Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 09:50 am GMT

PDB ID	:	6HUM
EMDB ID	:	EMD-0281
Title	:	Structure of the photosynthetic complex I from Thermosynechococcus elongatus
Authors	:	Schuller, J.M.; Schuller, S.K.; Kurisu, G.; Engel, B.D.; Nowaczyk, M.M.
Deposited on	:	2018-10-09
Resolution	:	3.34 Å(reported)

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 (i) 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 (1)) were used in the production of this report:

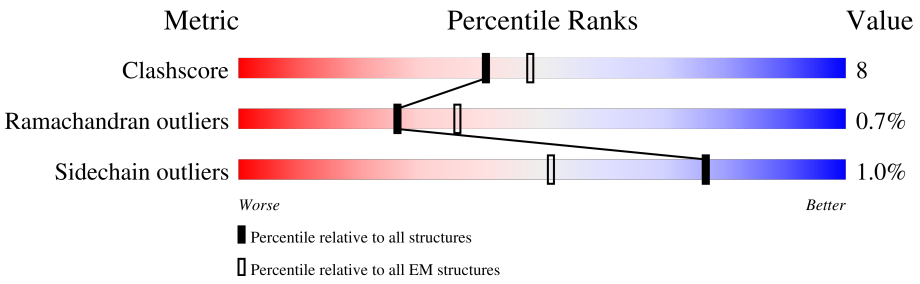
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.34 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	372	7% 78% 16% • 5%
2	C	132	5% 70% 16% • 14%
3	D	529	• 77% 15% • 8%
4	E	101	9% 86% 13% •
5	B	515	• 75% 16% • 8%
6	G	200	8% 74% 10% 16%
7	J	168	• 69% 23% • 7%
8	P	42	17% 88% 12%

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Mol	Chain	Length	Quality of chain
9	H	394	10% 84% 14%
10	I	196	6% 88% 10%
11	K	237	72% 14% 13%
12	L	76	24% 79% 21%
13	F	656	11% 84% 9% 7%
14	N	150	81% 15%
15	M	111	5% 90% 8%
16	S	110	48% 50%
17	O	70	24% 63% 30%
18	Q	39	77% 92% 8%

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 29521 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 NAD(P)H-quinone oxidoreductase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	352	2718	1833	421	454	10	0	0

- Molecule 2 is a protein called NAD(P)H-quinone oxidoreductase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	114	914	629	138	143	4	0	0

- Molecule 3 is a protein called NAD(P)H-quinone oxidoreductase chain 4 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	488	3706	2497	587	601	21	0	0

- Molecule 4 is a protein called NAD(P)H-quinone oxidoreductase subunit 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	100	769	506	126	133	4	0	0

- Molecule 5 is a protein called NAD(P)H-quinone oxidoreductase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	475	3541	2360	548	617	16	0	0

- Molecule 6 is a protein called NADH dehydrogenase subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	168	1262	844	196	218	4	0	0

- Molecule 7 is a protein called NAD(P)H-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	J	156	1278	817	218	238	5	0	0

- Molecule 8 is a protein called Proton-translocating NADH-quinone dehydrogenase subunit P NdhP.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	P	42	319	213	52	52	2	0	0

- Molecule 9 is a protein called NAD(P)H-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	H	393	3153	2035	540	559	19	0	0

- Molecule 10 is a protein called NAD(P)H-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	I	193	1520	970	260	277	13	0	0

- Molecule 11 is a protein called NAD(P)H-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	206	1594	1024	276	281	13	0	0

- Molecule 12 is a protein called NAD(P)H-quinone oxidoreductase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	76	609	417	93	97	2	0	0

- Molecule 13 is a protein called NADH dehydrogenase subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	F	611	4717	3148	736	796	37	0	0

- Molecule 14 is a protein called NAD(P)H-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	147	1160	755	200	204	1	0	0

- Molecule 15 is a protein called NAD(P)H-quinone oxidoreductase subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	M	110	879	548	160	169	2	0	0

- Molecule 16 is a protein called Tlr0636 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	S	55	432	280	69	82	1	0	0

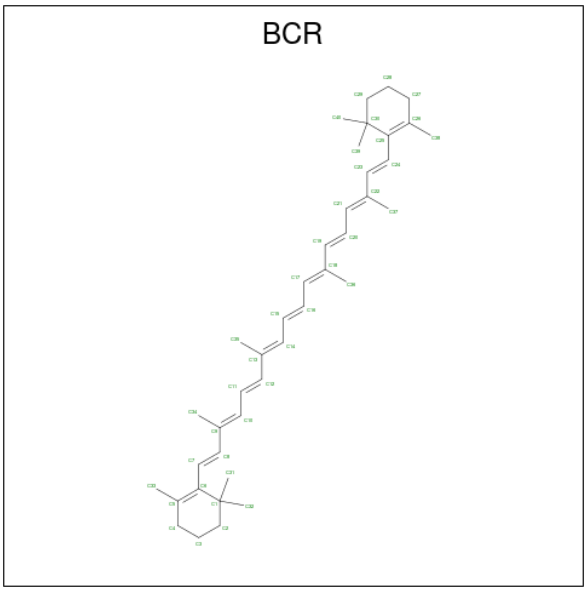
- Molecule 17 is a protein called NAD(P)H-quinone oxidoreductase subunit O.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	O	68	538	349	91	98	0	0

- Molecule 18 is a protein called Proton-translocating NADH-quinone dehydrogenase subunit Q NdhQ.

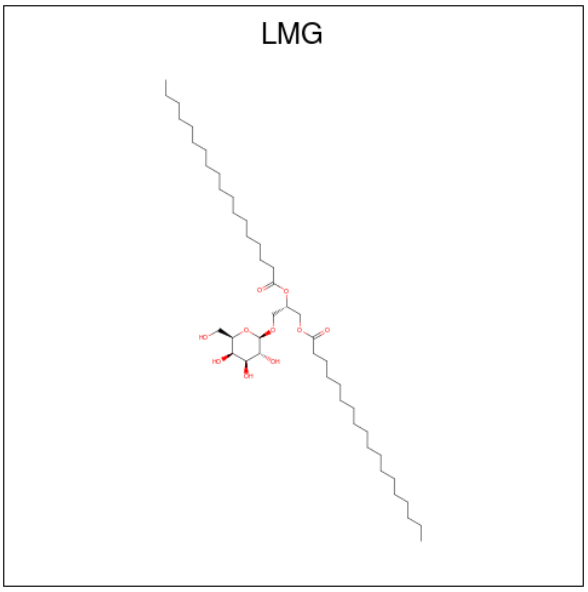
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Q	39	293	198	47	46	2	0	0

- Molecule 19 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



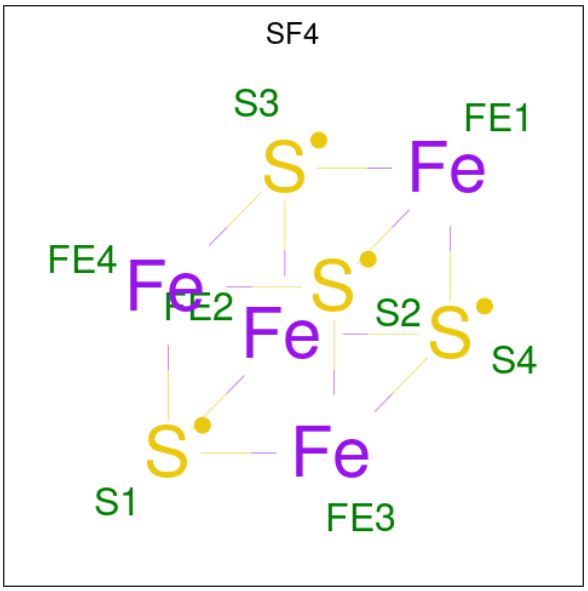
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
19	D	1	40	40	0

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
20	D	1	55	45	10	0

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



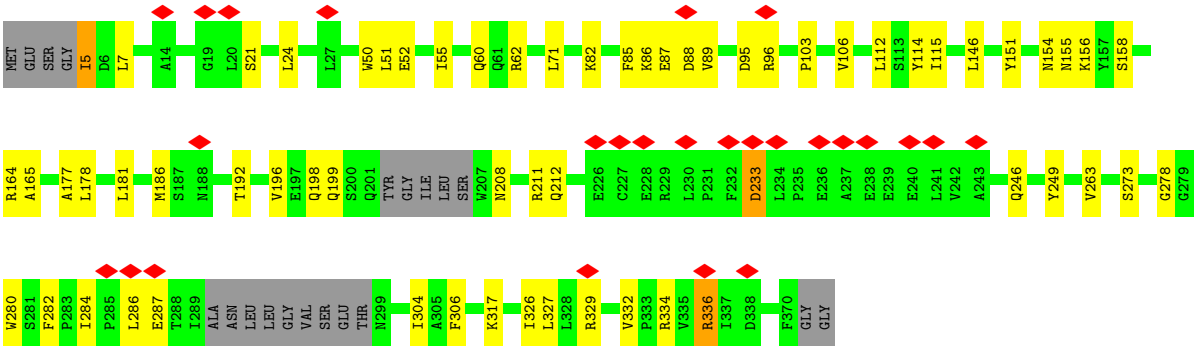
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
21	I	1	16	8	8	0
			Total	Fe	S	
21	I	1	16	8	8	0
			Total	Fe	S	
21	K	1	8	4	4	0

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.

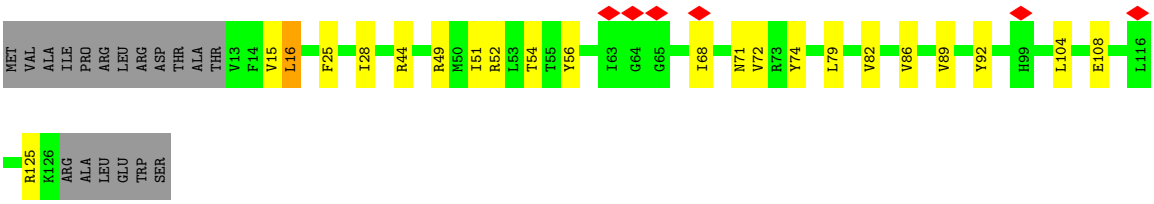
- Molecule 1: NAD(P)H-quinone oxidoreductase subunit 1

Chain A:



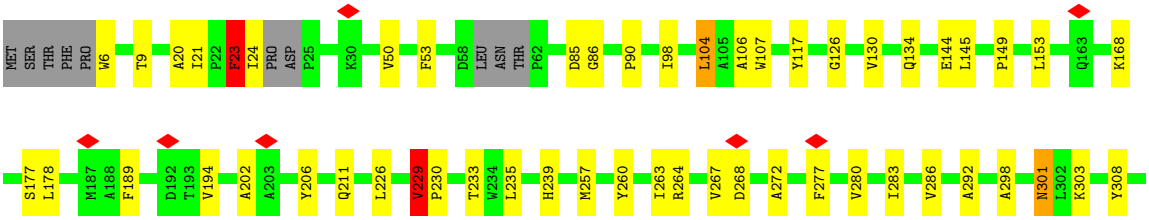
- Molecule 2: NAD(P)H-quinone oxidoreductase subunit 3

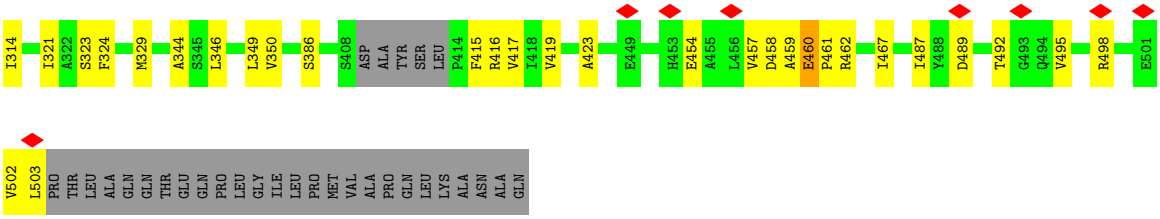
Chain C:



- Molecule 3: NAD(P)H-quinone oxidoreductase chain 4 1

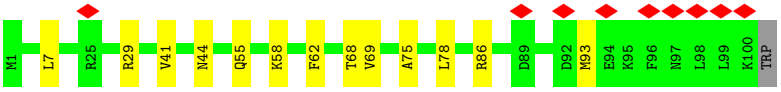
Chain D:





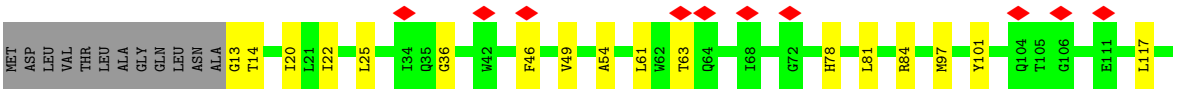
• Molecule 4: NAD(P)H-quinone oxidoreductase subunit 4L

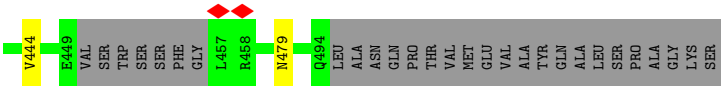
Chain E:



• Molecule 5: NAD(P)H-quinone oxidoreductase subunit 2

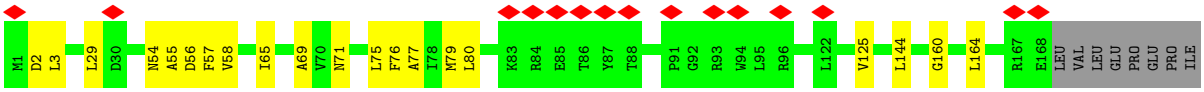
Chain B:





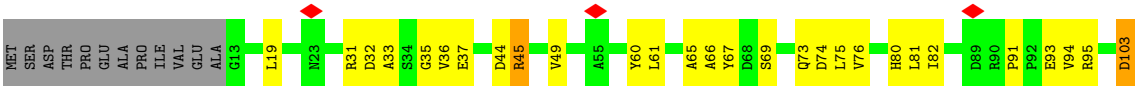
• Molecule 6: NADH dehydrogenase subunit 6

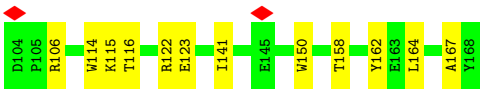
Chain G:



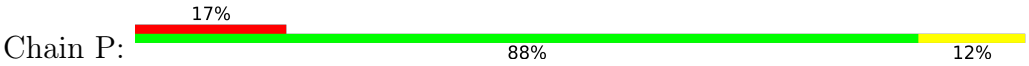
• Molecule 7: NAD(P)H-quinone oxidoreductase subunit J

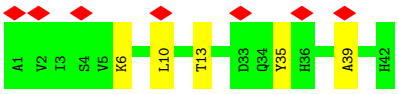
Chain J:



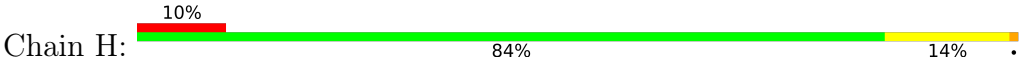


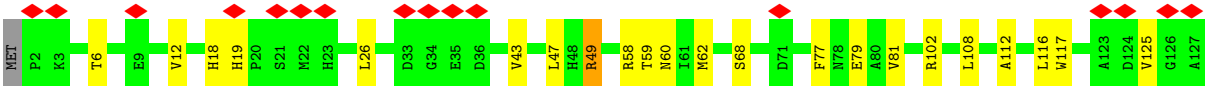
• Molecule 8: Proton-translocating NADH-quinone dehydrogenase subunit P NdhP

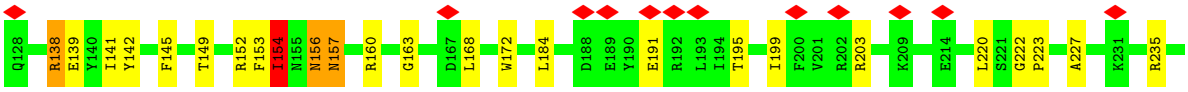


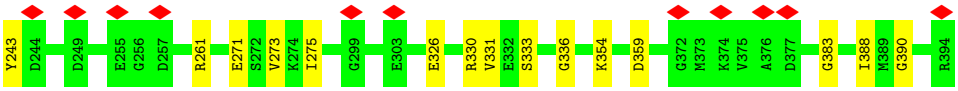


• Molecule 9: NAD(P)H-quinone oxidoreductase subunit H

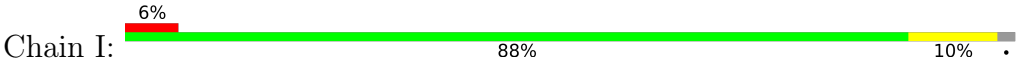


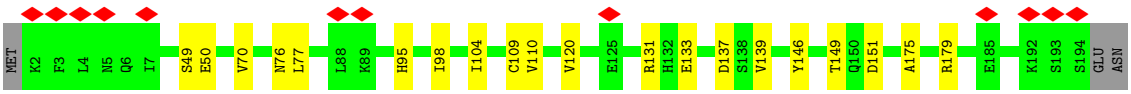




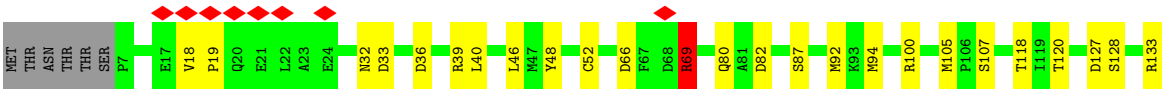


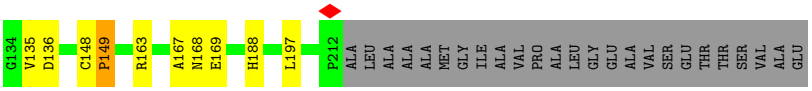
• Molecule 10: NAD(P)H-quinone oxidoreductase subunit I



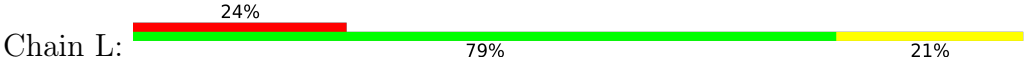


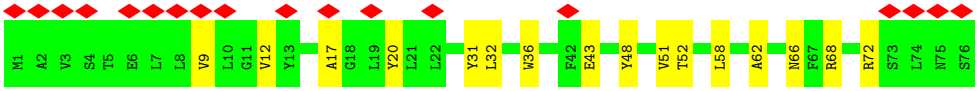
• Molecule 11: NAD(P)H-quinone oxidoreductase subunit K





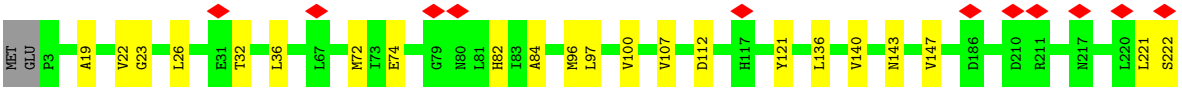
• Molecule 12: NAD(P)H-quinone oxidoreductase subunit L

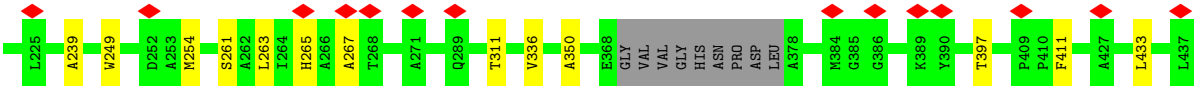


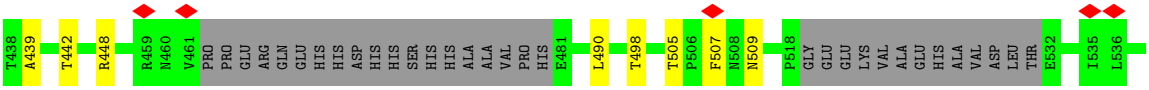


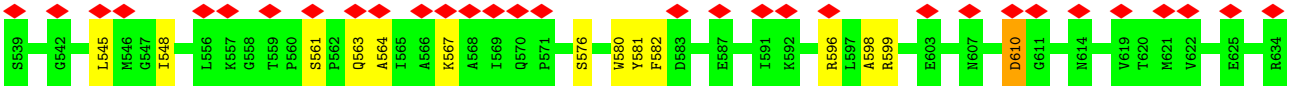
• Molecule 13: NADH dehydrogenase subunit 5

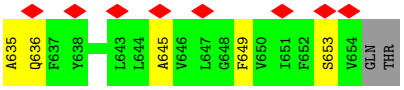
Chain F:





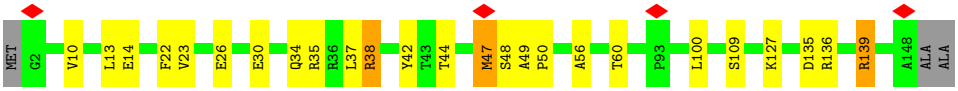






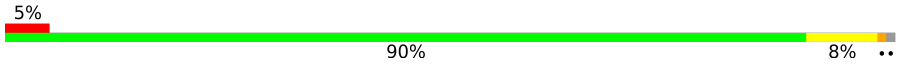
• Molecule 14: NAD(P)H-quinone oxidoreductase subunit N

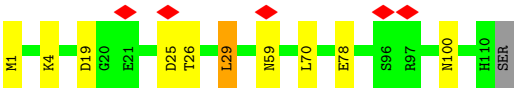
Chain N:



• Molecule 15: NAD(P)H-quinone oxidoreductase subunit M

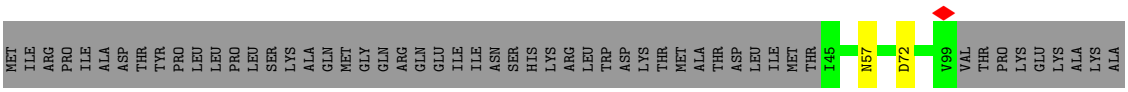
Chain M:





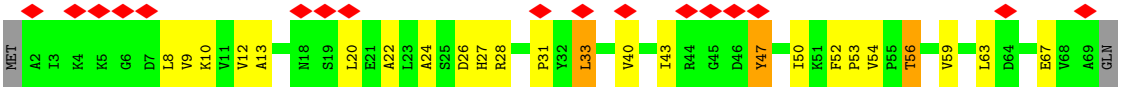
• Molecule 16: Tlr0636 protein

Chain S:



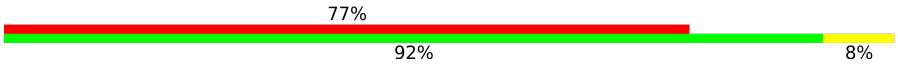
• Molecule 17: NAD(P)H-quinone oxidoreductase subunit O

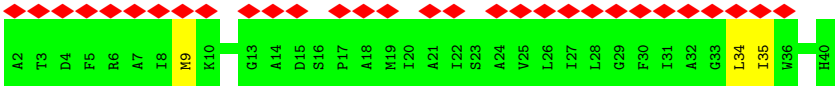
Chain O:



• Molecule 18: Proton-translocating NADH-quinone dehydrogenase subunit Q NdhQ

Chain Q:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133485	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 ($e^-/Å^2$)	49.93	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.659	Depositor
Minimum map value	-0.230	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	405.0, 405.0, 405.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, BCR, LMG

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	A	0.37	0/2788	0.60	0/3812
2	C	0.37	0/942	0.65	0/1285
3	D	0.38	0/3805	0.58	2/5189 (0.0%)
4	E	0.35	0/777	0.57	0/1054
5	B	0.38	0/3623	0.61	2/4947 (0.0%)
6	G	0.35	0/1288	0.55	0/1765
7	J	0.40	0/1314	0.72	3/1789 (0.2%)
8	P	0.39	0/328	0.59	0/447
9	H	0.39	0/3236	0.65	0/4389
10	I	0.41	0/1558	0.60	0/2116
11	K	0.40	0/1636	0.65	0/2228
12	L	0.36	0/629	0.62	0/860
13	F	0.33	0/4852	0.58	1/6603 (0.0%)
14	N	0.35	0/1192	0.66	1/1621 (0.1%)
15	M	0.35	0/895	0.72	2/1214 (0.2%)
16	S	0.34	0/441	0.55	0/601
17	O	0.45	0/550	1.26	12/748 (1.6%)
18	Q	0.27	0/301	0.48	0/409
All	All	0.37	0/30155	0.63	23/41077 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
3	D	0	2
5	B	0	1
11	K	0	3
17	O	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	9

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	23	PHE	O-C-N	-8.40	109.25	122.70
17	O	22	ALA	C-N-CA	7.50	140.45	121.70
17	O	50	ILE	CG1-CB-CG2	6.86	126.49	111.40
17	O	40	VAL	CG1-CB-CG2	6.79	121.77	110.90
17	O	9	VAL	CG1-CB-CG2	6.78	121.75	110.90
17	O	43	ILE	CG1-CB-CG2	6.51	125.72	111.40
17	O	59	VAL	CG1-CB-CG2	6.50	121.29	110.90
17	O	33	LEU	CB-CG-CD1	6.32	121.74	111.00
17	O	63	LEU	CB-CG-CD2	6.02	121.24	111.00
7	J	75	LEU	CB-CG-CD2	5.72	120.73	111.00
15	M	29	LEU	CB-CG-CD1	5.58	120.49	111.00
17	O	8	LEU	CB-CG-CD2	5.58	120.48	111.00
17	O	8	LEU	CB-CG-CD1	5.54	120.42	111.00
15	M	29	LEU	CB-CG-CD2	5.35	120.10	111.00
17	O	33	LEU	CB-CG-CD2	5.33	120.07	111.00
5	B	121	VAL	CG1-CB-CG2	5.22	119.25	110.90
7	J	103	ASP	CB-CG-OD2	5.21	122.99	118.30
14	N	38	ARG	NE-CZ-NH1	5.20	122.90	120.30
13	F	610	ASP	CB-CG-OD2	5.20	122.98	118.30
5	B	178	LEU	CA-CB-CG	5.18	127.21	115.30
17	O	47	TYR	C-N-CA	5.17	134.62	121.70
7	J	75	LEU	CB-CG-CD1	5.05	119.59	111.00
3	D	104	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	B	387	PRO	Peptide
2	C	16	LEU	Peptide
3	D	23	PHE	Mainchain
3	D	301	ASN	Peptide
11	K	148	CYS	Peptide
11	K	18	VAL	Peptide
11	K	69	ARG	Peptide

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Mol	Chain	Res	Type	Group
17	O	13	ALA	Peptide
17	O	56	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	A	2718	0	2838	47	0
2	C	914	0	945	24	0
3	D	3706	0	3835	66	0
4	E	769	0	827	17	0
5	B	3541	0	3650	119	0
6	G	1262	0	1334	17	0
7	J	1278	0	1233	48	0
8	P	319	0	319	4	0
9	H	3153	0	3116	51	0
10	I	1520	0	1467	13	0
11	K	1594	0	1627	34	0
12	L	609	0	625	12	0
13	F	4717	0	4784	46	0
14	N	1160	0	1171	21	0
15	M	879	0	859	8	0
16	S	432	0	430	2	0
17	O	538	0	549	15	0
18	Q	293	0	299	3	0
19	D	40	0	56	0	0
20	D	55	0	86	2	0
21	I	16	0	0	1	0
21	K	8	0	0	0	0
All	All	29521	0	30050	447	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 8.

All (447) 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:B:194:LEU:CB	5:B:266:ALA:HB2	1.35	1.55
5:B:194:LEU:HB3	5:B:266:ALA:CB	1.04	1.49
5:B:194:LEU:CB	5:B:266:ALA:CB	1.87	1.41
3:D:233:THR:CG2	13:F:610:ASP:OD1	1.68	1.39
7:J:103:ASP:OD2	17:O:20:LEU:CG	1.74	1.35
7:J:103:ASP:OD2	17:O:20:LEU:HG	1.13	1.25
7:J:162:TYR:CD2	15:M:78:GLU:OE1	1.90	1.24
5:B:267:PHE:CG	5:B:268:PRO:HD3	1.75	1.22
5:B:194:LEU:O	5:B:266:ALA:HA	1.36	1.21
5:B:198:ALA:HB2	5:B:267:PHE:O	1.08	1.20
7:J:32:ASP:OD2	7:J:95:ARG:NH1	1.73	1.19
5:B:198:ALA:CB	5:B:267:PHE:O	1.93	1.16
5:B:194:LEU:H	5:B:195:PRO:HD2	1.10	1.14
5:B:267:PHE:CD2	5:B:268:PRO:HD3	1.83	1.13
3:D:233:THR:HG23	13:F:610:ASP:OD1	1.48	1.10
3:D:233:THR:HG21	13:F:610:ASP:OD1	1.37	1.09
3:D:21:ILE:CA	3:D:24:ILE:HD12	1.80	1.09
5:B:130:GLN:CA	5:B:194:LEU:HD12	1.82	1.09
5:B:130:GLN:HA	5:B:194:LEU:HD12	1.21	1.08
5:B:267:PHE:CD2	5:B:268:PRO:CD	2.38	1.07
5:B:194:LEU:CB	5:B:266:ALA:HB1	1.74	1.04
7:J:32:ASP:OD1	7:J:36:VAL:CG1	2.05	1.03
3:D:21:ILE:HA	3:D:24:ILE:HD12	1.03	1.02
3:D:233:THR:HG21	13:F:610:ASP:CG	1.80	1.02
3:D:233:THR:CG2	13:F:610:ASP:CG	2.28	0.98
5:B:194:LEU:CD2	5:B:266:ALA:HB1	1.93	0.97
5:B:194:LEU:H	5:B:195:PRO:CD	1.79	0.96
7:J:162:TYR:CG	15:M:78:GLU:OE1	2.18	0.95
5:B:270:VAL:HG23	5:B:271:THR:N	1.80	0.95
5:B:194:LEU:HD22	5:B:266:ALA:CB	1.99	0.93
5:B:267:PHE:CG	5:B:268:PRO:CD	2.49	0.92
3:D:21:ILE:HA	3:D:24:ILE:CD1	1.99	0.92
13:F:267:ALA:HB3	13:F:350:ALA:HB2	1.51	0.91
3:D:283:ILE:HD11	18:Q:34:LEU:HD13	1.53	0.90
9:H:139:GLU:OE2	9:H:152:ARG:NH2	2.04	0.90
5:B:194:LEU:HB3	5:B:266:ALA:CA	2.04	0.88
5:B:194:LEU:O	5:B:266:ALA:CA	2.21	0.88
5:B:194:LEU:C	5:B:266:ALA:HA	1.93	0.87
5:B:194:LEU:CG	5:B:266:ALA:CB	2.52	0.87
5:B:194:LEU:CD2	5:B:266:ALA:CB	2.52	0.87
9:H:157:ASN:ND2	9:H:157:ASN:O	2.07	0.87
5:B:270:VAL:HG23	5:B:271:THR:H	1.34	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ILE:HG21	1:A:326:ILE:HD13	1.58	0.85
7:J:103:ASP:OD2	17:O:20:LEU:CD2	2.26	0.84
3:D:20:ALA:O	3:D:24:ILE:HG13	1.77	0.84
5:B:194:LEU:CA	5:B:266:ALA:HB1	2.07	0.83
5:B:267:PHE:CD2	5:B:268:PRO:HD2	2.12	0.83
5:B:310:GLN:OE1	5:B:332:TYR:OH	1.96	0.83
5:B:184:LEU:HG	5:B:197:ILE:HD13	1.60	0.82
5:B:130:GLN:C	5:B:194:LEU:HD12	2.01	0.81
5:B:268:PRO:HB2	5:B:270:VAL:HG22	1.63	0.81
5:B:270:VAL:CG2	5:B:271:THR:H	1.94	0.80
7:J:103:ASP:OD2	17:O:20:LEU:CD1	2.29	0.80
5:B:194:LEU:CA	5:B:266:ALA:CB	2.61	0.78
9:H:149:THR:HG21	9:H:156:ASN:HB3	1.63	0.78
5:B:20:ILE:HG23	5:B:54:ALA:HB1	1.66	0.78
7:J:103:ASP:CG	17:O:20:LEU:HG	2.03	0.77
1:A:60:GLN:OE1	1:A:62:ARG:NH1	2.17	0.77
11:K:33:ASP:OD1	14:N:35:ARG:NH2	2.18	0.77
9:H:157:ASN:HD22	9:H:160:ARG:HH12	1.32	0.76
11:K:48:TYR:OH	11:K:94:MET:SD	2.44	0.76
5:B:267:PHE:CB	5:B:268:PRO:CD	2.63	0.76
1:A:5:ILE:HD11	1:A:304:ILE:HG22	1.68	0.75
7:J:32:ASP:OD1	7:J:36:VAL:HG13	1.84	0.75
3:D:23:PHE:O	3:D:24:ILE:HG13	1.87	0.74
11:K:36:ASP:OD2	14:N:35:ARG:NH1	2.19	0.74
11:K:168:ASN:O	14:N:38:ARG:NH2	2.21	0.74
5:B:194:LEU:N	5:B:195:PRO:HD2	1.95	0.73
11:K:66:ASP:O	11:K:69:ARG:NH2	2.21	0.73
4:E:41:VAL:HG11	5:B:178:LEU:HD13	1.70	0.73
5:B:194:LEU:HD22	5:B:266:ALA:HB1	1.64	0.73
5:B:194:LEU:CG	5:B:266:ALA:HB2	2.16	0.73
1:A:5:ILE:HD11	1:A:304:ILE:CG2	2.19	0.73
12:L:66:ASN:O	14:N:136:ARG:NH1	2.22	0.73
3:D:280:VAL:HG22	18:Q:35:ILE:HD11	1.70	0.72
11:K:128:SER:O	11:K:133:ARG:NH2	2.22	0.72
5:B:130:GLN:HA	5:B:194:LEU:CD1	2.10	0.72
5:B:194:LEU:HD22	5:B:266:ALA:HB3	1.73	0.70
11:K:163:ARG:NH1	14:N:26:GLU:O	2.25	0.69
5:B:194:LEU:HA	5:B:266:ALA:HB1	1.74	0.69
5:B:46:PHE:HA	5:B:49:VAL:CG2	2.21	0.69
7:J:32:ASP:OD1	7:J:36:VAL:HG12	1.89	0.69
5:B:194:LEU:CG	5:B:266:ALA:HB1	2.20	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:270:VAL:HG23	5:B:271:THR:HG23	1.73	0.68
13:F:649:PHE:O	13:F:653:SER:OG	2.11	0.68
1:A:151:TYR:OH	6:G:75:LEU:O	2.10	0.68
1:A:21:SER:O	1:A:24:LEU:N	2.27	0.68
2:C:125:ARG:NH1	5:B:36:GLY:O	2.27	0.68
13:F:84:ALA:O	13:F:143:ASN:ND2	2.27	0.67
1:A:88:ASP:OD2	2:C:44:ARG:NH1	2.26	0.67
1:A:198:GLN:NE2	1:A:199:GLN:OE1	2.28	0.67
3:D:260:TYR:OH	3:D:264:ARG:NH1	2.28	0.67
11:K:48:TYR:O	11:K:87:SER:OG	2.13	0.67
2:C:49:ARG:NH2	15:M:19:ASP:O	2.27	0.66
5:B:130:GLN:C	5:B:194:LEU:CD1	2.64	0.66
3:D:53:PHE:O	8:P:6:LYS:NZ	2.29	0.66
7:J:82:ILE:HD11	7:J:91:PRO:HG2	1.77	0.66
3:D:21:ILE:N	3:D:24:ILE:HD12	2.11	0.66
3:D:233:THR:HG23	13:F:610:ASP:CG	2.02	0.66
4:E:62:PHE:CD1	5:B:133:VAL:HG22	2.30	0.66
7:J:32:ASP:CG	7:J:36:VAL:CG1	2.64	0.66
5:B:46:PHE:HA	5:B:49:VAL:HG23	1.76	0.66
5:B:117:LEU:O	5:B:121:VAL:HG23	1.96	0.66
5:B:188:SER:HB2	5:B:200:ALA:HB3	1.78	0.66
5:B:293:ALA:HB2	5:B:305:TYR:HB2	1.79	0.65
8:P:35:TYR:OH	8:P:39:ALA:N	2.30	0.65
13:F:254:MET:SD	13:F:261:SER:OG	2.51	0.65
1:A:5:ILE:CD1	1:A:304:ILE:CG2	2.76	0.64
5:B:267:PHE:HB3	5:B:268:PRO:CD	2.28	0.64
1:A:52:GLU:OE2	1:A:329:ARG:NH1	2.29	0.64
9:H:117:TRP:NE1	9:H:383:GLY:O	2.30	0.63
5:B:198:ALA:HB2	5:B:266:ALA:O	1.99	0.63
13:F:580:TRP:O	13:F:582:PHE:N	2.31	0.63
5:B:194:LEU:N	5:B:195:PRO:CD	2.52	0.63
11:K:136:ASP:OD1	15:M:100:ASN:ND2	2.30	0.63
3:D:292:ALA:HB1	3:D:308:TYR:O	1.99	0.63
5:B:260:ILE:HD11	5:B:329:MET:CE	2.29	0.63
5:B:140:GLU:OE2	5:B:174:SER:OG	2.06	0.62
5:B:335:VAL:HG12	5:B:339:MET:SD	2.40	0.62
20:D:602:LMG:O1	20:D:602:LMG:O3	2.08	0.62
5:B:193:GLN:HB3	5:B:195:PRO:HD2	1.81	0.61
11:K:188:HIS:CD2	15:M:29:LEU:HD13	2.35	0.61
3:D:202:ALA:O	3:D:498:ARG:NH2	2.34	0.61
1:A:196:VAL:HG11	1:A:280:TRP:CZ3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:82:VAL:HG22	6:G:69:ALA:HB1	1.81	0.60
5:B:97:MET:HG2	5:B:345:THR:HG22	1.83	0.60
5:B:135:ILE:HD11	5:B:194:LEU:HD11	1.82	0.60
13:F:439:ALA:O	13:F:442:THR:OG1	2.16	0.60
7:J:61:LEU:HD13	7:J:114:TRP:HE1	1.65	0.60
7:J:32:ASP:CG	7:J:36:VAL:HG13	2.21	0.60
5:B:158:ARG:NH1	5:B:237:GLU:OE1	2.35	0.60
1:A:87:GLU:OE1	11:K:107:SER:OG	2.13	0.60
4:E:29:ARG:NH2	6:G:29:LEU:O	2.34	0.60
5:B:266:ALA:O	5:B:267:PHE:O	2.18	0.60
12:L:48:TYR:O	12:L:52:THR:HG23	2.02	0.60
13:F:112:ASP:OD1	13:F:121:TYR:OH	2.17	0.59
5:B:132:LEU:HD13	5:B:192:THR:O	2.02	0.59
3:D:144:GLU:OE2	3:D:177:SER:OG	2.20	0.59
3:D:346:LEU:HD11	3:D:386:SER:OG	2.02	0.59
4:E:93:MET:SD	13:F:636:GLN:NE2	2.74	0.59
10:I:133:GLU:OE1	14:N:48:SER:OG	2.16	0.59
2:C:79:LEU:CD2	4:E:75:ALA:HB1	2.32	0.59
3:D:229:VAL:HG23	3:D:230:PRO:HD2	1.85	0.59
12:L:68:ARG:O	14:N:136:ARG:NH2	2.36	0.59
7:J:164:LEU:O	11:K:133:ARG:NH1	2.36	0.59
9:H:152:ARG:O	9:H:156:ASN:ND2	2.34	0.59
2:C:16:LEU:HD21	6:G:54:ASN:HA	1.83	0.59
3:D:263:ILE:HG12	3:D:321:ILE:HD13	1.85	0.58
5:B:197:ILE:C	5:B:199:GLN:H	2.05	0.58
17:O:54:VAL:O	17:O:56:THR:N	2.36	0.58
1:A:55:ILE:CG2	1:A:326:ILE:HD13	2.31	0.58
14:N:56:ALA:O	14:N:60:THR:OG1	2.21	0.58
9:H:58:ARG:NH1	11:K:127:ASP:OD2	2.36	0.58
1:A:156:LYS:NZ	9:H:12:VAL:O	2.33	0.58
1:A:332:VAL:HG13	9:H:199:ILE:HD13	1.85	0.58
5:B:276:LEU:O	5:B:279:THR:OG1	2.21	0.58
7:J:65:ALA:HB3	9:H:354:LYS:CE	2.33	0.57
3:D:20:ALA:C	3:D:24:ILE:CD1	2.73	0.57
5:B:270:VAL:CG2	5:B:271:THR:N	2.48	0.57
1:A:249:TYR:O	11:K:80:GLN:NE2	2.37	0.57
7:J:167:ALA:O	10:I:131:ARG:NH1	2.37	0.57
9:H:142:TYR:CE1	9:H:153:PHE:HB3	2.40	0.57
3:D:298:ALA:HB2	13:F:598:ALA:HB1	1.85	0.57
5:B:368:LYS:NZ	5:B:444:VAL:O	2.38	0.57
10:I:77:LEU:HD12	10:I:98:ILE:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:89:VAL:HG21	6:G:65:ILE:HD11	1.87	0.57
3:D:229:VAL:HG23	3:D:230:PRO:CD	2.35	0.57
9:H:154:ILE:HD11	11:K:149:PRO:HG3	1.87	0.57
7:J:32:ASP:O	7:J:33:ALA:HB3	2.05	0.57
1:A:51:LEU:O	1:A:55:ILE:HG22	2.05	0.57
5:B:130:GLN:O	5:B:194:LEU:HG	2.05	0.56
5:B:188:SER:HB3	5:B:201:LEU:HD23	1.86	0.56
2:C:74:TYR:OH	6:G:79:MET:SD	2.55	0.56
1:A:186:MET:SD	1:A:211:ARG:NH1	2.78	0.56
1:A:233:ASP:OD1	1:A:334:ARG:NH1	2.39	0.56
9:H:223:PRO:O	9:H:227:ALA:N	2.39	0.56
12:L:31:TYR:OH	12:L:43:GLU:OE2	2.15	0.55
5:B:179:TYR:O	5:B:182:SER:OG	2.16	0.55
5:B:212:LEU:HA	5:B:267:PHE:CZ	2.42	0.55
9:H:102:ARG:NH2	9:H:163:GLY:O	2.39	0.55
11:K:39:ARG:NH2	11:K:169:GLU:OE1	2.40	0.55
17:O:52:PHE:O	17:O:54:VAL:N	2.37	0.55
3:D:233:THR:CB	13:F:610:ASP:OD1	2.51	0.55
5:B:267:PHE:HD2	5:B:268:PRO:HD2	1.65	0.55
7:J:32:ASP:O	9:H:326:GLU:O	2.25	0.55
14:N:23:VAL:HG11	14:N:30:GLU:HB3	1.89	0.55
3:D:489:ASP:N	3:D:489:ASP:OD1	2.39	0.55
5:B:185:TYR:CD1	5:B:192:THR:HG22	2.41	0.55
7:J:61:LEU:HD12	7:J:80:HIS:O	2.07	0.55
3:D:21:ILE:N	3:D:24:ILE:CD1	2.69	0.54
7:J:103:ASP:OD2	17:O:20:LEU:HD21	2.06	0.54
2:C:52:ARG:NE	11:K:105:MET:O	2.41	0.54
3:D:20:ALA:C	3:D:24:ILE:HD11	2.27	0.54
6:G:55:ALA:HB1	6:G:58:VAL:HG12	1.89	0.54
10:I:146:TYR:OH	10:I:151:ASP:OD2	2.25	0.54
11:K:167:ALA:O	14:N:35:ARG:NH1	2.41	0.54
7:J:31:ARG:NH1	7:J:35:GLY:O	2.39	0.54
13:F:411:PHE:CE1	13:F:498:THR:HG22	2.43	0.54
9:H:271:GLU:O	9:H:275:ILE:HD12	2.08	0.53
7:J:103:ASP:OD2	17:O:20:LEU:HD11	2.09	0.53
3:D:329:MET:HG2	3:D:492:THR:HG23	1.90	0.53
2:C:108:GLU:CG	6:G:144:LEU:HD11	2.39	0.53
3:D:104:LEU:HD22	3:D:107:TRP:HE1	1.74	0.53
7:J:167:ALA:CB	11:K:120:THR:HG23	2.39	0.53
7:J:65:ALA:HB3	9:H:354:LYS:HE2	1.89	0.53
3:D:20:ALA:O	3:D:24:ILE:CG1	2.54	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:286:VAL:HG11	3:D:419:VAL:HG22	1.92	0.52
5:B:341:LEU:O	5:B:345:THR:HG23	2.10	0.52
9:H:19:HIS:NE2	9:H:26:LEU:O	2.43	0.52
13:F:221:LEU:O	13:F:222:SER:OG	2.23	0.52
9:H:47:LEU:HD23	9:H:47:LEU:O	2.09	0.52
9:H:108:LEU:HD23	9:H:145:PHE:HE1	1.75	0.52
3:D:286:VAL:HG12	3:D:423:ALA:HB2	1.90	0.52
9:H:157:ASN:ND2	9:H:160:ARG:HH12	2.02	0.52
3:D:189:PHE:CE1	3:D:194:VAL:HG12	2.44	0.51
9:H:116:LEU:HD13	9:H:138:ARG:HH12	1.75	0.51
1:A:208:ASN:O	1:A:212:GLN:N	2.42	0.51
7:J:115:LYS:O	7:J:116:THR:OG1	2.18	0.51
5:B:46:PHE:HA	5:B:49:VAL:HB	1.92	0.51
5:B:227:PRO:CG	13:F:645:ALA:HB1	2.41	0.51
13:F:74:GLU:OE2	13:F:82:HIS:ND1	2.42	0.51
13:F:599:ARG:NH2	18:Q:9:MET:O	2.44	0.51
12:L:17:ALA:O	12:L:20:TYR:N	2.44	0.51
4:E:78:LEU:HD12	6:G:77:ALA:CB	2.41	0.51
9:H:112:ALA:HB2	9:H:141:ILE:CD1	2.41	0.51
9:H:125:VAL:HG13	9:H:203:ARG:HG2	1.93	0.51
9:H:235:ARG:NH1	9:H:243:TYR:OH	2.43	0.51
5:B:227:PRO:HG3	13:F:645:ALA:HB1	1.93	0.51
9:H:359:ASP:OD2	9:H:388:ILE:N	2.43	0.51
13:F:561:SER:HB2	13:F:564:ALA:HB3	1.92	0.51
1:A:177:ALA:HB1	2:C:92:TYR:OH	2.10	0.50
7:J:36:VAL:HG23	7:J:93:GLU:O	2.12	0.50
1:A:82:LYS:O	1:A:85:PHE:N	2.45	0.50
1:A:55:ILE:HG21	1:A:326:ILE:CD1	2.36	0.50
3:D:21:ILE:CA	3:D:24:ILE:CD1	2.72	0.50
7:J:60:TYR:HD2	7:J:82:ILE:HG21	1.76	0.50
3:D:23:PHE:O	3:D:24:ILE:CG1	2.59	0.50
3:D:134:GLN:OE1	3:D:264:ARG:NH1	2.45	0.50
5:B:184:LEU:HG	5:B:197:ILE:HG21	1.93	0.50
7:J:167:ALA:HB3	11:K:120:THR:HG23	1.94	0.50
1:A:246:GLN:O	11:K:80:GLN:NE2	2.44	0.50
5:B:279:THR:HG23	5:B:319:VAL:HG21	1.94	0.50
1:A:112:LEU:HA	2:C:25:PHE:CE2	2.47	0.49
2:C:25:PHE:HA	2:C:28:ILE:HG22	1.94	0.49
3:D:267:VAL:HG21	3:D:321:ILE:HD11	1.93	0.49
3:D:460:GLU:O	3:D:462:ARG:N	2.45	0.49
7:J:60:TYR:O	7:J:82:ILE:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:194:LEU:HB3	5:B:266:ALA:HB2	0.50	0.49
9:H:125:VAL:HG12	9:H:125:VAL:O	2.12	0.49
3:D:126:GLY:HA3	3:D:145:LEU:HD11	1.92	0.49
9:H:168:LEU:HD13	9:H:172:TRP:CE3	2.48	0.49
6:G:76:PHE:O	6:G:80:LEU:HD23	2.12	0.49
13:F:97:LEU:HD12	13:F:136:LEU:HD22	1.94	0.49
1:A:86:LYS:NZ	11:K:82:ASP:OD1	2.35	0.49
10:I:70:VAL:O	10:I:76:ASN:ND2	2.43	0.49
10:I:175:ALA:O	16:S:57:ASN:ND2	2.44	0.49
5:B:267:PHE:HB3	5:B:268:PRO:HD2	1.94	0.49
13:F:147:VAL:HG12	13:F:147:VAL:O	2.12	0.49
1:A:146:LEU:HD13	1:A:165:ALA:HB1	1.94	0.49
14:N:34:GLN:OE1	14:N:44:THR:HG21	2.13	0.49
5:B:101:TYR:CD2	5:B:101:TYR:C	2.85	0.49
10:I:95:HIS:NE2	10:I:137:ASP:OD1	2.44	0.49
7:J:162:TYR:CB	15:M:78:GLU:OE1	2.61	0.48
2:C:104:LEU:HD13	2:C:104:LEU:O	2.13	0.48
5:B:46:PHE:HA	5:B:49:VAL:CB	2.43	0.48
5:B:268:PRO:O	5:B:274:TRP:CH2	2.66	0.48
1:A:164:ARG:NH2	1:A:336:ARG:O	2.45	0.48
7:J:65:ALA:HB2	7:J:123:GLU:OE2	2.13	0.48
13:F:505:THR:O	13:F:507:PHE:N	2.40	0.48
3:D:194:VAL:HG23	3:D:194:VAL:O	2.13	0.48
7:J:44:ASP:OD1	7:J:45:ARG:N	2.46	0.48
1:A:103:PRO:HA	1:A:106:VAL:HG12	1.96	0.48
3:D:149:PRO:O	3:D:153:LEU:HD13	2.13	0.48
7:J:164:LEU:HD21	11:K:92:MET:SD	2.54	0.48
13:F:261:SER:O	13:F:265:HIS:ND1	2.45	0.48
14:N:10:VAL:HG22	14:N:37:LEU:HD23	1.95	0.48
1:A:112:LEU:HA	2:C:25:PHE:HE2	1.79	0.48
1:A:326:ILE:HD12	1:A:327:LEU:N	2.29	0.48
9:H:43:VAL:HG21	11:K:197:LEU:HD11	1.95	0.48
1:A:286:LEU:HD21	1:A:306:PHE:CE1	2.50	0.47
5:B:135:ILE:CD1	5:B:194:LEU:HD11	2.44	0.47
3:D:286:VAL:HG11	3:D:419:VAL:CG2	2.45	0.47
6:G:55:ALA:HB1	6:G:58:VAL:CG1	2.44	0.47
13:F:239:ALA:O	13:F:249:TRP:NE1	2.47	0.47
7:J:69:SER:OG	7:J:74:ASP:OD1	2.26	0.47
1:A:286:LEU:HD13	1:A:287:GLU:N	2.29	0.47
4:E:78:LEU:HD12	6:G:77:ALA:HB1	1.97	0.47
9:H:77:PHE:O	9:H:81:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:56:ASP:OD1	6:G:57:PHE:N	2.47	0.47
3:D:303:LYS:HG2	3:D:350:VAL:HG11	1.96	0.47
11:K:118:THR:O	11:K:135:VAL:HG12	2.13	0.47
13:F:397:THR:HG21	13:F:490:LEU:HB3	1.96	0.47
4:E:55:GLN:NE2	6:G:125:VAL:HG11	2.28	0.47
4:E:93:MET:CE	13:F:635:ALA:HB3	2.45	0.47
5:B:266:ALA:C	5:B:267:PHE:O	2.53	0.47
6:G:160:GLY:O	6:G:164:LEU:HD23	2.15	0.47
3:D:50:VAL:HG11	8:P:13:THR:HG21	1.97	0.47
9:H:333:SER:N	9:H:336:GLY:O	2.46	0.46
14:N:135:ASP:OD1	14:N:136:ARG:N	2.49	0.46
7:J:158:THR:HG21	17:O:56:THR:HG22	1.97	0.46
3:D:6:TRP:O	3:D:9:THR:OG1	2.25	0.46
9:H:157:ASN:HD21	9:H:160:ARG:HH22	1.62	0.46
20:D:602:LMG:O5	20:D:602:LMG:O4	2.31	0.46
13:F:311:THR:OG1	13:F:576:SER:O	2.33	0.46
5:B:344:PHE:HA	5:B:347:VAL:HG12	1.98	0.46
3:D:277:PHE:CZ	3:D:280:VAL:HG11	2.50	0.46
7:J:150:TRP:HD1	17:O:24:ALA:HA	1.81	0.46
9:H:112:ALA:HB2	9:H:141:ILE:HD11	1.97	0.46
14:N:14:GLU:OE1	14:N:42:TYR:OH	2.33	0.46
14:N:47:MET:SD	14:N:100:LEU:HD21	2.56	0.46
3:D:206:TYR:O	3:D:211:GLN:NE2	2.49	0.46
5:B:22:ILE:HA	5:B:25:LEU:HB2	1.96	0.46
7:J:82:ILE:HD11	7:J:91:PRO:CG	2.44	0.46
14:N:13:LEU:HD21	14:N:127:LYS:HB3	1.98	0.46
5:B:63:THR:OG1	5:B:78:HIS:NE2	2.45	0.45
5:B:286:MET:HE1	5:B:316:ILE:HG21	1.97	0.45
7:J:66:ALA:HB1	7:J:76:VAL:O	2.16	0.45
6:G:2:ASP:OD1	6:G:3:LEU:N	2.49	0.45
14:N:22:PHE:HD2	14:N:139:ARG:HE	1.64	0.45
9:H:108:LEU:HD23	9:H:145:PHE:CE1	2.51	0.45
9:H:154:ILE:HD11	11:K:149:PRO:CG	2.46	0.45
13:F:19:ALA:O	13:F:23:GLY:N	2.42	0.45
1:A:71:LEU:HD11	12:L:32:LEU:HD22	1.99	0.45
10:I:110:VAL:HG21	10:I:120:VAL:HG13	1.99	0.45
15:M:29:LEU:HD21	15:M:70:LEU:HD21	1.99	0.45
3:D:460:GLU:O	3:D:461:PRO:C	2.55	0.45
5:B:196:ALA:O	5:B:199:GLN:HB3	2.16	0.45
9:H:47:LEU:HD22	9:H:390:GLY:HA2	1.97	0.45
5:B:164:LEU:O	5:B:168:LEU:HD23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:198:ALA:CB	5:B:266:ALA:O	2.65	0.45
5:B:419:VAL:O	5:B:422:ILE:HG22	2.17	0.45
9:H:153:PHE:O	9:H:153:PHE:CD1	2.70	0.45
13:F:107:VAL:HG11	13:F:263:LEU:CD1	2.46	0.45
1:A:114:TYR:OH	1:A:263:VAL:HG22	2.17	0.45
2:C:56:TYR:O	2:C:56:TYR:CD1	2.70	0.45
3:D:235:LEU:HD11	3:D:239:HIS:CE1	2.51	0.45
1:A:115:ILE:HG22	1:A:115:ILE:O	2.16	0.45
1:A:89:VAL:HG21	2:C:52:ARG:HG2	1.99	0.45
9:H:153:PHE:O	9:H:153:PHE:CG	2.70	0.45
9:H:154:ILE:HD11	11:K:52:CYS:SG	2.57	0.45
4:E:86:ARG:NH2	5:B:154:LYS:O	2.50	0.44
7:J:32:ASP:HB2	9:H:326:GLU:O	2.17	0.44
10:I:109:CYS:SG	10:I:110:VAL:N	2.90	0.44
4:E:7:LEU:HD13	4:E:44:ASN:OD1	2.17	0.44
4:E:41:VAL:HG11	5:B:178:LEU:CD1	2.45	0.44
17:O:26:ASP:OD1	17:O:27:HIS:N	2.50	0.44
5:B:185:TYR:CD1	5:B:192:THR:CG2	3.00	0.44
11:K:66:ASP:OD1	11:K:69:ARG:NH2	2.43	0.44
13:F:336:VAL:O	13:F:336:VAL:HG13	2.16	0.44
13:F:433:LEU:HD13	13:F:433:LEU:O	2.18	0.44
17:O:31:PRO:HA	17:O:33:LEU:HD23	1.99	0.44
5:B:197:ILE:C	5:B:199:GLN:N	2.70	0.44
7:J:73:GLN:NE2	17:O:47:TYR:OH	2.50	0.44
10:I:49:SER:OG	10:I:50:GLU:N	2.50	0.44
15:M:25:ASP:O	15:M:26:THR:OG1	2.22	0.44
3:D:130:VAL:HG11	3:D:257:MET:CG	2.48	0.44
3:D:178:LEU:HD21	5:B:415:LEU:HB3	2.00	0.44
5:B:288:LEU:O	5:B:292:VAL:HG12	2.17	0.44
13:F:140:VAL:HG23	13:F:140:VAL:O	2.17	0.44
14:N:47:MET:CE	14:N:100:LEU:HD21	2.48	0.44
1:A:155:ASN:O	1:A:158:SER:N	2.42	0.44
3:D:268:ASP:OD1	3:D:495:VAL:HG13	2.18	0.44
3:D:211:GLN:OE1	3:D:272:ALA:HB3	2.18	0.43
2:C:54:THR:HG21	11:K:100:ARG:HD2	1.99	0.43
14:N:109:SER:OG	16:S:72:ASP:OD2	2.26	0.43
1:A:273:SER:O	1:A:278:GLY:N	2.44	0.43
2:C:71:ASN:OD1	2:C:72:VAL:N	2.51	0.43
13:F:563:GLN:O	13:F:567:LYS:N	2.45	0.43
9:H:18:HIS:HE1	11:K:46:LEU:HD11	1.84	0.43
4:E:58:LYS:HD3	5:B:192:THR:OG1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:194:LEU:C	5:B:266:ALA:CA	2.77	0.43
5:B:226:VAL:O	5:B:281:LEU:HD22	2.17	0.43
12:L:32:LEU:HD21	12:L:36:TRP:CE3	2.53	0.43
3:D:85:ASP:OD1	3:D:86:GLY:N	2.49	0.43
3:D:226:LEU:HD11	3:D:314:ILE:HD12	2.01	0.43
3:D:233:THR:HG23	13:F:610:ASP:OD2	2.19	0.43
4:E:58:LYS:CD	5:B:192:THR:HG23	2.49	0.43
5:B:260:ILE:HD11	5:B:329:MET:HE1	1.98	0.43
7:J:81:LEU:HD21	7:J:114:TRP:HH2	1.84	0.43
9:H:59:THR:HG22	9:H:62:MET:SD	2.59	0.43
1:A:50:TRP:CZ3	12:L:51:VAL:HG11	2.54	0.42
3:D:502:VAL:HG23	3:D:503:LEU:HD23	2.01	0.42
5:B:314:VAL:HG13	5:B:329:MET:HG3	2.01	0.42
7:J:37:GLU:HG2	7:J:94:VAL:HG23	2.01	0.42
2:C:15:VAL:HG12	2:C:15:VAL:O	2.18	0.42
4:E:69:VAL:HG11	5:B:140:GLU:HG3	2.01	0.42
5:B:81:LEU:HD22	5:B:84:ARG:HH21	1.85	0.42
5:B:138:ALA:O	5:B:141:THR:OG1	2.30	0.42
13:F:411:PHE:HE1	13:F:498:THR:HG22	1.83	0.42
2:C:51:ILE:O	2:C:54:THR:HG22	2.19	0.42
1:A:282:PHE:O	1:A:284:ILE:N	2.51	0.42
2:C:68:ILE:HB	9:H:6:THR:HG22	2.01	0.42
9:H:81:VAL:HG22	9:H:331:VAL:CG2	2.48	0.42
9:H:191:GLU:HG2	9:H:195:THR:HG21	2.02	0.42
9:H:154:ILE:CD1	11:K:52:CYS:SG	3.07	0.42
3:D:168:LYS:NZ	3:D:233:THR:HG22	2.35	0.42
1:A:95:ASP:OD1	1:A:96:ARG:N	2.53	0.42
7:J:67:TYR:CE1	7:J:76:VAL:HG11	2.54	0.42
13:F:22:VAL:HG12	13:F:26:LEU:HD23	2.01	0.42
1:A:178:LEU:HD23	1:A:181:LEU:HD12	2.02	0.42
9:H:152:ARG:H	9:H:152:ARG:HG3	1.74	0.42
10:I:149:THR:O	12:L:72:ARG:NH1	2.52	0.42
3:D:90:PRO:HG3	3:D:487:ILE:HG21	2.02	0.42
3:D:98:ILE:HD11	3:D:344:ALA:CB	2.50	0.42
3:D:415:PHE:O	3:D:417:VAL:N	2.49	0.42
9:H:49:ARG:O	11:K:128:SER:OG	2.30	0.42
13:F:561:SER:CB	13:F:564:ALA:HB3	2.49	0.42
14:N:49:ALA:HB3	14:N:50:PRO:HD3	2.01	0.42
1:A:5:ILE:HG13	1:A:7:LEU:HD11	2.01	0.41
12:L:58:LEU:O	12:L:62:ALA:HB2	2.20	0.41
5:B:13:GLY:O	5:B:14:THR:OG1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:THR:O	1:A:196:VAL:HG12	2.20	0.41
5:B:196:ALA:HA	5:B:199:GLN:HB3	2.02	0.41
5:B:212:LEU:CA	5:B:267:PHE:CZ	3.03	0.41
9:H:68:SER:OG	9:H:79:GLU:OE2	2.37	0.41
13:F:96:MET:O	13:F:100:VAL:HG23	2.20	0.41
5:B:194:LEU:O	5:B:266:ALA:O	2.39	0.41
5:B:260:ILE:HD11	5:B:329:MET:HE3	2.01	0.41
7:J:19:LEU:CD1	7:J:49:VAL:HG13	2.50	0.41
13:F:32:THR:O	13:F:36:LEU:N	2.53	0.41
13:F:97:LEU:HD12	13:F:136:LEU:CD2	2.50	0.41
1:A:278:GLY:O	1:A:317:LYS:NZ	2.43	0.41
17:O:10:LYS:NZ	17:O:67:GLU:OE2	2.41	0.41
8:P:6:LYS:O	8:P:10:LEU:HD23	2.21	0.41
2:C:86:VAL:HG11	4:E:68:THR:HG23	2.02	0.41
11:K:40:LEU:HD11	11:K:163:ARG:HB3	2.03	0.41
13:F:545:LEU:HA	13:F:548:ILE:HG22	2.02	0.41
9:H:220:LEU:O	9:H:222:GLY:N	2.54	0.41
1:A:71:LEU:CD1	12:L:32:LEU:HD22	2.51	0.41
3:D:349:LEU:HD21	3:D:467:ILE:CD1	2.50	0.41
2:C:108:GLU:HG2	6:G:144:LEU:HD11	2.03	0.40
3:D:106:ALA:O	3:D:117:TYR:OH	2.37	0.40
5:B:262:PHE:CE2	5:B:267:PHE:CD1	3.09	0.40
9:H:184:LEU:HD21	9:H:273:VAL:HG11	2.03	0.40
12:L:9:VAL:HA	12:L:12:VAL:HG12	2.03	0.40
3:D:323:SER:OG	3:D:324:PHE:N	2.54	0.40
5:B:212:LEU:CA	5:B:267:PHE:HZ	2.34	0.40
11:K:120:THR:HG22	11:K:120:THR:O	2.20	0.40
5:B:61:LEU:HD12	5:B:81:LEU:HD11	2.03	0.40
5:B:130:GLN:O	5:B:194:LEU:CG	2.68	0.40
10:I:104:ILE:HG22	21:I:201:SF4:S2	2.61	0.40
10:I:139:VAL:O	10:I:139:VAL:HG22	2.22	0.40
5:B:196:ALA:C	5:B:199:GLN:HB3	2.42	0.40
7:J:122:ARG:NE	7:J:141:ILE:HG23	2.37	0.40
4:E:93:MET:HE2	13:F:635:ALA:HB3	2.03	0.40
7:J:32:ASP:O	7:J:33:ALA:CB	2.68	0.40
14:N:13:LEU:HD21	14:N:127:LYS:CB	2.50	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	A	346/372 (93%)	308 (89%)	36 (10%)	2 (1%)	25	60
2	C	112/132 (85%)	99 (88%)	13 (12%)	0	100	100
3	D	480/529 (91%)	437 (91%)	36 (8%)	7 (2%)	10	40
4	E	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
5	B	471/515 (92%)	423 (90%)	39 (8%)	9 (2%)	8	36
6	G	166/200 (83%)	156 (94%)	10 (6%)	0	100	100
7	J	154/168 (92%)	121 (79%)	33 (21%)	0	100	100
8	P	40/42 (95%)	32 (80%)	8 (20%)	0	100	100
9	H	391/394 (99%)	333 (85%)	57 (15%)	1 (0%)	41	72
10	I	191/196 (97%)	168 (88%)	22 (12%)	1 (0%)	29	63
11	K	204/237 (86%)	174 (85%)	28 (14%)	2 (1%)	15	49
12	L	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
13	F	603/656 (92%)	535 (89%)	67 (11%)	1 (0%)	47	78
14	N	145/150 (97%)	121 (83%)	24 (17%)	0	100	100
15	M	108/111 (97%)	87 (81%)	21 (19%)	0	100	100
16	S	53/110 (48%)	49 (92%)	4 (8%)	0	100	100
17	O	66/70 (94%)	47 (71%)	17 (26%)	2 (3%)	4	27
18	Q	37/39 (95%)	33 (89%)	4 (11%)	0	100	100
All	All	3739/4098 (91%)	3285 (88%)	429 (12%)	25 (1%)	26	57

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	187	LEU
5	B	194	LEU
5	B	267	PHE
9	H	154	ILE

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Mol	Chain	Res	Type
13	F	581	TYR
1	A	233	ASP
3	D	459	ALA
5	B	188	SER
5	B	189	GLY
5	B	191	HIS
1	A	336	ARG
5	B	268	PRO
3	D	454	GLU
3	D	458	ASP
5	B	193	GLN
10	I	179	ARG
11	K	19	PRO
3	D	229	VAL
3	D	301	ASN
3	D	416	ARG
17	O	12	VAL
3	D	457	VAL
5	B	388	PRO
11	K	149	PRO
17	O	53	PRO

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	A	284/302 (94%)	282 (99%)	2 (1%)	84 91
2	C	93/109 (85%)	93 (100%)	0	100 100
3	D	370/424 (87%)	368 (100%)	2 (0%)	88 93
4	E	81/82 (99%)	81 (100%)	0	100 100
5	B	367/413 (89%)	363 (99%)	4 (1%)	73 86
6	G	134/166 (81%)	133 (99%)	1 (1%)	84 91
7	J	138/148 (93%)	136 (99%)	2 (1%)	67 83
8	P	32/34 (94%)	32 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	H	331/338 (98%)	323 (98%)	8 (2%)	49	75
10	I	162/172 (94%)	162 (100%)	0	100	100
11	K	174/196 (89%)	172 (99%)	2 (1%)	73	86
12	L	63/63 (100%)	63 (100%)	0	100	100
13	F	487/527 (92%)	483 (99%)	4 (1%)	81	90
14	N	119/120 (99%)	117 (98%)	2 (2%)	60	80
15	M	95/96 (99%)	92 (97%)	3 (3%)	39	69
16	S	48/97 (50%)	48 (100%)	0	100	100
17	O	57/59 (97%)	56 (98%)	1 (2%)	59	79
18	Q	27/28 (96%)	27 (100%)	0	100	100
All	All	3062/3374 (91%)	3031 (99%)	31 (1%)	77	87

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	154	ASN
3	D	229	VAL
3	D	460	GLU
5	B	154	LYS
5	B	269	SER
5	B	340	ASN
5	B	479	ASN
6	G	71	ASN
7	J	45	ARG
7	J	106	ARG
9	H	49	ARG
9	H	60	ASN
9	H	138	ARG
9	H	154	ILE
9	H	156	ASN
9	H	157	ASN
9	H	261	ARG
9	H	330	ARG
11	K	32	ASN
11	K	69	ARG
13	F	72	MET
13	F	448	ARG

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Mol	Chain	Res	Type
13	F	509	ASN
13	F	596	ARG
14	N	47	MET
14	N	139	ARG
15	M	1	MET
15	M	4	LYS
15	M	59	ASN
17	O	28	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	GLN
1	A	208	ASN
7	J	73	GLN
9	H	18	HIS
9	H	155	ASN
9	H	157	ASN
11	K	104	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
21	SF4	I	202	10	0,12,12	-	-	-		
21	SF4	K	501	11	0,12,12	-	-	-		
20	LMG	D	602	-	55,55,55	0.80	2 (3%)	63,63,63	1.33	7 (11%)
21	SF4	I	201	10	0,12,12	-	-	-		
19	BCR	D	601	-	41,41,41	1.09	2 (4%)	56,56,56	1.48	9 (16%)

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	SF4	I	202	10	-	-	0/6/5/5
21	SF4	K	501	11	-	-	0/6/5/5
20	LMG	D	602	-	-	15/50/70/70	0/1/1/1
21	SF4	I	201	10	-	-	0/6/5/5
19	BCR	D	601	-	-	21/29/63/63	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	601	BCR	C1-C6	-3.52	1.48	1.53
20	D	602	LMG	C4-C5	2.73	1.58	1.53
20	D	602	LMG	O7-C8	-2.34	1.40	1.46
19	D	601	BCR	C30-C25	-2.12	1.50	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	D	601	BCR	C24-C23-C22	-4.23	119.84	126.23
19	D	601	BCR	C11-C10-C9	-3.73	121.98	127.31
20	D	602	LMG	O6-C5-C4	3.48	116.02	109.69
19	D	601	BCR	C15-C16-C17	-2.87	117.59	123.47
19	D	601	BCR	C33-C5-C6	-2.78	121.41	124.53
20	D	602	LMG	O7-C10-O9	-2.65	117.30	123.70
19	D	601	BCR	C28-C27-C26	-2.45	109.71	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	D	602	LMG	O1-C7-C8	-2.37	105.19	110.90
20	D	602	LMG	C1-O6-C5	2.36	118.31	113.69
19	D	601	BCR	C34-C9-C10	-2.25	119.77	122.92
20	D	602	LMG	O3-C3-C2	-2.24	105.18	110.35
19	D	601	BCR	C7-C8-C9	-2.21	122.89	126.23
20	D	602	LMG	O2-C2-C1	-2.19	104.72	110.05
19	D	601	BCR	C38-C26-C25	-2.12	122.15	124.53
20	D	602	LMG	O6-C1-O1	-2.10	104.99	109.97
19	D	601	BCR	C8-C7-C6	-2.09	121.34	127.20

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	D	601	BCR	C1-C6-C7-C8
19	D	601	BCR	C6-C7-C8-C9
19	D	601	BCR	C11-C10-C9-C8
19	D	601	BCR	C11-C10-C9-C34
19	D	601	BCR	C10-C11-C12-C13
19	D	601	BCR	C11-C12-C13-C35
19	D	601	BCR	C16-C17-C18-C19
19	D	601	BCR	C16-C17-C18-C36
19	D	601	BCR	C36-C18-C19-C20
19	D	601	BCR	C21-C22-C23-C24
19	D	601	BCR	C22-C23-C24-C25
19	D	601	BCR	C23-C24-C25-C26
19	D	601	BCR	C23-C24-C25-C30
20	D	602	LMG	C11-C10-O7-C8
20	D	602	LMG	O9-C10-O7-C8
19	D	601	BCR	C7-C8-C9-C34
19	D	601	BCR	C37-C22-C23-C24
19	D	601	BCR	C14-C15-C16-C17
19	D	601	BCR	C9-C10-C11-C12
19	D	601	BCR	C35-C13-C14-C15
19	D	601	BCR	C20-C21-C22-C37
19	D	601	BCR	C11-C12-C13-C14
20	D	602	LMG	C41-C42-C43-C44
20	D	602	LMG	C30-C31-C32-C33
19	D	601	BCR	C5-C6-C7-C8
20	D	602	LMG	C20-C21-C22-C23
20	D	602	LMG	C22-C23-C24-C25
20	D	602	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
20	D	602	LMG	O6-C5-C6-O5
20	D	602	LMG	C38-C39-C40-C41
20	D	602	LMG	C12-C13-C14-C15
20	D	602	LMG	O7-C8-C9-O8
20	D	602	LMG	C14-C15-C16-C17
20	D	602	LMG	C21-C22-C23-C24
20	D	602	LMG	C7-C8-C9-O8
20	D	602	LMG	C15-C16-C17-C18

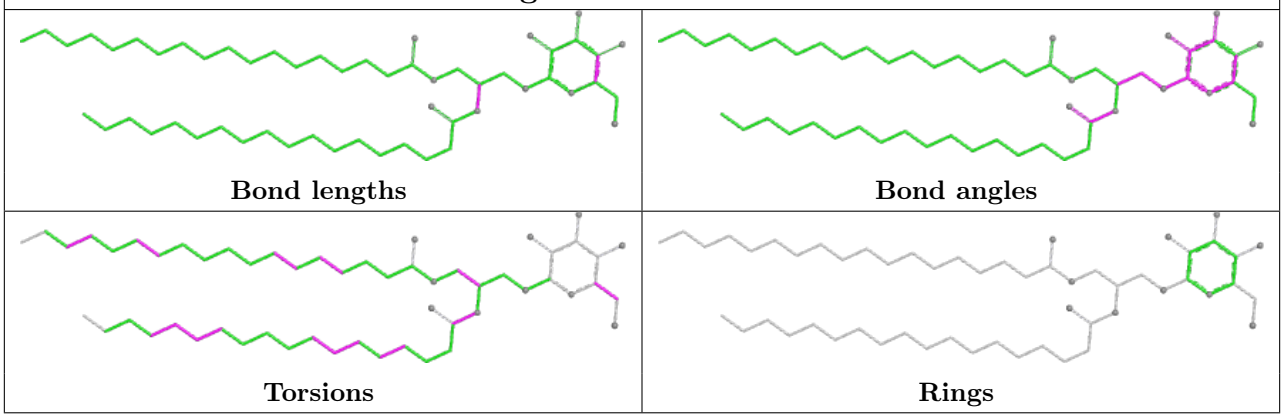
There are no ring outliers.

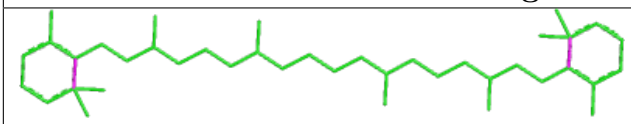
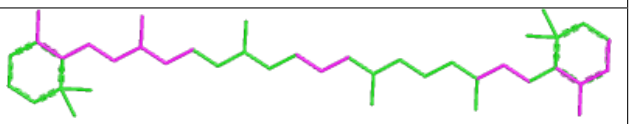
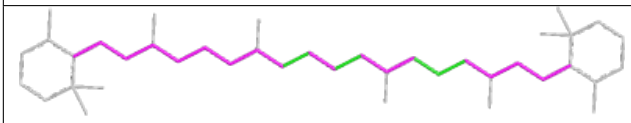
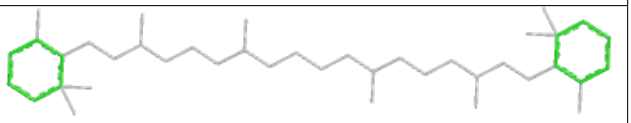
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	D	602	LMG	2	0
21	I	201	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 LMG D 602



Ligand BCR D 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

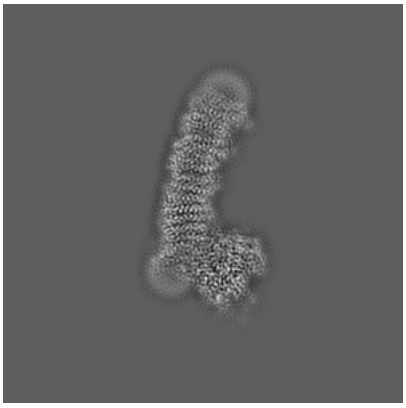
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0281. These allow visual inspection of the internal detail of the map and identification of artifacts.

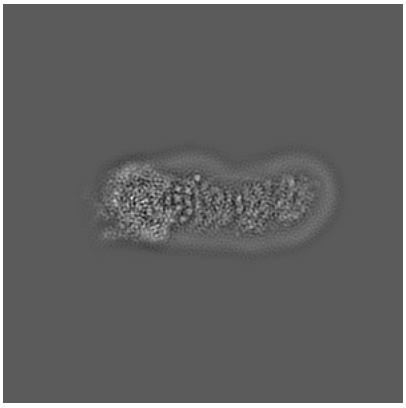
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

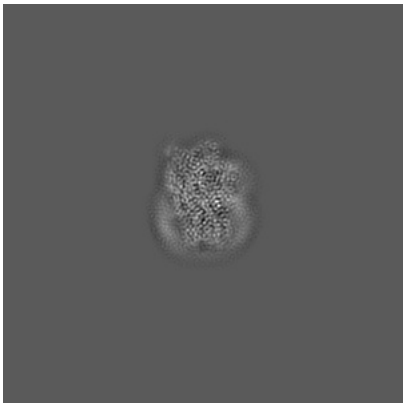
6.1.1 Primary map



X



Y

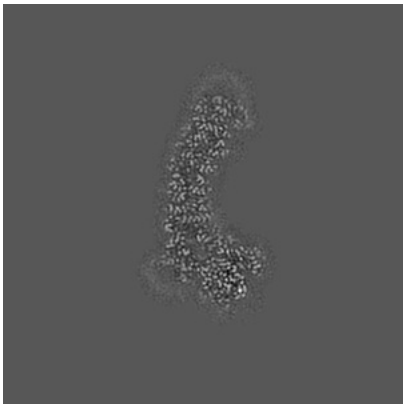


Z

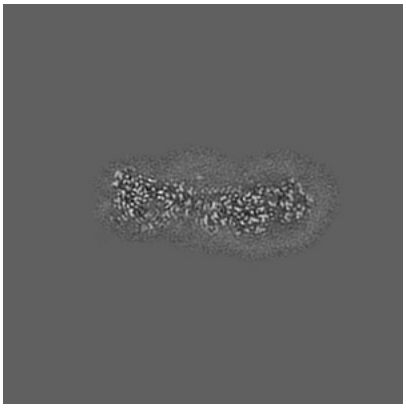
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

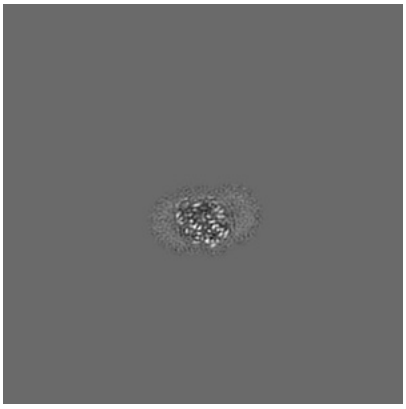
6.2.1 Primary map



X Index: 150



Y Index: 150

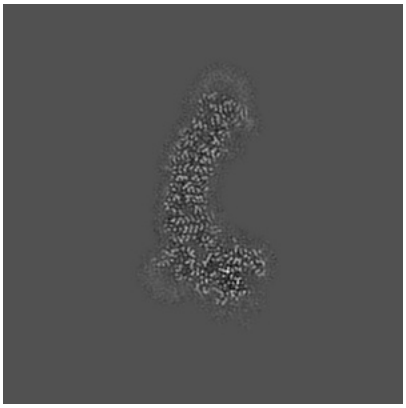


Z Index: 150

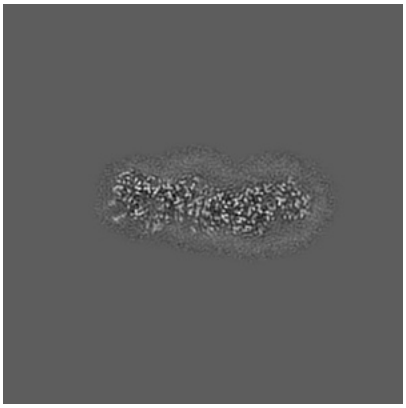
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

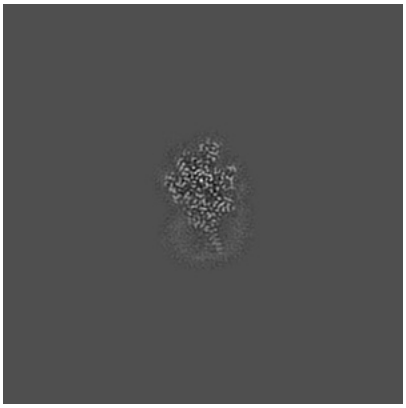
6.3.1 Primary map



X Index: 152



Y Index: 148



Z Index: 100

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

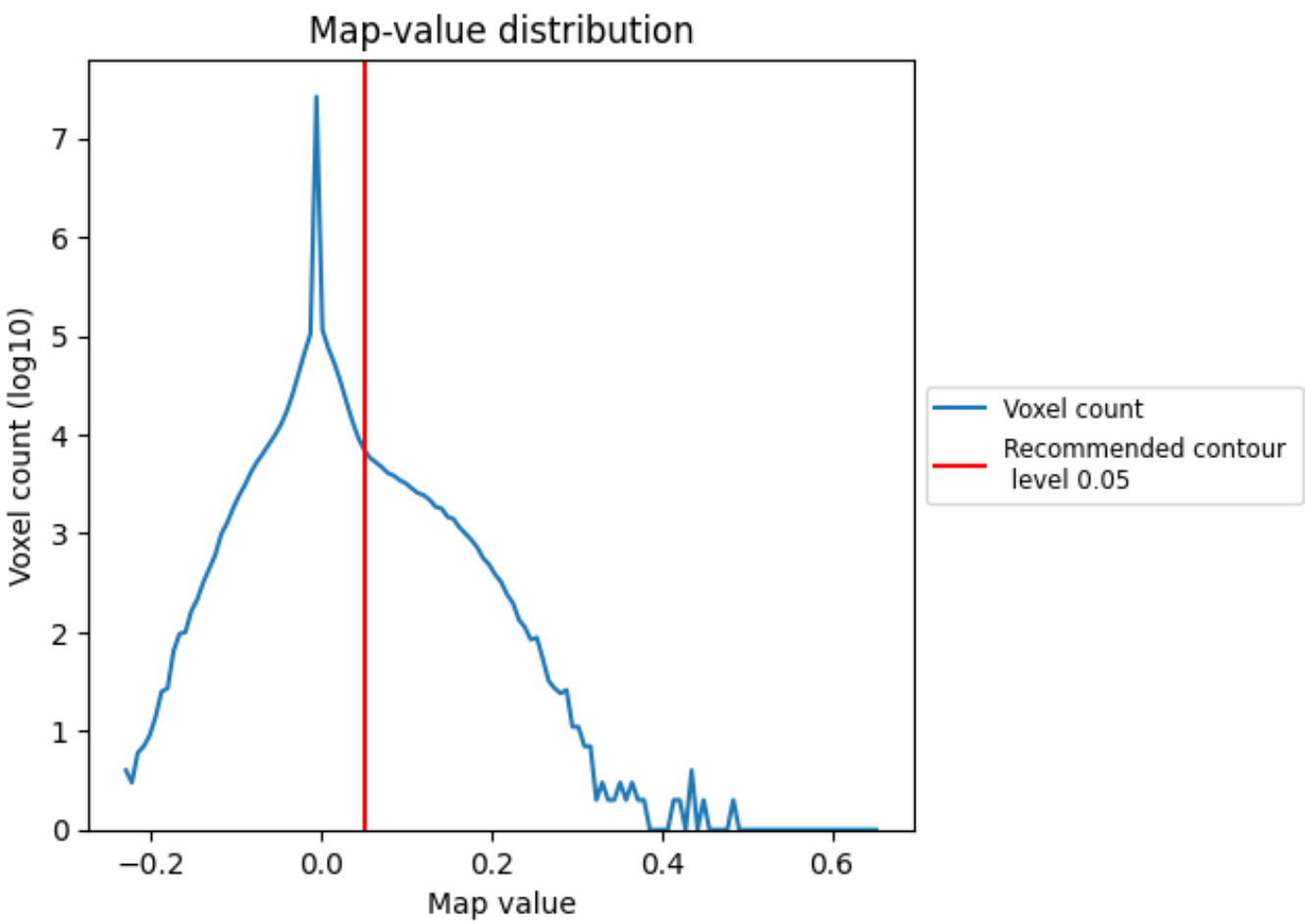
6.5 Mask visualisation (i)

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

7 Map analysis (i)

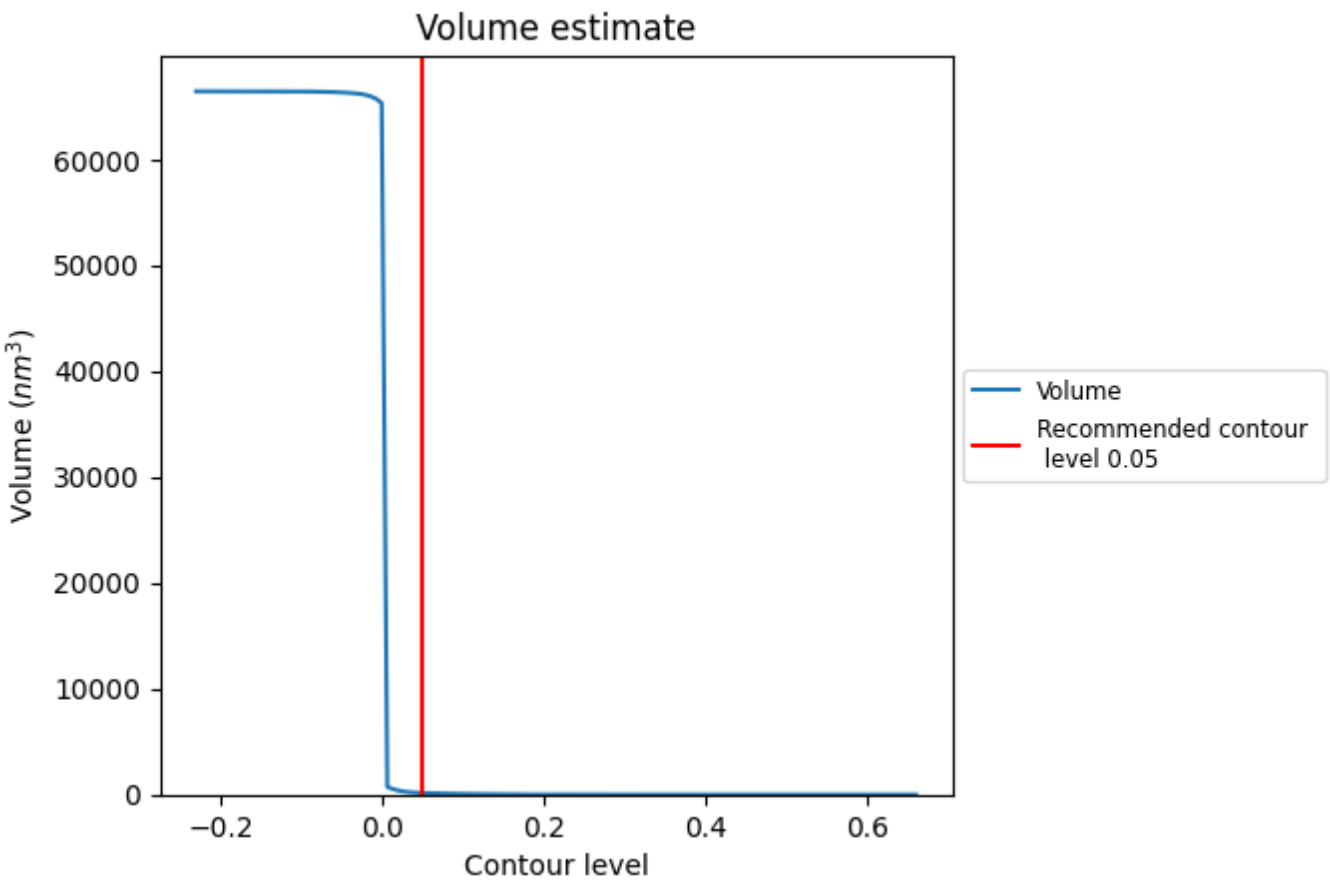
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

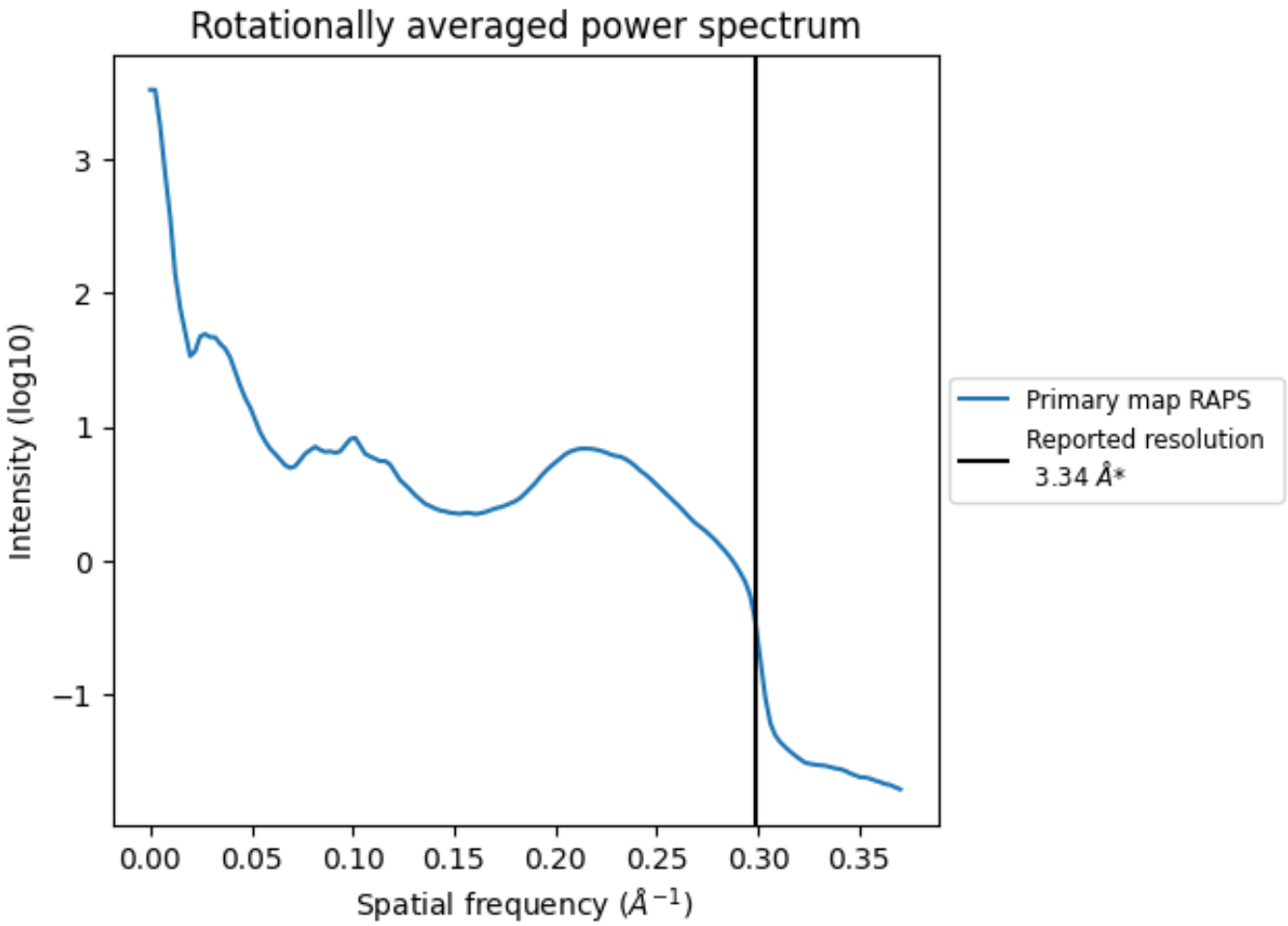
7.2 Volume estimate (i)



The volume at the recommended contour level is 150 nm^3; this corresponds to an approximate mass of 135 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 0.299 Å^{-1}

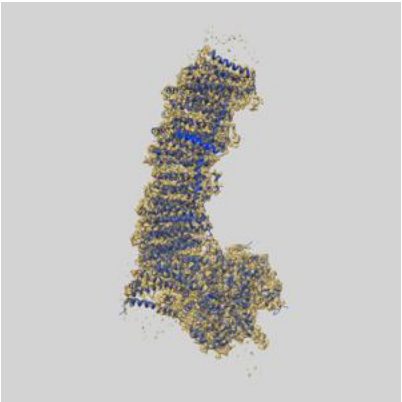
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

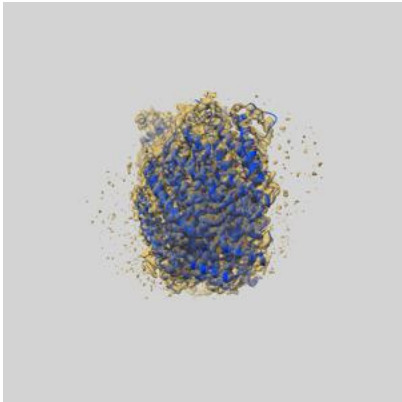
This section contains information regarding the fit between EMDB map EMD-0281 and PDB model 6HUM. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay (i)



X

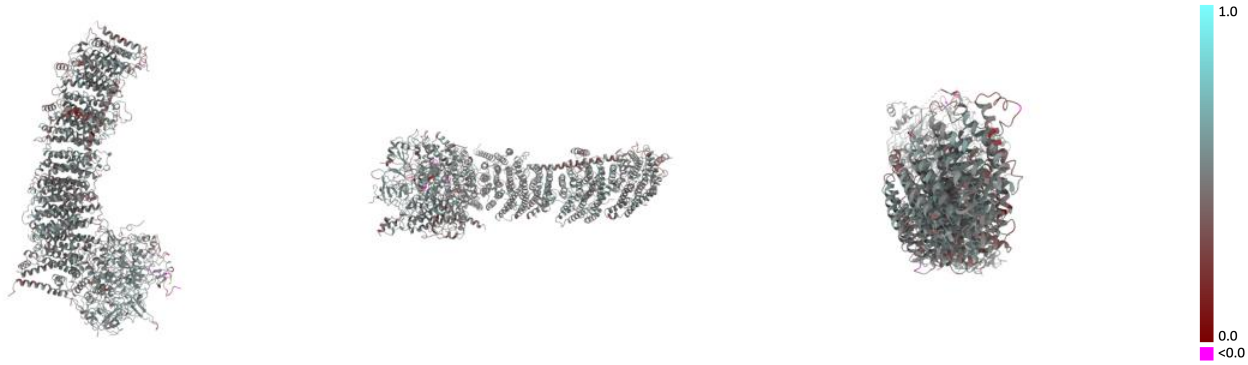
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

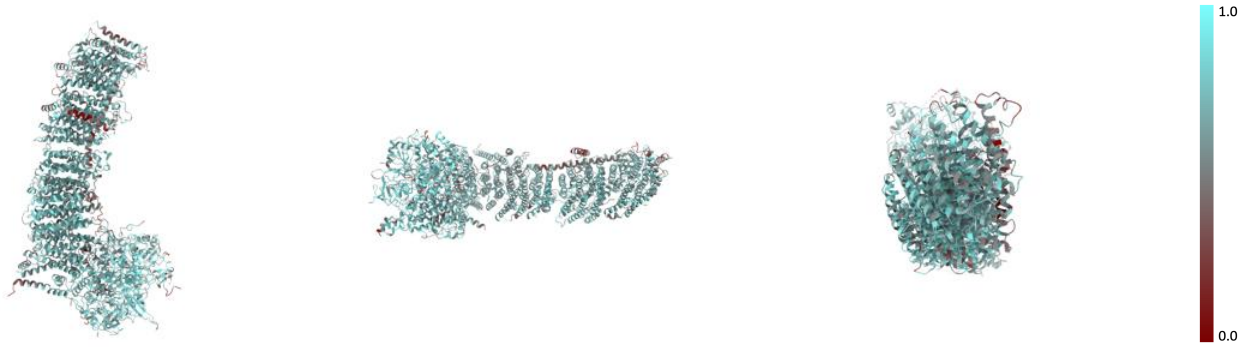
9.2 Q-score mapped to coordinate model (i)



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.

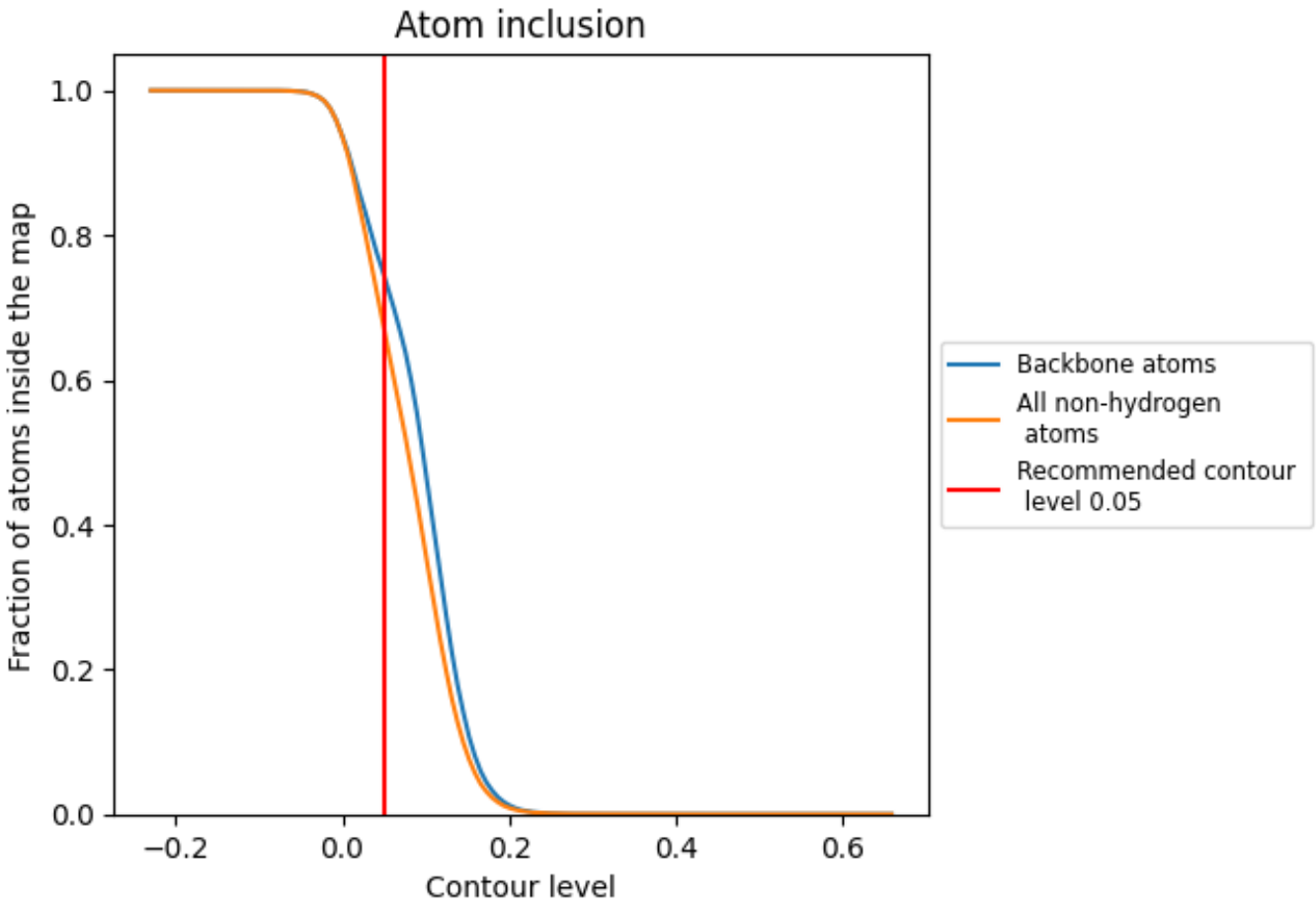
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6715	0.4820
A	0.6629	0.4820
B	0.7012	0.4880
C	0.6801	0.4760
D	0.7018	0.4960
E	0.6618	0.4970
F	0.6088	0.4610
G	0.6514	0.4980
H	0.6841	0.4840
I	0.7093	0.5050
J	0.7111	0.4740
K	0.7301	0.5060
L	0.5808	0.4550
M	0.7098	0.4850
N	0.7120	0.4910
O	0.6027	0.3740
P	0.6635	0.4780
Q	0.2457	0.3980
S	0.7237	0.5200