Full wwPDB EM Validation Report ⓘ

Aug 26, 2026 – 09:22 pm BST

PDB ID	:	7P63 / pdb_00007p63
EMDB ID	:	EMD-13216
Title	:	Complex I from E. coli, DDM/LMNG-purified, under Turnover at pH 6, Closed state
Authors	:	Kravchuk, V.; Kampjut, D.; Sazanov, L.
Deposited on	:	2021-07-15
Resolution	:	3.40 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:

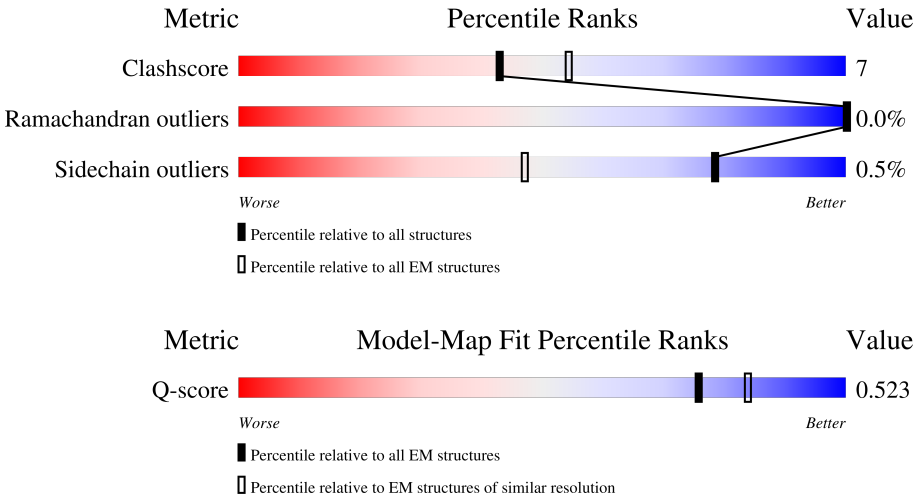
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.40 Å.

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



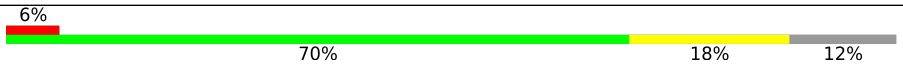
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	82% 16%
2	E	166	81% 13% 6%
3	G	908	85% 14%
4	C	600	79% 19%

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Mol	Chain	Length	Quality of chain
5	B	220	
6	I	180	
7	H	325	
8	A	147	
9	L	613	
10	M	509	
11	N	485	
12	K	100	
13	J	184	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 37770 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	7012	4384	1268	1323	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	589	4762	3050	828	860	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	210	1672	1059	291	306	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	322	Total	C	N	O	S	0	0
			2534	1702	398	416	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	129	Total	C	N	O	S	0	0
			1021	679	174	164	4		

- Molecule 9 is a protein called Proton-translocating NADH-quinone oxidoreductase, chain L.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	598	Total	C	N	O	S	0	0
			4560	3037	726	765	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
			3614	2414	571	609	20		

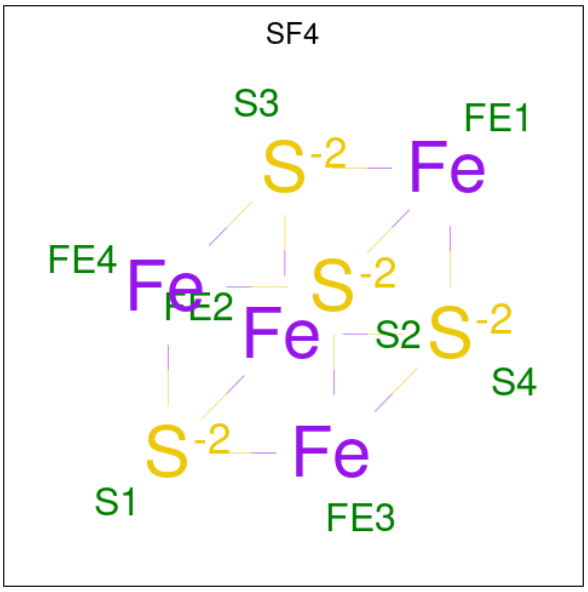
- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit K.

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.

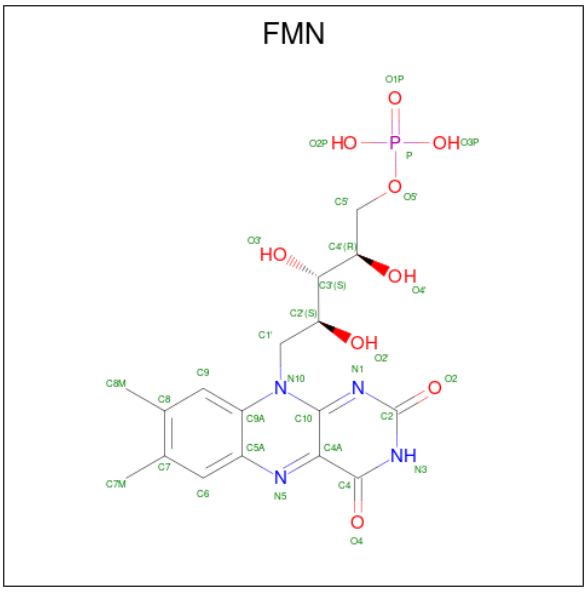
Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	162	Total	C	N	O	S	0	0
			1226	824	188	207	7		

- Molecule 14 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



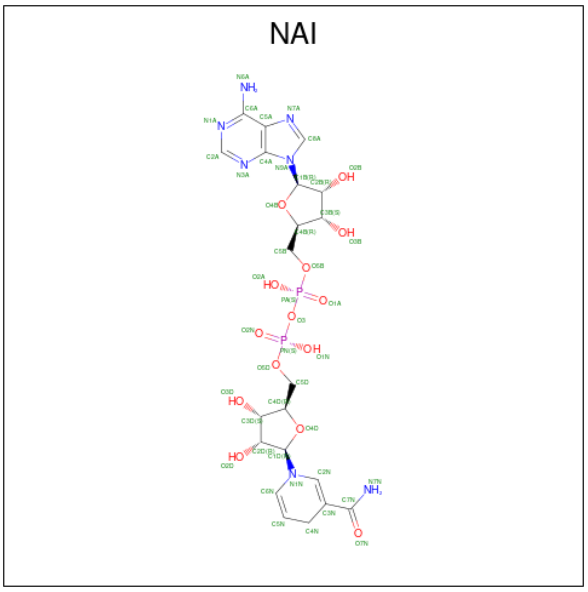
Mol	Chain	Residues	Atoms	AltConf
14	F	1	Total Fe S 8 4 4	0
14	G	1	Total Fe S 8 4 4	0
14	G	1	Total Fe S 8 4 4	0
14	G	1	Total Fe S 8 4 4	0
14	B	1	Total Fe S 8 4 4	0
14	I	1	Total Fe S 8 4 4	0
14	I	1	Total Fe S 8 4 4	0

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



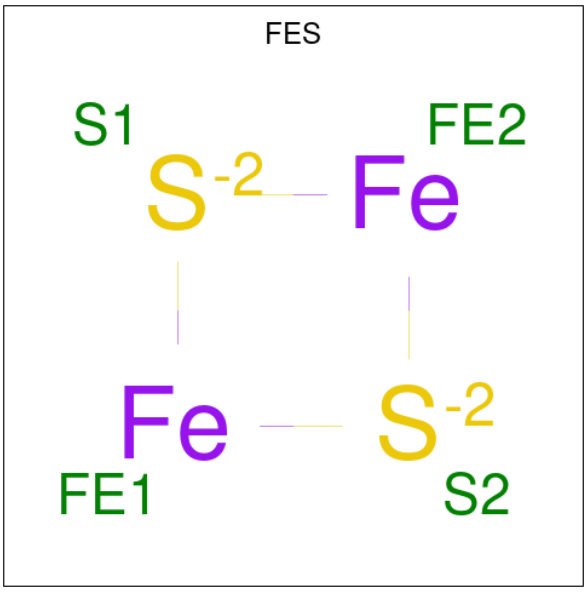
Mol	Chain	Residues	Atoms					AltConf
15	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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



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

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

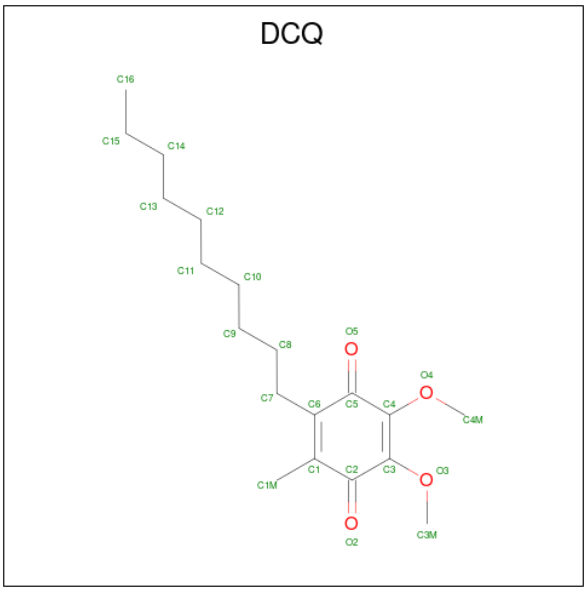


Mol	Chain	Residues	Atoms			AltConf
17	E	1	Total	Fe	S	0
			4	2	2	
17	G	1	Total	Fe	S	0
			4	2	2	

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

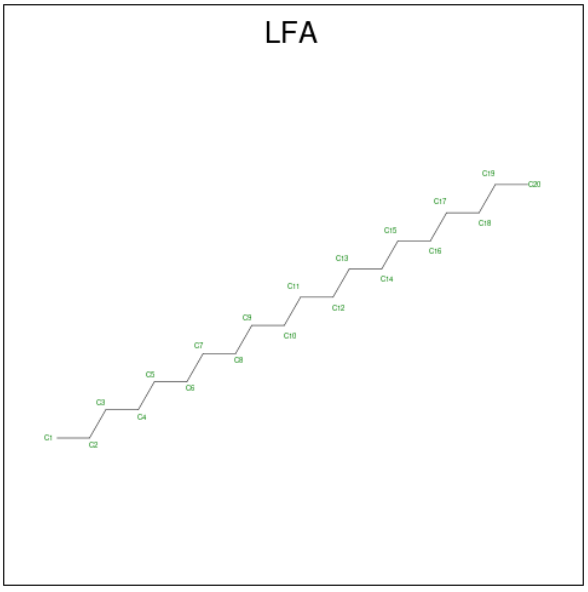
Mol	Chain	Residues	Atoms		AltConf
18	G	1	Total	Ca	0
			1	1	

- Molecule 19 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (CCD ID: DCQ) (formula: $C_{19}H_{30}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
19	C	1	Total C O 23 19 4	0

- Molecule 20 is EICOSANE (CCD ID: LFA) (formula: $C_{20}H_{42}$).



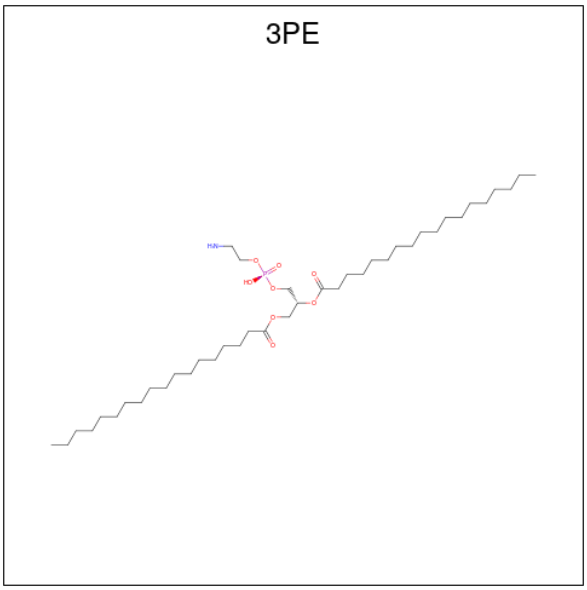
Mol	Chain	Residues	Atoms	AltConf
20	H	1	Total C 20 20	0
20	L	1	Total C 20 20	0
20	N	1	Total C 15 15	0

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Mol	Chain	Residues	Atoms	AltConf
20	N	1	Total C 14 14	0

- Molecule 21 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total C N O P 51 41 1 8 1	0
21	L	1	Total C N O P 51 41 1 8 1	0
21	L	1	Total C N O P 36 26 1 8 1	0
21	L	1	Total C N O P 51 41 1 8 1	0
21	M	1	Total C N O P 47 37 1 8 1	0
21	M	1	Total C N O P 47 37 1 8 1	0
21	J	1	Total C N O P 42 32 1 8 1	0
21	J	1	Total C N O P 36 26 1 8 1	0

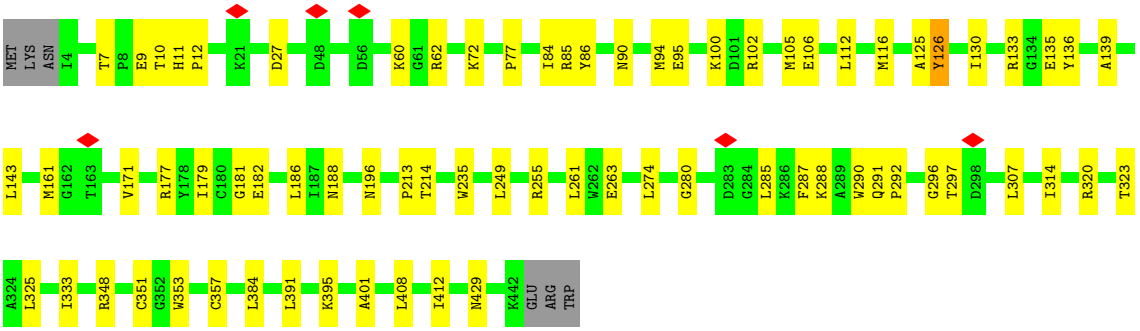
3 Residue-property plots (i)

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

• Molecule 1: NADH-quinone oxidoreductase subunit F

Chain F:

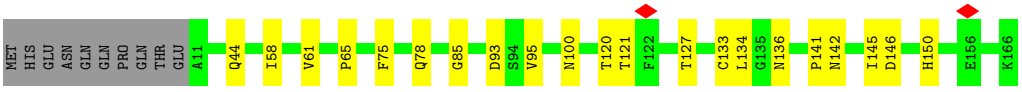




• Molecule 2: NADH dehydrogenase I subunit E

Chain E:

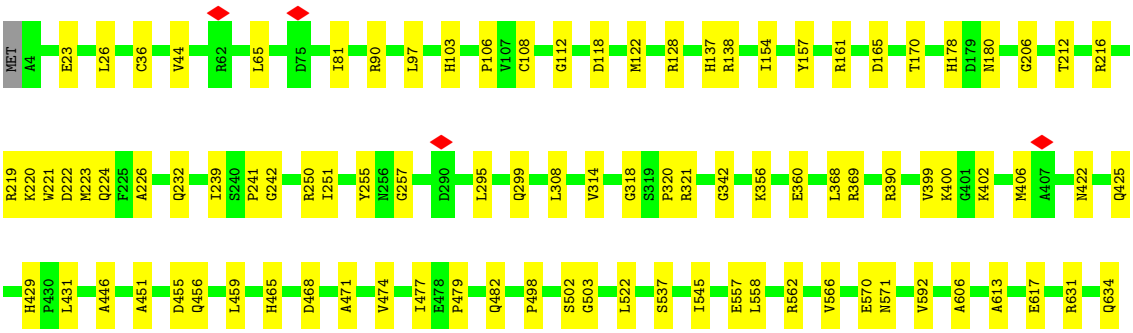


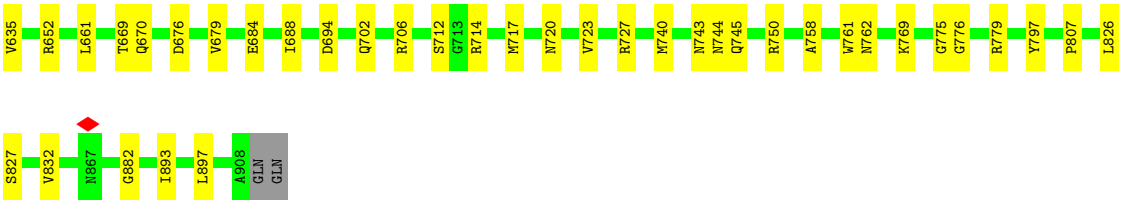


• Molecule 3: NADH-quinone oxidoreductase

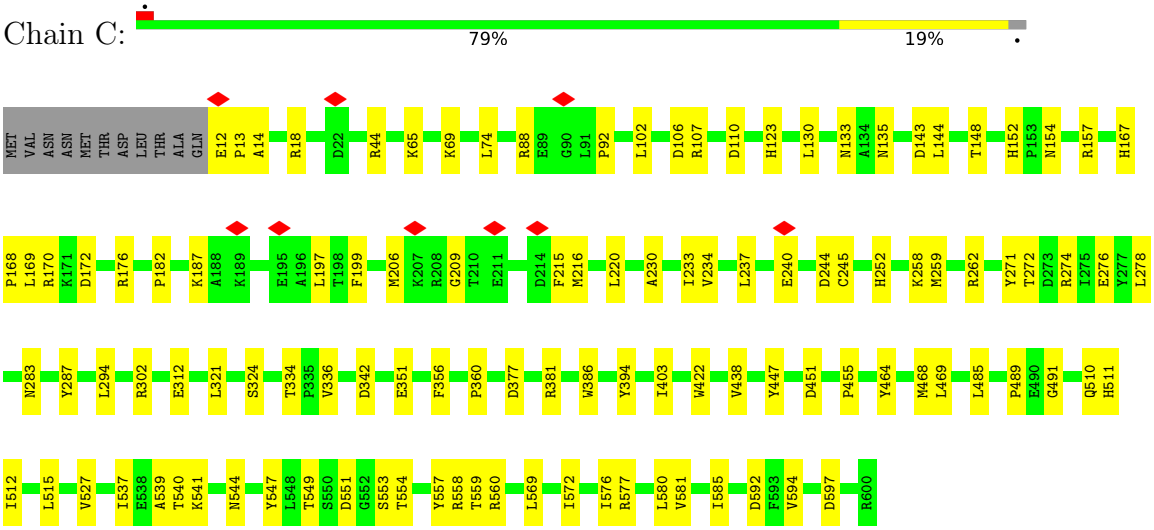
Chain G:



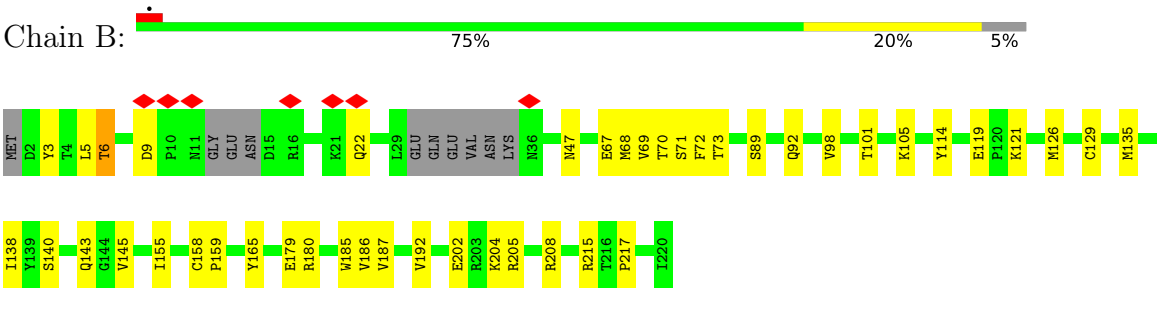




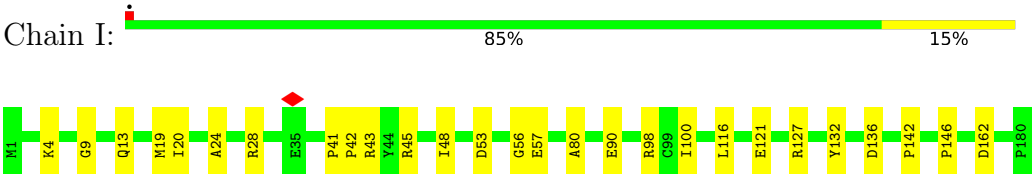
• Molecule 4: NADH-quinone oxidoreductase subunit C/D



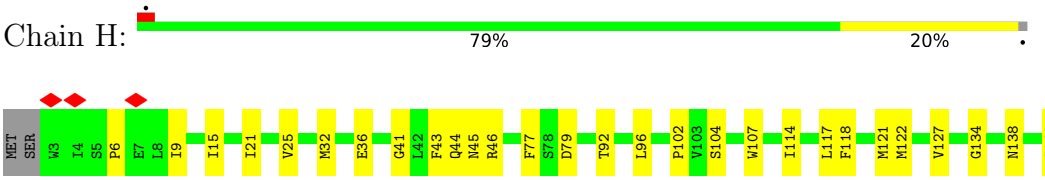
• Molecule 5: NADH-quinone oxidoreductase subunit B

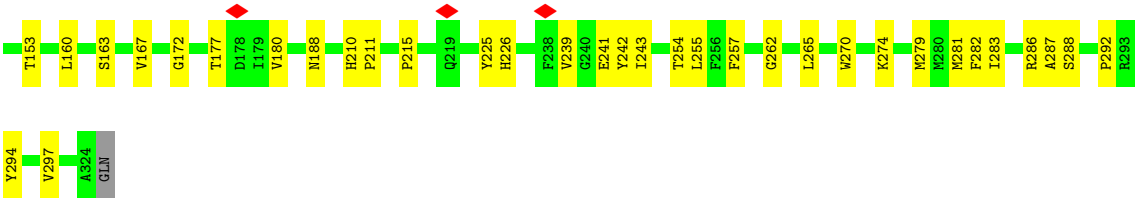


• Molecule 6: NADH-quinone oxidoreductase subunit I



• Molecule 7: NADH-quinone oxidoreductase subunit H

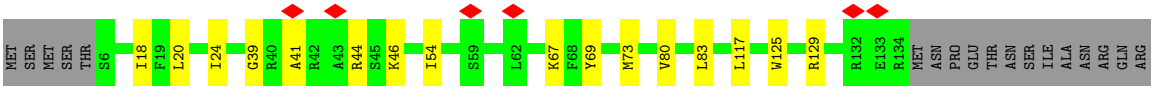




• Molecule 8: NADH-quinone oxidoreductase subunit A

Chain A:

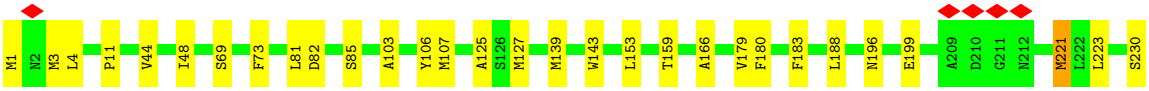


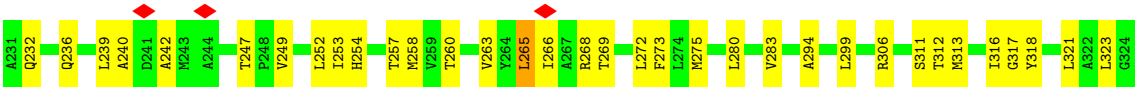


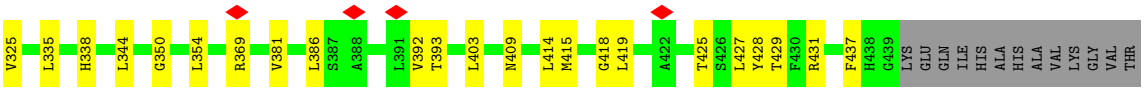
• Molecule 9: Proton-translocating NADH-quinone oxidoreductase, chain L

Chain L:







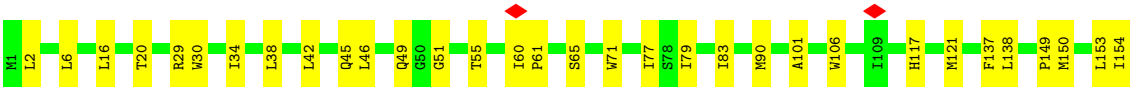


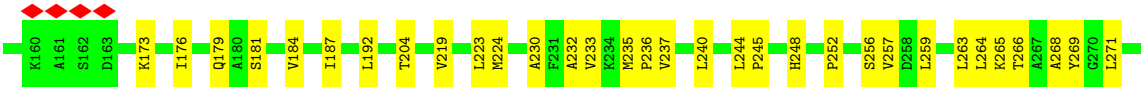


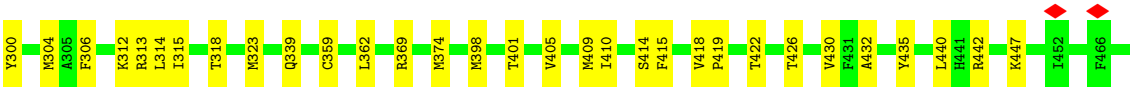
• Molecule 10: NADH dehydrogenase I subunit M

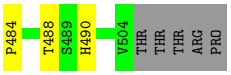
Chain M:





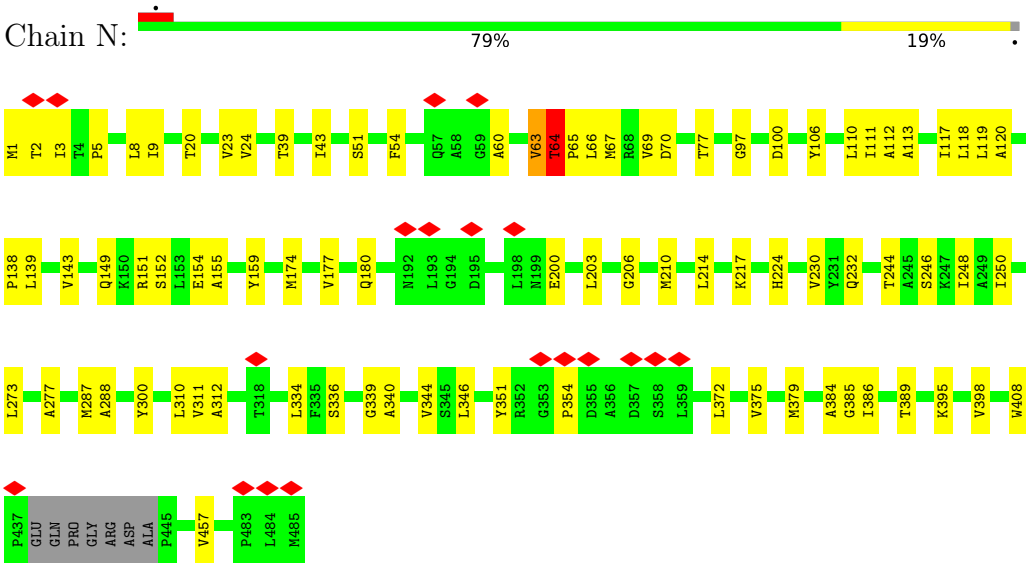






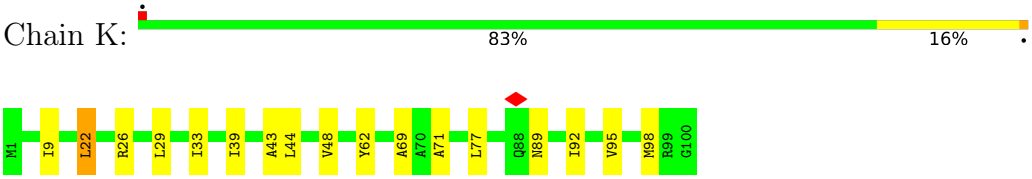
• Molecule 11: NADH-quinone oxidoreductase subunit N

Chain N:



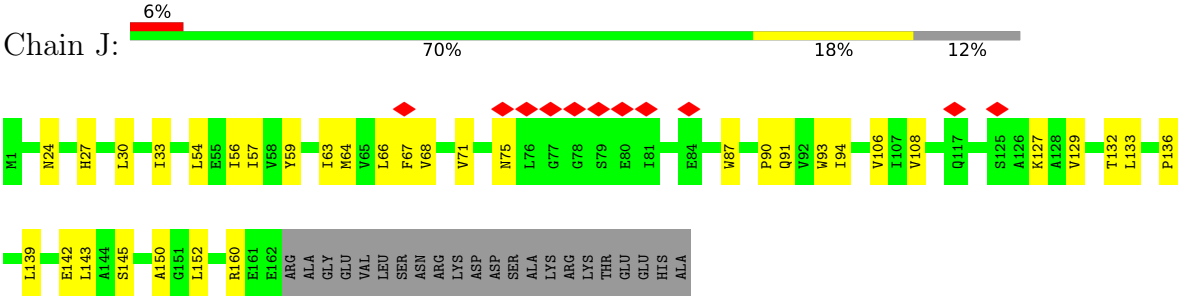
• Molecule 12: NADH-quinone oxidoreductase subunit K

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	8247	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 ($e^-/Å^2$)	78	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	0.247	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.026	Depositor
Map size (Å)	160.06, 213.05998, 238.49998	wwPDB
Map dimensions	225, 201, 151	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: CA, FMN, SF4, LFA, NAI, DCQ, 3PE, FES

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	0.16	0/3486	0.38	1/4713 (0.0%)
2	E	0.14	0/1248	0.35	0/1691
3	G	0.15	0/7163	0.37	0/9713
4	C	0.16	0/4893	0.38	0/6640
5	B	0.16	0/1708	0.40	0/2314
6	I	0.16	0/1470	0.37	0/1985
7	H	0.20	0/2610	0.42	0/3553
8	A	0.17	0/1049	0.41	0/1422
9	L	0.19	0/4677	0.43	0/6375
10	M	0.21	0/4074	0.45	0/5546
11	N	0.21	0/3703	0.49	1/5053 (0.0%)
12	K	0.21	0/769	0.48	0/1040
13	J	0.16	0/1252	0.38	0/1708
All	All	0.18	0/38102	0.41	2/51753 (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
11	N	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	161	MET	CA-CB-CG	5.20	124.49	114.10
11	N	64	THR	N-CA-C	-5.13	98.48	109.81

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	49	0
2	E	1220	0	1187	13	0
3	G	7012	0	6814	82	0
4	C	4762	0	4679	72	0
5	B	1672	0	1654	32	0
6	I	1436	0	1415	24	0
7	H	2534	0	2583	45	0
8	A	1021	0	1039	12	0
9	L	4560	0	4703	69	0
10	M	3953	0	4053	59	0
11	N	3614	0	3779	65	0
12	K	760	0	817	13	0
13	J	1226	0	1297	29	0
14	B	8	0	0	0	0
14	F	8	0	0	0	0
14	G	24	0	0	3	0
14	I	16	0	0	0	0
15	F	31	0	19	1	0
16	F	44	0	27	2	0
17	E	4	0	0	0	0
17	G	4	0	0	0	0
18	G	1	0	0	0	0
19	C	23	0	30	1	0
20	H	20	0	42	0	0
20	L	20	0	42	0	0
20	N	29	0	56	1	0
21	A	51	0	82	2	0
21	J	78	0	104	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	L	138	0	210	4	0
21	M	94	0	142	4	0
All	All	37770	0	38148	504	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 (504) 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	1.57	1.02
9:L:179:VAL:HG22	10:M:426:THR:HG22	1.70	0.74
7:H:121:MET:HG2	13:J:56:ILE:HB	1.75	0.67
5:B:135:MET:HB3	6:I:100:ILE:HG21	1.78	0.66
11:N:180:GLN:NE2	11:N:200:GLU:OE1	2.27	0.66
11:N:312:ALA:HB2	11:N:398:VAL:HG22	1.77	0.65
21:M:1001:3PE:H331	21:M:1001:3PE:H231	1.79	0.65
11:N:129:PHE:HB2	11:N:174:MET:HE1	1.77	0.65
12:K:9:ILE:HG12	13:J:108:VAL:HG22	1.78	0.65
9:L:153:LEU:HB3	9:L:249:VAL:HG21	1.79	0.64
10:M:6:LEU:HG	10:M:42:LEU:HD22	1.80	0.64
7:H:134:GLY:HA3	7:H:146:ALA:HB2	1.80	0.63
7:H:121:MET:HE3	13:J:56:ILE:HD12	1.80	0.63
11:N:111:ILE:HG21	13:J:150:ALA:HB2	1.80	0.63
3:G:356:LYS:O	3:G:360:GLU:HB2	1.99	0.62
10:M:362:LEU:HD21	10:M:374:MET:HE1	1.81	0.62
9:L:11:PRO:HB2	9:L:125:ALA:HB2	1.82	0.62
11:N:375:VAL:HG11	11:N:457:VAL:HB	1.81	0.62
8:A:117:LEU:HD11	13:J:152:LEU:HD11	1.82	0.61
1:F:291:GLN:NE2	1:F:297:THR:O	2.33	0.61
11:N:384:ALA:HB1	11:N:422:LEU:HD12	1.82	0.61
9:L:595:VAL:HG11	12:K:22:LEU:HD22	1.83	0.61
4:C:278:LEU:HD11	4:C:321:LEU:HD13	1.81	0.61
9:L:263:VAL:HG13	9:L:323:LEU:HD11	1.82	0.61
3:G:223:MET:HE1	3:G:250:ARG:HB3	1.83	0.60
5:B:215:ARG:HB2	6:I:42:PRO:HB3	1.82	0.60
4:C:276:GLU:O	4:C:283:ASN:ND2	2.34	0.60
3:G:239:ILE:HD12	3:G:251:ILE:HD12	1.81	0.60
1:F:249:LEU:HB3	1:F:261:LEU:HD11	1.82	0.60
9:L:223:LEU:HD13	9:L:283:VAL:HG22	1.84	0.60
11:N:120:ALA:O	11:N:256:ARG:NH2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:428:TYR:HA	9:L:431:ARG:HG2	1.84	0.60
10:M:235:MET:HG2	10:M:323:MET:HB3	1.84	0.60
9:L:3:MET:HG3	9:L:44:VAL:HG13	1.85	0.59
11:N:386:ILE:O	11:N:389:THR:OG1	2.19	0.59
3:G:23:GLU:HA	3:G:26:LEU:HB2	1.83	0.59
3:G:727:ARG:HB2	4:C:182:PRO:HD3	1.83	0.59
4:C:144:LEU:HA	4:C:168:PRO:HD2	1.83	0.59
10:M:264:LEU:HB2	10:M:266:THR:HG23	1.84	0.59
10:M:414:SER:O	10:M:418:VAL:N	2.31	0.59
3:G:239:ILE:HG13	3:G:241:PRO:HD3	1.84	0.59
4:C:569:LEU:HD13	4:C:572:ILE:HD12	1.84	0.59
7:H:32:MET:HE2	7:H:279:MET:HG2	1.84	0.58
10:M:150:MET:HE3	10:M:154:ILE:HD11	1.85	0.58
10:M:184:VAL:HA	10:M:187:ILE:HD12	1.86	0.58
1:F:112:LEU:HG	1:F:116:MET:HE2	1.85	0.58
4:C:455:PRO:HB2	4:C:469:LEU:HD22	1.84	0.58
1:F:136:TYR:HB3	1:F:139:ALA:HB3	1.86	0.58
6:I:28:ARG:HH21	7:H:45:ASN:HA	1.68	0.58
8:A:83:LEU:HB2	13:J:54:LEU:HD22	1.86	0.58
3:G:714:ARG:HH11	3:G:740:MET:HE3	1.68	0.58
1:F:105:MET:HG3	1:F:139:ALA:HB1	1.84	0.57
11:N:248:ILE:HD11	11:N:334:LEU:HB2	1.85	0.57
6:I:48:ILE:HG12	6:I:116:LEU:HG	1.87	0.57
9:L:570:ASN:OD1	10:M:173:LYS:NZ	2.38	0.57
9:L:82:ASP:N	9:L:82:ASP:OD1	2.38	0.56
1:F:95:GLU:HB2	16:F:503:NAI:H42N	1.85	0.56
7:H:210:HIS:HB3	7:H:286:ARG:HA	1.87	0.56
9:L:325:VAL:O	9:L:409:ASN:ND2	2.38	0.56
3:G:652:ARG:NH1	3:G:669:THR:O	2.37	0.56
5:B:92:GLN:NE2	7:H:226:HIS:O	2.38	0.56
10:M:359:CYS:SG	10:M:369:ARG:NH1	2.79	0.56
3:G:714:ARG:HA	3:G:717:MET:HE2	1.86	0.56
10:M:265:LYS:NZ	10:M:323:MET:SD	2.79	0.56
10:M:181:SER:HB2	10:M:230:ALA:HA	1.88	0.56
1:F:94:MET:HE2	1:F:133:ARG:HB2	1.87	0.55
4:C:274:ARG:NH2	5:B:158:CYS:SG	2.74	0.55
1:F:72:LYS:NZ	15:F:502:FMN:O3P	2.40	0.55
3:G:368:LEU:HD21	3:G:390:ARG:HB3	1.87	0.55
7:H:36:GLU:HG3	7:H:283:ILE:HD12	1.87	0.55
1:F:90:ASN:ND2	1:F:181:GLY:O	2.38	0.55
4:C:510:GLN:O	4:C:511:HIS:ND1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:41:GLY:HA2	7:H:46:ARG:HG3	1.89	0.55
11:N:217:LYS:HB3	11:N:250:ILE:HD13	1.88	0.55
9:L:519:VAL:HG13	21:L:803:3PE:H31	1.90	0.54
7:H:36:GLU:OE1	7:H:242:TYR:OH	2.26	0.54
7:H:211:PRO:HB2	7:H:292:PRO:HD3	1.90	0.54
3:G:758:ALA:HB3	3:G:761:TRP:HB2	1.89	0.54
7:H:167:VAL:HG11	7:H:255:LEU:HB3	1.88	0.54
11:N:385:GLY:HA3	11:N:395:LYS:HE2	1.90	0.54
10:M:252:PRO:HD2	10:M:257:VAL:HG11	1.90	0.54
11:N:180:GLN:HG3	11:N:203:LEU:HB2	1.88	0.54
5:B:114:TYR:O	5:B:121:LYS:NZ	2.41	0.54
5:B:208:ARG:NH1	6:I:132:TYR:OH	2.37	0.54
5:B:98:VAL:HG11	5:B:145:VAL:HG21	1.88	0.54
11:N:149:GLN:NE2	11:N:354:PRO:O	2.40	0.53
10:M:248:HIS:O	10:M:312:LYS:NZ	2.40	0.53
1:F:7:THR:HG22	1:F:10:THR:HG22	1.90	0.53
4:C:209:GLY:HA2	4:C:215:PHE:H	1.74	0.53
9:L:166:ALA:HB1	9:L:242:ALA:HA	1.89	0.53
1:F:85:ARG:HG2	1:F:213:PRO:HG2	1.91	0.53
1:F:357:CYS:HB2	1:F:401:ALA:HB2	1.91	0.53
4:C:216:MET:HE1	4:C:237:LEU:HD12	1.91	0.53
3:G:81:ILE:O	3:G:90:ARG:NH2	2.40	0.53
3:G:694:ASP:N	3:G:694:ASP:OD1	2.41	0.53
10:M:235:MET:HE3	10:M:268:ALA:HB2	1.90	0.53
1:F:177:ARG:NH2	2:E:75:PHE:O	2.42	0.53
5:B:217:PRO:HB3	6:I:43:ARG:HB3	1.91	0.53
21:J:201:3PE:H342	21:J:202:3PE:H351	1.90	0.53
3:G:106:PRO:HD3	4:C:515:LEU:HD21	1.91	0.53
3:G:103:HIS:HA	4:C:512:ILE:HD13	1.90	0.52
3:G:431:LEU:O	3:G:446:ALA:N	2.41	0.52
4:C:135:ASN:OD1	4:C:152:HIS:NE2	2.42	0.52
4:C:259:MET:SD	4:C:262:ARG:NE	2.82	0.52
1:F:296:GLY:O	1:F:320:ARG:NH2	2.42	0.52
5:B:186:VAL:HG23	5:B:187:VAL:HG23	1.91	0.52
9:L:546:ASP:HA	9:L:550:VAL:HB	1.89	0.52
13:J:91:GLN:HA	13:J:94:ILE:HG12	1.90	0.52
3:G:226:ALA:HB3	3:G:635:VAL:HG22	1.92	0.52
11:N:70:ASP:N	11:N:70:ASP:OD1	2.40	0.52
12:K:39:ILE:HG21	12:K:69:ALA:HB2	1.90	0.52
2:E:44:GLN:NE2	2:E:78:GLN:O	2.39	0.52
5:B:138:ILE:HG23	5:B:140:SER:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:24:ASN:HB3	13:J:27:HIS:HB2	1.91	0.52
4:C:334:THR:OG1	7:H:287:ALA:O	2.23	0.52
7:H:104:SER:HB3	7:H:107:TRP:HB2	1.91	0.52
1:F:77:PRO:O	1:F:85:ARG:NH2	2.42	0.52
7:H:149:ALA:HB2	7:H:215:PRO:HB3	1.91	0.52
9:L:247:THR:HG21	9:L:350:GLY:HA3	1.92	0.52
11:N:97:GLY:HA3	11:N:351:TYR:H	1.75	0.51
3:G:308:LEU:HG	3:G:314:VAL:HG21	1.92	0.51
9:L:159:THR:O	10:M:447:LYS:NZ	2.42	0.51
1:F:348:ARG:NH2	2:E:93:ASP:OD1	2.43	0.51
9:L:550:VAL:HG22	21:M:1001:3PE:H252	1.92	0.51
13:J:142:GLU:O	13:J:145:SER:OG	2.27	0.51
4:C:577:ARG:O	8:A:129:ARG:NH1	2.43	0.51
5:B:205:ARG:NE	6:I:136:ASP:OD2	2.41	0.51
3:G:613:ALA:HB1	3:G:617:GLU:HB2	1.92	0.51
10:M:77:ILE:HG21	10:M:137:PHE:HD2	1.75	0.51
10:M:245:PRO:HB2	10:M:313:ARG:HG3	1.93	0.51
11:N:1:MET:HE3	11:N:65:PRO:HD3	1.90	0.51
7:H:142:SER:HA	7:H:225:TYR:HA	1.92	0.51
3:G:165:ASP:O	3:G:400:LYS:NZ	2.39	0.51
4:C:65:LYS:NZ	4:C:130:LEU:O	2.44	0.51
9:L:179:VAL:HG21	10:M:430:VAL:HG23	1.93	0.51
10:M:236:PRO:HG3	10:M:244:LEU:HD22	1.92	0.51
3:G:108:CYS:O	3:G:219:ARG:NH1	2.41	0.51
4:C:351:GLU:HB3	6:I:41:PRO:HG3	1.92	0.51
5:B:185:TRP:HB3	8:A:39:GLY:HA2	1.91	0.51
5:B:204:LYS:NZ	6:I:121:GLU:O	2.43	0.51
9:L:611:VAL:HG23	9:L:612:LEU:HG	1.93	0.51
4:C:342:ASP:OD2	4:C:394:TYR:OH	2.26	0.51
9:L:425:THR:O	9:L:429:THR:HG23	2.11	0.51
11:N:106:TYR:O	11:N:110:LEU:HD12	2.11	0.51
11:N:386:ILE:HD11	11:N:426:LEU:HD21	1.92	0.51
3:G:321:ARG:NH1	3:G:570:GLU:O	2.44	0.50
4:C:14:ALA:HA	4:C:18:ARG:HH12	1.77	0.50
4:C:356:PHE:HE2	5:B:159:PRO:HD2	1.76	0.50
9:L:294:ALA:HB2	9:L:313:MET:HG2	1.93	0.50
10:M:432:ALA:HA	10:M:435:TYR:CE1	2.46	0.50
10:M:29:ARG:NH1	10:M:106:TRP:O	2.44	0.50
10:M:318:THR:HG22	10:M:435:TYR:CE2	2.46	0.50
3:G:893:ILE:HG23	3:G:897:LEU:HD22	1.93	0.50
1:F:288:LYS:NZ	1:F:333:ILE:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:527:VAL:HG22	4:C:554:THR:HG22	1.94	0.50
1:F:60:LYS:O	1:F:62:ARG:NH1	2.44	0.50
3:G:422:ASN:O	3:G:425:GLN:NE2	2.45	0.50
10:M:300:TYR:O	10:M:304:MET:HG2	2.11	0.50
3:G:308:LEU:HD23	3:G:661:LEU:HD22	1.94	0.50
4:C:176:ARG:HE	4:C:262:ARG:HD2	1.76	0.50
7:H:127:VAL:HG21	7:H:153:THR:HG21	1.93	0.50
1:F:130:ILE:HD12	1:F:171:VAL:HG22	1.93	0.50
6:I:20:ILE:HG13	7:H:288:SER:HA	1.94	0.50
1:F:255:ARG:HH11	1:F:285:LEU:HD21	1.76	0.50
11:N:51:SER:HA	11:N:54:PHE:HD1	1.77	0.50
3:G:222:ASP:OD1	3:G:712:SER:OG	2.30	0.49
4:C:403:ILE:HD13	7:H:292:PRO:HG3	1.94	0.49
10:M:79:ILE:HA	10:M:138:LEU:HD22	1.94	0.49
10:M:405:VAL:O	10:M:409:MET:HG3	2.11	0.49
11:N:246:SER:O	11:N:250:ILE:HD12	2.12	0.49
9:L:4:LEU:HD12	9:L:48:ILE:HD13	1.94	0.49
4:C:381:ARG:HG2	4:C:485:LEU:HD21	1.94	0.49
7:H:281:MET:HB3	21:A:201:3PE:H3E2	1.95	0.49
6:I:24:ALA:HB2	7:H:43:PHE:HD1	1.77	0.49
8:A:83:LEU:HD13	13:J:54:LEU:HD13	1.94	0.49
9:L:85:SER:OG	9:L:268:ARG:NH2	2.45	0.49
1:F:27:ASP:OD1	1:F:27:ASP:N	2.46	0.49
3:G:634:GLN:O	3:G:706:ARG:NE	2.44	0.49
4:C:106:ASP:OD1	4:C:106:ASP:N	2.43	0.49
11:N:177:VAL:HG21	11:N:210:MET:HE2	1.92	0.49
9:L:321:LEU:HD11	9:L:414:LEU:HB3	1.94	0.49
3:G:743:ASN:ND2	3:G:745:GLN:OE1	2.46	0.49
11:N:118:LEU:HD22	13:J:143:LEU:HD22	1.95	0.49
2:E:65:PRO:HB3	3:G:170:THR:HB	1.94	0.49
3:G:295:LEU:HB3	3:G:299:GLN:HG3	1.94	0.49
3:G:744:ASN:HA	3:G:750:ARG:HH21	1.78	0.49
10:M:176:ILE:HD11	11:N:423:TYR:HB2	1.95	0.49
11:N:339:GLY:HA3	11:N:379:MET:HE3	1.95	0.49
6:I:9:GLY:O	6:I:13:GLN:HG2	2.13	0.48
7:H:122:MET:HE1	21:J:202:3PE:H292	1.94	0.48
3:G:720:ASN:OD1	3:G:720:ASN:N	2.46	0.48
6:I:53:ASP:OD2	6:I:57:GLU:N	2.46	0.48
11:N:143:VAL:O	11:N:152:SER:OG	2.29	0.48
11:N:214:LEU:HD13	11:N:254:VAL:HG22	1.95	0.48
9:L:265:LEU:O	9:L:269:THR:OG1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:112:ALA:HB2	11:N:138:PRO:HB2	1.96	0.48
1:F:7:THR:HG23	1:F:9:GLU:H	1.79	0.48
3:G:807:PRO:HB3	3:G:882:GLY:HA3	1.95	0.48
5:B:119:GLU:HG3	5:B:121:LYS:HG2	1.95	0.48
9:L:230:SER:HB3	9:L:316:ILE:HG21	1.95	0.48
1:F:320:ARG:NH1	16:F:503:NAI:O2D	2.46	0.48
4:C:133:ASN:HB3	4:C:422:TRP:HA	1.95	0.48
5:B:9:ASP:N	5:B:9:ASP:OD1	2.44	0.48
7:H:239:VAL:O	7:H:243:ILE:HG13	2.13	0.48
9:L:180:PHE:HD1	9:L:221:MET:HE1	1.77	0.48
3:G:451:ALA:O	3:G:456:GLN:NE2	2.39	0.48
10:M:179:GLN:HB3	11:N:422:LEU:HD21	1.95	0.48
12:K:43:ALA:HB1	12:K:62:TYR:HD1	1.79	0.48
3:G:97:LEU:HD22	3:G:154:ILE:HB	1.96	0.48
9:L:403:LEU:HB3	9:L:493:LEU:HD11	1.95	0.48
11:N:224:HIS:CD2	11:N:287:MET:HE1	2.49	0.48
12:K:29:LEU:O	12:K:33:ILE:HD12	2.13	0.48
7:H:121:MET:HG3	13:J:57:ILE:HG13	1.95	0.48
10:M:30:TRP:O	10:M:34:ILE:HG13	2.14	0.48
4:C:154:ASN:OD1	4:C:154:ASN:N	2.46	0.48
5:B:47:ASN:ND2	5:B:179:GLU:O	2.35	0.48
2:E:142:ASN:HA	2:E:150:HIS:O	2.14	0.47
6:I:142:PRO:HB2	6:I:146:PRO:HA	1.96	0.47
11:N:60:ALA:HA	11:N:69:VAL:O	2.14	0.47
4:C:334:THR:HG21	6:I:20:ILE:HD12	1.96	0.47
6:I:53:ASP:OD2	6:I:56:GLY:N	2.48	0.47
7:H:77:PHE:HB2	7:H:138:ASN:HD22	1.78	0.47
5:B:5:LEU:O	5:B:22:GLN:HA	2.14	0.47
11:N:256:ARG:HD3	11:N:260:TYR:CE1	2.50	0.47
2:E:134:LEU:HD12	2:E:142:ASN:HB2	1.96	0.47
9:L:272:LEU:HA	9:L:275:MET:HE3	1.97	0.47
1:F:100:LYS:HE3	1:F:323:THR:HB	1.97	0.47
4:C:541:LYS:NZ	4:C:592:ASP:OD1	2.33	0.47
6:I:80:ALA:HB2	6:I:90:GLU:HB2	1.96	0.47
11:N:244:THR:O	11:N:248:ILE:HG13	2.14	0.47
12:K:44:LEU:O	12:K:48:VAL:HG23	2.14	0.47
4:C:553:SER:OG	4:C:554:THR:N	2.47	0.47
9:L:501:ALA:O	9:L:505:ILE:HG12	2.14	0.47
10:M:219:VAL:HG13	21:M:1002:3PE:H252	1.96	0.47
3:G:106:PRO:O	3:G:219:ARG:NH2	2.48	0.47
4:C:143:ASP:OD1	4:C:157:ARG:NH1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:475:LEU:HD22	9:L:479:LEU:HD12	1.96	0.47
1:F:353:TRP:HZ2	3:G:44:VAL:HB	1.80	0.47
3:G:474:VAL:HG23	3:G:477:ILE:HD11	1.97	0.47
5:B:126:MET:HE3	5:B:165:TYR:HB2	1.97	0.47
11:N:77:THR:HG23	11:N:117:ILE:HD12	1.97	0.47
1:F:85:ARG:HB2	1:F:125:ALA:HA	1.97	0.47
3:G:669:THR:OG1	3:G:670:GLN:N	2.47	0.47
10:M:90:MET:HE3	10:M:269:TYR:HB2	1.97	0.47
3:G:118:ASP:OD1	3:G:762:ASN:ND2	2.48	0.47
4:C:123:HIS:HA	4:C:148:THR:O	2.15	0.47
9:L:490:MET:HE2	9:L:490:MET:HB3	1.81	0.47
10:M:415:PHE:HB2	10:M:422:THR:HG21	1.96	0.47
3:G:122:MET:HE3	3:G:122:MET:HB2	1.75	0.46
3:G:318:GLY:O	3:G:571:ASN:ND2	2.42	0.46
5:B:69:VAL:HA	5:B:72:PHE:HB2	1.97	0.46
4:C:240:GLU:HG2	4:C:580:LEU:HD23	1.97	0.46
11:N:64:THR:HB	11:N:67:MET:H	1.80	0.46
7:H:172:GLY:O	13:J:127:LYS:NZ	2.47	0.46
9:L:232:GLN:HE22	9:L:317:GLY:HA2	1.80	0.46
9:L:260:THR:HB	9:L:335:LEU:HD11	1.97	0.46
9:L:311:SER:HB2	9:L:386:LEU:HD21	1.97	0.46
10:M:16:LEU:O	10:M:20:THR:OG1	2.18	0.46
1:F:12:PRO:HB3	1:F:235:TRP:HH2	1.79	0.46
2:E:85:GLY:H	2:E:127:THR:HG1	1.61	0.46
11:N:2:THR:OG1	11:N:3:ILE:N	2.45	0.46
3:G:402:LYS:O	3:G:406:MET:HG3	2.16	0.46
3:G:557:GLU:OE2	3:G:562:ARG:NH1	2.49	0.46
7:H:118:PHE:HE1	21:J:202:3PE:H251	1.80	0.46
4:C:312:GLU:OE2	4:C:447:TYR:OH	2.30	0.46
9:L:318:TYR:OH	9:L:418:GLY:O	2.28	0.46
9:L:606:LEU:HB3	13:J:106:VAL:HG11	1.97	0.46
11:N:155:ALA:HB1	11:N:230:VAL:HA	1.98	0.46
3:G:36:CYS:O	3:G:161:ARG:NH1	2.38	0.46
4:C:276:GLU:OE2	4:C:540:THR:OG1	2.34	0.46
5:B:126:MET:HG3	5:B:155:ILE:HD12	1.97	0.46
9:L:240:ALA:HB1	9:L:306:ARG:HE	1.80	0.46
11:N:66:LEU:HA	11:N:124:HIS:HB2	1.96	0.46
1:F:188:ASN:ND2	1:F:196:ASN:O	2.41	0.45
3:G:498:PRO:HG3	3:G:522:LEU:HD22	1.97	0.45
9:L:1:MET:HA	9:L:48:ILE:HG12	1.98	0.45
10:M:117:HIS:O	10:M:121:MET:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:549:THR:HB	4:C:558:ARG:HB3	1.99	0.45
7:H:15:ILE:HG23	8:A:18:ILE:HG21	1.98	0.45
9:L:488:GLY:O	9:L:492:THR:HG23	2.16	0.45
1:F:179:ILE:HG12	1:F:351:CYS:HB3	1.99	0.45
3:G:465:HIS:HA	3:G:471:ALA:HB3	1.98	0.45
10:M:268:ALA:HA	10:M:271:LEU:HD12	1.98	0.45
1:F:384:LEU:HD22	1:F:408:LEU:HD21	1.98	0.45
3:G:558:LEU:HD21	3:G:566:VAL:HB	1.98	0.45
4:C:69:LYS:HE3	4:C:107:ARG:HG2	1.98	0.45
7:H:262:GLY:HA3	7:H:270:TRP:CD1	2.52	0.45
9:L:354:LEU:HD12	9:L:354:LEU:HA	1.83	0.45
4:C:206:MET:HE1	4:C:244:ASP:HB3	1.98	0.45
4:C:230:ALA:HB3	4:C:252:HIS:HB2	1.97	0.45
11:N:151:ARG:NH1	11:N:232:GLN:O	2.49	0.45
21:J:201:3PE:H261	21:J:202:3PE:H241	1.98	0.45
1:F:429:ASN:ND2	3:G:128:ARG:O	2.50	0.45
4:C:220:LEU:HD11	4:C:585:ILE:HD11	1.99	0.45
9:L:392:VAL:HG23	9:L:393:THR:HG23	1.98	0.45
1:F:395:LYS:HE3	3:G:65:LEU:HD12	1.99	0.45
10:M:101:ALA:O	10:M:256:SER:OG	2.33	0.45
1:F:133:ARG:NE	1:F:135:GLU:OE1	2.50	0.45
4:C:302:ARG:NH1	4:C:489:PRO:O	2.50	0.45
4:C:547:TYR:HB3	4:C:560:ARG:HB3	1.99	0.45
9:L:183:PHE:HD2	9:L:221:MET:HE2	1.82	0.45
11:N:65:PRO:HG2	13:J:136:PRO:HB3	1.99	0.45
1:F:287:PHE:HZ	1:F:290:TRP:HB3	1.82	0.44
3:G:451:ALA:HB1	3:G:455:ASP:HB2	1.99	0.44
4:C:271:TYR:OH	5:B:135:MET:O	2.33	0.44
13:J:67:PHE:O	13:J:71:VAL:HG23	2.16	0.44
1:F:133:ARG:NH2	2:E:133:CYS:O	2.45	0.44
3:G:212:THR:HG22	3:G:832:VAL:HG21	1.99	0.44
3:G:232:GLN:HB2	14:G:1003:SF4:S3	2.56	0.44
3:G:321:ARG:HE	3:G:826:LEU:HD11	1.83	0.44
4:C:324:SER:HB2	4:C:336:VAL:HG23	1.99	0.44
6:I:19:MET:HE2	6:I:19:MET:HB3	1.88	0.44
11:N:340:ALA:O	11:N:344:VAL:HG23	2.16	0.44
11:N:20:THR:HA	11:N:23:VAL:HB	1.99	0.44
11:N:100:ASP:OD2	13:J:160:ARG:NH2	2.50	0.44
5:B:67:GLU:HG3	5:B:159:PRO:HB2	1.98	0.44
10:M:2:LEU:HD13	10:M:46:LEU:HD21	1.99	0.44
10:M:252:PRO:HD2	10:M:257:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:101:THR:HA	5:B:129:CYS:HB3	1.98	0.44
8:A:20:LEU:O	8:A:24:ILE:HG12	2.18	0.44
9:L:196:ASN:HB3	9:L:199:GLU:HB2	1.98	0.44
10:M:233:VAL:HG23	10:M:240:LEU:HB3	1.99	0.44
1:F:274:LEU:O	1:F:280:GLY:N	2.47	0.44
3:G:299:GLN:H	3:G:299:GLN:HG2	1.57	0.44
5:B:143:GLN:OE1	6:I:98:ARG:NH2	2.43	0.44
9:L:253:ILE:HG23	9:L:258:MET:HB3	1.99	0.44
13:J:64:MET:O	13:J:68:VAL:HG23	2.18	0.44
4:C:74:LEU:HA	4:C:102:LEU:HD23	1.98	0.44
4:C:187:LYS:HE2	8:A:44:ARG:HD2	1.99	0.44
5:B:6:THR:HG23	5:B:192:VAL:HB	2.00	0.44
6:I:4:LYS:HE3	6:I:4:LYS:HB2	1.88	0.44
7:H:177:THR:HA	7:H:180:VAL:HG22	1.98	0.44
9:L:344:LEU:HB2	9:L:460:LEU:HB3	2.00	0.44
9:L:369:ARG:HB3	9:L:437:PHE:HB3	1.99	0.44
10:M:418:VAL:HA	10:M:419:PRO:HD3	1.86	0.44
12:K:26:ARG:NH2	13:J:87:TRP:HB3	2.33	0.44
3:G:206:GLY:N	14:G:1001:SF4:S2	2.83	0.44
10:M:315:ILE:O	10:M:318:THR:OG1	2.24	0.44
1:F:391:LEU:HD22	1:F:401:ALA:HB1	1.98	0.44
4:C:576:ILE:HD12	4:C:576:ILE:HA	1.91	0.44
9:L:127:MET:HG2	9:L:257:THR:HG22	1.99	0.44
9:L:236:GLN:HB2	9:L:313:MET:HE2	2.00	0.44
10:M:45:GLN:O	10:M:49:GLN:HB2	2.16	0.44
10:M:398:MET:O	10:M:401:THR:OG1	2.32	0.44
11:N:39:THR:O	11:N:43:ILE:HD12	2.18	0.44
13:J:139:LEU:HD12	13:J:139:LEU:H	1.82	0.44
1:F:297:THR:HG23	1:F:320:ARG:HB2	1.99	0.43
3:G:676:ASP:HA	3:G:679:VAL:HG22	2.01	0.43
4:C:551:ASP:HB2	4:C:557:TYR:HB2	1.99	0.43
7:H:114:ILE:HG22	7:H:117:LEU:HD12	2.00	0.43
9:L:403:LEU:HD22	9:L:415:MET:HG3	2.00	0.43
10:M:60:ILE:HA	10:M:61:PRO:HA	1.86	0.43
1:F:307:LEU:HD23	1:F:314:ILE:HD13	2.00	0.43
7:H:102:PRO:HD2	7:H:254:THR:HG21	2.00	0.43
7:H:114:ILE:HB	7:H:117:LEU:HB2	2.00	0.43
2:E:145:ILE:HD12	2:E:150:HIS:CE1	2.53	0.43
4:C:464:TYR:O	4:C:468:MET:HG2	2.18	0.43
11:N:177:VAL:HG22	11:N:203:LEU:HD12	2.00	0.43
11:N:346:LEU:HD12	11:N:372:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:4:LEU:HD11	9:L:81:LEU:HD13	2.00	0.43
3:G:138:ARG:NH1	6:I:162:ASP:OD2	2.48	0.43
4:C:302:ARG:HD2	4:C:491:GLY:H	1.83	0.43
10:M:2:LEU:HB3	10:M:42:LEU:HD21	2.00	0.43
2:E:136:ASN:HB3	2:E:142:ASN:ND2	2.34	0.43
9:L:588:ASN:OD1	9:L:588:ASN:N	2.50	0.43
11:N:137:LEU:HD21	12:K:71:ALA:HB1	2.01	0.43
11:N:408:TRP:HB2	20:N:502:LFA:H102	2.00	0.43
4:C:272:THR:HG21	4:C:287:TYR:CG	2.54	0.43
8:A:41:ALA:HB3	8:A:46:LYS:HE3	2.01	0.43
11:N:277:ALA:HB1	11:N:311:VAL:HG23	2.00	0.43
1:F:177:ARG:HG3	1:F:179:ILE:HG22	2.00	0.43
2:E:100:ASN:HB3	2:E:141:PRO:HD3	2.01	0.43
4:C:233:ILE:HD11	4:C:245:CYS:HB3	2.01	0.43
7:H:6:PRO:HA	7:H:9:ILE:HG12	2.00	0.43
9:L:381:VAL:HG21	9:L:461:LEU:HG	2.01	0.43
3:G:369:ARG:NH2	3:G:775:GLY:O	2.47	0.42
10:M:314:LEU:O	10:M:318:THR:HG23	2.19	0.42
11:N:255:MET:HE3	11:N:255:MET:HB3	1.88	0.42
7:H:167:VAL:HG13	7:H:188:ASN:HD22	1.85	0.42
7:H:265:LEU:HB2	7:H:270:TRP:CD1	2.54	0.42
10:M:306:PHE:O	10:M:442:ARG:NH2	2.43	0.42
11:N:64:THR:HB	11:N:66:LEU:H	1.85	0.42
7:H:92:THR:O	7:H:96:LEU:HG	2.20	0.42
9:L:239:LEU:HD22	9:L:313:MET:HE3	2.01	0.42
2:E:58:ILE:HA	2:E:61:VAL:HG12	2.00	0.42
3:G:178:HIS:CD2	3:G:178:HIS:H	2.37	0.42
3:G:255:TYR:OH	3:G:776:GLY:O	2.26	0.42
4:C:169:LEU:HD23	4:C:169:LEU:HA	1.90	0.42
9:L:299:LEU:HD11	9:L:427:LEU:HD22	2.01	0.42
1:F:11:HIS:HD2	1:F:263:GLU:HB3	1.84	0.42
5:B:3:TYR:OH	5:B:180:ARG:NH2	2.49	0.42
7:H:21:ILE:O	7:H:25:VAL:HG12	2.20	0.42
11:N:288:ALA:HB2	11:N:300:TYR:HB2	2.02	0.42
3:G:232:GLN:OE1	3:G:827:SER:OG	2.35	0.42
3:G:342:GLY:HA3	3:G:571:ASN:HD21	1.85	0.42
4:C:170:ARG:O	4:C:258:LYS:NZ	2.52	0.42
4:C:438:VAL:HG11	4:C:537:ILE:HA	2.01	0.42
7:H:160:LEU:O	7:H:163:SER:OG	2.32	0.42
9:L:103:ALA:HA	9:L:106:TYR:HB3	2.02	0.42
9:L:252:LEU:O	9:L:257:THR:OG1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:484:PRO:O	10:M:488:THR:OG1	2.26	0.42
7:H:281:MET:HE2	21:A:201:3PE:H3D1	2.00	0.42
10:M:224:MET:HE3	10:M:224:MET:HB3	1.81	0.42
11:N:154:GLU:HG2	12:K:95:VAL:HG13	2.01	0.42
13:J:75:ASN:OD1	13:J:75:ASN:N	2.52	0.42
1:F:102:ARG:O	1:F:106:GLU:HB2	2.20	0.42
9:L:69:SER:HA	9:L:73:PHE:O	2.20	0.42
11:N:67:MET:HE3	13:J:139:LEU:HD22	2.02	0.42
11:N:113:ALA:O	11:N:117:ILE:HG12	2.19	0.42
13:J:90:PRO:HA	13:J:93:TRP:NE1	2.35	0.42
3:G:714:ARG:NH1	3:G:740:MET:HE3	2.33	0.42
7:H:257:PHE:O	7:H:274:LYS:NZ	2.53	0.42
21:L:804:3PE:H322	10:M:173:LYS:HA	2.02	0.42
10:M:192:LEU:HB2	10:M:223:LEU:HD13	2.02	0.42
2:E:145:ILE:HG22	2:E:146:ASP:H	1.85	0.42
3:G:137:HIS:NE2	3:G:180:ASN:OD1	2.48	0.42
8:A:80:VAL:HA	8:A:83:LEU:HD23	2.02	0.42
11:N:273:LEU:HD22	11:N:310:LEU:HD11	2.02	0.42
3:G:769:LYS:O	3:G:779:ARG:NH1	2.51	0.41
9:L:188:LEU:HD23	9:L:188:LEU:HA	1.96	0.41
11:N:5:PRO:HA	11:N:8:LEU:HB2	2.02	0.41
11:N:9:ILE:HD13	11:N:9:ILE:HA	1.89	0.41
12:K:26:ARG:CZ	13:J:87:TRP:HB3	2.50	0.41
12:K:92:ILE:HD12	12:K:92:ILE:HA	1.91	0.41
3:G:112:GLY:HA3	3:G:221:TRP:HZ3	1.85	0.41
3:G:502:SER:OG	3:G:503:GLY:N	2.53	0.41
4:C:594:VAL:HG23	4:C:597:ASP:HB2	2.02	0.41
9:L:139:MET:SD	9:L:265:LEU:HD11	2.60	0.41
11:N:139:LEU:HB3	11:N:159:TYR:HE2	1.84	0.41
13:J:129:VAL:O	13:J:133:LEU:HB2	2.20	0.41
3:G:220:LYS:NZ	3:G:762:ASN:O	2.51	0.41
5:B:202:GLU:OE1	5:B:205:ARG:NH1	2.53	0.41
9:L:431:ARG:NH2	21:L:803:3PE:O14	2.53	0.41
10:M:232:ALA:O	10:M:237:VAL:N	2.52	0.41
1:F:182:GLU:O	1:F:186:LEU:N	2.48	0.41
3:G:723:VAL:HG11	6:I:127:ARG:HG3	2.01	0.41
4:C:342:ASP:OD1	4:C:386:TRP:NE1	2.49	0.41
3:G:157:TYR:N	14:G:1002:SF4:S4	2.90	0.41
3:G:468:ASP:OD1	3:G:797:TYR:OH	2.31	0.41
4:C:88:ARG:NH2	4:C:92:PRO:O	2.42	0.41
4:C:199:PHE:CG	4:C:234:VAL:HG11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:558:ARG:NH1	4:C:559:THR:O	2.54	0.41
8:A:67:LYS:HB3	8:A:125:TRP:HB2	2.03	0.41
9:L:107:MET:HE3	9:L:107:MET:HB3	1.82	0.41
10:M:339:GLN:HE22	10:M:490:HIS:HA	1.86	0.41
13:J:132:THR:HA	13:J:136:PRO:HD2	2.02	0.41
3:G:224:GLN:O	3:G:242:GLY:HA2	2.21	0.41
3:G:479:PRO:HA	3:G:482:GLN:HB2	2.02	0.41
4:C:377:ASP:OD1	4:C:377:ASP:N	2.49	0.41
10:M:149:PRO:O	10:M:153:LEU:HG	2.20	0.41
3:G:216:ARG:NH1	6:I:90:GLU:OE1	2.37	0.41
3:G:702:GLN:HB3	4:C:172:ASP:HA	2.02	0.41
10:M:51:GLY:O	10:M:55:THR:OG1	2.39	0.41
12:K:98:MET:HE3	12:K:98:MET:HB2	1.93	0.41
4:C:167:HIS:HA	4:C:168:PRO:HD3	1.90	0.41
4:C:539:ALA:HB2	4:C:544:ASN:HB2	2.03	0.41
7:H:279:MET:O	7:H:283:ILE:HG12	2.21	0.41
21:L:804:3PE:H3H1	21:L:804:3PE:H2G1	2.02	0.41
11:N:97:GLY:HA3	11:N:351:TYR:N	2.35	0.41
1:F:84:ILE:HG23	1:F:126:TYR:CE1	2.56	0.41
1:F:412:ILE:HD13	1:F:412:ILE:HA	1.88	0.41
3:G:545:ILE:HG23	3:G:684:GLU:HG3	2.03	0.41
4:C:12:GLU:HA	4:C:13:PRO:HD3	1.87	0.41
4:C:172:ASP:OD1	4:C:172:ASP:N	2.50	0.41
4:C:451:ASP:OD1	4:C:451:ASP:N	2.43	0.41
5:B:89:SER:HB3	5:B:92:GLN:HG3	2.02	0.41
7:H:44:GLN:OE1	7:H:46:ARG:NH2	2.47	0.41
8:A:69:TYR:O	8:A:73:MET:HG3	2.21	0.41
9:L:485:LEU:HD12	9:L:485:LEU:HA	1.94	0.41
11:N:125:LEU:HB3	11:N:174:MET:SD	2.61	0.41
11:N:336:SER:HA	11:N:379:MET:SD	2.61	0.41
12:K:77:LEU:HD21	13:J:66:LEU:HD12	2.03	0.41
13:J:30:LEU:HA	13:J:33:ILE:HD12	2.03	0.41
1:F:86:TYR:O	1:F:214:THR:HA	2.21	0.41
1:F:291:GLN:HA	1:F:292:PRO:HD3	1.92	0.41
3:G:320:PRO:HB2	3:G:537:SER:HB2	2.03	0.41
4:C:44:ARG:NH1	4:C:294:LEU:O	2.54	0.41
4:C:336:VAL:HG21	19:C:701:DCQ:H10	2.03	0.41
5:B:70:THR:O	5:B:73:THR:OG1	2.38	0.41
1:F:325:LEU:HD23	1:F:325:LEU:HA	1.98	0.40
9:L:239:LEU:HG	9:L:254:HIS:HE1	1.86	0.40
9:L:312:THR:HG23	9:L:338:HIS:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:554:LEU:HD21	21:M:1001:3PE:H221	2.01	0.40
11:N:20:THR:O	11:N:24:VAL:HG22	2.20	0.40
3:G:592:VAL:HB	3:G:606:ALA:HA	2.02	0.40
3:G:631:ARG:NH2	3:G:688:ILE:O	2.55	0.40
4:C:197:LEU:HD11	5:B:105:LYS:HG2	2.03	0.40
9:L:266:ILE:HB	9:L:323:LEU:HD13	2.02	0.40
10:M:410:ILE:O	10:M:414:SER:OG	2.37	0.40
13:J:59:TYR:O	13:J:63:ILE:HG12	2.22	0.40
9:L:143:TRP:CZ3	9:L:265:LEU:HD13	2.56	0.40
10:M:65:SER:HB3	10:M:83:ILE:HG22	2.03	0.40
11:N:119:LEU:HD23	11:N:119:LEU:HA	1.88	0.40
3:G:257:GLY:O	3:G:369:ARG:NH1	2.52	0.40
3:G:399:VAL:HA	3:G:429:HIS:HB2	2.02	0.40
4:C:360:PRO:O	6:I:45:ARG:NH1	2.37	0.40
10:M:71:TRP:HB2	10:M:79:ILE:HG13	2.03	0.40
11:N:177:VAL:HG23	11:N:206:GLY:HA3	2.04	0.40
1:F:130:ILE:HD13	1:F:143:LEU:HD13	2.04	0.40
5:B:68:MET:O	5:B:71:SER:OG	2.33	0.40
7:H:79:ASP:OD1	7:H:79:ASP:N	2.55	0.40
7:H:294:TYR:HA	7:H:297:VAL:HB	2.04	0.40
9:L:273:PHE:HB3	9:L:280:LEU:HD13	2.03	0.40
10:M:259:LEU:HA	10:M:263:LEU:HD12	2.03	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%)	425 (97%)	12 (3%)	0	100	100
2	E	154/166 (93%)	147 (96%)	7 (4%)	0	100	100
3	G	903/908 (99%)	877 (97%)	26 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	C	587/600 (98%)	565 (96%)	22 (4%)	0	100	100
5	B	204/220 (93%)	195 (96%)	9 (4%)	0	100	100
6	I	178/180 (99%)	173 (97%)	5 (3%)	0	100	100
7	H	320/325 (98%)	309 (97%)	11 (3%)	0	100	100
8	A	127/147 (86%)	123 (97%)	4 (3%)	0	100	100
9	L	594/613 (97%)	572 (96%)	22 (4%)	0	100	100
10	M	502/509 (99%)	487 (97%)	15 (3%)	0	100	100
11	N	474/485 (98%)	461 (97%)	12 (2%)	1 (0%)	43	71
12	K	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
13	J	160/184 (87%)	157 (98%)	3 (2%)	0	100	100
All	All	4738/4882 (97%)	4587 (97%)	150 (3%)	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%)	352 (100%)	1 (0%)	86	84
2	E	129/139 (93%)	126 (98%)	3 (2%)	44	63
3	G	729/735 (99%)	728 (100%)	1 (0%)	88	89
4	C	509/519 (98%)	507 (100%)	2 (0%)	84	83
5	B	183/192 (95%)	182 (100%)	1 (0%)	81	81
6	I	154/154 (100%)	154 (100%)	0	100	100
7	H	266/269 (99%)	264 (99%)	2 (1%)	73	77
8	A	102/119 (86%)	101 (99%)	1 (1%)	68	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	L	472/486 (97%)	469 (99%)	3 (1%)	78 80
10	M	413/418 (99%)	410 (99%)	3 (1%)	76 78
11	N	378/385 (98%)	378 (100%)	0	100 100
12	K	79/79 (100%)	77 (98%)	2 (2%)	42 62
13	J	128/146 (88%)	128 (100%)	0	100 100
All	All	3895/4000 (97%)	3876 (100%)	19 (0%)	78 81

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	126	TYR
2	E	95	VAL
2	E	120	THR
2	E	121	THR
3	G	459	LEU
4	C	110	ASP
4	C	581	VAL
5	B	6	THR
7	H	241	GLU
7	H	282	PHE
8	A	54	ILE
9	L	221	MET
9	L	265	LEU
9	L	419	LEU
10	M	38	LEU
10	M	204	THR
10	M	440	LEU
12	K	22	LEU
12	K	89	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	53	GLN
1	F	218	ASN
1	F	291	GLN
3	G	16	ASN
3	G	253	ASN
3	G	348	GLN

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Mol	Chain	Res	Type
3	G	422	ASN
3	G	571	ASN
3	G	658	HIS
3	G	743	ASN
4	C	20	HIS
4	C	167	HIS
5	B	111	GLN
6	I	23	HIS
6	I	64	ASN
6	I	149	ASN
9	L	409	ASN
9	L	537	ASN
10	M	339	GLN
11	N	199	ASN
13	J	117	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 oligosaccharides 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	$\#\|Z\|>2$
21	3PE	J	202	-	35,35,50	0.36	0	38,40,55	0.33	0
17	FES	G	1004	3	0,4,4	-	-	-		
14	SF4	B	301	5	0,12,12	-	-	-		
21	3PE	M	1001	-	46,46,50	0.31	0	49,51,55	0.30	0
16	NAI	F	503	-	45,48,48	0.26	0	60,73,73	0.32	0
14	SF4	F	501	1	0,12,12	-	-	-		
17	FES	E	201	2	0,4,4	-	-	-		
20	LFA	N	502	-	13,13,19	0.14	0	12,12,18	0.12	0
20	LFA	H	601	-	19,19,19	0.14	0	18,18,18	0.10	0
21	3PE	J	201	-	41,41,50	0.33	0	44,46,55	0.31	0
21	3PE	M	1002	-	46,46,50	0.31	0	49,51,55	0.31	0
21	3PE	L	804	-	50,50,50	0.30	0	53,55,55	0.25	0
15	FMN	F	502	-	33,33,33	1.06	2 (6%)	48,50,50	1.21	6 (12%)
21	3PE	A	201	-	50,50,50	0.30	0	53,55,55	0.31	0
19	DCQ	C	701	-	23,23,23	0.25	0	26,29,29	0.45	0
20	LFA	N	501	-	14,14,19	0.16	0	13,13,18	0.12	0
21	3PE	L	803	-	35,35,50	0.36	0	38,40,55	0.35	0
14	SF4	G	1002	3	0,12,12	-	-	-		
20	LFA	L	802	-	19,19,19	0.15	0	18,18,18	0.10	0
14	SF4	G	1003	3	0,12,12	-	-	-		
14	SF4	I	202	6	0,12,12	-	-	-		
14	SF4	G	1001	3	0,12,12	-	-	-		
14	SF4	I	201	6	0,12,12	-	-	-		
21	3PE	L	801	-	50,50,50	0.30	0	53,55,55	0.27	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
21	3PE	J	202	-	-	8/39/39/54	-
17	FES	G	1004	3	-	-	0/1/1/1
21	3PE	M	1001	-	-	7/50/50/54	-
14	SF4	B	301	5	-	-	0/6/5/5
16	NAI	F	503	-	-	4/29/72/72	0/5/5/5
14	SF4	F	501	1	-	-	0/6/5/5
17	FES	E	201	2	-	-	0/1/1/1
20	LFA	N	502	-	-	0/11/11/17	-
20	LFA	H	601	-	-	2/17/17/17	-
21	3PE	J	201	-	-	10/45/45/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	3PE	M	1002	-	-	11/50/50/54	-
21	3PE	L	804	-	-	12/54/54/54	-
15	FMN	F	502	-	-	9/18/18/18	0/3/3/3
21	3PE	A	201	-	-	14/54/54/54	-
19	DCQ	C	701	-	-	0/14/38/38	0/1/1/1
20	LFA	N	501	-	-	0/12/12/17	-
21	3PE	L	803	-	-	6/39/39/54	-
14	SF4	G	1002	3	-	-	0/6/5/5
20	LFA	L	802	-	-	0/17/17/17	-
14	SF4	G	1003	3	-	-	0/6/5/5
14	SF4	I	202	6	-	-	0/6/5/5
14	SF4	G	1001	3	-	-	0/6/5/5
14	SF4	I	201	6	-	-	0/6/5/5
21	3PE	L	801	-	-	11/54/54/54	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	502	FMN	C4A-N5	3.73	1.38	1.30
15	F	502	FMN	C10-N1	2.37	1.38	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	502	FMN	C4-N3-C2	-3.16	119.81	125.64
15	F	502	FMN	C4A-C10-N10	2.73	120.47	116.48
15	F	502	FMN	C4A-C4-N3	2.65	119.93	113.19
15	F	502	FMN	O4-C4-C4A	-2.52	119.91	126.60
15	F	502	FMN	C10-C4A-N5	-2.31	119.94	124.86
15	F	502	FMN	C4A-C10-N1	-2.23	119.55	124.73

There are no chirality outliers.

All (94) 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'-O3'
15	F	502	FMN	C1'-C2'-C3'-C4'
15	F	502	FMN	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
15	F	502	FMN	C5'-O5'-P-O2P
21	A	201	3PE	C1-O11-P-O12
21	A	201	3PE	C11-O13-P-O11
21	A	201	3PE	C11-O13-P-O12
21	A	201	3PE	C11-O13-P-O14
21	A	201	3PE	O13-C11-C12-N
21	L	801	3PE	C11-O13-P-O14
21	L	803	3PE	C11-O13-P-O11
21	L	803	3PE	O13-C11-C12-N
21	L	804	3PE	C1-O11-P-O12
21	L	804	3PE	C1-O11-P-O13
21	L	804	3PE	C1-O11-P-O14
21	L	804	3PE	C11-O13-P-O11
21	L	804	3PE	O13-C11-C12-N
21	M	1001	3PE	C1-O11-P-O12
21	M	1002	3PE	C1-O11-P-O12
21	M	1002	3PE	C11-O13-P-O11
21	M	1002	3PE	C11-O13-P-O12
21	M	1002	3PE	C11-O13-P-O14
21	J	201	3PE	C1-O11-P-O12
21	J	201	3PE	C1-O11-P-O13
21	J	201	3PE	C11-O13-P-O12
21	J	201	3PE	O13-C11-C12-N
21	J	202	3PE	C11-O13-P-O11
21	J	202	3PE	C11-O13-P-O12
21	J	202	3PE	C11-O13-P-O14
21	J	202	3PE	O13-C11-C12-N
21	M	1002	3PE	C2-C1-O11-P
21	J	202	3PE	C21-C22-C23-C24
21	M	1001	3PE	C1-O11-P-O13
21	J	201	3PE	C11-O13-P-O11
15	F	502	FMN	O2'-C2'-C3'-O3'
21	M	1002	3PE	C3C-C3D-C3E-C3F
21	M	1002	3PE	C3E-C3F-C3G-C3H
15	F	502	FMN	O2'-C2'-C3'-C4'
21	L	804	3PE	C3B-C3C-C3D-C3E
21	A	201	3PE	C3D-C3E-C3F-C3G
21	L	801	3PE	C2C-C2D-C2E-C2F
21	L	804	3PE	O21-C21-C22-C23
21	L	801	3PE	C39-C3A-C3B-C3C
21	J	201	3PE	C2-C1-O11-P
21	M	1001	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
16	F	503	NAI	C5B-O5B-PA-O3
21	L	801	3PE	C23-C24-C25-C26
21	A	201	3PE	C27-C28-C29-C2A
21	L	801	3PE	C11-O13-P-O11
21	L	804	3PE	C2-C1-O11-P
21	L	803	3PE	C11-O13-P-O12
21	L	804	3PE	C11-O13-P-O12
21	J	201	3PE	C1-O11-P-O14
21	J	202	3PE	C12-C11-O13-P
21	L	801	3PE	C3A-C3B-C3C-C3D
21	J	201	3PE	O21-C21-C22-C23
21	L	801	3PE	C25-C26-C27-C28
21	M	1002	3PE	C26-C27-C28-C29
21	L	804	3PE	C25-C26-C27-C28
21	M	1001	3PE	C34-C35-C36-C37
21	J	202	3PE	C1-O11-P-O13
21	L	801	3PE	C31-C32-C33-C34
21	A	201	3PE	C29-C2A-C2B-C2C
21	J	201	3PE	C23-C24-C25-C26
16	F	503	NAI	O4D-C1D-N1N-C2N
20	H	601	LFA	C4-C5-C6-C7
16	F	503	NAI	PN-O3-PA-O5B
21	L	801	3PE	O13-C11-C12-N
15	F	502	FMN	C5'-O5'-P-O3P
20	H	601	LFA	C5-C6-C7-C8
21	L	803	3PE	O31-C31-C32-C33
21	L	801	3PE	C3D-C3E-C3F-C3G
21	M	1001	3PE	O21-C21-C22-C23
21	L	804	3PE	O22-C21-C22-C23
21	L	804	3PE	O21-C2-C3-O31
21	J	201	3PE	C22-C23-C24-C25
21	A	201	3PE	C1-O11-P-O13
21	M	1002	3PE	C1-O11-P-O13
21	A	201	3PE	O21-C21-C22-C23
21	A	201	3PE	C1-O11-P-O14
21	L	803	3PE	C1-O11-P-O14
21	M	1002	3PE	C1-O11-P-O14
21	J	202	3PE	C1-O11-P-O14
21	M	1001	3PE	O22-C21-C22-C23
21	L	801	3PE	O11-C1-C2-C3
21	M	1002	3PE	O13-C11-C12-N
21	L	803	3PE	O32-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
21	A	201	3PE	O31-C31-C32-C33
21	M	1001	3PE	O31-C31-C32-C33
21	A	201	3PE	O22-C21-C22-C23
21	A	201	3PE	O32-C31-C32-C33
16	F	503	NAI	C2D-C1D-N1N-C2N

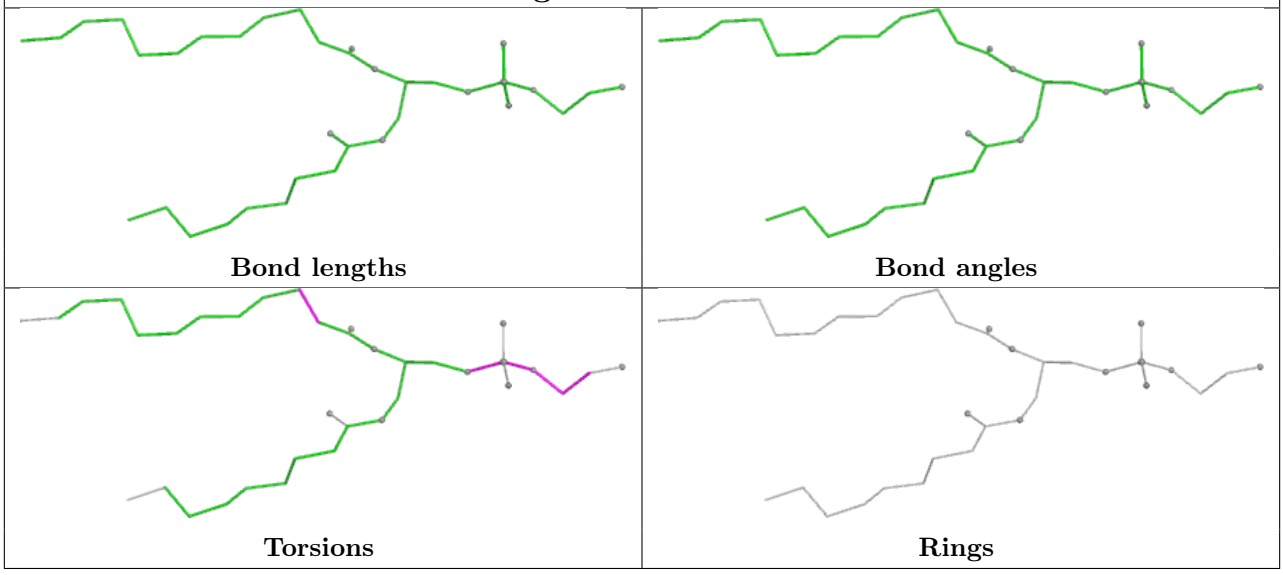
There are no ring outliers.

14 monomers are involved in 22 short contacts:

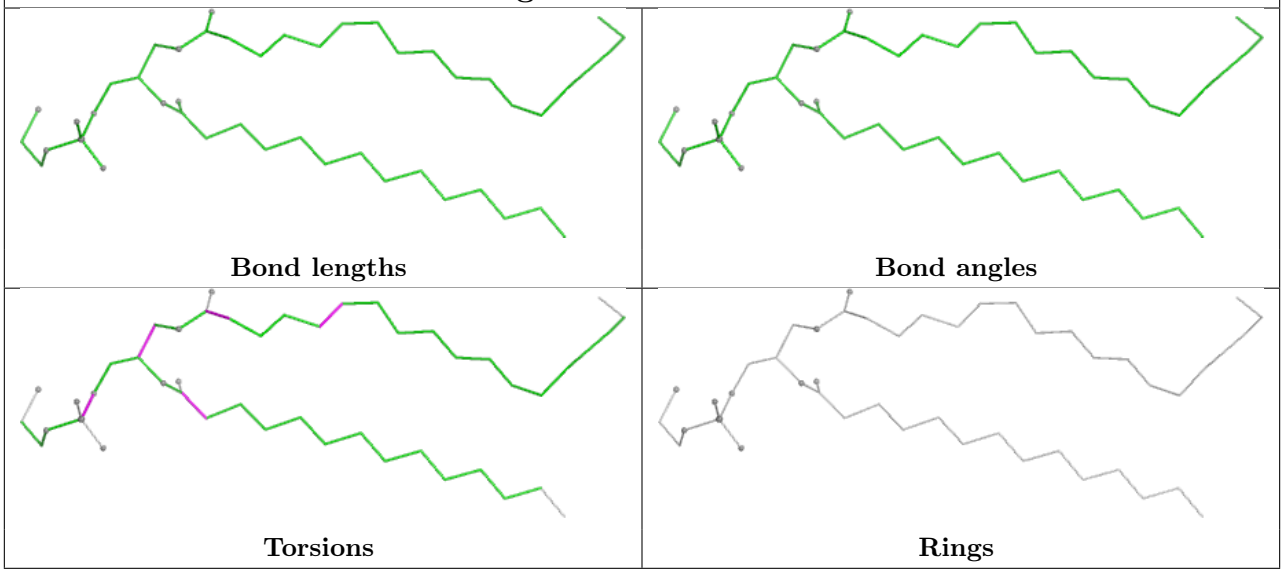
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	J	202	3PE	4	0
21	M	1001	3PE	3	0
16	F	503	NAI	2	0
20	N	502	LFA	1	0
21	J	201	3PE	2	0
21	M	1002	3PE	1	0
21	L	804	3PE	2	0
15	F	502	FMN	1	0
21	A	201	3PE	2	0
19	C	701	DCQ	1	0
21	L	803	3PE	2	0
14	G	1002	SF4	1	0
14	G	1003	SF4	1	0
14	G	1001	SF4	1	0

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.

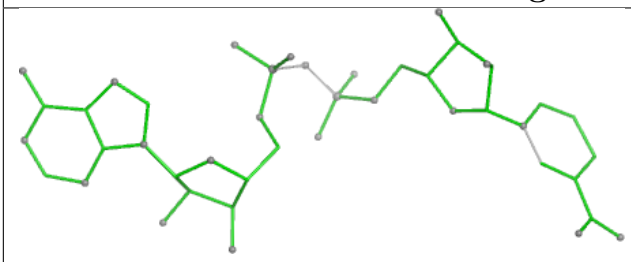
Ligand 3PE J 202



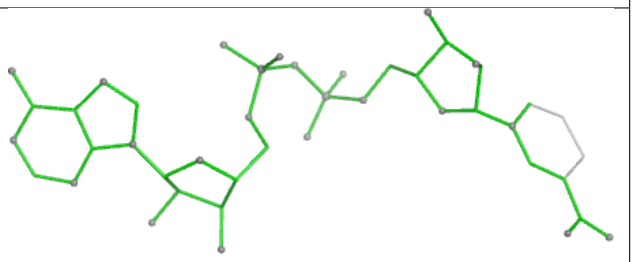
Ligand 3PE M 1001



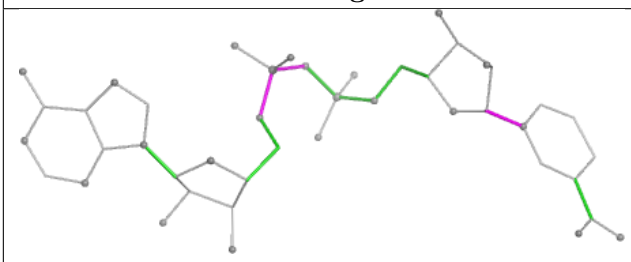
Ligand NAI F 503



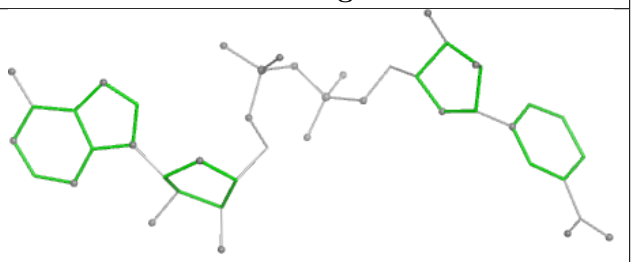
Bond lengths



Bond angles

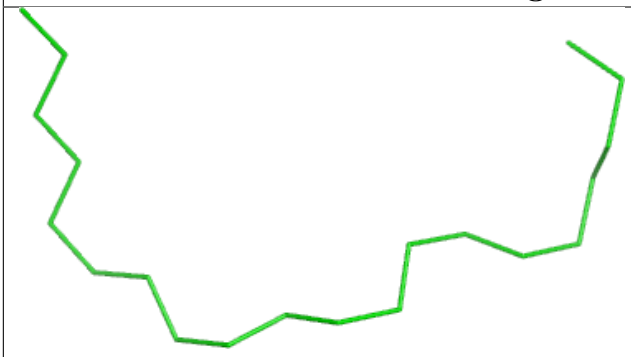


Torsions

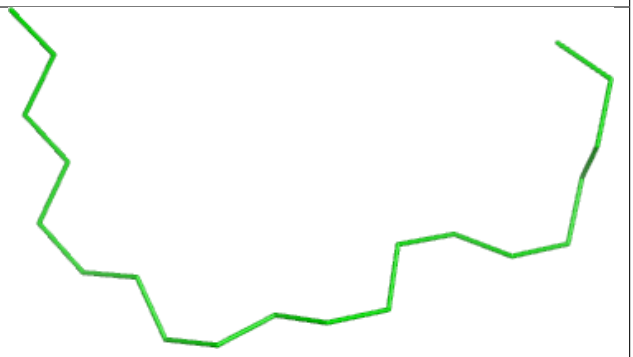


Rings

Ligand LFA H 601



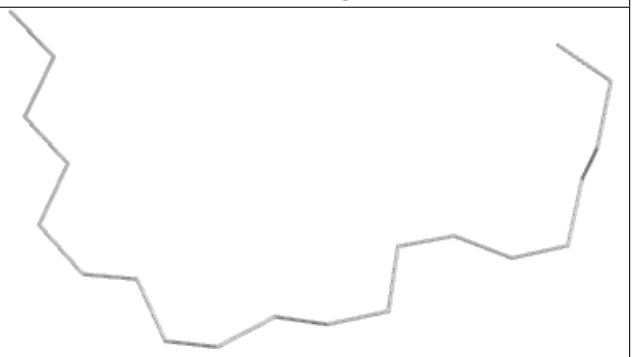
Bond lengths



Bond angles

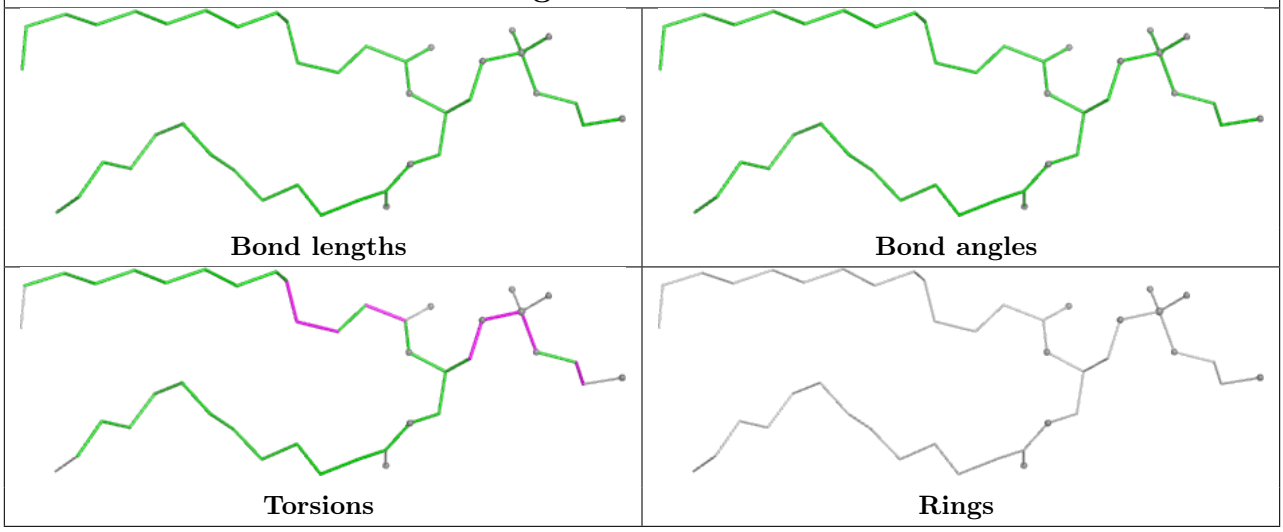


Torsions

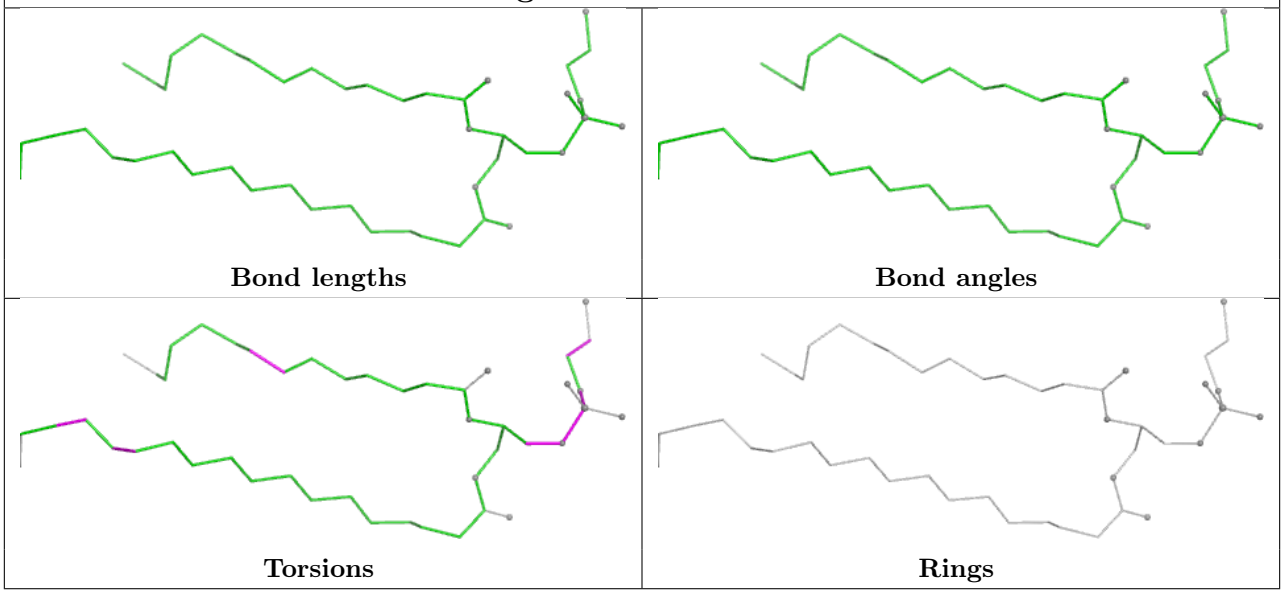


Rings

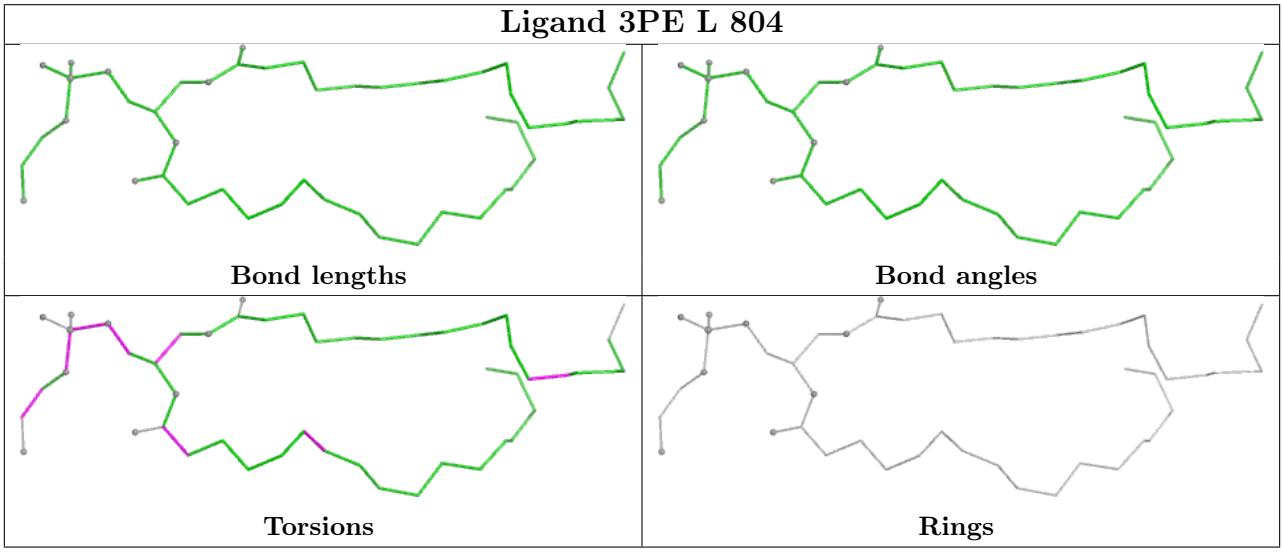
Ligand 3PE J 201



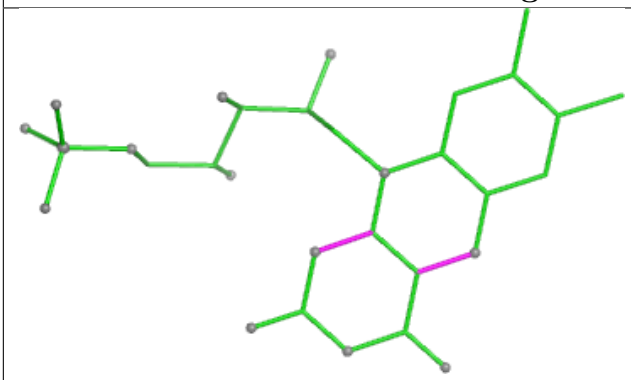
Ligand 3PE M 1002



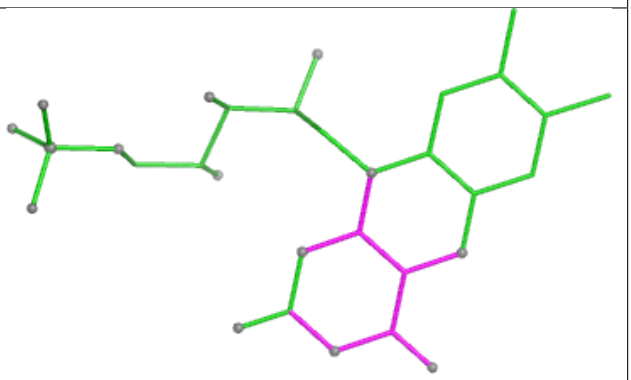
Ligand 3PE L 804



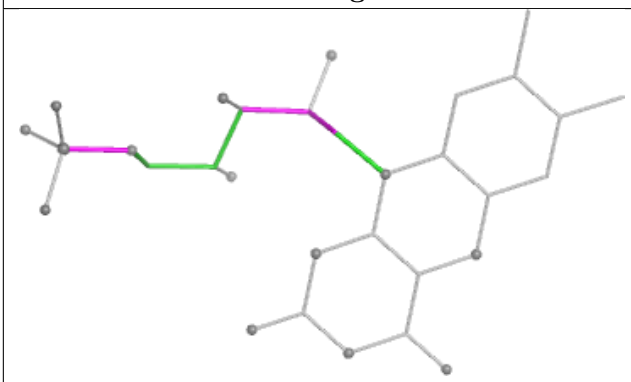
Ligand FMN F 502



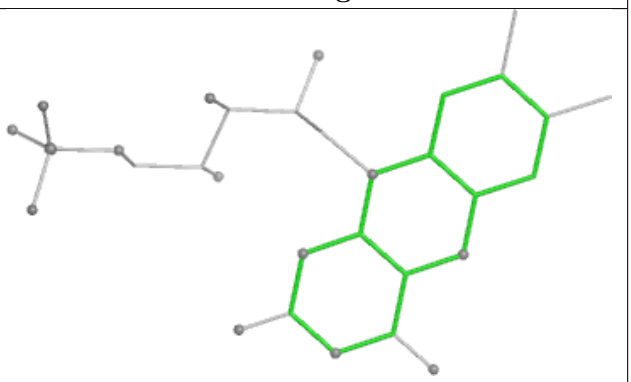
Bond lengths



Bond angles

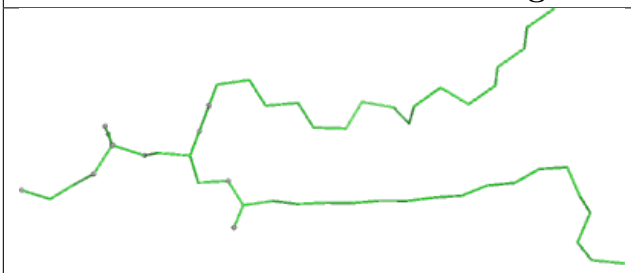


Torsions

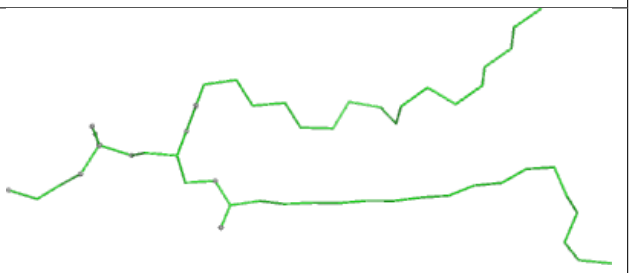


Rings

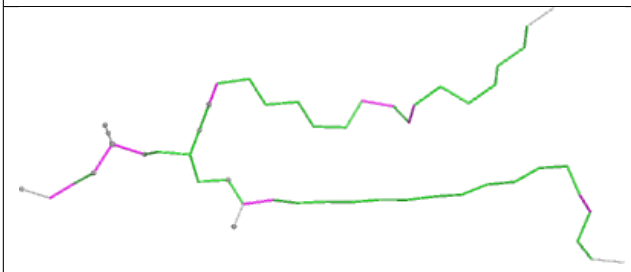
Ligand 3PE A 201



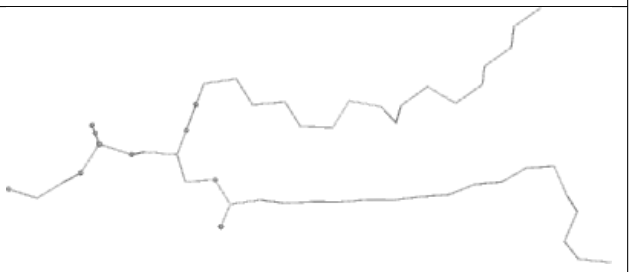
Bond lengths



Bond angles

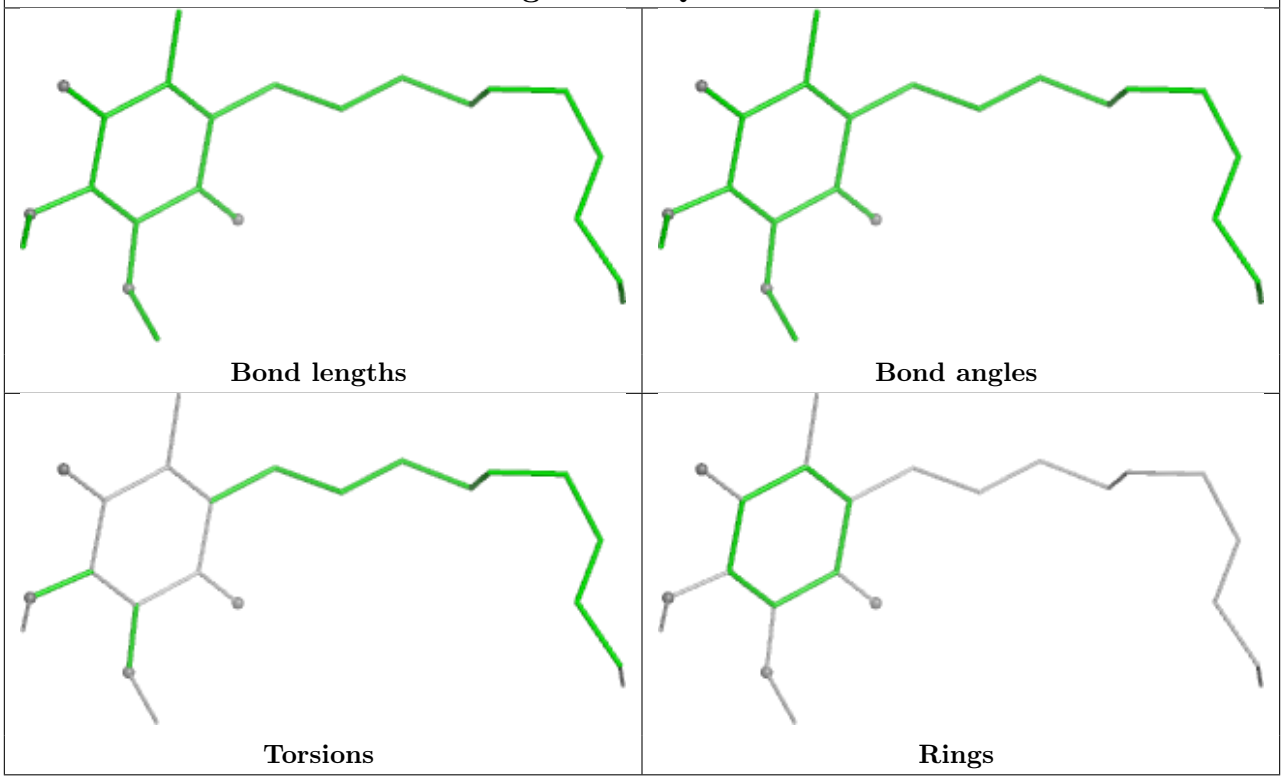


Torsions

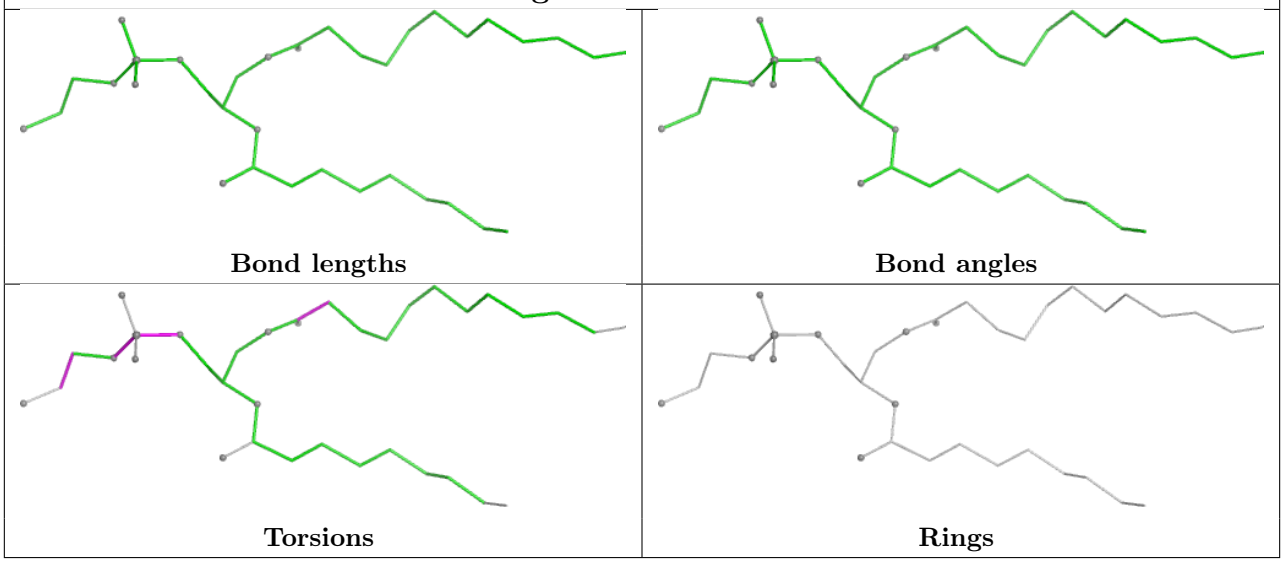


Rings

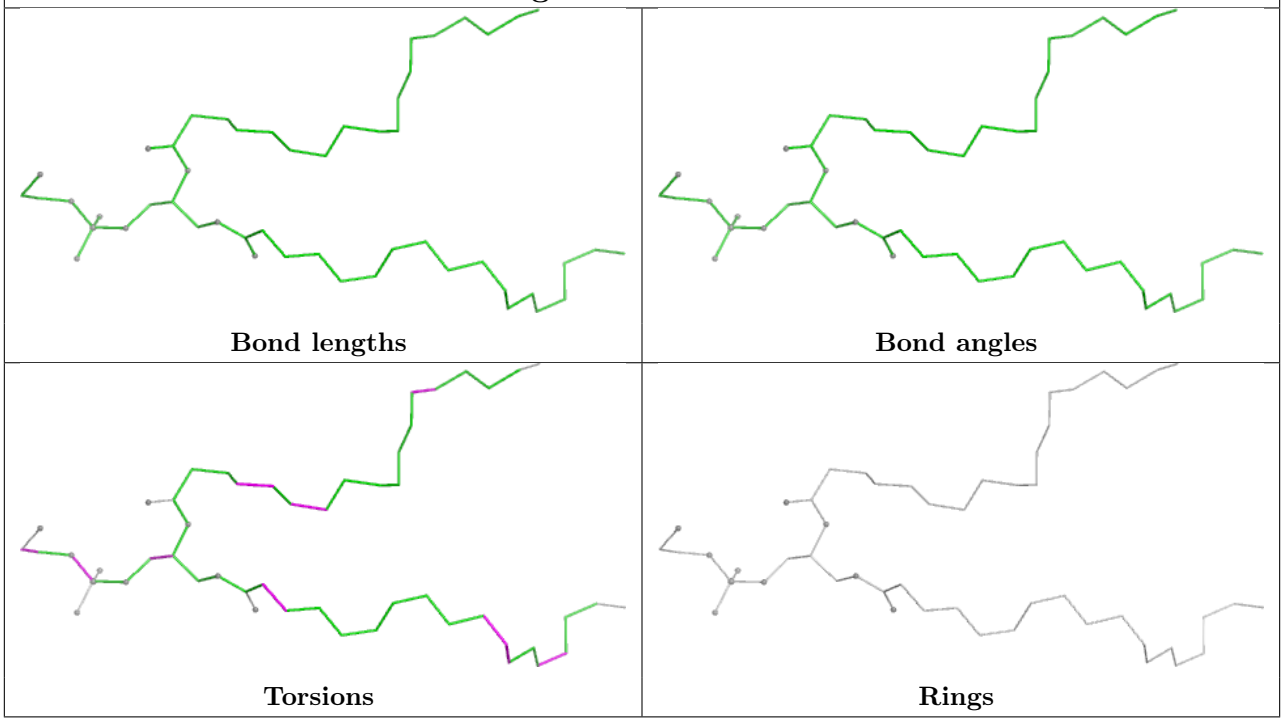
Ligand DCQ C 701



Ligand 3PE L 803



Ligand 3PE L 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

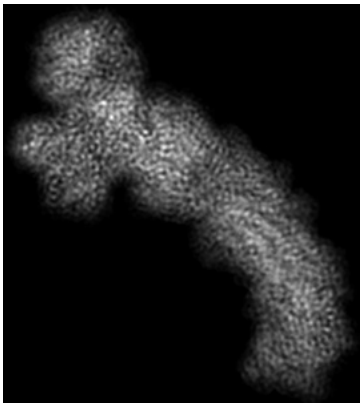
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13216. These allow visual inspection of the internal detail of the map and identification of artifacts.

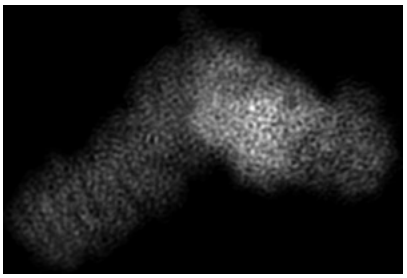
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

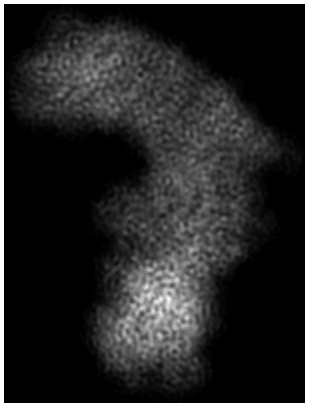
6.1.1 Primary map



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: 75



Y Index: 100



Z Index: 112

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

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 86



Y Index: 47

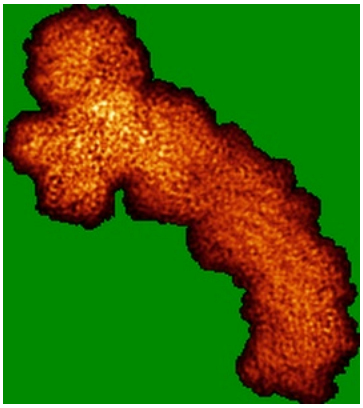


Z Index: 149

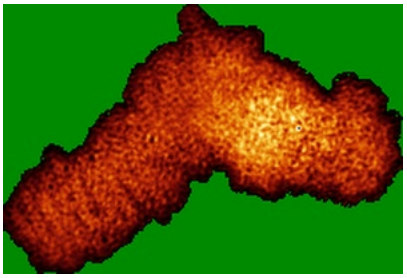
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X



Y

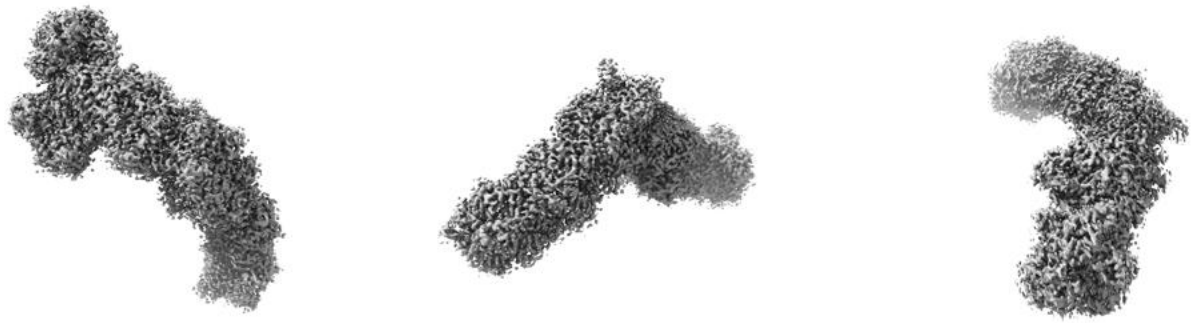


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.026. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

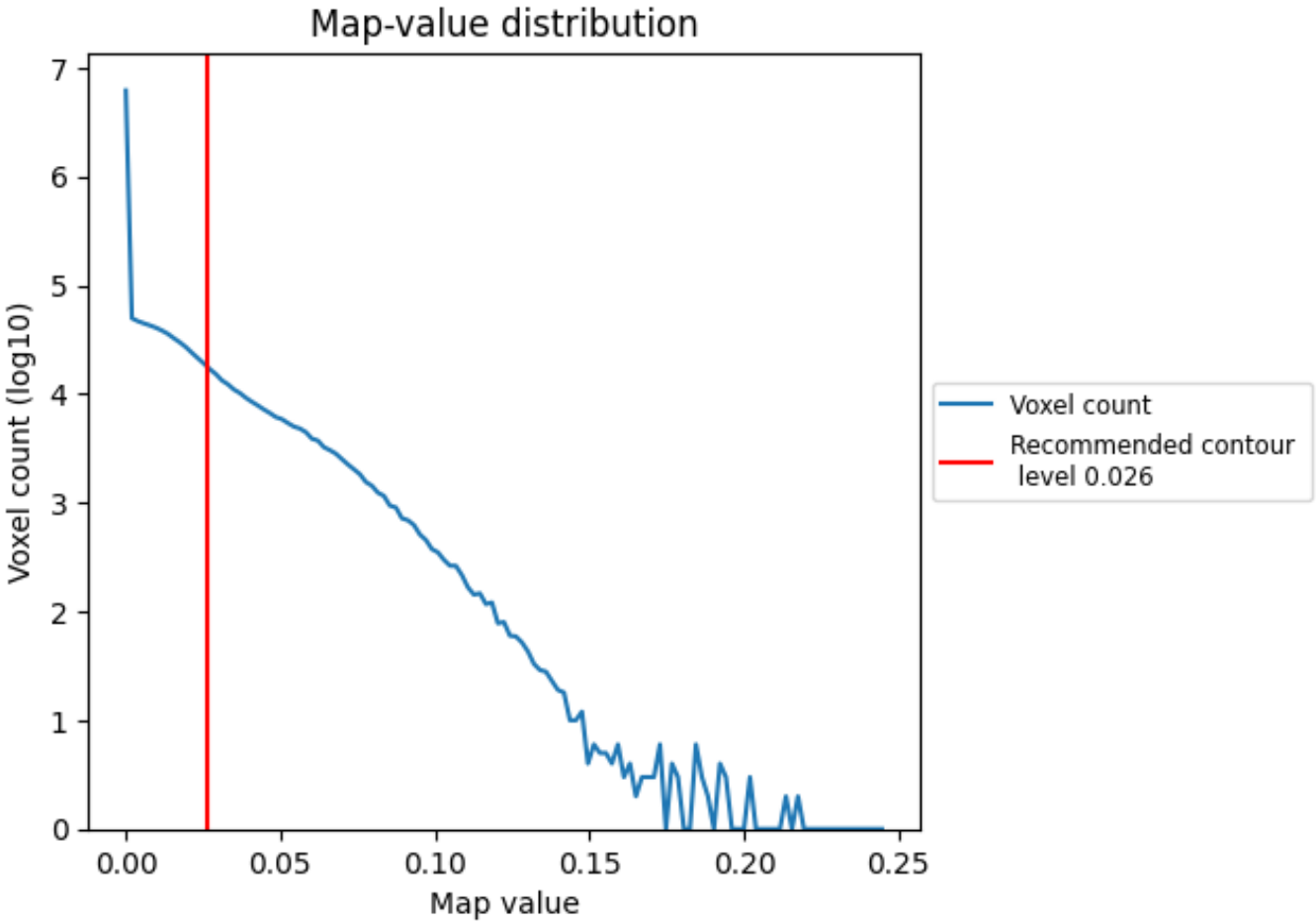
6.6 Mask visualisation (i)

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

7 Map analysis

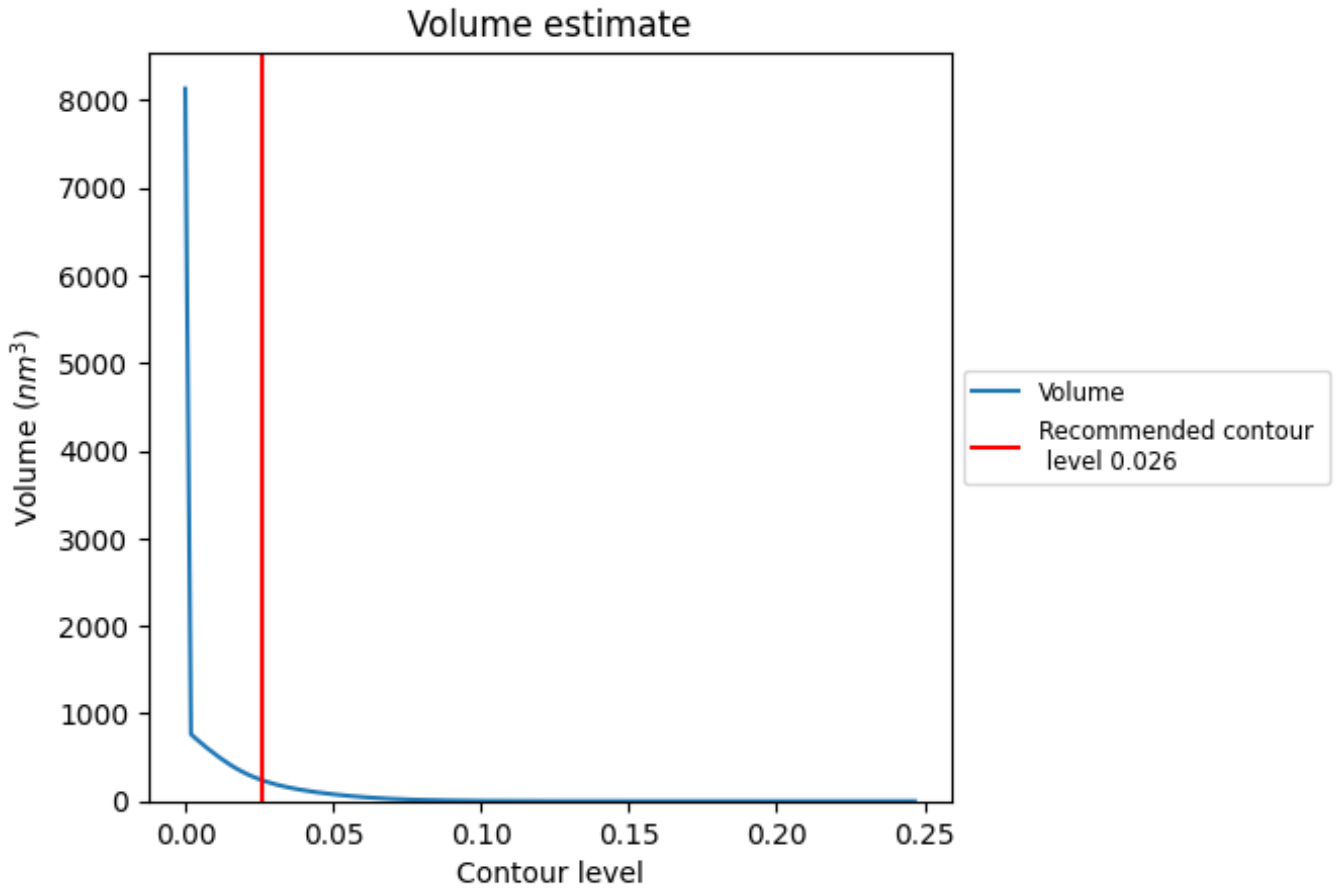
This section contains the results of statistical analysis of the map.

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 239 nm^3; this corresponds to an approximate mass of 216 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.

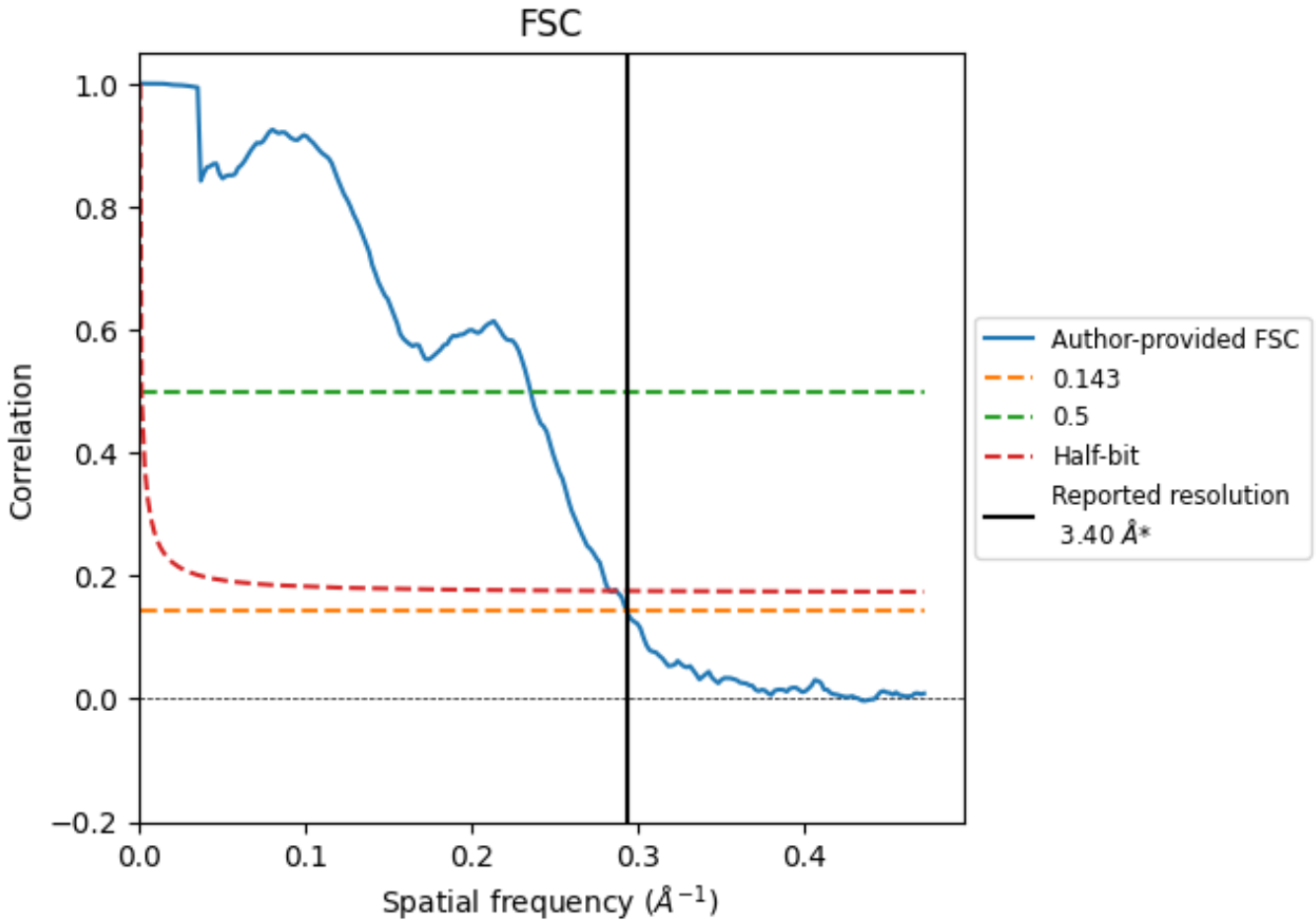
7.3 Rotationally averaged power spectrum

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

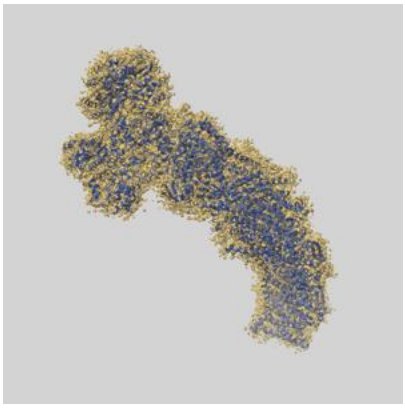
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.41	4.25	3.53
Unmasked-calculated*	-	-	-

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

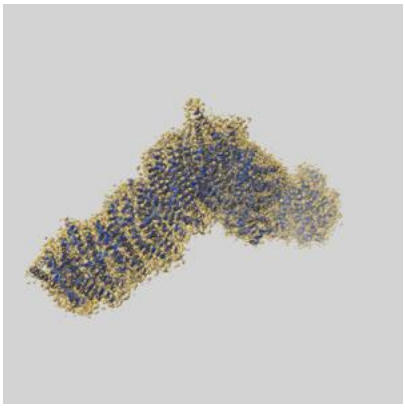
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13216 and PDB model 7P63. Per-residue inclusion information can be found in section 3 on page 11.

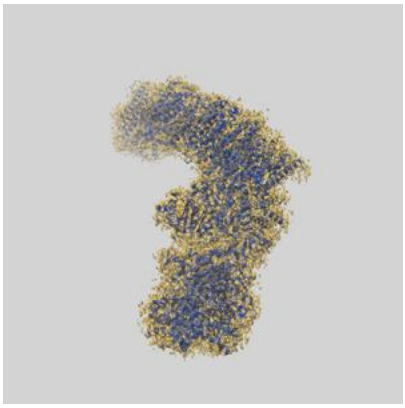
9.1 Map-model overlay



X



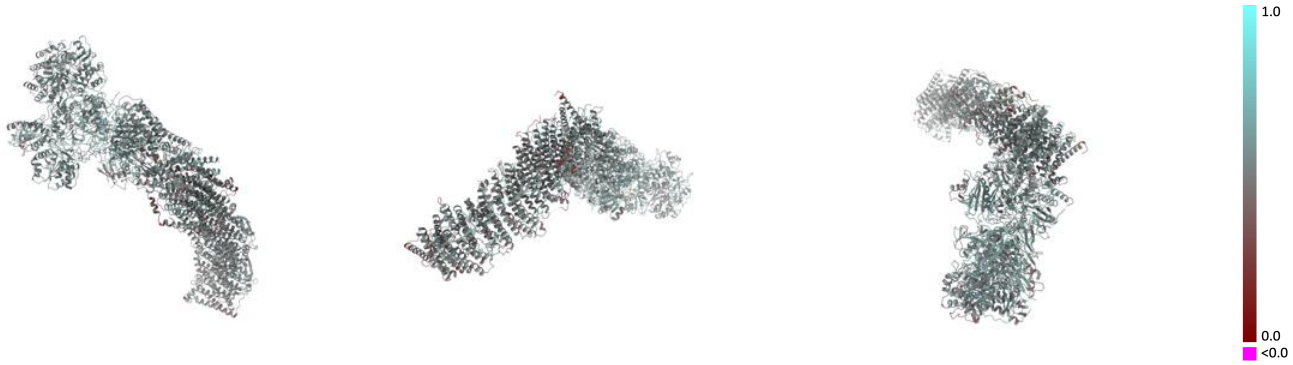
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.026 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.

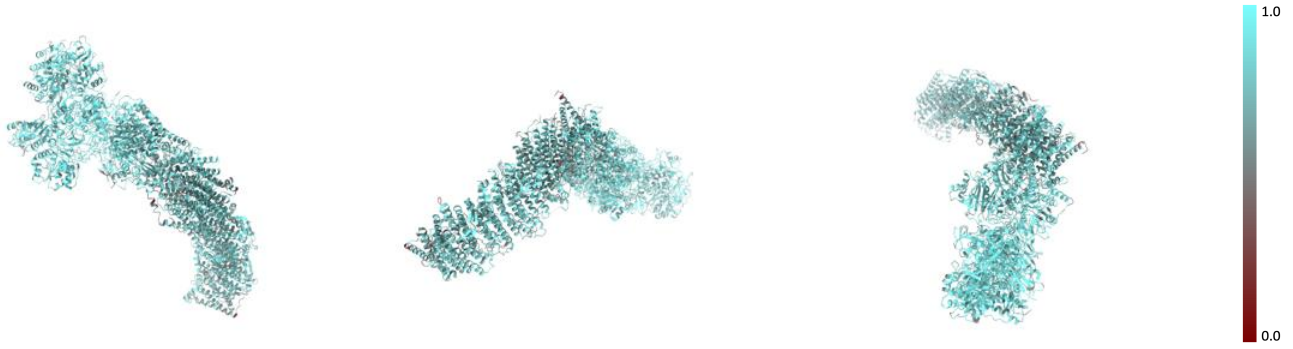
9.2 Q-score mapped to coordinate model (i)



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.

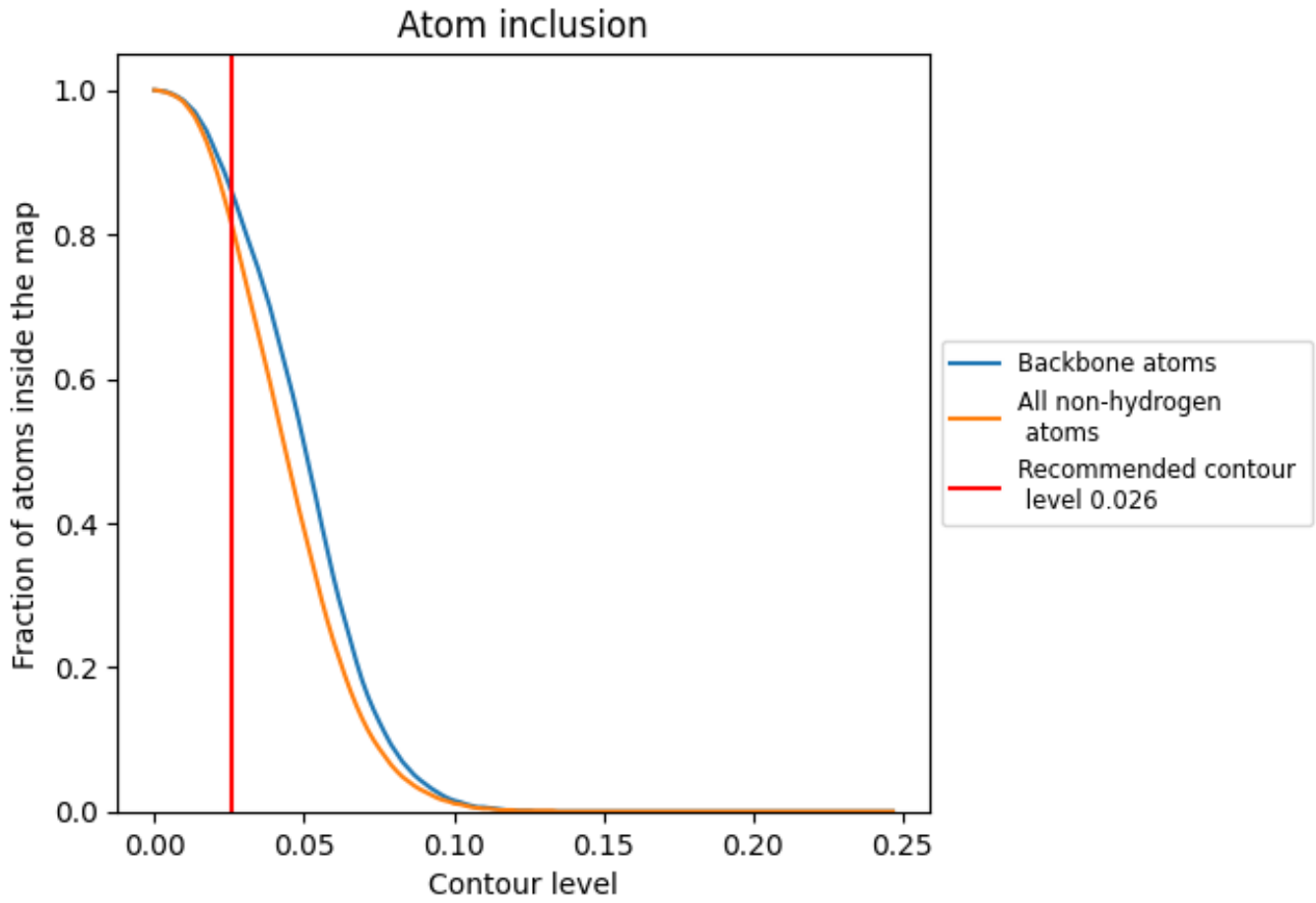
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.026).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 81% 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 (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8110	0.5230
A	0.7420	0.5070
B	0.8230	0.5430
C	0.8290	0.5420
E	0.8560	0.5270
F	0.8500	0.5290
G	0.8890	0.5550
H	0.7770	0.5180
I	0.8840	0.5590
J	0.6980	0.4830
K	0.7890	0.5180
L	0.7500	0.4920
M	0.7840	0.5020
N	0.7500	0.4920

