Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 11:14 pm GMT

PDB ID	:	7ZKP
EMDB ID	:	EMD-14764
Title	:	Late assembly intermediate of the proximal proton pumping module of complex I with assembly factors NDUFAF1 and CIA84
Authors	:	Schiller, J.; Laube, E.; Vonck, J.; Zickermann, V.
Deposited on	:	2022-04-13
Resolution	:	3.20 Å(reported)
Based on initial model	:	7O71

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:

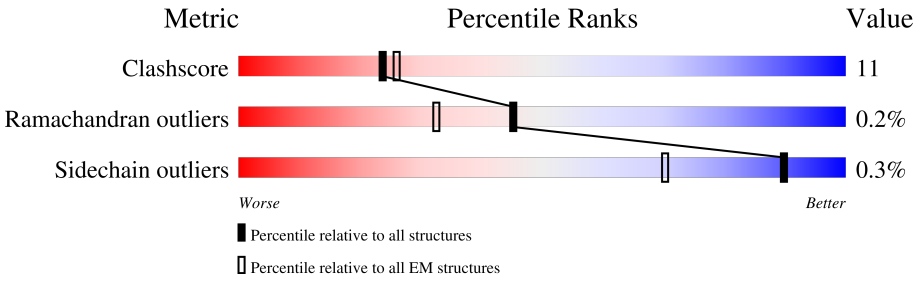
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	D	87	11% 77% 22%
2	L	89	9% 54% 45%
3	U	172	14% 72% 26%
4	W	123	7% 67% 7% 25%
5	X	169	10% 74% 21%
6	1	341	21% 65% 24% 11%
7	2	469	77% 23%
8	3	128	23% 50% 39% 11%

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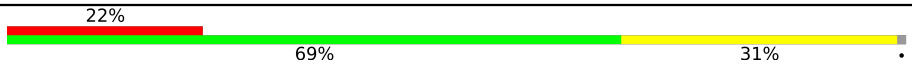
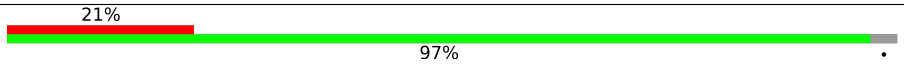
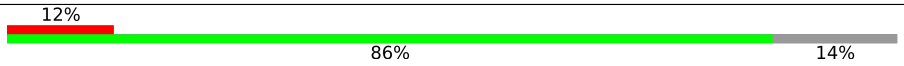
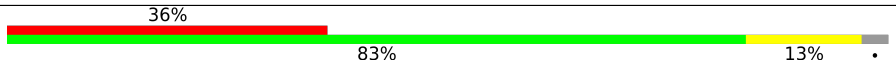
Mol	Chain	Length	Quality of chain
9	6	185	
10	g	78	
11	b	74	
12	9	89	
13	C	852	
14	A	290	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CDL	X	201	-	-	X	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 19929 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 Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	86	Total	C	N	O	S	0	0
			681	432	127	119	3		

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	89	Total	C	N	O	S	0	0
			693	465	109	116	3		

- Molecule 3 is a protein called Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	U	171	Total	C	N	O	S	0	0
			1345	847	236	252	10		

- Molecule 4 is a protein called Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	W	92	Total	C	N	O	S	0	0
			744	476	133	130	5		

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit -domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	X	164	Total	C	N	O	S	0	0
			1274	828	216	226	4		

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1	303	Total	C	N	O	S	0	0
			2426	1664	347	408	7		

- Molecule 7 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	2	469	Total	C	N	O	S	0	0
			3776	2558	550	656	12		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	3	114	Total	C	N	O	S	0	0
			909	626	131	150	2		

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	6	184	Total	C	N	O	S	0	0
			1453	985	208	251	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	1	FME	-	insertion	UNP S5U3X7

- Molecule 10 is a protein called subunit NI9M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
10	g	76	Total	C	N	O	0	0
			622	408	113	101		

- Molecule 11 is a protein called Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
11	b	64	Total	C	N	O	0	0
			490	326	83	81		

- Molecule 12 is a protein called Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	9	86	Total	C	N	O	S	0	0
			672	422	122	122	6		

- Molecule 13 is a protein called assembly factor CIA84.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	337	Total	C	N	O	S	0	0
			2763	1754	471	525	13		

- Molecule 14 is a protein called CIA30 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A	216	Total	C	N	O	S	0	0
			1749	1119	296	328	6		

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	GLU	-	expression tag	UNP A0A1D8NEL0
A	239	ASN	-	expression tag	UNP A0A1D8NEL0
A	240	LEU	-	expression tag	UNP A0A1D8NEL0
A	241	TYR	-	expression tag	UNP A0A1D8NEL0
A	242	PHE	-	expression tag	UNP A0A1D8NEL0
A	243	GLN	-	expression tag	UNP A0A1D8NEL0
A	244	GLY	-	expression tag	UNP A0A1D8NEL0
A	245	ALA	-	expression tag	UNP A0A1D8NEL0
A	246	GLU	-	expression tag	UNP A0A1D8NEL0
A	247	ALA	-	expression tag	UNP A0A1D8NEL0
A	248	ALA	-	expression tag	UNP A0A1D8NEL0
A	249	ALA	-	expression tag	UNP A0A1D8NEL0
A	250	LYS	-	expression tag	UNP A0A1D8NEL0
A	251	GLU	-	expression tag	UNP A0A1D8NEL0
A	252	ALA	-	expression tag	UNP A0A1D8NEL0
A	253	ALA	-	expression tag	UNP A0A1D8NEL0
A	254	ALA	-	expression tag	UNP A0A1D8NEL0
A	255	LYS	-	expression tag	UNP A0A1D8NEL0
A	256	ALA	-	expression tag	UNP A0A1D8NEL0
A	257	TRP	-	expression tag	UNP A0A1D8NEL0
A	258	SER	-	expression tag	UNP A0A1D8NEL0
A	259	HIS	-	expression tag	UNP A0A1D8NEL0
A	260	PRO	-	expression tag	UNP A0A1D8NEL0
A	261	GLN	-	expression tag	UNP A0A1D8NEL0
A	262	PHE	-	expression tag	UNP A0A1D8NEL0

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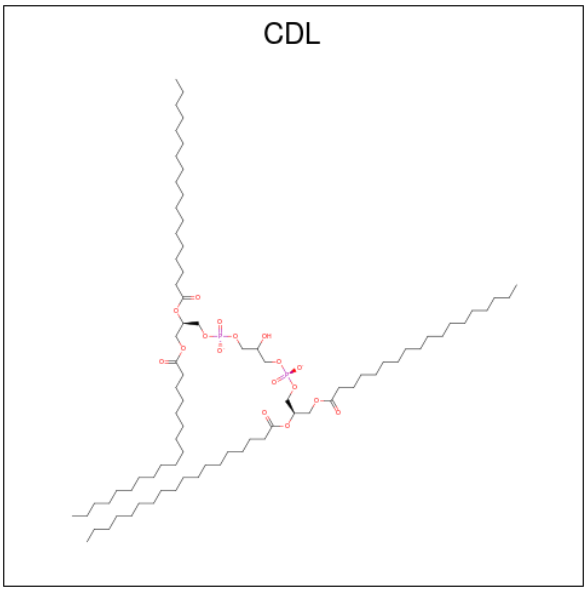
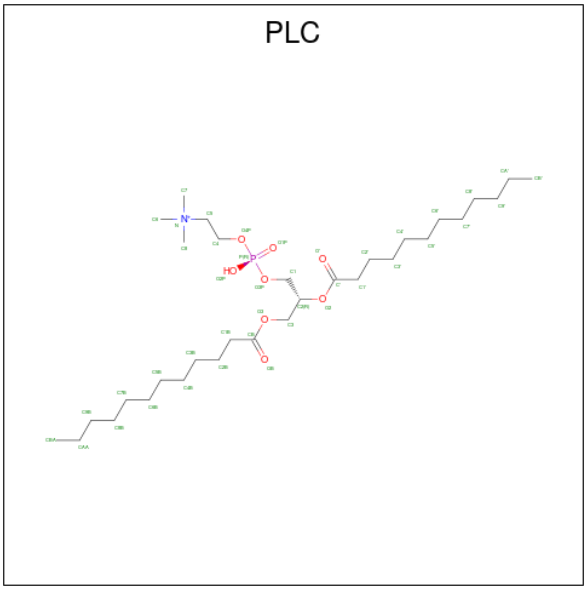
Chain	Residue	Modelled	Actual	Comment	Reference
A	263	GLU	-	expression tag	UNP A0A1D8NEL0
A	264	LYS	-	expression tag	UNP A0A1D8NEL0
A	265	GLY	-	expression tag	UNP A0A1D8NEL0
A	266	GLY	-	expression tag	UNP A0A1D8NEL0
A	267	GLY	-	expression tag	UNP A0A1D8NEL0
A	268	SER	-	expression tag	UNP A0A1D8NEL0
A	269	GLY	-	expression tag	UNP A0A1D8NEL0
A	270	GLY	-	expression tag	UNP A0A1D8NEL0
A	271	GLY	-	expression tag	UNP A0A1D8NEL0
A	272	SER	-	expression tag	UNP A0A1D8NEL0
A	273	GLY	-	expression tag	UNP A0A1D8NEL0
A	274	GLY	-	expression tag	UNP A0A1D8NEL0
A	275	SER	-	expression tag	UNP A0A1D8NEL0
A	276	ALA	-	expression tag	UNP A0A1D8NEL0
A	277	TRP	-	expression tag	UNP A0A1D8NEL0
A	278	SER	-	expression tag	UNP A0A1D8NEL0
A	279	HIS	-	expression tag	UNP A0A1D8NEL0
A	280	PRO	-	expression tag	UNP A0A1D8NEL0
A	281	GLN	-	expression tag	UNP A0A1D8NEL0
A	282	PHE	-	expression tag	UNP A0A1D8NEL0
A	283	GLU	-	expression tag	UNP A0A1D8NEL0
A	284	LYS	-	expression tag	UNP A0A1D8NEL0

- Molecule 15 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



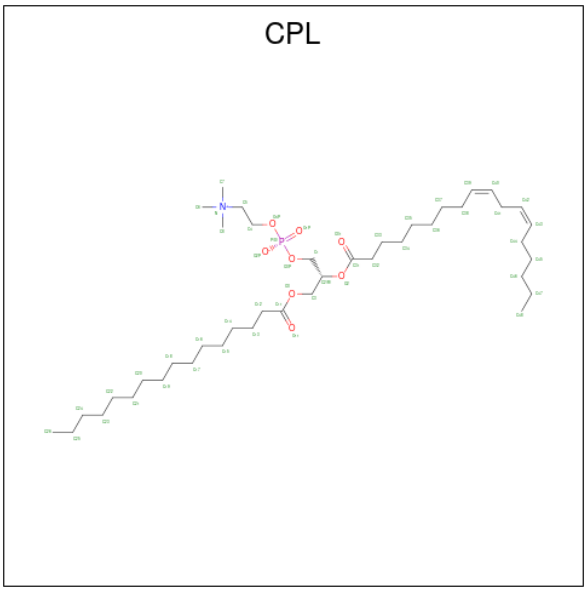
Mol	Chain	Residues	Atoms				AltConf
15	X	1	Total	C	O	P	0
			64	46	16	2	
15	g	1	Total	C	O	P	0
			83	64	17	2	

- Molecule 16 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: $C_{32}H_{65}NO_8P$).



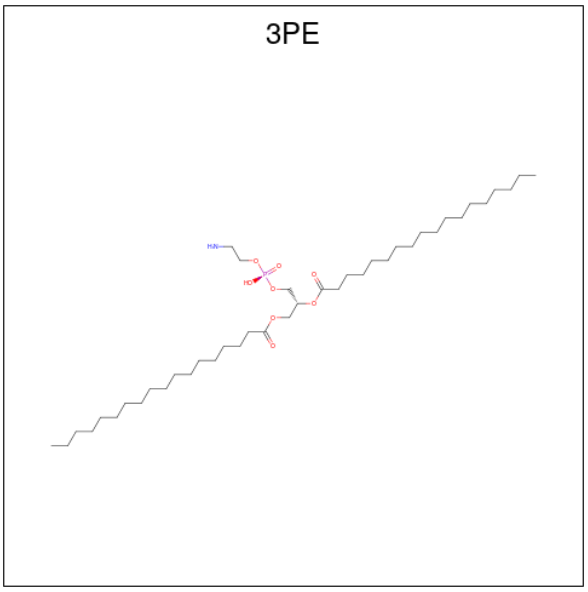
Mol	Chain	Residues	Atoms					AltConf
16	1	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 17 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: CPL) (formula: $C_{42}H_{80}NO_8P$).



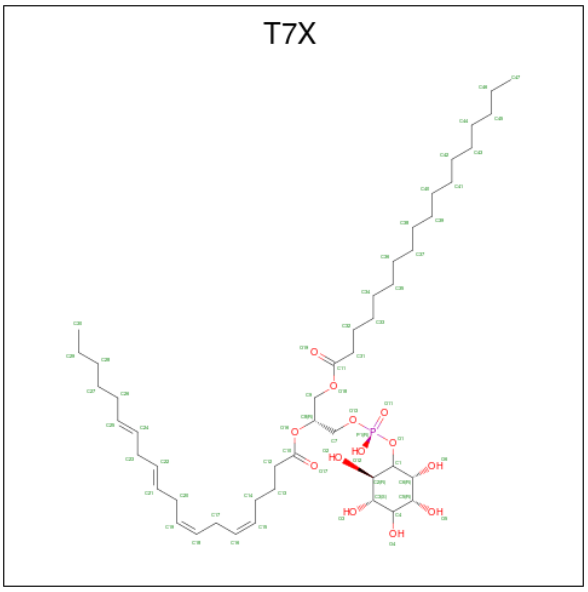
Mol	Chain	Residues	Atoms					AltConf
17	2	1	Total	C	N	O	P	0
			52	42	1	8	1	

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



Mol	Chain	Residues	Atoms					AltConf
18	g	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 19 is Phosphatidylinositol (three-letter code: T7X) (formula: $C_{47}H_{83}O_{13}P$).



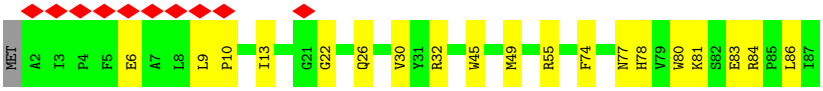
Mol	Chain	Residues	Atoms				AltConf
19	b	1	Total	C	O	P	0
			48	34	13	1	

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.

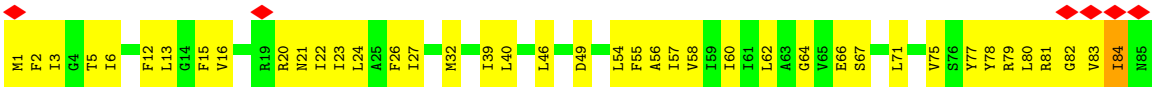
• Molecule 1: Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain D:



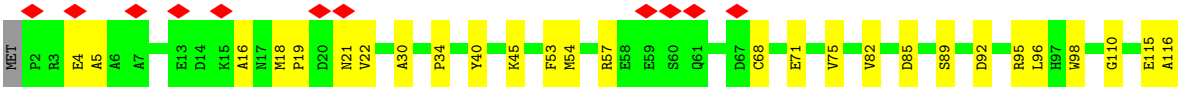
• Molecule 2: NADH-ubiquinone oxidoreductase chain 4L

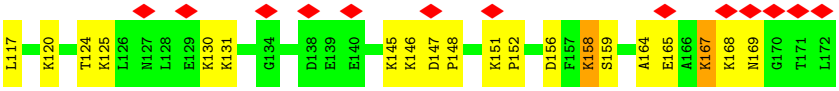
Chain L:



• Molecule 3: Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I)

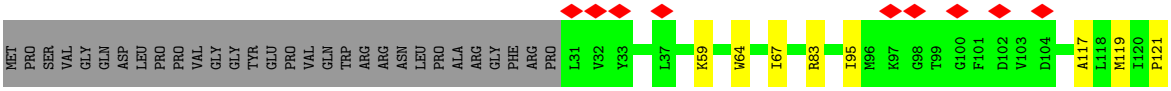
Chain U:





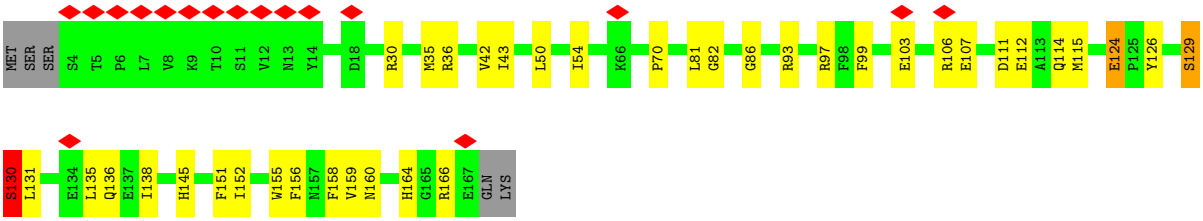
• Molecule 4: Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain W:



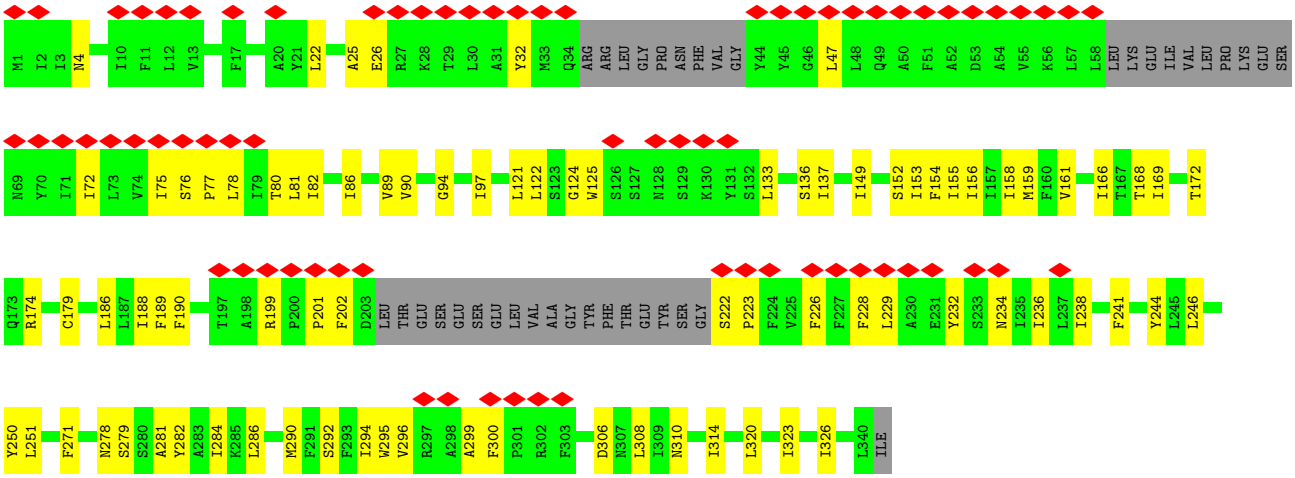
• Molecule 5: NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit-domain-containing protein

Chain X:



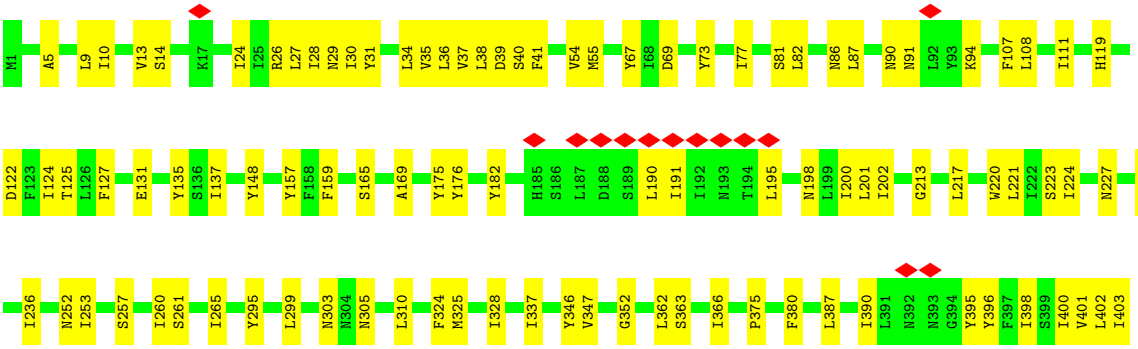
• Molecule 6: NADH-ubiquinone oxidoreductase chain 1

Chain 1:

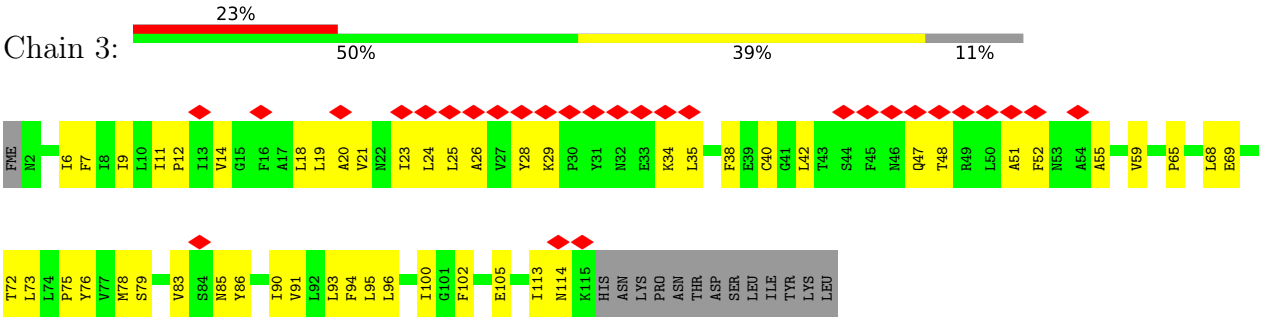


• Molecule 7: NADH dehydrogenase subunit 2

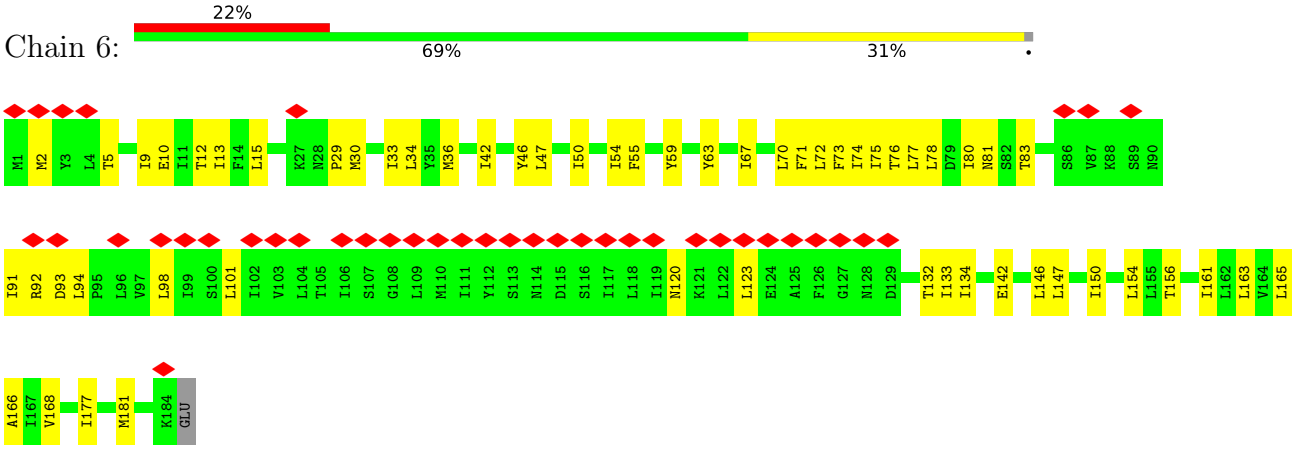
Chain 2:



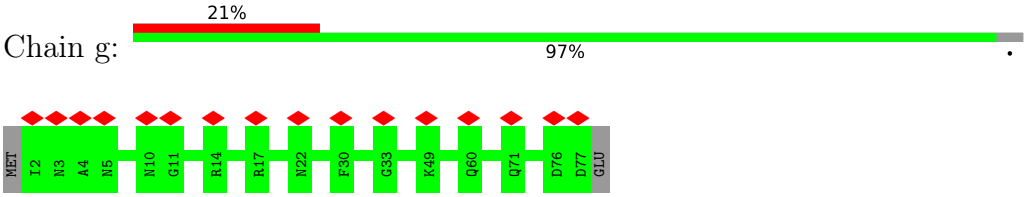
• Molecule 8: NADH-ubiquinone oxidoreductase chain 3



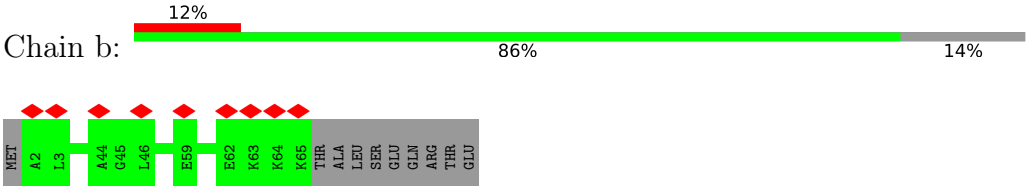
• Molecule 9: NADH-ubiquinone oxidoreductase chain 6



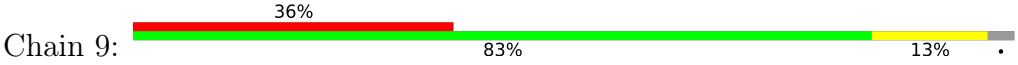
• Molecule 10: subunit NI9M of protein NADH:Ubiquinone Oxidoreductase (Complex I)

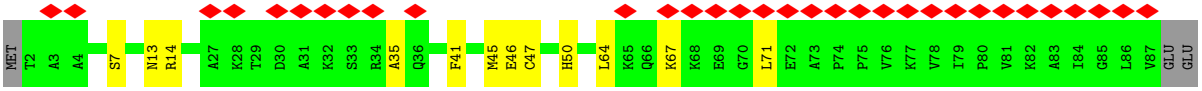


• Molecule 11: Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I)



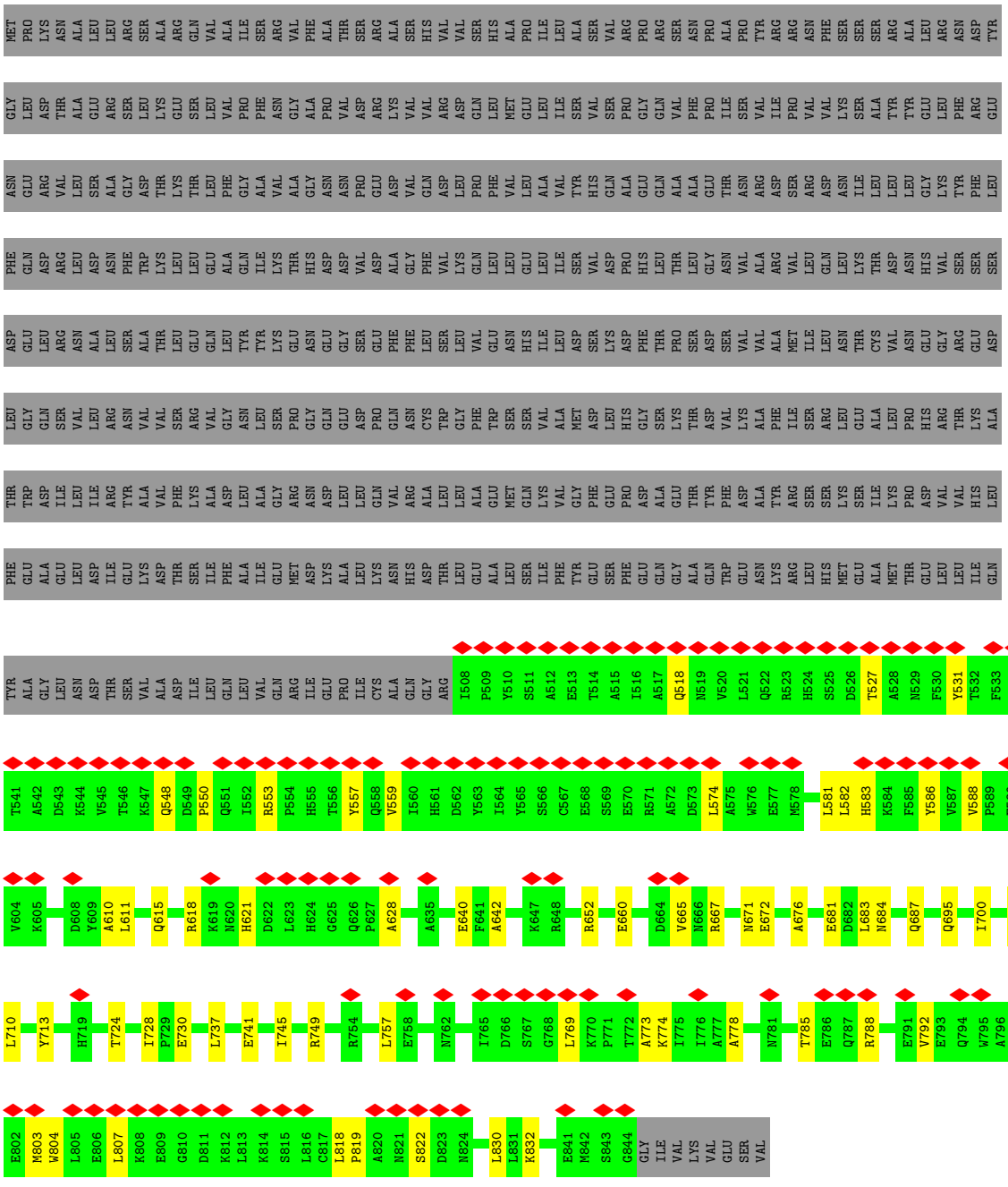
• Molecule 12: Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I)





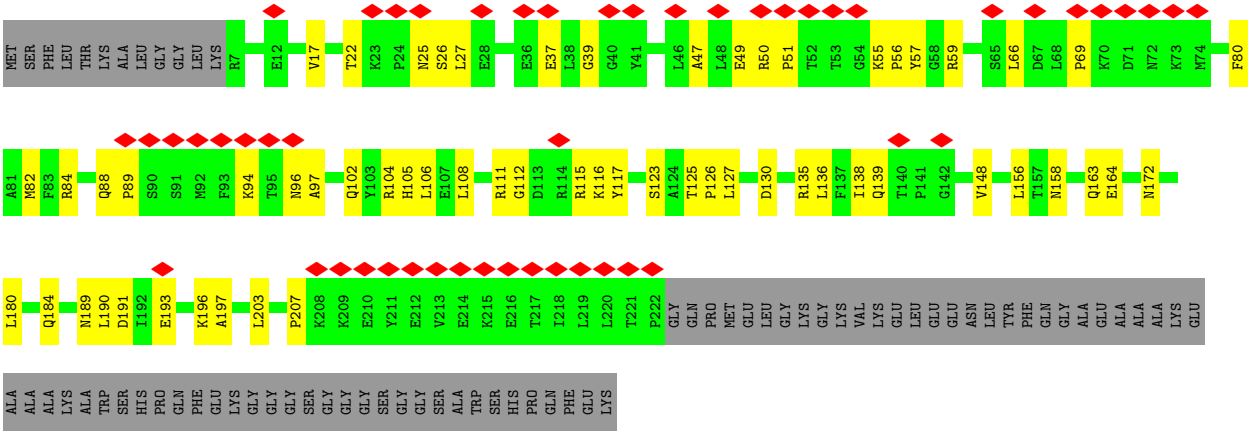
• Molecule 13: assembly factor CIA84

Chain C:



• Molecule 14: CIA30 domain-containing protein

Chain A:


MET SER PHE LEU THR LYS ALA LEU GLY GLY LEU LYS R7 E12 V17 T22 K23 P24 N25 S26 L27 E28 E36 E37 L38 G39 G40 Y41 L46 A47 L48 E49 R50 P51 T52 T53 G54 K55 P56 Y57 G58 R59 S65 L66 D67 L68 P69 K70 D71 N72 K73 M74 F80
A81 M82 F83 R84 Q88 P89 S90 S91 M92 F93 K94 T95 N96 A97 Q102 Y103 R104 H105 L106 E107 L108 R111 G112 D113 R114 R115 K116 Y117 S123 A124 T125 P126 L127 D130 R135 L136 F137 I138 Q139 T140 P141 G142 V148 L156 T157 N158 Q163 E164 N172
L180 Q184 N189 L190 D191 I192 E193 K196 A197 L203 P207 K208 K209 E210 Y211 E212 V213 E214 K215 E216 T217 I218 L219 L220 T221 P222 GLY GLN PRO MET GLU LEU GLY LYS GLY LYS VAL LYS GLU LEU GLU GLU ASN LEU TYR PHE GLN GLY ALA GLU ALA ALA ALA LYS GLU
ALA ALA ALA LYS ALA TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18279	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.341	Depositor
Minimum map value	-1.273	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.099	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	251.09967, 251.09967, 251.09967	wwPDB
Map dimensions	208, 208, 208	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.20721, 1.20721, 1.20721	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CPL, CDL, PLC, 3PE, FME, T7X

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	D	0.24	0/697	0.49	0/940
2	L	0.26	0/692	0.49	0/937
3	U	0.26	0/1374	0.51	0/1856
4	W	0.24	0/758	0.47	0/1017
5	X	0.34	0/1313	0.55	1/1782 (0.1%)
6	1	0.27	0/2482	0.44	0/3389
7	2	0.27	0/3846	0.42	0/5242
8	3	0.32	0/930	0.49	0/1269
9	6	0.26	0/1468	0.46	0/2003
10	g	0.25	0/648	0.49	0/887
11	b	0.25	0/503	0.38	0/679
12	9	0.24	0/684	0.45	0/918
13	C	0.25	0/2828	0.45	0/3832
14	A	0.26	0/1791	0.56	0/2435
All	All	0.27	0/20014	0.47	1/27186 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	X	130	SER	N-CA-CB	-5.17	102.74	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	681	0	671	16	0
2	L	693	0	753	44	0
3	U	1345	0	1327	28	0
4	W	744	0	761	7	0
5	X	1274	0	1245	46	0
6	1	2426	0	2522	56	0
7	2	3776	0	4004	85	0
8	3	909	0	970	35	0
9	6	1453	0	1576	54	0
10	g	622	0	602	0	0
11	b	490	0	509	0	0
12	9	672	0	683	8	0
13	C	2763	0	2672	47	0
14	A	1749	0	1731	45	0
15	X	64	0	78	26	0
15	g	83	0	116	0	0
16	1	42	0	64	2	0
17	2	52	0	79	4	0
18	g	43	0	63	0	0
19	b	48	0	0	0	0
All	All	19929	0	20426	400	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 11.

All (400) 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)
5:X:160:ASN:ND2	15:X:201:CDL:HA21	1.87	0.90
5:X:159:VAL:HG22	15:X:201:CDL:HA31	1.58	0.83
7:2:9:LEU:HD11	7:2:28:ILE:HD11	1.61	0.82
5:X:30:ARG:NH2	5:X:111:ASP:OD1	2.15	0.80
5:X:129:SER:HB2	5:X:136:GLN:NE2	1.96	0.79
14:A:130:ASP:OD1	14:A:158:ASN:ND2	2.14	0.79
5:X:30:ARG:NH1	5:X:114:GLN:OE1	2.17	0.78
15:X:201:CDL:H422	9:6:163:LEU:HD13	1.66	0.78
5:X:159:VAL:HG23	15:X:201:CDL:OA9	1.84	0.77
2:L:3:ILE:HB	9:6:13:ILE:HG12	1.65	0.76
13:C:601:ALA:HB1	13:C:640:GLU:HG2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:LYS:HB2	9:6:134:ILE:HB	1.68	0.73
8:3:34:LYS:HD3	14:A:37:GLU:HB3	1.71	0.73
7:2:54:VAL:HG12	7:2:55:MET:HG2	1.69	0.73
2:L:75:VAL:HA	2:L:80:LEU:HD23	1.70	0.72
7:2:299:LEU:O	7:2:305:ASN:ND2	2.24	0.71
13:C:745:ILE:HD11	13:C:778:ALA:HB1	1.72	0.70
6:1:161:VAL:HG21	6:1:169:ILE:HG23	1.72	0.70
6:1:323:ILE:HA	6:1:326:ILE:HG22	1.74	0.70
1:D:10:PRO:HB2	6:1:25:ALA:HB2	1.73	0.70
14:A:25:ASN:O	14:A:27:LEU:N	2.26	0.68
5:X:129:SER:HB2	5:X:136:GLN:HE22	1.58	0.68
2:L:62:LEU:HD13	7:2:131:GLU:HG3	1.74	0.68
8:3:73:LEU:HD21	8:3:95:LEU:HD11	1.76	0.68
2:L:79:ARG:NH1	7:2:148:TYR:OH	2.27	0.67
5:X:54:ILE:HD11	7:2:27:LEU:HA	1.76	0.67
5:X:151:PHE:O	7:2:73:TYR:OH	2.12	0.67
2:L:79:ARG:HD2	14:A:164:GLU:HB3	1.78	0.66
7:2:137:ILE:HD11	7:2:236:ILE:HG22	1.77	0.66
13:C:518:GLN:HA	13:C:559:VAL:HG21	1.77	0.66
15:X:201:CDL:HB61	15:X:201:CDL:OB7	1.94	0.66
13:C:665:VAL:O	14:A:139:GLN:NE2	2.29	0.66
9:6:92:ARG:NH1	14:A:94:LYS:O	2.29	0.66
3:U:115:GLU:OE2	3:U:130:LYS:NZ	2.27	0.65
6:1:22:LEU:HD13	6:1:236:ILE:HD11	1.78	0.64
14:A:108:LEU:HD11	14:A:136:LEU:HD11	1.78	0.64
6:1:296:VAL:HA	6:1:299:ALA:HB3	1.80	0.63
2:L:13:LEU:HD12	8:3:14:VAL:HG13	1.81	0.63
1:D:32:ARG:NH2	6:1:4:ASN:OD1	2.32	0.63
14:A:88:GLN:HG2	14:A:97:ALA:HA	1.81	0.63
2:L:60:ILE:HG23	9:6:63:TYR:HE1	1.64	0.63
6:1:174:ARG:HG2	6:1:251:LEU:HD21	1.79	0.63
7:2:29:ASN:ND2	7:2:81:SER:OG	2.30	0.63
1:D:86:LEU:HD13	9:6:50:ILE:HG23	1.81	0.63
3:U:95:ARG:HA	3:U:98:TRP:CD1	2.35	0.62
3:U:148:PRO:O	3:U:151:LYS:NZ	2.33	0.62
6:1:94:GLY:HA3	6:1:97:ILE:HD12	1.81	0.62
14:A:115:ARG:NH1	14:A:184:GLN:OE1	2.33	0.62
14:A:49:GLU:HG3	14:A:51:PRO:HD3	1.80	0.62
2:L:71:LEU:HD22	9:6:74:ILE:HG13	1.81	0.62
6:1:76:SER:HB3	6:1:122:LEU:HD13	1.82	0.62
14:A:22:THR:HG21	14:A:55:LYS:HE2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:80:LEU:HD11	9:6:78:LEU:HG	1.83	0.61
13:C:618:ARG:NH1	13:C:660:GLU:OE1	2.33	0.61
15:X:201:CDL:H562	15:X:201:CDL:H201	1.80	0.61
2:L:64:GLY:HA3	8:3:68:LEU:HD11	1.83	0.61
3:U:45:LYS:HD3	3:U:82:VAL:HB	1.83	0.61
7:2:9:LEU:HD21	7:2:28:ILE:HG13	1.81	0.61
13:C:818:LEU:HD22	13:C:830:LEU:HB3	1.83	0.60
2:L:23:ILE:HG21	9:6:29:PRO:HB3	1.83	0.60
14:A:50:ARG:HA	14:A:56:PRO:HB3	1.83	0.60
7:2:137:ILE:HG23	7:2:157:TYR:HE2	1.66	0.59
13:C:819:PRO:HB2	13:C:822:SER:HB3	1.83	0.59
13:C:800:HIS:ND1	13:C:803:MET:SD	2.75	0.59
2:L:26:PHE:HZ	2:L:67:SER:HA	1.66	0.59
6:1:295:TRP:O	6:1:299:ALA:HB2	2.03	0.59
2:L:79:ARG:NH2	14:A:163:GLN:OE1	2.35	0.58
5:X:99:PHE:HE2	5:X:145:HIS:HD2	1.49	0.58
3:U:21:ASN:OD1	3:U:22:VAL:N	2.36	0.58
6:1:168:THR:O	6:1:172:THR:HG23	2.02	0.58
13:C:557:TYR:HD1	13:C:582:LEU:HD11	1.68	0.58
6:1:72:ILE:HA	6:1:75:ILE:HG12	1.85	0.58
5:X:131:LEU:HD13	5:X:135:LEU:HB3	1.84	0.58
3:U:110:GLY:HA2	3:U:152:PRO:HG3	1.85	0.58
13:C:730:GLU:HG3	14:A:207:PRO:HD3	1.85	0.58
2:L:21:ASN:O	2:L:24:LEU:N	2.36	0.57
14:A:130:ASP:HB3	14:A:156:LEU:HD11	1.86	0.57
15:X:201:CDL:H441	9:6:163:LEU:HB3	1.85	0.57
13:C:785:THR:HB	13:C:788:ARG:HB2	1.87	0.57
2:L:54:LEU:HD11	9:6:154:LEU:HD13	1.85	0.57
14:A:111:ARG:HG2	14:A:191:ASP:HB2	1.87	0.57
5:X:42:VAL:HG13	7:2:38:LEU:HD11	1.87	0.57
5:X:138:ILE:HG21	9:6:156:THR:HB	1.86	0.57
7:2:223:SER:O	7:2:227:ASN:ND2	2.37	0.56
8:3:19:LEU:O	8:3:23:ILE:HG13	2.05	0.56
15:X:201:CDL:C42	9:6:163:LEU:HD13	2.34	0.56
8:3:52:PHE:CE2	9:6:80:ILE:HD11	2.40	0.56
3:U:4:GLU:HG2	3:U:5:ALA:H	1.69	0.56
3:U:30:ALA:HB1	3:U:34:PRO:HB2	1.88	0.56
6:1:149:ILE:HG23	6:1:320:LEU:HD11	1.87	0.56
8:3:28:TYR:O	8:3:29:LYS:C	2.44	0.56
13:C:687:GLN:HG2	14:A:203:LEU:HD21	1.88	0.56
5:X:130:SER:HB3	15:X:201:CDL:OA3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:59:LYS:NZ	9:6:142:GLU:OE2	2.38	0.55
14:A:116:LYS:HG2	14:A:135:ARG:HH21	1.71	0.55
12:9:14:ARG:NH1	12:9:47:CYS:O	2.34	0.55
5:X:151:PHE:HE1	7:2:39:ASP:HB2	1.70	0.55
4:W:64:TRP:HA	4:W:67:ILE:HD12	1.89	0.55
7:2:395:TYR:HB3	7:2:398:ILE:HB	1.89	0.55
8:3:96:LEU:O	8:3:100:ILE:HG12	2.07	0.55
2:L:83:VAL:HG11	14:A:163:GLN:HA	1.88	0.55
6:1:81:LEU:HD13	6:1:226:PHE:HD1	1.72	0.55
7:2:34:LEU:HA	7:2:37:VAL:HG22	1.89	0.54
5:X:50:LEU:HD23	7:2:30:ILE:HG22	1.89	0.54
7:2:265:ILE:HG23	7:2:401:VAL:HG11	1.88	0.54
6:1:121:LEU:HD23	9:6:72:LEU:HD23	1.88	0.54
8:3:18:LEU:HA	8:3:21:VAL:HG12	1.90	0.54
9:6:33:ILE:HD12	9:6:71:PHE:HB3	1.88	0.54
13:C:741:GLU:HG3	13:C:774:LYS:HD3	1.90	0.54
5:X:129:SER:CB	5:X:136:GLN:NE2	2.69	0.54
14:A:106:LEU:HA	14:A:197:ALA:HA	1.89	0.54
5:X:158:PHE:HB3	15:X:201:CDL:H512	1.89	0.54
6:1:306:ASP:O	6:1:310:ASN:ND2	2.41	0.54
8:3:47:GLN:CD	8:3:48:THR:H	2.11	0.54
3:U:145:LYS:HE2	3:U:148:PRO:HB3	1.90	0.54
8:3:78:MET:HG3	9:6:147:LEU:HD23	1.90	0.54
8:3:102:PHE:O	8:3:105:GLU:HG3	2.07	0.53
9:6:54:ILE:HD11	9:6:147:LEU:HD22	1.90	0.53
2:L:15:PHE:HZ	7:2:159:PHE:HB3	1.73	0.53
15:X:201:CDL:H401	8:3:93:LEU:HD13	1.89	0.53
5:X:126:TYR:HB3	5:X:164:HIS:HE1	1.74	0.53
9:6:15:LEU:HB3	9:6:42:ILE:HD13	1.90	0.53
3:U:116:ALA:O	3:U:120:LYS:HG3	2.08	0.53
9:6:91:ILE:HA	9:6:94:LEU:HD23	1.90	0.53
5:X:112:GLU:HA	5:X:115:MET:SD	2.49	0.53
7:2:325:MET:HE2	7:2:443:LEU:HB2	1.91	0.53
13:C:527:THR:HG21	13:C:574:LEU:HD22	1.90	0.53
15:X:201:CDL:CA6	15:X:201:CDL:H112	2.38	0.53
14:A:47:ALA:HB3	14:A:59:ARG:HB3	1.90	0.53
14:A:112:GLY:HA3	14:A:138:ILE:HG21	1.91	0.53
2:L:83:VAL:HG13	2:L:84:ILE:N	2.24	0.52
15:X:201:CDL:HB4	15:X:201:CDL:CB2	2.39	0.52
6:1:232:TYR:O	6:1:236:ILE:HG12	2.09	0.52
3:U:165:GLU:OE2	3:U:169:ASN:ND2	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1:179:CYS:SG	6:1:186:LEU:HD22	2.49	0.52
7:2:429:ILE:HD11	13:C:683:LEU:HD12	1.90	0.52
8:3:12:PRO:HA	9:6:101:LEU:HD11	1.92	0.52
5:X:126:TYR:OH	5:X:166:ARG:HB2	2.09	0.52
13:C:757:LEU:HD21	13:C:792:VAL:HA	1.92	0.52
1:D:84:ARG:NH2	9:6:10:GLU:OE2	2.35	0.52
5:X:126:TYR:HB3	5:X:164:HIS:CE1	2.44	0.52
9:6:33:ILE:HG13	9:6:75:ILE:HD12	1.92	0.52
13:C:601:ALA:HB2	13:C:610:ALA:HB2	1.91	0.52
7:2:36:LEU:O	7:2:40:SER:HB2	2.09	0.52
8:3:94:PHE:CD1	9:6:166:ALA:HB2	2.45	0.52
2:L:1:FME:HG3	2:L:39:ILE:HG12	1.91	0.51
7:2:10:ILE:O	7:2:14:SER:OG	2.17	0.51
5:X:158:PHE:CD1	15:X:201:CDL:H511	2.45	0.51
6:1:124:GLY:HA3	6:1:136:SER:HB3	1.92	0.51
7:2:363:SER:HB3	7:2:447:ILE:HG13	1.91	0.51
1:D:22:GLY:HA3	6:1:279:SER:OG	2.11	0.51
5:X:54:ILE:HG22	5:X:70:PRO:HG3	1.92	0.51
6:1:152:SER:HB2	6:1:320:LEU:HD13	1.93	0.51
13:C:672:GLU:OE1	13:C:705:ARG:NH2	2.42	0.51
8:3:20:ALA:O	8:3:24:LEU:HG	2.11	0.51
12:9:46:GLU:O	12:9:50:HIS:ND1	2.44	0.51
2:L:22:ILE:HG23	7:2:159:PHE:CZ	2.46	0.50
4:W:95:ILE:HD13	12:9:64:LEU:HD12	1.92	0.50
5:X:106:ARG:NH1	5:X:107:GLU:OE2	2.44	0.50
6:1:154:PHE:O	6:1:158:ILE:HG12	2.10	0.50
7:2:69:ASP:OD1	7:2:73:TYR:HE2	1.93	0.50
13:C:550:PRO:HG3	13:C:586:TYR:HB3	1.91	0.50
7:2:124:ILE:HG13	7:2:125:THR:N	2.27	0.50
8:3:40:CYS:SG	14:A:82:MET:HG2	2.52	0.50
3:U:54:MET:O	3:U:57:ARG:N	2.45	0.50
2:L:20:ARG:NH1	9:6:93:ASP:OD2	2.45	0.50
7:2:252:ASN:ND2	7:2:303:ASN:OD1	2.45	0.50
6:1:72:ILE:HG21	9:6:34:LEU:HB3	1.94	0.50
15:X:201:CDL:H112	15:X:201:CDL:HA62	1.94	0.49
7:2:175:TYR:HB2	7:2:200:ILE:HG21	1.94	0.49
5:X:50:LEU:HD12	5:X:82:GLY:N	2.27	0.49
13:C:600:PHE:O	13:C:610:ALA:HB2	2.13	0.49
14:A:22:THR:HG22	14:A:56:PRO:O	2.12	0.49
1:D:74:PHE:HD1	1:D:77:ASN:HD21	1.59	0.49
7:2:337:ILE:O	13:C:684:ASN:ND2	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:40:LEU:HD21	2:L:55:PHE:HB3	1.94	0.49
2:L:83:VAL:HG13	2:L:84:ILE:H	1.77	0.49
13:C:804:TRP:HD1	13:C:807:LEU:HD12	1.77	0.49
3:U:92:ASP:O	3:U:96:LEU:HD23	2.12	0.49
5:X:129:SER:HB3	5:X:131:LEU:H	1.78	0.49
6:1:295:TRP:O	6:1:299:ALA:CB	2.61	0.49
8:3:55:ALA:O	8:3:59:VAL:HG23	2.13	0.49
5:X:160:ASN:OD1	15:X:201:CDL:HB21	2.12	0.49
14:A:117:TYR:CE2	14:A:190:LEU:HD13	2.48	0.49
6:1:125:TRP:CE3	9:6:30:MET:HE1	2.48	0.48
6:1:228:PHE:HD2	6:1:229:LEU:HD12	1.77	0.48
15:X:201:CDL:HB4	15:X:201:CDL:OB2	2.13	0.48
7:2:233:THR:HA	7:2:236:ILE:HG12	1.95	0.48
7:2:387:LEU:HD23	7:2:390:ILE:HD11	1.95	0.48
7:2:13:VAL:HG22	7:2:24:ILE:HD13	1.94	0.48
7:2:107:PHE:O	7:2:111:ILE:HG12	2.14	0.48
7:2:460:ILE:HD13	17:2:501:CPL:H151	1.94	0.48
8:3:113:ILE:HG22	8:3:114:ASN:H	1.78	0.48
13:C:557:TYR:CD1	13:C:582:LEU:HD11	2.46	0.48
13:C:700:ILE:O	13:C:700:ILE:HG13	2.13	0.48
1:D:55:ARG:HB3	1:D:74:PHE:HE1	1.78	0.48
5:X:36:ARG:NH2	5:X:103:GLU:OE1	2.46	0.48
7:2:387:LEU:HD11	7:2:403:ILE:HD11	1.94	0.48
9:6:146:LEU:O	9:6:150:ILE:HG12	2.14	0.48
13:C:642:ALA:HB2	13:C:676:ALA:HA	1.95	0.48
2:L:66:GLU:HB2	7:2:135:TYR:CZ	2.49	0.48
3:U:53:PHE:HA	3:U:71:GLU:HG3	1.96	0.48
5:X:159:VAL:CG2	15:X:201:CDL:HA31	2.37	0.48
9:6:2:MET:HA	9:6:5:THR:HG22	1.96	0.48
14:A:116:LYS:HB3	14:A:135:ARG:HE	1.78	0.48
3:U:18:MET:SD	3:U:19:PRO:HD2	2.54	0.48
3:U:85:ASP:O	3:U:89:SER:CB	2.62	0.48
7:2:198:ASN:O	7:2:202:ILE:HG12	2.13	0.48
13:C:583:HIS:CE1	13:C:588:VAL:HG21	2.49	0.48
7:2:36:LEU:HD21	7:2:73:TYR:HB2	1.96	0.47
7:2:127:PHE:CE1	7:2:169:ALA:HB2	2.49	0.47
6:1:186:LEU:HA	6:1:246:LEU:HD13	1.95	0.47
14:A:104:ARG:O	14:A:105:HIS:ND1	2.47	0.47
8:3:19:LEU:HD11	9:6:98:LEU:HD22	1.96	0.47
9:6:80:ILE:HG13	9:6:81:ASN:H	1.80	0.47
13:C:531:TYR:HD1	13:C:581:LEU:HD21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:C:611:LEU:O	13:C:615:GLN:HG2	2.15	0.47
14:A:88:GLN:OE1	14:A:89:PRO:HD2	2.14	0.47
6:1:153:ILE:HD11	6:1:188:ILE:HG22	1.96	0.47
7:2:9:LEU:HD22	7:2:108:LEU:HD12	1.97	0.47
14:A:189:ASN:OD1	14:A:190:LEU:N	2.47	0.47
2:L:81:ARG:HD3	2:L:82:GLY:O	2.14	0.47
3:U:156:ASP:HB3	3:U:159:SER:HB3	1.96	0.47
13:C:741:GLU:O	13:C:745:ILE:HG12	2.15	0.47
15:X:201:CDL:HB4	15:X:201:CDL:HB22	1.96	0.46
3:U:164:ALA:O	3:U:167:LYS:HG3	2.15	0.46
6:1:310:ASN:HB3	6:1:314:ILE:HD12	1.96	0.46
13:C:737:LEU:HD22	13:C:769:LEU:HD13	1.98	0.46
2:L:5:THR:HG21	8:3:6:ILE:HB	1.98	0.46
7:2:82:LEU:HD21	7:2:325:MET:HG2	1.98	0.46
7:2:201:LEU:HD13	7:2:253:ILE:HB	1.98	0.46
2:L:78:TYR:HB2	2:L:80:LEU:CD2	2.46	0.46
7:2:90:ASN:O	7:2:94:LYS:HG2	2.15	0.46
8:3:52:PHE:HE2	9:6:80:ILE:HD11	1.81	0.46
9:6:80:ILE:HG13	9:6:81:ASN:N	2.31	0.46
5:X:81:LEU:HD12	7:2:27:LEU:HD21	1.98	0.46
6:1:137:ILE:HD11	9:6:76:THR:HB	1.96	0.46
6:1:241:PHE:HA	6:1:244:TYR:CE2	2.50	0.46
9:6:47:LEU:HD13	9:6:55:PHE:HB3	1.98	0.46
5:X:155:TRP:CD2	15:X:201:CDL:H362	2.52	0.45
6:1:77:PRO:O	6:1:80:THR:OG1	2.29	0.45
1:D:83:GLU:HB3	9:6:132:THR:HB	1.97	0.45
3:U:117:LEU:HA	3:U:120:LYS:HE2	1.97	0.45
8:3:72:THR:O	8:3:75:PRO:HD2	2.16	0.45
8:3:7:PHE:CE1	8:3:11:ILE:HD11	2.52	0.45
3:U:40:TYR:CG	3:U:130:LYS:HE3	2.51	0.45
6:1:133:LEU:O	6:1:137:ILE:HG12	2.16	0.45
6:1:202:PHE:HA	6:1:308:LEU:HD21	1.98	0.45
7:2:346:TYR:CE2	14:A:102:GLN:HB3	2.52	0.45
7:2:433:GLU:HG3	13:C:832:LYS:NZ	2.31	0.45
7:2:87:LEU:HD13	7:2:439:LEU:HD12	1.97	0.45
8:3:9:ILE:O	8:3:12:PRO:HD2	2.16	0.45
3:U:68:CYS:HB3	3:U:71:GLU:OE2	2.17	0.45
5:X:36:ARG:HH11	5:X:97:ARG:HD3	1.81	0.45
6:1:281:ALA:O	6:1:284:ILE:HG22	2.17	0.45
9:6:29:PRO:HB2	9:6:75:ILE:HD13	1.99	0.45
5:X:30:ARG:HG3	5:X:30:ARG:HH11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:124:GLU:HA	5:X:124:GLU:OE2	2.17	0.44
7:2:257:SER:HB2	7:2:260:ILE:HB	1.99	0.44
8:3:35:LEU:HD23	8:3:38:PHE:HD2	1.81	0.44
9:6:9:ILE:HG23	9:6:46:TYR:HE1	1.82	0.44
2:L:62:LEU:HD23	9:6:168:VAL:HG11	1.99	0.44
1:D:83:GLU:OE1	9:6:134:ILE:HD11	2.18	0.44
5:X:160:ASN:CG	15:X:201:CDL:HA21	2.36	0.44
6:1:47:LEU:HD11	6:1:229:LEU:HD22	1.99	0.44
7:2:5:ALA:O	7:2:9:LEU:HD13	2.17	0.44
7:2:37:VAL:HA	17:2:501:CPL:H472	1.98	0.44
7:2:67:TYR:CD2	7:2:310:LEU:HD22	2.52	0.44
7:2:190:LEU:HD12	12:9:35:ALA:HA	1.99	0.44
17:2:501:CPL:HC62	17:2:501:CPL:HC42	1.80	0.44
7:2:191:ILE:HG23	12:9:41:PHE:CZ	2.53	0.44
2:L:49:ASP:OD2	7:2:176:TYR:OH	2.23	0.44
6:1:152:SER:O	6:1:156:ILE:HG13	2.18	0.44
3:U:120:LYS:O	3:U:124:THR:OG1	2.21	0.44
8:3:86:TYR:O	8:3:90:ILE:HG12	2.18	0.44
2:L:12:PHE:HD1	2:L:32:MET:HE3	1.82	0.44
2:L:77:TYR:CZ	14:A:126:PRO:HG3	2.53	0.44
3:U:146:LYS:HD3	3:U:147:ASP:HB2	1.99	0.44
7:2:9:LEU:HD11	7:2:28:ILE:CD1	2.39	0.44
7:2:157:TYR:HB2	7:2:224:ILE:HD13	1.99	0.44
1:D:30:VAL:HG21	6:1:271:PHE:CG	2.53	0.44
2:L:57:ILE:HG13	2:L:58:VAL:N	2.32	0.44
3:U:85:ASP:O	3:U:89:SER:OG	2.31	0.44
6:1:26:GLU:OE2	6:1:199:ARG:NH1	2.47	0.43
12:9:7:SER:HB3	12:9:13:ASN:HA	2.00	0.43
13:C:667:ARG:O	13:C:671:ASN:ND2	2.51	0.43
2:L:60:ILE:HD11	9:6:59:TYR:HE1	1.83	0.43
7:2:122:ASP:OD1	7:2:182:TYR:HB3	2.18	0.43
8:3:25:LEU:O	8:3:26:ALA:C	2.55	0.43
13:C:695:GLN:NE2	14:A:148:VAL:HG12	2.32	0.43
13:C:621:HIS:CE1	13:C:628:ALA:HB2	2.53	0.43
5:X:155:TRP:CE2	15:X:201:CDL:H362	2.54	0.43
7:2:261:SER:O	7:2:265:ILE:HG12	2.19	0.43
14:A:123:SER:OG	14:A:172:ASN:O	2.30	0.43
1:D:9:LEU:O	1:D:13:ILE:HG12	2.19	0.43
2:L:80:LEU:HD12	9:6:77:LEU:HB3	1.99	0.43
6:1:222:SER:HB3	6:1:223:PRO:HD3	2.01	0.43
13:C:707:VAL:HG21	13:C:728:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:X:201:CDL:H112	15:X:201:CDL:HA4	1.66	0.43
7:2:213:GLY:HA3	7:2:221:LEU:HD12	2.00	0.43
14:A:116:LYS:CG	14:A:135:ARG:HH21	2.32	0.43
1:D:26:GLN:OE1	6:1:97:ILE:HD11	2.18	0.43
1:D:45:TRP:O	1:D:49:MET:HG2	2.19	0.43
7:2:91:ASN:N	13:C:681:GLU:OE1	2.49	0.43
7:2:429:ILE:HD12	13:C:713:TYR:OH	2.19	0.43
9:6:120:ASN:HA	9:6:123:LEU:HD12	2.00	0.43
13:C:548:GLN:OE1	13:C:553:ARG:NH2	2.51	0.43
2:L:26:PHE:CZ	2:L:67:SER:HA	2.52	0.43
5:X:131:LEU:HD21	8:3:85:ASN:HB2	2.00	0.43
6:1:86:ILE:O	6:1:89:VAL:HG12	2.19	0.43
5:X:156:PHE:HB2	5:X:158:PHE:CE2	2.54	0.42
15:X:201:CDL:H182	15:X:201:CDL:H211	1.48	0.42
9:6:81:ASN:O	9:6:83:THR:HG23	2.19	0.42
7:2:265:ILE:HD11	7:2:398:ILE:HG12	2.01	0.42
7:2:26:ARG:O	7:2:30:ILE:HD12	2.19	0.42
7:2:362:LEU:O	7:2:366:ILE:HG12	2.20	0.42
8:3:42:LEU:HD11	14:A:80:PHE:HB3	2.01	0.42
8:3:79:SER:O	8:3:83:VAL:HG22	2.20	0.42
7:2:157:TYR:CD1	7:2:224:ILE:HD13	2.54	0.42
13:C:695:GLN:HE22	14:A:148:VAL:HG12	1.85	0.42
13:C:773:ALA:HB1	13:C:807:LEU:HD21	2.01	0.42
5:X:43:ILE:HA	5:X:86:GLY:HA3	2.01	0.42
5:X:93:ARG:HG3	7:2:41:PHE:CZ	2.54	0.42
5:X:130:SER:OG	8:3:85:ASN:OD1	2.34	0.42
5:X:152:ILE:HD11	7:2:119:HIS:CE1	2.54	0.42
6:1:153:ILE:HG21	6:1:189:PHE:HD2	1.83	0.42
6:1:286:LEU:O	6:1:290:MET:HG3	2.18	0.42
4:W:117:ALA:HA	9:6:133:ILE:HD12	2.01	0.42
15:X:201:CDL:H171	15:X:201:CDL:H142	1.87	0.42
16:1:401:PLC:H1'1	16:1:401:PLC:H2	1.84	0.42
1:D:78:HIS:HE1	1:D:80:TRP:NE1	2.17	0.42
3:U:96:LEU:HD13	3:U:158:LYS:NZ	2.35	0.42
3:U:164:ALA:HB1	3:U:168:LYS:NZ	2.35	0.42
6:1:201:PRO:HB3	6:1:300:PHE:O	2.19	0.42
7:2:67:TYR:HD2	7:2:310:LEU:HD22	1.85	0.42
13:C:611:LEU:HD21	13:C:652:ARG:HG2	2.02	0.42
2:L:13:LEU:HD23	2:L:13:LEU:HA	1.84	0.42
7:2:195:LEU:HD11	12:9:45:MET:HG3	2.01	0.42
7:2:295:TYR:CE1	7:2:402:LEU:HG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2:347:VAL:HG13	7:2:416:LEU:HD23	2.02	0.42
6:1:306:ASP:OD1	6:1:306:ASP:N	2.52	0.42
7:2:31:TYR:O	7:2:35:VAL:HG23	2.20	0.42
7:2:86:ASN:O	7:2:436:SER:HB2	2.20	0.42
8:3:65:PRO:O	8:3:69:GLU:HG3	2.19	0.42
3:U:71:GLU:O	3:U:75:VAL:HG23	2.20	0.42
6:1:250:TYR:HB2	6:1:278:ASN:HB3	2.02	0.42
7:2:29:ASN:OD1	7:2:77:ILE:HG23	2.19	0.42
13:C:695:GLN:HE22	14:A:148:VAL:H	1.68	0.42
7:2:324:PHE:O	7:2:328:ILE:HG12	2.20	0.41
14:A:39:GLY:C	14:A:69:PRO:HB3	2.40	0.41
14:A:57:TYR:HB3	14:A:193:GLU:HB3	2.01	0.41
14:A:111:ARG:HD2	14:A:191:ASP:OD2	2.20	0.41
2:L:22:ILE:HG23	7:2:159:PHE:HZ	1.84	0.41
6:1:78:LEU:O	6:1:82:ILE:HG13	2.20	0.41
6:1:155:ILE:O	6:1:159:MET:HG3	2.20	0.41
6:1:290:MET:O	6:1:294:ILE:HD12	2.19	0.41
7:2:217:LEU:O	7:2:220:TRP:NE1	2.53	0.41
7:2:232:ILE:O	7:2:236:ILE:HG23	2.19	0.41
9:6:177:ILE:O	9:6:181:MET:HG2	2.20	0.41
14:A:82:MET:HE1	14:A:84:ARG:HB3	2.02	0.41
13:C:745:ILE:HG22	13:C:749:ARG:HD2	2.03	0.41
4:W:119:MET:HB3	9:6:133:ILE:HD11	2.03	0.41
5:X:129:SER:OG	15:X:201:CDL:PA1	2.78	0.41
7:2:131:GLU:OE2	7:2:165:SER:HB2	2.21	0.41
13:C:710:LEU:HD23	13:C:724:THR:HG23	2.02	0.41
14:A:66:LEU:HD11	14:A:184:GLN:N	2.35	0.41
2:L:46:LEU:HD23	2:L:46:LEU:HA	1.92	0.41
2:L:2:PHE:O	2:L:6:ILE:HG12	2.21	0.41
17:2:501:CPL:H341	17:2:501:CPL:H201	2.03	0.41
2:L:84:ILE:HD11	8:3:51:ALA:HB2	2.02	0.41
16:1:401:PLC:H83	16:1:401:PLC:H42	1.85	0.41
9:6:9:ILE:O	9:6:12:THR:OG1	2.31	0.41
2:L:71:LEU:HD13	9:6:70:LEU:HG	2.02	0.41
6:1:137:ILE:HG23	9:6:73:PHE:CE2	2.56	0.41
7:2:352:GLY:HA3	7:2:424:LYS:HG2	2.02	0.41
7:2:396:TYR:O	7:2:400:ILE:HG13	2.21	0.41
13:C:599:PHE:HA	13:C:603:ASP:HB2	2.03	0.41
1:D:6:GLU:HB2	6:1:32:TYR:CE2	2.56	0.41
2:L:12:PHE:O	2:L:16:VAL:HG23	2.21	0.41
6:1:90:VAL:HG22	6:1:166:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2:375:PRO:HG3	7:2:380:PHE:CD1	2.56	0.41
8:3:76:TYR:CD1	8:3:91:VAL:HG21	2.56	0.41
9:6:161:ILE:O	9:6:165:LEU:HD23	2.20	0.41
14:A:180:LEU:HD23	14:A:180:LEU:HA	1.90	0.41
14:A:125:THR:HG22	14:A:127:LEU:H	1.86	0.41
6:1:190:PHE:CZ	6:1:292:SER:HB3	2.56	0.40
7:2:28:ILE:HD13	7:2:28:ILE:HA	1.80	0.40
9:6:67:ILE:O	9:6:71:PHE:HD1	2.04	0.40
2:L:27:ILE:HG12	9:6:36:MET:SD	2.61	0.40
5:X:35:MET:HB2	5:X:35:MET:HE2	1.89	0.40
6:1:250:TYR:HA	6:1:282:TYR:HB2	2.02	0.40
12:9:67:LYS:HZ1	12:9:71:LEU:HD21	1.86	0.40
4:W:121:PRO:HA	4:W:122:PRO:HD3	1.83	0.40
5:X:50:LEU:HG	7:2:34:LEU:HD12	2.04	0.40
6:1:234:ASN:O	6:1:238:ILE:HG12	2.21	0.40
13:C:804:TRP:CD1	13:C:807:LEU:HD12	2.57	0.40
3:U:16:ALA:O	4:W:83:ARG:NH1	2.47	0.40
13:C:788:ARG:O	13:C:792:VAL:HG23	2.20	0.40
14:A:17:VAL:HG12	14:A:196:LYS:HE3	2.04	0.40
2:L:56:ALA:O	2:L:60:ILE:HG13	2.21	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	D	84/87 (97%)	83 (99%)	1 (1%)	0	100 100
2	L	87/89 (98%)	81 (93%)	5 (6%)	1 (1%)	12 44
3	U	169/172 (98%)	164 (97%)	5 (3%)	0	100 100
4	W	90/123 (73%)	89 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	X	162/169 (96%)	159 (98%)	3 (2%)	0	100	100
6	1	295/341 (86%)	286 (97%)	9 (3%)	0	100	100
7	2	467/469 (100%)	457 (98%)	10 (2%)	0	100	100
8	3	112/128 (88%)	94 (84%)	18 (16%)	0	100	100
9	6	182/185 (98%)	173 (95%)	9 (5%)	0	100	100
10	g	74/78 (95%)	70 (95%)	4 (5%)	0	100	100
11	b	62/74 (84%)	62 (100%)	0	0	100	100
12	9	84/89 (94%)	83 (99%)	1 (1%)	0	100	100
13	C	335/852 (39%)	318 (95%)	16 (5%)	1 (0%)	37	69
14	A	214/290 (74%)	190 (89%)	22 (10%)	2 (1%)	14	49
All	All	2417/3146 (77%)	2309 (96%)	104 (4%)	4 (0%)	45	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	A	26	SER
13	C	601	ALA
14	A	96	ASN
2	L	84	ILE

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	D	68/69 (99%)	68 (100%)	0	100	100
2	L	76/76 (100%)	76 (100%)	0	100	100
3	U	147/148 (99%)	143 (97%)	4 (3%)	40	69
4	W	76/102 (74%)	76 (100%)	0	100	100
5	X	127/133 (96%)	124 (98%)	3 (2%)	44	71
6	1	268/301 (89%)	268 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	2	432/432 (100%)	432 (100%)	0	100	100
8	3	100/113 (88%)	100 (100%)	0	100	100
9	6	165/166 (99%)	165 (100%)	0	100	100
10	g	63/65 (97%)	63 (100%)	0	100	100
11	b	50/59 (85%)	50 (100%)	0	100	100
12	9	73/76 (96%)	73 (100%)	0	100	100
13	C	297/745 (40%)	297 (100%)	0	100	100
14	A	193/245 (79%)	193 (100%)	0	100	100
All	All	2135/2730 (78%)	2128 (100%)	7 (0%)	90	96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	U	125	LYS
3	U	131	LYS
3	U	158	LYS
3	U	167	LYS
5	X	124	GLU
5	X	129	SER
5	X	130	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
7	2	29	ASN
8	3	107	ASN
13	C	583	HIS
13	C	695	GLN
13	C	739	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	FME	1	1	6	8,9,10	0.93	0	7,9,11	0.88	0
2	FME	L	1	2	8,9,10	0.91	0	7,9,11	0.90	0
7	FME	2	1	7	8,9,10	0.93	0	7,9,11	0.86	0
9	FME	6	1	9	8,9,10	0.92	0	7,9,11	0.90	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
6	FME	1	1	6	-	0/7/9/11	-
2	FME	L	1	2	-	2/7/9/11	-
7	FME	2	1	7	-	3/7/9/11	-
9	FME	6	1	9	-	5/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	2	1	FME	N-CA-CB-CG
7	2	1	FME	C-CA-CB-CG
9	6	1	FME	O1-CN-N-CA
9	6	1	FME	N-CA-CB-CG
9	6	1	FME	C-CA-CB-CG
9	6	1	FME	CB-CG-SD-CE
7	2	1	FME	CB-CG-SD-CE
2	L	1	FME	CB-CG-SD-CE
9	6	1	FME	CA-CB-CG-SD
2	L	1	FME	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	PLC	1	401	-	41,41,41	1.19	3 (7%)	47,49,49	1.10	3 (6%)
18	3PE	g	102	-	42,42,50	0.55	0	45,47,55	0.55	1 (2%)
15	CDL	g	101	-	82,82,99	0.30	0	88,94,111	0.38	0
17	CPL	2	501	-	51,51,51	1.14	3 (5%)	57,59,59	1.16	4 (7%)
15	CDL	X	201	-	63,63,99	0.47	0	68,74,111	0.77	2 (2%)
19	T7X	b	501	-	48,48,61	0.55	0	57,60,73	0.78	1 (1%)

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
16	PLC	1	401	-	-	25/45/45/45	-
18	3PE	g	102	-	-	21/46/46/54	-
15	CDL	g	101	-	-	30/93/93/110	-
17	CPL	2	501	-	-	25/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CDL	X	201	-	-	41/73/73/110	-
19	T7X	b	501	-	-	15/43/67/80	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	1	401	PLC	O3-CB	3.05	1.42	1.33
17	2	501	CPL	O3-C11	3.00	1.42	1.33
16	1	401	PLC	O2-C'	2.94	1.42	1.34
16	1	401	PLC	O2-C2	-2.45	1.40	1.46
17	2	501	CPL	O2-C2	-2.43	1.40	1.46
17	2	501	CPL	O2-C31	2.24	1.40	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	501	CPL	O2-C31-C32	4.11	120.35	111.50
16	1	401	PLC	O2-C'-C1'	4.08	120.30	111.50
17	2	501	CPL	C8-N-C7	3.96	119.16	108.97
16	1	401	PLC	C7-N-C6	3.84	118.84	108.97
17	2	501	CPL	C41-C40-C39	3.43	152.51	123.57
19	b	501	T7X	O1-C1-C6	2.81	115.20	108.66
16	1	401	PLC	O3-CB-C1B	2.57	119.98	111.91
15	X	201	CDL	OA4-PA1-OA5	-2.49	96.16	107.75
17	2	501	CPL	O3-C11-C12	2.47	119.65	111.91
18	g	102	3PE	O12-P-O14	2.31	123.67	112.24
15	X	201	CDL	OA4-PA1-OA3	2.19	123.06	112.24

There are no chirality outliers.

All (157) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	X	201	CDL	CA3-OA5-PA1-OA4
15	X	201	CDL	OA7-CA5-OA6-CA4
15	X	201	CDL	C11-CA5-OA6-CA4
15	X	201	CDL	CB4-CB3-OB5-PB2
15	X	201	CDL	CB3-CB4-CB6-OB8
15	X	201	CDL	OB6-CB4-CB6-OB8
15	g	101	CDL	CA2-C1-CB2-OB2
16	1	401	PLC	O4P-C4-C5-N
16	1	401	PLC	C1'-C'-O2-C2

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Mol	Chain	Res	Type	Atoms
16	1	401	PLC	O'-C'-O2-C2
16	1	401	PLC	C1-O3P-P-O1P
16	1	401	PLC	C4-O4P-P-O1P
16	1	401	PLC	C4-O4P-P-O2P
17	2	501	CPL	C1-O3P-P-O1P
17	2	501	CPL	C1-O3P-P-O2P
17	2	501	CPL	C4-O4P-P-O1P
17	2	501	CPL	C4-O4P-P-O2P
18	g	102	3PE	O13-C11-C12-N
18	g	102	3PE	C22-C21-O21-C2
19	b	501	T7X	C6-C1-O1-P1
19	b	501	T7X	C7-O13-P1-O11
19	b	501	T7X	C7-O13-P1-O12
19	b	501	T7X	C12-C10-O16-C8
19	b	501	T7X	C16-C17-C18-C19
15	X	201	CDL	C31-CA7-OA8-CA6
15	X	201	CDL	OA9-CA7-OA8-CA6
16	1	401	PLC	OB-CB-O3-C3
15	X	201	CDL	OB7-CB5-OB6-CB4
18	g	102	3PE	O22-C21-O21-C2
19	b	501	T7X	O17-C10-O16-C8
16	1	401	PLC	C1B-CB-O3-C3
15	X	201	CDL	C51-CB5-OB6-CB4
15	X	201	CDL	C12-C13-C14-C15
15	X	201	CDL	C18-C19-C20-C21
15	g	101	CDL	C1-CA2-OA2-PA1
15	X	201	CDL	C32-C33-C34-C35
15	g	101	CDL	O1-C1-CB2-OB2
15	X	201	CDL	CA7-C31-C32-C33
19	b	501	T7X	O16-C8-C9-O18
19	b	501	T7X	C10-C12-C13-C14
16	1	401	PLC	CB-C1B-C2B-C3B
15	X	201	CDL	CA5-C11-C12-C13
15	g	101	CDL	O1-C1-CA2-OA2
15	X	201	CDL	CA3-OA5-PA1-OA2
16	1	401	PLC	C1-O3P-P-O4P
16	1	401	PLC	C4-O4P-P-O3P
17	2	501	CPL	C1-O3P-P-O4P
17	2	501	CPL	C4-O4P-P-O3P
18	g	102	3PE	C11-O13-P-O11
19	b	501	T7X	C7-O13-P1-O1
15	g	101	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
15	g	101	CDL	C11-CA5-OA6-CA4
15	X	201	CDL	C41-C42-C43-C44
16	1	401	PLC	C2B-C3B-C4B-C5B
15	g	101	CDL	OA7-CA5-OA6-CA4
17	2	501	CPL	C18-C19-C20-C21
15	X	201	CDL	CB5-C51-C52-C53
17	2	501	CPL	C20-C21-C22-C23
15	X	201	CDL	C51-C52-C53-C54
15	X	201	CDL	C17-C18-C19-C20
15	X	201	CDL	C39-C40-C41-C42
16	1	401	PLC	C1B-C2B-C3B-C4B
15	X	201	CDL	C35-C36-C37-C38
15	g	101	CDL	C19-C20-C21-C22
16	1	401	PLC	C1'-C2'-C3'-C4'
15	X	201	CDL	C15-C16-C17-C18
17	2	501	CPL	C32-C33-C34-C35
16	1	401	PLC	C5'-C6'-C7'-C8'
17	2	501	CPL	C33-C34-C35-C36
17	2	501	CPL	C12-C11-O3-C3
18	g	102	3PE	C27-C28-C29-C2A
18	g	102	3PE	C21-C22-C23-C24
16	1	401	PLC	C6'-C7'-C8'-C9'
17	2	501	CPL	O11-C11-O3-C3
15	g	101	CDL	OB6-CB4-CB6-OB8
18	g	102	3PE	C24-C25-C26-C27
15	X	201	CDL	C13-C14-C15-C16
15	g	101	CDL	C11-C12-C13-C14
15	X	201	CDL	OB5-CB3-CB4-CB6
15	X	201	CDL	C34-C35-C36-C37
16	1	401	PLC	C1-C2-C3-O3
19	b	501	T7X	C7-C8-C9-O18
15	X	201	CDL	C16-C17-C18-C19
15	X	201	CDL	C14-C15-C16-C17
15	X	201	CDL	C19-C20-C21-C22
15	X	201	CDL	CB6-CB4-OB6-CB5
19	b	501	T7X	C7-C8-O16-C10
15	X	201	CDL	C1-CA2-OA2-PA1
18	g	102	3PE	O11-C1-C2-O21
18	g	102	3PE	C26-C27-C28-C29
15	g	101	CDL	OA5-CA3-CA4-CA6
17	2	501	CPL	O3P-C1-C2-C3
15	X	201	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
17	2	501	CPL	C44-C45-C46-C47
15	g	101	CDL	CB3-CB4-CB6-OB8
18	g	102	3PE	C33-C34-C35-C36
19	b	501	T7X	C22-C23-C24-C25
15	X	201	CDL	OA6-CA4-CA6-OA8
16	1	401	PLC	O2-C2-C3-O3
15	X	201	CDL	CB2-C1-CA2-OA2
15	g	101	CDL	C12-C13-C14-C15
18	g	102	3PE	O11-C1-C2-C3
15	X	201	CDL	O1-C1-CA2-OA2
15	X	201	CDL	CA3-CA4-CA6-OA8
15	g	101	CDL	CB4-CB3-OB5-PB2
15	g	101	CDL	OA5-CA3-CA4-OA6
15	g	101	CDL	OB5-CB3-CB4-OB6
18	g	102	3PE	C28-C29-C2A-C2B
18	g	102	3PE	C32-C31-O31-C3
15	X	201	CDL	C38-C39-C40-C41
15	X	201	CDL	CA3-OA5-PA1-OA3
18	g	102	3PE	C11-O13-P-O14
15	g	101	CDL	OB5-CB3-CB4-CB6
17	2	501	CPL	O3P-C1-C2-O2
17	2	501	CPL	O4P-C4-C5-N
18	g	102	3PE	C1-C2-C3-O31
18	g	102	3PE	O21-C2-C3-O31
18	g	102	3PE	O32-C31-O31-C3
15	X	201	CDL	C54-C55-C56-C57
15	g	101	CDL	C78-C79-C80-C81
19	b	501	T7X	C8-C7-O13-P1
15	X	201	CDL	OB5-CB3-CB4-OB6
15	g	101	CDL	CA2-OA2-PA1-OA5
15	g	101	CDL	CB2-OB2-PB2-OB5
15	g	101	CDL	C1-CB2-OB2-PB2
17	2	501	CPL	C42-C43-C44-C45
16	1	401	PLC	C7B-C8B-C9B-CAA
17	2	501	CPL	C43-C44-C45-C46
17	2	501	CPL	C12-C13-C14-C15
17	2	501	CPL	C39-C40-C41-C42
17	2	501	CPL	C40-C41-C42-C43
17	2	501	CPL	C35-C36-C37-C38
17	2	501	CPL	C15-C16-C17-C18
16	1	401	PLC	C5B-C6B-C7B-C8B
16	1	401	PLC	C4'-C5'-C6'-C7'

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Mol	Chain	Res	Type	Atoms
18	g	102	3PE	C32-C33-C34-C35
15	g	101	CDL	C34-C35-C36-C37
18	g	102	3PE	C25-C26-C27-C28
16	1	401	PLC	C4B-C5B-C6B-C7B
17	2	501	CPL	C45-C46-C47-C48
19	b	501	T7X	C13-C14-C15-C16
18	g	102	3PE	C29-C2A-C2B-C2C
15	g	101	CDL	C31-CA7-OA8-CA6
15	g	101	CDL	OB9-CB7-OB8-CB6
15	X	201	CDL	C53-C54-C55-C56
17	2	501	CPL	C36-C37-C38-C39
15	g	101	CDL	OA9-CA7-OA8-CA6
15	g	101	CDL	CA2-OA2-PA1-OA3
15	g	101	CDL	C32-C31-CA7-OA8
16	1	401	PLC	C5-C4-O4P-P
18	g	102	3PE	O31-C31-C32-C33
15	g	101	CDL	CB4-CB6-OB8-CB7
16	1	401	PLC	C8B-C9B-CAA-CBA
19	b	501	T7X	O16-C10-C12-C13
16	1	401	PLC	C2B-C1B-CB-O3
15	g	101	CDL	C71-CB7-OB8-CB6
15	g	101	CDL	C52-C51-CB5-OB6

There are no ring outliers.

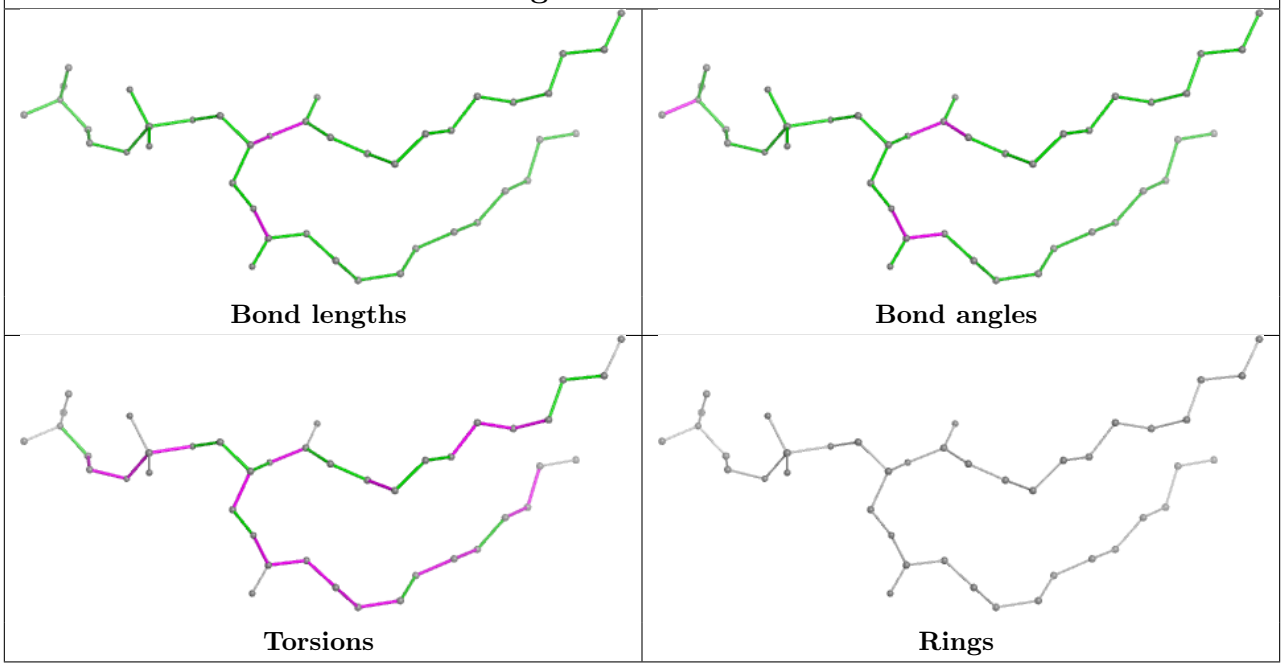
3 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	1	401	PLC	2	0
17	2	501	CPL	4	0
15	X	201	CDL	26	0

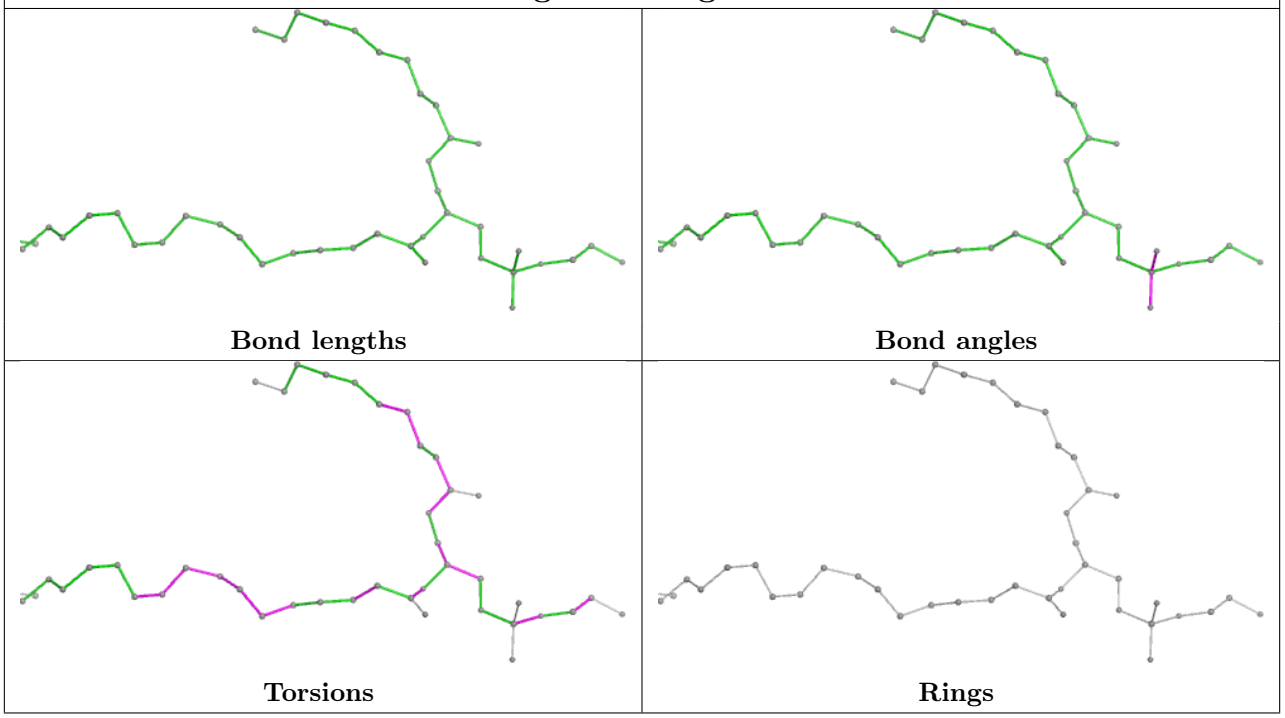
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

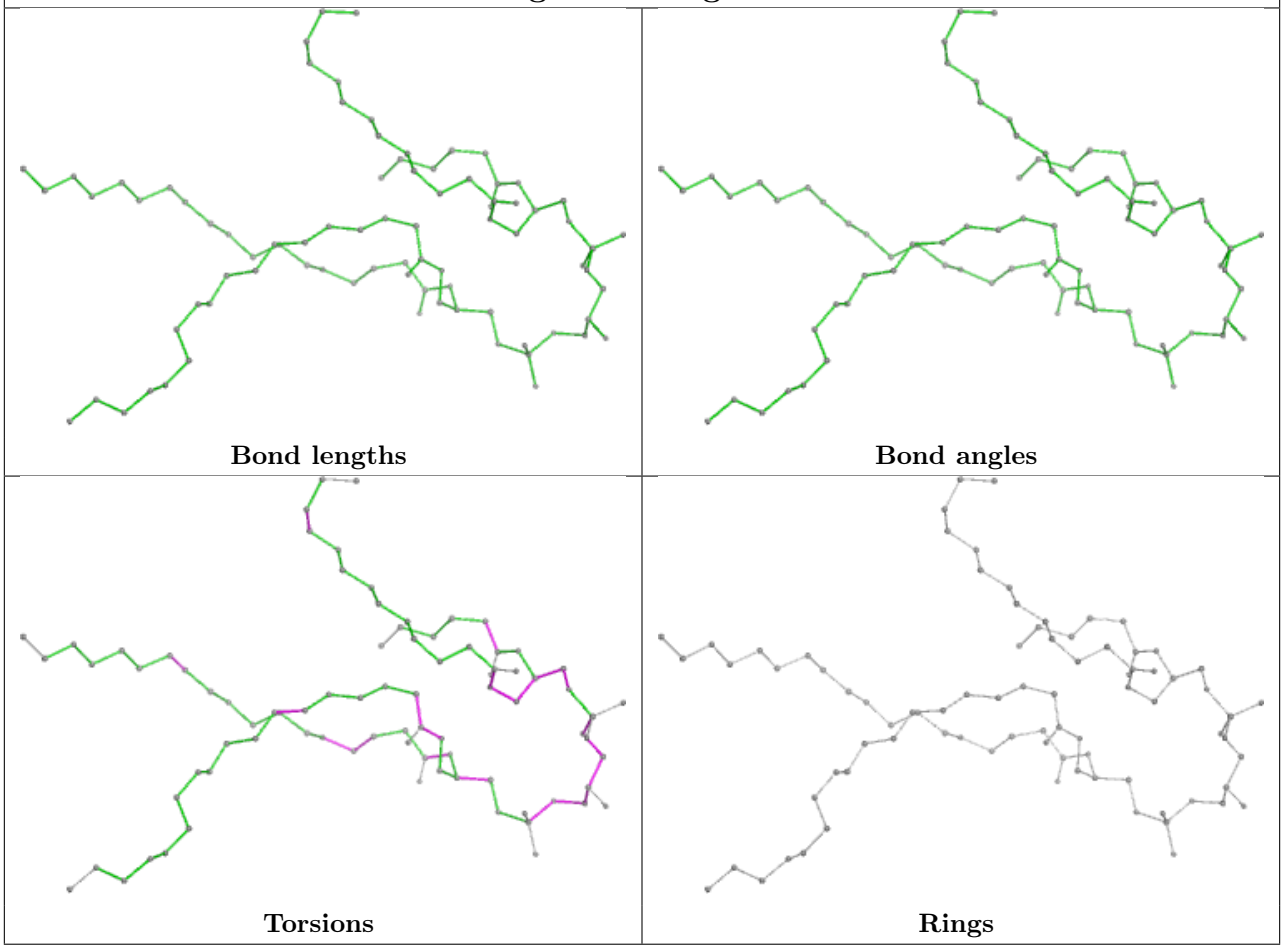
Ligand PLC 1 401



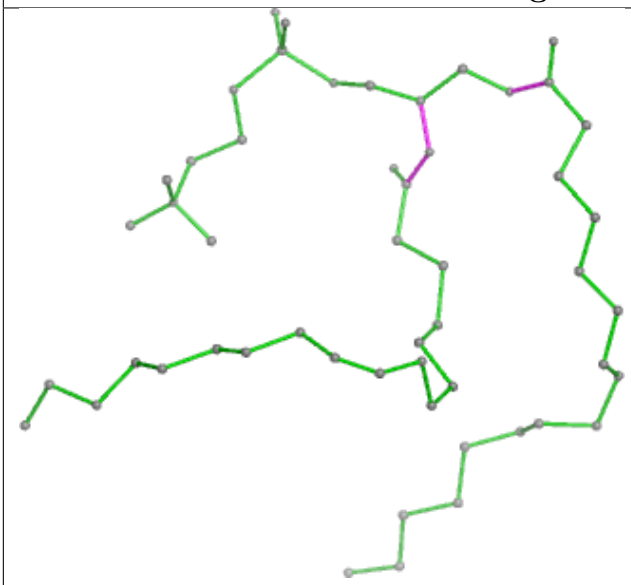
Ligand 3PE g 102



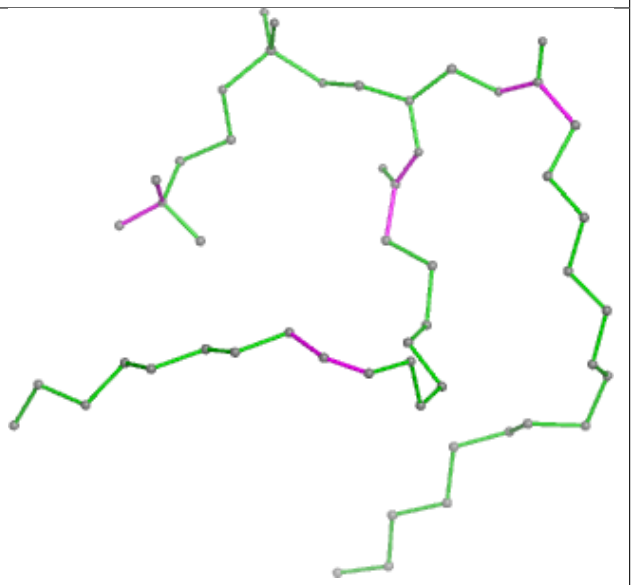
Ligand CDL g 101



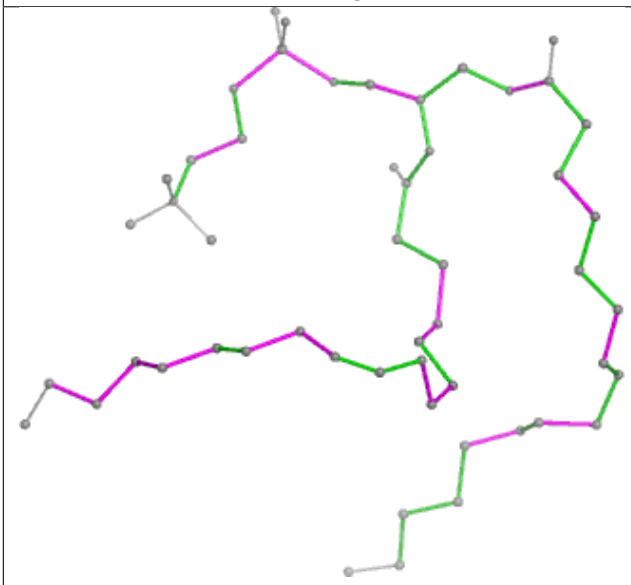
Ligand CPL 2 501



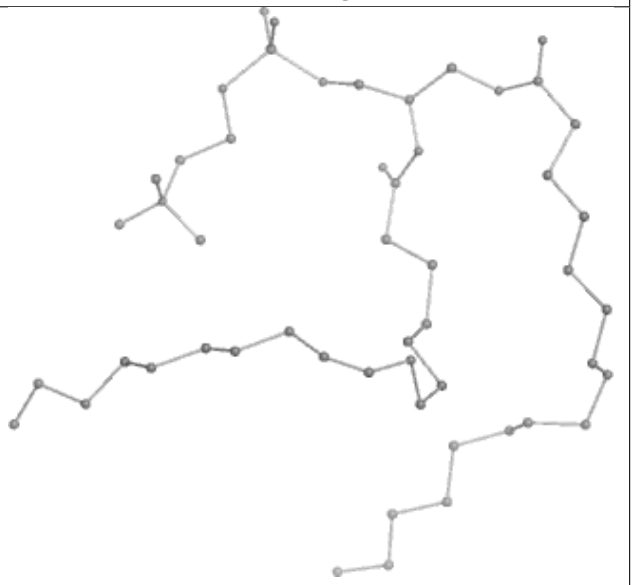
Bond lengths



Bond angles

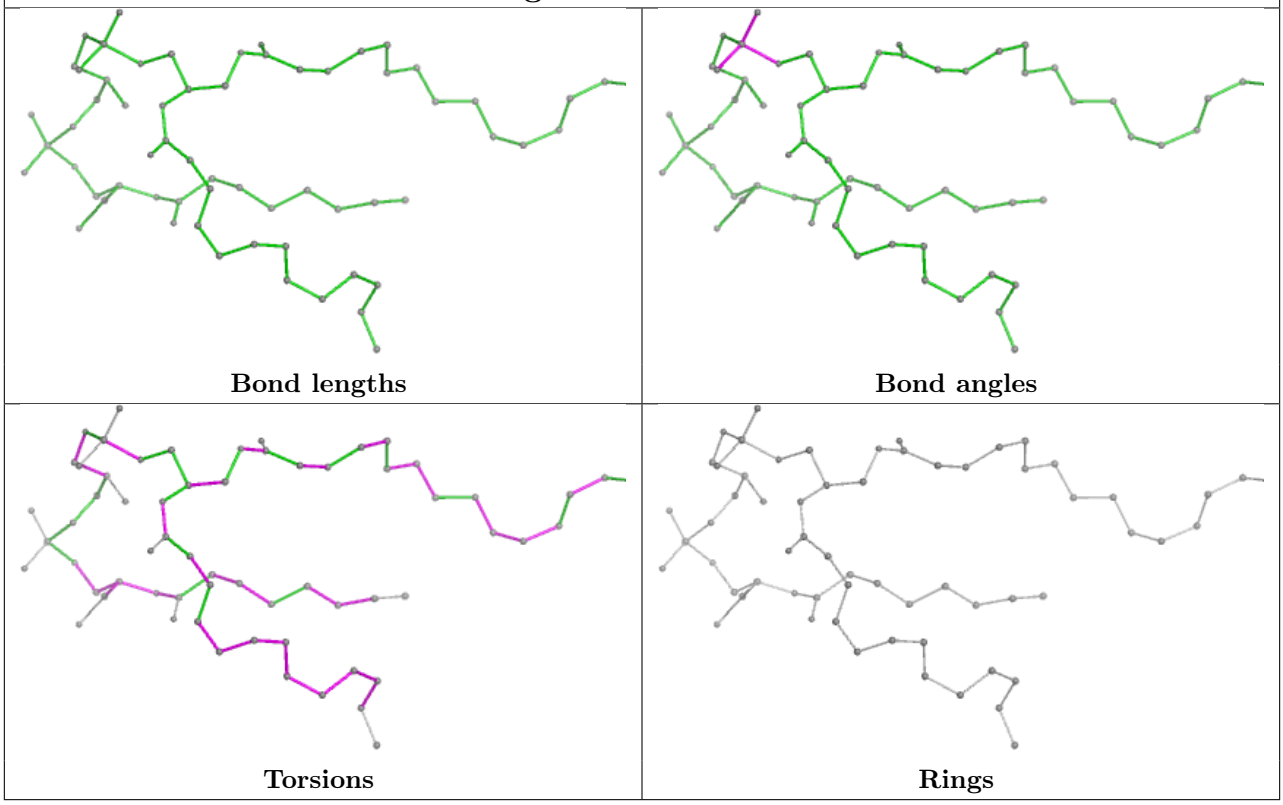


Torsions

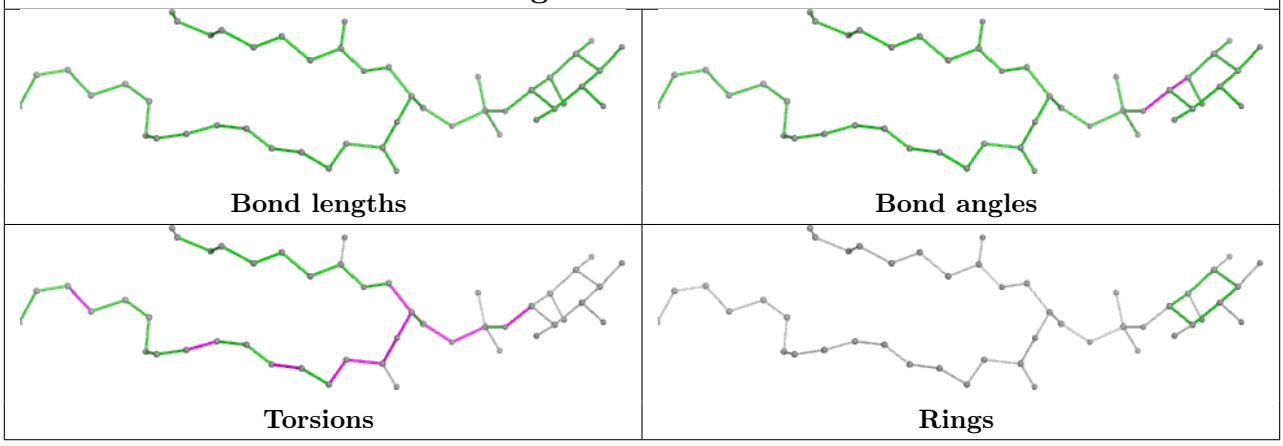


Rings

Ligand CDL X 201



Ligand T7X b 501



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.

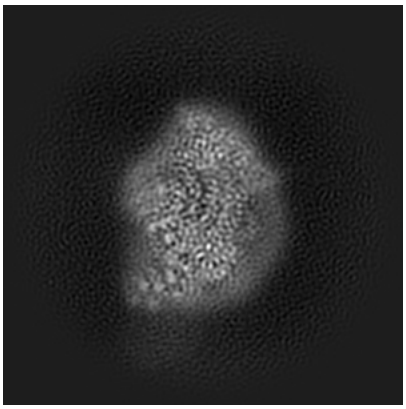
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14764. These allow visual inspection of the internal detail of the map and identification of artifacts.

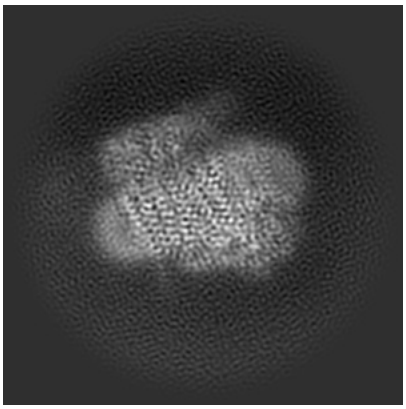
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

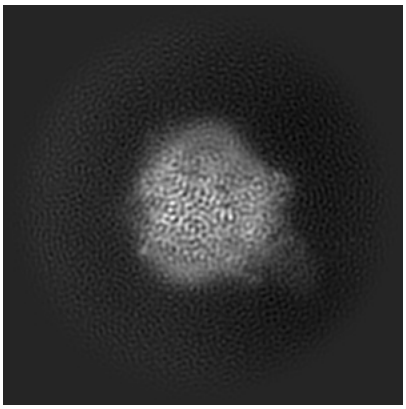
6.1.1 Primary map



X

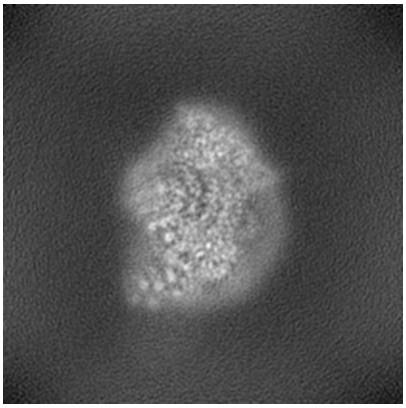


Y

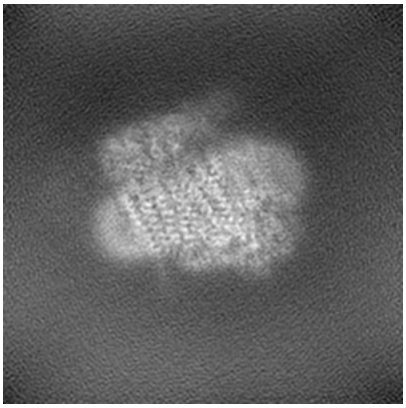


Z

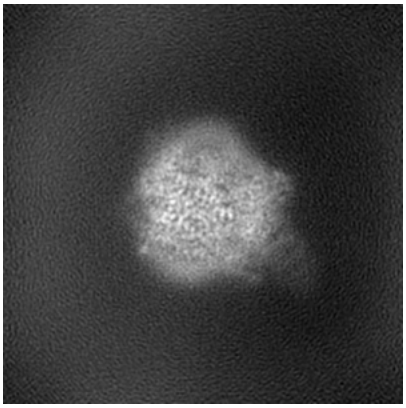
6.1.2 Raw map



X



Y

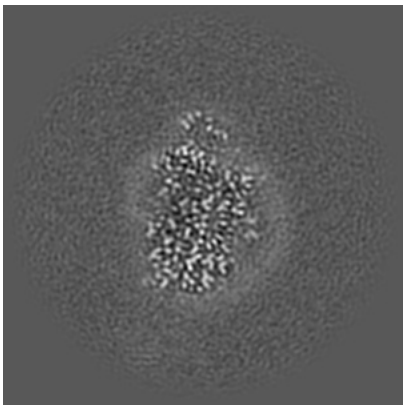


Z

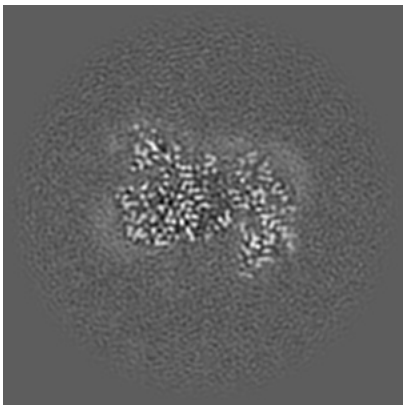
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

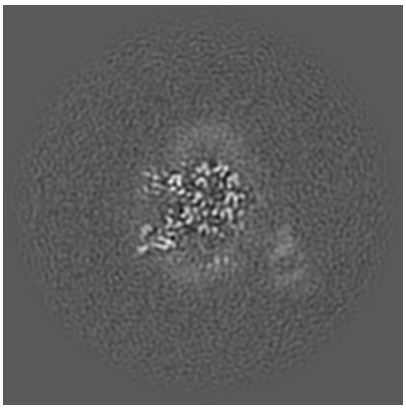
6.2.1 Primary map



X Index: 104

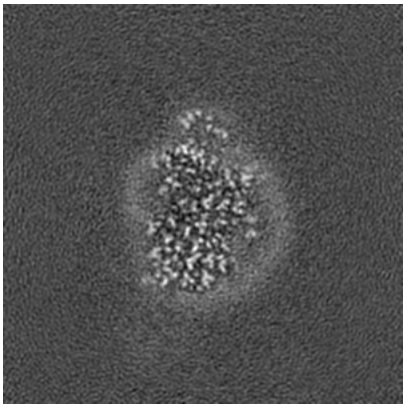


Y Index: 104

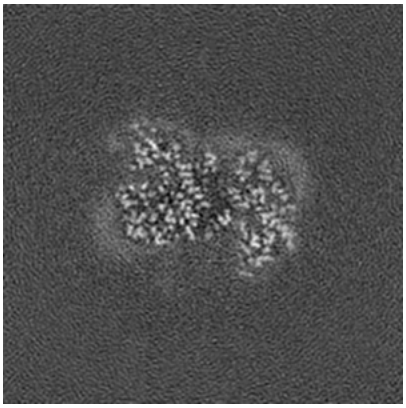


Z Index: 104

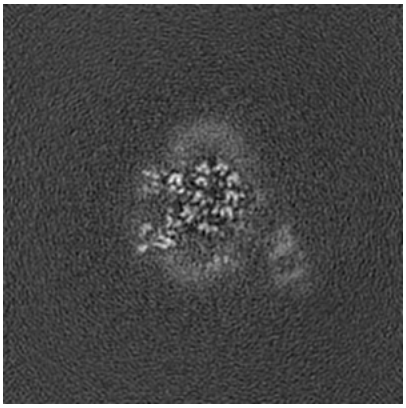
6.2.2 Raw map



X Index: 104



Y Index: 104

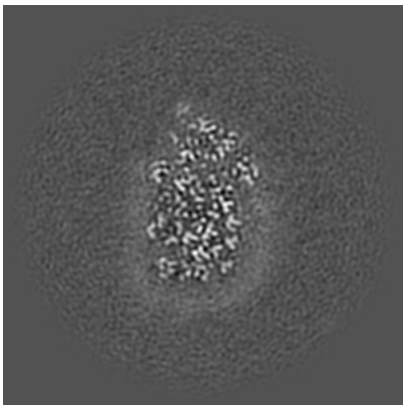


Z Index: 104

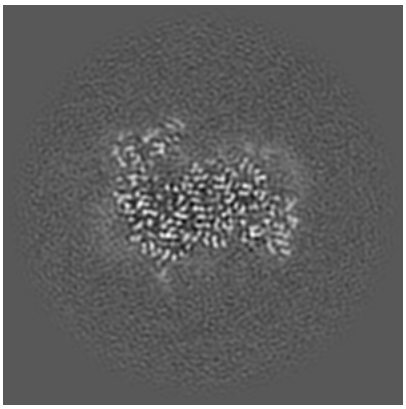
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

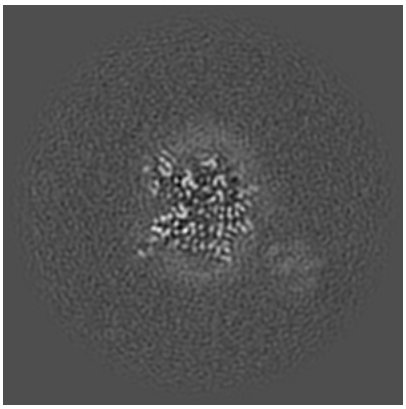
6.3.1 Primary map



X Index: 91

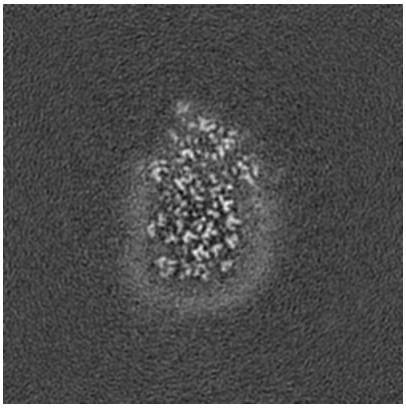


Y Index: 97

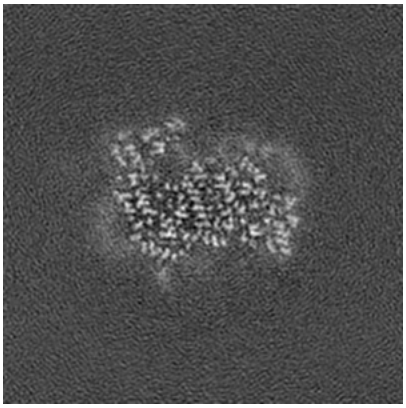


Z Index: 110

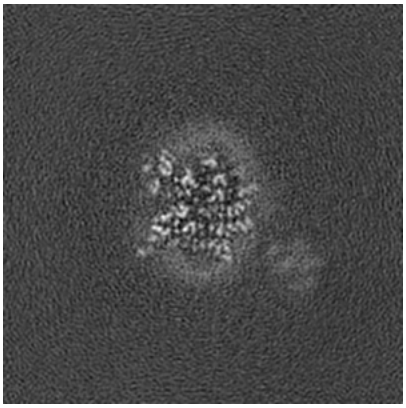
6.3.2 Raw map



X Index: 91



Y Index: 97

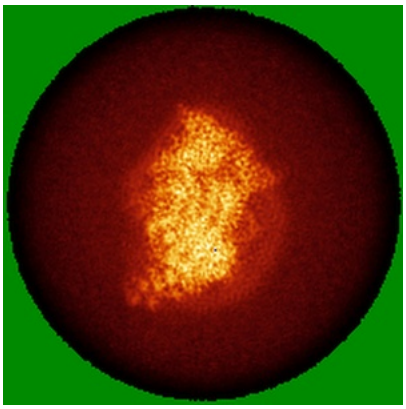


Z Index: 110

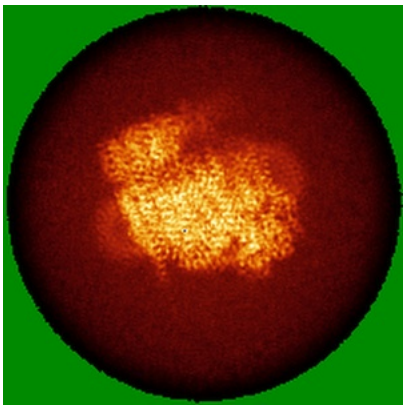
The images above show the largest variance slices of the map in three orthogonal directions.

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

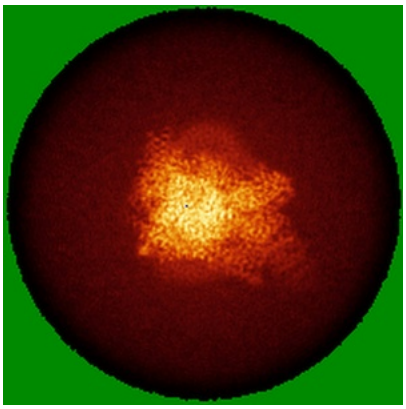
6.4.1 Primary map



X

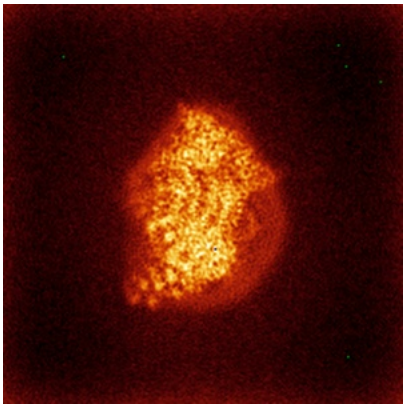


Y

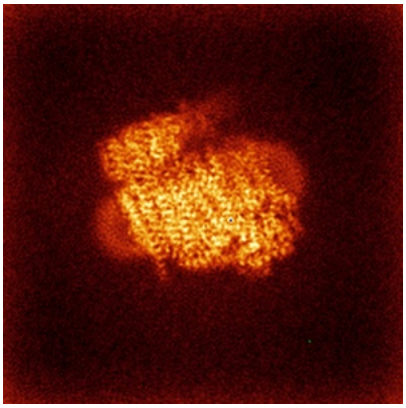


Z

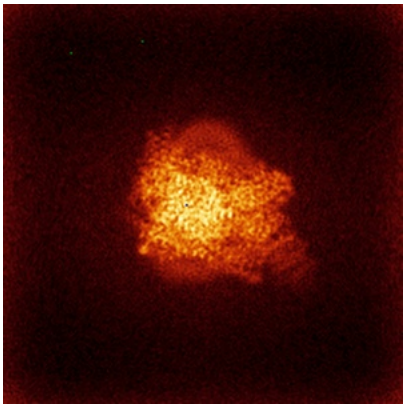
6.4.2 Raw map



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

6.5.2 Raw map

X

Y

Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

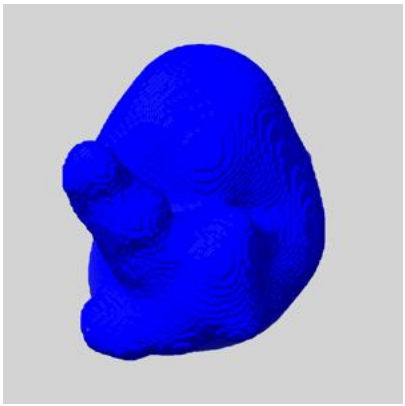
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

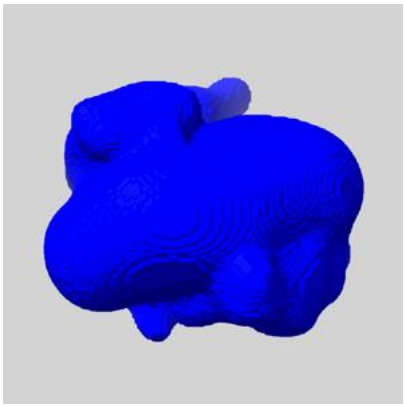
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

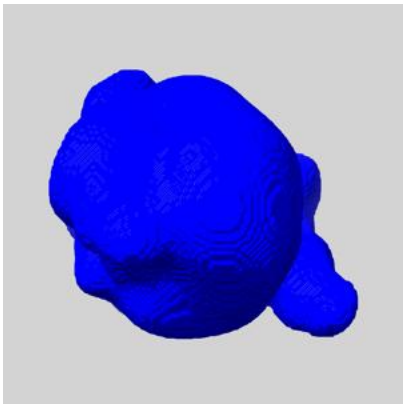
6.6.1 emd_14764_msk_1.map (i)



X



Y

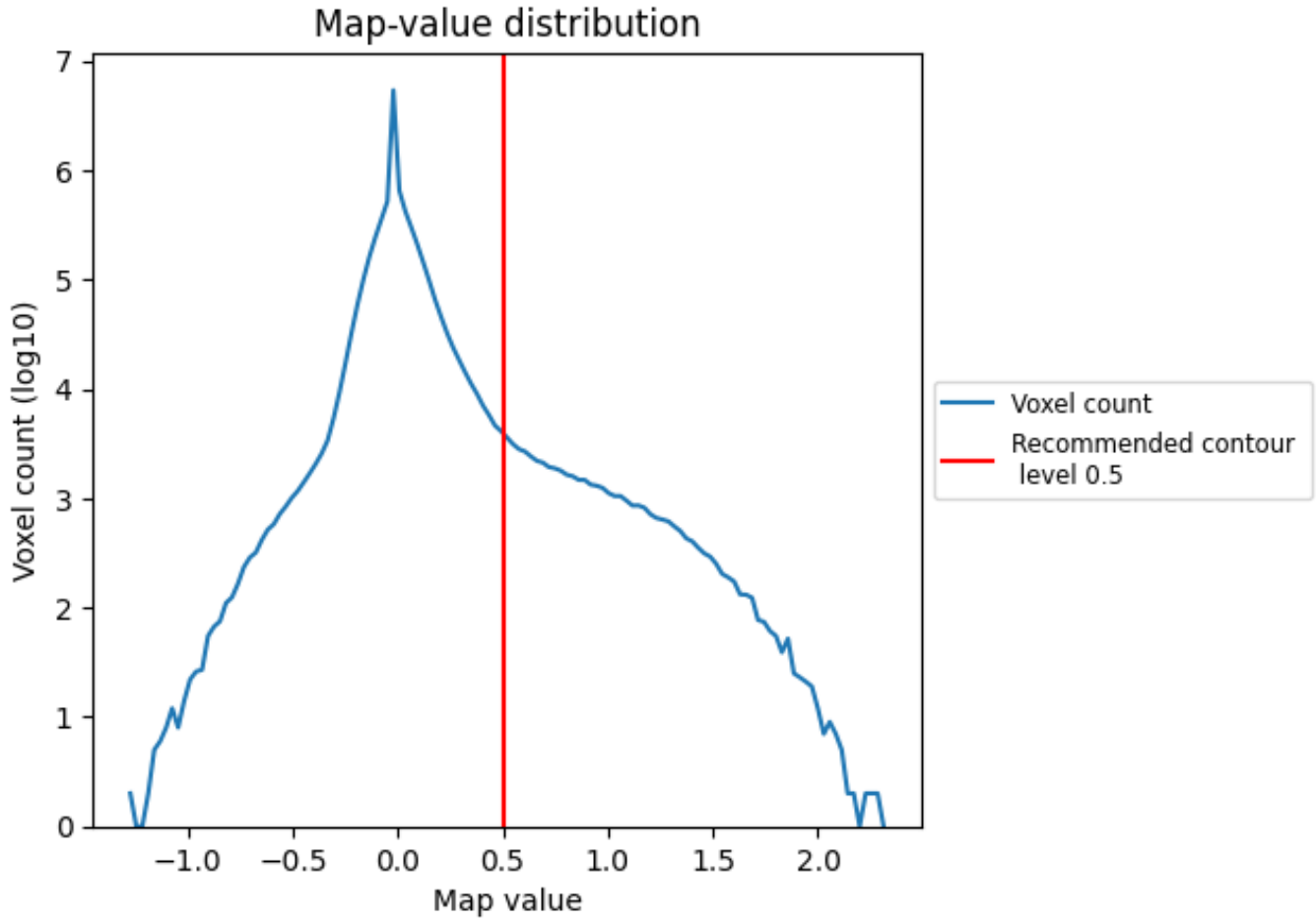


Z

7 Map analysis

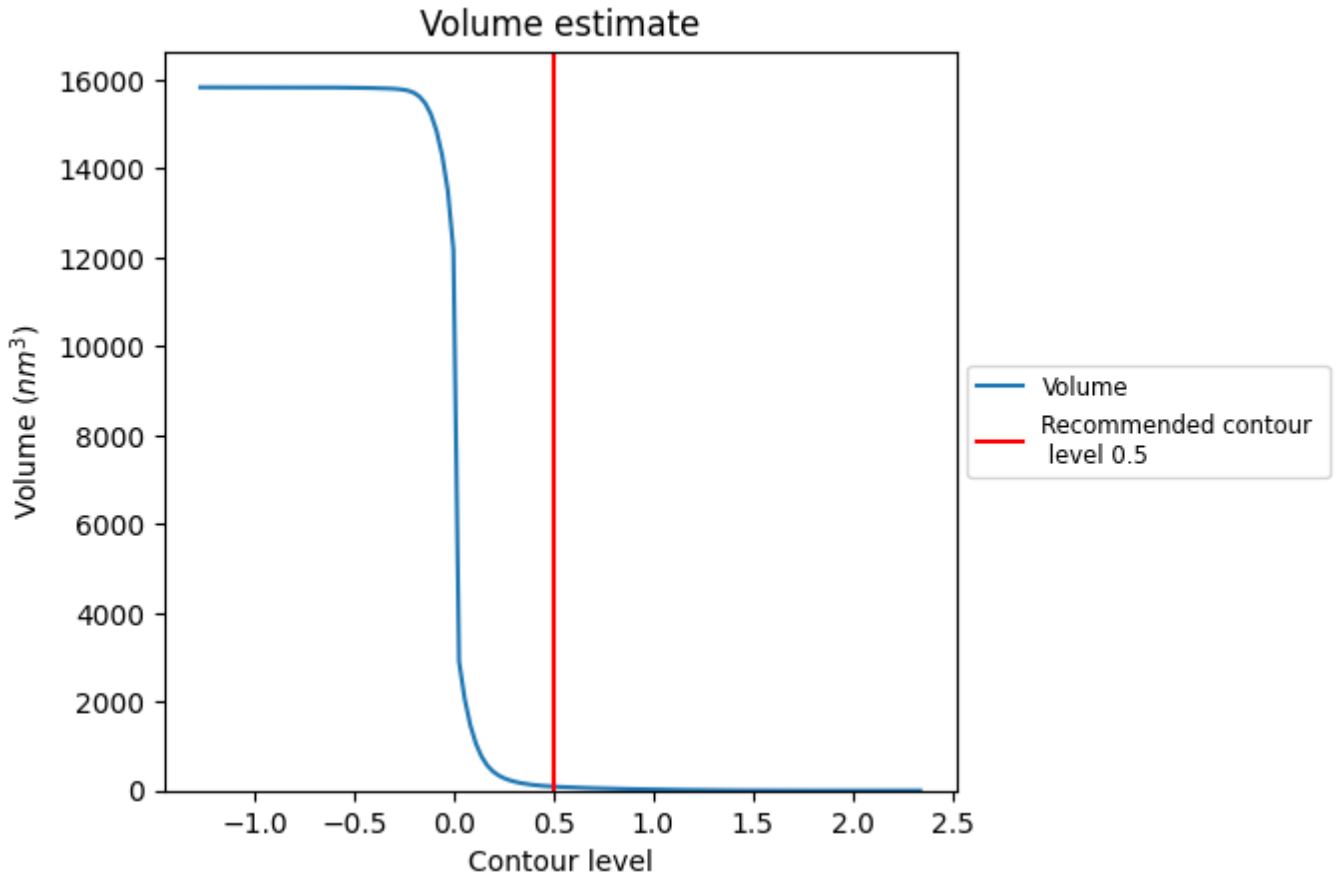
This section contains the results of statistical analysis of the map.

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.

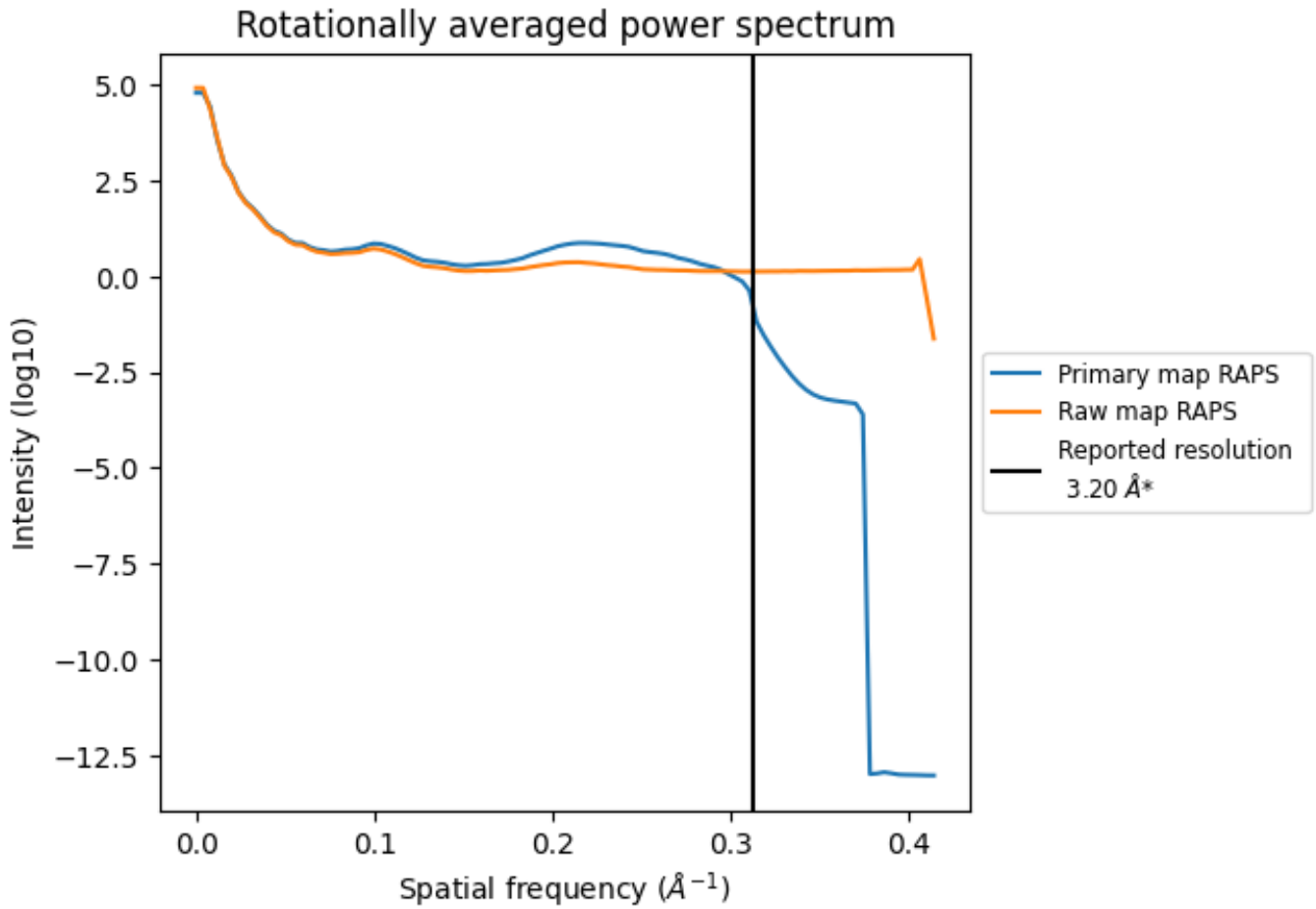
7.2 Volume estimate



The volume at the recommended contour level is 90 nm^3; this corresponds to an approximate mass of 81 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

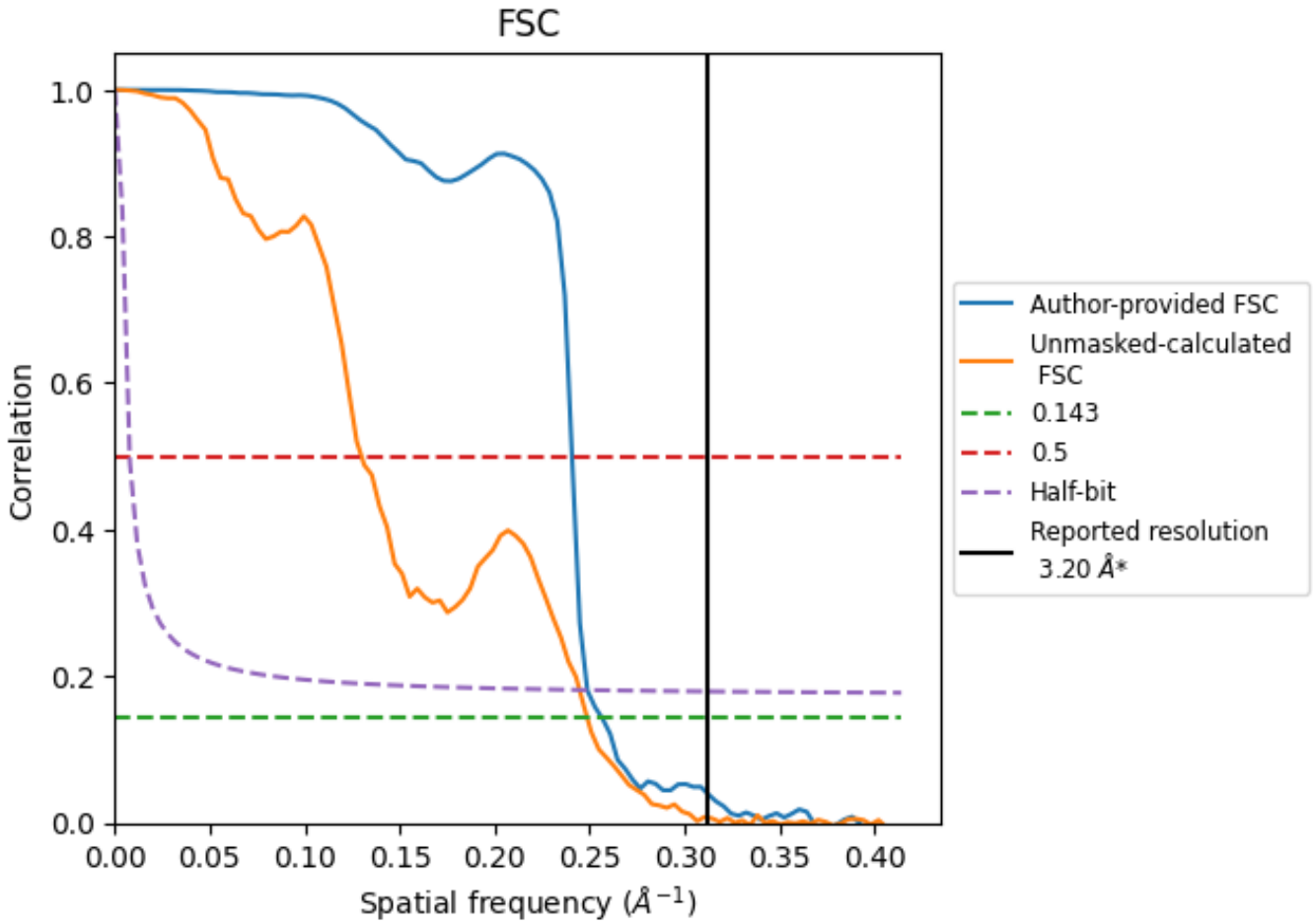


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.90	4.15	4.02
Unmasked-calculated*	4.02	7.70	4.08

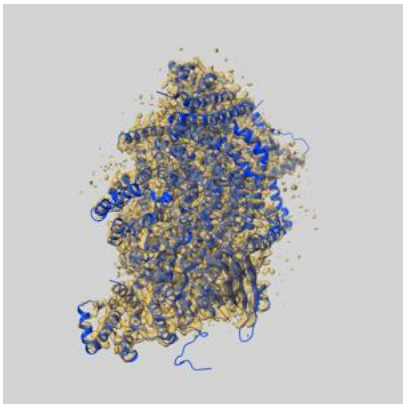
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.90 differs from the reported value 3.2 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.02 differs from the reported value 3.2 by more than 10 %

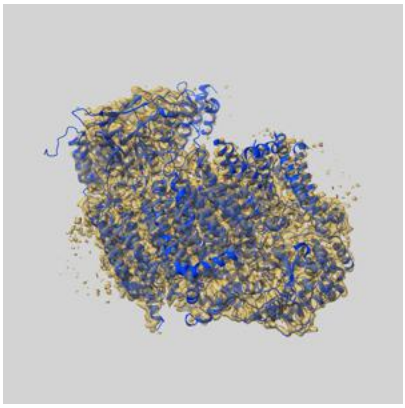
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14764 and PDB model 7ZKP. Per-residue inclusion information can be found in section 3 on page 11.

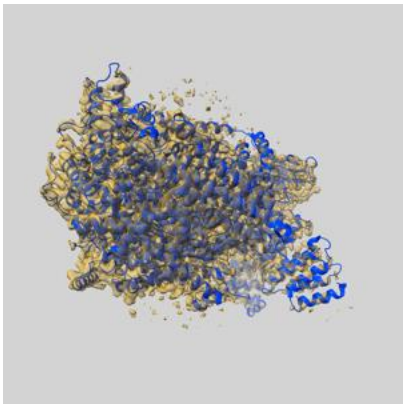
9.1 Map-model overlay



X



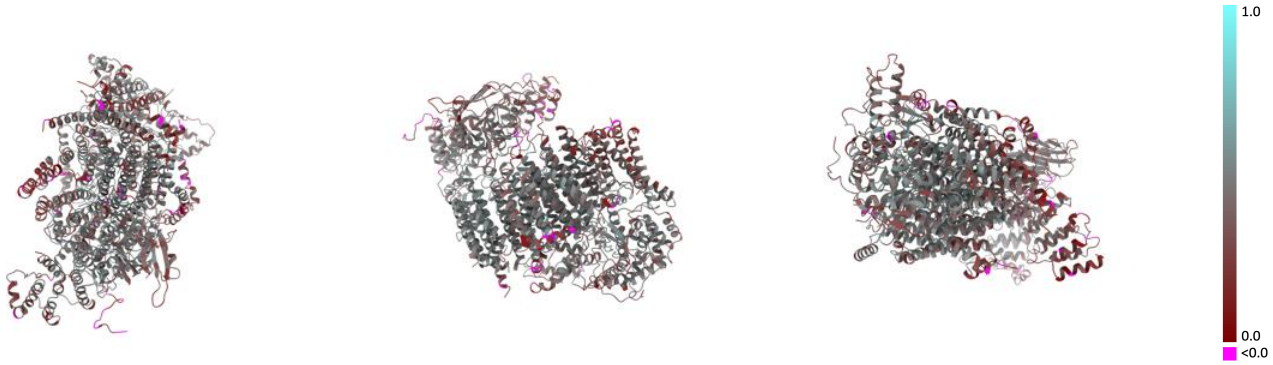
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

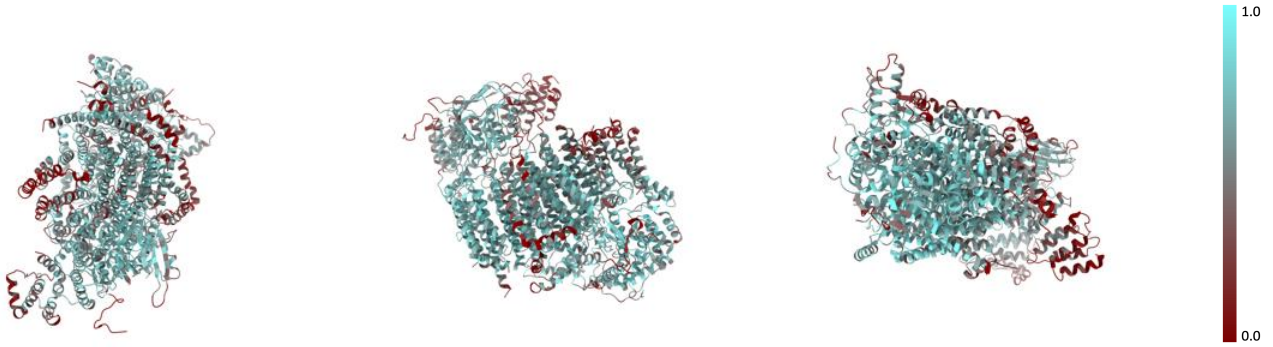
9.2 Q-score mapped to coordinate model (i)



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.

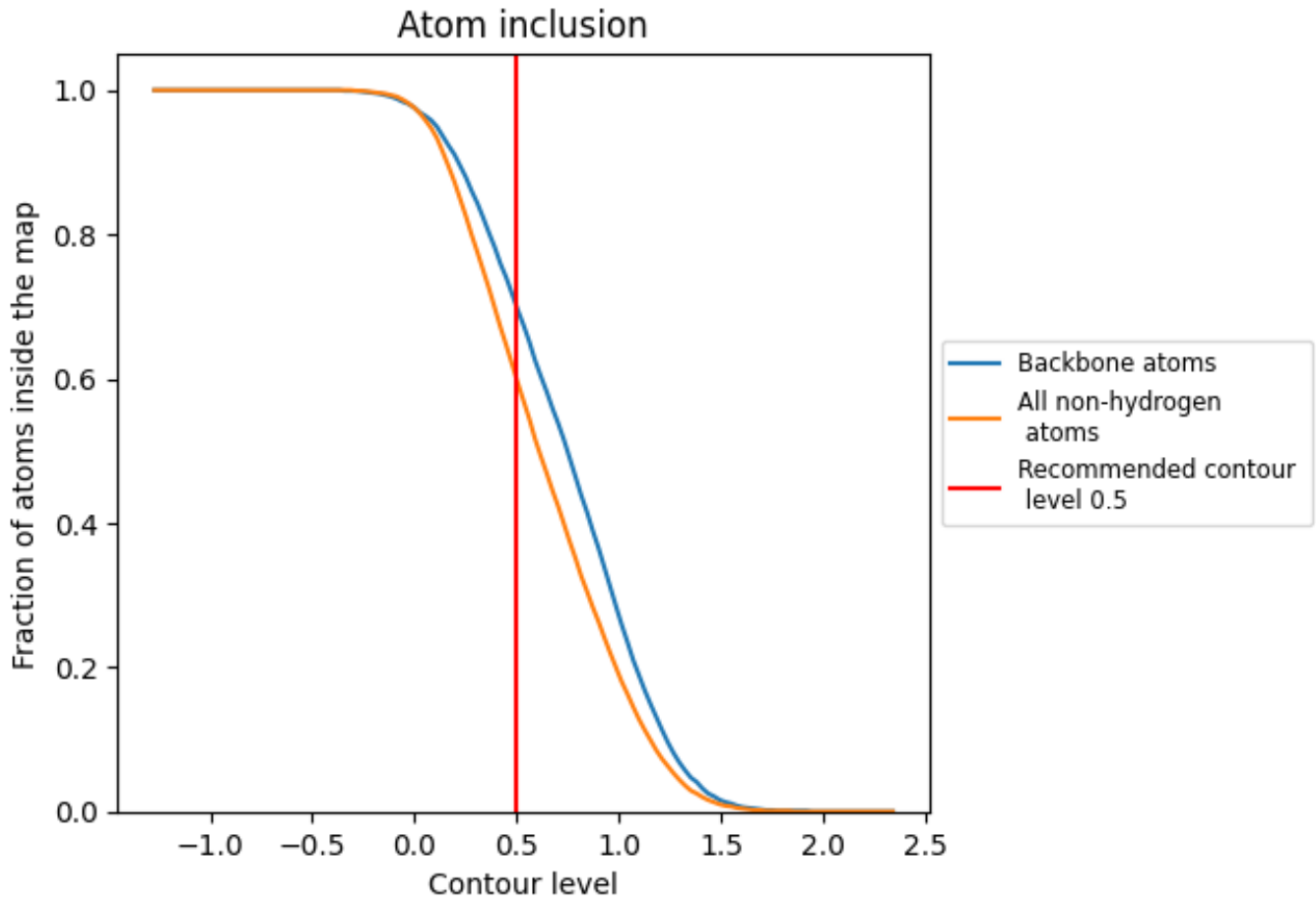
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 60% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5990	0.4150
1	0.5560	0.3870
2	0.7330	0.4850
3	0.5260	0.3940
6	0.5920	0.4090
9	0.4820	0.4010
A	0.5680	0.3700
C	0.4300	0.3620
D	0.6500	0.4340
L	0.6760	0.4620
U	0.6450	0.4120
W	0.6620	0.4300
X	0.6860	0.4390
b	0.6370	0.4290
g	0.4970	0.3660