Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 01:49 pm GMT

PDB ID	:	6QC5
EMDB ID	:	EMD-4497
Title	:	Ovine respiratory complex I FRC closed class 1
Authors	:	Letts, J.A.; Sazanov, L.A.
Deposited on	:	2018-12-26
Resolution	:	4.30 Å(reported)
Based on initial model	:	5LNK

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

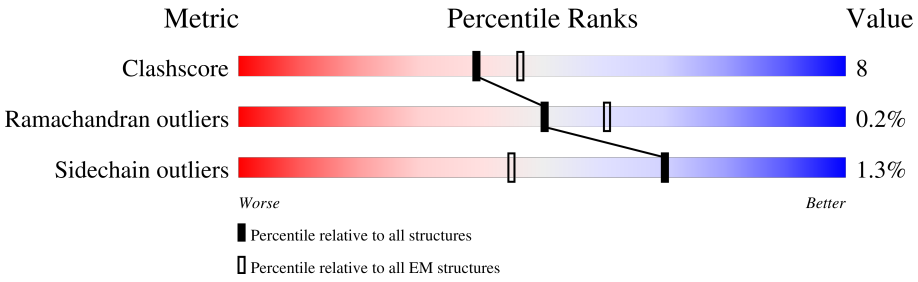
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.30 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	V1	445	22% 75% 21%
2	V2	217	25% 74% 22%
3	S1	704	23% 72% 25%
4	S2	430	27% 75% 24%
5	S3	228	20% 68% 22% 9%
6	S7	179	26% 65% 21% 13%
7	S8	176	17% 73% 24%
8	V3	75	20% 39% 12% 45%

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Mol	Chain	Length	Quality of chain
9	S6	96	26% 76% 23%
10	S4	133	26% 77% 18% 5%
11	A9	338	32% 71% 21% 8%
12	A2	98	20% 63% 20% 16%
13	A5	115	23% 79% 17%
14	A6	127	30% 79% 11% 10%
15	A7	112	44% 57% 27% 15%
16	AL	145	47% 60% 25% 15%
17	AA	88	51% 69% 22% 9%
17	AB	88	44% 86% 13%
18	AM	143	31% 80% 17%
19	D3	115	67% 84% 16%
20	D1	318	48% 68% 31%
21	D6	175	57% 88% 12%
22	4L	98	67% 81% 17%
23	D5	606	53% 78% 21%
24	D4	459	40% 81% 19%
25	D2	347	39% 77% 23%
26	AK	140	66% 88% 11%
27	B5	143	36% 80% 17%
28	A8	171	31% 80% 20%
29	BJ	175	34% 74% 23%
30	AJ	320	43% 82% 17%
31	S5	105	31% 73% 20% 6%
32	A3	83	36% 72% 17% 11%

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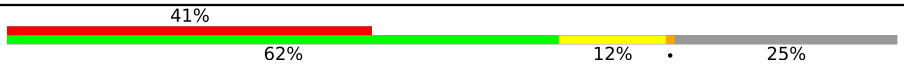
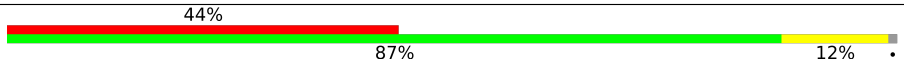
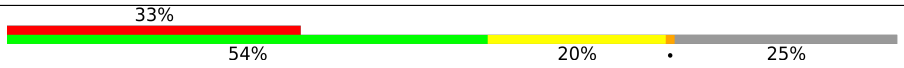
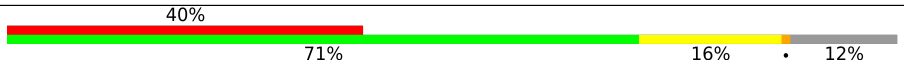
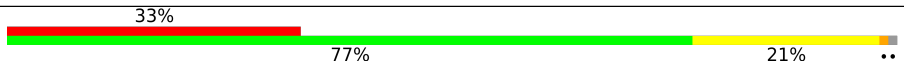
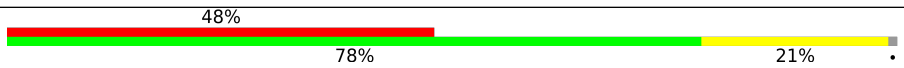
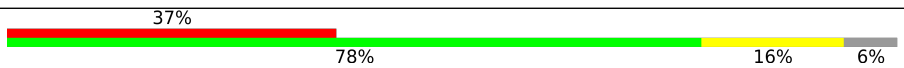
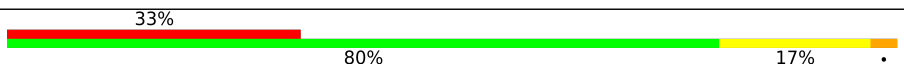
Mol	Chain	Length	Quality of chain
33	B3	97	
34	C2	120	
35	B4	128	
36	B6	127	
37	B7	136	
38	B9	178	
39	B2	72	
40	B8	158	
41	BK	125	
42	C1	49	
43	B1	57	
44	A1	70	

2 Entry composition (i)

There are 52 unique types of molecules in this entry. The entry contains 65691 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	V1	430	3312	2086	593	613	20	0	0

- Molecule 2 is a protein called NDUFV2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	V2	212	1647	1052	277	308	10	0	0

- Molecule 3 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	S1	688	5275	3301	922	1011	41	0	0

- Molecule 4 is a protein called NDUFS2,NADH:ubiquinone oxidoreductase core subunit S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	S2	430	3455	2205	594	631	25	0	0

- Molecule 5 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	S3	208	1726	1112	296	315	3	0	0

- Molecule 6 is a protein called NADH:ubiquinone oxidoreductase core subunit S7,NDUFS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	S7	156	1248	795	225	214	14	0	0

- Molecule 7 is a protein called NDUFS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S8	176	Total	C	N	O	S	0	0
			1415	889	243	271	12		

- Molecule 8 is a protein called NDUFV3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V3	41	Total	C	N	O	S	0	0
			345	215	63	66	1		

- Molecule 9 is a protein called NDUFS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S6	95	Total	C	N	O	S	0	0
			737	451	139	144	3		

- Molecule 10 is a protein called NADH:ubiquinone oxidoreductase subunit S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S4	126	Total	C	N	O	S	0	0
			1025	646	182	194	3		

- Molecule 11 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A9	311	Total	C	N	O	S	0	0
			2512	1614	451	442	5		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A2	82	Total	C	N	O	S	0	0
			665	419	124	120	2		

- Molecule 13 is a protein called NDUFA5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A5	111	Total	C	N	O	S	0	0
			901	583	151	165	2		

- Molecule 14 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A6	114	Total	C	N	O	S	0	0
			969	619	180	166	4		

- Molecule 15 is a protein called NDUFA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A7	95	Total	C	N	O	S	0	0
			757	473	144	137	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AL	123	Total	C	N	O	S	0	0
			1044	676	182	182	4		

- Molecule 17 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AA	80	Total	C	N	O	S	0	0
			645	416	96	128	5		
17	AB	87	Total	C	N	O	S	0	0
			702	451	103	143	5		

- Molecule 18 is a protein called NDUFA13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AM	139	Total	C	N	O	S	0	0
			1143	733	200	201	9		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	D3	115	Total	C	N	O	S	0	0
			923	621	133	162	7		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	D1	318	Total	C	N	O	S	0	0
			2529	1704	384	422	19		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	D6	175	Total	C	N	O	S	0	0
			1345	904	192	236	13		

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	4L	98	Total	C	N	O	S	0	0
			748	489	112	132	15		

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	D5	606	Total	C	N	O	S	0	0
			4805	3187	746	828	44		

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	D4	459	Total	C	N	O	S	0	0
			3646	2428	571	607	40		

- Molecule 25 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	D2	347	Total	C	N	O	S	0	0
			2724	1808	416	460	40		

- Molecule 26 is a protein called NDUFA11.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AK	140	Total	C	N	O	S	0	0
			1025	654	175	190	6		

- Molecule 27 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B5	139	Total	C	N	O	S	0	0
			1156	761	194	199	2		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A8	171	Total	C	N	O	S	0	0
			1404	889	253	252	10		

- Molecule 29 is a protein called NDUFB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BJ	171	Total	C	N	O	S	0	0
			1441	905	266	262	8		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AJ	319	Total	C	N	O	S	0	0
			2583	1653	430	490	10		

- Molecule 31 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	S5	99	Total	C	N	O	S	0	0
			822	520	154	142	6		

- Molecule 32 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	A3	74	Total	C	N	O	S	0	0
			582	379	96	105	2		

- Molecule 33 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	B3	73	Total	C	N	O	S	0	0
			578	378	100	98	2		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	C2	119	Total	C	N	O	S	0	0
			997	647	174	172	4		

- Molecule 35 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	B4	128	Total	C	N	O	S	0	0
			1059	675	189	194	1		

- Molecule 36 is a protein called NDUFB6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B6	95	Total	C	N	O	S	0	0
			804	530	135	138	1		

- Molecule 37 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	B7	119	Total	C	N	O	S	0	0
			1026	641	196	181	8		

- Molecule 38 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	B9	176	Total	C	N	O	S	0	0
			1515	970	278	261	6		

- Molecule 39 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	B2	64	Total	C	N	O	S	0	0
			555	368	92	94	1		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	B8	157	Total	C	N	O	S	0	0
			1324	855	217	243	9		

- Molecule 41 is a protein called NDUFB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BK	102	Total	C	N	O	S	0	0
			853	547	141	161	4		

- Molecule 42 is a protein called NDUFC1.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	C1	46	Total	C	N	O	0	0
			391	258	67	66		

- Molecule 43 is a protein called NDUFB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	B1	52	Total	C	N	O	0	0
			449	296	79	74		

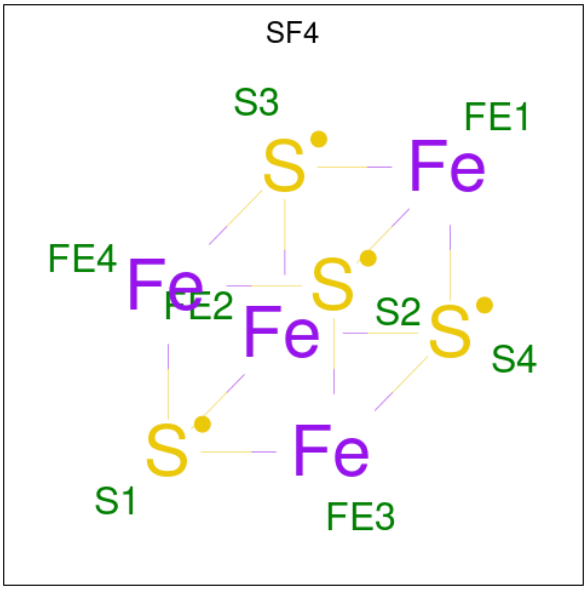
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	16	VAL	GLY	conflict	UNP W5QG39
B1	35	ALA	THR	conflict	UNP W5QG39
B1	38	ARG	TRP	conflict	UNP W5QG39

- Molecule 44 is a protein called NDUFA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	A1	70	Total	C	N	O	S	0	0
			577	369	106	97	5		

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
45	V1	1	Total	Fe	S	0
			8	4	4	

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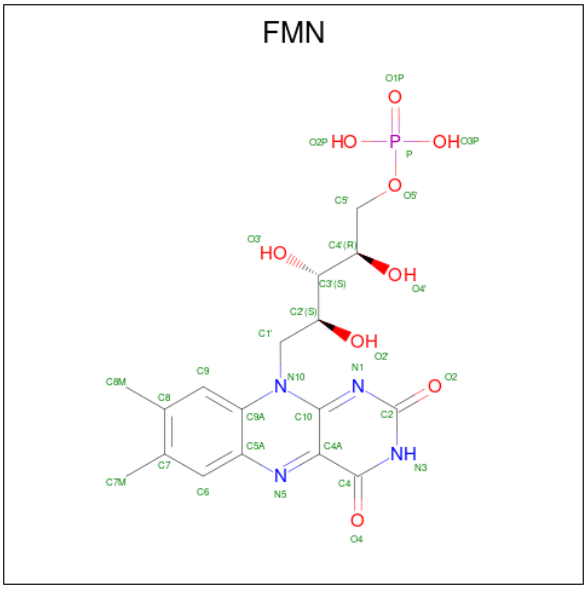
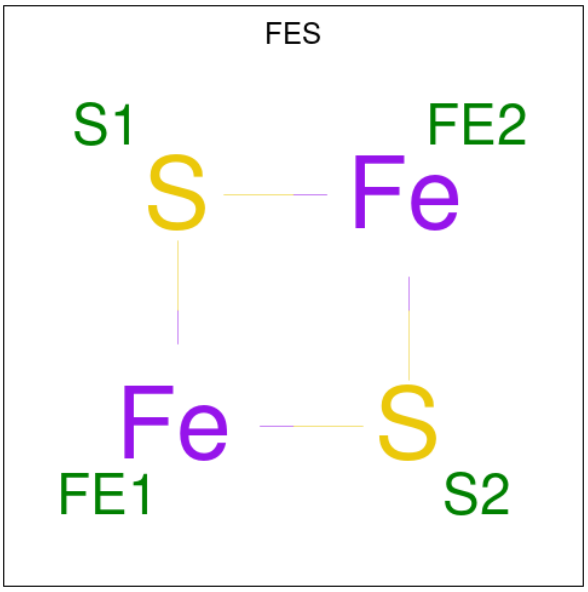
Mol	Chain	Residues	Atoms			AltConf
45	S1	1	Total 16	Fe 8	S 8	0
45	S1	1	Total 16	Fe 8	S 8	0
45	S7	1	Total 8	Fe 4	S 4	0
45	S8	1	Total 16	Fe 8	S 8	0
45	S8	1	Total 16	Fe 8	S 8	0

- Molecule 46 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



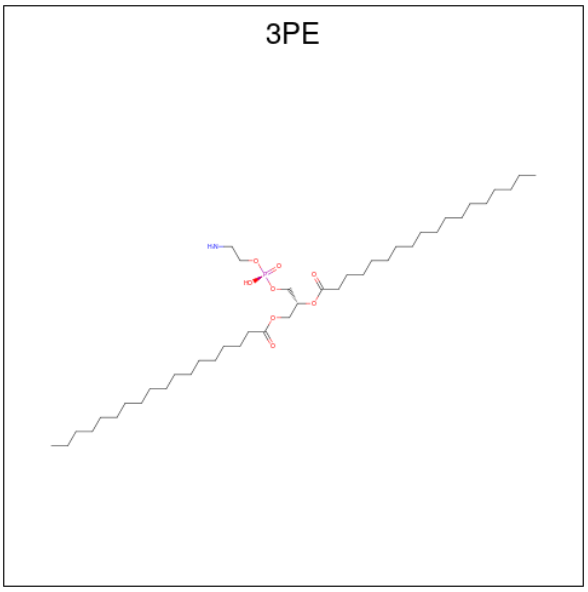
Mol	Chain	Residues	Atoms					AltConf
46	V1	1	Total 31	C 17	N 4	O 9	P 1	0

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
47	V2	1	Total	Fe	S	0
			4	2	2	
47	S1	1	Total	Fe	S	0
			4	2	2	

- Molecule 48 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
48	S2	1	Total	C	N	O	P	0
			40	30	1	8	1	

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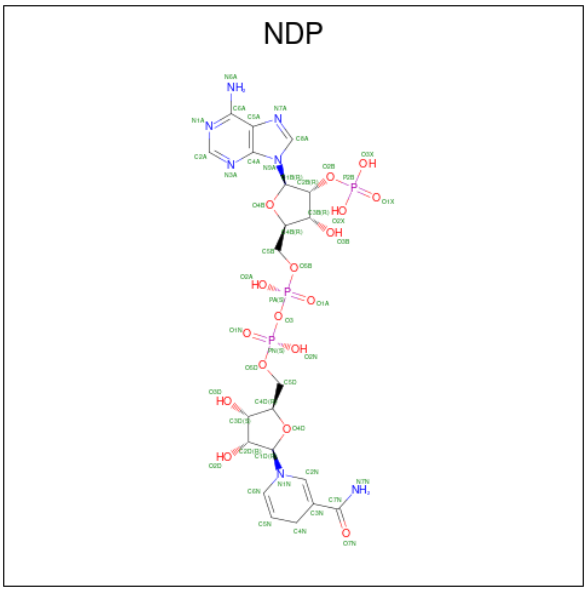
Mol	Chain	Residues	Atoms					AltConf
48	D5	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

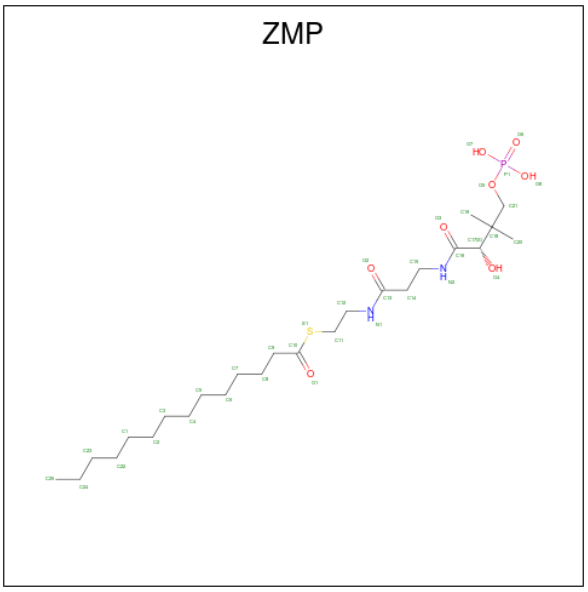
Mol	Chain	Residues	Atoms		AltConf
49	S6	1	Total	Zn	0
			1	1	

- Molecule 50 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



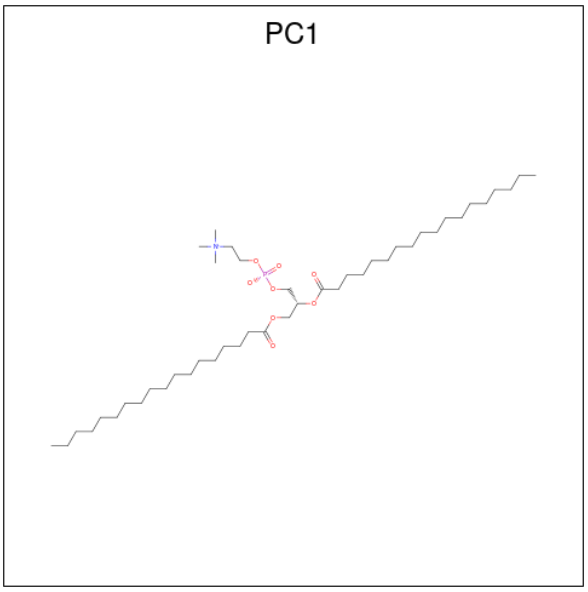
Mol	Chain	Residues	Atoms					AltConf
50	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 51 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



Mol	Chain	Residues	Atoms						AltConf
51	AA	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	
51	AB	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	

- Molecule 52 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



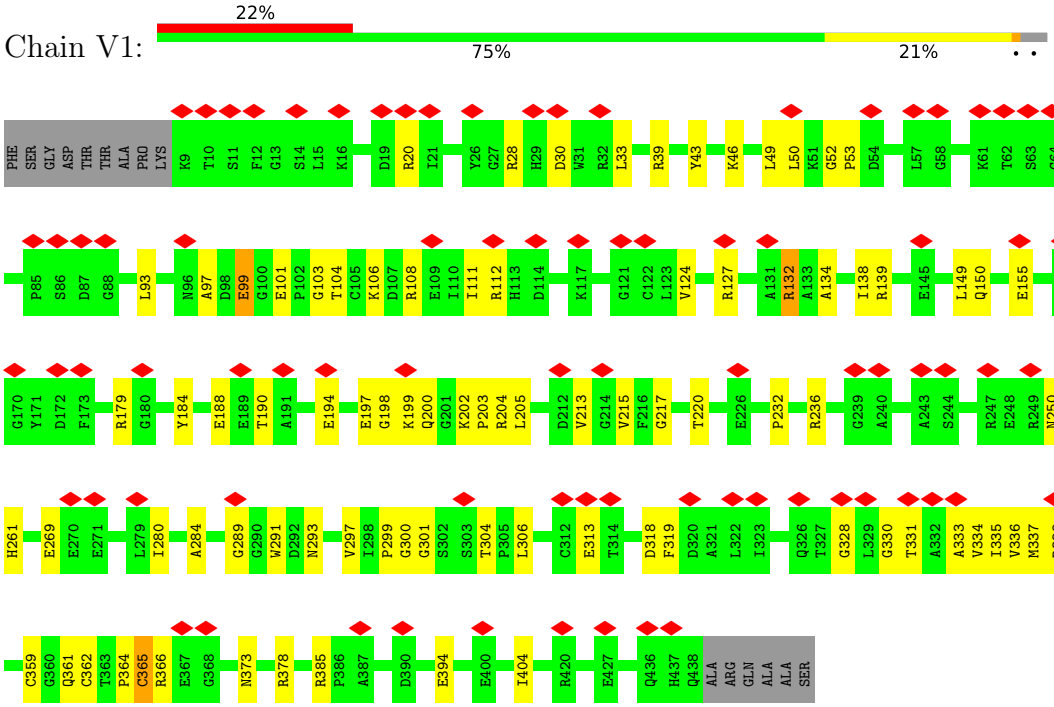
Mol	Chain	Residues	Atoms					AltConf
52	AK	1	Total	C	N	O	P	0
			28	18	1	8	1	

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.

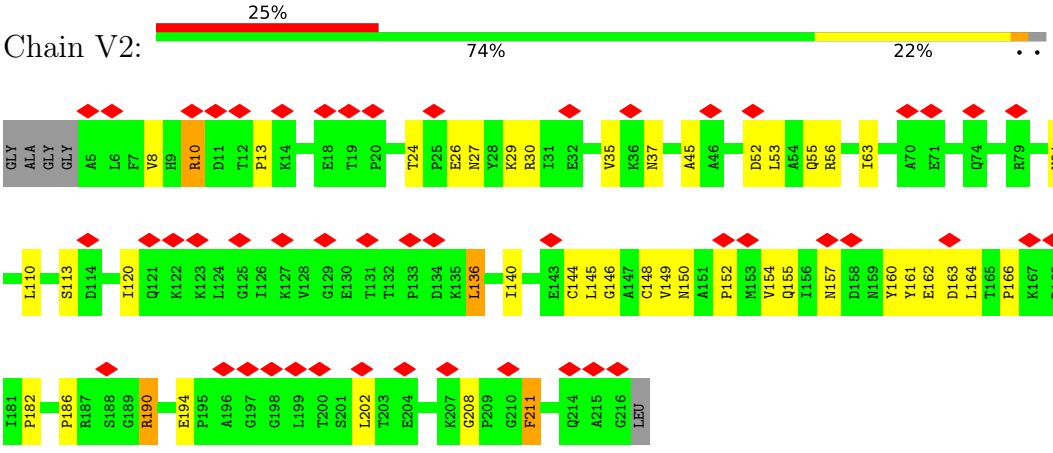
• Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain V1:



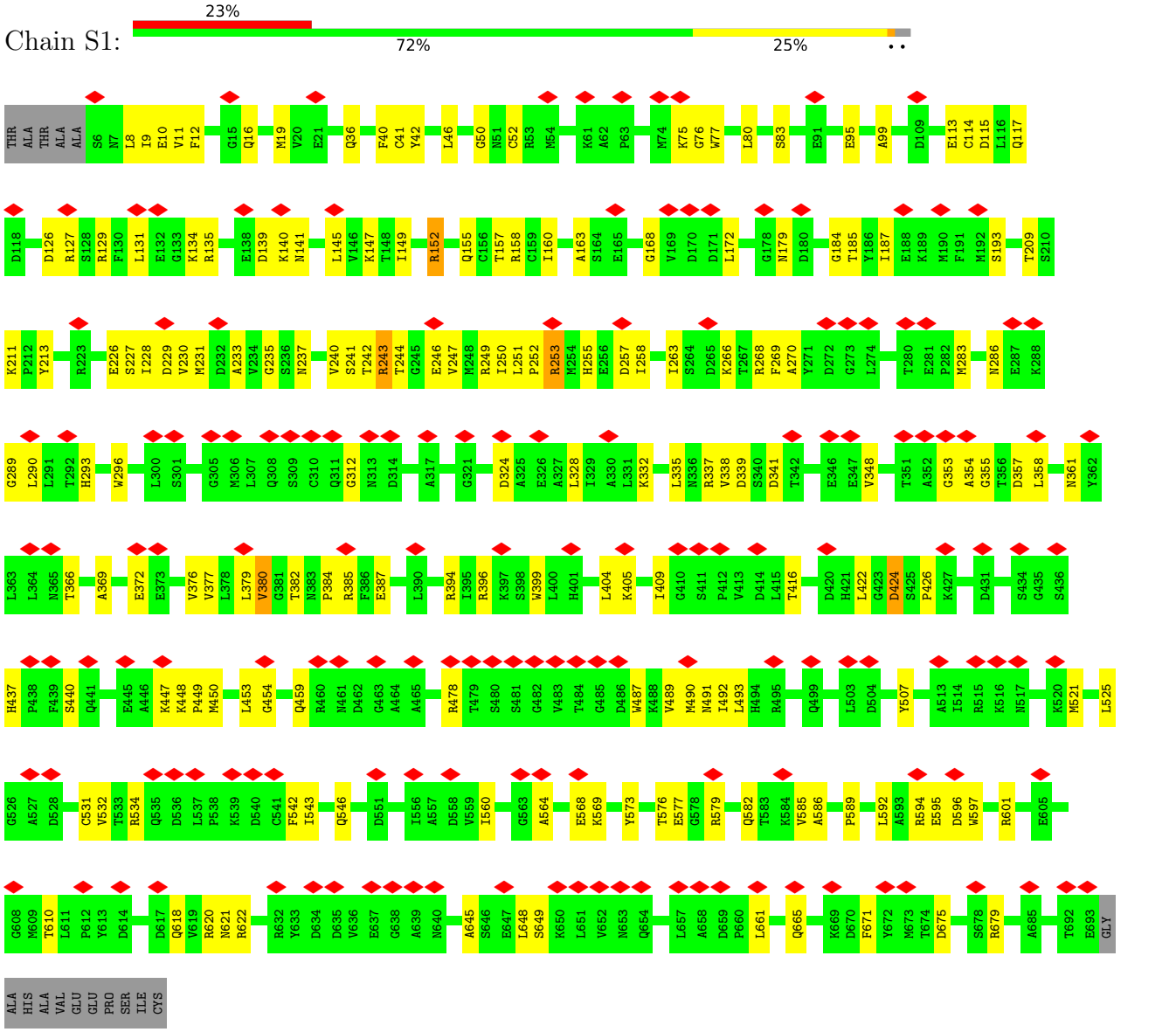
• Molecule 2: NDUFV2

Chain V2:



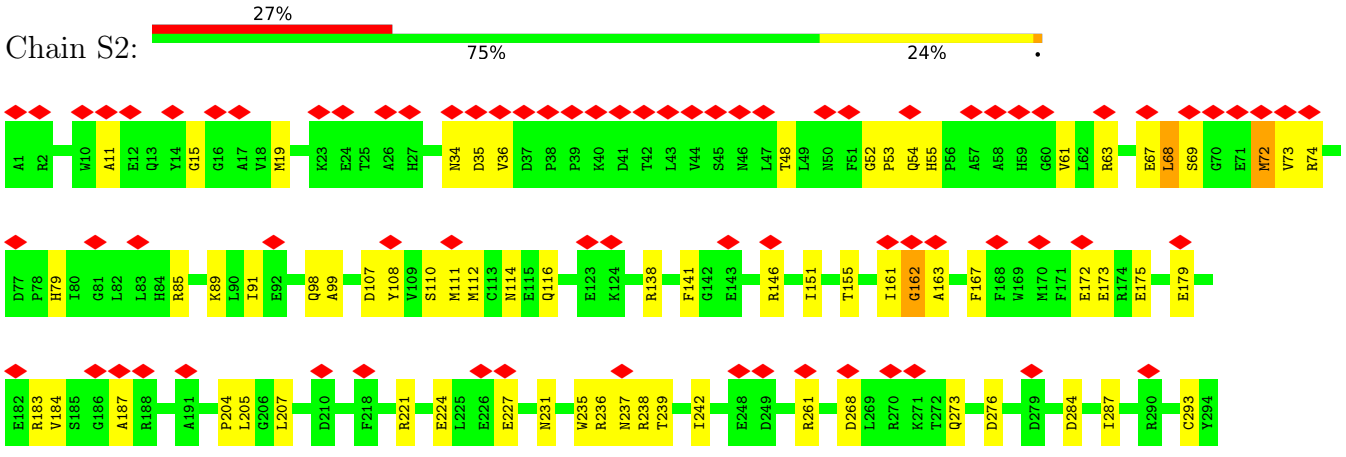
• Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

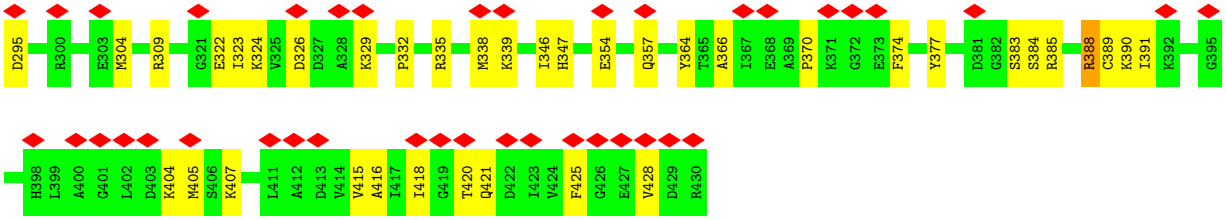
Chain S1:



• Molecule 4: NDUFS2,NADH:ubiquinone oxidoreductase core subunit S2

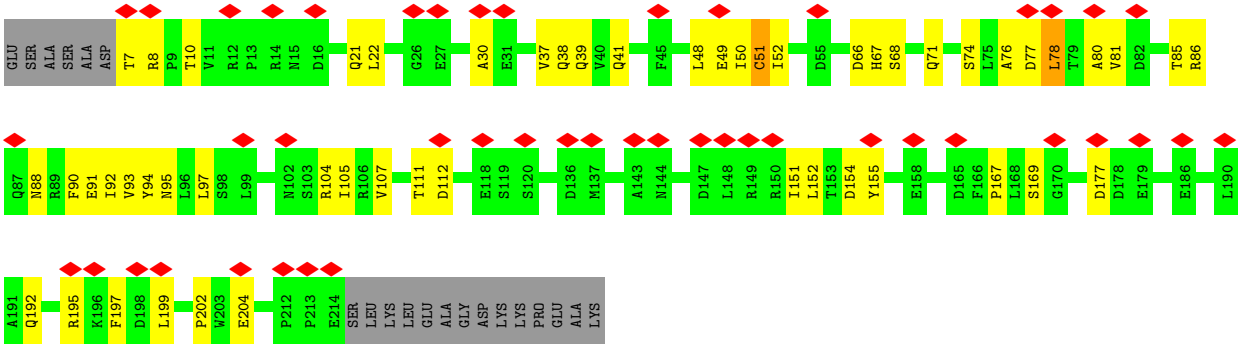
Chain S2:





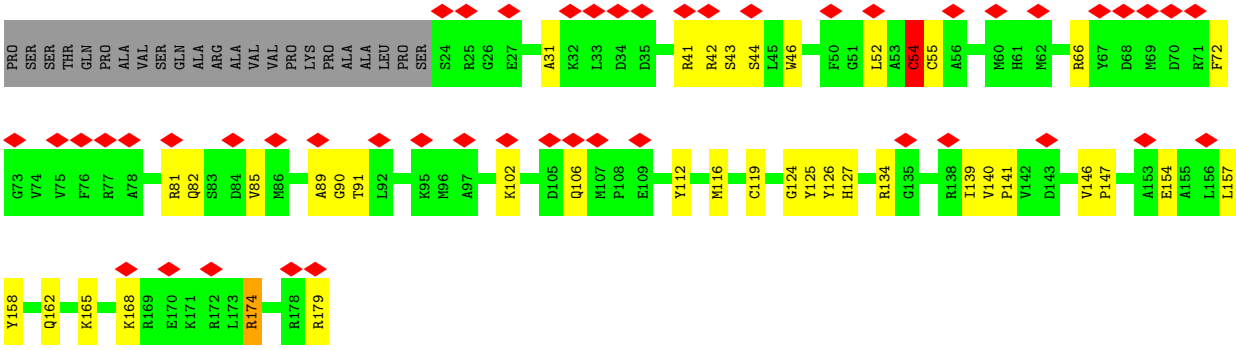
• Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3

Chain S3:



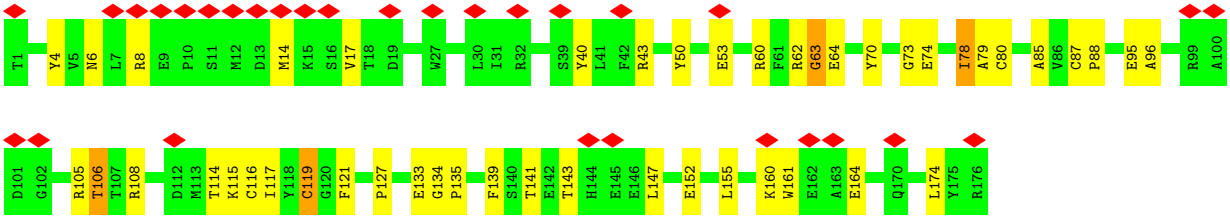
• Molecule 6: NADH:ubiquinone oxidoreductase core subunit S7,NDUFS7

Chain S7:



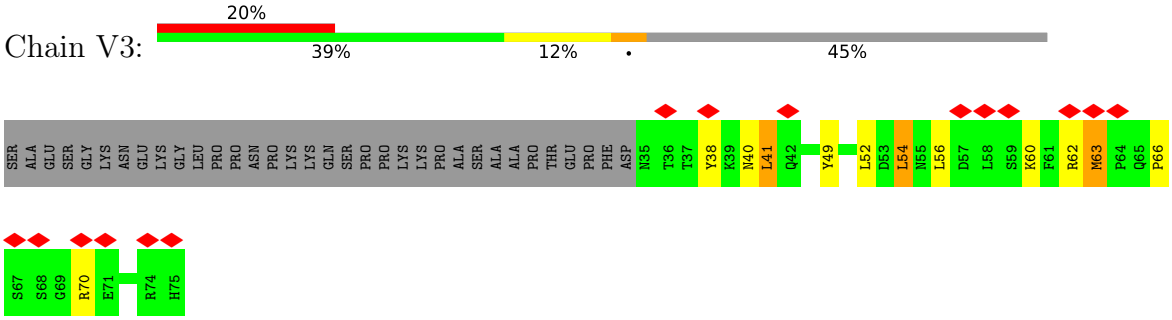
• Molecule 7: NDUFS8

Chain S8:



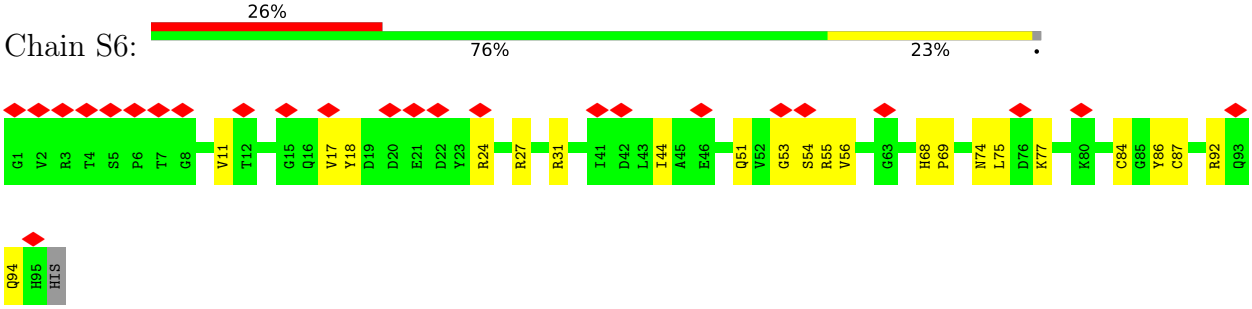
• Molecule 8: NDUFV3

Chain V3:



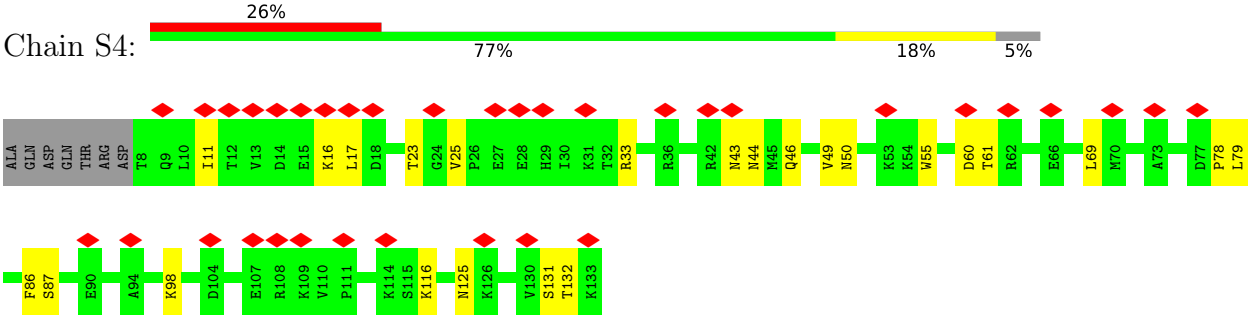
• Molecule 9: NDUFS6

Chain S6:



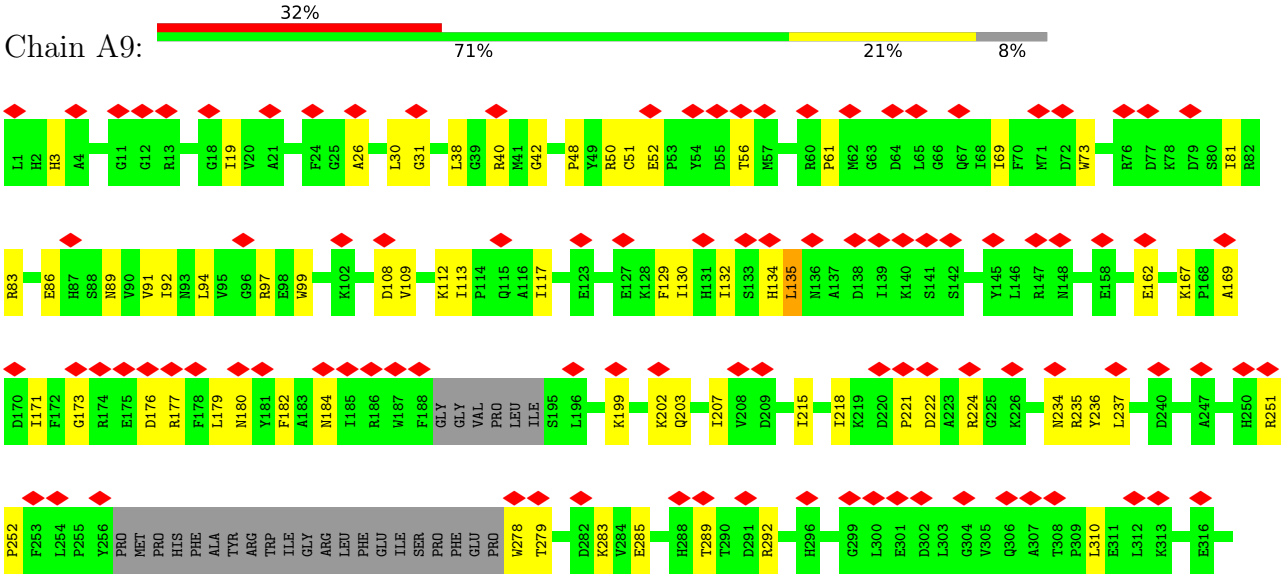
• Molecule 10: NADH:ubiquinone oxidoreductase subunit S4

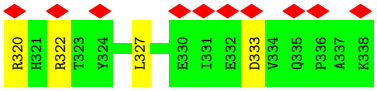
Chain S4:



• Molecule 11: NADH:ubiquinone oxidoreductase subunit A9

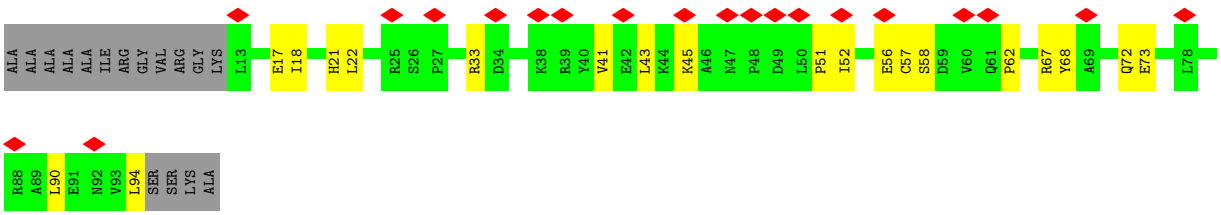
Chain A9:





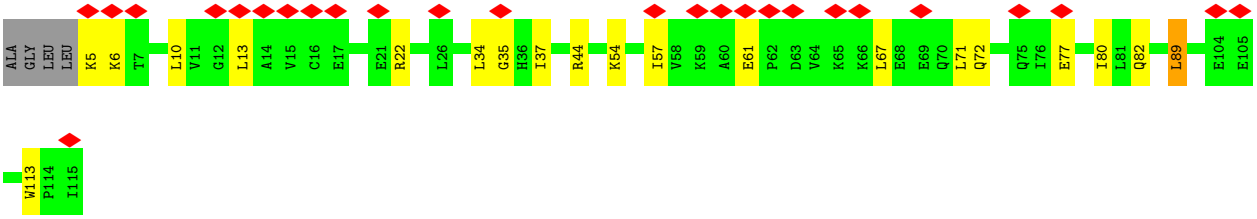
• Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain A2:



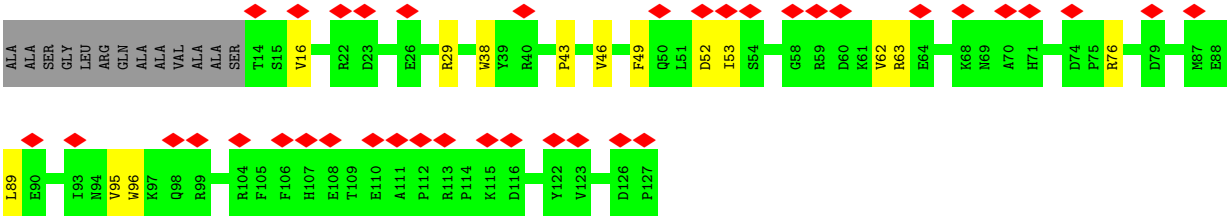
• Molecule 13: NDUFA5

Chain A5:



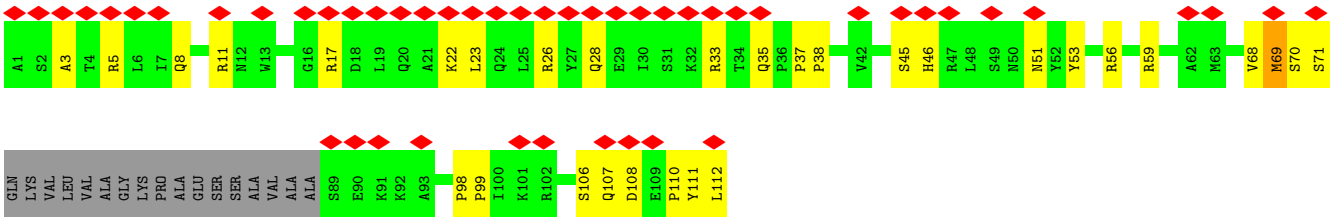
• Molecule 14: NADH:ubiquinone oxidoreductase subunit A6

Chain A6:



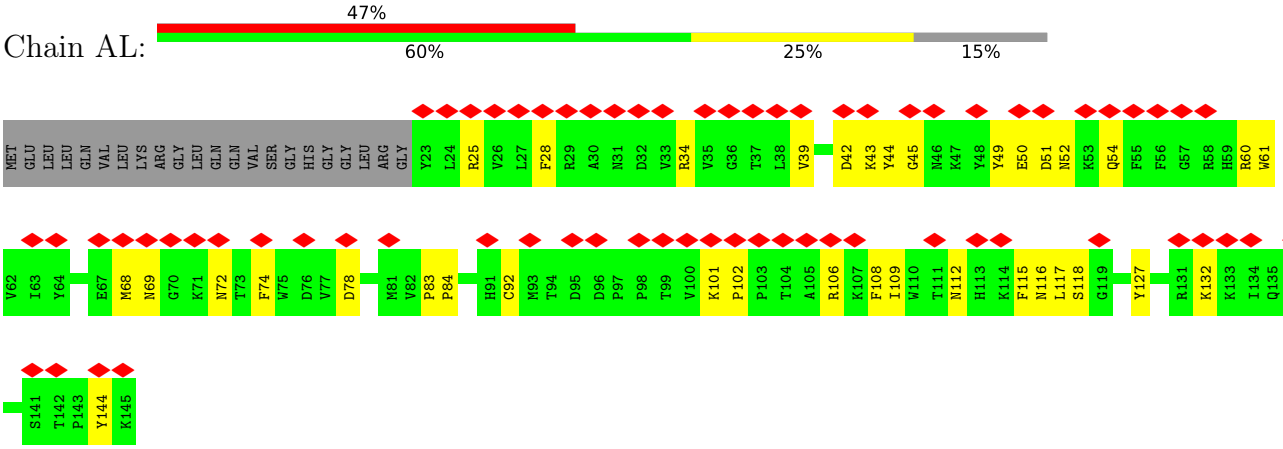
• Molecule 15: NDUFA7

Chain A7:



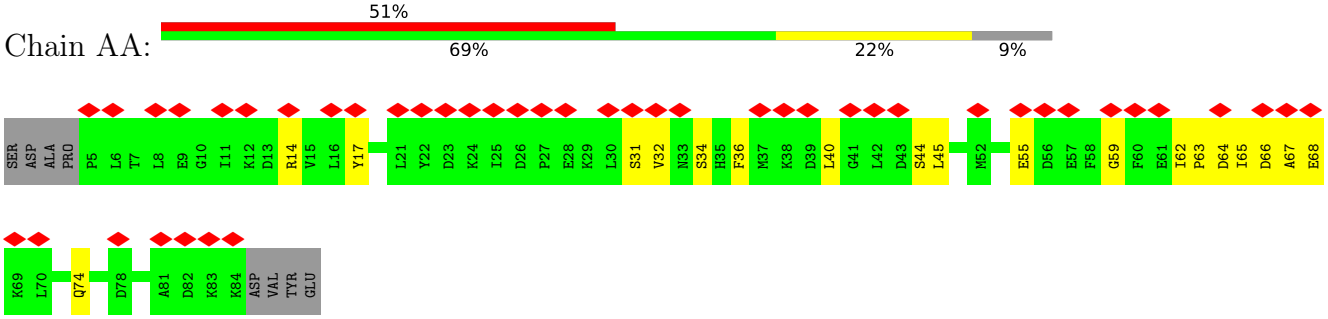
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain AL:



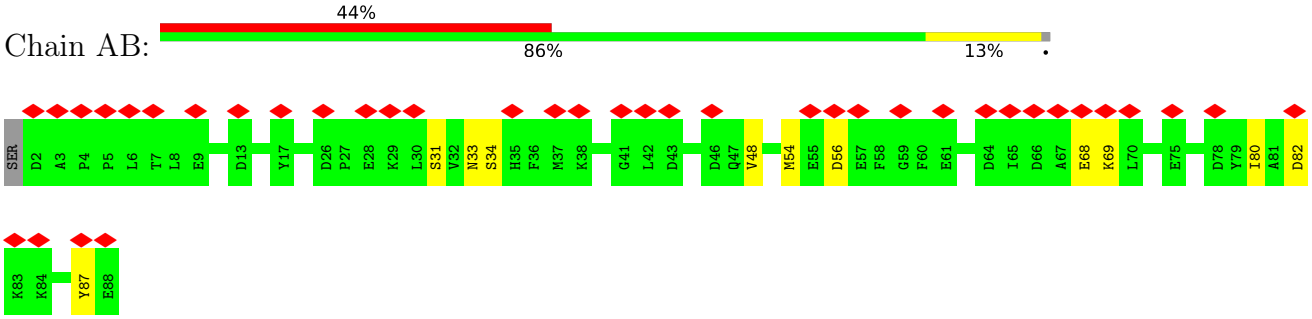
• Molecule 17: Acyl carrier protein

Chain AA:



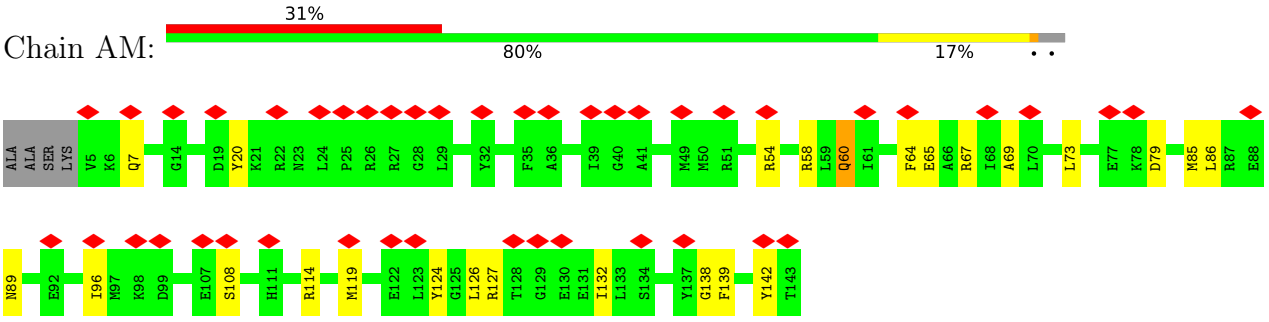
• Molecule 17: Acyl carrier protein

Chain AB:



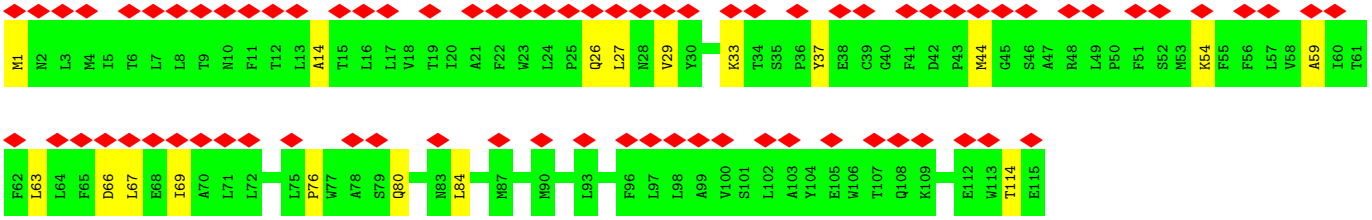
• Molecule 18: NDUFA13

Chain AM:



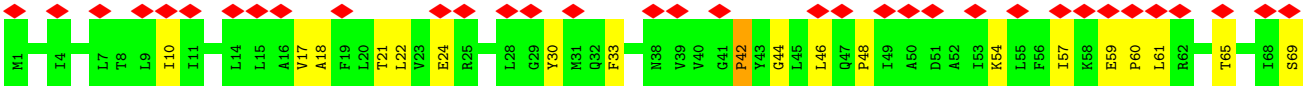
• Molecule 19: NADH-ubiquinone oxidoreductase chain 3

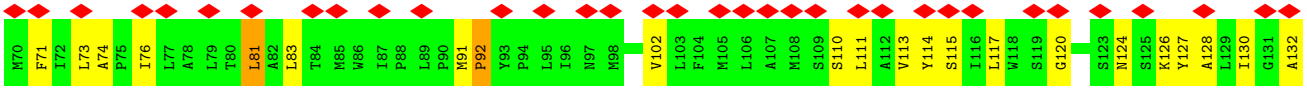
Chain D3:

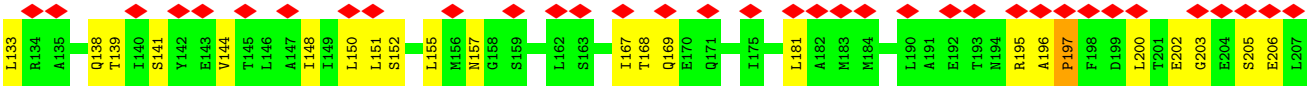


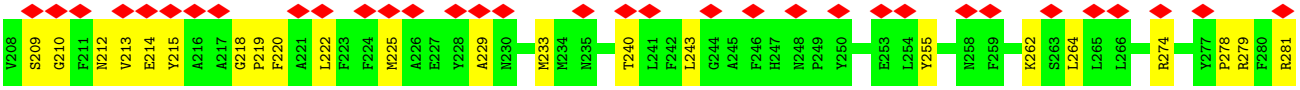
• Molecule 20: NADH-ubiquinone oxidoreductase chain 1

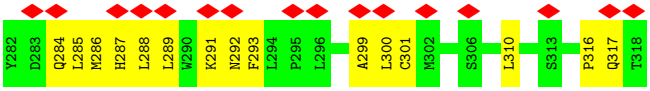
Chain D1:





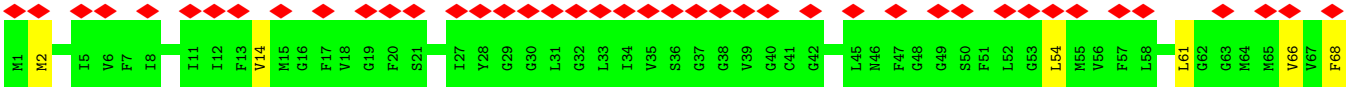


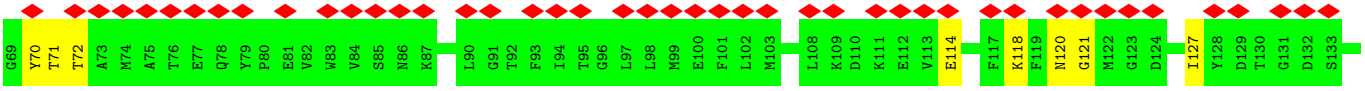


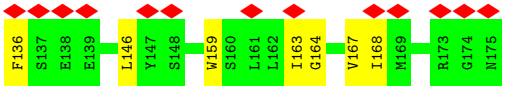


• Molecule 21: NADH-ubiquinone oxidoreductase chain 6

Chain D6:

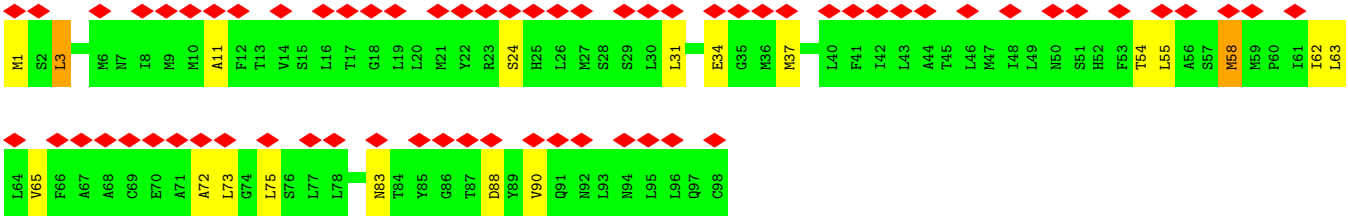






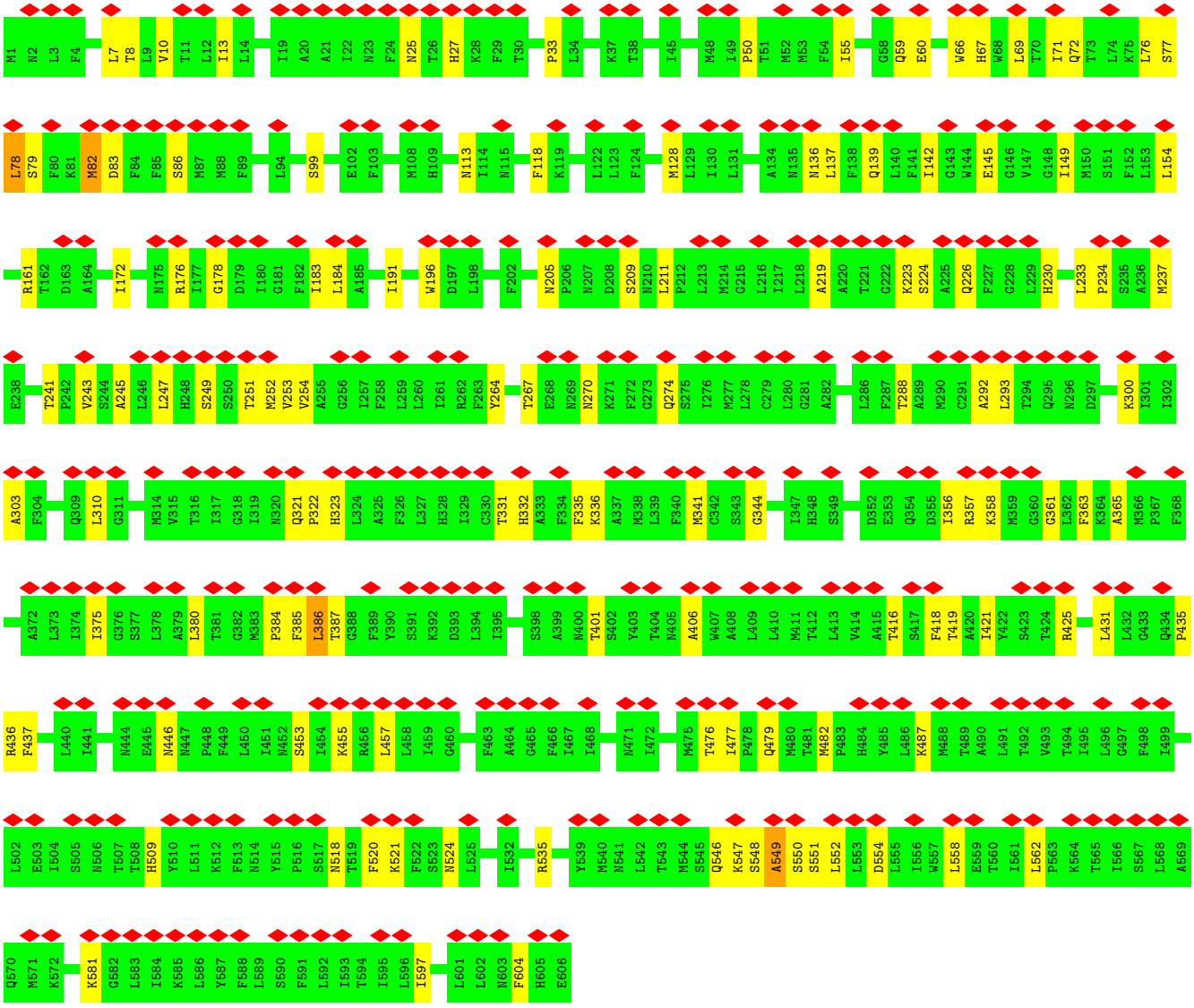
• Molecule 22: NADH-ubiquinone oxidoreductase chain 4L

Chain 4L:



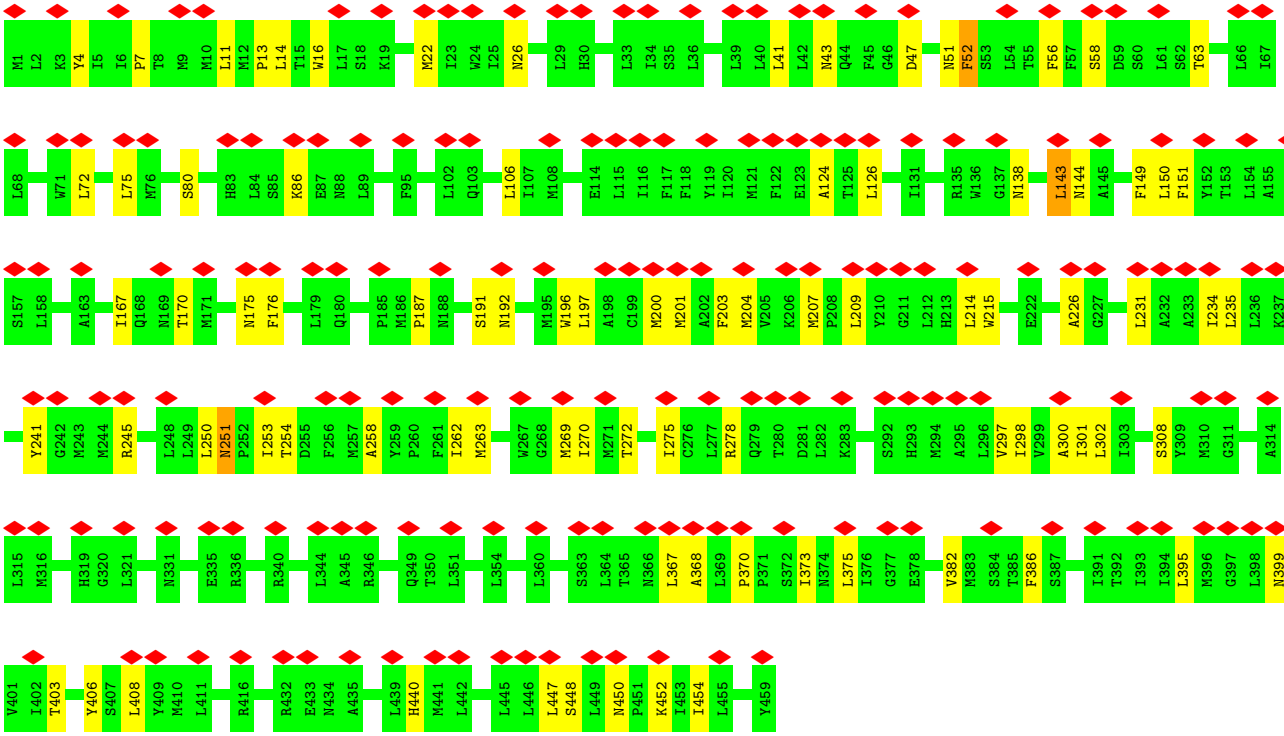
• Molecule 23: NADH-ubiquinone oxidoreductase chain 5

Chain D5:



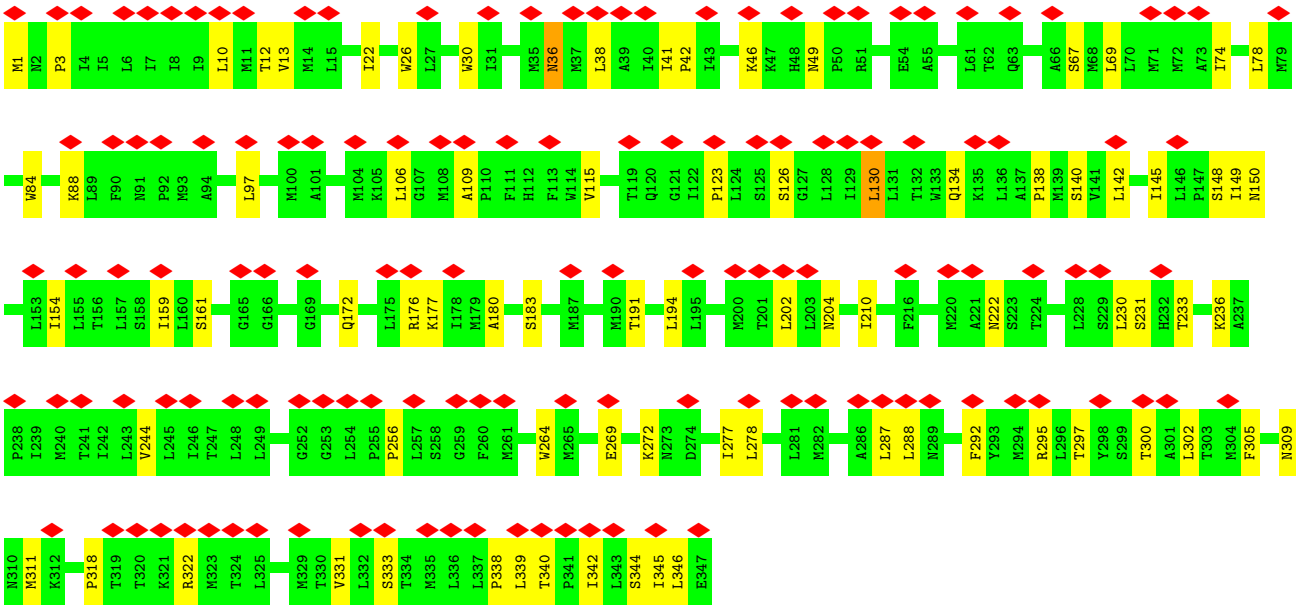
• Molecule 24: NADH-ubiquinone oxidoreductase chain 4

Chain D4:



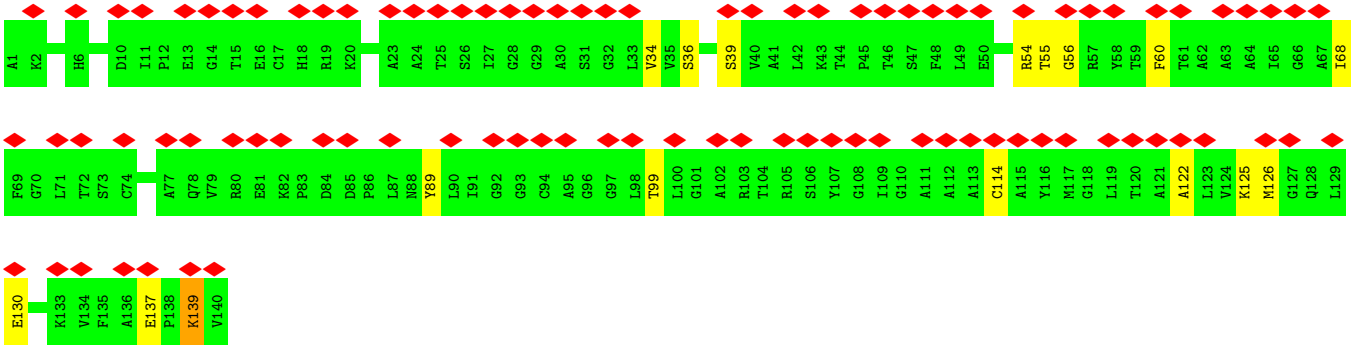
• Molecule 25: NADH-ubiquinone oxidoreductase chain 2

Chain D2:

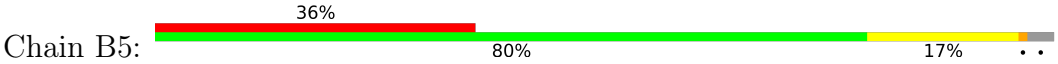


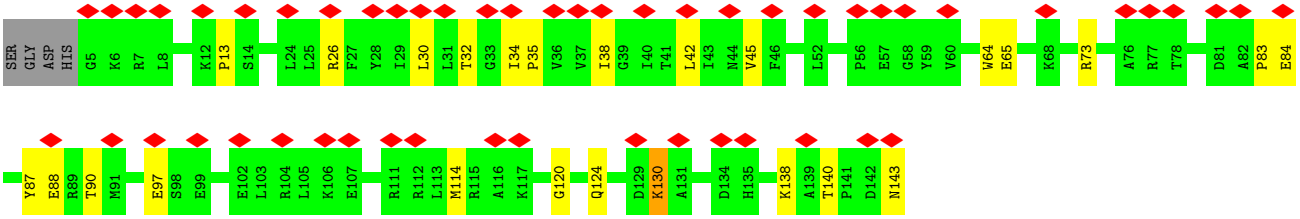
• Molecule 26: NDUFA11

Chain AK:

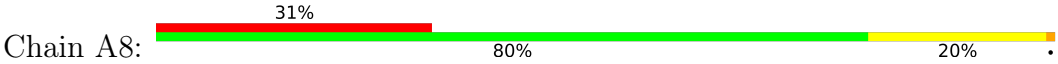


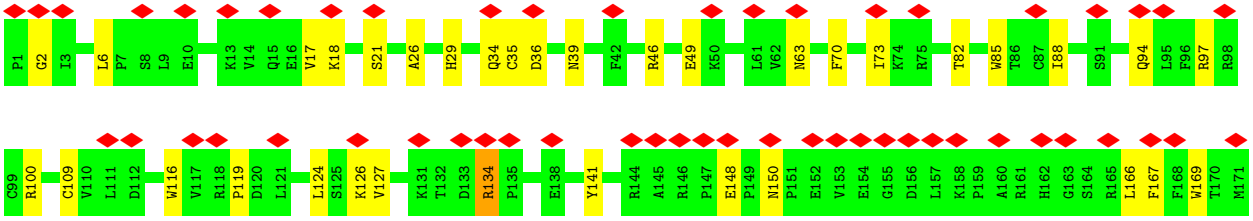
• Molecule 27: NADH:ubiquinone oxidoreductase subunit B5



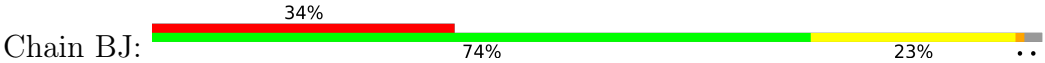


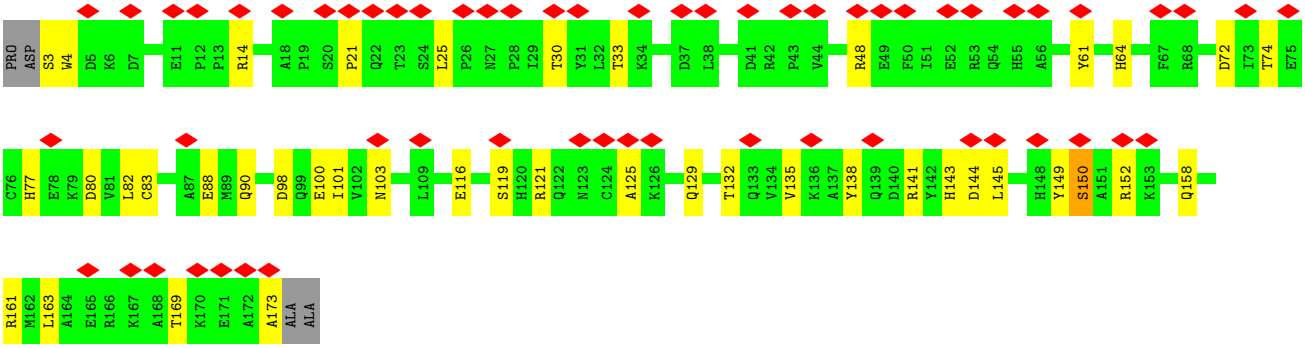
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8





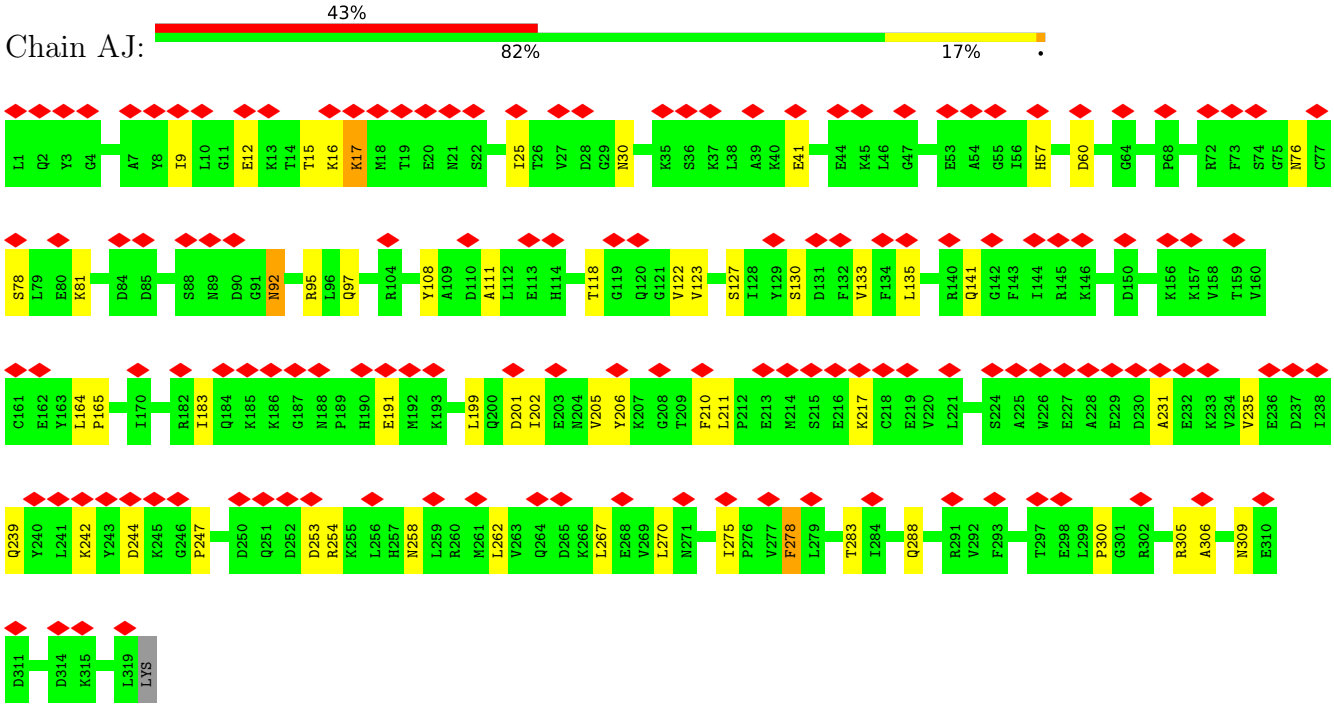
• Molecule 29: NDUFB10





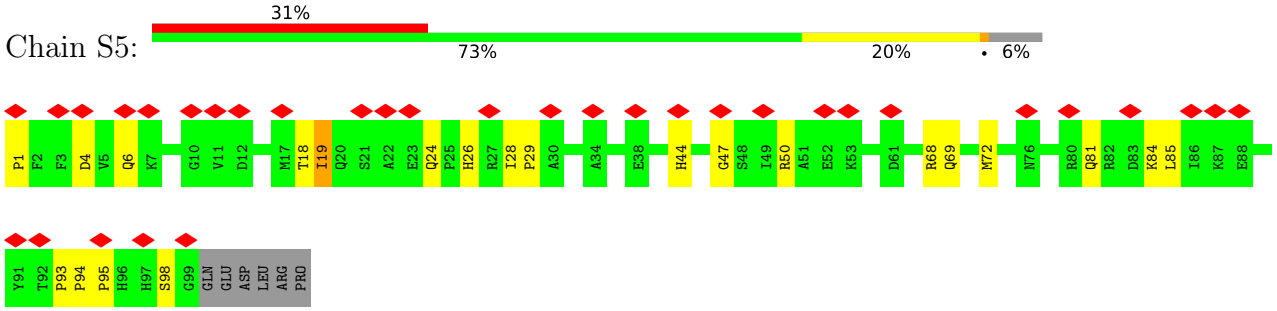
• Molecule 30: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain AJ:



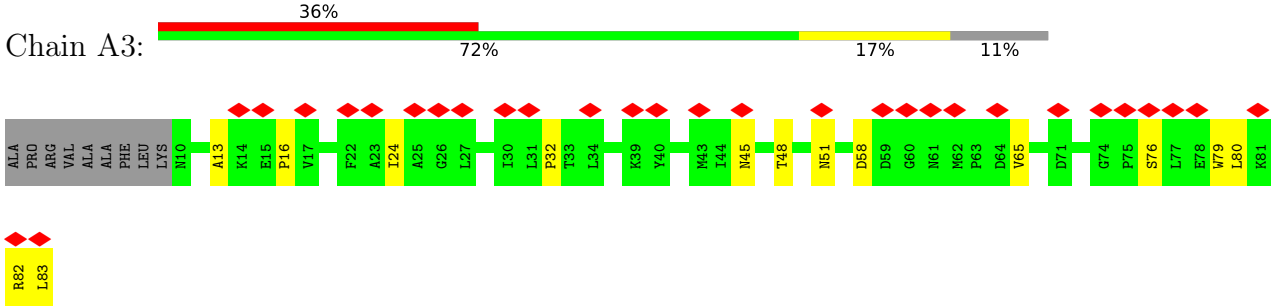
• Molecule 31: NADH:ubiquinone oxidoreductase subunit S5

Chain S5:



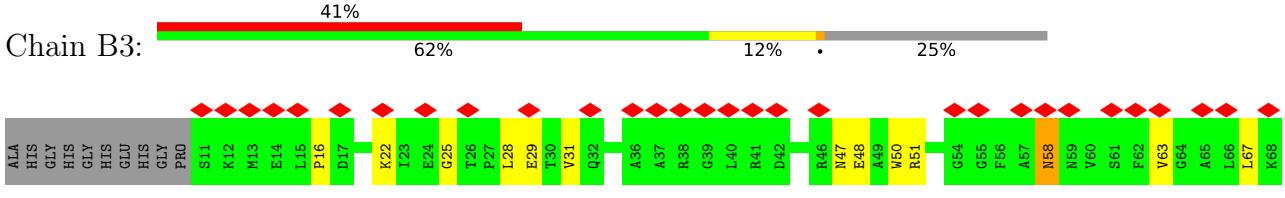
• Molecule 32: NADH:ubiquinone oxidoreductase subunit A3

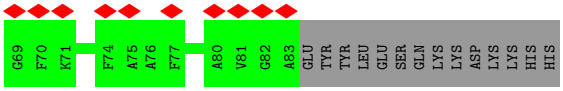
Chain A3:



• Molecule 33: NADH:ubiquinone oxidoreductase subunit B3

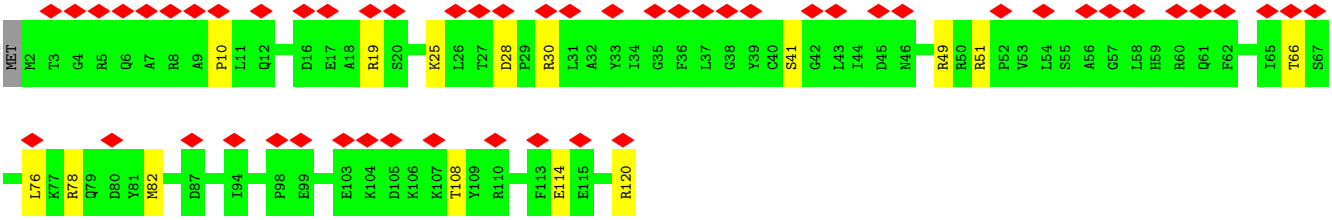
Chain B3:





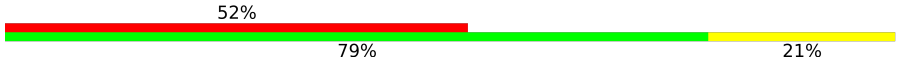
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 subunit C2

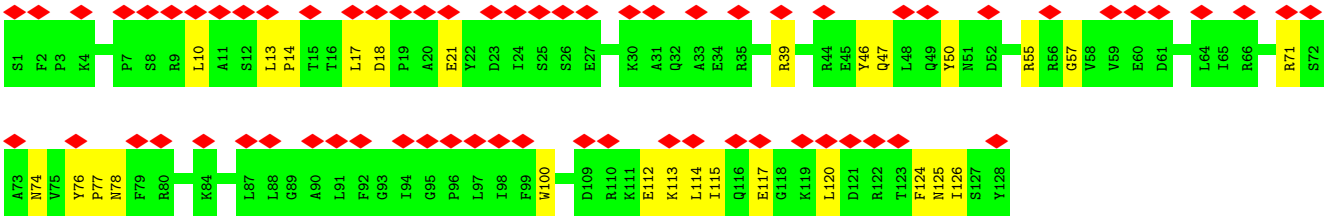
Chain C2:



• Molecule 35: NADH:ubiquinone oxidoreductase subunit B4

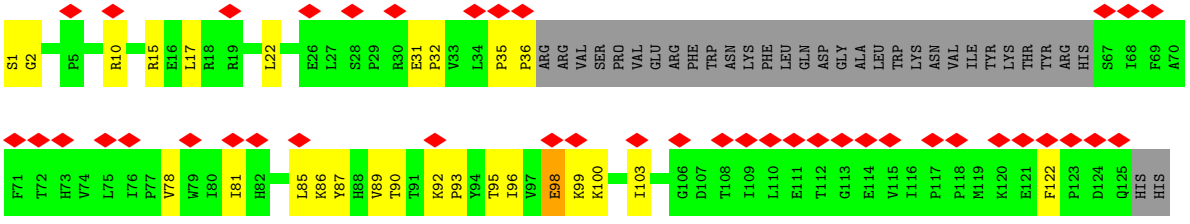
Chain B4:





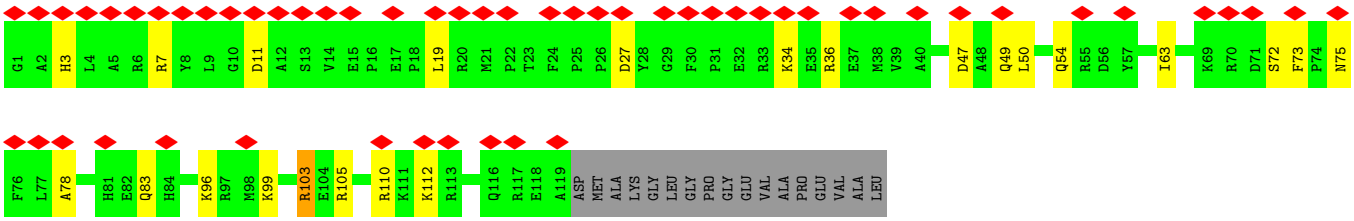
• Molecule 36: NDUFB6

Chain B6:



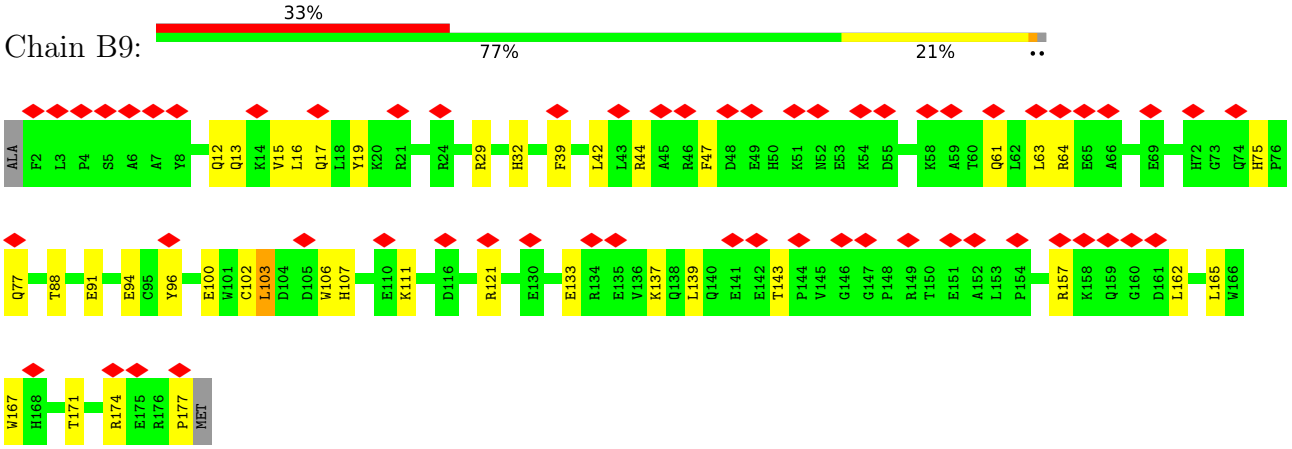
• Molecule 37: NADH:ubiquinone oxidoreductase subunit B7

Chain B7:



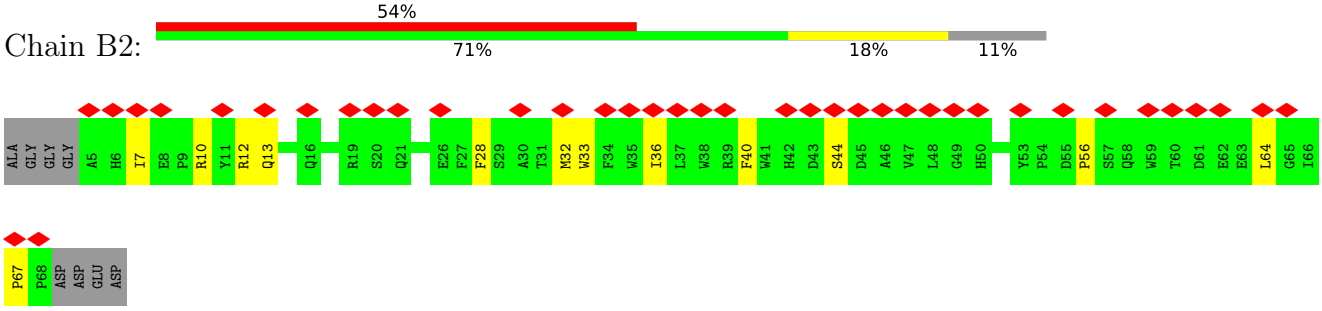
• Molecule 38: NADH:ubiquinone oxidoreductase subunit B9

Chain B9:



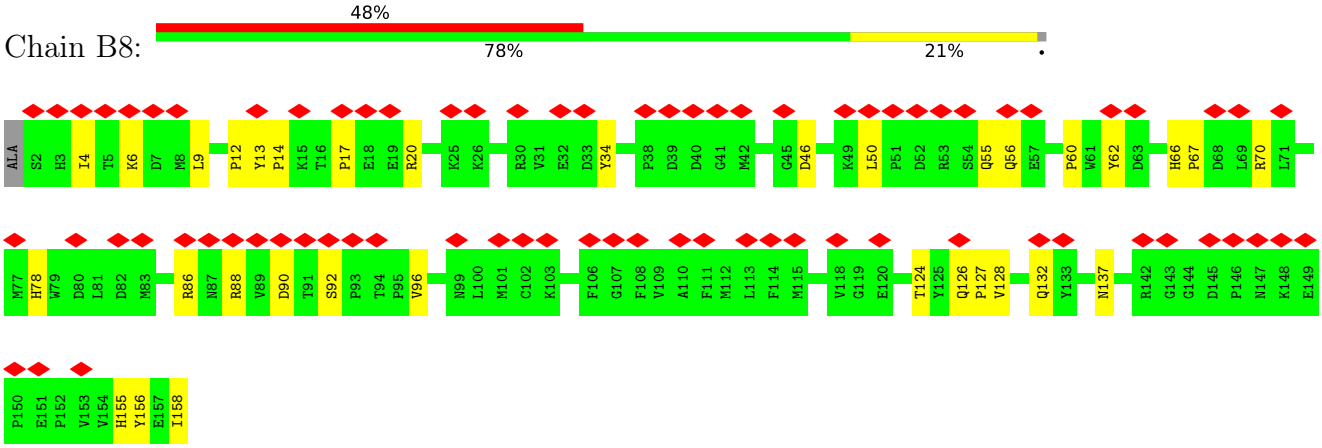
• Molecule 39: NADH:ubiquinone oxidoreductase subunit B2

Chain B2:



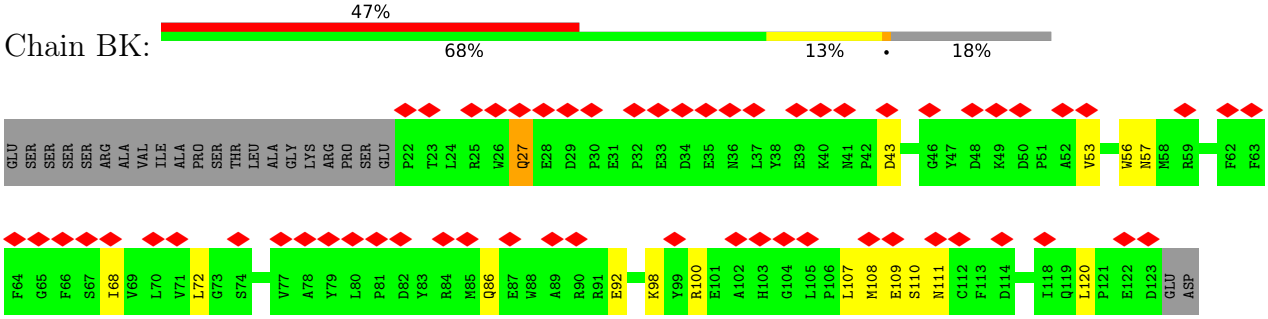
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain B8:



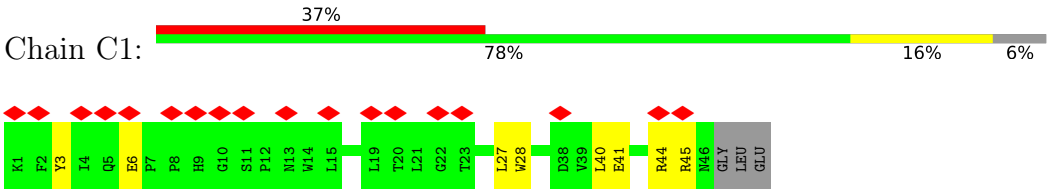
• Molecule 41: NDUFB11

Chain BK:



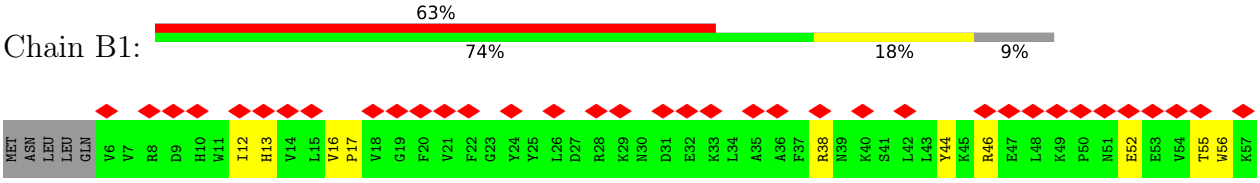
• Molecule 42: NDUFC1

Chain C1:



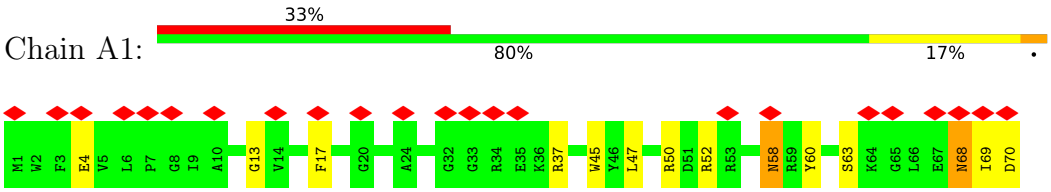
• Molecule 43: NDUFB1

Chain B1:



• Molecule 44: NDUFA1

Chain A1:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	22107	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 ($e^-/Å^2$)	51	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	100000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.214	Depositor
Minimum map value	-0.283	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	716.8, 716.8, 716.8	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	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: PC1, NDP, FMN, ZMP, 3PE, ZN, FES, SF4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	V1	0.45	0/3386	0.65	0/4575
2	V2	0.43	0/1687	0.73	1/2295 (0.0%)
3	S1	0.44	0/5362	0.66	1/7266 (0.0%)
4	S2	0.50	0/3547	0.68	1/4808 (0.0%)
5	S3	0.49	0/1776	0.65	0/2417
6	S7	0.50	0/1279	0.65	0/1728
7	S8	0.56	1/1446 (0.1%)	0.69	1/1956 (0.1%)
8	V3	0.35	0/355	0.69	1/480 (0.2%)
9	S6	0.47	0/749	0.62	0/1009
10	S4	0.43	0/1048	0.62	0/1415
11	A9	0.42	0/2574	0.67	2/3483 (0.1%)
12	A2	0.39	0/676	0.65	0/911
13	A5	0.40	0/921	0.71	2/1249 (0.2%)
14	A6	0.42	0/993	0.61	0/1336
15	A7	0.38	0/775	0.67	0/1048
16	AL	0.42	0/1084	0.66	0/1478
17	AA	0.36	0/655	0.69	0/881
17	AB	0.39	0/714	0.66	0/963
18	AM	0.42	0/1172	0.63	1/1579 (0.1%)
19	D3	0.44	0/948	0.74	0/1296
20	D1	0.48	0/2604	0.72	2/3561 (0.1%)
21	D6	0.46	0/1379	0.66	0/1868
22	4L	0.43	0/758	0.81	2/1024 (0.2%)
23	D5	0.42	0/4933	0.73	3/6710 (0.0%)
24	D4	0.45	0/3740	0.74	3/5095 (0.1%)
25	D2	0.46	0/2788	0.71	2/3795 (0.1%)
26	AK	0.37	0/1046	0.67	0/1419
27	B5	0.43	0/1189	0.60	0/1607
28	A8	0.42	0/1441	0.72	0/1942
29	BJ	0.40	0/1475	0.62	2/1989 (0.1%)
30	AJ	0.42	0/2644	0.65	1/3579 (0.0%)
31	S5	0.43	0/843	0.69	1/1128 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	A3	0.38	0/602	0.74	0/828
33	B3	0.41	0/595	0.69	0/803
34	C2	0.45	0/1028	0.61	0/1388
35	B4	0.42	0/1085	0.65	1/1467 (0.1%)
36	B6	0.42	0/830	0.72	1/1130 (0.1%)
37	B7	0.35	0/1051	0.68	2/1408 (0.1%)
38	B9	0.43	0/1568	0.63	1/2123 (0.0%)
39	B2	0.44	0/582	0.68	1/799 (0.1%)
40	B8	0.45	0/1379	0.72	1/1884 (0.1%)
41	BK	0.41	0/880	0.65	0/1196
42	C1	0.39	0/404	0.60	0/548
43	B1	0.37	0/462	0.63	0/624
44	A1	0.40	0/592	0.65	0/795
All	All	0.44	1/67045 (0.0%)	0.68	33/90883 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	V1	0	3
2	V2	0	4
3	S1	0	5
4	S2	0	2
5	S3	0	1
7	S8	0	2
10	S4	0	1
11	A9	0	2
13	A5	0	1
15	A7	0	2
16	AL	0	2
20	D1	0	5
23	D5	0	1
24	D4	0	2
28	A8	0	1
29	BJ	0	1
30	AJ	0	1
32	A3	0	1
33	B3	0	3
35	B4	0	2
36	B6	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
39	B2	0	1
40	B8	0	1
42	C1	0	1
43	B1	0	1
44	A1	0	1
All	All	0	49

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	S8	119	CYS	CB-SG	-5.61	1.72	1.81

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D5	69	LEU	CA-CB-CG	8.46	134.75	115.30
13	A5	89	LEU	CA-CB-CG	7.84	133.33	115.30
2	V2	136	LEU	CA-CB-CG	7.63	132.84	115.30
37	B7	19	LEU	CA-CB-CG	7.57	132.70	115.30
23	D5	78	LEU	CA-CB-CG	7.26	132.00	115.30
11	A9	222	ASP	CB-CG-OD1	6.92	124.53	118.30
13	A5	89	LEU	CB-CG-CD2	-6.87	99.32	111.00
37	B7	27	ASP	CB-CG-OD1	6.73	124.35	118.30
24	D4	126	LEU	CA-CB-CG	6.30	129.79	115.30
18	AM	126	LEU	CA-CB-CG	6.10	129.33	115.30
35	B4	17	LEU	CA-CB-CG	6.04	129.19	115.30
22	4L	31	LEU	CA-CB-CG	5.90	128.88	115.30
7	S8	78	ILE	CG1-CB-CG2	-5.89	98.44	111.40
29	BJ	21	PRO	C-N-CA	5.88	136.40	121.70
20	D1	81	LEU	CA-CB-CG	-5.82	101.91	115.30
25	D2	130	LEU	CA-CB-CG	5.69	128.39	115.30
38	B9	103	LEU	CA-CB-CG	5.67	128.34	115.30
39	B2	44	SER	C-N-CA	5.58	135.66	121.70
8	V3	41	LEU	CA-CB-CG	5.57	128.11	115.30
36	B6	96	ILE	CG1-CB-CG2	-5.57	99.15	111.40
3	S1	424	ASP	CB-CG-OD1	5.50	123.25	118.30
40	B8	86	ARG	C-N-CA	5.41	135.23	121.70
31	S5	19	ILE	CG1-CB-CG2	-5.38	99.57	111.40
23	D5	386	LEU	CA-CB-CG	5.32	127.53	115.30
24	D4	150	LEU	CA-CB-CG	5.31	127.52	115.30
30	AJ	275	ILE	C-N-CD	-5.17	109.23	120.60
11	A9	135	LEU	CA-CB-CG	5.16	127.17	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D4	143	LEU	CA-CB-CG	5.14	127.12	115.30
22	4L	63	LEU	CA-CB-CG	5.06	126.93	115.30
20	D1	148	ILE	CG1-CB-CG2	-5.05	100.30	111.40
29	BJ	25	LEU	C-N-CD	-5.04	109.52	120.60
4	S2	72	MET	C-N-CA	5.02	134.24	121.70
25	D2	287	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (49) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	A1	63	SER	Peptide
32	A3	58	ASP	Peptide
13	A5	113	TRP	Peptide
15	A7	68	VAL	Peptide
15	A7	69	MET	Peptide
28	A8	18	LYS	Peptide
11	A9	221	PRO	Peptide
11	A9	310	LEU	Peptide
30	AJ	278	PHE	Peptide
16	AL	102	PRO	Peptide
16	AL	43	LYS	Peptide
43	B1	52	GLU	Peptide
39	B2	56	PRO	Peptide
33	B3	16	PRO	Peptide
33	B3	22	LYS	Peptide
33	B3	58	ASN	Peptide
35	B4	21	GLU	Peptide
35	B4	76	TYR	Peptide
36	B6	122	PHE	Peptide
36	B6	98	GLU	Peptide
40	B8	56	GLN	Peptide
29	BJ	150	SER	Peptide
42	C1	6	GLU	Peptide
20	D1	293	PHE	Peptide
20	D1	42	PRO	Peptide
20	D1	44	GLY	Peptide
20	D1	57	ILE	Peptide
20	D1	91	MET	Peptide
24	D4	367	LEU	Peptide
24	D4	52	PHE	Peptide
23	D5	365	ALA	Peptide

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Mol	Chain	Res	Type	Group
3	S1	141	ASN	Peptide
3	S1	213	TYR	Peptide
3	S1	243	ARG	Peptide
3	S1	253	ARG	Peptide
3	S1	380	VAL	Peptide
4	S2	162	GLY	Peptide
4	S2	68	LEU	Peptide
5	S3	51	CYS	Peptide
10	S4	11	ILE	Peptide
7	S8	106	THR	Peptide
7	S8	63	GLY	Peptide
1	V1	28	ARG	Peptide
1	V1	331	THR	Peptide
1	V1	99	GLU	Peptide
2	V2	10	ARG	Peptide
2	V2	13	PRO	Peptide
2	V2	211	PHE	Peptide
2	V2	35	VAL	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	V1	3312	0	3266	68	0
2	V2	1647	0	1657	37	0
3	S1	5275	0	5300	121	0
4	S2	3455	0	3395	84	0
5	S3	1726	0	1676	48	0
6	S7	1248	0	1256	30	0
7	S8	1415	0	1371	41	0
8	V3	345	0	323	9	0
9	S6	737	0	710	16	0
10	S4	1025	0	1023	18	0
11	A9	2512	0	2527	43	0
12	A2	665	0	678	12	0
13	A5	901	0	936	17	0
14	A6	969	0	980	10	0
15	A7	757	0	771	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	AL	1044	0	1001	22	0
17	AA	645	0	649	10	0
17	AB	702	0	692	7	0
18	AM	1143	0	1137	21	0
19	D3	923	0	952	19	0
20	D1	2529	0	2641	65	0
21	D6	1345	0	1364	20	0
22	4L	748	0	794	18	0
23	D5	4805	0	4950	97	0
24	D4	3646	0	3850	59	0
25	D2	2724	0	2930	56	0
26	AK	1025	0	1033	10	0
27	B5	1156	0	1177	18	0
28	A8	1404	0	1384	25	0
29	BJ	1441	0	1417	29	0
30	AJ	2583	0	2547	36	0
31	S5	822	0	820	21	0
32	A3	582	0	583	12	0
33	B3	578	0	570	6	0
34	C2	997	0	983	13	0
35	B4	1059	0	1062	16	0
36	B6	804	0	824	20	0
37	B7	1026	0	995	18	0
38	B9	1515	0	1469	26	0
39	B2	555	0	505	9	0
40	B8	1324	0	1219	22	0
41	BK	853	0	800	13	0
42	C1	391	0	391	6	0
43	B1	449	0	453	8	0
44	A1	577	0	570	9	0
45	S1	16	0	0	1	0
45	S7	8	0	0	0	0
45	S8	16	0	0	1	0
45	V1	8	0	0	1	0
46	V1	31	0	19	4	0
47	S1	4	0	0	0	0
47	V2	4	0	0	1	0
48	D5	38	0	50	1	0
48	S2	40	0	54	3	0
49	S6	1	0	0	0	0
50	A9	48	0	26	4	0
51	AA	34	0	40	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	AB	31	0	34	1	0
52	AK	28	0	30	1	0
All	All	65691	0	65884	1025	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 (1025) 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:S3:80:ALA:HA	5:S3:91:GLU:O	1.19	1.26
5:S3:78:LEU:HA	5:S3:93:VAL:O	1.34	1.21
5:S3:38:GLN:O	15:A7:70:SER:HA	1.41	1.20
3:S1:449:PRO:O	3:S1:489:VAL:HA	1.51	1.11
12:A2:21:HIS:O	12:A2:62:PRO:HA	1.66	0.95
5:S3:38:GLN:O	15:A7:70:SER:CA	2.19	0.90
5:S3:38:GLN:HA	15:A7:70:SER:O	1.80	0.81
23:D5:554:ASP:O	23:D5:558:LEU:HB2	1.82	0.80
5:S3:80:ALA:CA	5:S3:91:GLU:O	2.16	0.80
3:S1:242:THR:HA	3:S1:247:VAL:O	1.83	0.78
3:S1:675:ASP:O	3:S1:679:ARG:HB2	1.84	0.76
31:S5:26:HIS:HB3	32:A3:51:ASN:HD21	1.54	0.73
6:S7:52:LEU:HB2	6:S7:90:GLY:HA3	1.71	0.72
25:D2:88:LYS:HG3	25:D2:148:SER:HB3	1.71	0.72
38:B9:133:GLU:O	38:B9:137:LYS:HB2	1.90	0.72
3:S1:36:GLN:HE22	10:S4:49:VAL:H	1.37	0.71
48:S2:501:3PE:H291	25:D2:288:LEU:HD23	1.72	0.71
12:A2:22:LEU:HB2	12:A2:56:GLU:HG2	1.71	0.71
12:A2:68:TYR:O	12:A2:72:GLN:HB2	1.89	0.71
23:D5:547:LYS:O	23:D5:552:LEU:HB2	1.89	0.71
20:D1:229:ALA:O	20:D1:233:MET:HB2	1.90	0.71
18:AM:138:GLY:O	18:AM:142:TYR:HB3	1.90	0.70
33:B3:25:GLY:O	33:B3:29:GLU:HB2	1.92	0.70
5:S3:78:LEU:CA	5:S3:93:VAL:O	2.28	0.70
5:S3:192:GLN:HE21	5:S3:195:ARG:HH12	1.39	0.69
19:D3:14:ALA:HB1	20:D1:76:ILE:HD12	1.74	0.69
35:B4:46:TYR:O	35:B4:50:TYR:HB2	1.93	0.69
15:A7:106:SER:HB3	15:A7:110:PRO:HB3	1.76	0.68
7:S8:43:ARG:NH1	15:A7:23:LEU:O	2.27	0.68
3:S1:113:GLU:HA	10:S4:46:GLN:HE21	1.57	0.68
3:S1:283:MET:HB2	3:S1:560:ILE:HB	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:AJ:111:ALA:HB1	30:AJ:122:VAL:HG21	1.77	0.67
4:S2:63:ARG:HB3	4:S2:79:HIS:O	1.93	0.67
40:B8:13:TYR:HB2	40:B8:20:ARG:HE	1.59	0.67
19:D3:80:GLN:HA	32:A3:45:ASN:HD21	1.60	0.66
19:D3:67:LEU:HB3	22:4L:65:VAL:HG23	1.77	0.66
23:D5:482:MET:SD	23:D5:487:LYS:NZ	2.68	0.66
24:D4:231:LEU:O	24:D4:235:LEU:HB2	1.95	0.66
5:S3:78:LEU:HA	5:S3:93:VAL:C	2.13	0.66
11:A9:51:CYS:SG	11:A9:52:GLU:N	2.68	0.66
17:AB:31:SER:HB3	17:AB:34:SER:HB2	1.78	0.66
31:S5:18:THR:HG22	31:S5:19:ILE:HG13	1.78	0.65
9:S6:68:HIS:HE1	9:S6:87:CYS:SG	2.14	0.65
3:S1:117:GLN:NE2	45:S1:801:SF4:S3	2.70	0.65
5:S3:80:ALA:HA	5:S3:91:GLU:C	2.14	0.65
2:V2:154:VAL:HB	2:V2:161:TYR:HB2	1.80	0.64
3:S1:250:ILE:HD11	3:S1:268:ARG:HA	1.79	0.64
12:A2:41:VAL:O	12:A2:45:LYS:HB2	1.97	0.64
19:D3:37:TYR:HB3	20:D1:214:GLU:HG2	1.80	0.64
23:D5:137:LEU:HB3	23:D5:196:TRP:HB2	1.79	0.64
23:D5:161:ARG:NH1	38:B9:88:THR:O	2.29	0.64
17:AA:64:ASP:O	17:AA:68:GLU:HB2	1.98	0.63
25:D2:130:LEU:O	25:D2:134:GLN:HB2	1.98	0.63
20:D1:203:GLY:HA2	20:D1:209:SER:HA	1.79	0.63
29:BJ:125:ALA:O	29:BJ:129:GLN:HB2	1.97	0.63
10:S4:78:PRO:HG2	10:S4:79:LEU:HG	1.79	0.63
20:D1:152:SER:OG	20:D1:301:CYS:SG	2.55	0.63
22:4L:1:MET:N	31:S5:72:MET:SD	2.72	0.63
24:D4:175:ASN:ND2	27:B5:97:GLU:OE1	2.32	0.63
20:D1:65:THR:OG1	20:D1:124:ASN:ND2	2.32	0.62
3:S1:8:LEU:HB3	3:S1:19:MET:HB3	1.81	0.62
21:D6:159:TRP:HE1	25:D2:12:THR:HG22	1.64	0.62
23:D5:293:LEU:HA	23:D5:425:ARG:HH22	1.63	0.62
4:S2:416:ALA:O	4:S2:420:THR:HB	1.99	0.62
30:AJ:306:ALA:HA	30:AJ:309:ASN:HB2	1.81	0.62
20:D1:22:LEU:HB2	20:D1:48:PRO:HG2	1.81	0.62
4:S2:388:ARG:NH1	4:S2:389:CYS:O	2.30	0.62
21:D6:14:VAL:HG22	22:4L:11:ALA:HB2	1.82	0.62
39:B2:36:ILE:O	39:B2:40:PHE:HB2	1.99	0.62
11:A9:199:LYS:HG2	11:A9:237:LEU:HD11	1.81	0.62
7:S8:64:GLU:H	7:S8:134:GLY:H	1.46	0.62
23:D5:82:MET:SD	23:D5:82:MET:N	2.72	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BJ:141:ARG:NH1	41:BK:109:GLU:O	2.33	0.61
20:D1:114:TYR:OH	21:D6:61:LEU:O	2.19	0.61
17:AB:82:ASP:OD1	36:B6:15:ARG:NH2	2.33	0.61
7:S8:74:GLU:OE1	7:S8:105:ARG:NH2	2.32	0.61
11:A9:176:ASP:O	11:A9:180:ASN:ND2	2.33	0.61
24:D4:197:LEU:O	24:D4:201:MET:HB2	2.00	0.61
35:B4:55:ARG:NH1	35:B4:57:GLY:O	2.34	0.61
1:V1:289:GLY:HA3	1:V1:293:ASN:HD22	1.64	0.61
4:S2:425:PHE:HA	4:S2:428:VAL:HB	1.82	0.61
12:A2:57:CYS:SG	12:A2:58:SER:N	2.71	0.61
24:D4:250:LEU:HB3	24:D4:253:ILE:HD11	1.83	0.61
24:D4:251:ASN:OD1	24:D4:251:ASN:N	2.27	0.61
4:S2:108:TYR:HB2	6:S7:54:CYS:HB3	1.82	0.61
11:A9:92:ILE:HG22	11:A9:130:ILE:HB	1.83	0.61
16:AL:51:ASP:OD2	16:AL:54:GLN:NE2	2.34	0.61
24:D4:51:ASN:HD22	27:B5:90:THR:HG22	1.66	0.61
36:B6:100:LYS:HB3	37:B7:49:GLN:HE22	1.65	0.61
4:S2:237:ASN:O	20:D1:284:GLN:NE2	2.34	0.60
25:D2:233:THR:HA	25:D2:236:LYS:HG2	1.83	0.60
15:A7:8:GLN:HA	15:A7:11:ARG:HE	1.65	0.60
13:A5:34:LEU:O	13:A5:44:ARG:NH1	2.34	0.60
23:D5:363:PHE:HB2	23:D5:431:LEU:HB3	1.83	0.60
2:V2:144:CYS:SG	2:V2:145:LEU:N	2.75	0.60
3:S1:592:LEU:O	3:S1:594:ARG:NH1	2.35	0.60
37:B7:72:SER:HB2	37:B7:75:ASN:HD22	1.66	0.60
2:V2:144:CYS:SG	2:V2:146:GLY:N	2.74	0.60
25:D2:202:LEU:HB3	25:D2:346:LEU:HD21	1.84	0.60
4:S2:48:THR:HG22	4:S2:67:GLU:HG2	1.84	0.60
18:AM:124:TYR:HB3	18:AM:132:ILE:HG22	1.83	0.60
3:S1:237:ASN:HB3	3:S1:253:ARG:O	2.02	0.60
6:S7:102:LYS:O	6:S7:106:GLN:NE2	2.35	0.60
7:S8:53:GLU:OE2	16:AL:34:ARG:NH2	2.34	0.60
23:D5:233:LEU:HG	23:D5:303:ALA:HB1	1.83	0.60
30:AJ:165:PRO:HD2	30:AJ:247:PRO:HG3	1.83	0.60
3:S1:229:ASP:HB3	3:S1:235:GLY:HA2	1.83	0.60
17:AA:55:GLU:HA	17:AA:59:GLY:HA3	1.83	0.60
30:AJ:12:GLU:OE1	30:AJ:16:LYS:NZ	2.35	0.60
38:B9:102:CYS:SG	38:B9:103:LEU:N	2.71	0.60
4:S2:36:VAL:HG22	25:D2:49:ASN:HB3	1.84	0.60
15:A7:51:ASN:HB2	15:A7:56:ARG:HH22	1.67	0.60
1:V1:99:GLU:OE2	1:V1:106:LYS:N	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:4L:34:GLU:HA	22:4L:37:MET:HE3	1.83	0.59
4:S2:179:GLU:OE2	4:S2:183:ARG:NH2	2.34	0.59
12:A2:17:GLU:OE1	12:A2:67:ARG:NH2	2.35	0.59
20:D1:288:LEU:O	20:D1:292:ASN:HB2	2.03	0.59
23:D5:597:ILE:HD11	26:AK:34:VAL:HG22	1.84	0.59
2:V2:113:SER:HA	2:V2:152:PRO:HG3	1.84	0.59
19:D3:63:LEU:HD22	22:4L:72:ALA:HB2	1.85	0.59
4:S2:261:ARG:NH2	4:S2:268:ASP:OD1	2.36	0.59
29:BJ:3:SER:OG	29:BJ:4:TRP:N	2.35	0.59
3:S1:266:LYS:O	3:S1:270:ALA:HB2	2.02	0.59
3:S1:372:GLU:OE2	3:S1:394:ARG:NH1	2.34	0.59
3:S1:531:CYS:SG	3:S1:532:VAL:N	2.75	0.59
4:S2:204:PRO:HD3	7:S8:60:ARG:HH22	1.66	0.59
20:D1:60:PRO:HB3	20:D1:218:GLY:H	1.67	0.59
20:D1:281:ARG:HB3	20:D1:284:GLN:HB2	1.84	0.59
6:S7:139:ILE:HG22	6:S7:140:VAL:HG13	1.84	0.59
23:D5:10:VAL:HA	23:D5:13:ILE:HG22	1.84	0.59
22:4L:58:MET:HB3	22:4L:62:ILE:HD12	1.85	0.59
29:BJ:158:GLN:OE1	29:BJ:161:ARG:NH2	2.36	0.59
1:V1:101:GLU:O	1:V1:104:THR:OG1	2.21	0.59
38:B9:107:HIS:NE2	41:BK:43:ASP:OD1	2.35	0.59
12:A2:17:GLU:HG2	12:A2:51:PRO:HG2	1.85	0.59
28:A8:34:GLN:OE1	28:A8:116:TRP:NE1	2.35	0.59
30:AJ:183:ILE:HD11	30:AJ:191:GLU:HB3	1.84	0.59
41:BK:100:ARG:HD3	41:BK:107:LEU:HA	1.85	0.59
3:S1:286:ASN:O	3:S1:289:GLY:N	2.29	0.58
3:S1:396:ARG:NH1	3:S1:416:THR:O	2.36	0.58
7:S8:119:CYS:HB2	7:S8:121:PHE:H	1.68	0.58
16:AL:60:ARG:NH1	16:AL:92:CYS:SG	2.76	0.58
5:S3:94:TYR:HB2	5:S3:107:VAL:HB	1.86	0.58
11:A9:173:GLY:H	11:A9:176:ASP:HB2	1.68	0.58
4:S2:339:LYS:NZ	7:S8:127:PRO:O	2.37	0.58
11:A9:180:ASN:OD1	11:A9:320:ARG:NH2	2.32	0.58
15:A7:3:ALA:O	15:A7:5:ARG:NH1	2.36	0.58
18:AM:79:ASP:OD2	28:A8:46:ARG:NH1	2.36	0.58
22:4L:55:LEU:HD13	31:S5:24:GLN:HA	1.84	0.58
24:D4:262:ILE:HD11	24:D4:302:LEU:HB2	1.86	0.58
36:B6:85:LEU:HD12	36:B6:89:VAL:HG21	1.84	0.58
3:S1:577:GLU:OE2	3:S1:579:ARG:NH1	2.37	0.58
5:S3:74:SER:HB3	5:S3:97:LEU:O	2.04	0.58
30:AJ:30:ASN:HD21	30:AJ:199:LEU:HD11	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S2:204:PRO:HD2	4:S2:207:LEU:HD22	1.86	0.58
48:S2:501:3PE:H372	24:D4:151:PHE:HB3	1.85	0.58
6:S7:158:TYR:OH	16:AL:116:ASN:ND2	2.37	0.58
5:S3:202:PRO:HA	10:S4:50:ASN:HB3	1.84	0.57
24:D4:270:ILE:HG13	24:D4:395:LEU:HD22	1.84	0.57
6:S7:162:GLN:HE22	16:AL:118:SER:HB3	1.69	0.57
20:D1:133:LEU:HD11	21:D6:72:THR:HG21	1.86	0.57
1:V1:150:GLN:HB3	8:V3:54:LEU:HD12	1.86	0.57
38:B9:91:GLU:HB3	38:B9:94:GLU:HB2	1.86	0.57
1:V1:299:PRO:HA	1:V1:334:VAL:HG12	1.86	0.57
3:S1:147:LYS:HB3	3:S1:209:THR:HG23	1.85	0.57
16:AL:25:ARG:HG3	16:AL:74:PHE:HE1	1.68	0.57
40:B8:60:PRO:HG3	40:B8:70:ARG:HH11	1.69	0.57
7:S8:95:GLU:OE1	7:S8:108:ARG:NH1	2.35	0.57
11:A9:251:ARG:HD3	11:A9:252:PRO:HD2	1.87	0.57
20:D1:202:GLU:O	20:D1:210:GLY:N	2.38	0.57
23:D5:10:VAL:HG11	36:B6:78:VAL:HG22	1.87	0.57
1:V1:297:VAL:HG22	1:V1:336:VAL:HG12	1.87	0.57
3:S1:380:VAL:HG12	3:S1:409:ILE:HB	1.87	0.57
4:S2:19:MET:SD	25:D2:295:ARG:NH2	2.73	0.57
11:A9:108:ASP:O	11:A9:112:LYS:HB2	2.05	0.57
16:AL:42:ASP:O	16:AL:45:GLY:N	2.37	0.57
3:S1:255:HIS:HD2	3:S1:258:ILE:H	1.51	0.57
23:D5:535:ARG:NH1	40:B8:90:ASP:O	2.38	0.57
4:S2:354:GLU:HA	5:S3:199:LEU:HD22	1.87	0.56
21:D6:127:ILE:HG21	31:S5:68:ARG:HD2	1.86	0.56
37:B7:99:LYS:HE2	40:B8:158:ILE:HG22	1.86	0.56
23:D5:288:THR:O	23:D5:292:ALA:HB2	2.05	0.56
23:D5:361:GLY:H	23:D5:435:PRO:HA	1.70	0.56
4:S2:238:ARG:HG3	4:S2:239:THR:HG23	1.87	0.56
19:D3:69:ILE:HD11	20:D1:144:VAL:HG13	1.87	0.56
23:D5:548:SER:OG	23:D5:549:ALA:N	2.37	0.56
18:AM:96:ILE:HD12	31:S5:93:PRO:HG3	1.85	0.56
4:S2:179:GLU:OE1	15:A7:26:ARG:NH2	2.38	0.56
23:D5:267:THR:O	23:D5:274:GLN:NE2	2.39	0.56
28:A8:36:ASP:OD1	28:A8:39:ASN:ND2	2.39	0.56
6:S7:46:TRP:NE1	6:S7:82:GLN:O	2.37	0.56
24:D4:300:ALA:O	24:D4:308:SER:OG	2.24	0.56
30:AJ:141:GLN:NE2	30:AJ:201:ASP:OD2	2.39	0.56
42:C1:41:GLU:OE2	42:C1:44:ARG:NH2	2.38	0.56
4:S2:227:GLU:OE1	15:A7:17:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S2:287:ILE:HB	7:S8:4:TYR:HB3	1.88	0.56
5:S3:177:ASP:OD2	11:A9:40:ARG:NH2	2.39	0.56
13:A5:22:ARG:HH22	30:AJ:239:GLN:HB3	1.71	0.56
30:AJ:300:PRO:O	30:AJ:309:ASN:ND2	2.39	0.56
3:S1:41:CYS:SG	3:S1:42:TYR:N	2.79	0.56
3:S1:257:ASP:O	3:S1:394:ARG:NH2	2.39	0.56
21:D6:146:LEU:HD12	22:4L:58:MET:HG3	1.87	0.56
22:4L:73:LEU:HD22	25:D2:38:LEU:HD23	1.87	0.56
35:B4:113:LYS:NZ	35:B4:117:GLU:OE2	2.39	0.56
37:B7:110:ARG:NH1	39:B2:67:PRO:O	2.39	0.56
3:S1:41:CYS:HB3	3:S1:52:CYS:HB3	1.88	0.55
13:A5:61:GLU:HB2	13:A5:67:LEU:HD12	1.88	0.55
3:S1:11:VAL:HG12	3:S1:77:TRP:HB2	1.88	0.55
13:A5:72:GLN:HE21	15:A7:99:PRO:HB2	1.72	0.55
21:D6:167:VAL:HG22	25:D2:42:PRO:HG2	1.87	0.55
25:D2:339:LEU:HD23	25:D2:342:ILE:HG13	1.87	0.55
11:A9:162:GLU:OE1	11:A9:224:ARG:NH1	2.40	0.55
20:D1:138:GLN:NE2	20:D1:202:GLU:OE2	2.39	0.55
30:AJ:288:GLN:HE22	41:BK:27:GLN:HE22	1.54	0.55
3:S1:546:GLN:NE2	3:S1:596:ASP:OD1	2.39	0.55
34:C2:66:THR:OG1	42:C1:28:TRP:NE1	2.39	0.55
1:V1:46:LYS:O	1:V1:50:LEU:HB2	2.06	0.55
6:S7:31:ALA:HA	6:S7:174:ARG:HD2	1.89	0.55
25:D2:222:ASN:HD22	25:D2:233:THR:HG21	1.71	0.55
27:B5:73:ARG:NH2	29:BJ:61:TYR:O	2.40	0.55
4:S2:183:ARG:HH21	15:A7:33:ARG:HH22	1.54	0.55
4:S2:273:GLN:OE1	5:S3:104:ARG:NH2	2.39	0.55
11:A9:135:LEU:HA	11:A9:167:LYS:HD3	1.88	0.55
1:V1:111:ILE:HD11	1:V1:149:LEU:HD22	1.89	0.55
1:V1:202:LYS:HB3	1:V1:361:GLN:HE21	1.72	0.55
2:V2:97:LYS:O	2:V2:157:ASN:ND2	2.40	0.54
10:S4:33:ARG:NH1	10:S4:60:ASP:OD1	2.37	0.54
11:A9:19:ILE:HA	11:A9:89:ASN:HD22	1.70	0.54
11:A9:333:ASP:OD1	11:A9:333:ASP:N	2.39	0.54
1:V1:43:TYR:O	1:V1:236:ARG:NH1	2.38	0.54
1:V1:394:GLU:OE1	3:S1:129:ARG:NH1	2.41	0.54
3:S1:377:VAL:HA	3:S1:450:MET:O	2.07	0.54
25:D2:338:PRO:O	28:A8:169:TRP:NE1	2.40	0.54
1:V1:304:THR:HG23	1:V1:328:GLY:H	1.72	0.54
20:D1:69:SER:O	20:D1:73:LEU:HB2	2.06	0.54
23:D5:33:PRO:HB3	23:D5:118:PHE:HE2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BJ:80:ASP:HB3	29:BJ:83:CYS:HB3	1.88	0.54
1:V1:362:CYS:HB3	1:V1:364:PRO:HD2	1.89	0.54
3:S1:114:CYS:SG	3:S1:115:ASP:N	2.80	0.54
20:D1:281:ARG:O	20:D1:285:LEU:N	2.39	0.54
35:B4:39:ARG:NH1	40:B8:62:TYR:OH	2.41	0.54
40:B8:55:GLN:O	40:B8:70:ARG:NH2	2.40	0.54
1:V1:213:VAL:HG13	1:V1:217:GLY:HA2	1.89	0.54
15:A7:28:GLN:NE2	16:AL:52:ASN:O	2.40	0.54
1:V1:205:LEU:HD11	3:S1:50:GLY:HA3	1.90	0.54
2:V2:27:ASN:OD1	2:V2:30:ARG:NH1	2.41	0.54
5:S3:80:ALA:HB2	5:S3:92:ILE:HD13	1.89	0.54
23:D5:547:LYS:O	23:D5:552:LEU:CB	2.54	0.54
24:D4:149:PHE:HD1	24:D4:215:TRP:HE1	1.56	0.54
26:AK:56:GLY:O	26:AK:60:PHE:HB2	2.07	0.54
26:AK:68:ILE:HG21	26:AK:99:THR:HG21	1.89	0.54
28:A8:49:GLU:OE2	28:A8:134:ARG:NH1	2.39	0.54
4:S2:172:GLU:HG3	20:D1:33:PHE:HE2	1.73	0.54
25:D2:292:PHE:HA	25:D2:295:ARG:HG2	1.90	0.54
43:B1:38:ARG:NH2	43:B1:56:TRP:O	2.41	0.54
4:S2:19:MET:HG2	25:D2:295:ARG:HH12	1.72	0.54
20:D1:243:LEU:HD13	20:D1:262:LYS:HD3	1.90	0.54
24:D4:231:LEU:HA	24:D4:235:LEU:HD13	1.89	0.54
30:AJ:108:TYR:OH	30:AJ:164:LEU:O	2.25	0.54
20:D1:81:LEU:HD13	20:D1:111:LEU:HB3	1.89	0.53
20:D1:102:VAL:HB	20:D1:150:LEU:HD21	1.91	0.53
16:AL:69:ASN:HD22	16:AL:115:PHE:HE1	1.56	0.53
25:D2:142:LEU:HB3	25:D2:194:LEU:HD21	1.90	0.53
4:S2:107:ASP:OD2	4:S2:110:SER:OG	2.26	0.53
1:V1:108:ARG:HH21	2:V2:160:TYR:HD2	1.55	0.53
3:S1:252:PRO:O	10:S4:44:ASN:ND2	2.42	0.53
3:S1:341:ASP:OD1	3:S1:341:ASP:N	2.40	0.53
13:A5:37:ILE:O	13:A5:44:ARG:NH1	2.41	0.53
25:D2:140:SER:HA	31:S5:1:PRO:H2	1.72	0.53
36:B6:92:LYS:HD3	36:B6:93:PRO:HD2	1.90	0.53
1:V1:215:VAL:HG23	1:V1:220:THR:HG21	1.91	0.53
1:V1:258:ILE:HD11	1:V1:280:ILE:HA	1.91	0.53
3:S1:157:THR:HG23	3:S1:160:ILE:HD12	1.91	0.53
4:S2:204:PRO:HB3	7:S8:60:ARG:HH12	1.73	0.53
1:V1:203:PRO:O	1:V1:361:GLN:NE2	2.40	0.53
3:S1:99:ALA:O	3:S1:134:LYS:NZ	2.32	0.53
16:AL:44:TYR:OH	16:AL:112:ASN:O	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:D4:22:MET:O	24:D4:26:ASN:ND2	2.42	0.53
24:D4:368:ALA:HB1	24:D4:375:LEU:HD12	1.90	0.53
25:D2:230:LEU:HB3	25:D2:300:THR:HG22	1.91	0.53
30:AJ:235:VAL:O	30:AJ:239:GLN:NE2	2.42	0.53
30:AJ:258:ASN:O	30:AJ:262:LEU:HB2	2.09	0.53
46:V1:501:FMN:O4'	46:V1:501:FMN:O2'	2.27	0.52
3:S1:332:LYS:HD3	3:S1:507:TYR:HE1	1.74	0.52
6:S7:124:GLY:HA2	7:S8:115:LYS:HA	1.90	0.52
11:A9:134:HIS:ND1	11:A9:135:LEU:O	2.31	0.52
13:A5:34:LEU:HD11	13:A5:44:ARG:HA	1.91	0.52
23:D5:8:THR:HG21	23:D5:82:MET:HG3	1.91	0.52
5:S3:39:GLN:HB3	5:S3:51:CYS:HB2	1.91	0.52
28:A8:126:LYS:HD2	32:A3:76:SER:HB2	1.92	0.52
44:A1:52:ARG:HE	44:A1:58:ASN:HD21	1.55	0.52
1:V1:106:LYS:HG3	1:V1:255:LEU:HD12	1.90	0.52
51:AB:101:ZMP:O5	38:B9:12:GLN:NE2	2.42	0.52
1:V1:46:LYS:HE3	1:V1:169:SER:HB3	1.92	0.52
26:AK:137:GLU:HB3	26:AK:139:LYS:HG3	1.91	0.52
1:V1:30:ASP:O	1:V1:39:ARG:NH2	2.43	0.52
3:S1:149:ILE:HG21	3:S1:152:ARG:HE	1.73	0.52
23:D5:245:ALA:O	23:D5:249:SER:CB	2.58	0.52
35:B4:124:PHE:HB2	35:B4:126:ILE:HD11	1.91	0.52
44:A1:68:ASN:ND2	44:A1:70:ASP:OXT	2.42	0.52
3:S1:127:ARG:HH11	15:A7:46:HIS:HB3	1.74	0.52
19:D3:54:LYS:HB3	19:D3:114:THR:HB	1.91	0.52
23:D5:154:LEU:HD13	23:D5:243:VAL:HG13	1.92	0.52
23:D5:535:ARG:HH12	40:B8:92:SER:H	1.56	0.52
23:D5:546:GLN:OE1	35:B4:71:ARG:NH2	2.39	0.52
25:D2:22:ILE:HD11	31:S5:6:GLN:H	1.75	0.52
27:B5:34:ILE:HG23	27:B5:38:ILE:HD12	1.92	0.52
37:B7:50:LEU:HD11	37:B7:63:ILE:HD11	1.91	0.52
23:D5:67:HIS:HA	23:D5:77:SER:HA	1.91	0.52
7:S8:80:CYS:N	45:S8:202:SF4:S1	2.82	0.52
25:D2:106:LEU:HD23	25:D2:138:PRO:HB2	1.92	0.52
27:B5:88:GLU:OE1	43:B1:56:TRP:NE1	2.40	0.52
31:S5:4:ASP:HB2	34:C2:10:PRO:HG2	1.92	0.52
2:V2:24:THR:HG22	2:V2:26:GLU:H	1.75	0.52
9:S6:54:SER:OG	9:S6:55:ARG:N	2.42	0.52
21:D6:70:TYR:HD2	22:4L:75:LEU:HD22	1.75	0.52
23:D5:77:SER:OG	23:D5:79:SER:OG	2.28	0.52
24:D4:373:ILE:HD11	24:D4:448:SER:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B5:84:GLU:OE1	43:B1:46:ARG:NH1	2.41	0.52
37:B7:36:ARG:NH1	40:B8:132:GLN:OE1	2.43	0.52
5:S3:30:ALA:HA	5:S3:37:VAL:HG21	1.92	0.52
14:A6:95:VAL:HG21	19:D3:44:MET:HB3	1.92	0.52
23:D5:520:PHE:HE2	38:B9:29:ARG:HH12	1.58	0.52
23:D5:224:SER:HB2	23:D5:310:LEU:HD23	1.92	0.51
30:AJ:41:GLU:HB3	30:AJ:231:ALA:HB2	1.92	0.51
35:B4:114:LEU:HD22	35:B4:120:LEU:HD23	1.91	0.51
4:S2:91:ILE:HG12	4:S2:99:ALA:HB1	1.91	0.51
4:S2:295:ASP:OD1	7:S8:6:ASN:ND2	2.41	0.51
11:A9:26:ALA:HA	11:A9:31:GLY:HA3	1.93	0.51
23:D5:245:ALA:O	23:D5:249:SER:HB3	2.11	0.51
23:D5:546:GLN:O	23:D5:551:SER:HB3	2.11	0.51
1:V1:291:TRP:HZ2	1:V1:313:GLU:HA	1.74	0.51
3:S1:534:ARG:HD2	16:AL:144:TYR:HE2	1.74	0.51
4:S2:61:VAL:HG11	6:S7:52:LEU:HD23	1.91	0.51
14:A6:63:ARG:HB2	17:AA:45:LEU:HD21	1.92	0.51
23:D5:25:ASN:ND2	23:D5:27:HIS:O	2.43	0.51
3:S1:230:VAL:HG23	3:S1:231:MET:HG3	1.92	0.51
3:S1:379:LEU:HD21	3:S1:384:PRO:HG2	1.92	0.51
5:S3:85:THR:HG21	10:S4:87:SER:H	1.75	0.51
9:S6:53:GLY:HA2	9:S6:94:GLN:H	1.76	0.51
36:B6:86:LYS:O	36:B6:90:THR:CB	2.58	0.51
1:V1:103:GLY:N	2:V2:148:CYS:SG	2.82	0.51
1:V1:200:GLN:NE2	10:S4:132:THR:O	2.42	0.51
2:V2:101:GLN:HB2	2:V2:155:GLN:HB3	1.93	0.51
5:S3:7:THR:OG1	5:S3:8:ARG:N	2.42	0.51
9:S6:18:TYR:OH	9:S6:24:ARG:NH1	2.44	0.51
15:A7:38:PRO:HA	18:AM:7:GLN:HB2	1.92	0.51
1:V1:258:ILE:HD12	1:V1:284:ALA:HB3	1.92	0.51
3:S1:582:GLN:OE1	3:S1:620:ARG:NH1	2.42	0.51
20:D1:74:ALA:O	20:D1:115:SER:OG	2.29	0.51
21:D6:136:PHE:HZ	31:S5:28:ILE:HG21	1.75	0.51
22:4L:62:ILE:HA	22:4L:65:VAL:HG12	1.92	0.51
29:BJ:14:ARG:NH1	36:B6:98:GLU:OE2	2.43	0.51
2:V2:37:ASN:OD1	8:V3:62:ARG:NH1	2.44	0.51
2:V2:172:ILE:HG23	2:V2:182:PRO:HG2	1.93	0.51
3:S1:382:THR:HB	3:S1:454:GLY:HA3	1.93	0.51
18:AM:69:ALA:HB2	28:A8:124:LEU:HD13	1.93	0.51
23:D5:226:GLN:O	23:D5:230:HIS:N	2.43	0.51
23:D5:241:THR:HG21	23:D5:344:GLY:HA3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:D5:546:GLN:HA	23:D5:550:SER:HB2	1.91	0.51
25:D2:109:ALA:HB2	25:D2:161:SER:HA	1.91	0.51
25:D2:222:ASN:OD1	25:D2:222:ASN:N	2.42	0.51
1:V1:101:GLU:H	1:V1:184:TYR:HE1	1.57	0.51
3:S1:193:SER:OG	3:S1:385:ARG:NH2	2.44	0.51
24:D4:447:LEU:HD11	24:D4:454:ILE:HG12	1.93	0.51
36:B6:81:ILE:O	36:B6:85:LEU:HB2	2.10	0.51
6:S7:116:MET:HA	6:S7:146:VAL:HG23	1.92	0.51
23:D5:243:VAL:O	23:D5:247:LEU:HB2	2.11	0.51
4:S2:111:MET:HG3	4:S2:112:MET:HG2	1.92	0.51
6:S7:179:ARG:HG3	11:A9:50:ARG:HH12	1.76	0.51
15:A7:70:SER:OG	15:A7:71:SER:N	2.43	0.51
20:D1:151:LEU:O	20:D1:155:LEU:HB2	2.10	0.51
23:D5:205:ASN:HD22	29:BJ:121:ARG:HH22	1.57	0.51
33:B3:63:VAL:O	33:B3:67:LEU:HB2	2.10	0.51
3:S1:233:ALA:HB1	3:S1:576:THR:HB	1.93	0.50
26:AK:122:ALA:O	26:AK:126:MET:HB2	2.11	0.50
31:S5:94:PRO:O	31:S5:98:SER:OG	2.28	0.50
3:S1:357:ASP:N	3:S1:357:ASP:OD1	2.43	0.50
4:S2:175:GLU:HB3	6:S7:66:ARG:HH11	1.77	0.50
23:D5:253:VAL:HG13	23:D5:254:VAL:HG13	1.92	0.50
24:D4:52:PHE:HB2	24:D4:56:PHE:HB2	1.93	0.50
3:S1:40:PHE:O	3:S1:158:ARG:NH2	2.43	0.50
3:S1:568:GLU:HB3	3:S1:589:PRO:HG3	1.93	0.50
13:A5:54:LYS:HE2	13:A5:71:LEU:HD11	1.93	0.50
20:D1:30:TYR:OH	44:A1:4:GLU:OE1	2.29	0.50
32:A3:13:ALA:HA	32:A3:16:PRO:HB3	1.93	0.50
2:V2:29:LYS:HE3	8:V3:56:LEU:HD11	1.93	0.50
5:S3:38:GLN:HG2	15:A7:71:SER:HB2	1.93	0.50
12:A2:41:VAL:O	12:A2:45:LYS:CB	2.59	0.50
20:D1:196:ALA:HA	20:D1:274:ARG:HG3	1.93	0.50
25:D2:154:ILE:HG23	25:D2:191:THR:HG22	1.92	0.50
30:AJ:306:ALA:O	42:C1:3:TYR:OH	2.28	0.50
1:V1:261:HIS:HB2	2:V2:110:LEU:HD21	1.94	0.50
3:S1:80:LEU:HB3	3:S1:83:SER:HB3	1.93	0.50
3:S1:353:GLY:HA3	3:S1:649:SER:HA	1.94	0.50
24:D4:254:THR:O	24:D4:258:ALA:CB	2.59	0.50
3:S1:242:THR:HG21	3:S1:586:ALA:HB1	1.93	0.50
5:S3:67:HIS:HB2	13:A5:89:LEU:HD21	1.93	0.50
23:D5:178:GLY:HA2	23:D5:219:ALA:HA	1.94	0.50
25:D2:309:ASN:HD21	30:AJ:95:ARG:HG3	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B5:42:LEU:HA	27:B5:45:VAL:HG12	1.94	0.50
4:S2:110:SER:OG	4:S2:114:ASN:OD1	2.30	0.50
4:S2:155:THR:HG23	4:S2:167:PHE:HA	1.93	0.50
11:A9:169:ALA:O	50:A9:401:NDP:N7N	2.45	0.50
20:D1:169:GLN:NE2	20:D1:240:THR:O	2.41	0.50
23:D5:332:HIS:CE1	23:D5:336:LYS:HD2	2.47	0.50
23:D5:535:ARG:NH2	35:B4:10:LEU:O	2.43	0.50
24:D4:26:ASN:OD1	43:B1:13:HIS:NE2	2.44	0.50
1:V1:259:SER:OG	2:V2:148:CYS:O	2.29	0.50
3:S1:145:LEU:HB3	3:S1:269:PHE:HE2	1.76	0.50
5:S3:86:ARG:NH1	5:S3:91:GLU:OE2	2.42	0.50
20:D1:181:LEU:HB2	20:D1:300:LEU:HD13	1.93	0.50
38:B9:96:TYR:HB2	38:B9:177:PRO:HB3	1.94	0.50
3:S1:9:ILE:HG23	3:S1:75:LYS:HA	1.93	0.49
5:S3:76:ALA:HB3	5:S3:95:ASN:HB3	1.94	0.49
12:A2:18:ILE:O	12:A2:52:ILE:HA	2.12	0.49
12:A2:90:LEU:O	12:A2:94:LEU:HB3	2.12	0.49
16:AL:28:PHE:HE1	20:D1:42:PRO:HD3	1.77	0.49
24:D4:403:THR:HA	24:D4:406:TYR:CE2	2.46	0.49
1:V1:355:LYS:HD3	1:V1:373:ASN:HD22	1.77	0.49
3:S1:226:GLU:OE1	3:S1:253:ARG:NH2	2.45	0.49
4:S2:35:ASP:O	25:D2:49:ASN:ND2	2.38	0.49
23:D5:401:THR:HG21	23:D5:479:GLN:HG2	1.94	0.49
24:D4:204:MET:HB3	24:D4:209:LEU:HD22	1.94	0.49
2:V2:120:ILE:HD11	2:V2:169:ILE:HD12	1.92	0.49
3:S1:665:GLN:HE22	3:S1:671:PHE:HA	1.77	0.49
23:D5:358:LYS:HA	23:D5:436:ARG:HG3	1.94	0.49
1:V1:20:ARG:NH1	1:V1:269:GLU:O	2.45	0.49
3:S1:622:ARG:NH2	12:A2:73:GLU:OE2	2.44	0.49
4:S2:55:HIS:NE2	20:D1:205:SER:O	2.45	0.49
48:S2:501:3PE:H3B1	23:D5:562:LEU:HD11	1.92	0.49
20:D1:113:VAL:HG11	20:D1:139:THR:HG21	1.94	0.49
23:D5:60:GLU:HB2	36:B6:99:LYS:HB3	1.95	0.49
25:D2:3:PRO:HD2	30:AJ:9:ILE:HD11	1.93	0.49
25:D2:26:TRP:HB3	25:D2:74:ILE:HD13	1.94	0.49
34:C2:66:THR:HG22	42:C1:27:LEU:HD23	1.93	0.49
1:V1:194:GLU:HA	1:V1:197:GLU:HB2	1.95	0.49
3:S1:324:ASP:HA	3:S1:573:TYR:HE1	1.77	0.49
4:S2:383:SER:OG	4:S2:384:SER:N	2.45	0.49
23:D5:518:ASN:HA	23:D5:521:LYS:HB2	1.94	0.49
24:D4:72:LEU:HD12	24:D4:75:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V1:366:ARG:NH1	3:S1:155:GLN:OE1	2.45	0.49
3:S1:243:ARG:HH22	7:S8:95:GLU:HA	1.77	0.49
25:D2:269:GLU:HA	25:D2:272:LYS:HE3	1.95	0.49
40:B8:12:PRO:HG2	40:B8:14:PRO:HD2	1.95	0.49
5:S3:71:GLN:HE21	13:A5:82:GLN:HE22	1.60	0.49
6:S7:147:PRO:HG2	7:S8:139:PHE:HD2	1.78	0.49
7:S8:74:GLU:HB3	9:S6:44:ILE:HD11	1.95	0.49
11:A9:48:PRO:HB2	11:A9:73:TRP:CD1	2.47	0.49
24:D4:196:TRP:CE2	24:D4:200:MET:HG3	2.48	0.49
28:A8:97:ARG:HA	28:A8:100:ARG:HH21	1.77	0.49
29:BJ:4:TRP:CG	36:B6:93:PRO:HB3	2.47	0.49
2:V2:190:ARG:HB2	2:V2:194:GLU:HB2	1.94	0.49
3:S1:117:GLN:HG2	4:S2:346:ILE:HG23	1.95	0.49
4:S2:63:ARG:HH22	14:A6:96:TRP:HA	1.78	0.49
4:S2:151:ILE:HD13	4:S2:304:MET:HE1	1.93	0.49
5:S3:22:LEU:HD23	5:S3:48:LEU:HB2	1.93	0.49
16:AL:106:ARG:HB2	16:AL:109:ILE:HD11	1.94	0.49
23:D5:524:ASN:O	38:B9:77:GLN:NE2	2.39	0.49
30:AJ:210:PHE:HD2	30:AJ:211:LEU:HD22	1.76	0.49
4:S2:357:GLN:HB2	15:A7:59:ARG:HH22	1.76	0.49
4:S2:364:TYR:HB2	4:S2:377:TYR:HD1	1.78	0.49
15:A7:28:GLN:NE2	16:AL:52:ASN:OD1	2.46	0.49
21:D6:121:GLY:HA2	22:4L:3:LEU:HD21	1.93	0.49
25:D2:244:VAL:HG11	25:D2:300:THR:HG21	1.95	0.49
3:S1:163:ALA:O	3:S1:168:GLY:N	2.39	0.49
6:S7:165:LYS:NZ	16:AL:78:ASP:OD1	2.37	0.49
14:A6:43:PRO:HA	14:A6:46:VAL:HG12	1.94	0.49
30:AJ:76:ASN:H	30:AJ:95:ARG:HD3	1.78	0.49
30:AJ:244:ASP:OD1	30:AJ:244:ASP:N	2.43	0.49
4:S2:68:LEU:HA	4:S2:74:ARG:H	1.77	0.48
4:S2:163:ALA:H	20:D1:278:PRO:HA	1.78	0.48
15:A7:45:SER:O	15:A7:46:HIS:ND1	2.45	0.48
28:A8:35:CYS:SG	28:A8:36:ASP:N	2.85	0.48
30:AJ:25:ILE:O	30:AJ:123:VAL:HA	2.12	0.48
38:B9:106:TRP:HB2	38:B9:111:LYS:HE3	1.95	0.48
1:V1:199:LYS:HE3	10:S4:131:SER:HA	1.95	0.48
3:S1:251:LEU:HD13	10:S4:44:ASN:HB3	1.94	0.48
23:D5:358:LYS:NZ	17:AB:56:ASP:O	2.46	0.48
37:B7:96:LYS:HD3	40:B8:132:GLN:HE22	1.78	0.48
1:V1:365:CYS:SG	1:V1:366:ARG:N	2.85	0.48
11:A9:30:LEU:HD22	11:A9:94:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AA:32:VAL:HG12	17:AA:74:GLN:HE21	1.79	0.48
18:AM:119:MET:HB2	21:D6:127:ILE:HG22	1.95	0.48
19:D3:33:LYS:HD3	20:D1:61:LEU:HD22	1.95	0.48
20:D1:141:SER:OG	20:D1:286:MET:SD	2.71	0.48
23:D5:604:PHE:O	25:D2:150:ASN:ND2	2.41	0.48
24:D4:58:SER:OG	24:D4:63:THR:OG1	2.31	0.48
4:S2:187:ALA:HB2	7:S8:62:ARG:HH22	1.78	0.48
6:S7:55:CYS:HB3	6:S7:89:ALA:HB1	1.94	0.48
7:S8:135:PRO:HG3	7:S8:164:GLU:HG2	1.96	0.48
11:A9:285:GLU:O	11:A9:289:THR:OG1	2.24	0.48
30:AJ:202:ILE:O	30:AJ:206:TYR:HB2	2.12	0.48
33:B3:25:GLY:O	33:B3:29:GLU:CB	2.60	0.48
43:B1:46:ARG:NH2	43:B1:55:THR:OG1	2.46	0.48
2:V2:24:THR:HB	2:V2:27:ASN:H	1.79	0.48
2:V2:53:LEU:HD12	8:V3:52:LEU:HD13	1.95	0.48
3:S1:185:THR:HG22	3:S1:187:ILE:H	1.78	0.48
3:S1:447:LYS:HG3	3:S1:448:LYS:HG3	1.96	0.48
11:A9:92:ILE:HD12	11:A9:94:LEU:HD13	1.96	0.48
23:D5:435:PRO:HB2	23:D5:437:PHE:HE2	1.77	0.48
24:D4:263:MET:HE1	35:B4:100:TRP:HB2	1.96	0.48
25:D2:115:VAL:HG12	25:D2:180:ALA:HB1	1.95	0.48
30:AJ:133:VAL:HG13	30:AJ:205:VAL:HG12	1.96	0.48
35:B4:13:LEU:HD11	35:B4:18:ASP:HA	1.96	0.48
7:S8:63:GLY:H	7:S8:133:GLU:HB3	1.78	0.48
9:S6:56:VAL:HG22	9:S6:74:ASN:HA	1.96	0.48
23:D5:71:ILE:HG13	23:D5:72:GLN:H	1.78	0.48
2:V2:56:ARG:HB3	8:V3:49:TYR:HE1	1.79	0.48
3:S1:283:MET:HA	3:S1:293:HIS:HA	1.94	0.48
3:S1:478:ARG:NH1	3:S1:487:TRP:O	2.35	0.48
4:S2:54:GLN:NE2	19:D3:37:TYR:OH	2.37	0.48
15:A7:51:ASN:HA	15:A7:56:ARG:HH12	1.78	0.48
24:D4:269:MET:SD	24:D4:399:ASN:ND2	2.86	0.48
3:S1:437:HIS:H	3:S1:440:SER:HB3	1.78	0.48
24:D4:241:TYR:OH	24:D4:245:ARG:NH2	2.46	0.48
25:D2:123:PRO:O	25:D2:126:SER:OG	2.32	0.48
3:S1:521:MET:HG3	3:S1:542:PHE:HD2	1.79	0.48
7:S8:152:GLU:OE1	16:AL:127:TYR:OH	2.32	0.48
37:B7:34:LYS:NZ	40:B8:155:HIS:O	2.40	0.48
1:V1:132:ARG:NH2	8:V3:63:MET:SD	2.86	0.48
3:S1:399:TRP:HD1	3:S1:404:LEU:HB2	1.79	0.48
6:S7:91:THR:OG1	6:S7:119:CYS:SG	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:S4:125:ASN:N	10:S4:125:ASN:OD1	2.47	0.48
21:D6:120:ASN:H	22:4L:1:MET:HG2	1.79	0.48
23:D5:139:GLN:HA	23:D5:142:ILE:HD12	1.95	0.48
23:D5:406:ALA:HB2	40:B8:124:THR:HG23	1.95	0.48
29:BJ:98:ASP:HA	29:BJ:101:ILE:HD12	1.96	0.48
15:A7:106:SER:OG	15:A7:107:GLN:N	2.48	0.47
20:D1:92:PRO:HG3	20:D1:255:TYR:HD2	1.79	0.47
24:D4:207:MET:HG3	24:D4:298:ILE:HD11	1.96	0.47
27:B5:64:TRP:HD1	27:B5:65:GLU:HG3	1.79	0.47
29:BJ:64:HIS:NE2	41:BK:92:GLU:OE1	2.47	0.47
38:B9:139:LEU:O	38:B9:143:THR:OG1	2.31	0.47
1:V1:198:GLY:HA3	2:V2:45:ALA:HA	1.97	0.47
3:S1:147:LYS:HB2	3:S1:211:LYS:HA	1.95	0.47
3:S1:227:SER:OG	3:S1:228:ILE:N	2.47	0.47
4:S2:69:SER:OG	4:S2:72:MET:O	2.22	0.47
4:S2:146:ARG:HG3	4:S2:370:PRO:HG3	1.96	0.47
4:S2:390:LYS:NZ	4:S2:391:ILE:O	2.42	0.47
4:S2:415:VAL:HG11	20:D1:206:GLU:HG2	1.95	0.47
14:A6:49:PHE:HE1	14:A6:95:VAL:HG13	1.79	0.47
24:D4:272:THR:HA	24:D4:275:ILE:HG22	1.95	0.47
30:AJ:202:ILE:O	30:AJ:206:TYR:CB	2.62	0.47
11:A9:322:ARG:NH1	11:A9:327:LEU:O	2.44	0.47
25:D2:180:ALA:O	25:D2:183:SER:OG	2.25	0.47
41:BK:110:SER:OG	41:BK:111:ASN:N	2.47	0.47
9:S6:51:GLN:HG2	9:S6:92:ARG:HB2	1.97	0.47
23:D5:341:MET:HE1	23:D5:457:LEU:HD22	1.97	0.47
30:AJ:57:HIS:HB2	30:AJ:60:ASP:HB2	1.96	0.47
40:B8:46:ASP:OD1	40:B8:46:ASP:N	2.48	0.47
11:A9:202:LYS:N	11:A9:236:TYR:O	2.47	0.47
18:AM:86:LEU:HB3	28:A8:6:LEU:HD13	1.97	0.47
30:AJ:267:LEU:HA	30:AJ:270:LEU:HB2	1.97	0.47
1:V1:301:GLY:HA2	1:V1:333:ALA:HB3	1.97	0.47
2:V2:97:LYS:HB3	2:V2:136:LEU:HB2	1.97	0.47
3:S1:46:LEU:O	10:S4:116:LYS:NZ	2.44	0.47
3:S1:312:GLY:N	3:S1:339:ASP:OD2	2.47	0.47
4:S2:85:ARG:NH1	6:S7:126:TYR:OH	2.47	0.47
6:S7:81:ARG:HG3	20:D1:214:GLU:HA	1.96	0.47
21:D6:163:ILE:HG13	25:D2:12:THR:HG21	1.97	0.47
25:D2:159:ILE:HD11	25:D2:278:LEU:HD21	1.96	0.47
1:V1:188:GLU:HG2	46:V1:501:FMN:C7	2.45	0.47
1:V1:338:ASP:HB3	1:V1:341:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V2:150:ASN:HB3	2:V2:163:ASP:H	1.80	0.47
3:S1:240:VAL:HG12	3:S1:250:ILE:HG22	1.96	0.47
3:S1:337:ARG:NH1	3:S1:610:THR:O	2.47	0.47
4:S2:339:LYS:HA	9:S6:69:PRO:HB3	1.97	0.47
5:S3:38:GLN:O	15:A7:70:SER:C	2.53	0.47
10:S4:23:THR:HG23	10:S4:25:VAL:HG12	1.96	0.47
11:A9:91:VAL:HG13	11:A9:129:PHE:HD1	1.79	0.47
20:D1:71:PHE:O	20:D1:215:TYR:OH	2.28	0.47
23:D5:172:ILE:HG21	24:D4:408:LEU:HD23	1.97	0.47
23:D5:223:LYS:NZ	23:D5:252:MET:SD	2.81	0.47
25:D2:1:MET:HG2	30:AJ:254:ARG:HD2	1.97	0.47
31:S5:81:GLN:HA	31:S5:84:LYS:HG2	1.97	0.47
37:B7:34:LYS:HG3	40:B8:156:TYR:HD1	1.80	0.47
37:B7:75:ASN:HB3	37:B7:78:ALA:HB2	1.96	0.47
40:B8:4:ILE:HG22	40:B8:6:LYS:H	1.80	0.47
2:V2:63:ILE:HD11	3:S1:187:ILE:HG22	1.96	0.47
3:S1:377:VAL:HG22	3:S1:450:MET:HB3	1.96	0.47
4:S2:238:ARG:HH11	20:D1:281:ARG:HB2	1.80	0.47
5:S3:80:ALA:HB1	5:S3:90:PHE:HB3	1.97	0.47
5:S3:151:ILE:HG22	5:S3:152:LEU:HG	1.96	0.47
17:AA:63:PRO:HG2	17:AA:66:ASP:HB2	1.97	0.47
36:B6:1:SER:OG	36:B6:2:GLY:N	2.47	0.47
38:B9:100:GLU:O	38:B9:121:ARG:NH2	2.48	0.47
40:B8:126:GLN:O	40:B8:128:VAL:N	2.47	0.47
1:V1:93:LEU:O	1:V1:134:ALA:HA	2.15	0.47
3:S1:283:MET:HG2	3:S1:293:HIS:HB3	1.97	0.47
6:S7:125:TYR:HE1	7:S8:88:PRO:HB2	1.79	0.47
14:A6:62:VAL:HG22	51:AA:101:ZMP:H2	1.96	0.47
25:D2:231:SER:HB2	25:D2:305:PHE:HB2	1.97	0.47
35:B4:47:GLN:HE21	38:B9:165:LEU:HD23	1.78	0.47
2:V2:149:VAL:O	2:V2:190:ARG:NH2	2.48	0.47
7:S8:116:CYS:SG	7:S8:117:ILE:N	2.88	0.47
9:S6:11:VAL:HG12	9:S6:17:VAL:HG21	1.96	0.47
9:S6:69:PRO:HG2	9:S6:86:TYR:HE2	1.80	0.47
9:S6:84:CYS:SG	9:S6:86:TYR:N	2.88	0.47
23:D5:55:ILE:HG22	37:B7:73:PHE:HE1	1.80	0.47
23:D5:386:LEU:HD23	23:D5:387:THR:H	1.80	0.47
23:D5:535:ARG:HH12	40:B8:92:SER:N	2.13	0.47
29:BJ:82:LEU:H	29:BJ:82:LEU:HG	1.56	0.47
29:BJ:116:GLU:OE1	29:BJ:119:SER:OG	2.24	0.47
29:BJ:163:LEU:HD12	41:BK:120:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S1:139:ASP:OD1	3:S1:139:ASP:N	2.43	0.46
5:S3:88:ASN:HA	5:S3:112:ASP:HB3	1.96	0.46
24:D4:167:ILE:HA	24:D4:170:THR:HG22	1.97	0.46
25:D2:30:TRP:NE1	25:D2:67:SER:OG	2.48	0.46
1:V1:33:LEU:HD23	1:V1:155:GLU:HB3	1.97	0.46
1:V1:99:GLU:O	1:V1:139:ARG:NH1	2.49	0.46
5:S3:39:GLN:NE2	5:S3:41:GLN:OE1	2.48	0.46
5:S3:154:ASP:OD1	5:S3:155:TYR:N	2.48	0.46
29:BJ:77:HIS:HA	34:C2:108:THR:HA	1.97	0.46
35:B4:13:LEU:HD22	35:B4:14:PRO:HD2	1.96	0.46
37:B7:3:HIS:CE1	40:B8:127:PRO:HD3	2.50	0.46
3:S1:140:LYS:HD2	9:S6:77:LYS:HG3	1.97	0.46
5:S3:68:SER:HA	13:A5:82:GLN:HE21	1.79	0.46
14:A6:29:ARG:HH21	17:AA:65:ILE:HD13	1.80	0.46
23:D5:79:SER:HB2	23:D5:136:ASN:HB2	1.98	0.46
28:A8:70:PHE:HB3	44:A1:69:ILE:HD12	1.96	0.46
31:S5:93:PRO:HB2	31:S5:95:PRO:HD3	1.98	0.46
3:S1:95:GLU:OE2	3:S1:129:ARG:NE	2.48	0.46
3:S1:255:HIS:CD2	3:S1:258:ILE:HG12	2.50	0.46
6:S7:154:GLU:HG3	7:S8:50:TYR:HE1	1.79	0.46
7:S8:14:MET:HA	7:S8:17:VAL:HG12	1.98	0.46
21:D6:120:ASN:HD21	31:S5:69:GLN:HG3	1.80	0.46
29:BJ:100:GLU:HA	29:BJ:103:ASN:HD22	1.80	0.46
29:BJ:145:LEU:HD13	29:BJ:149:TYR:HB3	1.97	0.46
30:AJ:217:LYS:HD3	30:AJ:247:PRO:HD3	1.98	0.46
1:V1:338:ASP:OD1	1:V1:339:ARG:N	2.49	0.46
4:S2:404:LYS:HA	4:S2:407:LYS:HG2	1.97	0.46
6:S7:125:TYR:CG	7:S8:117:ILE:HD12	2.50	0.46
16:AL:39:VAL:HG21	16:AL:50:GLU:HB3	1.98	0.46
18:AM:54:ARG:NH2	32:A3:83:LEU:O	2.48	0.46
18:AM:73:LEU:HD21	28:A8:17:VAL:HG21	1.96	0.46
19:D3:84:LEU:HD21	32:A3:45:ASN:HD22	1.80	0.46
23:D5:288:THR:O	23:D5:292:ALA:CB	2.63	0.46
24:D4:197:LEU:O	24:D4:201:MET:CB	2.63	0.46
43:B1:16:VAL:HG23	43:B1:17:PRO:HD3	1.97	0.46
3:S1:366:THR:OG1	3:S1:491:ASN:ND2	2.48	0.46
4:S2:141:PHE:HZ	4:S2:184:VAL:HG21	1.80	0.46
4:S2:231:ASN:OD1	4:S2:236:ARG:NH2	2.48	0.46
7:S8:174:LEU:HD12	15:A7:37:PRO:HB2	1.97	0.46
11:A9:215:ILE:HA	11:A9:218:ILE:HG22	1.97	0.46
19:D3:80:GLN:NE2	20:D1:317:GLN:O	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A8:26:ALA:HB2	28:A8:88:ILE:HG21	1.96	0.46
29:BJ:100:GLU:OE2	41:BK:86:GLN:NE2	2.49	0.46
38:B9:103:LEU:HB3	38:B9:121:ARG:NH1	2.31	0.46
1:V1:250:ASN:HD21	1:V1:318:ASP:HB3	1.80	0.46
4:S2:89:LYS:NZ	5:S3:167:PRO:O	2.49	0.46
11:A9:83:ARG:HA	11:A9:86:GLU:HG3	1.98	0.46
3:S1:595:GLU:OE1	3:S1:597:TRP:NE1	2.49	0.46
4:S2:284:ASP:OD1	4:S2:284:ASP:N	2.47	0.46
4:S2:357:GLN:O	15:A7:59:ARG:NH1	2.48	0.46
19:D3:66:ASP:HA	19:D3:69:ILE:HD12	1.97	0.46
20:D1:299:ALA:HB1	32:A3:24:ILE:HG23	1.98	0.46
23:D5:509:HIS:HD2	38:B9:32:HIS:HE1	1.63	0.46
29:BJ:161:ARG:NH2	41:BK:110:SER:OG	2.49	0.46
4:S2:324:LYS:NZ	4:S2:332:PRO:O	2.42	0.46
28:A8:29:HIS:HB3	28:A8:119:PRO:HD2	1.97	0.46
36:B6:17:LEU:HD11	38:B9:162:LEU:HD22	1.98	0.46
41:BK:68:ILE:HA	41:BK:72:LEU:HD13	1.97	0.46
7:S8:160:LYS:HD2	7:S8:161:TRP:CZ3	2.50	0.46
10:S4:55:TRP:HB2	10:S4:86:PHE:HB2	1.97	0.46
23:D5:356:ILE:HD13	23:D5:356:ILE:HA	1.85	0.46
23:D5:418:PHE:HA	23:D5:421:ILE:HG12	1.98	0.46
25:D2:345:ILE:HD12	34:C2:78:ARG:HG2	1.97	0.46
1:V1:362:CYS:N	45:V1:500:SF4:S2	2.76	0.45
3:S1:382:THR:HG21	3:S1:493:LEU:HD21	1.98	0.45
18:AM:65:GLU:HG2	28:A8:124:LEU:HB2	1.98	0.45
1:V1:250:ASN:HD22	1:V1:319:PHE:HD2	1.64	0.45
3:S1:426:PRO:HG3	3:S1:661:LEU:HD23	1.97	0.45
11:A9:38:LEU:O	11:A9:42:GLY:N	2.49	0.45
23:D5:234:PRO:HB3	23:D5:300:LYS:HG2	1.98	0.45
24:D4:13:PRO:HA	24:D4:16:TRP:HD1	1.81	0.45
28:A8:70:PHE:HA	28:A8:73:ILE:HG22	1.98	0.45
33:B3:48:GLU:HG2	33:B3:51:ARG:HD2	1.98	0.45
5:S3:48:LEU:HB3	5:S3:105:ILE:HG22	1.98	0.45
18:AM:108:SER:N	28:A8:2:GLY:O	2.50	0.45
3:S1:449:PRO:HB2	3:S1:489:VAL:HG23	1.98	0.45
19:D3:76:PRO:HB2	20:D1:317:GLN:HE22	1.81	0.45
23:D5:237:MET:HG3	23:D5:303:ALA:HB2	1.98	0.45
24:D4:254:THR:O	24:D4:258:ALA:HB2	2.16	0.45
29:BJ:30:THR:HA	29:BJ:33:THR:HG22	1.99	0.45
35:B4:112:GLU:HA	35:B4:115:ILE:HG12	1.98	0.45
1:V1:297:VAL:HA	1:V1:335:ILE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S2:116:GLN:HG3	4:S2:138:ARG:HD3	1.98	0.45
7:S8:70:TYR:HB2	7:S8:73:GLY:HA3	1.98	0.45
7:S8:160:LYS:HD2	7:S8:161:TRP:HZ3	1.81	0.45
11:A9:179:LEU:HA	11:A9:182:PHE:HD2	1.82	0.45
23:D5:76:LEU:HB2	23:D5:136:ASN:HD21	1.82	0.45
23:D5:331:THR:O	23:D5:335:PHE:HB2	2.16	0.45
35:B4:77:PRO:HA	35:B4:78:ASN:HA	1.72	0.45
42:C1:40:LEU:O	42:C1:44:ARG:HB2	2.16	0.45
2:V2:208:GLY:H	2:V2:211:PHE:HE1	1.65	0.45
19:D3:67:LEU:HD22	22:4L:65:VAL:HA	1.98	0.45
20:D1:197:PRO:HB3	20:D1:279:ARG:HG2	1.98	0.45
25:D2:264:TRP:HZ3	25:D2:340:THR:HG21	1.82	0.45
36:B6:86:LYS:O	36:B6:90:THR:OG1	2.26	0.45
36:B6:86:LYS:O	36:B6:90:THR:HB	2.17	0.45
4:S2:388:ARG:HD2	5:S3:81:VAL:HG12	1.99	0.45
17:AB:48:VAL:HG21	38:B9:16:LEU:HD21	1.99	0.45
28:A8:21:SER:HB2	44:A1:47:LEU:HG	1.99	0.45
6:S7:41:ARG:HA	20:D1:54:LYS:HD3	1.99	0.45
24:D4:187:PRO:O	24:D4:192:ASN:ND2	2.43	0.45
25:D2:344:SER:HB2	34:C2:82:MET:HG2	1.98	0.45
26:AK:89:TYR:CD2	26:AK:125:LYS:HB2	2.52	0.45
7:S8:79:ALA:HB2	7:S8:106:THR:HG22	1.99	0.45
23:D5:384:PRO:HA	23:D5:385:PHE:HA	1.68	0.45
29:BJ:144:ASP:OD2	34:C2:120:ARG:NE	2.46	0.45
30:AJ:78:SER:HB2	30:AJ:81:LYS:HD3	1.99	0.45
35:B4:46:TYR:O	35:B4:50:TYR:CB	2.63	0.45
44:A1:13:GLY:O	44:A1:17:PHE:N	2.50	0.45
1:V1:190:THR:HG21	1:V1:204:ARG:HB2	1.99	0.45
7:S8:114:THR:OG1	7:S8:115:LYS:N	2.50	0.45
11:A9:81:ILE:HG21	11:A9:117:ILE:HG22	1.99	0.45
16:AL:49:TYR:HD2	16:AL:61:TRP:HE1	1.65	0.45
23:D5:509:HIS:HD2	38:B9:32:HIS:CE1	2.35	0.45
3:S1:172:LEU:HA	3:S1:184:GLY:O	2.17	0.44
8:V3:38:TYR:HE2	8:V3:41:LEU:HB2	1.82	0.44
18:AM:96:ILE:HG12	31:S5:85:LEU:HD21	1.99	0.44
23:D5:128:MET:HG3	23:D5:251:THR:HB	1.99	0.44
24:D4:191:SER:N	26:AK:130:GLU:OE2	2.49	0.44
30:AJ:17:LYS:HG2	30:AJ:118:THR:HA	1.98	0.44
34:C2:19:ARG:HB2	42:C1:45:ARG:HH21	1.82	0.44
3:S1:328:LEU:HD22	3:S1:507:TYR:HE2	1.82	0.44
4:S2:98:GLN:NE2	7:S8:85:ALA:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AB:87:TYR:HB2	36:B6:22:LEU:HD23	1.99	0.44
1:V1:30:ASP:OD1	1:V1:30:ASP:N	2.51	0.44
3:S1:453:LEU:HD23	3:S1:492:ILE:HD12	1.99	0.44
3:S1:564:ALA:HB3	3:S1:569:LYS:HD3	2.00	0.44
9:S6:31:ARG:HH22	11:A9:69:ILE:HD11	1.82	0.44
23:D5:435:PRO:HB2	23:D5:437:PHE:CE2	2.52	0.44
26:AK:36:SER:HB2	26:AK:55:THR:HG22	1.98	0.44
34:C2:49:ARG:HB2	34:C2:51:ARG:HE	1.83	0.44
23:D5:99:SER:OG	23:D5:453:SER:OG	2.30	0.44
27:B5:140:THR:O	27:B5:143:ASN:ND2	2.50	0.44
3:S1:675:ASP:O	3:S1:679:ARG:CB	2.61	0.44
9:S6:27:ARG:HH12	10:S4:69:LEU:HA	1.83	0.44
11:A9:30:LEU:HG	11:A9:207:ILE:HD11	1.99	0.44
14:A6:38:TRP:CD2	14:A6:89:LEU:HD12	2.52	0.44
20:D1:287:HIS:ND1	20:D1:291:LYS:HD2	2.33	0.44
30:AJ:15:THR:OG1	30:AJ:253:ASP:OD1	2.31	0.44
1:V1:33:LEU:N	1:V1:155:GLU:OE1	2.50	0.44
17:AA:36:PHE:HA	17:AA:40:LEU:HD13	1.98	0.44
20:D1:10:ILE:HG22	20:D1:83:LEU:HD21	1.99	0.44
23:D5:558:LEU:HB3	24:D4:214:LEU:HD23	2.00	0.44
3:S1:354:ALA:HB3	3:S1:648:LEU:HD13	1.99	0.44
18:AM:60:GLN:HG3	20:D1:316:PRO:HB2	1.99	0.44
23:D5:172:ILE:O	23:D5:176:ARG:HG2	2.18	0.44
17:AB:68:GLU:OE1	17:AB:69:LYS:NZ	2.37	0.44
40:B8:34:TYR:OH	40:B8:46:ASP:O	2.30	0.44
1:V1:124:VAL:HG21	1:V1:232:PRO:HB3	2.00	0.44
3:S1:296:TRP:HE1	3:S1:592:LEU:HB3	1.82	0.44
4:S2:69:SER:O	4:S2:72:MET:O	2.36	0.44
13:A5:10:LEU:HB2	13:A5:13:LEU:HD22	2.00	0.44
17:AA:62:ILE:HG22	17:AA:67:ALA:HB2	1.98	0.44
20:D1:120:GLY:HA2	20:D1:128:ALA:HB1	2.00	0.44
23:D5:209:SER:O	23:D5:270:ASN:ND2	2.51	0.44
23:D5:321:GLN:NE2	23:D5:476:THR:OG1	2.36	0.44
38:B9:39:PHE:HA	38:B9:42:LEU:HB2	2.00	0.44
39:B2:10:ARG:HD3	39:B2:13:GLN:HB2	2.00	0.44
3:S1:241:SER:HB2	3:S1:249:ARG:HG3	1.99	0.44
4:S2:385:ARG:NH2	5:S3:197:PHE:O	2.47	0.44
5:S3:41:GLN:NE2	5:S3:49:GLU:OE1	2.50	0.44
21:D6:114:GLU:HG2	21:D6:118:LYS:HG2	2.00	0.44
23:D5:446:ASN:HD21	39:B2:7:ILE:HD13	1.83	0.44
27:B5:26:ARG:O	27:B5:30:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:A9:401:NDP:H8A	50:A9:401:NDP:H51A	2.00	0.43
1:V1:68:ARG:O	46:V1:501:FMN:O4'	2.30	0.43
3:S1:36:GLN:N	5:S3:204:GLU:OE2	2.51	0.43
4:S2:276:ASP:N	4:S2:276:ASP:OD1	2.50	0.43
4:S2:329:LYS:HD2	15:A7:53:TYR:CZ	2.53	0.43
11:A9:278:TRP:O	11:A9:283:LYS:NZ	2.46	0.43
27:B5:130:LYS:H	31:S5:44:HIS:CE1	2.35	0.43
27:B5:138:LYS:HB3	31:S5:29:PRO:HD3	2.00	0.43
3:S1:645:ALA:HA	3:S1:648:LEU:HD12	2.00	0.43
15:A7:108:ASP:OD2	18:AM:20:TYR:OH	2.35	0.43
18:AM:64:PHE:HE2	32:A3:48:THR:HB	1.83	0.43
20:D1:310:LEU:HD21	32:A3:32:PRO:HA	1.99	0.43
48:D5:701:3PE:H31	40:B8:88:ARG:HA	2.00	0.43
25:D2:30:TRP:HE1	25:D2:67:SER:HG	1.65	0.43
3:S1:135:ARG:NH2	3:S1:179:ASN:O	2.51	0.43
3:S1:369:ALA:HA	3:S1:394:ARG:HD3	2.00	0.43
3:S1:585:VAL:O	10:S4:61:THR:OG1	2.36	0.43
4:S2:221:ARG:HA	4:S2:221:ARG:HD3	1.89	0.43
15:A7:111:TYR:HA	15:A7:112:LEU:HA	1.79	0.43
24:D4:151:PHE:HD1	24:D4:151:PHE:HA	1.70	0.43
38:B9:13:GLN:HE21	38:B9:17:GLN:HE21	1.65	0.43
4:S2:69:SER:O	4:S2:72:MET:C	2.56	0.43
7:S8:53:GLU:HG2	16:AL:61:TRP:HB3	1.99	0.43
11:A9:3:HIS:CD2	16:AL:132:LYS:HE2	2.53	0.43
18:AM:58:ARG:NH2	32:A3:80:LEU:O	2.50	0.43
20:D1:264:LEU:HD13	20:D1:264:LEU:HA	1.80	0.43
24:D4:298:ILE:HD13	24:D4:298:ILE:HA	1.69	0.43
26:AK:39:SER:HB2	26:AK:54:ARG:HH22	1.84	0.43
27:B5:87:TYR:O	27:B5:90:THR:OG1	2.30	0.43
28:A8:166:LEU:HD23	28:A8:167:PHE:H	1.84	0.43
29:BJ:72:ASP:OD2	29:BJ:74:THR:OG1	2.29	0.43
40:B8:66:HIS:HA	40:B8:67:PRO:HD3	1.89	0.43
1:V1:378:ARG:HH12	3:S1:131:LEU:HD22	1.83	0.43
3:S1:618:GLN:HA	3:S1:621:ASN:HD22	1.84	0.43
7:S8:155:LEU:HA	7:S8:155:LEU:HD23	1.80	0.43
17:AA:31:SER:H	17:AA:34:SER:HB2	1.83	0.43
20:D1:110:SER:HB2	21:D6:61:LEU:HD21	2.01	0.43
24:D4:7:PRO:O	24:D4:11:LEU:HB2	2.18	0.43
25:D2:331:VAL:HG21	34:C2:41:SER:HB2	2.00	0.43
44:A1:52:ARG:HB3	44:A1:60:TYR:HB3	2.01	0.43
3:S1:355:GLY:HA2	3:S1:361:ASN:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:D1:17:VAL:HG11	20:D1:225:MET:HA	1.99	0.43
23:D5:191:ILE:HD12	24:D4:386:PHE:HD2	1.83	0.43
23:D5:322:PRO:HG2	23:D5:323:HIS:CD2	2.54	0.43
24:D4:14:LEU:HD11	43:B1:12:ILE:HG23	2.01	0.43
25:D2:297:THR:HG22	25:D2:302:LEU:HD13	2.00	0.43
37:B7:112:LYS:HD3	37:B7:112:LYS:HA	1.81	0.43
2:V2:162:GLU:HB2	2:V2:186:PRO:HA	2.01	0.43
12:A2:43:LEU:HD11	12:A2:90:LEU:HD21	2.01	0.43
14:A6:52:ASP:H	14:A6:53:ILE:HD12	1.83	0.43
22:4L:54:THR:HG21	31:S5:28:ILE:HD11	2.01	0.43
22:4L:73:LEU:HD21	25:D2:41:ILE:HG13	2.01	0.43
23:D5:455:LYS:HG3	39:B2:28:PHE:CZ	2.54	0.43
33:B3:50:TRP:CD1	39:B2:12:ARG:HD3	2.54	0.43
1:V1:20:ARG:HD2	2:V2:202:LEU:HD23	2.01	0.43
1:V1:300:GLY:HA2	1:V1:330:GLY:N	2.33	0.43
3:S1:525:LEU:HD13	3:S1:525:LEU:HA	1.90	0.43
4:S2:390:LYS:HZ2	4:S2:390:LYS:HG2	1.61	0.43
20:D1:117:LEU:HD12	20:D1:132:ALA:HB1	2.00	0.43
20:D1:197:PRO:HA	20:D1:200:LEU:HB3	2.01	0.43
21:D6:68:PHE:HA	21:D6:71:THR:HG22	2.01	0.43
25:D2:145:ILE:HD12	25:D2:149:ILE:HD11	2.01	0.43
36:B6:103:ILE:H	36:B6:103:ILE:HG13	1.72	0.43
40:B8:50:LEU:HB2	40:B8:78:HIS:CD2	2.54	0.43
11:A9:171:ILE:H	11:A9:171:ILE:HG13	1.71	0.43
20:D1:219:PRO:HB3	20:D1:222:LEU:HD12	2.01	0.43
24:D4:106:LEU:HD13	24:D4:234:ILE:HG21	2.01	0.43
25:D2:69:LEU:HD11	25:D2:97:LEU:HD22	2.00	0.43
29:BJ:143:HIS:NE2	35:B4:125:ASN:O	2.48	0.43
38:B9:61:GLN:HG3	38:B9:64:ARG:HH22	1.83	0.43
3:S1:41:CYS:N	3:S1:52:CYS:SG	2.91	0.42
3:S1:348:VAL:N	3:S1:459:GLN:OE1	2.43	0.42
4:S2:405:MET:SD	4:S2:421:GLN:NE2	2.92	0.42
5:S3:77:ASP:O	5:S3:93:VAL:O	2.37	0.42
6:S7:141:PRO:HB3	11:A9:61:PRO:HD3	2.01	0.42
23:D5:264:TYR:HA	23:D5:267:THR:HG22	2.01	0.42
4:S2:326:ASP:HB2	5:S3:10:THR:HG21	2.00	0.42
19:D3:27:LEU:HD13	19:D3:29:VAL:HG23	2.01	0.42
24:D4:75:LEU:HD11	24:D4:440:HIS:CE1	2.54	0.42
25:D2:210:ILE:HG22	25:D2:333:SER:HB3	2.01	0.42
36:B6:92:LYS:O	36:B6:95:THR:OG1	2.32	0.42
37:B7:103:ARG:NH2	39:B2:64:LEU:O	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S1:95:GLU:OE1	3:S1:129:ARG:NH2	2.50	0.42
5:S3:66:ASP:HB2	13:A5:89:LEU:HD23	2.01	0.42
18:AM:114:ARG:HD3	28:A8:141:TYR:HA	2.01	0.42
20:D1:18:ALA:O	20:D1:21:THR:OG1	2.27	0.42
21:D6:127:ILE:H	21:D6:127:ILE:HG13	1.66	0.42
23:D5:183:ILE:HD13	24:D4:382:VAL:HG11	2.00	0.42
23:D5:550:SER:HA	24:D4:275:ILE:HG13	2.01	0.42
29:BJ:138:TYR:HA	41:BK:108:MET:HE1	2.01	0.42
3:S1:10:GLU:O	3:S1:76:GLY:HA2	2.19	0.42
4:S2:335:ARG:NH1	4:S2:338:MET:SD	2.92	0.42
8:V3:38:TYR:CZ	8:V3:40:ASN:HB2	2.54	0.42
11:A9:177:ARG:NH2	50:A9:401:NDP:O1N	2.52	0.42
19:D3:26:GLN:HB2	20:D1:59:GLU:HG3	2.01	0.42
23:D5:335:PHE:HZ	23:D5:380:LEU:HB2	1.84	0.42
24:D4:4:TYR:HE2	24:D4:41:LEU:HD12	1.84	0.42
24:D4:297:VAL:O	24:D4:301:ILE:HG12	2.20	0.42
25:D2:318:PRO:HB2	30:AJ:305:ARG:HH11	1.85	0.42
27:B5:32:THR:HA	27:B5:35:PRO:HD2	2.01	0.42
28:A8:94:GLN:HE22	44:A1:37:ARG:CZ	2.33	0.42
27:B5:114:MET:HG3	27:B5:120:GLY:HA3	2.00	0.42
34:C2:30:ARG:HE	34:C2:76:LEU:HD11	1.83	0.42
41:BK:53:VAL:HA	41:BK:56:TRP:HB2	2.01	0.42
3:S1:376:VAL:HG22	3:S1:405:LYS:HB3	2.02	0.42
5:S3:21:GLN:HE22	15:A7:98:PRO:HD3	1.84	0.42
9:S6:75:LEU:HD23	9:S6:75:LEU:HA	1.91	0.42
13:A5:5:LYS:HB3	13:A5:6:LYS:H	1.55	0.42
38:B9:29:ARG:HD3	38:B9:75:HIS:HB2	2.01	0.42
1:V1:306:LEU:HD22	1:V1:343:ILE:HD11	2.00	0.42
2:V2:91:ASN:OD1	2:V2:91:ASN:N	2.52	0.42
3:S1:126:ASP:HA	4:S2:347:HIS:HE1	1.85	0.42
3:S1:243:ARG:HG2	3:S1:244:THR:HG23	2.01	0.42
4:S2:322:GLU:HG2	4:S2:323:ILE:H	1.84	0.42
11:A9:109:VAL:O	11:A9:113:ILE:HB	2.19	0.42
17:AA:14:ARG:HA	17:AA:17:TYR:CE2	2.54	0.42
25:D2:84:TRP:HB2	31:S5:18:THR:HA	2.01	0.42
29:BJ:169:THR:O	29:BJ:173:ALA:HB2	2.20	0.42
3:S1:113:GLU:OE2	10:S4:43:ASN:ND2	2.48	0.42
4:S2:162:GLY:HA3	20:D1:279:ARG:H	1.84	0.42
4:S2:309:ARG:HD2	18:AM:20:TYR:CE2	2.55	0.42
11:A9:94:LEU:HG	11:A9:132:ILE:HG12	2.00	0.42
16:AL:83:PRO:HA	16:AL:84:PRO:HD3	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AM:139:PHE:HB2	44:A1:45:TRP:CG	2.53	0.42
23:D5:66:TRP:CE3	23:D5:78:LEU:HD23	2.54	0.42
25:D2:10:LEU:HD23	25:D2:10:LEU:HA	1.86	0.42
33:B3:28:LEU:HA	33:B3:31:VAL:HG12	2.02	0.42
1:V1:404:ILE:HD13	1:V1:404:ILE:HA	1.81	0.42
3:S1:286:ASN:CB	3:S1:290:LEU:O	2.67	0.42
3:S1:409:ILE:HG12	3:S1:422:LEU:HB2	2.01	0.42
20:D1:24:GLU:OE2	20:D1:195:ARG:NH2	2.51	0.42
4:S2:173:GLU:OE2	4:S2:221:ARG:NH1	2.53	0.42
16:AL:106:ARG:HD2	16:AL:108:PHE:HE2	1.85	0.42
18:AM:127:ARG:HB2	18:AM:132:ILE:HG23	2.01	0.42
23:D5:375:ILE:HD12	39:B2:32:MET:HG3	2.01	0.42
28:A8:82:THR:HA	28:A8:85:TRP:NE1	2.35	0.42
7:S8:141:THR:HG22	7:S8:143:THR:H	1.85	0.41
24:D4:250:LEU:HD23	24:D4:250:LEU:HA	1.88	0.41
30:AJ:78:SER:OG	30:AJ:92:ASN:OD1	2.39	0.41
30:AJ:278:PHE:HA	30:AJ:283:THR:HG21	2.02	0.41
32:A3:79:TRP:HA	32:A3:82:ARG:HB2	2.00	0.41
1:V1:49:LEU:HB3	1:V1:127:ARG:HG2	2.02	0.41
2:V2:166:PRO:HA	2:V2:169:ILE:HB	2.01	0.41
4:S2:52:GLY:HA3	4:S2:53:PRO:HD3	1.79	0.41
13:A5:77:GLU:HA	13:A5:80:ILE:HD12	2.02	0.41
20:D1:141:SER:HB3	20:D1:289:LEU:HG	2.02	0.41
23:D5:546:GLN:HB2	24:D4:278:ARG:HD3	2.02	0.41
1:V1:132:ARG:HH12	8:V3:66:PRO:HG3	1.85	0.41
7:S8:147:LEU:HD23	7:S8:147:LEU:HA	1.87	0.41
19:D3:26:GLN:HB3	19:D3:27:LEU:H	1.74	0.41
23:D5:145:GLU:HB2	24:D4:370:PRO:HG3	2.01	0.41
25:D2:13:VAL:HG13	25:D2:36:ASN:HD21	1.84	0.41
17:AB:48:VAL:HG21	38:B9:16:LEU:HD11	2.02	0.41
29:BJ:88:GLU:OE2	29:BJ:150:SER:OG	2.33	0.41
2:V2:101:GLN:HA	2:V2:140:ILE:O	2.21	0.41
3:S1:252:PRO:HB3	3:S1:263:ILE:HB	2.02	0.41
3:S1:335:LEU:HA	3:S1:335:LEU:HD12	1.77	0.41
4:S2:161:ILE:HG21	4:S2:235:TRP:HE1	1.85	0.41
11:A9:234:ASN:HB3	11:A9:236:TYR:CD1	2.55	0.41
24:D4:47:ASP:OD1	24:D4:47:ASP:N	2.52	0.41
24:D4:203:PHE:O	24:D4:207:MET:HG2	2.21	0.41
41:BK:98:LYS:HB3	41:BK:98:LYS:HE3	1.87	0.41
3:S1:12:PHE:HA	3:S1:16:GLN:O	2.20	0.41
5:S3:50:ILE:HG22	5:S3:52:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S3:169:SER:OG	6:S7:134:ARG:NH2	2.53	0.41
11:A9:203:GLN:HB3	11:A9:235:ARG:HA	2.02	0.41
25:D2:172:GLN:HE21	25:D2:177:LYS:HD2	1.86	0.41
28:A8:148:GLU:O	31:S5:50:ARG:NH2	2.53	0.41
29:BJ:132:THR:HA	29:BJ:135:VAL:HG12	2.02	0.41
36:B6:103:ILE:HD11	37:B7:47:ASP:HB3	2.01	0.41
2:V2:161:TYR:HB3	2:V2:164:LEU:HD11	2.02	0.41
4:S2:205:LEU:HD22	15:A7:35:GLN:HG2	2.03	0.41
6:S7:42:ARG:HH12	6:S7:168:LYS:HD2	1.86	0.41
6:S7:85:VAL:HG12	6:S7:112:TYR:HB2	2.03	0.41
7:S8:87:CYS:HA	7:S8:88:PRO:HD3	1.87	0.41
22:4L:88:ASP:OD1	22:4L:88:ASP:N	2.52	0.41
24:D4:370:PRO:HA	24:D4:375:LEU:HD13	2.03	0.41
29:BJ:152:ARG:NH2	34:C2:114:GLU:OE2	2.54	0.41
37:B7:36:ARG:HD3	37:B7:36:ARG:HA	1.76	0.41
3:S1:243:ARG:O	3:S1:246:GLU:C	2.59	0.41
7:S8:105:ARG:HB3	7:S8:106:THR:H	1.56	0.41
11:A9:97:ARG:HG3	11:A9:99:TRP:H	1.86	0.41
19:D3:59:ALA:HB1	21:D6:66:VAL:HG13	2.02	0.41
20:D1:167:ILE:HD12	28:A8:97:ARG:HH21	1.86	0.41
25:D2:1:MET:SD	25:D2:46:LYS:NZ	2.82	0.41
1:V1:49:LEU:HD22	1:V1:127:ARG:HB3	2.02	0.41
9:S6:24:ARG:HG2	9:S6:27:ARG:NE	2.35	0.41
13:A5:10:LEU:HD22	13:A5:13:LEU:HD13	2.02	0.41
20:D1:126:LYS:O	20:D1:130:ILE:HG12	2.21	0.41
20:D1:157:ASN:HB3	20:D1:168:THR:HG21	2.02	0.41
23:D5:416:THR:HA	23:D5:419:THR:HG22	2.03	0.41
23:D5:477:ILE:HD11	37:B7:54:GLN:HG2	2.02	0.41
24:D4:80:SER:HB3	24:D4:226:ALA:HB2	2.02	0.41
29:BJ:48:ARG:HD2	36:B6:87:TYR:CE2	2.55	0.41
34:C2:25:LYS:N	34:C2:28:ASP:OD2	2.54	0.41
1:V1:52:GLY:HA2	1:V1:53:PRO:HD3	1.92	0.41
2:V2:8:VAL:H	2:V2:10:ARG:HH12	1.69	0.41
3:S1:358:LEU:HD13	3:S1:358:LEU:HA	1.95	0.41
4:S2:224:GLU:OE1	7:S8:40:TYR:OH	2.36	0.41
4:S2:242:ILE:H	4:S2:242:ILE:HG13	1.78	0.41
4:S2:366:ALA:HA	4:S2:374:PHE:O	2.21	0.41
6:S7:72:PHE:HE2	6:S7:157:LEU:HD11	1.86	0.41
7:S8:96:ALA:HA	7:S8:106:THR:HA	2.03	0.41
10:S4:17:LEU:HB2	10:S4:98:LYS:HG3	2.03	0.41
13:A5:35:GLY:HA2	13:A5:44:ARG:HH22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:D6:164:GLY:O	21:D6:168:ILE:HG12	2.21	0.41
23:D5:184:LEU:HD21	23:D5:211:LEU:HD12	2.01	0.41
23:D5:245:ALA:O	23:D5:249:SER:OG	2.35	0.41
23:D5:293:LEU:HA	23:D5:293:LEU:HD23	1.91	0.41
24:D4:253:ILE:H	24:D4:253:ILE:HG13	1.53	0.41
27:B5:124:GLN:HG2	31:S5:47:GLY:HA3	2.01	0.41
30:AJ:97:GLN:HG2	30:AJ:135:LEU:HD22	2.03	0.41
38:B9:19:TYR:HB2	38:B9:47:PHE:HE2	1.85	0.41
38:B9:167:TRP:O	38:B9:171:THR:OG1	2.24	0.41
39:B2:33:TRP:HA	39:B2:36:ILE:HG22	2.03	0.41
1:V1:202:LYS:HB3	1:V1:361:GLN:NE2	2.36	0.41
6:S7:127:HIS:CG	7:S8:115:LYS:HE3	2.55	0.41
22:4L:24:SER:HA	22:4L:90:VAL:HG23	2.03	0.41
1:V1:108:ARG:O	1:V1:112:ARG:HB2	2.21	0.40
1:V1:179:ARG:NH1	2:V2:52:ASP:OD2	2.54	0.40
1:V1:337:MET:SD	1:V1:337:MET:N	2.93	0.40
4:S2:11:ALA:O	4:S2:15:GLY:N	2.54	0.40
5:S3:77:ASP:OD1	5:S3:78:LEU:N	2.35	0.40
11:A9:177:ARG:NH1	50:A9:401:NDP:O2N	2.54	0.40
14:A6:16:VAL:HG11	14:A6:76:ARG:NH1	2.36	0.40
20:D1:212:ASN:HB3	20:D1:220:PHE:HE1	1.86	0.40
23:D5:83:ASP:H	23:D5:86:SER:HB3	1.86	0.40
27:B5:84:GLU:HG2	43:B1:44:TYR:CD2	2.57	0.40
2:V2:24:THR:H	2:V2:27:ASN:HB2	1.86	0.40
2:V2:105:THR:OG1	47:V2:300:FES:S2	2.75	0.40
5:S3:111:THR:OG1	5:S3:112:ASP:N	2.54	0.40
23:D5:7:LEU:HD23	23:D5:50:PRO:HG3	2.02	0.40
23:D5:558:LEU:HA	23:D5:558:LEU:HD13	1.86	0.40
25:D2:277:ILE:HD13	52:AK:201:PC1:H221	2.03	0.40
27:B5:83:PRO:O	27:B5:87:TYR:HB2	2.21	0.40
36:B6:35:PRO:HA	36:B6:36:PRO:HD3	1.91	0.40
1:V1:97:ALA:HB3	1:V1:138:ILE:HA	2.02	0.40
3:S1:266:LYS:O	3:S1:270:ALA:CB	2.68	0.40
3:S1:382:THR:OG1	3:S1:387:GLU:OE1	2.33	0.40
6:S7:43:SER:OG	6:S7:44:SER:N	2.53	0.40
28:A8:127:VAL:HG13	32:A3:65:VAL:HG23	2.02	0.40
30:AJ:127:SER:O	30:AJ:130:SER:OG	2.27	0.40
37:B7:11:ASP:N	37:B7:11:ASP:OD1	2.52	0.40
1:V1:184:TYR:CZ	46:V1:501:FMN:H6	2.57	0.40
2:V2:55:GLN:NE2	2:V2:91:ASN:OD1	2.54	0.40
3:S1:355:GLY:HA2	3:S1:361:ASN:ND2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A5:54:LYS:HA	13:A5:57:ILE:HD12	2.03	0.40
23:D5:149:ILE:HD13	23:D5:149:ILE:HA	1.86	0.40
26:AK:68:ILE:HD13	26:AK:99:THR:HG21	2.01	0.40
4:S2:407:LYS:HA	4:S2:407:LYS:HD2	1.94	0.40
11:A9:279:THR:HG22	11:A9:283:LYS:HZ2	1.86	0.40
20:D1:127:TYR:HB3	20:D1:213:VAL:HG21	2.03	0.40
24:D4:124:ALA:HA	25:D2:256:PRO:HG3	2.02	0.40
24:D4:175:ASN:OD1	24:D4:176:PHE:N	2.54	0.40
24:D4:450:ASN:HD21	24:D4:452:LYS:HE3	1.86	0.40
38:B9:15:VAL:HG22	38:B9:63:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V1	428/445 (96%)	382 (89%)	46 (11%)	0	100	100
2	V2	210/217 (97%)	175 (83%)	35 (17%)	0	100	100
3	S1	686/704 (97%)	604 (88%)	80 (12%)	2 (0%)	41	76
4	S2	428/430 (100%)	369 (86%)	57 (13%)	2 (0%)	29	68
5	S3	206/228 (90%)	181 (88%)	25 (12%)	0	100	100
6	S7	154/179 (86%)	135 (88%)	18 (12%)	1 (1%)	25	65
7	S8	174/176 (99%)	155 (89%)	19 (11%)	0	100	100
8	V3	39/75 (52%)	32 (82%)	7 (18%)	0	100	100
9	S6	93/96 (97%)	85 (91%)	8 (9%)	0	100	100
10	S4	124/133 (93%)	108 (87%)	16 (13%)	0	100	100
11	A9	305/338 (90%)	268 (88%)	37 (12%)	0	100	100
12	A2	80/98 (82%)	70 (88%)	10 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	A5	109/115 (95%)	96 (88%)	13 (12%)	0	100	100
14	A6	112/127 (88%)	104 (93%)	8 (7%)	0	100	100
15	A7	91/112 (81%)	73 (80%)	17 (19%)	1 (1%)	14	52
16	AL	121/145 (83%)	97 (80%)	24 (20%)	0	100	100
17	AA	78/88 (89%)	65 (83%)	13 (17%)	0	100	100
17	AB	85/88 (97%)	77 (91%)	8 (9%)	0	100	100
18	AM	137/143 (96%)	122 (89%)	15 (11%)	0	100	100
19	D3	113/115 (98%)	90 (80%)	23 (20%)	0	100	100
20	D1	316/318 (99%)	269 (85%)	45 (14%)	2 (1%)	25	65
21	D6	173/175 (99%)	150 (87%)	23 (13%)	0	100	100
22	4L	96/98 (98%)	86 (90%)	9 (9%)	1 (1%)	15	54
23	D5	604/606 (100%)	544 (90%)	59 (10%)	1 (0%)	47	81
24	D4	457/459 (100%)	422 (92%)	35 (8%)	0	100	100
25	D2	345/347 (99%)	315 (91%)	30 (9%)	0	100	100
26	AK	138/140 (99%)	128 (93%)	10 (7%)	0	100	100
27	B5	137/143 (96%)	124 (90%)	12 (9%)	1 (1%)	22	62
28	A8	169/171 (99%)	137 (81%)	32 (19%)	0	100	100
29	BJ	169/175 (97%)	155 (92%)	14 (8%)	0	100	100
30	AJ	317/320 (99%)	274 (86%)	43 (14%)	0	100	100
31	S5	97/105 (92%)	84 (87%)	13 (13%)	0	100	100
32	A3	72/83 (87%)	61 (85%)	11 (15%)	0	100	100
33	B3	71/97 (73%)	58 (82%)	13 (18%)	0	100	100
34	C2	117/120 (98%)	107 (92%)	10 (8%)	0	100	100
35	B4	126/128 (98%)	109 (86%)	17 (14%)	0	100	100
36	B6	91/127 (72%)	78 (86%)	12 (13%)	1 (1%)	14	52
37	B7	117/136 (86%)	99 (85%)	18 (15%)	0	100	100
38	B9	174/178 (98%)	145 (83%)	29 (17%)	0	100	100
39	B2	62/72 (86%)	57 (92%)	5 (8%)	0	100	100
40	B8	155/158 (98%)	118 (76%)	36 (23%)	1 (1%)	25	65
41	BK	100/125 (80%)	85 (85%)	15 (15%)	0	100	100
42	C1	44/49 (90%)	40 (91%)	4 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
43	B1	50/57 (88%)	37 (74%)	13 (26%)	0	100 100
44	A1	68/70 (97%)	64 (94%)	4 (6%)	0	100 100
All	All	8038/8509 (94%)	7034 (88%)	991 (12%)	13 (0%)	50 81

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	S2	293	CYS
6	S7	54	CYS
22	4L	3	LEU
15	A7	69	MET
4	S2	73	VAL
3	S1	424	ASP
23	D5	549	ALA
20	D1	92	PRO
27	B5	13	PRO
40	B8	17	PRO
3	S1	338	VAL
20	D1	197	PRO
36	B6	32	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	V1	344/354 (97%)	340 (99%)	4 (1%)	71 84
2	V2	182/183 (100%)	180 (99%)	2 (1%)	73 85
3	S1	578/588 (98%)	574 (99%)	4 (1%)	84 90
4	S2	371/371 (100%)	368 (99%)	3 (1%)	81 89
5	S3	189/204 (93%)	188 (100%)	1 (0%)	88 93
6	S7	132/150 (88%)	130 (98%)	2 (2%)	65 80
7	S8	151/151 (100%)	149 (99%)	2 (1%)	69 82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	V3	40/68 (59%)	36 (90%)	4 (10%)	7 28
9	S6	79/80 (99%)	79 (100%)	0	100 100
10	S4	113/119 (95%)	112 (99%)	1 (1%)	78 88
11	A9	269/292 (92%)	266 (99%)	3 (1%)	73 85
12	A2	73/81 (90%)	72 (99%)	1 (1%)	67 81
13	A5	99/101 (98%)	99 (100%)	0	100 100
14	A6	107/113 (95%)	107 (100%)	0	100 100
15	A7	83/94 (88%)	82 (99%)	1 (1%)	71 84
16	AL	114/131 (87%)	110 (96%)	4 (4%)	36 60
17	AA	74/81 (91%)	73 (99%)	1 (1%)	67 81
17	AB	80/81 (99%)	77 (96%)	3 (4%)	33 58
18	AM	119/121 (98%)	115 (97%)	4 (3%)	37 61
19	D3	103/103 (100%)	102 (99%)	1 (1%)	76 86
20	D1	278/278 (100%)	277 (100%)	1 (0%)	91 94
21	D6	144/144 (100%)	142 (99%)	2 (1%)	67 81
22	4L	87/87 (100%)	85 (98%)	2 (2%)	50 70
23	D5	539/539 (100%)	534 (99%)	5 (1%)	78 88
24	D4	412/412 (100%)	406 (98%)	6 (2%)	65 80
25	D2	315/315 (100%)	309 (98%)	6 (2%)	57 75
26	AK	101/101 (100%)	99 (98%)	2 (2%)	55 73
27	B5	122/125 (98%)	121 (99%)	1 (1%)	81 89
28	A8	154/154 (100%)	150 (97%)	4 (3%)	46 67
29	BJ	155/157 (99%)	154 (99%)	1 (1%)	86 92
30	AJ	283/284 (100%)	280 (99%)	3 (1%)	73 85
31	S5	88/94 (94%)	88 (100%)	0	100 100
32	A3	65/71 (92%)	65 (100%)	0	100 100
33	B3	55/75 (73%)	53 (96%)	2 (4%)	35 60
34	C2	106/107 (99%)	106 (100%)	0	100 100
35	B4	114/114 (100%)	113 (99%)	1 (1%)	78 88
36	B6	91/121 (75%)	89 (98%)	2 (2%)	52 71
37	B7	108/119 (91%)	104 (96%)	4 (4%)	34 59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
38	B9	159/160 (99%)	156 (98%)	3 (2%)	57 75
39	B2	58/62 (94%)	58 (100%)	0	100 100
40	B8	142/142 (100%)	139 (98%)	3 (2%)	53 72
41	BK	93/112 (83%)	91 (98%)	2 (2%)	52 71
42	C1	42/44 (96%)	42 (100%)	0	100 100
43	B1	48/53 (91%)	48 (100%)	0	100 100
44	A1	59/59 (100%)	56 (95%)	3 (5%)	24 51
All	All	7118/7395 (96%)	7024 (99%)	94 (1%)	70 82

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V1	132	ARG
1	V1	359	CYS
1	V1	365	CYS
1	V1	385	ARG
2	V2	104	THR
2	V2	190	ARG
3	S1	152	ARG
3	S1	490	MET
3	S1	543	ILE
3	S1	601	ARG
4	S2	34	ASN
4	S2	388	ARG
4	S2	418	ILE
5	S3	78	LEU
6	S7	54	CYS
6	S7	174	ARG
7	S8	8	ARG
7	S8	78	ILE
8	V3	54	LEU
8	V3	60	LYS
8	V3	63	MET
8	V3	70	ARG
10	S4	16	LYS
11	A9	56	THR
11	A9	184	ASN
11	A9	292	ARG
12	A2	33	ARG
15	A7	22	LYS

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Mol	Chain	Res	Type
16	AL	68	MET
16	AL	72	ASN
16	AL	101	LYS
16	AL	117	LEU
17	AA	44	SER
18	AM	60	GLN
18	AM	67	ARG
18	AM	85	MET
18	AM	89	ASN
19	D3	1	MET
20	D1	46	LEU
21	D6	2	MET
21	D6	54	LEU
22	4L	58	MET
22	4L	83	ASN
23	D5	59	GLN
23	D5	82	MET
23	D5	113	ASN
23	D5	357	ARG
23	D5	581	LYS
24	D4	43	ASN
24	D4	86	LYS
24	D4	138	ASN
24	D4	143	LEU
24	D4	144	ASN
24	D4	251	ASN
25	D2	36	ASN
25	D2	78	LEU
25	D2	176	ARG
25	D2	204	ASN
25	D2	311	MET
25	D2	322	ARG
26	AK	114	CYS
26	AK	139	LYS
27	B5	130	LYS
17	AB	33	ASN
17	AB	54	MET
17	AB	80	ILE
28	A8	63	ASN
28	A8	109	CYS
28	A8	134	ARG
28	A8	150	ASN

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Mol	Chain	Res	Type
29	BJ	90	GLN
30	AJ	17	LYS
30	AJ	92	ASN
30	AJ	242	LYS
33	B3	47	ASN
33	B3	58	ASN
35	B4	74	ASN
36	B6	10	ARG
36	B6	31	GLU
37	B7	7	ARG
37	B7	83	GLN
37	B7	103	ARG
37	B7	105	ARG
38	B9	44	ARG
38	B9	157	ARG
38	B9	174	ARG
40	B8	9	LEU
40	B8	96	VAL
40	B8	137	ASN
41	BK	27	GLN
41	BK	57	ASN
44	A1	50	ARG
44	A1	58	ASN
44	A1	68	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	V1	37	GLN
1	V1	200	GLN
1	V1	293	ASN
2	V2	55	GLN
2	V2	99	HIS
2	V2	159	ASN
3	S1	36	GLN
3	S1	336	ASN
3	S1	621	ASN
3	S1	665	GLN
4	S2	34	ASN
4	S2	84	HIS
4	S2	347	HIS
5	S3	39	GLN

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Mol	Chain	Res	Type
5	S3	88	ASN
5	S3	192	GLN
6	S7	162	GLN
8	V3	44	HIS
10	S4	46	GLN
11	A9	3	HIS
11	A9	58	HIS
11	A9	89	ASN
11	A9	288	HIS
12	A2	61	GLN
13	A5	72	GLN
13	A5	82	GLN
15	A7	28	GLN
16	AL	31	ASN
16	AL	46	ASN
16	AL	69	ASN
16	AL	72	ASN
17	AA	74	GLN
18	AM	60	GLN
18	AM	75	GLN
18	AM	89	ASN
20	D1	124	ASN
20	D1	138	GLN
21	D6	120	ASN
22	4L	7	ASN
22	4L	83	ASN
23	D5	113	ASN
23	D5	205	ASN
23	D5	354	GLN
23	D5	405	ASN
23	D5	446	ASN
23	D5	479	GLN
23	D5	509	HIS
23	D5	541	ASN
23	D5	570	GLN
23	D5	580	GLN
24	D4	43	ASN
24	D4	51	ASN
24	D4	144	ASN
24	D4	319	HIS
24	D4	390	ASN
25	D2	36	ASN

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Mol	Chain	Res	Type
25	D2	63	GLN
25	D2	204	ASN
25	D2	235	ASN
25	D2	316	GLN
27	B5	143	ASN
17	AB	33	ASN
17	AB	47	GLN
28	A8	63	ASN
28	A8	150	ASN
29	BJ	77	HIS
29	BJ	103	ASN
29	BJ	113	GLN
30	AJ	92	ASN
30	AJ	97	GLN
30	AJ	141	GLN
30	AJ	204	ASN
30	AJ	239	GLN
30	AJ	251	GLN
31	S5	44	HIS
31	S5	81	GLN
32	A3	45	ASN
32	A3	51	ASN
33	B3	47	ASN
33	B3	58	ASN
34	C2	59	HIS
34	C2	88	HIS
35	B4	47	GLN
35	B4	74	ASN
36	B6	25	GLN
36	B6	82	HIS
37	B7	75	ASN
37	B7	91	HIS
38	B9	17	GLN
38	B9	32	HIS
38	B9	168	HIS
40	B8	78	HIS
40	B8	104	HIS
40	B8	137	ASN
41	BK	27	GLN
41	BK	45	HIS
41	BK	57	ASN
44	A1	58	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
46	FMN	V1	501	-	33,33,33	0.37	0	48,50,50	0.49	1 (2%)
51	ZMP	AB	101	17	24,30,36	0.74	1 (4%)	29,37,45	0.87	0
51	ZMP	AA	101	17	27,33,36	0.68	1 (3%)	32,40,45	1.02	2 (6%)
48	3PE	D5	701	-	37,37,50	0.34	0	40,42,55	0.35	0
47	FES	V2	300	2	0,4,4	-	-	-		
45	SF4	S1	802	3	0,12,12	-	-	-		
50	NDP	A9	401	-	45,52,52	0.74	2 (4%)	53,80,80	0.57	1 (1%)
52	PC1	AK	201	-	27,27,53	0.40	0	33,35,61	0.37	0
45	SF4	S1	801	3	0,12,12	-	-	-		
45	SF4	S8	202	7	0,12,12	-	-	-		
47	FES	S1	803	3	0,4,4	-	-	-		
45	SF4	S8	201	7	0,12,12	-	-	-		
45	SF4	S7	300	6	0,12,12	-	-	-		
48	3PE	S2	501	-	39,39,50	0.34	0	42,44,55	0.36	0
45	SF4	V1	500	1	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	FMN	V1	501	-	-	5/18/18/18	0/3/3/3
51	ZMP	AB	101	17	-	8/35/37/43	-
51	ZMP	AA	101	17	-	9/38/40/43	-
48	3PE	D5	701	-	-	10/41/41/54	-
47	FES	V2	300	2	-	-	0/1/1/1
45	SF4	S1	802	3	-	-	0/6/5/5
50	NDP	A9	401	-	-	16/30/77/77	0/5/5/5
52	PC1	AK	201	-	-	7/31/31/57	-
45	SF4	S1	801	3	-	-	0/6/5/5
45	SF4	S8	202	7	-	-	0/6/5/5
47	FES	S1	803	3	-	-	0/1/1/1
45	SF4	S8	201	7	-	-	0/6/5/5
45	SF4	S7	300	6	-	-	0/6/5/5
48	3PE	S2	501	-	-	9/43/43/54	-
45	SF4	V1	500	1	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	AA	101	ZMP	C9-C10	2.37	1.53	1.50
50	A9	401	NDP	P2B-O2B	2.35	1.63	1.59
51	AB	101	ZMP	C9-C10	2.28	1.53	1.50
50	A9	401	NDP	C8A-N7A	-2.08	1.31	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	A9	401	NDP	C5A-C6A-N6A	2.44	124.06	120.35
46	V1	501	FMN	P-O5'-C5'	2.42	124.96	118.30
51	AA	101	ZMP	C15-C14-C13	-2.30	108.53	112.36
51	AA	101	ZMP	O1-C10-C9	-2.21	121.38	123.99

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	V1	501	FMN	C4'-C5'-O5'-P
46	V1	501	FMN	C5'-O5'-P-O2P
46	V1	501	FMN	C5'-O5'-P-O3P
48	S2	501	3PE	C11-O13-P-O12
48	S2	501	3PE	O13-C11-C12-N
48	D5	701	3PE	C11-O13-P-O14
48	D5	701	3PE	O13-C11-C12-N
48	D5	701	3PE	O21-C2-C3-O31
50	A9	401	NDP	C5B-O5B-PA-O1A
50	A9	401	NDP	C5B-O5B-PA-O2A
50	A9	401	NDP	C2N-C3N-C7N-O7N
50	A9	401	NDP	C2N-C3N-C7N-N7N
51	AA	101	ZMP	C12-C11-S1-C10
51	AB	101	ZMP	C7-C8-C9-C10
51	AA	101	ZMP	C14-C13-N1-C12
51	AB	101	ZMP	C14-C13-N1-C12
51	AA	101	ZMP	O2-C13-N1-C12
51	AB	101	ZMP	O2-C13-N1-C12
50	A9	401	NDP	C3B-C2B-O2B-P2B
48	S2	501	3PE	C11-O13-P-O11
48	D5	701	3PE	C11-O13-P-O11
48	D5	701	3PE	C21-C22-C23-C24
50	A9	401	NDP	C1B-C2B-O2B-P2B
50	A9	401	NDP	C4B-C5B-O5B-PA
48	S2	501	3PE	C35-C36-C37-C38
51	AB	101	ZMP	C13-C14-C15-N2
48	D5	701	3PE	C22-C23-C24-C25
50	A9	401	NDP	C2D-C1D-N1N-C2N
52	AK	201	PC1	O11-C1-C2-C3
48	D5	701	3PE	C1-C2-C3-O31
50	A9	401	NDP	O4B-C4B-C5B-O5B
46	V1	501	FMN	C5'-O5'-P-O1P
51	AB	101	ZMP	C5-C6-C7-C8
51	AA	101	ZMP	C4-C5-C6-C7
51	AB	101	ZMP	C4-C5-C6-C7
48	S2	501	3PE	C25-C26-C27-C28
52	AK	201	PC1	O11-C1-C2-O21
51	AA	101	ZMP	O1-C10-S1-C11
50	A9	401	NDP	C2D-C1D-N1N-C6N
51	AA	101	ZMP	C9-C10-S1-C11
50	A9	401	NDP	O4D-C1D-N1N-C2N
52	AK	201	PC1	C11-O13-P-O11
48	D5	701	3PE	C11-O13-P-O12

Continued on next page...

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Mol	Chain	Res	Type	Atoms
51	AA	101	ZMP	C11-C12-N1-C13
52	AK	201	PC1	O13-C11-C12-N
50	A9	401	NDP	O4D-C1D-N1N-C6N
48	S2	501	3PE	C34-C35-C36-C37
52	AK	201	PC1	C1-O11-P-O13
51	AB	101	ZMP	C6-C7-C8-C9
52	AK	201	PC1	C2-C1-O11-P
48	S2	501	3PE	C1-C2-C3-O31
51	AA	101	ZMP	C19-C18-C21-O5
51	AB	101	ZMP	C12-C11-S1-C10
48	S2	501	3PE	O21-C2-C3-O31
50	A9	401	NDP	PA-O3-PN-O1N
50	A9	401	NDP	C2B-O2B-P2B-O1X
51	AA	101	ZMP	C22-C1-C2-C3
50	A9	401	NDP	C5B-O5B-PA-O3
50	A9	401	NDP	C2B-O2B-P2B-O3X
48	D5	701	3PE	C29-C2A-C2B-C2C
48	S2	501	3PE	C2-C1-O11-P
46	V1	501	FMN	C3'-C4'-C5'-O5'
52	AK	201	PC1	C1-O11-P-O14
48	D5	701	3PE	C12-C11-O13-P

There are no ring outliers.

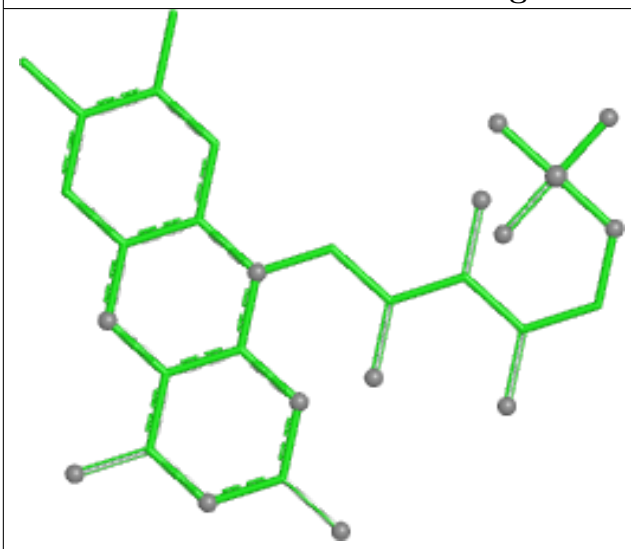
11 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	V1	501	FMN	4	0
51	AB	101	ZMP	1	0
51	AA	101	ZMP	1	0
48	D5	701	3PE	1	0
47	V2	300	FES	1	0
50	A9	401	NDP	4	0
52	AK	201	PC1	1	0
45	S1	801	SF4	1	0
45	S8	202	SF4	1	0
48	S2	501	3PE	3	0
45	V1	500	SF4	1	0

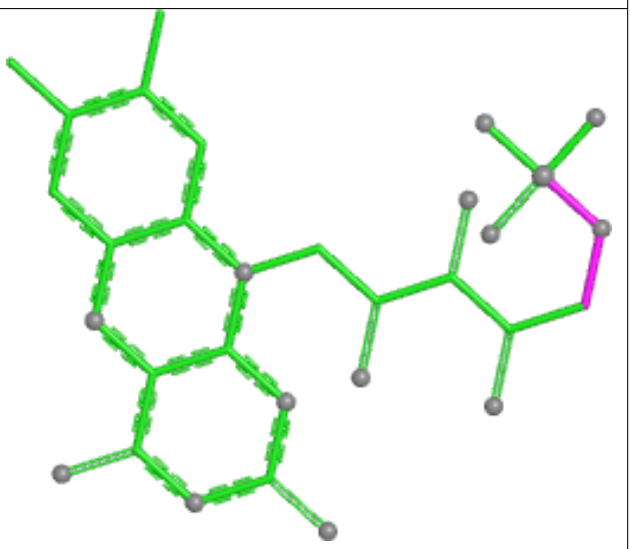
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

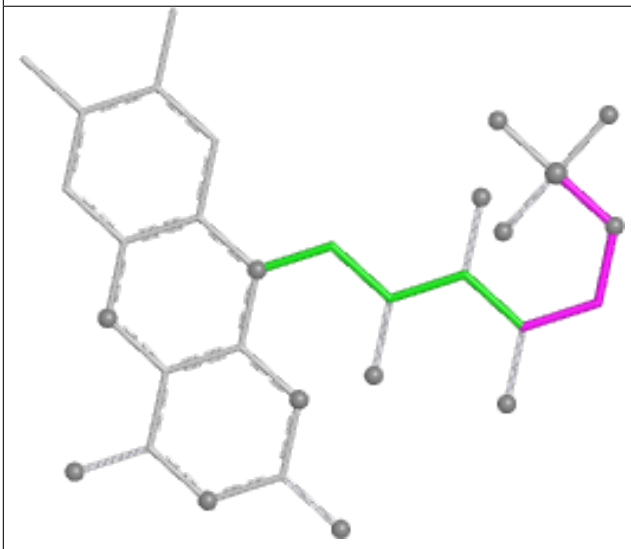
Ligand FMN V1 501



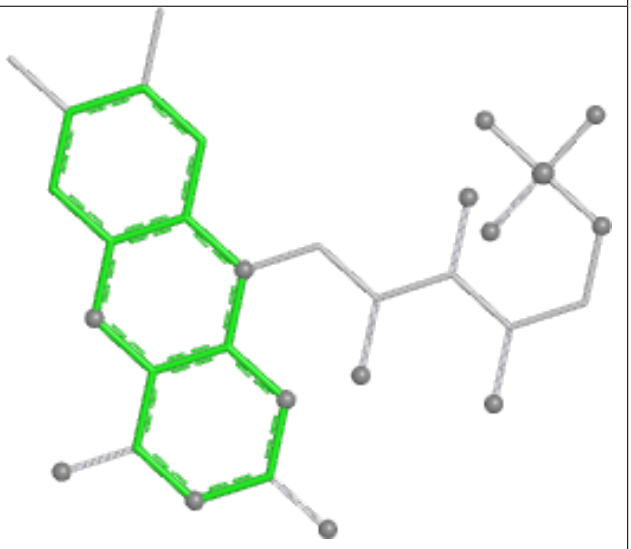
Bond lengths



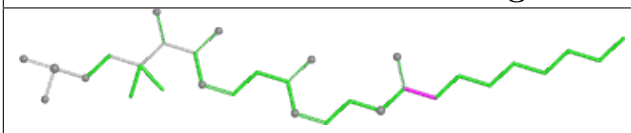
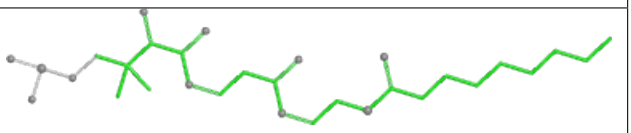
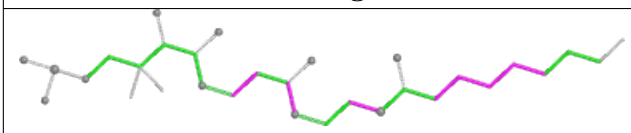
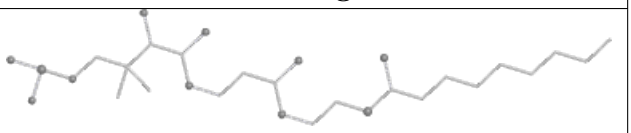
Bond angles

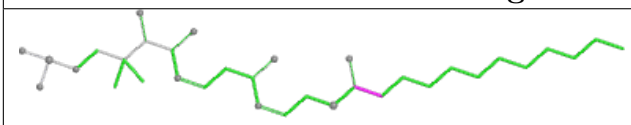
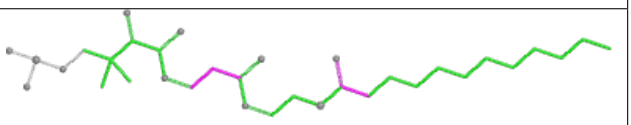
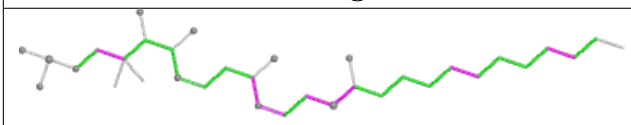
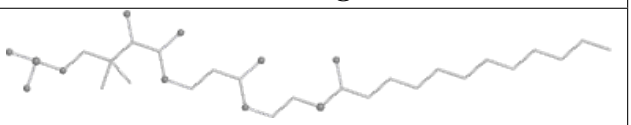


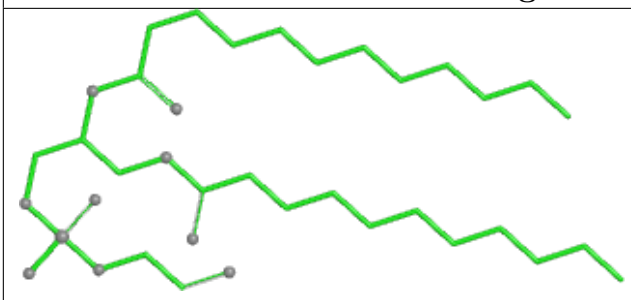
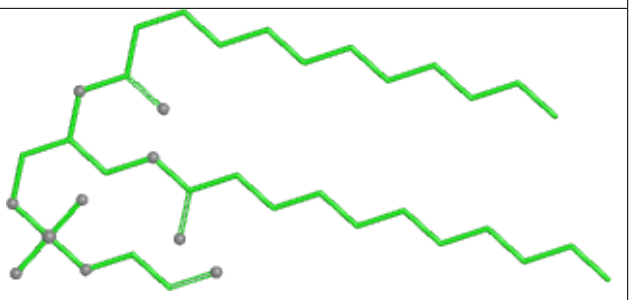
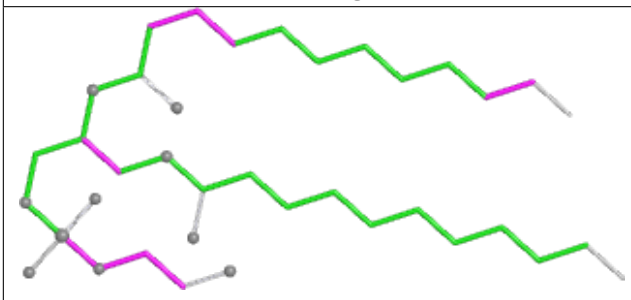
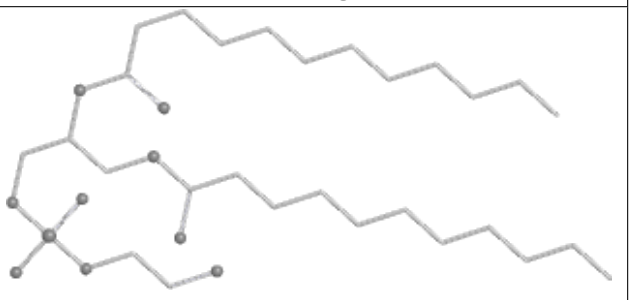
Torsions

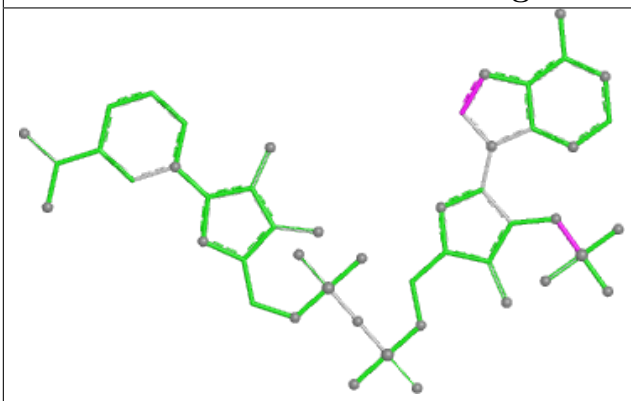
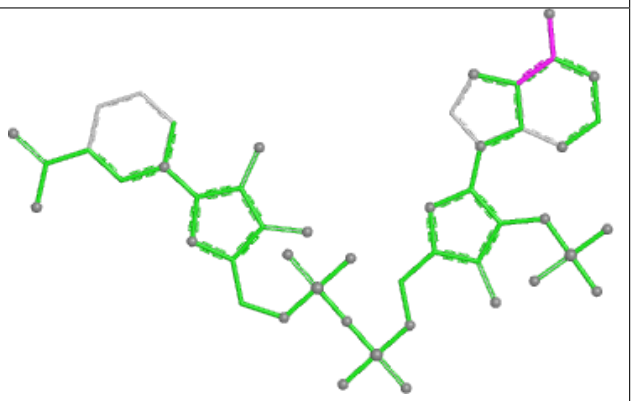
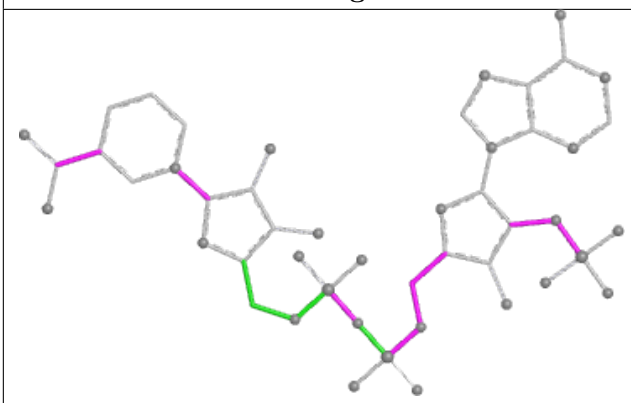
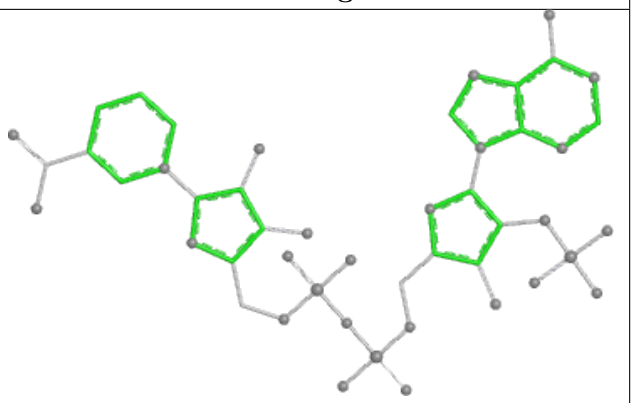


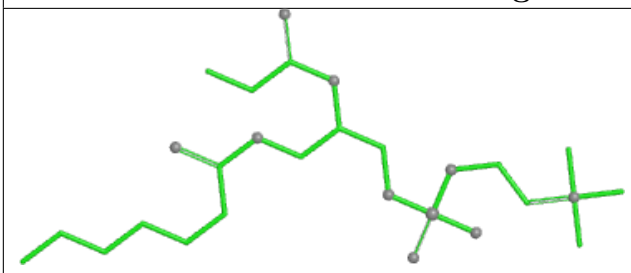
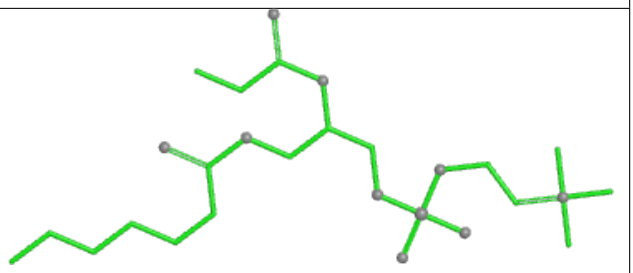
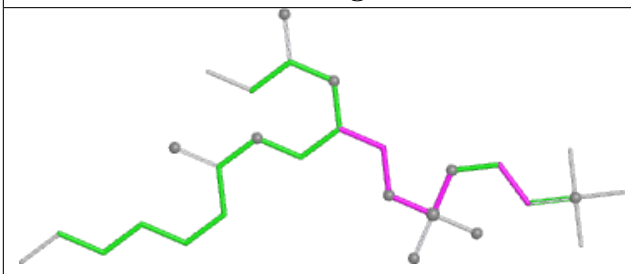
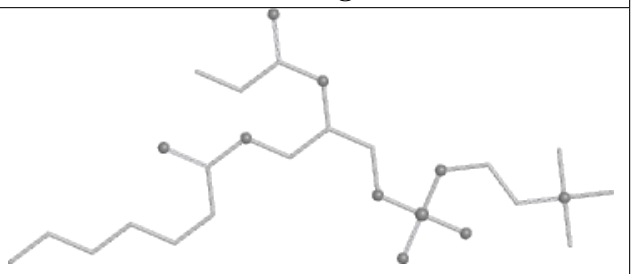
Rings

Ligand ZMP AB 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

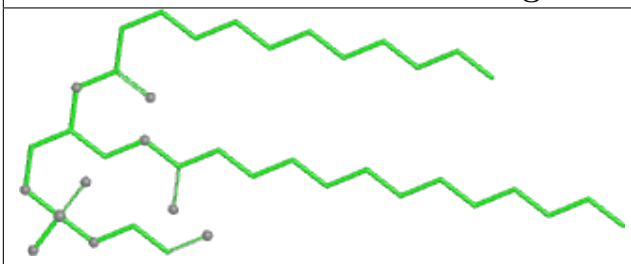
Ligand ZMP AA 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE D5 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

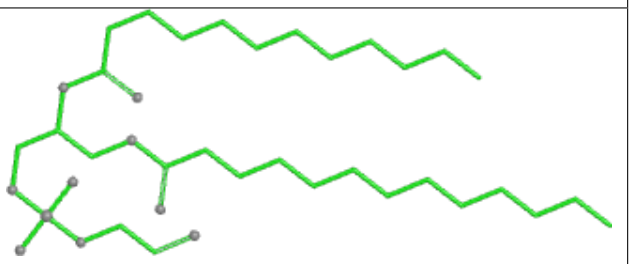
Ligand NDP A9 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 AK 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

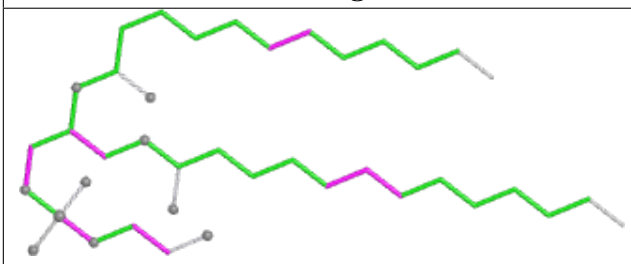
Ligand 3PE S2 501



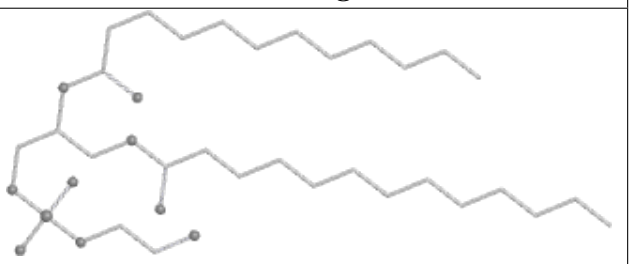
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

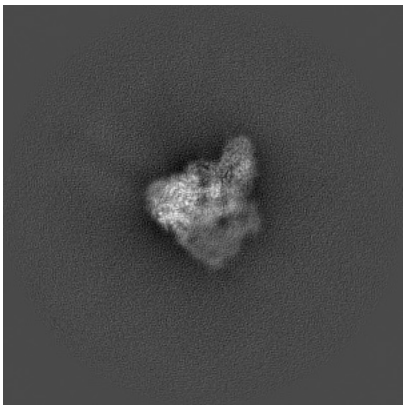
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4497. These allow visual inspection of the internal detail of the map and identification of artifacts.

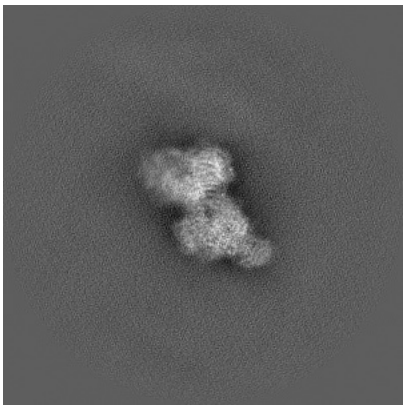
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

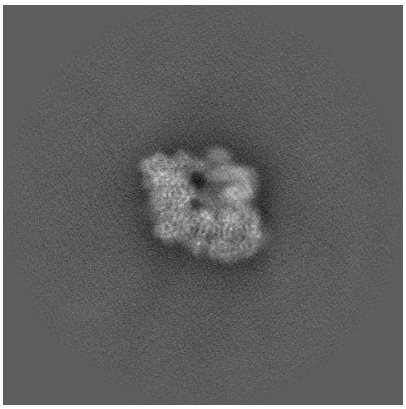
6.1.1 Primary map



X

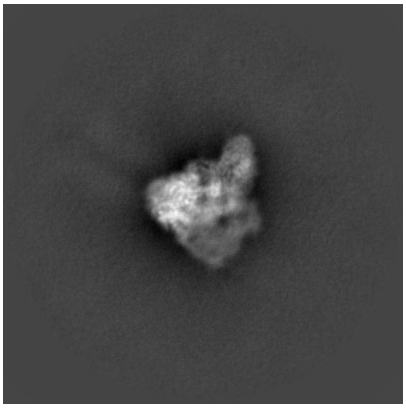


Y

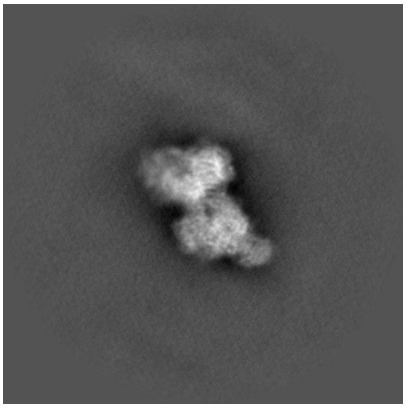


Z

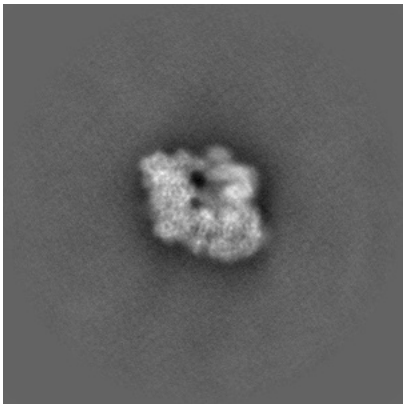
6.1.2 Raw map



X



Y

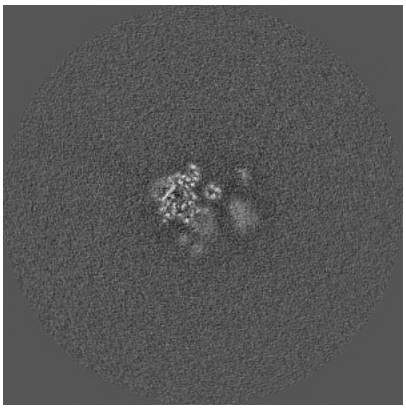


Z

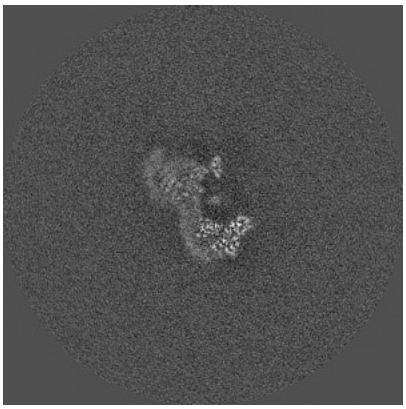
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

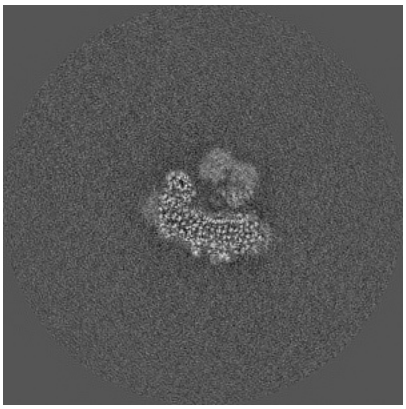
6.2.1 Primary map



X Index: 256

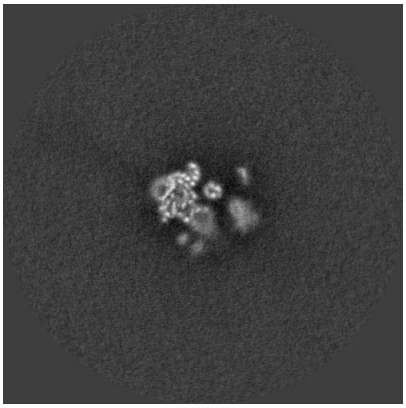


Y Index: 256

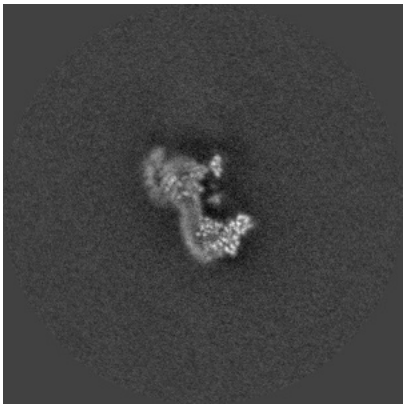


Z Index: 256

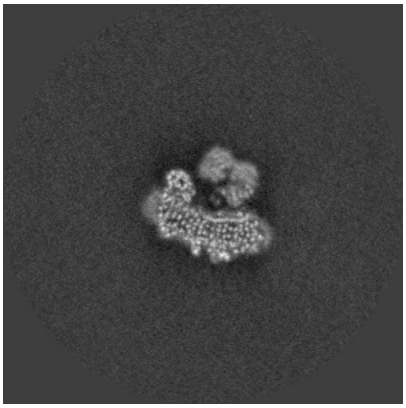
6.2.2 Raw map



X Index: 256



Y Index: 256

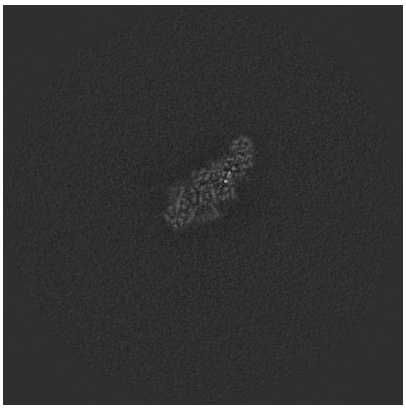


Z Index: 256

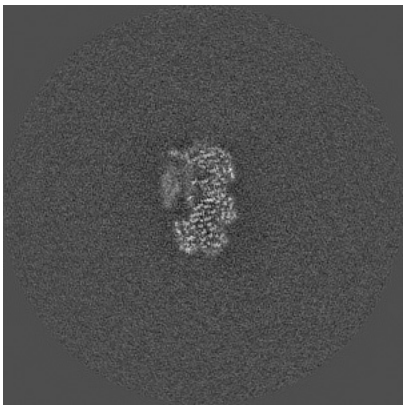
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

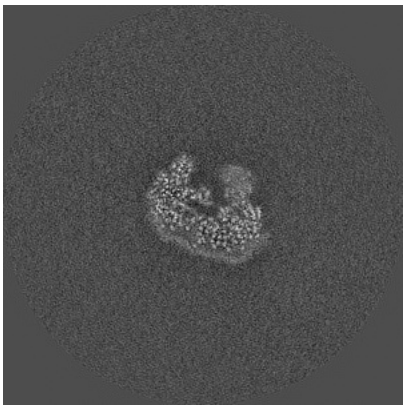
6.3.1 Primary map



X Index: 205

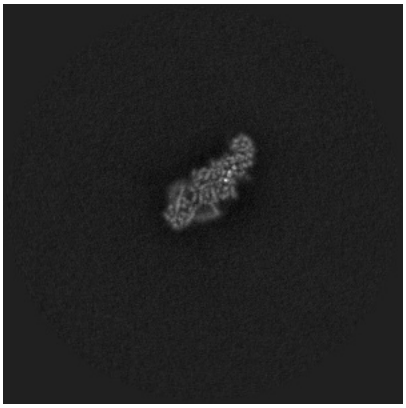


Y Index: 229

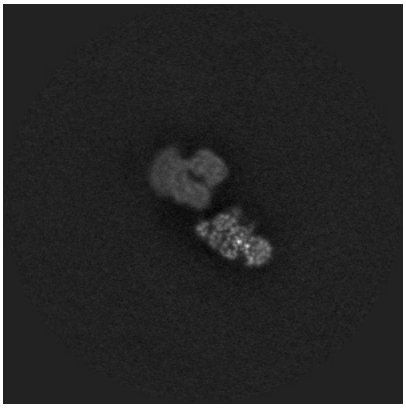


Z Index: 272

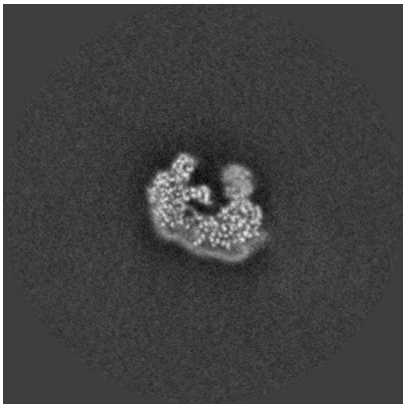
6.3.2 Raw map



X Index: 205



Y Index: 296



Z Index: 274

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

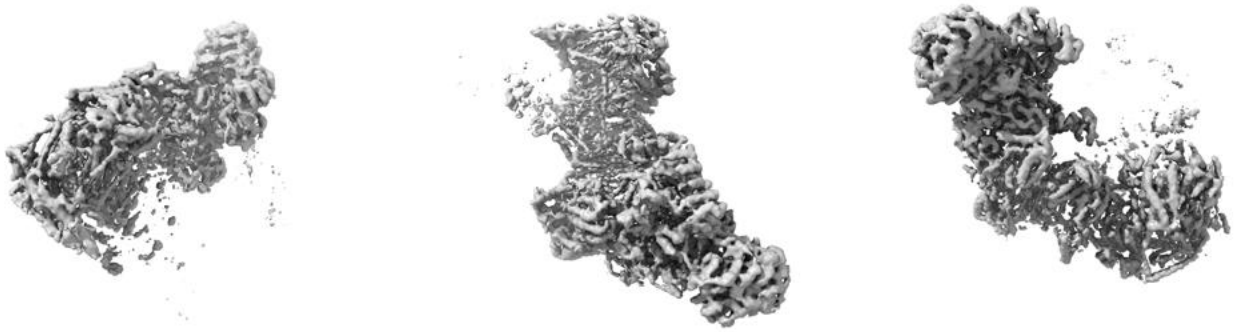
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

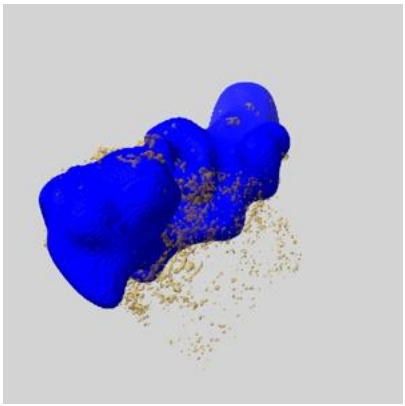
6.5 Mask visualisation (i)

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

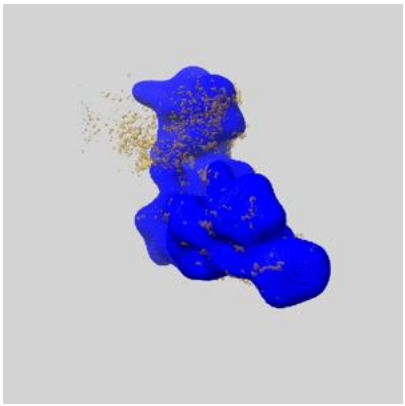
A mask typically either:

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

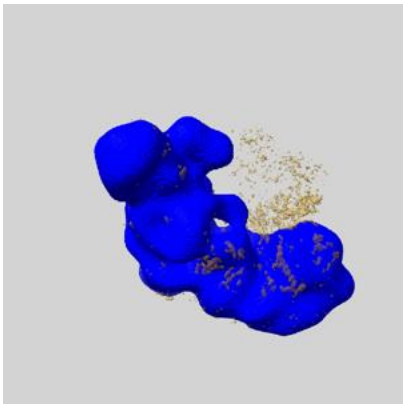
6.5.1 emd_4497_msk_1.map (i)



X



Y

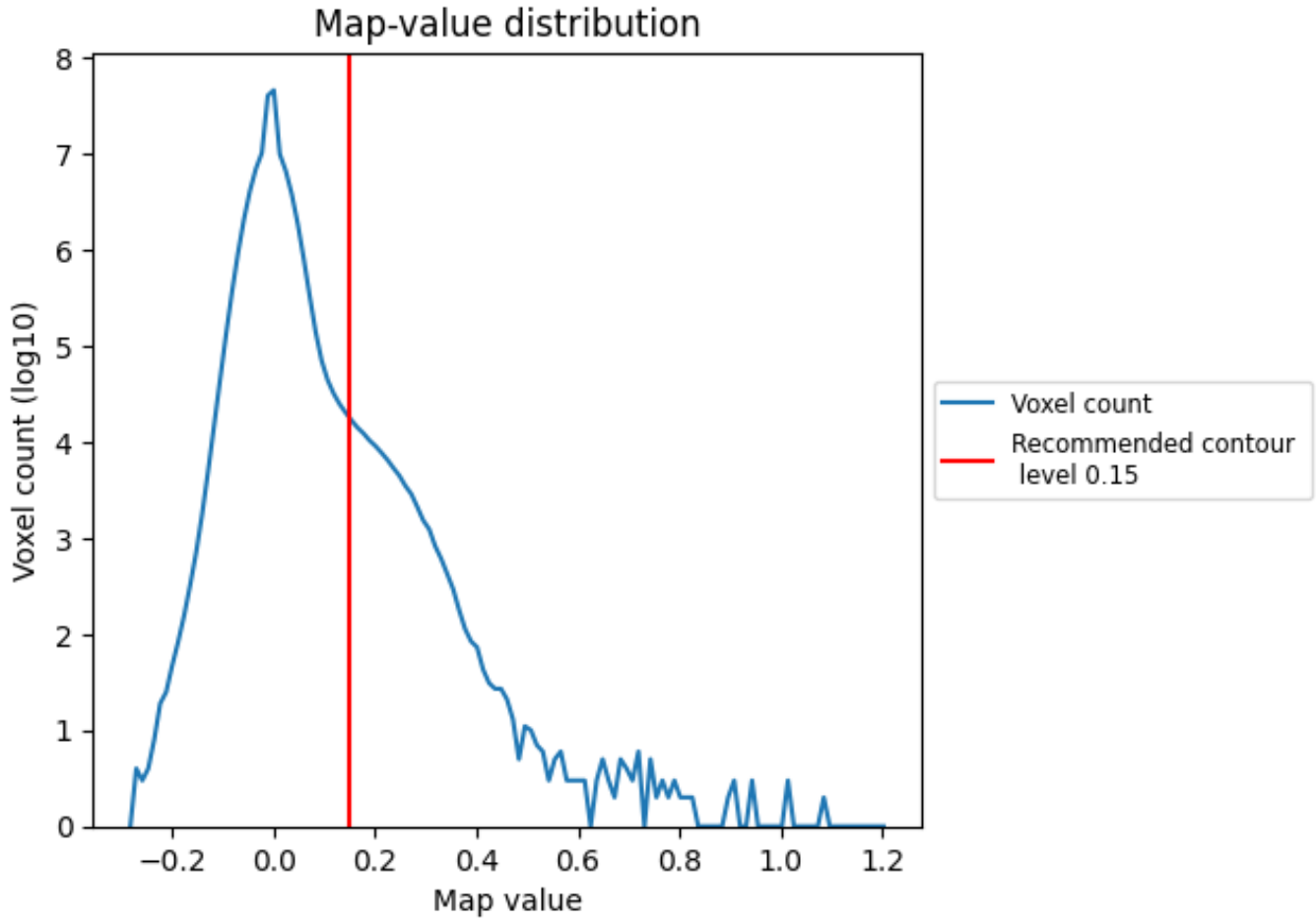


Z

7 Map analysis

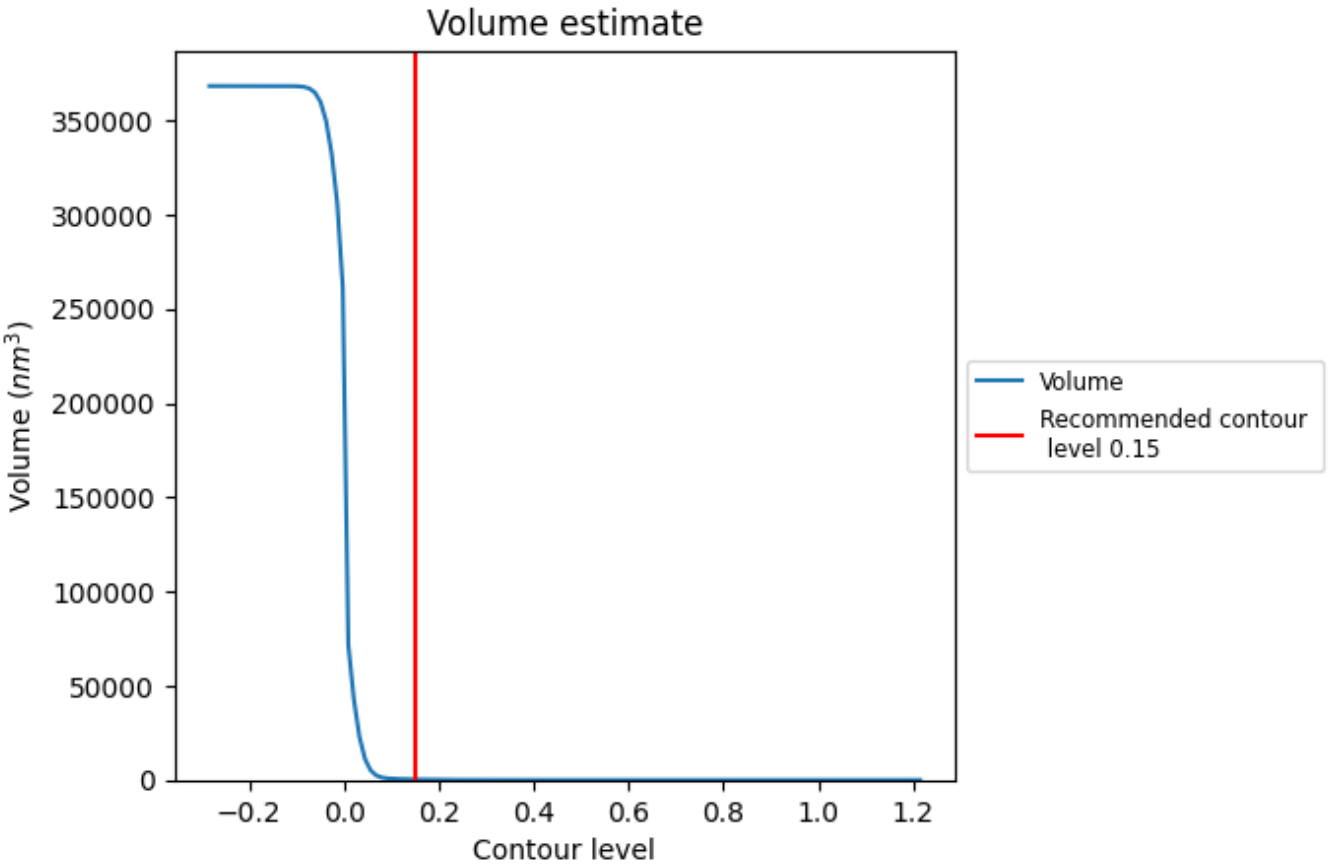
This section contains the results of statistical analysis of the map.

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.

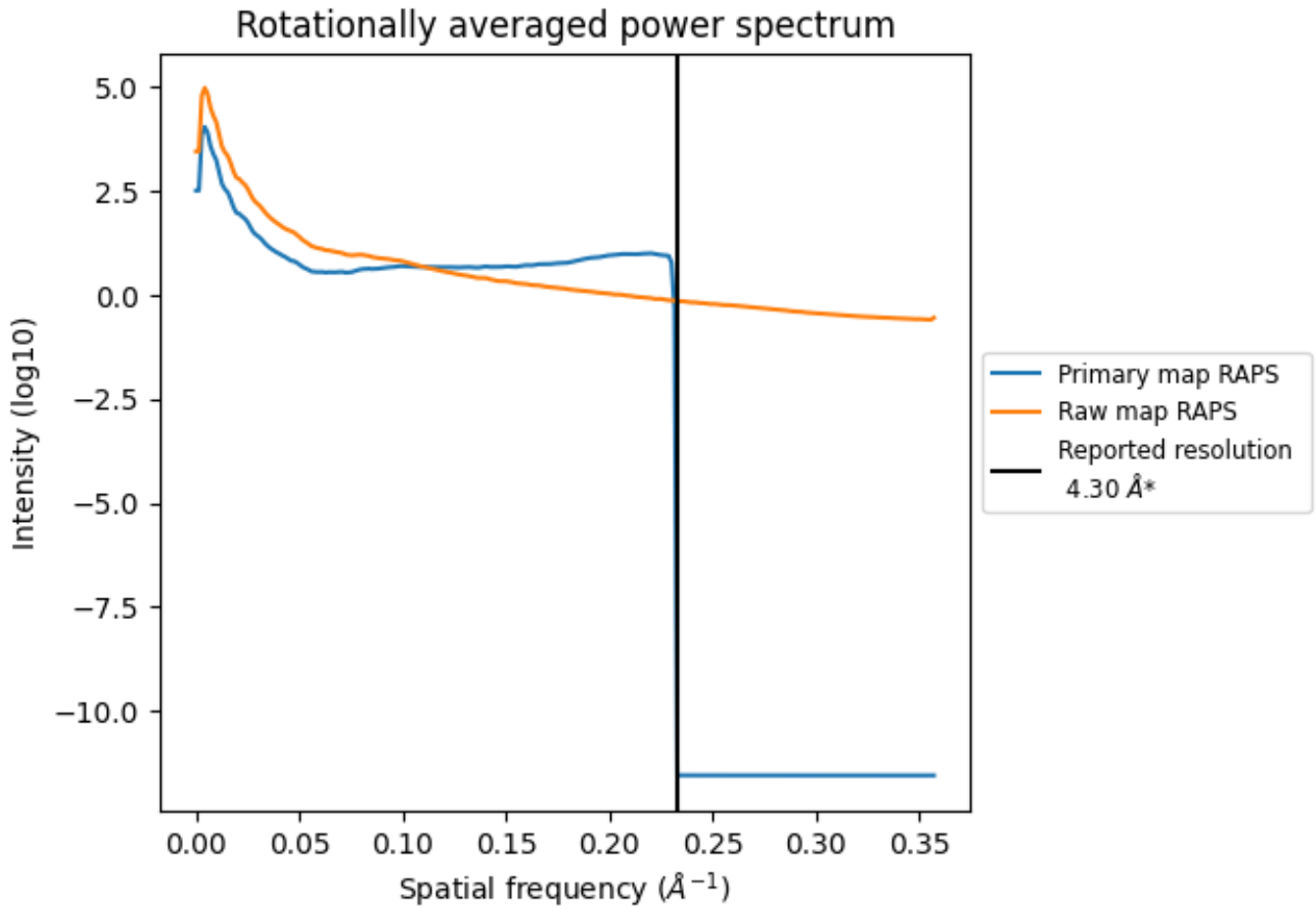
7.2 Volume estimate



The volume at the recommended contour level is 291 nm^3; this corresponds to an approximate mass of 263 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)

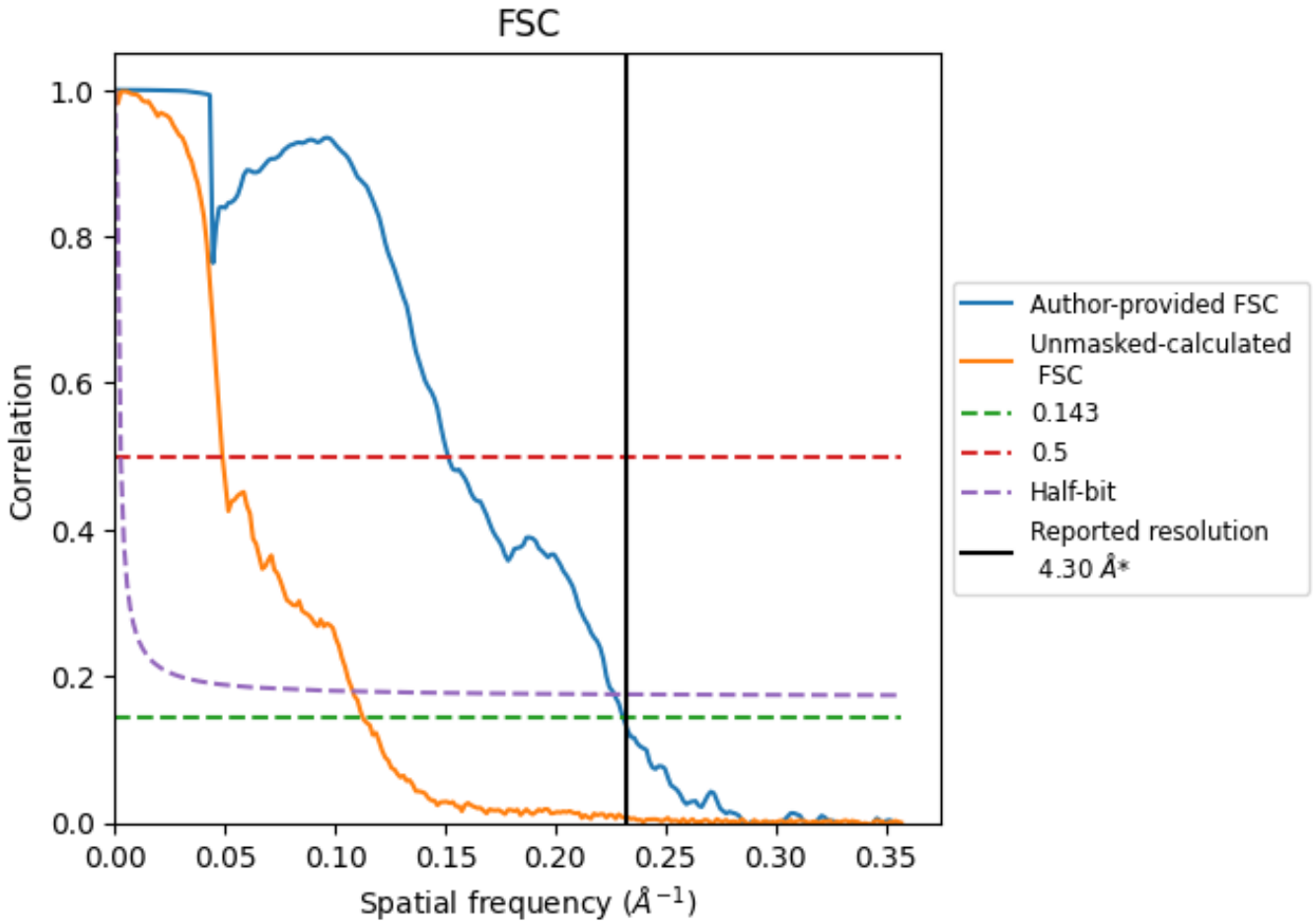


*Reported resolution corresponds to spatial frequency of 0.233 $Å^{-1}$

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 0.233 Å^{-1}

8.2 Resolution estimates (i)

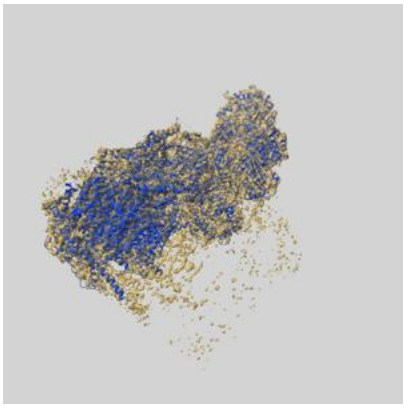
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.33	6.61	4.41
Unmasked-calculated*	8.87	20.45	9.25

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.87 differs from the reported value 4.3 by more than 10 %

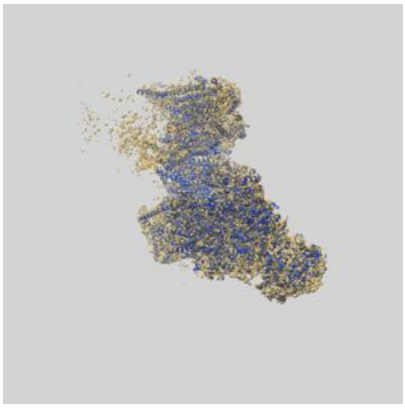
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4497 and PDB model 6QC5. Per-residue inclusion information can be found in section 3 on page 16.

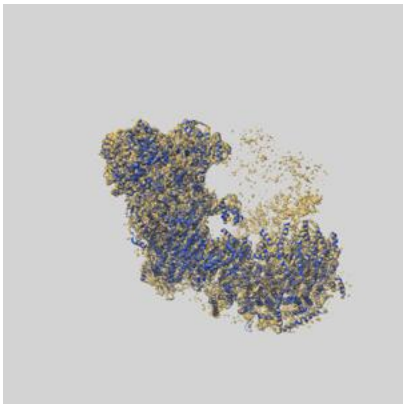
9.1 Map-model overlay



X



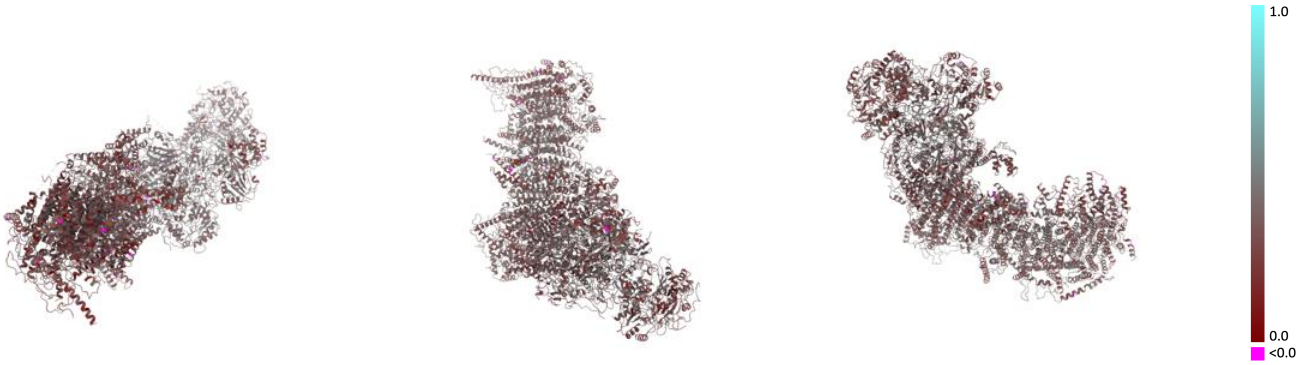
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

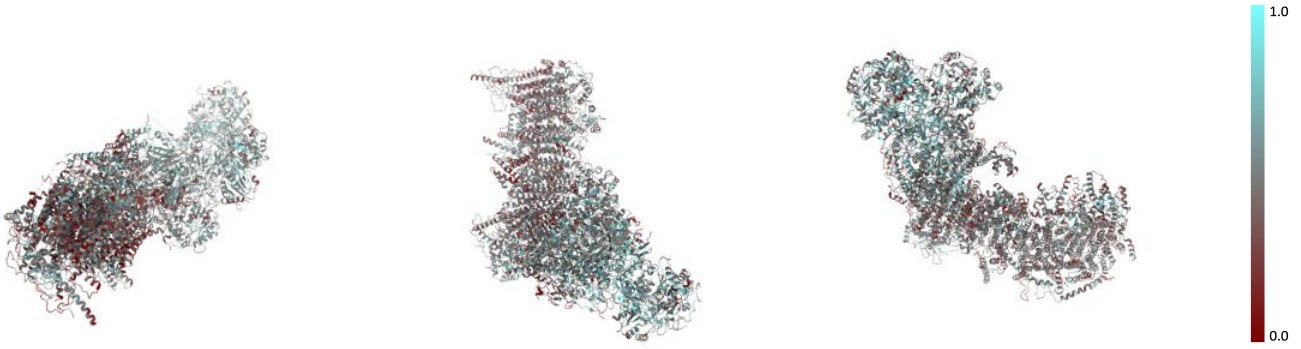
9.2 Q-score mapped to coordinate model (i)



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.

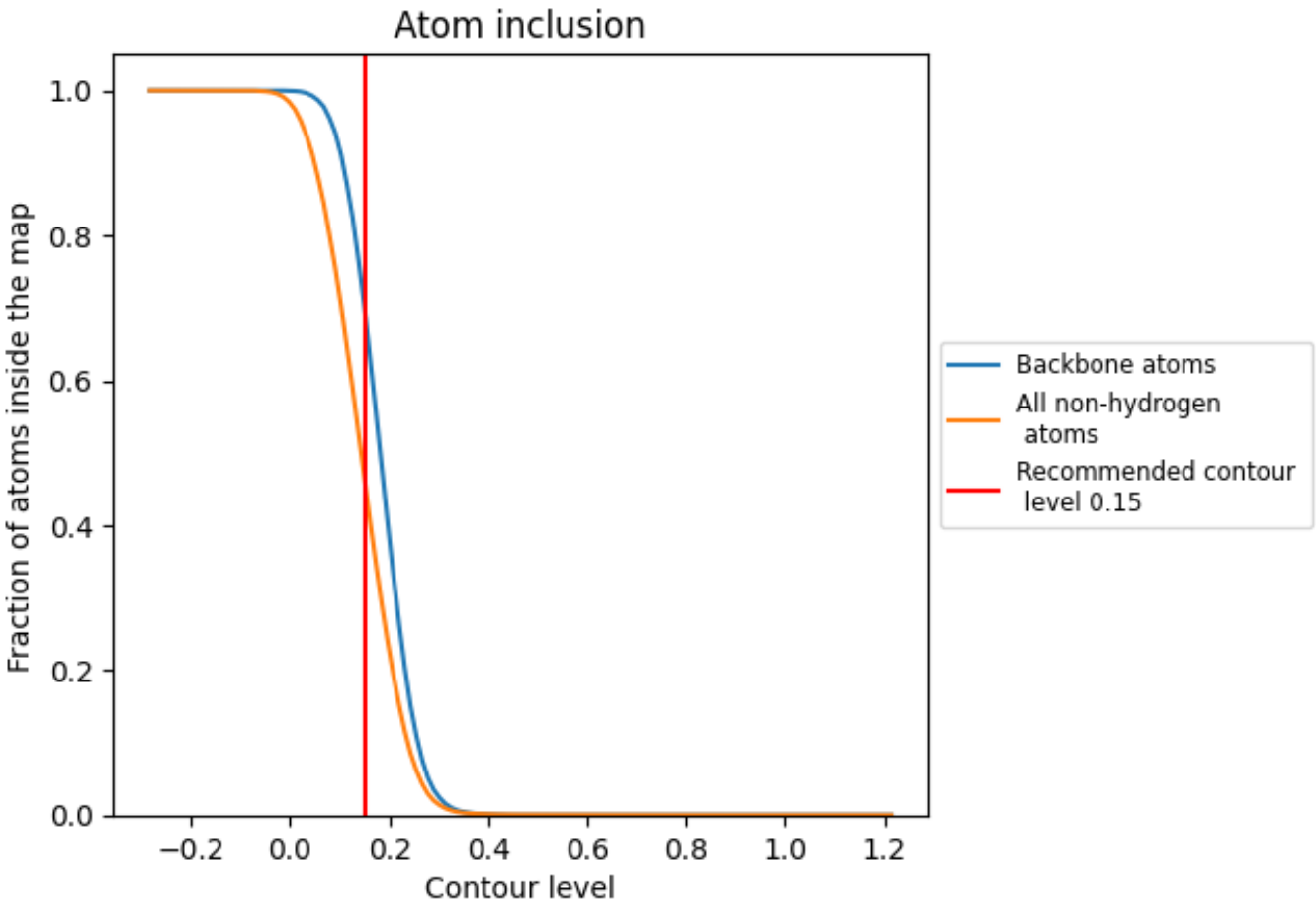
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 47% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4657	0.3510
4L	0.3491	0.3440
A1	0.5072	0.3460
A2	0.5588	0.3490
A3	0.4386	0.3500
A5	0.5304	0.3450
A6	0.4628	0.3730
A7	0.3639	0.3590
A8	0.5066	0.3490
A9	0.4946	0.3750
AA	0.3635	0.2980
AB	0.4237	0.3280
AJ	0.4353	0.3390
AK	0.3110	0.3090
AL	0.3708	0.3460
AM	0.4896	0.3360
B1	0.3257	0.3270
B2	0.3722	0.3100
B3	0.4007	0.3040
B4	0.4163	0.3360
B5	0.4747	0.3440
B6	0.4240	0.3170
B7	0.4154	0.2910
B8	0.4146	0.3400
B9	0.4884	0.3340
BJ	0.4710	0.3260
BK	0.4043	0.3230
C1	0.4084	0.3240
C2	0.4461	0.3620
D1	0.4230	0.3500
D2	0.4514	0.3620
D3	0.3315	0.3330
D4	0.4364	0.3600
D5	0.3929	0.3360
D6	0.3469	0.3390

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Chain	Atom inclusion	Q-score
S1	0.5461	0.3700
S2	0.5139	0.3810
S3	0.5456	0.3900
S4	0.5090	0.3890
S5	0.5044	0.3610
S6	0.5446	0.3820
S7	0.5463	0.3760
S8	0.5830	0.3820
V1	0.5638	0.3440
V2	0.5554	0.3580
V3	0.5030	0.3200