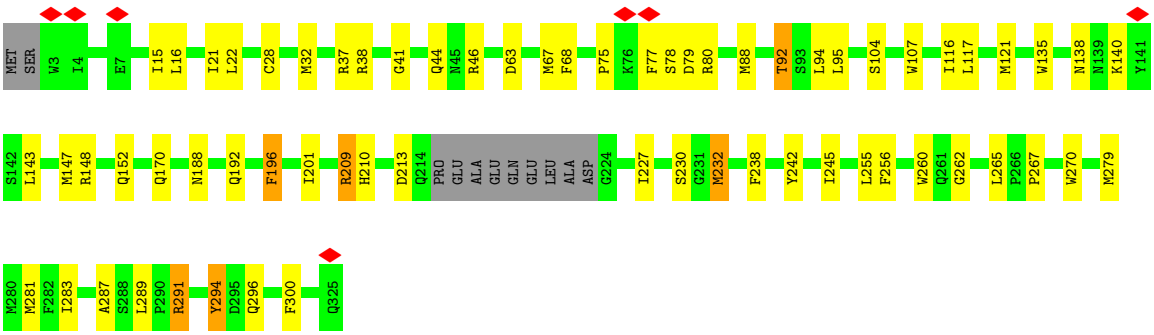
• Molecule 6: NADH-quinone oxidoreductase subunit I

Chain I:



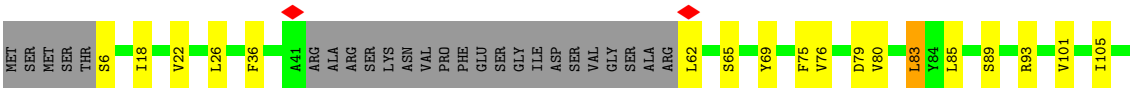
• Molecule 7: NADH-quinone oxidoreductase subunit H

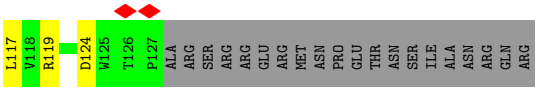
Chain H:



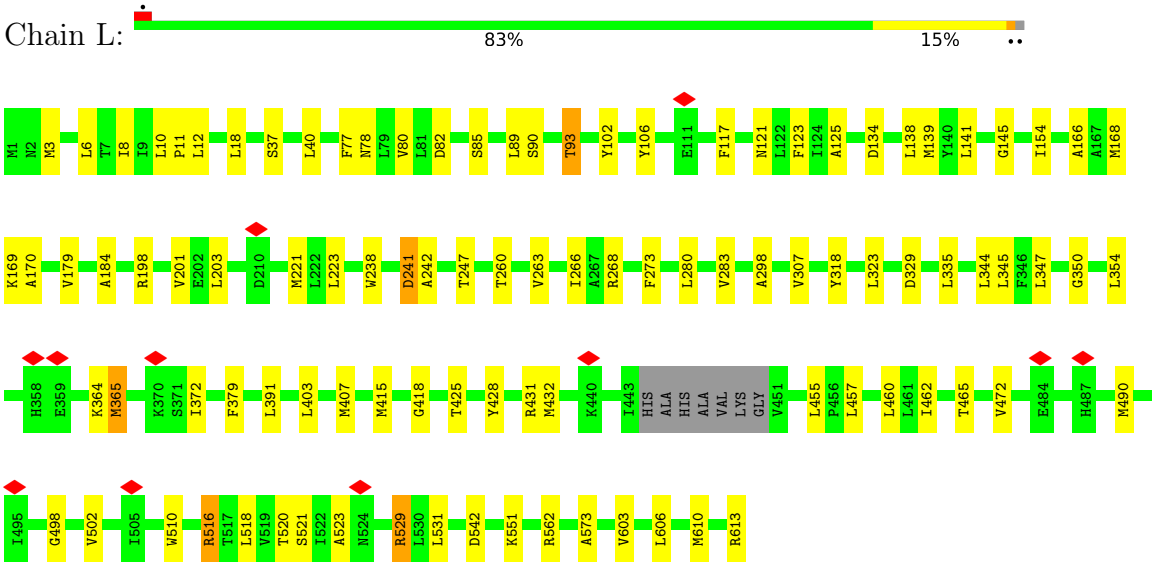
• Molecule 8: NADH-quinone oxidoreductase subunit A

Chain A:

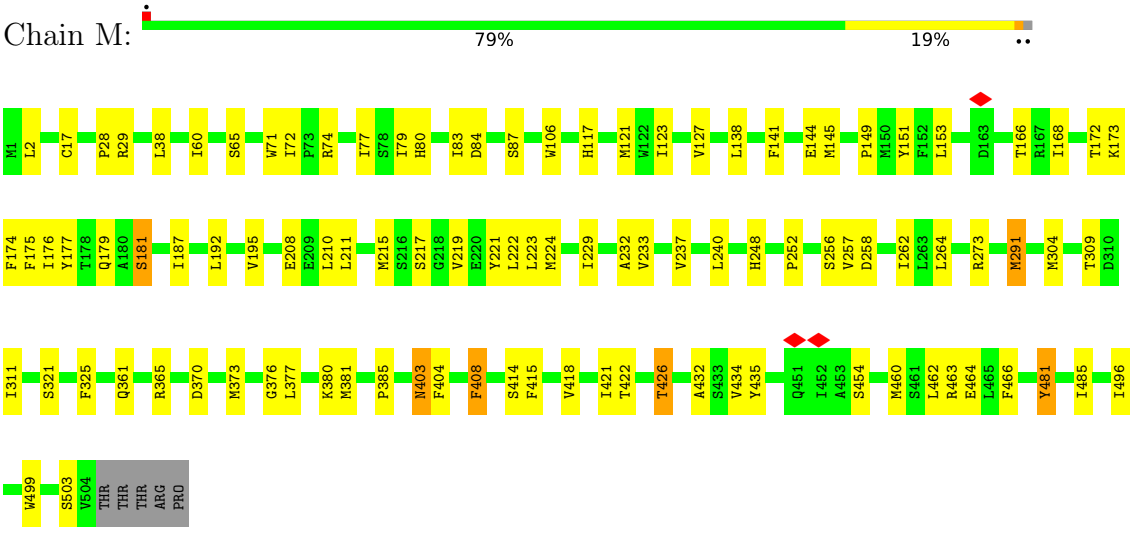




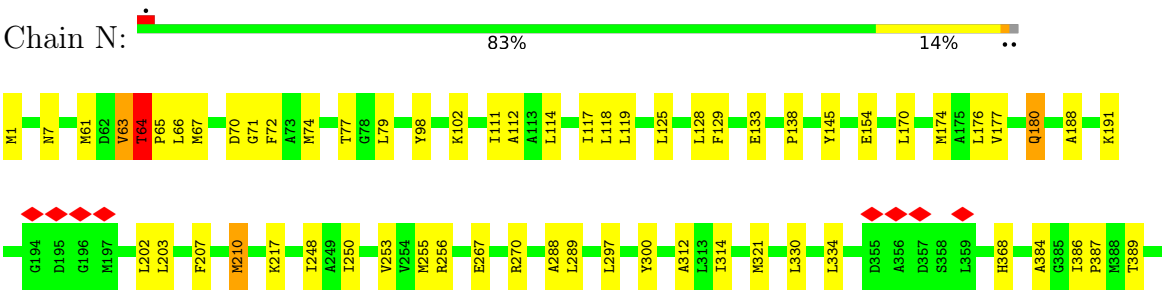
• Molecule 9: NADH-quinone oxidoreductase subunit L

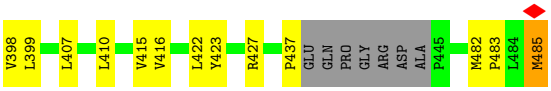


• Molecule 10: NADH dehydrogenase I subunit M



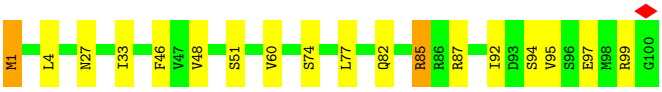
• Molecule 11: NADH-quinone oxidoreductase subunit N





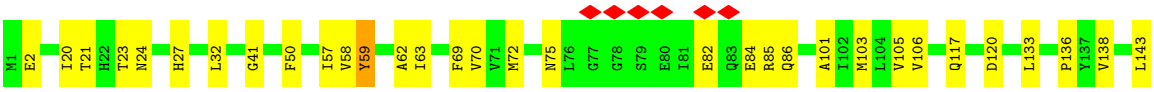
• Molecule 12: NADH-quinone oxidoreductase subunit K

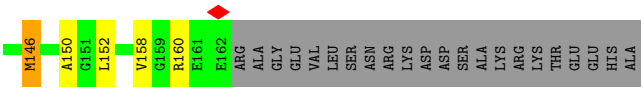
Chain K:



• Molecule 13: NADH-quinone oxidoreductase subunit J

Chain J:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	67274	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.403	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	153.7, 211.99998, 240.61998	wwPDB
Map dimensions	145, 200, 227	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.28	0/3486	0.52	0/4713
2	E	0.29	0/1248	0.50	0/1691
3	G	0.29	0/7173	0.54	0/9726
4	C	0.29	0/4871	0.56	1/6610 (0.0%)
5	B	0.29	0/1601	0.56	0/2168
6	I	0.29	0/1470	0.54	1/1985 (0.1%)
7	H	0.29	0/2549	0.55	3/3466 (0.1%)
8	A	0.26	0/833	0.48	1/1134 (0.1%)
9	L	0.28	0/4755	0.54	4/6479 (0.1%)
10	M	0.28	0/4074	0.53	1/5546 (0.0%)
11	N	0.31	0/3709	0.56	3/5061 (0.1%)
12	K	0.27	0/769	0.54	0/1040
13	J	0.29	0/1252	0.50	1/1708 (0.1%)
All	All	0.29	0/37790	0.54	15/51327 (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
2	E	0	1
3	G	0	2
11	N	0	2
All	All	0	5

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	N	437	PRO	CA-N-CD	-12.00	94.70	111.50
11	N	437	PRO	N-CD-CG	-7.43	92.05	103.20
7	H	213	ASP	CB-CG-OD1	6.73	124.35	118.30
9	L	455	LEU	CA-CB-CG	6.09	129.30	115.30
7	H	16	LEU	CA-CB-CG	6.00	129.10	115.30
7	H	232	MET	CB-CG-SD	5.79	129.76	112.40
8	A	83	LEU	CA-CB-CG	5.78	128.60	115.30
13	J	120	ASP	CB-CG-OD2	5.61	123.35	118.30
10	M	304	MET	CB-CG-SD	5.33	128.39	112.40
11	N	64	THR	N-CA-C	-5.30	96.69	111.00
4	C	200	LYS	CB-CG-CD	5.28	125.33	111.60
9	L	403	LEU	CA-CB-CG	5.28	127.44	115.30
9	L	403	LEU	CB-CG-CD2	5.07	119.62	111.00
9	L	391	LEU	CA-CB-CG	5.06	126.94	115.30
6	I	27	LYS	CB-CG-CD	5.06	124.75	111.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	145	ILE	Peptide
3	G	668	TRP	Peptide
3	G	669	THR	Peptide
11	N	63	VAL	Peptide
11	N	64	THR	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	3407	0	3374	29	0
2	E	1220	0	1187	12	0
3	G	7022	0	6824	60	0
4	C	4741	0	4652	50	0
5	B	1568	0	1553	27	0
6	I	1436	0	1415	14	0
7	H	2475	0	2532	37	0
8	A	808	0	821	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	L	4637	0	4783	51	0
10	M	3953	0	4053	54	0
11	N	3620	0	3790	48	0
12	K	760	0	817	12	0
13	J	1226	0	1297	24	0
14	B	8	0	0	0	0
14	F	8	0	0	0	0
14	G	24	0	0	1	0
14	I	16	0	0	0	0
15	F	31	0	19	0	0
16	F	44	0	27	2	0
17	E	4	0	0	1	0
17	G	4	0	0	0	0
18	G	1	0	0	0	0
19	H	51	0	82	4	0
19	J	102	0	164	5	0
19	L	204	0	328	10	0
19	M	102	0	164	6	0
20	H	20	0	42	1	0
20	M	20	0	42	2	0
20	N	34	0	69	0	0
All	All	37546	0	38035	387	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (387) 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)
11:N:63:VAL:O	11:N:67:MET:HB2	1.69	0.92
1:F:95:GLU:HB2	16:F:503:NAI:H42N	1.71	0.72
5:B:77:ASP:HB3	5:B:80:ARG:HE	1.54	0.71
10:M:123:ILE:HG13	10:M:149:PRO:HB2	1.76	0.66
11:N:154:GLU:HG3	12:K:95:VAL:HG22	1.76	0.66
7:H:242:TYR:HA	7:H:245:ILE:HD12	1.78	0.66
11:N:65:PRO:HG2	13:J:136:PRO:HB3	1.78	0.65
9:L:223:LEU:HD13	9:L:283:VAL:HG22	1.79	0.65
11:N:77:THR:HG23	11:N:117:ILE:HG12	1.80	0.64
7:H:140:LYS:HD3	8:A:62:LEU:HB2	1.79	0.64
4:C:215:PHE:HA	4:C:237:LEU:O	1.98	0.64
1:F:249:LEU:HB3	1:F:261:LEU:HD11	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:263:VAL:HG13	9:L:323:LEU:HD11	1.80	0.63
4:C:594:VAL:HG23	4:C:597:ASP:HB2	1.81	0.63
19:J:202:3PE:H2C1	19:J:202:3PE:H3E1	1.80	0.62
7:H:209:ARG:HD3	7:H:245:ILE:HD11	1.82	0.61
11:N:217:LYS:HB3	11:N:250:ILE:HD13	1.82	0.61
9:L:523:ALA:O	9:L:529:ARG:NH1	2.34	0.61
10:M:414:SER:O	10:M:418:VAL:N	2.32	0.60
4:C:274:ARG:NH2	5:B:158:CYS:SG	2.71	0.60
1:F:357:CYS:HB2	1:F:401:ALA:HB2	1.82	0.60
4:C:123:HIS:HA	4:C:148:THR:O	2.01	0.59
10:M:258:ASP:HA	10:M:262:ILE:HD12	1.84	0.59
9:L:85:SER:OG	9:L:268:ARG:NH2	2.35	0.59
5:B:101:THR:HA	5:B:129:CYS:HB3	1.85	0.58
10:M:177:TYR:O	10:M:181:SER:OG	2.21	0.58
9:L:154:ILE:HD13	9:L:242:ALA:HB1	1.86	0.58
11:N:71:GLY:HA2	11:N:74:MET:HG3	1.85	0.58
5:B:124:ILE:HG12	5:B:153:VAL:HB	1.86	0.58
11:N:98:TYR:O	11:N:102:LYS:NZ	2.36	0.58
4:C:133:ASN:OD1	4:C:133:ASN:N	2.31	0.58
5:B:72:PHE:HE1	5:B:84:GLU:HA	1.69	0.58
7:H:104:SER:HB3	7:H:107:TRP:HB2	1.86	0.58
3:G:668:TRP:O	3:G:669:THR:OG1	2.22	0.57
7:H:15:ILE:HG23	8:A:18:ILE:HG21	1.86	0.57
13:J:57:ILE:HG22	13:J:58:VAL:HG23	1.85	0.57
4:C:276:GLU:O	4:C:283:ASN:ND2	2.34	0.57
1:F:106:GLU:O	1:F:142:ASN:ND2	2.37	0.57
11:N:188:ALA:HA	11:N:191:LYS:HD3	1.87	0.56
7:H:77:PHE:O	7:H:138:ASN:ND2	2.39	0.56
3:G:828:GLN:NE2	3:G:889:GLY:O	2.39	0.56
4:C:455:PRO:HB2	4:C:469:LEU:HD22	1.87	0.56
3:G:331:ARG:NH2	3:G:336:GLU:OE1	2.38	0.56
9:L:241:ASP:N	9:L:241:ASP:OD1	2.38	0.56
9:L:318:TYR:OH	9:L:418:GLY:O	2.20	0.56
11:N:118:LEU:HD22	13:J:143:LEU:HD13	1.86	0.55
1:F:395:LYS:HE3	3:G:65:LEU:HD12	1.86	0.55
3:G:368:LEU:HD21	3:G:390:ARG:HB3	1.88	0.55
1:F:176:GLY:HA3	2:E:78:GLN:HG2	1.89	0.55
3:G:165:ASP:OD1	3:G:165:ASP:N	2.40	0.55
3:G:807:PRO:HB3	3:G:882:GLY:HA3	1.88	0.55
3:G:218:ASN:HD21	3:G:223:MET:HG2	1.72	0.55
9:L:169:LYS:HD3	9:L:238:TRP:HA	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:87:SER:OG	10:M:273:ARG:NH2	2.40	0.54
1:F:340:ARG:NE	1:F:372:GLU:OE1	2.41	0.54
9:L:168:MET:HB3	19:L:802:3PE:H321	1.88	0.54
11:N:1:MET:HB3	11:N:65:PRO:HD3	1.88	0.54
3:G:834:GLN:HA	3:G:837:MET:HE2	1.89	0.54
9:L:11:PRO:HB2	9:L:125:ALA:HB2	1.89	0.54
11:N:170:LEU:HD12	11:N:210:MET:HB3	1.90	0.54
4:C:77:LEU:HB3	4:C:137:TYR:HB3	1.89	0.54
2:E:86:ARG:NH2	2:E:166:LYS:O	2.41	0.54
4:C:186:THR:HB	4:C:187:LYS:HE2	1.90	0.54
7:H:210:HIS:NE2	7:H:289:LEU:O	2.37	0.53
9:L:166:ALA:HB1	9:L:242:ALA:HA	1.90	0.53
9:L:260:THR:HB	9:L:335:LEU:HD11	1.90	0.53
10:M:377:LEU:HA	10:M:380:LYS:HE2	1.90	0.53
11:N:289:LEU:O	11:N:427:ARG:NH1	2.42	0.53
4:C:232:ARG:HB2	4:C:248:ASP:HB3	1.89	0.53
10:M:481:TYR:HD2	20:M:1201:LFA:H122	1.73	0.53
1:F:296:GLY:O	1:F:320:ARG:NH2	2.41	0.53
3:G:57:ASN:ND2	3:G:59:GLU:O	2.41	0.53
3:G:862:PHE:HB3	3:G:905:LEU:HD23	1.90	0.53
5:B:69:VAL:HA	5:B:72:PHE:HB2	1.89	0.53
6:I:48:ILE:HG12	6:I:116:LEU:HG	1.91	0.53
8:A:117:LEU:HD11	13:J:152:LEU:HD11	1.92	0.52
3:G:226:ALA:HB3	3:G:635:VAL:HG22	1.91	0.52
3:G:694:ASP:N	3:G:694:ASP:OD1	2.41	0.52
2:E:84:VAL:HB	2:E:127:THR:HG21	1.90	0.52
4:C:110:ASP:OD1	4:C:110:ASP:N	2.42	0.52
5:B:186:VAL:HG23	5:B:187:VAL:HG23	1.91	0.52
8:A:69:TYR:OH	12:K:74:SER:O	2.27	0.52
13:J:20:ILE:HG13	13:J:21:THR:HG23	1.91	0.52
3:G:723:VAL:HG11	6:I:127:ARG:HB3	1.90	0.52
7:H:196:PHE:HZ	19:H:401:3PE:H2I1	1.75	0.52
11:N:180:GLN:HG3	11:N:203:LEU:HB2	1.92	0.52
2:E:138:ASP:OD1	2:E:138:ASP:N	2.42	0.52
7:H:148:ARG:O	7:H:294:TYR:OH	2.25	0.52
10:M:415:PHE:HB2	10:M:422:THR:HG21	1.92	0.52
10:M:370:ASP:HB3	10:M:373:MET:HG2	1.92	0.52
3:G:772:ASP:HB3	3:G:779:ARG:HA	1.92	0.52
8:A:75:PHE:O	8:A:79:ASP:HB2	2.09	0.52
8:A:76:VAL:HG22	13:J:62:ALA:HB1	1.92	0.52
1:F:136:TYR:HB3	1:F:139:ALA:HB3	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:804:3PE:H2F1	19:M:1202:3PE:H3D2	1.92	0.51
10:M:365:ARG:HH21	10:M:460:MET:HA	1.75	0.51
8:A:85:LEU:O	8:A:89:SER:OG	2.27	0.51
9:L:179:VAL:HG22	10:M:426:THR:HG22	1.92	0.51
19:J:201:3PE:H3B2	19:J:202:3PE:H3B1	1.90	0.51
6:I:154:ALA:O	6:I:161:LYS:NZ	2.35	0.51
9:L:307:VAL:HG11	9:L:432:MET:HG3	1.93	0.51
4:C:334:THR:OG1	7:H:287:ALA:O	2.28	0.51
7:H:117:LEU:O	7:H:121:MET:HG3	2.11	0.51
3:G:431:LEU:O	3:G:446:ALA:N	2.43	0.51
4:C:65:LYS:NZ	4:C:130:LEU:O	2.43	0.51
3:G:501:ILE:HG12	3:G:532:THR:HB	1.92	0.51
10:M:187:ILE:HD11	11:N:399:LEU:HD22	1.91	0.51
10:M:208:GLU:HA	10:M:211:LEU:HD12	1.91	0.50
19:L:802:3PE:H331	19:L:802:3PE:H231	1.94	0.50
3:G:74:SER:O	3:G:77:THR:OG1	2.27	0.50
4:C:333:MET:SD	7:H:44:GLN:NE2	2.85	0.50
10:M:219:VAL:HG13	19:M:1203:3PE:H252	1.94	0.50
3:G:617:GLU:HG2	3:G:638:PRO:HG3	1.94	0.50
10:M:17:CYS:HB3	10:M:28:PRO:HB3	1.93	0.50
10:M:361:GLN:NE2	10:M:464:GLU:OE2	2.44	0.50
12:K:82:GLN:NE2	13:J:158:VAL:O	2.45	0.50
1:F:98:THR:HA	1:F:325:LEU:HD12	1.94	0.50
10:M:127:VAL:HG11	10:M:264:LEU:HD13	1.93	0.50
11:N:154:GLU:OE2	12:K:97:GLU:N	2.39	0.50
3:G:397:GLN:O	3:G:404:ARG:NH2	2.38	0.50
9:L:329:ASP:OD1	9:L:329:ASP:N	2.41	0.50
10:M:195:VAL:HG11	10:M:215:MET:HG2	1.94	0.50
7:H:41:GLY:HA2	7:H:46:ARG:HG3	1.94	0.49
10:M:79:ILE:HA	10:M:138:LEU:HD22	1.94	0.49
11:N:64:THR:HB	11:N:67:MET:H	1.77	0.49
13:J:84:GLU:HB3	13:J:86:GLN:HG2	1.94	0.49
2:E:87:HIS:ND1	2:E:146:ASP:OD2	2.46	0.49
3:G:379:VAL:HB	3:G:433:VAL:HG12	1.94	0.49
9:L:10:LEU:HD13	9:L:40:LEU:HB3	1.94	0.49
1:F:291:GLN:O	1:F:326:ALA:HA	2.13	0.49
4:C:144:LEU:HB3	4:C:169:LEU:HB2	1.95	0.49
7:H:121:MET:HG2	13:J:57:ILE:HG13	1.94	0.49
9:L:542:ASP:OD1	9:L:542:ASP:N	2.45	0.49
11:N:386:ILE:O	11:N:389:THR:OG1	2.26	0.49
3:G:103:HIS:HA	4:C:512:ILE:HD13	1.92	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:138:ILE:HG23	5:B:140:SER:H	1.78	0.49
9:L:18:LEU:HD13	9:L:117:PHE:HB3	1.94	0.49
1:F:356:PRO:HB2	1:F:396:THR:HG22	1.93	0.49
4:C:190:GLN:O	4:C:194:MET:HG2	2.13	0.49
11:N:112:ALA:HB2	11:N:138:PRO:HB2	1.94	0.49
11:N:119:LEU:HD22	11:N:253:VAL:HG11	1.95	0.49
3:G:466:ALA:HB3	3:G:489:VAL:HG21	1.95	0.49
5:B:217:PRO:HB3	6:I:43:ARG:HB3	1.94	0.49
9:L:298:ALA:HB1	9:L:307:VAL:HG23	1.95	0.49
11:N:64:THR:HB	11:N:66:LEU:H	1.77	0.49
10:M:144:GLU:HB2	11:N:387:PRO:HG2	1.94	0.49
4:C:501:THR:HG23	4:C:521:GLN:HB3	1.94	0.48
7:H:22:LEU:HD11	7:H:95:LEU:HD21	1.94	0.48
3:G:212:THR:HG22	3:G:832:VAL:HG21	1.95	0.48
3:G:267:ARG:HB2	3:G:820:LEU:HG	1.96	0.48
9:L:364:LYS:HD3	9:L:365:MET:HG3	1.95	0.48
3:G:309:ARG:NH2	3:G:660:THR:O	2.46	0.48
11:N:176:LEU:HD22	11:N:202:LEU:HD11	1.94	0.48
4:C:201:PRO:HG3	4:C:209:GLY:HA3	1.96	0.48
7:H:21:ILE:HG12	20:H:402:LFA:H62	1.95	0.48
7:H:116:ILE:HD13	7:H:255:LEU:HD21	1.95	0.48
1:F:182:GLU:O	1:F:186:LEU:N	2.42	0.48
10:M:381:MET:HB2	10:M:385:PRO:HD3	1.96	0.48
2:E:68:ASP:N	2:E:68:ASP:OD1	2.47	0.47
3:G:399:VAL:HG13	3:G:428:LYS:HB2	1.95	0.47
9:L:606:LEU:HB3	13:J:106:VAL:HG11	1.96	0.47
12:K:85:ARG:NH1	13:J:160:ARG:O	2.47	0.47
3:G:106:PRO:HD3	4:C:515:LEU:HD21	1.95	0.47
7:H:88:MET:O	7:H:92:THR:OG1	2.30	0.47
4:C:344:GLN:HG2	5:B:75:VAL:HG21	1.96	0.47
10:M:29:ARG:NH1	10:M:106:TRP:O	2.44	0.47
19:M:1203:3PE:H3H2	11:N:415:VAL:HG11	1.96	0.47
3:G:97:LEU:HD22	3:G:154:ILE:HB	1.96	0.47
10:M:192:LEU:HG	10:M:210:LEU:HD22	1.96	0.47
4:C:221:GLY:HA3	4:C:232:ARG:HG2	1.96	0.47
4:C:312:GLU:OE2	4:C:447:TYR:OH	2.31	0.47
7:H:79:ASP:OD2	13:J:27:HIS:NE2	2.47	0.47
9:L:3:MET:HB3	9:L:6:LEU:HD12	1.97	0.47
11:N:485:MET:SD	11:N:485:MET:N	2.87	0.47
3:G:361:GLY:HA2	3:G:795:LEU:HG	1.97	0.47
5:B:53:SER:O	5:B:53:SER:OG	2.31	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:27:LYS:HE2	6:I:27:LYS:HA	1.97	0.47
11:N:248:ILE:HG12	11:N:330:LEU:HD22	1.96	0.47
5:B:67:GLU:HG3	5:B:159:PRO:HB2	1.96	0.47
9:L:37:SER:OG	9:L:121:ASN:OD1	2.33	0.47
9:L:85:SER:HG	9:L:268:ARG:HH22	1.60	0.47
10:M:432:ALA:HA	10:M:435:TYR:CE2	2.50	0.47
9:L:273:PHE:HB3	9:L:280:LEU:HD13	1.96	0.46
11:N:79:LEU:HD22	11:N:334:LEU:HD22	1.97	0.46
11:N:111:ILE:HG21	13:J:150:ALA:HB2	1.96	0.46
1:F:282:ARG:HB2	1:F:285:LEU:HD12	1.97	0.46
4:C:189:LYS:NZ	5:B:115:ASP:OD1	2.48	0.46
13:J:24:ASN:HB3	13:J:27:HIS:HB2	1.97	0.46
1:F:105:MET:HG3	1:F:139:ALA:HB1	1.97	0.46
7:H:28:CYS:O	7:H:32:MET:HB2	2.15	0.46
4:C:74:LEU:HA	4:C:102:LEU:HD23	1.98	0.46
12:K:33:ILE:HG23	13:J:32:LEU:HD22	1.98	0.46
1:F:38:ALA:HB2	1:F:114:GLU:HG3	1.98	0.46
1:F:330:ASP:OD1	1:F:330:ASP:N	2.42	0.46
3:G:55:TYR:HB3	3:G:60:ASP:HB3	1.97	0.46
3:G:307:ILE:HG21	3:G:591:LEU:HD13	1.97	0.46
13:J:59:TYR:HA	13:J:63:ILE:HD12	1.98	0.46
4:C:569:LEU:HD13	4:C:572:ILE:HD12	1.98	0.46
3:G:845:ASN:ND2	3:G:879:LEU:O	2.38	0.46
5:B:89:SER:HB2	7:H:227:ILE:HG22	1.98	0.46
5:B:91:ARG:HB3	7:H:230:SER:HB3	1.98	0.46
4:C:254:ARG:HG3	5:B:103:PHE:HE1	1.81	0.46
3:G:320:PRO:HB2	3:G:537:SER:HB2	1.97	0.46
9:L:551:LYS:HA	9:L:551:LYS:HD3	1.70	0.46
10:M:65:SER:HB3	10:M:83:ILE:HG22	1.96	0.46
4:C:407:ARG:NH1	7:H:291:ARG:O	2.49	0.45
1:F:308:PRO:O	1:F:313:SER:OG	2.32	0.45
7:H:94:LEU:HD12	7:H:94:LEU:HA	1.82	0.45
9:L:516:ARG:O	9:L:520:THR:OG1	2.26	0.45
10:M:71:TRP:HB2	10:M:79:ILE:HG13	1.98	0.45
8:A:22:VAL:O	8:A:26:LEU:HB2	2.15	0.45
10:M:192:LEU:HB2	10:M:223:LEU:HD13	1.98	0.45
13:J:101:ALA:O	13:J:105:VAL:HG23	2.17	0.45
2:E:117:PRO:HB3	2:E:130:PRO:HD3	1.99	0.45
3:G:569:LEU:HD13	3:G:654:LEU:HD11	1.96	0.45
19:J:201:3PE:H342	19:J:202:3PE:H351	1.98	0.45
5:B:74:ALA:O	6:I:30:THR:OG1	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:222:LEU:HD13	19:M:1203:3PE:H381	1.98	0.45
19:J:201:3PE:H321	19:J:202:3PE:H341	1.99	0.45
1:F:61:GLY:N	1:F:67:PHE:O	2.46	0.45
7:H:262:GLY:HA3	7:H:270:TRP:CD1	2.51	0.45
9:L:170:ALA:HA	9:L:238:TRP:HB2	1.97	0.45
10:M:153:LEU:HD23	10:M:153:LEU:HA	1.81	0.45
11:N:288:ALA:HB2	11:N:300:TYR:HB2	1.97	0.45
19:L:804:3PE:H2A2	11:N:416:VAL:HG13	1.98	0.45
9:L:531:LEU:HD23	9:L:531:LEU:HA	1.86	0.45
10:M:291:MET:HE3	10:M:421:ILE:HD13	1.98	0.45
11:N:270:ARG:HG2	11:N:314:ILE:HG23	1.99	0.45
3:G:227:PRO:HD3	3:G:754:PRO:HB3	1.99	0.45
5:B:6:THR:OG1	5:B:194:ARG:NH2	2.50	0.45
4:C:176:ARG:HA	4:C:176:ARG:HD3	1.83	0.44
1:F:178:TYR:HE2	1:F:400:HIS:HD2	1.64	0.44
3:G:626:GLU:OE1	3:G:786:ARG:NH1	2.49	0.44
4:C:200:LYS:HE3	4:C:200:LYS:HA	1.98	0.44
9:L:82:ASP:OD1	9:L:82:ASP:N	2.50	0.44
19:H:401:3PE:H341	19:H:401:3PE:H251	2.00	0.44
3:G:433:VAL:HG23	3:G:448:THR:HG23	1.99	0.44
3:G:806:GLN:HA	3:G:806:GLN:NE2	2.33	0.44
7:H:38:ARG:HD2	7:H:38:ARG:HA	1.83	0.44
10:M:179:GLN:HG2	11:N:422:LEU:HD11	2.00	0.44
11:N:312:ALA:HB2	11:N:398:VAL:HG22	2.00	0.44
13:J:82:GLU:HG2	13:J:85:ARG:HH22	1.83	0.44
3:G:210:ASP:HB3	3:G:213:HIS:HB3	2.00	0.44
6:I:59:ARG:NH2	6:I:142:PRO:O	2.51	0.44
10:M:485:ILE:HD11	20:M:1201:LFA:H61	2.00	0.44
9:L:102:TYR:O	9:L:106:TYR:HB2	2.18	0.44
10:M:141:PHE:O	10:M:145:MET:HB2	2.18	0.44
12:K:60:VAL:HG22	13:J:133:LEU:HD13	2.00	0.44
3:G:114:CYS:HB3	3:G:117:GLN:HB2	2.00	0.43
5:B:64:CYS:HB3	5:B:126:MET:HG2	2.00	0.43
7:H:279:MET:O	7:H:283:ILE:HG12	2.18	0.43
9:L:12:LEU:HD11	19:L:801:3PE:H3I1	2.00	0.43
10:M:176:ILE:HD11	11:N:423:TYR:HB2	1.99	0.43
11:N:125:LEU:HD13	11:N:174:MET:HG2	2.00	0.43
2:E:142:ASN:ND2	17:E:201:FES:S1	2.92	0.43
5:B:215:ARG:HB2	6:I:42:PRO:HB3	2.01	0.43
6:I:53:ASP:OD2	6:I:57:GLU:N	2.51	0.43
10:M:365:ARG:HG3	10:M:381:MET:HE1	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:102:PRO:HG3	3:G:151:ASN:HB3	2.00	0.43
4:C:351:GLU:HB3	6:I:41:PRO:HG3	2.00	0.43
7:H:143:LEU:O	7:H:147:MET:HG2	2.19	0.43
11:N:70:ASP:N	11:N:70:ASP:OD1	2.48	0.43
2:E:44:GLN:NE2	2:E:78:GLN:O	2.44	0.43
4:C:225:PRO:HA	5:B:58:ASN:HD21	1.82	0.43
6:I:161:LYS:HE3	6:I:166:ALA:HB2	1.99	0.43
10:M:84:ASP:N	10:M:84:ASP:OD1	2.51	0.43
11:N:74:MET:HE2	11:N:74:MET:HB3	1.89	0.43
1:F:102:ARG:O	1:F:106:GLU:HB2	2.19	0.43
8:A:119:ARG:HA	8:A:119:ARG:HD2	1.82	0.43
10:M:117:HIS:O	10:M:121:MET:HG2	2.18	0.43
10:M:217:SER:O	19:M:1202:3PE:N	2.45	0.43
1:F:182:GLU:OE1	1:F:184:THR:OG1	2.30	0.43
3:G:390:ARG:HA	3:G:390:ARG:HD2	1.88	0.43
3:G:592:VAL:HB	3:G:606:ALA:HA	2.00	0.43
4:C:67:LEU:HB2	4:C:70:PRO:HA	2.00	0.43
10:M:72:ILE:HB	10:M:77:ILE:HB	2.00	0.43
4:C:587:TYR:O	4:C:591:ILE:HG13	2.19	0.43
5:B:57:TYR:HE1	5:B:113:LEU:HD13	1.82	0.43
9:L:247:THR:HG21	9:L:350:GLY:HA3	2.00	0.43
10:M:60:ILE:HD11	10:M:496:ILE:HA	2.01	0.43
5:B:47:ASN:ND2	5:B:179:GLU:O	2.48	0.43
19:L:802:3PE:H262	10:M:434:VAL:HG21	2.00	0.43
10:M:248:HIS:ND1	10:M:258:ASP:OD1	2.51	0.43
11:N:98:TYR:OH	11:N:145:TYR:O	2.36	0.43
11:N:114:LEU:HD23	13:J:146:MET:HG2	2.00	0.43
12:K:77:LEU:HD22	13:J:70:VAL:HG11	2.00	0.43
4:C:120:ASN:OD1	4:C:120:ASN:N	2.42	0.42
4:C:172:ASP:OD1	4:C:172:ASP:N	2.52	0.42
4:C:333:MET:H	4:C:333:MET:HG3	1.71	0.42
4:C:377:ASP:OD1	4:C:377:ASP:N	2.52	0.42
9:L:138:LEU:HD12	9:L:141:LEU:HD23	2.01	0.42
11:N:330:LEU:HD23	11:N:330:LEU:HA	1.87	0.42
1:F:63:GLY:O	16:F:503:NAI:H2N	2.18	0.42
4:C:169:LEU:HD23	4:C:169:LEU:HA	1.89	0.42
9:L:184:ALA:HB2	9:L:221:MET:HB2	2.00	0.42
11:N:7:ASN:HB3	11:N:63:VAL:HG13	2.00	0.42
3:G:216:ARG:NH1	6:I:90:GLU:OE1	2.42	0.42
10:M:233:VAL:HG23	10:M:240:LEU:HD23	2.00	0.42
1:F:177:ARG:HD3	1:F:177:ARG:HA	1.77	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:80:VAL:O	8:A:83:LEU:HG	2.18	0.42
3:G:36:CYS:O	3:G:161:ARG:NH1	2.42	0.42
3:G:125:HIS:NE2	4:C:513:GLU:OE2	2.51	0.42
4:C:52:ILE:HD12	4:C:60:VAL:HG21	2.01	0.42
7:H:265:LEU:HB2	7:H:270:TRP:CD1	2.55	0.42
6:I:66:CYS:HB2	6:I:105:CYS:HB2	2.02	0.42
9:L:603:VAL:HG22	13:J:103:MET:HB2	2.00	0.42
11:N:177:VAL:HG22	11:N:203:LEU:HD12	2.00	0.42
7:H:170:GLN:OE1	7:H:192:GLN:NE2	2.43	0.42
9:L:266:ILE:HB	9:L:323:LEU:HD13	2.02	0.42
5:B:185:TRP:CD1	5:B:186:VAL:HG13	2.55	0.42
9:L:344:LEU:HB2	9:L:460:LEU:HB3	2.01	0.42
4:C:38:PHE:HB3	4:C:52:ILE:HD13	2.02	0.42
5:B:5:LEU:HD23	5:B:5:LEU:HA	1.79	0.42
9:L:457:LEU:HD13	9:L:457:LEU:HA	1.89	0.42
12:K:92:ILE:HD12	12:K:92:ILE:HA	1.93	0.42
3:G:5:THR:O	3:G:76:GLY:N	2.53	0.41
3:G:42:GLY:O	3:G:161:ARG:NH2	2.52	0.41
3:G:843:LYS:HB2	3:G:885:GLY:HA3	2.02	0.41
4:C:12:GLU:HA	4:C:13:PRO:HD3	1.93	0.41
8:A:101:VAL:O	8:A:105:ILE:HG12	2.20	0.41
19:L:804:3PE:H322	10:M:173:LYS:HA	2.01	0.41
10:M:168:ILE:O	10:M:172:THR:OG1	2.32	0.41
11:N:255:MET:HA	11:N:255:MET:HE2	2.01	0.41
13:J:41:GLY:HA2	19:J:201:3PE:H251	2.01	0.41
19:H:401:3PE:H292	19:H:401:3PE:H361	2.02	0.41
12:K:4:LEU:HD12	12:K:48:VAL:HG12	2.02	0.41
3:G:232:GLN:HB2	14:G:1003:SF4:S3	2.61	0.41
7:H:260:TRP:HB2	7:H:267:PRO:HB3	2.01	0.41
9:L:145:GLY:HA3	19:L:801:3PE:H3E1	2.01	0.41
3:G:610:LEU:HD13	3:G:653:TRP:CD2	2.56	0.41
4:C:387:MET:HG2	4:C:478:LEU:HD21	2.03	0.41
6:I:80:ALA:HB2	6:I:90:GLU:HB2	2.02	0.41
7:H:209:ARG:HE	7:H:209:ARG:HB3	1.37	0.41
9:L:498:GLY:O	9:L:502:VAL:HG22	2.20	0.41
11:N:129:PHE:O	11:N:133:GLU:HG2	2.20	0.41
11:N:384:ALA:HB1	11:N:422:LEU:HD23	2.02	0.41
4:C:41:GLN:HG2	4:C:43:THR:HG23	2.02	0.41
9:L:89:LEU:O	9:L:93:THR:OG1	2.31	0.41
10:M:229:ILE:HD11	19:M:1202:3PE:H2C2	2.01	0.41
10:M:403:ASN:OD1	10:M:403:ASN:N	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:1:MET:SD	12:K:1:MET:N	2.87	0.41
1:F:88:LEU:HD22	1:F:129:TYR:HB2	2.03	0.41
3:G:731:ASP:OD2	3:G:734:THR:OG1	2.31	0.41
3:G:828:GLN:H	3:G:828:GLN:HG3	1.64	0.41
3:G:843:LYS:HD2	3:G:876:ALA:HB2	2.02	0.41
9:L:345:LEU:HD23	9:L:345:LEU:HA	1.94	0.41
10:M:376:GLY:O	10:M:380:LYS:NZ	2.46	0.41
10:M:404:PHE:O	10:M:408:PHE:HB2	2.21	0.41
11:N:248:ILE:HD11	11:N:334:LEU:HB2	2.03	0.41
1:F:50:ILE:HG23	1:F:229:LEU:HD21	2.03	0.41
2:E:87:HIS:NE2	2:E:166:LYS:OXT	2.43	0.41
3:G:431:LEU:HB3	3:G:445:ALA:HA	2.01	0.41
4:C:549:THR:HB	4:C:558:ARG:HB3	2.02	0.41
7:H:188:ASN:HB2	7:H:256:PHE:HA	2.03	0.41
1:F:78:LYS:HB3	1:F:78:LYS:HE3	1.77	0.41
2:E:93:ASP:OD2	2:E:93:ASP:N	2.53	0.41
3:G:741:GLU:OE2	4:C:262:ARG:NE	2.49	0.41
9:L:80:VAL:HB	9:L:134:ASP:HB3	2.01	0.41
9:L:102:TYR:CD1	9:L:347:LEU:HD22	2.56	0.41
9:L:425:THR:HA	9:L:428:TYR:CE2	2.55	0.41
10:M:151:TYR:HB2	10:M:175:PHE:HD2	1.86	0.41
4:C:103:ILE:HG12	4:C:110:ASP:HB3	2.03	0.41
10:M:252:PRO:HG2	10:M:257:VAL:HG21	2.02	0.41
3:G:428:LYS:HB3	3:G:428:LYS:HE3	1.86	0.40
3:G:465:HIS:HA	3:G:471:ALA:HB3	2.03	0.40
4:C:254:ARG:HD3	5:B:136:TYR:CZ	2.56	0.40
7:H:75:PRO:HB2	7:H:78:SER:HB3	2.03	0.40
7:H:201:ILE:HG12	19:H:401:3PE:H382	2.03	0.40
9:L:117:PHE:O	9:L:121:ASN:ND2	2.51	0.40
10:M:232:ALA:HB1	10:M:237:VAL:HB	2.02	0.40
4:C:271:TYR:OH	5:B:135:MET:O	2.32	0.40
9:L:462:ILE:O	9:L:465:THR:OG1	2.36	0.40
12:K:77:LEU:HD23	12:K:77:LEU:HA	1.96	0.40
1:F:177:ARG:HG3	1:F:179:ILE:HG22	2.03	0.40
2:E:65:PRO:HB3	3:G:170:THR:HB	2.04	0.40
9:L:198:ARG:HA	9:L:201:VAL:HG22	2.03	0.40
19:L:801:3PE:H3I2	19:L:801:3PE:H3F2	1.95	0.40
10:M:422:THR:O	10:M:426:THR:OG1	2.38	0.40
11:N:407:LEU:HB3	11:N:410:LEU:HD12	2.04	0.40
1:F:196:ASN:ND2	1:F:351:CYS:SG	2.91	0.40
7:H:135:TRP:CD1	13:J:72:MET:HG2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:201:ILE:HD13	7:H:300:PHE:HE2	1.87	0.40
9:L:518:LEU:HA	9:L:521:SER:HB3	2.02	0.40
11:N:72:PHE:HB2	11:N:483:PRO:HB3	2.02	0.40
11:N:217:LYS:HD2	11:N:217:LYS:HA	1.83	0.40
9:L:573:ALA:HB2	19:L:804:3PE:H341	2.02	0.40
10:M:499:TRP:O	10:M:503:SER:OG	2.32	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	437/445 (98%)	429 (98%)	8 (2%)	0	100	100
2	E	154/166 (93%)	150 (97%)	4 (3%)	0	100	100
3	G	903/908 (99%)	874 (97%)	29 (3%)	0	100	100
4	C	584/600 (97%)	571 (98%)	13 (2%)	0	100	100
5	B	192/220 (87%)	185 (96%)	7 (4%)	0	100	100
6	I	178/180 (99%)	175 (98%)	3 (2%)	0	100	100
7	H	310/325 (95%)	301 (97%)	9 (3%)	0	100	100
8	A	98/147 (67%)	96 (98%)	2 (2%)	0	100	100
9	L	602/613 (98%)	588 (98%)	14 (2%)	0	100	100
10	M	502/509 (99%)	491 (98%)	11 (2%)	0	100	100
11	N	474/485 (98%)	463 (98%)	10 (2%)	1 (0%)	47	76
12	K	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
13	J	160/184 (87%)	160 (100%)	0	0	100	100
All	All	4692/4882 (96%)	4579 (98%)	112 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	N	64	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	353/359 (98%)	341 (97%)	12 (3%)	37	69
2	E	129/139 (93%)	123 (95%)	6 (5%)	26	57
3	G	732/735 (100%)	702 (96%)	30 (4%)	30	62
4	C	505/519 (97%)	480 (95%)	25 (5%)	24	54
5	B	171/192 (89%)	159 (93%)	12 (7%)	15	39
6	I	154/154 (100%)	148 (96%)	6 (4%)	32	64
7	H	260/269 (97%)	245 (94%)	15 (6%)	20	48
8	A	80/119 (67%)	75 (94%)	5 (6%)	18	44
9	L	482/486 (99%)	458 (95%)	24 (5%)	24	54
10	M	413/418 (99%)	390 (94%)	23 (6%)	21	49
11	N	380/385 (99%)	368 (97%)	12 (3%)	39	71
12	K	79/79 (100%)	71 (90%)	8 (10%)	7	21
13	J	128/146 (88%)	119 (93%)	9 (7%)	15	39
All	All	3866/4000 (97%)	3679 (95%)	187 (5%)	29	56

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	21	LYS
1	F	103	LEU
1	F	104	LEU
1	F	126	TYR
1	F	158	LYS
1	F	243	LYS
1	F	252	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	255	ARG
1	F	351	CYS
1	F	373	ARG
1	F	398	CYS
1	F	440	LEU
2	E	13	GLU
2	E	60	ASP
2	E	68	ASP
2	E	127	THR
2	E	144	MET
2	E	149	THR
3	G	31	ASP
3	G	61	THR
3	G	107	VAL
3	G	135	ARG
3	G	165	ASP
3	G	181	VAL
3	G	195	PHE
3	G	238	ASN
3	G	265	CYS
3	G	312	LYS
3	G	326	SER
3	G	411	LYS
3	G	434	THR
3	G	438	ASP
3	G	470	SER
3	G	475	ASP
3	G	496	LYS
3	G	586	LEU
3	G	631	ARG
3	G	643	SER
3	G	735	MET
3	G	737	THR
3	G	740	MET
3	G	750	ARG
3	G	785	VAL
3	G	791	SER
3	G	832	VAL
3	G	841	TYR
3	G	884	VAL
3	G	906	LYS
4	C	19	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	C	62	ASP
4	C	65	LYS
4	C	110	ASP
4	C	112	MET
4	C	124	VAL
4	C	127	PHE
4	C	129	LYS
4	C	133	ASN
4	C	156	ARG
4	C	183	PHE
4	C	184	GLU
4	C	190	GLN
4	C	191	ASP
4	C	215	PHE
4	C	228	HIS
4	C	273	ASP
4	C	333	MET
4	C	377	ASP
4	C	487	ASN
4	C	513	GLU
4	C	536	MET
4	C	545	SER
4	C	569	LEU
4	C	594	VAL
5	B	39	MET
5	B	45	MET
5	B	53	SER
5	B	63	CYS
5	B	77	ASP
5	B	78	VAL
5	B	94	ASP
5	B	101	THR
5	B	145	VAL
5	B	152	ASP
5	B	185	TRP
5	B	219	GLU
6	I	16	SER
6	I	27	LYS
6	I	32	MET
6	I	77	LEU
6	I	153	MET
6	I	159	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	H	37	ARG
7	H	63	ASP
7	H	67	MET
7	H	68	PHE
7	H	80	ARG
7	H	92	THR
7	H	152	GLN
7	H	196	PHE
7	H	209	ARG
7	H	232	MET
7	H	238	PHE
7	H	281	MET
7	H	291	ARG
7	H	294	TYR
7	H	296	GLN
8	A	6	SER
8	A	36	PHE
8	A	65	SER
8	A	93	ARG
8	A	124	ASP
9	L	8	ILE
9	L	77	PHE
9	L	78	ASN
9	L	90	SER
9	L	93	THR
9	L	123	PHE
9	L	139	MET
9	L	203	LEU
9	L	241	ASP
9	L	354	LEU
9	L	365	MET
9	L	372	ILE
9	L	379	PHE
9	L	407	MET
9	L	415	MET
9	L	431	ARG
9	L	472	VAL
9	L	490	MET
9	L	510	TRP
9	L	516	ARG
9	L	529	ARG
9	L	562	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	L	610	MET
9	L	613	ARG
10	M	2	LEU
10	M	38	LEU
10	M	74	ARG
10	M	80	HIS
10	M	166	THR
10	M	174	PHE
10	M	181	SER
10	M	221	TYR
10	M	224	MET
10	M	256	SER
10	M	291	MET
10	M	309	THR
10	M	311	ILE
10	M	321	SER
10	M	325	PHE
10	M	403	ASN
10	M	408	PHE
10	M	426	THR
10	M	454	SER
10	M	462	LEU
10	M	463	ARG
10	M	466	PHE
10	M	481	TYR
11	N	61	MET
11	N	128	LEU
11	N	180	GLN
11	N	207	PHE
11	N	210	MET
11	N	256	ARG
11	N	267	GLU
11	N	297	LEU
11	N	321	MET
11	N	368	HIS
11	N	482	MET
11	N	485	MET
12	K	1	MET
12	K	27	ASN
12	K	46	PHE
12	K	51	SER
12	K	85	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	K	87	ARG
12	K	94	SER
12	K	99	ARG
13	J	2	GLU
13	J	23	THR
13	J	50	PHE
13	J	59	TYR
13	J	69	PHE
13	J	75	ASN
13	J	117	GLN
13	J	138	VAL
13	J	146	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	218	ASN
3	G	386	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 25 ligands modelled in this entry, 1 is monoatomic - leaving 24 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	I	201	6	0,12,12	-	-	-		
14	SF4	G	1003	3	0,12,12	-	-	-		
17	FES	G	1004	3	0,4,4	-	-	-		
19	3PE	L	801	-	50,50,50	0.30	0	53,55,55	0.28	0
17	FES	E	201	2	0,4,4	-	-	-		
19	3PE	L	802	-	50,50,50	0.30	0	53,55,55	0.26	0
16	NAI	F	503	-	42,48,48	0.51	0	47,73,73	0.59	1 (2%)
19	3PE	J	201	-	50,50,50	0.30	0	53,55,55	0.27	0
19	3PE	M	1202	-	50,50,50	0.30	0	53,55,55	0.28	0
19	3PE	H	401	-	50,50,50	0.30	0	53,55,55	0.30	0
15	FMN	F	502	-	33,33,33	1.06	2 (6%)	48,50,50	1.26	7 (14%)
14	SF4	F	501	1	0,12,12	-	-	-		
19	3PE	M	1203	-	50,50,50	0.30	0	53,55,55	0.27	0
14	SF4	G	1002	3	0,12,12	-	-	-		
20	LFA	N	501	-	19,19,19	0.14	0	18,18,18	0.12	0
19	3PE	J	202	-	50,50,50	0.31	0	53,55,55	0.29	0
14	SF4	G	1001	3	0,12,12	-	-	-		
14	SF4	B	301	5	0,12,12	-	-	-		
19	3PE	L	804	-	50,50,50	0.31	0	53,55,55	0.30	0
20	LFA	N	502	-	13,13,19	0.16	0	12,12,18	0.11	0
20	LFA	M	1201	-	19,19,19	0.14	0	18,18,18	0.11	0
19	3PE	L	803	-	50,50,50	0.31	0	53,55,55	0.29	0
14	SF4	I	202	6	0,12,12	-	-	-		
20	LFA	H	402	-	19,19,19	0.17	0	18,18,18	0.13	0

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	I	201	6	-	-	0/6/5/5
14	SF4	G	1003	3	-	-	0/6/5/5
17	FES	G	1004	3	-	-	0/1/1/1
19	3PE	L	801	-	-	14/54/54/54	-
17	FES	E	201	2	-	-	0/1/1/1
19	3PE	L	802	-	-	8/54/54/54	-
16	NAI	F	503	-	-	5/25/72/72	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	3PE	J	201	-	-	11/54/54/54	-
19	3PE	M	1202	-	-	11/54/54/54	-
19	3PE	H	401	-	-	15/54/54/54	-
15	FMN	F	502	-	-	6/18/18/18	0/3/3/3
14	SF4	F	501	1	-	-	0/6/5/5
19	3PE	M	1203	-	-	10/54/54/54	-
14	SF4	G	1002	3	-	-	0/6/5/5
20	LFA	N	501	-	-	0/17/17/17	-
19	3PE	J	202	-	-	6/54/54/54	-
14	SF4	G	1001	3	-	-	0/6/5/5
19	3PE	L	804	-	-	14/54/54/54	-
20	LFA	N	502	-	-	0/11/11/17	-
14	SF4	B	301	5	-	-	0/6/5/5
20	LFA	M	1201	-	-	1/17/17/17	-
19	3PE	L	803	-	-	12/54/54/54	-
14	SF4	I	202	6	-	-	0/6/5/5
20	LFA	H	402	-	-	3/17/17/17	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	502	FMN	C4A-N5	3.59	1.37	1.30
15	F	502	FMN	C10-N1	2.24	1.37	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	502	FMN	C4-N3-C2	-3.29	119.56	125.64
15	F	502	FMN	C4A-C10-N10	2.85	120.65	116.48
15	F	502	FMN	C4A-C4-N3	2.71	120.08	113.19
15	F	502	FMN	O4-C4-C4A	-2.57	119.78	126.60
15	F	502	FMN	C4A-C10-N1	-2.42	119.12	124.73
16	F	503	NAI	C5A-C6A-N6A	2.33	123.89	120.35
15	F	502	FMN	C10-C4A-N5	-2.32	119.93	124.86
15	F	502	FMN	C4-C4A-C10	2.01	120.17	116.79

There are no chirality outliers.

All (116) 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	H	401	3PE	C1-O11-P-O12
19	H	401	3PE	C1-O11-P-O14
19	H	401	3PE	C11-O13-P-O11
19	H	401	3PE	C11-O13-P-O12
19	H	401	3PE	C11-O13-P-O14
19	L	801	3PE	C1-O11-P-O12
19	L	801	3PE	C11-O13-P-O12
19	L	801	3PE	C11-O13-P-O14
19	L	802	3PE	C1-O11-P-O12
19	L	802	3PE	C1-O11-P-O14
19	L	803	3PE	C1-O11-P-O14
19	L	803	3PE	C11-O13-P-O11
19	L	803	3PE	C11-O13-P-O14
19	L	803	3PE	C2-C1-O11-P
19	L	804	3PE	C1-O11-P-O12
19	L	804	3PE	C11-O13-P-O11
19	L	804	3PE	C11-O13-P-O14
19	L	804	3PE	O13-C11-C12-N
19	M	1202	3PE	C11-O13-P-O14
19	M	1202	3PE	O13-C11-C12-N
19	M	1203	3PE	C1-O11-P-O12
19	M	1203	3PE	C11-O13-P-O11
19	M	1203	3PE	C11-O13-P-O12
19	M	1203	3PE	C11-O13-P-O14
19	J	201	3PE	C1-O11-P-O12
19	J	201	3PE	C1-O11-P-O14
19	J	201	3PE	O13-C11-C12-N
19	J	202	3PE	C11-O13-P-O14
19	J	202	3PE	O13-C11-C12-N
19	M	1203	3PE	C2-C1-O11-P
19	H	401	3PE	C1-O11-P-O13
19	L	801	3PE	C1-O11-P-O13
19	L	801	3PE	C11-O13-P-O11
19	L	802	3PE	C1-O11-P-O13
19	L	804	3PE	C1-O11-P-O13
19	M	1202	3PE	C1-O11-P-O13
19	J	201	3PE	C1-O11-P-O13
19	J	201	3PE	C11-O13-P-O11
19	L	803	3PE	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	J	201	3PE	C2-C1-O11-P
19	H	401	3PE	O13-C11-C12-N
19	L	801	3PE	C37-C38-C39-C3A
19	L	801	3PE	C2C-C2D-C2E-C2F
19	L	804	3PE	C3B-C3C-C3D-C3E
19	M	1203	3PE	C26-C27-C28-C29
19	L	804	3PE	C2A-C2B-C2C-C2D
20	H	402	LFA	C13-C14-C15-C16
19	M	1202	3PE	C24-C25-C26-C27
15	F	502	FMN	C5'-O5'-P-O1P
19	L	803	3PE	O21-C2-C3-O31
19	L	801	3PE	C3E-C3F-C3G-C3H
19	L	804	3PE	C1-C2-C3-O31
19	H	401	3PE	C3D-C3E-C3F-C3G
19	L	803	3PE	C39-C3A-C3B-C3C
19	L	804	3PE	O21-C2-C3-O31
16	F	503	NAI	PN-O3-PA-O5B
19	J	202	3PE	C3C-C3D-C3E-C3F
19	L	801	3PE	C34-C35-C36-C37
19	M	1202	3PE	C2-C1-O11-P
19	L	803	3PE	C3E-C3F-C3G-C3H
19	M	1202	3PE	C35-C36-C37-C38
19	L	802	3PE	C11-O13-P-O11
19	M	1202	3PE	C11-O13-P-O11
19	L	801	3PE	C23-C24-C25-C26
20	H	402	LFA	C7-C8-C9-C10
19	L	801	3PE	C1-O11-P-O14
19	L	804	3PE	C1-O11-P-O14
19	M	1202	3PE	C1-O11-P-O14
19	J	201	3PE	C11-O13-P-O14
19	L	801	3PE	C25-C26-C27-C28
19	J	201	3PE	O21-C21-C22-C23
19	J	202	3PE	C21-C22-C23-C24
19	J	202	3PE	C11-O13-P-O11
19	L	803	3PE	C1-C2-C3-O31
19	L	801	3PE	C33-C34-C35-C36
15	F	502	FMN	C4'-C5'-O5'-P
20	H	402	LFA	C14-C15-C16-C17
19	J	201	3PE	O11-C1-C2-C3
16	F	503	NAI	O4D-C1D-N1N-C2N
19	L	803	3PE	C3D-C3E-C3F-C3G
19	M	1203	3PE	C3C-C3D-C3E-C3F

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	L	803	3PE	C34-C35-C36-C37
19	L	804	3PE	C31-C32-C33-C34
19	H	401	3PE	C1-C2-C3-O31
19	J	201	3PE	O11-C1-C2-O21
19	J	201	3PE	C23-C24-C25-C26
19	H	401	3PE	O31-C31-C32-C33
19	H	401	3PE	O21-C21-C22-C23
19	M	1203	3PE	O31-C31-C32-C33
19	L	804	3PE	C25-C26-C27-C28
19	M	1202	3PE	C3B-C3C-C3D-C3E
19	H	401	3PE	C28-C29-C2A-C2B
19	H	401	3PE	O21-C2-C3-O31
19	L	801	3PE	O21-C2-C3-O31
19	L	802	3PE	O21-C2-C3-O31
19	M	1202	3PE	C2F-C2G-C2H-C2I
16	F	503	NAI	C5B-O5B-PA-O3
19	M	1202	3PE	C25-C26-C27-C28
16	F	503	NAI	PN-O3-PA-O1A
19	L	804	3PE	C2F-C2G-C2H-C2I
19	L	803	3PE	C3C-C3D-C3E-C3F
19	M	1203	3PE	O32-C31-C32-C33
19	H	401	3PE	O32-C31-C32-C33
19	J	202	3PE	C2F-C2G-C2H-C2I
19	L	802	3PE	C11-O13-P-O12
19	M	1203	3PE	C1-O11-P-O14
19	H	401	3PE	O22-C21-C22-C23
20	M	1201	LFA	C6-C7-C8-C9
19	L	802	3PE	C3B-C3C-C3D-C3E
19	L	804	3PE	C23-C24-C25-C26
19	L	802	3PE	O21-C21-C22-C23
16	F	503	NAI	C2D-C1D-N1N-C2N

There are no ring outliers.

13 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	G	1003	SF4	1	0
19	L	801	3PE	3	0
17	E	201	FES	1	0
19	L	802	3PE	3	0
16	F	503	NAI	2	0
19	J	201	3PE	4	0

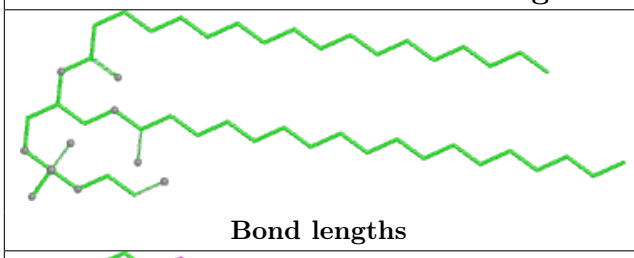
Continued on next page...

Continued from previous page...

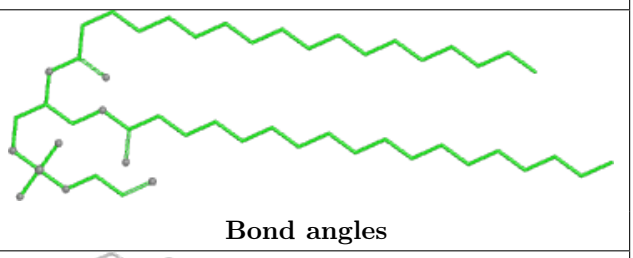
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	M	1202	3PE	3	0
19	H	401	3PE	4	0
19	M	1203	3PE	3	0
19	J	202	3PE	4	0
19	L	804	3PE	4	0
20	M	1201	LFA	2	0
20	H	402	LFA	1	0

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

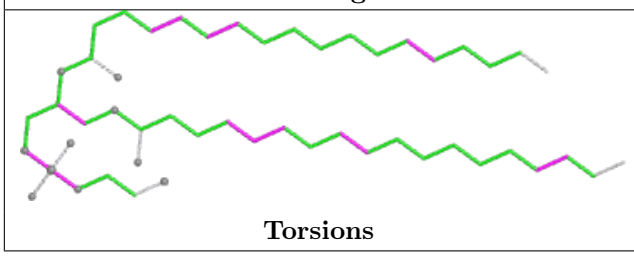
Ligand 3PE L 801



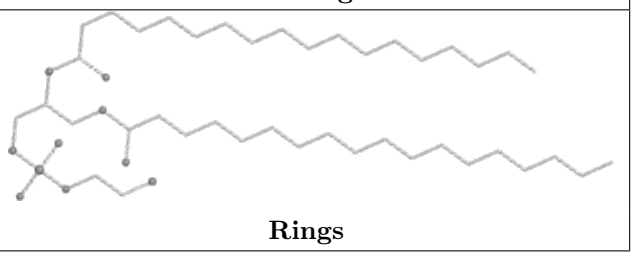
Bond lengths



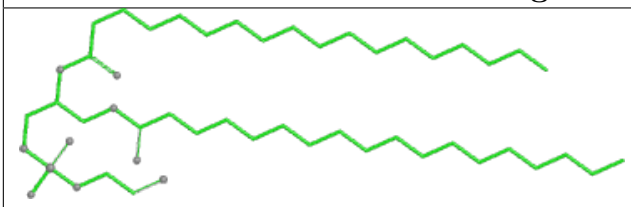
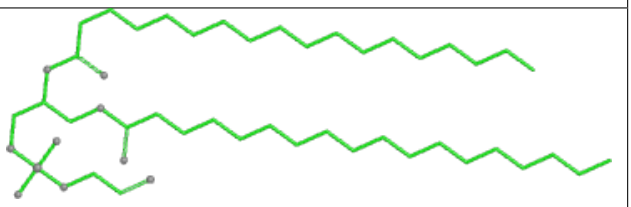
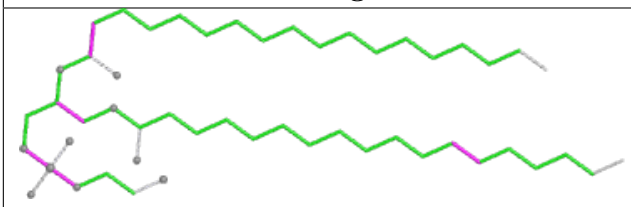
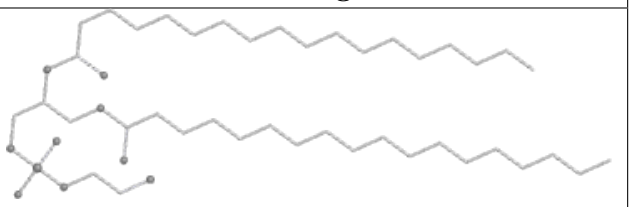
Bond angles

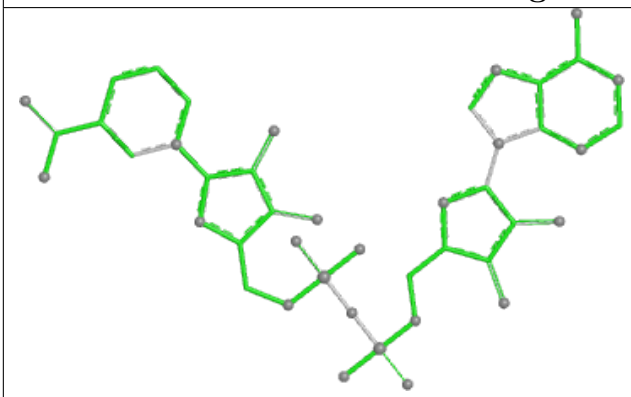
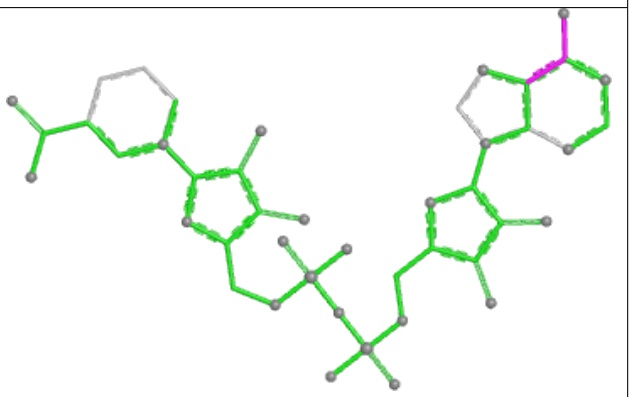
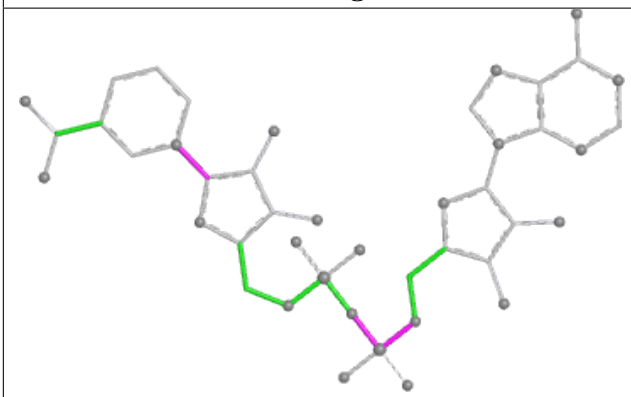
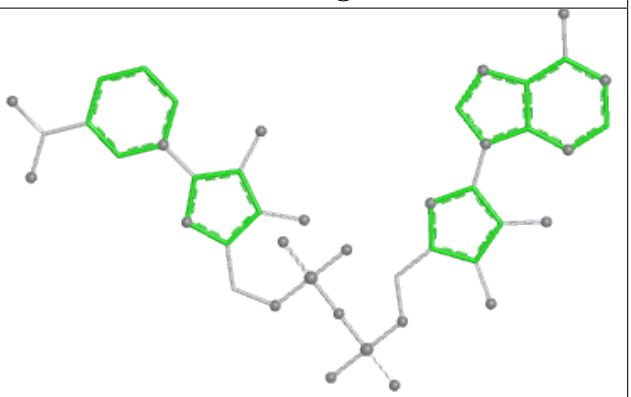


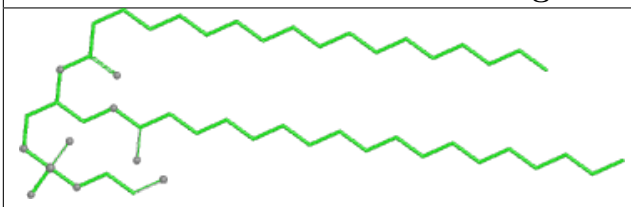
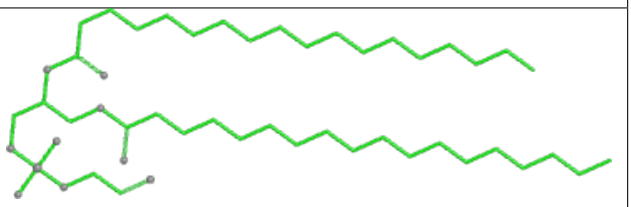
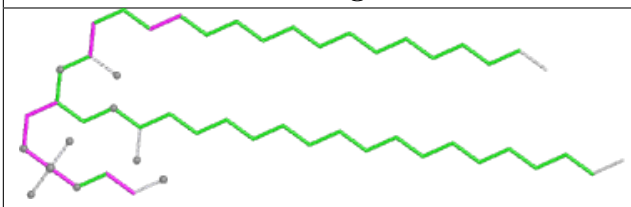
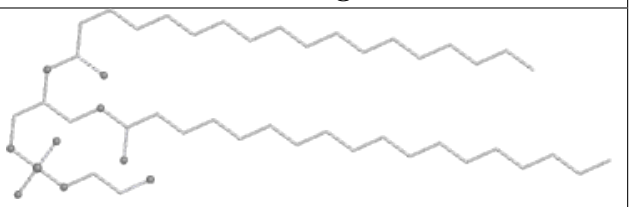
Torsions

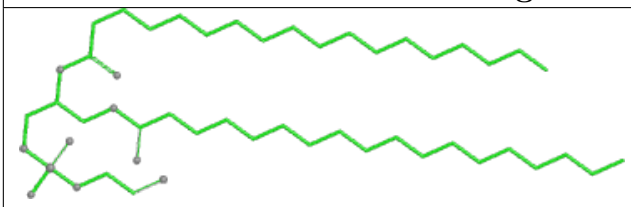
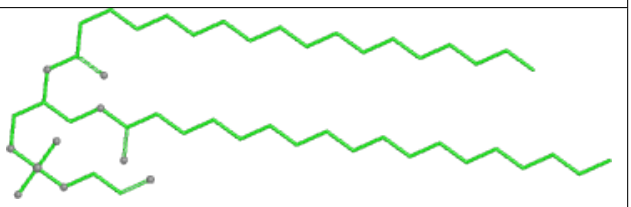
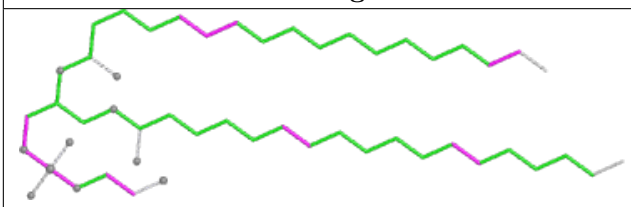
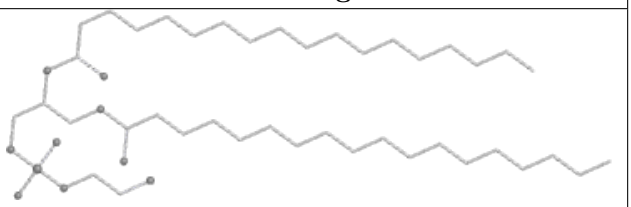


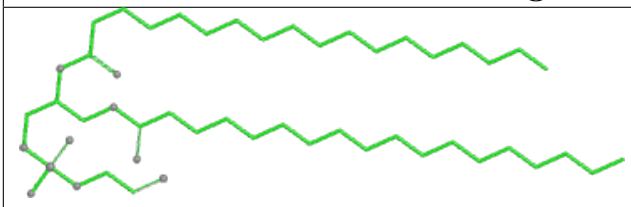
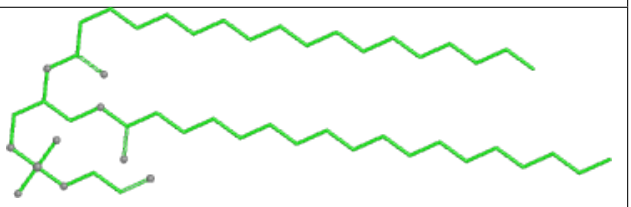
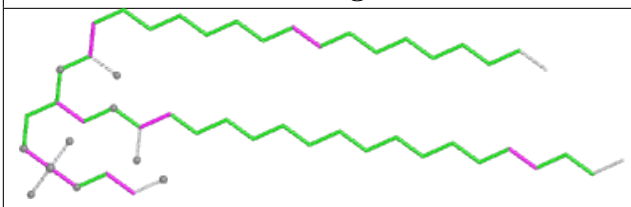
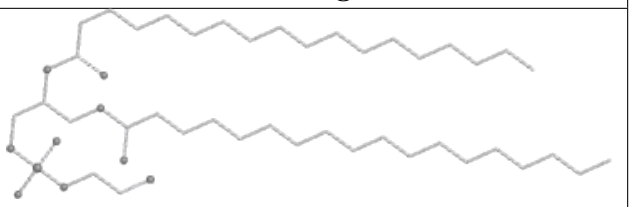
Rings

Ligand 3PE L 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

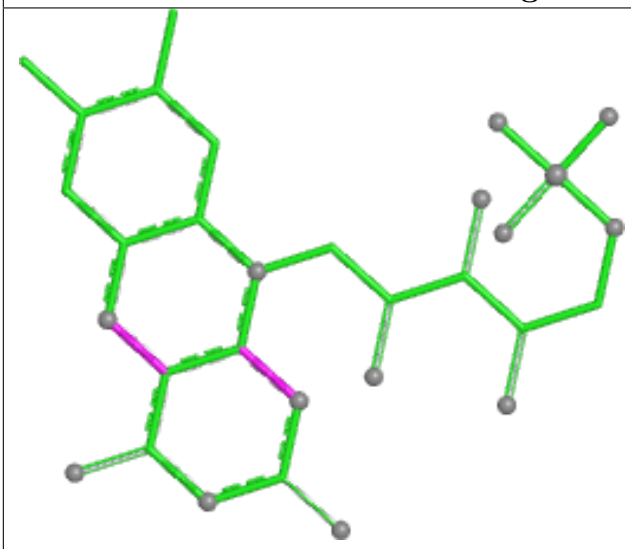
Ligand NAI F 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE J 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

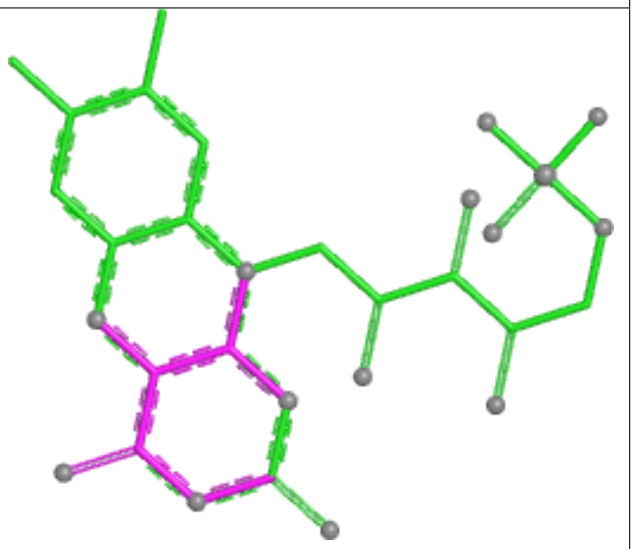
Ligand 3PE M 1202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE H 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

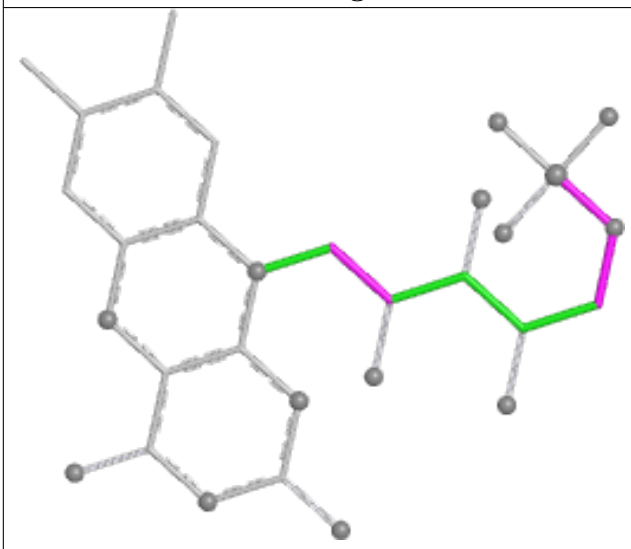
Ligand FMN F 502



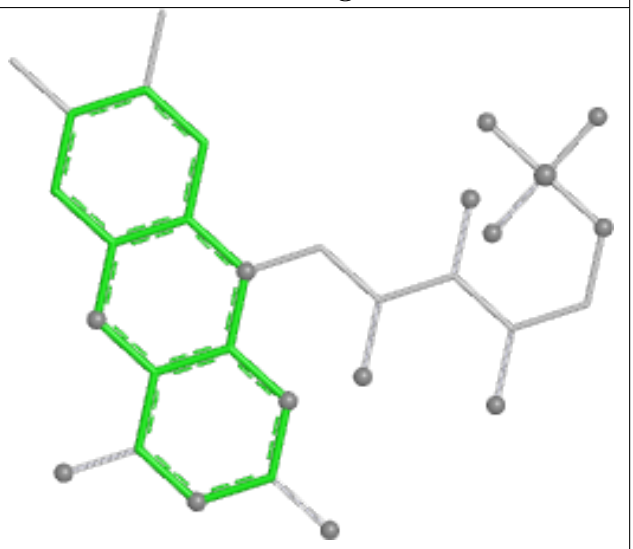
Bond lengths



Bond angles

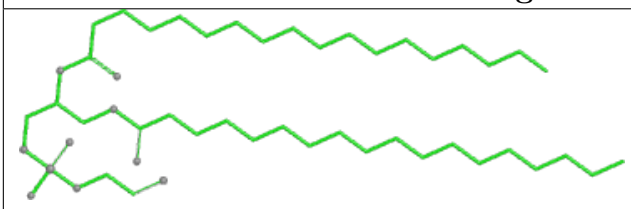


Torsions

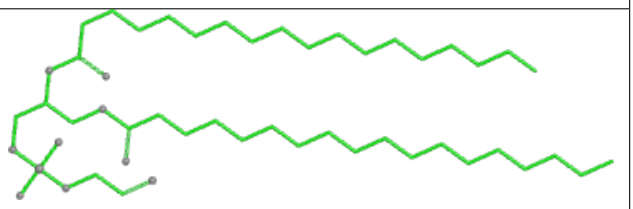


Rings

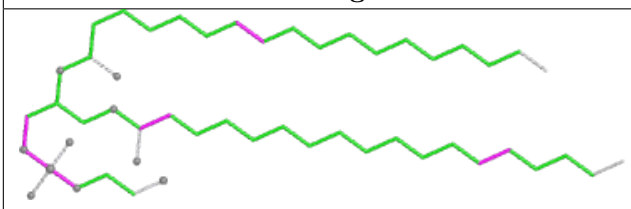
Ligand 3PE M 1203



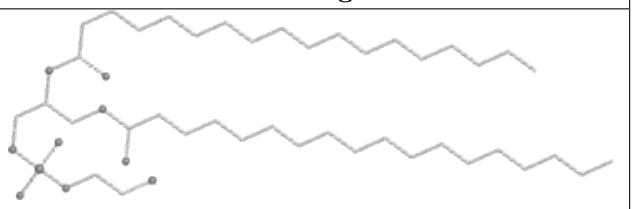
Bond lengths



Bond angles

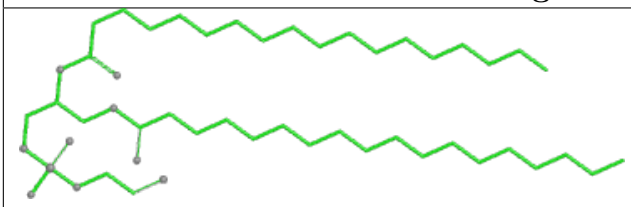


Torsions

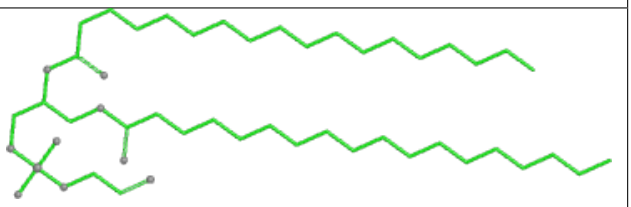


Rings

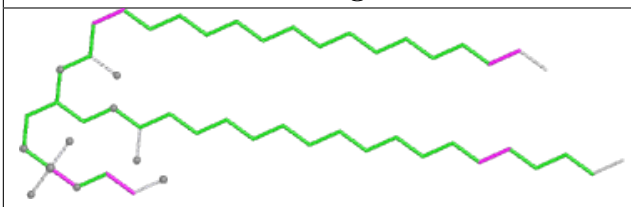
Ligand 3PE J 202



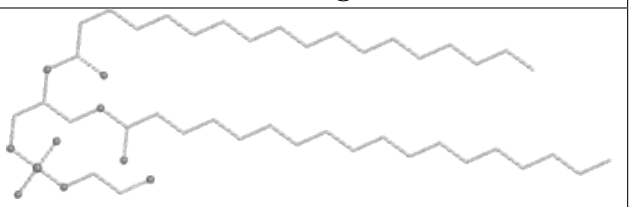
Bond lengths



Bond angles

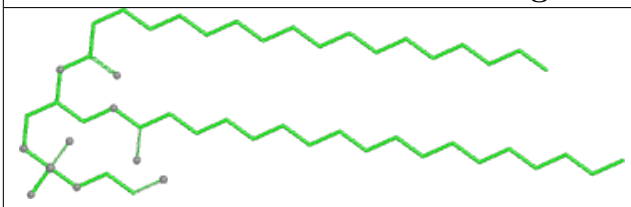


Torsions

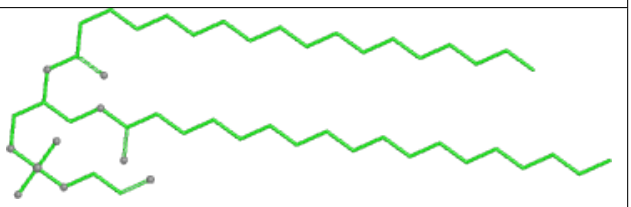


Rings

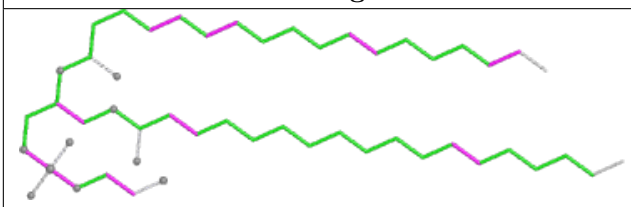
Ligand 3PE L 804



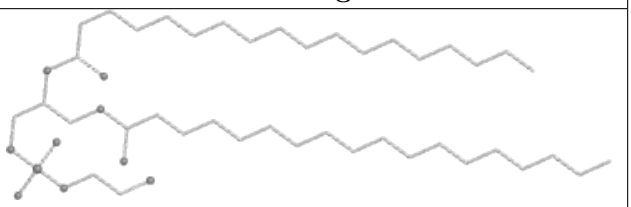
Bond lengths



Bond angles

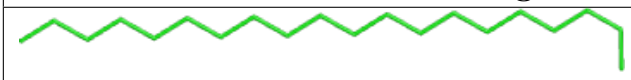


Torsions

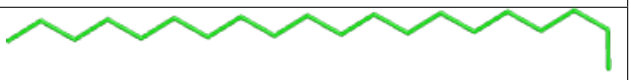


Rings

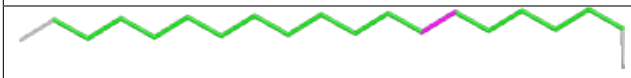
Ligand LFA M 1201



Bond lengths



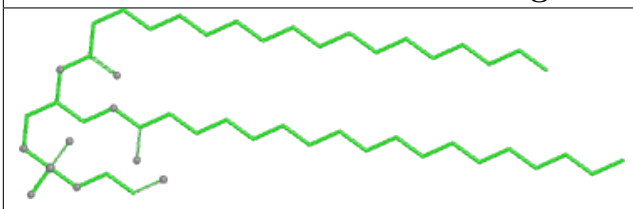
Bond angles



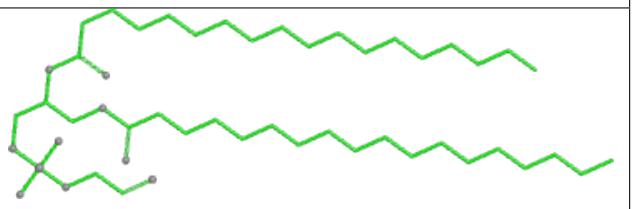
Torsions

Rings

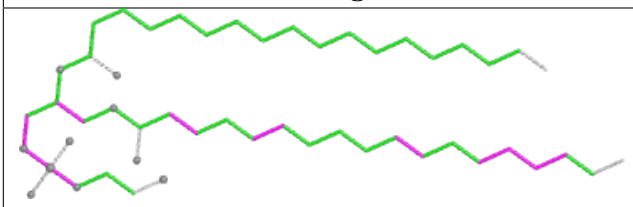
Ligand 3PE L 803



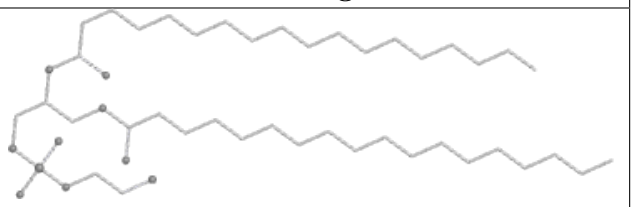
Bond lengths



Bond angles

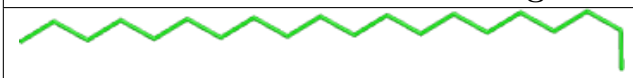


Torsions

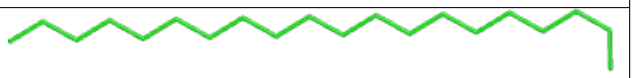


Rings

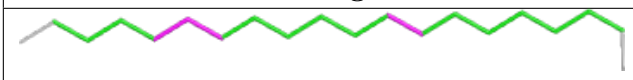
Ligand LFA H 402



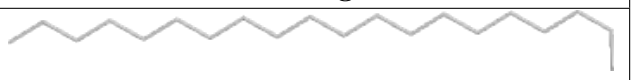
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

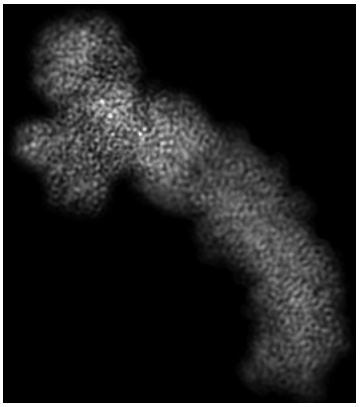
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14541. These allow visual inspection of the internal detail of the map and identification of artifacts.

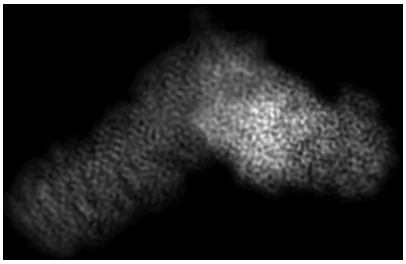
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

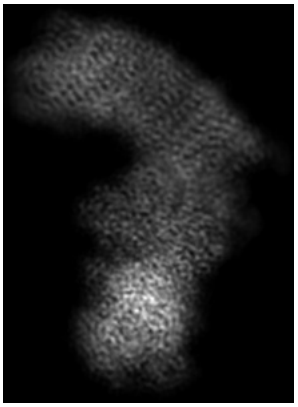
6.1.1 Primary map



X



Y



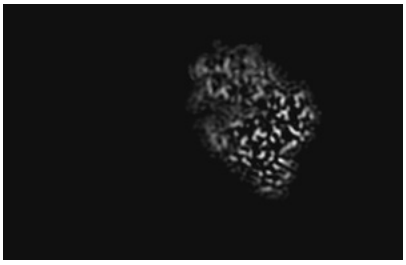
Z

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

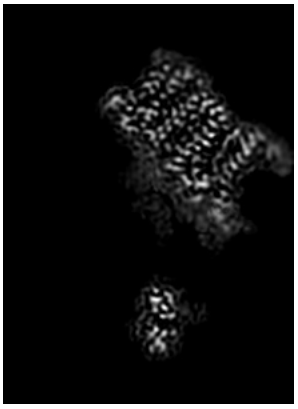
6.2 Central slices

6.2.1 Primary map

X Index: 72



Y Index: 100



Z Index: 113

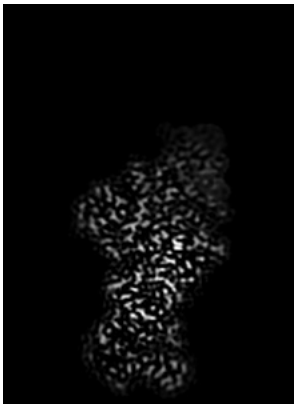
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 73

Y Index: 53



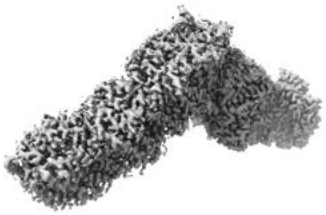
Z Index: 152

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

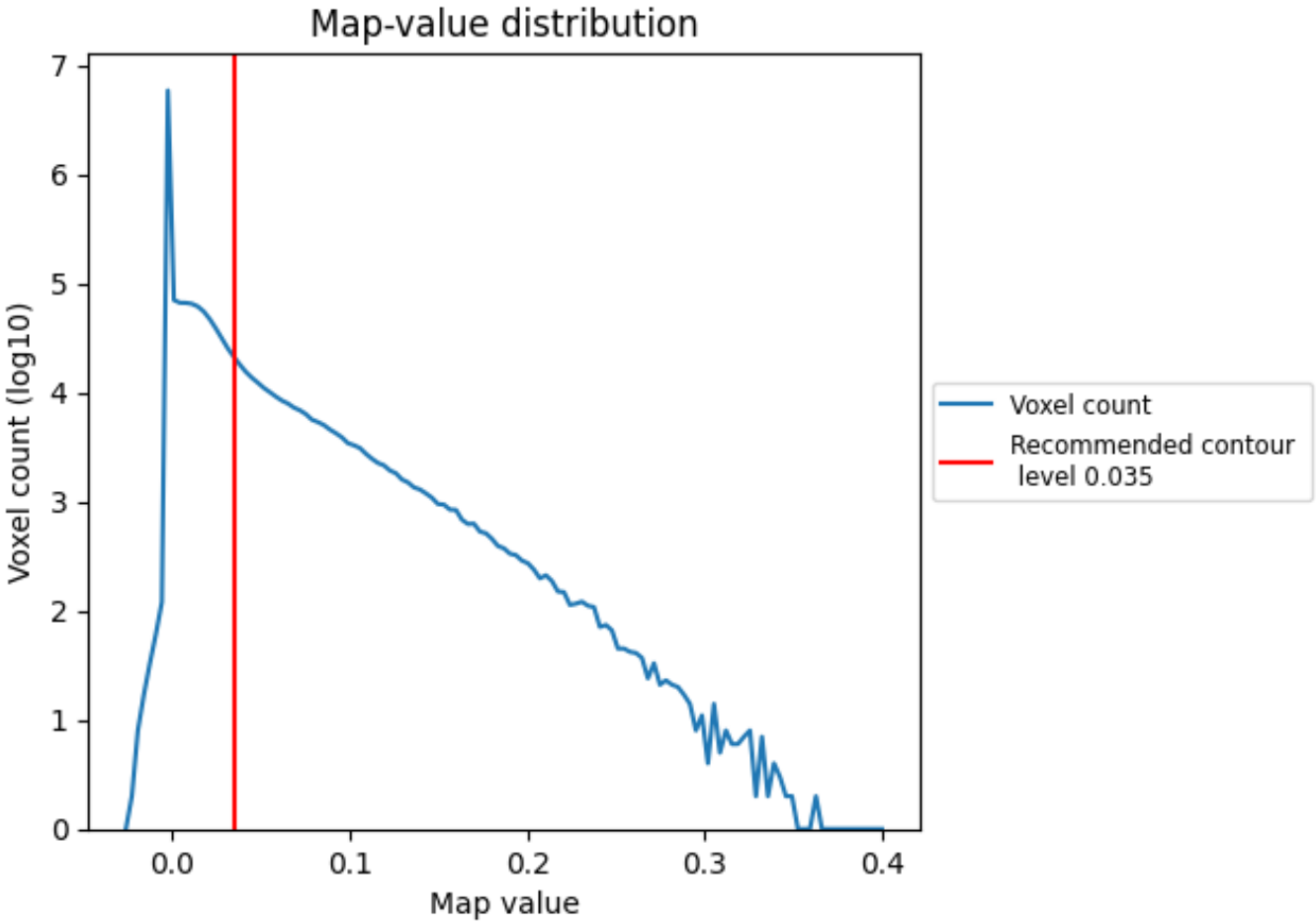
6.5 Mask visualisation (i)

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

7 Map analysis

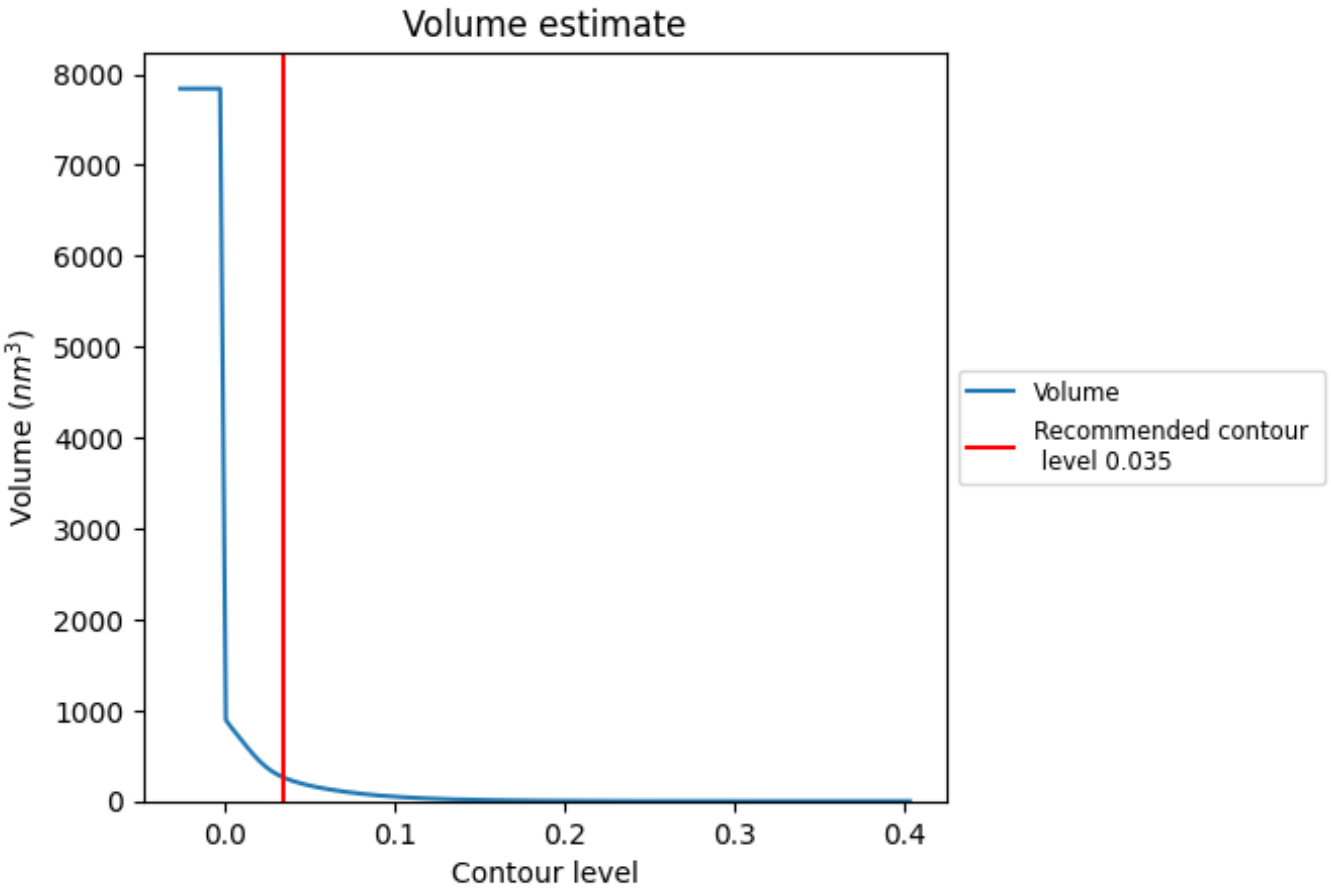
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate



The volume at the recommended contour level is 261 nm^3; this corresponds to an approximate mass of 236 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.

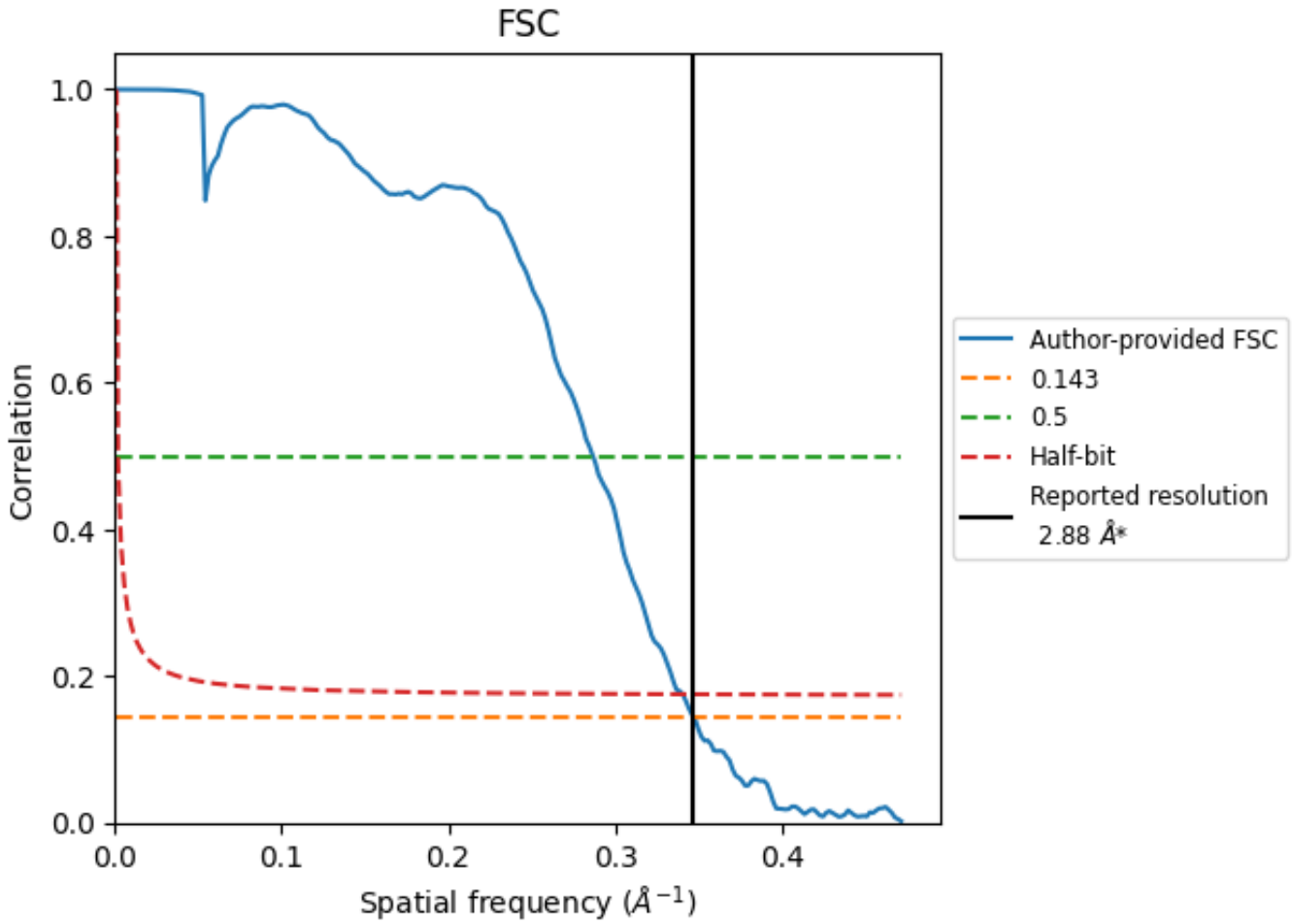
7.3 Rotationally averaged power spectrum

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

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.347 Å^{-1}

8.2 Resolution estimates (i)

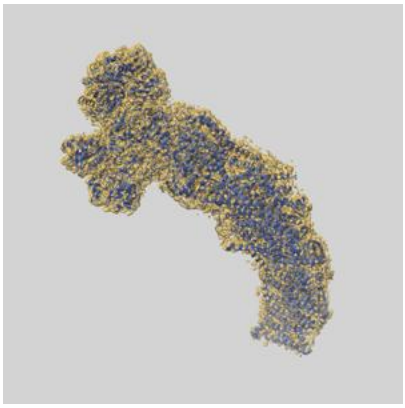
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	2.88	3.49	2.94
Unmasked-calculated*	-	-	-

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

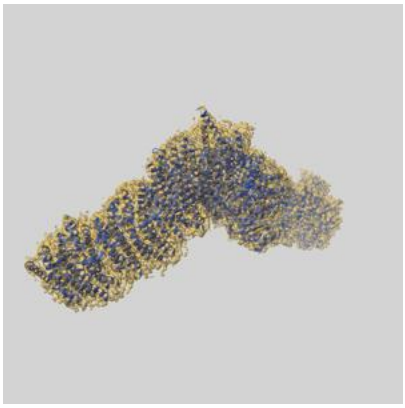
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14541 and PDB model 7Z83. Per-residue inclusion information can be found in section 3 on page 11.

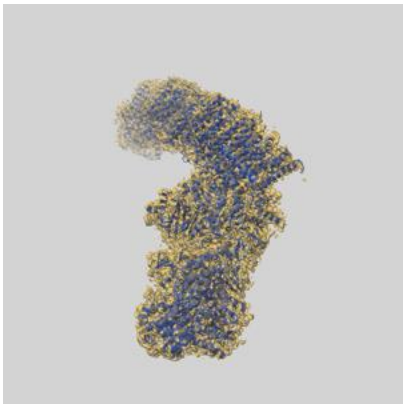
9.1 Map-model overlay



X



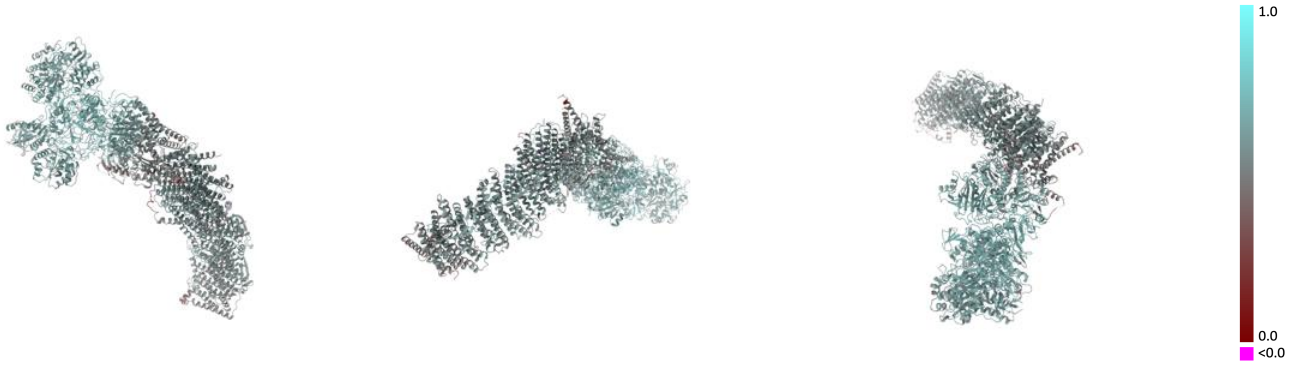
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

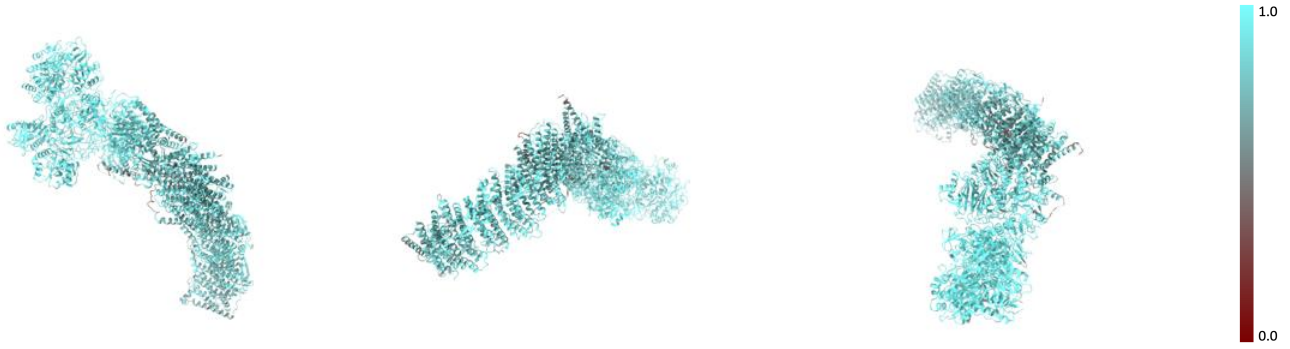
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

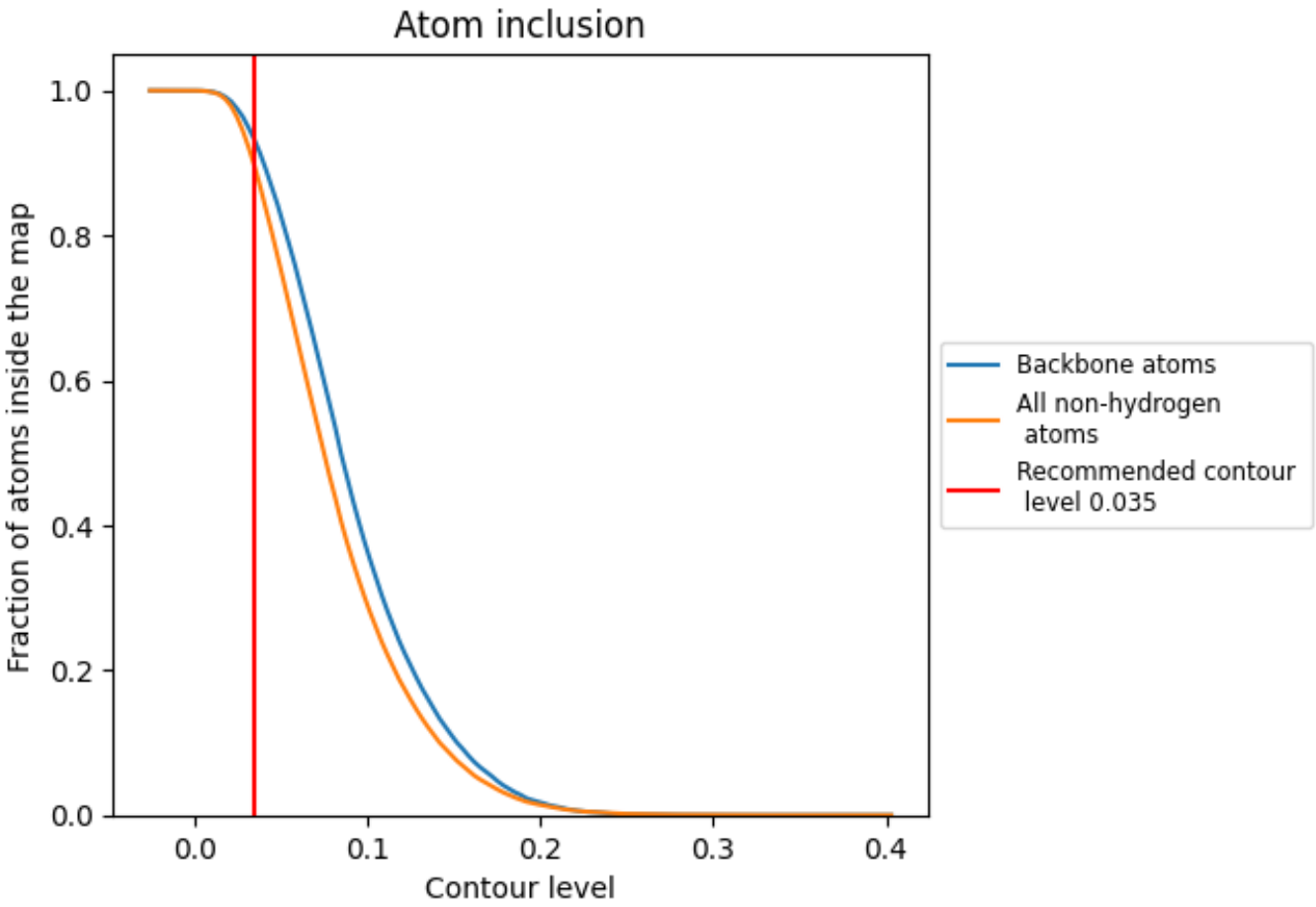
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 89% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8932	0.5770
A	0.7917	0.5170
B	0.9054	0.5710
C	0.9219	0.6050
E	0.9509	0.6120
F	0.9529	0.6140
G	0.9679	0.6410
H	0.8152	0.5060
I	0.9307	0.6320
J	0.8115	0.5240
K	0.8872	0.5560
L	0.8124	0.5100
M	0.8805	0.5530
N	0.8463	0.5500